



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 10:46 am BST

PDB ID : 2TMD
Title : CORRELATION OF X-RAY DEDUCED AND EXPERIMENTAL AMINO ACID SEQUENCES OF TRIMETHYLAMINE DEHYDROGENASE
Authors : Mathews, F.S.; Lim, L.W.; White, S.
Deposited on : 1993-10-15
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

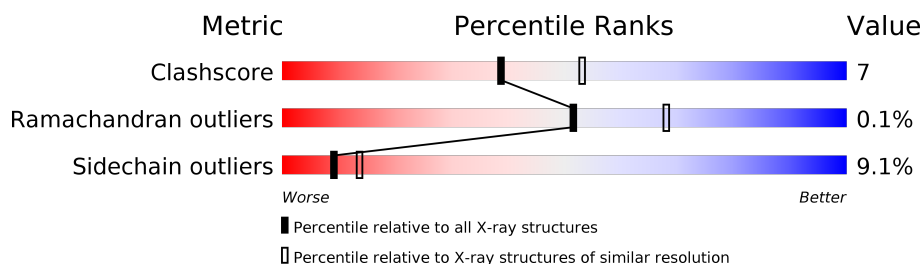
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	729	
1	B	729	

2 Entry composition [i](#)

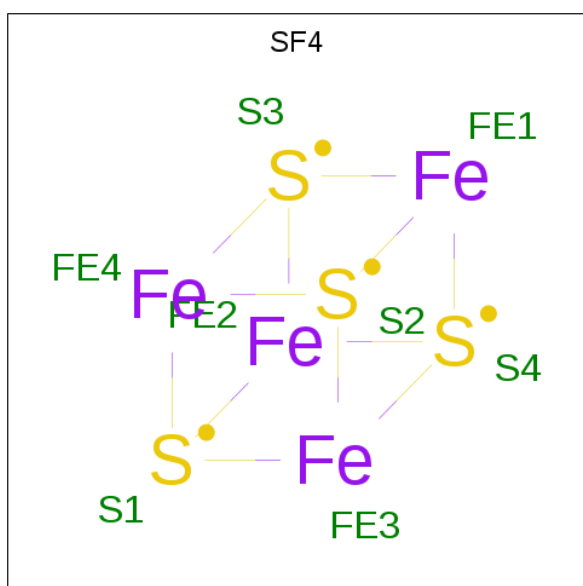
There are 5 unique types of molecules in this entry. The entry contains 12195 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 TRIMETHYLAMINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5741	3617	1012	1084	28			
1	B	729	Total	C	N	O	S	0	0	0
			5741	3617	1012	1084	28			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



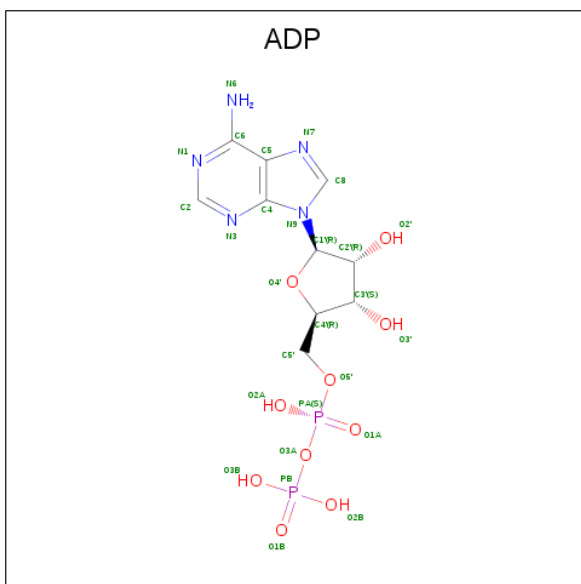
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

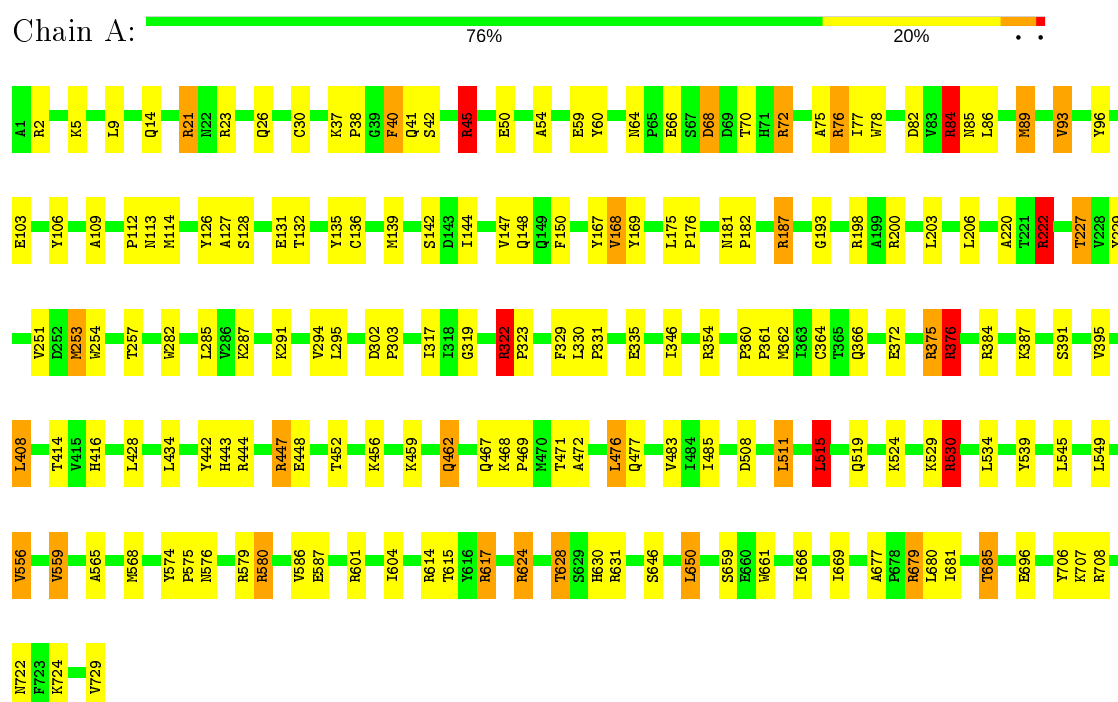
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	287	Total	O	0	0
			287	287		
5	B	294	Total	O	0	0
			294	294		

3 Residue-property plots [i](#)

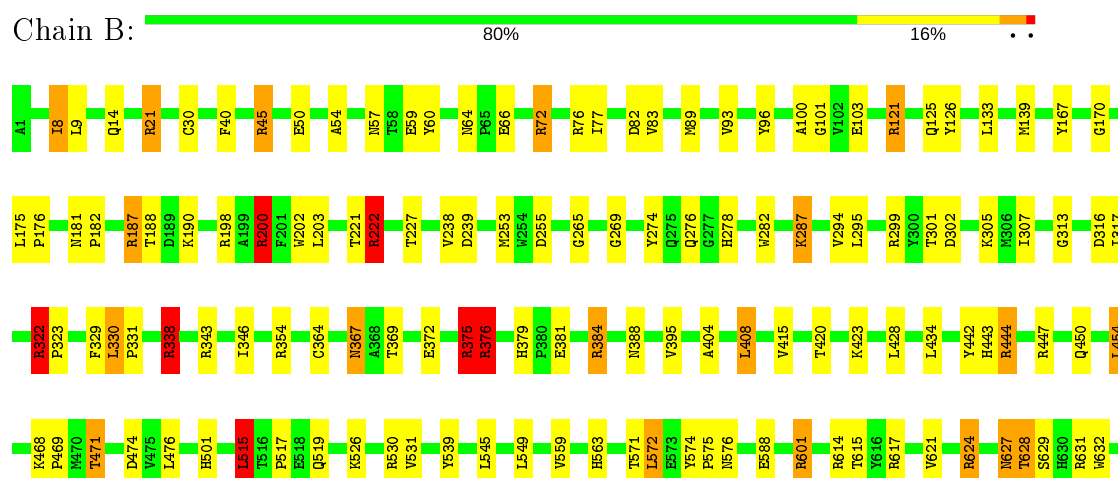
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

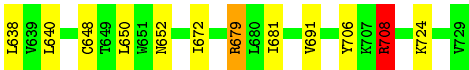
Note EDS was not executed.

• Molecule 1: TRIMETHYLAMINE DEHYDROGENASE



• Molecule 1: TRIMETHYLAMINE DEHYDROGENASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.75Å 71.95Å 83.82Å 90.00° 97.69° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12195	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

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: FMN, SF4, ADP

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	0/5885	0.58	2/7980 (0.0%)
1	B	0.37	0/5885	0.59	4/7980 (0.1%)
All	All	0.38	0/11770	0.58	6/15960 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
1	B	0	16
All	All	0	34

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	708	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	515	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	515	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	322	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	72	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	322	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	TYR	Sidechain
1	A	135	TYR	Sidechain
1	A	169	TYR	Sidechain
1	A	187	ARG	Sidechain
1	A	200	ARG	Sidechain
1	A	222	ARG	Sidechain
1	A	23	ARG	Sidechain
1	A	322	ARG	Sidechain
1	A	376	ARG	Sidechain
1	A	447	ARG	Sidechain
1	A	45	ARG	Sidechain
1	A	530	ARG	Sidechain
1	A	579	ARG	Sidechain
1	A	580	ARG	Sidechain
1	A	624	ARG	Sidechain
1	A	679	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	84	ARG	Sidechain
1	B	121	ARG	Sidechain
1	B	126	TYR	Sidechain
1	B	187	ARG	Mainchain
1	B	200	ARG	Sidechain
1	B	222	ARG	Sidechain
1	B	322	ARG	Sidechain
1	B	338	ARG	Sidechain
1	B	375	ARG	Sidechain
1	B	376	ARG	Sidechain
1	B	447	ARG	Sidechain
1	B	45	ARG	Sidechain
1	B	530	ARG	Sidechain
1	B	624	ARG	Sidechain
1	B	679	ARG	Sidechain
1	B	708	ARG	Sidechain
1	B	72	ARG	Sidechain

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	5741	0	5574	99	0
1	B	5741	0	5574	86	0
2	A	8	0	0	1	0
2	B	8	0	0	1	0
3	A	31	0	18	1	0
3	B	31	0	18	3	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	287	0	0	6	0
5	B	294	0	0	10	0
All	All	12195	0	11208	171	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (171) 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:646:SER:H	1:B:125:GLN:HE22	1.12	0.90
1:B:276:GLN:HE22	1:B:302:ASP:H	1.24	0.81
1:B:379:HIS:HD2	1:B:381:GLU:H	1.33	0.74
1:A:646:SER:H	1:B:125:GLN:NE2	1.89	0.69
1:B:627:ASN:HD22	1:B:628:THR:N	1.89	0.69
1:A:372:GLU:OE1	1:A:376:ARG:HD3	1.94	0.67
1:B:372:GLU:OE1	1:B:376:ARG:HD3	1.94	0.67
1:B:428:LEU:HD21	1:B:443:HIS:HB3	1.78	0.66
1:B:375:ARG:HB2	1:B:706:TYR:HB2	1.78	0.65
1:B:103:GLU:HA	1:B:167:TYR:HB2	1.79	0.64
1:B:372:GLU:OE1	1:B:375:ARG:HD2	1.98	0.64
1:A:614:ARG:HD3	1:B:282:TRP:CH2	2.33	0.63
1:A:68:ASP:H	1:A:113:ASN:ND2	1.95	0.63
1:A:41:GLN:O	1:A:45:ARG:HG3	1.99	0.63
1:A:282:TRP:CH2	1:B:614:ARG:HD3	2.34	0.63
1:A:64:ASN:HD22	1:A:66:GLU:HG2	1.62	0.63
1:A:84:ARG:HG3	1:A:85:ASN:N	2.14	0.62
1:A:722:ASN:OD1	1:A:724:LYS:HG2	1.99	0.62
1:A:508:ASP:HB3	1:A:511:LEU:HD22	1.81	0.62
1:A:448:GLU:O	1:A:452:THR:HG23	2.01	0.61
1:A:372:GLU:OE1	1:A:375:ARG:HD2	2.00	0.60
5:A:1019:HOH:O	1:B:624:ARG:HD2	2.00	0.60
1:A:375:ARG:HB2	1:A:706:TYR:HB2	1.84	0.59
1:A:354:ARG:HD2	5:A:966:HOH:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LYS:HG2	1:B:313:GLY:O	2.01	0.59
1:A:103:GLU:HA	1:A:167:TYR:HB2	1.85	0.59
1:A:661:TRP:CE2	1:A:669:ILE:HD12	2.38	0.58
1:B:139:MET:O	1:B:187:ARG:NH2	2.37	0.58
1:B:322:ARG:HG3	3:B:802:FMN:O3P	2.04	0.58
1:A:21:ARG:HD3	1:A:54:ALA:HA	1.86	0.58
1:B:276:GLN:NE2	1:B:302:ASP:H	2.00	0.57
1:A:624:ARG:NH2	1:B:576:ASN:OD1	2.37	0.57
1:A:346:ILE:HG22	1:A:442:TYR:HB2	1.87	0.56
1:B:30:CYS:HA	1:B:59:GLU:HB3	1.87	0.56
1:A:354:ARG:O	1:A:360:PRO:HD2	2.06	0.55
1:A:556:VAL:HG22	1:A:586:VAL:HG13	1.88	0.55
1:A:416:HIS:ND1	1:A:462:GLN:HB2	2.21	0.55
1:A:483:VAL:HB	1:A:669:ILE:HG12	1.88	0.55
1:B:222:ARG:HA	1:B:255:ASP:O	2.06	0.54
1:A:139:MET:O	1:A:187:ARG:NH2	2.35	0.54
1:A:468:LYS:HG2	1:A:469:PRO:HD2	1.89	0.54
1:A:574:TYR:HB3	1:A:575:PRO:HD3	1.89	0.54
1:A:530:ARG:HB2	1:A:530:ARG:HH11	1.71	0.53
1:B:468:LYS:HG2	1:B:469:PRO:HD2	1.89	0.53
1:B:354:ARG:HD3	5:B:968:HOH:O	2.09	0.53
1:A:576:ASN:OD1	1:B:624:ARG:NH2	2.42	0.52
1:A:64:ASN:ND2	1:A:66:GLU:HG2	2.24	0.52
1:A:615:THR:HB	1:A:617:ARG:HH11	1.75	0.52
1:A:114:MET:O	1:B:354:ARG:NH2	2.43	0.51
1:A:64:ASN:HD22	1:A:66:GLU:H	1.57	0.51
1:A:708:ARG:HD2	5:B:978:HOH:O	2.09	0.51
1:A:251:VAL:HG21	1:A:254:TRP:CE2	2.47	0.50
1:A:41:GLN:OE1	1:A:45:ARG:HD2	2.12	0.50
1:B:515:LEU:HA	1:B:519:GLN:OE1	2.12	0.50
1:A:72:ARG:NH2	1:A:131:GLU:OE2	2.44	0.50
1:A:361:PRO:HG2	5:B:1044:HOH:O	2.11	0.50
1:A:515:LEU:HA	1:A:519:GLN:OE1	2.12	0.50
1:B:64:ASN:HD22	1:B:66:GLU:HG2	1.77	0.50
1:B:346:ILE:HG22	1:B:442:TYR:HB2	1.94	0.50
1:B:50:GLU:HG2	1:B:329:PHE:CZ	2.47	0.49
1:B:450:GLN:O	1:B:454:LEU:HD22	2.12	0.49
1:A:106:TYR:CD1	1:A:175:LEU:HD22	2.47	0.49
1:B:428:LEU:CD2	1:B:443:HIS:HB3	2.41	0.49
1:A:428:LEU:HD21	1:A:443:HIS:HB3	1.95	0.49
1:A:624:ARG:HD2	5:B:1000:HOH:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLY:O	1:A:198:ARG:HD3	2.12	0.49
1:B:121:ARG:HB2	1:B:139:MET:HE2	1.95	0.49
1:A:322:ARG:HB2	1:A:323:PRO:HD3	1.95	0.48
1:B:679:ARG:NE	5:B:843:HOH:O	2.46	0.48
1:A:456:LYS:HE3	5:A:1072:HOH:O	2.13	0.48
1:B:601:ARG:HG3	1:B:632:TRP:CE3	2.49	0.48
1:B:627:ASN:ND2	1:B:629:SER:H	2.10	0.48
1:A:729:VAL:O	1:B:384:ARG:HD3	2.14	0.47
1:B:77:ILE:O	1:B:77:ILE:HG23	2.13	0.47
1:B:93:VAL:HG21	1:B:100:ALA:HB2	1.96	0.47
1:B:338:ARG:HG2	1:B:338:ARG:HH11	1.79	0.47
1:A:679:ARG:NE	5:A:1067:HOH:O	2.47	0.47
1:B:364:CYS:HA	2:B:801:SF4:S1	2.55	0.47
1:B:190:LYS:O	1:B:200:ARG:HD2	2.15	0.47
1:A:282:TRP:HH2	1:B:614:ARG:HD3	1.79	0.47
1:A:681:ILE:O	1:A:685:THR:HG23	2.14	0.47
1:A:443:HIS:NE2	1:A:685:THR:HG21	2.30	0.46
1:B:30:CYS:HA	1:B:59:GLU:CB	2.46	0.46
1:A:175:LEU:HB3	1:A:176:PRO:HD3	1.97	0.46
1:A:89:MET:O	1:A:93:VAL:HG13	2.15	0.46
1:B:563:HIS:CE1	5:B:838:HOH:O	2.67	0.46
1:B:627:ASN:C	1:B:627:ASN:HD22	2.18	0.46
1:B:343:ARG:NH2	5:B:867:HOH:O	2.47	0.46
1:B:423:LYS:HE2	1:B:444:ARG:NH2	2.31	0.46
1:A:38:PRO:O	1:A:42:SER:HB2	2.15	0.46
1:A:77:ILE:HG23	1:A:77:ILE:O	2.15	0.46
1:A:295:LEU:HB3	1:A:317:ILE:HB	1.97	0.46
1:B:274:TYR:O	1:B:299:ARG:NH2	2.32	0.45
1:A:76:ARG:HD2	1:A:78:TRP:CZ2	2.51	0.45
1:A:322:ARG:HG3	3:A:802:FMN:O3P	2.17	0.45
1:A:30:CYS:HA	1:A:59:GLU:HB3	1.96	0.45
1:B:367:ASN:ND2	1:B:369:THR:H	2.13	0.45
1:A:109:ALA:HB2	1:A:136:CYS:HB3	1.98	0.45
1:A:565:ALA:O	1:A:568:MET:HB2	2.17	0.45
1:B:21:ARG:NH2	1:B:96:TYR:O	2.50	0.45
1:B:420:THR:HG21	1:B:469:PRO:HG3	1.98	0.45
1:A:471:THR:HG22	1:A:472:ALA:N	2.31	0.45
1:A:227:THR:O	1:A:229:TYR:HD1	1.99	0.45
1:A:364:CYS:HA	2:A:801:SF4:S1	2.57	0.44
1:A:82:ASP:CG	1:B:708:ARG:HH22	2.21	0.44
1:A:128:SER:O	1:A:132:THR:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:THR:HG22	1:B:474:ASP:H	1.83	0.44
1:B:531:VAL:HG11	1:B:549:LEU:HD13	2.00	0.44
1:A:21:ARG:NH2	1:A:96:TYR:O	2.51	0.44
1:A:476:LEU:HD12	1:A:666:ILE:HD12	2.00	0.44
1:B:198:ARG:HH22	1:B:239:ASP:CG	2.21	0.44
1:A:222:ARG:HD2	1:A:257:THR:HG23	1.99	0.44
1:A:366:GLN:OE1	1:A:447:ARG:NH1	2.49	0.44
1:A:75:ALA:C	1:A:76:ARG:HG2	2.37	0.44
1:B:64:ASN:HD22	1:B:66:GLU:H	1.66	0.44
1:A:708:ARG:HH22	1:B:82:ASP:CG	2.21	0.44
1:A:220:ALA:HB2	1:A:253:MET:HE3	2.00	0.44
1:B:57:ASN:OD1	1:B:101:GLY:HA3	2.18	0.44
1:B:8:ILE:HD11	1:B:307:ILE:HB	1.99	0.44
1:A:376:ARG:HB3	5:A:900:HOH:O	2.18	0.43
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.84	0.43
1:A:70:THR:O	1:A:112:PRO:HG2	2.19	0.43
1:A:330:LEU:HB3	1:A:331:PRO:HD3	1.99	0.43
1:A:21:ARG:CD	1:A:54:ALA:HA	2.47	0.43
1:A:646:SER:N	1:B:125:GLN:HE22	1.95	0.43
1:B:202:TRP:HB2	5:B:857:HOH:O	2.18	0.43
1:A:295:LEU:HD13	1:A:319:GLY:HA3	2.01	0.43
1:A:50:GLU:HG3	1:A:329:PHE:CZ	2.54	0.43
1:B:322:ARG:HB2	1:B:323:PRO:HD3	2.00	0.43
1:B:574:TYR:HB3	1:B:575:PRO:HD3	2.01	0.43
1:A:677:ALA:O	1:A:679:ARG:HG2	2.19	0.43
1:B:627:ASN:HD22	1:B:628:THR:H	1.64	0.43
1:A:287:LYS:HD2	1:A:294:VAL:HG13	2.00	0.43
1:B:322:ARG:NH1	3:B:802:FMN:O2P	2.52	0.43
1:B:276:GLN:NE2	1:B:301:THR:H	2.18	0.42
1:B:278:HIS:HE1	5:B:861:HOH:O	2.01	0.42
1:B:672:ILE:HG21	1:B:691:VAL:HG21	2.01	0.42
1:A:144:ILE:O	1:A:148:GLN:HG3	2.18	0.42
1:A:147:VAL:O	1:A:150:PHE:HB2	2.19	0.42
1:A:724:LYS:HE2	1:A:724:LYS:HB3	1.87	0.42
1:B:265:GLY:O	1:B:269:GLY:HA2	2.19	0.42
1:A:391:SER:HA	1:A:414:THR:O	2.19	0.42
1:B:295:LEU:HB3	1:B:317:ILE:HB	2.01	0.42
1:A:2:ARG:HB2	1:A:335:GLU:O	2.20	0.42
1:B:322:ARG:HH11	3:B:802:FMN:P	2.43	0.42
1:A:302:ASP:HA	1:A:303:PRO:HD2	1.97	0.42
1:B:181:ASN:HA	1:B:182:PRO:HD2	1.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ASN:ND2	1:B:66:GLU:H	2.17	0.42
1:A:614:ARG:HD2	5:A:914:HOH:O	2.19	0.42
1:B:404:ALA:O	1:B:408:LEU:HB2	2.19	0.42
1:A:485:ILE:HD12	1:A:650:LEU:HD13	2.02	0.41
1:A:628:THR:HG23	1:A:628:THR:O	2.19	0.41
1:B:287:LYS:HE3	1:B:316:ASP:OD1	2.20	0.41
1:B:648:CYS:HA	5:B:844:HOH:O	2.20	0.41
1:A:604:ILE:O	1:A:630:HIS:HA	2.21	0.41
1:A:40:PHE:C	1:A:40:PHE:CD1	2.94	0.41
1:A:127:ALA:O	1:B:501:HIS:HE1	2.04	0.41
1:A:534:LEU:HD12	1:A:559:VAL:HG22	2.03	0.41
1:A:707:LYS:NZ	1:B:724:LYS:O	2.54	0.41
1:B:330:LEU:HB3	1:B:331:PRO:HD3	2.03	0.41
1:B:338:ARG:CG	1:B:338:ARG:HH11	2.33	0.41
1:B:652:ASN:HA	1:B:652:ASN:HD22	1.74	0.41
1:B:428:LEU:HD13	1:B:681:ILE:HD13	2.03	0.41
1:B:170:GLY:HA3	1:B:202:TRP:CH2	2.56	0.40
1:B:175:LEU:HB3	1:B:176:PRO:HD3	2.03	0.40
1:A:168:VAL:HG11	1:A:206:LEU:HD23	2.03	0.40
1:B:21:ARG:HD3	1:B:54:ALA:HA	2.04	0.40
1:B:571:THR:O	1:B:572:LEU:HB2	2.21	0.40
1:A:181:ASN:HA	1:A:182:PRO:HD2	1.87	0.40
1:A:408:LEU:HA	1:A:408:LEU:HD12	1.91	0.40
1:B:517:PRO:HD3	1:B:640:LEU:O	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 X-ray entries followed by that with respect to entries of similar resolution.

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	727/729 (100%)	698 (96%)	29 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	727/729 (100%)	704 (97%)	22 (3%)	1 (0%)	51	68
All	All	1454/1458 (100%)	1402 (96%)	51 (4%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	602/602 (100%)	545 (90%)	57 (10%)	8	12
1	B	602/602 (100%)	549 (91%)	53 (9%)	10	15
All	All	1204/1204 (100%)	1094 (91%)	110 (9%)	9	14

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	9	LEU
1	A	14	GLN
1	A	21	ARG
1	A	26	GLN
1	A	37	LYS
1	A	40	PHE
1	A	45	ARG
1	A	60	TYR
1	A	68	ASP
1	A	76	ARG
1	A	84	ARG
1	A	86	LEU
1	A	89	MET
1	A	93	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	142	SER
1	A	168	VAL
1	A	203	LEU
1	A	222	ARG
1	A	227	THR
1	A	253	MET
1	A	285	LEU
1	A	291	LYS
1	A	362	MET
1	A	375	ARG
1	A	376	ARG
1	A	384	ARG
1	A	387	LYS
1	A	395	VAL
1	A	408	LEU
1	A	434	LEU
1	A	444	ARG
1	A	459	LYS
1	A	462	GLN
1	A	467	GLN
1	A	476	LEU
1	A	477	GLN
1	A	511	LEU
1	A	515	LEU
1	A	524	LYS
1	A	529	LYS
1	A	530	ARG
1	A	539	TYR
1	A	545	LEU
1	A	556	VAL
1	A	559	VAL
1	A	580	ARG
1	A	587	GLU
1	A	601	ARG
1	A	617	ARG
1	A	628	THR
1	A	631	ARG
1	A	650	LEU
1	A	659	SER
1	A	680	LEU
1	A	685	THR
1	A	696	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	8	ILE
1	B	9	LEU
1	B	14	GLN
1	B	21	ARG
1	B	40	PHE
1	B	45	ARG
1	B	60	TYR
1	B	76	ARG
1	B	83	VAL
1	B	89	MET
1	B	133	LEU
1	B	188	THR
1	B	200	ARG
1	B	203	LEU
1	B	221	THR
1	B	222	ARG
1	B	227	THR
1	B	253	MET
1	B	287	LYS
1	B	294	VAL
1	B	305	LYS
1	B	330	LEU
1	B	338	ARG
1	B	367	ASN
1	B	375	ARG
1	B	376	ARG
1	B	384	ARG
1	B	388	ASN
1	B	395	VAL
1	B	408	LEU
1	B	415	VAL
1	B	434	LEU
1	B	444	ARG
1	B	454	LEU
1	B	471	THR
1	B	476	LEU
1	B	515	LEU
1	B	526	LYS
1	B	539	TYR
1	B	545	LEU
1	B	559	VAL
1	B	572	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	588	GLU
1	B	601	ARG
1	B	615	THR
1	B	617	ARG
1	B	621	VAL
1	B	627	ASN
1	B	628	THR
1	B	631	ARG
1	B	638	LEU
1	B	650	LEU
1	B	708	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	64	ASN
1	A	113	ASN
1	A	467	GLN
1	A	535	ASN
1	A	563	HIS
1	B	26	GLN
1	B	64	ASN
1	B	125	GLN
1	B	241	GLN
1	B	276	GLN
1	B	278	HIS
1	B	288	GLN
1	B	367	ASN
1	B	379	HIS
1	B	388	ASN
1	B	458	ASN
1	B	566	ASN
1	B	627	ASN
1	B	630	HIS
1	B	652	ASN
1	B	664	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	ADP	A	803	-	24,29,29	1.20	3 (12%)	29,45,45	1.03	2 (6%)
2	SF4	A	801	1	0,12,12	0.00	-	-		
4	ADP	B	803	-	24,29,29	1.33	1 (4%)	29,45,45	0.91	0
3	FMN	B	802	-	31,33,33	2.26	6 (19%)	40,50,50	3.29	12 (30%)
2	SF4	B	801	1	0,12,12	0.00	-	-		
3	FMN	A	802	-	31,33,33	2.48	8 (25%)	40,50,50	3.22	12 (30%)

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	ADP	A	803	-	-	3/12/32/32	0/3/3/3
2	SF4	A	801	1	-	-	0/6/5/5
4	ADP	B	803	-	-	3/12/32/32	0/3/3/3
3	FMN	B	802	-	-	1/18/18/18	0/3/3/3
2	SF4	B	801	1	-	-	0/6/5/5
3	FMN	A	802	-	-	1/18/18/18	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	FMN	C1'-N10	-10.79	1.37	1.48
3	B	802	FMN	C1'-N10	-9.86	1.38	1.48
4	B	803	ADP	C2'-C1'	-3.95	1.47	1.53
3	B	802	FMN	C10-N1	3.47	1.37	1.33
3	A	802	FMN	C10-N1	3.07	1.37	1.33
3	B	802	FMN	C4-C4A	3.03	1.46	1.41
3	A	802	FMN	C4A-N5	3.03	1.37	1.33
3	A	802	FMN	C7M-C7	2.93	1.56	1.51
3	B	802	FMN	C4A-N5	2.64	1.37	1.33
3	A	802	FMN	C6-C5A	-2.45	1.38	1.41
4	A	803	ADP	C8-N7	-2.24	1.30	1.34
4	A	803	ADP	PB-O2B	-2.22	1.46	1.54
3	A	802	FMN	P-O3P	-2.18	1.46	1.54
4	A	803	ADP	C5-C4	-2.08	1.35	1.40
3	A	802	FMN	C4'-C3'	2.07	1.57	1.53
3	B	802	FMN	C9-C9A	-2.06	1.36	1.40
3	A	802	FMN	C9-C9A	-2.04	1.36	1.40
3	B	802	FMN	P-O2P	-2.01	1.47	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	FMN	C4-N3-C2	12.83	125.97	115.14
3	B	802	FMN	C4-N3-C2	12.81	125.95	115.14
3	B	802	FMN	C4A-C4-N3	-7.54	113.12	123.43
3	A	802	FMN	C1'-N10-C9A	7.46	124.17	118.29
3	A	802	FMN	C4A-C4-N3	-7.19	113.60	123.43
3	B	802	FMN	C4-C4A-C10	7.07	124.63	119.95
3	B	802	FMN	C1'-N10-C9A	6.86	123.69	118.29
3	A	802	FMN	C4-C4A-C10	6.64	124.34	119.95
3	B	802	FMN	C5A-C9A-N10	5.30	121.56	117.72
3	B	802	FMN	C6-C5A-N5	4.28	123.77	119.05
3	A	802	FMN	C5A-C9A-N10	3.51	120.26	117.72
3	A	802	FMN	C10-C4A-N5	-3.46	118.86	121.26
3	B	802	FMN	C10-C4A-N5	-3.28	118.99	121.26
3	B	802	FMN	C9A-C5A-N5	-3.24	117.29	122.36
3	A	802	FMN	O3'-C3'-C4'	3.20	116.54	108.81
3	A	802	FMN	C6-C5A-N5	3.10	122.47	119.05
3	A	802	FMN	O3P-P-O2P	2.93	118.83	107.64
4	A	803	ADP	O4'-C1'-C2'	-2.73	102.94	106.93
3	B	802	FMN	C9A-N10-C10	-2.67	118.42	121.91
3	A	802	FMN	C4A-N5-C5A	2.50	119.27	116.77
3	A	802	FMN	C9A-C5A-N5	-2.48	118.48	122.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	FMN	O3'-C3'-C4'	2.26	114.28	108.81
3	A	802	FMN	C9A-N10-C10	-2.24	118.97	121.91
3	B	802	FMN	C4-C4A-N5	-2.09	116.20	118.60
3	B	802	FMN	O2P-P-O5'	-2.06	101.24	106.73
4	A	803	ADP	O3B-PB-O2B	2.06	115.51	107.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

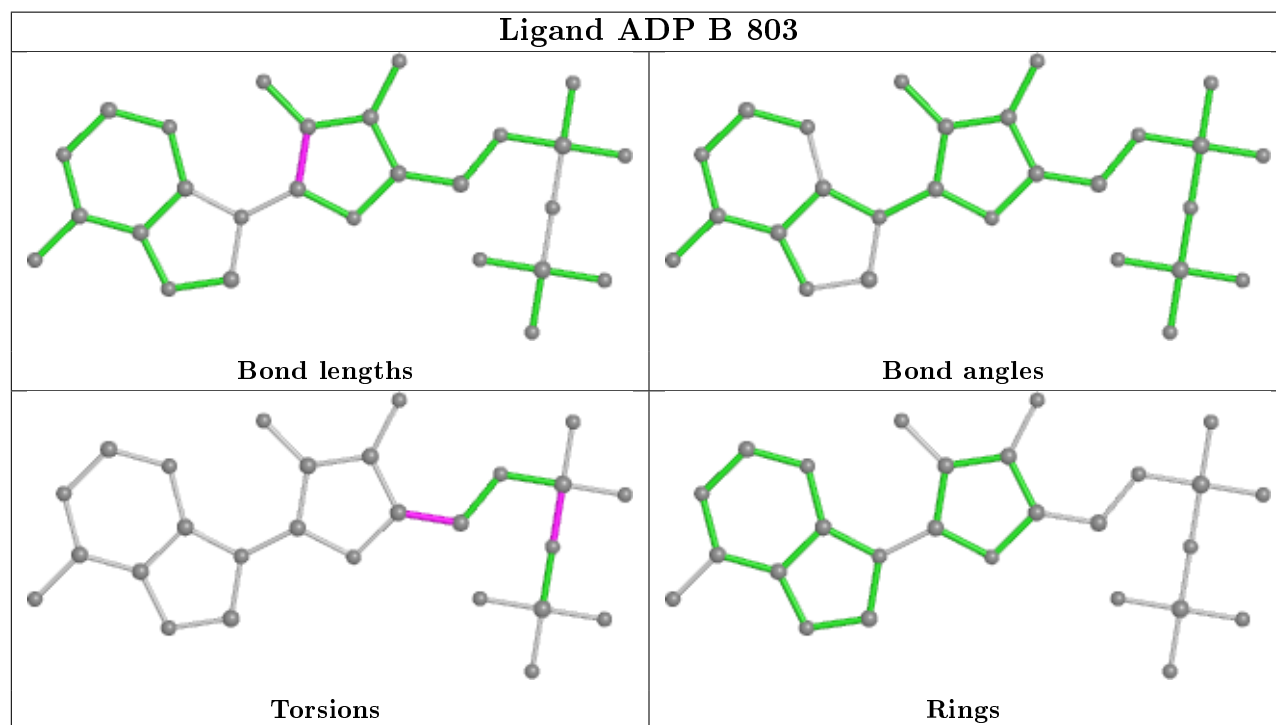
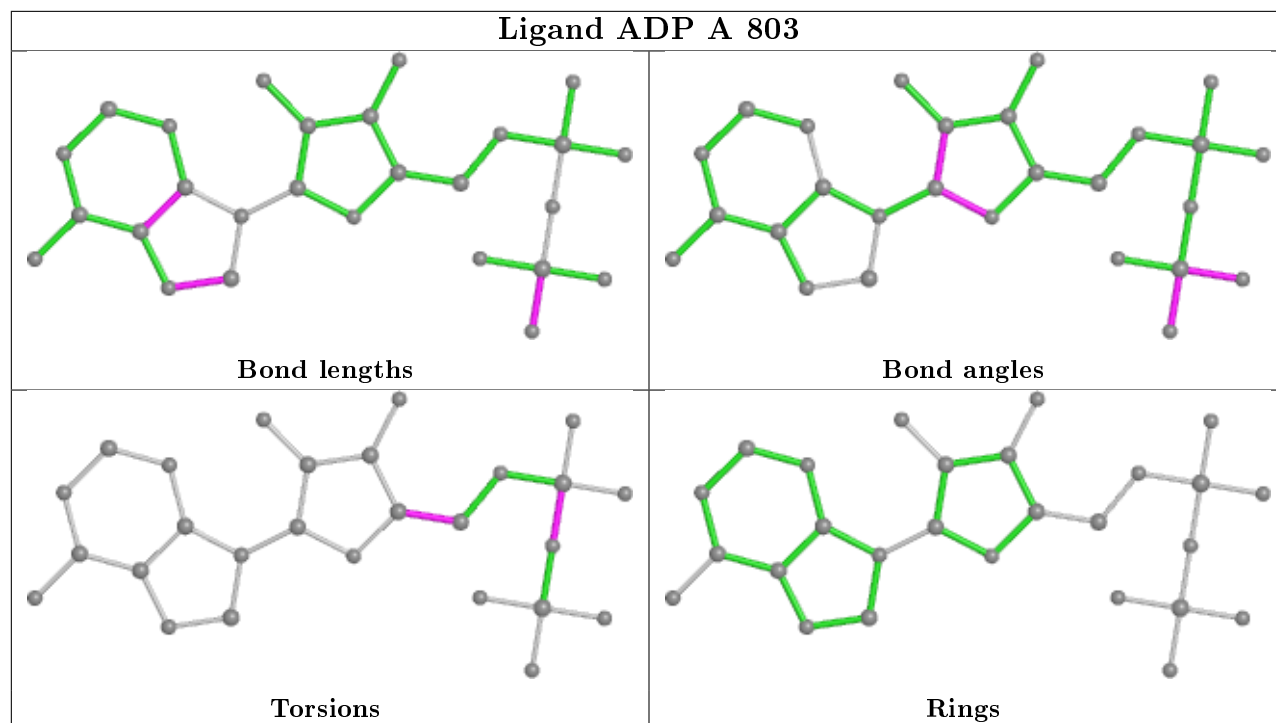
Mol	Chain	Res	Type	Atoms
4	A	803	ADP	PB-O3A-PA-O1A
4	B	803	ADP	PB-O3A-PA-O2A
3	B	802	FMN	C4'-C5'-O5'-P
4	A	803	ADP	PB-O3A-PA-O2A
4	B	803	ADP	PB-O3A-PA-O1A
3	A	802	FMN	C4'-C5'-O5'-P
4	A	803	ADP	O4'-C4'-C5'-O5'
4	B	803	ADP	O4'-C4'-C5'-O5'

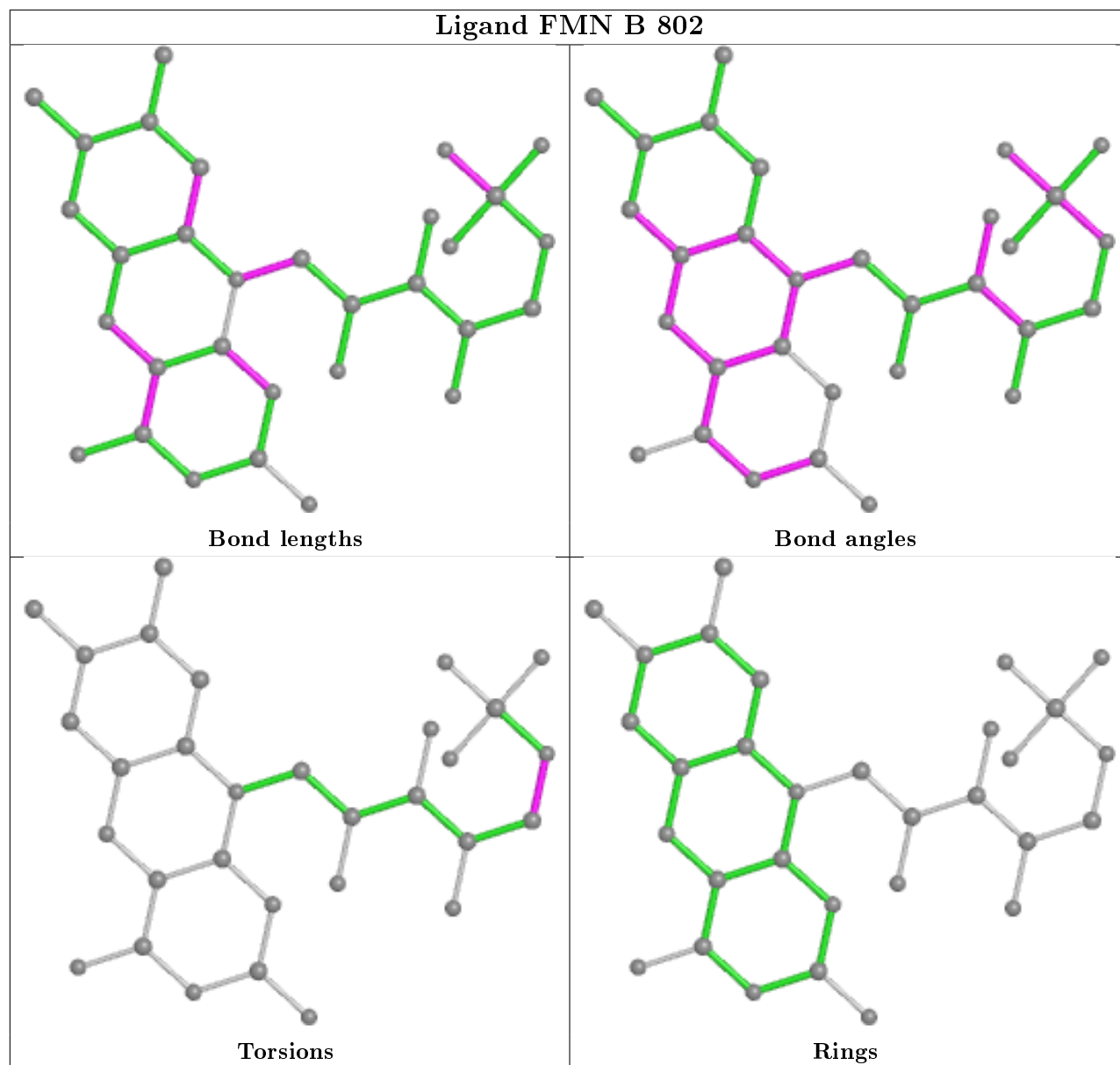
There are no ring outliers.

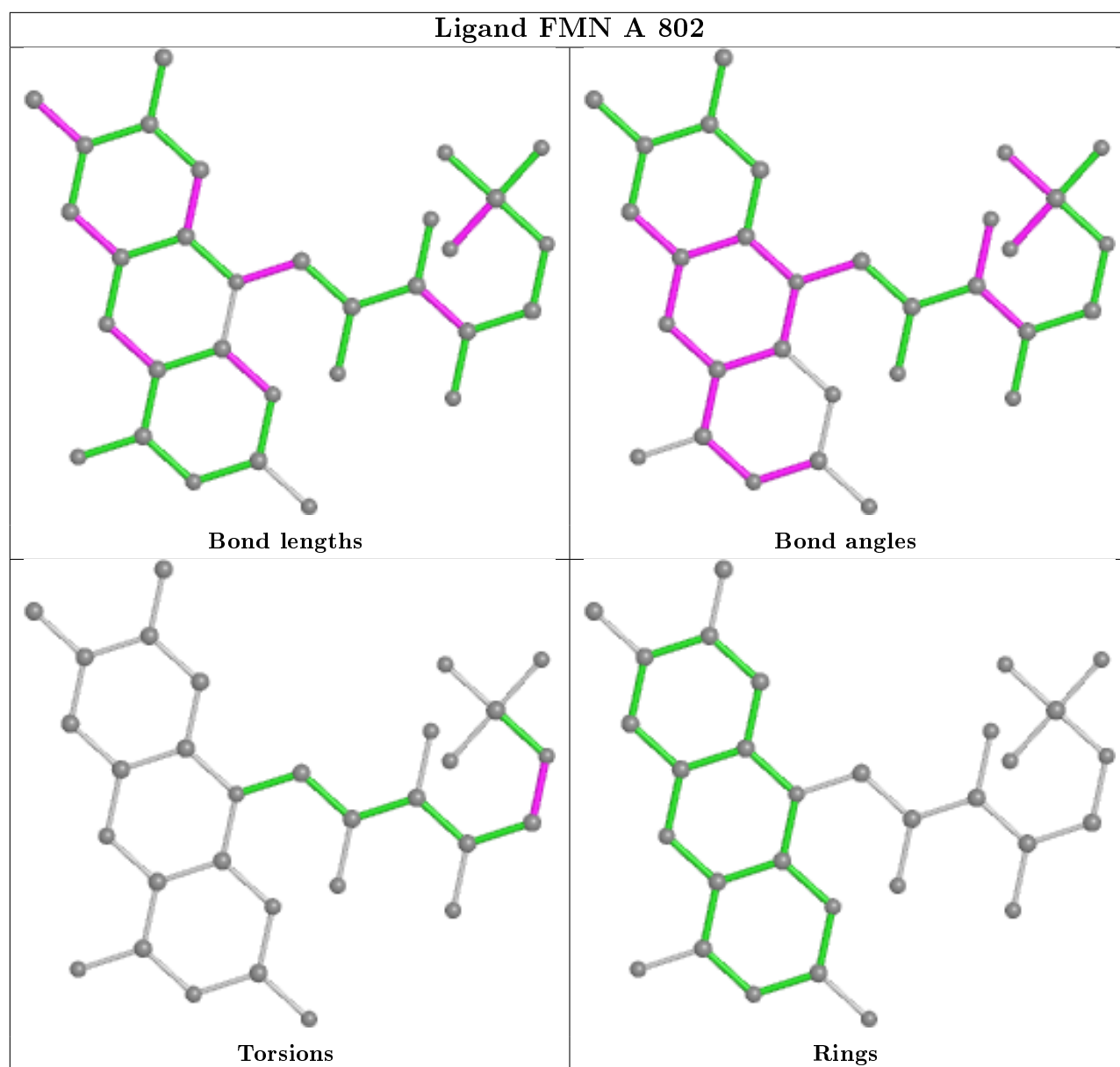
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SF4	1	0
3	B	802	FMN	3	0
2	B	801	SF4	1	0
3	A	802	FMN	1	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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.