



Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 02:24 PM EDT

PDB ID : 9YND / pdb_00009ynd
EMDB ID : EMD-73174
Title : Motor domain of human dynein-1 in pre-power stroke bound to dynactin-p15
0glued-CC1B and LIS1
Authors : Yang, J.; Rao, Q.; Chai, P.; Zhang, K.
Deposited on : 2025-10-10
Resolution : 4.26 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:

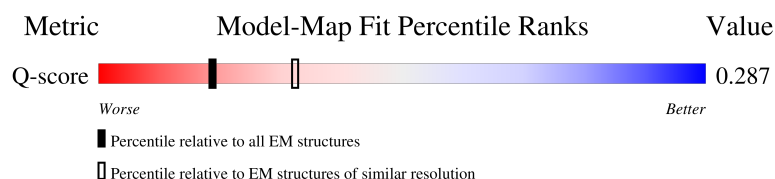
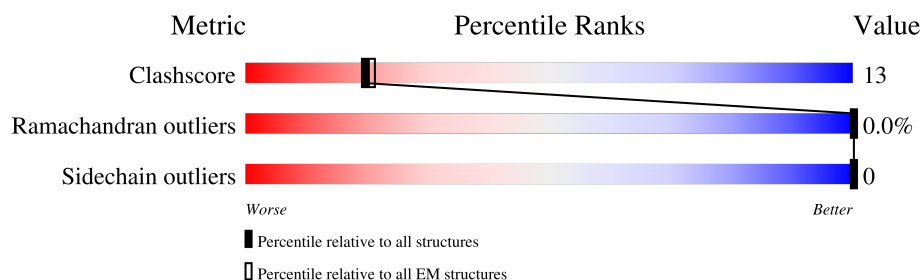
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.26 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.




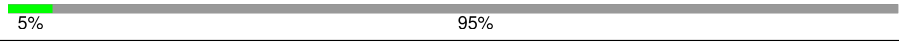
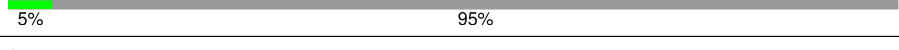
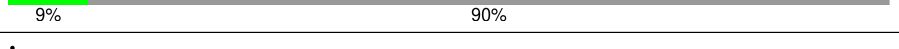
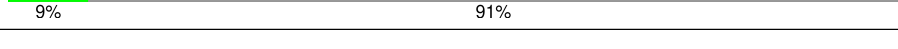
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4601 (3.76 - 4.76)

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	
2	B	410	
2	C	410	
2	D	410	

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ADP	A	4701	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32118 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	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	B	322	Total	C	N	O	S	0	0
			2557	1608	452	477	20		
2	C	313	Total	C	N	O	S	0	0
			2494	1571	440	463	20		
2	D	75	Total	C	N	O		0	0
			373	223	75	75			
2	E	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	F	34	Total	C	N	O	0	0
			170	102	34	34		
3	G	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	H	122	Total	C	N	O	0	0
			607	363	122	122		
4	I	120	Total	C	N	O	1	0
			602	360	121	121		

There are 56 discrepancies between the modelled and reference sequences:

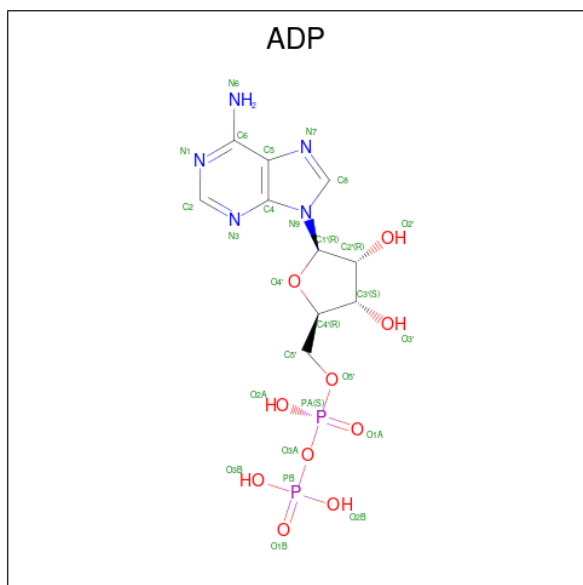
Chain	Residue	Modelled	Actual	Comment	Reference
H	118	ARG	LYS	conflict	UNP Q14203
H	124	SER	THR	conflict	UNP Q14203
H	125	ASN	THR	conflict	UNP Q14203
H	134	PRO	LEU	conflict	UNP Q14203
H	200	ALA	VAL	conflict	UNP Q14203
H	207	ALA	VAL	conflict	UNP Q14203
H	631	ASP	GLU	conflict	UNP Q14203
H	742	SER	CYS	conflict	UNP Q14203
H	778	SER	THR	conflict	UNP Q14203
H	821	ALA	PRO	conflict	UNP Q14203
H	862	PRO	LEU	conflict	UNP Q14203
H	1048	ILE	LEU	conflict	UNP Q14203
H	1072	GLY	ALA	conflict	UNP Q14203
H	1073	ALA	ILE	conflict	UNP Q14203
H	1080	ILE	SER	conflict	UNP Q14203
H	1113	VAL	ILE	conflict	UNP Q14203
H	1125	ALA	SER	conflict	UNP Q14203
H	1136	LEU	-	insertion	UNP Q14203
H	1137	PRO	-	insertion	UNP Q14203
H	1138	PRO	-	insertion	UNP Q14203
H	1147	ALA	PRO	conflict	UNP Q14203
H	1156	ASN	SER	conflict	UNP Q14203
H	1177	SER	THR	conflict	UNP Q14203
H	1189	LEU	MET	conflict	UNP Q14203
H	1193	THR	ALA	conflict	UNP Q14203
H	1202	ILE	VAL	conflict	UNP Q14203
H	1259	LEU	PHE	conflict	UNP Q14203
H	1277	ASP	SER	conflict	UNP Q14203
I	118	ARG	LYS	conflict	UNP Q14203
I	124	SER	THR	conflict	UNP Q14203
I	125	ASN	THR	conflict	UNP Q14203
I	134	PRO	LEU	conflict	UNP Q14203
I	200	ALA	VAL	conflict	UNP Q14203
I	207	ALA	VAL	conflict	UNP Q14203
I	631	ASP	GLU	conflict	UNP Q14203
I	742	SER	CYS	conflict	UNP Q14203
I	778	SER	THR	conflict	UNP Q14203
I	821	ALA	PRO	conflict	UNP Q14203
I	862	PRO	LEU	conflict	UNP Q14203
I	1048	ILE	LEU	conflict	UNP Q14203
I	1072	GLY	ALA	conflict	UNP Q14203
I	1073	ALA	ILE	conflict	UNP Q14203
I	1080	ILE	SER	conflict	UNP Q14203

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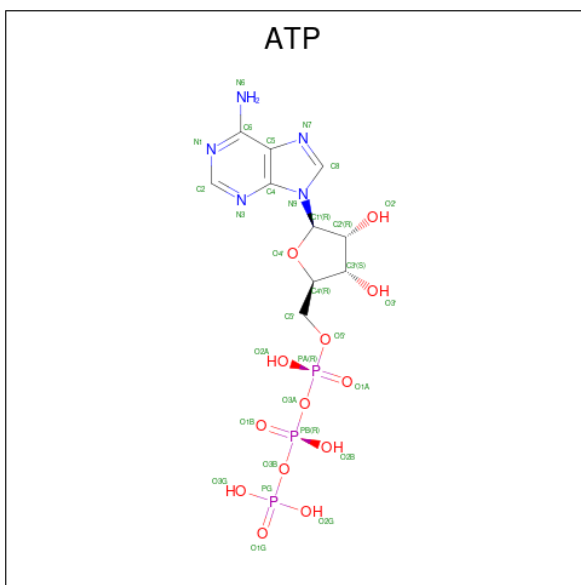
Chain	Residue	Modelled	Actual	Comment	Reference
I	1113	VAL	ILE	conflict	UNP Q14203
I	1125	ALA	SER	conflict	UNP Q14203
I	1136	LEU	-	insertion	UNP Q14203
I	1137	PRO	-	insertion	UNP Q14203
I	1138	PRO	-	insertion	UNP Q14203
I	1147	ALA	PRO	conflict	UNP Q14203
I	1156	ASN	SER	conflict	UNP Q14203
I	1177	SER	THR	conflict	UNP Q14203
I	1189	LEU	MET	conflict	UNP Q14203
I	1193	THR	ALA	conflict	UNP Q14203
I	1202	ILE	VAL	conflict	UNP Q14203
I	1259	LEU	PHE	conflict	UNP Q14203
I	1277	ASP	SER	conflict	UNP Q14203

- 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	

- 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	

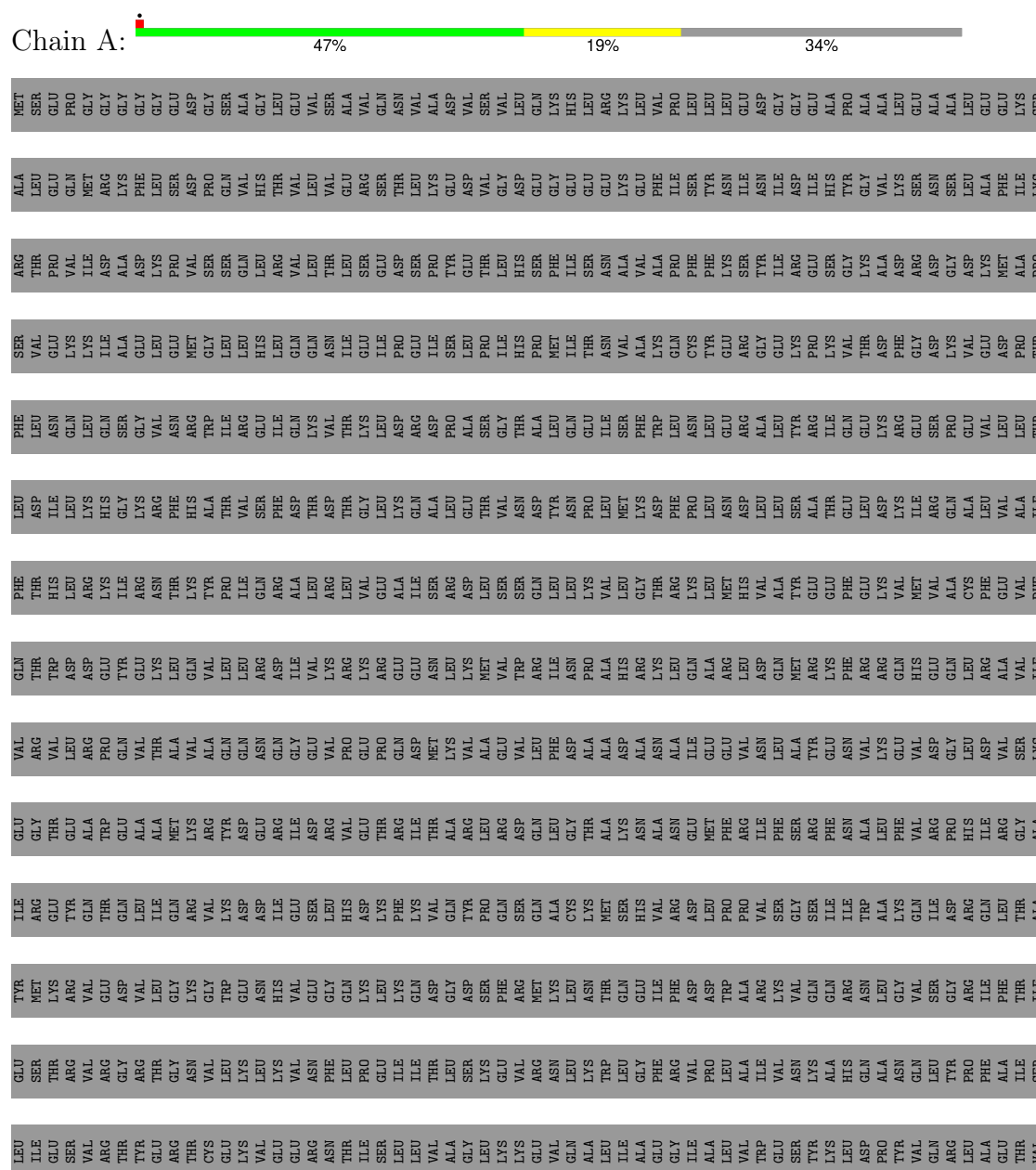
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

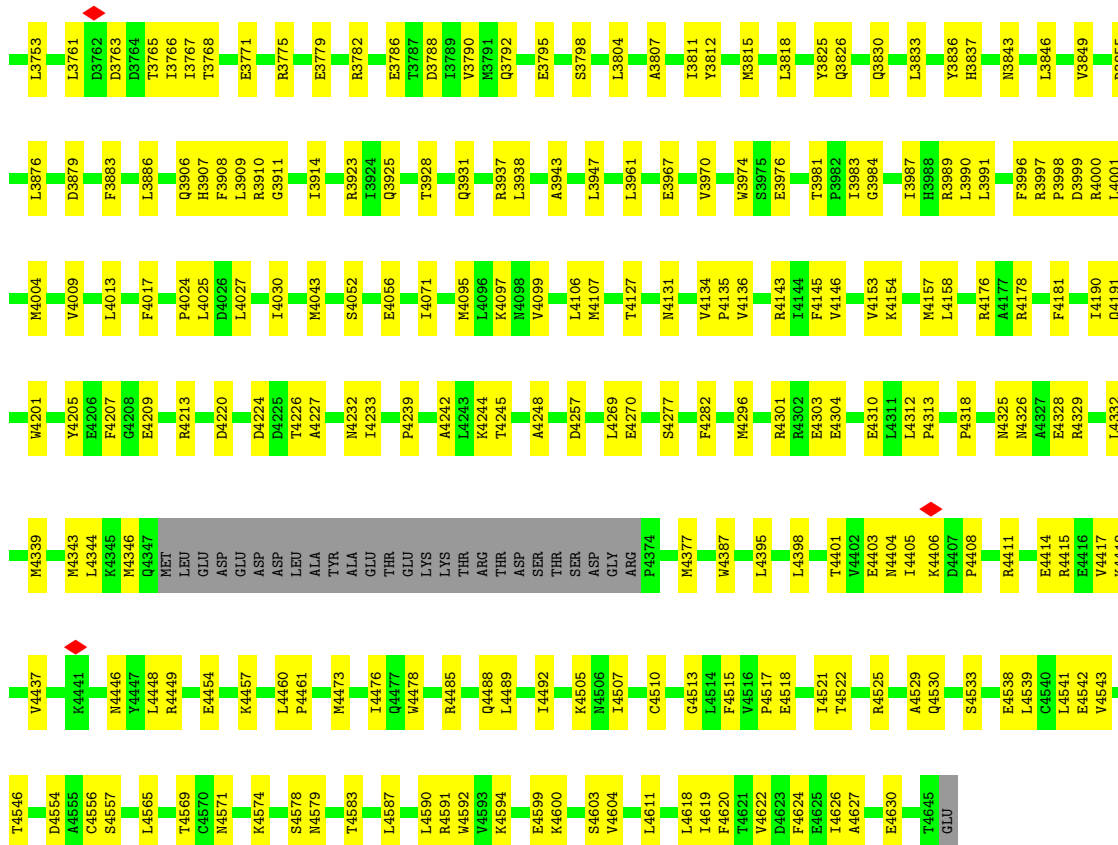
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

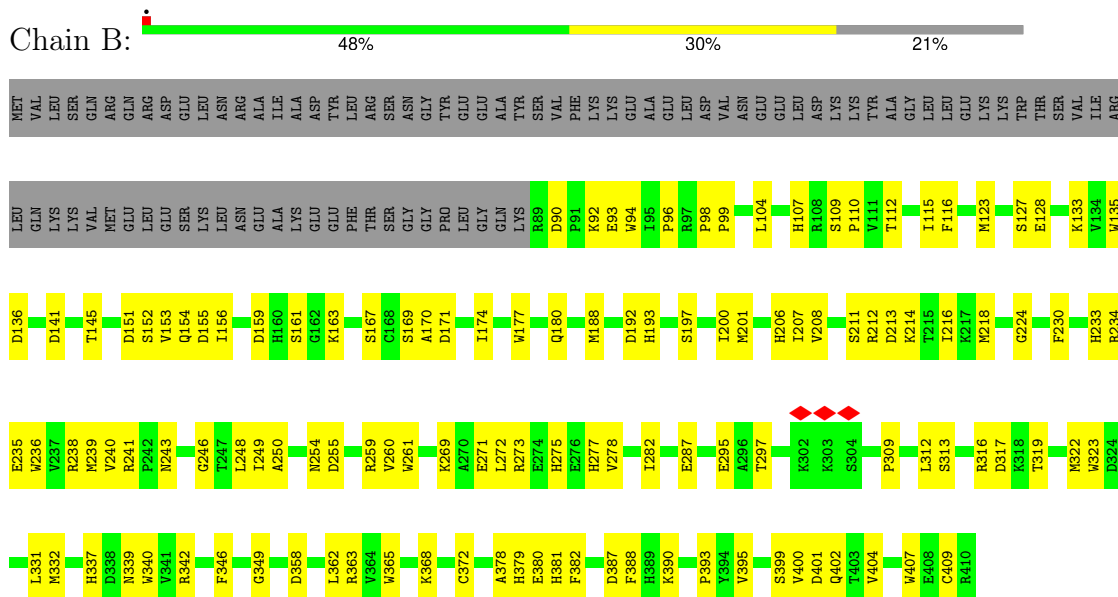


F2072	R1962	M1867	E1700	N1593	C1484	K1395	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
F2073	L1963	Y1868	W1701	I1594	R1485	I1396	ALA	GLU	PHE	PHE	LEU	LEU	LEU	LEU	ASN
R2074	E1964	L1873	E1708	I1594	L1486	L1399	LEU	THR	THR	THR	VAL	THR	THR	GLN	LEU
L2075	E1965	L1873	E1708	I1594	L1486	L1399	GLU	LYS	LYS	GLN	ILE	MET	GLN	GLY	LYS
R2077	L1968	V1880	K1715	V1597	D1491	L1403	LEU	VAL	PRO	ILE	ILE	MET	PRO	ASN	GLY
E2078	Q1881	Q1881	E1723	L1601	D1492	K1404	GLN	THR	TRP	SER	ARG	ARG	VAL	GLN	VAL
Q2079	P1883	P1883	E1723	E1620	L1493	S1405	ASP	LYS	TRP	LYS	LYS	ASP	VAL	GLU	ASP
L2080	C1977	C1977	I1739	E1620	F1494	E1406	LEU	THR	LYS	SER	ALA	GLY	ILE	ILE	ASP
S2081	I1978	D1886	T1740	R1623	N1495	A1407	LYS	ASN	TYR	GLN	ARG	VAL	VAL	GLY	LEU
R2091	L1982	Y1889	W1741	R1623	K1498	L1408	VAL	ARG	ASP	GLU	THR	ALA	ASN	ILE	ILE
E2092	L1982	Y1889	I1742	P1627	E1499	K1409	TRP	PRO	ASN	LEU	PHE	LEU	PRO	VAL	VAL
L2093	D1991	M1892	Q1746	R1628	H1500	D1410	SER	GLU	ILE	GLU	ASP	GLU	PRO	ARG	GLU
R2094	K1992	H1892	A1747	F1629	V1504	H1411	GLU	GLU	GLU	GLN	ASN	GLU	ILE	LEU	LYS
S2095	T1993	R1899	Q1748	D1634	W1413	H1412	LEU	ALA	GLY	GLN	ALA	SER	ILE	GLY	LYS
L2097	S1994	P1904	L1749	E1635	M1507	K1414	LYS	GLN	ASP	THR	THR	GLY	ALA	ILE	ILE
W2098	F1905	F1905	L1782	D1636	K1508	Q1415	VAL	VAL	GLY	ASP	ASP	SER	GLY	ASP	ASP
S2099	L2001	F1905	L1782	D1636	K1508	Q1415	TRP	LEU	ALA	THR	LYS	ALA	LEU	LEU	LEU
N2102	L2002	A1908	E1763	E1639	Y1512	M1417	GLU	THR	PHE	ALA	GLU	VAL	ARG	GLU	VAL
R2105	N2003	G1911	S1767	I1650	Y1513	K1418	ILE	ILE	ASN	PHE	GLY	GLY	THR	GLY	ALA
E2106	K2004	T1913	A1776	H1653	R1523	R1419	GLN	GLY	ILE	ASP	VAL	VAL	GLN	THR	THR
R2107	D2011	E1914	H1779	M1657	R1529	V1426	LYS	LYS	ARG	GLY	VAL	VAL	VAL	GLU	THR
E2120	L2016	K1917	H1779	M1657	R1529	V1426	GLY	PHE	ARG	VAL	ILE	VAL	VAL	LEU	LEU
D2123	T2017	A1918	M1798	V1661	A1532	S1427	THR	THR	LYS	THR	ASP	GLY	GLY	GLY	CYS
E2126	M2018	L1919	E1798	E1668	L1533	E1428	LEU	ARG	ASP	PHE	THR	GLN	ALA	ALA	GLY
L2127	P2020	G1920	Q1800	I1664	F1534	E1428	LYS	LYS	SER	ILE	THR	VAL	LYS	LYS	TYR
A2128	G2021	H1921	Q1800	I1664	F1534	E1428	ASP	ASP	ILE	THR	VAL	VAL	VAL	VAL	ASP
E2129	Y2022	H1921	Q1800	I1664	F1534	E1428	GLN	ASP	ILE	THR	VAL	VAL	VAL	VAL	ASP
Q2139	R2025	F1926	E1809	D1668	V1540	W1435	LYS	CYS	ALA	LEU	ASN	ASN	PRO	ASP	LEU
C2142	S2026	F1926	R1805	D1668	V1540	W1435	LEU	GLY	ALA	LEU	ASN	ASN	PRO	ASP	LEU
V2146	N2027	V1927	E1809	D1668	V1540	W1435	LYS	LYS	LYS	ILE	THR	CTR	ILE	ASP	ASP
R2147	L2028	C1932	S1824	V1672	Y1546	M1442	ALA	ALA	LYS	ILE	THR	CTR	ILE	ASP	ASP
K2148	N2031	D1933	S1824	V1672	Y1546	M1442	LYS	LYS	LYS	ILE	THR	CTR	ILE	ASP	ASP
L2149	K2034	F1936	K1827	I1676	S1554	V1446	ALA	ALA	LYS	PHE	THR	MET	ARG	PRO	ALA
D2153	A2040	D1937	F1836	R1679	I1557	V1449	GLU	GLU	VAL	GLU	LYS	ALA	GLN	VAL	VAL
L2157	L2048	Q1938	L1839	E1680	K1558	L1450	GLN	GLU	GLU	GLU	GLU	SER	VAL	SER	ASP
R2172	L2049	A1940	R1843	E1682	L1561	V1452	ASP	VAL	ASP	VAL	VAL	ASN	GLY	HIS	ASP
G2173	M2053	M1941	R1843	E1682	L1561	V1452	GLU	GLU	ARG	GLU	LEU	ILE	VAL	LYS	LEU
L2174	L2054	G1942	Q1850	F1686	E1564	Q1454	VAL	GLY	VAL	VAL	TYR	SER	SER	ASN	ASN
Y2190	R2060	L1948	Q1856	K1687	L1576	E1456	GLU	LEU	GLU	ARG	ASN	ARG	GLY	GLY	HIS
E2197	E2063	Q1950	L1857	T1688	L1576	E1456	LEU	LEU	SER	THR	GLY	GLY	GLY	GLY	SER
Y2211	N2067	D1958	Q1860	E1694	K1580	R1467	GLY	GLY	THR	THR	GLY	GLY	GLY	GLY	TYR
L2220	V2070	F1960	K1865	K1697	S1583	N1471	LEU	GLU	ASP	LEU	LEU	ASP	GLY	LEU	LEU
	P2071	N1961	F1866	N1699	D1590	Y1480	THR	VAL	THR	LEU	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	ASP	THR	LYS	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
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							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
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							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							THR	GLN	THR	GLY	GLY	ASN	GLY	LEU	LEU
							ASP	GLN	THR						

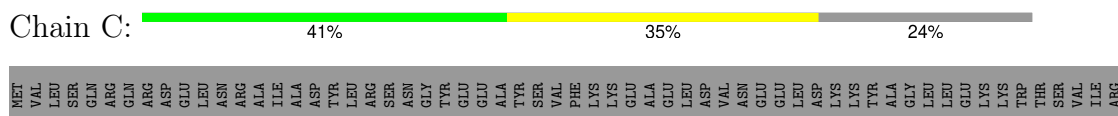




• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta



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





ARG	GLY	THR	PHE
THR	THR	THR	THR
GLY	GLY	GLY	GLY
ILE	ILE	ILE	HIS
LEU	LEU	GLU	ARG
CYS	CYS	ALA	TRP
ASP	ALA	THR	VAL
ASP	ASP	GLY	ARG
LYS	LYS	GLU	VAL
THR	THR	THR	ARG
LEU	LEU	LYS	PRO
ARG	ARG	LYS	ASN
VAL	VAL	GLN	ASN
TRP	TRP	GLY	ASP
ASP	ASP	LYS	THR
THR	THR	GLY	LEU
LYS	LYS	ILE	LEU
ASN	ASN	PRO	ILE
ARG	ARG	PHE	ALA
CYS	CYS	LEU	SER
MET	MET	SER	CYS
LYS	LYS	GLY	SER
THR	THR	SER	ASN
LEU	LEU	ARG	ASP
ASN	ASN	GLN	THR
ALA	ALA	LYS	VAL
HIS	HIS	THR	ARG
GLU	GLU	ILE	VAL
PHE	PHE	LYS	TRP
VAL	VAL	MET	VAL
THR	THR	TRP	VAL
SER	SER	ASP	ALA
LEU	LEU	VAL	THR
ALA	ALA	MET	GLU
PRO	PRO	THR	LYS
TYR	TYR	LEU	GLU
VAL	VAL	LEU	CYS
VAL	VAL	VAL	LYS
THR	THR	GLY	ALA
GLY	GLY	HIS	GLU
SER	SER	GLS	HIS
ASP	ASP	VAL	VAL
ASN	ASN	ASP	VAL
GLN	GLN	ARG	GLY
THR	THR	GLY	SER
VAL	VAL	VAL	TRP
LYS	LYS	LEU	ALA
VAL	VAL	PHE	ALA
TRP	TRP	HIS	PRO
GLU	GLU	SER	GLU
CYS	CYS	THR	SER

- Molecule 3: Cytoplasmic dynein 1 intermediate chain 2

Chain F:  5% 95%

[illegible]

- Molecule 3: Cytoplasmic dynein 1 intermediate chain 2

Chain G: 5% 95%

MET S2 K35
 GLU THR
 ASP ASP
 GLN GLN
 LYS LYS
 LYS LYS
 GLU GLU
 ALA VAL
 VAL VAL
 ALA ALA
 PRO PRO
 VAL VAL
 GLN GLN
 GLU GLU
 GLU GLU
 SER SER
 ASP ASP
 LEU LEU
 GLU GLU
 LYS LYS
 LYS LYS
 ARG ARG
 ARG ARG
 GLU GLU
 ALA ALA
 GLU GLU
 ALA ALA
 LEU LEU
 LEU LEU
 GLN GLN
 SER SER
 MET MET
 GLY GLY
 THR THR
 PRO PRO
 GLU GLU
 SER SER
 PRO PRO
 VAL VAL
 ILE ILE
 VAL VAL
 PHE PHE
 SER SER
 GLU GLU
 TYR TYR
 TRP TRP
 VAL VAL
 PRO PRO
 PRO PRO
 PRO PRO
 MET MET
 SER SER
 PRO PRO
 SER SER

[illegible]

- Molecule 4: Dynactin subunit 1

Chain H:  9% 90%

[illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37109	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	0.853	Depositor
Minimum map value	-0.366	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	444.416, 444.416, 444.416	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.736, 1.736, 1.736	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.10	0/25177	0.28	0/34112
2	B	0.12	0/2624	0.36	0/3555
2	C	0.11	0/2560	0.31	0/3470
2	D	0.06	0/372	0.19	0/518
2	E	0.07	0/372	0.17	0/518
3	F	0.04	0/169	0.13	0/235
3	G	0.05	0/169	0.13	0/235
4	H	0.19	0/606	0.29	0/845
4	I	0.40	0/601	0.54	0/838
All	All	0.12	0/32650	0.30	0/44326

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	I	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	533[A]	GLU	Mainchain
4	I	533[B]	GLU	Mainchain

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	24658	0	24763	598	0
2	B	2557	0	2487	90	0
2	C	2494	0	2419	102	0
2	D	373	0	172	0	0
2	E	373	0	172	1	0
3	F	170	0	73	0	0
3	G	170	0	73	0	0
4	H	607	0	285	1	0
4	I	602	0	282	3	0
5	A	81	0	36	14	0
6	A	31	0	12	2	0
7	A	2	0	0	0	0
All	All	32118	0	30774	788	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 13.

All (788) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2965:ARG:NH2	1:A:3640:SER:O	2.00	0.94
2:C:174:ILE:HB	2:C:188:MET:HB3	1.60	0.82
1:A:2503:SER:HB3	1:A:2511:ARG:HG2	1.60	0.81
2:C:207:ILE:HB	2:C:219:TRP:HB2	1.64	0.79
1:A:3039:LYS:O	2:B:273:ARG:NH2	2.16	0.79
1:A:3981:THR:HG23	1:A:3984:GLY:H	1.51	0.75
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.22	0.72
2:C:196:SER:H	2:C:211:SER:HA	1.55	0.71
1:A:4398:LEU:HG	1:A:4417:VAL:HG11	1.72	0.71
2:C:186:ARG:NH1	2:C:221:VAL:O	2.21	0.70
1:A:4343:MET:HA	1:A:4346:MET:HB2	1.73	0.70
2:C:197:SER:HB3	2:C:210:ALA:HB3	1.73	0.70
1:A:2988:GLU:OE1	2:B:234:ARG:NH2	2.25	0.70
1:A:4542:GLU:HB3	1:A:4591:ARG:HB2	1.74	0.70
1:A:2828:GLU:HG2	1:A:2832:LEU:HD23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4095:MET:HE1	1:A:4097:LYS:HE2	1.72	0.69
2:C:165:LEU:HB3	2:C:177:TRP:HB2	1.74	0.69
1:A:1439:LEU:HA	1:A:1442:ASN:HB3	1.73	0.69
1:A:3655:ARG:HH21	1:A:3660:VAL:HA	1.56	0.69
1:A:2347:ASP:OD1	1:A:2349:LYS:NZ	2.24	0.69
1:A:2222:MET:HE1	1:A:2342:MET:HB3	1.74	0.69
1:A:2060:ARG:NH1	1:A:2128:ALA:O	2.27	0.68
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.25	0.68
2:C:324:ASP:HB3	2:C:327:THR:HG22	1.76	0.68
1:A:3167:ARG:NH1	1:A:3687:GLU:OE2	2.27	0.67
1:A:3478:LEU:HD12	1:A:3771:GLU:HG3	1.76	0.67
2:C:174:ILE:HD11	2:C:195:VAL:HG11	1.75	0.67
1:A:2081:SER:HA	1:A:4415:ARG:HH21	1.59	0.67
1:A:2953:MET:O	2:B:277:HIS:NE2	2.26	0.67
1:A:4301:ARG:NH1	1:A:4303:GLU:OE2	2.27	0.67
1:A:2569:VAL:HG11	1:A:2747:ILE:HA	1.76	0.67
2:C:104:LEU:HB2	2:C:404:VAL:HB	1.77	0.67
1:A:2315:LEU:HB3	1:A:2319:LEU:HD23	1.76	0.66
2:B:297:THR:HG21	2:B:331:LEU:HD13	1.78	0.66
1:A:4492:ILE:HG13	1:A:4507:ILE:HD13	1.77	0.66
1:A:2813:LEU:HD21	1:A:2816:LEU:HB2	1.78	0.66
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.78	0.66
1:A:1396:ILE:HG21	1:A:1439:LEU:HD22	1.77	0.65
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.13	0.65
1:A:3931:GLN:NE2	1:A:3996:PHE:O	2.28	0.65
1:A:1415:GLN:HA	1:A:1418:LYS:HE2	1.77	0.65
1:A:2260:SER:OG	1:A:2262:ASP:OD1	2.14	0.65
1:A:2306:ASP:OD1	1:A:2307:VAL:N	2.28	0.65
1:A:3771:GLU:HB3	1:A:3775:ARG:HH21	1.60	0.65
1:A:1911:GLY:H	5:A:4701:ADP:H5'2	1.62	0.65
1:A:2271:ASN:OD1	1:A:2272:THR:N	2.29	0.65
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	1.78	0.65
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.78	0.65
1:A:1672:VAL:HA	1:A:1691:SER:HA	1.78	0.64
1:A:3782:ARG:NH1	1:A:3786:GLU:OE2	2.30	0.64
2:B:174:ILE:HB	2:B:188:MET:HB3	1.80	0.64
2:C:209:SER:OG	2:C:219:TRP:NE1	2.24	0.64
1:A:3638:VAL:HG22	1:A:3681:THR:HB	1.79	0.64
2:C:149:HIS:ND1	2:C:171:ASP:OD2	2.23	0.64
1:A:1892:MET:HE1	1:A:1904:PRO:HD3	1.80	0.64
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:GLU:OE2	2:B:368:LYS:NZ	2.31	0.64
1:A:2094:LYS:NZ	5:A:4701:ADP:O2'	2.31	0.64
1:A:2956:LEU:HD13	1:A:2989:LYS:HB3	1.79	0.64
2:C:234:ARG:HH22	2:C:273:ARG:HH21	1.45	0.64
1:A:1667:ASN:ND2	1:A:1671:SER:OG	2.29	0.64
1:A:2076:CYS:HA	1:A:2080:LEU:HD23	1.80	0.64
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.80	0.63
1:A:4153:VAL:HG12	1:A:4157:MET:HE1	1.80	0.63
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.31	0.63
1:A:3914:ILE:O	1:A:3937:ARG:NH1	2.32	0.63
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.32	0.63
1:A:2694:ARG:NH1	1:A:2697:ASP:OD2	2.31	0.63
2:B:193:HIS:HB3	2:B:212:ARG:HB3	1.79	0.63
1:A:2664:ASP:HA	1:A:2711:ALA:HB3	1.79	0.63
2:B:233:HIS:ND1	2:B:255:ASP:OD2	2.22	0.63
2:B:379:HIS:ND1	2:B:401:ASP:OD2	2.30	0.63
1:A:2254:ILE:HD12	1:A:2279:LEU:HD21	1.80	0.63
1:A:2419:ALA:HA	1:A:2422:ILE:HD12	1.81	0.63
1:A:2261:LYS:NZ	1:A:2310:GLU:O	2.29	0.62
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.32	0.62
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.80	0.62
1:A:4154:LYS:HE3	1:A:4310:GLU:HA	1.81	0.62
1:A:1931:ASN:ND2	1:A:2313:GLU:O	2.28	0.62
1:A:2684:ARG:NH1	1:A:2688:GLU:OE1	2.31	0.62
2:C:152:SER:O	2:C:154:GLN:NE2	2.32	0.62
1:A:4097:LYS:HA	1:A:4127:THR:HB	1.80	0.62
2:C:94:TRP:O	2:C:347:HIS:NE2	2.30	0.62
1:A:4301:ARG:HB2	1:A:4304:GLU:HG3	1.81	0.62
1:A:2564:ALA:HA	1:A:2804:ARG:HH22	1.65	0.62
1:A:2767:GLU:OE1	1:A:2767:GLU:N	2.30	0.61
1:A:1620:GLU:OE2	1:A:1943:ARG:NH1	2.34	0.61
1:A:3645:LEU:HB3	1:A:3649:LEU:HD23	1.81	0.61
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.34	0.61
2:B:112:THR:HG21	2:B:154:GLN:HA	1.83	0.61
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	1.82	0.61
1:A:3502:THR:HG22	1:A:3542:GLN:HB3	1.81	0.61
2:C:206:HIS:HB3	2:C:218:MET:HE1	1.81	0.61
1:A:3716:VAL:HG21	1:A:3804:LEU:HD21	1.83	0.60
1:A:4518:GLU:N	1:A:4518:GLU:OE1	2.33	0.60
2:C:178:ASP:HB2	2:C:185:ILE:HD11	1.82	0.60
1:A:1914:GLU:OE1	1:A:1914:GLU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:SER:HB3	2:B:128:GLU:HB3	1.81	0.60
2:B:365:TRP:HA	2:B:372:CYS:HA	1.83	0.60
2:C:109:SER:HB3	2:C:128:GLU:HB3	1.83	0.60
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.66	0.60
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.32	0.60
1:A:2965:ARG:NH2	1:A:3614:PHE:HB3	2.15	0.60
1:A:3990:LEU:HD12	1:A:4004:MET:HG3	1.81	0.60
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.82	0.60
1:A:2447:MET:HE3	1:A:2447:MET:HA	1.84	0.60
1:A:2944:THR:N	5:A:4704:ADP:O1B	2.34	0.60
1:A:2123:ASP:HB3	1:A:2126:GLU:HG2	1.83	0.60
2:C:330:CYS:SG	2:C:333:THR:OG1	2.60	0.60
1:A:1933:ASP:HB2	1:A:1962:ARG:HH21	1.66	0.59
1:A:2992:PHE:HB3	1:A:3064:VAL:HG22	1.83	0.59
1:A:2174:GLU:N	1:A:2174:GLU:OE2	2.35	0.59
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.36	0.59
2:C:216:ILE:HB	2:C:230:PHE:HB2	1.83	0.59
1:A:1628:ARG:NH1	1:A:1657:MET:O	2.30	0.59
2:C:244:GLN:N	2:C:244:GLN:OE1	2.35	0.59
1:A:3588:LEU:HD11	1:A:3638:VAL:HG21	1.85	0.59
1:A:1535:ASP:OD1	1:A:2292:ARG:NH2	2.29	0.59
1:A:1800:GLN:HB3	1:A:1804:ARG:HD2	1.85	0.59
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.35	0.59
1:A:1917:LYS:NZ	1:A:2322:ASN:OD1	2.24	0.58
2:B:192:ASP:HB3	2:B:213:ASP:HB3	1.85	0.58
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.84	0.58
1:A:3128:VAL:HG23	1:A:3133:LEU:HD12	1.86	0.58
1:A:3117:LYS:NZ	1:A:3542:GLN:OE1	2.36	0.58
1:A:2232:MET:HA	1:A:2235:ARG:HB2	1.84	0.58
1:A:2562:VAL:O	1:A:2804:ARG:NH1	2.36	0.58
2:C:94:TRP:CE2	2:C:393:PRO:HB3	2.38	0.58
2:C:369:ASN:ND2	2:C:373:MET:SD	2.67	0.58
1:A:1471:ASN:HA	1:A:1589:MET:HE1	1.86	0.58
1:A:3083:PRO:O	1:A:3087:ASN:ND2	2.37	0.58
1:A:4226:THR:HG21	1:A:4239:PRO:HD3	1.86	0.58
1:A:1936:PHE:HD2	1:A:1941:MET:HE1	1.69	0.58
2:B:98:PRO:HG2	2:B:99:PRO:HD3	1.85	0.58
1:A:1390:LEU:O	1:A:1395:LYS:N	2.36	0.57
1:A:1540:VAL:HG11	1:A:1601:LEU:HD12	1.86	0.57
1:A:3653:VAL:HG12	1:A:3662:ILE:HD13	1.85	0.57
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.86	0.57
1:A:1399:LEU:HA	1:A:1403:LEU:HB3	1.84	0.57
1:A:1409:LYS:O	1:A:1412:HIS:ND1	2.37	0.57
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.39	0.57
1:A:3558:GLU:HG2	1:A:3561:ARG:HH21	1.69	0.57
2:B:395:VAL:HB	2:B:407:TRP:HB2	1.86	0.57
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.37	0.57
1:A:2623:SER:N	1:A:2626:THR:OG1	2.37	0.57
1:A:2654:GLN:NE2	1:A:2657:LYS:O	2.35	0.57
1:A:4181:PHE:HE2	1:A:4296:MET:HE1	1.69	0.57
1:A:4543:VAL:HG11	1:A:4622:VAL:HB	1.85	0.57
2:B:275:HIS:HE2	2:B:313:SER:HG	1.51	0.57
1:A:2107:ARG:NH1	1:A:2139:GLN:OE1	2.37	0.57
1:A:3510:SER:HB3	1:A:3553:LEU:HD11	1.86	0.57
1:A:3907:HIS:O	1:A:3911:GLY:N	2.37	0.56
2:C:243:ASN:ND2	2:C:248:LEU:HB2	2.20	0.56
1:A:1533:LEU:HD11	1:A:1597:VAL:HG22	1.88	0.56
1:A:2839:GLU:OE1	1:A:2841:GLU:N	2.34	0.56
1:A:3043:MET:HE3	1:A:3044:LEU:N	2.20	0.56
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.86	0.56
2:C:322:MET:O	2:C:331:LEU:N	2.38	0.56
1:A:1491:ASP:OD1	1:A:1492:ASP:N	2.38	0.56
1:A:3174:ARG:HA	1:A:3177:LEU:HD12	1.87	0.56
1:A:3175:HIS:CE1	1:A:3585:ARG:HH12	2.23	0.56
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.70	0.56
1:A:2797:ARG:NH1	5:A:4703:ADP:O2B	2.35	0.56
2:B:107:HIS:O	2:B:402:GLN:NE2	2.36	0.56
1:A:1412:HIS:HB2	1:A:1449:VAL:HG13	1.88	0.56
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.71	0.55
1:A:3013:ALA:HA	1:A:3088:ARG:HG3	1.88	0.55
1:A:3229:LEU:O	1:A:3233:ASN:ND2	2.38	0.55
2:C:101:LYS:N	2:C:406:VAL:O	2.39	0.55
1:A:1363:LEU:HG	1:A:1390:LEU:HD22	1.88	0.55
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.34	0.55
1:A:2223:VAL:HG13	1:A:2363:TRP:HE3	1.70	0.55
1:A:2372:ASP:OD1	1:A:2373:MET:N	2.40	0.55
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.87	0.55
1:A:2148:LYS:HB2	1:A:2361:MET:HB2	1.89	0.55
1:A:3638:VAL:HG12	1:A:3679:LEU:HD12	1.87	0.55
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.88	0.55
1:A:3035:GLU:HA	1:A:3038:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3886:LEU:HD21	1:A:4343:MET:HG3	1.89	0.55
1:A:1880:VAL:O	5:A:4701:ADP:N6	2.35	0.55
1:A:2387:LEU:O	1:A:2467:ARG:NH2	2.40	0.55
1:A:3037:ALA:HB1	1:A:3042:LEU:HB2	1.88	0.55
1:A:2962:LYS:HG2	1:A:3665:GLY:HA2	1.88	0.55
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.89	0.55
2:B:180:GLN:OE1	2:B:180:GLN:N	2.40	0.54
2:B:277:HIS:ND1	2:B:316:ARG:HB2	2.22	0.54
1:A:1411:ARG:NE	1:A:1456:GLU:OE1	2.40	0.54
1:A:4446:ASN:OD1	1:A:4449:ARG:NH1	2.37	0.54
2:C:218:MET:HE3	2:C:219:TRP:N	2.22	0.54
1:A:1687:LYS:HG3	1:A:1715:LYS:HD2	1.88	0.54
1:A:4485:ARG:HD3	1:A:4515:PHE:HE1	1.73	0.54
2:C:154:GLN:HG2	2:C:169:SER:HA	1.88	0.54
2:C:393:PRO:O	2:C:409:CYS:N	2.35	0.54
1:A:2262:ASP:OD1	1:A:2263:HIS:N	2.41	0.54
1:A:2452:LEU:HD23	1:A:2729:ARG:HH21	1.73	0.54
1:A:4191:GLN:NE2	1:A:4207:PHE:O	2.41	0.54
1:A:4414:GLU:HG3	1:A:4418:LYS:HZ3	1.72	0.54
2:B:188:MET:HE1	2:B:224:GLY:HA2	1.89	0.54
2:B:243:ASN:HD21	2:B:248:LEU:H	1.55	0.54
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.89	0.54
2:B:154:GLN:HE22	2:B:170:ALA:HB2	1.72	0.54
1:A:2301:ILE:O	1:A:2342:MET:N	2.35	0.54
1:A:2910:VAL:N	5:A:4704:ADP:N1	2.48	0.54
1:A:2950:VAL:HA	1:A:2953:MET:HG2	1.89	0.54
1:A:1968:LEU:HD13	1:A:2028:LEU:HD23	1.89	0.53
2:C:197:SER:HB2	2:C:239:MET:HA	1.89	0.53
1:A:1620:GLU:HA	1:A:1623:ARG:HD2	1.91	0.53
1:A:1913:THR:OG1	5:A:4701:ADP:O2B	2.25	0.53
1:A:1351:TRP:HZ2	1:A:1399:LEU:HD21	1.74	0.53
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	1.90	0.53
2:B:243:ASN:OD1	2:B:246:GLY:N	2.38	0.53
1:A:3143:ILE:HD13	1:A:3541:ILE:HD13	1.89	0.53
1:A:4485:ARG:HG2	1:A:4513:GLY:HA2	1.89	0.53
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.34	0.53
1:A:4541:LEU:HD11	1:A:4590:LEU:HB2	1.90	0.53
1:A:1978:ILE:HD11	1:A:2001:LEU:HD21	1.89	0.53
1:A:1982:LEU:HD21	1:A:2012:MET:HB3	1.90	0.53
1:A:4387:TRP:HZ2	1:A:4476:ILE:HG22	1.73	0.53
1:A:2285:ARG:NH1	1:A:2331:GLU:OE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2307:VAL:HG23	1:A:2312:VAL:HG11	1.89	0.53
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.90	0.53
1:A:4131:ASN:HB3	1:A:4134:VAL:HG23	1.91	0.53
2:B:212:ARG:HA	2:B:236:TRP:CD1	2.44	0.53
1:A:1817:HIS:CD2	1:A:1881:GLN:HG2	2.43	0.53
1:A:3478:LEU:HD13	1:A:3767:ILE:HG23	1.91	0.53
2:B:96:PRO:HA	2:B:409:CYS:HA	1.91	0.53
1:A:1958:ASP:HA	1:A:2017:THR:HB	1.91	0.53
1:A:4027:LEU:HD13	1:A:4030:ILE:HD11	1.91	0.53
2:B:92:LYS:HG2	2:B:349:GLY:HA3	1.90	0.53
2:C:216:ILE:O	2:C:230:PHE:N	2.42	0.52
1:A:2855:LEU:HD11	1:A:2863:ARG:HH21	1.72	0.52
1:A:1889:TYR:CD1	1:A:1919:LEU:HD12	2.44	0.52
1:A:2614:ASP:O	1:A:2615:MET:HE2	2.09	0.52
2:C:212:ARG:HA	2:C:236:TRP:CD1	2.44	0.52
2:C:366:ASP:HB2	2:C:373:MET:HE1	1.91	0.52
2:C:387:ASP:OD1	2:C:388:PHE:N	2.42	0.52
1:A:1492:ASP:HA	1:A:1495:ASN:HD22	1.74	0.52
2:C:350:GLY:O	2:C:367:TYR:OH	2.27	0.52
1:A:1392:GLY:HA3	1:A:1435:TRP:HE1	1.75	0.52
1:A:2934:LEU:HD22	1:A:3085:LEU:HG	1.90	0.52
2:C:168:CYS:HB3	2:C:198:VAL:HB	1.90	0.52
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.90	0.52
1:A:2363:TRP:HE1	1:A:2365:SER:HB2	1.75	0.52
2:B:163:LYS:HA	2:B:180:GLN:HE22	1.75	0.52
1:A:1963:LEU:O	1:A:2026:SER:OG	2.23	0.52
1:A:2075:LEU:O	1:A:2079:GLN:N	2.33	0.52
1:A:3715:GLU:O	1:A:3719:ALA:N	2.39	0.52
1:A:3243:MET:HE3	1:A:3243:MET:HA	1.90	0.52
1:A:2596:PRO:O	1:A:2601:LYS:NZ	2.43	0.52
1:A:2796:PRO:HA	1:A:2799:MET:HB3	1.92	0.52
2:B:104:LEU:N	2:B:404:VAL:O	2.43	0.52
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.42	0.51
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.32	0.51
2:B:110:PRO:HB3	2:B:400:VAL:HA	1.91	0.51
1:A:2386:PRO:HG3	1:A:2413:LEU:HD22	1.92	0.51
1:A:2488:ARG:HG2	1:A:2492:ARG:HH12	1.73	0.51
1:A:3151:HIS:ND1	1:A:3516:TYR:OH	2.35	0.51
2:C:89:ARG:HH12	2:C:410:ARG:HG2	1.75	0.51
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.44	0.51
1:A:2964:HIS:H	1:A:2967:TYR:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4517:PRO:HG3	1:A:4611:LEU:HD13	1.92	0.51
1:A:2806:ILE:HG22	1:A:2824:ILE:HG22	1.92	0.51
2:B:216:ILE:O	2:B:230:PHE:N	2.43	0.51
2:C:95:ILE:HB	2:C:97:ARG:HH12	1.75	0.51
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.27	0.51
2:C:240:VAL:O	2:C:241:ARG:HD2	2.11	0.51
2:B:239:MET:SD	2:B:240:VAL:N	2.83	0.51
2:B:309:PRO:HG2	2:B:325:VAL:HB	1.92	0.51
2:C:277:HIS:HB3	2:C:316:ARG:HB2	1.92	0.51
1:A:1857:LEU:HD23	1:A:1868:TYR:HB2	1.92	0.51
2:C:174:ILE:O	2:C:188:MET:N	2.32	0.51
1:A:1667:ASN:ND2	1:A:1669:ASP:OD1	2.44	0.51
1:A:2012:MET:HE2	1:A:2012:MET:HA	1.93	0.51
2:B:297:THR:HG22	2:B:332:MET:HE1	1.92	0.51
1:A:3517:ALA:O	1:A:3525:ARG:NE	2.44	0.51
1:A:1359:LEU:HD11	1:A:1393:TYR:HE2	1.76	0.50
1:A:2667:ASN:ND2	1:A:2713:ASN:O	2.44	0.50
1:A:2793:ILE:O	1:A:2836:ARG:NH1	2.44	0.50
1:A:3189:GLU:OE2	1:A:3582:ARG:NH2	2.40	0.50
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.92	0.50
1:A:4414:GLU:O	1:A:4418:LYS:HG2	2.11	0.50
1:A:2220:LEU:HD12	1:A:2342:MET:HE2	1.93	0.50
1:A:2221:MET:HG3	1:A:2343:PHE:HB2	1.92	0.50
1:A:1880:VAL:HG11	1:A:2049:ILE:HA	1.92	0.50
1:A:2091:ARG:NH2	5:A:4701:ADP:O3A	2.44	0.50
2:B:211:SER:OG	2:B:213:ASP:OD1	2.23	0.50
1:A:2603:MET:HE1	5:A:4703:ADP:C5	2.47	0.50
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.45	0.50
1:A:2414:GLN:NE2	1:A:2418:ASP:OD2	2.31	0.50
1:A:2684:ARG:HD2	1:A:2726:ARG:HG2	1.93	0.50
1:A:4043:MET:HB2	1:A:4127:THR:HA	1.93	0.50
2:B:287:GLU:N	2:B:287:GLU:OE1	2.41	0.50
2:B:380:GLU:OE1	2:B:380:GLU:N	2.31	0.50
2:C:131:THR:HG22	2:C:147:LYS:HG2	1.93	0.50
1:A:1349:GLN:HE22	1:A:1353:SER:H	1.58	0.50
1:A:1636:ASP:O	1:A:1640:ILE:HG12	2.12	0.50
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	1.93	0.50
1:A:2018:MET:HG3	1:A:2020:PRO:HD3	1.93	0.50
1:A:3239:LYS:HB3	1:A:3451:TYR:CD2	2.46	0.50
1:A:3732:LEU:O	1:A:3736:GLY:N	2.43	0.50
1:A:1723:GLU:OE2	1:A:1741:TRP:NE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2232:MET:HA	1:A:2235:ARG:HD2	1.92	0.50
1:A:1763:GLU:O	1:A:1767:SER:N	2.41	0.49
1:A:2022:TYR:OH	1:A:2354:ALA:N	2.45	0.49
1:A:3826:GLN:HG3	1:A:4136:VAL:HG13	1.93	0.49
1:A:4403:GLU:HA	1:A:4406:LYS:HE3	1.94	0.49
2:C:110:PRO:HB3	2:C:400:VAL:HA	1.93	0.49
1:A:3763:ASP:HB3	1:A:3766:ILE:HG12	1.93	0.49
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.35	0.49
2:B:239:MET:SD	2:B:241:ARG:HG2	2.53	0.49
1:A:1416:LEU:HA	1:A:1445:ILE:HD11	1.94	0.49
1:A:1739:ILE:HA	1:A:1742:ILE:HG22	1.95	0.49
1:A:2221:MET:HA	1:A:2343:PHE:HB2	1.95	0.49
1:A:3473:ASN:OD1	1:A:3474:ARG:N	2.44	0.49
1:A:2897:LEU:HA	1:A:2900:PHE:HB3	1.95	0.49
1:A:3586:TYR:HD2	1:A:3649:LEU:HD13	1.76	0.49
2:C:236:TRP:O	2:C:254:ASN:N	2.35	0.49
1:A:2869:ARG:O	1:A:2871:ILE:HD12	2.12	0.49
2:C:395:VAL:O	2:C:407:TRP:N	2.42	0.49
1:A:1494:PHE:C	1:A:1498:LYS:HZ2	2.20	0.49
1:A:2933:LEU:HB2	1:A:3065:VAL:HG13	1.93	0.49
1:A:3833:LEU:O	1:A:3837:HIS:ND1	2.45	0.49
1:A:4525:ARG:NH2	1:A:4539:LEU:O	2.43	0.49
1:A:4599:GLU:CD	1:A:4600:LYS:H	2.20	0.49
1:A:1409:LYS:H	1:A:1412:HIS:CE1	2.30	0.49
1:A:3908:PHE:HB2	1:A:3991:LEU:HD11	1.94	0.49
2:B:200:ILE:HG12	2:B:207:ILE:HG12	1.94	0.49
2:C:104:LEU:HD22	2:C:135:TRP:CE3	2.47	0.49
2:C:362:LEU:HD21	2:C:383:VAL:HG11	1.94	0.49
1:A:1880:VAL:N	5:A:4701:ADP:N1	2.54	0.49
1:A:2756:LEU:HD13	1:A:2762:LEU:O	2.13	0.49
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.13	0.49
2:C:132:ILE:HG13	2:C:146:LEU:HB2	1.94	0.49
2:C:153:VAL:HA	2:C:169:SER:HB2	1.94	0.49
2:C:206:HIS:NE2	2:C:220:GLU:OE1	2.46	0.49
1:A:4052:SER:O	1:A:4056:GLU:HG2	2.13	0.48
2:C:123:MET:SD	2:C:135:TRP:HB2	2.53	0.48
1:A:1507:MET:N	1:A:1507:MET:HE2	2.28	0.48
1:A:2660:VAL:HG22	1:A:2707:GLN:HB3	1.94	0.48
1:A:3619:PHE:HZ	1:A:3645:LEU:HD21	1.78	0.48
1:A:3923:ARG:HH12	1:A:3925:GLN:HA	1.78	0.48
1:A:3943:ALA:HB1	1:A:3974:TRP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:SER:OG	2:B:128:GLU:N	2.46	0.48
2:C:96:PRO:HA	2:C:409:CYS:HA	1.94	0.48
1:A:2197:GLU:OE2	1:A:2197:GLU:N	2.42	0.48
1:A:2423:MET:HG2	1:A:2427:PHE:HD2	1.77	0.48
1:A:2548:TRP:CE2	1:A:2576:ARG:HG2	2.48	0.48
1:A:3938:LEU:HD23	1:A:3947:LEU:HD22	1.95	0.48
2:B:151:ASP:H	2:B:171:ASP:HB3	1.78	0.48
2:B:174:ILE:O	2:B:188:MET:N	2.36	0.48
2:C:312:LEU:HG	2:C:346:PHE:CZ	2.48	0.48
1:A:1411:ARG:HA	1:A:1414:LYS:HG2	1.96	0.48
1:A:1539:ASP:HB3	1:A:1543:ARG:HH21	1.78	0.48
1:A:3779:GLU:HA	1:A:3782:ARG:HB3	1.94	0.48
1:A:3999:ASP:HB3	1:A:4329:ARG:HD2	1.95	0.48
2:B:362:LEU:HD23	2:B:378:ALA:HB2	1.96	0.48
2:C:157:SER:HB3	2:C:166:ALA:HB3	1.94	0.48
1:A:2987:ASN:OD1	1:A:3060:ARG:NH2	2.46	0.48
1:A:3190:LYS:NZ	1:A:3552:TYR:O	2.31	0.48
2:C:260:VAL:HG13	2:C:269:LYS:HB3	1.94	0.48
1:A:1554:SER:O	1:A:1558:LYS:NZ	2.39	0.48
1:A:1561:LEU:HB3	1:A:1564:GLU:CD	2.38	0.48
1:A:2221:MET:HB2	1:A:2361:MET:HE1	1.95	0.48
1:A:2893:VAL:O	1:A:2897:LEU:HD12	2.13	0.48
1:A:2973:ASP:OD2	1:A:3007:ARG:NH2	2.44	0.48
1:A:3519:TYR:HA	1:A:3700:ASN:OD1	2.13	0.48
1:A:4154:LYS:HB2	1:A:4312:LEU:HD23	1.95	0.48
2:C:114:VAL:HG12	2:C:125:SER:HA	1.96	0.48
2:C:239:MET:HE2	2:C:241:ARG:NH1	2.29	0.48
1:A:3471:LYS:HE3	1:A:3761:LEU:HD13	1.96	0.48
2:B:201:MET:HE3	2:B:208:VAL:HG13	1.95	0.48
1:A:1446:VAL:HA	1:A:1449:VAL:HB	1.96	0.48
1:A:1579:MET:O	1:A:1583:SER:N	2.41	0.48
1:A:2354:ALA:O	1:A:2358:ARG:HG3	2.14	0.48
1:A:2628:PRO:HG3	1:A:2679:VAL:HA	1.96	0.48
1:A:2648:VAL:HG11	1:A:2694:ARG:HH22	1.78	0.48
1:A:2957:SER:HB2	1:A:2990:ILE:HD12	1.96	0.48
2:C:383:VAL:HA	2:C:399:SER:HB2	1.95	0.48
1:A:1664:ILE:HA	1:A:1676:ILE:HA	1.96	0.48
1:A:2953:MET:C	2:B:277:HIS:HE2	2.20	0.48
1:A:4604:VAL:HG23	1:A:4624:PHE:C	2.39	0.48
2:B:381:HIS:CE1	2:B:382:PHE:HD2	2.32	0.47
2:C:95:ILE:O	2:C:410:ARG:N	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2488:ARG:O	1:A:2492:ARG:HG2	2.14	0.47
1:A:2976:LEU:HD21	1:A:3008:MET:HE1	1.97	0.47
1:A:3196:GLU:O	1:A:3199:MET:HG3	2.14	0.47
1:A:1419:ARG:HD2	1:A:1445:ILE:HG13	1.96	0.47
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.95	0.47
1:A:2650:LEU:O	1:A:2704:GLU:N	2.47	0.47
1:A:1411:ARG:HA	1:A:1414:LYS:HE3	1.95	0.47
1:A:1452:VAL:HA	1:A:1512:TYR:CE1	2.49	0.47
1:A:1991:ASP:O	1:A:1994:SER:OG	2.31	0.47
1:A:2965:ARG:NH1	1:A:3642:ASP:HB2	2.29	0.47
1:A:3214:GLN:O	1:A:3218:LEU:N	2.48	0.47
1:A:1948:LEU:HB3	1:A:2012:MET:HE1	1.95	0.47
1:A:2867:MET:SD	1:A:2869:ARG:NH2	2.87	0.47
1:A:3537:GLN:NE2	1:A:3538:GLN:HG3	2.30	0.47
1:A:4401:THR:H	1:A:4404:ASN:HB2	1.80	0.47
2:B:233:HIS:CE1	2:B:259:ARG:HD2	2.50	0.47
1:A:1356:PRO:O	1:A:1360:ARG:N	2.43	0.47
1:A:1484:CYS:SG	1:A:1485:ARG:N	2.84	0.47
1:A:1861:MET:HE1	1:A:1889:TYR:HB3	1.96	0.47
1:A:2172:ARG:NH1	1:A:2174:GLU:HA	2.30	0.47
1:A:2304:ASP:OD1	1:A:2684:ARG:NH2	2.48	0.47
1:A:2581:LEU:HD13	1:A:2591:LEU:HD11	1.97	0.47
1:A:2791:HIS:ND1	1:A:3075:LEU:HD21	2.30	0.47
1:A:3626:ALA:HA	1:A:3631:ASN:HB2	1.97	0.47
1:A:4205:TYR:OH	1:A:4257:ASP:OD1	2.30	0.47
1:A:4554:ASP:OD2	1:A:4557:SER:OG	2.24	0.47
2:B:123:MET:HE3	2:B:135:TRP:HB2	1.96	0.47
2:B:155:ASP:HB2	2:B:197:SER:HA	1.96	0.47
2:B:188:MET:HB2	2:B:188:MET:HE2	1.75	0.47
2:C:145:THR:O	2:C:147:LYS:NZ	2.48	0.47
2:C:272:LEU:HB3	2:C:323:TRP:CZ3	2.50	0.47
1:A:3811:ILE:O	1:A:3815:MET:N	2.41	0.47
1:A:1691:SER:OG	1:A:1694:GLU:OE1	2.27	0.47
1:A:3222:LEU:HD22	1:A:3472:VAL:HG21	1.94	0.47
1:A:3457:GLU:O	1:A:3461:ILE:HG12	2.15	0.47
1:A:4405:ILE:O	1:A:4411:ARG:NE	2.48	0.47
2:B:110:PRO:HB3	2:B:400:VAL:HG13	1.97	0.47
2:C:279:VAL:HA	2:C:315:SER:HA	1.97	0.47
1:A:3161:LEU:HD23	1:A:3168:THR:HG22	1.97	0.47
1:A:3715:GLU:HB2	1:A:3836:TYR:HE2	1.79	0.47
1:A:4244:LYS:HE3	1:A:4270:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1965:GLU:OE1	1:A:2026:SER:HB3	2.15	0.46
1:A:3833:LEU:HB3	1:A:3837:HIS:HE1	1.80	0.46
1:A:2648:VAL:HG11	1:A:2694:ARG:NH2	2.30	0.46
2:C:320:ILE:HB	2:C:334:LEU:HD12	1.97	0.46
1:A:2283:VAL:O	1:A:2287:ILE:HG12	2.16	0.46
1:A:2616:GLU:N	1:A:2616:GLU:OE1	2.49	0.46
1:A:3459:GLN:HA	1:A:3462:LYS:NZ	2.30	0.46
1:A:1467:ARG:HA	1:A:1523:TRP:HZ2	1.80	0.46
1:A:1487:ILE:O	1:A:1541:GLN:NE2	2.41	0.46
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.97	0.46
1:A:1937:ASP:O	1:A:1941:MET:HG2	2.15	0.46
1:A:2875:ASN:HD21	1:A:2927:ARG:HD3	1.80	0.46
1:A:3967:GLU:OE2	1:A:4000:ARG:NH2	2.43	0.46
1:A:2294:GLU:HB2	1:A:2297:LYS:HD2	1.97	0.46
1:A:4417:VAL:HA	1:A:4489:LEU:HD21	1.98	0.46
1:A:4538:GLU:OE1	1:A:4594:LYS:NZ	2.49	0.46
1:A:1504:VAL:HA	1:A:1507:MET:HG2	1.97	0.46
1:A:1576:LEU:O	1:A:1580:LYS:N	2.39	0.46
1:A:2358:ARG:NH1	5:A:4701:ADP:O3B	2.42	0.46
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.97	0.46
1:A:3846:LEU:HD22	1:A:3855:ARG:HE	1.81	0.46
2:B:388:PHE:O	2:B:390:LYS:NZ	2.47	0.46
2:C:197:SER:N	2:C:210:ALA:O	2.49	0.46
1:A:1746:GLN:HB2	1:A:1749:LEU:HD12	1.97	0.46
1:A:3175:HIS:HB3	1:A:3516:TYR:CE1	2.51	0.46
2:C:340:TRP:HB2	2:C:358:ASP:OD2	2.16	0.46
1:A:1667:ASN:ND2	1:A:1672:VAL:HG12	2.31	0.46
1:A:1679:ARG:NH2	1:A:1680:GLU:OE2	2.49	0.46
1:A:2307:VAL:HG11	1:A:2348:LEU:HD13	1.98	0.46
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.51	0.46
1:A:2556:GLU:OE2	1:A:2753:ARG:NH1	2.49	0.46
1:A:2896:ARG:HD2	1:A:2953:MET:HE1	1.98	0.46
1:A:4339:MET:SD	1:A:4343:MET:HE1	2.55	0.46
1:A:4600:LYS:HD2	1:A:4604:VAL:HG13	1.98	0.46
2:B:322:MET:HE1	2:B:331:LEU:HD12	1.98	0.46
2:C:249:ILE:O	2:C:261:TRP:N	2.40	0.46
1:A:2982:ARG:HB3	1:A:2988:GLU:OE2	2.15	0.45
1:A:3812:TYR:HA	1:A:3815:MET:HB3	1.99	0.45
2:C:214:LYS:HA	2:C:237:VAL:HG23	1.98	0.45
1:A:1540:VAL:HG11	1:A:1601:LEU:CD1	2.46	0.45
1:A:1932:CYS:HB3	1:A:1963:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2579:ALA:O	1:A:2583:THR:N	2.49	0.45
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.97	0.45
1:A:4556:CYS:SG	1:A:4591:ARG:NH2	2.90	0.45
2:B:136:ASP:HB3	2:B:141:ASP:OD1	2.16	0.45
2:C:272:LEU:HD13	2:C:323:TRP:CD2	2.52	0.45
1:A:1370:LEU:HD22	1:A:1387:GLN:CD	2.42	0.45
1:A:1590:ASP:O	1:A:1594:ILE:HG13	2.16	0.45
1:A:2313:GLU:N	1:A:2313:GLU:OE1	2.50	0.45
1:A:2654:GLN:NE2	1:A:2657:LYS:HB3	2.31	0.45
1:A:4488:GLN:OE1	1:A:4510:CYS:N	2.45	0.45
1:A:4603:SER:O	1:A:4626:ILE:HG12	2.16	0.45
1:A:3771:GLU:HB3	1:A:3775:ARG:NH2	2.31	0.45
1:A:4248:ALA:HB2	1:A:4269:LEU:HD12	1.99	0.45
2:C:120:PHE:HD2	2:C:179:PHE:HE1	1.64	0.45
2:C:236:TRP:HB3	2:C:254:ASN:CG	2.42	0.45
1:A:2231:SER:N	6:A:4702:ATP:O2B	2.43	0.45
1:A:3974:TRP:NE1	1:A:3976:GLU:OE1	2.40	0.45
2:B:236:TRP:HB3	2:B:254:ASN:OD1	2.17	0.45
2:B:340:TRP:HB2	2:B:358:ASP:OD2	2.16	0.45
1:A:2629:GLU:N	1:A:2629:GLU:OE1	2.50	0.45
1:A:3653:VAL:HG23	1:A:3655:ARG:HH12	1.81	0.45
1:A:4178:ARG:HH21	1:A:4296:MET:HG3	1.81	0.45
1:A:1477:LEU:C	1:A:1485:ARG:HE	2.24	0.45
1:A:1798:MET:SD	1:A:1800:GLN:NE2	2.90	0.45
1:A:2448:ASP:O	1:A:2453:ARG:NH2	2.50	0.45
1:A:3727:LYS:O	1:A:3731:LEU:HG	2.17	0.45
1:A:2003:ASN:O	1:A:2004:LYS:HD2	2.17	0.45
1:A:2840:ASP:OD1	1:A:2841:GLU:N	2.50	0.45
1:A:4437:VAL:HG21	1:A:4448:LEU:HD13	1.99	0.45
1:A:1682:GLU:OE2	1:A:1747:ALA:N	2.49	0.45
1:A:1930:PHE:HA	1:A:2326:THR:HG21	1.99	0.45
1:A:2839:GLU:HG3	1:A:2842:GLU:OE2	2.16	0.45
1:A:4473:MET:HE1	1:A:4478:TRP:HB2	1.98	0.45
1:A:1824:SER:HA	1:A:1827:LYS:HG2	1.99	0.45
1:A:2221:MET:HE2	1:A:2361:MET:HE1	1.99	0.45
1:A:2273:ARG:HA	1:A:2273:ARG:HD2	1.80	0.45
1:A:3520:PHE:HB3	1:A:3524:MET:HB2	1.99	0.45
1:A:3788:ASP:O	1:A:3792:GLN:N	2.46	0.45
2:C:385:SER:OG	2:C:386:LEU:N	2.50	0.45
1:A:2654:GLN:HE22	1:A:2657:LYS:HB3	1.81	0.44
1:A:3044:LEU:HB3	1:A:3049:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3635:VAL:HB	1:A:3679:LEU:HD13	1.99	0.44
2:B:275:HIS:CD2	2:B:313:SER:HG	2.35	0.44
1:A:2054:LEU:HD21	1:A:2097:LEU:HD22	1.98	0.44
1:A:3208:ILE:HD11	1:A:3486:ARG:HD2	1.98	0.44
1:A:3983:ILE:O	1:A:3987:ILE:HD12	2.17	0.44
1:A:3998:PRO:HA	1:A:4001:LEU:HG	1.99	0.44
1:A:4627:ALA:O	1:A:4630:GLU:HG3	2.17	0.44
2:B:322:MET:HE3	2:B:332:MET:SD	2.57	0.44
1:A:1399:LEU:HG	1:A:1403:LEU:HD22	1.98	0.44
1:A:1904:PRO:HD2	1:A:2016:ILE:O	2.17	0.44
1:A:2615:MET:HE1	1:A:2658:TRP:HB2	1.99	0.44
1:A:3044:LEU:HD12	1:A:3050:LEU:HD23	1.99	0.44
1:A:3113:MET:HB3	1:A:3115:LEU:HD13	1.99	0.44
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.82	0.44
2:B:159:ASP:OD2	2:B:161:SER:OG	2.36	0.44
2:C:353:ILE:N	2:C:365:TRP:O	2.46	0.44
1:A:1480:TYR:HB2	1:A:1486:LEU:HD23	2.00	0.44
1:A:1836:PHE:CG	1:A:4242:ALA:HA	2.52	0.44
1:A:3717:LEU:HG	1:A:3725:ASP:HB2	1.99	0.44
1:A:4025:LEU:HG	1:A:4027:LEU:HD22	1.99	0.44
2:C:155:ASP:OD2	2:C:197:SER:HA	2.17	0.44
1:A:1589:MET:O	1:A:1593:ASN:N	2.51	0.44
1:A:2976:LEU:HD23	1:A:2976:LEU:HA	1.87	0.44
1:A:4618:LEU:HD23	1:A:4618:LEU:H	1.83	0.44
2:C:123:MET:HG2	2:C:137:TYR:HB3	2.00	0.44
1:A:1939:GLN:HB2	1:A:2273:ARG:NH2	2.33	0.44
1:A:2220:LEU:O	1:A:2343:PHE:N	2.51	0.44
1:A:2294:GLU:OE1	1:A:2294:GLU:N	2.35	0.44
1:A:3655:ARG:HA	1:A:3655:ARG:NE	2.31	0.44
1:A:3830:GLN:HA	1:A:3833:LEU:HB2	1.99	0.44
1:A:1873:LEU:HD13	1:A:1921:HIS:ND1	2.31	0.44
1:A:2265:TYR:O	1:A:2281:THR:OG1	2.26	0.44
1:A:2369:LEU:O	1:A:2451:ARG:NH2	2.51	0.44
2:B:260:VAL:O	2:B:269:LYS:N	2.51	0.44
1:A:1867:ASN:O	1:A:1925:ARG:NH1	2.38	0.44
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.99	0.44
1:A:3520:PHE:O	1:A:3525:ARG:NE	2.50	0.44
1:A:4571:ASN:O	1:A:4574:LYS:N	2.43	0.44
2:B:90:ASP:HB3	2:B:93:GLU:HB3	1.99	0.44
2:B:278:VAL:HB	2:B:316:ARG:HD2	1.99	0.44
1:A:2969:GLY:HA2	1:A:3004:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3818:LEU:HD11	1:A:3883:PHE:CE1	2.53	0.44
2:B:116:PHE:N	2:B:387:ASP:OD2	2.51	0.44
2:B:212:ARG:HG3	2:B:236:TRP:CG	2.53	0.44
2:C:90:ASP:OD1	2:C:90:ASP:N	2.51	0.44
1:A:4296:MET:HE2	1:A:4296:MET:HA	2.00	0.43
2:B:94:TRP:CD2	2:B:393:PRO:HB3	2.54	0.43
4:I:427:LYS:O	4:I:431:ASP:N	2.41	0.43
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	2.00	0.43
1:A:4569:THR:HG23	1:A:4578:SER:HB2	2.00	0.43
2:C:384:THR:H	2:C:399:SER:HA	1.83	0.43
1:A:1843:ARG:NH1	1:A:1861:MET:HA	2.33	0.43
1:A:1959:GLU:OE2	1:A:2025:ARG:NH1	2.30	0.43
1:A:2756:LEU:HB3	1:A:2763:ARG:HA	2.00	0.43
1:A:4406:LYS:O	1:A:4530:GLN:NE2	2.51	0.43
2:C:153:VAL:HG21	2:C:156:ILE:HD11	2.00	0.43
2:C:351:LYS:HG3	2:C:352:PHE:CD2	2.53	0.43
1:A:1351:TRP:CH2	1:A:1359:LEU:HD22	2.54	0.43
1:A:1666:LEU:HD23	1:A:1673:VAL:HA	2.00	0.43
1:A:1905:PHE:CZ	1:A:2040:ALA:HB2	2.53	0.43
1:A:1925:ARG:NE	1:A:2011:ASP:HB2	2.33	0.43
1:A:2952:TRP:NE1	2:B:316:ARG:HH12	2.15	0.43
1:A:3106:GLY:O	1:A:3110:THR:OG1	2.32	0.43
2:B:382:PHE:O	2:B:399:SER:OG	2.20	0.43
2:C:206:HIS:HB3	2:C:218:MET:CE	2.48	0.43
1:A:1912:LYS:HE2	5:A:4701:ADP:O2B	2.13	0.43
1:A:2078:GLU:OE1	1:A:2079:GLN:NE2	2.51	0.43
1:A:2335:LEU:HD23	1:A:2336:PRO:O	2.18	0.43
2:C:101:LYS:O	2:C:102:TYR:HD2	2.00	0.43
2:E:41:GLU:O	2:E:45:LYS:N	2.46	0.43
1:A:2679:VAL:O	1:A:2683:ILE:HG12	2.19	0.43
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.83	0.43
2:B:238:ARG:HH11	2:B:254:ASN:HD21	1.66	0.43
1:A:1431:LEU:O	1:A:1434:ILE:HG22	2.18	0.43
1:A:1676:ILE:HG23	1:A:1686:PHE:HZ	1.84	0.43
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.50	0.43
1:A:2790:PRO:HG3	1:A:3076:LYS:HG2	2.01	0.43
2:B:271:GLU:OE1	2:B:273:ARG:NH1	2.47	0.43
2:C:258:VAL:HB	2:C:272:LEU:HD12	2.00	0.43
1:A:1404:LYS:O	1:A:1404:LYS:HD3	2.19	0.43
1:A:1409:LYS:H	1:A:1412:HIS:HD1	1.66	0.43
1:A:1557:ILE:HD11	1:A:1561:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1805:ARG:O	1:A:1809:GLU:HG3	2.19	0.43
1:A:3459:GLN:HA	1:A:3462:LYS:HZ3	1.82	0.43
1:A:3741:ARG:NH2	1:A:3745:LEU:HD21	2.33	0.43
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.54	0.43
1:A:1508:LYS:NZ	1:A:1513:TYR:OH	2.49	0.43
1:A:4328:GLU:HG2	1:A:4332:LEU:HG	2.00	0.43
1:A:4525:ARG:HB2	1:A:4592:TRP:CE2	2.54	0.43
4:I:533[A]:GLU:O	4:I:537:GLN:N	2.51	0.43
4:I:533[B]:GLU:O	4:I:537:GLN:N	2.51	0.43
1:A:2440:ALA:HB2	1:A:2502:LEU:HD13	2.01	0.43
1:A:2994:MET:HE1	1:A:3064:VAL:HG13	2.01	0.43
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	2.01	0.43
1:A:3609:ILE:HA	1:A:3632:PRO:O	2.19	0.43
2:C:158:PHE:CE1	2:C:165:LEU:HD13	2.54	0.43
2:C:396:VAL:HG12	2:C:406:VAL:HG22	2.01	0.43
1:A:1351:TRP:HH2	1:A:1359:LEU:HB2	1.84	0.42
1:A:2060:ARG:NH2	1:A:2129:GLU:O	2.52	0.42
1:A:2264:LEU:O	1:A:2280:PHE:N	2.47	0.42
2:C:254:ASN:HA	2:C:278:VAL:HG13	2.01	0.42
1:A:1451:LEU:HD12	1:A:1454:GLN:HE21	1.85	0.42
1:A:1892:MET:CE	1:A:1904:PRO:HD3	2.47	0.42
1:A:2031:ASN:O	1:A:2034:LYS:HG2	2.19	0.42
1:A:2457:SER:HB3	1:A:2732:PRO:HB3	2.00	0.42
1:A:3514:ILE:HG13	1:A:3579:MET:SD	2.59	0.42
1:A:3779:GLU:OE1	1:A:3779:GLU:N	2.35	0.42
1:A:3849:VAL:HG12	1:A:3855:ARG:HG2	2.01	0.42
2:B:133:LYS:HG2	2:B:145:THR:OG1	2.19	0.42
1:A:1529:ARG:HA	1:A:1532:ALA:HB3	2.01	0.42
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	2.01	0.42
1:A:2142:CYS:O	1:A:2146:VAL:HB	2.20	0.42
1:A:2254:ILE:HB	1:A:2303:PHE:CD1	2.54	0.42
1:A:2560:HIS:NE2	1:A:2561:LYS:HE2	2.34	0.42
1:A:2609:LEU:HD13	1:A:2617:VAL:HB	2.00	0.42
1:A:3108:GLU:O	1:A:3111:SER:OG	2.37	0.42
1:A:3495:THR:O	1:A:3499:GLN:HG3	2.19	0.42
1:A:3843:ASN:HB3	1:A:3846:LEU:HG	2.02	0.42
1:A:4377:MET:HE2	1:A:4377:MET:HB3	1.84	0.42
2:B:339:ASN:CG	2:B:340:TRP:H	2.26	0.42
1:A:1417:MET:SD	1:A:1417:MET:N	2.91	0.42
1:A:1500:HIS:O	1:A:1504:VAL:HG23	2.19	0.42
1:A:1623:ARG:NH1	1:A:1629:PHE:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1880:VAL:HG22	1:A:2053:MET:HE3	2.00	0.42
1:A:1908:ALA:HA	1:A:1912:LYS:NZ	2.34	0.42
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.36	0.42
2:B:167:SER:OG	2:B:177:TRP:NE1	2.45	0.42
2:B:272:LEU:HD22	2:B:323:TRP:CE3	2.55	0.42
2:B:337:HIS:CE1	2:B:363:ARG:HD2	2.55	0.42
2:C:163:LYS:HA	2:C:180:GLN:HE22	1.83	0.42
1:A:2080:LEU:HD12	1:A:2153:ASP:HB3	2.02	0.42
1:A:2228:SER:N	6:A:4702:ATP:O1B	2.50	0.42
1:A:2504:GLY:O	1:A:2735:TYR:N	2.38	0.42
1:A:3723:ASP:OD1	1:A:3724:VAL:N	2.52	0.42
1:A:4346:MET:HE3	1:A:4346:MET:O	2.19	0.42
2:C:154:GLN:HE21	2:C:170:ALA:H	1.66	0.42
2:C:196:SER:HB3	2:C:236:TRP:HE1	1.84	0.42
1:A:2873:TYR:CE2	1:A:2883:PRO:HD3	2.54	0.42
1:A:2965:ARG:HH12	1:A:3642:ASP:HB2	1.84	0.42
1:A:2984:GLY:HA3	1:A:3054:PHE:CE1	2.55	0.42
1:A:3928:THR:HB	1:A:3931:GLN:HB2	2.00	0.42
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.53	0.42
1:A:1883:PRO:HA	1:A:1886:ASP:HB2	2.01	0.42
1:A:1974:GLN:O	1:A:1977:CYS:N	2.49	0.42
1:A:1982:LEU:HD11	1:A:2012:MET:HB3	2.02	0.42
1:A:2703:LEU:HD13	1:A:2706:ILE:HB	2.02	0.42
1:A:1413:TRP:O	1:A:1416:LEU:HG	2.19	0.42
1:A:1836:PHE:HE2	1:A:4245:THR:HB	1.84	0.42
1:A:2839:GLU:O	1:A:2843:ARG:HG3	2.20	0.42
1:A:2896:ARG:HD3	1:A:2896:ARG:HA	1.91	0.42
1:A:2922:ILE:HG22	1:A:2950:VAL:HG11	2.01	0.42
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.52	0.42
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	2.02	0.42
2:C:111:VAL:O	2:C:384:THR:OG1	2.32	0.42
4:H:519:LYS:O	4:H:523:LEU:N	2.48	0.42
1:A:1423:ASN:OD1	1:A:1424:TRP:N	2.51	0.42
1:A:1546:TYR:HB2	1:A:1639:GLU:HA	2.01	0.42
1:A:1688:THR:OG1	1:A:1708:GLU:OE1	2.37	0.42
1:A:2980:LEU:HB3	1:A:3054:PHE:HZ	1.85	0.42
1:A:3191:ARG:HG2	1:A:3195:GLU:OE1	2.20	0.42
1:A:4232:ASN:OD1	1:A:4233:ILE:N	2.52	0.42
2:B:115:ILE:HD13	2:B:156:ILE:HG13	2.02	0.42
1:A:2230:LYS:HG2	1:A:2364:PHE:CD2	2.55	0.42
1:A:2903:GLU:O	2:B:212:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3012:LEU:HD23	1:A:3012:LEU:HA	1.93	0.42
1:A:3069:ASN:O	1:A:3071:SER:N	2.52	0.42
1:A:4107:MET:HE3	1:A:4135:PRO:HB2	2.02	0.42
1:A:4542:GLU:O	1:A:4591:ARG:N	2.43	0.42
1:A:4546:THR:OG1	1:A:4587:LEU:HB3	2.20	0.42
2:B:206:HIS:HB3	2:B:218:MET:HE3	2.01	0.42
2:B:272:LEU:HD13	2:B:323:TRP:CG	2.55	0.42
2:C:324:ASP:HB2	2:C:331:LEU:HD11	2.02	0.42
1:A:2713:ASN:OD1	1:A:2720:ARG:NH2	2.51	0.41
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.02	0.41
2:B:239:MET:HE3	2:B:282:ILE:H	1.85	0.41
2:C:148:GLY:HA3	2:C:175:LYS:HE2	2.01	0.41
2:C:318:LYS:HG2	2:C:339:ASN:O	2.20	0.41
1:A:2073:PHE:HA	1:A:2076:CYS:HB2	2.02	0.41
1:A:2096:VAL:O	1:A:2099:SER:OG	2.38	0.41
1:A:2568:VAL:HG22	1:A:2603:MET:SD	2.60	0.41
1:A:2755:MET:CE	1:A:2806:ILE:HG13	2.50	0.41
1:A:2834:GLN:HA	1:A:2837:LEU:HG	2.00	0.41
1:A:2848:GLU:O	1:A:2851:ASP:HB2	2.19	0.41
2:C:203:ASN:OD1	2:C:204:GLY:N	2.52	0.41
1:A:3072:SER:O	1:A:3076:LYS:HG3	2.20	0.41
1:A:3623:LEU:HD12	1:A:3624:GLU:N	2.35	0.41
1:A:3624:GLU:O	1:A:3628:ARG:HG2	2.21	0.41
1:A:3734:LEU:HA	1:A:3737:GLU:OE1	2.21	0.41
1:A:3909:LEU:O	1:A:4344:LEU:HD21	2.20	0.41
1:A:4411:ARG:O	1:A:4415:ARG:HG3	2.20	0.41
1:A:4485:ARG:HH11	1:A:4515:PHE:HD1	1.67	0.41
1:A:1369:GLN:HG2	1:A:1373:PHE:CZ	2.56	0.41
1:A:2022:TYR:CZ	1:A:2352:THR:HB	2.56	0.41
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	2.03	0.41
1:A:3765:THR:O	1:A:3768:THR:OG1	2.26	0.41
1:A:3906:GLN:HG2	1:A:3910:ARG:NH1	2.35	0.41
1:A:3961:LEU:HD11	1:A:3996:PHE:HB3	2.02	0.41
2:C:133:LYS:HB3	2:C:135:TRP:HE1	1.86	0.41
2:C:159:ASP:OD2	2:C:161:SER:OG	2.33	0.41
1:A:1513:TYR:CZ	1:A:1517:GLU:HA	2.55	0.41
1:A:1697:LYS:HG2	1:A:1699:ASN:OD1	2.21	0.41
1:A:2072:PHE:HZ	1:A:2157:LEU:HD11	1.85	0.41
1:A:2290:SER:HB2	1:A:2295:LEU:HG	2.01	0.41
1:A:4024:PRO:HD3	1:A:4158:LEU:HB3	2.02	0.41
1:A:4521:ILE:HG13	1:A:4522:THR:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ILE:HG13	2:B:261:TRP:HB2	2.03	0.41
1:A:1917:LYS:HG2	1:A:1927:VAL:HG11	2.01	0.41
1:A:2622:PHE:HB3	1:A:2669:PRO:HD3	2.03	0.41
1:A:3807:ALA:O	1:A:3811:ILE:HD12	2.20	0.41
2:B:214:LYS:HG2	2:B:235:GLU:C	2.45	0.41
2:B:243:ASN:ND2	2:B:248:LEU:H	2.19	0.41
2:B:277:HIS:CG	2:B:316:ARG:HB2	2.56	0.41
2:B:342:ARG:HD2	2:B:342:ARG:HA	1.91	0.41
2:C:94:TRP:CD2	2:C:393:PRO:HB3	2.55	0.41
2:C:172:MET:HE1	2:C:192:ASP:C	2.45	0.41
1:A:1914:GLU:OE2	5:A:4701:ADP:H3'	2.20	0.41
1:A:2190:TYR:CE2	1:A:2385:ILE:HD11	2.55	0.41
1:A:2796:PRO:O	1:A:2800:THR:N	2.44	0.41
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.31	0.41
1:A:3970:VAL:HB	1:A:3989:ARG:HH11	1.85	0.41
1:A:4209:GLU:HG3	1:A:4213:ARG:HD3	2.03	0.41
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	2.01	0.41
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.54	0.41
1:A:1880:VAL:HG21	1:A:2049:ILE:HG23	2.03	0.41
1:A:1905:PHE:HB3	1:A:2018:MET:HB3	2.02	0.41
1:A:3126:MET:HE1	1:A:3128:VAL:HA	2.02	0.41
1:A:3163:LYS:HB3	1:A:3163:LYS:HE2	1.84	0.41
1:A:3717:LEU:HD11	1:A:3724:VAL:HB	2.03	0.41
2:B:317:ASP:OD1	2:B:319:THR:HG22	2.21	0.41
2:B:395:VAL:O	2:B:407:TRP:N	2.37	0.41
1:A:1373:PHE:HD2	1:A:1383:TYR:HD1	1.69	0.41
1:A:1466:ILE:HG12	1:A:1500:HIS:CE1	2.55	0.41
1:A:1752:LEU:HD11	1:A:1857:LEU:HD21	2.03	0.41
1:A:1776:ALA:HB3	1:A:1779:HIS:CE1	2.56	0.41
1:A:2823:ARG:NH2	1:A:2871:ILE:HA	2.34	0.41
1:A:2848:GLU:HA	1:A:2851:ASP:OD2	2.21	0.41
1:A:4143:ARG:HG2	1:A:4145:PHE:CE2	2.56	0.41
1:A:4485:ARG:HD3	1:A:4515:PHE:CE1	2.54	0.41
1:A:4565:LEU:HB3	1:A:4583:THR:HB	2.03	0.41
2:B:153:VAL:HA	2:B:169:SER:HA	2.03	0.41
1:A:2172:ARG:CZ	1:A:2174:GLU:HA	2.51	0.41
1:A:3114:ASP:O	1:A:3116:GLU:HG2	2.21	0.41
1:A:3442:ALA:O	1:A:3446:ARG:HG2	2.21	0.41
1:A:4312:LEU:HD12	1:A:4313:PRO:HD2	2.02	0.41
2:B:240:VAL:HG23	2:B:250:ALA:O	2.21	0.41
2:C:102:TYR:HB2	2:C:406:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:238:ARG:HA	2:C:238:ARG:HD3	1.89	0.41
2:C:239:MET:SD	2:C:282:ILE:HG12	2.60	0.41
2:C:253:SER:OG	2:C:254:ASN:N	2.54	0.41
2:C:363:ARG:HB3	2:C:372:CYS:SG	2.61	0.41
1:A:2915:VAL:HG13	1:A:2946:LEU:HD11	2.02	0.40
1:A:2944:THR:H	5:A:4704:ADP:PB	2.44	0.40
1:A:3521:ASP:N	1:A:3521:ASP:OD1	2.54	0.40
1:A:3606:ASP:OD1	1:A:3607:ARG:N	2.55	0.40
2:C:327:THR:HG23	2:C:329:MET:HG3	2.03	0.40
1:A:1351:TRP:CD1	1:A:1404:LYS:HB2	2.56	0.40
1:A:1357:ARG:HH21	1:A:1360:ARG:HD2	1.86	0.40
1:A:3753:LEU:HD23	1:A:3753:LEU:HA	1.86	0.40
1:A:4529:ALA:O	1:A:4533:SER:N	2.54	0.40
2:B:128:GLU:HA	2:B:152:SER:HB2	2.03	0.40
1:A:2221:MET:HE2	1:A:2361:MET:CE	2.51	0.40
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.22	0.40
1:A:3740:LEU:HD23	1:A:3743:ARG:HH12	1.87	0.40
1:A:4013:LEU:HD13	1:A:4017:PHE:CE2	2.56	0.40
1:A:4395:LEU:HD21	1:A:4489:LEU:HD22	2.04	0.40
1:A:4408:PRO:HA	1:A:4411:ARG:HD2	2.04	0.40
2:C:91:PRO:HB3	2:C:94:TRP:CZ3	2.56	0.40
1:A:1650:LEU:HA	1:A:1653:HIS:HD2	1.86	0.40
1:A:1961:ASN:OD1	1:A:1961:ASN:N	2.54	0.40
1:A:2432:LEU:HD11	1:A:2522:THR:HA	2.03	0.40
1:A:2823:ARG:HH12	1:A:2868:SER:N	2.19	0.40
1:A:3145:ASN:HA	1:A:3148:VAL:HG22	2.03	0.40
1:A:3239:LYS:HD3	1:A:3451:TYR:CD1	2.57	0.40
1:A:4454:GLU:HA	1:A:4457:LYS:NZ	2.36	0.40
2:B:312:LEU:HD11	2:B:346:PHE:CZ	2.57	0.40
1:A:1899:ARG:HD2	1:A:1982:LEU:HB3	2.02	0.40
1:A:2756:LEU:HD23	1:A:2756:LEU:HA	1.78	0.40
1:A:3126:MET:HA	1:A:3127:PRO:HD3	1.90	0.40
1:A:3657:GLY:HA3	2:B:193:HIS:CE1	2.56	0.40
1:A:3795:GLU:HA	1:A:3798:SER:OG	2.22	0.40
1:A:4521:ILE:HD13	1:A:4620:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	3057/4646 (66%)	2977 (97%)	79 (3%)	1 (0%)	100	100
2	B	320/410 (78%)	306 (96%)	14 (4%)	0	100	100
2	C	309/410 (75%)	289 (94%)	20 (6%)	0	100	100
2	D	73/410 (18%)	73 (100%)	0	0	100	100
2	E	73/410 (18%)	72 (99%)	1 (1%)	0	100	100
3	F	32/638 (5%)	32 (100%)	0	0	100	100
3	G	32/638 (5%)	32 (100%)	0	0	100	100
4	H	120/1281 (9%)	119 (99%)	1 (1%)	0	100	100
4	I	119/1281 (9%)	119 (100%)	0	0	100	100
All	All	4135/10124 (41%)	4019 (97%)	115 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1374	PRO

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	2721/4125 (66%)	2721 (100%)	0	100	100
2	B	287/364 (79%)	287 (100%)	0	100	100
2	C	280/364 (77%)	280 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3288/4853 (68%)	3288 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1349	GLN
1	A	1421	HIS
1	A	1433	GLN
1	A	1454	GLN
1	A	1569	GLN
1	A	1755	GLN
1	A	1841	GLN
1	A	2212	GLN
1	A	2296	GLN
1	A	2299	GLN
1	A	2588	HIS
1	A	2685	GLN
1	A	3014	ASN
1	A	3057	GLN
1	A	3069	ASN
1	A	3119	ASN
1	A	3522	GLN
1	A	3535	HIS
1	A	3711	GLN
1	A	3735	GLN
1	A	3792	GLN
1	A	3820	GLN
1	A	4295	GLN
1	A	4335	GLN
1	A	4530	GLN
1	A	4566	GLN
2	C	194	ASN
2	C	277	HIS

5.3.3 RNA ⓘ

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	4701	7	28,29,29	1.45	5 (17%)	43,45,45	1.83	8 (18%)
5	ADP	A	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.89	8 (18%)
6	ATP	A	4702	7	32,33,33	0.31	0	48,52,52	0.30	0
5	ADP	A	4704	-	28,29,29	1.41	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	4701	7	-	4/16/32/32	0/3/3/3
5	ADP	A	4703	-	-	2/16/32/32	0/3/3/3
6	ATP	A	4702	7	-	0/22/38/38	0/3/3/3
5	ADP	A	4704	-	-	2/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4703	ADP	C5-C4	4.79	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4701	ADP	C5-C4	4.76	1.47	1.39
5	A	4704	ADP	C5-C4	4.69	1.47	1.39
5	A	4704	ADP	C5-C6	2.75	1.48	1.41
5	A	4703	ADP	C5-C6	2.72	1.48	1.41
5	A	4701	ADP	C5-C6	2.68	1.48	1.41
5	A	4703	ADP	C5-N7	-2.37	1.34	1.39
5	A	4701	ADP	C5-N7	-2.36	1.34	1.39
5	A	4704	ADP	C8-N7	2.34	1.36	1.31
5	A	4704	ADP	C5-N7	-2.28	1.34	1.39
5	A	4701	ADP	C8-N7	2.27	1.36	1.31
5	A	4701	ADP	PA-O3A	2.25	1.61	1.59
5	A	4703	ADP	C8-N7	2.22	1.36	1.31

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4703	ADP	C5-C4-N3	-6.38	117.93	126.72
5	A	4701	ADP	C5-C4-N3	-6.02	118.42	126.72
5	A	4704	ADP	C5-C4-N3	-5.87	118.63	126.72
5	A	4703	ADP	N3-C4-N9	5.10	135.84	127.17
5	A	4701	ADP	N3-C4-N9	4.74	135.23	127.17
5	A	4704	ADP	N3-C4-N9	4.57	134.94	127.17
5	A	4703	ADP	C2-N3-C4	3.93	121.44	111.83
5	A	4701	ADP	C2-N3-C4	3.74	120.96	111.83
5	A	4704	ADP	C2-N3-C4	3.71	120.90	111.83
5	A	4704	ADP	C4-C5-N7	-3.52	106.56	110.58
5	A	4701	ADP	C4-C5-N7	-3.42	106.67	110.58
5	A	4703	ADP	C4-C5-N7	-3.36	106.74	110.58
5	A	4703	ADP	N3-C2-N1	-3.26	123.65	128.58
5	A	4704	ADP	N3-C2-N1	-3.18	123.77	128.58
5	A	4701	ADP	N3-C2-N1	-3.17	123.78	128.58
5	A	4704	ADP	C5-N7-C8	2.49	107.37	103.45
5	A	4703	ADP	C5-N7-C8	2.49	107.37	103.45
5	A	4704	ADP	C4-N9-C8	2.49	108.35	105.74
5	A	4704	ADP	C3'-C2'-C1'	2.47	106.14	101.46
5	A	4701	ADP	C5-N7-C8	2.42	107.25	103.45
5	A	4703	ADP	C3'-C2'-C1'	2.37	105.95	101.46
5	A	4701	ADP	C4-N9-C8	2.36	108.22	105.74
5	A	4703	ADP	C4-N9-C8	2.26	108.11	105.74
5	A	4701	ADP	C3'-C2'-C1'	2.19	105.61	101.46
5	A	4704	ADP	C6-C5-N7	2.10	136.15	132.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

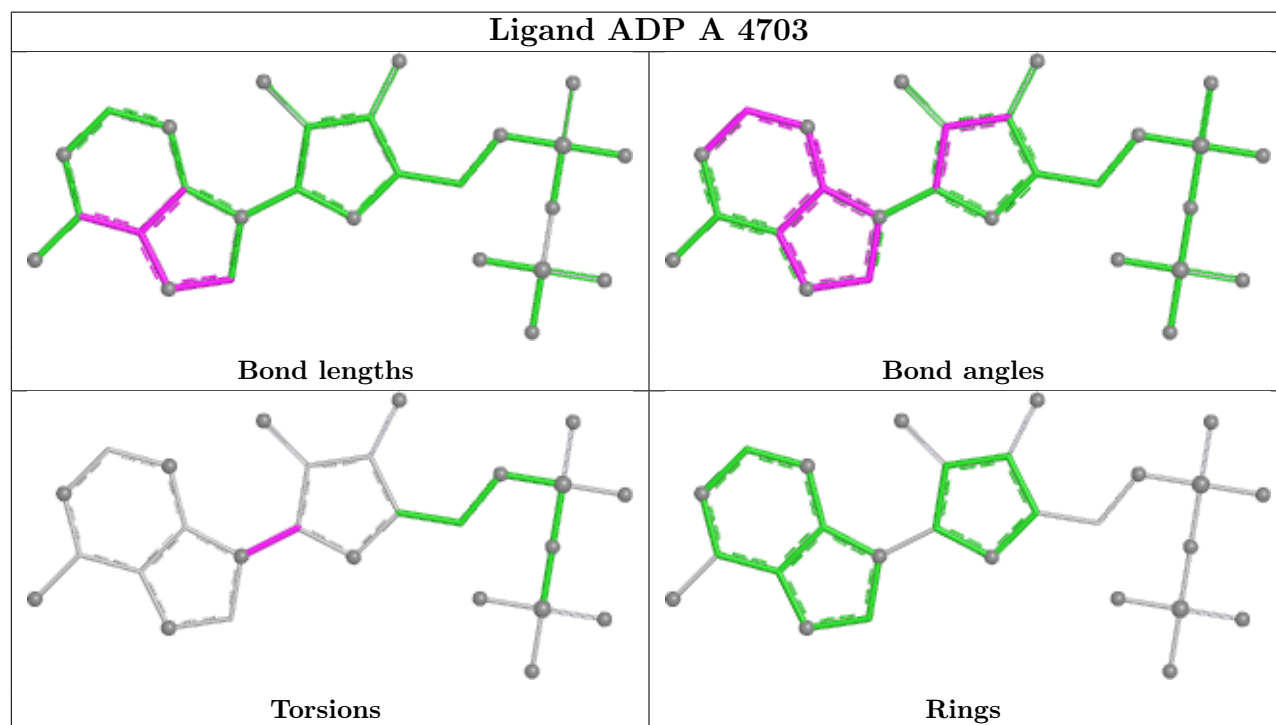
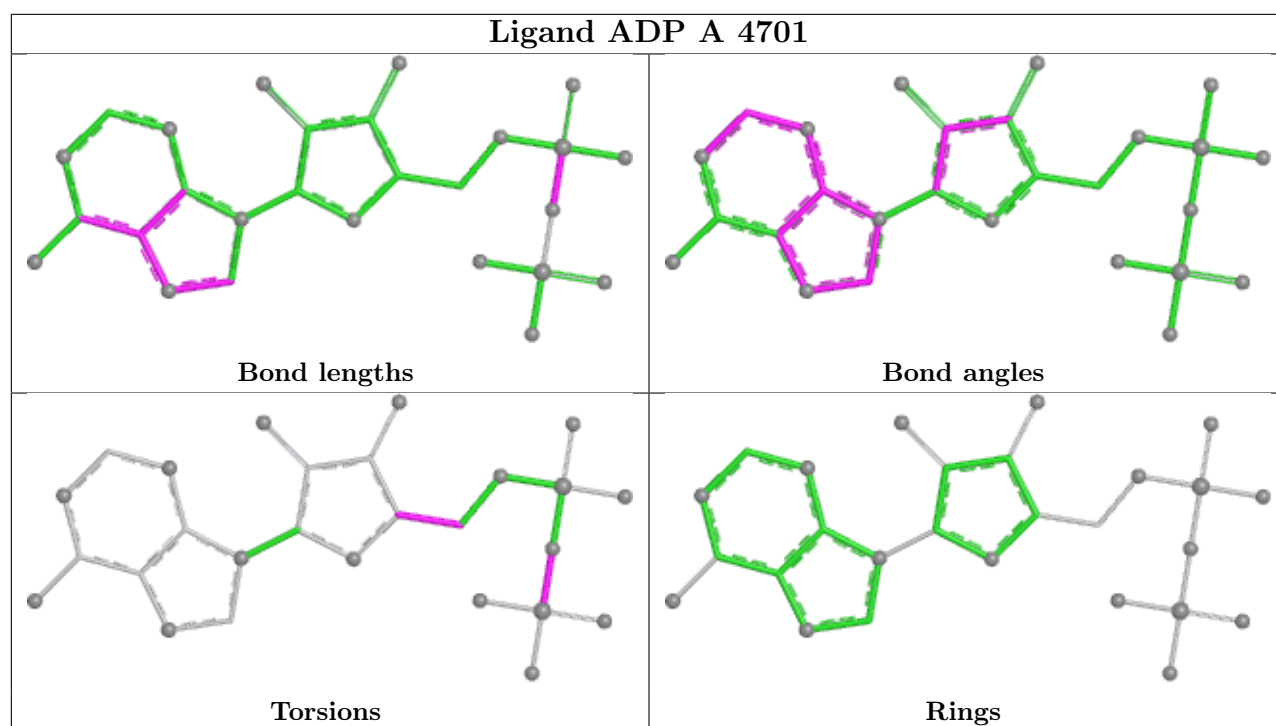
Mol	Chain	Res	Type	Atoms
5	A	4701	ADP	PA-O3A-PB-O2B
5	A	4701	ADP	PA-O3A-PB-O3B
5	A	4701	ADP	O4'-C4'-C5'-O5'
5	A	4701	ADP	C3'-C4'-C5'-O5'
5	A	4704	ADP	C3'-C4'-C5'-O5'
5	A	4704	ADP	O4'-C4'-C5'-O5'
5	A	4703	ADP	C2'-C1'-N9-C8
5	A	4703	ADP	C2'-C1'-N9-C4

There are no ring outliers.

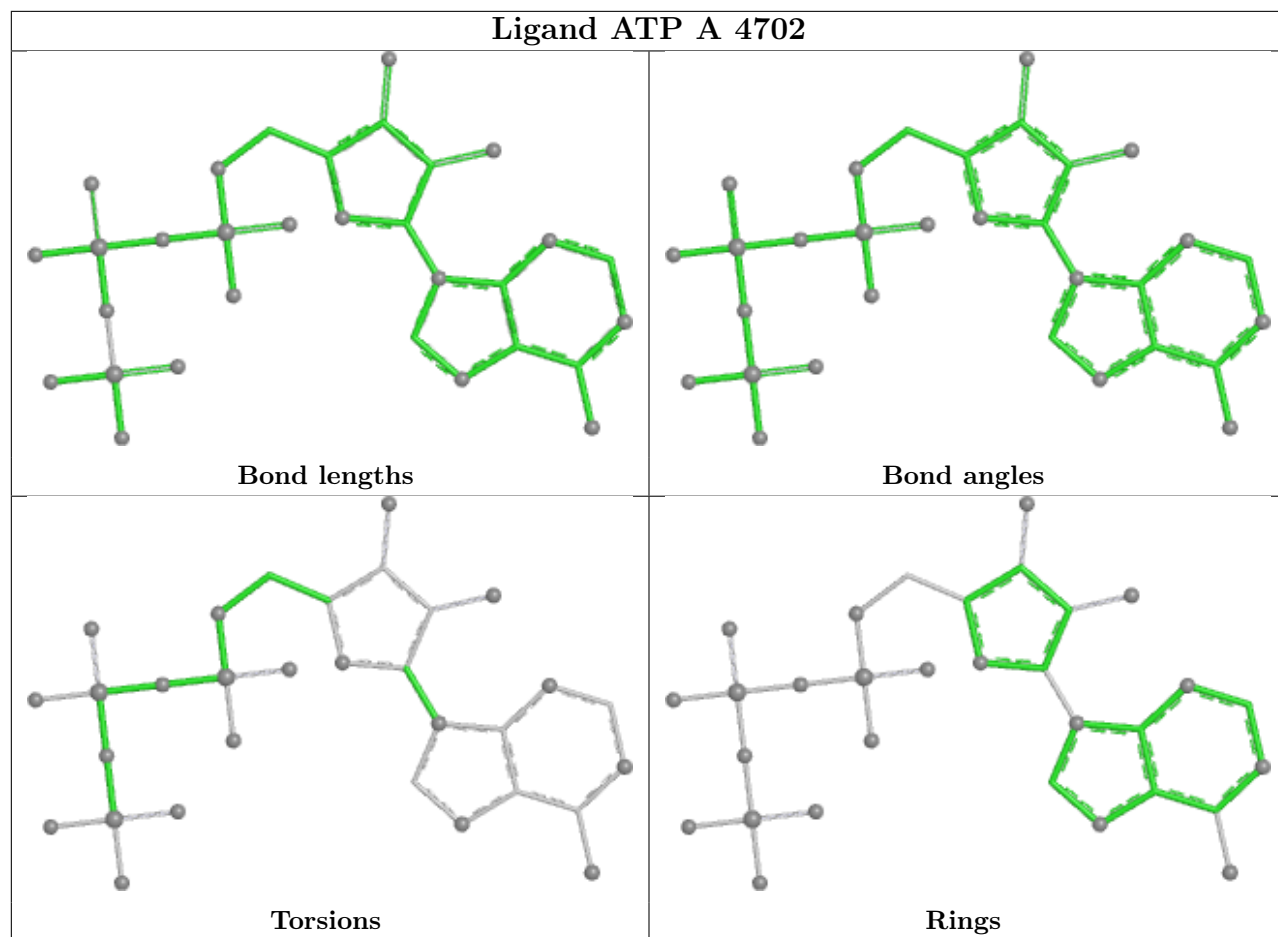
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4701	ADP	9	0
5	A	4703	ADP	2	0
6	A	4702	ATP	2	0
5	A	4704	ADP	3	0

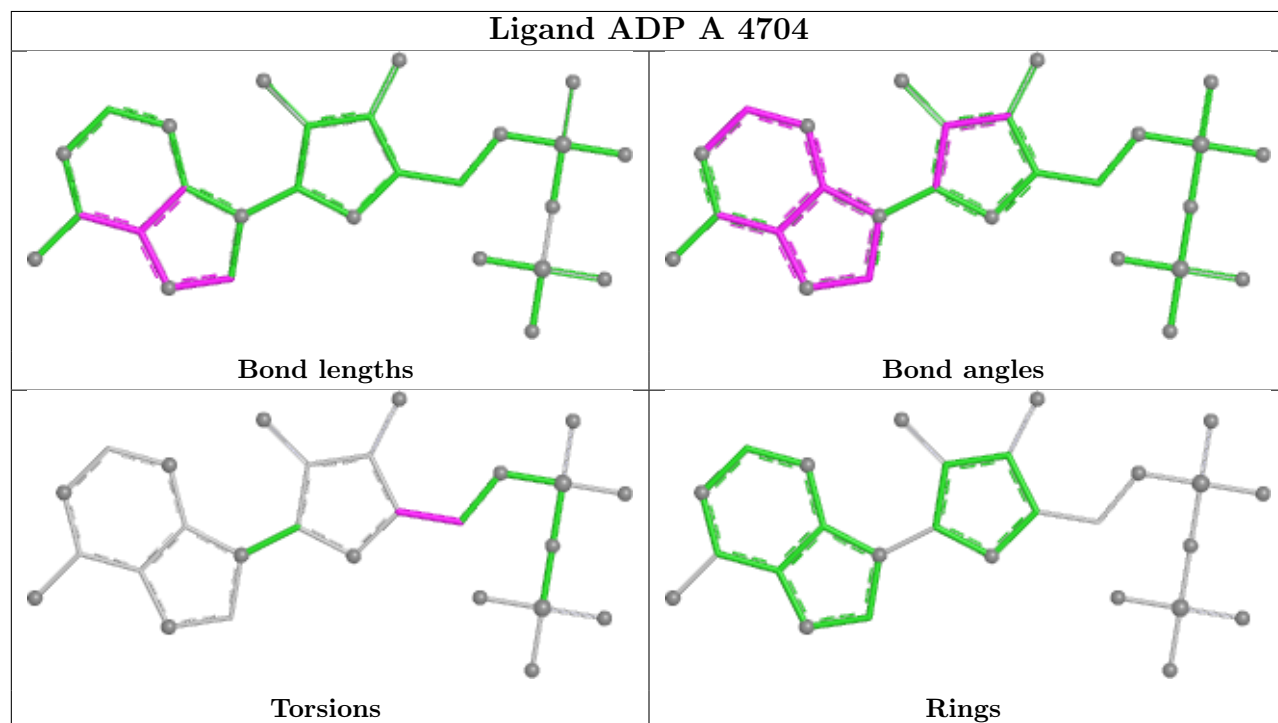
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand ATP A 4702



Ligand ADP A 4704



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

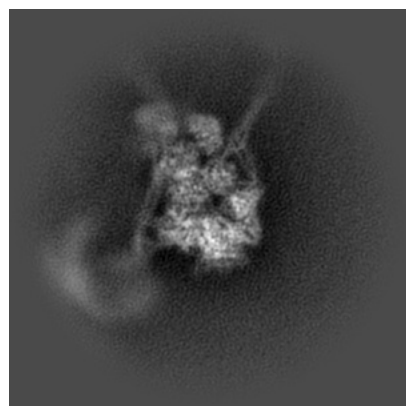
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73174. These allow visual inspection of the internal detail of the map and identification of artifacts.

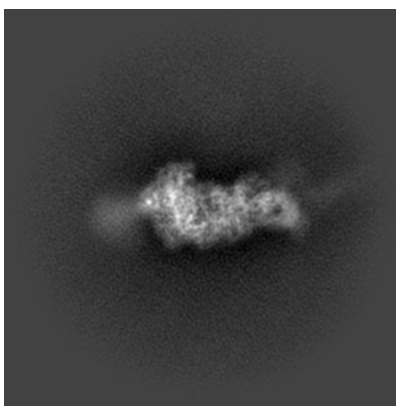
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

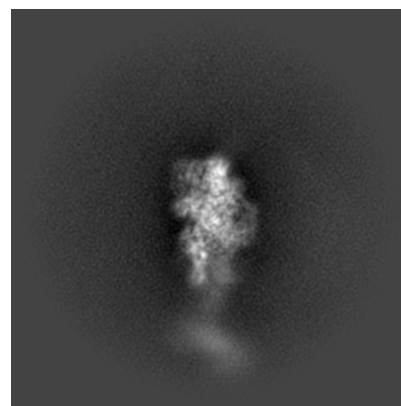
6.1.1 Primary map



X

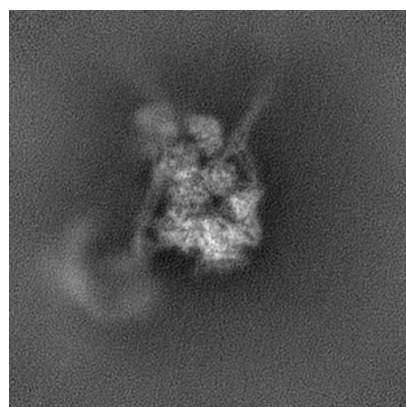


Y

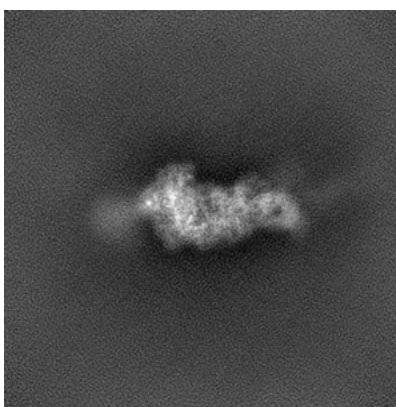


Z

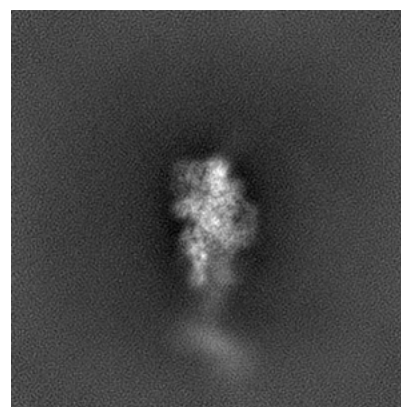
6.1.2 Raw map



X



Y

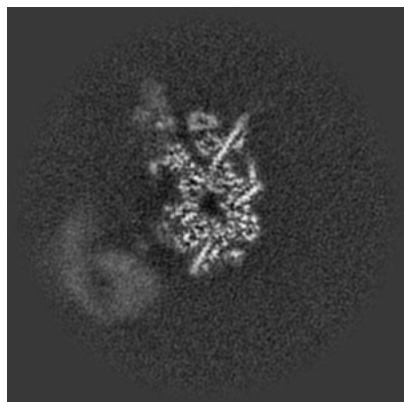


Z

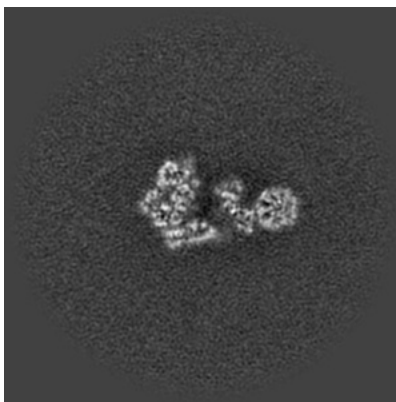
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

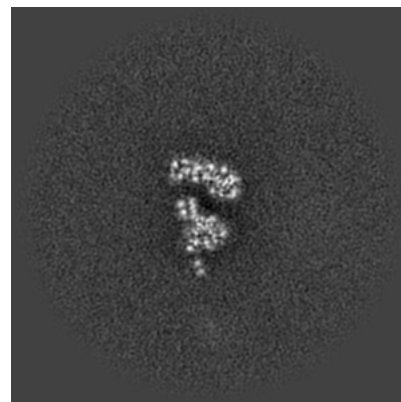
6.2.1 Primary map



X Index: 128

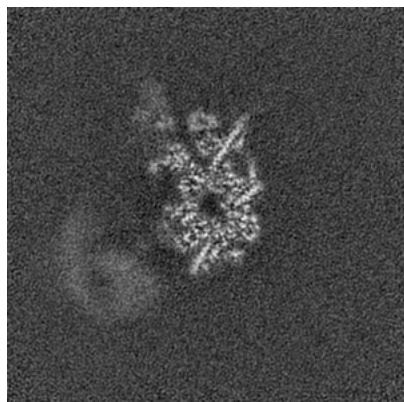


Y Index: 128

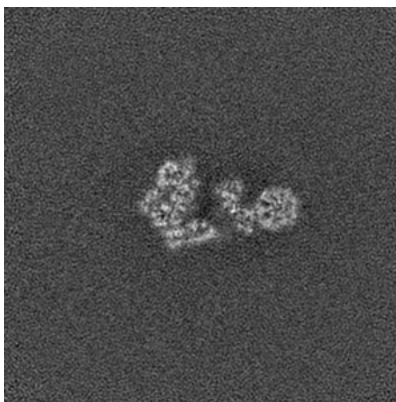


Z Index: 128

6.2.2 Raw map



X Index: 128



Y Index: 128

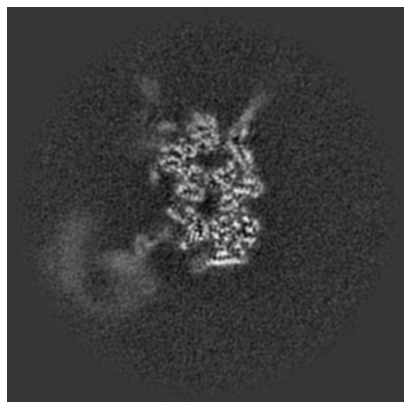


Z Index: 128

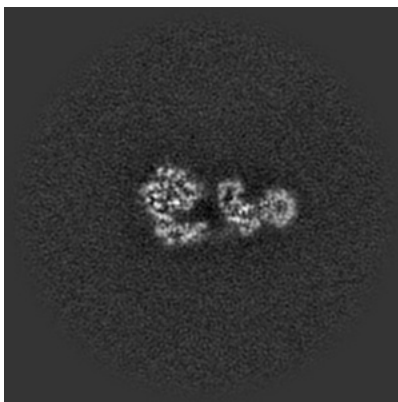
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

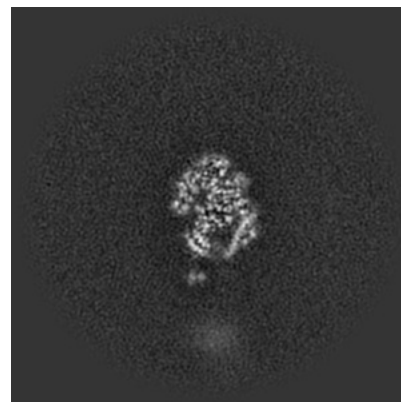
6.3.1 Primary map



X Index: 132

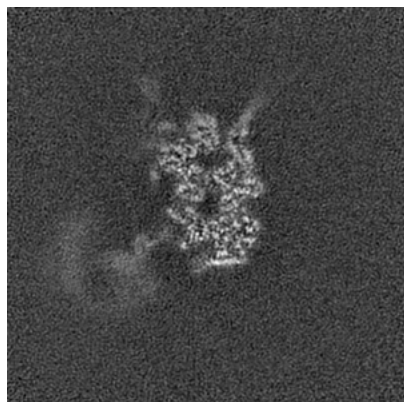


Y Index: 132

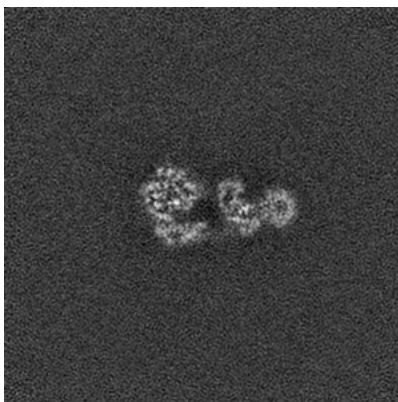


Z Index: 112

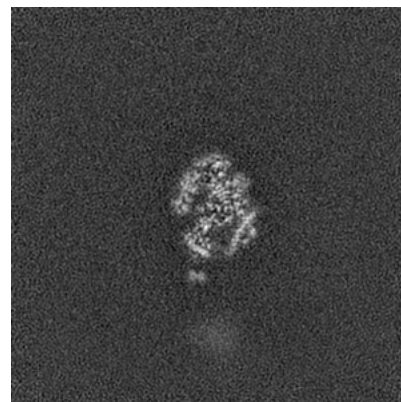
6.3.2 Raw map



X Index: 132



Y Index: 132

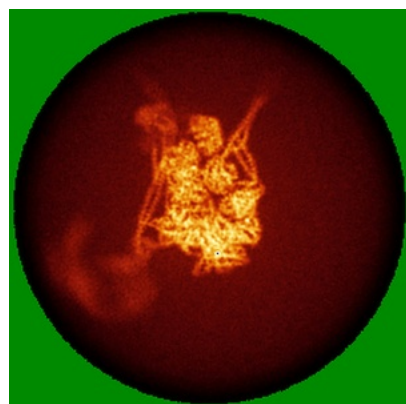


Z Index: 113

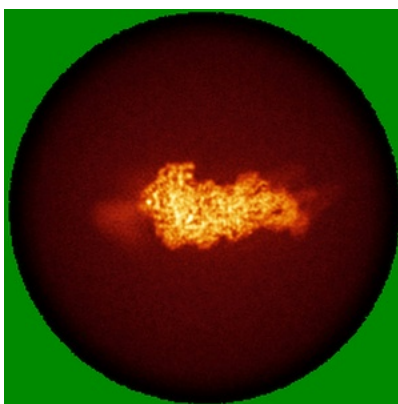
The images above show the largest variance slices of the map in three orthogonal directions.

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

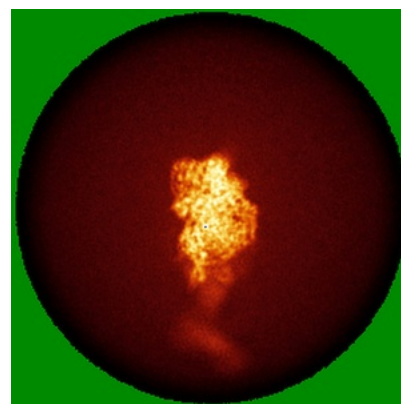
6.4.1 Primary map



X

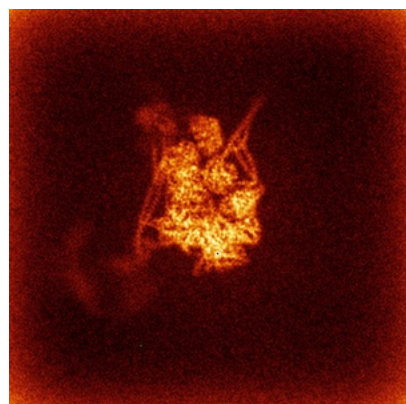


Y

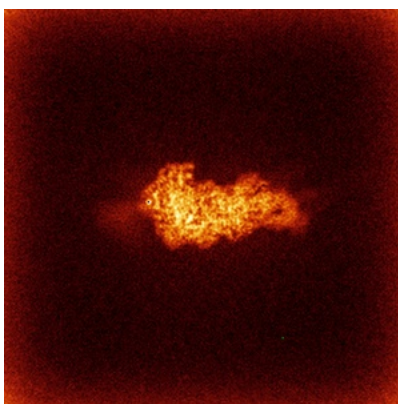


Z

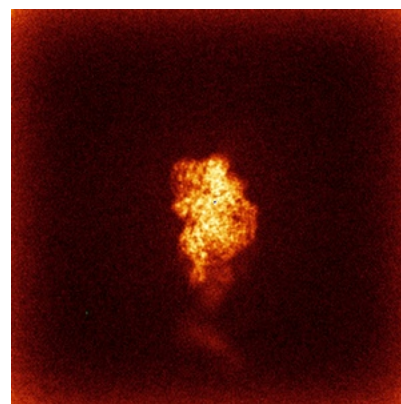
6.4.2 Raw map



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.

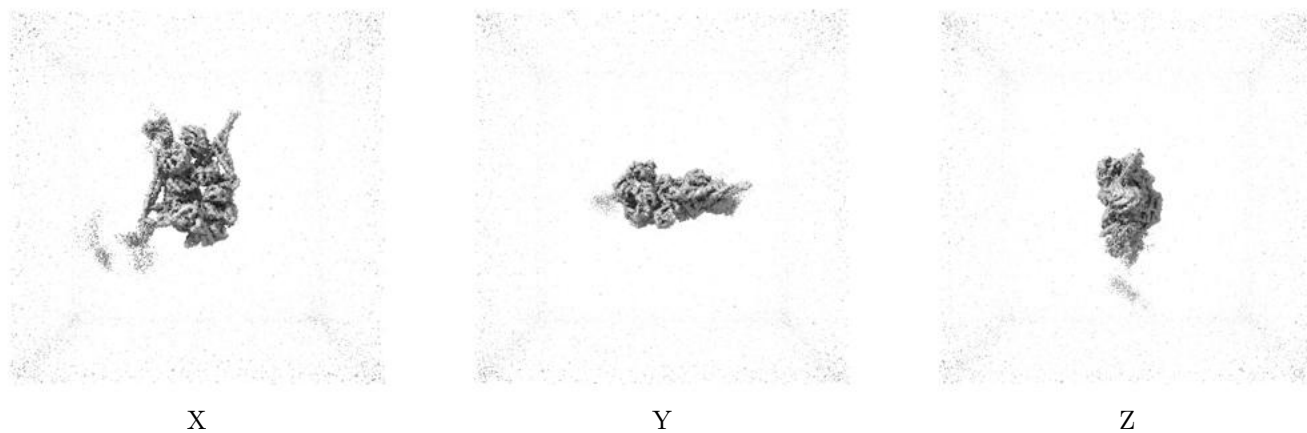
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

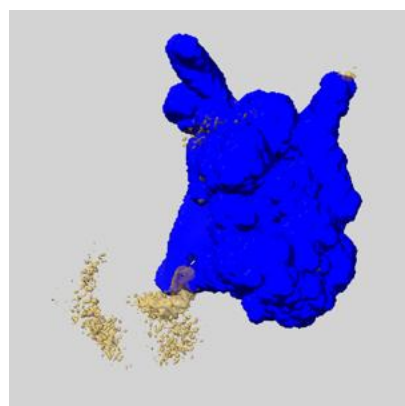
6.6 Mask visualisation [i](#)

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

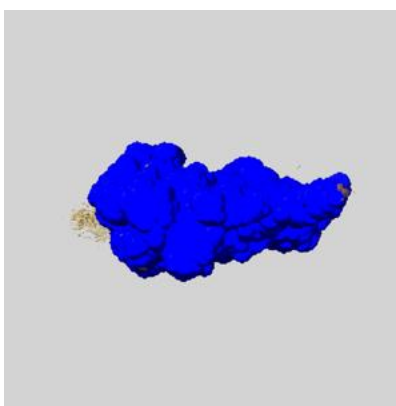
A mask typically either:

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

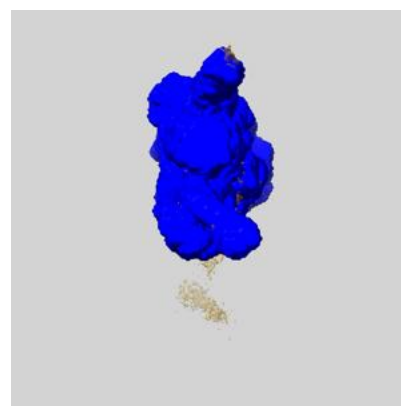
6.6.1 emd_73174_msk_1.map [i](#)



X



Y

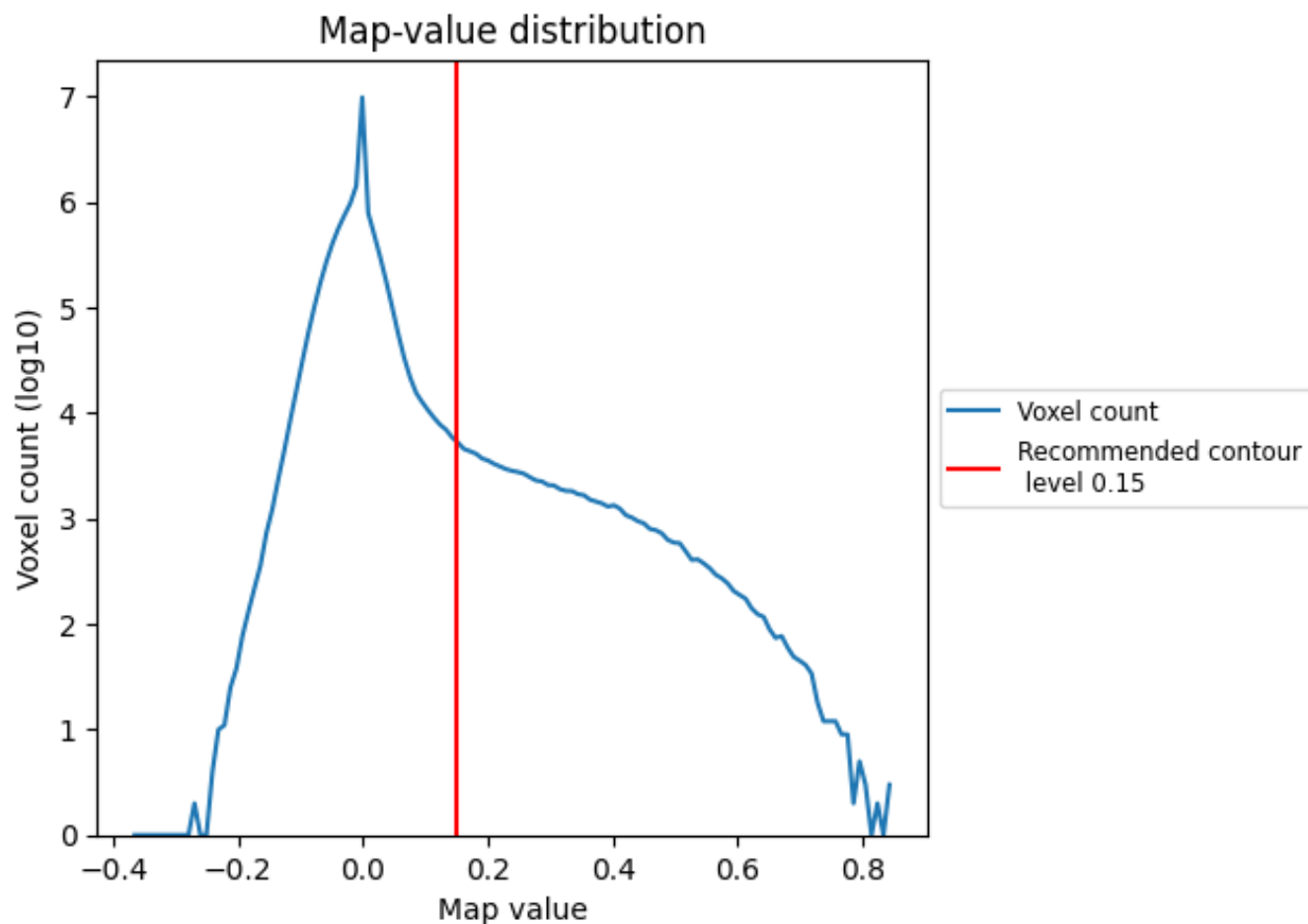


Z

7 Map analysis [i](#)

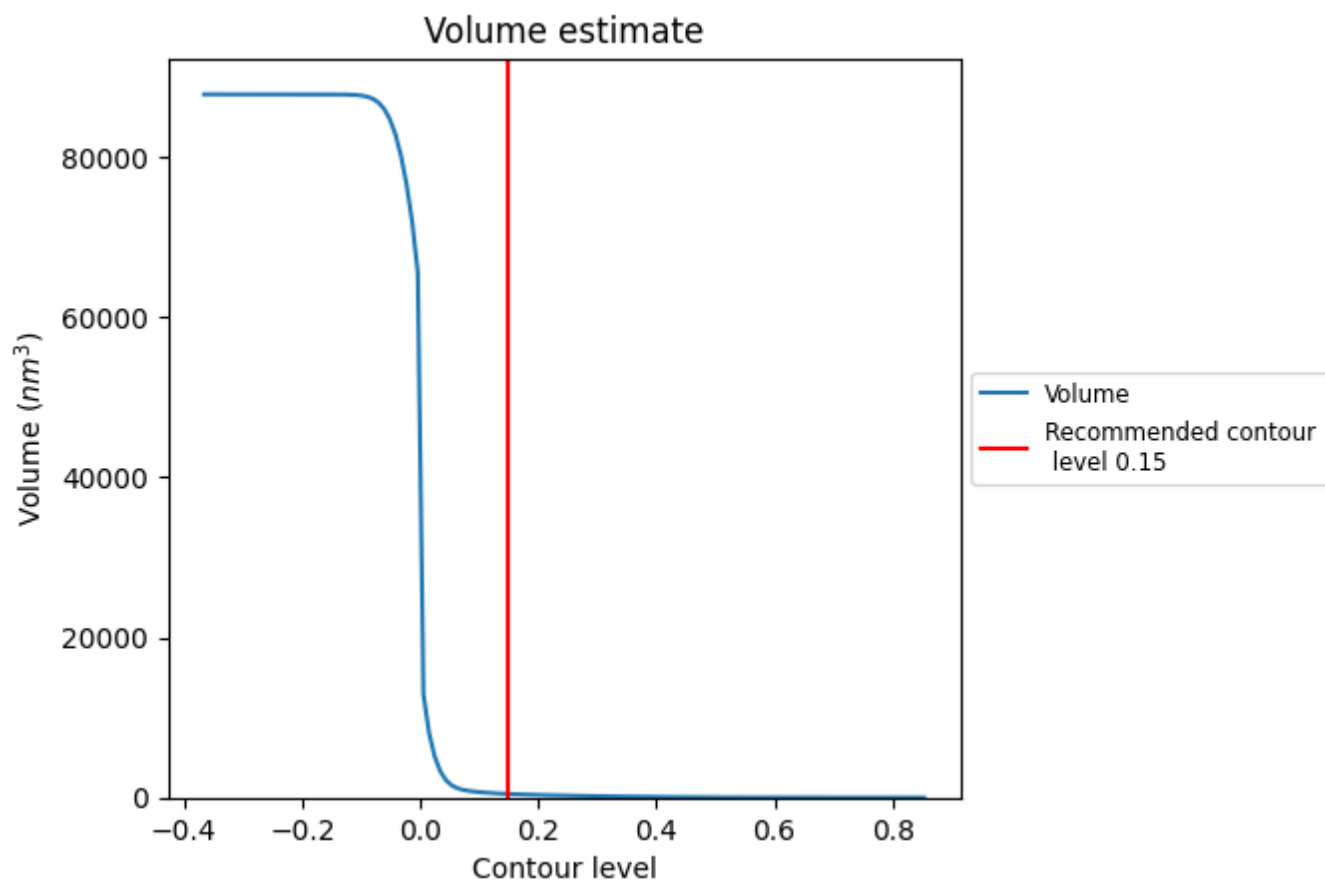
This section contains the results of statistical analysis of the map.

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.

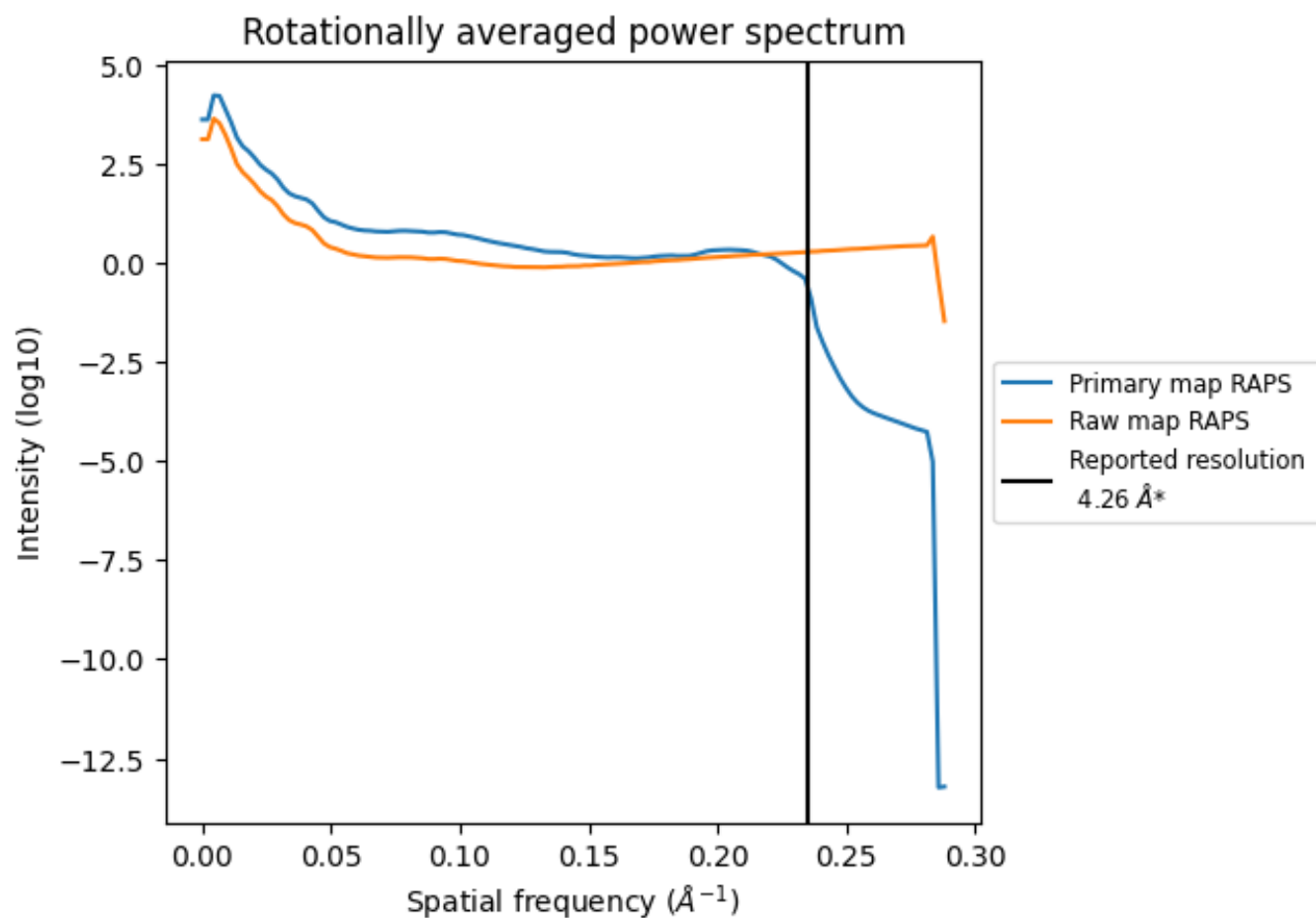
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 447 nm³; this corresponds to an approximate mass of 404 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 ⓘ

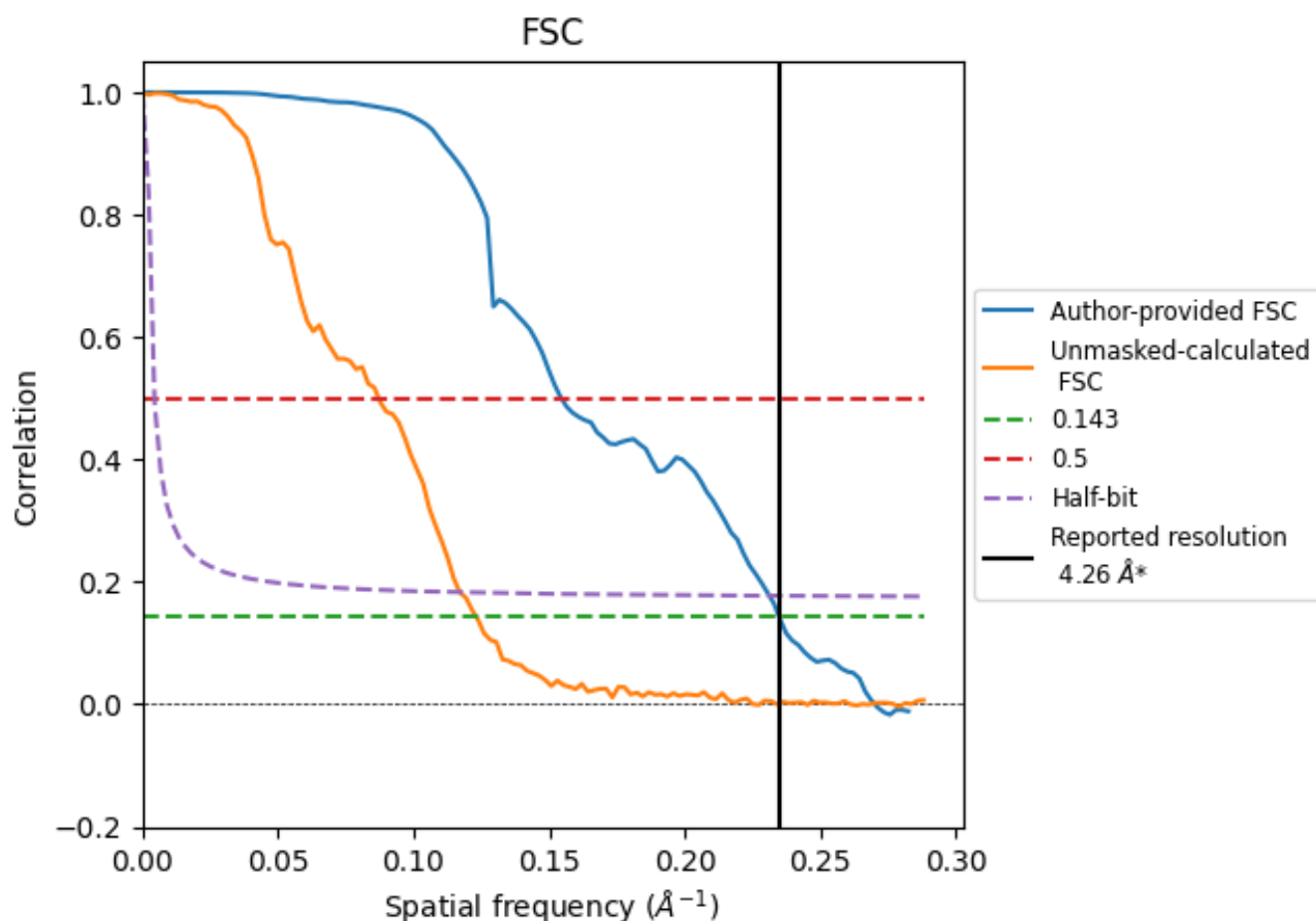


*Reported resolution corresponds to spatial frequency of 0.235 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.235 \AA^{-1}

8.2 Resolution estimates [i](#)

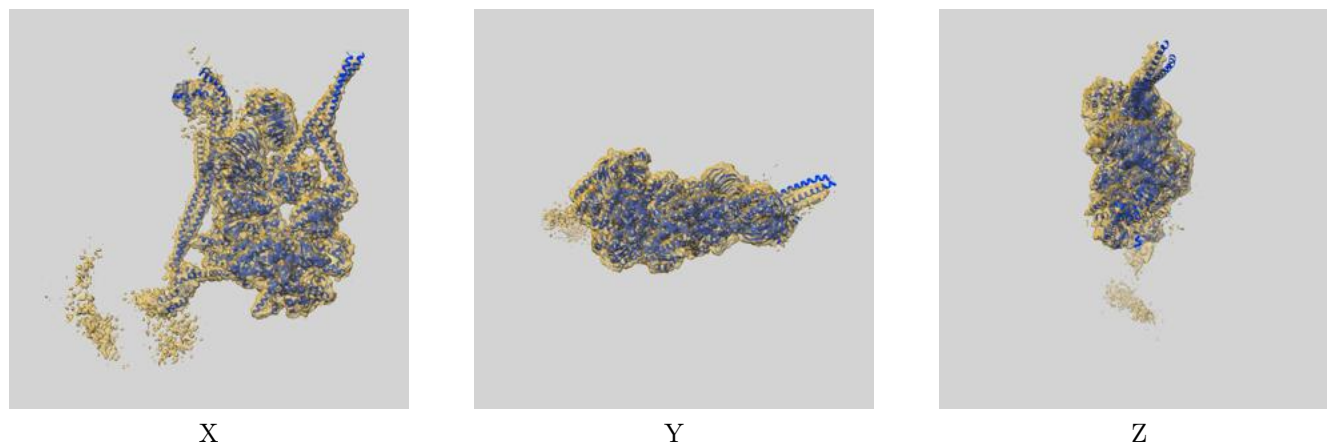
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.26	-	-
Author-provided FSC curve	4.26	6.47	4.33
Unmasked-calculated*	8.13	11.48	8.54

*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 8.13 differs from the reported value 4.26 by more than 10 %

9 Map-model fit [i](#)

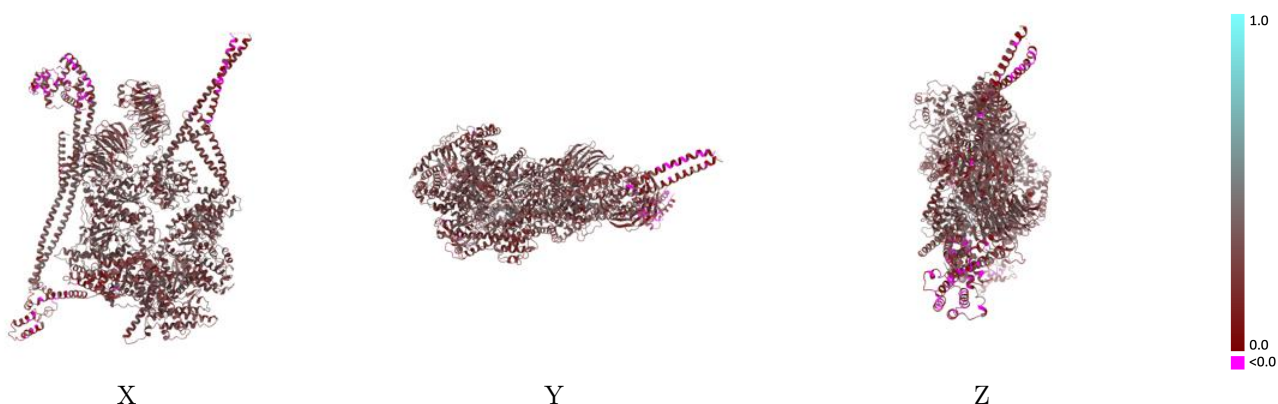
This section contains information regarding the fit between EMDB map EMD-73174 and PDB model 9YND. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



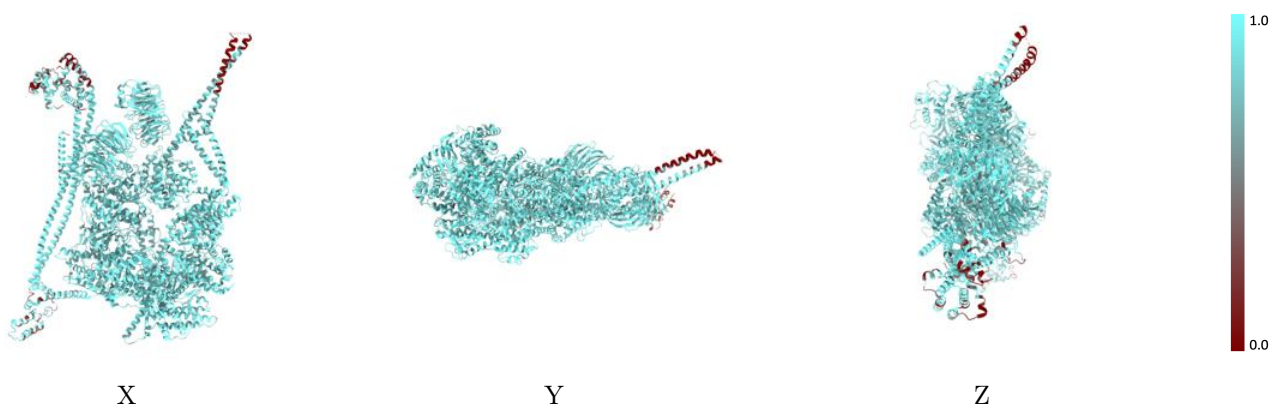
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



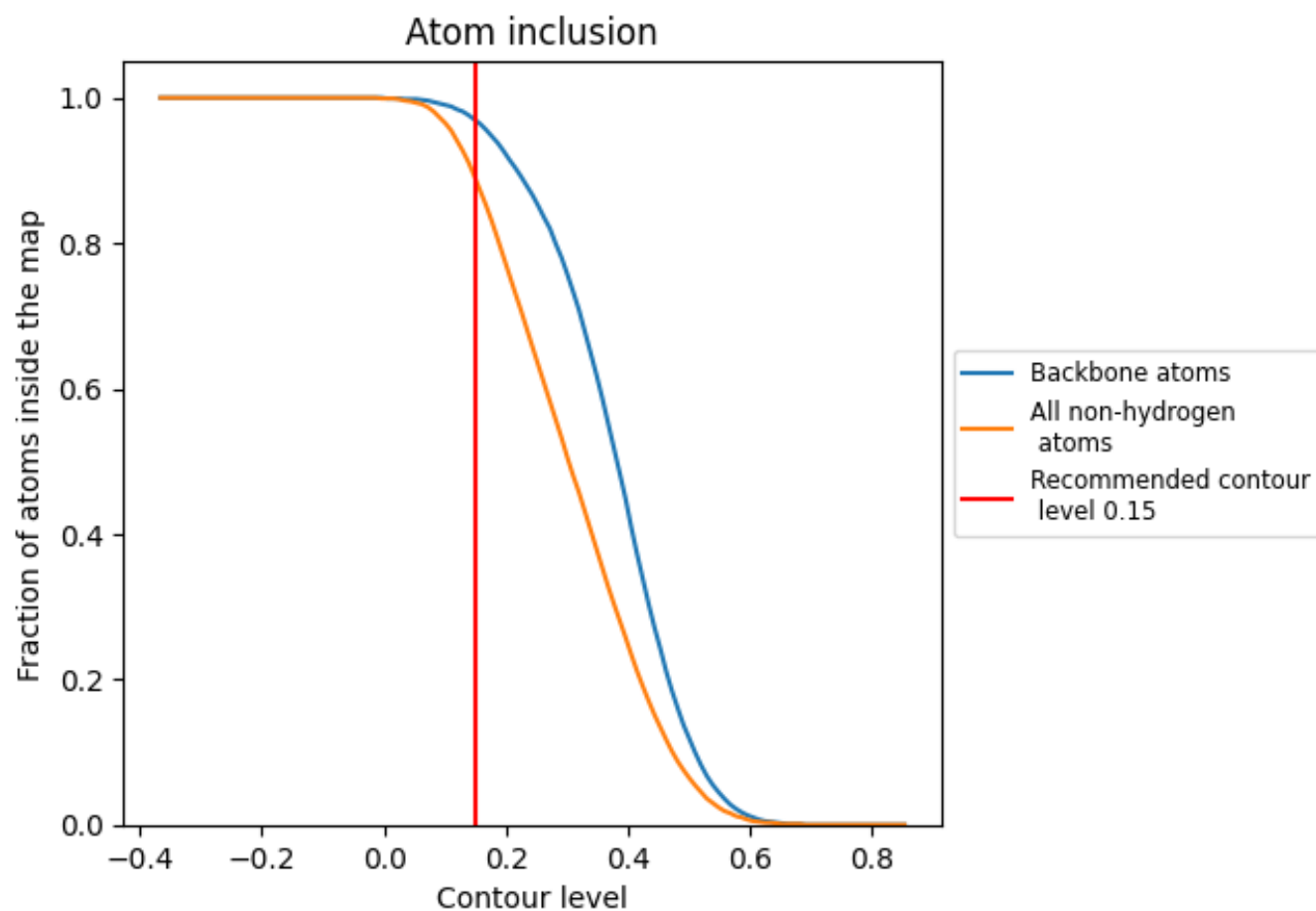
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8890</div>	<div><div></div>0.2870</div>
A	<div><div></div>0.8920</div>	<div><div></div>0.2930</div>
B	<div><div></div>0.8950</div>	<div><div></div>0.3020</div>
C	<div><div></div>0.9050</div>	<div><div></div>0.2610</div>
D	<div><div></div>0.6700</div>	<div><div></div>0.1660</div>
E	<div><div></div>0.7400</div>	<div><div></div>0.1450</div>
F	<div><div></div>0.9410</div>	<div><div></div>0.2990</div>
G	<div><div></div>0.9590</div>	<div><div></div>0.3040</div>
H	<div><div></div>0.8900</div>	<div><div></div>0.2630</div>
I	<div><div></div>0.8880</div>	<div><div></div>0.2740</div>

1.0

0.0

<0.0