



Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 01:25 PM EDT

PDB ID : 9YNC / pdb_00009ync
EMDB ID : EMD-73173
Title : Motor domains of phi-like human dynein-1 bound to dynactin-p150glued and LIS1
Authors : Yang, J.; Rao, Q.; Chai, P.; Zhang, K.
Deposited on : 2025-10-10
Resolution : 3.93 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

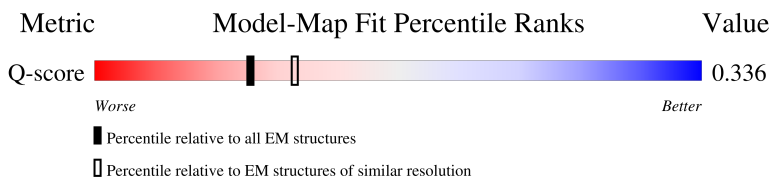
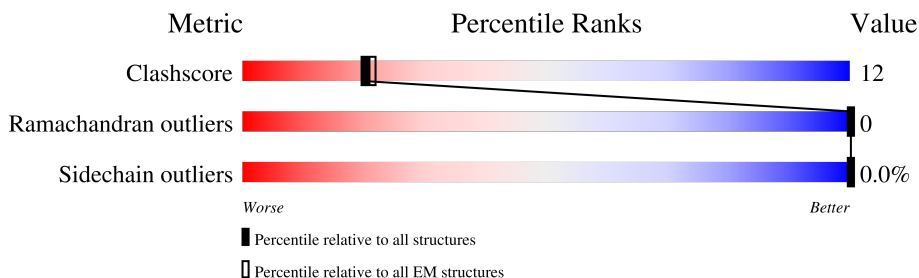
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.93 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.





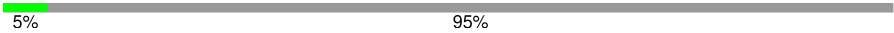
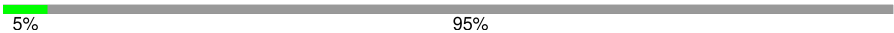


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7811 (3.43 - 4.43)

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

Mol	Chain	Length	Quality of chain
1	A	4646	 45% 21% 34%
1	B	4646	 49% 17% 34%
2	C	410	 54% 25% 21%
2	D	410	 48% 29% 24%

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Mol	Chain	Length	Quality of chain
2	E	410	 13% 18% 82%
2	F	410	 8% 18% 82%
3	G	638	 5% 95%
3	H	638	 5% 95%
4	I	1281	 10% 90%
4	J	1281	 9% 91%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 56882 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	3064	Total	C	N	O	S	0	0
			24650	15707	4259	4563	121		
1	B	3065	Total	C	N	O	S	0	0
			24658	15711	4260	4566	121		

- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	322	Total	C	N	O	S	0	0
			2557	1608	452	477	20		
2	D	313	Total	C	N	O	S	0	0
			2494	1571	440	463	20		
2	E	75	Total	C	N	O		0	0
			373	223	75	75			
2	F	75	Total	C	N	O		0	0
			373	223	75	75			

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	34	Total	C	N	O	0	0
			170	102	34	34		
3	H	34	Total	C	N	O	0	0
			170	102	34	34		

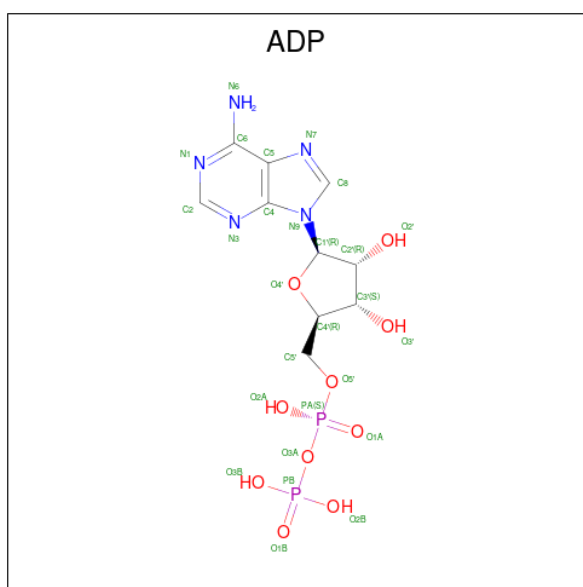
- Molecule 4 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	122	Total	C	N	O	0	0
			607	363	122	122		
4	J	120	Total	C	N	O	1	0
			602	360	121	121		

There are 6 discrepancies between the modelled and reference sequences:

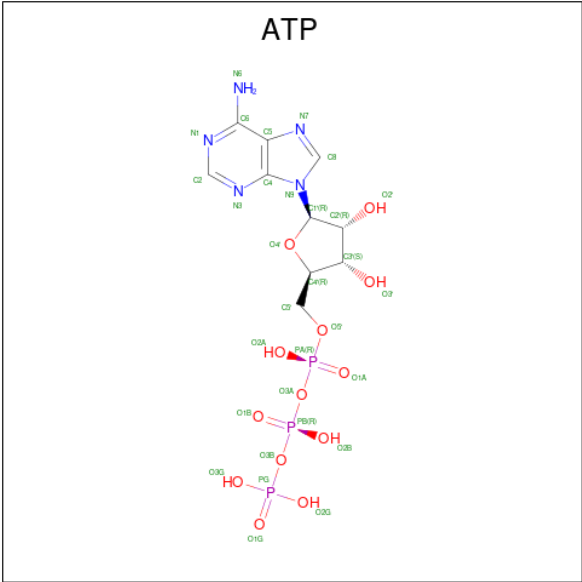
Chain	Residue	Modelled	Actual	Comment	Reference
I	1279	LEU	-	expression tag	UNP A0A287B8J2
I	1280	ILE	-	expression tag	UNP A0A287B8J2
I	1281	SER	-	expression tag	UNP A0A287B8J2
J	1279	LEU	-	expression tag	UNP A0A287B8J2
J	1280	ILE	-	expression tag	UNP A0A287B8J2
J	1281	SER	-	expression tag	UNP A0A287B8J2

- Molecule 5 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
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 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
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

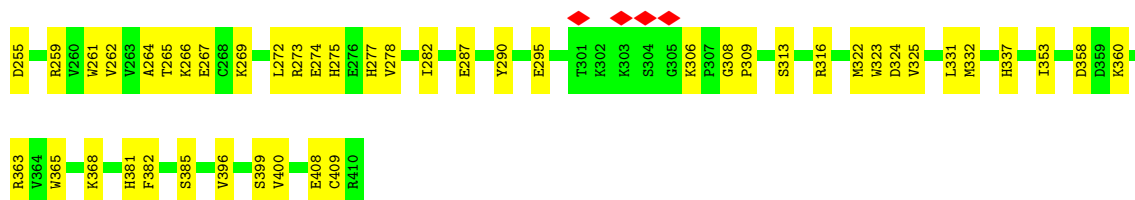
Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Mg	0
			2	2	
7	B	2	Total	Mg	0
			2	2	

G1942	S1835	E1706		M1457	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
R1943	F1836	K1707		A1458	ALA	GLU	PHE	PHE	LEU	LEU	LEU	LEU	PHE
I1944	E1837	E1708		L1459	GLU	THR	PHE	THR	VAL	THR	THR	ASP	GLN
L1948	V1838	T1712	◆	K1391	GLU	LYS	GLN	GLN	ILE	MET	GLN	GLY	LYS
C1949	L1839	E1622		G1392	LEU	PRO	PRO	ILE	ILE	MET	ASN	VAL	VAL
Q1950	S1840	R1623		Y1393	GLN	VAL	TRP	SER	ARG	PRO	GLN	ILE	GLY
V1951	Q1841	A1532	◆	M1394	ASP	THR	TRP	LYS	LYS	ASP	VAL	GLU	ASP
	M1842	F1534		K1395	GLN	GLY	TRP	THR	ASP	GLY	VAL	GLU	ASP
	Q1850	D1535		L1396	LEU	ASN	LYR	LEU	ALA	ASP	VAL	LEU	LEU
W1954	Q1856	I1538		N1397	GLY	ARG	ILE	GLN	THR	VAL	ASN	GLY	ILE
G1955	Q1857	R1542		R1467	TRP	PRO	ASN	GLU	PHE	LEU	PRO	VAL	ILE
C1956	F1857	R1543		E1468	VAL	GLU	ILE	LEU	THR	LEU	ARG	GLU	GLU
F1957	V1630	R1544		M1470	SER	GLU	GLY	GLN	ASP	GLU	PRO	VAL	GLU
D1958	Y1631	V1544		N1471	LEU	ALA	GLY	GLN	THR	LEU	PRO	VAL	GLU
E1959	V1632	Y1545		T1472	LEU	ALA	GLY	GLN	THR	LEU	PRO	VAL	GLU
F1960	Y1633	Y1546		Y1473	SER	GLN	GLY	GLN	THR	LEU	PRO	VAL	GLU
F1961	E1635	L1547		D1476	VAL	ALA	GLY	GLN	THR	LEU	PRO	VAL	GLU
R1962	D1636			L1477	TRP	LEU	ALA	GLY	THR	LEU	PRO	VAL	GLU
L1963	L1637			V1478	TRP	LEU	ALA	GLY	THR	LEU	PRO	VAL	GLU
E1964	L1638			V1479	TRP	LEU	ALA	GLY	THR	LEU	PRO	VAL	GLU
E1965	E1639			N1482	GLN	ILE	ASN	THR	PHE	GLY	VAL	ALA	GLU
R1966	I1641				GLN	LYS	ILE	THR	PHE	GLY	VAL	ALA	GLU
Q1974	V1647				MET	LYS	ARG	ALA	THR	GLY	VAL	ALA	GLU
L1978	L1650			R1485	GLY	PHE	ARG	ALA	THR	GLY	VAL	ALA	GLU
Q1979	L1651			L1486	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
H1985	E1653			R1487	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
A1992	F1654		◆	G1488	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
T1993	M1655		◆	W1490	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
S1994	R1656		◆	D1491	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
A1995	K1657		◆	D1492	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
P1996	M1657		◆	L1493	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
I1997	S1662			F1494	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
L2001	I1663			N1495	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
P2010	I1664			V1496	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
D2011	E1668		◆	V1497	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
M2012	D1673			K1498	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
F2015	V1673			E1499	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
I2016	T1676			I1501	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
T2017	T1677			V1504	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
M2018	M1679			M1507	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
D2030	R1679		◆	K1508	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
K2034	M1685			L1509	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
L2035	T1682		◆	P1510	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
L2039	H1695			Y1511	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
L2043	T1698			Y1512	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
L2048	N1699		◆	Y1513	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
L2049	E1700			K1514	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
T2042	E1701			E1518	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
Q2047	L1702			D1519	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
L2048	L1703			Y1521	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
L2049	T1704			L1521	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
L2049	V1705			E1524	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU
L2049	V1705			D1525	GLY	THR	ARG	ALA	THR	GLY	VAL	ALA	GLU

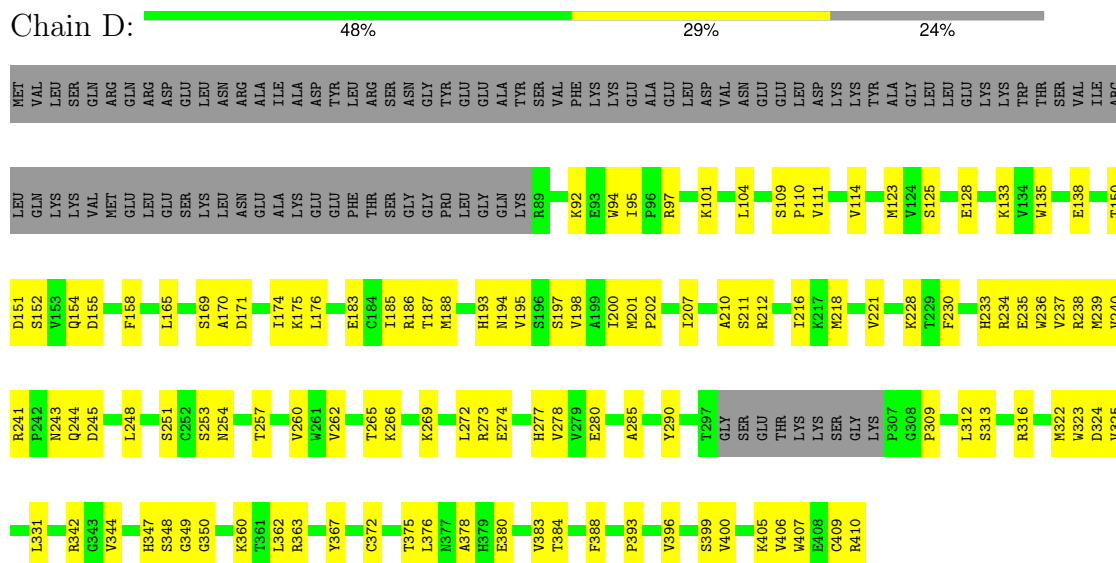


Y1393	VAL	THR	ARG	GLN	ASN	PHE	LEU	ILE	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
M1394	ALA	GLU	PHE	GLN	LEU	GLU	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
K1395	GLU	THR	PHE	GLN	LEU	GLU	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1399	GLU	THR	PHE	GLN	LEU	GLU	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1403	GLN	PRO	PRO	LEU	GLN	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
K1404	ASP	VAL	SER	SER	ASP	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
S1405	LEU	THR	THR	GLU	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1408	GLY	LEU	ILE	GLN	ASN	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
K1409	VAL	PRO	ASP	ASN	LEU	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
D1410	TRP	GLU	ILE	GLN	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
R1411	SER	GLU	GLN	GLU	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
H1412	GLU	ALA	GLY	GLN	SER	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
W1413	LEU	LEU	GLY	GLN	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
R1419	LYS	GLN	TRP	GLN	SER	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
W1424	VAL	ALA	ALA	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
V1425	TRP	LEU	ALA	LYS	VAL	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
V1426	GLU	THR	PHE	GLN	MET	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
S1427	ILE	ILE	ASP	PHE	ILE	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
E1428	GLY	THR	ASP	THR	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
T1429	ASP	GLY	ILE	GLN	SER	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1431	MET	LYS	ARG	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
I1434	GLY	PHE	ARG	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
W1435	LEU	ILE	ASP	ASN	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
D1436	LYS	THR	ALA	LYS	VAL	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
V1437	ASP	ASP	ILE	GLN	TRP	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
D1438	GLU	GLN	GLN	GLN	TRP	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1439	GLU	GLN	GLN	GLN	TRP	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
Q1355	GLY	LYS	VAL	VAL	GLN	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
Q1356	CYS	LYS	VAL	VAL	GLN	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
H1357	ALA	ALA	ASN	GLN	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
K1358	LYS	LYS	LYS	CYS	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1359	ALA	ALA	LYS	TRP	TRP	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
M1362	GLY	ALA	ILE	LYS	MET	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1363	LEU	LEU	ILE	GLN	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
D1364	GLY	GLU	PHE	GLN	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
A1365	LEU	GLN	GLY	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1370	ASP	THR	ARG	ILE	ILE	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
K1371	THR	THR	VAL	ALA	ASN	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
A1375	GLY	GLY	GLY	LYS	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
E1460	LEU	LEU	ASN	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
E1461	SER	LEU	SER	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
F1462	GLY	GLY	ARG	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1463	THR	THR	THR	GLN	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
K1464	SER	SER	THR	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
W1470	GLU	GLU	LEU	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
W1478	ARG	ARG	LEU	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
V1478	THR	THR	THR	GLY	GLY	LEU	GLU	LEU	GLU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1389	GLN	GLN	ASP	THR	THR	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU
L1390	GLN	GLN	ASP	THR	THR	GLY	LEU	GLU	LEU	THR	GLY	VAL	GLN	ASP	GLY	LEU	ASP	LEU

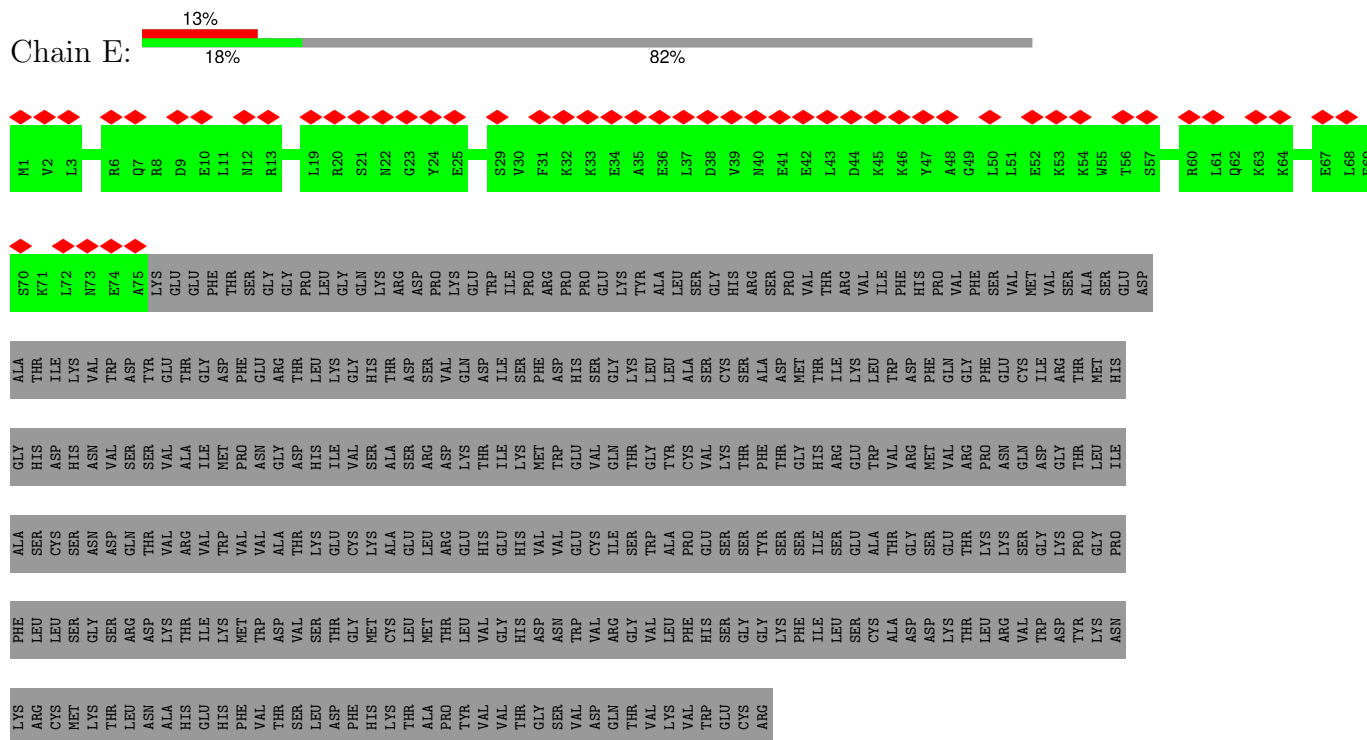
LYS	Q3214	T3081	L2993	Q2834	E2688	W2545	W2545	ASP	V2307	E2188	S2303	S1903	V1724	L1485
VAL	V3216	R3088	M2994	E2839	R2694	W2548	W2548	GLY	D2308	M2189	S2038	S1903	E1725	R1488
PRO	E3216	C3089	E2996	E2842	D2697	W2562	W2562	GLY	E2310	Y2190	T2042	T1910	F1727	R1603
ALA	E3217	F3094	V2999	R2843	K2702	W2563	W2563	ALA	W2311	T2192	K2043	G1911	K1729	W1490
VAL	R3219	G3095	G3003	L2885	K2702	W2564	W2564	ALA	E2313	E2197	Q2047	E1914	S1753	H1500
ILE	R3220	D3096	F3004	L2885	Q2707	P2565	P2565	ALA	M2322	W2203	R2060	S1916	S1753	V1504
GLU	R3223	W3097	L3006	L2885	V2708	D2566	D2566	ALA	T2326	K2206	E2063	K1917	I1756	M1507
ASN	Q3227	T3110	E3006	L2885	V2709	V2567	V2567	ALA	W2329	L2210	A2066	V1929	L1766	K1508
ALA	E3228	S3111	R3007	L2885	N2713	D2573	D2573	ALA	R2332	Y2211	R2067	F1930	M1769	Y1513
VAL	L3229	K3112	M3008	L2885	P2714	R2576	R2576	ALA	L2333	I2213	R2068	D1933	E1517	E1517
LYS	E3230	K3113	L3012	L2885	R2720	T2583	T2583	ALA	L2333	T2069	P2070	F1936	P1627	E1518
SER	V3231	D3114	A3013	L2885	R2726	W2584	W2584	ALA	W2338	Q2215	P2071	F1938	R1628	D1519
ILE	K3232	D3124	V3017	L2885	R2726	L2585	L2585	ALA	W2339	Q2216	S2081	Q1939	F1629	A1520
LYS	N3233	Y3125	V3017	L2885	R2726	L2585	L2585	ALA	R2340	I2216	S2081	A1940	L1521	L1522
GLN	K3239	V3129	L3020	L2885	R2729	P2590	P2590	ALA	R2341	L2220	S2081	M1941	D1634	L1527
HIS	M3243	Y3130	D3024	L2885	V2733	L2591	L2591	ALA	M2342	M2221	H2085	V1946	L1797	I1530
VAL	V3244	D3131	E2903	L2885	V2733	V2592	V2592	ALA	F2343	M2222	H2085	C1949	M1798	D1535
GLU	K3245	K3132	E3025	L2885	Y2738	V2592	V2592	ALA	E2344	M2222	H2085	Q1950	Q1800	I1640
VAL	L3246	L3133	L2905	L2885	Y2738	V2592	V2592	ALA	V2345	S2228	R2091	V1946	E1814	I1538
ARG	Q3247	P3134	T3028	L2885	Y2748	P2596	P2596	ALA	T2352	M2232	S2099	C1949	L1797	R1543
SER	Q3248	Q3135	T3031	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1530
MET	E3249	P3136	Q3032	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	D1535
ALA	K3252	P3137	C3033	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
PRO	LYS	R3140	K3034	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
PRO	LYS	E3141	G3035	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
ALA	VAL	V3144	G3036	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
VAL	SER	F3149	G3038	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
LYS	GLU	V3150	K3039	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
LEU	ILE	L3154	L3042	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
LEU	GLN	T3172	M3043	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
SER	GLN	P3173	S3046	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
ILE	LEU	R3174	H3047	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
CYS	HIS	R3175	E3048	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
LEU	LYS	H3176	E3049	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
LEU	GLN	V3177	L3050	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
LEU	GLN	L3177	Y3051	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
GLY	GLU	D3178	K3052	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
ILE	VAL	H3182	F3054	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
SER	ALA	Q3197	R3060	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
THR	ASP	Q3198	R3060	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
ASP	LYS	Q3199	R3060	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
THR	GLN	R3200	V3065	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
LYS	MET	L3201	S3072	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
GLN	SER	E3073	E3073	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
ILE	VAL	K3207	E3073	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
ARG	LYS	T3208	K3076	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
SER	GLU	L3208	R3077	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
ILE	ASP	T3211	D3077	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
ILE	LEU	T3211	R3077	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538
MET	ASP	T3211	R3077	L2885	Y2748	P2596	P2596	ALA	R2358	M2232	S2099	C1949	M1798	I1538



• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta



• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta



• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90591	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	0.483	Depositor
Minimum map value	-0.187	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size (\AA)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.12	0/25169	0.32	0/34101
1	B	0.12	0/25177	0.30	0/34112
2	C	0.12	0/2624	0.39	0/3555
2	D	0.10	0/2560	0.31	0/3470
2	E	0.06	0/372	0.20	0/518
2	F	0.06	0/372	0.17	0/518
3	G	0.05	0/169	0.14	0/235
3	H	0.05	0/169	0.13	0/235
4	I	0.21	0/606	0.30	0/845
4	J	0.35	0/601	0.44	0/838
All	All	0.12	0/57819	0.32	0/78427

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	24650	0	24762	653	0
1	B	24658	0	24766	577	0
2	C	2557	0	2487	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2494	0	2419	89	0
2	E	373	0	172	0	0
2	F	373	0	172	0	0
3	G	170	0	73	1	0
3	H	170	0	73	0	0
4	I	607	0	285	0	0
4	J	602	0	282	0	0
5	A	81	0	36	9	0
5	B	81	0	36	10	0
6	A	31	0	12	4	0
6	B	31	0	12	6	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
All	All	56882	0	55587	1380	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 12.

All (1380) 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)
2:C:275:HIS:HE2	2:C:313:SER:HG	1.16	0.93
1:A:1892:MET:HE1	1:A:1902:GLY:HA3	1.53	0.90
1:A:2096:VAL:HG22	1:A:2144:THR:HG21	1.53	0.90
1:A:2633:LYS:HZ3	1:A:3019:GLY:H	1.20	0.88
1:A:4473:MET:HE1	1:A:4478:TRP:HB2	1.58	0.84
1:A:1356:PRO:HG2	1:A:1404:LYS:HE3	1.59	0.84
1:B:4043:MET:HE1	1:B:4125:PHE:HB3	1.59	0.83
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.59	0.83
1:A:4157:MET:HE1	1:A:4185:TRP:HA	1.59	0.83
1:A:2644:THR:HG22	1:A:2646:ASN:H	1.42	0.83
1:A:2503:SER:HB3	1:A:2511:ARG:HG2	1.61	0.82
1:B:1437:VAL:HG12	1:B:1442:ASN:HD21	1.45	0.81
1:A:2770:THR:O	1:A:2773:MET:HB2	1.82	0.80
1:A:1464:LYS:HA	1:A:1467:ARG:HG2	1.63	0.79
1:B:2081:SER:HA	1:B:4415:ARG:HH21	1.48	0.79
1:B:3048:GLU:OE1	1:B:3052:LYS:NZ	2.16	0.78
1:A:1695:HIS:HB3	1:A:1700:GLU:HG3	1.65	0.78
1:A:3239:LYS:HA	1:A:3242:LYS:HG2	1.65	0.77
1:A:2189:MET:HG3	1:A:2191:LEU:HD23	1.68	0.76
1:B:1843:ARG:HH12	1:B:1862:ALA:H	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3810:SER:HB3	1:A:3890:ILE:HD12	1.70	0.73
1:A:4336:GLY:O	1:A:4339:MET:HB3	1.89	0.73
2:D:234:ARG:HH22	2:D:273:ARG:HH21	1.35	0.73
1:A:1612:GLN:NE2	1:A:1635:GLU:OE1	2.22	0.73
2:D:186:ARG:NH1	2:D:221:VAL:O	2.21	0.72
1:A:3113:MET:HB3	1:A:3115:LEU:HD23	1.70	0.72
1:B:4505:LYS:NZ	1:B:4554:ASP:O	2.22	0.72
1:B:2816:LEU:HD11	1:B:2820:GLY:HA3	1.71	0.72
1:A:1397:ASN:HA	1:A:1400:VAL:HB	1.71	0.72
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.23	0.72
1:B:1439:LEU:HA	1:B:1442:ASN:HB2	1.72	0.71
1:B:4326:ASN:ND2	1:B:4579:ASN:O	2.23	0.71
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.23	0.71
1:B:4336:GLY:O	1:B:4339:MET:HB3	1.91	0.70
1:A:3741:ARG:NH1	1:A:3744:GLN:OE1	2.25	0.70
1:B:2503:SER:HB3	1:B:2511:ARG:HG2	1.74	0.70
1:B:3028:THR:O	1:B:3031:THR:HB	1.91	0.70
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.25	0.69
2:D:101:LYS:N	2:D:406:VAL:O	2.26	0.69
1:A:1879:LEU:HD13	1:A:1918:ALA:HB2	1.75	0.69
1:B:2047:GLN:NE2	1:B:2067:ASN:OD1	2.24	0.69
1:B:3601:MET:HE1	1:B:3611:ARG:HB2	1.73	0.69
1:B:1672:VAL:HA	1:B:1691:SER:HA	1.75	0.69
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.74	0.69
1:B:1627:PRO:HB3	1:B:1950:GLN:HB3	1.75	0.69
1:B:1640:ILE:HG13	1:B:1650:LEU:HD22	1.75	0.69
1:A:1930:PHE:HA	1:A:2326:THR:HG21	1.74	0.69
2:C:197:SER:HB2	2:C:239:MET:HA	1.75	0.69
1:A:1451:LEU:HD13	1:A:1454:GLN:HE21	1.57	0.68
1:A:1623:ARG:NH1	1:A:1632:VAL:O	2.25	0.68
2:D:193:HIS:HB3	2:D:212:ARG:HB3	1.74	0.68
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.75	0.68
1:B:3032:GLN:O	1:B:3036:GLY:N	2.27	0.68
1:B:2872:LEU:HD12	1:B:2920:LEU:HD12	1.74	0.68
1:B:4099:VAL:HB	1:B:4106:LEU:HD21	1.76	0.67
1:A:3820:GLN:HB2	1:A:4346:MET:HE1	1.75	0.67
1:B:3110:THR:O	1:B:3140:ARG:NH1	2.28	0.67
1:B:3039:LYS:O	2:C:273:ARG:NH2	2.27	0.67
1:B:4543:VAL:HG11	1:B:4622:VAL:HB	1.74	0.67
1:B:2684:ARG:HD2	1:B:2726:ARG:HG2	1.76	0.67
1:B:3638:VAL:HG22	1:B:3681:THR:HB	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4150:PRO:O	1:B:4195:ARG:NH2	2.27	0.67
1:B:4301:ARG:NH1	1:B:4303:GLU:OE2	2.27	0.67
1:B:2660:VAL:HG22	1:B:2707:GLN:HB3	1.77	0.67
1:A:1894:GLN:HG3	1:A:4246:LEU:HD11	1.76	0.67
1:B:2925:ILE:HG21	1:B:2933:LEU:HG	1.77	0.67
1:A:4323:LEU:HD12	1:A:4324:PRO:HD2	1.76	0.66
1:A:4541:LEU:HD11	1:A:4590:LEU:HD13	1.77	0.66
1:B:1399:LEU:HB2	1:B:1439:LEU:HD11	1.77	0.66
1:A:1363:LEU:HD13	1:A:1394:MET:HA	1.77	0.66
1:B:1623:ARG:NH1	1:B:1629:PHE:O	2.29	0.66
1:B:2573:ASP:OD1	1:B:2576:ARG:NH2	2.28	0.66
1:B:3914:ILE:O	1:B:3937:ARG:NH1	2.29	0.66
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.76	0.66
1:B:3459:GLN:HG3	1:B:3462:LYS:NZ	2.11	0.66
1:A:1535:ASP:HA	1:A:2292:ARG:HH12	1.59	0.65
1:A:2566:ASP:OD1	1:A:2610:ARG:NH2	2.29	0.65
1:A:2578:GLU:OE2	1:A:2607:SER:OG	2.13	0.65
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.30	0.65
1:B:1839:LEU:O	1:B:1843:ARG:NH1	2.29	0.65
1:B:2060:ARG:NH1	1:B:2128:ALA:O	2.29	0.65
1:B:2222:MET:HE1	1:B:2234:TRP:CD1	2.32	0.65
1:B:1424:TRP:HE1	1:B:1429:LEU:HA	1.60	0.65
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.29	0.65
1:B:2452:LEU:HD13	1:B:2729:ARG:HH21	1.62	0.65
1:B:2605:LEU:HD13	1:B:2709:VAL:HG11	1.77	0.65
1:A:1943:ARG:NH1	1:A:2329:ASN:O	2.30	0.65
1:A:1966:ARG:HB2	1:A:4072:GLY:HA2	1.77	0.65
1:A:1439:LEU:HB2	1:A:1443:GLU:HB2	1.78	0.65
1:A:2221:MET:HE3	1:A:2361:MET:HE1	1.79	0.65
1:A:4395:LEU:HD23	1:A:4421:ALA:HB2	1.78	0.65
1:B:1390:LEU:HA	1:B:1394:MET:SD	2.36	0.65
1:B:2271:ASN:OD1	1:B:2272:THR:N	2.29	0.65
2:D:152:SER:O	2:D:154:GLN:NE2	2.29	0.65
1:A:2304:ASP:OD1	1:A:2726:ARG:NH1	2.30	0.64
1:A:3763:ASP:OD2	1:A:3765:THR:OG1	2.15	0.64
1:B:3036:GLY:O	1:B:3039:LYS:HB3	1.97	0.64
1:B:3481:SER:HB3	1:B:3774:LYS:HE2	1.79	0.64
1:A:1352:VAL:HG22	1:B:1353:SER:HB3	1.77	0.64
1:B:3455:ILE:HG12	1:B:3459:GLN:HE22	1.61	0.64
1:B:2770:THR:O	1:B:2773:MET:HB2	1.97	0.64
1:B:3239:LYS:HB3	1:B:3451:TYR:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3517:ALA:HB1	1:B:3525:ARG:HG2	1.79	0.64
1:B:3981:THR:HG23	1:B:3984:GLY:H	1.63	0.64
1:A:3946:ASP:OD2	1:A:3950:LYS:NZ	2.30	0.64
1:A:4154:LYS:HE3	1:A:4310:GLU:HA	1.78	0.64
2:D:324:ASP:HB2	2:D:331:LEU:HD11	1.80	0.64
1:B:2590:PRO:HA	1:B:2708:PHE:O	1.98	0.64
1:B:1561:LEU:O	1:B:1565:THR:OG1	2.14	0.64
1:A:3247:GLN:OE1	1:B:3248:GLN:NE2	2.31	0.64
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.31	0.64
1:B:2684:ARG:NH1	1:B:2688:GLU:OE1	2.31	0.64
1:B:3835:ILE:HG12	1:B:3870:ARG:HD2	1.80	0.64
1:B:1370:LEU:HD13	1:B:1386:VAL:HB	1.80	0.63
1:B:2265:TYR:OH	1:B:2311:TRP:O	2.15	0.63
1:A:1370:LEU:HD21	1:A:1386:VAL:HG23	1.81	0.63
1:B:1409:LYS:H	1:B:1412:HIS:CE1	2.15	0.63
1:A:1628:ARG:NH1	1:A:1657:MET:O	2.27	0.63
1:B:3219:ARG:HH21	1:B:3472:VAL:HG22	1.63	0.63
1:B:1599:ARG:HH12	1:B:1603:ARG:HD2	1.63	0.63
1:B:2976:LEU:HD11	1:B:3008:MET:HE1	1.81	0.63
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.32	0.63
1:A:4542:GLU:OE1	1:A:4591:ARG:NH2	2.31	0.63
2:C:218:MET:HB3	2:C:228:LYS:HB2	1.81	0.63
1:A:2506:SER:HB2	1:A:2510:MET:HE2	1.81	0.63
1:B:2536:ASP:OD1	1:B:2576:ARG:NH1	2.32	0.63
1:A:2452:LEU:HD13	1:A:2729:ARG:HH21	1.63	0.62
1:A:3113:MET:HE3	1:A:3184:ALA:HA	1.80	0.62
1:B:3561:ARG:NH1	1:B:3603:GLU:OE2	2.32	0.62
1:B:4492:ILE:HG13	1:B:4507:ILE:HD13	1.81	0.62
1:A:1391:LYS:HA	1:A:1394:MET:HE2	1.81	0.62
1:A:1582:VAL:HG13	1:A:1591:VAL:HG11	1.80	0.62
1:A:1704:LEU:HD22	1:A:1707:LYS:HZ3	1.65	0.62
1:B:4099:VAL:HG11	1:B:4126:LEU:HD22	1.81	0.62
1:A:3242:LYS:HA	1:A:3245:LYS:HD2	1.82	0.62
1:B:2694:ARG:NH1	1:B:2697:ASP:OD2	2.33	0.62
2:C:89:ARG:NH2	2:C:409:CYS:O	2.31	0.62
1:A:2065:LEU:HD22	1:A:2137:LEU:HD22	1.80	0.62
1:A:2540:SER:O	1:A:2543:GLY:N	2.32	0.62
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.32	0.62
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.33	0.62
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.31	0.62
1:B:2507:ARG:HH21	1:B:2509:LYS:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2242:GLU:HG3	1:B:2248:GLU:HA	1.81	0.61
1:B:2903:GLU:O	2:C:212:ARG:NH2	2.33	0.61
1:B:4318:PRO:HG2	1:B:4325:ASN:HA	1.81	0.61
1:A:1462:PHE:O	1:A:1466:ILE:HD12	1.99	0.61
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.33	0.61
1:A:3602:ASN:HA	1:A:3605:LYS:HD2	1.82	0.61
1:B:2174:GLU:OE1	1:B:2179:ARG:NH1	2.33	0.61
1:B:2755:MET:HE1	1:B:2810:LEU:HD12	1.81	0.61
1:A:1443:GLU:OE2	1:A:1447:LYS:NZ	2.33	0.61
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	1.81	0.61
1:B:2232:MET:HA	1:B:2235:ARG:HB2	1.82	0.61
1:A:3753:LEU:HD21	1:A:3770:LEU:HD21	1.83	0.61
1:B:1558:LYS:HG3	1:B:1565:THR:HG21	1.83	0.61
2:D:174:ILE:HB	2:D:188:MET:HB2	1.83	0.61
1:A:2716:THR:O	1:A:4449:ARG:NH2	2.34	0.61
2:C:211:SER:OG	2:C:213:ASP:OD1	2.19	0.61
1:B:2307:VAL:HG23	1:B:2345:VAL:HG11	1.81	0.61
1:A:2388:ASP:OD1	1:A:2389:GLU:N	2.33	0.61
1:A:3872:ALA:HA	1:A:3875:MET:HE3	1.81	0.61
1:B:2066:ALA:HA	1:B:2069:ILE:HG22	1.83	0.61
2:C:154:GLN:HE22	2:C:170:ALA:HB2	1.65	0.61
1:A:2956:LEU:HD23	1:A:2989:LYS:HB3	1.82	0.60
1:B:2091:ARG:NH2	5:B:4701:ADP:O3A	2.34	0.60
1:B:2294:GLU:OE1	1:B:2294:GLU:N	2.33	0.60
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.82	0.60
1:A:3222:LEU:HD23	1:A:3223:ARG:HH12	1.65	0.60
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.83	0.60
1:B:4174:ASN:OD1	1:B:4231:GLN:NE2	2.32	0.60
1:A:1395:LYS:HB2	1:A:1398:MET:HE1	1.84	0.60
1:B:3017:VAL:HB	1:B:3020:LEU:HB2	1.83	0.60
1:A:1402:GLU:HB2	1:A:1450:LEU:HD21	1.82	0.60
1:B:4518:GLU:OE1	1:B:4518:GLU:N	2.33	0.60
1:B:1933:ASP:HB2	1:B:1962:ARG:HH21	1.66	0.60
1:A:1396:ILE:HG13	1:A:1435:TRP:CD1	2.37	0.60
1:B:1665:ILE:O	1:B:1674:LEU:N	2.30	0.60
1:B:3182:HIS:NE2	1:B:3582:ARG:O	2.32	0.60
1:A:1477:LEU:HA	1:A:1486:LEU:O	2.01	0.60
1:A:1662:SER:HB2	1:A:1679:ARG:HD3	1.84	0.60
1:A:2373:MET:HE3	6:A:4702:ATP:C6	2.36	0.60
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.82	0.60
1:B:3825:TYR:CZ	1:B:3875:MET:HG3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.37	0.60
1:A:3654:ARG:NH1	1:A:3655:ARG:O	2.35	0.60
1:A:3923:ARG:NH1	1:A:3924:ILE:O	2.35	0.60
1:B:2616:GLU:N	1:B:2616:GLU:OE1	2.35	0.60
1:B:3967:GLU:HB2	1:B:4004:MET:HG2	1.84	0.60
1:A:2519:ARG:NH2	1:A:2527:PRO:O	2.34	0.60
1:B:1836:PHE:HA	1:B:1839:LEU:HB2	1.83	0.60
1:A:4004:MET:HA	1:A:4007:MET:HE3	1.84	0.59
1:B:2993:ILE:HG22	1:B:3065:VAL:HB	1.83	0.59
1:A:1625:SER:HB2	1:A:1699:ASN:HD22	1.67	0.59
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	1.84	0.59
1:B:4172:SER:O	1:B:4231:GLN:NE2	2.35	0.59
2:D:151:ASP:HB2	2:D:171:ASP:HB3	1.82	0.59
1:A:1491:ASP:O	1:A:1495:ASN:ND2	2.35	0.59
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.34	0.59
1:A:3239:LYS:HE3	1:A:3454:LEU:HD12	1.84	0.59
1:B:3178:ASP:OD2	1:B:3585:ARG:NE	2.35	0.59
1:B:3727:LYS:O	1:B:3731:LEU:HG	2.01	0.59
1:A:1647:VAL:HA	1:A:1650:LEU:HD12	1.84	0.59
1:A:1842:MET:HE1	1:A:1922:GLN:HG2	1.84	0.59
1:A:1880:VAL:HG11	1:A:2049:ILE:HA	1.84	0.59
1:A:2222:MET:HE3	1:A:2230:LYS:HB3	1.84	0.59
1:B:1623:ARG:NH2	1:B:1634:ASP:OD1	2.36	0.59
1:B:3471:LYS:NZ	1:B:3761:LEU:O	2.35	0.59
1:B:4385:SER:O	1:B:4389:HIS:ND1	2.31	0.59
2:C:113:ARG:NH1	2:C:154:GLN:O	2.35	0.59
2:C:295:GLU:OE2	2:C:368:LYS:NZ	2.35	0.59
1:A:1430:THR:HG23	1:A:1433:GLN:H	1.68	0.59
1:B:3558:GLU:HG2	1:B:3561:ARG:HH21	1.67	0.59
1:B:3779:GLU:OE2	1:B:3782:ARG:NH2	2.34	0.59
1:B:3510:SER:HB3	1:B:3553:LEU:HD21	1.83	0.59
2:C:206:HIS:HB3	2:C:218:MET:HE3	1.84	0.59
2:C:353:ILE:HB	2:C:365:TRP:HB2	1.85	0.59
2:D:109:SER:HB3	2:D:128:GLU:HB3	1.83	0.59
1:A:2386:PRO:HG3	1:A:2413:LEU:HD12	1.84	0.59
1:A:3239:LYS:HD2	1:A:3451:TYR:CD1	2.36	0.59
1:B:3442:ALA:O	1:B:3446:ARG:HG2	2.03	0.59
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.35	0.59
1:A:3240:LEU:HD13	1:B:3448:LYS:HZ3	1.68	0.59
1:A:4470:PRO:HG3	1:A:4612:ASN:HD22	1.67	0.59
1:B:2220:LEU:HB2	1:B:2342:MET:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1985:HIS:CD2	1:A:1997:ILE:HG13	2.38	0.59
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.68	0.58
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.84	0.58
1:A:2683:ILE:HA	1:A:2686:MET:SD	2.44	0.58
1:B:3033:CYS:HB3	1:B:3050:LEU:HD22	1.85	0.58
1:B:4178:ARG:NH2	1:B:4297:PRO:O	2.35	0.58
1:A:3559:ARG:O	1:A:3563:GLN:HG2	2.02	0.58
1:B:2816:LEU:HD12	1:B:2817:PRO:HD2	1.84	0.58
1:B:4037:PRO:HB2	1:B:4118:PRO:HG2	1.84	0.58
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.84	0.58
1:A:3689:PRO:HG2	1:A:3692:LEU:HD23	1.85	0.58
1:A:4179:LEU:HD21	1:A:4238:ILE:HD13	1.85	0.58
1:B:3024:ASP:OD1	1:B:3025:GLU:N	2.36	0.58
2:D:97:ARG:HG3	2:D:410:ARG:HD2	1.86	0.58
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.84	0.58
1:A:2138:ILE:HD12	1:A:2161:LEU:HD12	1.85	0.58
1:B:4150:PRO:HB3	1:B:4159:ARG:HE	1.69	0.58
2:C:101:LYS:NZ	2:C:408:GLU:OE2	2.29	0.58
1:A:1511:PRO:O	1:A:1514:LYS:NZ	2.33	0.58
1:A:4209:GLU:OE1	1:A:4213:ARG:NH1	2.37	0.58
1:B:1547:LEU:HD12	1:B:1608:LEU:HD22	1.86	0.58
1:B:2025:ARG:NH2	1:B:2313:GLU:OE1	2.36	0.58
1:B:3133:LEU:HD11	1:B:3141:GLU:HB3	1.86	0.58
1:A:2441:PHE:HZ	1:A:2451:ARG:HB2	1.69	0.58
1:A:4049:TYR:OH	1:A:4191:GLN:OE1	2.18	0.58
1:B:2683:ILE:HA	1:B:2686:MET:HE2	1.86	0.58
1:A:3040:GLU:OE2	1:A:3053:TRP:NE1	2.37	0.58
1:A:4408:PRO:HG3	1:A:4526:GLN:HB3	1.85	0.58
1:B:4169:ILE:HG21	1:B:4302:ARG:HD2	1.84	0.58
1:A:2302:VAL:HA	1:A:2342:MET:HB2	1.86	0.57
1:B:2232:MET:HE2	6:B:4702:ATP:H2'	1.86	0.57
1:B:3708:LEU:HD23	1:B:3809:SER:HA	1.85	0.57
1:B:4226:THR:O	1:B:4230:ARG:NH2	2.37	0.57
2:C:265:THR:OG1	2:C:267:GLU:OE1	2.22	0.57
2:D:290:TYR:HE1	2:D:309:PRO:HA	1.68	0.57
1:B:1411:ARG:HD2	1:B:1412:HIS:N	2.19	0.57
1:A:1461:GLU:HA	1:A:1464:LYS:HG2	1.85	0.57
1:B:2974:GLU:OE1	1:B:2977:ARG:NH1	2.38	0.57
1:B:3818:LEU:HA	1:B:4346:MET:HE2	1.85	0.57
1:B:3869:ASN:HD21	1:B:4020:ILE:HG13	1.69	0.57
1:A:1397:ASN:O	1:A:1401:ILE:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1912:LYS:NZ	5:A:4701:ADP:O3B	2.36	0.57
1:A:1933:ASP:OD2	1:A:2314:ASN:ND2	2.35	0.57
1:B:2800:THR:OG1	5:B:4703:ADP:O2'	2.17	0.57
1:B:3499:GLN:O	1:B:3503:ILE:HG12	2.03	0.57
1:B:4191:GLN:HA	1:B:4194:LEU:HD12	1.86	0.57
1:A:1396:ILE:HG23	1:A:1438:ASP:OD2	2.05	0.57
1:A:1985:HIS:HD2	1:A:1997:ILE:HG13	1.69	0.57
1:A:2387:LEU:HD21	1:A:2463:HIS:HB3	1.87	0.57
1:B:1353:SER:HA	1:B:1404:LYS:HD2	1.86	0.57
1:B:3807:ALA:O	1:B:3811:ILE:HG12	2.04	0.57
1:A:1948:LEU:HG	1:A:2012:MET:HE2	1.86	0.57
2:C:207:ILE:HG23	2:C:219:TRP:HB2	1.87	0.57
2:D:175:LYS:NZ	2:D:187:THR:OG1	2.34	0.57
1:A:1958:ASP:HA	1:A:2017:THR:HB	1.87	0.57
1:B:2987:ASN:OD1	1:B:3060:ARG:NH2	2.38	0.57
1:B:3474:ARG:NH1	1:B:3764:ASP:OD1	2.38	0.57
1:B:3606:ASP:OD1	1:B:3607:ARG:N	2.38	0.57
1:B:2562:VAL:HG11	1:B:2755:MET:HB3	1.87	0.56
1:B:3129:VAL:HG21	1:B:3149:PHE:HB2	1.87	0.56
1:B:4411:ARG:O	1:B:4415:ARG:HG3	2.05	0.56
1:B:1666:LEU:HD23	1:B:1673:VAL:HA	1.86	0.56
1:B:4525:ARG:NH2	1:B:4539:LEU:O	2.38	0.56
2:D:254:ASN:HA	2:D:278:VAL:HG13	1.87	0.56
1:A:1408:LEU:HD12	1:A:1412:HIS:CD2	2.40	0.56
1:A:1607:LEU:HD23	1:A:1610:LYS:HZ3	1.70	0.56
1:A:2071:PRO:HB3	1:A:4536:LEU:HD23	1.86	0.56
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	1.87	0.56
1:A:3960:TRP:HZ2	1:A:3970:VAL:HG22	1.69	0.56
1:B:2213:ILE:HA	1:B:2216:ILE:HG22	1.86	0.56
1:B:2288:ILE:HD12	1:B:2333:LEU:HD23	1.87	0.56
1:B:3130:TYR:CZ	1:B:3132:LYS:HB2	2.41	0.56
1:A:3838:ASN:ND2	1:A:3842:GLU:OE1	2.28	0.56
1:A:4457:LYS:HZ2	1:A:4459:ILE:HD13	1.70	0.56
1:B:1798:MET:SD	1:B:1800:GLN:NE2	2.79	0.56
1:B:1936:PHE:HB3	1:B:1941:MET:HE3	1.87	0.56
1:B:2623:SER:N	1:B:2626:THR:OG1	2.30	0.56
1:B:3588:LEU:HD11	1:B:3638:VAL:HG21	1.86	0.56
1:A:3441:GLU:HA	1:A:3444:ILE:HD12	1.87	0.56
1:A:4105:TRP:HE3	1:A:4106:LEU:HD22	1.69	0.56
1:B:1911:GLY:N	5:B:4701:ADP:O1A	2.31	0.56
1:B:2654:GLN:NE2	1:B:2657:LYS:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3172:THR:HG21	1:B:3694:SER:HB3	1.87	0.56
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.88	0.56
1:B:1599:ARG:HH22	1:B:1603:ARG:HD2	1.71	0.56
1:B:1964:GLU:N	1:B:1964:GLU:OE1	2.39	0.56
1:B:4528:VAL:HG11	1:B:4592:TRP:HB2	1.87	0.56
1:A:1380:TYR:HD2	1:A:1382:SER:H	1.52	0.56
1:A:2134:GLN:HE21	1:A:2165:PHE:HD2	1.53	0.56
1:A:2717:ASP:O	1:A:4446:ASN:ND2	2.33	0.56
1:A:2918:HIS:O	1:A:2922:ILE:HG12	2.06	0.56
1:B:2222:MET:HE1	1:B:2234:TRP:HD1	1.71	0.56
1:B:3983:ILE:O	1:B:3987:ILE:HD12	2.05	0.56
2:D:272:LEU:HD13	2:D:323:TRP:CD2	2.41	0.56
1:B:1766:LEU:HD13	1:B:1833:ALA:HA	1.87	0.56
1:B:2419:ALA:O	1:B:2423:MET:HG2	2.06	0.56
1:B:2488:ARG:O	1:B:2492:ARG:HG2	2.06	0.56
1:A:3073:GLU:OE1	1:A:3073:GLU:N	2.27	0.56
1:A:3875:MET:O	1:A:3880:HIS:NE2	2.39	0.56
2:C:233:HIS:CE1	2:C:259:ARG:HD2	2.41	0.56
1:A:2649:VAL:HG13	1:A:2704:GLU:OE1	2.06	0.55
1:A:3196:GLU:O	1:A:3200:HIS:ND1	2.28	0.55
1:A:4518:GLU:OE1	1:A:4518:GLU:N	2.33	0.55
1:B:2592:VAL:HB	1:B:2733:VAL:HG22	1.88	0.55
1:B:3782:ARG:NH1	1:B:3786:GLU:OE2	2.39	0.55
2:C:243:ASN:OD1	2:C:246:GLY:N	2.36	0.55
2:D:396:VAL:HG12	2:D:406:VAL:HG22	1.88	0.55
1:A:2877:LEU:HD11	1:A:2884:VAL:HG13	1.88	0.55
1:B:3825:TYR:OH	1:B:3879:ASP:OD2	2.18	0.55
2:C:112:THR:HG21	2:C:154:GLN:HA	1.87	0.55
1:A:1623:ARG:NH1	1:A:1629:PHE:O	2.35	0.55
1:A:2494:LEU:O	1:A:2498:ILE:HG12	2.06	0.55
1:A:3875:MET:SD	1:A:3879:ASP:HB2	2.45	0.55
1:B:4176:ARG:NH1	1:B:4220:ASP:OD1	2.40	0.55
2:D:378:ALA:O	2:D:405:LYS:NZ	2.32	0.55
1:A:2260:SER:OG	1:A:2262:ASP:OD1	2.19	0.55
1:A:2793:ILE:O	1:A:2836:ARG:NH1	2.39	0.55
1:A:2910:VAL:N	5:A:4704:ADP:N1	2.53	0.55
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.88	0.55
1:B:1404:LYS:HA	1:B:1408:LEU:HD21	1.87	0.55
1:A:3795:GLU:O	1:A:3799:GLN:HG2	2.07	0.55
1:B:2358:ARG:NH2	5:B:4701:ADP:O3B	2.23	0.55
1:A:3024:ASP:OD1	1:A:3025:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:GLY:O	2:D:367:TYR:OH	2.24	0.55
1:A:1579:MET:HE3	1:A:1579:MET:O	2.06	0.55
1:A:2211:TYR:O	1:A:2215:GLN:HG3	2.07	0.55
1:A:3997:ARG:HH21	1:A:4329:ARG:HH12	1.55	0.55
1:B:2914:GLU:OE1	1:B:2914:GLU:N	2.38	0.55
1:B:2965:ARG:NH2	1:B:3614:PHE:O	2.40	0.55
1:A:2585:LEU:HD12	1:A:2591:LEU:HD21	1.87	0.55
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.41	0.55
1:B:3445:ALA:O	1:B:3449:GLU:HG2	2.07	0.55
1:A:1355:GLN:HG3	1:A:1358:LYS:H	1.72	0.55
1:B:1543:ARG:HB3	1:B:1608:LEU:HD13	1.89	0.55
2:C:109:SER:HB3	2:C:128:GLU:HB2	1.89	0.55
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.89	0.54
1:A:1521:LEU:O	1:A:1524:GLU:HB2	2.06	0.54
1:A:2660:VAL:HG22	1:A:2707:GLN:HB3	1.88	0.54
1:A:4161:PHE:O	1:A:4302:ARG:NH2	2.36	0.54
1:B:2802:TRP:CZ2	1:B:2829:ALA:HB2	2.42	0.54
1:B:3839:VAL:HG21	1:B:3863:LEU:HA	1.89	0.54
2:C:337:HIS:CE1	2:C:363:ARG:HD2	2.42	0.54
1:A:1618:TYR:HD1	1:A:1621:ARG:HH21	1.54	0.54
1:A:1861:MET:HE3	1:A:1890:LEU:HA	1.90	0.54
1:A:3135:GLN:HG3	1:A:3136:PRO:HD3	1.89	0.54
1:B:1938:PHE:HB2	1:B:1967:MET:HE1	1.89	0.54
1:B:4004:MET:HA	1:B:4007:MET:HG3	1.89	0.54
1:A:1408:LEU:HD12	1:A:1412:HIS:HD2	1.73	0.54
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.41	0.54
1:A:3045:ASP:OD1	1:A:3046:SER:N	2.41	0.54
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.19	0.54
2:C:123:MET:SD	2:C:135:TRP:HB2	2.47	0.54
1:A:2943:LYS:N	5:A:4704:ADP:O1B	2.36	0.54
2:D:362:LEU:HD21	2:D:383:VAL:HG11	1.90	0.54
1:A:1454:GLN:HA	1:A:1457:MET:HG2	1.90	0.54
1:A:2180:GLU:O	1:A:2184:LYS:HG2	2.08	0.54
1:A:2650:LEU:HG	1:A:2703:LEU:HA	1.89	0.54
1:A:3517:ALA:O	1:A:3525:ARG:NE	2.41	0.54
1:B:3459:GLN:HG3	1:B:3462:LYS:HZ1	1.73	0.54
1:B:3882:THR:HA	1:B:4339:MET:HE1	1.89	0.54
2:D:94:TRP:O	2:D:347:HIS:NE2	2.35	0.54
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.90	0.54
1:A:1889:TYR:CD1	1:A:1919:LEU:HD12	2.43	0.54
1:A:1932:CYS:HB3	1:A:1963:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2091:ARG:HG2	5:A:4701:ADP:H4'	1.90	0.54
1:A:2978:THR:O	1:A:2982:ARG:HG3	2.07	0.54
1:A:3499:GLN:O	1:A:3503:ILE:HG12	2.08	0.54
1:B:1569:GLN:O	1:B:1573:THR:HG23	2.08	0.54
1:B:4339:MET:HG3	1:B:4343:MET:HE1	1.89	0.54
1:A:3875:MET:HE1	1:A:3880:HIS:HA	1.89	0.53
1:B:2373:MET:HE1	6:B:4702:ATP:C5	2.43	0.53
2:C:219:TRP:HA	2:C:226:CYS:HA	1.90	0.53
1:A:1860:GLN:OE1	1:A:1865:LYS:NZ	2.34	0.53
1:A:2377:ASN:HB2	6:A:4702:ATP:H2	1.74	0.53
1:A:2556:GLU:OE2	1:A:2753:ARG:NH1	2.41	0.53
1:B:2232:MET:SD	1:B:2232:MET:N	2.81	0.53
1:B:4377:MET:HE1	1:B:4438:CYS:HA	1.89	0.53
1:A:1766:LEU:HD13	1:A:1833:ALA:HA	1.89	0.53
1:A:4525:ARG:NH2	1:A:4536:LEU:O	2.41	0.53
1:B:2999:VAL:HG11	1:B:3005:LEU:HG	1.91	0.53
1:A:1529:ARG:HE	1:A:1592:LEU:HD11	1.73	0.53
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.72	0.53
1:A:2091:ARG:HD2	1:A:2357:SER:HB2	1.91	0.53
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.89	0.53
1:A:4409:LEU:HB3	1:A:4504:LEU:HD21	1.90	0.53
2:D:372:CYS:SG	2:D:375:THR:OG1	2.66	0.53
1:A:1554:SER:O	1:A:1558:LYS:NZ	2.39	0.53
1:A:2262:ASP:OD1	1:A:2263:HIS:N	2.41	0.53
1:A:4338:ASP:OD1	1:A:4342:LYS:HE3	2.08	0.53
2:C:153:VAL:HG22	2:C:169:SER:HB2	1.89	0.53
1:B:2307:VAL:HG13	1:B:2312:VAL:HG11	1.90	0.53
1:A:2179:ARG:NH2	1:A:2195:ASP:OD1	2.42	0.53
1:A:2538:GLU:OE2	1:A:2551:LYS:NZ	2.32	0.53
1:A:3820:GLN:HB3	1:A:4345:LYS:NZ	2.23	0.53
1:A:3825:TYR:CZ	1:A:3875:MET:HG2	2.44	0.53
1:A:4173:PRO:HG2	1:A:4176:ARG:HH21	1.73	0.53
1:A:4392:PRO:O	1:A:4428:ARG:NH1	2.42	0.53
1:B:2221:MET:HB2	1:B:2361:MET:SD	2.49	0.53
1:A:1476:ASP:HB3	1:A:1488:ARG:NH1	2.24	0.53
1:A:2775:GLU:HG2	1:A:2779:MET:HE1	1.91	0.53
1:B:3612:THR:HG23	1:B:3633:LEU:HD11	1.91	0.53
1:A:1365:ALA:HA	1:A:1368:ASN:HD21	1.73	0.53
1:A:1547:LEU:HD12	1:A:1608:LEU:HD22	1.90	0.53
1:A:2016:ILE:HB	1:A:2018:MET:HE3	1.91	0.53
1:A:2786:GLN:HG3	1:A:2793:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3548:ALA:HB3	1:A:3551:GLU:HG2	1.91	0.53
1:B:3135:GLN:O	1:B:3137:PRO:HD3	2.09	0.53
2:C:306:LYS:HD2	2:C:308:GLY:H	1.74	0.53
2:D:197:SER:HB3	2:D:210:ALA:HB3	1.91	0.53
1:A:1543:ARG:HA	1:A:1546:TYR:CE2	2.44	0.52
1:A:3485:GLU:CD	1:A:3488:ARG:HH12	2.17	0.52
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.44	0.52
1:B:4157:MET:HE2	1:B:4157:MET:HA	1.91	0.52
2:D:169:SER:OG	2:D:170:ALA:N	2.42	0.52
1:B:1351:TRP:NE1	1:B:1354:VAL:O	2.43	0.52
1:B:1959:GLU:OE1	1:B:2025:ARG:NH1	2.41	0.52
2:C:228:LYS:HD2	2:C:266:LYS:HG3	1.90	0.52
1:A:1639:GLU:OE1	1:A:1653:HIS:NE2	2.41	0.52
1:B:2839:GLU:OE1	1:B:2839:GLU:N	2.35	0.52
1:A:1936:PHE:HB3	1:A:1941:MET:HE3	1.91	0.52
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.91	0.52
1:A:4492:ILE:HD13	1:A:4507:ILE:HG21	1.92	0.52
1:B:4030:ILE:HG21	1:B:4145:PHE:HZ	1.74	0.52
2:D:280:GLU:OE2	2:D:316:ARG:NH2	2.39	0.52
1:A:1664:ILE:HA	1:A:1676:ILE:HA	1.90	0.52
1:A:2147:PRO:HG3	1:A:2209:GLN:HB3	1.92	0.52
1:A:2284:LEU:HD12	1:A:2287:ILE:HD11	1.92	0.52
1:A:3603:GLU:O	1:A:3607:ARG:NH2	2.41	0.52
1:B:1657:MET:HG3	1:B:1658:PHE:CD1	2.45	0.52
1:B:4541:LEU:HD11	1:B:4590:LEU:HB2	1.91	0.52
1:A:1914:GLU:HG3	5:A:4701:ADP:H2'	1.91	0.52
1:A:4287:LYS:H	1:A:4293:ASP:HB3	1.75	0.52
1:B:1599:ARG:HA	1:B:1602:GLU:CD	2.35	0.52
1:B:3005:LEU:HD13	1:B:3081:THR:HG21	1.91	0.52
2:C:309:PRO:HG2	2:C:325:VAL:HB	1.90	0.52
2:C:278:VAL:HB	2:C:316:ARG:HD2	1.91	0.52
1:A:1473:TYR:CZ	1:A:1493:LEU:HD13	2.45	0.52
1:A:1558:LYS:HG3	1:A:1565:THR:HG21	1.91	0.52
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.92	0.52
1:B:1897:GLU:O	1:B:1899:ARG:NH1	2.43	0.52
1:B:2562:VAL:O	1:B:2804:ARG:NH1	2.43	0.52
1:B:3230:GLU:HA	1:B:3233:ASN:HD21	1.74	0.52
1:B:3998:PRO:HA	1:B:4001:LEU:HG	1.90	0.52
2:D:240:VAL:O	2:D:241:ARG:NH1	2.43	0.52
1:A:1351:TRP:HZ2	1:A:1356:PRO:HG3	1.74	0.52
1:A:1458:ALA:HA	1:A:1461:GLU:CD	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2621:ASN:HA	1:A:2664:ASP:HB3	1.92	0.52
1:B:1438:ASP:O	1:B:1442:ASN:ND2	2.43	0.52
1:A:1892:MET:HE2	1:A:2015:PHE:CE2	2.45	0.52
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.40	0.52
1:A:2964:HIS:H	1:A:2967:TYR:HB2	1.75	0.52
1:B:2211:TYR:HB2	1:B:2237:LEU:HD11	1.92	0.52
1:B:3217:GLU:O	1:B:3220:ARG:HG2	2.09	0.52
1:B:4485:ARG:HD3	1:B:4515:PHE:HE1	1.74	0.52
1:A:2148:LYS:HB2	1:A:2361:MET:HB2	1.92	0.51
1:A:2560:HIS:CD2	1:A:2561:LYS:HG2	2.45	0.51
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.75	0.51
1:A:4427:VAL:HG21	1:A:4478:TRP:HH2	1.75	0.51
1:B:2465:ALA:HB2	1:B:2493:TYR:CD2	2.44	0.51
1:A:2481:MET:HE1	1:A:2486:LEU:HD13	1.92	0.51
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.43	0.51
1:B:2944:THR:N	5:B:4704:ADP:O1B	2.42	0.51
1:B:4413:PHE:CD1	1:B:4492:ILE:HG21	2.45	0.51
2:C:233:HIS:ND1	2:C:255:ASP:OD2	2.25	0.51
1:A:1401:ILE:HA	1:A:1404:LYS:NZ	2.25	0.51
1:A:1452:VAL:HA	1:A:1512:TYR:CE2	2.46	0.51
1:A:2590:PRO:HB2	1:A:2731:VAL:HG22	1.92	0.51
1:A:3845:ASN:ND2	1:A:3862:ASP:OD2	2.38	0.51
1:B:1411:ARG:NH2	1:B:1452:VAL:HG12	2.25	0.51
1:B:1937:ASP:CG	1:B:2273:ARG:HH22	2.18	0.51
1:B:1939:GLN:HB2	1:B:2273:ARG:NH2	2.25	0.51
1:B:2190:TYR:O	1:B:2377:ASN:ND2	2.39	0.51
1:B:3717:LEU:HD12	1:B:3801:TYR:HD2	1.75	0.51
1:A:1360:ARG:HD2	1:A:1363:LEU:HD12	1.92	0.51
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	1.92	0.51
1:B:1508:LYS:HG2	1:B:1513:TYR:CZ	2.46	0.51
2:C:207:ILE:CG2	2:C:219:TRP:HB2	2.41	0.51
1:A:1954:TRP:NE1	1:A:2011:ASP:O	2.43	0.51
1:A:2202:MET:HE2	1:A:2202:MET:HA	1.93	0.51
1:A:3731:LEU:HD23	1:A:3787:THR:HG23	1.92	0.51
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.93	0.51
1:A:4511:LEU:HD23	1:A:4560:VAL:HG13	1.91	0.51
1:B:1393:TYR:CD1	1:B:1435:TRP:HB2	2.45	0.51
1:B:1667:ASN:ND2	1:B:1671:SER:OG	2.27	0.51
1:B:1667:ASN:ND2	1:B:1672:VAL:HG12	2.24	0.51
2:D:277:HIS:HB3	2:D:316:ARG:HB2	1.92	0.51
1:B:1836:PHE:O	1:B:1840:SER:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1861:MET:HG3	1:B:1893:THR:HG21	1.91	0.51
1:B:2063:GLU:O	1:B:2067:ASN:ND2	2.44	0.51
1:B:2591:LEU:HG	1:B:2709:VAL:HG22	1.92	0.51
1:B:3207:LYS:HB3	1:B:3760:ILE:HD11	1.92	0.51
2:D:133:LYS:HB3	2:D:135:TRP:HE1	1.76	0.51
1:A:1897:GLU:O	1:A:1899:ARG:NH1	2.43	0.51
1:A:2191:LEU:HD12	6:A:4702:ATP:C6	2.44	0.51
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.91	0.51
1:B:4030:ILE:HG23	1:B:4034:GLU:HB2	1.93	0.51
1:B:4157:MET:HE1	1:B:4184:ALA:C	2.36	0.51
1:B:4398:LEU:HG	1:B:4417:VAL:HG11	1.91	0.51
2:C:212:ARG:HA	2:C:236:TRP:CD1	2.46	0.51
1:A:1478:VAL:HG23	1:A:1488:ARG:NH1	2.26	0.51
1:B:2134:GLN:O	1:B:2138:ILE:HG12	2.11	0.51
1:B:2156:LEU:HD22	1:B:4411:ARG:HD2	1.92	0.51
1:B:3983:ILE:HG13	1:B:4011:THR:HG22	1.92	0.51
1:A:3469:GLU:OE2	1:A:3473:ASN:ND2	2.43	0.51
1:A:4339:MET:HE3	1:A:4343:MET:HE1	1.92	0.51
1:A:1769:MET:SD	1:A:1777:PRO:HD2	2.51	0.51
1:A:2773:MET:HB3	1:A:2799:MET:HE1	1.91	0.51
1:B:1408:LEU:HA	1:B:1412:HIS:HE1	1.76	0.51
1:B:2682:PHE:CD2	1:B:2686:MET:HE1	2.46	0.51
1:A:1964:GLU:OE1	1:A:1966:ARG:HG2	2.10	0.50
1:A:4039:THR:HG23	1:A:4142:GLY:HA2	1.92	0.50
1:A:4069:ILE:HD13	1:A:4079:GLN:HG3	1.92	0.50
1:B:2304:ASP:OD1	1:B:2684:ARG:NH2	2.45	0.50
1:B:3457:GLU:O	1:B:3461:ILE:HG12	2.11	0.50
2:D:348:SER:H	2:D:388:PHE:HE2	1.59	0.50
1:A:1974:GLN:O	1:A:1978:ILE:HG12	2.11	0.50
1:B:1349:GLN:HE21	1:B:1351:TRP:H	1.57	0.50
1:B:1453:ALA:O	1:B:1456:GLU:HG2	2.11	0.50
1:B:3725:ASP:OD1	1:B:3728:ARG:NH2	2.33	0.50
1:A:1571:ILE:HG12	1:A:1607:LEU:HD13	1.94	0.50
1:B:1589:MET:SD	1:B:1589:MET:N	2.84	0.50
1:B:1589:MET:O	1:B:1593:ASN:N	2.39	0.50
1:B:1835:SER:OG	1:B:1837:GLU:OE1	2.30	0.50
1:B:2449:LEU:HA	1:B:2453:ARG:HH21	1.76	0.50
2:C:90:ASP:HB3	2:C:93:GLU:HB3	1.93	0.50
1:A:3731:LEU:HB2	1:A:3791:MET:HE3	1.93	0.50
1:B:4487:LYS:O	1:B:4490:GLN:HG2	2.11	0.50
2:D:278:VAL:HB	2:D:316:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1390:LEU:HD23	1:A:1393:TYR:HD2	1.77	0.50
1:A:2441:PHE:HA	1:A:2449:LEU:HD23	1.94	0.50
1:B:1917:LYS:NZ	1:B:2322:ASN:OD1	2.31	0.50
1:B:2648:VAL:HG11	1:B:2694:ARG:NH2	2.27	0.50
2:C:136:ASP:N	2:C:143:GLU:OE1	2.45	0.50
2:C:243:ASN:HD22	2:C:248:LEU:HB2	1.77	0.50
2:D:155:ASP:HB3	2:D:198:VAL:HG12	1.93	0.50
1:A:3928:THR:H	1:A:3931:GLN:HE21	1.58	0.50
1:B:4168:ARG:NH2	1:B:4217:ASP:OD1	2.44	0.50
1:A:1519:ASP:OD1	1:A:1520:ALA:N	2.44	0.50
1:B:1785:VAL:O	1:B:1789:LEU:HG	2.11	0.50
1:B:2495:VAL:HG11	1:B:2526:LEU:HD21	1.94	0.50
1:B:2566:ASP:OD1	1:B:2567:VAL:N	2.44	0.50
1:B:4419:MET:HA	1:B:4422:LYS:HG2	1.92	0.50
2:C:110:PRO:HB3	2:C:400:VAL:HA	1.93	0.50
1:B:2387:LEU:HB2	1:B:2412:MET:HE2	1.94	0.50
1:B:3229:LEU:O	1:B:3233:ASN:ND2	2.45	0.50
1:A:2909:LEU:HD21	1:A:2945:THR:HG21	1.93	0.50
1:B:1674:LEU:HB3	1:B:1685:MET:HE1	1.93	0.50
1:B:4544:ASN:OD1	1:B:4589:GLN:HB2	2.12	0.50
2:C:153:VAL:HA	2:C:169:SER:HA	1.92	0.50
1:A:1798:MET:SD	1:A:1800:GLN:NE2	2.85	0.49
1:A:1860:GLN:HB3	1:A:1865:LYS:NZ	2.27	0.49
1:A:2060:ARG:HH22	1:A:2129:GLU:HA	1.76	0.49
1:A:3131:ASP:OD1	1:A:3132:LYS:N	2.45	0.49
1:A:3793:GLU:HA	1:A:3796:THR:HG22	1.92	0.49
1:A:4018:MET:SD	1:A:4018:MET:N	2.84	0.49
1:B:3175:HIS:CE1	1:B:3585:ARG:HH12	2.30	0.49
2:C:91:PRO:HA	2:C:94:TRP:CZ3	2.47	0.49
2:D:257:THR:HA	2:D:272:LEU:O	2.12	0.49
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.94	0.49
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.94	0.49
1:B:1911:GLY:O	1:B:1915:SER:N	2.34	0.49
1:B:2176:THR:O	1:B:2179:ARG:N	2.45	0.49
1:B:4488:GLN:O	1:B:4492:ILE:HD12	2.11	0.49
1:B:4554:ASP:OD2	1:B:4557:SER:OG	2.27	0.49
1:A:2159:SER:OG	1:A:4411:ARG:NH1	2.45	0.49
1:A:3175:HIS:CE1	1:A:3585:ARG:HH12	2.30	0.49
1:B:1688:THR:OG1	1:B:1708:GLU:OE1	2.30	0.49
2:C:198:VAL:HG22	2:C:207:ILE:HD11	1.93	0.49
1:A:1457:MET:HA	1:A:1460:GLU:CD	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1755:GLN:NE2	1:A:1814:GLU:OE2	2.32	0.49
1:B:1992:LYS:O	1:B:1992:LYS:NZ	2.31	0.49
1:B:2564:ALA:HB3	1:B:2567:VAL:HG22	1.93	0.49
1:B:2085:HIS:HB2	1:B:2361:MET:HE2	1.94	0.49
1:B:3839:VAL:HG11	1:B:3863:LEU:HB2	1.94	0.49
2:D:274:GLU:HB2	2:D:323:TRP:HH2	1.77	0.49
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.95	0.49
1:A:4308:TRP:CH2	1:A:4312:LEU:HD21	2.48	0.49
1:B:1978:ILE:HD11	1:B:2001:LEU:HD11	1.94	0.49
1:B:2060:ARG:NH2	1:B:2129:GLU:O	2.46	0.49
1:B:2641:TYR:CE1	1:B:2650:LEU:HD13	2.47	0.49
1:B:4405:ILE:O	1:B:4411:ARG:NH1	2.45	0.49
1:A:1507:MET:O	1:A:1510:SER:OG	2.23	0.49
1:A:1563:VAL:O	1:A:1567:ARG:HG2	2.13	0.49
1:A:2628:PRO:HG3	1:A:2679:VAL:HA	1.95	0.49
1:B:2009:SER:O	1:B:2012:MET:HG3	2.13	0.49
1:A:1415:GLN:NE2	1:A:1449:VAL:HG13	2.28	0.49
1:A:1495:ASN:HA	1:A:1498:LYS:HE3	1.95	0.49
1:A:2641:TYR:CE2	1:A:2694:ARG:HD3	2.48	0.49
1:A:4136:VAL:O	1:A:4140:ARG:HG3	2.12	0.49
1:B:1991:ASP:O	1:B:1994:SER:OG	2.29	0.49
1:A:1454:GLN:HA	1:A:1457:MET:HE3	1.94	0.49
1:A:1960:PHE:HB3	1:A:2018:MET:HE1	1.95	0.49
1:A:2478:ASP:OD1	1:A:2479:PHE:N	2.45	0.49
1:A:2903:GLU:OE1	1:A:2952:TRP:NE1	2.46	0.49
1:A:4093:TRP:CD1	1:A:4123:ARG:HB2	2.48	0.49
1:B:1399:LEU:HD23	1:B:1403:LEU:HB2	1.93	0.49
1:A:1518:GLU:OE1	1:A:1518:GLU:N	2.37	0.49
1:A:1627:PRO:HB2	1:A:1951:VAL:HG23	1.95	0.49
1:A:1929:VAL:HG12	1:A:1956:CYS:HB3	1.95	0.49
1:A:3822:HIS:HE1	1:A:4130:ILE:HD11	1.77	0.49
1:A:3856:LEU:O	1:A:3859:ILE:HG22	2.13	0.49
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.95	0.49
1:B:3931:GLN:NE2	1:B:3996:PHE:O	2.40	0.49
1:B:4009:VAL:HG13	1:B:4013:LEU:HD12	1.94	0.49
1:A:2053:MET:O	1:A:2056:SER:OG	2.23	0.48
1:A:4335:GLN:O	1:A:4339:MET:N	2.35	0.48
1:B:1698:ILE:HD12	1:B:1701:TRP:HE1	1.78	0.48
1:B:3219:ARG:CZ	1:B:3472:VAL:HG13	2.42	0.48
2:C:186:ARG:HG2	2:C:188:MET:SD	2.53	0.48
1:A:1451:LEU:HD13	1:A:1454:GLN:NE2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2047:GLN:NE2	1:A:2051:GLN:OE1	2.44	0.48
1:A:2935:LEU:HB2	1:A:3067:THR:HG22	1.96	0.48
1:A:2963:VAL:HG13	1:A:3643:PRO:HG2	1.95	0.48
1:B:1490:TRP:CG	1:B:1538:ILE:HD12	2.48	0.48
1:B:2139:GLN:HG3	1:B:2170:TYR:CE1	2.48	0.48
1:B:3548:ALA:HB3	1:B:3551:GLU:HG2	1.95	0.48
1:B:4069:ILE:O	1:B:4096:LEU:HA	2.13	0.48
2:D:197:SER:HB2	2:D:239:MET:HA	1.94	0.48
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.40	0.48
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.77	0.48
1:B:1484:CYS:SG	1:B:1485:ARG:N	2.86	0.48
1:B:1600:SER:O	1:B:1603:ARG:HG2	2.14	0.48
1:B:3622:ASN:O	1:B:3625:SER:OG	2.24	0.48
2:D:92:LYS:HG3	2:D:349:GLY:HA3	1.96	0.48
2:D:309:PRO:HG2	2:D:325:VAL:HB	1.95	0.48
1:A:1407:ALA:HB2	1:A:1457:MET:HE1	1.95	0.48
1:A:2092:ALA:O	1:A:2096:VAL:HG23	2.13	0.48
1:A:2384:SER:HB2	1:A:2385:ILE:HD12	1.95	0.48
1:B:2210:LEU:HD13	1:B:2362:VAL:HG21	1.95	0.48
1:B:2213:ILE:HG22	1:B:2220:LEU:HD21	1.93	0.48
1:B:3239:LYS:HB3	1:B:3451:TYR:CE2	2.48	0.48
1:B:4052:SER:O	1:B:4056:GLU:HG2	2.13	0.48
2:C:216:ILE:HB	2:C:230:PHE:HB2	1.96	0.48
2:C:254:ASN:HD22	2:C:278:VAL:HG21	1.78	0.48
1:A:1417:MET:HE1	1:A:1423:ASN:HA	1.95	0.48
1:A:2430:ASN:O	1:A:2435:LYS:NZ	2.46	0.48
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.94	0.48
1:A:3761:LEU:HA	1:A:3767:ILE:HD11	1.95	0.48
2:D:200:ILE:HG12	2:D:207:ILE:HG12	1.95	0.48
2:D:201:MET:SD	2:D:201:MET:N	2.85	0.48
1:A:1668:GLU:N	1:A:1668:GLU:OE1	2.44	0.48
1:A:2239:LYS:O	1:A:2242:GLU:HB3	2.14	0.48
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.38	0.48
1:A:4393:GLN:HG3	1:A:4428:ARG:CZ	2.43	0.48
1:A:4525:ARG:HH21	1:A:4537:GLU:HA	1.78	0.48
1:A:4529:ALA:O	1:A:4533:SER:N	2.47	0.48
1:B:1413:TRP:HZ2	1:B:1424:TRP:CE2	2.31	0.48
1:B:2047:GLN:HA	1:B:2070:VAL:HG21	1.95	0.48
1:B:3459:GLN:HG3	1:B:3462:LYS:HZ3	1.78	0.48
1:B:4397:HIS:CE1	1:B:4418:LYS:HG3	2.49	0.48
2:C:91:PRO:HA	2:C:94:TRP:HZ3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.79	0.48
1:A:2230:LYS:HG2	1:A:2364:PHE:CG	2.49	0.48
1:A:2232:MET:HE3	1:A:2232:MET:H	1.77	0.48
1:A:4156:ASN:ND2	1:A:4188:ALA:HA	2.29	0.48
1:B:4190:ILE:HD12	1:B:4201:TRP:HZ2	1.79	0.48
1:A:1491:ASP:OD1	1:A:1492:ASP:N	2.47	0.48
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.14	0.48
1:A:3243:MET:HE1	1:A:3444:ILE:HG23	1.95	0.48
1:B:1437:VAL:HG12	1:B:1442:ASN:ND2	2.23	0.48
1:B:1850:GLN:HB3	1:B:1856:GLN:HG2	1.96	0.48
1:B:1929:VAL:H	1:B:2332:ARG:HH21	1.60	0.48
1:B:2956:LEU:HD13	1:B:2989:LYS:HB3	1.95	0.48
1:B:3073:GLU:OE1	1:B:3073:GLU:N	2.45	0.48
1:B:4110:GLU:OE1	1:B:4137:ASN:ND2	2.47	0.48
1:A:1364:ASP:O	1:A:1368:ASN:ND2	2.47	0.48
1:A:2156:LEU:O	1:A:2159:SER:OG	2.27	0.48
1:A:2277:ASP:OD2	1:A:2285:ARG:NE	2.44	0.48
1:A:2534:ILE:HD12	1:A:2534:ILE:H	1.79	0.48
1:A:3826:GLN:HG3	1:A:4136:VAL:HG13	1.96	0.48
1:A:3989:ARG:HB3	1:A:4004:MET:HE1	1.96	0.48
1:B:1375:ALA:HA	1:B:1378:ARG:HB2	1.96	0.48
1:B:1451:LEU:HD13	1:B:1454:GLN:NE2	2.28	0.48
1:A:2533:PRO:HB2	1:A:2535:ILE:HG22	1.95	0.48
1:B:2488:ARG:HG2	1:B:2492:ARG:HH12	1.79	0.48
1:B:3154:LEU:HD11	1:B:3516:TYR:HB3	1.95	0.48
1:B:3872:ALA:HA	1:B:3875:MET:HB3	1.96	0.48
2:C:358:ASP:C	2:C:360:LYS:H	2.21	0.48
1:A:1492:ASP:OD1	1:A:1493:LEU:N	2.47	0.47
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.14	0.47
1:A:4078:ASN:HB3	1:A:4082:LYS:NZ	2.29	0.47
1:A:4289:ASP:OD1	1:A:4292:LYS:N	2.45	0.47
1:A:4525:ARG:HE	1:A:4536:LEU:HG	1.79	0.47
1:B:1363:LEU:HB2	1:B:1394:MET:HG2	1.96	0.47
1:B:4446:ASN:OD1	1:B:4449:ARG:NH1	2.43	0.47
2:C:159:ASP:OD2	2:C:161:SER:OG	2.32	0.47
1:A:1415:GLN:HE21	1:A:1449:VAL:HG13	1.78	0.47
1:A:1817:HIS:CE1	1:A:1881:GLN:HG2	2.49	0.47
1:A:4525:ARG:NH2	1:A:4537:GLU:HA	2.29	0.47
1:B:2995:ASP:OD1	1:B:2996:GLU:N	2.47	0.47
1:B:3124:ASP:OD1	1:B:3125:TYR:N	2.45	0.47
1:B:3597:THR:O	1:B:3601:MET:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:183:GLU:OE1	2:D:183:GLU:N	2.47	0.47
1:A:1448:ASP:OD1	1:A:1449:VAL:N	2.48	0.47
1:A:3967:GLU:HB2	1:A:4004:MET:SD	2.54	0.47
1:B:1358:LYS:O	1:B:1362:ASN:ND2	2.47	0.47
1:B:1443:GLU:HG2	1:B:1447:LYS:NZ	2.28	0.47
1:B:1698:ILE:HD12	1:B:1701:TRP:NE1	2.29	0.47
1:B:2654:GLN:OE1	1:B:2657:LYS:HB2	2.14	0.47
1:B:3517:ALA:O	1:B:3525:ARG:NE	2.48	0.47
1:B:3826:GLN:HG3	1:B:4136:VAL:HG13	1.96	0.47
1:B:3942:PRO:O	1:B:3945:LYS:NZ	2.40	0.47
2:D:262:VAL:HB	2:D:265:THR:OG1	2.14	0.47
1:A:3459:GLN:O	1:A:3462:LYS:HG2	2.15	0.47
1:A:3731:LEU:HG	1:A:3734:LEU:HD12	1.96	0.47
1:A:3820:GLN:HB3	1:A:4345:LYS:HZ2	1.77	0.47
1:B:2042:THR:HG22	1:B:2043:LYS:HG3	1.95	0.47
1:B:3072:SER:O	1:B:3076:LYS:HG3	2.14	0.47
1:A:1836:PHE:O	1:A:1840:SER:N	2.47	0.47
1:A:1892:MET:HE2	1:A:2015:PHE:HE2	1.80	0.47
1:A:3244:VAL:O	1:A:3248:GLN:HG3	2.15	0.47
1:B:1964:GLU:HB2	1:B:1967:MET:HB2	1.96	0.47
2:D:123:MET:SD	2:D:135:TRP:HB2	2.54	0.47
1:B:1409:LYS:O	1:B:1412:HIS:ND1	2.47	0.47
1:B:1910:THR:N	5:B:4701:ADP:O1A	2.47	0.47
1:B:3459:GLN:HA	1:B:3462:LYS:HZ3	1.80	0.47
1:B:3786:GLU:O	1:B:3790:VAL:HG23	2.15	0.47
1:B:4277:SER:HA	1:B:4282:PHE:CD2	2.49	0.47
1:A:1441:LYS:HE3	1:A:1442:ASN:HD22	1.80	0.47
1:A:1526:LYS:HD2	1:A:1529:ARG:HH22	1.79	0.47
1:A:2603:MET:HE3	5:A:4703:ADP:H5'1	1.96	0.47
1:A:2934:LEU:HD13	1:A:3085:LEU:HD11	1.96	0.47
1:A:4305:PHE:O	1:A:4309:VAL:HG23	2.15	0.47
1:B:2138:ILE:HD12	1:B:2161:LEU:HD12	1.97	0.47
1:B:2270:PRO:HA	1:B:2273:ARG:HH11	1.80	0.47
1:B:2465:ALA:HB2	1:B:2493:TYR:CE2	2.50	0.47
1:B:2596:PRO:HB2	1:B:2738:TYR:CZ	2.49	0.47
1:B:3150:VAL:HG22	1:B:3532:TRP:CD1	2.50	0.47
1:B:3647:PRO:HA	1:B:3652:GLU:OE2	2.14	0.47
1:B:3876:LEU:HD23	1:B:4146:VAL:HG11	1.96	0.47
2:C:287:GLU:HA	2:C:290:TYR:CE2	2.50	0.47
2:C:381:HIS:CG	2:C:382:PHE:H	2.33	0.47
2:D:218:MET:HE3	2:D:228:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1360:ARG:HH12	1:A:1364:ASP:HB3	1.80	0.47
1:A:1455:GLY:HA3	1:A:1512:TYR:HD2	1.79	0.47
1:A:2601:LYS:N	5:A:4703:ADP:O1B	2.48	0.47
1:B:2969:GLY:HA2	1:B:3004:PHE:HE1	1.80	0.47
1:A:1350:PRO:HA	1:A:1429:LEU:O	2.15	0.47
1:A:3635:VAL:HB	1:A:3679:LEU:HD13	1.95	0.47
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.80	0.47
1:B:1451:LEU:O	1:B:1454:GLN:HG2	2.15	0.47
1:B:1518:GLU:HG2	1:B:1519:ASP:N	2.29	0.47
1:B:3249:GLU:HA	1:B:3252:LYS:HD2	1.96	0.47
1:A:2628:PRO:HG2	1:A:2678:ARG:HG2	1.97	0.47
1:A:3236:ALA:HA	1:A:3239:LYS:NZ	2.30	0.47
1:A:4248:ALA:HB2	1:A:4269:LEU:HD12	1.96	0.47
1:B:3003:GLY:O	1:B:3007:ARG:HG2	2.14	0.47
1:B:4462:ARG:NE	1:B:4462:ARG:HA	2.30	0.47
2:D:94:TRP:CE2	2:D:393:PRO:HB3	2.50	0.47
2:D:313:SER:OG	2:D:323:TRP:NE1	2.40	0.47
1:A:1359:LEU:O	1:A:1363:LEU:HG	2.15	0.46
1:A:1497:VAL:HG21	1:A:1531:MET:HE3	1.95	0.46
1:A:2210:LEU:HD12	1:A:2362:VAL:HG11	1.97	0.46
1:A:3154:LEU:HD11	1:A:3516:TYR:HB3	1.97	0.46
1:B:2238:LEU:HD13	1:B:2300:TRP:CE3	2.51	0.46
1:B:2446:ILE:HD11	1:B:2714:PRO:HB3	1.98	0.46
2:D:257:THR:HG22	2:D:273:ARG:HG2	1.97	0.46
1:A:1626:PHE:HB3	1:A:1629:PHE:CE2	2.50	0.46
1:A:1750:VAL:HG12	1:A:1811:LEU:HD21	1.96	0.46
1:A:2447:MET:HE3	1:A:2447:MET:HA	1.97	0.46
1:A:3617:ASP:OD1	2:C:226:CYS:HB3	2.15	0.46
1:B:4404:ASN:HB3	1:B:4410:PHE:CD2	2.51	0.46
1:A:2574:THR:O	1:A:2578:GLU:HG2	2.16	0.46
1:A:2633:LYS:NZ	1:A:3019:GLY:H	2.03	0.46
1:A:2671:MET:HB2	1:A:2721:LYS:HG2	1.97	0.46
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	1.97	0.46
1:B:3753:LEU:HD21	1:B:3770:LEU:HD21	1.97	0.46
1:B:4044:CYS:SG	1:B:4144:ILE:HG23	2.56	0.46
1:A:1471:ASN:HA	1:A:1589:MET:HE1	1.97	0.46
1:A:1561:LEU:O	1:A:1565:THR:OG1	2.22	0.46
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.31	0.46
1:A:2269:ASP:HB3	1:A:2274:GLU:H	1.80	0.46
1:A:2315:LEU:HB3	1:A:2319:LEU:HD13	1.97	0.46
1:A:3451:TYR:O	1:A:3455:ILE:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4599:GLU:HG3	1:A:4600:LYS:H	1.80	0.46
1:B:1390:LEU:O	1:B:1395:LYS:HB3	2.15	0.46
1:B:1996:PRO:HB3	1:B:2007:LYS:HD3	1.98	0.46
1:B:2855:LEU:HD21	1:B:2863:ARG:HG3	1.96	0.46
1:A:3456:SER:HB2	1:B:3459:GLN:NE2	2.31	0.46
1:A:3484:ALA:HA	1:A:3487:GLU:OE1	2.15	0.46
1:A:3769:THR:O	1:A:3773:LEU:HG	2.15	0.46
1:B:1399:LEU:HD11	1:B:1434:ILE:HG12	1.97	0.46
1:B:1478:VAL:HG11	1:B:1488:ARG:HH21	1.80	0.46
1:B:2943:LYS:HG2	1:B:3094:PHE:CD2	2.49	0.46
1:A:1745:TYR:O	1:A:1807:LYS:NZ	2.43	0.46
1:A:1860:GLN:CD	1:A:1865:LYS:HZ3	2.18	0.46
1:A:3518:GLY:O	1:A:3525:ARG:NH2	2.49	0.46
1:A:3537:GLN:NE2	1:A:3538:GLN:HG3	2.31	0.46
1:A:3606:ASP:OD1	1:A:3607:ARG:N	2.48	0.46
1:A:4445:THR:H	1:A:4448:LEU:HB2	1.81	0.46
1:B:1424:TRP:HH2	1:B:1434:ILE:HB	1.81	0.46
1:B:1470:TRP:HE1	1:B:1527:LEU:HD21	1.79	0.46
1:B:2430:ASN:O	1:B:2435:LYS:NZ	2.49	0.46
1:B:2628:PRO:HB3	1:B:2682:PHE:CD2	2.51	0.46
1:A:1466:ILE:HG13	1:A:1500:HIS:ND1	2.30	0.46
1:A:2616:GLU:HG3	1:A:2659:LEU:HD12	1.98	0.46
1:A:2658:TRP:CE2	1:A:2705:ARG:HA	2.51	0.46
1:A:3251:GLU:OE2	1:B:3248:GLN:HG2	2.16	0.46
1:B:1903:SER:HB3	1:B:2038:SER:HA	1.98	0.46
1:B:1949:CYS:HA	1:B:2012:MET:SD	2.56	0.46
1:B:3174:ARG:HA	1:B:3177:LEU:HD12	1.98	0.46
1:B:3960:TRP:O	1:B:3966:PRO:HB3	2.16	0.46
1:A:1438:ASP:CG	1:A:1439:LEU:H	2.24	0.46
1:A:1637:LEU:O	1:A:1641:ILE:HG12	2.16	0.46
1:A:1673:VAL:HG23	1:A:1692:ILE:HD11	1.98	0.46
1:A:1685:MET:O	1:A:1712:THR:HG21	2.16	0.46
1:A:1985:HIS:CE1	1:A:2010:PRO:HB3	2.50	0.46
1:A:2492:ARG:HG2	1:A:2545:TRP:CE2	2.51	0.46
1:B:2177:ALA:O	1:B:2181:GLU:HG2	2.16	0.46
1:B:2369:LEU:HD21	6:B:4702:ATP:C8	2.51	0.46
1:B:2464:GLN:HG2	1:B:2583:THR:HG23	1.98	0.46
2:D:233:HIS:NE2	2:D:251:SER:OG	2.45	0.46
1:A:3021:PHE:CD2	1:A:3029:LEU:HD22	2.51	0.46
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.98	0.46
1:B:1965:GLU:HG2	1:B:2026:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:MET:SD	2:C:241:ARG:HG2	2.56	0.46
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.51	0.46
1:A:3221:ASP:O	1:A:3225:LYS:HG2	2.16	0.46
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.16	0.46
1:A:4469:VAL:HG21	1:A:4473:MET:HE2	1.97	0.46
1:B:1451:LEU:HD13	1:B:1454:GLN:HE21	1.81	0.46
1:B:2221:MET:HE2	1:B:2361:MET:SD	2.55	0.46
1:B:2519:ARG:NH2	1:B:2527:PRO:O	2.45	0.46
1:B:2538:GLU:HB3	1:B:2548:TRP:CE2	2.51	0.46
1:B:2964:HIS:H	1:B:2967:TYR:HB2	1.80	0.46
1:A:2063:GLU:HG2	1:A:2064:VAL:N	2.30	0.45
1:A:2269:ASP:OD2	1:A:2272:THR:OG1	2.30	0.45
1:A:2548:TRP:CE2	1:A:2576:ARG:HG2	2.50	0.45
1:A:2657:LYS:O	1:A:2705:ARG:NH1	2.44	0.45
1:A:3489:TRP:HH2	1:A:3753:LEU:HD12	1.80	0.45
1:A:4194:LEU:HA	1:A:4201:TRP:HD1	1.81	0.45
1:B:1351:TRP:CD2	1:B:1354:VAL:HB	2.51	0.45
1:B:1478:VAL:HG11	1:B:1488:ARG:HE	1.80	0.45
1:B:2667:ASN:ND2	1:B:2713:ASN:O	2.48	0.45
1:B:2784:PHE:HB3	1:B:2792:TYR:CD2	2.51	0.45
2:C:98:PRO:HG2	3:G:2:SER:HA	1.98	0.45
1:A:1526:LYS:HB3	1:A:1526:LYS:HE2	1.70	0.45
1:A:2592:VAL:HB	1:A:2733:VAL:HG22	1.99	0.45
1:A:3222:LEU:HD13	1:A:3468:VAL:HG12	1.97	0.45
1:A:4307:GLN:HA	1:A:4310:GLU:CD	2.41	0.45
1:A:4518:GLU:HA	1:A:4521:ILE:HG22	1.98	0.45
1:B:1393:TYR:CE2	1:B:1431:LEU:HD13	2.52	0.45
1:B:1519:ASP:O	1:B:1522:SER:OG	2.17	0.45
1:B:1606:ASP:HB3	1:B:1610:LYS:NZ	2.31	0.45
1:B:2221:MET:HE1	1:B:2359:CYS:HB2	1.98	0.45
1:B:3211:THR:O	1:B:3215:VAL:HG23	2.16	0.45
1:B:4412:PHE:CZ	1:B:4520:TYR:HB2	2.51	0.45
2:D:138:GLU:N	2:D:138:GLU:OE1	2.48	0.45
2:D:360:LYS:HE3	2:D:380:GLU:HA	1.99	0.45
1:A:1393:TYR:CD1	1:A:1435:TRP:HD1	2.35	0.45
1:A:1598:GLN:NE2	1:A:1602:GLU:OE2	2.41	0.45
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.17	0.45
1:A:3235:ALA:O	1:A:3239:LYS:HG2	2.16	0.45
1:A:3873:ARG:HD2	1:A:4025:LEU:HD13	1.98	0.45
1:A:4028:THR:HG23	1:A:4062:GLN:HE21	1.81	0.45
1:B:1637:LEU:HA	1:B:1640:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1946:VAL:HG22	1:B:2006:VAL:HG21	1.99	0.45
1:B:3883:PHE:O	1:B:3887:LEU:HD23	2.16	0.45
2:D:312:LEU:HD13	2:D:344:VAL:HG12	1.98	0.45
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.98	0.45
1:B:1554:SER:O	1:B:1558:LYS:NZ	2.37	0.45
1:B:3215:VAL:HG13	1:B:3219:ARG:HH12	1.81	0.45
1:A:1420:LEU:HD23	1:A:1445:ILE:HD11	1.98	0.45
1:A:3882:THR:HG21	1:A:4342:LYS:HB3	1.98	0.45
1:A:4043:MET:HB2	1:A:4127:THR:HA	1.97	0.45
1:B:1462:PHE:HB2	1:B:1507:MET:HE2	1.99	0.45
1:B:1561:LEU:HB3	1:B:1564:GLU:CD	2.41	0.45
1:B:2385:ILE:O	1:B:2416:GLN:NE2	2.38	0.45
1:B:2980:LEU:HB3	1:B:3054:PHE:HZ	1.81	0.45
1:B:2104:LYS:HG3	1:B:2131:LEU:HD21	1.98	0.45
2:C:151:ASP:OD1	2:C:152:SER:N	2.42	0.45
1:A:2603:MET:HE1	5:A:4703:ADP:N9	2.31	0.45
1:A:3792:GLN:O	1:A:3795:GLU:HG3	2.16	0.45
1:B:2377:ASN:HB2	6:B:4702:ATP:H2	1.80	0.45
1:A:1741:TRP:CH2	1:A:1750:VAL:HG13	2.52	0.45
1:A:3630:GLY:HA2	1:A:3675:PHE:HB2	1.99	0.45
1:B:4470:PRO:HG3	1:B:4612:ASN:HD22	1.82	0.45
1:A:4172:SER:OG	1:A:4173:PRO:HD3	2.17	0.45
1:B:1490:TRP:CD1	1:B:1538:ILE:HD12	2.52	0.45
1:A:1476:ASP:HB3	1:A:1488:ARG:CZ	2.46	0.45
1:A:1835:SER:OG	1:A:1837:GLU:OE1	2.35	0.45
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.17	0.45
1:A:2739:PRO:HB2	1:A:2744:LEU:HG	1.98	0.45
1:A:3167:ARG:HH22	1:A:3687:GLU:HA	1.83	0.45
2:C:239:MET:HE1	2:C:282:ILE:H	1.82	0.45
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.99	0.44
1:A:3117:LYS:HB3	1:A:3120:TYR:HB2	1.99	0.44
1:A:4297:PRO:HG3	1:A:4308:TRP:CE2	2.52	0.44
1:B:2232:MET:HE1	6:B:4702:ATP:H5'1	2.00	0.44
1:B:3621:LYS:O	1:B:3621:LYS:NZ	2.46	0.44
1:A:1365:ALA:HA	1:A:1368:ASN:ND2	2.32	0.44
1:A:1756:ILE:O	1:A:1760:GLU:HG2	2.16	0.44
1:A:3071:SER:O	1:A:3075:LEU:N	2.46	0.44
1:A:4549:GLN:OE1	1:A:4587:LEU:HB2	2.17	0.44
1:B:2300:TRP:CD1	1:B:2340:ARG:HB2	2.53	0.44
1:B:3078:ARG:HD3	1:B:3078:ARG:HA	1.73	0.44
1:A:1455:GLY:HA3	1:A:1512:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1547:LEU:HD23	1:B:1547:LEU:HA	1.82	0.44
1:B:1576:LEU:HA	1:B:1579:MET:HG3	1.98	0.44
1:B:1599:ARG:HH12	1:B:1603:ARG:CD	2.30	0.44
1:B:2309:PRO:HB3	1:B:2352:THR:HG23	1.99	0.44
1:A:1604:LEU:HD23	1:A:1604:LEU:HA	1.85	0.44
1:A:2354:ALA:HB1	1:A:2358:ARG:NH1	2.32	0.44
1:B:1814:GLU:OE2	1:B:1818:GLN:NE2	2.50	0.44
1:B:3468:VAL:O	1:B:3472:VAL:HG23	2.16	0.44
1:B:4117:GLN:O	1:B:4117:GLN:HG2	2.17	0.44
2:C:262:VAL:HG23	2:C:269:LYS:HB2	1.98	0.44
2:D:237:VAL:HA	2:D:253:SER:HA	1.99	0.44
1:A:1458:ALA:HA	1:A:1461:GLU:OE2	2.18	0.44
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.99	0.44
1:A:2091:ARG:NH1	1:A:2320:ASP:OD1	2.50	0.44
1:A:3588:LEU:HD23	1:A:3698:PHE:CE1	2.53	0.44
1:A:3814:THR:O	1:A:3818:LEU:HG	2.17	0.44
1:B:1444:ALA:HA	1:B:1447:LYS:HG2	2.00	0.44
1:B:2894:LYS:HE3	1:B:2894:LYS:HB2	1.84	0.44
1:B:3818:LEU:HD23	1:B:3827:TYR:HE2	1.81	0.44
2:D:228:LYS:HB3	2:D:266:LYS:NZ	2.32	0.44
1:A:2185:VAL:HG13	1:A:2239:LYS:HD2	1.99	0.44
1:A:2472:TYR:CD2	1:A:2481:MET:HB2	2.52	0.44
1:B:1363:LEU:HD13	1:B:1395:LYS:HB2	1.99	0.44
1:B:1442:ASN:HA	1:B:1445:ILE:HD13	1.99	0.44
1:B:2713:ASN:HB2	1:B:2720:ARG:HE	1.82	0.44
1:B:3131:ASP:OD1	1:B:3132:LYS:N	2.51	0.44
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	2.00	0.44
1:A:4445:THR:O	1:A:4449:ARG:N	2.37	0.44
1:A:4601:LYS:HB2	1:A:4604:VAL:HG23	1.99	0.44
1:B:1518:GLU:O	1:B:1521:LEU:HG	2.18	0.44
1:B:1527:LEU:HA	1:B:1530:ILE:HD12	1.99	0.44
1:B:3239:LYS:HD3	1:B:3451:TYR:CE1	2.53	0.44
1:B:4227:ALA:HA	1:B:4230:ARG:HH21	1.83	0.44
1:B:4603:SER:O	1:B:4626:ILE:HG12	2.18	0.44
1:A:1378:ARG:HG3	1:A:1383:TYR:CE2	2.53	0.44
1:A:2312:VAL:HG13	1:A:2355:THR:HG21	1.99	0.44
1:A:2584:TRP:HE3	1:A:2591:LEU:HD22	1.83	0.44
1:A:2874:SER:HB3	1:A:2884:VAL:HG21	1.99	0.44
1:A:2976:LEU:O	1:A:2980:LEU:HD23	2.17	0.44
2:D:158:PHE:CE1	2:D:165:LEU:HD13	2.53	0.44
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2012:MET:HE2	1:B:2012:MET:HB3	1.82	0.44
1:B:3872:ALA:HA	1:B:3875:MET:HE2	2.00	0.44
1:B:4247:MET:HE1	1:B:4252:TYR:CD1	2.53	0.44
1:A:3790:VAL:O	1:A:3793:GLU:HG2	2.19	0.43
1:B:1817:HIS:CD2	1:B:1881:GLN:HG2	2.52	0.43
1:B:2773:MET:HE1	1:B:2802:TRP:CG	2.53	0.43
1:B:2976:LEU:O	1:B:2980:LEU:HD23	2.18	0.43
1:B:3198:GLN:HG2	2:D:150:THR:OG1	2.19	0.43
1:B:3223:ARG:O	1:B:3227:GLN:HG2	2.17	0.43
1:B:4529:ALA:O	1:B:4533:SER:N	2.51	0.43
2:D:110:PRO:HB3	2:D:400:VAL:HA	2.00	0.43
2:D:312:LEU:HD23	2:D:322:MET:HB3	2.00	0.43
1:A:1508:LYS:HG3	1:A:1513:TYR:CE2	2.53	0.43
1:A:1567:ARG:HG3	1:A:1567:ARG:HH11	1.84	0.43
1:A:2232:MET:HE2	6:A:4702:ATP:H2'	1.99	0.43
1:A:2905:LEU:HD11	1:A:3652:GLU:HB2	1.99	0.43
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.99	0.43
1:B:1350:PRO:HB2	1:B:1352:VAL:HG23	2.00	0.43
1:B:1411:ARG:HH21	1:B:1456:GLU:CD	2.26	0.43
1:B:1793:ALA:O	1:B:1797:LEU:HG	2.18	0.43
1:B:3478:LEU:HD13	1:B:3767:ILE:HG23	2.00	0.43
2:C:104:LEU:HD12	2:C:135:TRP:CZ3	2.53	0.43
2:D:383:VAL:HA	2:D:399:SER:HB2	2.00	0.43
1:A:2901:TYR:HA	1:A:2905:LEU:O	2.17	0.43
1:A:3115:LEU:HD12	1:A:3143:ILE:HG13	1.99	0.43
1:A:3211:THR:O	1:A:3215:VAL:HG23	2.19	0.43
1:A:3247:GLN:HE22	1:B:3247:GLN:HB2	1.82	0.43
1:A:3728:ARG:HA	1:A:3791:MET:HE1	2.00	0.43
1:B:3034:LYS:HA	1:B:3034:LYS:HD3	1.70	0.43
1:B:4007:MET:O	1:B:4011:THR:N	2.47	0.43
1:B:4377:MET:CE	1:B:4438:CYS:HA	2.47	0.43
1:B:4452:ILE:O	1:B:4456:VAL:HG23	2.18	0.43
1:B:4541:LEU:HB2	1:B:4592:TRP:CZ3	2.54	0.43
2:D:238:ARG:HA	2:D:238:ARG:HD3	1.87	0.43
2:D:239:MET:SD	2:D:241:ARG:HG2	2.58	0.43
2:D:245:ASP:OD1	2:D:245:ASP:N	2.50	0.43
1:A:1447:LYS:O	1:A:1451:LEU:HD23	2.18	0.43
1:A:3921:THR:HA	1:A:3936:VAL:HG21	1.99	0.43
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.50	0.43
1:B:1431:LEU:O	1:B:1434:ILE:HG22	2.19	0.43
1:B:1484:CYS:SG	1:B:1579:MET:HE3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3912:ASN:O	1:B:3937:ARG:NH1	2.51	0.43
1:B:4025:LEU:HG	1:B:4027:LEU:HD22	2.01	0.43
1:B:4190:ILE:HG23	1:B:4201:TRP:HZ2	1.84	0.43
1:B:4481:ASP:O	1:B:4484:GLU:HG3	2.19	0.43
2:D:260:VAL:HG13	2:D:269:LYS:HB3	2.00	0.43
1:A:1490:TRP:CD2	1:A:1538:ILE:HD12	2.54	0.43
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	2.01	0.43
1:A:2075:LEU:O	1:A:2079:GLN:HB2	2.18	0.43
1:A:2206:LYS:HA	1:A:2206:LYS:HD3	1.79	0.43
1:A:3226:SER:O	1:A:3230:GLU:HG2	2.19	0.43
1:A:3839:VAL:O	1:A:3843:ASN:HB2	2.18	0.43
1:B:2726:ARG:O	1:B:2729:ARG:HG2	2.19	0.43
1:B:2972:PHE:CZ	1:B:3008:MET:HE3	2.54	0.43
2:D:187:THR:O	2:D:188:MET:HE2	2.19	0.43
1:A:1351:TRP:HZ3	1:A:1435:TRP:HH2	1.65	0.43
1:A:1490:TRP:CG	1:A:1538:ILE:HD12	2.53	0.43
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	2.01	0.43
1:A:1949:CYS:SG	1:A:2012:MET:HE1	2.58	0.43
1:A:2186:CYS:HA	1:A:2191:LEU:HB2	2.00	0.43
1:A:2792:TYR:OH	1:A:2842:GLU:OE1	2.29	0.43
1:A:3457:GLU:O	1:A:3461:ILE:HG13	2.18	0.43
1:A:3772:ASN:OD1	1:A:3775:ARG:NH1	2.52	0.43
1:A:4413:PHE:CE1	1:A:4492:ILE:HG12	2.54	0.43
1:B:1543:ARG:HA	1:B:1546:TYR:CE2	2.54	0.43
1:B:1721:VAL:O	1:B:1725:GLU:HG2	2.18	0.43
1:B:1817:HIS:NE2	1:B:1881:GLN:HG2	2.33	0.43
2:C:259:ARG:HD3	2:C:261:TRP:CZ2	2.54	0.43
2:D:216:ILE:HB	2:D:230:PHE:HB2	2.00	0.43
2:D:243:ASN:HD22	2:D:248:LEU:HB2	1.84	0.43
1:A:1361:GLN:HA	1:A:1364:ASP:OD2	2.19	0.43
1:A:1469:VAL:O	1:A:1473:TYR:HB2	2.18	0.43
1:A:1907:PRO:HD2	1:A:2042:THR:HA	2.00	0.43
1:A:2819:GLU:HB3	1:A:2865:LYS:HD2	2.01	0.43
1:A:3555:ASN:OD1	1:A:3558:GLU:HG2	2.19	0.43
1:A:3839:VAL:HG22	1:A:3859:ILE:HD12	2.01	0.43
1:B:2070:VAL:HB	1:B:2071:PRO:HD3	2.01	0.43
1:B:2228:SER:HB2	1:B:2364:PHE:HB3	2.00	0.43
1:B:2726:ARG:NE	6:B:4702:ATP:O1G	2.51	0.43
2:D:241:ARG:HD3	2:D:241:ARG:HA	1.83	0.43
2:D:363:ARG:HG2	2:D:375:THR:HG23	2.01	0.43
1:A:1798:MET:HB2	1:A:2124:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2773:MET:HE1	1:A:2802:TRP:CE2	2.54	0.43
1:A:3048:GLU:HG2	1:A:3049:GLU:N	2.33	0.43
1:A:3174:ARG:HA	1:A:3177:LEU:HD12	2.00	0.43
1:A:3825:TYR:CE1	1:A:3875:MET:HG2	2.54	0.43
1:A:4199:LEU:HB3	1:A:4323:LEU:HD11	2.00	0.43
1:B:1724:VAL:HG23	1:B:1727:PHE:HD2	1.84	0.43
1:B:2188:GLU:OE1	1:B:2243:ARG:NH2	2.38	0.43
1:B:2834:GLN:NE2	1:B:2843:ARG:HB3	2.33	0.43
1:B:4234:SER:HB3	1:B:4237:LYS:HG2	1.99	0.43
2:D:193:HIS:CD2	2:D:212:ARG:HH21	2.36	0.43
1:A:1396:ILE:HG22	1:A:1400:VAL:HG23	1.99	0.43
1:A:2030:ASP:O	1:A:2034:LYS:HG2	2.19	0.43
1:A:2446:ILE:HG13	1:A:2735:TYR:CD1	2.54	0.43
1:A:2605:LEU:O	1:A:2609:LEU:HD23	2.18	0.43
1:A:3772:ASN:O	1:A:3775:ARG:HG2	2.17	0.43
1:A:4017:PHE:HB3	1:A:4018:MET:SD	2.58	0.43
1:B:1939:GLN:HB2	1:B:2273:ARG:CZ	2.49	0.43
1:B:3580:LEU:HD11	1:B:3589:ILE:HD11	2.01	0.43
1:B:3652:GLU:OE1	1:B:3652:GLU:N	2.38	0.43
2:C:272:LEU:HD13	2:C:323:TRP:CD2	2.53	0.43
2:C:277:HIS:ND1	2:C:316:ARG:HB2	2.33	0.43
2:D:384:THR:H	2:D:399:SER:HA	1.84	0.43
1:A:2150:VAL:O	1:A:2154:ILE:HG13	2.18	0.43
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.54	0.43
1:A:3575:GLU:O	1:A:3579:MET:HG2	2.19	0.43
1:A:4187:HIS:ND1	1:A:4252:TYR:OH	2.36	0.43
1:B:1699:ASN:OD1	1:B:1700:GLU:N	2.51	0.43
1:B:1842:MET:HG3	1:B:1844:PHE:CE1	2.54	0.43
1:B:3112:LYS:HE3	1:B:3112:LYS:HA	2.01	0.43
1:A:1778:LEU:HA	1:A:1781:VAL:HG12	2.01	0.42
1:A:1979:GLN:HE22	1:A:2035:LEU:HB3	1.84	0.42
1:A:3997:ARG:NH2	1:A:4329:ARG:HH12	2.16	0.42
1:A:4418:LYS:HA	1:A:4418:LYS:HD3	1.74	0.42
1:B:1930:PHE:HA	1:B:2326:THR:HG21	2.00	0.42
1:B:2702:LYS:HE2	1:B:2702:LYS:HB2	1.92	0.42
1:B:2819:GLU:HG3	1:B:2861:ILE:HG12	2.00	0.42
1:B:3473:ASN:OD1	1:B:3474:ARG:N	2.52	0.42
1:A:1360:ARG:NH2	1:A:1394:MET:SD	2.92	0.42
1:A:1443:GLU:O	1:A:1446:VAL:HG22	2.20	0.42
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	2.01	0.42
1:A:2300:TRP:CD1	1:A:2340:ARG:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4004:MET:O	1:A:4007:MET:HG2	2.19	0.42
1:B:2973:ASP:OD2	1:B:3007:ARG:NH2	2.49	0.42
1:B:3038:GLN:NE2	1:B:3043:MET:HE1	2.34	0.42
1:B:3567:LEU:HB2	1:B:3599:PHE:CD1	2.54	0.42
1:B:4388:LEU:HG	1:B:4431:LEU:HB3	2.01	0.42
2:D:133:LYS:HB3	2:D:135:TRP:NE1	2.35	0.42
2:D:202:PRO:HG2	2:D:244:GLN:O	2.19	0.42
2:D:236:TRP:HD1	2:D:237:VAL:N	2.17	0.42
2:D:236:TRP:O	2:D:254:ASN:N	2.38	0.42
1:A:2290:SER:HA	1:A:2294:GLU:HB2	2.01	0.42
1:A:3584:ASN:O	1:A:3651:ARG:NH1	2.53	0.42
1:A:3753:LEU:HD23	1:A:3753:LEU:HA	1.84	0.42
1:B:1470:TRP:NE1	1:B:1527:LEU:HD21	2.33	0.42
1:B:1967:MET:HE3	1:B:1970:ALA:HB3	2.01	0.42
1:B:2896:ARG:HD3	1:B:2896:ARG:HA	1.82	0.42
1:B:3492:THR:HA	1:B:3495:THR:HG22	2.00	0.42
1:B:3741:ARG:HA	1:B:3741:ARG:HD2	1.88	0.42
2:D:94:TRP:CD2	2:D:393:PRO:HB3	2.54	0.42
2:D:234:ARG:NH2	2:D:273:ARG:HH21	2.09	0.42
1:A:1424:TRP:HH2	1:A:1434:ILE:HA	1.84	0.42
1:A:1708:GLU:OE2	1:A:1712:THR:OG1	2.38	0.42
1:A:3114:ASP:O	1:A:3116:GLU:HG2	2.20	0.42
1:A:4324:PRO:HB3	1:A:4638:ARG:NH2	2.34	0.42
1:A:4432:ALA:O	1:A:4436:GLN:HG2	2.18	0.42
1:B:1513:TYR:CE2	1:B:1517:GLU:HG2	2.54	0.42
1:B:3751:GLN:O	1:B:3754:ASN:N	2.47	0.42
1:B:4445:THR:H	1:B:4448:LEU:HB2	1.84	0.42
2:C:113:ARG:HH11	2:C:155:ASP:HA	1.84	0.42
2:D:195:VAL:HA	2:D:211:SER:HA	1.99	0.42
1:A:1655:LYS:HB2	1:A:1679:ARG:NH2	2.34	0.42
1:A:2584:TRP:CH2	1:A:2732:PRO:HB2	2.54	0.42
1:A:3046:SER:OG	1:A:3048:GLU:OE1	2.33	0.42
1:B:1370:LEU:HD11	1:B:1383:TYR:HA	2.01	0.42
1:B:1386:VAL:HA	1:B:1389:LEU:HD13	2.02	0.42
1:B:1550:ILE:HG12	1:B:1641:ILE:HG22	2.02	0.42
1:B:1728:GLY:O	1:B:1729:LYS:HG3	2.19	0.42
1:B:2103:VAL:HA	1:B:2106:GLU:HG3	2.01	0.42
1:B:3906:GLN:HG2	1:B:3910:ARG:NH1	2.35	0.42
2:C:238:ARG:HH11	2:C:254:ASN:HD21	1.68	0.42
1:A:1542:ARG:O	1:A:1545:VAL:HB	2.18	0.42
1:A:3175:HIS:HB3	1:A:3516:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3222:LEU:HD12	1:A:3465:LEU:HD12	2.01	0.42
1:B:1460:GLU:HG3	1:B:1464:LYS:NZ	2.35	0.42
1:B:1698:ILE:O	1:B:1702:LEU:HD23	2.20	0.42
1:B:2773:MET:HE1	1:B:2802:TRP:CD2	2.54	0.42
2:C:114:VAL:HG12	2:C:125:SER:HB2	2.01	0.42
2:C:123:MET:HE3	2:C:396:VAL:HG21	2.00	0.42
2:D:95:ILE:HB	2:D:97:ARG:HH12	1.83	0.42
2:D:114:VAL:HG12	2:D:125:SER:HA	2.01	0.42
1:A:2538:GLU:HB3	1:A:2548:TRP:CZ2	2.55	0.42
1:A:4404:ASN:HB3	1:A:4410:PHE:CD2	2.54	0.42
1:B:1356:PRO:O	1:B:1359:LEU:HB2	2.19	0.42
1:B:1961:ASN:OD1	1:B:1961:ASN:N	2.53	0.42
1:B:2999:VAL:HG13	1:B:3004:PHE:HB2	2.01	0.42
1:B:3551:GLU:HA	1:B:3559:ARG:NH1	2.35	0.42
1:B:4039:THR:HG23	1:B:4142:GLY:HA2	2.02	0.42
2:D:155:ASP:HB2	2:D:197:SER:HA	2.01	0.42
1:A:1497:VAL:O	1:A:1501:ILE:HG12	2.19	0.42
1:A:1497:VAL:HG11	1:A:1531:MET:HE3	2.01	0.42
1:A:1518:GLU:O	1:A:1521:LEU:HG	2.20	0.42
1:A:1703:THR:HA	1:A:1706:GLU:HG2	2.02	0.42
1:A:1905:PHE:HB3	1:A:2018:MET:HB2	2.02	0.42
1:A:3783:LYS:O	1:A:3786:GLU:HG2	2.19	0.42
1:B:2760:PRO:HB3	1:B:2763:ARG:HH21	1.84	0.42
1:B:3873:ARG:HD3	1:B:3873:ARG:HA	1.91	0.42
1:A:1828:SER:HB2	1:A:1830:ILE:HG12	2.02	0.42
1:A:2983:SER:HB2	1:A:2990:ILE:HD12	2.02	0.42
1:A:3824:LEU:HD21	1:A:4144:ILE:HG21	2.02	0.42
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.80	0.42
1:B:1668:GLU:OE1	1:B:1668:GLU:N	2.46	0.42
1:B:1721:VAL:HA	1:B:1724:VAL:HG12	2.02	0.42
1:B:3228:GLU:HA	1:B:3231:VAL:HG12	2.01	0.42
1:B:3588:LEU:HD23	1:B:3698:PHE:CE1	2.55	0.42
1:B:4071:ILE:HG13	1:B:4099:VAL:HG12	2.02	0.42
1:B:4173:PRO:HG2	1:B:4176:ARG:HH21	1.85	0.42
1:B:4401:THR:O	1:B:4405:ILE:HG12	2.20	0.42
2:C:151:ASP:CG	2:C:152:SER:H	2.24	0.42
1:A:1930:PHE:CZ	1:A:1944:ILE:HD11	2.55	0.42
1:A:2935:LEU:HB3	1:A:2943:LYS:HD2	2.02	0.42
1:A:3586:TYR:HA	1:A:3587:PRO:HD3	1.90	0.42
1:A:3911:GLY:O	1:A:3937:ARG:HD3	2.20	0.42
1:B:1378:ARG:HA	1:B:1383:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1600:SER:O	1:B:1604:LEU:HD23	2.20	0.42
1:B:2099:SER:OG	1:B:2140:SER:HB3	2.20	0.42
1:B:2519:ARG:HG3	1:B:2526:LEU:HD12	2.02	0.42
1:B:3096:ASP:OD1	1:B:3097:TRP:N	2.53	0.42
1:B:3114:ASP:O	1:B:3140:ARG:NH2	2.53	0.42
1:B:3624:GLU:O	1:B:3628:ARG:HG2	2.20	0.42
1:B:4288:VAL:HB	1:B:4320:TRP:CD1	2.55	0.42
2:C:113:ARG:HA	2:C:385:SER:OG	2.20	0.42
2:D:176:LEU:O	2:D:185:ILE:HG22	2.20	0.42
2:D:210:ALA:HB2	2:D:240:VAL:HB	2.02	0.42
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.54	0.41
1:A:2290:SER:OG	1:A:2294:GLU:N	2.53	0.41
1:A:2559:THR:OG1	1:A:2757:ARG:HD2	2.20	0.41
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	2.02	0.41
1:A:3005:LEU:HD23	1:A:3005:LEU:HA	1.88	0.41
1:A:3510:SER:O	1:A:3514:ILE:HG12	2.20	0.41
1:A:3653:VAL:HG12	1:A:3662:ILE:HD13	2.02	0.41
1:A:3723:ASP:OD1	1:A:3724:VAL:N	2.50	0.41
1:A:4071:ILE:HG23	1:A:4077:PHE:CE1	2.55	0.41
1:A:4105:TRP:CE3	1:A:4106:LEU:HD22	2.54	0.41
1:B:1619:LEU:HD22	1:B:1637:LEU:HG	2.01	0.41
1:B:2197:GLU:N	1:B:2197:GLU:OE1	2.53	0.41
1:B:2413:LEU:O	1:B:2417:ARG:HG3	2.19	0.41
1:B:2467:ARG:O	1:B:2471:GLN:HG2	2.20	0.41
1:B:3208:ILE:HG21	1:B:3486:ARG:HD3	2.02	0.41
1:B:4485:ARG:HH11	1:B:4515:PHE:HD1	1.68	0.41
1:A:1589:MET:O	1:A:1593:ASN:N	2.51	0.41
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.02	0.41
1:A:2341:ILE:O	1:A:2342:MET:HE2	2.20	0.41
1:A:2825:TRP:CZ3	1:A:2850:ILE:HG23	2.56	0.41
1:A:4078:ASN:HB3	1:A:4082:LYS:HZ3	1.85	0.41
1:A:4421:ALA:HB1	1:A:4425:GLN:HE22	1.85	0.41
1:B:1513:TYR:O	1:B:1517:GLU:HG3	2.20	0.41
1:B:1914:GLU:HG3	5:B:4701:ADP:H2'	2.02	0.41
1:B:2527:PRO:HD3	1:B:2545:TRP:CE2	2.54	0.41
1:B:2797:ARG:HG2	5:B:4703:ADP:H4'	2.02	0.41
1:B:3200:HIS:HD2	1:B:3754:ASN:OD1	2.02	0.41
1:B:4546:THR:OG1	1:B:4587:LEU:HB3	2.21	0.41
2:C:382:PHE:O	2:C:399:SER:OG	2.31	0.41
1:A:1400:VAL:HA	1:A:1403:LEU:HB3	2.03	0.41
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2541:ILE:C	1:A:2543:GLY:H	2.27	0.41
1:A:2775:GLU:O	1:A:2778:THR:HB	2.21	0.41
1:A:3085:LEU:O	1:A:3089:CYS:HB2	2.20	0.41
1:A:3856:LEU:HA	1:A:3859:ILE:HG22	2.02	0.41
1:B:1527:LEU:HD23	1:B:1530:ILE:HD12	2.02	0.41
1:B:2222:MET:HE3	1:B:2344:GLU:HG3	2.01	0.41
1:B:2628:PRO:HG3	1:B:2679:VAL:HA	2.02	0.41
1:B:2792:TYR:OH	1:B:2842:GLU:OE1	2.38	0.41
1:B:2910:VAL:HG22	5:B:4704:ADP:N1	2.35	0.41
1:B:3197:GLN:O	1:B:3201:LEU:HG	2.21	0.41
1:B:3630:GLY:H	1:B:3672:SER:HB3	1.85	0.41
1:B:3720:GLU:OE1	1:B:3801:TYR:OH	2.33	0.41
2:D:376:LEU:HD21	2:D:407:TRP:CZ3	2.55	0.41
1:A:1623:ARG:HD3	1:A:1630:TYR:HA	2.03	0.41
1:A:1752:LEU:HD12	1:A:1752:LEU:HA	1.94	0.41
1:A:3194:LEU:HD12	1:A:3194:LEU:HA	1.89	0.41
1:A:3194:LEU:O	1:A:3197:GLN:HG3	2.20	0.41
1:A:3567:LEU:HB2	1:A:3599:PHE:CD1	2.55	0.41
1:B:3046:SER:OG	1:B:3047:HIS:N	2.53	0.41
1:B:3219:ARG:NH2	1:B:3472:VAL:HG22	2.31	0.41
1:B:3452:ALA:O	1:B:3455:ILE:HG22	2.20	0.41
1:B:3923:ARG:HH12	1:B:3925:GLN:HA	1.84	0.41
1:B:4106:LEU:HD23	1:B:4106:LEU:HA	1.86	0.41
1:B:4209:GLU:O	1:B:4213:ARG:HG2	2.20	0.41
1:B:4316:GLN:HA	1:B:4320:TRP:CE2	2.56	0.41
2:D:150:THR:HG23	2:D:171:ASP:HB2	2.03	0.41
1:A:2183:LYS:HB3	1:A:2184:LYS:HZ2	1.85	0.41
1:A:4234:SER:OG	1:A:4236:ASP:OD1	2.33	0.41
1:B:1350:PRO:O	1:B:1429:LEU:HB3	2.20	0.41
1:B:3013:ALA:HA	1:B:3088:ARG:HG3	2.02	0.41
2:C:236:TRP:HB3	2:C:254:ASN:OD1	2.21	0.41
2:C:274:GLU:HB2	2:C:323:TRP:CH2	2.55	0.41
2:D:274:GLU:HB2	2:D:323:TRP:CH2	2.55	0.41
1:A:1434:ILE:O	1:A:1438:ASP:HB2	2.21	0.41
1:A:2222:MET:HE1	1:A:2234:TRP:HD1	1.86	0.41
1:A:2468:ASN:ND2	1:A:2489:TYR:OH	2.54	0.41
1:A:2500:TRP:CE2	1:A:2535:ILE:HD11	2.55	0.41
1:A:2756:LEU:HD23	1:A:2756:LEU:HA	1.81	0.41
1:A:3204:GLY:O	1:A:3208:ILE:HG12	2.20	0.41
1:A:3243:MET:HE1	1:A:3444:ILE:HA	2.03	0.41
1:A:3970:VAL:HB	1:A:3989:ARG:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4541:LEU:HB2	1:A:4592:TRP:CZ3	2.55	0.41
1:B:3012:LEU:HD13	1:B:3089:CYS:SG	2.60	0.41
1:B:3214:GLN:NE2	1:B:3761:LEU:HB2	2.36	0.41
1:B:3243:MET:O	1:B:3247:GLN:HG3	2.19	0.41
1:B:3521:ASP:OD1	1:B:3521:ASP:N	2.54	0.41
2:C:129:ASP:OD1	2:C:131:THR:OG1	2.28	0.41
2:C:233:HIS:NE2	2:C:259:ARG:HB2	2.35	0.41
1:A:1408:LEU:HA	1:A:1412:HIS:CD2	2.56	0.41
1:A:1735:PRO:O	1:A:1739:ILE:HG12	2.21	0.41
1:A:1788:THR:O	1:A:1792:LEU:HD23	2.20	0.41
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.21	0.41
1:A:2571:THR:H	1:A:2574:THR:HB	1.85	0.41
1:A:2623:SER:N	1:A:2626:THR:OG1	2.27	0.41
1:A:2942:GLY:N	5:A:4704:ADP:O1B	2.54	0.41
1:A:4027:LEU:HD11	1:A:4043:MET:HE1	2.02	0.41
1:A:4236:ASP:OD1	1:A:4237:LYS:N	2.54	0.41
1:B:1405:SER:O	1:B:1408:LEU:HG	2.20	0.41
1:B:2192:THR:HB	1:B:2373:MET:SD	2.61	0.41
1:B:2221:MET:HG3	1:B:2343:PHE:HB2	2.03	0.41
1:B:2901:TYR:HA	1:B:2905:LEU:O	2.20	0.41
1:B:3049:GLU:HA	1:B:3052:LYS:HG2	2.03	0.41
1:B:3230:GLU:HA	1:B:3233:ASN:ND2	2.36	0.41
1:B:3551:GLU:HA	1:B:3559:ARG:HH12	1.84	0.41
1:B:4324:PRO:HG2	1:B:4327:ALA:HB2	2.02	0.41
1:B:4473:MET:HE1	1:B:4478:TRP:HB2	2.03	0.41
2:D:393:PRO:O	2:D:409:CYS:N	2.51	0.41
1:A:1507:MET:O	1:A:1513:TYR:HB2	2.21	0.41
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	2.02	0.41
1:A:3482:LEU:HD11	1:A:3770:LEU:HD23	2.03	0.41
1:A:3720:GLU:OE1	1:A:3855:ARG:NE	2.53	0.41
1:A:4122:PHE:CZ	1:A:4124:LEU:HB2	2.56	0.41
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	2.03	0.41
1:A:4215:ALA:HB2	1:A:4251:ILE:HG21	2.02	0.41
1:A:4564:LYS:HD3	1:A:4584:ALA:HA	2.02	0.41
1:B:2562:VAL:HG21	1:B:2755:MET:HB3	2.01	0.41
1:B:3576:ASN:HA	1:B:3579:MET:HE3	2.02	0.41
2:C:262:VAL:HG12	2:C:264:ALA:H	1.86	0.41
2:C:322:MET:HE2	2:C:332:MET:HG3	2.03	0.41
2:D:243:ASN:HB2	2:D:248:LEU:HB2	2.03	0.41
1:A:1422:VAL:HG21	1:A:1437:VAL:HG11	2.03	0.41
1:A:1468:GLU:O	1:A:1472:THR:OG1	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1766:LEU:HD23	1:A:1766:LEU:HA	1.88	0.41
1:A:2060:ARG:HH12	1:A:2129:GLU:HA	1.86	0.41
1:A:2232:MET:SD	1:A:2232:MET:N	2.93	0.41
1:A:2921:ARG:O	1:A:2925:ILE:HG12	2.21	0.41
1:A:3113:MET:HE1	1:A:3183:TYR:CD2	2.55	0.41
1:A:3190:LYS:HE3	1:A:3552:TYR:CZ	2.56	0.41
1:A:3488:ARG:HA	1:A:3491:LYS:HE2	2.03	0.41
1:A:3818:LEU:HD11	1:A:3883:PHE:CE1	2.56	0.41
1:A:4405:ILE:O	1:A:4411:ARG:NH1	2.54	0.41
1:B:1419:ARG:HD3	1:B:1445:ILE:HG23	2.02	0.41
1:B:1546:TYR:OH	1:B:1612:GLN:OE1	2.19	0.41
1:B:1862:ALA:HB1	1:B:4222:TRP:HZ2	1.85	0.41
1:B:2748:TYR:CZ	1:B:2799:MET:HG3	2.56	0.41
1:B:3042:LEU:O	1:B:3043:MET:HE2	2.21	0.41
1:B:4227:ALA:HB2	1:B:4233:ILE:HD12	2.02	0.41
2:D:111:VAL:O	2:D:384:THR:OG1	2.33	0.41
2:D:194:ASN:O	2:D:212:ARG:N	2.36	0.41
1:A:1354:VAL:HG11	1:A:1359:LEU:HD12	2.03	0.41
1:A:1557:ILE:HG23	1:A:1558:LYS:HD3	2.03	0.41
1:A:2186:CYS:HB3	1:A:2191:LEU:O	2.21	0.41
1:A:2892:TYR:HE2	1:A:2953:MET:HE1	1.86	0.41
1:A:4521:ILE:O	1:A:4524:THR:OG1	2.34	0.41
1:B:1535:ASP:OD1	1:B:2292:ARG:NH2	2.31	0.41
1:B:1841:GLN:O	1:B:1843:ARG:HG3	2.21	0.41
1:B:2203:TRP:HE1	1:B:2233:ALA:HB2	1.86	0.41
1:B:2268:LEU:HD13	1:B:2329:ASN:HB3	2.02	0.41
1:B:2297:LYS:O	1:B:2338:ASN:ND2	2.42	0.41
1:B:2603:MET:HE1	5:B:4703:ADP:C4	2.56	0.41
1:B:3723:ASP:OD1	1:B:3724:VAL:N	2.52	0.41
1:B:3932:ALA:HA	1:B:3935:VAL:HG22	2.03	0.41
2:C:324:ASP:HB2	2:C:331:LEU:HD21	2.03	0.41
2:D:104:LEU:HB3	2:D:135:TRP:CZ3	2.56	0.41
2:D:342:ARG:HB3	2:D:384:THR:O	2.21	0.41
1:A:1504:VAL:HA	1:A:1507:MET:HG3	2.02	0.40
1:A:1533:LEU:HD11	1:A:1597:VAL:HG22	2.02	0.40
1:A:2667:ASN:ND2	1:A:2720:ARG:HD2	2.36	0.40
1:B:1411:ARG:HH22	1:B:1452:VAL:C	2.29	0.40
1:B:1500:HIS:O	1:B:1504:VAL:HG23	2.21	0.40
1:B:1543:ARG:HD2	1:B:1608:LEU:HB3	2.03	0.40
1:B:1769:MET:HA	1:B:1769:MET:HE3	2.02	0.40
1:B:2206:LYS:HA	1:B:2206:LYS:HD3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3140:ARG:O	1:B:3144:VAL:HG23	2.21	0.40
1:B:3154:LEU:HG	1:B:3516:TYR:CD1	2.56	0.40
1:B:3653:VAL:HG12	1:B:3662:ILE:HD13	2.03	0.40
1:B:4030:ILE:HA	1:B:4034:GLU:HG3	2.03	0.40
1:B:4068:SER:HA	1:B:4095:MET:HG3	2.03	0.40
1:B:4485:ARG:HD3	1:B:4515:PHE:CE1	2.55	0.40
1:B:4600:LYS:HE3	1:B:4600:LYS:HA	2.03	0.40
1:A:1360:ARG:HA	1:A:1363:LEU:HD12	2.03	0.40
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.57	0.40
1:A:2875:ASN:HD21	1:A:2927:ARG:HD3	1.86	0.40
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.87	0.40
1:B:1518:GLU:HA	1:B:1521:LEU:HG	2.03	0.40
1:B:2211:TYR:O	1:B:2214:THR:OG1	2.29	0.40
1:B:2748:TYR:CD2	1:B:2799:MET:HE2	2.57	0.40
1:B:3576:ASN:O	1:B:3580:LEU:HD23	2.22	0.40
2:D:235:GLU:HB3	2:D:254:ASN:HB2	2.03	0.40
2:D:244:GLN:NE2	2:D:285:ALA:O	2.54	0.40
1:A:1355:GLN:HB3	1:A:1358:LYS:HB3	2.04	0.40
1:A:2349:LYS:HB3	1:A:2349:LYS:HE2	1.95	0.40
1:B:1411:ARG:HH22	1:B:1452:VAL:HG12	1.86	0.40
1:B:1619:LEU:HD21	1:B:1638:LEU:HD23	2.02	0.40
1:B:2585:LEU:HD23	1:B:2707:GLN:OE1	2.21	0.40
1:B:3245:LYS:HA	1:B:3248:GLN:OE1	2.22	0.40
1:B:3478:LEU:HD13	1:B:3767:ILE:HD12	2.04	0.40
1:B:3478:LEU:O	1:B:3482:LEU:HG	2.22	0.40
1:B:4115:SER:O	1:B:4116:LEU:HD12	2.21	0.40
1:B:4556:CYS:O	1:B:4591:ARG:HA	2.22	0.40
2:C:273:ARG:HG3	2:C:273:ARG:O	2.21	0.40
1:A:1389:LEU:HG	1:A:1393:TYR:CE2	2.56	0.40
1:A:2221:MET:HB2	1:A:2361:MET:HE1	2.03	0.40
1:A:2558:GLU:HG3	1:A:2560:HIS:CE1	2.57	0.40
1:B:1445:ILE:HD12	1:B:1445:ILE:H	1.87	0.40
1:B:1753:SER:HA	1:B:1756:ILE:HG22	2.03	0.40
1:B:3211:THR:OG1	1:B:3760:ILE:HD13	2.22	0.40
1:B:4556:CYS:SG	1:B:4591:ARG:NH2	2.94	0.40
2:D:212:ARG:HA	2:D:236:TRP:CD1	2.56	0.40
1:A:1477:LEU:HD23	1:A:1487:ILE:HG13	2.03	0.40
1:A:1961:ASN:N	1:A:1961:ASN:OD1	2.53	0.40
1:A:2999:VAL:HG11	1:A:3005:LEU:HG	2.03	0.40
1:A:3723:ASP:HA	1:A:3726:GLU:OE2	2.22	0.40
1:A:4281:GLU:O	1:A:4283:LYS:NZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4340:ILE:HA	1:A:4343:MET:SD	2.61	0.40
1:B:2413:LEU:HD12	1:B:2413:LEU:HA	1.93	0.40
1:B:3174:ARG:NH1	1:B:3650:ASN:OD1	2.54	0.40
1:B:3215:VAL:HG13	1:B:3219:ARG:NH1	2.37	0.40
1:B:3637:ASP:OD1	1:B:4111:LYS:HE3	2.22	0.40
1:B:3787:THR:O	1:B:3791:MET:HG2	2.22	0.40
2:C:214:LYS:HG2	2:C:235:GLU:C	2.46	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	3056/4646 (66%)	2984 (98%)	72 (2%)	0	100	100
1	B	3057/4646 (66%)	2974 (97%)	83 (3%)	0	100	100
2	C	320/410 (78%)	301 (94%)	19 (6%)	0	100	100
2	D	309/410 (75%)	294 (95%)	15 (5%)	0	100	100
2	E	73/410 (18%)	73 (100%)	0	0	100	100
2	F	73/410 (18%)	73 (100%)	0	0	100	100
3	G	32/638 (5%)	32 (100%)	0	0	100	100
3	H	32/638 (5%)	32 (100%)	0	0	100	100
4	I	120/1281 (9%)	120 (100%)	0	0	100	100
4	J	119/1281 (9%)	119 (100%)	0	0	100	100
All	All	7191/14770 (49%)	7002 (97%)	189 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2720/4125 (66%)	2720 (100%)	0	100	100
1	B	2721/4125 (66%)	2721 (100%)	0	100	100
2	C	287/364 (79%)	286 (100%)	1 (0%)	86	86
2	D	280/364 (77%)	280 (100%)	0	100	100
All	All	6008/8978 (67%)	6007 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	222	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1361	GLN
1	A	1368	ASN
1	A	1412	HIS
1	A	1415	GLN
1	A	1440	GLN
1	A	1442	ASN
1	A	1454	GLN
1	A	1541	GLN
1	A	1646	ASN
1	A	1818	GLN
1	A	1950	GLN
1	A	1974	GLN
1	A	1985	HIS
1	A	1987	ASN
1	A	2005	GLN
1	A	2134	GLN
1	A	2430	ASN
1	A	2439	HIS

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Mol	Chain	Res	Type
1	A	2476	HIS
1	A	2485	GLN
1	A	2549	GLN
1	A	2560	HIS
1	A	2588	HIS
1	A	2685	GLN
1	A	2707	GLN
1	A	3152	GLN
1	A	3459	GLN
1	A	3499	GLN
1	A	3526	GLN
1	A	3754	ASN
1	A	3952	GLN
1	A	3968	GLN
1	A	4098	ASN
1	A	4100	HIS
1	A	4156	ASN
1	A	4490	GLN
1	A	4549	GLN
1	A	4566	GLN
1	B	1349	GLN
1	B	1362	ASN
1	B	1387	GLN
1	B	1412	HIS
1	B	1423	ASN
1	B	1433	GLN
1	B	1442	ASN
1	B	1471	ASN
1	B	1541	GLN
1	B	1559	HIS
1	B	1569	GLN
1	B	1818	GLN
1	B	1867	ASN
1	B	1939	GLN
1	B	2047	GLN
1	B	2067	ASN
1	B	2296	GLN
1	B	2468	ASN
1	B	2482	GLN
1	B	2549	GLN
1	B	2685	GLN
1	B	3061	ASN

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Mol	Chain	Res	Type
1	B	3119	ASN
1	B	3200	HIS
1	B	3227	GLN
1	B	3459	GLN
1	B	3820	GLN
1	B	3877	HIS
1	B	4098	ASN
1	B	4386	ASN
1	B	4566	GLN
2	C	206	HIS
2	D	277	HIS

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
5	ADP	A	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.87	8 (18%)
5	ADP	B	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	B	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.92	8 (18%)
6	ATP	A	4702	7	32,33,33	0.29	0	48,52,52	0.29	0
5	ADP	A	4701	7	28,29,29	1.44	4 (14%)	43,45,45	1.77	8 (18%)
6	ATP	B	4702	7	32,33,33	0.37	0	48,52,52	0.30	0
5	ADP	B	4701	7	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
5	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.82	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	4703	-	-	0/16/32/32	0/3/3/3
5	ADP	B	4704	-	-	2/16/32/32	0/3/3/3
5	ADP	B	4703	-	-	2/16/32/32	0/3/3/3
6	ATP	A	4702	7	-	7/22/38/38	0/3/3/3
5	ADP	A	4701	7	-	0/16/32/32	0/3/3/3
6	ATP	B	4702	7	-	5/22/38/38	0/3/3/3
5	ADP	B	4701	7	-	2/16/32/32	0/3/3/3
5	ADP	A	4704	-	-	1/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4701	ADP	C5-C4	4.90	1.47	1.39
5	A	4703	ADP	C5-C4	4.75	1.47	1.39
5	B	4703	ADP	C5-C4	4.75	1.47	1.39
5	A	4704	ADP	C5-C4	4.73	1.47	1.39
5	B	4704	ADP	C5-C4	4.72	1.47	1.39
5	B	4701	ADP	C5-C4	4.67	1.47	1.39
5	B	4704	ADP	C5-C6	2.71	1.48	1.41
5	B	4703	ADP	C5-C6	2.70	1.48	1.41
5	B	4701	ADP	C5-C6	2.69	1.48	1.41
5	A	4704	ADP	C5-C6	2.69	1.48	1.41
5	A	4703	ADP	C5-C6	2.68	1.48	1.41
5	A	4701	ADP	C5-C6	2.59	1.48	1.41
5	B	4703	ADP	C5-N7	-2.43	1.34	1.39
5	A	4701	ADP	C5-N7	-2.41	1.34	1.39
5	A	4703	ADP	C8-N7	2.32	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4701	ADP	C5-N7	-2.32	1.34	1.39
5	A	4703	ADP	C5-N7	-2.30	1.34	1.39
5	B	4704	ADP	C8-N7	2.28	1.36	1.31
5	B	4704	ADP	C5-N7	-2.28	1.34	1.39
5	A	4704	ADP	C5-N7	-2.28	1.34	1.39
5	A	4704	ADP	C8-N7	2.27	1.36	1.31
5	B	4701	ADP	C8-N7	2.24	1.36	1.31
5	A	4701	ADP	C8-N7	2.22	1.36	1.31
5	B	4703	ADP	C8-N7	2.21	1.35	1.31

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	4703	ADP	C5-C4-N3	-6.52	117.74	126.72
5	A	4703	ADP	C5-C4-N3	-6.10	118.32	126.72
5	A	4704	ADP	C5-C4-N3	-5.92	118.56	126.72
5	B	4701	ADP	C5-C4-N3	-5.90	118.59	126.72
5	B	4704	ADP	C5-C4-N3	-5.87	118.64	126.72
5	A	4701	ADP	C5-C4-N3	-5.72	118.84	126.72
5	B	4703	ADP	N3-C4-N9	5.27	136.13	127.17
5	A	4701	ADP	N3-C4-N9	4.89	135.48	127.17
5	A	4703	ADP	N3-C4-N9	4.84	135.40	127.17
5	B	4701	ADP	N3-C4-N9	4.67	135.11	127.17
5	A	4704	ADP	N3-C4-N9	4.66	135.09	127.17
5	B	4704	ADP	N3-C4-N9	4.64	135.06	127.17
5	B	4703	ADP	C2-N3-C4	3.96	121.51	111.83
5	A	4703	ADP	C2-N3-C4	3.79	121.09	111.83
5	A	4704	ADP	C2-N3-C4	3.71	120.90	111.83
5	B	4704	ADP	C2-N3-C4	3.70	120.87	111.83
5	B	4701	ADP	C2-N3-C4	3.65	120.73	111.83
5	A	4704	ADP	C4-C5-N7	-3.45	106.64	110.58
5	B	4704	ADP	C4-C5-N7	-3.44	106.65	110.58
5	B	4701	ADP	C4-C5-N7	-3.40	106.69	110.58
5	A	4703	ADP	C4-C5-N7	-3.36	106.74	110.58
5	B	4704	ADP	N3-C2-N1	-3.27	123.63	128.58
5	B	4703	ADP	C4-C5-N7	-3.25	106.87	110.58
5	B	4703	ADP	N3-C2-N1	-3.24	123.67	128.58
5	A	4704	ADP	N3-C2-N1	-3.23	123.70	128.58
5	A	4701	ADP	C2-N3-C4	3.21	119.66	111.83
5	A	4703	ADP	N3-C2-N1	-3.20	123.74	128.58
5	A	4701	ADP	C4-C5-N7	-3.13	107.00	110.58
5	B	4701	ADP	N3-C2-N1	-3.09	123.90	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4701	ADP	C4-N9-C8	2.88	108.77	105.74
5	A	4703	ADP	C3'-C2'-C1'	2.66	106.50	101.46
5	B	4703	ADP	C3'-C2'-C1'	2.65	106.48	101.46
5	A	4701	ADP	N3-C2-N1	-2.63	124.60	128.58
5	B	4704	ADP	C4-N9-C8	2.54	108.40	105.74
5	B	4701	ADP	C4-N9-C8	2.47	108.33	105.74
5	B	4704	ADP	C5-N7-C8	2.46	107.32	103.45
5	A	4703	ADP	C5-N7-C8	2.46	107.31	103.45
5	B	4701	ADP	C5-N7-C8	2.46	107.31	103.45
5	B	4704	ADP	C3'-C2'-C1'	2.45	106.10	101.46
5	B	4703	ADP	C5-N7-C8	2.44	107.29	103.45
5	A	4703	ADP	C4-N9-C8	2.44	108.30	105.74
5	A	4704	ADP	C5-N7-C8	2.44	107.29	103.45
5	A	4704	ADP	C4-N9-C8	2.44	108.30	105.74
5	A	4701	ADP	C5-N7-C8	2.41	107.23	103.45
5	B	4701	ADP	C3'-C2'-C1'	2.37	105.94	101.46
5	A	4704	ADP	C3'-C2'-C1'	2.34	105.89	101.46
5	B	4703	ADP	C4-N9-C8	2.25	108.10	105.74
5	A	4701	ADP	C3'-C2'-C1'	2.05	105.35	101.46
5	B	4704	ADP	C6-C5-N7	2.03	136.00	132.09
5	A	4704	ADP	C6-C5-N7	2.01	135.96	132.09

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	4701	ADP	C5'-O5'-PA-O2A
5	B	4701	ADP	C5'-O5'-PA-O3A
6	A	4702	ATP	C5'-O5'-PA-O1A
6	A	4702	ATP	C5'-O5'-PA-O2A
6	A	4702	ATP	C5'-O5'-PA-O3A
6	B	4702	ATP	PB-O3B-PG-O2G
6	A	4702	ATP	O4'-C4'-C5'-O5'
6	A	4702	ATP	C3'-C4'-C5'-O5'
5	B	4704	ADP	C3'-C4'-C5'-O5'
5	B	4704	ADP	O4'-C4'-C5'-O5'
6	B	4702	ATP	PB-O3B-PG-O3G
6	A	4702	ATP	PG-O3B-PB-O2B
5	A	4704	ADP	C5'-O5'-PA-O1A
5	B	4703	ADP	C2'-C1'-N9-C8
5	B	4703	ADP	C2'-C1'-N9-C4
6	A	4702	ATP	PG-O3B-PB-O1B

Continued on next page...

Continued from previous page...

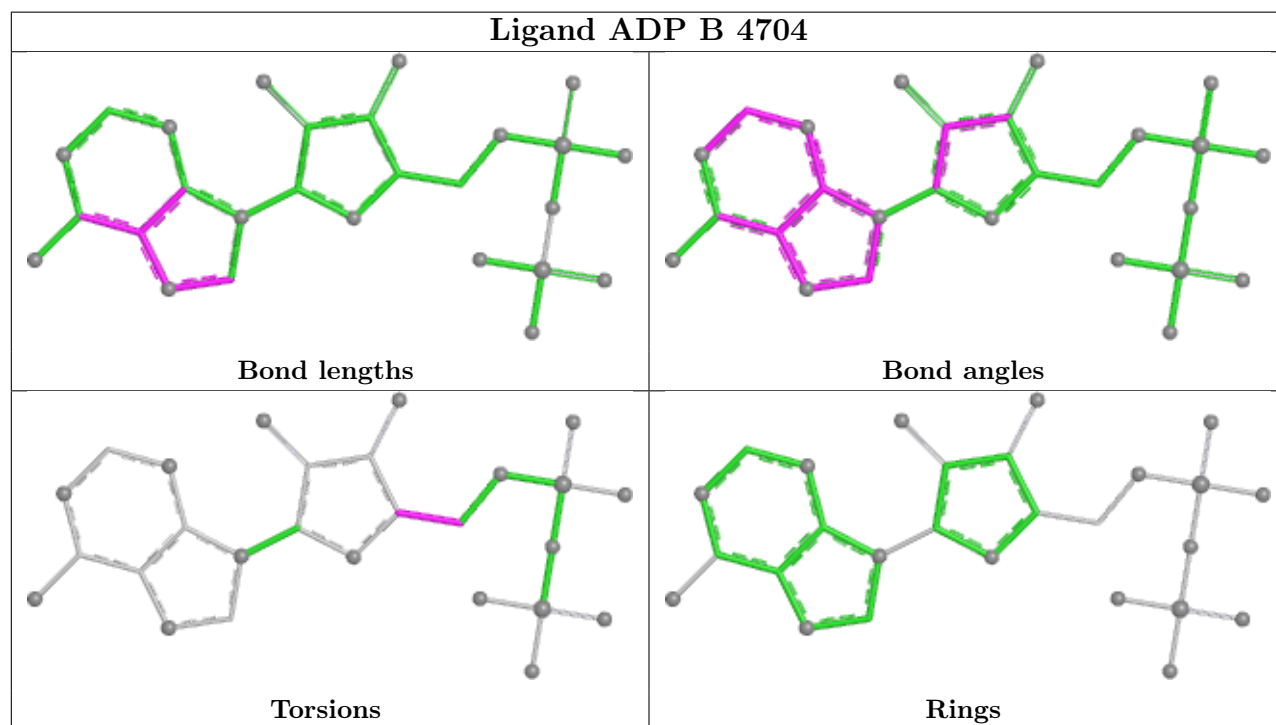
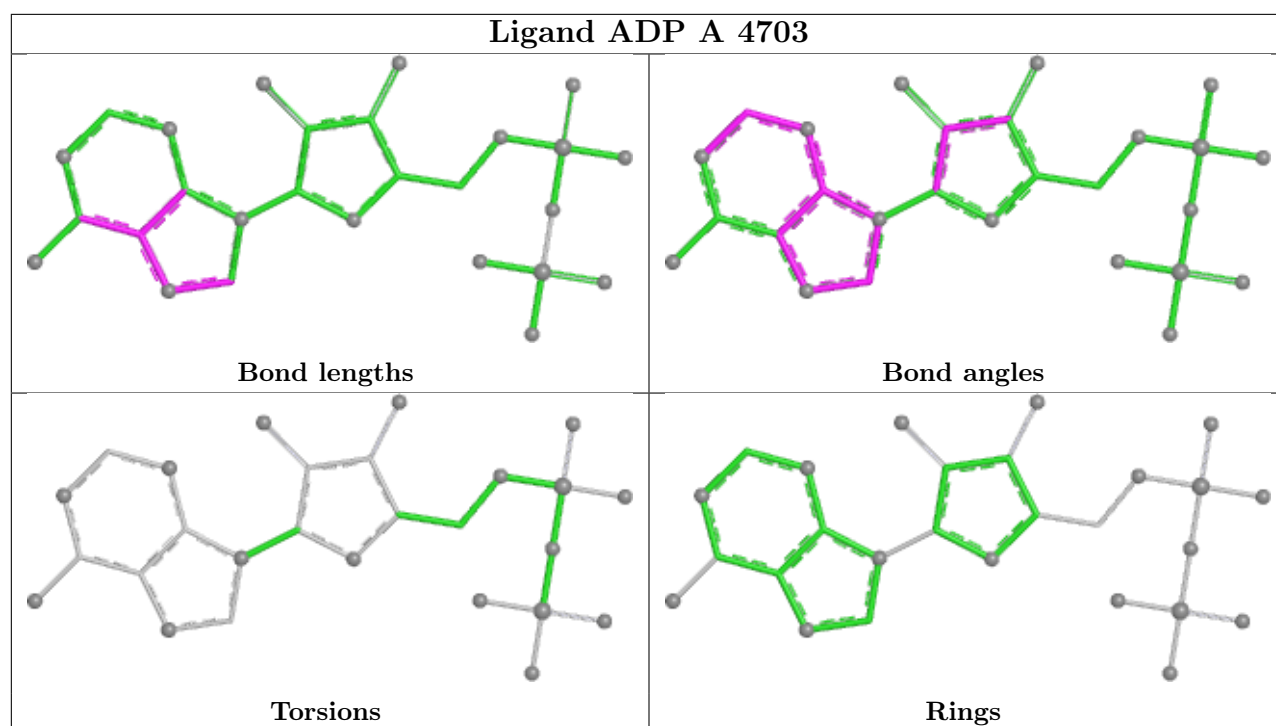
Mol	Chain	Res	Type	Atoms
6	B	4702	ATP	PA-O3A-PB-O2B
6	B	4702	ATP	PB-O3B-PG-O1G
6	B	4702	ATP	PA-O3A-PB-O1B

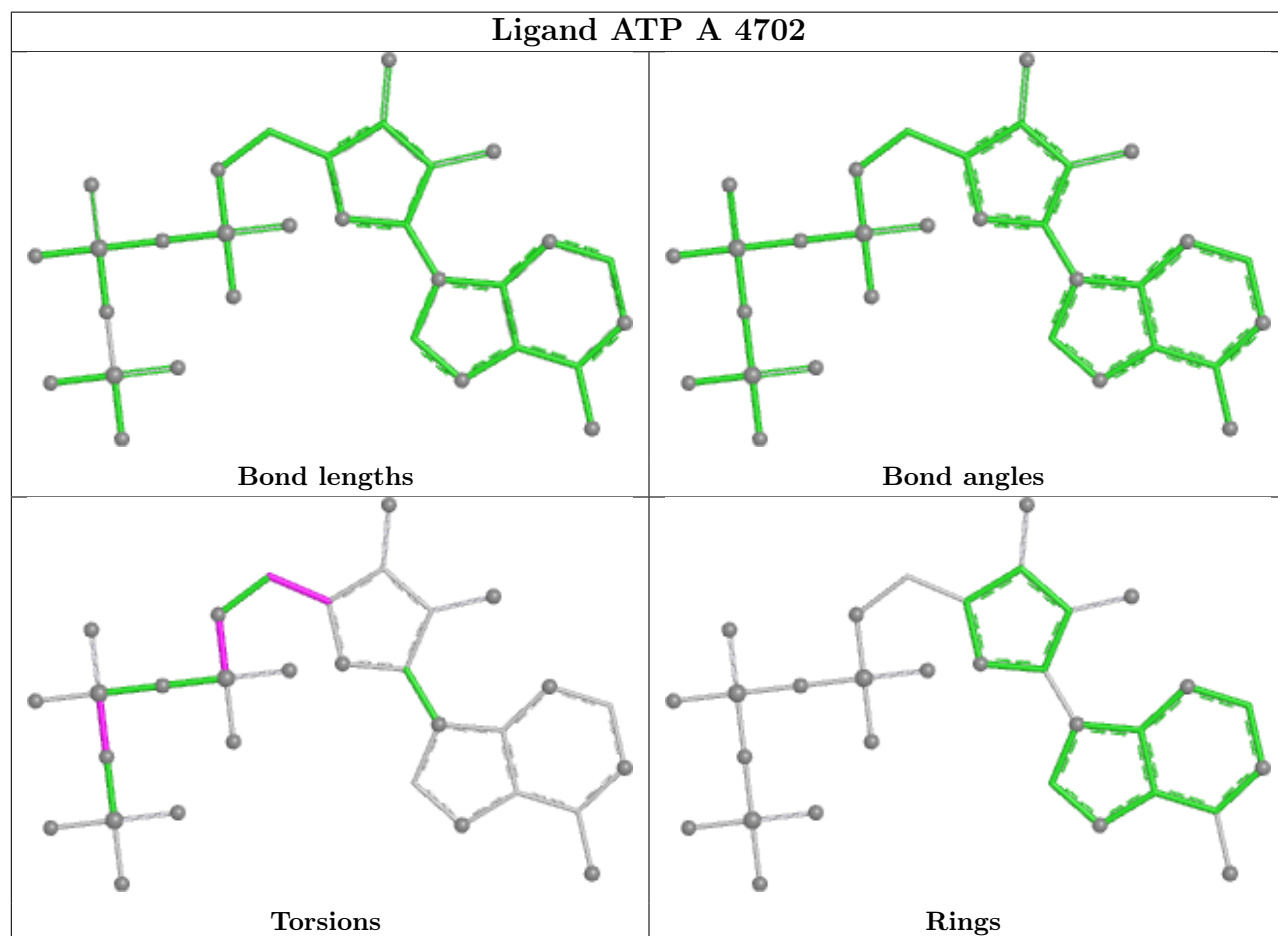
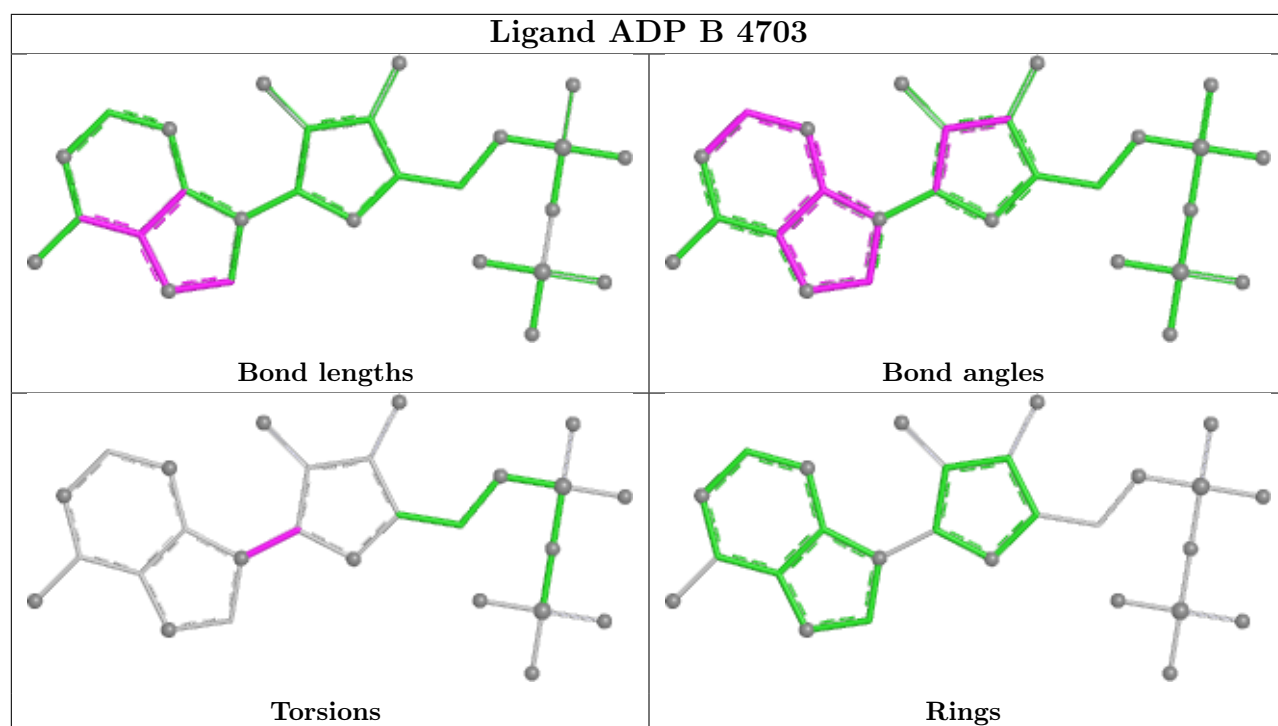
There are no ring outliers.

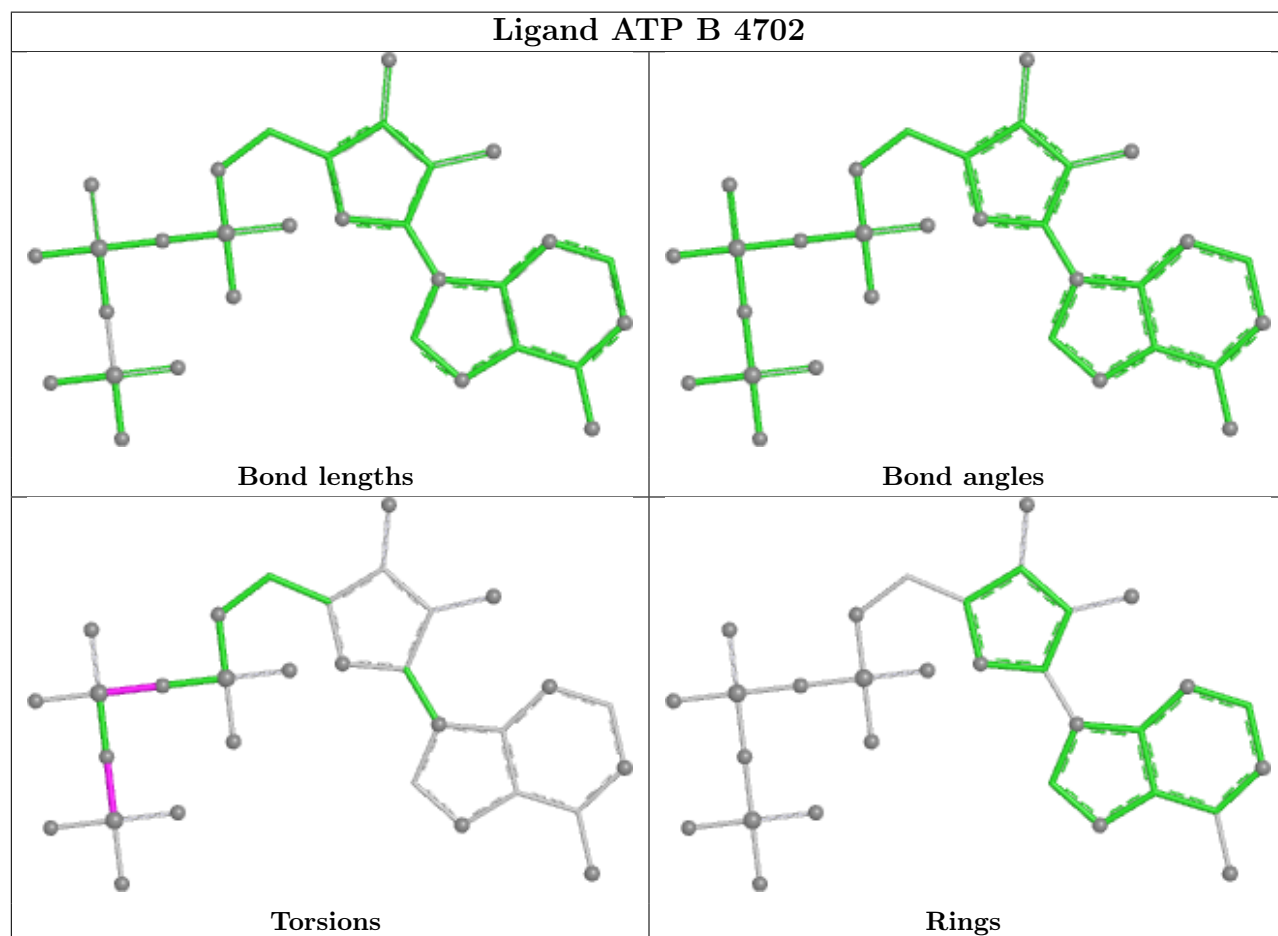
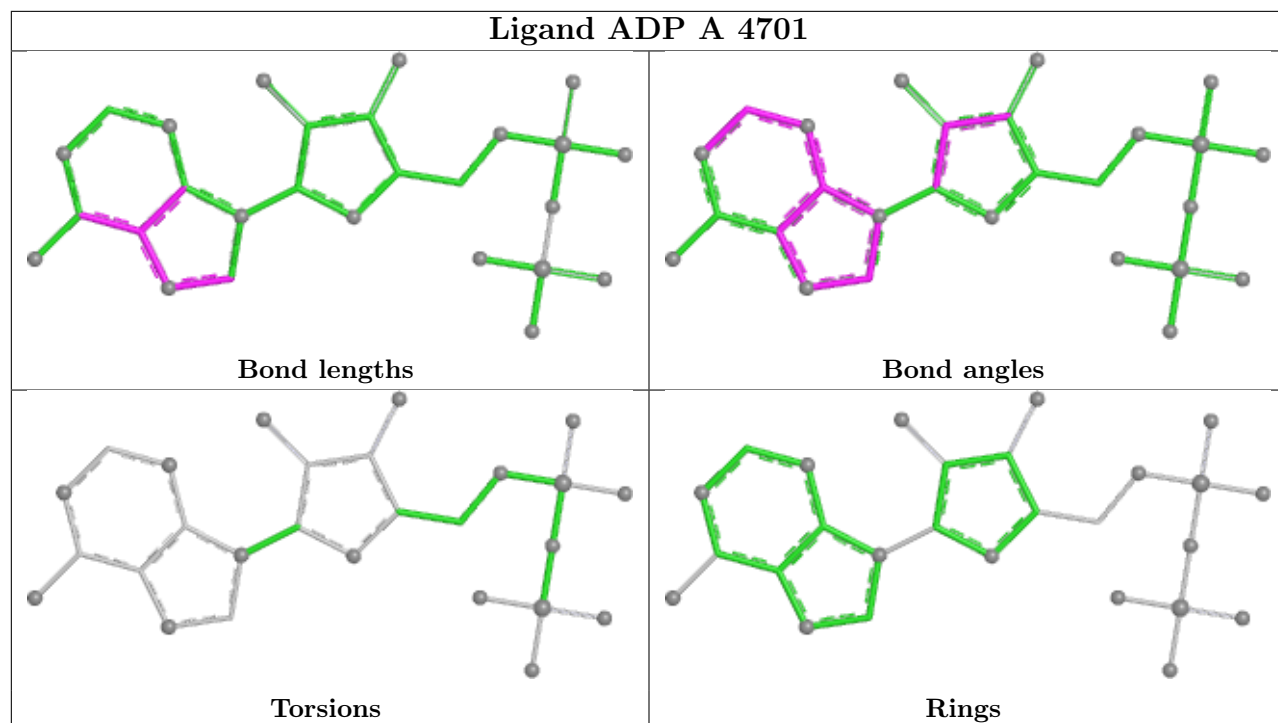
8 monomers are involved in 29 short contacts:

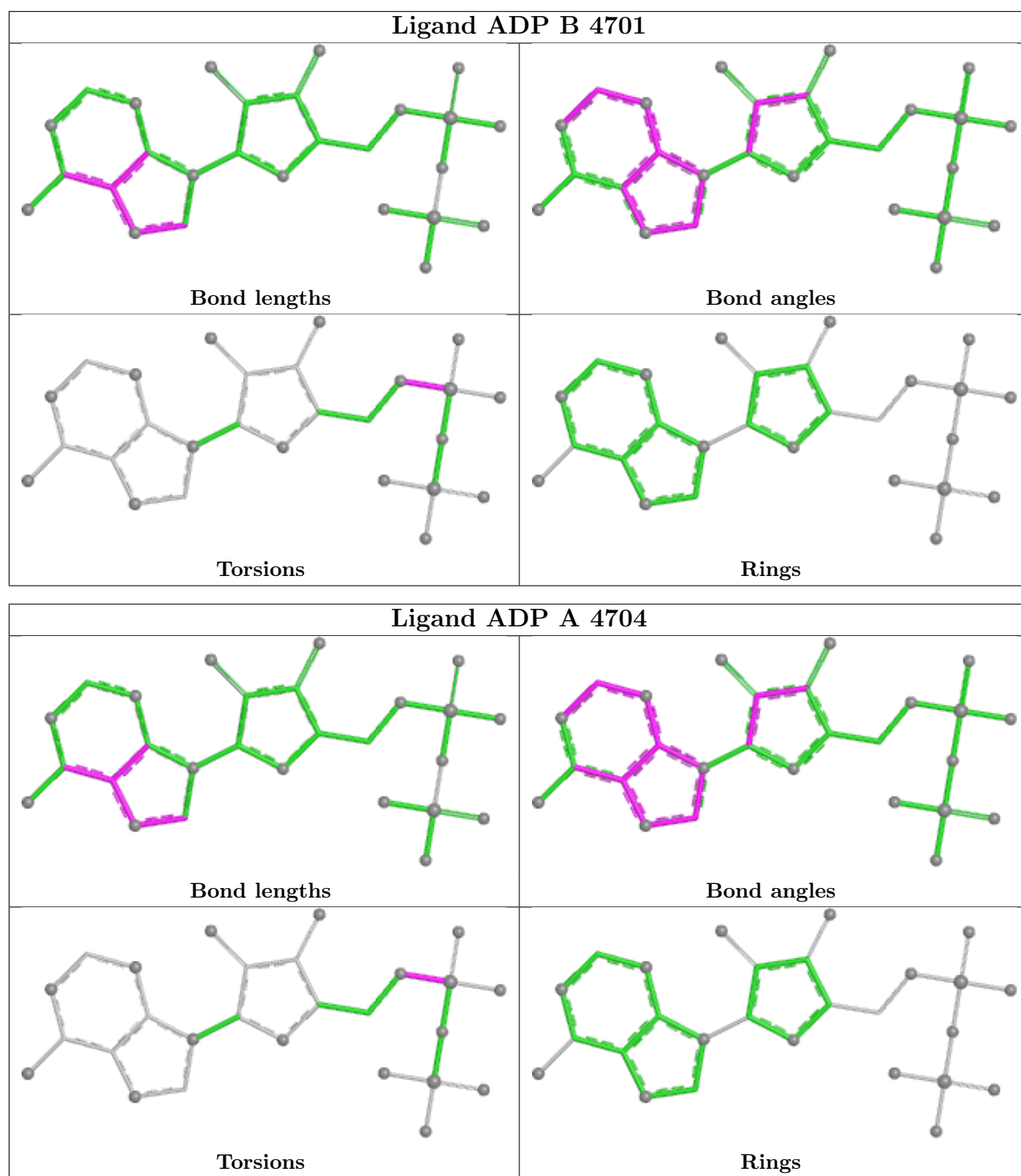
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4703	ADP	3	0
5	B	4704	ADP	2	0
5	B	4703	ADP	3	0
6	A	4702	ATP	4	0
5	A	4701	ADP	3	0
6	B	4702	ATP	6	0
5	B	4701	ADP	5	0
5	A	4704	ADP	3	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

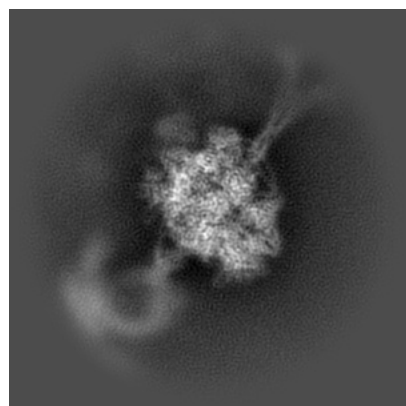
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73173. These allow visual inspection of the internal detail of the map and identification of artifacts.

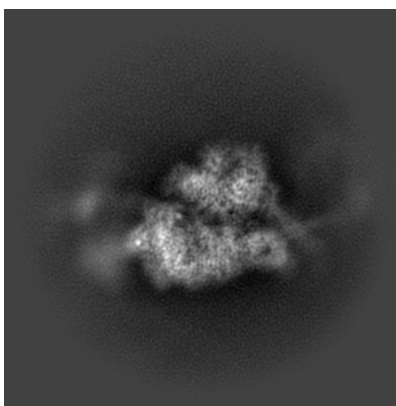
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

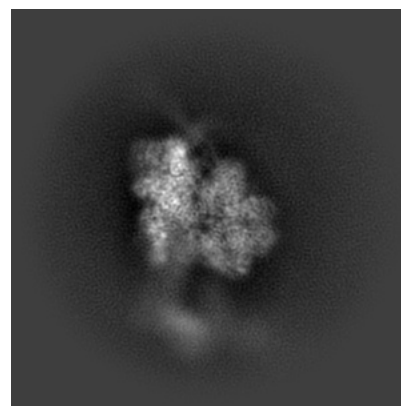
6.1.1 Primary map



X

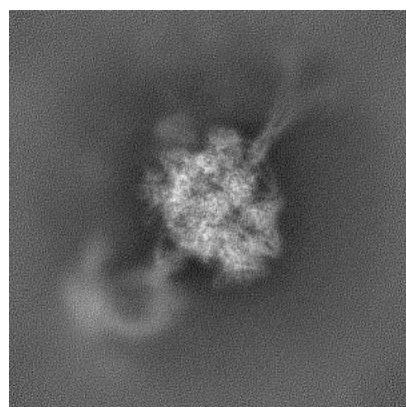


Y

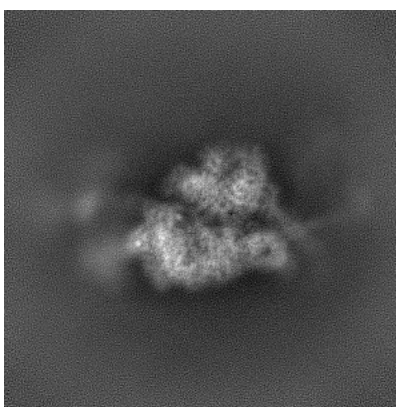


Z

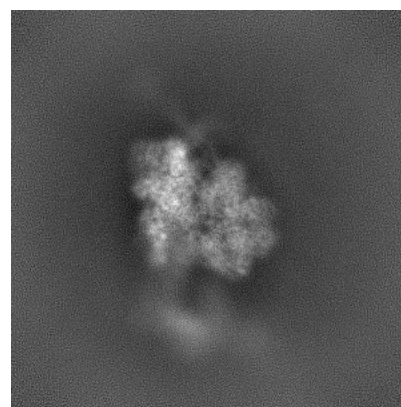
6.1.2 Raw map



X



Y

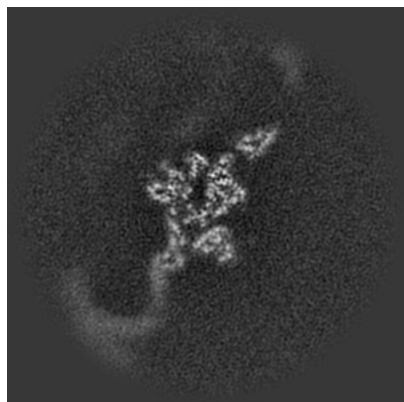


Z

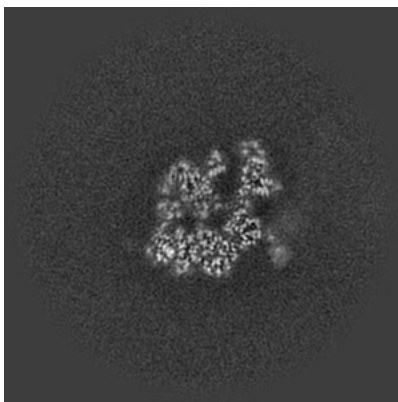
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

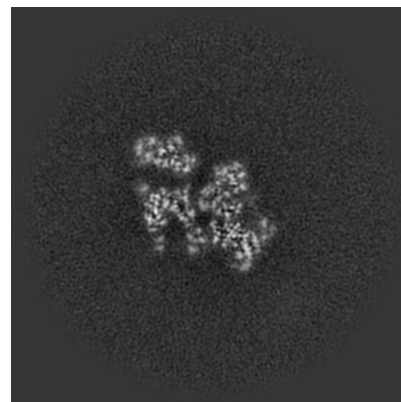
6.2.1 Primary map



X Index: 192

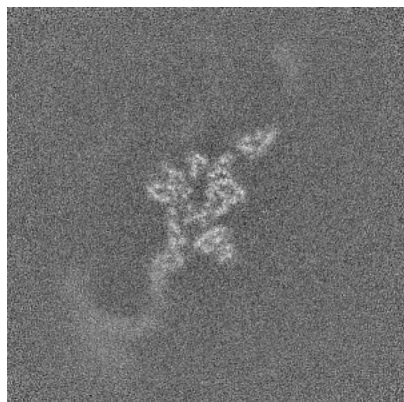


Y Index: 192

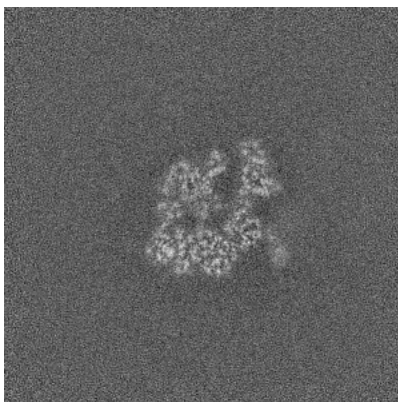


Z Index: 192

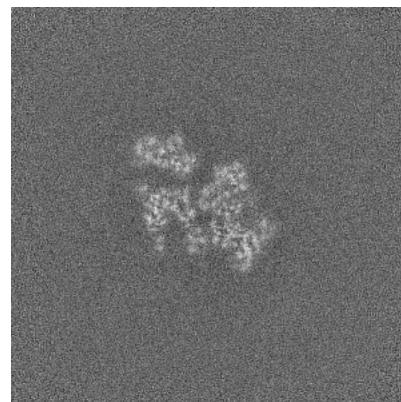
6.2.2 Raw map



X Index: 192



Y Index: 192

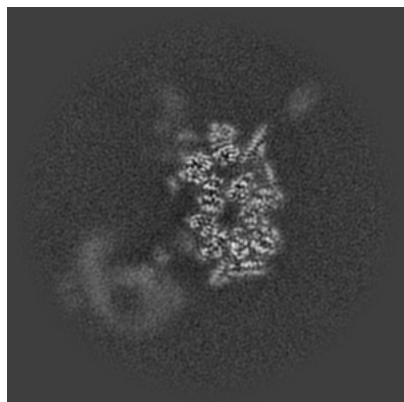


Z Index: 192

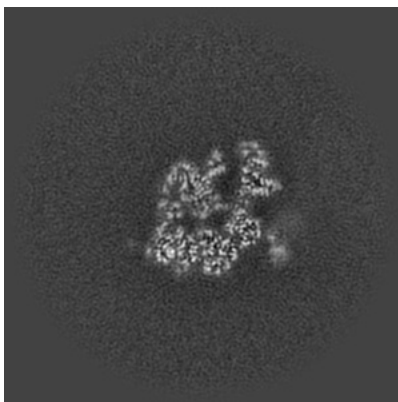
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

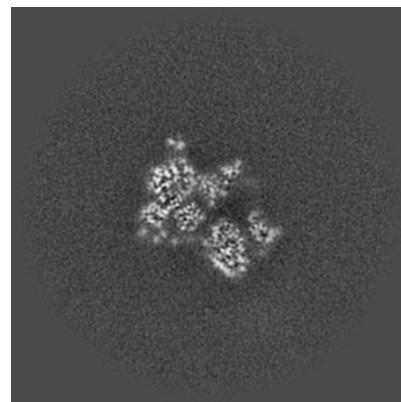
6.3.1 Primary map



X Index: 157

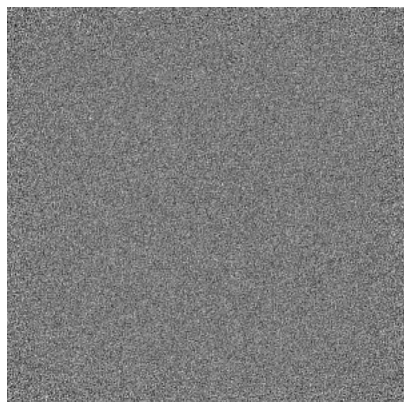


Y Index: 193

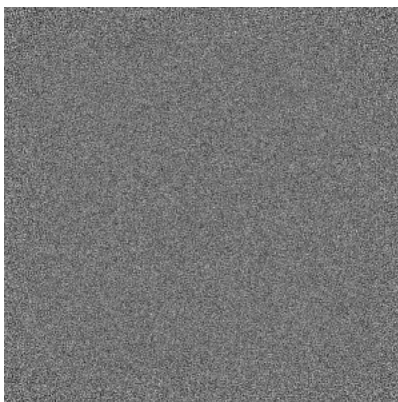


Z Index: 214

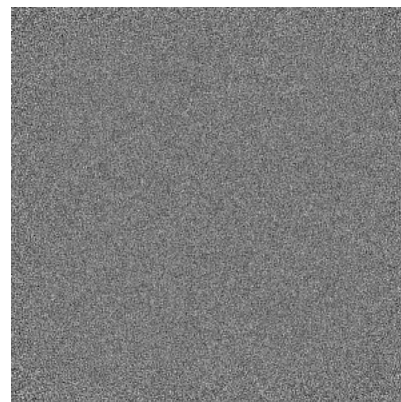
6.3.2 Raw map



X Index: 0



Y Index: 0

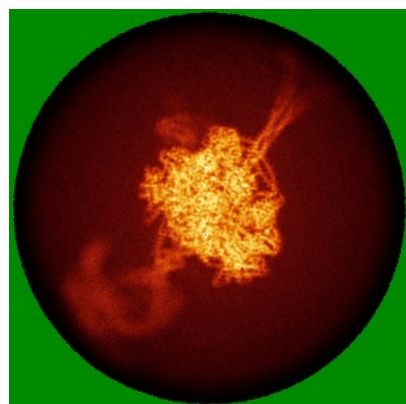


Z Index: 0

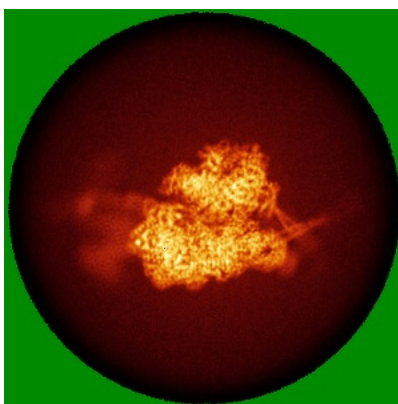
The images above show the largest variance slices of the map in three orthogonal directions.

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

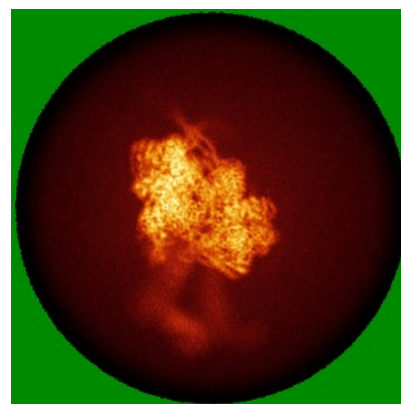
6.4.1 Primary map



X

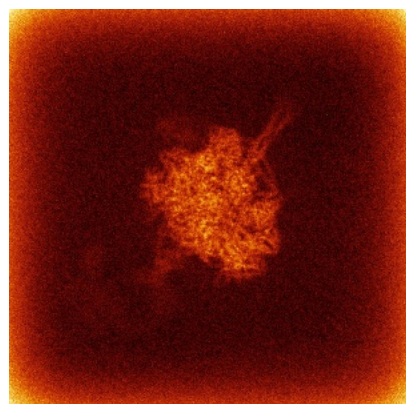


Y

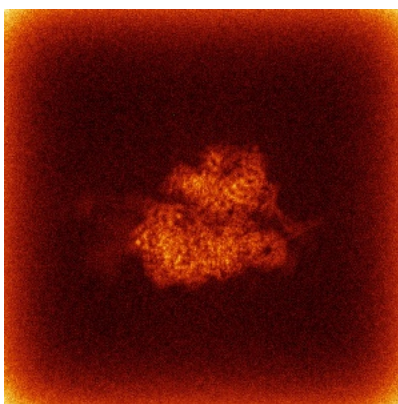


Z

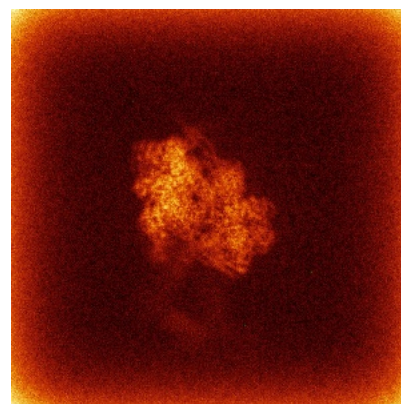
6.4.2 Raw map



X



Y

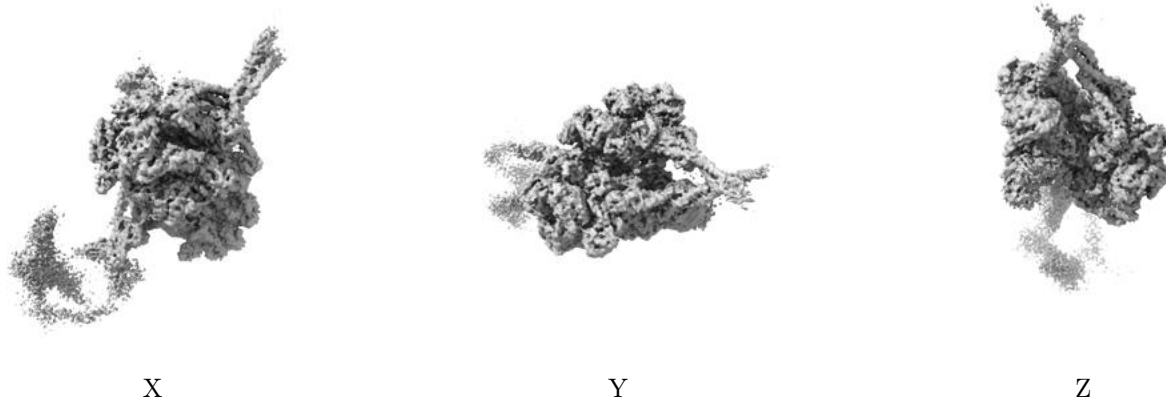


Z

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

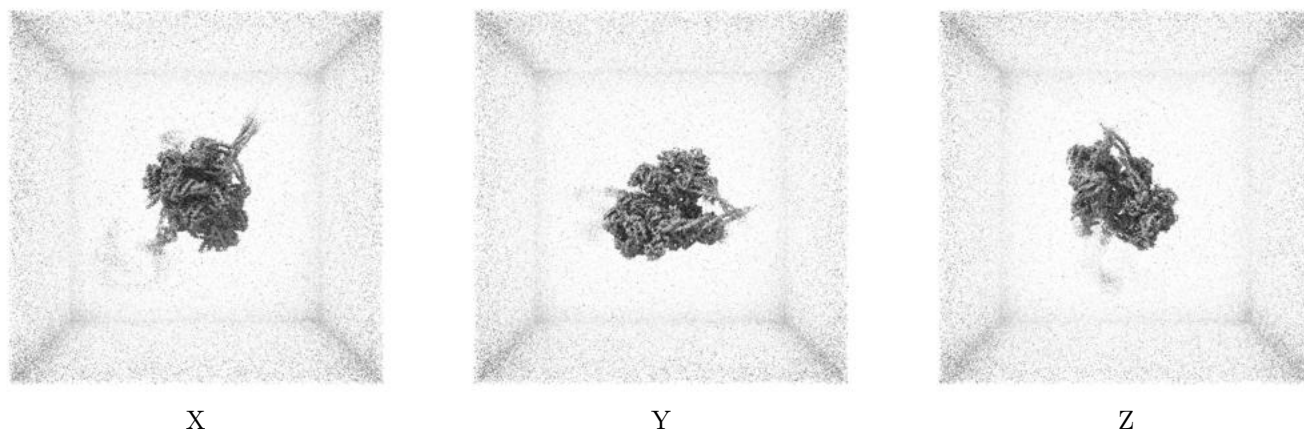
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

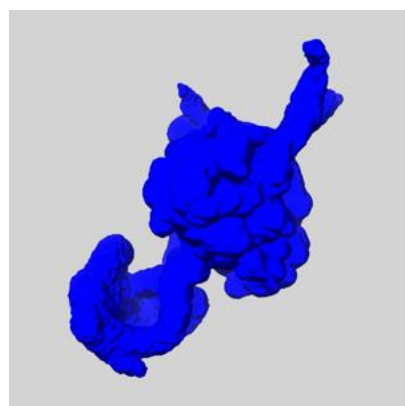
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

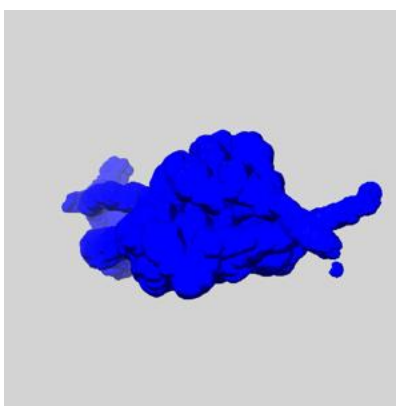
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

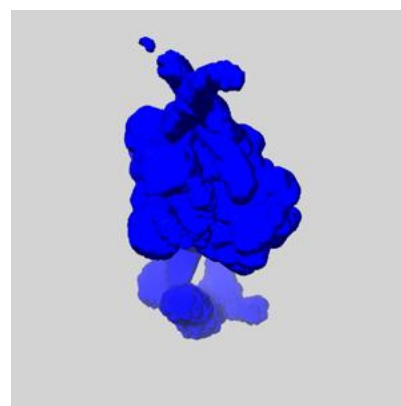
6.6.1 emd_73173_msk_1.map [i](#)



X



Y

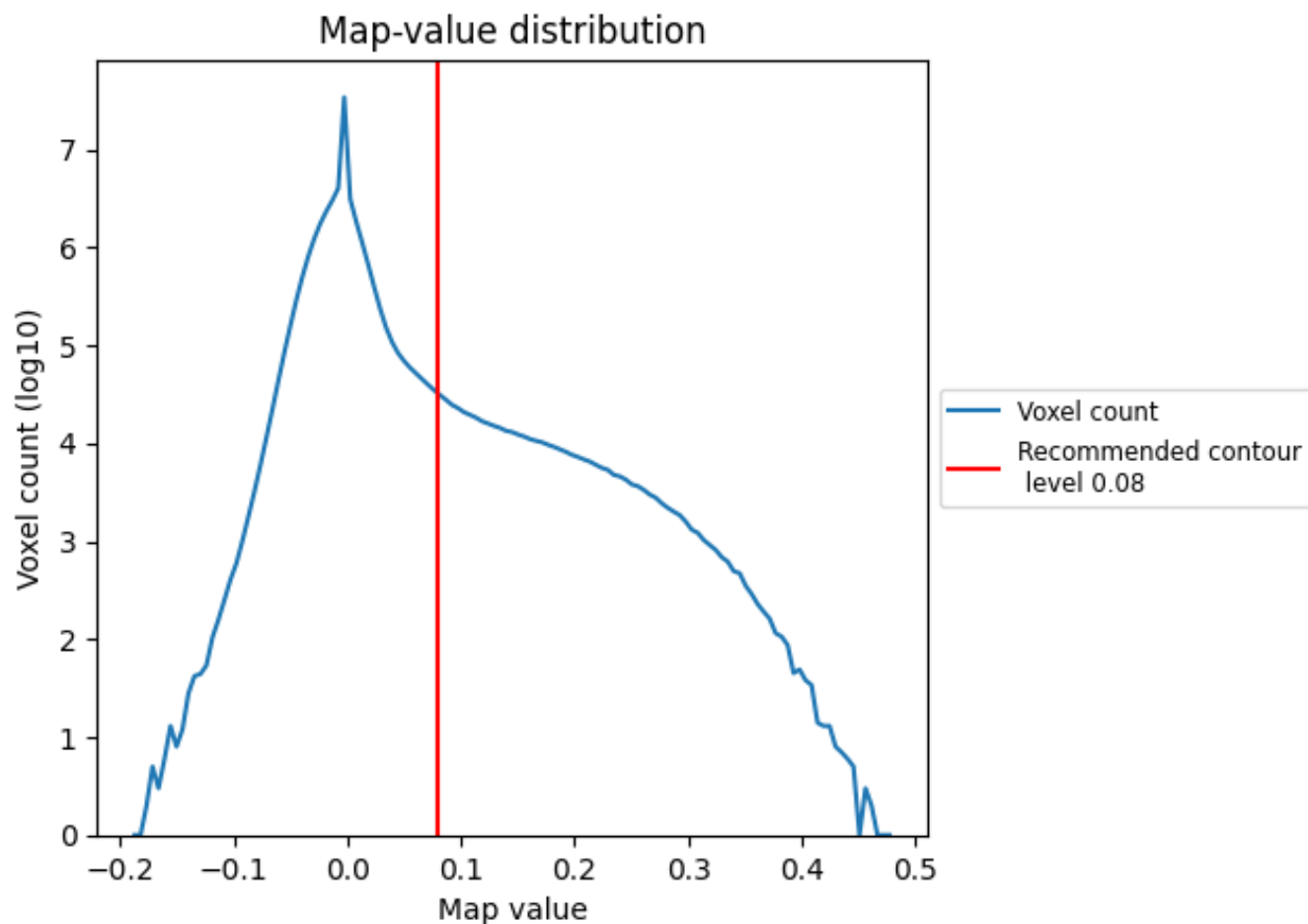


Z

7 Map analysis [i](#)

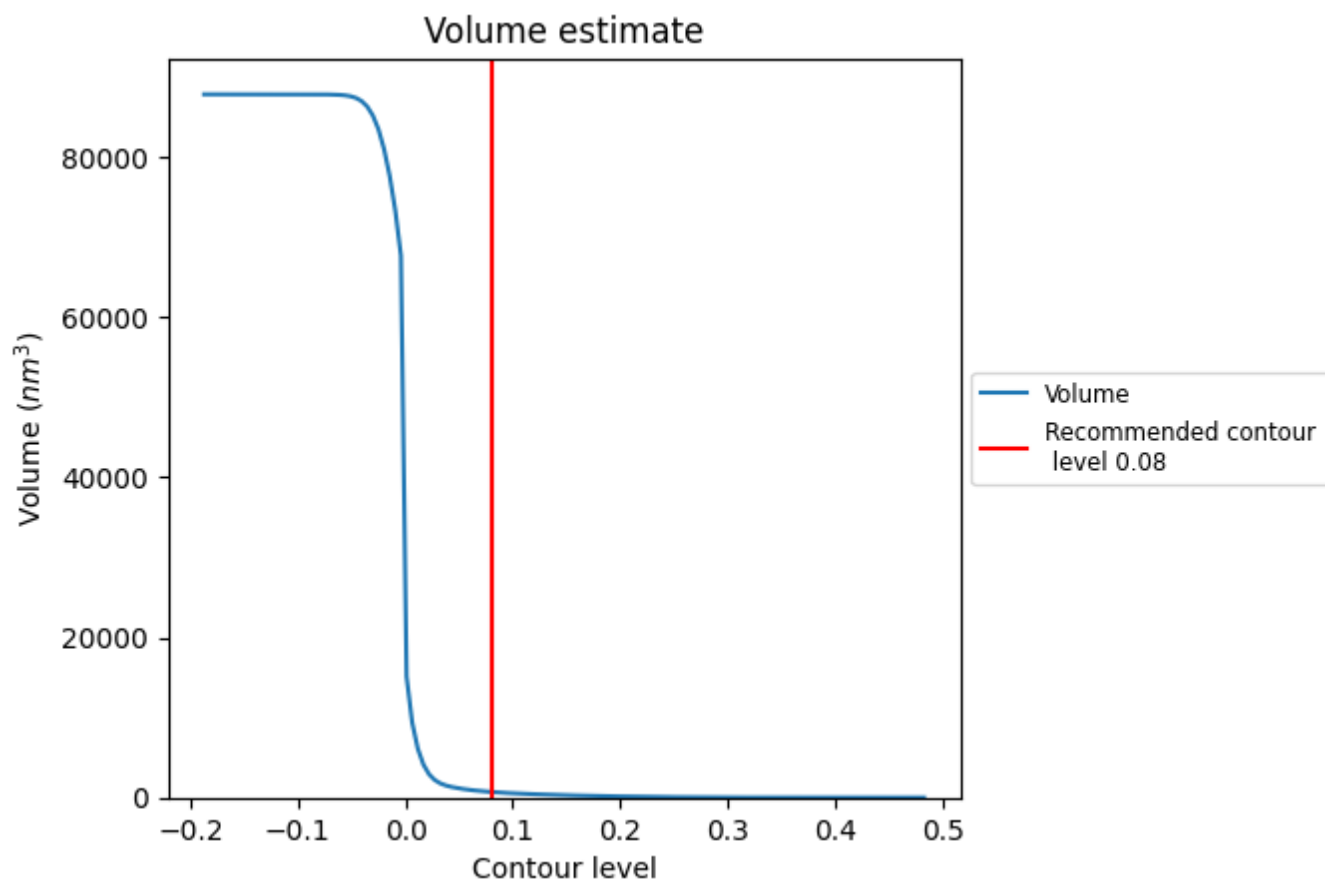
This section contains the results of statistical analysis of the map.

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.

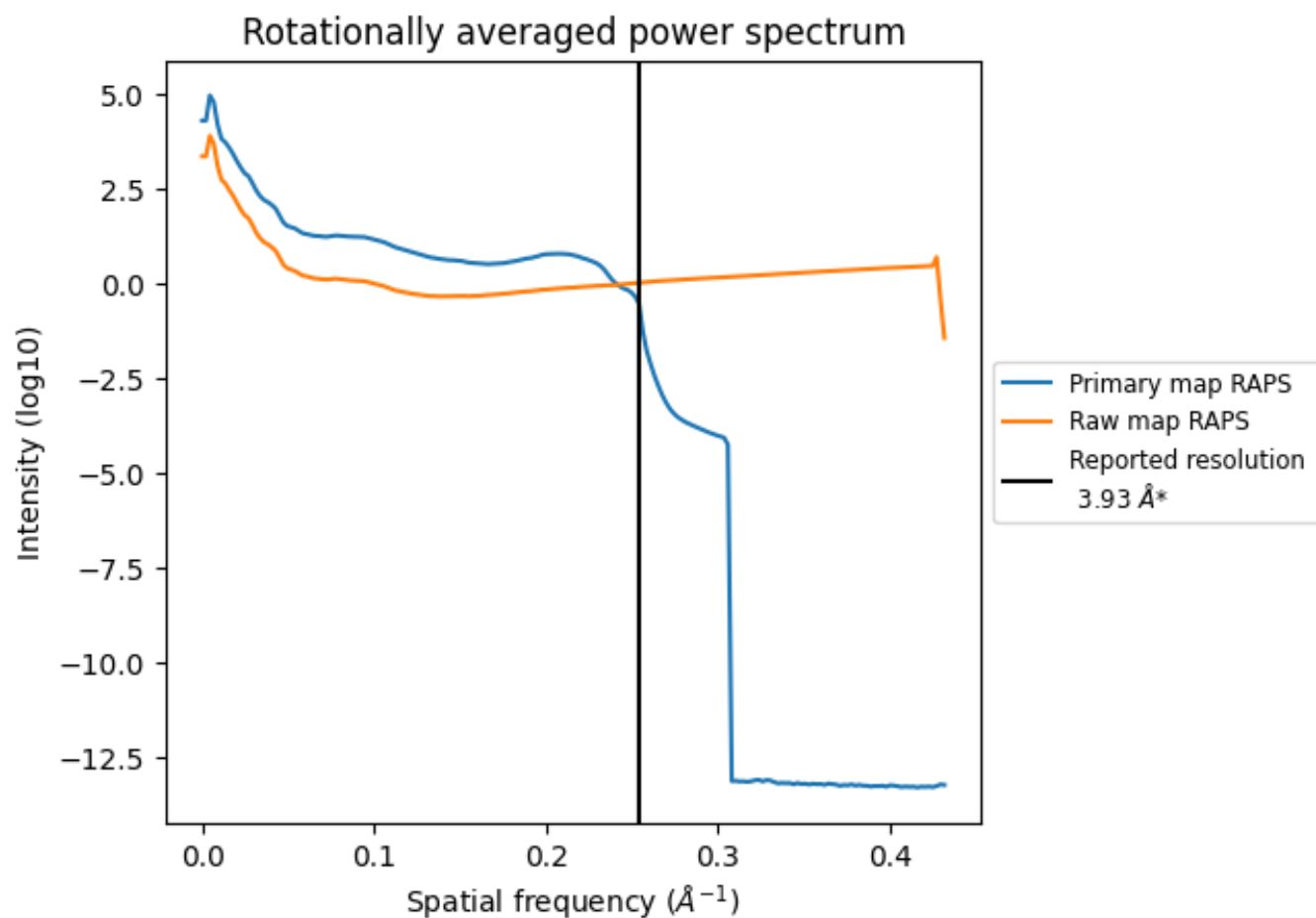
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 698 nm³; this corresponds to an approximate mass of 631 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 ⓘ

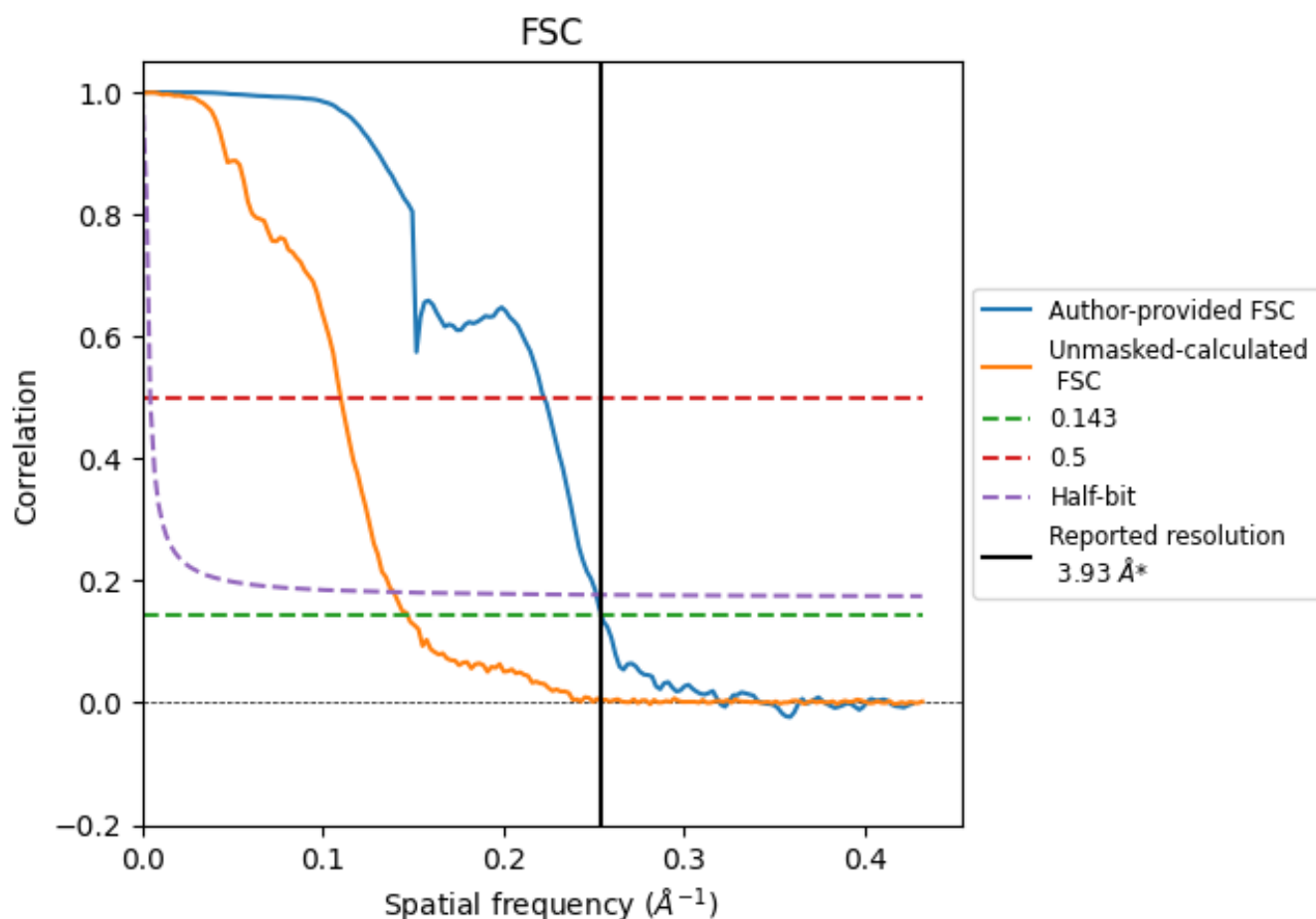


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.254 \AA^{-1}

8.2 Resolution estimates [i](#)

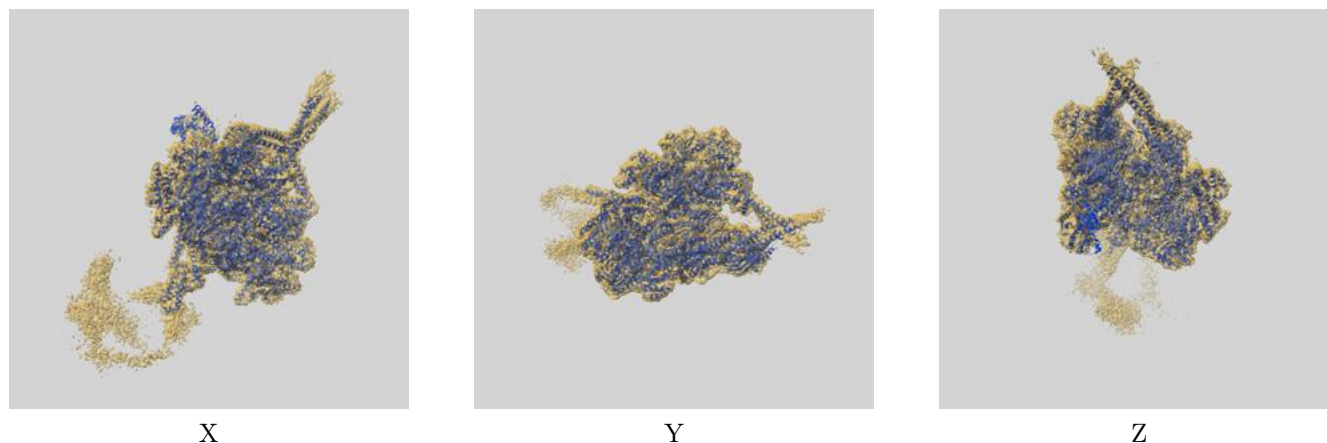
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.93	4.49	3.98
Unmasked-calculated*	6.81	9.10	7.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.81 differs from the reported value 3.93 by more than 10 %

9 Map-model fit [i](#)

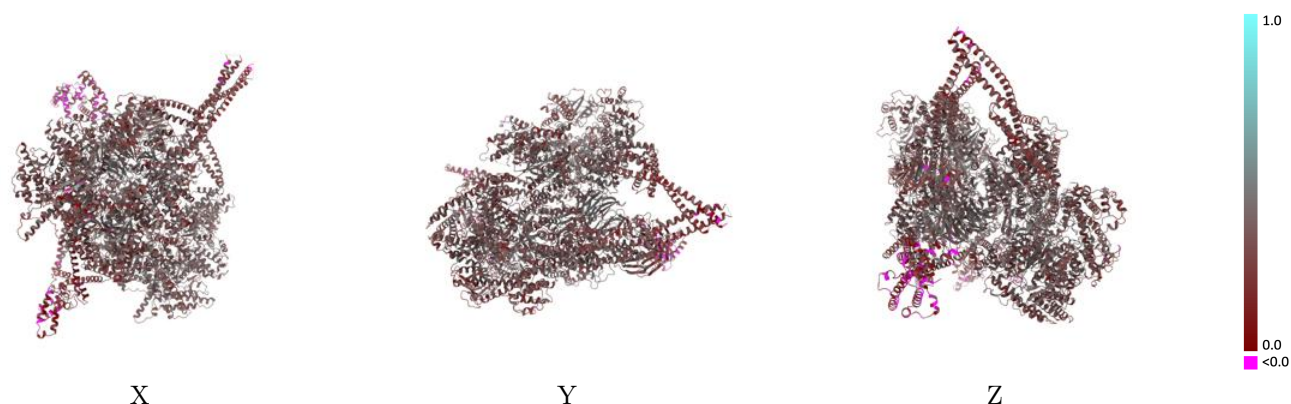
This section contains information regarding the fit between EMDB map EMD-73173 and PDB model 9YNC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



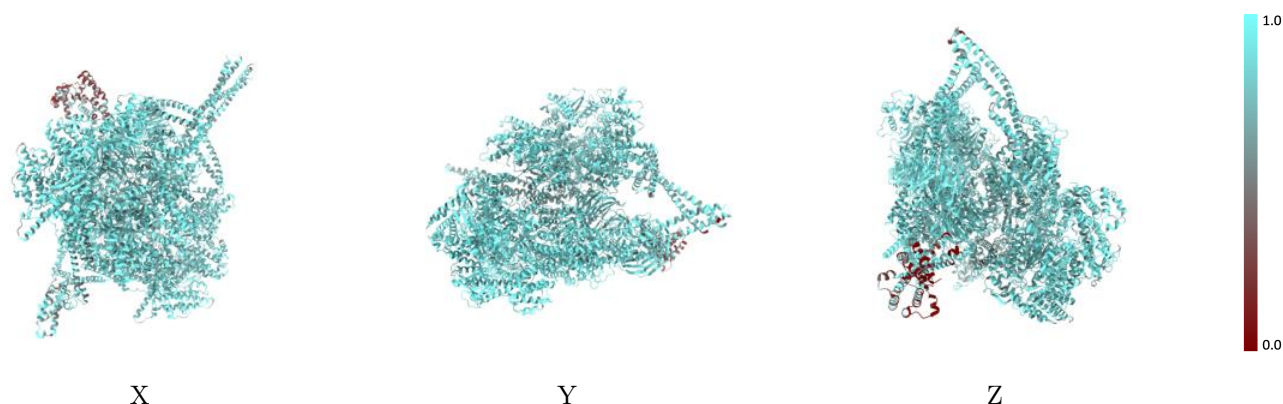
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



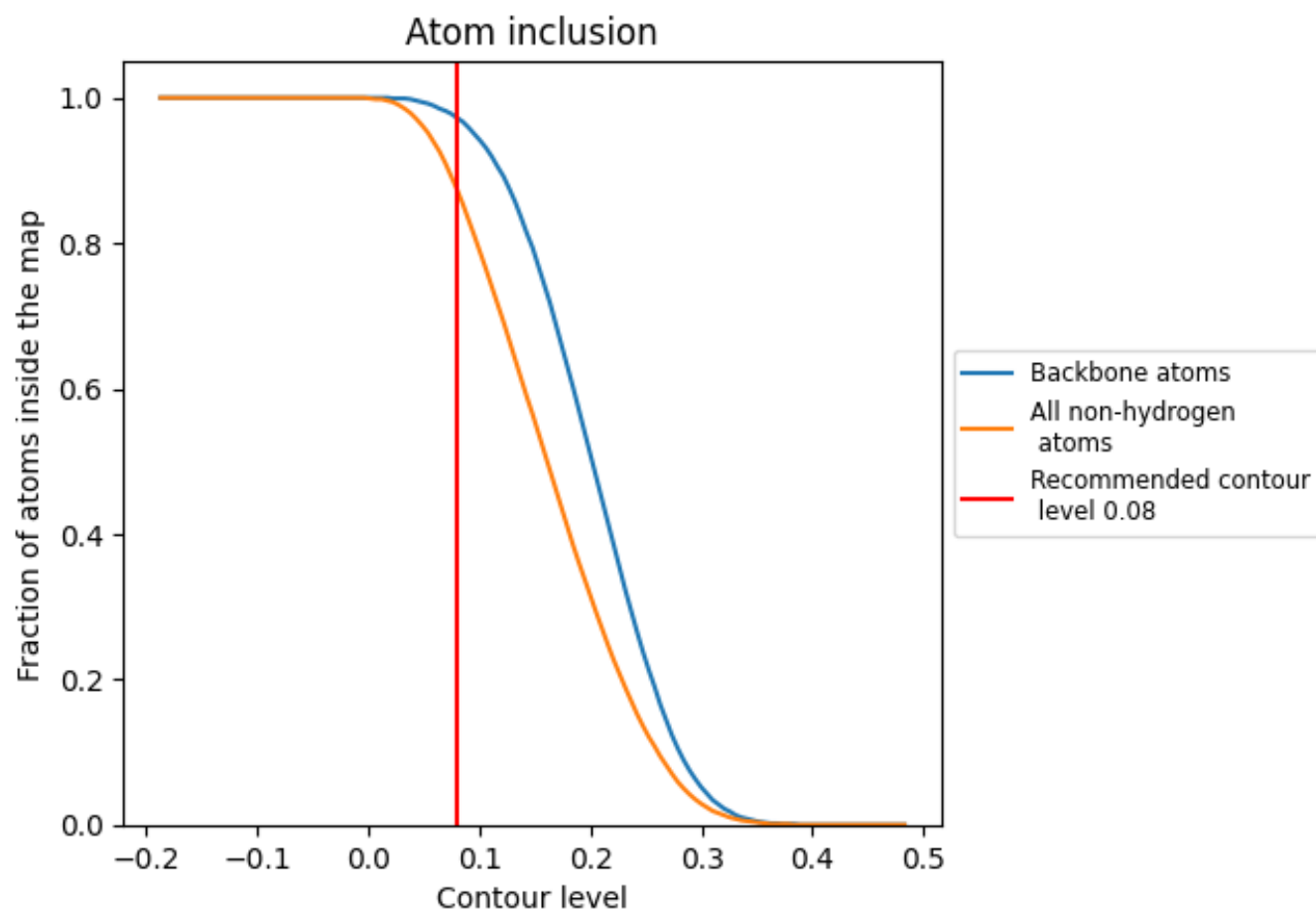
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 87% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8730	<div></div> 0.3360
A	<div></div> 0.8620	<div></div> 0.3330
B	<div></div> 0.8990	<div></div> 0.3430
C	<div></div> 0.8750	<div></div> 0.3970
D	<div></div> 0.9010	<div></div> 0.3220
E	<div></div> 0.3240	<div></div> 0.1010
F	<div></div> 0.5500	<div></div> 0.1330
G	<div></div> 0.8760	<div></div> 0.2920
H	<div></div> 0.8470	<div></div> 0.3090
I	<div></div> 0.7760	<div></div> 0.2370
J	<div></div> 0.8280	<div></div> 0.2870

1.0

0.0

<0.0