



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:21 AM UTC

PDB ID : 7R78 / pdb_00007r78
EMDB ID : EMD-24295
Title : cryo-EM structure of DNMT5 quaternary complex with hemimethylated DNA, AMP-PNP and SAH
Authors : Wang, J.; Patel, D.J.
Deposited on : 2021-06-24
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

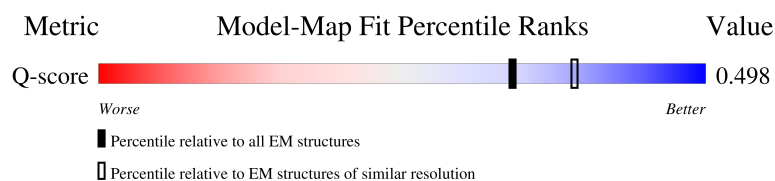
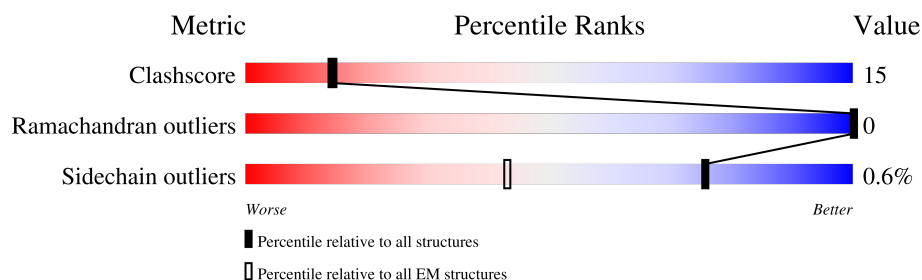
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	 54% 26% 20%
2	D	36	 17% 78%
3	E	36	 11% 17% 72%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15238 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	1880	Total	C	N	O	S	0	0
			14810	9284	2675	2780	71		

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

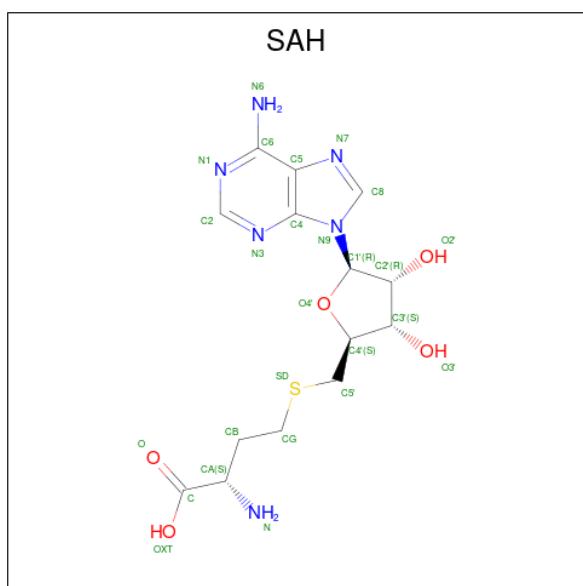
- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*AP*GP*(5CM)P*GP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	8	Total	C	N	O	P	0
			164	78	31	47	8	

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	10	Total	C	N	O	P	0
			201	97	38	57	9	

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).



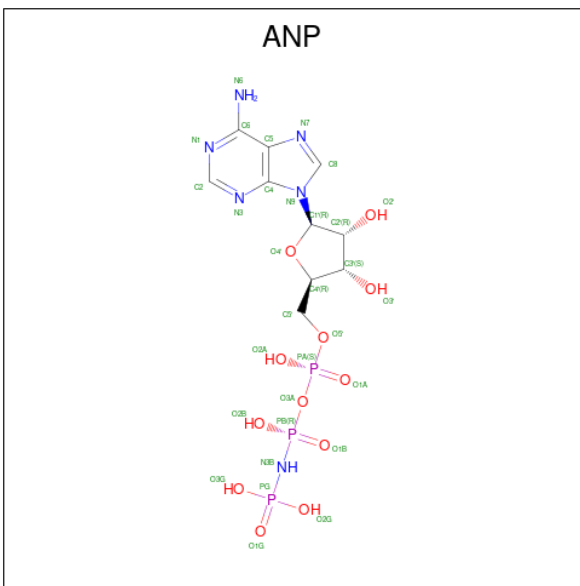
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	S
			26	14	6	5	1

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID:

ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total 31	C 10	N 6	O 12	P 3	0

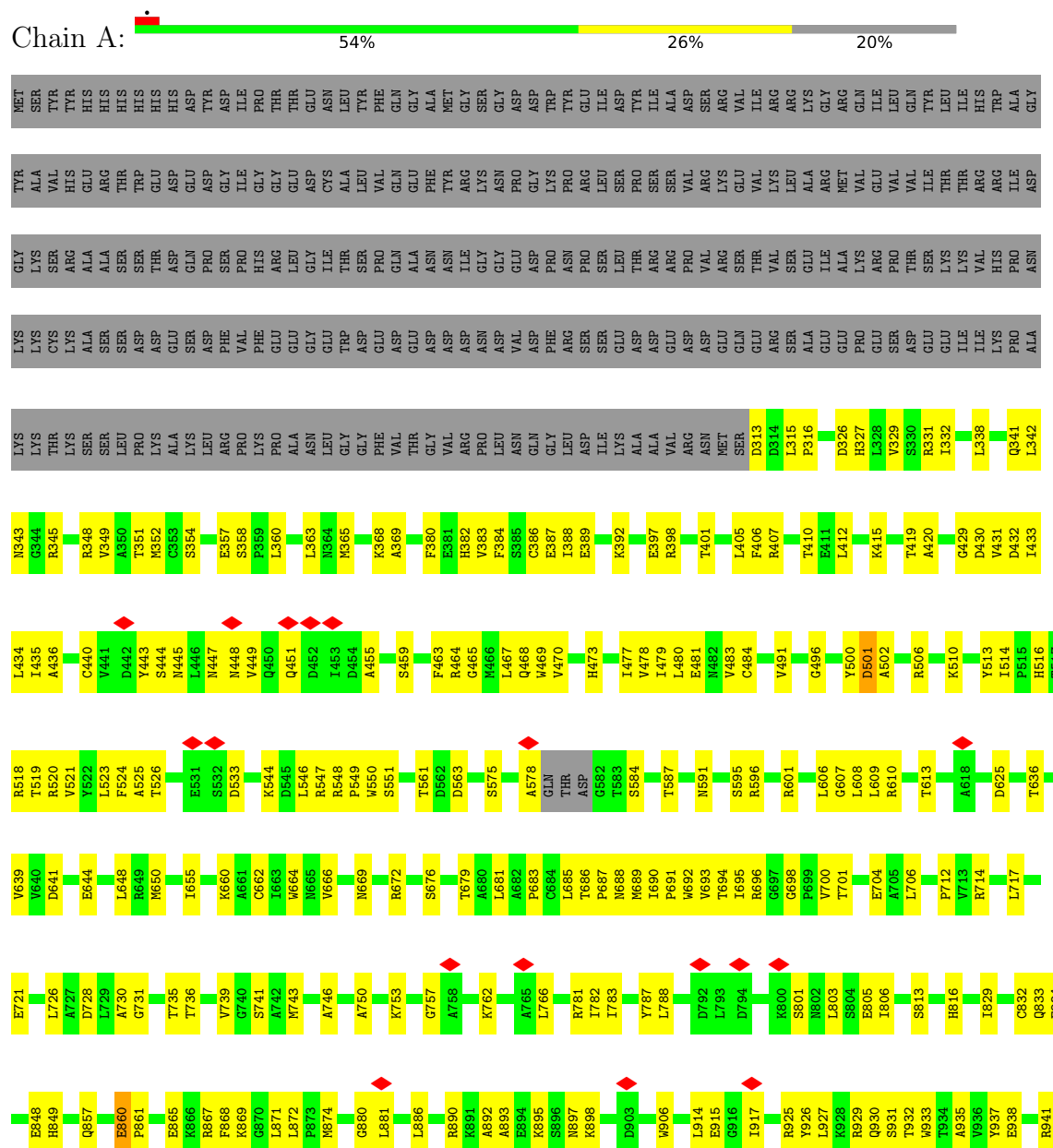
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total Mg 1 1	0

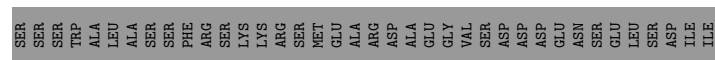
3 Residue-property plots

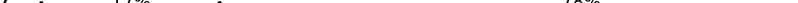
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

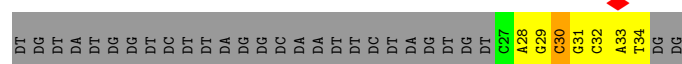
• Molecule 1: DNA repair protein Rad8

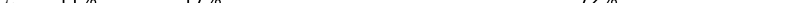


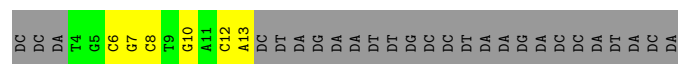
R2109	C2117	V2118	T2130	K2134	L2138	L2144	S2145	R2148	Y2149	E2167	R2168	V2169	L2170	L2173	S2183	S2187	R2190	H2193	K2201	S2202	N2205	T2206	L2207	Q2211	V2220	L2221	L2222	D2227	A2228	S2233	N2234	L2235	N2239	H2240	L2244	G2245	C2099	L2247																			
D2016	K2017	Q2018	S2019	P2020	S2021	L2022	A2023	S2024	G2025	A2026	K2027	M2028	V2031	R2036	K2043	V2046	V2053	L2056	R2057	F2058	F2059	V2062	K2067	G2068	K2069	S2070	Q2073	I2074	V2075	L2076	S2078	S2079	E2080	K2084	P2085	S2086	T2087	N2088	P2089	I2095	L2096	D2007	G2008	N2009	I2010	P2011	W2108										
E1923	R1932	A1933	A1938	E1941	D1942	L1943	V1947	N1948	I1951	G1955	V1956	I1957	K1958	K1959	K1960	G1961	G1962	F1963	S1964	K1965	N1966	D1967	L1968	E1969	R1970	Q1971	P1972	W1976	I1983	H1986	D1989	I1990	E1991	A1992	A1993	L1997	L2000	E2001	V2005	K2006	D2007	G2008	N2009	I2010	P2011												
Q1818	L1821	N1822	V1825	R1826	T1832	E1833	P1836	T1837	Y1854	L1855	E1856	L1857	E1858	Q1862	R1869	K1870	E1871	THR	LYS	PHE	LYS	N1876	D1881	R1882	L1886	E1887	E1888	S1891	D1892	S1893	E1898	C1904	L1909	D1910	L1911	S1912	D1913	K1914	T1915	Q1916	D1917	A1918	K1919	S1920	A1921	Q1922											
LYS	ASP	TYR	K1707	L1708	L1709	P1712	V1713	L1714	H1715	M1716	F1717	R1718	F1719	R1720	R1721	K1732	A1736	L1739	R1740	Y1745	L1749	P1754	V1755	S1756	D1757	A1760	I1761	I1770	H1771	D1777	G1780	D1781	VAL	GLN	TYR	GLN	LYS	ALA	ARG	ALA	LYS	D1791	Q1792	T1793	Q1794	W1809											
GLN	ALA	TYR	ARG	ASP	LYS	HIS	ASP	SER	ASP	SER	LYS	ALA	LYS	PRO	ILE	THR	LYS	GLU	GLU	LEU	GLU	ARG	K1605	G1606	E1607	E1608	A1609	R1612	M1613	M1614	E1615	D1616	K1617	K1618	K1619	X1620	L1621	V1622	D1623	N1624	S1627	K1628	K1629	E1630	V1631	L1632	L1633	ALA	VAL	ASN	ALA	SER	PHE	GLY	ARG	MET	GLY
V1460	I1461	D1463	G1468	K1469	T1470	I1471	I1472	A1475	T1480	P1486	E1487	P1488	A1489	T1490	P1491	L1493	L1496	K1497	A1498	T1499	L1500	I1501	P1504	G1505	H1506	L1507	F1518	T1519	I1528	K1532	D1533	L1534	E1535	E1536	K1537	T1538	I1539	I1547	W1548	V1549	A1550	A1551	I1554	S1557													
T1358	K1362	L1363	S1364	L1365	S1366	W1367	R1368	G1372	H1373	E1376	S1377	Q1378	P1379	L1386	P1387	S1388	N1389	K1390	S1396	Q1397	F1401	R1406	K1407	E1408	Q1409	L1410	R1411	S1412	W1415	E1420	E1432	E1433	I1434	S1435	E1436	V1442	G1443	R1445	A1446	E1447	G1448	K1449	V1456	R1457													
H1261	I1262	A1263	D1264	D1265	V1266	S1267	E1268	H1269	R1272	R1273	R1286	GLU	GLY	LYS	ALA	ASN	LYS	GLY	ASN	LYS	THR	LYS	SER	THR	ILE	A1303	F1304	E1305	A1310	E1314	P1321	Q1327	L1328	R1329	L1330	D1331	Q1332	D1333	I1334	G1335	S1336	F1337	R1338	N1342	I1343	V1344	A1347	L1351									
VAL	VAL	ALA	ASN	ASP	ALA	ALA	ALA	ASN	GLU	ILE	HIS	ARG	ASP	R1179	S1186	S1187	D1092	S1099	R1100	E1101	D1102	R1103	T1107	S1108	E1111	R1112	L1113	R1124	L1125	D1126	S1127	H1128	W1129	R1137	K1138	V1139	K1140	L1141	W1147	V1148	K1149	C1150	P1151	H1154	L1155	T1158	GLY	GLY	ASP	ASP	ILE	ALA					
L944	S945	L946	Y947	L948	R949	R950	Q951	L952	P953	E954	R955	R956	A980	R981	L982	A987	V991	P995	A996	E997	L998	C999	I1000	I1008	E1009	I1010	S1019	G1025	R1035	E1038	I1041	Q1044	A1045	E1046	T1050	L1051	D1052	R1053	K1054	Y1059	Q1060	L1061	L1062	P1063	R1064												



- Chain D:  17% 78%



- Chain E:  11% 17% 72%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23621	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	0.146	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SAH, ANP, 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	0.32	1/15111 (0.0%)	0.49	1/20456 (0.0%)
2	D	0.30	0/160	0.39	0/242
3	E	0.26	0/225	0.35	0/346
All	All	0.32	1/15496 (0.0%)	0.48	1/21044 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	681	LEU	C-N	-5.01	1.24	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	861	PRO	N-CA-C	-5.72	105.93	113.65

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	14810	0	14758	453	0
2	D	164	0	92	12	0
3	E	201	0	111	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	26	0	19	5	0
5	A	5	0	0	0	0
6	A	31	0	13	2	0
7	A	1	0	0	0	0
All	All	15238	0	14993	465	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 15.

All (465) 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:1379:GLN:HG3	1:A:1380:PRO:HD3	1.54	0.87
1:A:739:VAL:HG12	1:A:743:MET:HE2	1.59	0.84
1:A:2265:ARG:HG2	1:A:2265:ARG:HH21	1.40	0.84
1:A:636:THR:HG21	2:D:28:DA:H5'	1.61	0.83
1:A:2265:ARG:HG2	1:A:2265:ARG:NH2	1.98	0.79
1:A:880:GLY:HA3	1:A:917:ILE:HD11	1.64	0.78
1:A:1713:VAL:H	1:A:1716:MET:HE3	1.51	0.76
1:A:519:THR:O	1:A:520:ARG:NH1	2.19	0.76
1:A:874:MET:HB2	1:A:1249:ARG:HH21	1.50	0.75
1:A:1420:GLU:OE2	1:A:1721:ARG:NH2	2.21	0.74
1:A:897:ASN:ND2	1:A:1046:GLU:OE1	2.20	0.74
1:A:444:SER:HA	1:A:451:GLN:HG2	1.69	0.74
1:A:2005:VAL:HA	1:A:2009:ASN:HB2	1.69	0.73
1:A:1038:GLU:OE2	1:A:1076:ARG:NH1	2.21	0.73
1:A:429:GLY:HA3	1:A:473:HIS:HD2	1.54	0.73
1:A:1564:LEU:HD13	1:A:1713:VAL:HG11	1.69	0.73
1:A:587:THR:HG22	1:A:1869:ARG:HH11	1.53	0.72
1:A:1351:LEU:HD13	1:A:1363:ILE:HD13	1.69	0.72
1:A:1818:GLN:O	1:A:1822:ASN:ND2	2.23	0.72
1:A:980:ALA:HB2	1:A:998:LEU:HD12	1.71	0.72
1:A:548:ARG:NH2	1:A:551:SER:OG	2.24	0.71
1:A:546:LEU:HD11	1:A:741:SER:HB2	1.73	0.71
1:A:445:ASN:O	1:A:448:ASN:N	2.21	0.70
1:A:357:GLU:HG2	1:A:360:LEU:HD12	1.74	0.68
1:A:1445:ARG:NH2	1:A:1447:GLU:OE2	2.21	0.68
1:A:639:VAL:HG13	1:A:666:VAL:HG11	1.75	0.67
1:A:2169:VAL:HB	1:A:2220:VAL:HG12	1.75	0.67
1:A:501:ASP:OD1	1:A:501:ASP:N	2.23	0.67
1:A:650:MET:HE1	1:A:664:TRP:HE1	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1916:GLN:OE1	1:A:2148:ARG:NH2	2.28	0.67
1:A:516:HIS:HD2	1:A:518:ARG:HB3	1.59	0.66
1:A:1053:ARG:HD3	1:A:1084:LEU:HD13	1.77	0.66
1:A:1231:ASP:HB2	1:A:1234:HIS:HD2	1.61	0.66
1:A:484:CYS:SG	1:A:506:ARG:NH2	2.65	0.66
1:A:1964:SER:O	1:A:1966:ASN:ND2	2.29	0.66
1:A:2201:LYS:NZ	1:A:2205:ASN:OD1	2.29	0.66
1:A:925:ARG:NH1	1:A:938:GLU:OE1	2.29	0.65
1:A:2285:THR:HG22	1:A:2286:ILE:H	1.61	0.65
1:A:2300:GLU:OE1	1:A:2301:LYS:NZ	2.25	0.65
1:A:1222:TRP:HB3	1:A:1330:LEU:HB2	1.76	0.65
1:A:687:PRO:HB3	1:A:728:ASP:HA	1.78	0.64
1:A:1533:ASP:OD1	1:A:1537:LYS:NZ	2.30	0.64
1:A:949:ARG:NH2	1:A:954:GLU:OE2	2.31	0.64
1:A:1463:ASP:O	1:A:1469:LYS:NZ	2.29	0.64
1:A:2173:LEU:HD21	1:A:2222:LEU:HD21	1.80	0.63
1:A:672:ARG:HG2	2:D:32:DC:N4	2.14	0.63
1:A:1406:ARG:NH2	1:A:1409:GLN:OE1	2.32	0.63
1:A:526:THR:OG1	1:A:753:LYS:NZ	2.26	0.62
2:D:29:DG:H4'	2:D:29:DG:OP1	1.99	0.62
1:A:1582:ARG:NH1	1:A:1583:PHE:H	1.97	0.62
1:A:1989:ASP:OD2	1:A:2057:ARG:NH1	2.31	0.61
1:A:1328:LEU:HB3	1:A:1337:PHE:HB3	1.82	0.61
1:A:1904:CYS:HB3	1:A:2285:THR:HG21	1.81	0.61
1:A:691:PRO:HG2	1:A:700:VAL:HG22	1.83	0.61
1:A:655:ILE:HG22	1:A:1099:SER:HB3	1.83	0.61
1:A:662:CYS:HB3	1:A:679:THR:HG22	1.82	0.61
1:A:636:THR:CG2	2:D:28:DA:H5'	2.28	0.61
1:A:881:LEU:HD23	1:A:881:LEU:O	2.00	0.61
1:A:1951:ILE:HD11	1:A:2011:PRO:HD2	1.82	0.61
1:A:1818:GLN:OE1	1:A:1822:ASN:ND2	2.34	0.61
1:A:1067:GLN:HG3	1:A:1068:ALA:H	1.65	0.60
1:A:1579:GLN:HG3	1:A:1732:LYS:HD2	1.81	0.60
1:A:443:TYR:HH	1:A:459:SER:HG	1.45	0.60
1:A:2298:LEU:HB3	1:A:2304:TRP:CD1	2.37	0.60
1:A:383:VAL:HG11	1:A:431:VAL:HG12	1.83	0.60
1:A:1986:HIS:CD2	1:A:1993:ALA:HB2	2.37	0.60
1:A:2167:GLU:CD	1:A:2239:ASN:HD21	2.10	0.59
1:A:429:GLY:HA3	1:A:473:HIS:CD2	2.35	0.59
1:A:929:ARG:HG3	1:A:933:TRP:CZ2	2.37	0.59
1:A:1227:TRP:HA	1:A:1329:ARG:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ARG:NH2	1:A:731:GLY:O	2.33	0.58
1:A:801:SER:OG	1:A:805:GLU:OE2	2.21	0.58
1:A:1386:LEU:HD11	1:A:1755:VAL:HG21	1.85	0.58
1:A:1754:PRO:HB2	1:A:1760:ALA:HB1	1.85	0.58
1:A:874:MET:HB2	1:A:1249:ARG:NH2	2.17	0.58
1:A:2193:HIS:HB3	1:A:2220:VAL:HG23	1.85	0.58
1:A:516:HIS:CD2	1:A:518:ARG:HB3	2.37	0.58
1:A:803:LEU:HA	1:A:806:ILE:HG22	1.85	0.58
1:A:813:SER:O	1:A:933:TRP:NE1	2.26	0.58
1:A:1972:PRO:HG2	1:A:2036:ARG:HG3	1.85	0.58
1:A:455:ALA:HA	1:A:459:SER:HB2	1.85	0.58
1:A:463:PHE:CZ	1:A:491:VAL:HG13	2.37	0.58
1:A:1564:LEU:HD11	1:A:1595:LEU:HD22	1.85	0.58
1:A:2297:GLU:OE1	1:A:2301:LYS:NZ	2.33	0.58
1:A:1434:ILE:O	1:A:1809:TRP:NE1	2.34	0.58
1:A:1736:ALA:O	1:A:1740:ARG:NH1	2.37	0.58
1:A:343:ASN:HB3	1:A:757:GLY:H	1.68	0.57
1:A:2239:ASN:HD22	1:A:2273:LYS:HD3	1.69	0.57
1:A:860:GLU:HA	1:A:860:GLU:OE2	2.03	0.57
1:A:860:GLU:HG3	1:A:1376:GLU:HB3	1.86	0.57
1:A:1460:VAL:HB	1:A:1825:VAL:HG22	1.84	0.57
1:A:2266:VAL:O	1:A:2271:GLN:NE2	2.37	0.57
1:A:500:TYR:HB3	1:A:525:ALA:HB1	1.86	0.57
1:A:2265:ARG:HH21	1:A:2265:ARG:CG	2.13	0.57
1:A:687:PRO:HD3	3:E:6:DC:H2"	1.85	0.57
1:A:951:GLN:HB3	1:A:952:ILE:HD12	1.87	0.57
1:A:1486:PRO:HB2	1:A:1488:PRO:HD2	1.86	0.57
1:A:816:HIS:HB3	1:A:829:ILE:HG21	1.86	0.57
1:A:342:LEU:HD12	1:A:345:ARG:HG3	1.87	0.57
1:A:686:THR:OG1	1:A:688:ASN:OD1	2.21	0.57
1:A:1266:VAL:HG22	1:A:1362:LYS:HE2	1.85	0.57
1:A:1504:PRO:HD2	1:A:1507:LEU:HD22	1.87	0.57
1:A:1832:ILE:HG13	1:A:1833:GLU:H	1.70	0.57
1:A:1943:LEU:O	1:A:1947:VAL:HG23	2.05	0.56
1:A:591:ASN:OD1	1:A:2043:ARG:NH1	2.38	0.56
1:A:613:THR:OG1	1:A:644:GLU:OE2	2.23	0.56
1:A:1078:ASP:OD1	1:A:1080:SER:N	2.37	0.56
1:A:1468:GLY:HA2	6:A:2407:ANP:O2A	2.06	0.56
1:A:1566:TYR:HD2	1:A:1567:LEU:HD22	1.69	0.56
1:A:714:ARG:HD2	1:A:1235:GLN:HB3	1.87	0.56
1:A:1126:ASP:OD1	1:A:1127:SER:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ARG:NH2	1:A:641:ASP:OD1	2.38	0.56
1:A:2022:ILE:HD12	1:A:2031:VAL:HG22	1.87	0.56
1:A:2261:GLN:HG2	1:A:2265:ARG:HH22	1.69	0.56
1:A:2265:ARG:NH1	6:A:2407:ANP:O3G	2.39	0.56
3:E:10:DG:H8	3:E:10:DG:H5"	1.70	0.56
1:A:587:THR:HG22	1:A:1869:ARG:NH1	2.18	0.56
1:A:683:PRO:HG2	1:A:689:MET:HE1	1.88	0.56
1:A:351:THR:HG22	1:A:435:ILE:HG23	1.88	0.56
1:A:2006:LYS:H	1:A:2009:ASN:CG	2.13	0.56
1:A:1457:ARG:NH1	1:A:1487:GLU:OE1	2.38	0.55
1:A:313:ASP:OD1	1:A:313:ASP:N	2.39	0.55
1:A:1992:ALA:HB2	1:A:2053:VAL:HG11	1.89	0.55
1:A:1989:ASP:OD1	1:A:1990:ILE:N	2.40	0.55
1:A:1273:ARG:O	1:A:1321:PRO:HD3	2.06	0.55
1:A:1310:ALA:O	1:A:1314:GLU:HG2	2.05	0.55
1:A:1539:ILE:HD11	1:A:1712:PRO:HB3	1.87	0.55
1:A:1577:ASP:OD2	1:A:1587:ARG:NH2	2.40	0.55
1:A:2183:SER:O	1:A:2187:SER:HB2	2.07	0.55
1:A:331:ARG:NH2	1:A:546:LEU:HA	2.22	0.54
1:A:349:VAL:HG13	1:A:433:ILE:HG23	1.88	0.54
2:D:30:5CM:H2'	2:D:31:DG:C8	2.42	0.54
1:A:510:LYS:HA	1:A:514:ILE:O	2.07	0.54
1:A:2096:LEU:HB2	1:A:2108:MET:HE1	1.88	0.54
1:A:613:THR:N	1:A:644:GLU:OE2	2.41	0.54
1:A:1202:HIS:O	1:A:1342:ASN:ND2	2.40	0.54
1:A:1347:ALA:HB1	1:A:1365:LEU:HD13	1.90	0.54
1:A:1881:ASP:OD1	1:A:1932:ARG:NH2	2.40	0.54
2:D:28:DA:N6	3:E:8:DC:N4	2.56	0.54
1:A:464:ARG:NH1	1:A:468:GLN:HE21	2.05	0.54
1:A:1983:ILE:HD12	1:A:1983:ILE:H	1.72	0.54
1:A:610:ARG:HA	1:A:644:GLU:HG2	1.90	0.54
1:A:650:MET:HE1	1:A:664:TRP:NE1	2.22	0.54
1:A:1223:ARG:HD3	1:A:1228:ALA:HB2	1.88	0.54
1:A:1957:ILE:HG23	1:A:2028:MET:HE3	1.90	0.54
1:A:1618:LYS:O	1:A:1622:VAL:HG13	2.08	0.53
1:A:1532:LYS:O	1:A:1536:GLU:HG2	2.07	0.53
1:A:348:ARG:N	1:A:432:ASP:OD2	2.38	0.53
1:A:591:ASN:O	1:A:2043:ARG:NH1	2.41	0.53
1:A:2247:LEU:HD23	1:A:2255:TYR:CD2	2.43	0.53
1:A:1432:GLU:HG3	1:A:1449:LYS:HE3	1.90	0.53
1:A:2144:LEU:H	1:A:2144:LEU:HD23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:TYR:CE1	1:A:548:ARG:HB3	2.44	0.53
1:A:833:GLN:O	1:A:834:GLU:HG2	2.07	0.53
1:A:1592:MET:HE1	1:A:1715:HIS:HB3	1.90	0.53
1:A:516:HIS:CE1	1:A:685:LEU:HD13	2.44	0.52
1:A:1208:SER:HA	1:A:1337:PHE:O	2.08	0.52
1:A:1212:PRO:HA	1:A:1334:ILE:HG22	1.89	0.52
1:A:1976:TRP:CH2	1:A:2046:VAL:HG21	2.44	0.52
1:A:2105:HIS:O	1:A:2109:ARG:HG3	2.10	0.52
1:A:608:LEU:HD23	1:A:608:LEU:H	1.75	0.52
1:A:996:TRP:CD1	1:A:1154:HIS:HA	2.43	0.52
1:A:1010:ILE:HG21	1:A:1129:TRP:CZ2	2.44	0.52
1:A:1436:GLU:OE2	1:A:1445:ARG:NH2	2.43	0.52
1:A:1269:HIS:O	1:A:1269:HIS:ND1	2.42	0.52
1:A:1268:GLU:HG3	1:A:1351:LEU:HD11	1.91	0.52
1:A:2117:CYS:SG	1:A:2118:VAL:N	2.82	0.52
1:A:1195:LEU:HD12	1:A:1344:VAL:HG22	1.92	0.52
1:A:2244:LEU:HD12	1:A:2245:GLY:N	2.25	0.52
1:A:1139:VAL:HG22	1:A:1140:LYS:H	1.75	0.51
1:A:1493:LEU:HD23	1:A:1596:VAL:HG23	1.92	0.51
1:A:1582:ARG:C	1:A:1584:PHE:H	2.17	0.51
1:A:2261:GLN:CG	1:A:2265:ARG:HH22	2.23	0.51
1:A:890:ARG:HB2	1:A:906:TRP:CH2	2.46	0.51
1:A:947:VAL:HG21	1:A:956:ARG:HD2	1.92	0.51
1:A:480:LEU:HB2	1:A:523:LEU:HB3	1.92	0.51
1:A:999:CYS:HB2	1:A:1147:TRP:CE3	2.45	0.51
1:A:1231:ASP:HB2	1:A:1234:HIS:CD2	2.45	0.51
1:A:578:ALA:O	1:A:584:SER:HA	2.10	0.51
1:A:701:THR:OG1	1:A:704:GLU:OE1	2.28	0.51
1:A:516:HIS:HE1	1:A:685:LEU:HD22	1.75	0.51
1:A:1101:GLU:OE1	1:A:1101:GLU:N	2.44	0.50
1:A:2069:LYS:O	1:A:2073:GLN:HG2	2.11	0.50
2:D:29:DG:H2''	2:D:30:5CM:H5'	1.93	0.50
2:D:33:DA:H2''	2:D:34:DT:H5''	1.92	0.50
1:A:955:TRP:CD1	1:A:982:LEU:HD22	2.47	0.50
1:A:1401:PHE:HZ	1:A:1475:ALA:HA	1.76	0.50
1:A:1917:ASP:N	1:A:1917:ASP:OD1	2.45	0.50
1:A:388:ILE:H	4:A:2401:SAH:C8	2.24	0.50
1:A:388:ILE:H	4:A:2401:SAH:H8	1.76	0.50
1:A:1386:LEU:HD23	1:A:1825:VAL:HG11	1.93	0.50
1:A:445:ASN:O	1:A:447:ASN:N	2.45	0.50
1:A:386:CYS:HB3	1:A:406:PHE:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ASN:O	1:A:1050:THR:OG1	2.30	0.49
1:A:915:GLU:N	1:A:915:GLU:OE1	2.44	0.49
1:A:1858:GLU:O	1:A:1862:GLN:HG2	2.13	0.49
1:A:332:ILE:HG13	1:A:332:ILE:O	2.12	0.49
1:A:783:ILE:HD13	1:A:1202:HIS:CD2	2.47	0.49
1:A:806:ILE:HD13	1:A:867:ARG:HD2	1.94	0.49
1:A:1261:HIS:HE1	1:A:1263:ALA:HB2	1.78	0.49
1:A:342:LEU:O	1:A:345:ARG:HG2	2.12	0.49
1:A:685:LEU:HA	1:A:689:MET:SD	2.53	0.49
1:A:857:GLN:N	1:A:857:GLN:OE1	2.46	0.49
1:A:2202:SER:O	1:A:2206:THR:HG23	2.13	0.49
1:A:1389:ASN:ND2	1:A:1412:SER:HA	2.27	0.49
1:A:431:VAL:HG21	1:A:469:TRP:HH2	1.78	0.49
1:A:701:THR:N	1:A:704:GLU:OE1	2.35	0.49
1:A:1038:GLU:HG2	1:A:1060:GLN:HA	1.94	0.48
1:A:1528:ILE:HD11	1:A:1550:MET:HG3	1.95	0.48
1:A:1938:ALA:O	1:A:1941:GLU:HG3	2.12	0.48
1:A:477:ILE:HD11	1:A:750:ALA:HB3	1.93	0.48
1:A:762:LYS:NZ	1:A:766:LEU:HB2	2.28	0.48
1:A:1997:LEU:HA	1:A:2000:ILE:HG22	1.96	0.48
1:A:1107:SER:OG	1:A:1108:THR:N	2.46	0.48
3:E:10:DG:H5"	3:E:10:DG:C8	2.47	0.48
1:A:625:ASP:OD1	1:A:625:ASP:N	2.40	0.48
1:A:898:LYS:HD3	1:A:1000:ILE:HD11	1.95	0.48
1:A:1837:THR:HG21	1:A:2267:ARG:NH1	2.28	0.48
1:A:1420:GLU:HG3	1:A:1745:TYR:CD1	2.48	0.48
1:A:1496:LEU:HD13	1:A:1717:PHE:HB3	1.96	0.48
1:A:2006:LYS:N	1:A:2009:ASN:OD1	2.46	0.48
1:A:666:VAL:HB	1:A:690:ILE:HG13	1.95	0.48
1:A:931:SER:O	1:A:932:THR:OG1	2.30	0.48
1:A:360:LEU:HD11	1:A:382:HIS:CD2	2.49	0.48
1:A:706:LEU:HD23	1:A:730:ALA:HB2	1.95	0.48
1:A:595:SER:HB2	1:A:2043:ARG:NH1	2.29	0.48
1:A:946:LEU:HA	1:A:955:TRP:HA	1.96	0.48
1:A:1891:SER:OG	1:A:1892:ASP:N	2.46	0.48
1:A:2088:ASN:HB3	1:A:2089:PRO:HD2	1.95	0.48
1:A:2227:ASP:OD1	1:A:2228:ALA:N	2.47	0.48
1:A:1498:ALA:O	1:A:1719:PHE:HB3	2.13	0.47
1:A:1554:ILE:HA	1:A:1557:SER:HB2	1.96	0.47
1:A:533:ASP:N	1:A:533:ASP:OD1	2.48	0.47
1:A:1588:LEU:O	1:A:1592:MET:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:LEU:C	1:A:610:ARG:HD2	2.39	0.47
1:A:1125:LEU:HD23	1:A:1126:ASP:N	2.29	0.47
1:A:368:LYS:HD2	1:A:368:LYS:HA	1.70	0.47
1:A:550:TRP:CG	1:A:550:TRP:O	2.67	0.47
1:A:516:HIS:CE1	1:A:685:LEU:HB2	2.50	0.47
1:A:1125:LEU:HA	1:A:1141:LEU:HD12	1.96	0.47
1:A:1186:SER:OG	1:A:1187:SER:N	2.47	0.47
1:A:1886:LEU:C	1:A:1888:GLU:H	2.22	0.47
1:A:2207:LEU:HD11	1:A:2211:GLN:HE21	1.79	0.47
1:A:996:TRP:O	1:A:1151:PRO:HD2	2.15	0.47
1:A:1922:GLN:HE22	1:A:2067:LYS:HG3	1.80	0.47
1:A:2076:LEU:HD12	1:A:2076:LEU:HA	1.77	0.47
1:A:550:TRP:O	1:A:550:TRP:CD2	2.68	0.47
1:A:1396:SER:HA	1:A:1410:LEU:HD13	1.97	0.47
1:A:1593:GLU:O	1:A:1596:VAL:HG12	2.15	0.47
1:A:1609:ALA:HA	1:A:1612:ARG:HE	1.79	0.47
1:A:316:PRO:O	1:A:548:ARG:NH2	2.48	0.46
1:A:548:ARG:HA	1:A:549:PRO:HD3	1.66	0.46
1:A:1389:ASN:HD21	1:A:1415:TRP:HB3	1.80	0.46
1:A:1407:LYS:O	1:A:1411:ARG:HG3	2.15	0.46
1:A:406:PHE:HA	1:A:419:THR:HA	1.95	0.46
1:A:782:ILE:HG23	1:A:1205:ALA:HB2	1.97	0.46
1:A:1372:GLY:N	1:A:1443:GLY:O	2.48	0.46
1:A:1539:ILE:HD13	1:A:1709:LEU:HD23	1.96	0.46
1:A:363:LEU:HD23	1:A:380:PHE:CD1	2.51	0.46
1:A:735:THR:O	1:A:739:VAL:HG23	2.16	0.46
1:A:1506:HIS:NE2	1:A:2228:ALA:O	2.28	0.46
1:A:1008:ILE:HG21	1:A:1141:LEU:HB2	1.96	0.46
1:A:1086:GLN:OE1	1:A:1087:LEU:N	2.35	0.46
1:A:516:HIS:HE1	1:A:685:LEU:HD13	1.80	0.46
1:A:606:LEU:HD22	1:A:648:LEU:HB3	1.96	0.46
1:A:927:LEU:HD13	1:A:935:ALA:HB2	1.97	0.46
1:A:407:ARG:HG2	1:A:420:ALA:HA	1.98	0.46
1:A:479:ILE:HD11	1:A:746:ALA:HB2	1.96	0.46
1:A:1113:LEU:HD23	1:A:1113:LEU:HA	1.70	0.46
1:A:1919:LYS:HB3	1:A:1923:GLU:HG2	1.97	0.46
1:A:410:THR:HA	1:A:465:GLY:HA3	1.97	0.46
1:A:692:TRP:CD1	1:A:694:THR:HG22	2.51	0.46
1:A:1195:LEU:HD23	1:A:1195:LEU:H	1.80	0.46
1:A:1286:ARG:NH1	1:A:1629:LYS:HD2	2.31	0.46
1:A:1854:TYR:CZ	1:A:2285:THR:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2250:ASN:O	1:A:2294:ARG:NH2	2.48	0.46
1:A:449:VAL:HG22	3:E:7:DG:H21	1.80	0.46
1:A:348:ARG:NH1	1:A:430:ASP:HB3	2.31	0.46
1:A:696:ARG:NH2	1:A:704:GLU:OE2	2.33	0.46
1:A:781:ARG:HB3	1:A:1327:GLN:HE22	1.79	0.46
1:A:1862:GLN:HB3	1:A:2130:THR:HG21	1.98	0.46
1:A:398:ARG:HD2	1:A:717:LEU:HD22	1.97	0.45
1:A:1061:LEU:HD23	1:A:1062:LEU:N	2.31	0.45
1:A:1155:LEU:HD23	1:A:1155:LEU:H	1.82	0.45
1:A:1605:LYS:O	1:A:1607:SER:N	2.49	0.45
1:A:561:THR:HG22	1:A:561:THR:O	2.17	0.45
1:A:1261:HIS:O	1:A:1366:SER:HA	2.16	0.45
1:A:1388:SER:OG	1:A:1389:ASN:N	2.48	0.45
1:A:2078:SER:OG	1:A:2079:SER:N	2.49	0.45
1:A:358:SER:OG	1:A:736:THR:HG22	2.16	0.45
1:A:575:SER:O	1:A:575:SER:OG	2.29	0.45
1:A:929:ARG:O	1:A:929:ARG:HG2	2.16	0.45
1:A:1456:VAL:HG11	1:A:1770:ILE:HD11	1.98	0.45
1:A:2105:HIS:CE1	1:A:2134:LYS:HG2	2.51	0.45
1:A:2138:LEU:H	1:A:2138:LEU:HD23	1.81	0.45
1:A:1223:ARG:O	1:A:1330:LEU:N	2.34	0.45
1:A:352:MET:HB2	1:A:436:ALA:CB	2.47	0.45
1:A:365:MET:HE1	1:A:712:PRO:HD3	1.97	0.45
1:A:383:VAL:HG22	1:A:384:PHE:HD2	1.82	0.45
4:A:2401:SAH:H4'	4:A:2401:SAH:HG2	1.63	0.45
1:A:664:TRP:CD1	1:A:676:SER:HG	2.34	0.45
1:A:502:ALA:HA	1:A:524:PHE:O	2.16	0.45
1:A:1019:SER:HA	1:A:1035:ARG:HD3	1.99	0.45
1:A:1933:ALA:HA	1:A:2056:LEU:HD11	1.98	0.45
1:A:2235:LEU:HD12	1:A:2235:LEU:O	2.16	0.45
1:A:467:LEU:HA	1:A:470:VAL:HG12	1.99	0.45
1:A:2084:LYS:HB2	1:A:2085:PRO:HD2	1.98	0.45
1:A:2261:GLN:HG2	1:A:2265:ARG:NH2	2.32	0.45
1:A:1501:ILE:HD11	1:A:1547:ILE:HD11	1.98	0.44
1:A:2084:LYS:HG3	1:A:2086:SER:H	1.82	0.44
1:A:412:LEU:HG	1:A:469:TRP:HB2	2.00	0.44
1:A:1837:THR:HG21	1:A:2267:ARG:HH11	1.81	0.44
1:A:848:GLU:O	1:A:1064:ARG:HB3	2.17	0.44
1:A:1390:LYS:HG3	1:A:1411:ARG:HH12	1.83	0.44
1:A:1480:THR:HG21	1:A:1721:ARG:HH22	1.81	0.44
2:D:33:DA:H2''	2:D:34:DT:C5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:CYS:SG	1:A:833:GLN:N	2.90	0.44
1:A:980:ALA:HA	1:A:997:GLU:O	2.17	0.44
1:A:1254:ASP:OD1	1:A:1257:LYS:NZ	2.51	0.44
1:A:1261:HIS:HB3	1:A:1367:TRP:HD1	1.82	0.44
1:A:1566:TYR:CD2	1:A:1567:LEU:HD22	2.51	0.44
1:A:1836:PRO:HB2	1:A:2274:LYS:HG3	1.98	0.44
1:A:2005:VAL:HG23	1:A:2009:ASN:H	1.83	0.44
1:A:1148:VAL:HG13	1:A:1149:LYS:O	2.17	0.44
1:A:1893:SER:HA	1:A:1898:GLU:OE1	2.18	0.44
1:A:893:ALA:HB2	1:A:1148:VAL:HG23	1.98	0.44
1:A:941:ARG:HB3	1:A:941:ARG:NH1	2.33	0.44
1:A:2170:LEU:HD13	1:A:2235:LEU:HD11	1.99	0.44
1:A:496:GLY:HA2	1:A:500:TYR:O	2.18	0.44
1:A:929:ARG:O	1:A:930:GLN:C	2.60	0.44
1:A:1129:TRP:HD1	1:A:1137:ARG:HD2	1.82	0.44
1:A:1390:LYS:HG3	1:A:1411:ARG:NH1	2.33	0.44
1:A:354:SER:OG	1:A:357:GLU:OE1	2.34	0.43
1:A:832:CYS:SG	1:A:849:HIS:HB3	2.57	0.43
1:A:1550:MET:HG2	1:A:1551:ALA:O	2.18	0.43
1:A:1761:ILE:HD12	1:A:1821:LEU:HD11	2.00	0.43
1:A:914:LEU:HD13	1:A:917:ILE:HG21	1.99	0.43
1:A:1111:GLU:N	1:A:1111:GLU:OE1	2.51	0.43
1:A:1396:SER:O	1:A:1397:GLN:HB2	2.18	0.43
1:A:1856:GLU:CD	1:A:1882:ARG:HH21	2.26	0.43
1:A:1092:ASP:OD1	1:A:1092:ASP:N	2.51	0.43
1:A:1224:ARG:HD2	1:A:1224:ARG:N	2.33	0.43
1:A:1254:ASP:HA	1:A:1257:LYS:NZ	2.33	0.43
1:A:2006:LYS:O	1:A:2009:ASN:ND2	2.51	0.43
1:A:1713:VAL:O	1:A:1716:MET:HG2	2.18	0.43
1:A:1471:VAL:HG22	1:A:1518:PHE:CE2	2.53	0.43
1:A:2304:TRP:O	1:A:2304:TRP:CG	2.71	0.43
1:A:1041:ILE:HD12	1:A:1059:TYR:CE1	2.53	0.43
1:A:1259:TRP:CE2	1:A:1368:ARG:HD3	2.54	0.43
1:A:447:ASN:O	2:D:31:DG:N2	2.50	0.43
1:A:1247:THR:HG23	1:A:1442:VAL:HG22	2.01	0.43
1:A:1519:THR:O	1:A:1519:THR:OG1	2.32	0.43
1:A:1909:LEU:HD12	1:A:1910:ASP:H	1.83	0.43
1:A:865:GLU:O	1:A:869:LYS:HG2	2.19	0.43
1:A:2259:GLU:O	1:A:2263:ILE:HG12	2.18	0.43
1:A:464:ARG:HH12	1:A:468:GLN:HE21	1.67	0.43
1:A:484:CYS:HA	1:A:521:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:LYS:HZ3	1:A:766:LEU:HB2	1.84	0.43
1:A:926:TYR:O	1:A:926:TYR:CG	2.72	0.43
1:A:1257:LYS:O	1:A:1368:ARG:HD2	2.19	0.43
1:A:1433:GLU:OE2	1:A:1771:HIS:ND1	2.48	0.43
1:A:1461:ILE:HG23	1:A:1749:LEU:HD23	1.99	0.43
1:A:2169:VAL:HG22	1:A:2240:HIS:CE1	2.53	0.43
1:A:352:MET:HE1	1:A:384:PHE:HE1	1.84	0.43
1:A:607:GLY:HA3	1:A:1025:GLY:O	2.18	0.43
1:A:338:LEU:HG	1:A:342:LEU:HD23	2.01	0.42
1:A:1010:ILE:HD13	1:A:1041:ILE:HG12	2.01	0.42
1:A:1227:TRP:CZ3	1:A:1338:ARG:HG3	2.54	0.42
1:A:1245:TRP:CE2	1:A:1246:ILE:HG13	2.54	0.42
1:A:326:ASP:OD1	1:A:327:HIS:N	2.52	0.42
1:A:801:SER:HB3	1:A:871:LEU:HD13	2.01	0.42
1:A:2070:SER:O	1:A:2074:ILE:HG13	2.18	0.42
1:A:329:VAL:HG11	1:A:369:ALA:HB1	2.00	0.42
1:A:352:MET:HG2	1:A:434:LEU:HD11	2.00	0.42
1:A:389:GLU:HG3	1:A:392:LYS:HD2	2.00	0.42
1:A:1550:MET:HE1	1:A:1714:LEU:HG	2.00	0.42
1:A:1826:ARG:HA	1:A:1826:ARG:HD3	1.82	0.42
1:A:440:CYS:SG	1:A:483:VAL:HB	2.59	0.42
1:A:544:LYS:HE3	1:A:547:ARG:NH1	2.34	0.42
1:A:1125:LEU:HD21	1:A:1139:VAL:HG11	2.00	0.42
1:A:1487:GLU:N	1:A:1488:PRO:HD2	2.34	0.42
1:A:388:ILE:HG23	4:A:2401:SAH:N7	2.34	0.42
1:A:872:LEU:HD13	1:A:937:TYR:OH	2.19	0.42
1:A:660:LYS:HE2	1:A:660:LYS:HB2	1.82	0.42
1:A:869:LYS:O	1:A:1249:ARG:NH1	2.52	0.42
1:A:1498:ALA:HB1	1:A:1548:ILE:HG23	2.02	0.42
1:A:1500:LEU:HD22	1:A:1719:PHE:CD1	2.54	0.42
1:A:2148:ARG:HD2	1:A:2149:TYR:N	2.35	0.42
1:A:636:THR:HG21	2:D:28:DA:C5'	2.38	0.42
1:A:995:PRO:HB2	1:A:1150:CYS:HB3	2.01	0.42
1:A:436:ALA:O	1:A:480:LEU:HA	2.20	0.42
1:A:693:VAL:HG23	1:A:698:GLY:O	2.20	0.42
1:A:893:ALA:HB2	1:A:1148:VAL:CG2	2.50	0.42
1:A:1460:VAL:O	1:A:1825:VAL:HA	2.19	0.42
1:A:1209:CYS:O	1:A:1336:SER:HA	2.19	0.42
3:E:7:DG:H5'	3:E:7:DG:C8	2.55	0.42
1:A:868:PHE:O	1:A:872:LEU:HG	2.20	0.42
1:A:1129:TRP:CD1	1:A:1137:ARG:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1963:PHE:C	1:A:1965:LYS:H	2.28	0.42
1:A:2057:ARG:NH2	1:A:2099:CYS:O	2.53	0.42
1:A:349:VAL:O	1:A:383:VAL:HG12	2.20	0.41
1:A:991:VAL:HG12	1:A:991:VAL:O	2.20	0.41
1:A:1148:VAL:HG22	1:A:1149:LYS:H	1.85	0.41
1:A:1468:GLY:O	1:A:1472:ILE:HG13	2.20	0.41
1:A:1832:ILE:HG13	1:A:1833:GLU:N	2.34	0.41
1:A:1948:ASN:O	1:A:1951:ILE:HG22	2.19	0.41
1:A:721:GLU:HB3	1:A:726:LEU:CD2	2.50	0.41
1:A:886:LEU:HD11	1:A:914:LEU:HD21	2.02	0.41
1:A:1739:LEU:HA	1:A:1739:LEU:HD23	1.75	0.41
1:A:544:LYS:HE3	1:A:547:ARG:HH12	1.84	0.41
1:A:1078:ASP:OD1	1:A:1079:LEU:N	2.54	0.41
1:A:315:LEU:HD22	1:A:548:ARG:HE	1.85	0.41
1:A:1920:SER:HA	1:A:2145:SER:OG	2.19	0.41
1:A:481:GLU:HA	1:A:521:VAL:O	2.21	0.41
1:A:1054:LYS:HD3	1:A:1080:SER:OG	2.21	0.41
1:A:1207:LEU:HD23	1:A:1208:SER:N	2.35	0.41
1:A:1248:GLU:O	1:A:1249:ARG:HB2	2.21	0.41
1:A:479:ILE:HA	1:A:523:LEU:O	2.21	0.41
1:A:596:ARG:HD2	1:A:669:ASN:HD21	1.86	0.41
1:A:892:ALA:O	1:A:895:LYS:HB2	2.19	0.41
1:A:995:PRO:HB2	1:A:1150:CYS:CB	2.51	0.41
2:D:29:DG:C2'	2:D:30:5CM:H5'	2.51	0.41
1:A:693:VAL:HG12	1:A:695:ILE:HG22	2.03	0.41
1:A:1103:ARG:HD2	1:A:1124:ARG:HD3	2.01	0.41
1:A:1264:ASP:HB3	1:A:1362:LYS:HD3	2.02	0.41
1:A:1582:ARG:O	1:A:1583:PHE:HB2	2.21	0.41
1:A:1713:VAL:HG12	1:A:1715:HIS:H	1.86	0.41
1:A:1976:TRP:CZ2	1:A:2046:VAL:HG21	2.56	0.41
1:A:2306:GLU:HG3	1:A:2307:ILE:N	2.36	0.41
1:A:388:ILE:N	4:A:2401:SAH:H8	2.36	0.41
1:A:415:LYS:HE3	1:A:415:LYS:HB2	1.89	0.41
1:A:434:LEU:O	1:A:478:VAL:HA	2.21	0.41
1:A:2303:ASP:O	1:A:2304:TRP:C	2.63	0.41
1:A:401:THR:O	1:A:401:THR:OG1	2.29	0.41
1:A:915:GLU:HB2	1:A:941:ARG:NH1	2.36	0.41
1:A:1044:GLN:CD	1:A:1045:ALA:H	2.28	0.41
1:A:1108:THR:O	1:A:1108:THR:OG1	2.37	0.41
1:A:1221:MET:HE2	1:A:1221:MET:HB2	1.99	0.41
1:A:1331:ASP:CG	1:A:1332:GLN:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2016:ASP:OD1	1:A:2018:GLN:HB2	2.20	0.41
1:A:2239:ASN:HD22	1:A:2273:LYS:CD	2.32	0.41
3:E:12:DC:H1'	3:E:13:DA:H8	1.86	0.41
1:A:338:LEU:O	1:A:341:GLN:N	2.54	0.41
1:A:937:TYR:N	1:A:944:LEU:O	2.42	0.41
1:A:1063:PRO:HG2	1:A:1064:ARG:HD2	2.03	0.41
1:A:1777:ASP:OD1	1:A:1777:ASP:N	2.53	0.41
1:A:2239:ASN:ND2	1:A:2273:LYS:HD3	2.35	0.41
1:A:787:TYR:C	1:A:788:LEU:HD12	2.45	0.40
1:A:806:ILE:HD12	1:A:806:ILE:HA	1.89	0.40
1:A:1960:LYS:HB2	1:A:2028:MET:HE1	2.02	0.40
1:A:2211:GLN:NE2	1:A:2233:SER:O	2.54	0.40
1:A:2303:ASP:OD1	1:A:2304:TRP:N	2.45	0.40
1:A:397:GLU:HG2	1:A:405:LEU:HD22	2.03	0.40
1:A:1532:LYS:HA	1:A:1535:GLN:HG2	2.03	0.40
1:A:2027:LYS:O	1:A:2031:VAL:HG23	2.21	0.40
1:A:563:ASP:OD1	1:A:563:ASP:N	2.53	0.40
1:A:1052:ASP:OD1	1:A:1052:ASP:N	2.55	0.40
1:A:1837:THR:HA	1:A:2275:VAL:HG23	2.03	0.40
1:A:2059:PHE:HA	1:A:2062:VAL:HG12	2.03	0.40
1:A:2298:LEU:HB3	1:A:2304:TRP:HD1	1.83	0.40
1:A:1272:GLU:O	1:A:1273:ARG:HB2	2.22	0.40
1:A:1955:GLY:O	1:A:1959:LYS:HG2	2.21	0.40
1:A:2148:ARG:HD2	1:A:2149:TYR:H	1.87	0.40
1:A:352:MET:HB2	1:A:436:ALA:HB1	2.03	0.40
1:A:386:CYS:O	1:A:387:GLU:HG2	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	1866/2348 (80%)	1622 (87%)	244 (13%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1607/2015 (80%)	1598 (99%)	9 (1%)	78	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	501	ASP
1	A	860	GLU
1	A	944	LEU
1	A	1249	ARG
1	A	1373	HIS
1	A	1461	ILE
1	A	2095	ILE
1	A	2187	SER
1	A	2265	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	451	GLN
1	A	468	GLN
1	A	473	HIS
1	A	516	HIS
1	A	598	GLN
1	A	673	GLN
1	A	1067	GLN
1	A	1202	HIS
1	A	1242	ASN

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Mol	Chain	Res	Type
1	A	1342	ASN
1	A	1427	HIS
1	A	1570	GLN
1	A	1715	HIS
1	A	1818	GLN
1	A	1822	ASN
1	A	1827	GLN
1	A	1859	HIS
1	A	1922	GLN
1	A	1927	HIS
1	A	1940	GLN
1	A	2038	GLN
1	A	2101	HIS
1	A	2115	GLN
1	A	2158	ASN
1	A	2161	HIS
1	A	2211	GLN
1	A	2239	ASN
1	A	2240	HIS
1	A	2271	GLN
1	A	2272	GLN
1	A	2276	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	D	30	2,3	18,21,22	1.75	3 (16%)	24,30,33	1.33	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	D	30	2,3	-	2/7/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	30	5CM	C5-C4	6.17	1.48	1.44
2	D	30	5CM	C6-C5	2.85	1.39	1.34
2	D	30	5CM	C6-N1	-2.18	1.34	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	30	5CM	C5-C6-N1	-3.37	119.66	123.31
2	D	30	5CM	C5-C4-N3	-2.71	118.98	121.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	30	5CM	C3'-C4'-C5'-O5'
2	D	30	5CM	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SAH	A	2401	-	27,28,28	0.44	0	36,40,40	0.29	0
6	ANP	A	2407	7	33,33,33	1.12	5 (15%)	45,52,52	0.85	3 (6%)

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
4	SAH	A	2401	-	-	8/15/31/31	0/3/3/3
6	ANP	A	2407	7	-	6/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2407	ANP	PG-O1G	3.33	1.51	1.46
6	A	2407	ANP	PB-O1B	3.09	1.50	1.46
6	A	2407	ANP	PB-O2B	-2.26	1.50	1.56
6	A	2407	ANP	PG-O3G	-2.09	1.51	1.56
6	A	2407	ANP	PG-O2G	-2.08	1.51	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2407	ANP	O2B-PB-O1B	4.01	118.48	109.87
6	A	2407	ANP	O3G-PG-O1G	-2.02	108.37	113.45
6	A	2407	ANP	O2G-PG-O1G	-2.01	108.41	113.45

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2401	SAH	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	2401	SAH	C-CA-CB-CG
4	A	2401	SAH	O4'-C4'-C5'-SD
4	A	2401	SAH	C3'-C4'-C5'-SD
6	A	2407	ANP	C5'-O5'-PA-O2A
6	A	2407	ANP	C5'-O5'-PA-O3A
6	A	2407	ANP	O4'-C4'-C5'-O5'
4	A	2401	SAH	CA-CB-CG-SD
6	A	2407	ANP	C3'-C4'-C5'-O5'
6	A	2407	ANP	C5'-O5'-PA-O1A
4	A	2401	SAH	C4'-C5'-SD-CG
4	A	2401	SAH	OXT-C-CA-N
4	A	2401	SAH	O-C-CA-N
6	A	2407	ANP	PG-N3B-PB-O3A

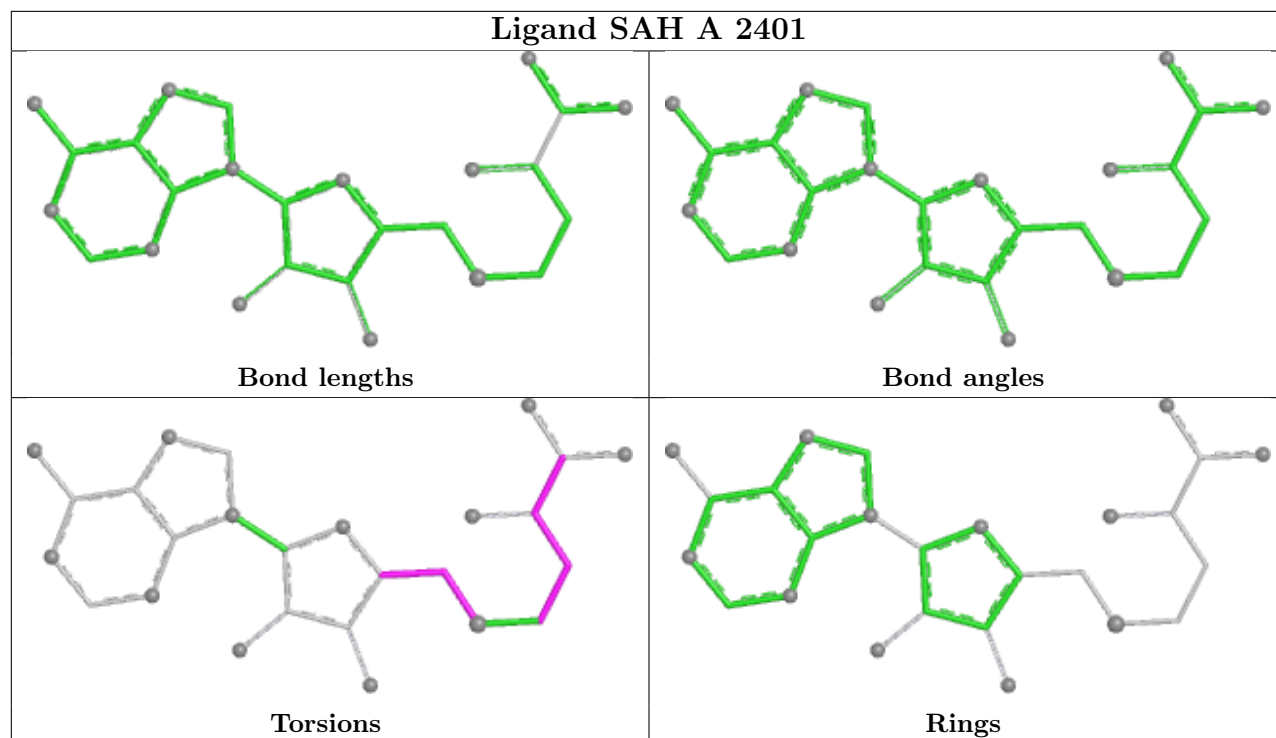
There are no ring outliers.

2 monomers are involved in 7 short contacts:

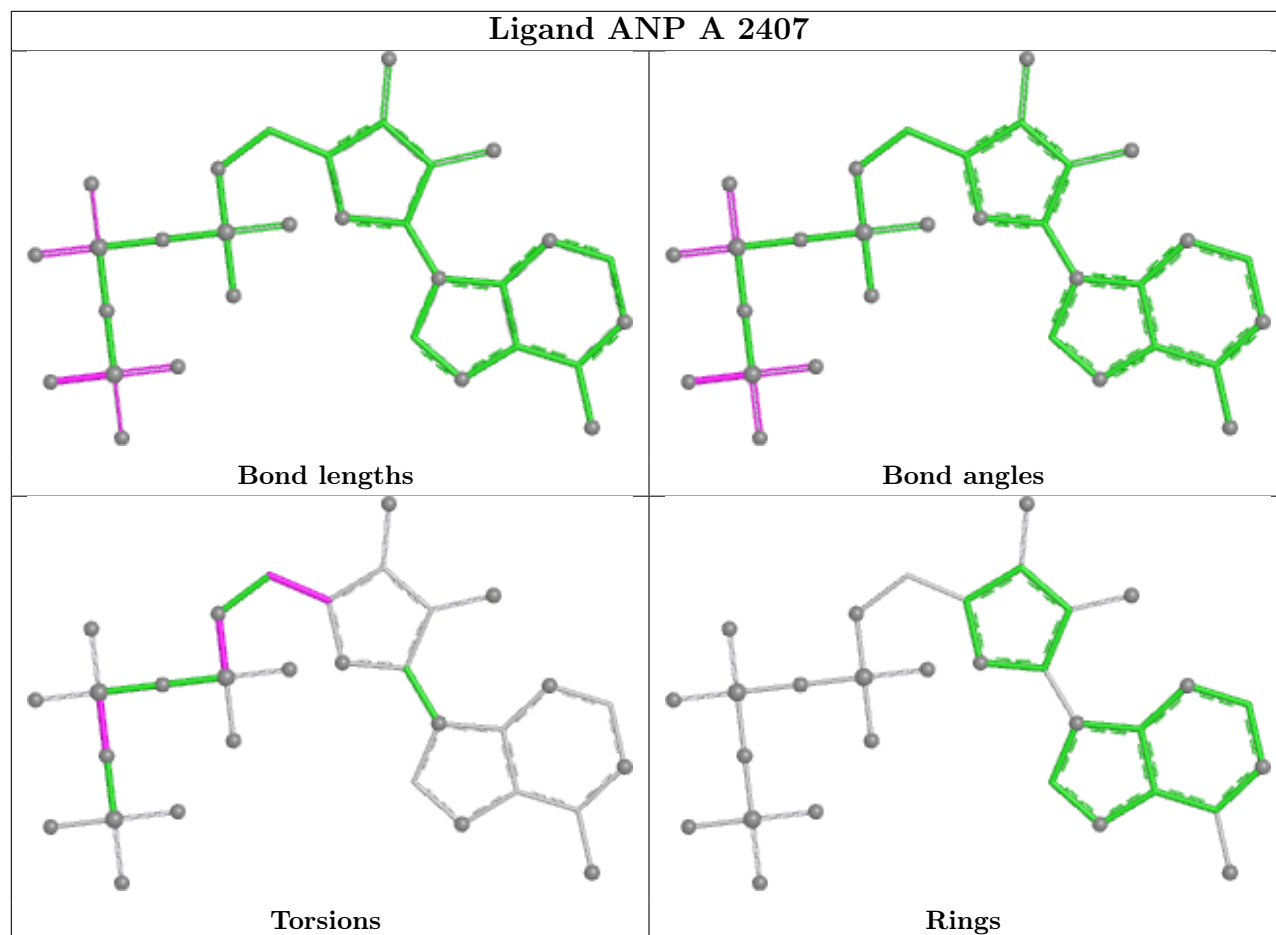
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2401	SAH	5	0
6	A	2407	ANP	2	0

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

Ligand SAH A 2401



Ligand ANP A 2407



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.

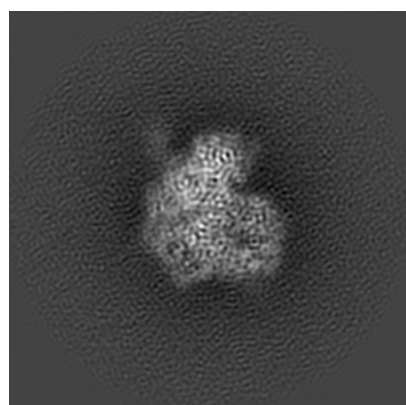
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24295. These allow visual inspection of the internal detail of the map and identification of artifacts.

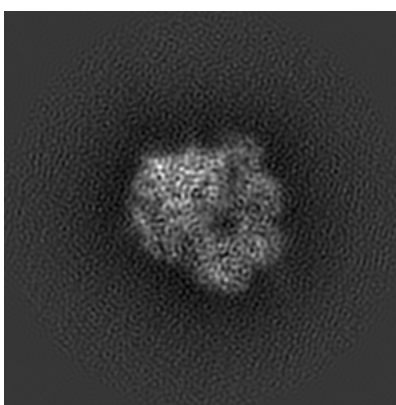
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

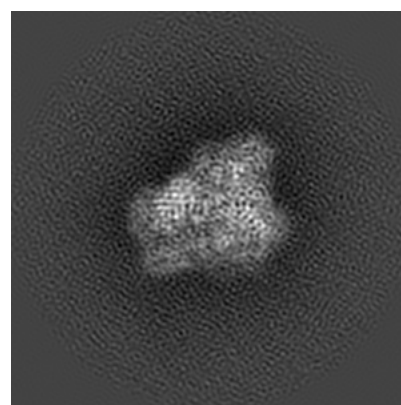
6.1.1 Primary map



X



Y

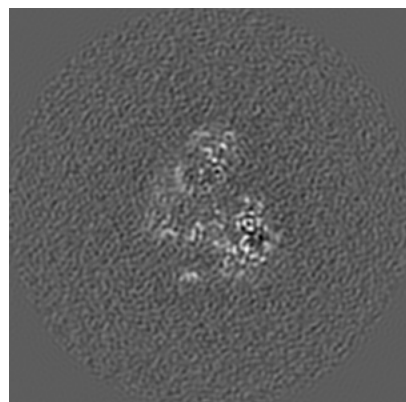


Z

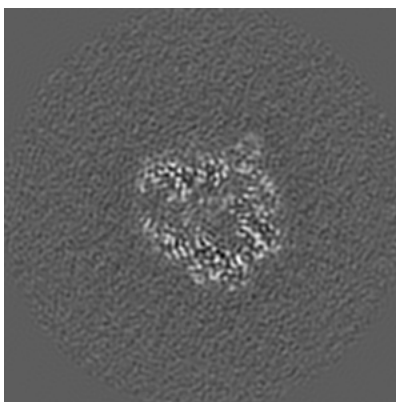
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

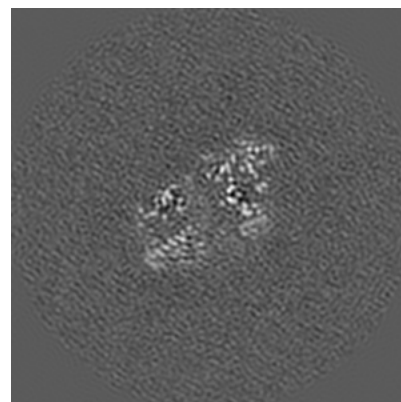
6.2.1 Primary map



X Index: 128



Y Index: 128

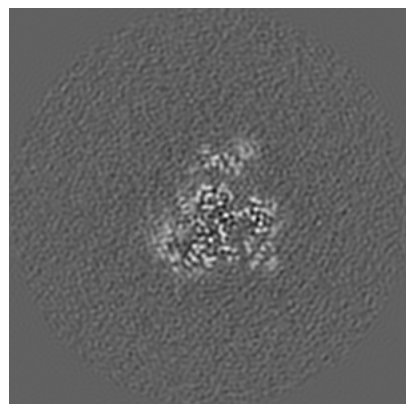


Z Index: 128

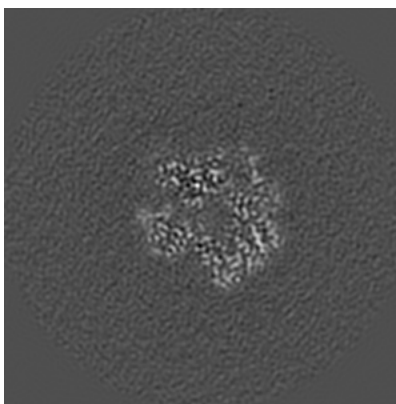
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

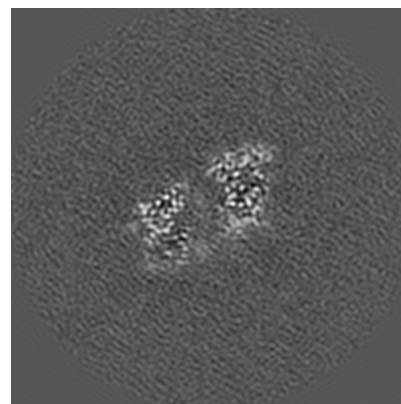
6.3.1 Primary map



X Index: 149



Y Index: 133

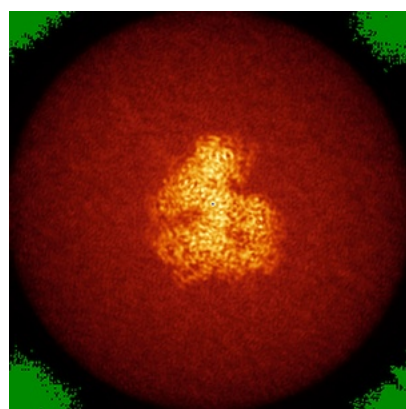


Z Index: 132

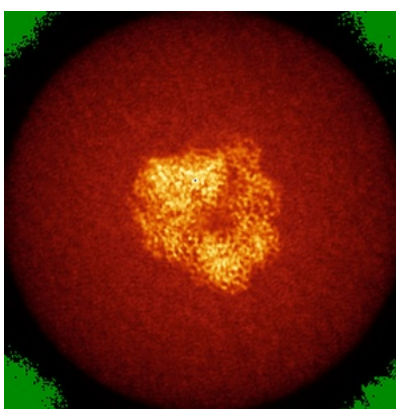
The images above show the largest variance slices of the map in three orthogonal directions.

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

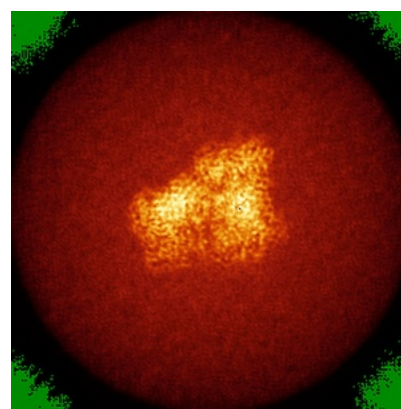
6.4.1 Primary map



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

This section was not generated.

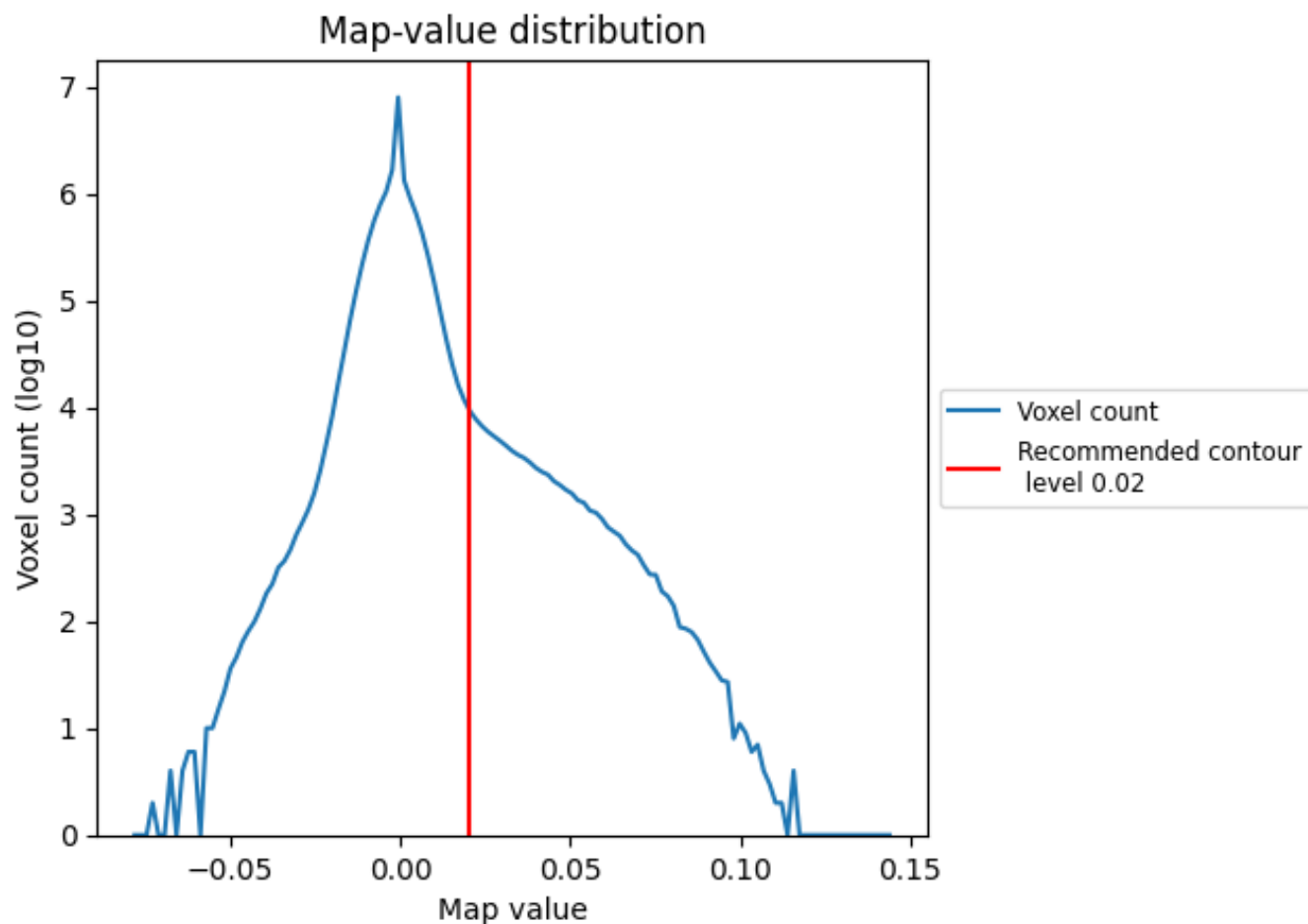
6.6 Mask visualisation

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

7 Map analysis [i](#)

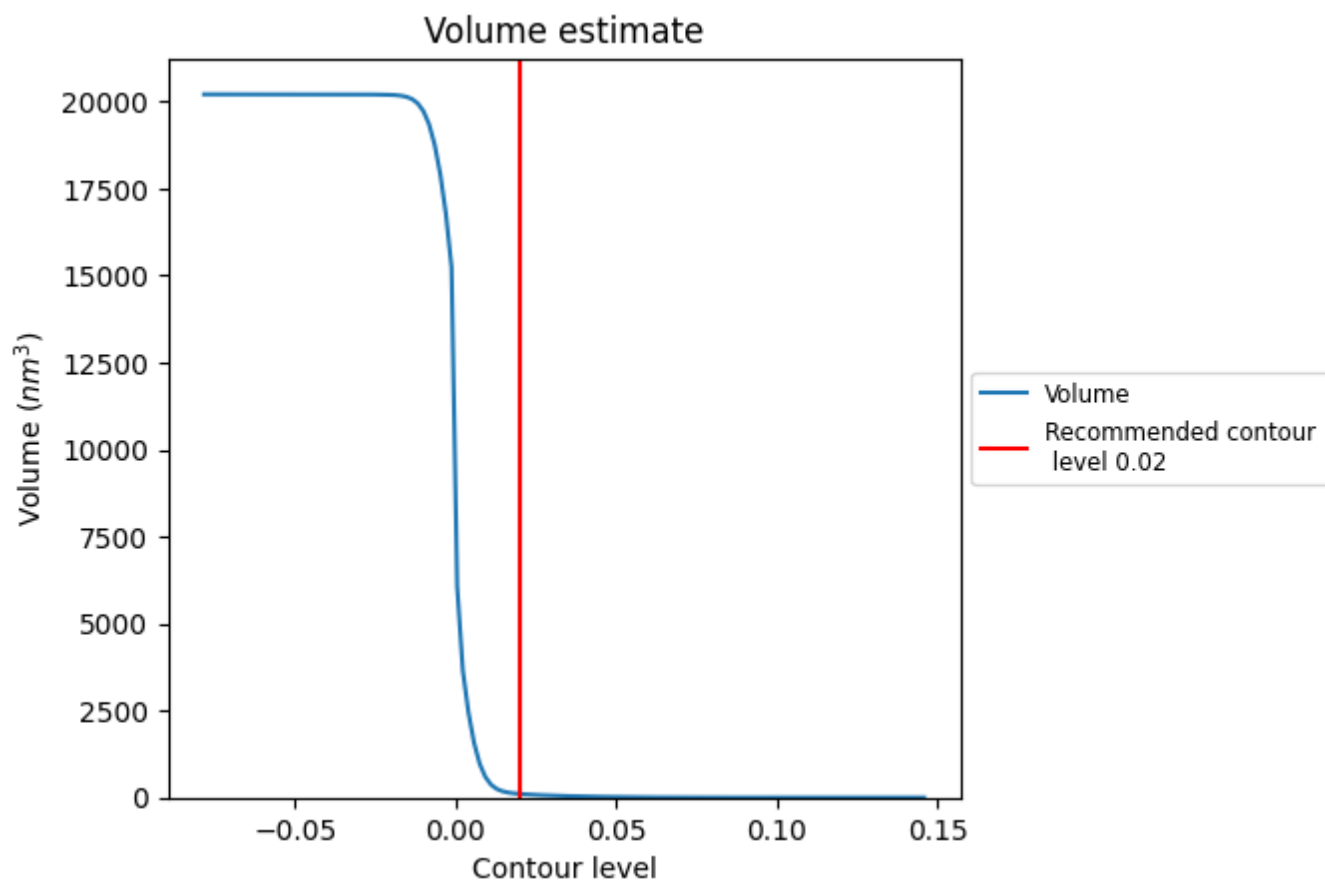
This section contains the results of statistical analysis of the map.

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.

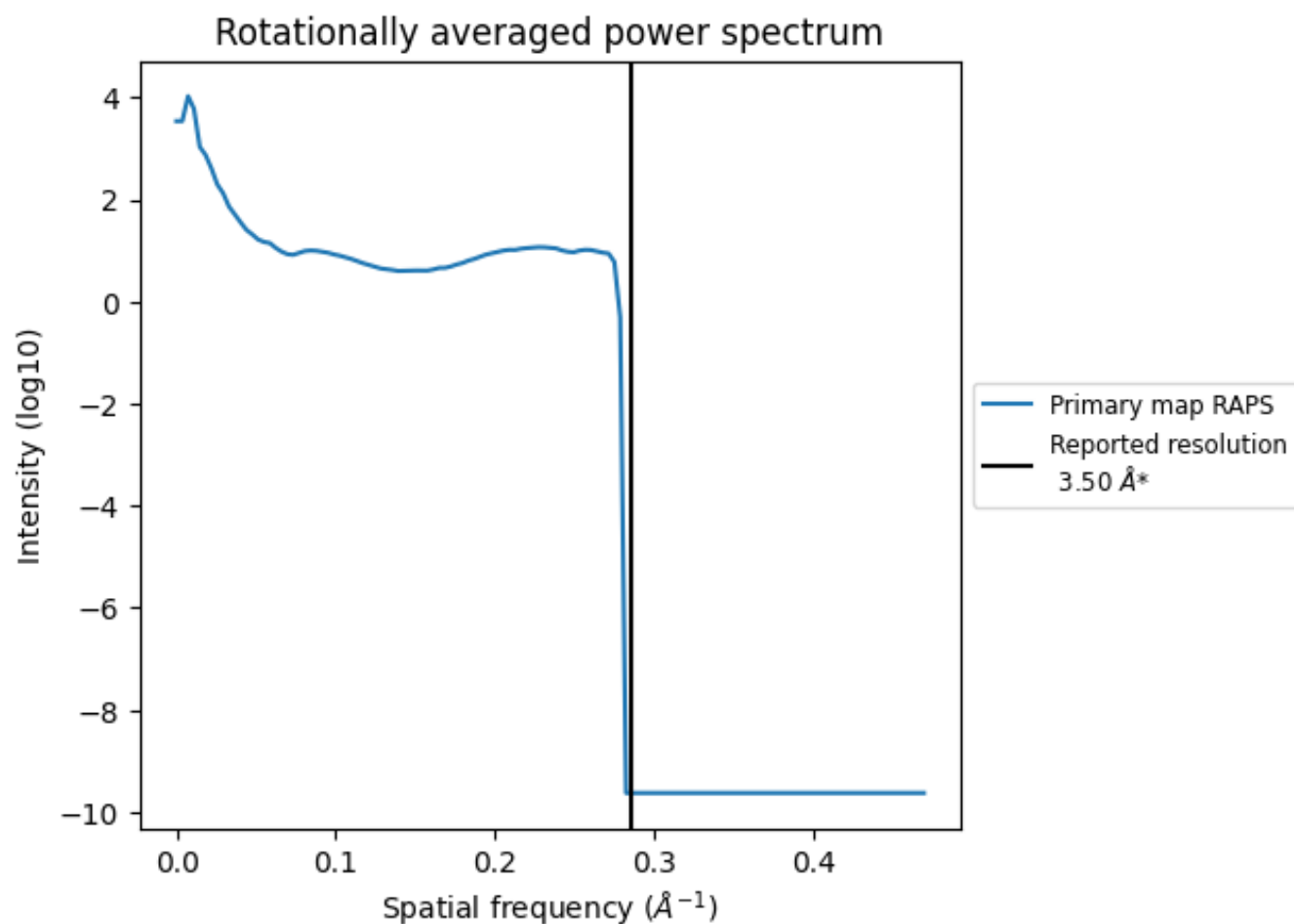
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 95 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 0.286 Å⁻¹

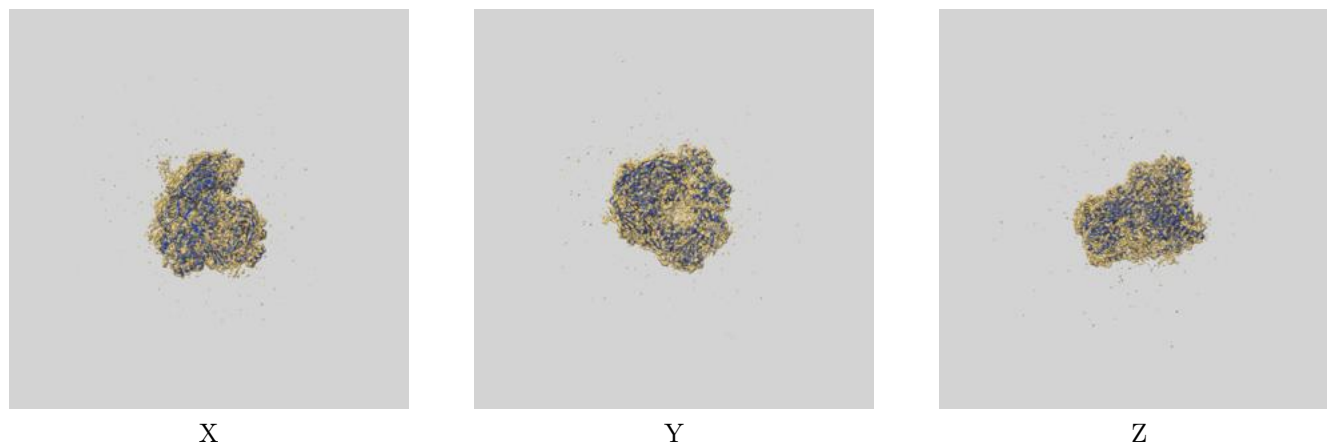
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

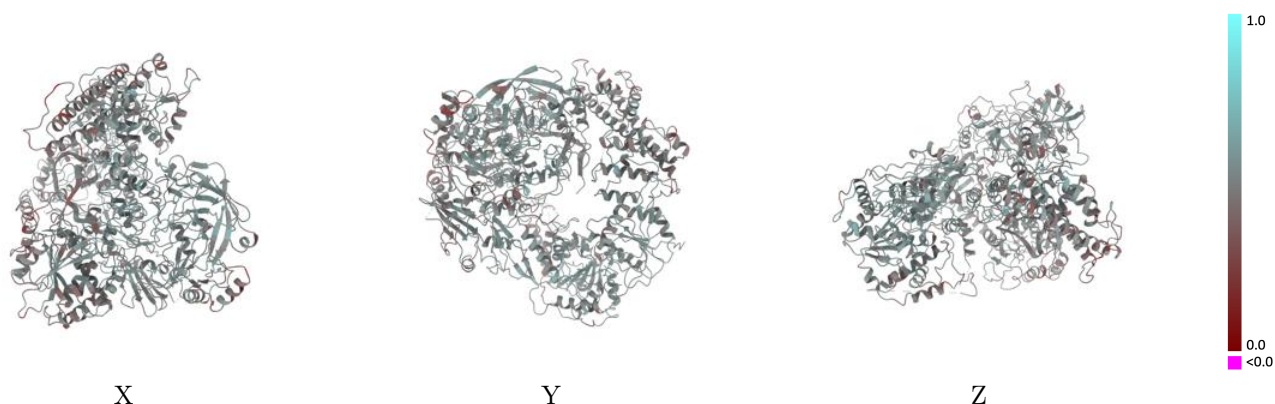
This section contains information regarding the fit between EMDB map EMD-24295 and PDB model 7R78. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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](#)

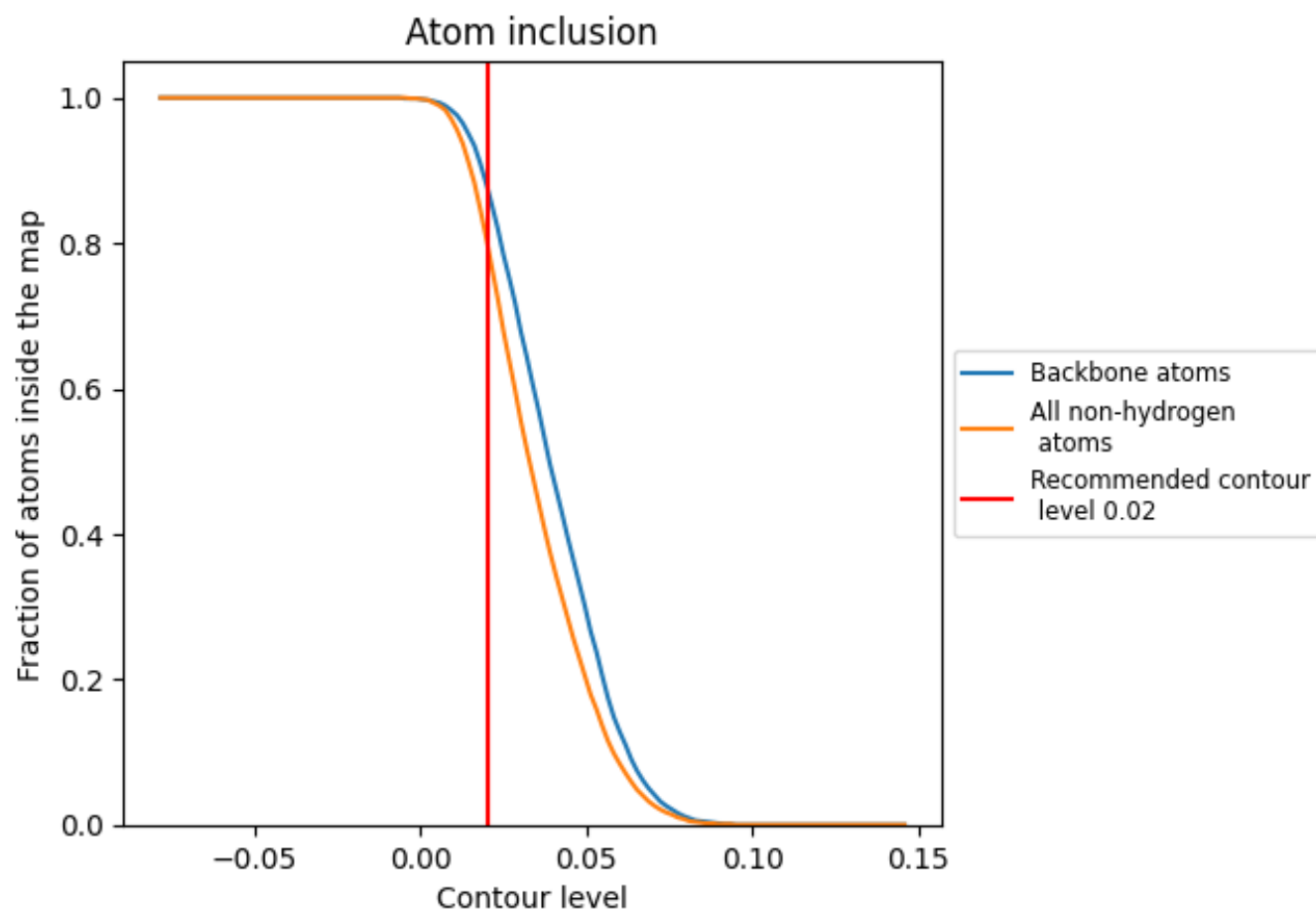


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.4980
A	0.8030	0.4990
D	0.7870	0.4410
E	0.8360	0.4690

