



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:59 AM UTC

PDB ID : 7R77 / pdb_00007r77
EMDB ID : EMD-24294
Title : Cryo-EM structure of DNMT5 binary complex with hemimethylated DNA
Authors : Wang, J.; Patel, D.J.
Deposited on : 2021-06-24
Resolution : 3.00 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

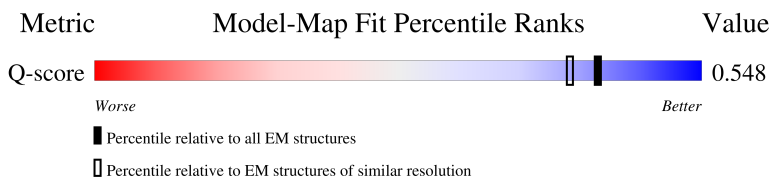
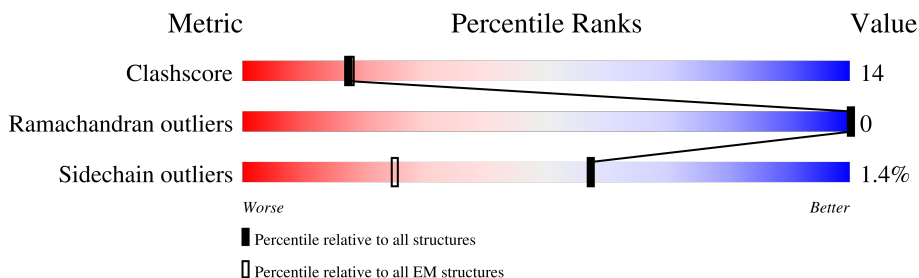
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	2348	
2	B	36	
3	D	36	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14980 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 DNA repair protein Rad8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1830	Total	C	N	O	S	0	0
			14464	9095	2612	2687	70		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP J9VI03
A	31	SER	-	expression tag	UNP J9VI03
A	32	TYR	-	expression tag	UNP J9VI03
A	33	TYR	-	expression tag	UNP J9VI03
A	34	HIS	-	expression tag	UNP J9VI03
A	35	HIS	-	expression tag	UNP J9VI03
A	36	HIS	-	expression tag	UNP J9VI03
A	37	HIS	-	expression tag	UNP J9VI03
A	38	HIS	-	expression tag	UNP J9VI03
A	39	HIS	-	expression tag	UNP J9VI03
A	40	ASP	-	expression tag	UNP J9VI03
A	41	TYR	-	expression tag	UNP J9VI03
A	42	ASP	-	expression tag	UNP J9VI03
A	43	ILE	-	expression tag	UNP J9VI03
A	44	PRO	-	expression tag	UNP J9VI03
A	45	THR	-	expression tag	UNP J9VI03
A	46	THR	-	expression tag	UNP J9VI03
A	47	GLU	-	expression tag	UNP J9VI03
A	48	ASN	-	expression tag	UNP J9VI03
A	49	LEU	-	expression tag	UNP J9VI03
A	50	TYR	-	expression tag	UNP J9VI03
A	51	PHE	-	expression tag	UNP J9VI03
A	52	GLN	-	expression tag	UNP J9VI03
A	53	GLY	-	expression tag	UNP J9VI03
A	54	ALA	-	expression tag	UNP J9VI03
A	55	MET	-	expression tag	UNP J9VI03
A	56	GLY	-	expression tag	UNP J9VI03
A	57	SER	-	expression tag	UNP J9VI03

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*TP*CP*AP*GP*(5CM)P*GP*CP*AP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	12	Total	C	N	O	P	0	0
			250	118	48	72	12		

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*TP*CP*AP*GP*(5CM)P*GP*CP*AP*TP*GP*G)-3').

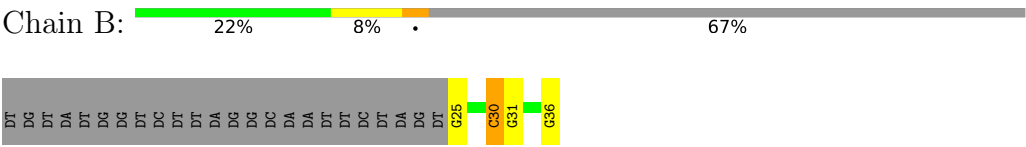
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	13	Total	C	N	O	P	0	0
			261	125	49	75	12		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

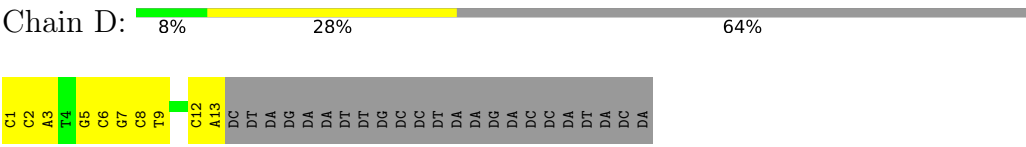
Mol	Chain	Residues	Atoms		AltConf
4	A	5	Total	Zn	0
			5	5	

LYS	Q2271	H2192	K2084	G1988	K1870	S1742	ASP	L1534	V1460	E1360	N1242	H1154
ARG	H2278	H2193	P2085	D1989	E1871	S1743	ASP	Q1535	I1461	H1361	L1243	L1155
SER	G2196	V2194	S2086	I1990	F1874	S1744	GLU	K1536	V1465	S1366	L1245	L1158
GLU	L2283	G2198	T2087	I1994	K1875	I1748	LYS	K1537	G1466	W1367	W1245	GLY
ALA	D2284	S2199	N2088	I1995	K1876	D1757	LYS	I1538	Y1487	T1375	E1248	ASP
ARG	T2285	A2200	P2089	V1999	Q1879	R1762	SER	I1539	Y1470	E1376	L1249	ASP
ASP	I2286	K2201	D2090	V2007	Q1888	R1763	LEU	A1540	I1471	S1377	L1250	ASP
ALA	D2287	I2091	I2092	K2002	A1884	I1770	VAL	I1547	I1472	P1378	L1256	ILE
GLY	M2288	S2092	M2093	K2003	R1885	I1771	ASN	V1548	I1473	Q1379	L1261	ALA
VAL	L2298	A2204	A2094	V2007	R1886	G1778	GLY	M1550	I1474	P1380	I1262	VAL
SER	T2302	D2208	I2095	S2007	E1888	V1774	LYS	S1552	L1476	K1390	A1263	ALA
ASP	W2303	H2209	H2101	I2010	A1889	E1775	LYS	S1553	T1480	P1393	D1264	ASN
ASP	W2304	V2210	P2011	P2011	L1890	D1776	LYS	I1554	I1481	E1394	D1265	ASP
GLU	A2103	A2103	P2012	P2012	D1777	G1778	GLU	I1554	S1482	P1394	V1266	ALA
ASN	E2310	K2106	S2013	S2013	S1893	D1781	VAL	V1559	L1483	E1397	S1267	ALA
SER	E2311	C2107	P2014	P2014	T1894	E1796	THR	R1563	P1484	PRO	E1268	GLU
GLU	Y2312	M2108	K2017	K2017	T1895	R1788	ALA	L1567	A1485	GLU	C1271	ILE
LEU	G2313	C2107	Q2018	Q2018	A1897	E1799	VAL	S1568	P1486	ALA	E1272	ARG
SER	G2314	C2107	P2020	P2020	E1898	S1806	PHE	S1568	P1486	ALA	R1273	ARG
ASP	Q2315	C2117	S2021	S2021	K1902	T1793	GLY	P1571	E1487	K1402	H1282	ASP
ILE	A2316	V2118	TLE	TLE	F1907	E1796	ARG	R1572	P1488	L1403	I1184	ASP
SER	R2219	K2119	ALA	ALA	T1908	E1796	THR	R1573	A1489	P1404	I1184	ASP
ILE	V2220	E2122	ALA	ALA	L1909	S1806	VAL	W1574	T1490	L1405	I1184	ASP
SER	L2221	C2123	SER	SER	T1909	S1806	VAL	L1575	T1490	R1406	I1184	ASP
THR	L2222	Q2124	GLY	GLY	L1909	S1806	VAL	L1575	T1490	K1407	I1184	ASP
THR	L2223	Q2124	GLY	GLY	L1909	S1806	VAL	L1575	T1490	E1408	I1184	ASP
ASN	K2224	V2127	ALA	ALA	C1925	H1810	GLN	L1575	T1490	Q1409	I1184	ASP
GLU	M2225	R2128	M2028	M2028	I1928	R1813	ALA	L1575	T1490	L1410	I1191	ASP
LYS	N2226	E2143	V2031	V2031	T1929	V1825	THR	L1575	T1490	L1410	I1191	ASP
ARG	D2227	E2143	K2032	K2032	T1929	V1825	THR	L1575	T1490	L1410	I1191	ASP
THR	ALA	E2143	L2042	L2042	L1936	I1829	THR	L1575	T1490	L1410	I1191	ASP
THR	ALA	R2148	L2042	L2042	Q1940	A1830	ASP	L1575	T1490	L1410	I1191	ASP
LEU	ALA	Y2149	L2042	L2042	E1941	I1832	ASP	L1575	T1490	L1410	I1191	ASP
THR	ALA	L2153	V2046	V2046	D1942	E1833	SER	L1575	T1490	L1410	I1191	ASP
VAL	L2233	L2153	R2047	R2047	V1947	D1834	SER	L1575	T1490	L1410	I1191	ASP
LYS	L2234	L2153	E2048	E2048	N1948	E1833	SER	L1575	T1490	L1410	I1191	ASP
SER	L2235	L2153	R2052	R2052	I1951	V1838	SER	L1575	T1490	L1410	I1191	ASP
ASN	H2240	V2169	V2053	V2053	I1951	E1839	SER	L1575	T1490	L1410	I1191	ASP
PRO	H2240	L2170	R2054	R2054	W1956	H1840	SER	L1575	T1490	L1410	I1191	ASP
PHE	H2240	V2171	R2057	R2057	W1956	H1841	SER	L1575	T1490	L1410	I1191	ASP
LYS	P2246	F2172	R2057	R2057	W1956	H1841	SER	L1575	T1490	L1410	I1191	ASP
ARG	L2247	L2173	R2057	R2057	W1956	H1841	SER	L1575	T1490	L1410	I1191	ASP
SER	F2248	Q2174	R2057	R2057	W1956	H1841	SER	L1575	T1490	L1410	I1191	ASP
SER	T2249	Q2175	R2057	R2057	W1956	H1841	SER	L1575	T1490	L1410	I1191	ASP
SER	T2249	Q2175	R2057	R2057	W1956	H1841	SER	L1575	T1490	L1410	I1191	ASP
TRP	N2254	E2176	K2064	K2064	G1962	A1848	LEU	L1600	A1516	H1427	P1212	ASP
ALA	Y2255	D2177	I2065	I2065	F1963	S1849	GLU	I1601	R1517	E1430	P1212	ASP
LEU	R2256	L2178	Q2066	Q2066	SER	E1850	GLU	LYS	R1517	E1431	P1212	ASP
ALA	Q2261	K2181	S2070	S2070	LYS	V1853	LEU	LYS	R1517	E1432	P1212	ASP
SER	Q2261	V2182	L2074	L2074	LYS	V1853	LEU	LYS	R1517	E1432	P1212	ASP
SER	Q2261	V2182	L2074	L2074	LYS	V1853	LEU	LYS	R1517	E1432	P1212	ASP
PHE	Q2264	A2185	L2186	L2186	ASP	L1864	GLU	ALA	R1517	E1432	P1212	ASP
ARG	R2265	A2185	L2186	L2186	ASP	L1864	GLU	ALA	R1517	E1432	P1212	ASP
SER	V2266	L2186	S2079	S2079	GLU	E1865	GLU	ALA	R1517	E1432	P1212	ASP
ARG	R2267	L2186	E2080	E2080	GLU	M1866	GLU	ALA	R1517	E1432	P1212	ASP
LYS	R2268	L2186	C2081	C2081	Q1971	R1869	ASP	ALA	R1517	E1432	P1212	ASP
								MET	R1517	E1432	P1212	ASP

● Molecule 2: DNA (5'-D(P*GP*TP*CP*AP*GP*(5CM)P*GP*CP*AP*TP*GP*G)-3')



● Molecule 3: DNA (5'-D(P*GP*TP*CP*AP*GP*(5CM)P*GP*CP*AP*TP*GP*G)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78477	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	47262	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.071	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size ($\text{\AA}$)	272.384, 272.384, 272.384	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.064, 1.064, 1.064	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5CM, 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	0.47	0/14759	0.57	4/19976 (0.0%)
2	B	0.52	0/257	0.49	0/393
3	D	0.53	0/292	0.49	0/448
All	All	0.47	0/15308	0.56	4/20817 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	847	PRO	N-CA-C	-6.23	99.64	112.47
1	A	847	PRO	CA-C-N	-5.88	114.00	123.23
1	A	847	PRO	C-N-CA	-5.88	114.00	123.23
1	A	1533	ASP	N-CA-C	-5.43	108.43	114.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14464	0	14458	392	0
2	B	250	0	137	8	0
3	D	261	0	147	9	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14980	0	14742	403	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (403) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:5CM:O4'	2:B:30:5CM:C1'	1.63	1.20
1:A:2011:PRO:HG2	1:A:2012:PRO:CD	1.70	1.19
1:A:2011:PRO:CG	1:A:2012:PRO:HD2	1.72	1.18
1:A:2011:PRO:HG2	1:A:2012:PRO:HD2	1.07	1.05
1:A:846:ARG:HB3	1:A:847:PRO:HD3	1.46	0.94
1:A:1948:ASN:CG	1:A:2014:PRO:HG3	1.96	0.91
1:A:2221:LEU:HD21	1:A:2223:LEU:HD23	1.55	0.87
1:A:562:ASP:OD2	1:A:822:GLN:NE2	2.09	0.84
1:A:2011:PRO:CG	1:A:2012:PRO:CD	2.46	0.82
2:B:25:DG:N2	3:D:12:DC:O2	2.09	0.82
1:A:2221:LEU:HD23	1:A:2221:LEU:O	1.80	0.82
1:A:846:ARG:HG3	1:A:846:ARG:HH11	1.45	0.81
1:A:441:VAL:HB	1:A:482:ASN:HD22	1.43	0.81
2:B:36:DG:N1	3:D:1:DC:N3	2.27	0.81
1:A:846:ARG:CB	1:A:847:PRO:HD3	2.11	0.79
1:A:1831:GLU:HG3	1:A:1834:ASP:HB3	1.65	0.79
1:A:2011:PRO:CD	1:A:2012:PRO:HD2	2.13	0.78
1:A:2013:SER:HB3	1:A:2014:PRO:HD2	1.65	0.78
1:A:713:VAL:HA	1:A:716:LEU:HD23	1.64	0.78
1:A:1774:VAL:O	1:A:1813:ARG:NH1	2.16	0.78
1:A:789:GLU:HG3	1:A:791:HIS:HB3	1.67	0.77
1:A:1948:ASN:OD1	1:A:2014:PRO:HG3	1.84	0.77
1:A:1394:GLU:HG2	1:A:1411:ARG:HG2	1.67	0.77
1:A:2013:SER:HB3	1:A:2014:PRO:CD	2.15	0.77
1:A:2085:PRO:HD3	1:A:2093:MET:HE2	1.67	0.75
1:A:2117:CYS:SG	1:A:2118:VAL:N	2.60	0.74
1:A:1397:GLN:H	1:A:1405:LEU:HD21	1.51	0.74
1:A:1893:SER:OG	1:A:1894:LYS:N	2.15	0.74
2:B:36:DG:N2	3:D:1:DC:O2	2.17	0.73
1:A:2011:PRO:HG2	1:A:2012:PRO:HD3	1.67	0.73
1:A:2080:GLU:HG2	1:A:2119:LYS:HD2	1.71	0.73
2:B:25:DG:N1	3:D:12:DC:N3	2.28	0.72
1:A:1777:ASP:HB3	1:A:1788:ARG:HH11	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:HD22	1:A:345:ARG:HB3	1.73	0.71
1:A:2127:VAL:O	1:A:2128:ARG:NH1	2.24	0.71
1:A:846:ARG:HG3	1:A:846:ARG:NH1	2.05	0.71
1:A:1261:HIS:CD2	1:A:1262:ILE:HG12	2.25	0.71
1:A:1460:VAL:HG22	1:A:1748:ILE:HB	1.74	0.70
1:A:1353:ARG:NH1	1:A:1434:ILE:O	2.24	0.70
1:A:555:GLU:OE2	1:A:1095:ARG:NH1	2.25	0.69
1:A:959:ILE:HG22	1:A:975:LEU:HD13	1.74	0.69
1:A:1095:ARG:NH2	1:A:1113:LEU:O	2.26	0.69
1:A:2266:VAL:O	1:A:2271:GLN:NE2	2.25	0.68
1:A:2221:LEU:HD23	1:A:2221:LEU:C	2.18	0.68
1:A:1936:LEU:HG	1:A:1940:GLN:HE21	1.58	0.68
1:A:1909:LEU:HD13	1:A:1928:ILE:HG12	1.76	0.67
1:A:308:VAL:HB	1:A:510:LYS:HE2	1.76	0.67
1:A:997:GLU:HA	1:A:1149:LYS:HA	1.75	0.67
1:A:2095:ILE:HG22	1:A:2102:VAL:HB	1.77	0.67
1:A:2149:TYR:CE2	1:A:2185:ALA:HA	2.29	0.67
1:A:2186:LEU:HD11	1:A:2193:HIS:CD2	2.30	0.67
1:A:998:LEU:N	1:A:1148:VAL:O	2.26	0.67
1:A:1456:VAL:HG11	1:A:1770:ILE:HD11	1.78	0.66
1:A:669:ASN:ND2	1:A:671:ASP:OD1	2.27	0.66
1:A:869:LYS:NZ	1:A:1248:GLU:OE1	2.20	0.65
1:A:513:TYR:CE2	1:A:548:ARG:HD2	2.31	0.65
1:A:1019:SER:OG	1:A:1033:THR:OG1	2.13	0.65
1:A:1512:PRO:HA	1:A:1515:ILE:HG22	1.79	0.65
1:A:1200:CYS:HB2	1:A:1273:ARG:HH11	1.62	0.64
1:A:660:LYS:NZ	1:A:1094:THR:O	2.30	0.64
1:A:658:GLY:H	1:A:694:THR:HG22	1.63	0.64
1:A:2119:LYS:HE2	1:A:2122:GLU:HB2	1.80	0.64
1:A:1743:SER:OG	1:A:1744:SER:N	2.29	0.64
1:A:832:CYS:SG	1:A:849:HIS:HB3	2.38	0.63
1:A:622:LYS:O	1:A:846:ARG:HG2	1.98	0.63
1:A:2283:LEU:O	1:A:2285:THR:OG1	2.17	0.63
1:A:309:ARG:O	1:A:678:LYS:HG3	1.99	0.63
1:A:2013:SER:CB	1:A:2014:PRO:CD	2.76	0.63
1:A:2249:THR:HG21	1:A:2254:ASN:HB3	1.80	0.62
1:A:1053:ARG:NH1	1:A:1085:PRO:O	2.31	0.62
1:A:1113:LEU:HD11	1:A:1119:ARG:HB3	1.81	0.62
1:A:2170:LEU:HD21	1:A:2223:LEU:HD21	1.81	0.62
3:D:6:DC:H4'	3:D:7:DG:H5'	1.82	0.61
1:A:762:LYS:O	1:A:766:LEU:HG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2081:CYS:HB2	1:A:2103:ALA:HB1	1.80	0.61
1:A:1575:LEU:HB2	1:A:1587:ARG:CZ	2.30	0.61
1:A:1902:LYS:NZ	1:A:2177:ASP:OD2	2.33	0.61
1:A:484:CYS:HA	1:A:521:VAL:HG23	1.82	0.61
1:A:658:GLY:H	1:A:694:THR:CG2	2.13	0.61
1:A:2298:LEU:O	1:A:2302:THR:OG1	2.18	0.61
1:A:1282:HIS:HB2	1:A:1304:PHE:HB3	1.83	0.61
1:A:1864:LEU:O	1:A:1866:MET:N	2.34	0.61
1:A:2194:VAL:HG21	1:A:2218:ALA:CB	2.31	0.60
1:A:1567:LEU:HD13	1:A:1716:MET:HE1	1.82	0.60
1:A:1430:VAL:HA	1:A:1453:PRO:HA	1.83	0.60
1:A:2087:THR:OG1	1:A:2088:ASN:N	2.33	0.60
1:A:2017:LYS:NZ	1:A:2020:PRO:HB3	2.17	0.60
1:A:2220:VAL:HG23	1:A:2220:VAL:O	2.01	0.60
1:A:1493:LEU:HD21	1:A:1596:VAL:HG22	1.84	0.59
1:A:907:GLN:NE2	1:A:911:THR:OG1	2.36	0.58
1:A:2233:SER:HB2	1:A:2265:ARG:NH2	2.18	0.58
1:A:1266:VAL:HG22	1:A:1268:GLU:H	1.69	0.58
1:A:696:ARG:NH1	1:A:704:GLU:OE1	2.33	0.58
1:A:2013:SER:CB	1:A:2014:PRO:HD2	2.32	0.58
1:A:480:LEU:HD22	1:A:523:LEU:HD22	1.86	0.58
1:A:1719:PHE:HB2	1:A:1743:SER:HB2	1.85	0.58
1:A:846:ARG:CB	1:A:847:PRO:CD	2.82	0.58
1:A:2233:SER:HB2	1:A:2265:ARG:HH22	1.70	0.57
1:A:510:LYS:HA	1:A:514:ILE:O	2.04	0.57
1:A:2174:GLN:O	1:A:2224:LYS:NZ	2.21	0.57
1:A:1196:THR:OG1	1:A:1197:THR:N	2.38	0.57
1:A:608:LEU:HD11	1:A:2124:GLN:HB3	1.86	0.56
1:A:473:HIS:O	1:A:475:PRO:HD3	2.05	0.56
1:A:1845:LYS:NZ	1:A:2284:ASP:OD2	2.39	0.56
1:A:1553:GLU:OE1	1:A:1553:GLU:N	2.36	0.56
1:A:2021:SER:O	1:A:2021:SER:OG	2.24	0.56
1:A:1533:ASP:O	1:A:1537:LYS:HD3	2.04	0.56
1:A:1580:GLY:HA3	1:A:1733:LYS:HD2	1.88	0.56
1:A:1408:GLU:HA	1:A:1411:ARG:HE	1.71	0.56
1:A:1494:ILE:HD12	1:A:1494:ILE:H	1.71	0.56
1:A:2194:VAL:HG21	1:A:2218:ALA:HB1	1.88	0.56
1:A:813:SER:HB2	1:A:859:VAL:HG13	1.88	0.55
1:A:1531:MET:HG2	1:A:1559:VAL:HG23	1.87	0.55
1:A:806:ILE:HG13	1:A:871:LEU:HD21	1.89	0.55
1:A:1105:VAL:HG23	1:A:1124:ARG:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:VAL:HB	1:A:482:ASN:ND2	2.19	0.55
1:A:1403:LEU:HB2	1:A:1404:PRO:HD3	1.88	0.55
1:A:1261:HIS:HB3	1:A:1366:SER:HA	1.88	0.55
1:A:1472:ILE:HG13	1:A:1473:SER:N	2.22	0.55
1:A:1869:ARG:NH2	1:A:1890:LEU:O	2.38	0.55
1:A:766:LEU:O	1:A:770:LYS:HG2	2.05	0.55
1:A:1180:ALA:HB2	1:A:1212:PRO:HD2	1.90	0.54
1:A:1575:LEU:HD13	1:A:1587:ARG:HG3	1.89	0.54
1:A:1730:LEU:HD13	1:A:1738:VAL:HG11	1.90	0.54
1:A:2048:GLU:OE2	1:A:2052:ARG:NE	2.40	0.54
1:A:885:CYS:O	1:A:889:VAL:HG23	2.06	0.54
1:A:1055:LEU:O	1:A:1059:TYR:OH	2.22	0.54
1:A:800:LYS:O	1:A:989:GLN:NE2	2.41	0.54
1:A:1406:ARG:O	1:A:1410:LEU:HD13	2.08	0.54
1:A:1507:LEU:O	1:A:1510:GLN:HG3	2.08	0.54
1:A:382:HIS:CE1	1:A:402:PRO:HB3	2.42	0.54
1:A:1397:GLN:N	1:A:1405:LEU:HD21	2.21	0.53
1:A:1925:CYS:O	1:A:1929:THR:HG23	2.07	0.53
1:A:623:GLY:H	1:A:629:ASN:ND2	2.06	0.53
1:A:2199:SER:O	1:A:2203:ARG:HG3	2.09	0.53
1:A:518:ARG:NH2	1:A:733:ALA:O	2.41	0.53
1:A:1500:LEU:HD21	1:A:1502:VAL:HG23	1.91	0.53
1:A:1897:GLU:HG3	1:A:2248:PHE:CZ	2.44	0.53
3:D:2:DC:H2"	3:D:3:DA:C8	2.44	0.53
1:A:1284:ILE:HD11	1:A:1304:PHE:CD1	2.44	0.53
1:A:897:ASN:O	1:A:1050:THR:HG23	2.10	0.52
1:A:1970:ARG:HG3	1:A:1971:GLN:HG3	1.90	0.52
1:A:1587:ARG:HH12	1:A:1591:ALA:HB2	1.74	0.52
1:A:720:SER:O	1:A:720:SER:OG	2.25	0.52
1:A:1414:TRP:O	1:A:1418:GLU:HG2	2.09	0.52
1:A:2084:LYS:C	1:A:2086:SER:H	2.18	0.52
1:A:1485:ALA:HB3	1:A:1486:PRO:HD3	1.91	0.51
1:A:1876:ASN:HB3	1:A:1879:GLN:HB3	1.91	0.51
1:A:2028:MET:HG3	1:A:2032:LYS:HD2	1.93	0.51
1:A:1895:THR:O	1:A:1898:GLU:N	2.37	0.51
1:A:2170:LEU:HD22	1:A:2172:PHE:CE1	2.45	0.51
1:A:409:VAL:HG23	1:A:412:LEU:HD12	1.92	0.51
1:A:538:LYS:O	1:A:542:THR:HG23	2.10	0.51
1:A:1219:GLU:OE1	1:A:1219:GLU:N	2.42	0.51
1:A:510:LYS:HD2	1:A:517:THR:HB	1.93	0.51
1:A:875:ARG:NE	1:A:921:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:GLU:O	1:A:1064:ARG:HB3	2.09	0.51
1:A:2101:HIS:CE1	1:A:2119:LYS:HD3	2.46	0.51
1:A:1832:ILE:C	1:A:1834:ASP:H	2.19	0.51
1:A:1377:SER:OG	1:A:1378:PRO:HD3	2.11	0.50
1:A:794:ASP:OD1	1:A:794:ASP:N	2.43	0.50
3:D:8:DC:H2"	3:D:9:DT:C5	2.46	0.50
1:A:596:ARG:HD3	1:A:669:ASN:HD21	1.77	0.50
1:A:1214:ASP:OD1	1:A:1214:ASP:N	2.44	0.50
1:A:1956:TRP:CZ3	1:A:2031:VAL:HG11	2.47	0.50
1:A:471:LYS:HG3	1:A:498:ILE:HD11	1.93	0.50
1:A:1052:ASP:OD1	1:A:1052:ASP:N	2.43	0.50
1:A:904:ASN:O	1:A:908:LEU:HG	2.12	0.50
1:A:2194:VAL:CG2	1:A:2218:ALA:HB1	2.42	0.50
1:A:992:LEU:HB2	1:A:1155:LEU:HD23	1.93	0.50
1:A:1436:GLU:CD	1:A:1806:SER:HG	2.20	0.50
1:A:2091:ILE:HG23	1:A:2092:GLU:H	1.77	0.50
1:A:1271:CYS:C	1:A:1273:ARG:H	2.19	0.50
1:A:990:ASP:HB3	1:A:993:CYS:HB3	1.93	0.49
1:A:1460:VAL:HB	1:A:1825:VAL:HG22	1.94	0.49
1:A:1842:HIS:CD2	1:A:2278:HIS:HB3	2.47	0.49
1:A:1536:GLU:N	1:A:1536:GLU:OE1	2.42	0.49
1:A:1995:ILE:O	1:A:1999:VAL:HG23	2.12	0.49
1:A:1221:MET:HG2	1:A:1328:LEU:HD22	1.95	0.49
1:A:513:TYR:CD2	1:A:548:ARG:HD2	2.48	0.49
1:A:783:ILE:HG22	1:A:1202:HIS:HB3	1.93	0.49
1:A:495:PHE:HA	1:A:498:ILE:HG22	1.94	0.49
1:A:2011:PRO:CB	1:A:2012:PRO:CD	2.90	0.49
1:A:1284:ILE:HD11	1:A:1304:PHE:HD1	1.77	0.49
1:A:2013:SER:HB2	1:A:2018:GLN:HE22	1.76	0.49
1:A:384:PHE:CD2	1:A:428:PRO:HG2	2.48	0.49
1:A:640:VAL:O	1:A:644:GLU:HG2	2.12	0.49
1:A:1793:THR:HB	1:A:1796:GLU:HG3	1.95	0.49
1:A:1048:GLU:OE1	1:A:1056:SER:OG	2.25	0.49
1:A:1359:SER:OG	1:A:1361:HIS:ND1	2.33	0.49
1:A:1848:ALA:HB1	1:A:2066:GLN:HE21	1.77	0.49
1:A:693:VAL:HB	1:A:696:ARG:HB3	1.94	0.48
1:A:1869:ARG:HB2	1:A:1894:LYS:HG2	1.96	0.48
1:A:2256:ARG:HE	1:A:2304:TRP:HB2	1.78	0.48
1:A:801:SER:O	1:A:989:GLN:NE2	2.42	0.48
1:A:1261:HIS:CG	1:A:1262:ILE:H	2.30	0.48
1:A:1408:GLU:HB2	1:A:1411:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASN:HB3	1:A:678:LYS:HD2	1.95	0.48
1:A:835:CYS:SG	1:A:835:CYS:O	2.71	0.48
1:A:1227:TRP:CE3	1:A:1329:ARG:HB3	2.48	0.48
1:A:1480:THR:OG1	1:A:1721:ARG:NH2	2.33	0.48
1:A:319:SER:O	1:A:319:SER:OG	2.31	0.48
1:A:1568:SER:O	1:A:1594:SER:OG	2.29	0.48
1:A:1947:VAL:O	1:A:1951:ILE:HG12	2.14	0.48
1:A:1470:THR:HG22	1:A:1511:TRP:CZ3	2.48	0.48
1:A:1840:HIS:ND1	1:A:2310:GLU:O	2.46	0.48
1:A:596:ARG:NH1	2:B:31:DG:OP2	2.47	0.48
1:A:1214:ASP:O	1:A:1218:SER:HB2	2.14	0.48
1:A:1357:THR:HG22	1:A:1358:THR:H	1.78	0.48
1:A:1587:ARG:NH1	1:A:1591:ALA:HB2	2.29	0.47
1:A:1713:VAL:HB	1:A:1716:MET:HE3	1.96	0.47
1:A:2256:ARG:NE	1:A:2304:TRP:HB2	2.29	0.47
1:A:345:ARG:NH2	1:A:432:ASP:OD2	2.35	0.47
1:A:1988:GLY:HA2	1:A:2054:ARG:NH2	2.29	0.47
1:A:484:CYS:HA	1:A:521:VAL:CG2	2.43	0.47
1:A:1005:THR:HG22	1:A:1142:ASP:OD1	2.15	0.47
1:A:1073:HIS:HE1	1:A:1131:GLU:OE2	1.97	0.47
1:A:1494:ILE:HB	1:A:1717:PHE:HB3	1.97	0.47
1:A:901:VAL:HG11	1:A:906:TRP:HB2	1.95	0.47
1:A:1840:HIS:ND1	1:A:2312:TYR:HB2	2.29	0.47
1:A:2085:PRO:HA	1:A:2089:PRO:O	2.15	0.47
1:A:2148:ARG:O	1:A:2149:TYR:CG	2.67	0.47
1:A:1212:PRO:HA	1:A:1334:ILE:HD13	1.95	0.47
1:A:1217:HIS:O	1:A:1217:HIS:ND1	2.47	0.47
1:A:1575:LEU:HA	1:A:1587:ARG:HG2	1.96	0.47
1:A:610:ARG:NH2	1:A:615:TRP:O	2.45	0.47
1:A:1521:SER:O	1:A:1521:SER:OG	2.29	0.47
1:A:1538:THR:HG23	1:A:1709:LEU:O	2.15	0.47
1:A:1716:MET:HE2	1:A:1716:MET:HB3	1.80	0.47
1:A:346:LYS:HD2	1:A:381:GLU:HB2	1.95	0.47
1:A:789:GLU:N	1:A:1184:ILE:O	2.44	0.47
1:A:2163:ILE:HG22	1:A:2312:TYR:CE2	2.50	0.47
1:A:643:LEU:O	1:A:647:THR:HG23	2.14	0.46
1:A:1011:THR:HG23	1:A:1136:GLN:HB3	1.97	0.46
1:A:1885:ARG:NH2	1:A:1942:ASP:OD2	2.37	0.46
1:A:1421:LYS:HZ2	1:A:1423:THR:HG22	1.80	0.46
1:A:360:LEU:HD22	1:A:380:PHE:HE2	1.80	0.46
1:A:959:ILE:CG2	1:A:975:LEU:HD13	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:SER:O	1:A:1075:LYS:NZ	2.40	0.46
1:A:1219:GLU:CD	1:A:1219:GLU:H	2.21	0.46
1:A:1256:LEU:O	1:A:1256:LEU:HD12	2.15	0.46
1:A:982:LEU:HD22	1:A:996:TRP:NE1	2.31	0.46
1:A:1589:ASP:O	1:A:1593:GLU:HG2	2.15	0.46
1:A:2175:TRP:HB2	1:A:2178:LEU:HD23	1.97	0.46
1:A:1390:LYS:HA	1:A:1411:ARG:HH22	1.81	0.46
1:A:1875:LYS:HD3	1:A:1875:LYS:HA	1.75	0.46
1:A:2186:LEU:HB2	1:A:2191:ILE:HD11	1.97	0.46
1:A:438:THR:HG21	1:A:732:ASN:O	2.16	0.46
1:A:902:ASN:HB3	1:A:905:ASP:OD2	2.16	0.46
1:A:2169:VAL:HG12	1:A:2170:LEU:N	2.31	0.46
1:A:1588:LEU:HD23	1:A:1592:MET:HG2	1.97	0.46
1:A:2178:LEU:O	1:A:2182:VAL:HG13	2.16	0.46
1:A:430:ASP:OD1	1:A:430:ASP:N	2.49	0.45
1:A:622:LYS:O	1:A:846:ARG:CG	2.64	0.45
1:A:2283:LEU:HA	1:A:2288:MET:HE3	1.99	0.45
1:A:778:VAL:CG2	1:A:1229:GLU:HG2	2.46	0.45
1:A:1015:GLU:OE1	1:A:1015:GLU:N	2.34	0.45
1:A:1776:ASP:OD1	1:A:1778:GLY:N	2.32	0.45
1:A:875:ARG:HD3	1:A:1245:TRP:CZ3	2.51	0.45
1:A:440:CYS:O	1:A:463:PHE:HD2	2.00	0.45
1:A:881:LEU:HD13	1:A:1153:ALA:HB2	1.99	0.45
1:A:2264:GLY:O	1:A:2268:ARG:HG2	2.17	0.45
1:A:896:SER:OG	1:A:897:ASN:N	2.50	0.45
1:A:1188:ALA:HB2	1:A:1256:LEU:HB3	1.98	0.45
1:A:1850:GLU:O	1:A:1853:VAL:HG22	2.17	0.45
1:A:1532:LYS:HD3	1:A:1532:LYS:HA	1.79	0.45
1:A:1465:VAL:HG21	1:A:2268:ARG:HA	1.98	0.45
1:A:1884:ALA:O	1:A:1888:GLU:HG3	2.16	0.45
1:A:383:VAL:HG12	1:A:384:PHE:HD2	1.81	0.45
1:A:1393:PRO:HD2	1:A:1414:TRP:CD2	2.52	0.45
1:A:1735:LEU:HA	1:A:1738:VAL:HG12	1.99	0.45
1:A:2153:LEU:HD22	1:A:2182:VAL:HG12	1.98	0.45
1:A:807:LEU:HD21	1:A:953:PRO:HG3	1.99	0.45
1:A:1406:ARG:HD2	1:A:1406:ARG:HA	1.69	0.45
1:A:1907:PHE:O	1:A:1908:THR:OG1	2.35	0.45
1:A:917:ILE:HD11	1:A:957:LEU:HD21	1.99	0.44
1:A:1525:VAL:O	1:A:1526:ILE:HD13	2.17	0.44
1:A:735:THR:O	1:A:739:VAL:HG23	2.16	0.44
1:A:1776:ASP:OD2	1:A:1810:HIS:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:ARG:HB2	2:B:30:5CM:P	2.57	0.44
1:A:1436:GLU:OE1	1:A:1445:ARG:NE	2.38	0.44
1:A:477:ILE:HD11	1:A:750:ALA:HB3	2.00	0.44
1:A:1059:TYR:HB3	1:A:1073:HIS:HB3	2.00	0.44
1:A:1140:LYS:HB3	1:A:1140:LYS:HE3	1.72	0.44
1:A:1870:LYS:HD3	1:A:1874:PHE:HZ	1.82	0.44
1:A:333:PRO:O	1:A:336:VAL:HG12	2.18	0.44
1:A:787:TYR:CE1	1:A:1191:ILE:HG12	2.52	0.44
1:A:1494:ILE:O	1:A:1718:ARG:N	2.45	0.44
1:A:997:GLU:HB3	1:A:1149:LYS:HB3	1.99	0.44
1:A:2079:SER:HB3	1:A:2103:ALA:HA	1.99	0.44
1:A:739:VAL:HG12	1:A:743:MET:HE2	1.99	0.44
1:A:2089:PRO:HB2	1:A:2091:ILE:HG22	2.00	0.44
1:A:675:GLY:O	1:A:676:SER:OG	2.24	0.44
1:A:1375:THR:HG22	1:A:1376:GLU:H	1.82	0.44
1:A:1390:LYS:HA	1:A:1411:ARG:NH2	2.32	0.44
1:A:1261:HIS:CB	1:A:1366:SER:HA	2.48	0.43
1:A:1539:ILE:HG13	1:A:1540:ALA:N	2.33	0.43
1:A:1988:GLY:HA2	1:A:2054:ARG:HH21	1.83	0.43
1:A:2240:HIS:CD2	1:A:2278:HIS:HE1	2.35	0.43
1:A:613:THR:OG1	1:A:644:GLU:OE2	2.14	0.43
1:A:1504:PRO:HG2	1:A:1726:GLU:HG3	2.00	0.43
1:A:1571:PRO:HB2	1:A:1574:TRP:HB2	2.00	0.43
1:A:1757:ASP:N	1:A:1757:ASP:OD1	2.51	0.43
1:A:400:PHE:O	1:A:402:PRO:HD3	2.18	0.43
1:A:1535:GLN:OE1	1:A:1535:GLN:N	2.51	0.43
1:A:1465:VAL:HG23	1:A:2268:ARG:HE	1.84	0.43
1:A:1470:THR:O	1:A:1474:ILE:HG12	2.17	0.43
1:A:1048:GLU:OE2	1:A:1048:GLU:HA	2.18	0.43
1:A:2246:PRO:HD3	1:A:2287:ASP:HB2	2.01	0.43
1:A:442:ASP:HB3	1:A:460:GLY:HA2	1.99	0.43
1:A:1476:LEU:O	1:A:1480:THR:HG23	2.19	0.43
1:A:2064:LYS:HE3	1:A:2064:LYS:HB2	1.75	0.43
2:B:30:5CM:H2'	2:B:30:5CM:H6	1.61	0.43
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.78	0.43
1:A:481:GLU:HG3	1:A:522:TYR:CZ	2.53	0.43
1:A:1285:LYS:HD2	1:A:1300:THR:HG22	2.01	0.43
1:A:1588:LEU:HD23	1:A:1588:LEU:O	2.19	0.43
1:A:1230:ILE:HD13	1:A:1230:ILE:HA	1.79	0.43
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.82	0.42
1:A:989:GLN:HG3	1:A:989:GLN:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1741:LEU:HD12	1:A:1742:SER:H	1.84	0.42
1:A:1838:VAL:HG21	1:A:2310:GLU:HB2	2.01	0.42
1:A:808:ASP:O	1:A:812:ARG:HG3	2.19	0.42
1:A:2169:VAL:HB	1:A:2220:VAL:HA	2.00	0.42
1:A:2194:VAL:HG21	1:A:2218:ALA:HB2	2.00	0.42
1:A:783:ILE:CG2	1:A:1202:HIS:HB3	2.48	0.42
1:A:816:HIS:CD2	1:A:858:ARG:NH2	2.87	0.42
1:A:1989:ASP:OD2	1:A:2057:ARG:NH2	2.53	0.42
1:A:2042:LEU:O	1:A:2046:VAL:HG23	2.19	0.42
1:A:2201:LYS:NZ	1:A:2204:ALA:HB3	2.34	0.42
1:A:554:PHE:CD1	1:A:554:PHE:C	2.97	0.42
1:A:1550:MET:HG3	1:A:1551:ALA:N	2.34	0.42
1:A:1574:TRP:CZ2	1:A:1587:ARG:HD3	2.55	0.42
1:A:641:ASP:O	1:A:645:ILE:HG13	2.20	0.42
1:A:778:VAL:HG21	1:A:1229:GLU:HG2	2.00	0.42
1:A:1427:HIS:HB2	1:A:1453:PRO:HB2	2.01	0.42
1:A:1528:ILE:HB	1:A:1533:ASP:HB3	2.02	0.42
1:A:2149:TYR:CZ	1:A:2185:ALA:HA	2.55	0.42
1:A:398:ARG:NH2	1:A:717:LEU:O	2.48	0.42
1:A:930:GLN:O	1:A:931:SER:HB3	2.20	0.42
1:A:981:ARG:HD3	1:A:997:GLU:OE2	2.19	0.42
1:A:1192:SER:HB3	1:A:1367:TRP:HE1	1.85	0.42
1:A:2181:LYS:HD3	1:A:2181:LYS:HA	1.65	0.42
1:A:888:ALA:HA	1:A:891:LYS:HG2	2.02	0.42
1:A:925:ARG:HD3	1:A:938:GLU:HB3	2.02	0.42
1:A:1008:ILE:HD12	1:A:1141:LEU:HD22	2.02	0.42
1:A:1432:GLU:HG3	1:A:1449:LYS:HD2	2.02	0.42
1:A:2240:HIS:HD2	1:A:2278:HIS:CE1	2.36	0.42
1:A:925:ARG:HH22	1:A:1242:ASN:HA	1.85	0.42
1:A:1244:ALA:O	1:A:1248:GLU:HG2	2.19	0.42
1:A:498:ILE:HG13	1:A:498:ILE:O	2.20	0.42
3:D:5:DG:H2'	3:D:6:DC:C5	2.55	0.42
1:A:2002:LYS:HB3	1:A:2002:LYS:HE3	1.78	0.42
1:A:846:ARG:HH11	1:A:846:ARG:CG	2.20	0.41
1:A:1261:HIS:CG	1:A:1262:ILE:N	2.88	0.41
1:A:1574:TRP:CE2	1:A:1587:ARG:HD3	2.55	0.41
1:A:2182:VAL:HG21	1:A:2222:LEU:HD11	2.02	0.41
1:A:579:GLN:OE1	1:A:580:THR:N	2.53	0.41
1:A:1526:ILE:HB	1:A:1548:ILE:HD13	2.01	0.41
1:A:2010:ILE:HG13	1:A:2011:PRO:HD2	2.02	0.41
1:A:1403:LEU:HD12	1:A:1403:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1535:GLN:HA	1:A:1711:ASN:OD1	2.20	0.41
1:A:2163:ILE:HD11	1:A:2169:VAL:HG22	2.01	0.41
1:A:325:PHE:O	1:A:329:VAL:HG23	2.20	0.41
1:A:477:ILE:HG23	1:A:524:PHE:HE1	1.86	0.41
1:A:803:LEU:HD23	1:A:986:ILE:HA	2.03	0.41
1:A:2172:PHE:HB3	1:A:2225:MET:HE2	2.02	0.41
1:A:774:ASP:O	1:A:778:VAL:HG12	2.20	0.41
1:A:846:ARG:HD2	1:A:846:ARG:HA	1.52	0.41
1:A:1397:GLN:O	1:A:1397:GLN:NE2	2.54	0.41
1:A:1016:LEU:H	1:A:1016:LEU:HD23	1.85	0.41
1:A:1407:LYS:O	1:A:1410:LEU:HB2	2.21	0.41
1:A:2070:SER:O	1:A:2074:ILE:HG13	2.20	0.41
1:A:816:HIS:CD2	1:A:858:ARG:CZ	3.03	0.41
1:A:875:ARG:HH21	1:A:1245:TRP:HZ3	1.68	0.41
1:A:1379:GLN:NE2	1:A:1380:PRO:HD2	2.35	0.41
1:A:1829:ILE:HD12	1:A:1829:ILE:HA	1.89	0.41
1:A:2057:ARG:O	1:A:2060:GLU:HG2	2.20	0.41
1:A:2173:LEU:HD21	1:A:2182:VAL:HG21	2.03	0.41
1:A:308:VAL:HG11	1:A:511:GLU:OE1	2.21	0.41
1:A:882:THR:OG1	1:A:883:ASP:N	2.54	0.41
1:A:1421:LYS:NZ	1:A:1423:THR:HG22	2.36	0.41
1:A:2106:LYS:C	1:A:2108:MET:H	2.28	0.41
1:A:886:LEU:HD11	1:A:914:LEU:HD21	2.03	0.40
1:A:955:TRP:CD1	1:A:984:ILE:HD11	2.56	0.40
1:A:1209:CYS:O	1:A:1336:SER:HA	2.21	0.40
1:A:1963:PHE:HD1	1:A:1963:PHE:HA	1.76	0.40
1:A:2170:LEU:HD11	1:A:2235:LEU:HD22	2.03	0.40
1:A:1284:ILE:CG1	1:A:1302:ILE:HB	2.51	0.40
1:A:1831:GLU:CG	1:A:1834:ASP:HB3	2.42	0.40
1:A:1936:LEU:HG	1:A:1940:GLN:NE2	2.31	0.40
3:D:12:DC:H2"	3:D:13:DA:C8	2.56	0.40
1:A:999:CYS:HB2	1:A:1147:TRP:CZ3	2.57	0.40
1:A:1563:ARG:NH2	1:A:1711:ASN:HB2	2.36	0.40
1:A:875:ARG:HD3	1:A:1245:TRP:CE3	2.57	0.40
1:A:1481:LEU:HD12	1:A:1481:LEU:HA	1.92	0.40
1:A:2153:LEU:CD2	1:A:2182:VAL:HG12	2.52	0.40
1:A:2261:GLN:O	1:A:2265:ARG:HG3	2.20	0.40
1:A:1082:ASP:OD1	1:A:1083:GLY:N	2.55	0.40
1:A:1150:CYS:HA	1:A:1151:PRO:HD3	1.97	0.40
1:A:1525:VAL:HG13	1:A:1547:ILE:HG23	2.02	0.40
1:A:1936:LEU:HD13	1:A:2052:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1990:ILE:O	1:A:1994:ARG:HD3	2.22	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	1806/2348 (77%)	1661 (92%)	145 (8%)	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	1569/2015 (78%)	1547 (99%)	22 (1%)	59	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	467	LEU
1	A	517	THR
1	A	717	LEU
1	A	846	ARG
1	A	850	VAL

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Mol	Chain	Res	Type
1	A	959	ILE
1	A	1105	VAL
1	A	1196	THR
1	A	1232	LEU
1	A	1250	LEU
1	A	1256	LEU
1	A	1357	THR
1	A	1430	VAL
1	A	1461	ILE
1	A	1554	ILE
1	A	1762	ARG
1	A	1775	GLU
1	A	1963	PHE
1	A	2010	ILE
1	A	2220	VAL
1	A	2221	LEU
1	A	2285	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	HIS
1	A	473	HIS
1	A	474	GLN
1	A	482	ASN
1	A	602	GLN
1	A	629	ASN
1	A	669	ASN
1	A	802	ASN
1	A	833	GLN
1	A	849	HIS
1	A	857	GLN
1	A	907	GLN
1	A	918	HIS
1	A	1234	HIS
1	A	1261	HIS
1	A	1319	HIS
1	A	1342	ASN
1	A	1379	GLN
1	A	1389	ASN
1	A	1409	GLN
1	A	1792	GLN

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Mol	Chain	Res	Type
1	A	1810	HIS
1	A	1811	ASN
1	A	1827	GLN
1	A	1927	HIS
1	A	1940	GLN
1	A	1949	GLN
1	A	2009	ASN
1	A	2066	GLN
1	A	2101	HIS
1	A	2115	GLN
1	A	2124	GLN
1	A	2131	ASN
1	A	2155	HIS
1	A	2158	ASN
1	A	2193	HIS
1	A	2211	GLN
1	A	2254	ASN
1	A	2278	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
2	5CM	B	30	2,3	18,21,22	5.06	13 (72%)	24,30,33	1.25	2 (8%)

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
2	5CM	B	30	2,3	-	6/7/21/22	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	30	5CM	O4'-C1'	9.60	1.63	1.42
2	B	30	5CM	C6-C5	8.35	1.48	1.34
2	B	30	5CM	O4'-C4'	-7.68	1.27	1.45
2	B	30	5CM	C2'-C1'	-7.58	1.31	1.52
2	B	30	5CM	C4-N3	6.40	1.44	1.34
2	B	30	5CM	C2-N3	5.86	1.48	1.36
2	B	30	5CM	O3'-C3'	-4.78	1.33	1.43
2	B	30	5CM	C5-C4	4.06	1.47	1.44
2	B	30	5CM	C4-N4	3.95	1.44	1.34
2	B	30	5CM	C6-N1	3.86	1.44	1.38
2	B	30	5CM	C2-N1	3.62	1.47	1.40
2	B	30	5CM	O2-C2	-3.31	1.17	1.23
2	B	30	5CM	C1'-N1	-2.80	1.41	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	30	5CM	C5-C6-N1	-2.91	120.16	123.31
2	B	30	5CM	C5A-C5-C6	-2.35	119.67	122.85

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	30	5CM	C3'-C4'-C5'-O5'
2	B	30	5CM	O4'-C4'-C5'-O5'
2	B	30	5CM	C2'-C1'-N1-C6
2	B	30	5CM	C2'-C1'-N1-C2
2	B	30	5CM	O4'-C1'-N1-C6
2	B	30	5CM	O4'-C1'-N1-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	30	5CM	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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.

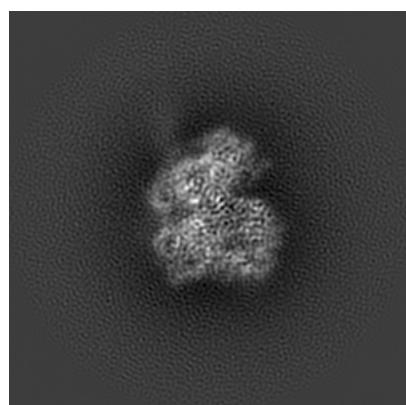
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24294. These allow visual inspection of the internal detail of the map and identification of artifacts.

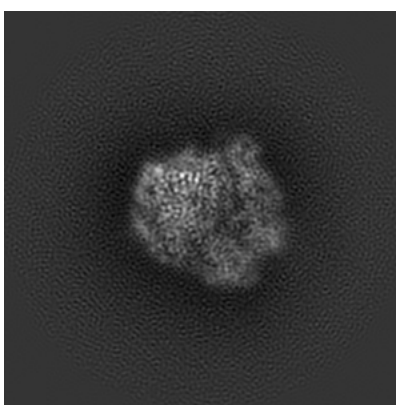
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

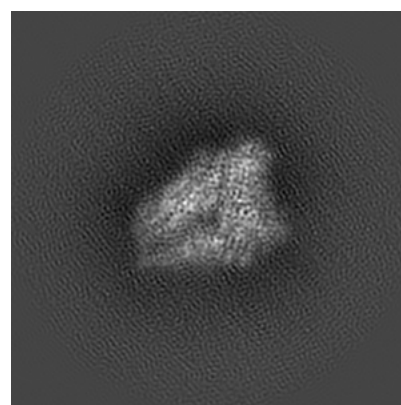
6.1.1 Primary map



X



Y

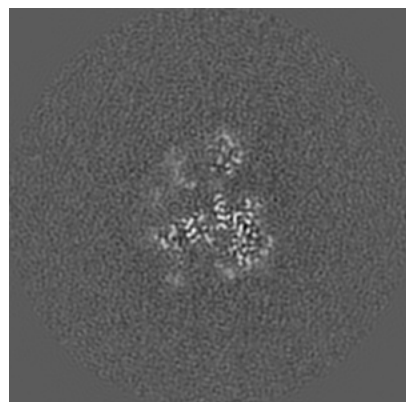


Z

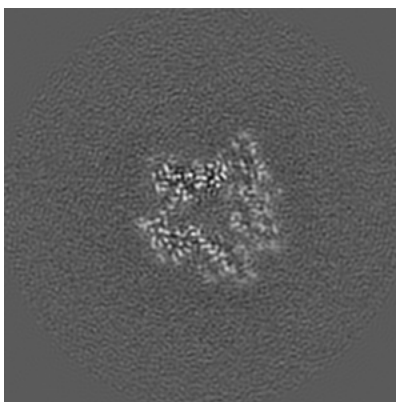
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

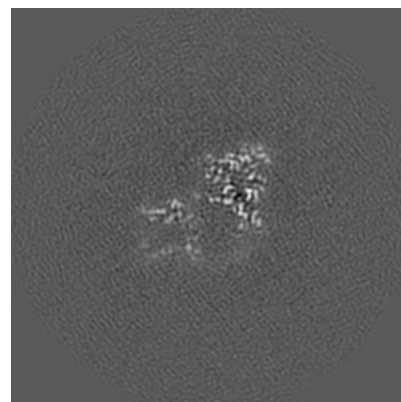
6.2.1 Primary map



X Index: 128



Y Index: 128

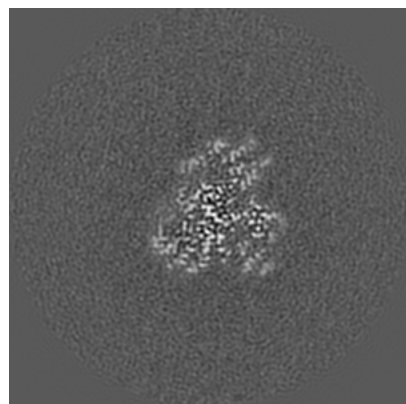


Z Index: 128

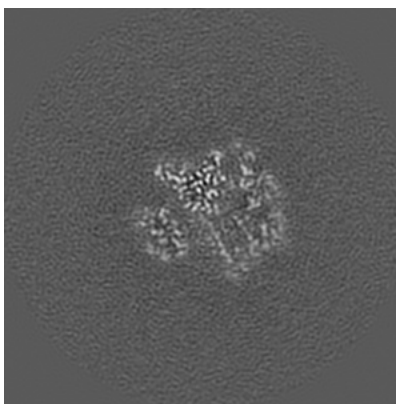
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

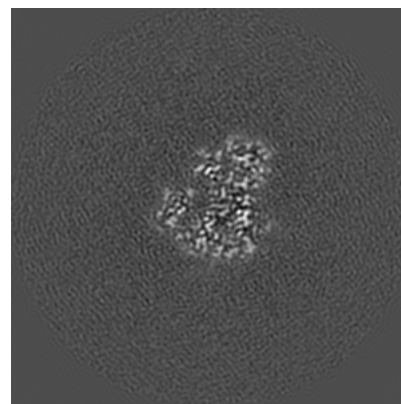
6.3.1 Primary map



X Index: 147



Y Index: 134

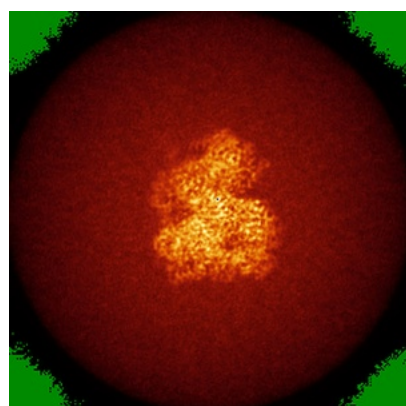


Z Index: 114

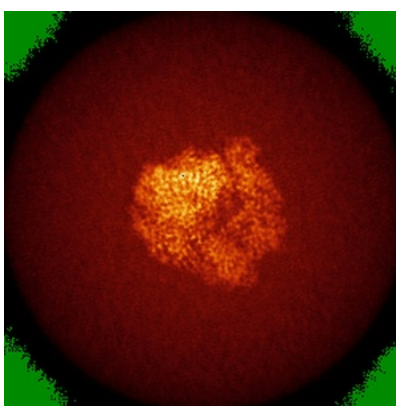
The images above show the largest variance slices of the map in three orthogonal directions.

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

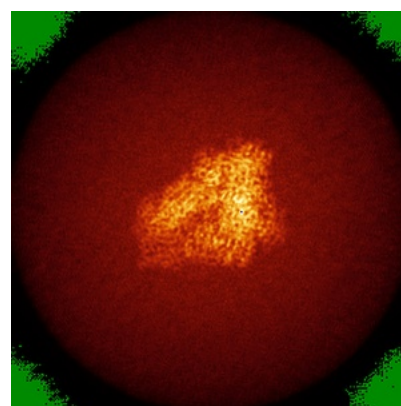
6.4.1 Primary map



X



Y

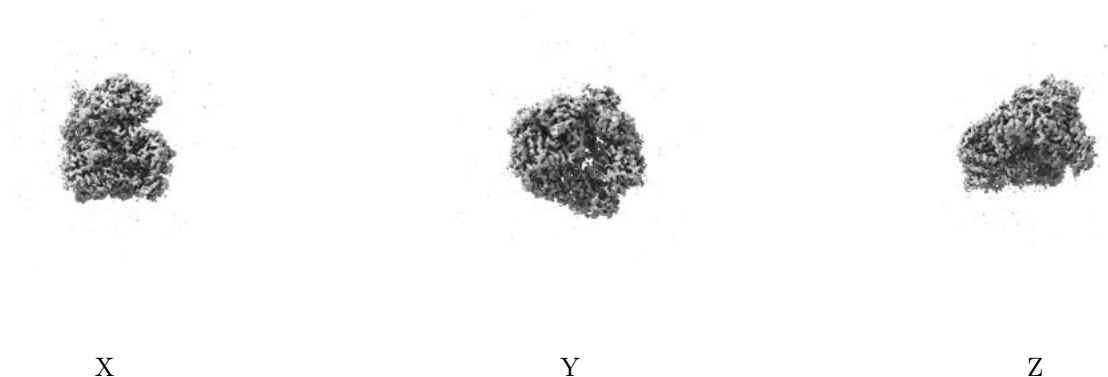


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

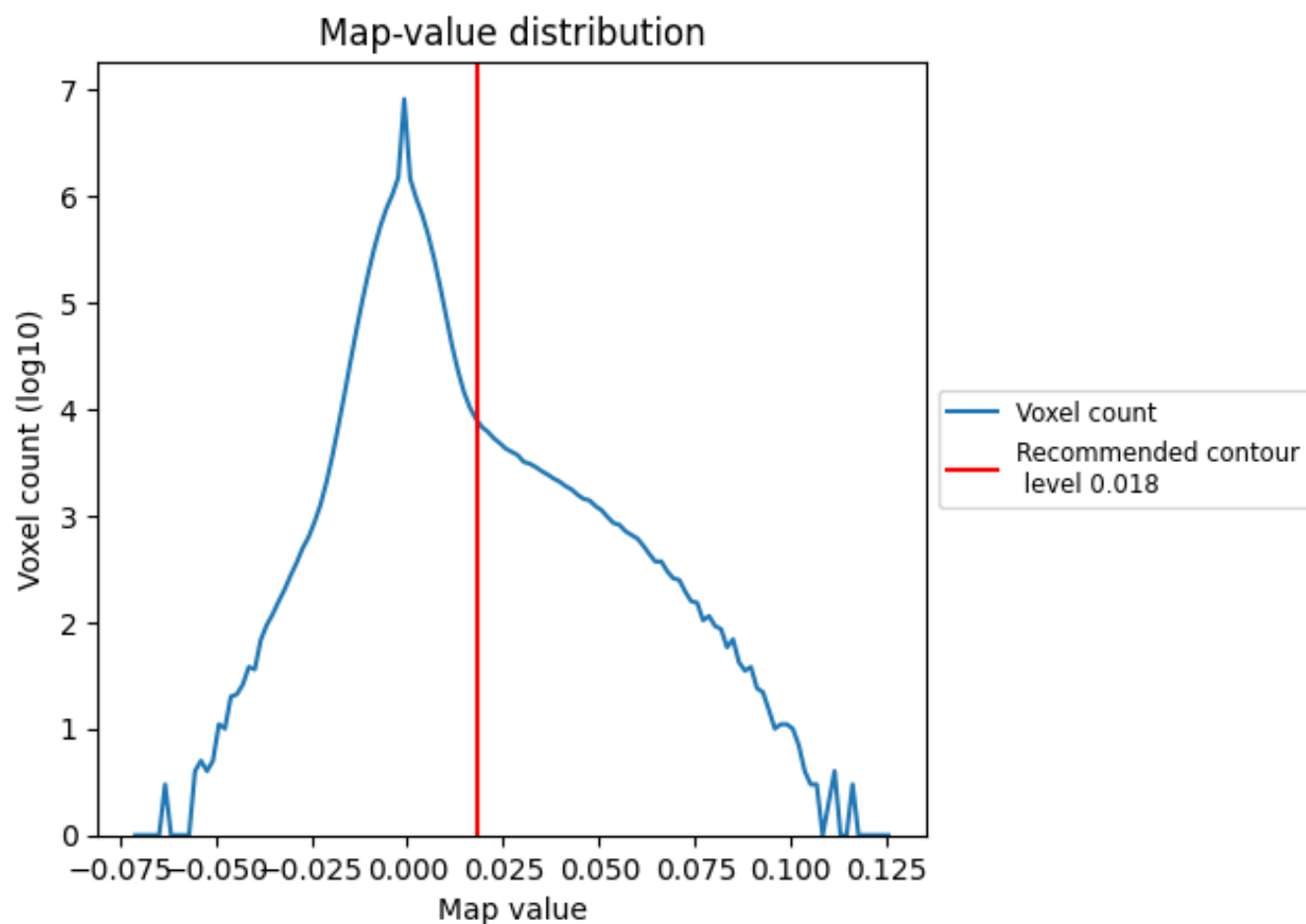
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

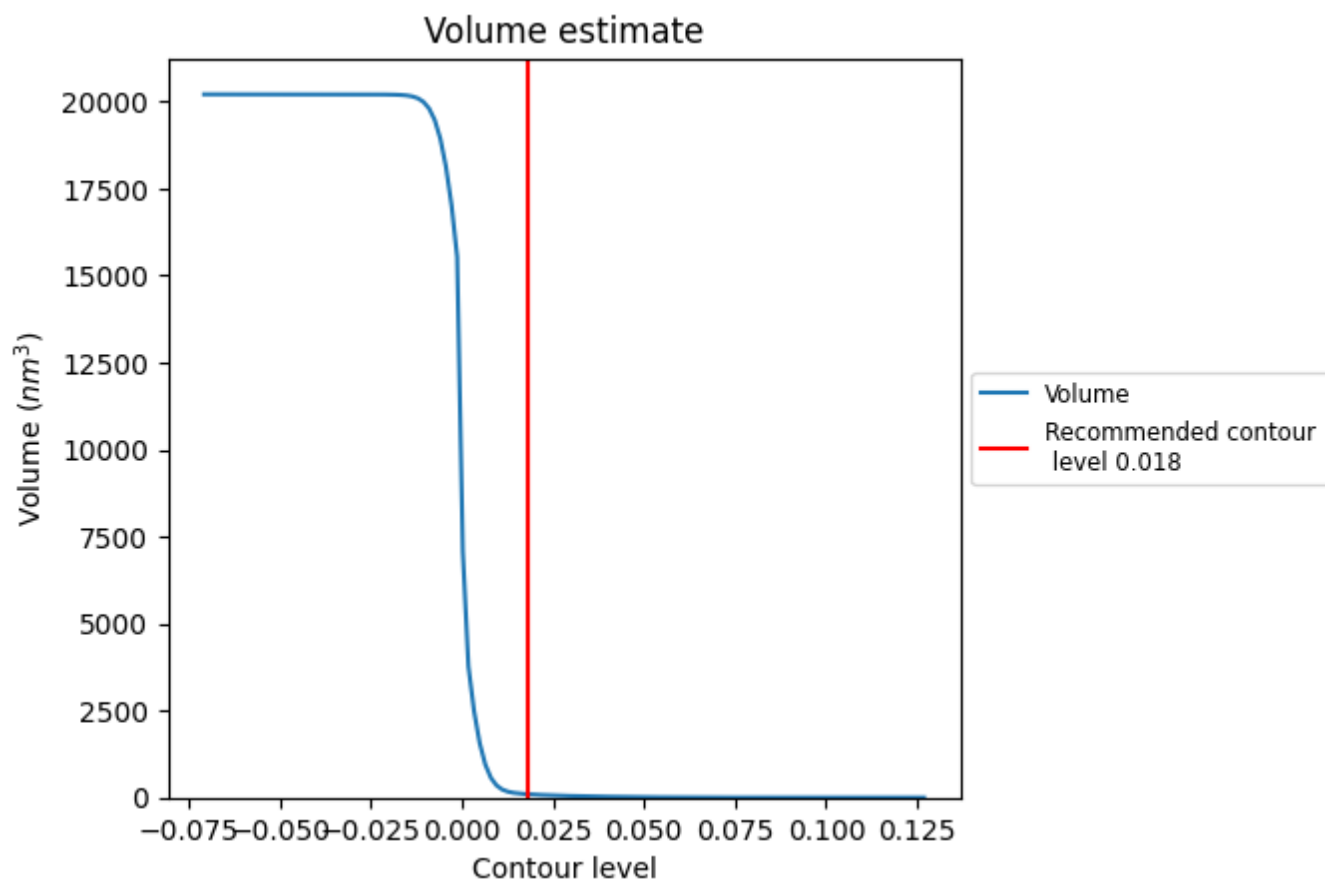
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

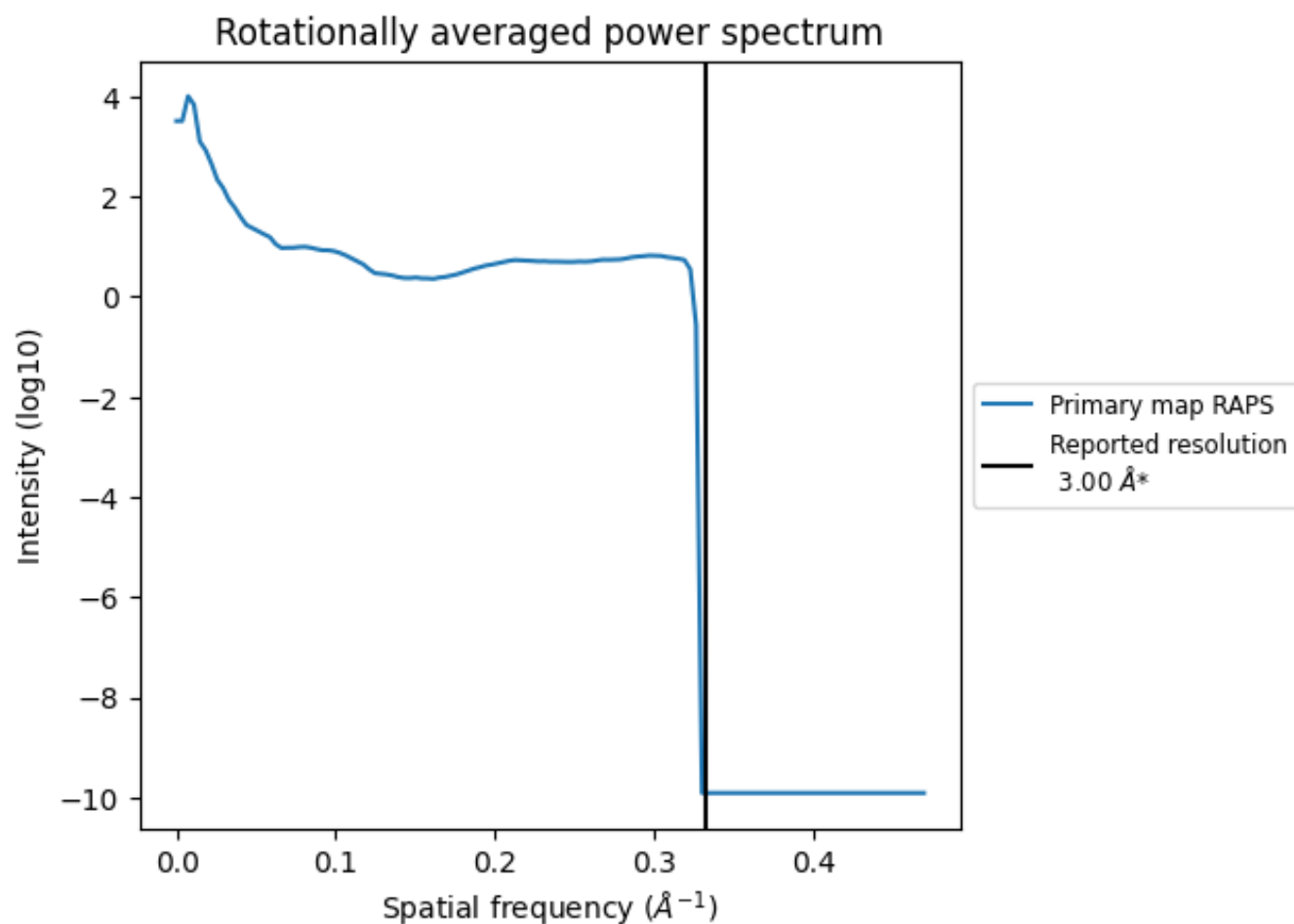
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm^3 ; this corresponds to an approximate mass of 87 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 0.333 Å⁻¹

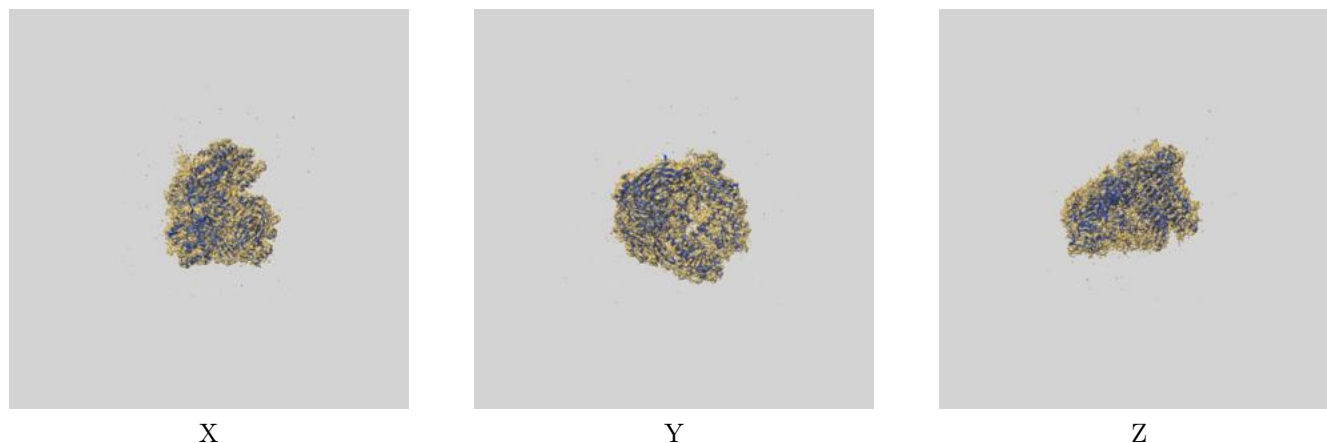
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

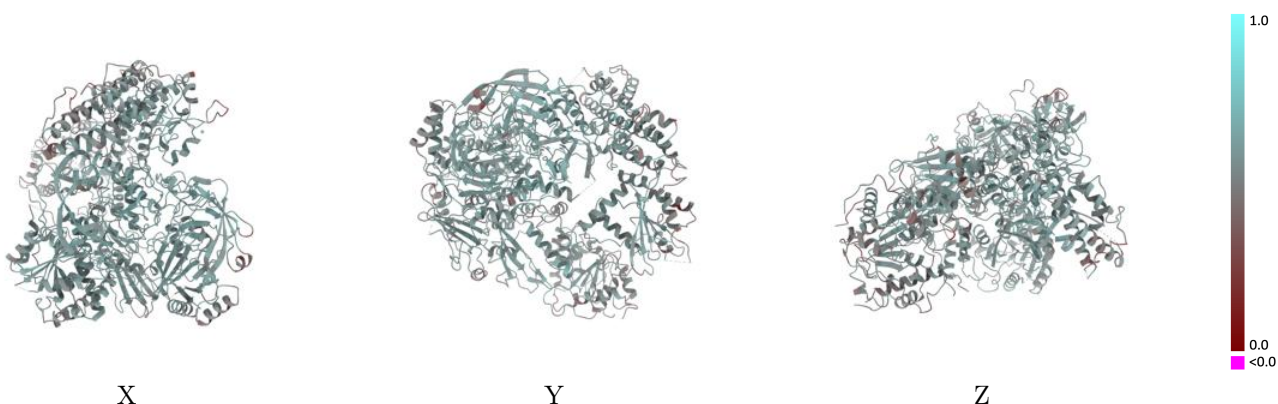
This section contains information regarding the fit between EMDB map EMD-24294 and PDB model 7R77. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



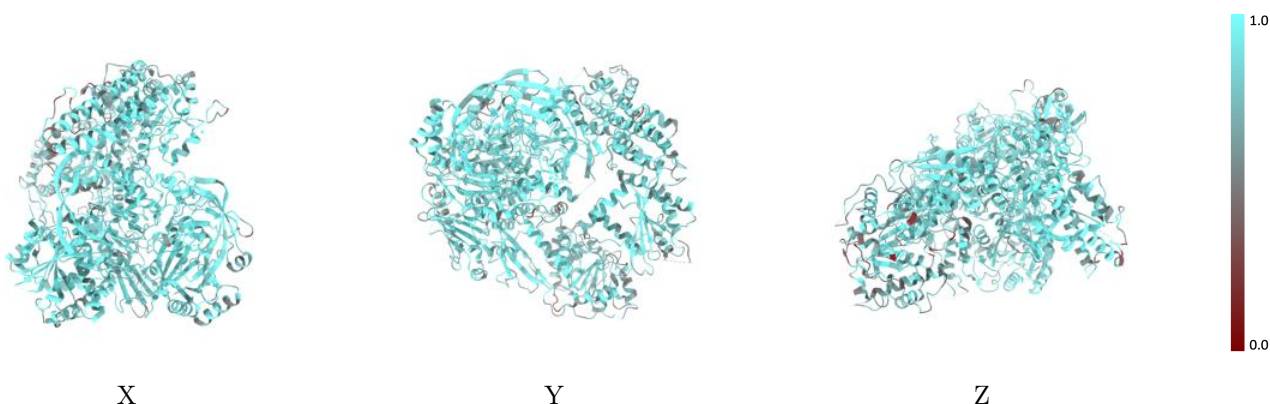
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



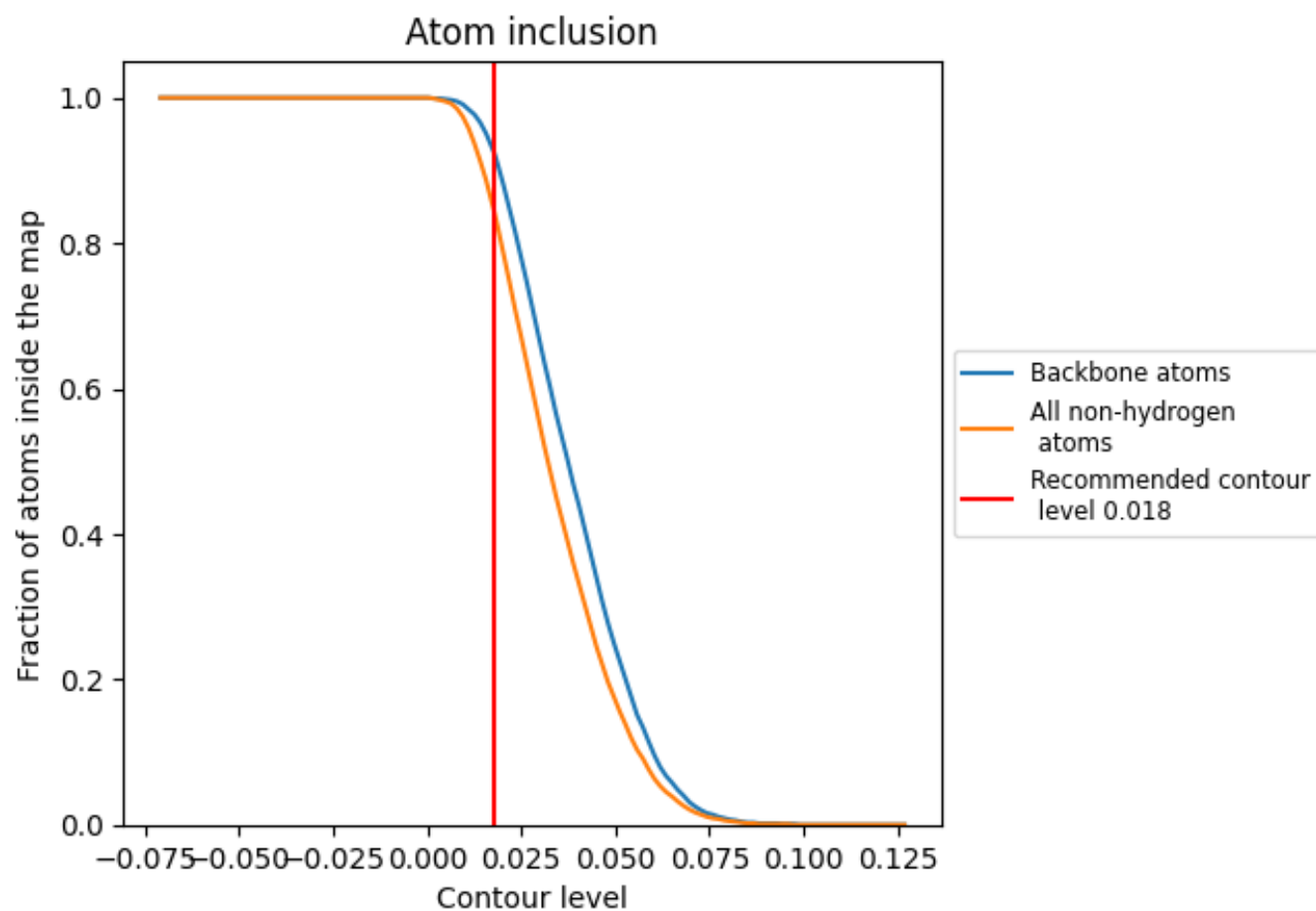
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.5480
A	0.8370	0.5470
B	0.9440	0.5910
D	0.9350	0.5770

