



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 12:03 PM EST

PDB ID : 7R78  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

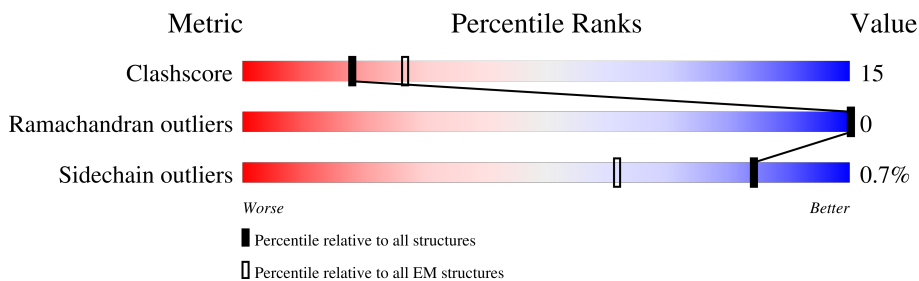
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	 55% 25% 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
			Total	C	N	O	S		
1	A	1880	14810	9284	2675	2780	71	0	0

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

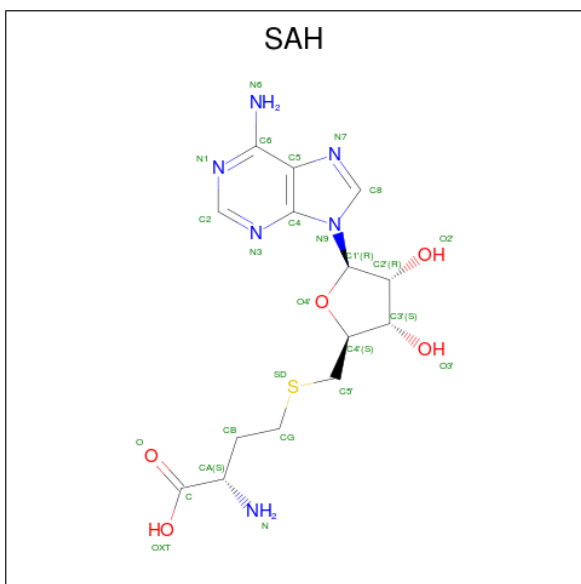
- Molecule 2 is a DNA chain called DNA (5'-D(P\*CP\*AP\*GP\*(5CM)P\*GP\*CP\*AP\*T)-3').

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

- 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	
			Total	C	N	O			P
3	E	10	201	97	38	57	9	0	0

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



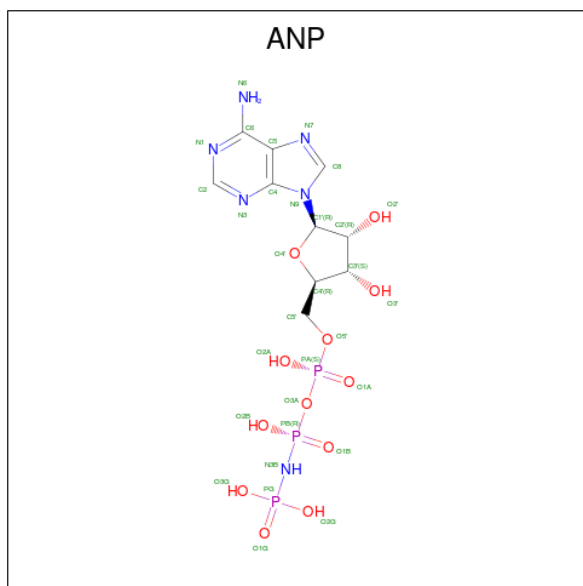
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		S
4	A	1	26	14	6	5	1	0

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

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

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

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



S2202	S2205	S2206	T2206	L2207	Q2211	V2062	D1967	E1871	Y1745	GLU	G1606	S1396	SER	L1206	T1108	P986
N2206	T2206	K2067	Q2068	K2069	S2070	K2073	D1968	THR	L1749	ALA	S1607	Q1397	THR	L1207	THR	4996
T2206	L2207	K2069	R1970	Q1971	P1972	W1976	E1969	GLU	A1498	SER	A1609	F1401	ILE	C1209	ILE	E997
L2207	L2075	S2070	R1971	Q1971	P1972	W1976	A1609	ASP	T1499	ASP	F1401	F1406	ASP	L1113	ASP	L998
L2222	L2076	E2077	Q1971	Q1971	P1972	W1976	R1612	ASP	I1501	ASP	R1406	R1407	ASP	R1124	ASP	C999
D2227	L2077	S2079	Q1971	Q1971	P1972	W1976	A1613	ASP	P1504	ASP	K1407	K1407	ASP	L1126	ASP	I1000
A2228	L2078	E2080	Q1971	Q1971	P1972	W1976	M1614	ASP	H1506	ASP	K1407	K1407	ASP	H1127	ASP	I1008
S2233	L2235	K2084	Q1971	Q1971	P1972	W1976	E1615	ASP	G1506	ASP	K1407	K1407	ASP	H1128	ASP	E1009
N2239	L2235	P2085	Q1971	Q1971	P1972	W1976	L1616	ASN	H1507	ASN	K1407	K1407	ASN	W1129	ASN	I1010
H2240	L2235	E2087	Q1971	Q1971	P1972	W1976	K1617	SER	L1507	SER	K1407	K1407	SER	S1019	SER	S1019
L2244	L2235	L2088	Q1971	Q1971	P1972	W1976	K1618	THR	F1518	THR	K1407	K1407	THR	R1137	THR	G1025
G2245	L2235	P2088	Q1971	Q1971	P1972	W1976	K1619	THR	T1519	THR	K1407	K1407	THR	K1139	THR	E1009
L2247	L2235	P2089	Q1971	Q1971	P1972	W1976	S1620	TYR	T1519	TYR	K1407	K1407	TYR	V1139	TYR	I1010
N2250	L2235	L2089	Q1971	Q1971	P1972	W1976	L1621	PRO	I1528	PRO	K1407	K1407	PRO	K1140	PRO	S1019
Y2255	L2235	L2089	Q1971	Q1971	P1972	W1976	L1622	ILE	I1528	ILE	K1407	K1407	ILE	L1141	ILE	S1019
E2259	L2235	P2089	Q1971	Q1971	P1972	W1976	L1623	PRO	K1592	PRO	K1407	K1407	PRO	E1038	PRO	S1019
T2260	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	LYS	D1593	LYS	K1407	K1407	LYS	I1041	LYS	S1019
A2262	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	PHE	L1594	PHE	K1407	K1407	PHE	E1046	PHE	S1019
I2263	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	HIS	G1595	HIS	K1407	K1407	HIS	E1046	HIS	S1019
G2264	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	THR	E1536	THR	K1407	K1407	THR	E1046	THR	S1019
R2285	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	GLY	K1537	GLY	K1407	K1407	GLY	E1046	GLY	S1019
V2286	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	VAL	T1538	VAL	K1407	K1407	VAL	E1046	VAL	S1019
R2287	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ASN	I1539	ASN	K1407	K1407	ASN	E1046	ASN	S1019
Q2271	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	LYS	I1547	LYS	K1407	K1407	LYS	E1046	LYS	S1019
Q2272	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ALA	T1548	ALA	K1407	K1407	ALA	E1046	ALA	S1019
K2273	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ARG	V1549	ARG	K1407	K1407	ARG	E1046	ARG	S1019
K2274	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	PHE	M1550	PHE	K1407	K1407	PHE	E1046	PHE	S1019
V2275	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	SER	A1551	SER	K1407	K1407	SER	E1046	SER	S1019
T2285	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	VAL	I1554	VAL	K1407	K1407	VAL	E1046	VAL	S1019
V2169	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	GLY	S1557	GLY	K1407	K1407	GLY	E1046	GLY	S1019
L2170	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ARG	L1564	ARG	K1407	K1407	ARG	E1046	ARG	S1019
L2173	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	MET	E1565	MET	K1407	K1407	MET	E1046	MET	S1019
R2294	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	LYS	Y1566	LYS	K1407	K1407	LYS	E1046	LYS	S1019
E2297	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	GLM	L1567	GLM	K1407	K1407	GLM	E1046	GLM	S1019
L2298	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ALA	D1577	ALA	K1407	K1407	ALA	E1046	ALA	S1019
K2299	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ARG	T1578	ARG	K1407	K1407	ARG	E1046	ARG	S1019
E2300	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ASP	Q1579	ASP	K1407	K1407	ASP	E1046	ASP	S1019
K2301	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	LYS	R1582	LYS	K1407	K1407	LYS	E1046	LYS	S1019
T2302	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	HIS	F1583	HIS	K1407	K1407	HIS	E1046	HIS	S1019
D2303	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	SER	F1584	SER	K1407	K1407	SER	E1046	SER	S1019
T2304	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ASP	R1587	ASP	K1407	K1407	ASP	E1046	ASP	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	SER	L1588	SER	K1407	K1407	SER	E1046	SER	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ALA	M1592	ALA	K1407	K1407	ALA	E1046	ALA	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	PRO	E1593	PRO	K1407	K1407	PRO	E1046	PRO	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ILE	S1594	ILE	K1407	K1407	ILE	E1046	ILE	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	THR	L1595	THR	K1407	K1407	THR	E1046	THR	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	LYS	V1596	LYS	K1407	K1407	LYS	E1046	LYS	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	GLU	K1605	GLU	K1407	K1407	GLU	E1046	GLU	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	LEU		LEU	K1407	K1407	LEU	E1046	LEU	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	GLU		GLU	K1407	K1407	GLU	E1046	GLU	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	ARG		ARG	K1407	K1407	ARG	E1046	ARG	S1019
	L2235	P2089	Q1971	Q1971	P1972	W1976	L1624	TRP		TRP	K1407	K1407	TRP	E1046	TRP	S1019





## 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 (Å)	272.384, 272.384, 272.384	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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, ZN, 5CM, ANP, SAH

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	0.38	0/15111	0.50	0/20456
2	D	0.55	0/160	0.85	0/242
3	E	0.64	0/225	0.87	0/346
All	All	0.39	0/15496	0.52	0/21044

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	434	0
2	D	164	0	92	12	0
3	E	201	0	111	7	0
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	446	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 (446) 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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:443:TYR:HH	1:A:459:SER:HG	1.48	0.59
1:A:1227:TRP:HA	1:A:1329:ARG:HB2	1.85	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:A:1376:GLU:HB3	1.86	0.57
1:A:860:GLU:HA	1:A:860:GLU:OE2	2.03	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
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:351:THR:HG22	1:A:435:ILE:HG23	1.88	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:2167:GLU:CD	1:A:2239:ASN:HD21	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1223:ARG:HD3	1:A:1228:ALA:HB2	1.88	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
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: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:2117:CYS:SG	1:A:2118:VAL:N	2.82	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: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:2261:GLN:CG	1:A:2265:ARG:HH22	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:ARG:HB2	1:A:906:TRP:CH2	2.46	0.51
1:A:2006:LYS:H	1:A:2009:ASN:CG	2.13	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: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:701:THR:OG1	1:A:704:GLU:OE1	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1416:MET:HE3	1:A:1476:LEU:HD22	1.96	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
1:A:1186:SER:OG	1:A:1187:SER:N	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1582:ARG:C	1:A:1584:PHE:H	2.17	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
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:693:VAL:O	1:A:694:THR:OG1	2.32	0.45
1:A:1388:SER:OG	1:A:1389:ASN:N	2.48	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: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:1254:ASP:HA	1:A:1257:LYS:HZ2	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:609:LEU:C	1:A:610:ARG:HD2	2.39	0.43
1:A:1471:VAL:HG22	1:A:1518:PHE:CE2	2.53	0.43
1:A:2304:TRP:CG	1:A:2304:TRP:O	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
1:A:926:TYR:CG	1:A:926:TYR:O	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1886:LEU:C	1:A:1888:GLU:H	2.22	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:452:ASP:N	1:A:452:ASP:OD1	2.53	0.42
1:A:563:ASP:N	1:A:563:ASP:OD1	2.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:401:THR:O	1:A:401:THR:OG1	2.29	0.41
1:A:443:TYR:OH	1:A:459:SER:OG	2.28	0.41
1:A:915:GLU:HB2	1:A:941:ARG:NH1	2.36	0.41
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:806:ILE:HD12	1:A:806:ILE:HA	1.89	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: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:1713:VAL:H	1:A:1716:MET:CE	2.35	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 [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	1607/2015 (80%)	1596 (99%)	11 (1%)	84	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	501	ASP
1	A	860	GLU
1	A	881	LEU
1	A	898	LYS
1	A	930	GLN
1	A	944	LEU
1	A	1373	HIS
1	A	1532	LYS
1	A	1797	LYS
1	A	2187	SER
1	A	2265	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	GLN
1	A	473	HIS
1	A	516	HIS
1	A	1067	GLN
1	A	1202	HIS
1	A	1242	ASN
1	A	1342	ASN
1	A	1348	HIS
1	A	1427	HIS
1	A	1715	HIS
1	A	1818	GLN
1	A	1822	ASN
1	A	1827	GLN
1	A	1859	HIS
1	A	1879	GLN
1	A	1940	GLN
1	A	2038	GLN
1	A	2101	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 [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	17,21,22	1.01	2 (11%)	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	30	5CM	C6-C5	2.84	1.39	1.34
2	D	30	5CM	C6-N1	-2.20	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	-3.58	119.66	123.34
2	D	30	5CM	C5-C4-N3	-2.50	118.98	121.67

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 monosaccharides in this entry.



## 5.6 Ligand geometry

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	-	24,28,28	0.66	0	25,40,40	0.66	0
6	ANP	A	2407	7	29,33,33	1.20	5 (17%)	31,52,52	1.07	4 (12%)

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	-	-	8/11/31/31	0/3/3/3
6	ANP	A	2407	7	-	6/14/38/38	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	3.20	1.51	1.46
6	A	2407	ANP	PB-O1B	2.97	1.50	1.46
6	A	2407	ANP	PB-O2B	-2.21	1.50	1.56
6	A	2407	ANP	PG-O3G	-2.04	1.51	1.56
6	A	2407	ANP	PG-O2G	-2.03	1.51	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2407	ANP	O2B-PB-O1B	4.08	118.48	109.92
6	A	2407	ANP	C5-C6-N6	2.07	123.49	120.35
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:

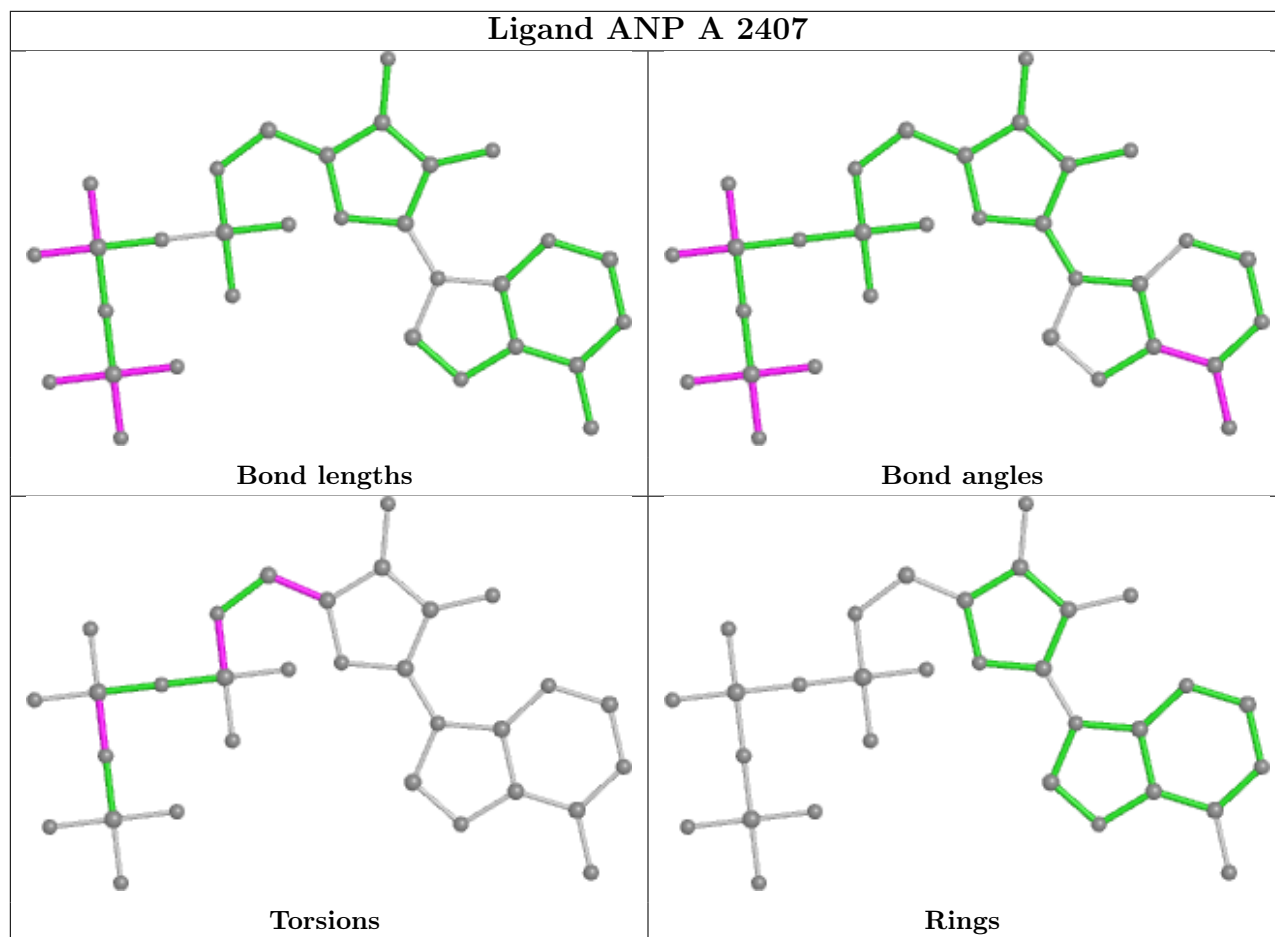
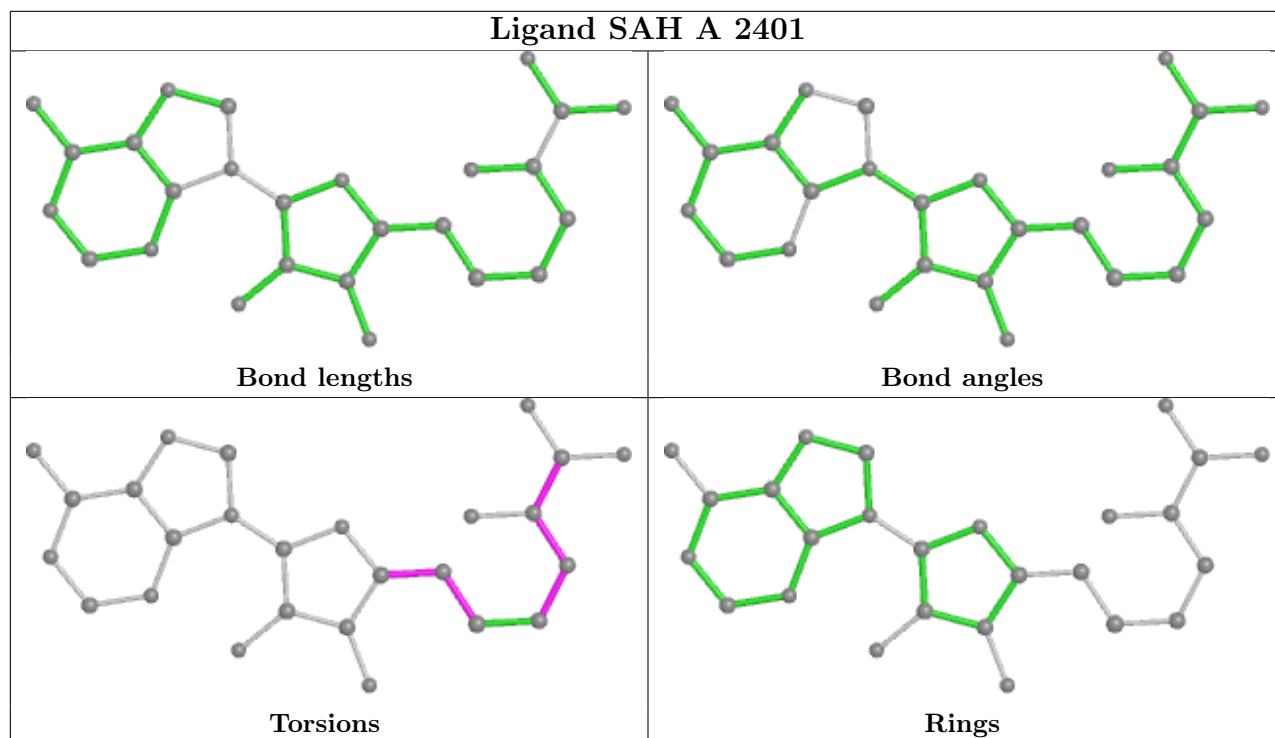
Mol	Chain	Res	Type	Atoms
4	A	2401	SAH	N-CA-CB-CG
4	A	2401	SAH	C-CA-CB-CG
4	A	2401	SAH	O4'-C4'-C5'-SD
4	A	2401	SAH	C3'-C4'-C5'-SD
6	A	2407	ANP	C5'-O5'-PA-O2A
6	A	2407	ANP	O4'-C4'-C5'-O5'
4	A	2401	SAH	CA-CB-CG-SD
6	A	2407	ANP	C5'-O5'-PA-O3A
6	A	2407	ANP	C5'-O5'-PA-O1A
6	A	2407	ANP	C3'-C4'-C5'-O5'
4	A	2401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



## 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.

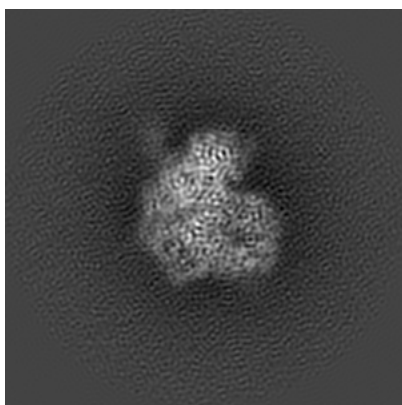
## 6 Map visualisation [i](#)

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.

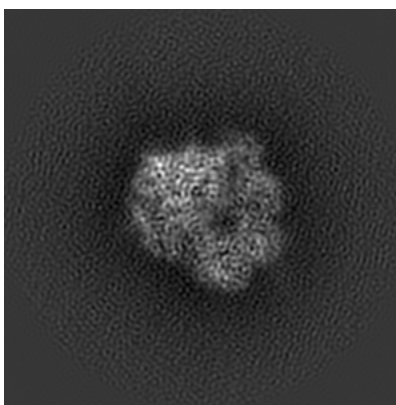
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

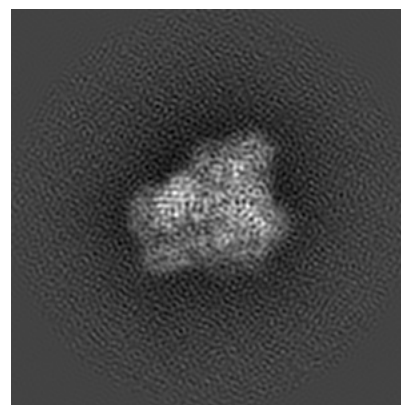
#### 6.1.1 Primary map



X



Y

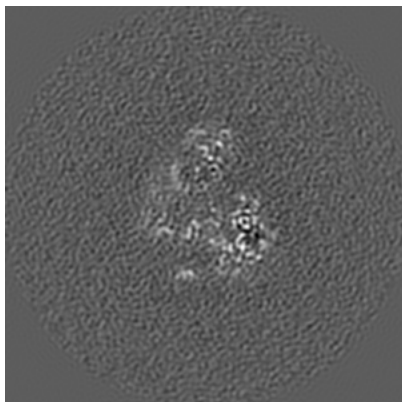


Z

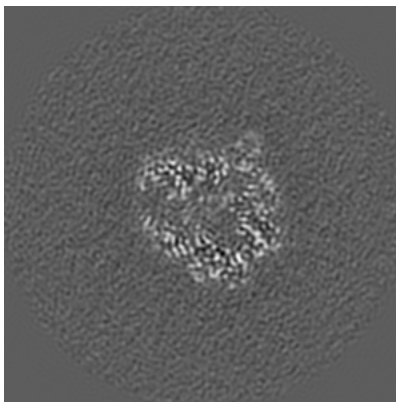
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

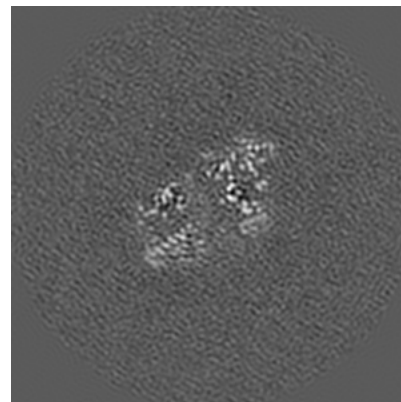
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

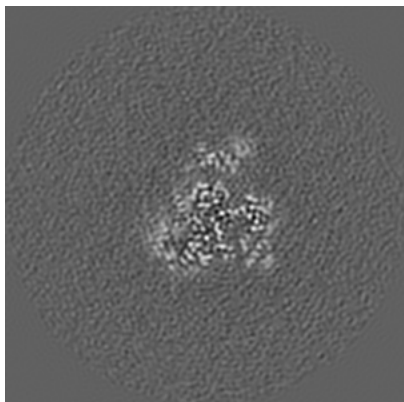


Z Index: 128

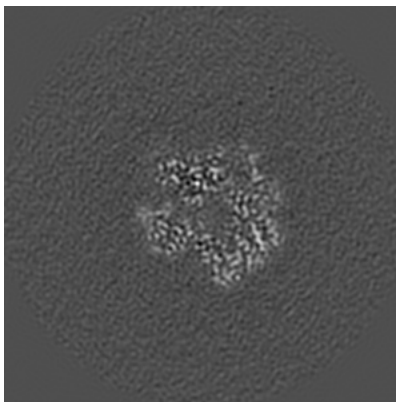
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

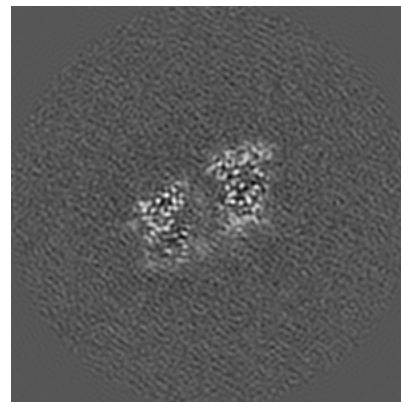
### 6.3.1 Primary map



X Index: 149



Y Index: 133

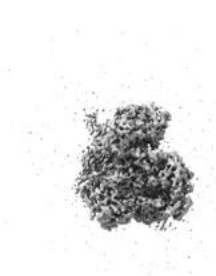


Z Index: 132

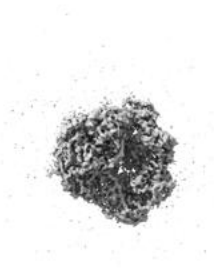
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

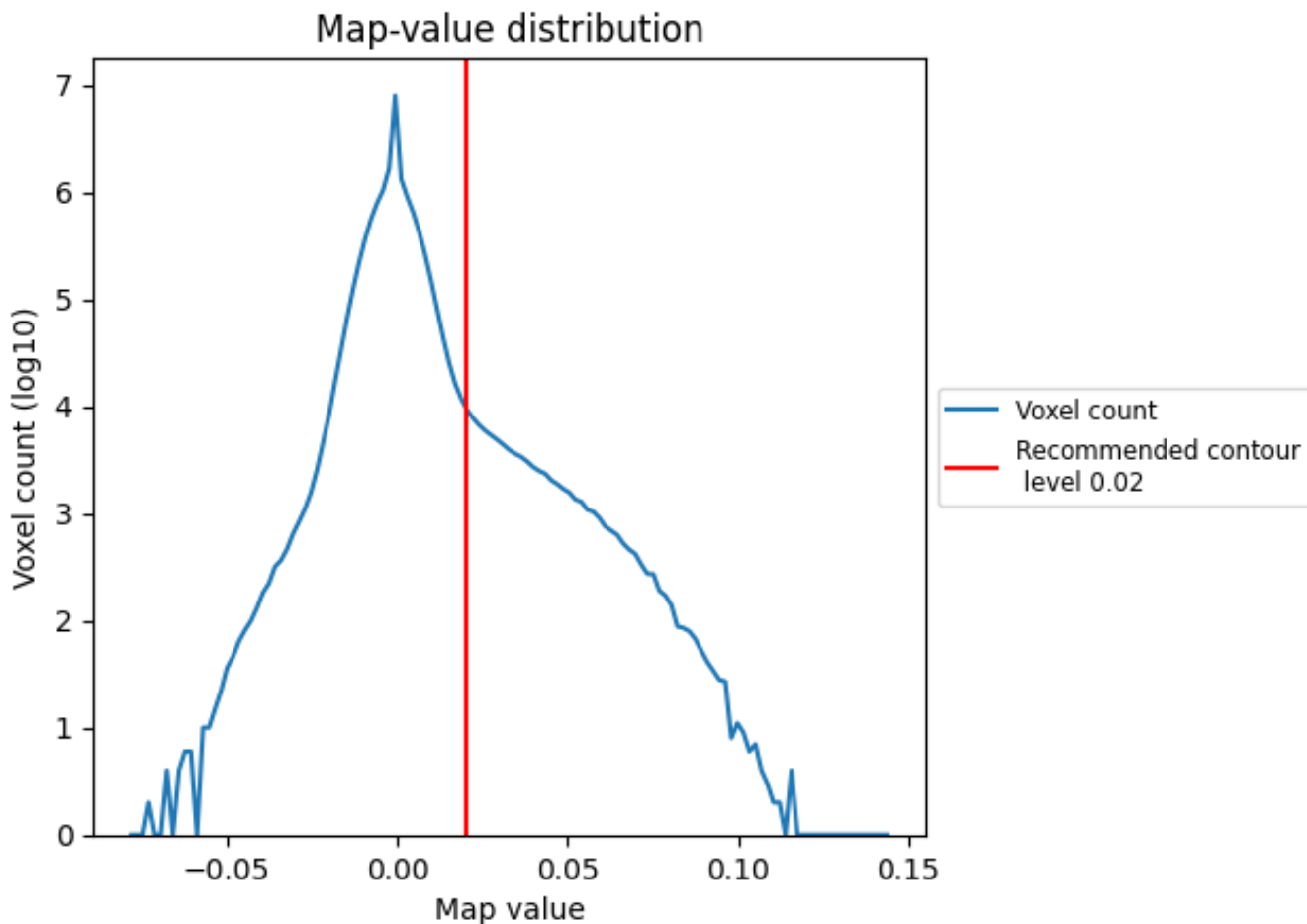
## 6.5 Mask visualisation

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.

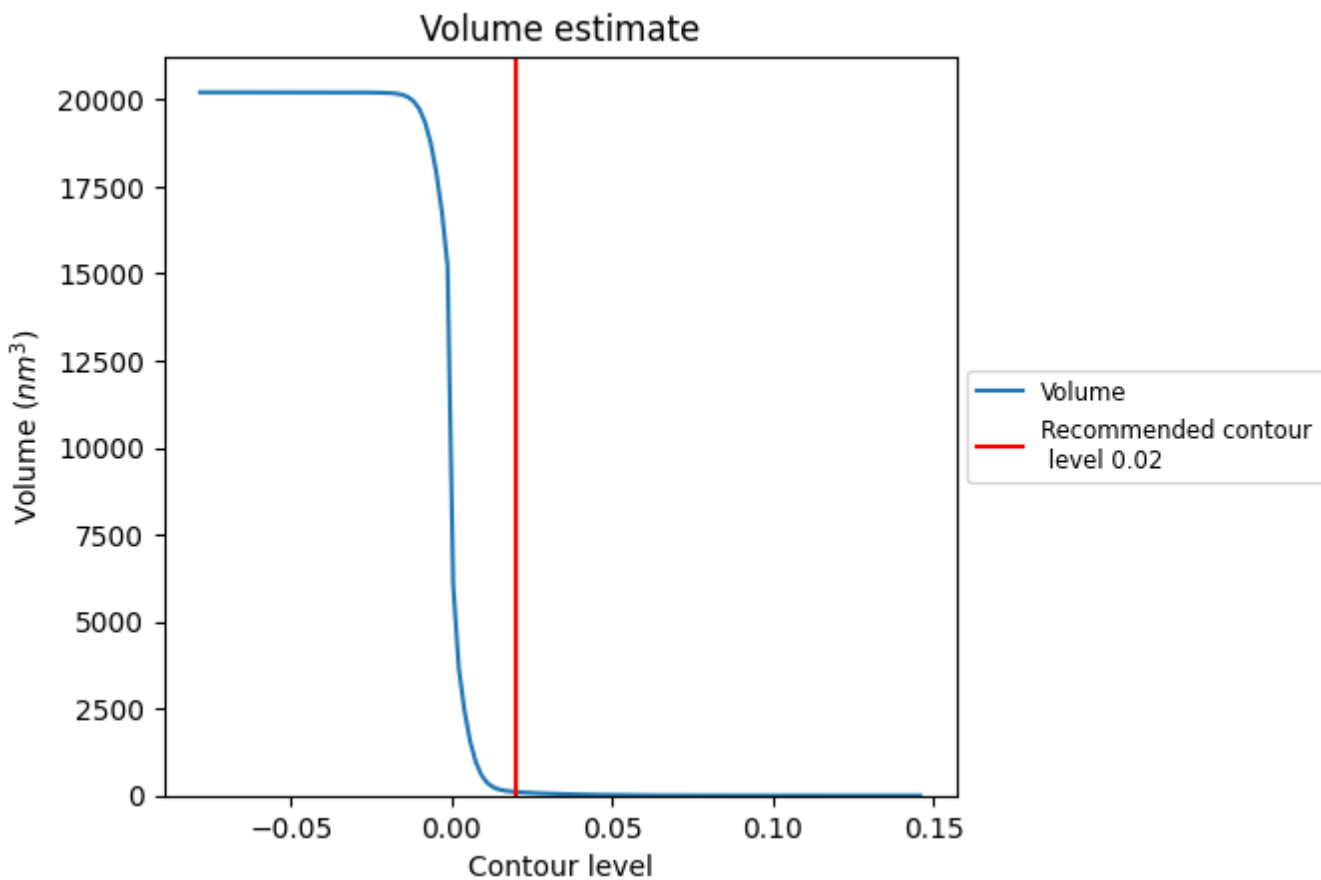
### 7.1 Map-value distribution [i](#)



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.



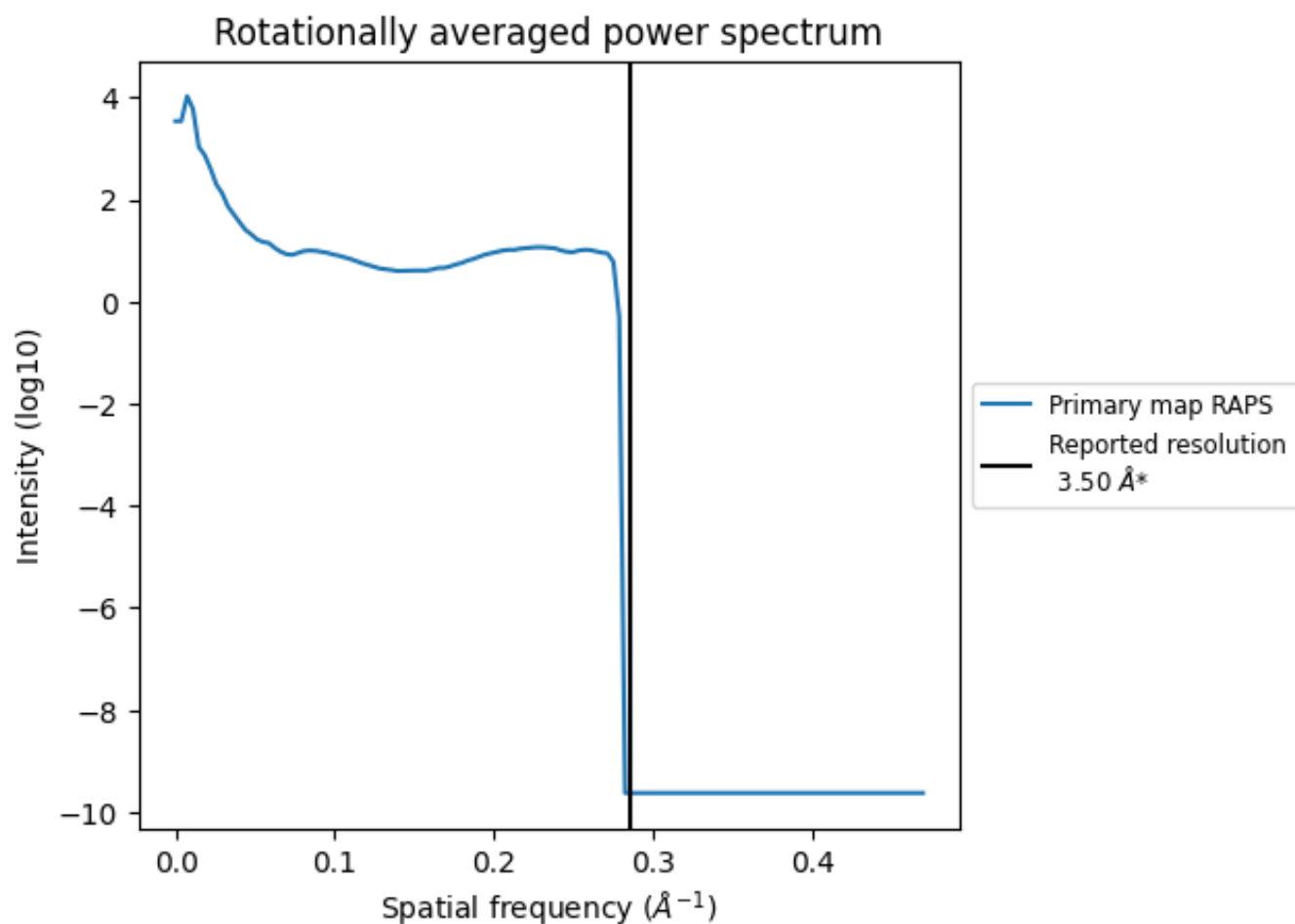
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm<sup>3</sup>; 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 [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of  $0.286 \text{\AA}^{-1}$

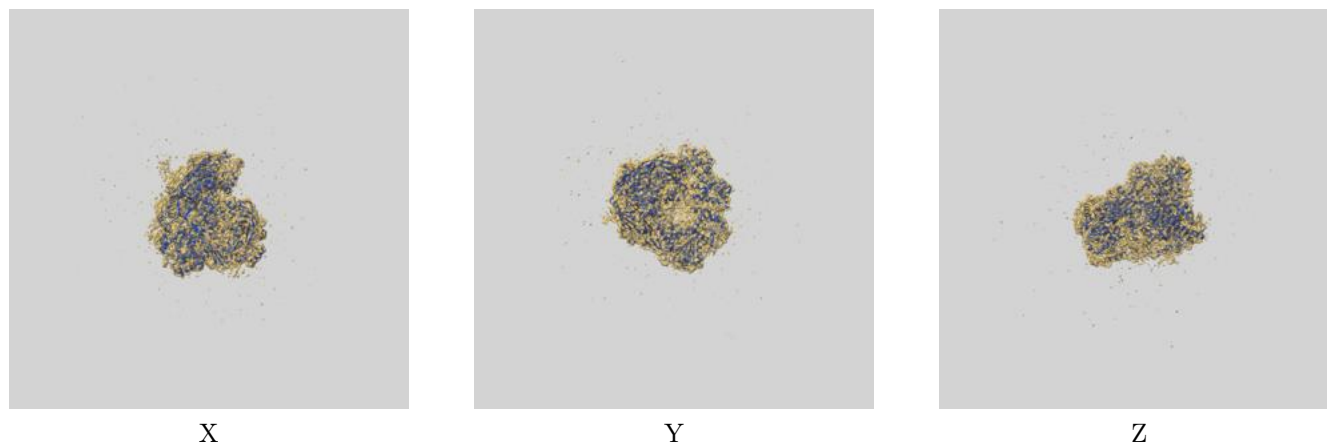
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

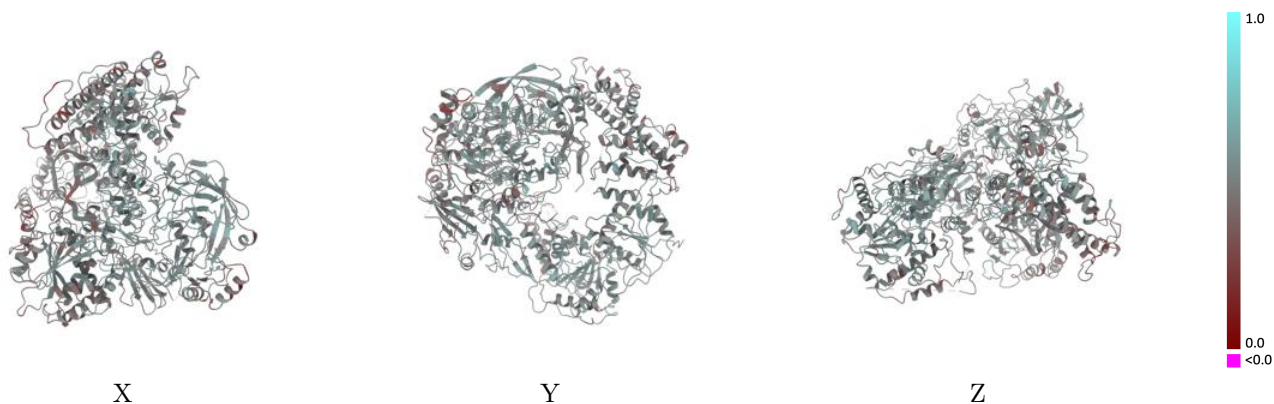
This section contains information regarding the fit between EMDB map EMD-24295 and PDB model 7R78. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



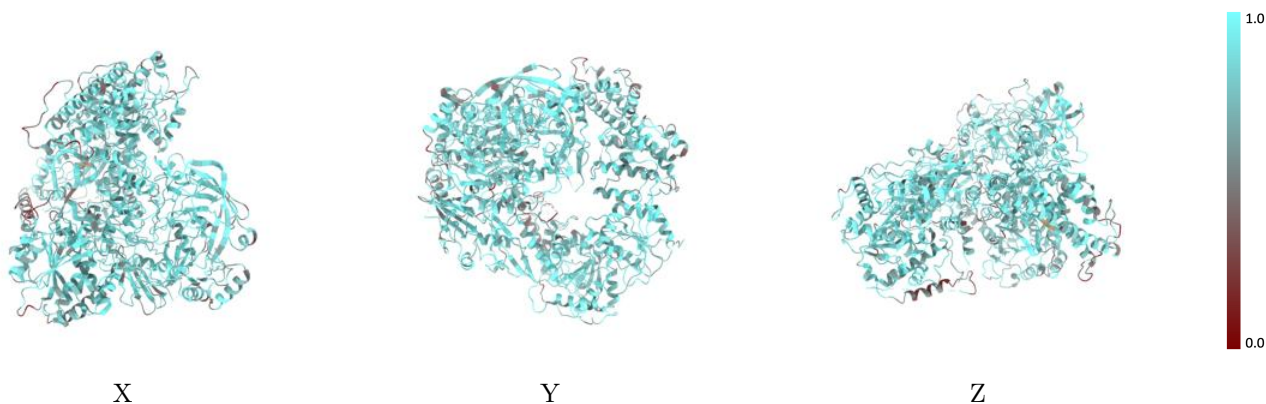
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



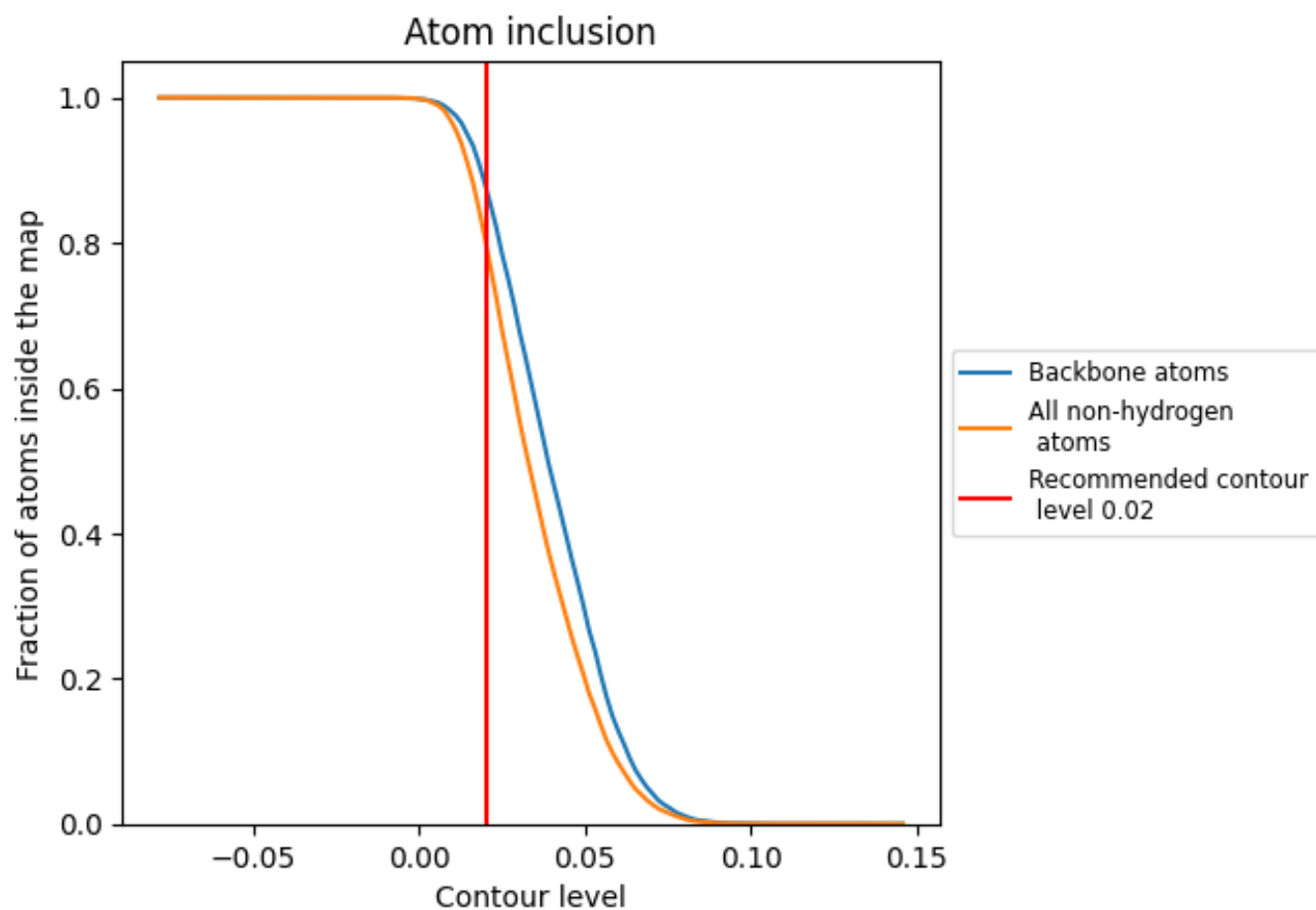
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.02).






## 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	 0.8032	 0.4980
A	 0.8029	 0.4990
D	 0.7866	 0.4410
E	 0.8358	 0.4690

