



Full wwPDB EM Validation Report ⓘ

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PDB ID : 8ATU / pdb_00008atu
EMDB ID : EMD-15663
Title : Cryo-EM structure of human BIRC6
Authors : Ehrmann, J.F.; Grabarczyk, D.B.; Clausen, T.
Deposited on : 2022-08-24
Resolution : 3.30 Å(reported)

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

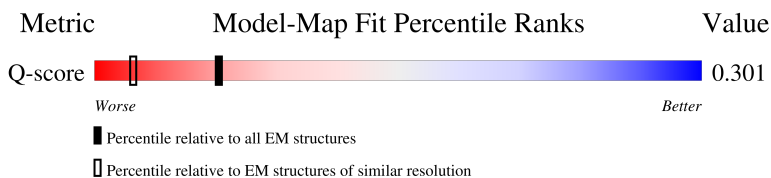
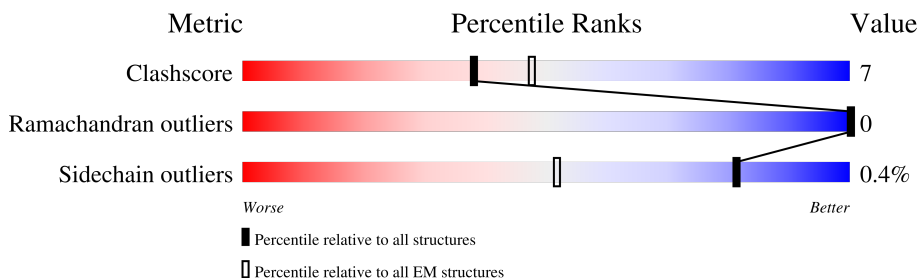
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	4867	34% 47% 11% 42%
1	B	4867	34% 47% 11% 42%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 43882 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 Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2837	Total	C	N	O	S	0	0
			21940	14019	3711	4059	151		
1	B	2837	Total	C	N	O	S	0	0
			21940	14019	3711	4059	151		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1332	VAL	LEU	conflict	UNP Q9NR09
A	4858	SER	-	expression tag	UNP Q9NR09
A	4859	ALA	-	expression tag	UNP Q9NR09
A	4860	TRP	-	expression tag	UNP Q9NR09
A	4861	SER	-	expression tag	UNP Q9NR09
A	4862	HIS	-	expression tag	UNP Q9NR09
A	4863	PRO	-	expression tag	UNP Q9NR09
A	4864	GLN	-	expression tag	UNP Q9NR09
A	4865	PHE	-	expression tag	UNP Q9NR09
A	4866	GLU	-	expression tag	UNP Q9NR09
A	4867	LYS	-	expression tag	UNP Q9NR09
B	1332	VAL	LEU	conflict	UNP Q9NR09
B	4858	SER	-	expression tag	UNP Q9NR09
B	4859	ALA	-	expression tag	UNP Q9NR09
B	4860	TRP	-	expression tag	UNP Q9NR09
B	4861	SER	-	expression tag	UNP Q9NR09
B	4862	HIS	-	expression tag	UNP Q9NR09
B	4863	PRO	-	expression tag	UNP Q9NR09
B	4864	GLN	-	expression tag	UNP Q9NR09
B	4865	PHE	-	expression tag	UNP Q9NR09
B	4866	GLU	-	expression tag	UNP Q9NR09
B	4867	LYS	-	expression tag	UNP Q9NR09

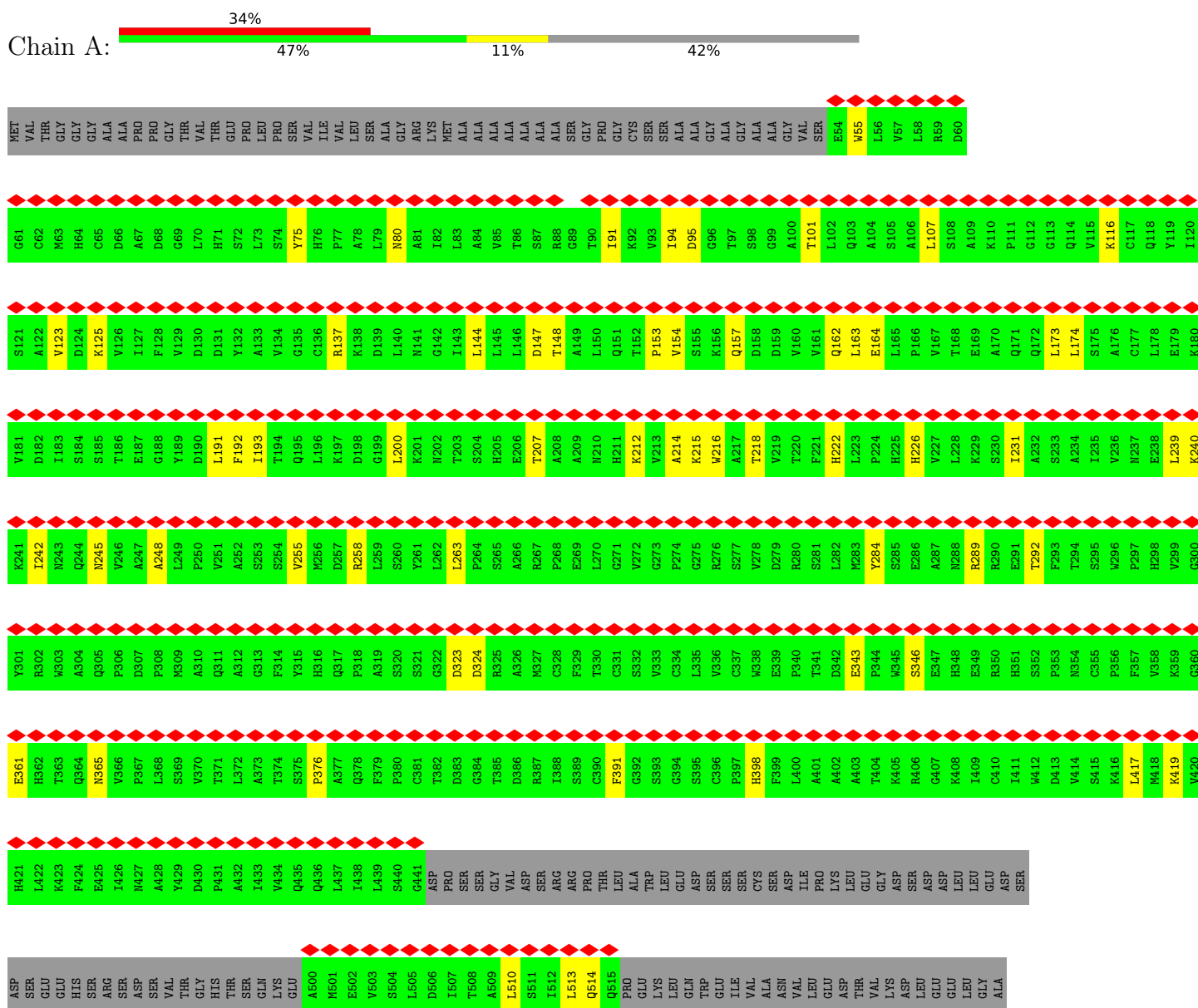
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	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: Baculoviral IAP repeat-containing protein 6





VAL	HIS	GLY	V2162	HIS	S2041	GLY	H1840	I1780	VAL	THR	SER	V1537	D1460	R1382	L1322
HIS	GLN	GLY	V2162	HIS	S2042	GLY	S1841	E1781	ILE	ALA	THR	L1538	E1461	K1383	Q1323
LYS	GLN	GLY	M2167	LYS	S2043	SER	L1842	R1782	ASN	ALA	VAL	GLY	D1462	F1384	F1324
GLN	GLN	GLY	M2173	GLN	H2044	ALA	L1843	M1783	GLU	ALA	ALA	GLY	ASN	L1385	S1325
LEU	LEU	GLY	M2173	LEU	S2045	ALA	L1844	H1784	LEU	ALA	GLY	GLY	GLY	S1386	E1326
ASN	ASN	GLY	L2174	ASN	S2046	ALA	H1845	S1785	GLN	ALA	ALA	LYS	D1387	F1327	F1327
LEU	LEU	GLY	V2175	LEU	P2047	ALA	D1846	G1786	VAL	ALA	THR	VAL	L1473	H1328	H1328
ALA	ALA	GLY	D2180	ALA	S2048	ALA	L1847	A1787	PHE	ALA	SER	SER	L1474	E1329	E1329
ALA	ALA	GLY	V2185	ALA	S2049	ALA	P1849	R1788	PRO	VAL	LEU	CYS	V1477	K1330	K1330
GLN	GLN	GLY	E2186	GLN	L2050	ALA	V1852	F1789	GLY	PRO	SER	THR	S1478	L1331	L1331
LYS	LYS	GLY	D2187	LYS	T2053	ALA	C1853	V1791	ILE	VAL	ALA	ALA	R1479	V1332	V1332
ALA	ALA	GLY	E2188	ALA	Q1981	ALA	R1854	T1792	ASP	HIS	ASN	GLN	E1396	G1397	G1397
LEU	LEU	GLY	A2189	LEU	L1982	ALA	F1855	L1793	PRO	SER	VAL	ALA	R1398	R1398	R1398
VAL	VAL	GLY	L2189	VAL	Q1983	ALA	M1856	D1794	PRO	VAL	ALA	ALA	S1399	L1335	L1335
GLY	GLY	GLY	L2189	GLY	L1984	ALA	M1856	F1795	ALA	PRO	LEU	GLN	I1400	C1336	C1336
GLN	GLN	GLY	L2189	GLN	L1985	ALA	K1857	G1796	VAL	SER	ASN	SER	T1486	R1337	R1337
MET	MET	GLY	L2189	MET	L1986	ALA	I1858	G1797	ASN	ASN	SER	THR	E1489	K1338	K1338
GLY	GLY	GLY	L2189	GLY	L1987	ALA	T1859	P1798	LEU	PRO	LEU	LEU	A1405	T1339	T1339
LYS	LYS	GLY	L2189	LYS	L1988	ALA	V1860	I1799	ALA	VAL	SER	LEU	L1490	D1340	D1340
GLY	GLY	GLY	L2189	GLY	L1989	ALA	I1861	L1800	ALA	ALA	HIS	ALA	L1492	G1342	G1342
ILE	ILE	GLY	L2189	ILE	L1990	ALA	G1862	L1801	ASN	ALA	MET	ALA	T1493	Q1343	Q1343
GLN	GLN	GLY	L2189	GLN	L1991	ALA	R1863	L1802	LYS	GLY	SER	SER	R1495	I1344	I1344
ASN	ASN	GLY	L2189	ASN	L1992	ALA	G1864	D1803	ASN	ILE	GLU	GLU	L1498	T1345	T1345
GLY	GLY	GLY	L2189	GLY	L1993	ALA	I1865	V1804	LYS	HIS	GLN	GLN	E1346	E1346	E1346
LYS	LYS	GLY	L2189	LYS	L1994	ALA	S1866	L1805	SER	PRO	GLN	GLN	D1504	H1347	H1347
GLY	GLY	GLY	L2189	GLY	L1995	ALA	T1867	I1806	ARG	SER	LEU	LEU	P1505	A1348	A1348
GLY	GLY	GLY	L2189	GLY	L1996	ALA	L1868	P1807	MET	ASP	GLN	GLN	K1416	Q1349	Q1349
GLY	GLY	GLY	L2189	GLY	L1997	ALA	M1868	T1808	ASN	VAL	VAL	VAL	D1509	S1350	S1350
GLY	GLY	GLY	L2189	GLY	L1998	ALA	R1870	G1810	PRO	ILE	LEU	LEU	L1510	L1351	L1351
GLY	GLY	GLY	L2189	GLY	L1999	ALA	A1871	L1811	GLY	PRO	GLU	GLU	E1511	V1352	V1352
GLY	GLY	GLY	L2189	GLY	L2000	ALA	K1872	D1812	SER	THR	THR	THR	M1512	L1353	L1353
GLY	GLY	GLY	L2189	GLY	L2001	ALA	L1873	L1813	GLY	LYS	LYS	LYS	S1513	D1354	D1354
GLY	GLY	GLY	L2189	GLY	L2002	ALA	P1874	A1814	GLY	THR	THR	THR	G1514	T1355	T1355
GLY	GLY	GLY	L2189	GLY	L2003	ALA	G1875	S1814	GLY	PRO	LEU	LEU	S1515	L1356	L1356
GLY	GLY	GLY	L2189	GLY	L2004	ALA	G1876	L1815	GLY	PRO	LEU	LEU	C1357	C1357	C1357
GLY	GLY	GLY	L2189	GLY	L2005	ALA	F1877	S1816	GLY	PRO	LEU	LEU	F1424	V1358	V1358
GLY	GLY	GLY	L2189	GLY	L2006	ALA	F1878	I1817	GLY	PRO	LEU	LEU	G1426	L1359	L1359
GLY	GLY	GLY	L2189	GLY	L2007	ALA	X1879	D1818	GLY	PRO	LEU	LEU	P1427	A1360	A1360
GLY	GLY	GLY	L2189	GLY	L2008	ALA	G1880	I1819	GLY	PRO	LEU	LEU	L1428	G1361	G1361
GLY	GLY	GLY	L2189	GLY	L2009	ALA	H1881	V1820	GLY	PRO	LEU	LEU	L1429	V1362	V1362
GLY	GLY	GLY	L2189	GLY	L2010	ALA	T1882	T1821	GLY	PRO	LEU	LEU	K1430	H1363	H1363
GLY	GLY	GLY	L2189	GLY	L2011	ALA	T1883	L1822	GLY	PRO	LEU	LEU	A1431	S1364	S1364
GLY	GLY	GLY	L2189	GLY	L2012	ALA	L1884	G1823	GLY	PRO	LEU	LEU	L1432	N1365	N1365
GLY	GLY	GLY	L2189	GLY	L2013	ALA	L1885	E1824	GLY	PRO	LEU	LEU	VAL	G1366	G1366
GLY	GLY	GLY	L2189	GLY	L2014	ALA	E1888	E1825	GLY	PRO	LEU	LEU	L1433	P1367	P1367
GLY	GLY	GLY	L2189	GLY	L2015	ALA	S1889	V1826	GLY	PRO	LEU	LEU	L1439	G1368	G1368
GLY	GLY	GLY	L2189	GLY	L2016	ALA	S1890	D1827	GLY	PRO	LEU	LEU	P1440	S1369	S1369
GLY	GLY	GLY	L2189	GLY	L2017	ALA	E1890	G1828	GLY	PRO	LEU	LEU	A1441	S1370	S1370
GLY	GLY	GLY	L2189	GLY	L2018	ALA	L1891	R1829	GLY	PRO	LEU	LEU	G1445	K1371	K1371
GLY	GLY	GLY	L2189	GLY	L2019	ALA	K1892	I1778	GLY	PRO	LEU	LEU	F1452	E1372	E1372
GLY	GLY	GLY	L2189	GLY	L2020	ALA	LEU	S1777	GLY	PRO	LEU	LEU	N1456	N1374	N1374
GLY	GLY	GLY	L2189	GLY	L2021	ALA	MET	P1774	GLY	PRO	LEU	LEU	Y1457	E1375	E1375
GLY	GLY	GLY	L2189	GLY	L2022	ALA	HIS	H1775	GLY	PRO	LEU	LEU	V1458	N1376	N1376
GLY	GLY	GLY	L2189	GLY	L2023	ALA	ASP	Q1776	GLY	PRO	LEU	LEU	K1459	L1377	L1377
GLY	GLY	GLY	L2189	GLY	L2024	ALA	PRO	I1776	GLY	PRO	LEU	LEU	Y1457	E1378	E1378
GLY	GLY	GLY	L2189	GLY	L2025	ALA	LEU	S1777	GLY	PRO	LEU	LEU	N1456	N1379	N1379
GLY	GLY	GLY	L2189	GLY	L2026	ALA	GLY	I1778	GLY	PRO	LEU	LEU	Y1457	E1380	E1380
GLY	GLY	GLY	L2189	GLY	L2027	ALA	GLY	I1779	GLY	PRO	LEU	LEU	V1458	N1381	N1381
GLY	GLY	GLY	L2189	GLY	L2028	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2029	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2030	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2031	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2032	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2033	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2034	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2035	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2036	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2037	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2038	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2039	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2040	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2041	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2042	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2043	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2044	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2045	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2046	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2047	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2048	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2049	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2050	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2051	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2052	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
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GLY	GLY	GLY	L2189	GLY	L2055	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
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GLY	GLY	GLY	L2189	GLY	L2059	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2060	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2061	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2062	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2063	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2064	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2065	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY	GLY	GLY	L2189	GLY	L2066	ALA	GLY	I1779	GLY	PRO	LEU	LEU	K1459	T1381	T1381
GLY															





K241	K242	N243	N244	N245	N246	A247	A248	L249	P250	V251	A252	S253	S254	V255	M256	D257	R258	L259	S260	Y261	L262	L263	P264	S265	A266	R267	P268	E269	L270	G271	V272	G273	P274	G275	R276	S277	V278	D279	R280	S281	L282	M283	Y284	S285	E286	A287	N288	R289	R290	E291	T292	F293	T294	S295	P296	H297	V298	V299	G300		
Y301	R302	W303	A304	Q305	P306	D307	P308	M309	A310	Q311	A312	G313	F314	Y315	H316	Q317	P318	A319	S320	S321	G322	D323	D324	R325	A326	M327	C328	F329	T330	C331	S332	V333	C334	L335	V336	C337	W338	E339	P340	T341	L342	E343	P344	W345	S346	E347	H348	E349	R350	H351	S352	P353	N354	C355	P356	F357	V358	K359	G360		
E361	H362	T363	Q364	N365	V366	P367	L368	V369	S370	T371	L372	A373	T374	S375	P376	A377	Q378	F379	P380	C381	L382	D383	G384	T385	L386	R387	I388	S389	C390	F391	G392	S393	G394	S395	C396	P397	H398	F399	L400	A401	A402	A403	T404	K405	R406	G407	K408	I409	C410	I411	W412	D413	V414	S415	K416	L417	M418	K419	V420		
H421	L422	K423	F424	E425	I426	M427	A428	Y429	D430	P431	A432	I433	V434	Q435	Q436	L437	I438	L439	S440	G441	ASP	PRO	SER	SER	GLY	VAL	SER	ARG	PRO	THR	ALA	GLU	TRP	LEU	GLU	SER	SER	CYS	SER	ASN	VAL	PRO	PRO	LEU	ASP	THR	LEU	GLY	ASP	LEU	GLU	GLY	ALA	SER							
ASP	SER	GLU	THR	HIS	SER	ARG	SER	SER	VAL	THR	GLY	HIS	THR	GLN	LYS	A500	M501	E502	V503	S504	L505	D506	I507	T508	A509	L510	S511	I512	ARG	S389	C390	F391	G392	S393	G394	S395	C396	P397	H398	F399	L400	A401	A402	A403	T404	K405	R406	G407	K408	I409	C410	I411	W412	D413	V414	S415	K416	L417	M418	K419	V420
ASN	PRO	CYS	LEU	THR	ASN	SER	LYS	GLU	VAL	THR	GLY	HIS	THR	GLN	LYS	A500	M501	E502	V503	S504	L505	D506	I507	T508	A509	L510	S511	I512	ARG	S389	C390	F391	G392	S393	G394	S395	C396	P397	H398	F399	L400	A401	A402	A403	T404	K405	R406	G407	K408	I409	C410	I411	W412	D413	V414	S415	K416	L417	M418	K419	V420
SER	ILE	GLU	GLY	GLY	SER	THR	ASP	ASN	GLU	SER	THR	ASN	GLU	ASN	SER	P621	L622	V623	R624	R625	T626	L627	P628	V629	L630	L631	L632	V633	S634	L635	K636	E637	P578	A579	T580	GLU	LYS	PRO	ALA	GLY	ILE	ILE	ASN	THR	GLN	GLY	MET	LYS	SER	THR	HIS	ASP	ASP								
GLY	PHE	THR	VAL	PRO	GLN	ILE	ILE	MET	LEU	SER	GLU	GLN	GLN	LEU	LEU	P621	L622	V623	R624	R625	T626	L627	P628	V629	L630	L631	L632	V633	S634	L635	K636	E637	P578	A579	T580	GLU	LYS	PRO	ALA	GLY	ILE	ILE	ASN	THR	GLN	GLY	MET	LYS	SER	THR	HIS	ASP	ASP								
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														
L722	P723	K724	F725	A726	E727	E728	E729	N730	L731	C732	I733	D734	S735	I736	P737	C739	A740	D741	G742	I743	H744	L745	L746	V747	G748	L749	R750	T751	C752	P753	V754	E755	SER	LEU	SER	ASN	SER	ALA	ILE	ASN	GLN	VAL	GLU	ALA	LEU	ASN	ARG														









LEU
MET
HIS
ASP
GLN
VAL
LYS
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SER
SER
LYS
GLU
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PRO
SER
ASP
PHE
GLN
LEU
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	136799	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	425.87997, 425.87997, 425.87997	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.17, 1.17, 1.17	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/22350	0.39	4/30362 (0.0%)
1	B	0.15	0/22350	0.39	4/30362 (0.0%)
All	All	0.15	0/44700	0.39	8/60724 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1807	PRO	CA-N-CD	-12.75	94.15	112.00
1	B	1807	PRO	CA-N-CD	-12.74	94.16	112.00
1	B	1426	PRO	CA-N-CD	-9.63	98.52	112.00
1	A	1426	PRO	CA-N-CD	-9.60	98.56	112.00
1	B	2850	VAL	N-CA-C	-5.30	108.11	113.20
1	A	2850	VAL	N-CA-C	-5.27	108.14	113.20
1	A	1807	PRO	N-CD-CG	-5.17	95.44	103.20
1	B	1807	PRO	N-CD-CG	-5.16	95.47	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21940	0	22350	343	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	21940	0	22350	334	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	43882	0	44700	658	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 7.

All (658) 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:3984:ALA:HB1	1:A:4067:ILE:H	1.52	0.74
1:B:3984:ALA:HB1	1:B:4067:ILE:H	1.51	0.72
1:A:3547:CYS:HG	1:A:3846:HIS:HE2	1.40	0.69
1:B:3547:CYS:HG	1:B:3846:HIS:HE2	1.41	0.68
1:A:2145:LEU:HD21	1:A:2167:MET:HG3	1.75	0.68
1:B:2145:LEU:HD21	1:B:2167:MET:HG3	1.75	0.67
1:B:3224:HIS:HB2	1:B:3297:LYS:HB2	1.77	0.66
1:A:3224:HIS:HB2	1:A:3297:LYS:HB2	1.77	0.66
1:A:3429:ASP:HA	1:A:3432:ILE:HD12	1.79	0.65
1:B:3429:ASP:HA	1:B:3432:ILE:HD12	1.79	0.65
1:B:1193:ASP:OD1	1:B:2565:GLN:NE2	2.30	0.65
1:A:3242:GLU:HG2	1:A:3252:PRO:HA	1.79	0.65
1:B:3242:GLU:HG2	1:B:3252:PRO:HA	1.79	0.64
1:B:343:GLU:HG2	1:B:346:SER:H	1.63	0.64
1:A:1193:ASP:OD1	1:A:2565:GLN:NE2	2.30	0.63
1:A:343:GLU:HG2	1:A:346:SER:H	1.63	0.63
1:A:1819:ILE:HD12	1:A:1853:CYS:HB2	1.80	0.63
1:A:3462:ARG:HG3	1:A:3524:LEU:HD21	1.81	0.63
1:A:1456:ASN:HD21	1:A:2033:THR:HG22	1.64	0.62
1:B:75:TYR:HB2	1:B:944:ILE:HD12	1.82	0.62
1:A:55:TRP:HE1	1:A:966:ILE:HG23	1.64	0.62
1:B:3462:ARG:HG3	1:B:3524:LEU:HD21	1.81	0.62
1:B:1819:ILE:HD12	1:B:1853:CYS:HB2	1.80	0.62
1:B:55:TRP:HE1	1:B:966:ILE:HG23	1.64	0.61
1:A:75:TYR:HB2	1:A:944:ILE:HD12	1.82	0.61
1:A:2658:GLU:HB2	1:A:2718:THR:HG22	1.82	0.61
1:B:1456:ASN:HD21	1:B:2033:THR:HG22	1.65	0.61
1:B:1853:CYS:SG	1:B:1854:ARG:N	2.74	0.61
1:B:2658:GLU:HB2	1:B:2718:THR:HG22	1.82	0.61
1:A:1980:LEU:HA	1:A:1983:GLN:HE21	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3639:LEU:HD11	1:A:3711:LEU:HG	1.82	0.61
1:B:3639:LEU:HD11	1:B:3711:LEU:HG	1.82	0.61
1:A:1853:CYS:SG	1:A:1854:ARG:N	2.74	0.60
1:B:1980:LEU:HA	1:B:1983:GLN:HE21	1.66	0.60
1:A:2397:ILE:HD12	1:B:3325:LYS:HB2	1.84	0.60
1:B:3720:CYS:SG	1:B:3721:HIS:N	2.75	0.60
1:B:1844:LEU:HD21	1:B:1847:LEU:HD21	1.85	0.59
1:A:1099:CYS:SG	1:A:1100:MET:N	2.75	0.59
1:A:1329:GLU:HB3	1:A:1380:LYS:HG3	1.85	0.59
1:B:1329:GLU:HB3	1:B:1380:LYS:HG3	1.85	0.59
1:A:2668:SER:HA	1:A:2693:VAL:HG22	1.85	0.59
1:B:3095:LEU:HD12	1:B:3348:MET:HE1	1.85	0.59
1:A:3325:LYS:HB2	1:B:2397:ILE:HD12	1.85	0.58
1:B:1813:ALA:HB2	1:B:1863:ARG:HA	1.85	0.58
1:A:1844:LEU:HD21	1:A:1847:LEU:HD21	1.85	0.58
1:A:3396:LEU:HD11	1:A:3438:LEU:HD11	1.85	0.58
1:A:3534:CYS:HA	1:A:3539:LYS:HD2	1.85	0.58
1:A:3720:CYS:SG	1:A:3721:HIS:N	2.75	0.58
1:A:417:LEU:HD23	1:A:419:LYS:HE3	1.85	0.58
1:A:2768:GLY:HA3	1:A:2831:GLY:HA2	1.86	0.58
1:B:3534:CYS:HA	1:B:3539:LYS:HD2	1.85	0.58
1:A:3095:LEU:HD12	1:A:3348:MET:HE1	1.85	0.58
1:A:1813:ALA:HB2	1:A:1863:ARG:HA	1.85	0.58
1:B:1452:PHE:O	1:B:1456:ASN:ND2	2.36	0.58
1:B:3396:LEU:HD11	1:B:3438:LEU:HD11	1.85	0.58
1:B:2768:GLY:HA3	1:B:2831:GLY:HA2	1.86	0.57
1:A:1829:ARG:NH2	1:A:1852:VAL:O	2.38	0.57
1:A:1771:GLN:NE2	1:A:1983:GLN:OE1	2.35	0.57
1:B:1099:CYS:SG	1:B:1100:MET:N	2.75	0.57
1:B:2668:SER:HA	1:B:2693:VAL:HG22	1.85	0.57
1:B:1328:HIS:HA	1:B:1331:LEU:HD12	1.87	0.57
1:A:1799:ILE:HD11	1:A:1882:THR:HA	1.87	0.57
1:B:2349:ASP:N	1:B:2349:ASP:OD1	2.38	0.57
1:B:1829:ARG:NH2	1:B:1852:VAL:O	2.38	0.56
1:A:1328:HIS:HA	1:A:1331:LEU:HD12	1.86	0.56
1:A:2180:ASP:OD1	1:A:2356:LYS:NZ	2.38	0.56
1:B:417:LEU:HD23	1:B:419:LYS:HE3	1.85	0.56
1:A:3242:GLU:HB2	1:A:3279:CYS:HB3	1.88	0.56
1:A:3396:LEU:HA	1:A:3399:ILE:HG12	1.87	0.56
1:A:630:LEU:HD12	1:A:720:LEU:HD22	1.88	0.56
1:B:3396:LEU:HA	1:B:3399:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3627:LEU:HD12	1:A:3698:ILE:HD12	1.88	0.56
1:B:1015:GLN:HG3	1:B:1021:ILE:HD13	1.87	0.56
1:A:2349:ASP:OD1	1:A:2349:ASP:N	2.38	0.56
1:A:1452:PHE:O	1:A:1456:ASN:ND2	2.36	0.56
1:B:630:LEU:HD12	1:B:720:LEU:HD22	1.88	0.56
1:B:3242:GLU:HB2	1:B:3279:CYS:HB3	1.88	0.56
1:B:1883:TYR:O	1:B:1993:ARG:NH2	2.39	0.56
1:B:1494:THR:HG21	1:B:2111:ILE:HG22	1.88	0.56
1:B:1557:LEU:HD22	1:B:1805:LEU:HD13	1.87	0.56
1:B:3774:HIS:HB3	1:B:3777:ASN:HB2	1.88	0.56
1:A:1015:GLN:HG3	1:A:1021:ILE:HD13	1.87	0.55
1:A:1494:THR:HG21	1:A:2111:ILE:HG22	1.88	0.55
1:A:1883:TYR:O	1:A:1993:ARG:NH2	2.39	0.55
1:B:1799:ILE:HD11	1:B:1882:THR:HA	1.87	0.55
1:B:3716:LEU:HD13	1:B:3788:LEU:HD11	1.88	0.55
1:A:1429:LEU:HD23	1:A:1433:LEU:HD23	1.88	0.55
1:A:1885:LEU:HB2	1:A:1888:GLU:HG3	1.89	0.55
1:B:1885:LEU:HB2	1:B:1888:GLU:HG3	1.89	0.55
1:B:3627:LEU:HD12	1:B:3698:ILE:HD12	1.88	0.55
1:B:1817:ILE:HD11	1:B:1856:MET:HE3	1.89	0.55
1:A:1557:LEU:HD22	1:A:1805:LEU:HD13	1.87	0.55
1:A:1817:ILE:HD11	1:A:1856:MET:HE3	1.89	0.55
1:A:3716:LEU:HD13	1:A:3788:LEU:HD11	1.88	0.55
1:A:3774:HIS:HB3	1:A:3777:ASN:HB2	1.88	0.55
1:B:1771:GLN:NE2	1:B:1983:GLN:OE1	2.35	0.55
1:A:576:LYS:HE3	1:A:624:ARG:HE	1.72	0.55
1:B:1429:LEU:HD23	1:B:1433:LEU:HD23	1.88	0.55
1:A:2374:ILE:HG22	1:A:2375:VAL:HG13	1.88	0.54
1:A:2384:LEU:HB3	1:A:2646:LEU:HD11	1.89	0.54
1:A:1346:GLU:HA	1:A:1349:GLN:HE21	1.73	0.54
1:B:576:LYS:HE3	1:B:624:ARG:HE	1.72	0.54
1:B:2374:ILE:HG22	1:B:2375:VAL:HG13	1.88	0.54
1:B:2384:LEU:HB3	1:B:2646:LEU:HD11	1.89	0.54
1:A:2336:VAL:HG22	1:A:2358:LEU:HD11	1.90	0.54
1:A:2582:MET:HA	1:A:2585:MET:HG3	1.90	0.54
1:A:1124:LEU:HB3	1:A:1183:CYS:HB2	1.89	0.54
1:B:2582:MET:HA	1:B:2585:MET:HG3	1.90	0.54
1:A:3700:LYS:NZ	1:A:3769:GLN:O	2.41	0.54
1:B:514:GLN:HA	1:B:837:VAL:HG21	1.90	0.54
1:B:1806:ILE:HB	1:B:1842:LEU:HB3	1.90	0.54
1:A:3209:ASP:OD1	1:A:3209:ASP:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:VAL:HG23	1:A:263:LEU:HD13	1.91	0.53
1:A:2084:GLN:NE2	1:A:2600:ASN:O	2.41	0.53
1:A:2566:ALA:O	1:A:2584:LYS:NZ	2.41	0.53
1:B:1124:LEU:HB3	1:B:1183:CYS:HB2	1.89	0.53
1:B:1346:GLU:HA	1:B:1349:GLN:HE21	1.73	0.53
1:B:2775:ASN:O	1:B:2777:HIS:ND1	2.42	0.53
1:A:239:LEU:HD23	1:A:242:ILE:HD11	1.91	0.53
1:B:239:LEU:HD23	1:B:242:ILE:HD11	1.91	0.53
1:B:2084:GLN:NE2	1:B:2600:ASN:O	2.41	0.53
1:B:2934:LEU:HA	1:B:2942:ALA:HA	1.90	0.53
1:B:3700:LYS:NZ	1:B:3769:GLN:O	2.41	0.53
1:B:3616:SER:O	1:B:3616:SER:OG	2.26	0.53
1:A:3828:SER:HB2	1:A:4006:VAL:HB	1.91	0.53
1:B:3450:ILE:HA	1:B:3453:LEU:HD12	1.90	0.53
1:A:514:GLN:HA	1:A:837:VAL:HG21	1.90	0.53
1:A:2826:PHE:O	1:A:2915:ARG:NH2	2.42	0.53
1:B:2336:VAL:HG22	1:B:2358:LEU:HD11	1.90	0.53
1:A:1806:ILE:HB	1:A:1842:LEU:HB3	1.90	0.52
1:A:2775:ASN:O	1:A:2777:HIS:ND1	2.42	0.52
1:A:2713:ASN:HB2	1:B:2869:HIS:CE1	2.45	0.52
1:A:2934:LEU:HA	1:A:2942:ALA:HA	1.90	0.52
1:B:2777:HIS:CD2	1:B:2778:SER:H	2.28	0.52
1:B:2826:PHE:O	1:B:2915:ARG:NH2	2.42	0.52
1:B:154:VAL:HG23	1:B:263:LEU:HD13	1.91	0.52
1:A:80:ASN:HD21	1:A:948:GLY:HA3	1.75	0.52
1:B:1100:MET:HE1	1:B:1315:ARG:HG3	1.90	0.52
1:B:3828:SER:HB2	1:B:4006:VAL:HB	1.91	0.52
1:A:1100:MET:HE1	1:A:1315:ARG:HG3	1.91	0.52
1:A:2813:LEU:HD12	1:A:2851:VAL:HG11	1.92	0.52
1:A:2777:HIS:CD2	1:A:2778:SER:H	2.28	0.51
1:B:80:ASN:HD21	1:B:948:GLY:HA3	1.75	0.51
1:B:1556:SER:HB2	1:B:1843:ILE:HG21	1.92	0.51
1:A:2688:ALA:O	1:A:2731:ASN:ND2	2.43	0.51
1:B:2927:ASN:HB2	1:B:3039:ILE:HG22	1.92	0.51
1:A:2869:HIS:CE1	1:B:2713:ASN:HB2	2.46	0.51
1:B:2121:LEU:HD23	1:B:2124:ILE:HD11	1.92	0.51
1:B:2813:LEU:HD12	1:B:2851:VAL:HG11	1.92	0.51
1:A:1556:SER:HB2	1:A:1843:ILE:HG21	1.92	0.51
1:B:1917:MET:HB3	1:B:1991:VAL:HG12	1.93	0.51
1:B:2688:ALA:O	1:B:2731:ASN:ND2	2.43	0.51
1:B:3494:LEU:HB2	1:B:3541:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:LYS:HB2	1:A:1182:LEU:HD12	1.92	0.51
1:A:1182:LEU:HD13	1:A:1208:LEU:HD23	1.92	0.51
1:A:3169:ILE:HB	1:A:3183:LEU:HD11	1.93	0.51
1:B:3512:ASP:OD1	1:B:3512:ASP:N	2.40	0.51
1:A:2416:LEU:HD21	1:A:2639:LEU:HD11	1.93	0.51
1:A:2927:ASN:HB2	1:A:3039:ILE:HG22	1.92	0.51
1:B:1126:LYS:HB2	1:B:1182:LEU:HD12	1.92	0.51
1:B:3002:ASN:ND2	1:B:3321:ASP:OD2	2.42	0.51
1:A:1364:SER:HA	1:A:1414:ASN:HD22	1.76	0.51
1:A:3401:LEU:HD11	1:A:3453:LEU:HD23	1.93	0.51
1:A:3494:LEU:HB2	1:A:3541:ALA:HB1	1.92	0.51
1:A:3819:ASP:OD1	1:A:3819:ASP:N	2.43	0.51
1:B:2390:THR:HB	1:B:2656:GLN:HG2	1.93	0.51
1:A:2121:LEU:HD23	1:A:2124:ILE:HD11	1.92	0.51
1:A:4068:GLN:O	1:A:4072:GLN:NE2	2.40	0.51
1:B:1356:LEU:HD23	1:B:1359:LEU:HD21	1.92	0.51
1:A:914:ILE:HB	1:A:924:ALA:HB3	1.93	0.51
1:A:3450:ILE:HA	1:A:3453:LEU:HD12	1.91	0.51
1:B:3401:LEU:HD11	1:B:3453:LEU:HD23	1.93	0.51
1:A:2175:VAL:HG23	1:A:2357:VAL:HG21	1.93	0.50
1:B:1364:SER:HA	1:B:1414:ASN:HD22	1.76	0.50
1:B:2416:LEU:HD21	1:B:2639:LEU:HD11	1.93	0.50
1:A:945:TYR:OH	1:A:950:ASP:OD1	2.28	0.50
1:A:1356:LEU:HD23	1:A:1359:LEU:HD21	1.92	0.50
1:A:2390:THR:HB	1:A:2656:GLN:HG2	1.93	0.50
1:B:289:ARG:O	1:B:292:THR:OG1	2.29	0.50
1:A:2880:ARG:HA	1:A:2880:ARG:HH11	1.76	0.50
1:B:2566:ALA:O	1:B:2584:LYS:NZ	2.40	0.50
1:B:153:PRO:HG3	1:B:376:PRO:HB2	1.93	0.50
1:A:3262:LEU:HD11	1:B:3286:ARG:HH21	1.76	0.50
1:A:3616:SER:O	1:A:3616:SER:OG	2.26	0.50
1:B:3169:ILE:HB	1:B:3183:LEU:HD11	1.93	0.50
1:B:914:ILE:HB	1:B:924:ALA:HB3	1.93	0.50
1:A:95:ASP:OD2	1:A:212:LYS:NZ	2.45	0.50
1:A:163:LEU:HD11	1:A:255:VAL:HG13	1.94	0.50
1:A:2872:THR:HG22	1:A:3000:LEU:HD12	1.94	0.50
1:B:163:LEU:HD11	1:B:255:VAL:HG13	1.94	0.50
1:B:1331:LEU:HD22	1:B:1352:VAL:HG23	1.94	0.50
1:B:2006:SER:HG	1:B:2009:SER:HG	1.52	0.50
1:A:164:GLU:HG3	1:A:258:ARG:HH12	1.77	0.50
1:A:1917:MET:HB3	1:A:1991:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2389:GLY:HA2	1:B:2655:VAL:HA	1.94	0.50
1:A:289:ARG:O	1:A:292:THR:OG1	2.29	0.49
1:A:3429:ASP:OD2	1:A:3853:HIS:ND1	2.42	0.49
1:B:1182:LEU:HD13	1:B:1208:LEU:HD23	1.93	0.49
1:A:2389:GLY:HA2	1:A:2655:VAL:HA	1.94	0.49
1:B:1914:LEU:HD12	1:B:1994:LEU:HB3	1.92	0.49
1:A:1122:VAL:HG22	1:A:1224:VAL:HG22	1.94	0.49
1:B:3124:SER:OG	1:B:3125:MET:N	2.45	0.49
1:B:3209:ASP:OD1	1:B:3209:ASP:N	2.36	0.49
1:A:153:PRO:HG3	1:A:376:PRO:HB2	1.93	0.49
1:A:3286:ARG:HH21	1:B:3262:LEU:HD11	1.78	0.49
1:B:2180:ASP:OD1	1:B:2356:LYS:NZ	2.38	0.49
1:B:2872:THR:HG22	1:B:3000:LEU:HD12	1.94	0.49
1:A:1914:LEU:HD12	1:A:1994:LEU:HB3	1.92	0.49
1:B:1510:LEU:HB3	1:B:1560:LEU:HB2	1.95	0.49
1:B:2690:ARG:O	1:B:2731:ASN:ND2	2.45	0.49
1:B:164:GLU:HG3	1:B:258:ARG:HH12	1.77	0.49
1:B:1335:LEU:HB3	1:B:1388:ILE:HG22	1.94	0.49
1:B:3778:GLN:HG2	1:B:4070:PRO:HG3	1.95	0.49
1:B:4173:VAL:HG11	1:B:4220:LEU:HB2	1.94	0.49
1:A:3002:ASN:ND2	1:A:3321:ASP:OD2	2.42	0.49
1:B:749:LEU:HD12	1:B:824:TYR:HB2	1.95	0.49
1:B:2713:ASN:OD1	1:B:2772:HIS:ND1	2.37	0.49
1:B:2852:SER:HA	1:B:2940:TYR:HA	1.95	0.49
1:B:3429:ASP:OD2	1:B:3853:HIS:ND1	2.42	0.49
1:A:2690:ARG:O	1:A:2731:ASN:ND2	2.45	0.49
1:B:240:LYS:NZ	1:B:284:TYR:OH	2.45	0.49
1:B:1101:VAL:HA	1:B:1305:ARG:HH21	1.78	0.49
1:B:2354:VAL:O	1:B:2358:LEU:HB2	2.13	0.49
1:B:3819:ASP:N	1:B:3819:ASP:OD1	2.43	0.49
1:B:137:ARG:NH2	1:B:148:THR:O	2.46	0.49
1:B:2880:ARG:HH11	1:B:2880:ARG:HA	1.76	0.49
1:B:2175:VAL:HG23	1:B:2357:VAL:HG21	1.93	0.48
1:A:1510:LEU:HB3	1:A:1560:LEU:HB2	1.95	0.48
1:A:3773:CYS:O	1:A:3991:TYR:OH	2.30	0.48
1:A:3778:GLN:HG2	1:A:4070:PRO:HG3	1.95	0.48
1:B:1075:ARG:HH21	1:B:1077:TRP:HZ2	1.61	0.48
1:A:240:LYS:NZ	1:A:284:TYR:OH	2.45	0.48
1:A:1075:ARG:HH21	1:A:1077:TRP:HZ2	1.61	0.48
1:A:1335:LEU:HB3	1:A:1388:ILE:HG22	1.94	0.48
1:A:1505:PRO:O	1:A:1985:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2755:ASP:OD1	1:A:2755:ASP:N	2.46	0.48
1:A:1331:LEU:HD22	1:A:1352:VAL:HG23	1.94	0.48
1:A:4173:VAL:HG11	1:A:4220:LEU:HB2	1.94	0.48
1:B:1505:PRO:O	1:B:1985:ASN:ND2	2.46	0.48
1:A:3039:ILE:O	1:A:3043:LEU:HB2	2.13	0.48
1:B:2755:ASP:OD1	1:B:2755:ASP:N	2.46	0.48
1:B:1122:VAL:HG22	1:B:1224:VAL:HG22	1.94	0.48
1:A:1101:VAL:HA	1:A:1305:ARG:HH21	1.78	0.48
1:A:2354:VAL:O	1:A:2358:LEU:HB2	2.13	0.48
1:A:2371:LEU:HA	1:A:2374:ILE:HB	1.95	0.48
1:A:2852:SER:HA	1:A:2940:TYR:HA	1.95	0.48
1:A:4060:SER:N	1:A:4063:GLU:OE1	2.47	0.48
1:B:2371:LEU:HA	1:B:2374:ILE:HB	1.95	0.48
1:A:3755:GLN:O	1:A:3759:ILE:HG12	2.14	0.48
1:A:1938:LEU:O	1:A:1941:SER:OG	2.30	0.48
1:A:2601:THR:OG1	1:A:2602:SER:N	2.47	0.48
1:B:2820:SER:HB3	1:B:2826:PHE:HD2	1.79	0.48
1:B:3755:GLN:O	1:B:3759:ILE:HG12	2.14	0.48
1:A:137:ARG:NH2	1:A:148:THR:O	2.46	0.48
1:A:3338:LEU:HD12	1:A:3381:VAL:HG23	1.96	0.48
1:B:3196:ALA:HB3	1:B:3294:SER:HA	1.96	0.48
1:B:3443:ASP:OD1	1:B:3446:THR:OG1	2.27	0.48
1:A:1027:GLU:HA	1:A:1030:ARG:HE	1.79	0.47
1:A:1359:LEU:HA	1:A:1362:VAL:HG22	1.96	0.47
1:A:1398:ARG:NH1	1:A:1846:ASP:OD1	2.47	0.47
1:B:3039:ILE:O	1:B:3043:LEU:HB2	2.13	0.47
1:B:3338:LEU:HD12	1:B:3381:VAL:HG23	1.96	0.47
1:B:1791:VAL:HG23	1:B:1858:ILE:HB	1.97	0.47
1:B:157:GLN:HB3	1:B:226:HIS:HB3	1.96	0.47
1:B:1359:LEU:HA	1:B:1362:VAL:HG22	1.96	0.47
1:B:1412:ILE:HD13	1:B:1424:PHE:HB3	1.96	0.47
1:B:4260:ARG:NH1	1:B:4367:SER:O	2.47	0.47
1:B:4441:LYS:HE3	1:B:4482:GLN:HG2	1.96	0.47
1:A:749:LEU:HD12	1:A:824:TYR:HB2	1.95	0.47
1:A:2820:SER:HB3	1:A:2826:PHE:HD2	1.79	0.47
1:A:3124:SER:OG	1:A:3125:MET:N	2.45	0.47
1:A:4441:LYS:HE3	1:A:4482:GLN:HG2	1.96	0.47
1:B:2362:ALA:HA	1:B:2369:ILE:HD12	1.97	0.47
1:A:147:ASP:OD2	1:A:218:THR:OG1	2.32	0.47
1:A:916:ASP:HB2	1:A:923:LEU:HD11	1.97	0.47
1:A:1353:LEU:HD21	1:A:1404:CYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2697:ASN:OD1	1:A:2698:GLN:N	2.48	0.47
1:A:3481:THR:HA	1:B:2162:VAL:HG13	1.96	0.47
1:B:95:ASP:OD2	1:B:212:LYS:NZ	2.45	0.47
1:B:215:LYS:HD2	1:B:215:LYS:HA	1.73	0.47
1:B:2687:ASN:HB3	1:B:2690:ARG:HG3	1.97	0.47
1:B:2750:HIS:O	1:B:2754:SER:OG	2.33	0.47
1:A:323:ASP:OD1	1:A:323:ASP:N	2.42	0.47
1:A:3623:ILE:HG23	1:A:3698:ILE:HD11	1.95	0.47
1:B:147:ASP:OD2	1:B:218:THR:OG1	2.32	0.47
1:B:945:TYR:OH	1:B:950:ASP:OD1	2.28	0.47
1:B:1398:ARG:NH1	1:B:1846:ASP:OD1	2.47	0.47
1:B:2601:THR:OG1	1:B:2602:SER:N	2.47	0.47
1:A:513:LEU:HD11	1:A:568:LEU:HD22	1.96	0.47
1:A:1811:ASP:HA	1:A:1863:ARG:HD3	1.96	0.47
1:A:2162:VAL:HG13	1:B:3481:THR:HA	1.96	0.47
1:A:2697:ASN:OD1	1:A:2699:ALA:N	2.45	0.47
1:A:2726:LEU:HD22	1:A:2752:LEU:HD21	1.97	0.47
1:A:3196:ALA:HB3	1:A:3294:SER:HA	1.96	0.47
1:A:3709:ASN:HD21	1:A:3780:LEU:HD21	1.79	0.47
1:A:3967:LEU:HD12	1:A:4004:LEU:HB3	1.97	0.47
1:B:513:LEU:HD11	1:B:568:LEU:HD22	1.96	0.47
1:B:912:VAL:HB	1:B:926:VAL:HB	1.96	0.47
1:B:1378:LEU:HD13	1:B:1382:ARG:HH21	1.79	0.47
1:B:2697:ASN:OD1	1:B:2698:GLN:N	2.48	0.47
1:A:1331:LEU:O	1:A:1334:THR:OG1	2.31	0.47
1:A:4260:ARG:NH1	1:A:4367:SER:O	2.47	0.47
1:B:123:VAL:HB	1:B:125:LYS:HZ3	1.80	0.47
1:B:2579:ALA:HA	1:B:2582:MET:HE2	1.97	0.47
1:B:3709:ASN:HD21	1:B:3780:LEU:HD21	1.79	0.47
1:A:1791:VAL:HG23	1:A:1858:ILE:HB	1.96	0.47
1:B:1027:GLU:HA	1:B:1030:ARG:HE	1.79	0.47
1:A:2834:ASP:OD1	1:A:2834:ASP:N	2.47	0.47
1:A:4396:LEU:HB3	1:A:4484:THR:HG21	1.97	0.47
1:B:1353:LEU:HD21	1:B:1404:CYS:HB2	1.96	0.47
1:B:2726:LEU:HD22	1:B:2752:LEU:HD21	1.97	0.47
1:B:3433:ASP:OD2	1:B:3853:HIS:NE2	2.48	0.47
1:B:4060:SER:N	1:B:4063:GLU:OE1	2.47	0.47
1:A:157:GLN:HB3	1:A:226:HIS:HB3	1.96	0.46
1:A:912:VAL:HB	1:A:926:VAL:HB	1.97	0.46
1:A:1077:TRP:HB2	1:A:1299:VAL:HG12	1.97	0.46
1:A:1213:ALA:HA	1:A:1315:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2109:LEU:H	1:A:2109:LEU:HD23	1.81	0.46
1:A:3433:ASP:OD2	1:A:3853:HIS:NE2	2.48	0.46
1:B:174:LEU:HD22	1:B:200:LEU:HD12	1.98	0.46
1:B:916:ASP:HB2	1:B:923:LEU:HD11	1.97	0.46
1:B:1504:ASP:O	1:B:1981:GLN:NE2	2.44	0.46
1:B:1811:ASP:HA	1:B:1863:ARG:HD3	1.96	0.46
1:B:3279:CYS:SG	1:B:3281:ARG:NH1	2.89	0.46
1:A:4244:LEU:HA	1:A:4247:ILE:HG22	1.97	0.46
1:B:1091:PHE:HB2	1:B:1222:ILE:HG13	1.97	0.46
1:A:3279:CYS:SG	1:A:3281:ARG:NH1	2.89	0.46
1:B:1302:THR:HG21	1:B:1304:ARG:HH21	1.80	0.46
1:B:3623:ILE:HG23	1:B:3698:ILE:HD11	1.95	0.46
1:B:3967:LEU:HD12	1:B:4004:LEU:HB3	1.97	0.46
1:A:1091:PHE:HB2	1:A:1222:ILE:HG13	1.97	0.46
1:A:1378:LEU:HD13	1:A:1382:ARG:HH21	1.79	0.46
1:A:3856:ARG:HD2	1:A:3856:ARG:HA	1.75	0.46
1:B:1089:HIS:HB2	1:B:1224:VAL:HB	1.98	0.46
1:A:174:LEU:HD22	1:A:200:LEU:HD12	1.98	0.46
1:A:1412:ILE:HD13	1:A:1424:PHE:HB3	1.96	0.46
1:A:2926:VAL:HA	1:A:2929:LEU:HB2	1.97	0.46
1:B:323:ASP:OD1	1:B:323:ASP:N	2.43	0.46
1:B:900:LEU:HB2	1:B:917:LEU:HB3	1.98	0.46
1:B:1569:THR:OG1	1:B:1794:ASP:O	2.34	0.46
1:B:2834:ASP:OD1	1:B:2834:ASP:N	2.47	0.46
1:A:1439:LEU:HD22	1:A:2026:ILE:HD11	1.98	0.46
1:A:2687:ASN:HB3	1:A:2690:ARG:HG3	1.97	0.46
1:B:1782:ARG:O	1:B:1789:ARG:NH2	2.48	0.46
1:B:2863:VAL:HG11	1:B:2926:VAL:HG11	1.98	0.46
1:B:4244:LEU:HA	1:B:4247:ILE:HG22	1.97	0.46
1:A:1089:HIS:HB2	1:A:1224:VAL:HB	1.98	0.46
1:A:2362:ALA:HA	1:A:2369:ILE:HD12	1.97	0.46
1:A:4153:ILE:HG23	1:A:4210:PRO:HG3	1.98	0.46
1:A:3846:HIS:CD2	1:A:3847:PRO:HD2	2.51	0.46
1:B:1439:LEU:HD22	1:B:2026:ILE:HD11	1.98	0.46
1:B:4396:LEU:HB3	1:B:4484:THR:HG21	1.97	0.46
1:A:1490:ALA:O	1:A:1494:THR:HG23	2.15	0.46
1:A:2671:SER:O	1:A:2690:ARG:NH1	2.49	0.46
1:A:2863:VAL:HG11	1:A:2926:VAL:HG11	1.98	0.46
1:B:2204:ILE:HD13	1:B:2356:LYS:HD2	1.98	0.46
1:B:3846:HIS:CD2	1:B:3847:PRO:HD2	2.51	0.46
1:A:2579:ALA:HA	1:A:2582:MET:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2750:HIS:O	1:A:2754:SER:OG	2.33	0.45
1:B:1490:ALA:O	1:B:1494:THR:HG23	2.15	0.45
1:B:2109:LEU:HD23	1:B:2109:LEU:H	1.80	0.45
1:B:3502:TRP:HH2	1:B:3619:SER:HB3	1.81	0.45
1:A:900:LEU:HB2	1:A:917:LEU:HB3	1.98	0.45
1:B:4068:GLN:O	1:B:4072:GLN:NE2	2.40	0.45
1:A:3684:ALA:HB2	1:A:3759:ILE:HD13	1.99	0.45
1:B:1388:ILE:HA	1:B:1391:VAL:HG22	1.99	0.45
1:B:1456:ASN:HA	1:B:1459:LYS:HD3	1.99	0.45
1:B:3817:LEU:HD11	1:B:4185:LEU:HD23	1.98	0.45
1:A:245:ASN:ND2	1:A:361:GLU:OE1	2.50	0.45
1:A:2173:MET:HE1	1:B:3129:ILE:HG13	1.98	0.45
1:A:3225:ILE:HB	1:A:3265:ILE:HB	1.98	0.45
1:B:3331:LEU:HD21	1:B:3378:ILE:HG23	1.98	0.45
1:A:1302:THR:HG21	1:A:1304:ARG:HH21	1.80	0.45
1:B:245:ASN:ND2	1:B:361:GLU:OE1	2.50	0.45
1:B:1077:TRP:HB2	1:B:1299:VAL:HG12	1.97	0.45
1:B:1213:ALA:HA	1:B:1315:ARG:HD3	1.97	0.45
1:B:3530:MET:HE2	1:B:3609:HIS:CD2	2.52	0.45
1:A:324:ASP:OD1	1:A:324:ASP:N	2.50	0.45
1:A:1489:GLU:HA	1:A:1492:LEU:HD12	1.98	0.45
1:B:1780:ILE:HD11	1:B:1873:ILE:HD11	1.99	0.45
1:A:391:PHE:HA	1:A:510:LEU:HD12	1.99	0.45
1:A:1388:ILE:HA	1:A:1391:VAL:HG22	1.99	0.45
1:B:2926:VAL:HA	1:B:2929:LEU:HB2	1.97	0.45
1:A:3530:MET:HE2	1:A:3609:HIS:CD2	2.52	0.45
1:B:94:ILE:HG12	1:B:101:THR:HG23	1.99	0.45
1:B:4153:ILE:HG23	1:B:4210:PRO:HG3	1.98	0.45
1:A:116:LYS:HE2	1:A:116:LYS:HB2	1.86	0.45
1:A:2655:VAL:HG11	1:A:2660:LEU:HD12	1.99	0.45
1:B:3684:ALA:HB2	1:B:3759:ILE:HD13	1.99	0.45
1:A:162:GLN:OE1	1:A:222:HIS:ND1	2.48	0.45
1:A:1504:ASP:O	1:A:1981:GLN:NE2	2.44	0.45
1:A:2028:ARG:HB2	1:A:2074:ILE:HG22	1.99	0.45
1:A:2204:ILE:HD13	1:A:2356:LYS:HD2	1.98	0.45
1:A:2368:THR:HG21	1:A:2418:GLY:HA3	1.99	0.45
1:A:2713:ASN:HD21	1:A:2772:HIS:HB3	1.82	0.45
1:B:2655:VAL:HG11	1:B:2660:LEU:HD12	1.99	0.45
1:B:3220:LEU:HD21	1:B:3223:ILE:HD11	1.99	0.45
1:A:1015:GLN:HG3	1:A:1021:ILE:HG21	1.99	0.44
1:A:3817:LEU:HD11	1:A:4185:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2713:ASN:HD21	1:B:2772:HIS:HB3	1.82	0.44
1:A:3258:VAL:HG23	1:B:2777:HIS:CD2	2.53	0.44
1:A:3502:TRP:HH2	1:A:3619:SER:HB3	1.81	0.44
1:A:1473:LEU:HB3	1:A:2030:LEU:HD11	1.99	0.44
1:A:1809:CYS:H	1:A:1837:ILE:HG22	1.82	0.44
1:A:3602:PRO:HB2	1:A:3603:LEU:H	1.59	0.44
1:B:1473:LEU:HB3	1:B:2030:LEU:HD11	1.99	0.44
1:A:144:LEU:HD12	1:A:216:TRP:HH2	1.82	0.44
1:A:1557:LEU:HD11	1:A:1803:ASP:HB3	2.00	0.44
1:A:2039:HIS:HB2	1:A:2597:ALA:HB2	1.99	0.44
1:A:2771:PRO:HG2	1:B:2869:HIS:HE1	1.82	0.44
1:B:3773:CYS:O	1:B:3991:TYR:OH	2.30	0.44
1:A:1456:ASN:HA	1:A:1459:LYS:HD3	1.98	0.44
1:A:1569:THR:OG1	1:A:1794:ASP:O	2.34	0.44
1:A:2985:LEU:HD13	1:A:3052:MET:HG3	2.00	0.44
1:A:3220:LEU:HD21	1:A:3223:ILE:HD11	1.99	0.44
1:B:1429:LEU:HD11	1:B:1462:ASP:H	1.83	0.44
1:B:2671:SER:O	1:B:2690:ARG:NH1	2.49	0.44
1:B:2985:LEU:HD13	1:B:3052:MET:HG3	2.00	0.44
1:B:3526:PHE:O	1:B:3530:MET:HG2	2.18	0.44
1:A:2324:ALA:HB3	1:A:2327:ARG:HE	1.82	0.44
1:B:1489:GLU:HA	1:B:1492:LEU:HD12	1.98	0.44
1:B:1809:CYS:H	1:B:1837:ILE:HG22	1.82	0.44
1:B:3225:ILE:HB	1:B:3265:ILE:HB	1.98	0.44
1:A:1377:LEU:O	1:A:1381:THR:OG1	2.34	0.44
1:A:1429:LEU:HD11	1:A:1462:ASP:H	1.83	0.44
1:A:1780:ILE:HD11	1:A:1873:ILE:HD11	1.99	0.44
1:A:2027:ILE:HD13	1:A:2066:LEU:HD21	1.99	0.44
1:A:2366:ARG:HA	1:A:2366:ARG:HD3	1.85	0.44
1:A:3129:ILE:HG13	1:B:2173:MET:HE1	1.98	0.44
1:B:2039:HIS:HB2	1:B:2597:ALA:HB2	1.99	0.44
1:A:3331:LEU:HD21	1:A:3378:ILE:HG23	1.98	0.44
1:B:1943:ASP:OD1	1:B:1943:ASP:N	2.51	0.44
1:B:2028:ARG:HB2	1:B:2074:ILE:HG22	1.99	0.44
1:A:94:ILE:HG12	1:A:101:THR:HG23	1.99	0.44
1:A:1943:ASP:OD1	1:A:1943:ASP:N	2.51	0.44
1:A:3813:LEU:HA	1:A:3817:LEU:HD22	2.00	0.44
1:A:3547:CYS:HB2	1:A:3616:SER:HA	2.00	0.43
1:A:1782:ARG:O	1:A:1789:ARG:NH2	2.48	0.43
1:A:2713:ASN:OD1	1:A:2772:HIS:ND1	2.37	0.43
1:B:1767:SER:HB3	1:B:1920:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2820:SER:HA	1:A:2826:PHE:HB2	2.01	0.43
1:A:4080:LEU:HD12	1:A:4165:LEU:HD13	2.00	0.43
1:B:827:LEU:HB3	1:B:845:LYS:HB3	2.01	0.43
1:B:1026:VAL:HG21	1:B:1351:LEU:HD22	2.01	0.43
1:B:1563:VAL:HG12	1:B:1879:TYR:HD1	1.83	0.43
1:B:2027:ILE:HD13	1:B:2066:LEU:HD21	1.99	0.43
1:B:2324:ALA:HB3	1:B:2327:ARG:HE	1.82	0.43
1:B:3179:ALA:HB1	1:B:3182:LEU:HD12	2.01	0.43
1:B:3679:THR:OG1	1:B:3680:ALA:N	2.51	0.43
1:A:2717:ARG:NH2	1:B:2876:LYS:HB3	2.33	0.43
1:A:3111:MET:HE1	1:A:3334:LEU:HD12	2.00	0.43
1:A:3512:ASP:OD1	1:A:3512:ASP:N	2.40	0.43
1:A:3526:PHE:O	1:A:3530:MET:HG2	2.18	0.43
1:A:3981:MET:HE1	1:A:3989:LEU:HD12	2.01	0.43
1:B:2368:THR:HG21	1:B:2418:GLY:HA3	1.99	0.43
1:B:2864:THR:HA	1:B:2867:VAL:HG12	2.00	0.43
1:B:3521:LEU:HD23	1:B:3525:LEU:HD13	2.01	0.43
1:B:3813:LEU:HD22	1:B:4189:LEU:HD22	2.01	0.43
1:B:4184:LEU:HD11	1:B:4212:LEU:HB3	2.01	0.43
1:A:1380:LYS:HA	1:A:1380:LYS:HD3	1.87	0.43
1:A:2869:HIS:HE1	1:B:2771:PRO:HG2	1.83	0.43
1:A:3521:LEU:HD23	1:A:3525:LEU:HD13	2.01	0.43
1:B:144:LEU:HD12	1:B:216:TRP:HH2	1.82	0.43
1:B:391:PHE:HA	1:B:510:LEU:HD12	1.99	0.43
1:B:1015:GLN:HG3	1:B:1021:ILE:HG21	1.99	0.43
1:B:3856:ARG:HD2	1:B:3856:ARG:HA	1.75	0.43
1:A:2876:LYS:HB3	1:B:2717:ARG:NH2	2.34	0.43
1:A:3756:ARG:HE	1:A:3756:ARG:HB3	1.64	0.43
1:B:324:ASP:OD1	1:B:324:ASP:N	2.50	0.43
1:B:2820:SER:HA	1:B:2826:PHE:HB2	2.01	0.43
1:A:1026:VAL:HG21	1:A:1351:LEU:HD22	2.01	0.43
1:B:3981:MET:HE1	1:B:3989:LEU:HD12	2.01	0.43
1:A:568:LEU:HD11	1:A:630:LEU:HB3	2.01	0.43
1:A:827:LEU:HB3	1:A:845:LYS:HB3	2.00	0.43
1:A:1777:SER:HA	1:A:1874:PRO:HA	2.01	0.43
1:A:3813:LEU:HD22	1:A:4189:LEU:HD22	2.01	0.43
1:B:1498:LEU:HD13	1:B:1974:TYR:CG	2.54	0.43
1:B:3813:LEU:HA	1:B:3817:LEU:HD22	2.00	0.43
1:A:2777:HIS:CD2	1:B:3258:VAL:HG23	2.54	0.43
1:B:162:GLN:OE1	1:B:222:HIS:ND1	2.48	0.43
1:B:2697:ASN:OD1	1:B:2699:ALA:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1563:VAL:HG12	1:A:1879:TYR:HD1	1.83	0.43
1:A:2034:LEU:HD23	1:A:2034:LEU:HA	1.88	0.43
1:A:3179:ALA:HB1	1:A:3182:LEU:HD12	2.01	0.43
1:A:3443:ASP:OD1	1:A:3446:THR:OG1	2.27	0.43
1:A:3679:THR:OG1	1:A:3680:ALA:N	2.51	0.43
1:B:1030:ARG:HH12	1:B:1891:LEU:HD22	1.83	0.43
1:B:1557:LEU:HD11	1:B:1803:ASP:HB3	2.00	0.43
1:B:2665:LEU:HD12	1:B:2728:LEU:HD22	2.00	0.43
1:A:1992:GLN:O	1:A:1996:VAL:HG22	2.19	0.42
1:A:2864:THR:HA	1:A:2867:VAL:HG12	2.00	0.42
1:B:1500:SER:O	1:B:1974:TYR:OH	2.36	0.42
1:B:3400:LEU:HD23	1:B:3400:LEU:HA	1.88	0.42
1:B:4080:LEU:HD12	1:B:4165:LEU:HD13	2.00	0.42
1:A:1030:ARG:HH12	1:A:1891:LEU:HD22	1.83	0.42
1:B:192:PHE:HD2	1:B:231:ILE:HG21	1.84	0.42
1:B:2351:LEU:HD11	1:B:2399:TRP:CZ3	2.54	0.42
1:B:3982:THR:HG22	1:B:3985:GLN:HG3	2.00	0.42
1:A:632:LEU:HD23	1:A:632:LEU:HA	1.89	0.42
1:A:1034:LEU:HD23	1:A:1038:PHE:HD2	1.85	0.42
1:B:2669:LEU:O	1:B:2690:ARG:NH1	2.51	0.42
1:A:1396:ALA:HB1	1:A:1400:ILE:HB	2.02	0.42
1:B:1193:ASP:HA	1:B:2581:LEU:HD21	2.02	0.42
1:B:1992:GLN:O	1:B:1996:VAL:HG22	2.20	0.42
1:B:3111:MET:HE1	1:B:3334:LEU:HD12	2.00	0.42
1:B:3253:LEU:HB3	1:B:3254:SER:H	1.70	0.42
1:B:4260:ARG:NH2	1:B:4364:LEU:O	2.53	0.42
1:A:1445:GLY:HA3	1:A:1509:ASP:HB3	2.02	0.42
1:A:1498:LEU:HD13	1:A:1974:TYR:CG	2.54	0.42
1:A:1831:LEU:HD23	1:A:1831:LEU:HA	1.86	0.42
1:A:2099:VAL:HG22	1:A:2103:LEU:HD12	2.01	0.42
1:A:2665:LEU:HD12	1:A:2728:LEU:HD22	2.00	0.42
1:A:2669:LEU:O	1:A:2690:ARG:NH1	2.51	0.42
1:A:3683:VAL:HA	1:A:3686:ILE:HG22	2.02	0.42
1:B:568:LEU:HD11	1:B:630:LEU:HB3	2.01	0.42
1:B:2099:VAL:HG22	1:B:2103:LEU:HD12	2.01	0.42
1:B:3547:CYS:HB2	1:B:3616:SER:HA	2.00	0.42
1:B:4260:ARG:HH21	1:B:4365:SER:HA	1.84	0.42
1:A:191:LEU:HD12	1:A:191:LEU:HA	1.90	0.42
1:A:630:LEU:HB2	1:A:720:LEU:HB3	2.00	0.42
1:A:853:GLN:HE21	1:A:909:GLY:HA3	1.85	0.42
1:A:1473:LEU:HD12	1:A:1473:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:LEU:HD12	1:A:2062:LEU:HD11	2.02	0.42
1:A:2029:TYR:O	1:A:2033:THR:HG23	2.20	0.42
1:A:2705:LEU:HD23	1:A:2705:LEU:HA	1.94	0.42
1:A:3124:SER:HB2	1:B:2347:HIS:CG	2.55	0.42
1:A:3432:ILE:HG23	1:A:3496:CYS:HB2	2.01	0.42
1:A:3982:THR:HG22	1:A:3985:GLN:HG3	2.00	0.42
1:A:4260:ARG:HH21	1:A:4365:SER:HA	1.85	0.42
1:A:123:VAL:HG11	1:A:398:HIS:HA	2.02	0.42
1:A:193:ILE:HD13	1:A:193:ILE:HA	1.92	0.42
1:B:1337:ARG:NH2	1:B:1349:GLN:OE1	2.53	0.42
1:B:2650:LEU:HD13	1:B:2707:VAL:HG11	2.01	0.42
1:A:834:THR:OG1	1:A:835:ARG:N	2.53	0.42
1:A:1935:LEU:O	1:A:1939:LEU:HB2	2.20	0.42
1:A:1978:ILE:HD13	1:A:1978:ILE:HA	1.92	0.42
1:B:630:LEU:HB2	1:B:720:LEU:HB3	2.00	0.42
1:B:3127:SER:O	1:B:3131:LYS:HB2	2.20	0.42
1:A:1767:SER:HB3	1:A:1920:LEU:HD11	2.00	0.42
1:A:1800:LEU:HB2	1:A:1881:HIS:HB2	2.02	0.42
1:A:2795:ARG:HA	1:A:2795:ARG:HD2	1.84	0.42
1:A:4184:LEU:HD11	1:A:4212:LEU:HB3	2.01	0.42
1:A:4260:ARG:NH2	1:A:4364:LEU:O	2.53	0.42
1:B:1396:ALA:HB1	1:B:1400:ILE:HB	2.02	0.42
1:B:2029:TYR:O	1:B:2033:THR:HG23	2.20	0.42
1:B:3525:LEU:HD21	1:B:3545:LEU:HD23	2.02	0.42
1:A:192:PHE:HD2	1:A:231:ILE:HG21	1.84	0.42
1:A:1193:ASP:HA	1:A:2581:LEU:HD21	2.02	0.42
1:A:1353:LEU:HD23	1:A:1403:LYS:HB3	2.01	0.42
1:A:2142:LEU:O	1:A:2146:LEU:HD23	2.20	0.42
1:A:2351:LEU:HD11	1:A:2399:TRP:CZ3	2.54	0.42
1:A:3127:SER:O	1:A:3131:LYS:HB2	2.20	0.42
1:B:853:GLN:HE21	1:B:909:GLY:HA3	1.85	0.42
1:B:2142:LEU:O	1:B:2146:LEU:HD23	2.20	0.42
1:B:2582:MET:O	1:B:2586:MET:HG3	2.20	0.42
1:B:2705:LEU:HD23	1:B:2705:LEU:HA	1.94	0.42
1:B:3865:THR:HA	1:B:3982:THR:HA	2.02	0.42
1:A:3525:LEU:HD21	1:A:3545:LEU:HD23	2.02	0.41
1:B:834:THR:OG1	1:B:835:ARG:N	2.53	0.41
1:B:3085:ILE:HA	1:B:3088:VAL:HG12	2.02	0.41
1:B:3432:ILE:HG23	1:B:3496:CYS:HB2	2.02	0.41
1:A:123:VAL:HB	1:A:125:LYS:HZ3	1.85	0.41
1:A:1337:ARG:NH2	1:A:1349:GLN:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2840:LEU:HD11	1:A:2922:LEU:HD23	2.02	0.41
1:A:3169:ILE:HG13	1:A:3212:ILE:HG12	2.01	0.41
1:A:3689:PHE:O	1:A:3693:VAL:HG22	2.20	0.41
1:B:1038:PHE:HA	1:B:1096:PRO:HD3	2.02	0.41
1:B:1353:LEU:HD23	1:B:1403:LYS:HB3	2.01	0.41
1:B:1777:SER:HA	1:B:1874:PRO:HA	2.01	0.41
1:B:1939:LEU:HD23	1:B:1939:LEU:HA	1.92	0.41
1:A:1182:LEU:HD23	1:A:1182:LEU:HA	1.91	0.41
1:A:1477:VAL:HG13	1:A:2023:LEU:HD22	2.03	0.41
1:B:173:LEU:HD23	1:B:248:ALA:HB1	2.02	0.41
1:B:1377:LEU:O	1:B:1381:THR:OG1	2.34	0.41
1:B:3169:ILE:HG13	1:B:3212:ILE:HG12	2.01	0.41
1:A:91:ILE:HD12	1:A:107:LEU:HD21	2.02	0.41
1:A:365:ASN:OD1	1:A:365:ASN:N	2.54	0.41
1:A:1783:MET:SD	1:A:1783:MET:N	2.94	0.41
1:A:1812:LEU:HD13	1:A:1862:GLY:HA2	2.02	0.41
1:B:2840:LEU:HD11	1:B:2922:LEU:HD23	2.02	0.41
1:B:3030:ILE:N	1:B:3034:ASP:OD1	2.54	0.41
1:A:3085:ILE:HA	1:A:3088:VAL:HG12	2.02	0.41
1:A:3695:ASN:OD1	1:A:3769:GLN:NE2	2.43	0.41
1:A:4241:ILE:HD12	1:A:4241:ILE:HA	1.94	0.41
1:B:1935:LEU:O	1:B:1939:LEU:HB2	2.20	0.41
1:B:2099:VAL:O	1:B:2103:LEU:HB2	2.21	0.41
1:A:1290:LEU:HD22	1:A:1294:ASP:HB3	2.01	0.41
1:A:2347:HIS:CG	1:B:3124:SER:HB2	2.56	0.41
1:A:2764:LYS:HA	1:A:2764:LYS:HD3	1.81	0.41
1:B:246:VAL:HG23	1:B:248:ALA:H	1.86	0.41
1:B:858:SER:OG	1:B:906:THR:OG1	2.35	0.41
1:B:1445:GLY:HA3	1:B:1509:ASP:HB3	2.02	0.41
1:B:1477:VAL:HG13	1:B:2023:LEU:HD22	2.03	0.41
1:B:1783:MET:SD	1:B:1783:MET:N	2.94	0.41
1:A:1190:SER:O	1:A:1190:SER:OG	2.38	0.41
1:A:2099:VAL:O	1:A:2103:LEU:HB2	2.21	0.41
1:A:2582:MET:O	1:A:2586:MET:HG3	2.20	0.41
1:A:3823:THR:HB	1:A:4001:SER:HA	2.01	0.41
1:A:3865:THR:HA	1:A:3982:THR:HA	2.01	0.41
1:B:91:ILE:HD12	1:B:107:LEU:HD21	2.02	0.41
1:B:2812:LEU:HD12	1:B:2812:LEU:HA	1.92	0.41
1:B:3484:TYR:HA	1:B:3487:LEU:HG	2.02	0.41
1:B:3823:THR:HB	1:B:4001:SER:HA	2.01	0.41
1:A:1038:PHE:HA	1:A:1096:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1398:ARG:HD2	1:A:1562:GLU:HB2	2.03	0.41
1:A:2354:VAL:HA	1:A:2357:VAL:HG12	2.03	0.41
1:A:3035:GLY:O	1:A:3039:ILE:HG23	2.21	0.41
1:A:3074:THR:OG1	1:A:3075:CYS:N	2.53	0.41
1:A:3175:THR:OG1	1:A:3177:GLN:O	2.33	0.41
1:B:1309:THR:HG23	1:B:1311:ILE:H	1.85	0.41
1:B:1812:LEU:HD13	1:B:1862:GLY:HA2	2.02	0.41
1:B:3689:PHE:O	1:B:3693:VAL:HG22	2.21	0.41
1:A:215:LYS:HD2	1:A:215:LYS:HA	1.73	0.41
1:A:1863:ARG:HG2	1:A:1866:SER:HB3	2.03	0.41
1:A:2650:LEU:HD13	1:A:2707:VAL:HG11	2.01	0.41
1:A:2797:GLN:O	1:A:2801:SER:OG	2.33	0.41
1:A:2873:CYS:O	1:B:2713:ASN:ND2	2.54	0.41
1:A:3130:MET:HE2	1:A:3130:MET:HB2	1.98	0.41
1:A:3454:LEU:HA	1:A:3457:VAL:HG12	2.03	0.41
1:B:1474:LEU:HD12	1:B:2062:LEU:HD11	2.02	0.41
1:B:2354:VAL:HA	1:B:2357:VAL:HG12	2.03	0.41
1:B:3175:THR:OG1	1:B:3177:GLN:O	2.33	0.41
1:B:3561:MET:HE2	1:B:3561:MET:HA	2.02	0.41
1:B:3635:LEU:HD11	1:B:3690:LEU:HD21	2.02	0.41
1:B:3683:VAL:HA	1:B:3686:ILE:HG22	2.02	0.41
1:A:173:LEU:HD23	1:A:248:ALA:HB1	2.02	0.41
1:A:1309:THR:HG23	1:A:1311:ILE:H	1.85	0.41
1:A:3030:ILE:N	1:A:3034:ASP:OD1	2.54	0.41
1:B:1398:ARG:HD2	1:B:1562:GLU:HB2	2.03	0.41
1:B:2716:LEU:HA	1:B:2719:TRP:HB2	2.03	0.41
1:B:3870:LEU:HD21	1:B:3967:LEU:HD21	2.02	0.41
1:A:934:THR:HG23	1:A:936:GLU:H	1.86	0.40
1:A:2096:LEU:HD23	1:A:2096:LEU:HA	1.91	0.40
1:A:3561:MET:HE2	1:A:3561:MET:HA	2.02	0.40
1:A:3635:LEU:HD11	1:A:3690:LEU:HD21	2.02	0.40
1:B:207:THR:HA	1:B:214:ALA:HB2	2.03	0.40
1:B:510:LEU:HD22	1:B:567:LEU:HD11	2.03	0.40
1:B:2050:LEU:HA	1:B:2053:THR:HG22	2.03	0.40
1:A:207:THR:HA	1:A:214:ALA:HB2	2.03	0.40
1:A:2050:LEU:HA	1:A:2053:THR:HG22	2.03	0.40
1:A:2716:LEU:HA	1:A:2719:TRP:HB2	2.03	0.40
1:B:123:VAL:HG11	1:B:398:HIS:HA	2.02	0.40
1:B:1034:LEU:HD23	1:B:1038:PHE:HD2	1.85	0.40
1:B:1290:LEU:HD22	1:B:1294:ASP:HB3	2.01	0.40
1:B:1989:ASN:HD22	1:B:1989:ASN:HA	1.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2172:VAL:HA	1:B:2175:VAL:HG22	2.03	0.40
1:B:3990:LEU:HD12	1:B:3995:LEU:HB2	2.04	0.40
1:A:1799:ILE:HD12	1:A:1799:ILE:HA	1.97	0.40
1:B:1207:LYS:HD3	1:B:1207:LYS:HA	1.87	0.40
1:B:3167:GLY:HA2	1:B:3215:PRO:HD3	2.04	0.40
1:B:3454:LEU:HA	1:B:3457:VAL:HG12	2.03	0.40
1:B:3627:LEU:HD23	1:B:3627:LEU:HA	1.88	0.40
1:B:3035:GLY:O	1:B:3039:ILE:HG23	2.21	0.40
1:B:3198:SER:HA	1:B:3291:LEU:O	2.22	0.40
1:B:3224:HIS:HD2	1:B:3299:LEU:HG	1.87	0.40
1:B:3335:HIS:O	1:B:3339:THR:OG1	2.32	0.40
1:A:1009:VAL:HG12	1:A:1313:LYS:HE2	2.03	0.40
1:B:3074:THR:OG1	1:B:3075:CYS:N	2.53	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	2745/4867 (56%)	2649 (96%)	96 (4%)	0	100	100
1	B	2745/4867 (56%)	2650 (96%)	95 (4%)	0	100	100
All	All	5490/9734 (56%)	5299 (96%)	191 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2497/4225 (59%)	2488 (100%)	9 (0%)	84	84
1	B	2497/4225 (59%)	2488 (100%)	9 (0%)	84	84
All	All	4994/8450 (59%)	4976 (100%)	18 (0%)	81	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1433	LEU
1	A	1474	LEU
1	A	1805	LEU
1	A	1833	VAL
1	A	2030	LEU
1	A	2582	MET
1	A	3204	GLU
1	A	3333	LEU
1	A	3690	LEU
1	B	1433	LEU
1	B	1474	LEU
1	B	1805	LEU
1	B	1833	VAL
1	B	2030	LEU
1	B	2582	MET
1	B	3204	GLU
1	B	3333	LEU
1	B	3690	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	514	GLN
1	A	744	HIS
1	A	869	ASN
1	A	1111	ASN
1	A	1297	GLN
1	A	1343	GLN
1	A	1907	GLN
1	A	1989	ASN

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Mol	Chain	Res	Type
1	A	2200	GLN
1	A	2205	ASN
1	A	2333	GLN
1	A	2363	ASN
1	A	2577	GLN
1	A	2830	GLN
1	A	2869	HIS
1	A	3451	GLN
1	A	3527	ASN
1	A	3709	ASN
1	A	3777	ASN
1	A	3790	GLN
1	A	3966	HIS
1	A	4180	HIS
1	A	4215	HIS
1	B	514	GLN
1	B	744	HIS
1	B	869	ASN
1	B	1111	ASN
1	B	1297	GLN
1	B	1343	GLN
1	B	1402	HIS
1	B	1907	GLN
1	B	1988	HIS
1	B	1989	ASN
1	B	2200	GLN
1	B	2205	ASN
1	B	2333	GLN
1	B	2363	ASN
1	B	2577	GLN
1	B	2656	GLN
1	B	2817	HIS
1	B	2830	GLN
1	B	2869	HIS
1	B	3451	GLN
1	B	3519	GLN
1	B	3527	ASN
1	B	3709	ASN
1	B	3777	ASN
1	B	3966	HIS
1	B	4180	HIS
1	B	4215	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

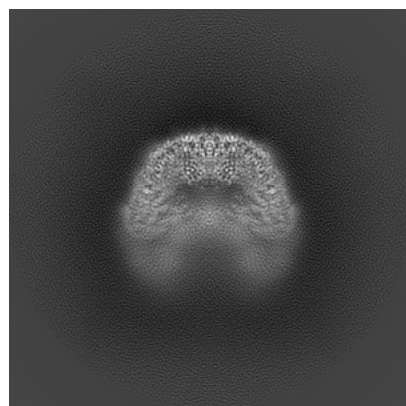
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15663. These allow visual inspection of the internal detail of the map and identification of artifacts.

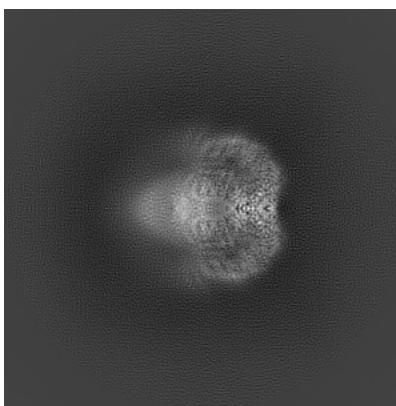
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

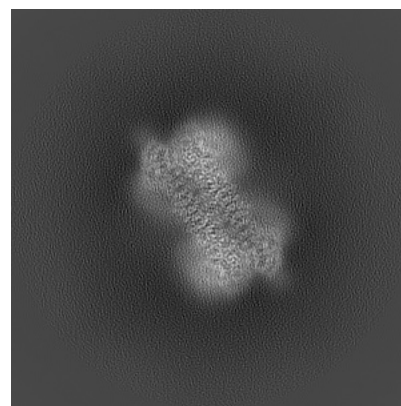
6.1.1 Primary map



X

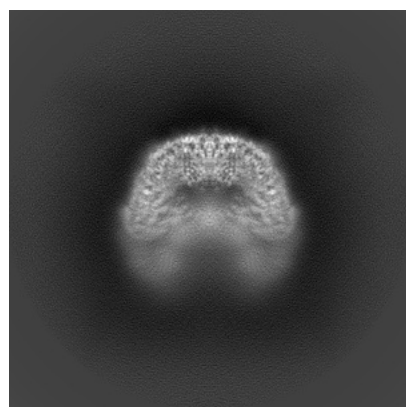


Y

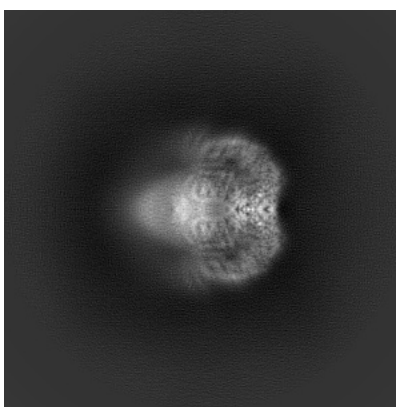


Z

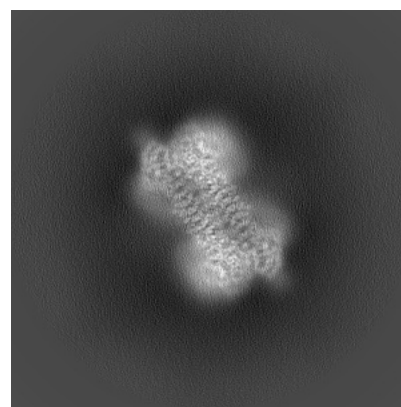
6.1.2 Raw map



X



Y

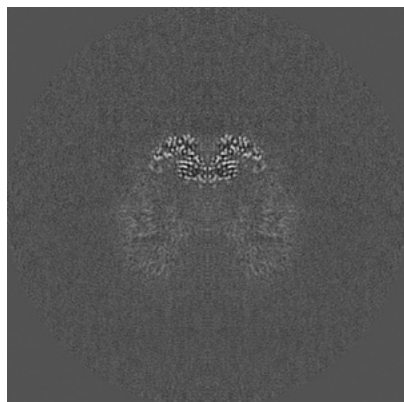


Z

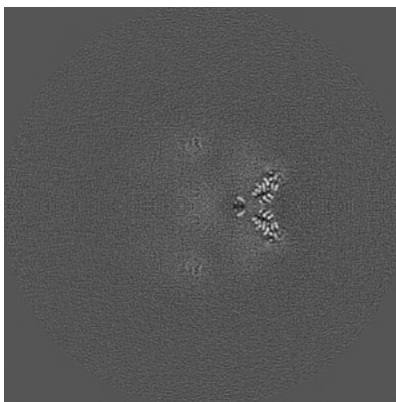
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

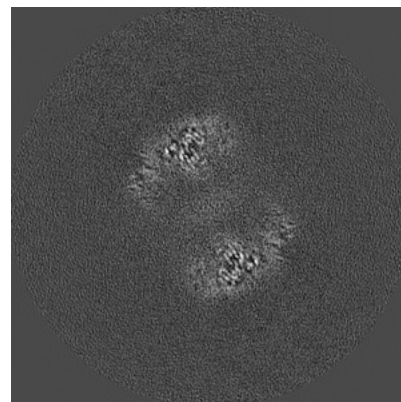
6.2.1 Primary map



X Index: 182

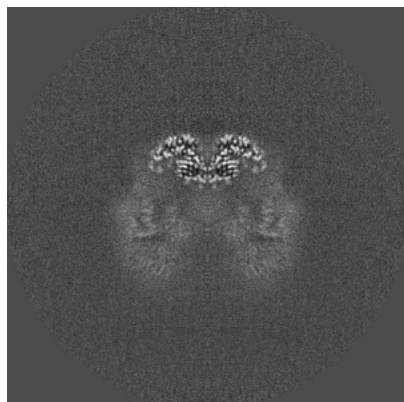


Y Index: 182

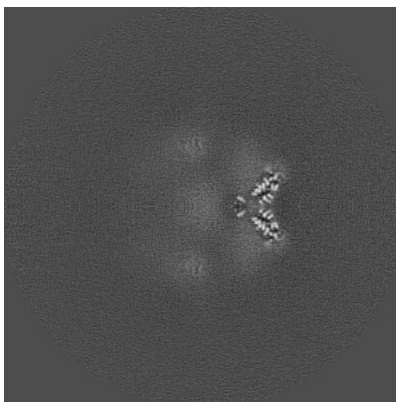


Z Index: 182

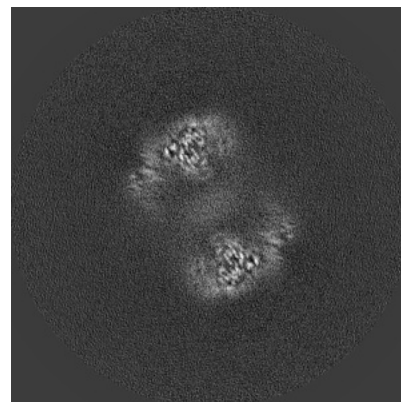
6.2.2 Raw map



X Index: 182



Y Index: 182

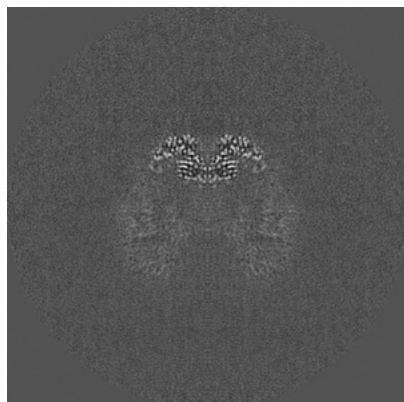


Z Index: 182

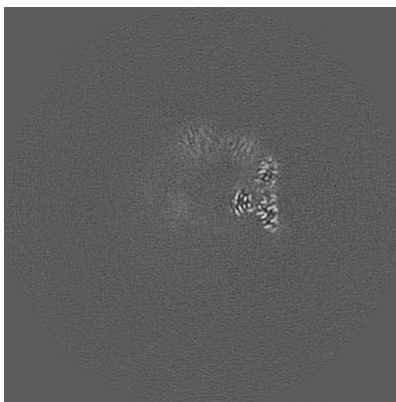
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

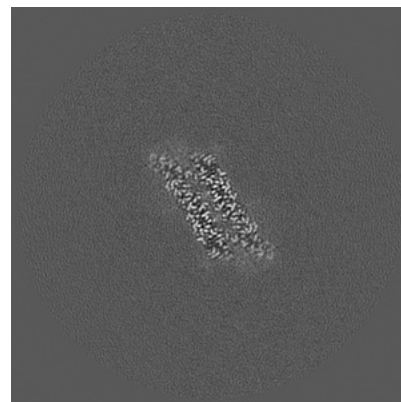
6.3.1 Primary map



X Index: 182

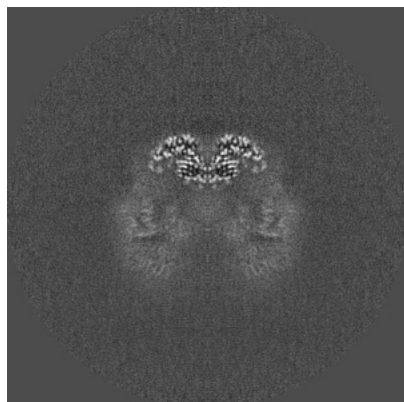


Y Index: 161

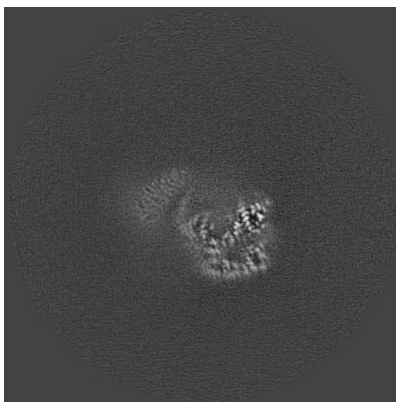


Z Index: 236

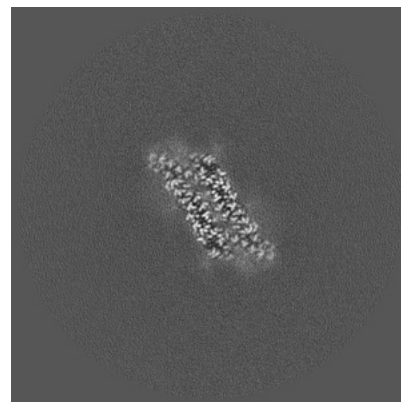
6.3.2 Raw map



X Index: 182



Y Index: 227

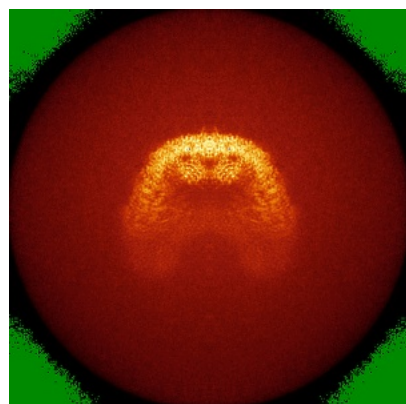


Z Index: 236

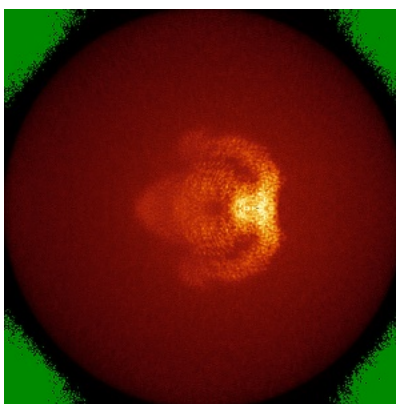
The images above show the largest variance slices of the map in three orthogonal directions.

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

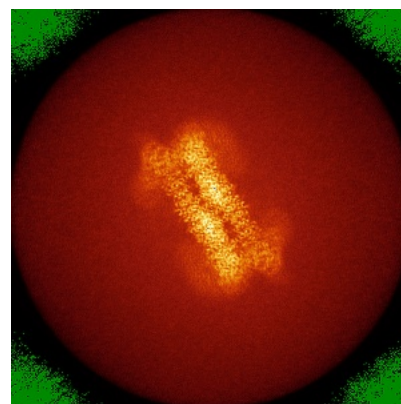
6.4.1 Primary map



X

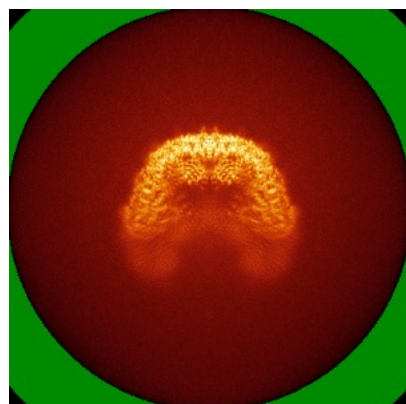


Y

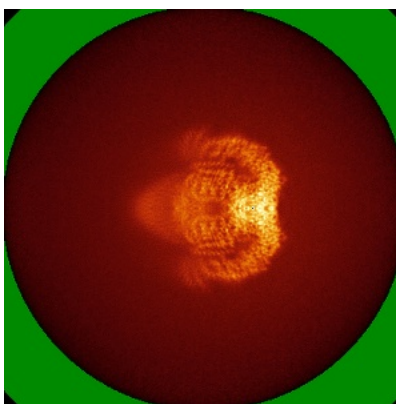


Z

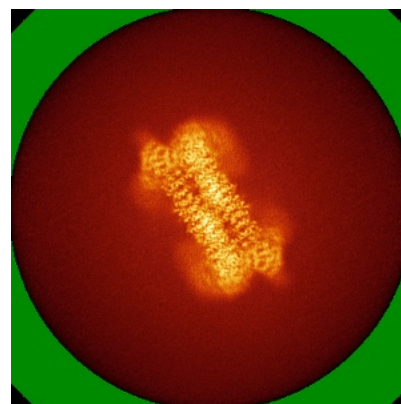
6.4.2 Raw map



X



Y

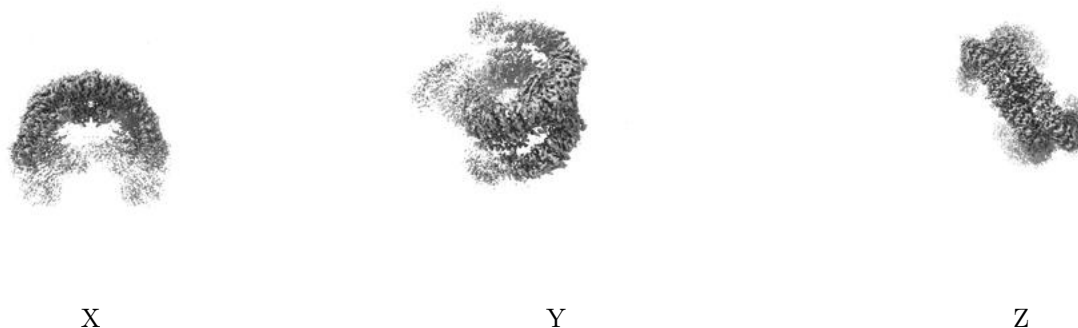


Z

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.

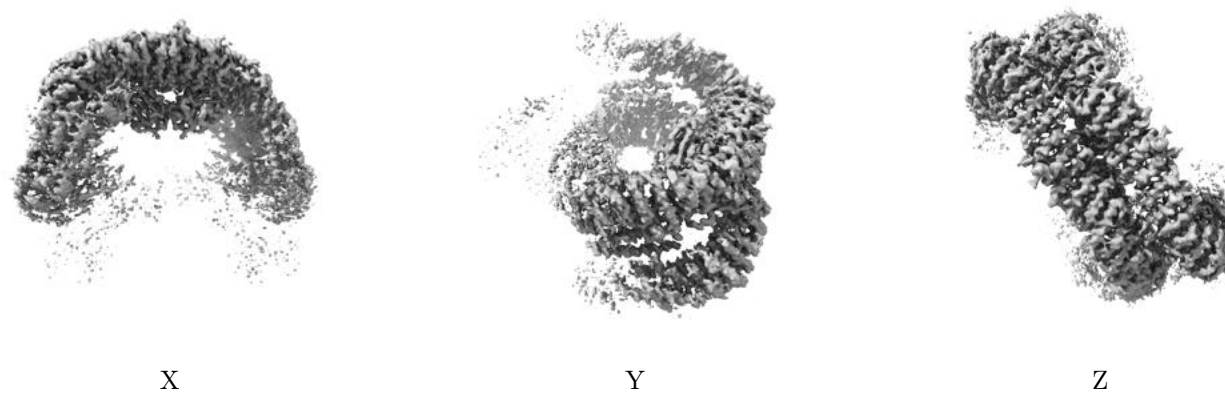
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

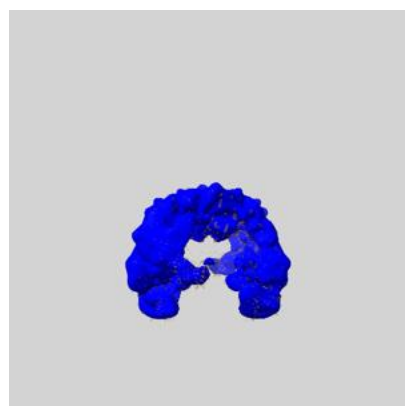
6.6 Mask visualisation [i](#)

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

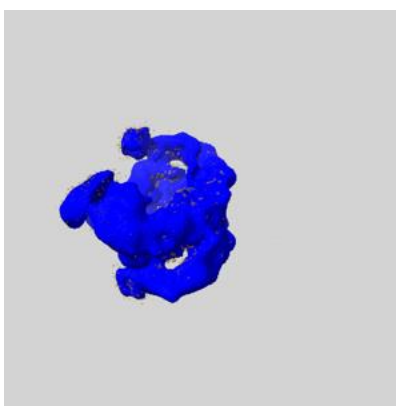
A mask typically either:

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

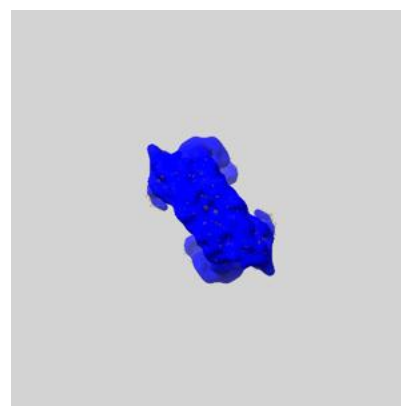
6.6.1 emd_15663_msk_1.map [i](#)



X



Y

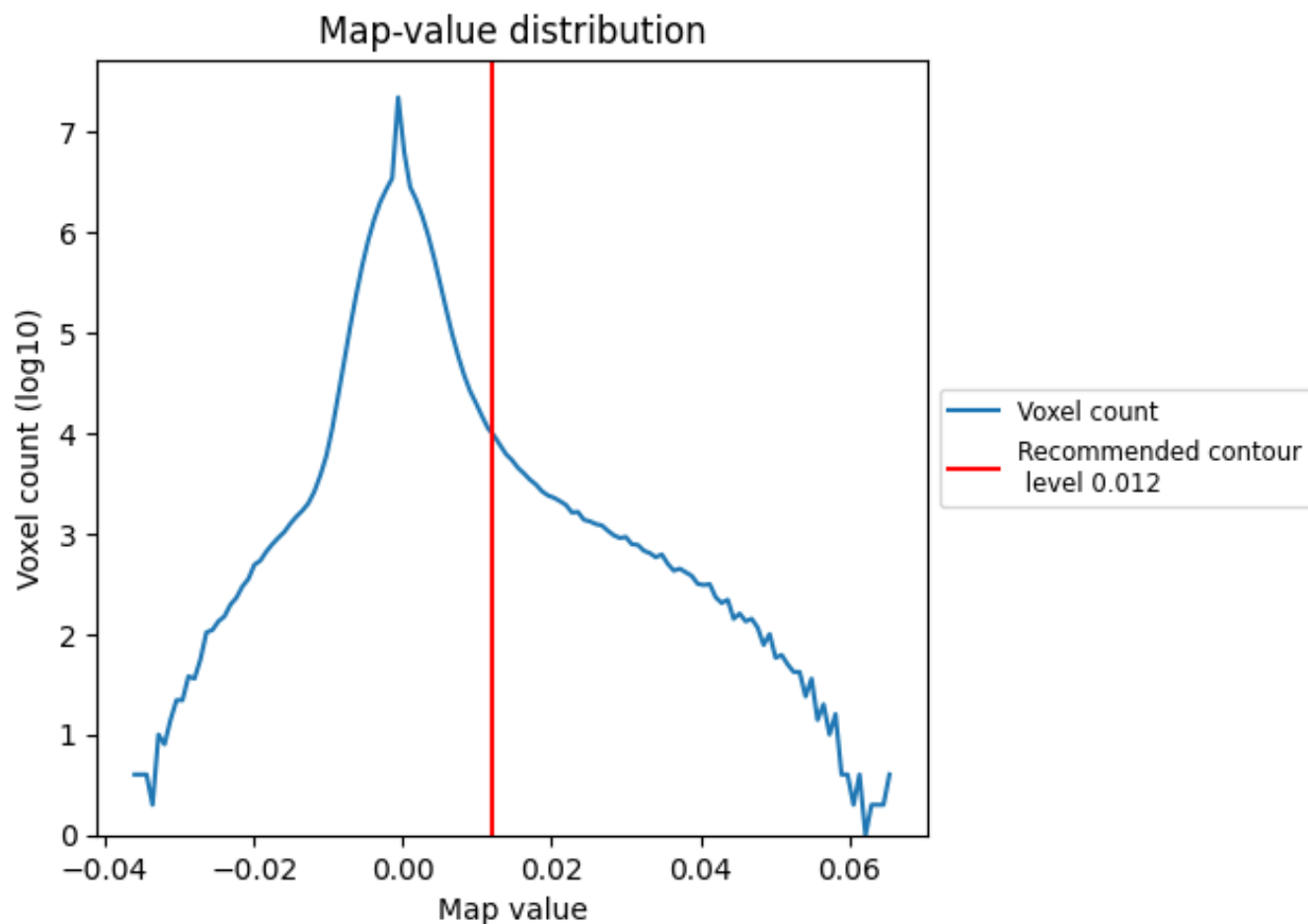


Z

7 Map analysis [i](#)

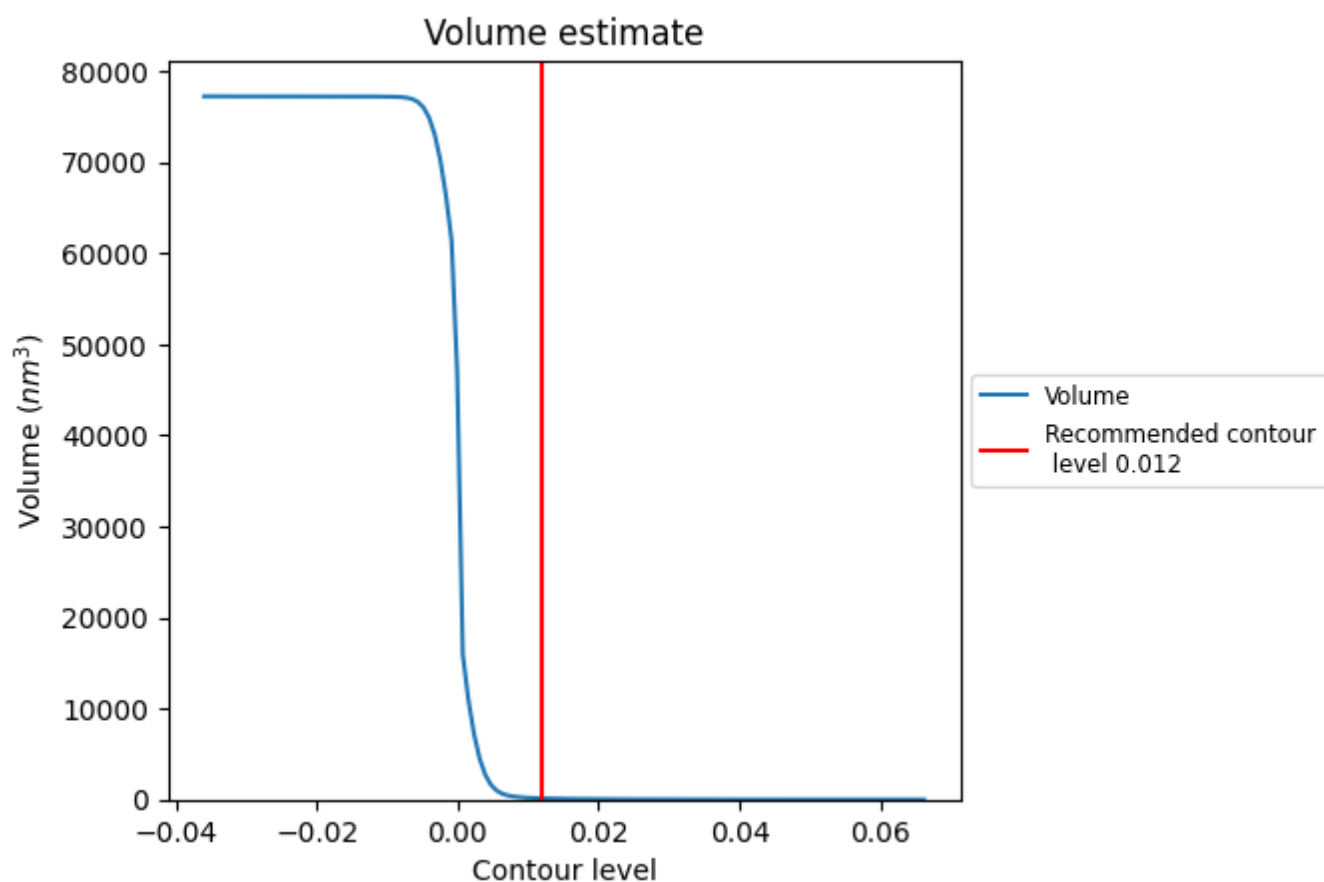
This section contains the results of statistical analysis of the map.

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.

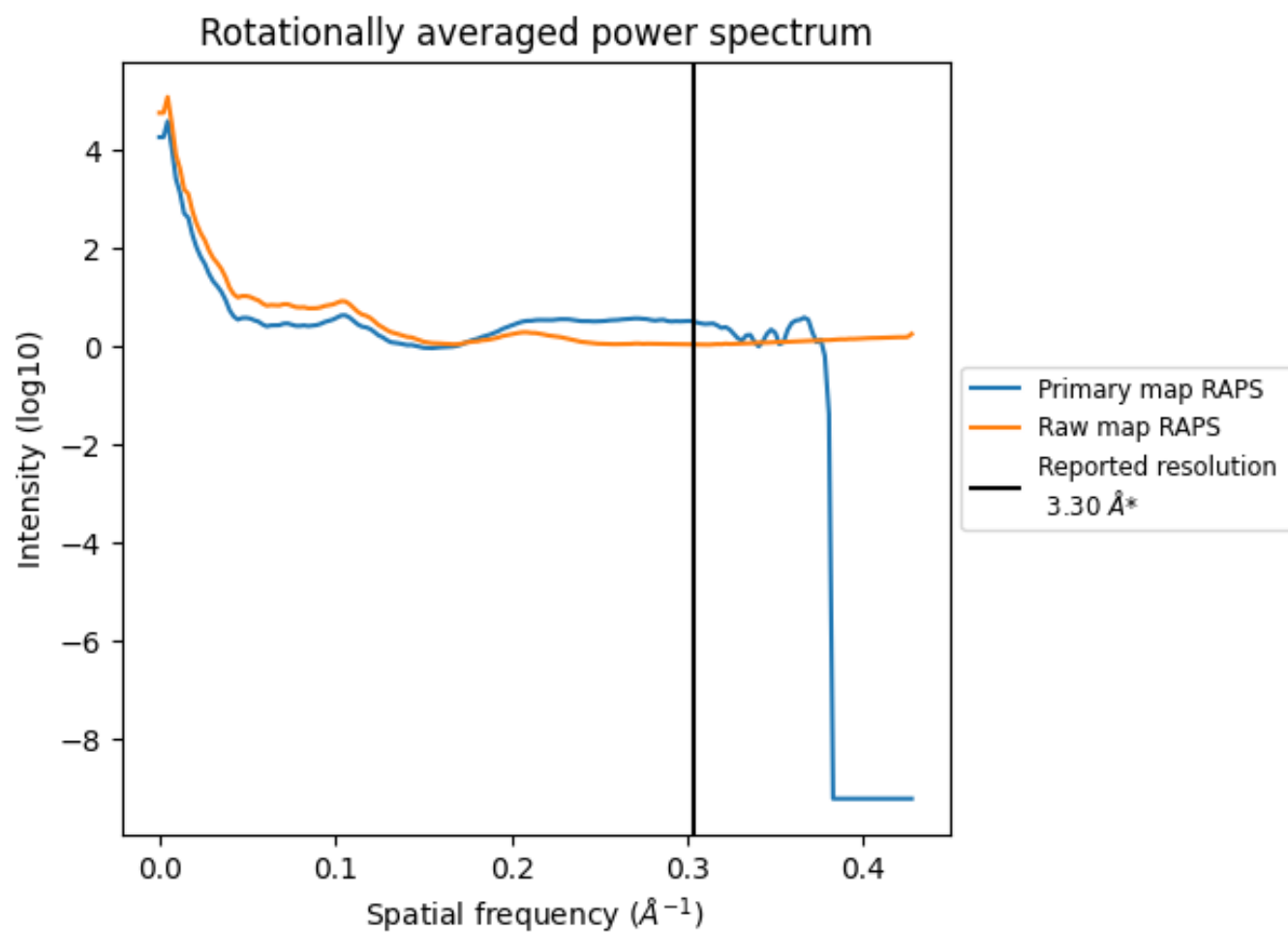
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 116 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 ⓘ

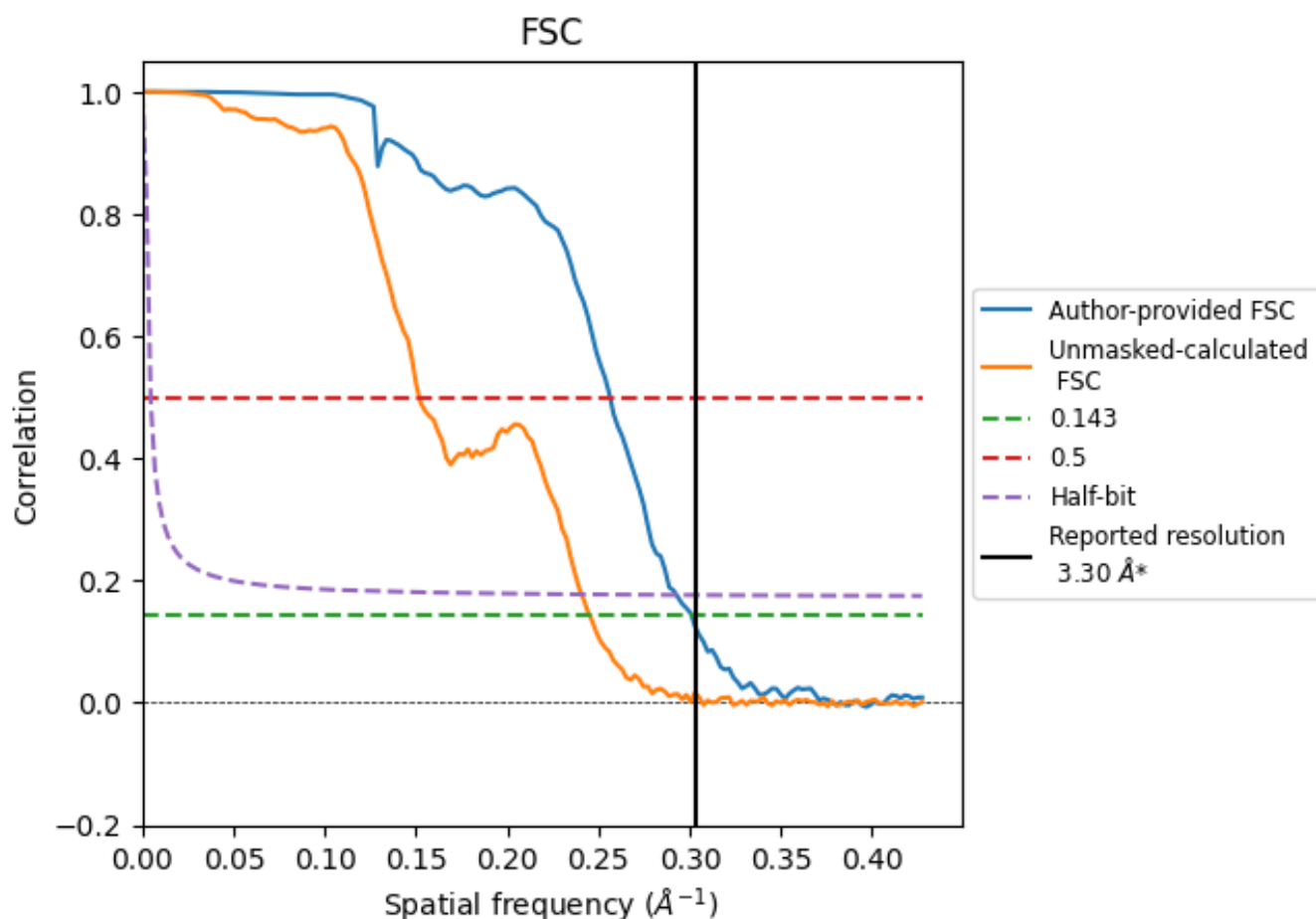


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

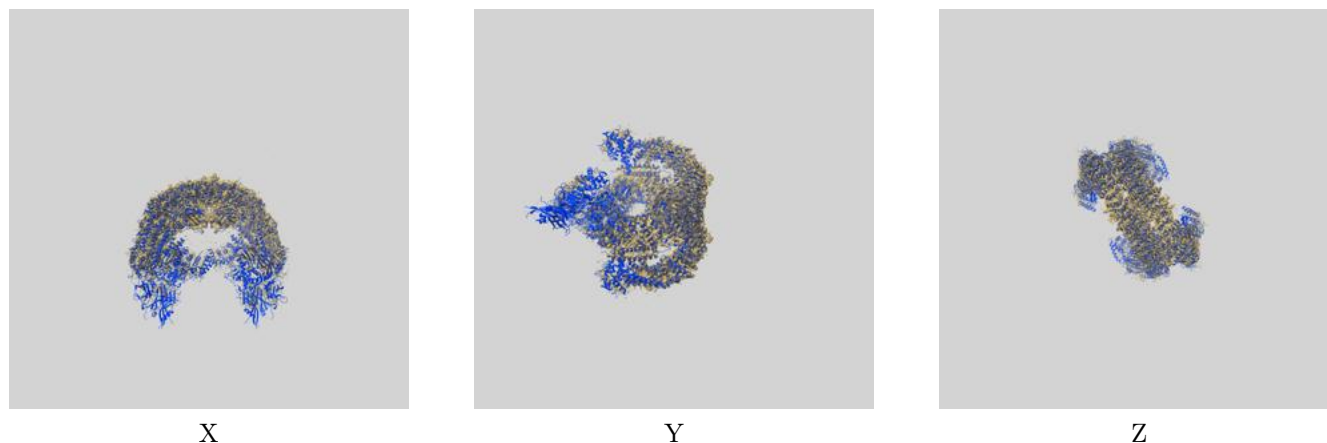
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.90	3.42
Unmasked-calculated*	4.08	6.59	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

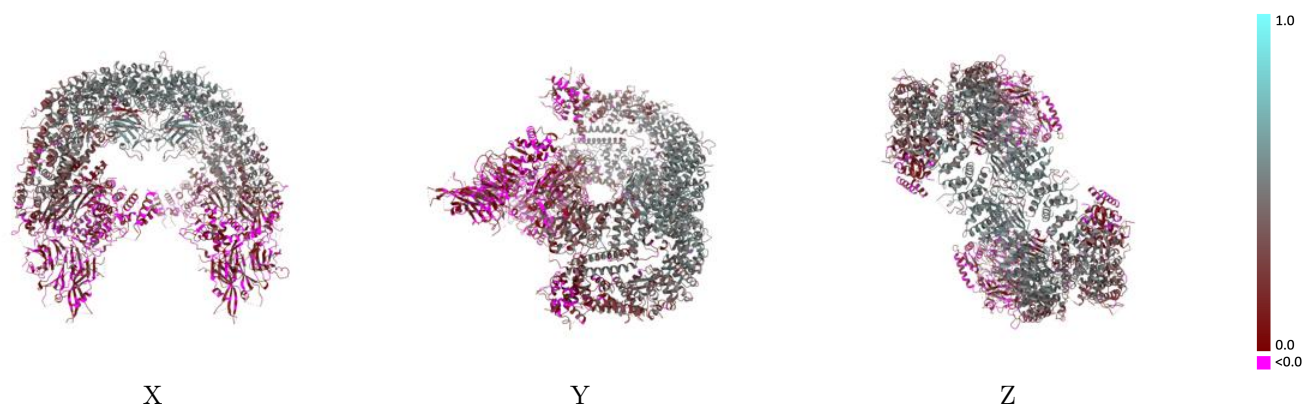
This section contains information regarding the fit between EMDB map EMD-15663 and PDB model 8ATU. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



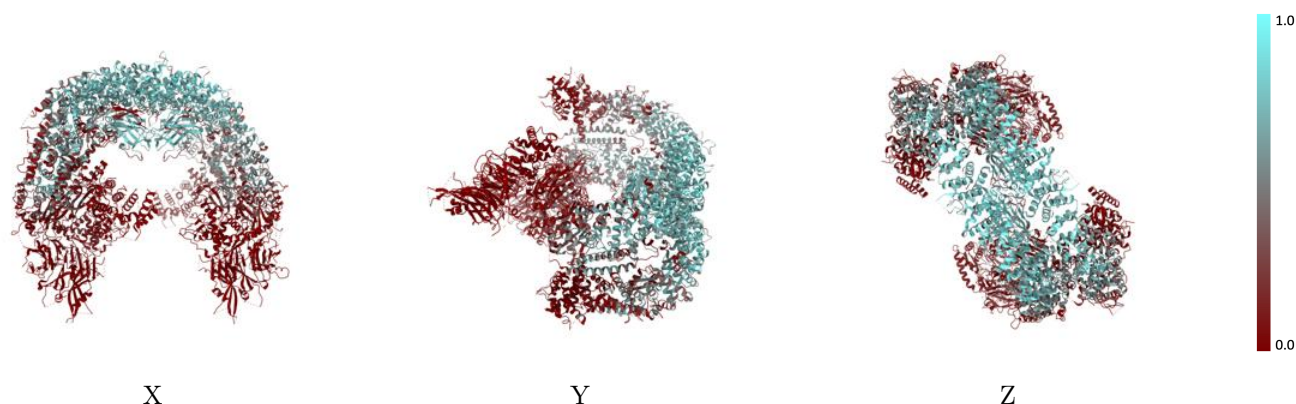
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



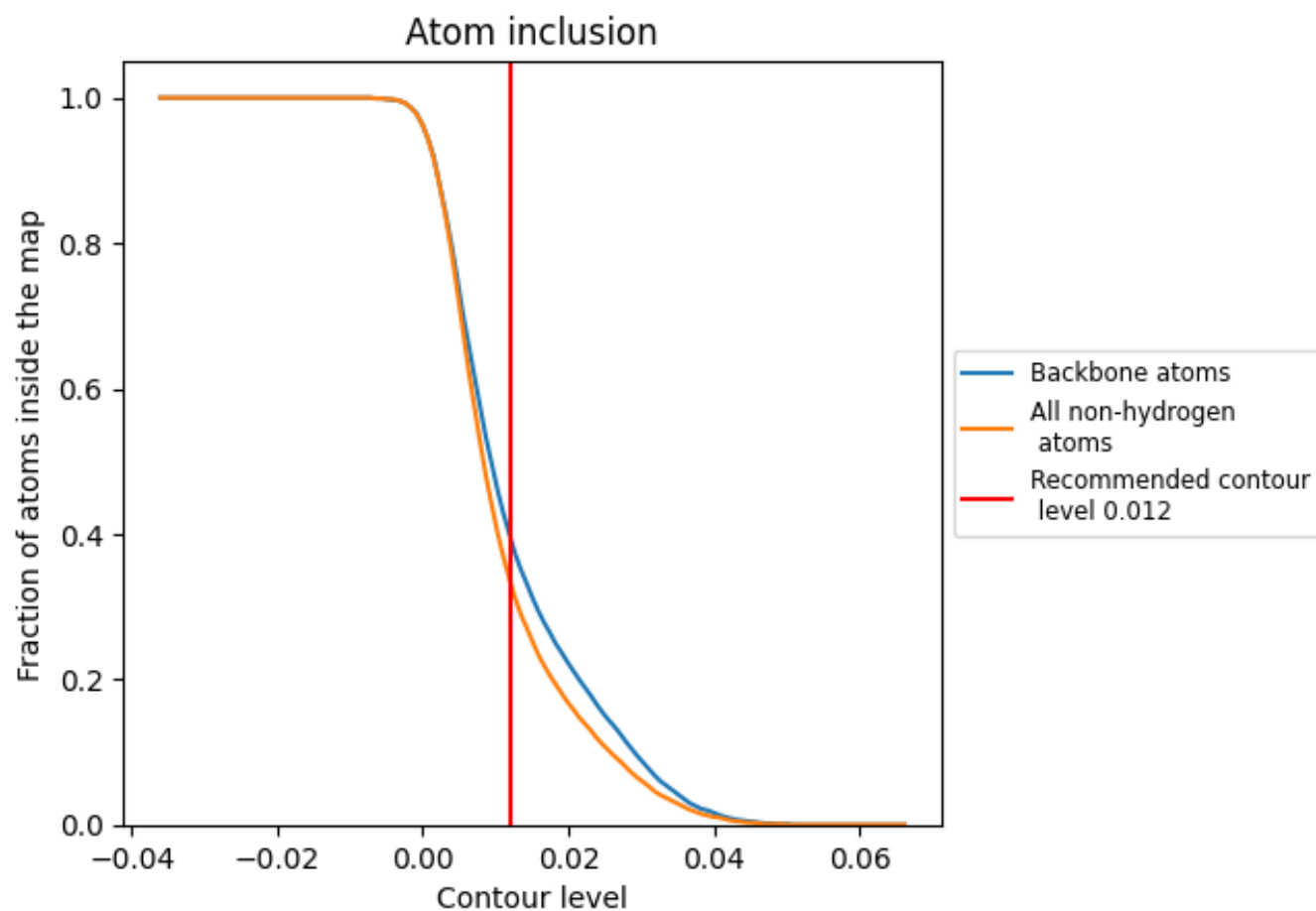
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 34% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3350	0.3010
A	0.3350	0.3010
B	0.3350	0.3010

