



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:16 pm BST

PDB ID : 2C3C  
Title : 2.01 Angstrom X-ray crystal structure of a mixed disulfide between coenzyme M and NADPH-dependent oxidoreductase 2-ketopropyl coenzyme M carboxylase  
Authors : Pandey, A.S.; Nocek, B.; Clark, D.D.; Ensign, S.A.; Peters, J.W.  
Deposited on : 2005-10-05  
Resolution : 2.15 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](mailto: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.

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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

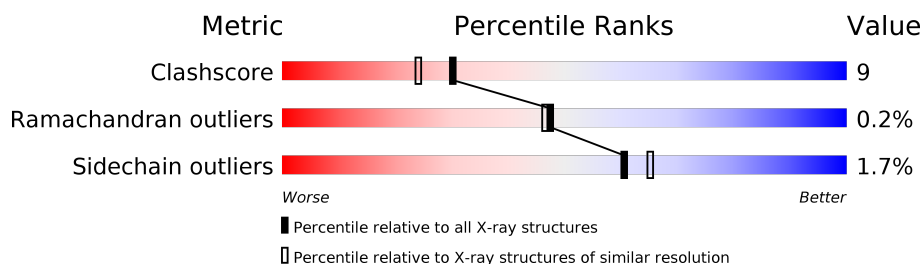
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	523	
1	B	523	

## 2 Entry composition [i](#)

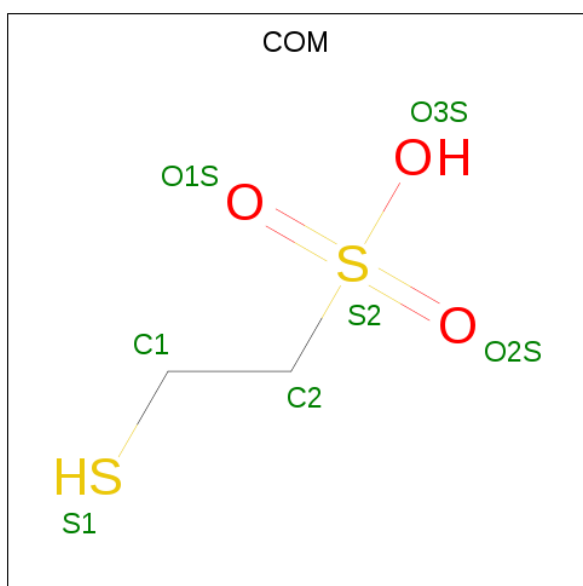
There are 6 unique types of molecules in this entry. The entry contains 8981 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-OXOPROPYL-COM REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	B	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			

- Molecule 2 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula:  $C_2H_6O_3S_2$ ).



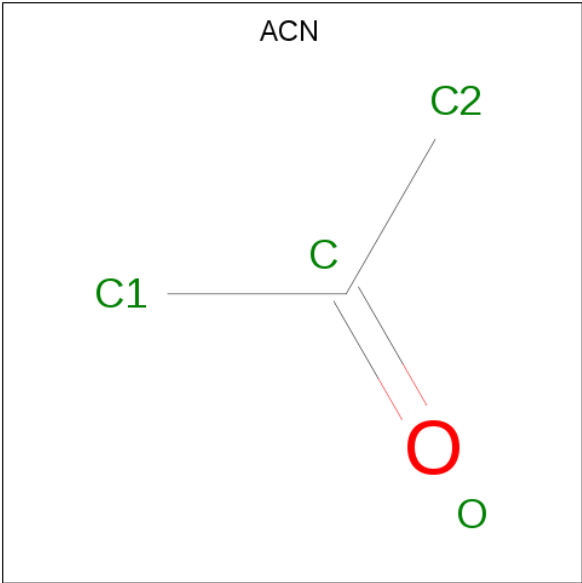
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			7	2	3	2		
2	B	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



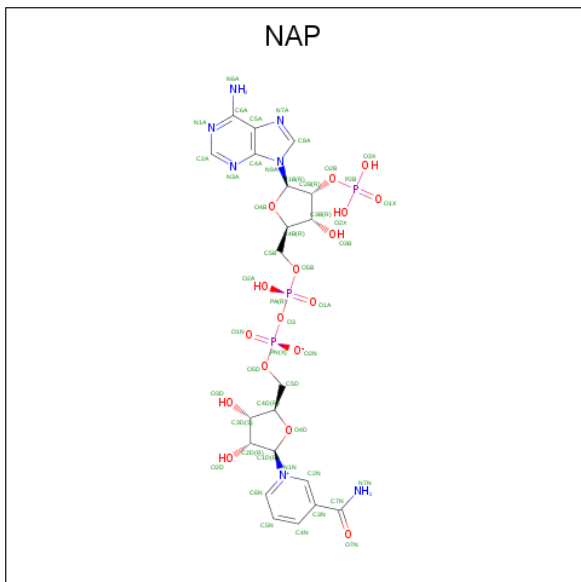
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is ACETONE (three-letter code: ACN) (formula: C<sub>3</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 17	P 3	19	0
5	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 6 is water.

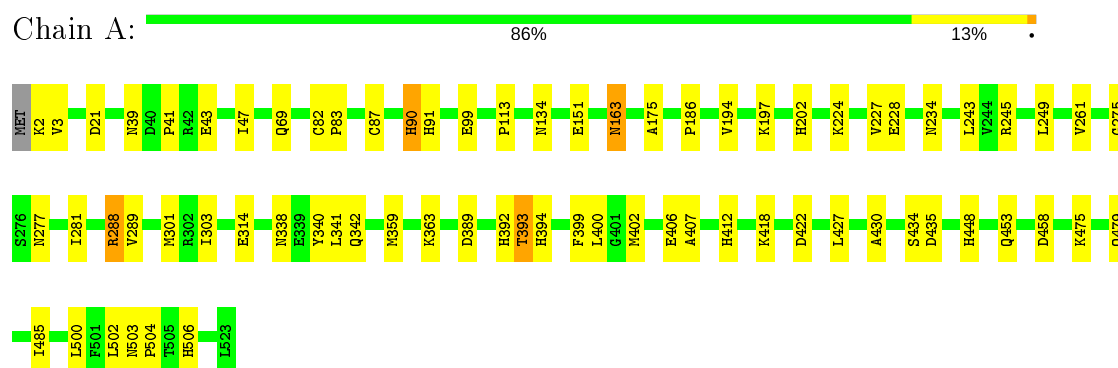
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	375	Total O 375 375	0	0
6	B	336	Total O 336 336	0	0

### 3 Residue-property plots [i](#)

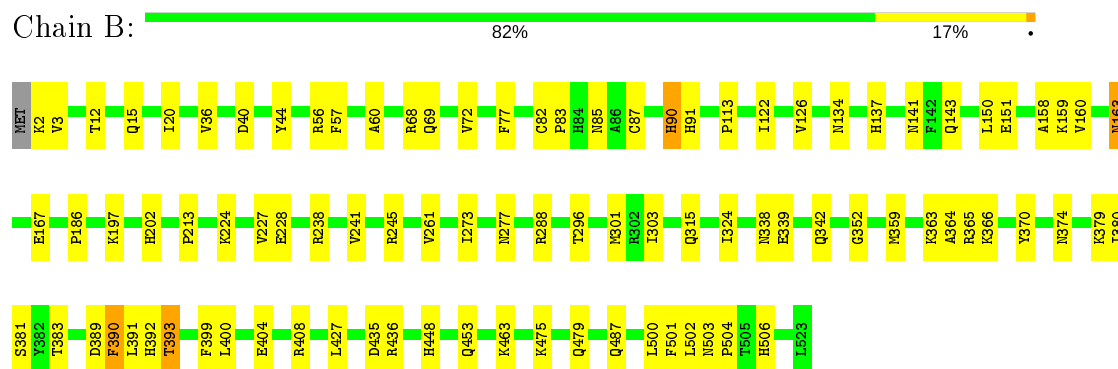
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 2-OXOPROPYL-COM REDUCTASE



#### • Molecule 1: 2-OXOPROPYL-COM REDUCTASE



## 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, $\alpha$ , $\beta$ , $\gamma$	88.06 Å   60.02 Å   105.96 Å 90.00°   102.43°   90.00°	Depositor
Resolution (Å)	36.99 – 2.15	Depositor
% Data completeness (in resolution range)	97.3 (36.99-2.15)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.181 , 0.226	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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: NAP, COM, ACN, FAD

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	0.40	0/4106	0.66	1/5556 (0.0%)
1	B	0.39	0/4106	0.64	1/5556 (0.0%)
All	All	0.40	0/8212	0.65	2/11112 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	THR	N-CA-C	-6.42	93.68	111.00
1	B	393	THR	N-CA-C	-6.18	94.31	111.00

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	4023	0	3982	70	0
1	B	4023	0	3982	93	0
2	A	7	0	6	2	0
2	B	7	0	6	2	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
4	A	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	6	1	0
5	A	48	0	25	5	0
5	B	48	0	25	4	0
6	A	375	0	0	4	0
6	B	336	0	0	6	0
All	All	8981	0	8100	152	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 9.

All (152) 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:338:ASN:HD21	1:A:342:GLN:HE21	1.05	0.97
1:B:453:GLN:HE22	1:B:506:HIS:H	0.97	0.97
1:A:453:GLN:HE22	1:A:506:HIS:H	0.98	0.95
1:A:500:LEU:H	1:B:479:GLN:HE21	1.16	0.92
1:A:69:GLN:HE22	1:A:151:GLU:H	1.18	0.91
1:A:479:GLN:HE22	1:B:503:ASN:HD22	1.11	0.90
1:A:82:CYS:HG	2:A:1000:COM:HS1	0.91	0.88
1:B:69:GLN:HE22	1:B:151:GLU:H	1.24	0.84
1:B:90:HIS:HE1	1:B:392:HIS:HD2	1.24	0.83
1:B:453:GLN:NE2	1:B:506:HIS:H	1.79	0.79
1:A:301:MET:CE	1:A:303:ILE:HD11	2.12	0.78
1:B:374:ASN:HD21	1:B:380:ILE:H	1.29	0.78
1:B:90:HIS:CE1	1:B:392:HIS:HD2	2.01	0.78
1:A:338:ASN:HD21	1:A:342:GLN:NE2	1.83	0.76
1:B:296:THR:HG21	1:B:301:MET:CE	2.17	0.75
1:A:503:ASN:HD22	1:B:479:GLN:HE22	1.32	0.75
1:B:296:THR:HG21	1:B:301:MET:HE3	1.69	0.74
1:B:56:ARG:HH12	1:B:143:GLN:HE21	1.33	0.73
1:A:479:GLN:HE21	1:B:500:LEU:H	1.34	0.73
1:A:43:GLU:HG3	6:A:2119:HOH:O	1.87	0.73
1:A:453:GLN:NE2	1:A:506:HIS:H	1.80	0.73
1:A:479:GLN:NE2	1:B:503:ASN:HD22	1.87	0.71
1:B:159:LYS:HB2	1:B:167:GLU:HB3	1.73	0.70
1:B:90:HIS:HE1	1:B:392:HIS:CD2	2.10	0.69
1:A:301:MET:HE3	1:A:303:ILE:HD11	1.73	0.69
1:B:338:ASN:HD21	1:B:342:GLN:HE21	1.40	0.68
1:A:301:MET:HE1	1:A:303:ILE:HD11	1.78	0.65
1:A:163:ASN:HD22	1:A:163:ASN:N	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:HD2	1:A:3:VAL:HG23	1.80	0.64
1:B:56:ARG:HH12	1:B:143:GLN:NE2	1.96	0.64
1:B:374:ASN:ND2	1:B:380:ILE:H	1.95	0.64
1:B:85:ASN:O	1:B:202:HIS:HD2	1.81	0.63
1:B:374:ASN:ND2	1:B:379:LYS:HA	2.13	0.63
1:B:453:GLN:HE22	1:B:506:HIS:N	1.83	0.62
1:B:463:LYS:HE2	6:B:2295:HOH:O	1.98	0.62
1:B:338:ASN:HD21	1:B:342:GLN:NE2	1.98	0.61
1:B:241:VAL:HG11	1:B:303:ILE:HD13	1.83	0.61
1:A:500:LEU:N	1:B:479:GLN:HE21	1.94	0.60
1:A:453:GLN:HE22	1:A:506:HIS:N	1.83	0.60
1:B:213:PRO:HD2	6:B:2115:HOH:O	2.00	0.60
1:A:500:LEU:H	1:B:479:GLN:NE2	1.95	0.60
1:A:90:HIS:HE1	1:A:392:HIS:HD2	1.48	0.59
1:B:273:ILE:HG21	1:B:301:MET:HE3	1.83	0.59
1:A:228:GLU:OE2	5:A:1526:NAP:H4N	2.02	0.59
1:B:2:LYS:HG3	1:B:3:VAL:HG23	1.83	0.59
1:A:163:ASN:HD22	1:A:163:ASN:H	1.49	0.59
1:A:288:ARG:HG3	1:A:289:VAL:N	2.17	0.58
1:B:390:PHE:HZ	1:B:392:HIS:CE1	2.22	0.58
1:B:389:ASP:HB3	1:B:399:PHE:CE1	2.40	0.57
1:B:90:HIS:CE1	1:B:392:HIS:CD2	2.88	0.57
1:B:163:ASN:HD22	1:B:163:ASN:N	2.02	0.57
1:A:90:HIS:CE1	1:A:392:HIS:HD2	2.23	0.57
1:A:90:HIS:HE1	1:A:392:HIS:CD2	2.23	0.56
1:B:273:ILE:HD13	1:B:301:MET:CE	2.37	0.55
1:A:113:PRO:HB3	1:B:113:PRO:HB3	1.87	0.55
1:A:227:VAL:HG21	1:A:249:LEU:HD21	1.89	0.55
1:B:352:GLY:HA2	1:B:364:ALA:HA	1.88	0.55
1:A:245:ARG:O	1:A:275:GLY:HA2	2.08	0.54
1:B:366:LYS:O	1:B:370:TYR:HD1	1.91	0.54
1:B:374:ASN:HD22	1:B:379:LYS:HA	1.72	0.54
1:B:91:HIS:HE1	1:B:475:LYS:NZ	2.05	0.54
1:B:20:ILE:HD13	1:B:137:HIS:HB3	1.89	0.53
1:B:228:GLU:OE2	5:B:1526:NAP:H4N	2.09	0.53
1:B:40:ASP:HB3	1:B:68:ARG:CZ	2.39	0.53
4:A:1525:ACN:H22	2:B:1000:COM:H11	1.91	0.53
1:A:234:ASN:HD22	1:A:394:HIS:CE1	2.27	0.52
1:B:77:PHE:HA	1:B:141:ASN:HD21	1.74	0.52
1:A:82:CYS:HB3	1:A:83:PRO:HD3	1.90	0.52
1:B:238:ARG:CZ	6:B:2115:HOH:O	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:CYS:HB3	1:B:83:PRO:HD3	1.91	0.52
1:A:359:MET:O	5:A:1526:NAP:H1D	2.10	0.52
1:A:91:HIS:HE1	1:A:475:LYS:NZ	2.08	0.52
1:B:374:ASN:HD21	1:B:380:ILE:N	2.03	0.51
1:A:389:ASP:HB3	1:A:399:PHE:CE1	2.45	0.51
1:A:82:CYS:HB3	1:A:83:PRO:CD	2.39	0.51
1:B:296:THR:HG21	1:B:301:MET:HE2	1.89	0.51
1:A:400:LEU:HD11	1:A:485:ILE:CD1	2.41	0.51
1:A:261:VAL:CG1	1:A:393:THR:HG21	2.41	0.51
1:B:245:ARG:HG3	1:B:277:ASN:HD21	1.75	0.51
1:A:234:ASN:HD22	1:A:394:HIS:HE1	1.58	0.50
1:B:160:VAL:O	1:B:324:ILE:HG21	2.11	0.50
1:A:400:LEU:C	1:A:400:LEU:HD12	2.32	0.49
1:B:82:CYS:HB3	1:B:83:PRO:CD	2.42	0.49
1:A:314:GLU:HG3	6:A:2254:HOH:O	2.11	0.49
1:B:338:ASN:ND2	1:B:342:GLN:HE21	2.10	0.49
1:B:339:GLU:HB2	1:B:381:SER:HB2	1.94	0.48
1:B:224:LYS:HD2	5:B:1526:NAP:C2N	2.42	0.48
1:B:359:MET:O	5:B:1526:NAP:H1D	2.14	0.48
1:B:36:VAL:HG13	1:B:44:TYR:OH	2.14	0.48
1:B:241:VAL:HG11	1:B:303:ILE:CD1	2.43	0.47
1:A:412:HIS:HD2	1:A:458:ASP:OD2	1.96	0.47
1:B:261:VAL:CG1	1:B:393:THR:HG21	2.45	0.47
1:A:479:GLN:HE22	1:B:503:ASN:ND2	1.94	0.47
1:A:402:MET:HE2	1:A:407:ALA:HA	1.96	0.47
1:A:197:LYS:O	1:A:289:VAL:HG23	2.15	0.46
6:A:2074:HOH:O	1:B:113:PRO:HD2	2.16	0.46
5:A:1526:NAP:O2N	5:A:1526:NAP:H52A	2.15	0.46
1:A:91:HIS:CD2	1:B:502:LEU:HD13	2.50	0.46
1:A:90:HIS:CE1	1:A:392:HIS:CD2	3.02	0.46
1:B:82:CYS:SG	2:B:1000:COM:S1	2.72	0.46
1:A:502:LEU:H	1:B:91:HIS:CE1	2.34	0.46
1:A:87:CYS:O	1:A:91:HIS:HD2	1.99	0.46
1:B:404:GLU:HG2	1:B:408:ARG:NH1	2.31	0.45
1:A:90:HIS:HD2	3:A:1524:FAD:N5	2.15	0.45
1:B:134:ASN:HB2	6:B:2073:HOH:O	2.16	0.45
1:B:227:VAL:HG11	1:B:393:THR:HG22	1.99	0.45
1:B:60:ALA:HA	1:B:150:LEU:HD21	1.97	0.45
1:B:261:VAL:HG13	1:B:393:THR:HG21	1.99	0.45
1:B:12:THR:OG1	1:B:15:GLN:HG3	2.16	0.45
1:B:56:ARG:HH22	1:B:143:GLN:HE22	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:PRO:HG3	1:B:202:HIS:CE1	2.52	0.45
1:B:57:PHE:CD2	1:B:365:ARG:HG2	2.52	0.45
1:A:427:LEU:O	1:A:448:HIS:HA	2.17	0.44
1:A:224:LYS:HD2	5:A:1526:NAP:C2N	2.47	0.44
2:A:1000:COM:H11	4:B:1525:ACN:H12	2.00	0.44
1:A:186:PRO:HG3	1:A:202:HIS:CE1	2.52	0.44
1:B:487:GLN:HG3	6:B:2291:HOH:O	2.17	0.44
1:A:245:ARG:HG3	1:A:277:ASN:HD21	1.81	0.44
1:B:227:VAL:CG1	1:B:393:THR:HG22	2.47	0.44
1:B:390:PHE:CG	1:B:391:LEU:N	2.85	0.44
1:A:39:ASN:O	1:A:41:PRO:HD3	2.17	0.44
1:B:197:LYS:HE3	6:B:2113:HOH:O	2.17	0.44
1:A:479:GLN:NE2	1:B:500:LEU:H	2.07	0.44
1:B:90:HIS:HD2	3:B:1524:FAD:N5	2.15	0.44
1:B:91:HIS:HE1	1:B:475:LYS:HZ1	1.64	0.44
1:A:194:VAL:HA	1:A:281:ILE:HD12	2.00	0.44
1:B:87:CYS:O	1:B:91:HIS:HD2	2.00	0.44
1:A:243:LEU:HD21	1:A:301:MET:CE	2.48	0.43
1:A:47:ILE:HG13	1:A:175:ALA:HB2	1.99	0.43
1:B:390:PHE:C	1:B:390:PHE:CD2	2.92	0.43
1:A:402:MET:HE3	1:A:406:GLU:HG2	2.01	0.43
1:A:435:ASP:OD1	1:B:392:HIS:HE1	2.01	0.43
1:A:90:HIS:C	1:A:90:HIS:ND1	2.72	0.43
5:A:1526:NAP:H51A	6:A:2375:HOH:O	2.19	0.43
1:B:400:LEU:C	1:B:400:LEU:HD12	2.39	0.43
1:B:134:ASN:HA	1:B:137:HIS:CD2	2.54	0.42
1:A:228:GLU:HG2	1:A:392:HIS:HB2	2.01	0.42
1:A:340:TYR:O	1:A:341:LEU:HB2	2.19	0.42
1:A:99:GLU:OE2	1:B:436:ARG:NH1	2.53	0.42
1:A:21:ASP:OD2	1:A:134:ASN:ND2	2.53	0.42
3:B:1524:FAD:H1'1	3:B:1524:FAD:H9	1.86	0.41
1:A:392:HIS:HE1	1:B:435:ASP:OD1	2.03	0.41
1:A:82:CYS:SG	1:B:501:PHE:HE2	2.43	0.41
1:B:427:LEU:O	1:B:448:HIS:HA	2.20	0.41
1:A:400:LEU:HD11	1:A:485:ILE:HD13	2.03	0.41
1:A:261:VAL:HG13	1:A:393:THR:HG21	2.02	0.41
1:B:390:PHE:CE1	1:B:475:LYS:HD3	2.56	0.41
1:B:245:ARG:HD2	5:B:1526:NAP:O3X	2.21	0.40
1:B:228:GLU:HG2	1:B:392:HIS:HB2	2.03	0.40
1:A:418:LYS:HB2	1:A:453:GLN:O	2.21	0.40
1:B:72:VAL:CG1	1:B:158:ALA:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:O	1:B:126:VAL:HG23	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	520/523 (99%)	499 (96%)	19 (4%)	2 (0%)	34	29
1	B	520/523 (99%)	496 (95%)	24 (5%)	0	100	100
All	All	1040/1046 (99%)	995 (96%)	43 (4%)	2 (0%)	47	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	430	ALA
1	A	434	SER

### 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 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	423/424 (100%)	417 (99%)	6 (1%)	67	72
1	B	423/424 (100%)	415 (98%)	8 (2%)	57	61
All	All	846/848 (100%)	832 (98%)	14 (2%)	60	65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	163	ASN
1	A	288	ARG
1	A	363	LYS
1	A	422	ASP
1	A	504	PRO
1	B	90	HIS
1	B	163	ASN
1	B	288	ARG
1	B	315	GLN
1	B	363	LYS
1	B	383	THR
1	B	390	PHE
1	B	504	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	39	ASN
1	A	69	GLN
1	A	90	HIS
1	A	91	HIS
1	A	134	ASN
1	A	163	ASN
1	A	164	HIS
1	A	202	HIS
1	A	234	ASN
1	A	277	ASN
1	A	290	GLN
1	A	315	GLN
1	A	342	GLN
1	A	374	ASN
1	A	392	HIS
1	A	394	HIS
1	A	412	HIS
1	A	453	GLN
1	A	479	GLN
1	A	487	GLN
1	B	14	ASN
1	B	69	GLN

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Mol	Chain	Res	Type
1	B	90	HIS
1	B	91	HIS
1	B	137	HIS
1	B	141	ASN
1	B	143	GLN
1	B	163	ASN
1	B	202	HIS
1	B	234	ASN
1	B	255	ASN
1	B	277	ASN
1	B	290	GLN
1	B	298	ASN
1	B	342	GLN
1	B	374	ASN
1	B	392	HIS
1	B	412	HIS
1	B	453	GLN
1	B	479	GLN
1	B	487	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	ACN	A	1525	-	3,3,3	0.74	0	3,3,3	0.87	0
3	FAD	B	1524	-	51,58,58	2.68	17 (33%)	60,89,89	2.33	8 (13%)
4	ACN	B	1525	-	3,3,3	0.78	0	3,3,3	0.86	0
3	FAD	A	1524	-	51,58,58	2.68	16 (31%)	60,89,89	2.39	9 (15%)
2	COM	A	1000	-	6,6,6	1.79	1 (16%)	7,8,8	1.50	2 (28%)
2	COM	B	1000	-	6,6,6	1.60	1 (16%)	7,8,8	1.34	1 (14%)
5	NAP	B	1526	-	45,52,52	2.44	10 (22%)	56,80,80	1.66	12 (21%)
5	NAP	A	1526	-	45,52,52	2.44	14 (31%)	56,80,80	1.55	10 (17%)

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
5	NAP	A	1526	-	-	7/31/67/67	0/5/5/5
3	FAD	B	1524	-	-	1/30/50/50	0/6/6/6
3	FAD	A	1524	-	-	1/30/50/50	0/6/6/6
2	COM	A	1000	-	-	0/4/4/4	-
2	COM	B	1000	-	-	0/4/4/4	-
5	NAP	B	1526	-	-	7/31/67/67	0/5/5/5

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1524	FAD	C9A-N10	8.54	1.50	1.38
5	B	1526	NAP	C2N-N1N	8.41	1.45	1.35
5	A	1526	NAP	C2N-N1N	8.33	1.45	1.35
3	B	1524	FAD	C9A-N10	8.04	1.49	1.38
3	B	1524	FAD	C4X-N5	7.50	1.44	1.33
3	A	1524	FAD	C4X-N5	7.18	1.43	1.33
3	B	1524	FAD	C4A-N3A	6.31	1.44	1.35
3	B	1524	FAD	C2A-N3A	5.94	1.41	1.32
5	B	1526	NAP	C4N-C3N	5.71	1.49	1.39
3	A	1524	FAD	C4A-N3A	5.64	1.43	1.35
5	A	1526	NAP	C4N-C3N	5.58	1.48	1.39
5	B	1526	NAP	O4D-C1D	5.45	1.48	1.41
3	A	1524	FAD	C2A-N3A	5.42	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1524	FAD	C1'-N10	-5.27	1.42	1.48
5	A	1526	NAP	O4D-C1D	5.10	1.48	1.41
3	A	1524	FAD	C4-N3	5.00	1.41	1.33
3	B	1524	FAD	C4-N3	5.00	1.41	1.33
5	A	1526	NAP	C2A-N3A	4.99	1.40	1.32
3	A	1524	FAD	C1'-N10	-4.96	1.43	1.48
5	B	1526	NAP	C6N-N1N	4.73	1.47	1.35
5	B	1526	NAP	C2A-N3A	4.59	1.39	1.32
5	A	1526	NAP	C6N-N1N	4.44	1.46	1.35
3	B	1524	FAD	C5X-N5	4.27	1.42	1.35
3	A	1524	FAD	C5X-N5	3.85	1.41	1.35
5	A	1526	NAP	C2A-N1A	3.84	1.41	1.33
5	B	1526	NAP	C2A-N1A	3.84	1.41	1.33
3	A	1524	FAD	C10-N1	3.83	1.38	1.33
3	A	1524	FAD	C5A-C4A	-3.78	1.30	1.40
3	B	1524	FAD	C4X-C10	3.70	1.42	1.38
5	B	1526	NAP	C4A-N3A	3.70	1.40	1.35
5	A	1526	NAP	C3N-C7N	3.66	1.56	1.50
2	A	1000	COM	C2-S2	3.59	1.82	1.77
3	B	1524	FAD	C5A-C4A	-3.59	1.31	1.40
3	A	1524	FAD	C4X-C10	3.55	1.42	1.38
5	B	1526	NAP	C3N-C7N	3.31	1.55	1.50
3	A	1524	FAD	C5'-C4'	-3.23	1.47	1.51
2	B	1000	COM	C2-S2	2.95	1.81	1.77
3	B	1524	FAD	C10-N1	2.89	1.37	1.33
3	A	1524	FAD	C2'-C3'	-2.70	1.48	1.53
5	A	1526	NAP	C4A-N3A	2.70	1.39	1.35
3	A	1524	FAD	C8A-N7A	-2.46	1.30	1.34
5	B	1526	NAP	C5N-C4N	2.43	1.44	1.38
3	B	1524	FAD	C2'-C3'	-2.43	1.48	1.53
5	A	1526	NAP	C5N-C4N	2.40	1.44	1.38
3	B	1524	FAD	O4B-C1B	2.40	1.44	1.41
5	A	1526	NAP	PA-O1A	-2.29	1.42	1.50
3	B	1524	FAD	C5'-C4'	-2.27	1.48	1.51
3	B	1524	FAD	C2B-C3B	-2.26	1.47	1.53
3	A	1524	FAD	O4B-C1B	2.24	1.44	1.41
3	B	1524	FAD	C4-C4X	-2.23	1.37	1.41
5	A	1526	NAP	O4B-C4B	2.19	1.49	1.45
3	A	1524	FAD	C6-C7	2.15	1.43	1.37
3	B	1524	FAD	C9A-C5X	2.13	1.46	1.42
5	A	1526	NAP	P2B-O2B	2.13	1.63	1.59
3	A	1524	FAD	C2B-C3B	-2.10	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1526	NAP	C6N-C5N	2.10	1.43	1.38
5	A	1526	NAP	P2B-O2X	-2.07	1.46	1.54
3	B	1524	FAD	C8A-N7A	-2.06	1.31	1.34
5	B	1526	NAP	P2B-O2B	2.06	1.63	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1524	FAD	C4-N3-C2	12.00	125.27	115.14
3	B	1524	FAD	C4-N3-C2	11.87	125.16	115.14
3	B	1524	FAD	C4X-C4-N3	-6.30	114.82	123.43
3	A	1524	FAD	C4X-C4-N3	-6.28	114.84	123.43
3	A	1524	FAD	C1'-N10-C10	5.54	123.37	118.41
3	A	1524	FAD	C1'-N10-C9A	-5.42	114.03	118.29
3	B	1524	FAD	C1'-N10-C10	5.16	123.03	118.41
3	B	1524	FAD	C1'-N10-C9A	-4.89	114.45	118.29
5	A	1526	NAP	C5A-C6A-N6A	4.33	126.93	120.35
5	B	1526	NAP	C5A-C6A-N6A	4.27	126.84	120.35
5	B	1526	NAP	N3A-C2A-N1A	-4.23	122.06	128.68
5	A	1526	NAP	N3A-C2A-N1A	-4.17	122.17	128.68
5	B	1526	NAP	C3N-C7N-N7N	4.05	122.61	117.75
3	A	1524	FAD	C5X-C9A-N10	-3.71	115.03	117.72
5	A	1526	NAP	C3N-C7N-N7N	3.69	122.18	117.75
3	B	1524	FAD	C5X-C9A-N10	-3.62	115.09	117.72
5	B	1526	NAP	O7N-C7N-C3N	-3.43	115.52	119.63
5	B	1526	NAP	C3D-C2D-C1D	3.24	105.85	100.98
3	A	1524	FAD	C10-C4X-N5	3.02	123.35	121.26
5	B	1526	NAP	C3N-C2N-N1N	-2.87	117.62	120.43
3	B	1524	FAD	N3A-C2A-N1A	-2.75	124.38	128.68
3	A	1524	FAD	N3A-C2A-N1A	-2.74	124.40	128.68
5	A	1526	NAP	O7N-C7N-C3N	-2.72	116.37	119.63
3	B	1524	FAD	C10-C4X-N5	2.68	123.11	121.26
5	A	1526	NAP	C3D-C2D-C1D	2.64	104.95	100.98
5	A	1526	NAP	O2A-PA-O1A	2.57	124.93	112.24
5	A	1526	NAP	O3X-P2B-O2X	2.52	117.26	107.64
5	B	1526	NAP	O2A-PA-O1A	2.51	124.63	112.24
5	B	1526	NAP	O5B-C5B-C4B	-2.49	100.43	108.99
3	B	1524	FAD	C1'-C2'-C3'	2.41	116.52	109.79
2	A	1000	COM	O1S-S2-C2	2.38	109.78	106.92
5	B	1526	NAP	C2N-C3N-C4N	2.34	120.91	118.26
5	A	1526	NAP	C3N-C2N-N1N	-2.32	118.16	120.43
2	A	1000	COM	O3S-S2-C2	2.32	109.52	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1524	FAD	O2B-C2B-C3B	2.27	119.17	111.82
5	A	1526	NAP	C1B-N9A-C4A	-2.23	122.72	126.64
2	B	1000	COM	O3S-S2-C2	2.19	109.31	105.77
5	A	1526	NAP	C2N-C3N-C4N	2.17	120.71	118.26
5	B	1526	NAP	C1B-N9A-C4A	-2.15	122.86	126.64
5	B	1526	NAP	O3X-P2B-O2X	2.15	115.85	107.64
3	A	1524	FAD	C1'-C2'-C3'	2.12	115.72	109.79
5	B	1526	NAP	O4B-C4B-C5B	-2.11	102.44	109.37

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1526	NAP	C5B-O5B-PA-O1A
5	B	1526	NAP	C2B-O2B-P2B-O3X
5	B	1526	NAP	PN-O3-PA-O5B
5	A	1526	NAP	PN-O3-PA-O5B
5	B	1526	NAP	C5B-O5B-PA-O3
5	A	1526	NAP	C2B-O2B-P2B-O2X
5	B	1526	NAP	PA-O3-PN-O2N
5	A	1526	NAP	PA-O3-PN-O2N
5	A	1526	NAP	C5B-O5B-PA-O1A
3	B	1524	FAD	O4B-C4B-C5B-O5B
3	A	1524	FAD	O4B-C4B-C5B-O5B
5	B	1526	NAP	O4B-C4B-C5B-O5B
5	A	1526	NAP	O4B-C4B-C5B-O5B
5	A	1526	NAP	C5B-O5B-PA-O3
5	B	1526	NAP	PA-O3-PN-O1N
5	A	1526	NAP	PA-O3-PN-O1N

There are no ring outliers.

8 monomers are involved in 16 short contacts:

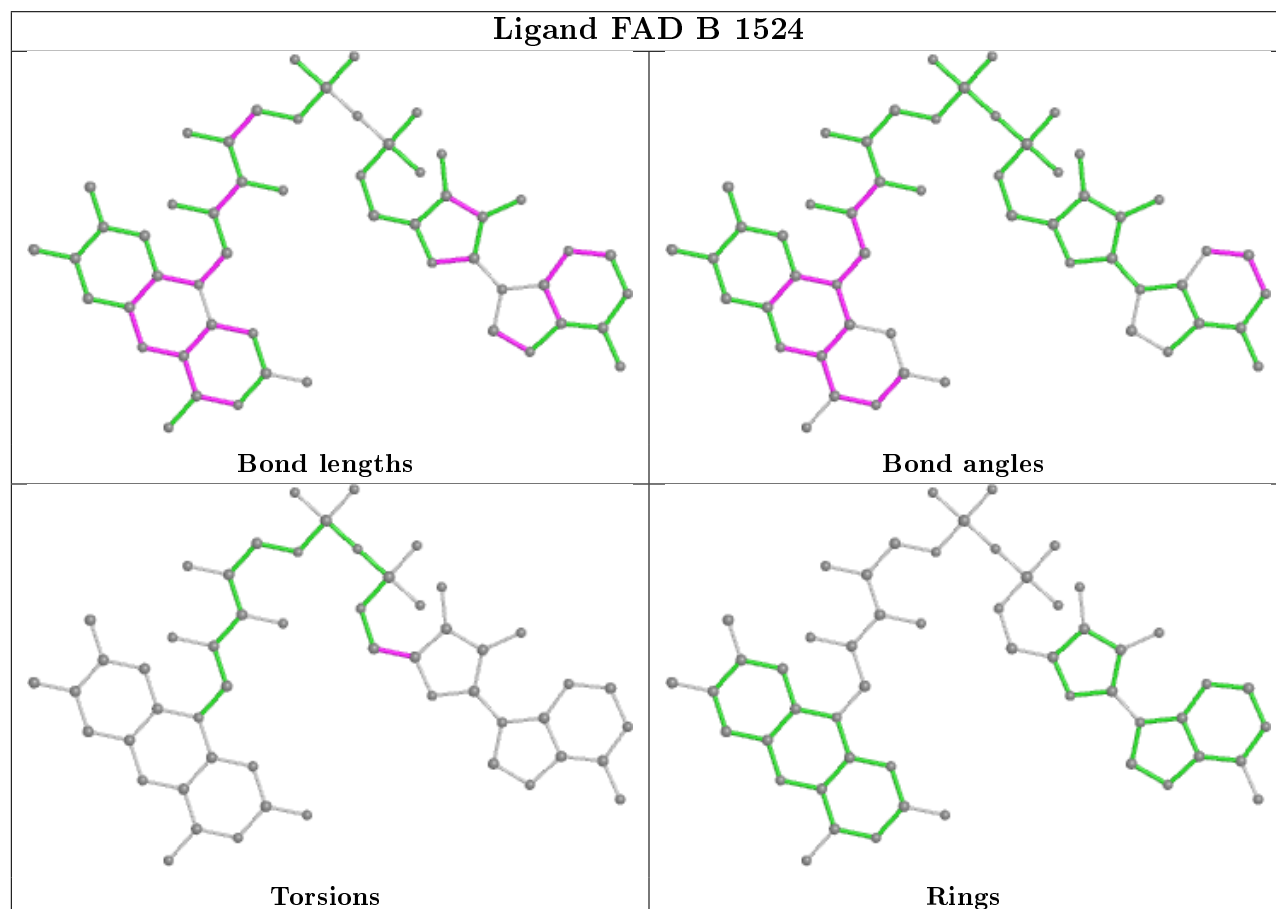
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1525	ACN	1	0
3	B	1524	FAD	2	0
4	B	1525	ACN	1	0
3	A	1524	FAD	1	0
2	A	1000	COM	2	0
2	B	1000	COM	2	0
5	B	1526	NAP	4	0

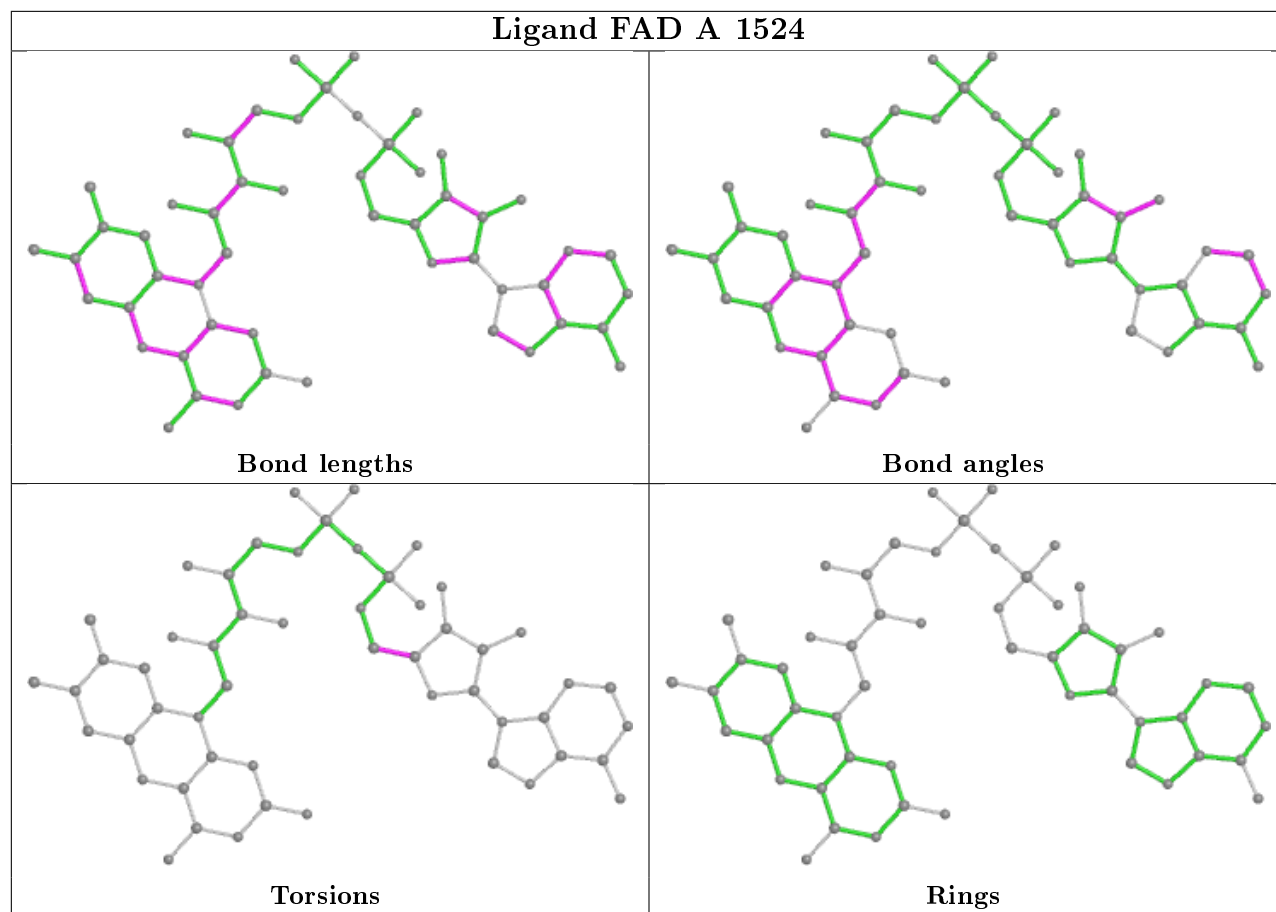
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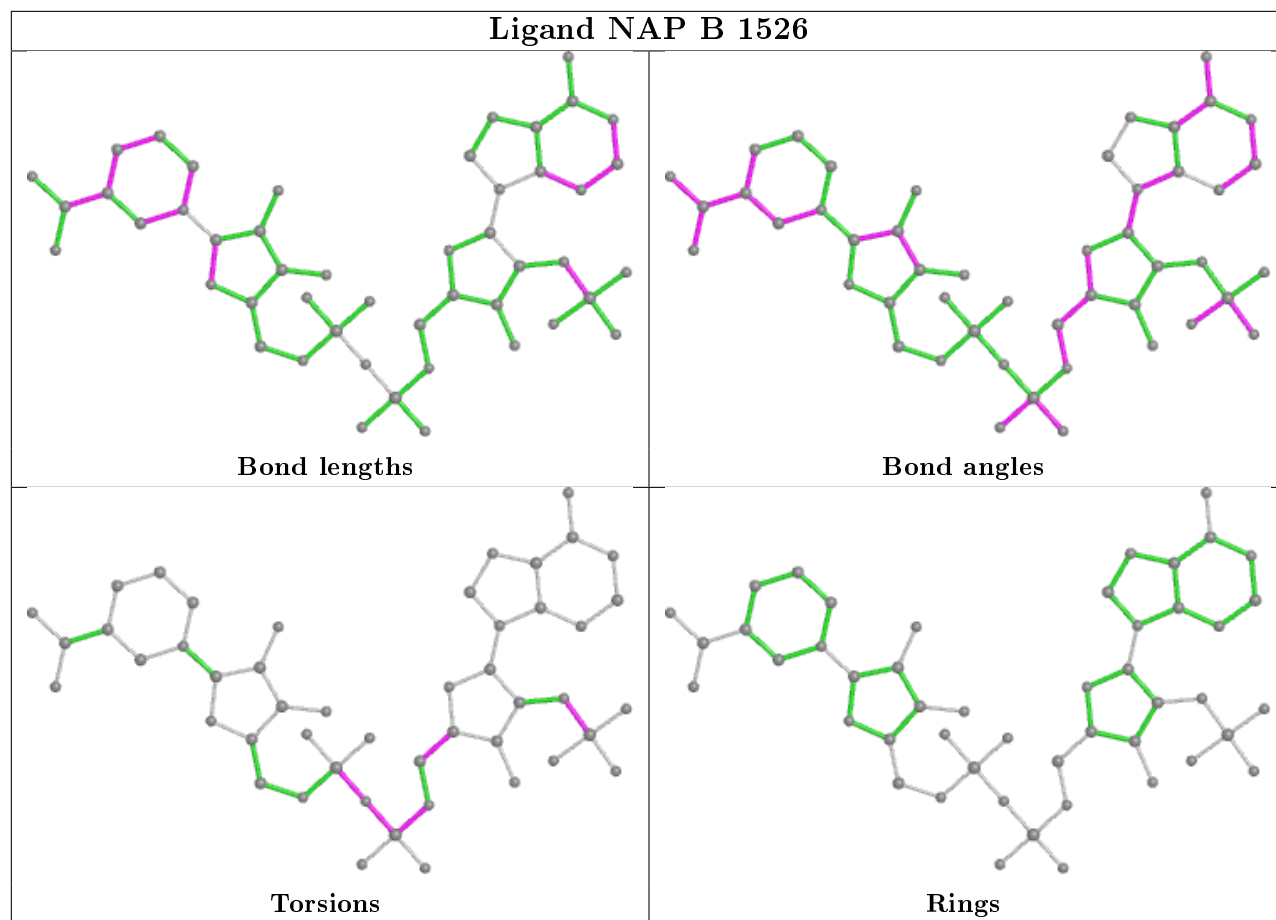
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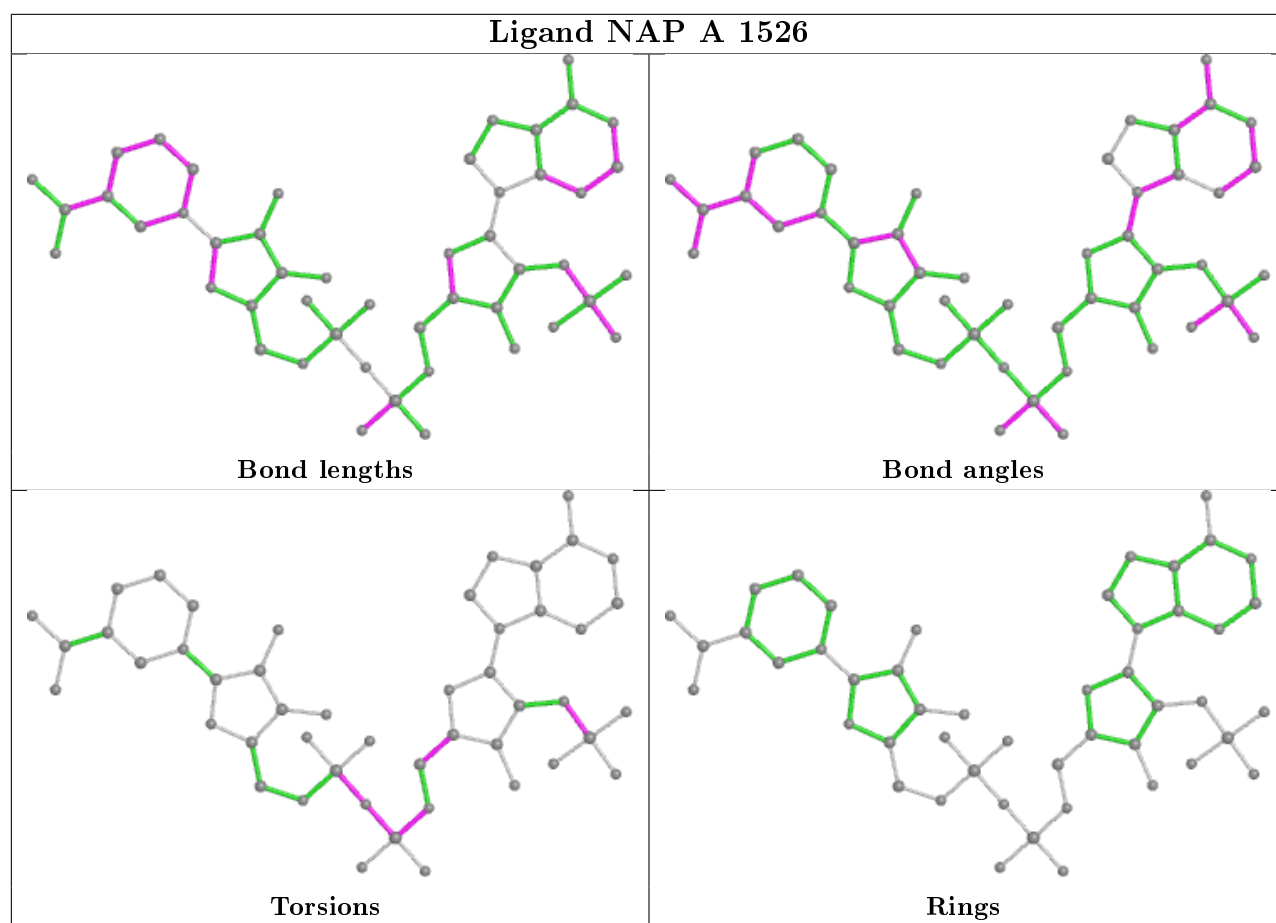
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1526	NAP	5	0

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.