



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:18 AM UTC

PDB ID : 8PS1 / pdb_00008ps1
EMDB ID : EMD-17842
Title : Asymmetric unit of the yeast fatty acid synthase in the non-rotated state with ACP at the ketosynthase domain (FASamn sample)
Authors : Singh, K.; Bunzel, G.; Graf, B.; Yip, K.M.; Stark, H.; Chari, A.
Deposited on : 2023-07-13
Resolution : 2.80 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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

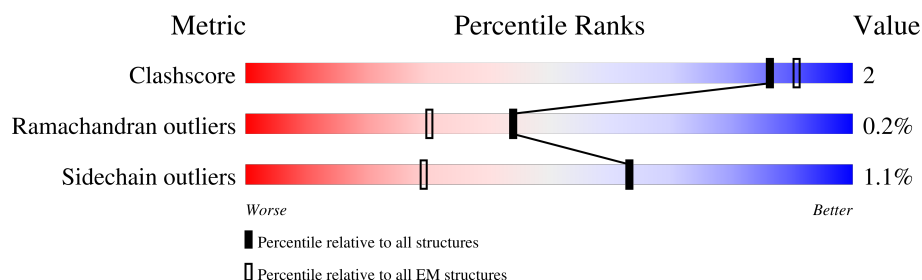
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1887	 77% 7% 16%
1	B	1887	 8% 91%
2	G	2051	 93% 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 29787 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.

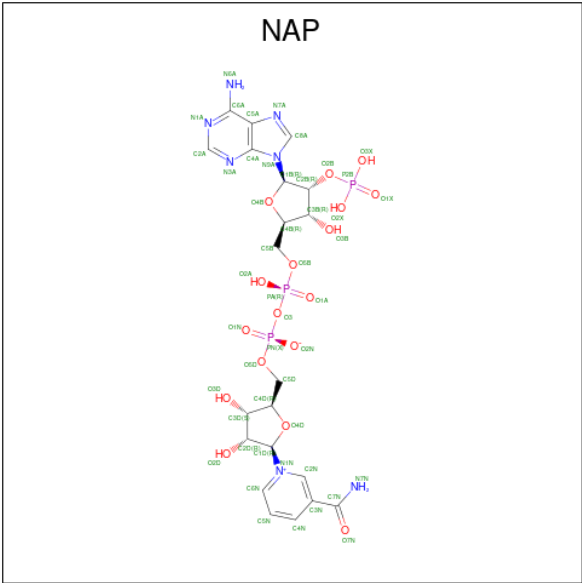
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1584	12379	7837	2089	2405	48	0	0
1	B	163	1223	775	205	240	3	0	0

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	2034	16010	10261	2661	3032	56	0	0

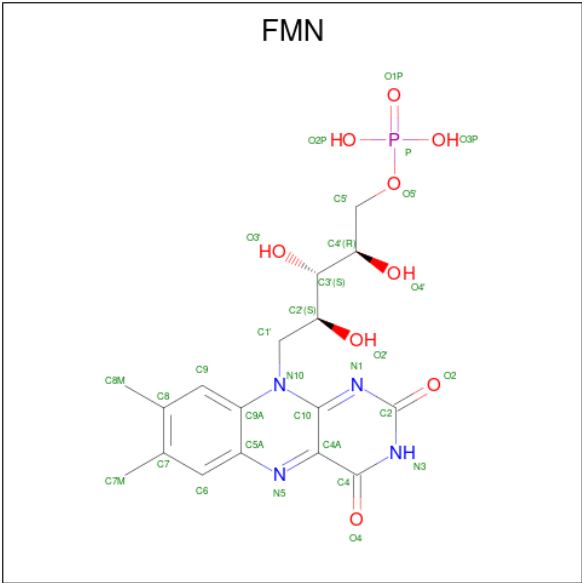
- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	G	1	48	21	7	17	3	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
5	G	1	48	21	7	16	3	1	0





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121299	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	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: NAP, J8W, FMN, COA

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	1.07	6/12613 (0.0%)	1.51	16/17048 (0.1%)
1	B	1.02	0/1241	1.64	7/1675 (0.4%)
2	G	1.02	1/16362 (0.0%)	1.48	19/22199 (0.1%)
All	All	1.04	7/30216 (0.0%)	1.50	42/40922 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	733	ILE	C-O	-6.55	1.16	1.24
1	A	1690	ASN	C-O	-6.42	1.16	1.24
1	A	1386	ILE	C-O	-6.32	1.17	1.24
1	A	1029	PRO	C-O	-6.16	1.16	1.24
1	A	703	VAL	C-O	-5.62	1.18	1.24
1	A	677	TYR	C-O	-5.28	1.17	1.24
2	G	1562	PRO	C-O	-5.20	1.17	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1417	SER	CA-C-N	8.46	125.57	120.24
1	A	1417	SER	C-N-CA	8.46	125.57	120.24
1	A	1288	ASN	CA-CB-CG	-7.80	104.80	112.60
2	G	1150	ARG	CB-CA-C	-6.64	99.77	110.79
1	A	1370	THR	CB-CA-C	6.35	120.28	109.80
1	B	179	LYS	CA-C-N	6.29	129.34	120.28
1	B	179	LYS	C-N-CA	6.29	129.34	120.28
1	B	237	MET	CA-C-N	-6.22	114.33	120.98
1	B	237	MET	C-N-CA	-6.22	114.33	120.98
2	G	799	PHE	CA-CB-CG	-6.00	107.80	113.80
2	G	460	TYR	CA-C-N	5.87	129.44	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	460	TYR	C-N-CA	5.87	129.44	121.05
1	B	272	GLU	CA-C-N	-5.70	114.13	120.45
1	B	272	GLU	C-N-CA	-5.70	114.13	120.45
1	A	1601	ASN	CA-CB-CG	-5.64	106.96	112.60
2	G	830	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	1875	ASP	CA-CB-CG	5.60	118.20	112.60
2	G	684	GLY	CA-C-O	-5.57	118.38	122.23
2	G	1587	ALA	CA-C-N	5.53	128.15	120.63
2	G	1587	ALA	C-N-CA	5.53	128.15	120.63
1	A	764	ASP	CB-CA-C	5.45	118.18	111.43
1	A	1612	ASP	CA-CB-CG	5.40	118.00	112.60
2	G	880	LEU	CA-C-N	5.37	124.62	120.33
2	G	880	LEU	C-N-CA	5.37	124.62	120.33
2	G	52	ASP	CA-CB-CG	5.33	117.93	112.60
2	G	65	LEU	CA-C-N	5.30	125.87	119.98
2	G	65	LEU	C-N-CA	5.30	125.87	119.98
1	B	276	ARG	N-CA-C	-5.26	99.60	110.80
1	A	904	ASN	CA-C-N	5.23	127.29	120.28
1	A	904	ASN	C-N-CA	5.23	127.29	120.28
2	G	637	VAL	N-CA-C	-5.20	105.53	110.42
2	G	484	ILE	CA-C-O	-5.19	114.70	120.46
2	G	1423	PHE	CA-C-O	-5.17	115.90	121.38
2	G	1820	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	1874	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	1208	VAL	CA-C-N	5.10	127.48	120.39
1	A	1208	VAL	C-N-CA	5.10	127.48	120.39
2	G	589	ARG	CB-CA-C	5.09	116.97	110.76
1	A	452	GLU	N-CA-C	-5.09	105.01	111.11
1	A	1219	VAL	CA-C-O	-5.08	115.41	121.05
2	G	1801	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	424	VAL	N-CA-C	-5.03	106.89	111.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12379	0	12317	59	0
1	B	1223	0	1265	3	0
2	G	16010	0	15979	64	0
3	A	48	0	25	0	0
3	G	48	0	25	0	0
4	G	31	0	19	2	0
5	G	48	0	32	0	0
All	All	29787	0	29662	123	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 2.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1150:ARG:HD2	2:G:1193:THR:HG21	1.72	0.71
1:A:865:CYS:HB2	1:A:917:CYS:SG	2.30	0.71
2:G:1838:MET:HE1	2:G:1976:PHE:HD1	1.58	0.69
1:A:1189:ILE:H	1:A:1380:GLN:HE21	1.42	0.67
2:G:806:MET:HE1	2:G:1054:LEU:O	1.96	0.65
2:G:1838:MET:CE	2:G:1976:PHE:HD1	2.10	0.64
2:G:1736:MET:HG2	2:G:1751:ILE:HD13	1.83	0.61
1:A:706:THR:HB	1:A:737:PHE:HB3	1.82	0.61
1:A:41:THR:HG21	2:G:1663:THR:HG22	1.85	0.59
1:A:1186:ALA:HB3	1:A:1188:GLN:HE21	1.68	0.58
1:A:790:PHE:CE2	1:A:794:ILE:HD11	2.38	0.58
2:G:1838:MET:HE1	2:G:1976:PHE:CD1	2.37	0.57
2:G:597:MET:HA	4:G:2101:FMN:N5	2.20	0.57
2:G:1638:ILE:HD13	2:G:1657:ILE:CG1	2.35	0.56
2:G:1782:THR:HG22	2:G:1827:LEU:HD21	1.89	0.55
1:A:1592:MET:HE2	1:A:1641:ILE:HG23	1.88	0.54
2:G:1789:PHE:CD2	2:G:1817:SER:HB3	2.41	0.54
2:G:915:ALA:HA	2:G:1000:ILE:HD11	1.89	0.54
2:G:864:LEU:HD11	2:G:868:PHE:CZ	2.43	0.54
1:A:826:MET:HE1	1:A:850:PHE:CE2	2.43	0.53
1:A:1411:THR:HA	1:A:1648:GLN:O	2.07	0.53
1:A:451:MET:HE1	1:A:480:CYS:SG	2.49	0.53
2:G:145:LEU:HD21	2:G:156:LEU:HD21	1.91	0.53
2:G:1201:VAL:HG11	2:G:1226:ASN:HB2	1.89	0.53
1:A:771:PHE:CE1	1:A:825:PRO:HB3	2.44	0.53
1:A:413:LEU:HD11	1:A:451:MET:SD	2.49	0.52
2:G:234:ILE:N	2:G:235:PRO:CD	2.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1629:VAL:HG12	2:G:1637:LEU:O	2.09	0.52
1:A:35:PHE:CD1	2:G:1663:THR:HG21	2.45	0.52
2:G:1838:MET:CE	2:G:1976:PHE:CD1	2.92	0.52
2:G:1782:THR:CG2	2:G:1827:LEU:HD21	2.40	0.51
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.45	0.51
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.45	0.51
1:A:17:LEU:HD23	2:G:2014:LEU:HD23	1.93	0.51
1:A:518:LYS:HG3	1:A:519:VAL:HG23	1.93	0.51
1:B:249:TYR:CE1	1:B:284:LYS:HD2	2.46	0.50
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.47	0.50
1:A:529:MET:HE1	1:A:894:ARG:HG2	1.92	0.50
1:A:995:LEU:HD13	1:A:1674:VAL:HG22	1.94	0.50
2:G:653:TYR:HA	2:G:659:LEU:HD11	1.94	0.50
2:G:1339:PHE:N	2:G:1340:PRO:HD2	2.27	0.50
1:A:1248:GLY:O	1:A:1331:GLY:HA2	2.12	0.49
2:G:679:LEU:HD21	2:G:681:ILE:HD11	1.94	0.49
1:A:1600:LEU:HD11	1:A:1655:VAL:HG12	1.95	0.49
2:G:1890:ASN:HB2	2:G:1899:VAL:HB	1.94	0.49
1:A:1533:ILE:HD11	1:A:1561:MET:HE1	1.95	0.49
2:G:767:PHE:HD2	2:G:771:PHE:CE2	2.31	0.49
1:A:891:MET:SD	1:A:939:PHE:CE2	3.06	0.49
2:G:1638:ILE:HD13	2:G:1657:ILE:HG13	1.95	0.48
2:G:808:ALA:HB3	2:G:811:VAL:HG23	1.96	0.48
1:A:1815:ALA:HB2	1:A:1871:ILE:HD11	1.96	0.47
2:G:848:SER:HB3	2:G:854:ILE:HD11	1.96	0.47
1:A:443:SER:HA	1:A:447:LEU:HD23	1.97	0.47
1:A:704:VAL:HG23	1:A:763:TRP:CZ3	2.51	0.46
2:G:528:ILE:HG21	2:G:547:ILE:HG13	1.97	0.46
2:G:1048:VAL:O	2:G:1051:THR:OG1	2.28	0.46
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.77	0.46
2:G:965:SER:O	2:G:968:GLN:NE2	2.48	0.46
1:A:1030:TRP:O	1:A:1035:THR:OG1	2.34	0.46
2:G:1323:MET:HE2	2:G:1357:TYR:HB2	1.98	0.46
2:G:369:SER:HB2	2:G:428:HIS:HB2	1.98	0.45
1:A:1592:MET:HE1	1:A:1642:THR:O	2.16	0.45
2:G:1323:MET:CE	2:G:1357:TYR:HB2	2.45	0.45
1:A:1246:CYS:SG	1:A:1327:CYS:SG	3.07	0.45
1:A:702:LYS:HG3	1:A:731:THR:HB	1.99	0.45
2:G:1546:THR:HG21	2:G:1616:VAL:HG11	1.99	0.45
1:A:1791:PHE:HZ	1:A:1813:TRP:HB2	1.81	0.44
2:G:602:VAL:HG12	2:G:620:ALA:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1816:LYS:HB3	1:A:1834:LEU:HD12	1.99	0.44
1:A:671:VAL:HG21	1:A:910:THR:HG22	1.99	0.44
2:G:593:LEU:HB3	2:G:616:THR:OG1	2.17	0.44
1:A:1600:LEU:CD1	1:A:1655:VAL:HG12	2.48	0.44
2:G:250:VAL:O	2:G:251:VAL:C	2.61	0.44
2:G:1638:ILE:HD13	2:G:1657:ILE:HG12	1.98	0.43
1:A:413:LEU:CD1	1:A:451:MET:HG2	2.49	0.43
1:B:184:ASN:OD1	1:B:184:ASN:C	2.61	0.43
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	2.00	0.43
1:A:1544:THR:O	1:A:1545:SER:HB3	2.18	0.43
1:A:655:LEU:HD22	1:A:916:LEU:HD21	2.01	0.43
2:G:648:GLY:HA3	2:G:678:PHE:CZ	2.54	0.43
2:G:827:VAL:HG11	2:G:840:THR:HG22	2.01	0.43
1:A:1293:SER:O	1:A:1293:SER:OG	2.28	0.43
1:A:1470:LEU:HD13	1:A:1489:ARG:HG2	2.01	0.43
2:G:233:SER:OG	2:G:235:PRO:HD2	2.18	0.43
1:A:1531:LEU:HD21	1:A:1660:TYR:CE1	2.54	0.43
2:G:105:ALA:HB1	2:G:119:THR:CG2	2.48	0.43
2:G:372:ASN:HB3	2:G:515:LEU:HD21	2.01	0.43
2:G:598:THR:HA	2:G:599:PRO:HA	1.79	0.43
1:A:1367:ARG:O	1:A:1370:THR:HB	2.20	0.42
2:G:1804:PHE:CE2	2:G:2010:TYR:HB2	2.54	0.42
1:A:451:MET:O	1:A:452:GLU:C	2.60	0.42
1:A:852:ARG:HA	1:A:855:SER:OG	2.19	0.42
1:A:1138:LYS:HG3	1:A:1163:TYR:CE1	2.53	0.42
2:G:176:LEU:HD13	2:G:247:ALA:HB3	2.02	0.42
2:G:615:TYR:OH	2:G:1075:ASP:OD1	2.33	0.42
2:G:738:GLY:HA3	4:G:2101:FMN:HM83	2.02	0.42
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	2.02	0.42
1:B:150:LEU:HD21	1:B:193:GLU:OE2	2.19	0.42
2:G:159:ILE:HA	2:G:271:THR:O	2.19	0.42
2:G:370:LEU:HB2	2:G:378:VAL:HB	2.01	0.42
1:A:413:LEU:HD11	1:A:451:MET:HG2	2.01	0.42
1:A:1186:ALA:HB3	1:A:1188:GLN:NE2	2.35	0.41
1:A:719:GLN:HG3	1:A:1612:ASP:HA	2.02	0.41
1:A:1181:PHE:CE2	1:A:1183:ARG:HB2	2.55	0.41
2:G:1778:GLN:HB2	2:G:1779:PRO:HD3	2.02	0.41
1:A:1752:THR:O	1:A:1756:ILE:HG12	2.21	0.41
2:G:64:PHE:O	2:G:68:VAL:HG23	2.21	0.41
2:G:730:LEU:C	2:G:730:LEU:HD23	2.46	0.41
2:G:1313:SER:N	2:G:1319:MET:HE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:ILE:HD13	1:A:1283:MET:HE3	2.03	0.41
1:A:1523:ARG:NH2	1:A:1564:LEU:O	2.49	0.41
2:G:1784:MET:SD	2:G:1784:MET:C	3.04	0.41
1:A:334:ASP:HA	1:A:337:VAL:HG12	2.03	0.41
2:G:767:PHE:HD1	2:G:796:PHE:CE2	2.39	0.41
1:A:1787:ILE:HD12	1:A:1809:PHE:CE1	2.56	0.40
1:A:1842:VAL:HG23	1:A:1845:ASN:HB2	2.03	0.40
2:G:844:VAL:HG21	2:G:866:LYS:HD2	2.03	0.40
1:A:821:GLN:HA	1:A:863:THR:OG1	2.22	0.40
1:A:1541:PHE:CD2	1:A:1553:GLU:HG2	2.55	0.40
1:A:447:LEU:HG	1:A:451:MET:HE2	2.02	0.40
1:A:1305:CYS:HB2	1:A:1645:GLY:HA2	2.04	0.40
2:G:1773:ALA:O	2:G:1774:THR:C	2.65	0.40
2:G:1878:VAL:HG22	2:G:1944:ILE:HG12	2.04	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	1576/1887 (84%)	1491 (95%)	81 (5%)	4 (0%)	36	66
1	B	161/1887 (8%)	143 (89%)	16 (10%)	2 (1%)	10	34
2	G	2029/2051 (99%)	1907 (94%)	119 (6%)	3 (0%)	48	77
All	All	3766/5825 (65%)	3541 (94%)	216 (6%)	9 (0%)	44	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	1091	GLY
2	G	2034	GLY
1	A	22	PHE

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Mol	Chain	Res	Type
1	A	829	ASN
1	A	1545	SER
1	B	276	ARG
1	A	951	SER
1	B	178	GLY
2	G	185	GLY

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	1340/1566 (86%)	1324 (99%)	16 (1%)	63	87
1	B	135/1566 (9%)	133 (98%)	2 (2%)	57	84
2	G	1772/1788 (99%)	1755 (99%)	17 (1%)	68	88
All	All	3247/4920 (66%)	3212 (99%)	35 (1%)	63	87

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	413	LEU
1	A	523	SER
1	A	855	SER
1	A	940	THR
1	A	967	VAL
1	A	1001	VAL
1	A	1164	SER
1	A	1284	SER
1	A	1332	TYR
1	A	1333	ASP
1	A	1370	THR
1	A	1391	ASP
1	A	1643	SER
1	A	1735	SER
1	A	1850	GLU

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Mol	Chain	Res	Type
1	B	230	SER
1	B	236	LYS
2	G	193	GLU
2	G	233	SER
2	G	318	SER
2	G	340	SER
2	G	380	SER
2	G	481	ASP
2	G	599	PRO
2	G	784	GLU
2	G	843	ILE
2	G	1348	LEU
2	G	1373	SER
2	G	1381	VAL
2	G	1551	GLU
2	G	1585	SER
2	G	1586	SER
2	G	1638	ILE
2	G	1650	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	GLN
1	A	356	ASN
1	A	379	ASN
1	A	618	ASN
1	A	669	ASN
1	A	743	GLN
1	A	851	ASN
1	A	854	HIS
1	A	1188	GLN
1	A	1380	GLN
1	A	1444	ASN
1	A	1549	ASN
1	A	1558	ASN
1	A	1695	ASN
1	A	1794	GLN
1	A	1845	ASN
1	B	214	GLN
2	G	99	ASN
2	G	245	GLN

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Mol	Chain	Res	Type
2	G	500	HIS
2	G	650	ASN
2	G	655	ASN
2	G	718	ASN
2	G	723	HIS
2	G	747	HIS
2	G	760	HIS
2	G	1008	GLN
2	G	1151	HIS
2	G	1202	GLN
2	G	1217	ASN
2	G	1220	GLN
2	G	1226	ASN
2	G	1341	ASN
2	G	1352	HIS
2	G	1355	ASN
2	G	1561	ASN
2	G	1595	ASN
2	G	1619	ASN
2	G	1669	GLN
2	G	1697	HIS
2	G	1720	HIS
2	G	1851	ASN
2	G	1872	GLN
2	G	1890	ASN
2	G	1912	ASN
2	G	1983	ASN
2	G	1995	ASN
2	G	2020	GLN
2	G	2027	GLN

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	J8W	G	1808	2	10,11,12	1.76	1 (10%)	8,13,15	1.36	2 (25%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	J8W	G	1808	2	-	3/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1808	J8W	OG-C2	4.86	1.47	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1808	J8W	C3-C1-C2	-2.26	105.07	113.18
2	G	1808	J8W	OG-C2-C1	2.02	117.45	111.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1808	J8W	C-CA-CB-OG
2	G	1808	J8W	O7-C2-OG-CB
2	G	1808	J8W	C1-C2-OG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are 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$
4	FMN	G	2101	-	33,33,33	1.44	4 (12%)	48,50,50	1.65	10 (20%)
5	COA	G	2102	-	47,50,50	0.72	1 (2%)	69,75,75	0.54	0
3	NAP	G	2103	-	50,52,52	1.57	8 (16%)	71,80,80	1.75	11 (15%)
3	NAP	A	1901	-	50,52,52	1.41	8 (16%)	71,80,80	1.74	16 (22%)

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	FMN	G	2101	-	-	5/18/18/18	0/3/3/3
5	COA	G	2102	-	-	5/48/64/64	0/3/3/3
3	NAP	G	2103	-	-	7/35/67/67	0/5/5/5
3	NAP	A	1901	-	-	1/35/67/67	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2103	NAP	C5A-C4A	6.05	1.49	1.39
4	G	2101	FMN	C9A-C5A	4.50	1.48	1.41
3	A	1901	NAP	C8A-N9A	-3.81	1.31	1.37
3	A	1901	NAP	C5A-N7A	-3.72	1.32	1.39
3	A	1901	NAP	C4A-N9A	-3.56	1.30	1.37
3	G	2103	NAP	PN-O3	3.23	1.63	1.59
3	G	2103	NAP	C5A-C6A	3.13	1.49	1.41
5	G	2102	COA	P3B-O3B	2.95	1.64	1.59
3	A	1901	NAP	PN-O3	2.89	1.62	1.59
3	G	2103	NAP	O4D-C1D	2.83	1.44	1.40
3	A	1901	NAP	C8A-N7A	2.78	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1901	NAP	C5A-C4A	2.73	1.44	1.39
3	G	2103	NAP	C8A-N7A	2.66	1.36	1.31
3	G	2103	NAP	PA-O3	2.63	1.62	1.59
4	G	2101	FMN	C9-C8	-2.57	1.36	1.39
4	G	2101	FMN	O2-C2	2.47	1.29	1.24
3	A	1901	NAP	C5N-C4N	2.44	1.43	1.38
3	G	2103	NAP	C4A-N3A	2.32	1.38	1.34
3	A	1901	NAP	PA-O3	2.24	1.61	1.59
4	G	2101	FMN	C5A-N5	-2.19	1.35	1.39
3	G	2103	NAP	C5A-N7A	-2.07	1.35	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2103	NAP	C5A-C4A-N3A	-6.14	118.26	126.72
3	A	1901	NAP	C5A-C4A-N3A	-5.64	118.94	126.72
3	G	2103	NAP	N3A-C4A-N9A	5.39	136.33	127.17
4	G	2101	FMN	O3P-P-O5'	-4.81	94.12	106.67
3	G	2103	NAP	N3A-C2A-N1A	-4.33	122.03	128.58
3	G	2103	NAP	C2A-N3A-C4A	4.18	122.03	111.83
3	G	2103	NAP	C3N-C7N-N7N	4.12	122.81	117.74
4	G	2101	FMN	O2P-P-O5'	3.84	116.67	106.67
3	A	1901	NAP	N3A-C4A-N9A	3.73	133.50	127.17
3	A	1901	NAP	N3A-C2A-N1A	-3.66	123.04	128.58
3	A	1901	NAP	C2A-N3A-C4A	3.65	120.74	111.83
3	A	1901	NAP	C4A-C5A-N7A	-3.59	106.48	110.58
4	G	2101	FMN	C4'-C3'-C2'	-3.50	107.74	113.57
3	A	1901	NAP	O7N-C7N-N7N	-3.45	117.63	122.62
3	A	1901	NAP	C3N-C7N-N7N	3.36	121.88	117.74
4	G	2101	FMN	C10-N1-C2	2.91	123.15	116.85
3	A	1901	NAP	O3-PA-O1A	2.89	119.41	110.70
4	G	2101	FMN	O4-C4-C4A	-2.82	119.09	126.53
3	A	1901	NAP	O2X-P2B-O1X	2.77	121.62	110.83
3	G	2103	NAP	C4A-C5A-N7A	-2.71	107.48	110.58
3	G	2103	NAP	C2B-C1B-N9A	2.68	118.16	113.75
3	A	1901	NAP	O3-PN-O1N	-2.67	102.68	110.70
3	A	1901	NAP	C4A-N9A-C8A	2.66	108.53	105.74
3	A	1901	NAP	C5N-C4N-C3N	-2.48	117.93	120.36
4	G	2101	FMN	C4-C4A-N5	2.42	121.55	118.21
3	G	2103	NAP	C5A-N7A-C8A	2.31	107.08	103.45
4	G	2101	FMN	C4A-C10-N10	2.30	119.78	116.48
3	A	1901	NAP	O2N-PN-O1N	2.30	123.13	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2103	NAP	C4A-N9A-C8A	2.28	108.14	105.74
3	G	2103	NAP	C2A-N1A-C6A	2.24	122.42	118.73
4	G	2101	FMN	O2-C2-N3	2.21	122.83	118.58
4	G	2101	FMN	O2-C2-N1	-2.20	118.15	121.80
3	G	2103	NAP	N6A-C6A-N1A	2.13	123.13	118.38
3	A	1901	NAP	N9A-C8A-N7A	-2.12	110.92	113.94
3	A	1901	NAP	O5B-PA-O1A	-2.09	100.66	108.94
4	G	2101	FMN	O2'-C2'-C3'	2.07	114.08	109.25
3	A	1901	NAP	O2B-P2B-O1X	-2.04	102.06	109.33

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2103	NAP	C5B-O5B-PA-O1A
3	G	2103	NAP	C5B-O5B-PA-O2A
3	G	2103	NAP	C5B-O5B-PA-O3
5	G	2102	COA	CCP-O6A-P2A-O4A
4	G	2101	FMN	O3'-C3'-C4'-C5'
4	G	2101	FMN	C2'-C3'-C4'-C5'
4	G	2101	FMN	C2'-C3'-C4'-O4'
5	G	2102	COA	P1A-O3A-P2A-O5A
5	G	2102	COA	C3B-O3B-P3B-O7A
4	G	2101	FMN	O3'-C3'-C4'-O4'
5	G	2102	COA	S1P-C2P-C3P-N4P
3	A	1901	NAP	O4D-C4D-C5D-O5D
4	G	2101	FMN	C4'-C5'-O5'-P
3	G	2103	NAP	O4B-C4B-C5B-O5B
3	G	2103	NAP	C4B-C5B-O5B-PA
3	G	2103	NAP	PA-O3-PN-O1N
5	G	2102	COA	P1A-O3A-P2A-O4A
3	G	2103	NAP	PA-O3-PN-O2N

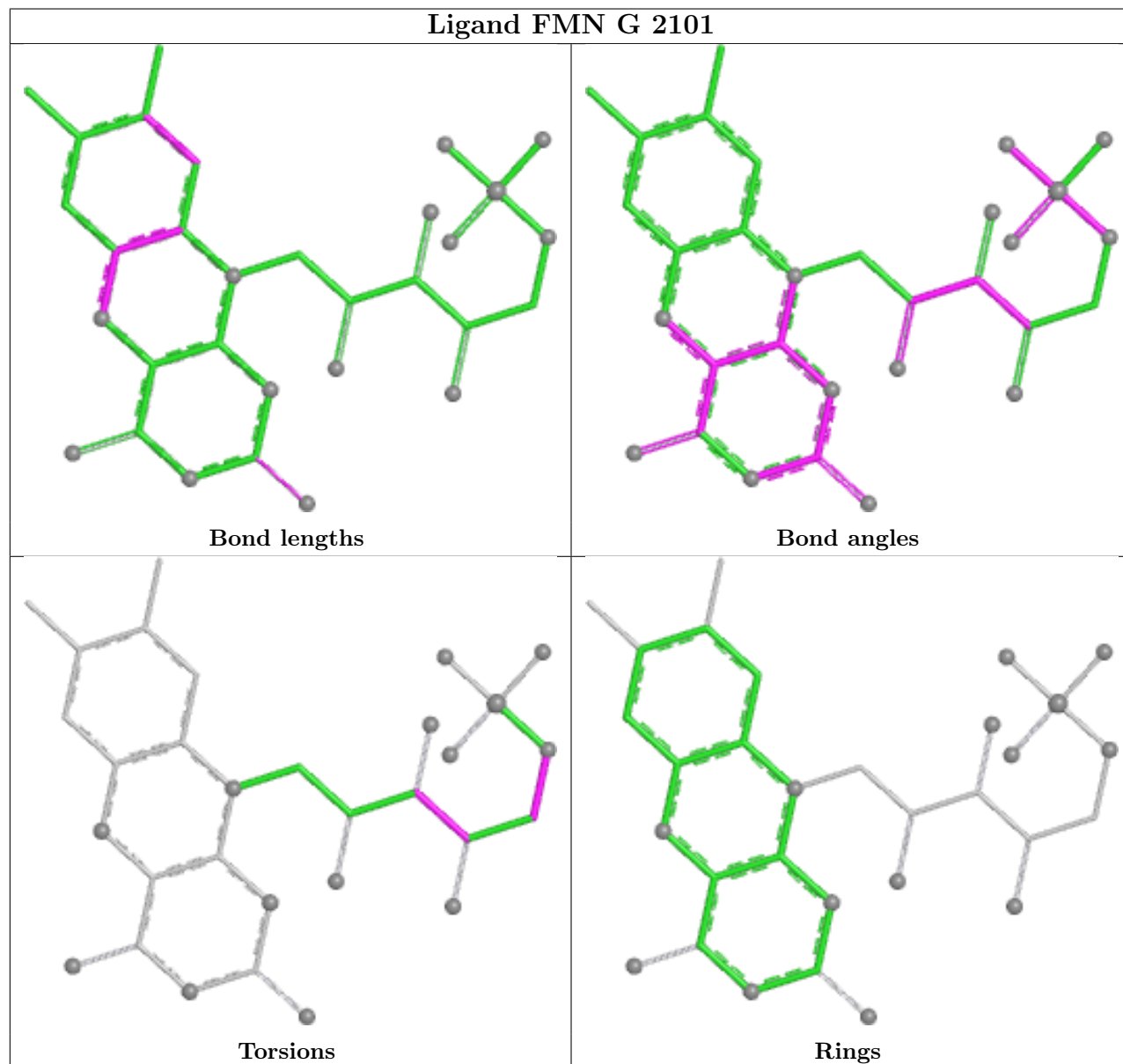
There are no ring outliers.

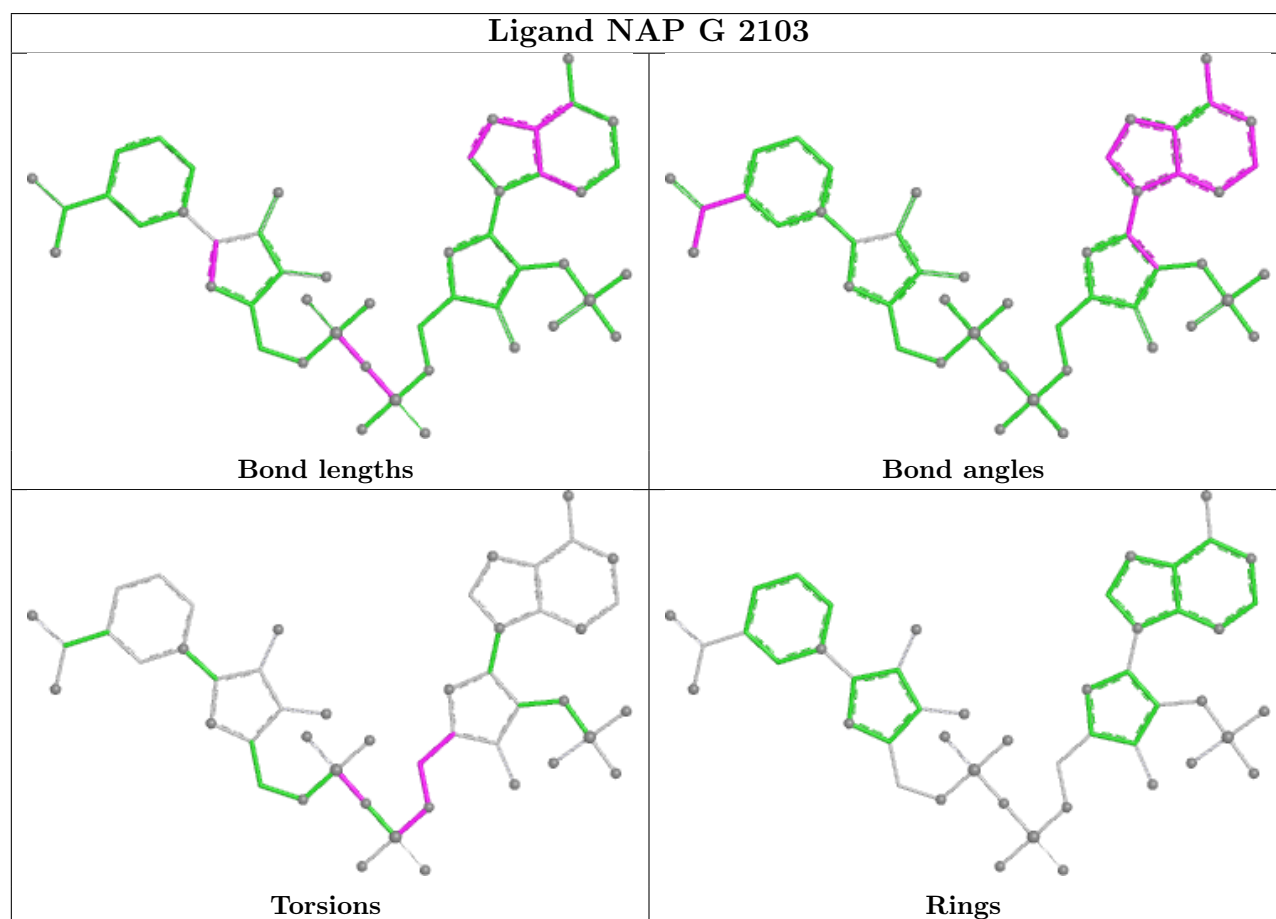
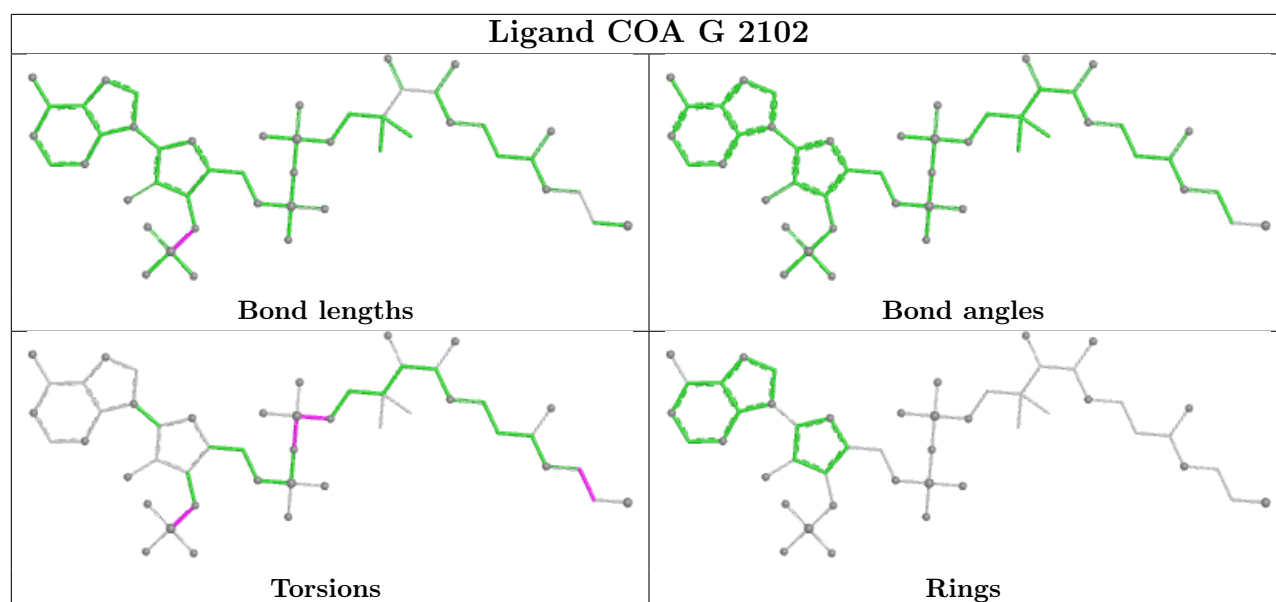
1 monomer is involved in 2 short contacts:

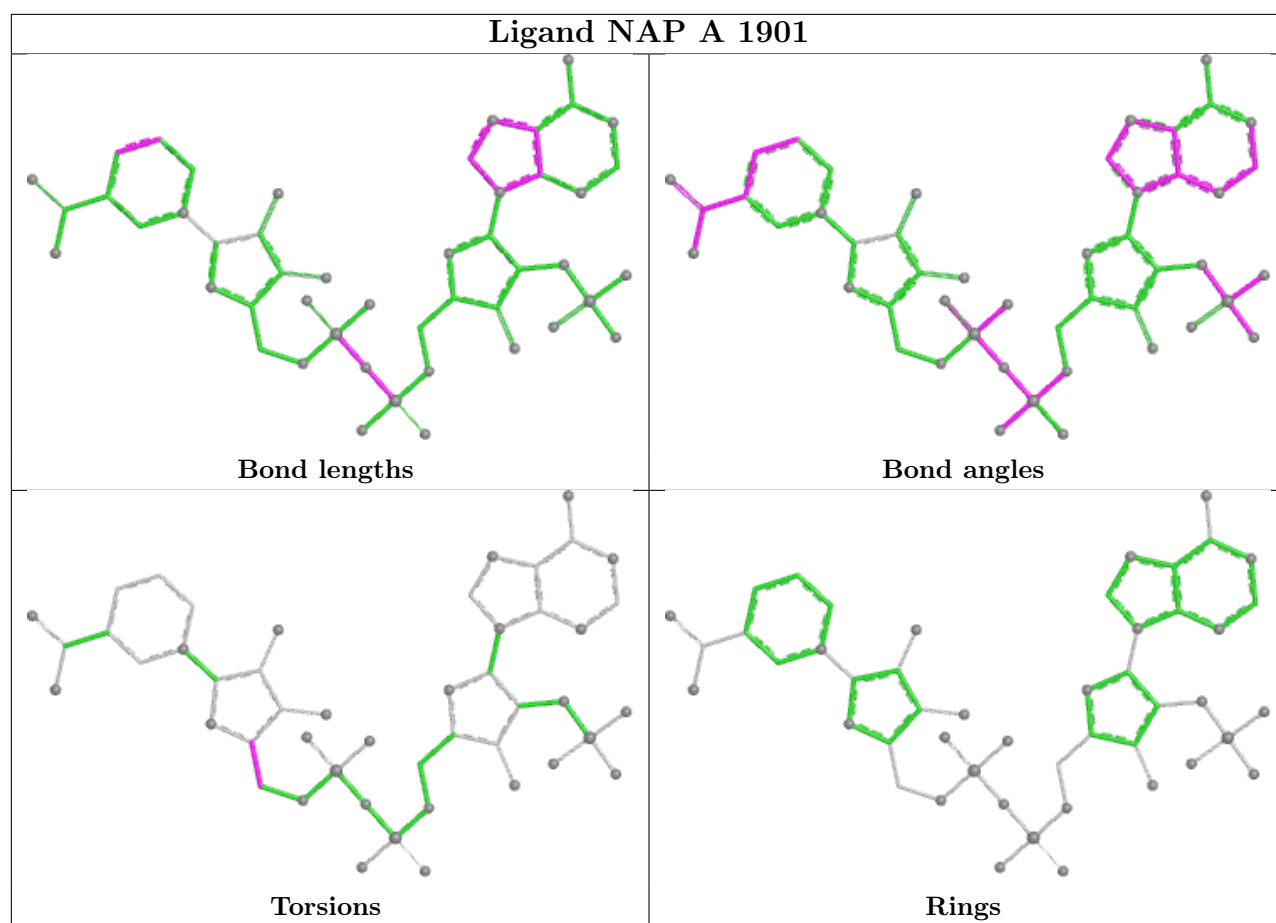
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2101	FMN	2	0

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

This section contains visualisations of the EMDB entry EMD-17842. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

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 ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.