



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:22 AM UTC

PDB ID : 2C3C / pdb_00002c3c
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

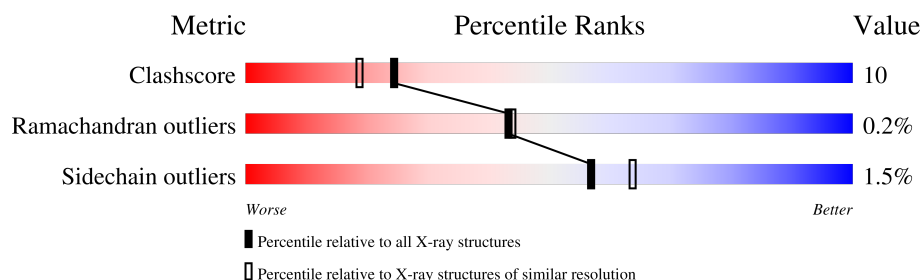
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (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 of 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	523	 84% 15% .
1	B	523	 82% 17% .

2 Entry composition [i](#)

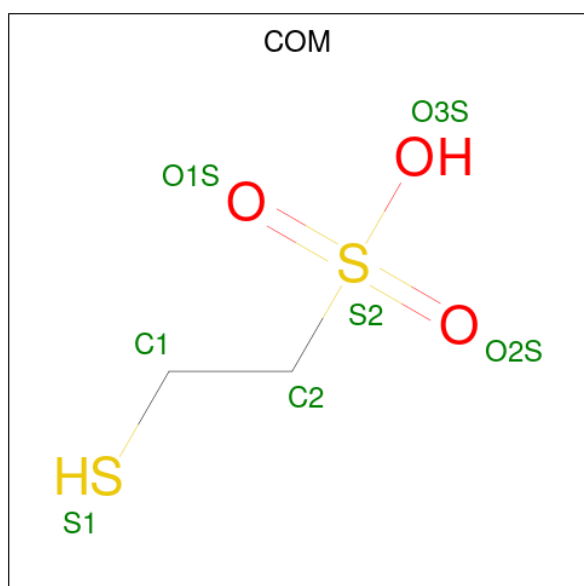
There are 6 unique types of molecules in this entry. The entry contains 8981 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

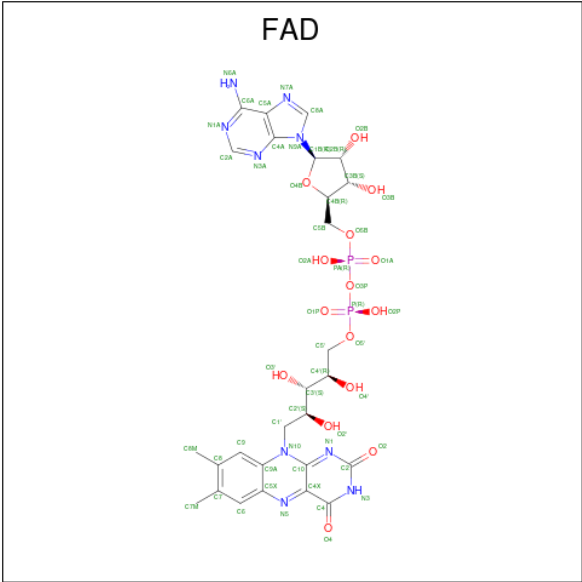
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	B	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			

- Molecule 2 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



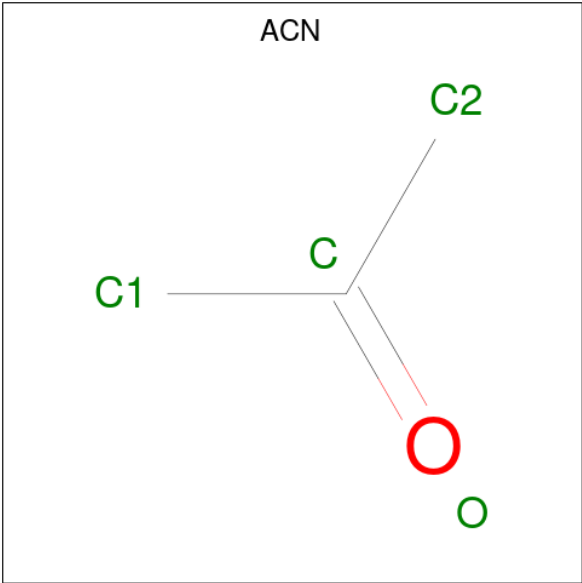
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			7	2	3	2		
2	B	1	Total	C	O	S	0	0
			7	2	3	2		

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



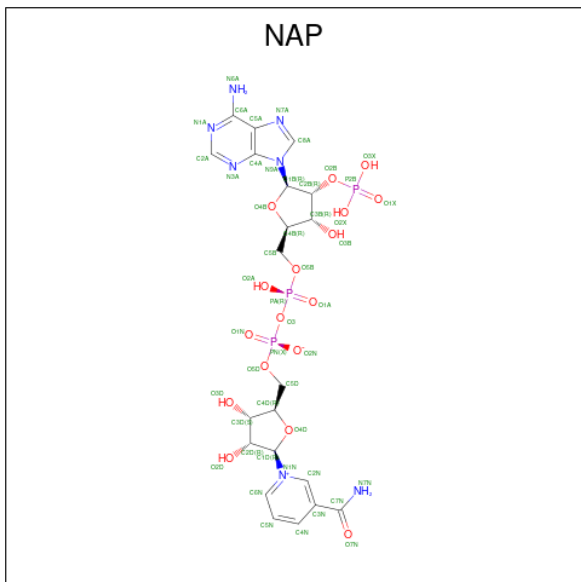
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is ACETONE (CCD ID: ACN) (formula: C₃H₆O).



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 (CCD ID: 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.

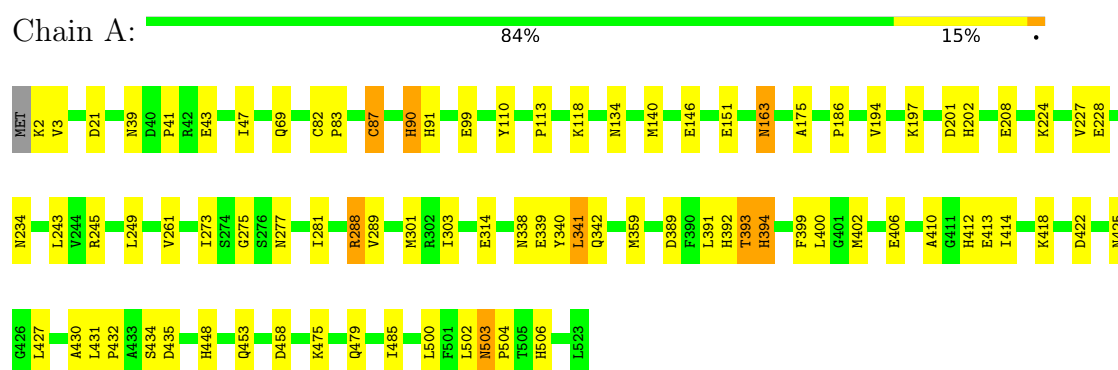
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	375	Total O 375 375	0	0
6	B	336	Total O 336 336	0	0

3 Residue-property plots [i](#)

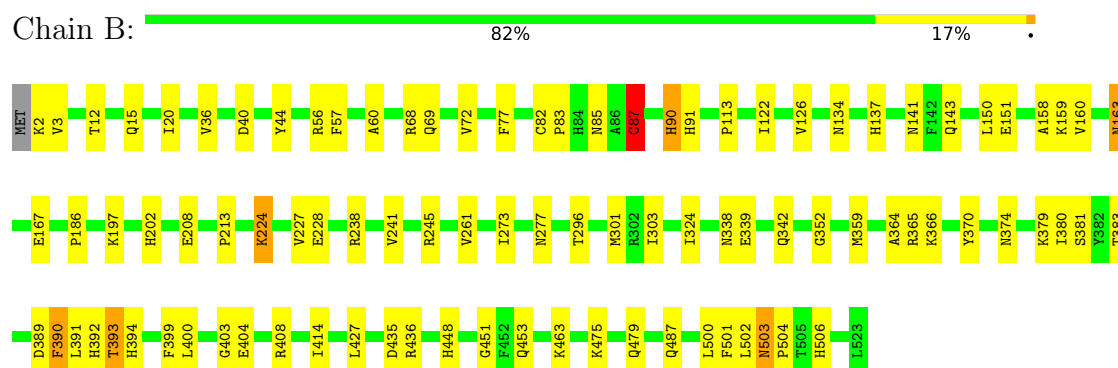
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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, α , β , γ	88.06Å 60.02Å 105.96Å 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 ²)	23.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACN, NAP, COM, 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	0.46	0/4106	0.94	12/5556 (0.2%)
1	B	0.46	0/4106	0.94	9/5556 (0.2%)
All	All	0.46	0/8212	0.94	21/11112 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	HIS	N-CA-C	-9.43	101.79	113.38
1	A	394	HIS	N-CA-C	-9.14	101.66	113.17
1	A	393	THR	N-CA-C	-8.04	93.68	110.80
1	B	393	THR	N-CA-C	-7.74	94.31	110.80
1	A	208	GLU	N-CA-C	6.95	121.45	112.41
1	A	414	ILE	N-CA-C	6.39	118.12	108.80
1	B	224	LYS	N-CA-C	5.97	118.30	111.02
1	B	87	CYS	N-CA-C	5.93	118.23	111.11
1	A	413	GLU	N-CA-C	-5.93	99.54	108.96
1	B	208	GLU	N-CA-C	5.78	119.93	112.41
1	B	414	ILE	N-CA-C	5.70	118.36	108.90
1	B	403	GLY	N-CA-C	-5.52	103.97	112.85
1	A	87	CYS	N-CA-C	5.39	117.58	111.11
1	A	110	TYR	CB-CA-C	-5.38	110.36	116.54
1	A	146	GLU	N-CA-C	5.38	119.00	112.23
1	A	503	ASN	N-CA-C	5.27	117.59	110.31
1	B	503	ASN	N-CA-C	5.27	117.58	110.31
1	A	425	ASN	N-CA-C	-5.26	106.82	113.18
1	A	201	ASP	N-CA-C	-5.08	101.70	108.86
1	B	451	GLY	N-CA-C	5.05	117.44	111.63
1	A	118	LYS	N-CA-C	5.04	116.98	108.96

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	4023	0	3982	76	0
1	B	4023	0	3982	97	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
4	B	4	0	6	1	0
5	A	48	0	25	5	0
5	B	48	0	25	5	0
6	A	375	0	0	4	0
6	B	336	0	0	8	0
All	All	8981	0	8100	162	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 10.

All (162) 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:B:296:THR:HG21	1:B:301:MET:HE3	1.27	1.10
1:A:301:MET:HE3	1:A:303:ILE:HD11	1.41	1.00
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: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:A:82:CYS:HG	2:A:1000:COM:HS1	1.01	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:GLN:NE2	1:B:506:HIS:H	1.79	0.79
1:B:90:HIS:CE1	1:B:392:HIS:HD2	2.01	0.78
1:B:374:ASN:HD21	1:B:380:ILE:H	1.29	0.78
1:B:273:ILE:HD13	1:B:301:MET:HE1	1.66	0.78
1:A:301:MET:CE	1:A:303:ILE:HD11	2.12	0.76
1:A:338:ASN:HD21	1:A:342:GLN:NE2	1.83	0.76
1:A:503:ASN:HD22	1:B:479:GLN:HE22	1.32	0.75
1:B:296:THR:CG2	1:B:301:MET:HE3	2.14	0.75
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:402:MET:HE2	1:A:406:GLU:HG2	1.72	0.72
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:B:338:ASN:HD21	1:B:342:GLN:HE21	1.40	0.68
1:A:163:ASN:HD22	1:A:163:ASN:N	1.95	0.65
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:296:THR:HG21	1:B:301:MET:CE	2.17	0.61
1:B:359:MET:HE3	5:B:1526:NAP:H4D	1.82	0.61
1:B:338:ASN:HD21	1:B:342:GLN:NE2	1.98	0.61
1:A:301:MET:HE3	1:A:303:ILE:CD1	2.25	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: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:90:HIS:CE1	1:B:392:HIS:CD2	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ASP:HB3	1:B:399:PHE:CE1	2.40	0.57
1:B:163:ASN:N	1:B:163:ASN:HD22	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: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:A:400:LEU:C	1:A:400:LEU:HD12	2.32	0.54
1:B:366:LYS:O	1:B:370:TYR:HD1	1.91	0.54
1:A:273:ILE:CD1	1:A:301:MET:HE1	2.38	0.54
1:B:273:ILE:HD13	1:B:301:MET:CE	2.37	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:359:MET:HE2	6:B:2208:HOH:O	2.08	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
1:B:82:CYS:HB3	1:B:83:PRO:HD3	1.91	0.52
1:A:91:HIS:HE1	1:A:475:LYS:NZ	2.08	0.52
1:A:359:MET:O	5:A:1526:NAP:H1D	2.10	0.52
1:B:374:ASN:HD21	1:B:380:ILE:N	2.03	0.51
1:A:82:CYS:HB3	1:A:83:PRO:CD	2.39	0.51
1:A:389:ASP:HB3	1:A:399:PHE:CE1	2.45	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:B:359:MET:HE1	6:B:2335:HOH:O	2.11	0.50
1:A:402:MET:HE1	1:A:410:ALA:HB2	1.95	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:A:402:MET:HE1	1:A:410:ALA:CB	2.43	0.49
1:B:339:GLU:HB2	1:B:381:SER:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:390:PHE:CD2	1:B:390:PHE:C	2.92	0.48
1:A:90:HIS:ND1	1:A:90:HIS:C	2.72	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:B:400:LEU:HD12	1:B:400:LEU:C	2.39	0.47
1:A:479:GLN:HE22	1:B:503:ASN:ND2	1.94	0.47
1:A:273:ILE:HD12	1:A:301:MET:HE1	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:H52A	5:A:1526:NAP:O2N	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:91:HIS:HE1	1:B:475:LYS:HZ1	1.63	0.45
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
1:B:57:PHE:CD2	1:B:365:ARG:HG2	2.52	0.45
1:B:186:PRO:HG3	1:B:202:HIS:CE1	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
1:A:186:PRO:HG3	1:A:202:HIS:CE1	2.52	0.44
2:A:1000:COM:H11	4:B:1525:ACN:H12	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LYS:HE3	6:B:2113:HOH:O	2.17	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:A:140:MET:HA	1:A:140:MET:HE2	2.00	0.43
1:A:435:ASP:OD1	1:B:392:HIS:HE1	2.01	0.43
5:A:1526:NAP:H51A	6:A:2375:HOH:O	2.19	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:391:LEU:C	1:A:391:LEU:HD12	2.45	0.42
1:A:21:ASP:OD2	1:A:134:ASN:ND2	2.53	0.42
1:A:431:LEU:HA	1:A:432:PRO:C	2.45	0.41
3:B:1524:FAD:H9	3:B:1524:FAD:H1'1	1.86	0.41
1:A:82:CYS:SG	1:B:501:PHE:HE2	2.43	0.41
1:A:392:HIS:HE1	1:B:435:ASP:OD1	2.03	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:228:GLU:HG2	1:B:392:HIS:HB2	2.03	0.40
1:B:245:ARG:HD2	5:B:1526:NAP:O3X	2.21	0.40
1:B:90:HIS:ND1	1:B:90:HIS:C	2.79	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
1:B:122:ILE:O	1:B:126:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	30	26
1	B	520/523 (99%)	496 (95%)	24 (5%)	0	100	100
All	All	1040/1046 (99%)	995 (96%)	43 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

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

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	423/424 (100%)	416 (98%)	7 (2%)	53	60
1	B	423/424 (100%)	417 (99%)	6 (1%)	59	66
All	All	846/848 (100%)	833 (98%)	13 (2%)	57	64

All (13) 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	339	GLU
1	A	341	LEU
1	A	422	ASP
1	A	504	PRO
1	B	87	CYS
1	B	90	HIS
1	B	163	ASN
1	B	383	THR
1	B	390	PHE
1	B	504	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) 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	149	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	482	ASN
1	A	487	GLN
1	B	14	ASN
1	B	69	GLN
1	B	90	HIS
1	B	91	HIS
1	B	109	GLN
1	B	137	HIS
1	B	141	ASN
1	B	143	GLN
1	B	149	ASN
1	B	163	ASN
1	B	177	ASN
1	B	195	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

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Mol	Chain	Res	Type
1	B	374	ASN
1	B	392	HIS
1	B	428	ASN
1	B	453	GLN
1	B	479	GLN
1	B	487	GLN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	COM	B	1000	-	6,6,6	1.62	2 (33%)	8,8,8	1.09	0
2	COM	A	1000	-	6,6,6	1.81	1 (16%)	8,8,8	1.21	1 (12%)
3	FAD	B	1524	-	58,58,58	2.01	13 (22%)	85,89,89	1.54	11 (12%)
4	ACN	A	1525	-	3,3,3	0.75	0	3,3,3	0.91	0
5	NAP	B	1526	-	50,52,52	2.53	14 (28%)	71,80,80	1.37	9 (12%)
4	ACN	B	1525	-	3,3,3	0.80	0	3,3,3	0.90	0
5	NAP	A	1526	-	50,52,52	2.52	16 (32%)	71,80,80	1.30	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	A	1524	-	58,58,58	1.98	13 (22%)	85,89,89	1.53	11 (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
2	COM	B	1000	-	-	0/4/4/4	-
2	COM	A	1000	-	-	0/4/4/4	-
3	FAD	B	1524	-	-	1/34/50/50	0/6/6/6
5	NAP	B	1526	-	-	7/35/67/67	0/5/5/5
5	NAP	A	1526	-	-	6/35/67/67	0/5/5/5
3	FAD	A	1524	-	-	1/34/50/50	0/6/6/6

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1526	NAP	C2N-N1N	9.30	1.45	1.35
5	A	1526	NAP	C2N-N1N	9.22	1.45	1.35
5	B	1526	NAP	C4N-C3N	6.37	1.49	1.39
5	A	1526	NAP	C4N-C3N	6.23	1.48	1.39
3	B	1524	FAD	C4X-N5	6.15	1.44	1.30
3	A	1524	FAD	C4X-N5	5.95	1.43	1.30
5	B	1526	NAP	O4D-C1D	5.94	1.48	1.40
5	A	1526	NAP	O4D-C1D	5.56	1.48	1.40
3	B	1524	FAD	C4A-N3A	5.31	1.44	1.34
3	A	1524	FAD	C9A-N10	5.14	1.50	1.41
5	B	1526	NAP	C6N-N1N	5.10	1.47	1.35
3	A	1524	FAD	C4A-N3A	4.82	1.43	1.34
5	A	1526	NAP	C6N-N1N	4.79	1.46	1.35
3	B	1524	FAD	C9A-N10	4.75	1.49	1.41
3	A	1524	FAD	C5A-C4A	-4.57	1.30	1.39
3	B	1524	FAD	C2A-N3A	4.36	1.41	1.33
3	B	1524	FAD	C5A-C4A	-4.29	1.31	1.39
5	B	1526	NAP	PN-O3	4.17	1.64	1.59
5	A	1526	NAP	C2A-N1A	4.01	1.41	1.33
5	B	1526	NAP	C2A-N1A	4.01	1.41	1.33
3	A	1524	FAD	C2A-N3A	3.89	1.40	1.33
5	A	1526	NAP	PN-O3	3.84	1.63	1.59
5	A	1526	NAP	C3N-C7N	3.68	1.56	1.50
2	A	1000	COM	C2-S2	3.59	1.82	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1524	FAD	C9A-C5X	3.51	1.46	1.41
5	A	1526	NAP	C2A-N3A	3.50	1.40	1.33
5	B	1526	NAP	C4A-N3A	3.39	1.40	1.34
3	A	1524	FAD	C5'-C4'	-3.37	1.47	1.51
3	A	1524	FAD	C9A-C5X	3.34	1.46	1.41
5	B	1526	NAP	C3N-C7N	3.32	1.55	1.50
5	B	1526	NAP	C2A-N3A	3.13	1.39	1.33
5	B	1526	NAP	C5N-C4N	3.00	1.44	1.38
5	A	1526	NAP	C5N-C4N	2.96	1.44	1.38
3	B	1524	FAD	C8A-N9A	2.94	1.42	1.37
2	B	1000	COM	C2-S2	2.93	1.81	1.77
3	A	1524	FAD	C2'-C3'	-2.88	1.48	1.53
3	A	1524	FAD	C8A-N9A	2.74	1.42	1.37
5	A	1526	NAP	C4A-N3A	2.65	1.39	1.34
3	A	1524	FAD	C6-C7	2.62	1.43	1.39
3	B	1524	FAD	C2'-C3'	-2.59	1.48	1.53
5	B	1526	NAP	C6A-N1A	2.53	1.42	1.35
3	A	1524	FAD	C10-N1	2.45	1.38	1.33
3	B	1524	FAD	C5'-C4'	-2.37	1.48	1.51
5	A	1526	NAP	C6A-N1A	2.32	1.42	1.35
5	A	1526	NAP	PA-O1A	-2.32	1.42	1.50
3	A	1524	FAD	C9-C9A	2.30	1.43	1.39
3	B	1524	FAD	C2B-C3B	-2.29	1.47	1.53
3	B	1524	FAD	PA-O3P	2.27	1.62	1.59
5	A	1526	NAP	C6N-C5N	2.24	1.43	1.38
5	A	1526	NAP	O4B-C4B	2.21	1.49	1.45
5	A	1526	NAP	P2B-O2B	2.17	1.63	1.59
3	A	1524	FAD	C2B-C3B	-2.13	1.47	1.53
5	A	1526	NAP	P2B-O2X	-2.13	1.46	1.54
3	B	1524	FAD	C6-C7	2.12	1.42	1.39
5	B	1526	NAP	P2B-O2B	2.09	1.63	1.59
3	B	1524	FAD	C1'-N10	-2.08	1.42	1.47
5	B	1526	NAP	C6N-C5N	2.05	1.42	1.38
2	B	1000	COM	O1S-S2	2.05	1.50	1.45
5	B	1526	NAP	PA-O1A	-2.02	1.43	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1524	FAD	C4A-N9A-C8A	-5.32	100.15	105.74
3	B	1524	FAD	C5A-C4A-N9A	5.15	111.42	105.81
3	A	1524	FAD	C5A-C4A-N9A	5.14	111.42	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1524	FAD	C4A-N9A-C8A	-5.09	100.39	105.74
3	A	1524	FAD	N3A-C4A-N9A	-4.76	119.08	127.17
3	B	1524	FAD	N3A-C4A-N9A	-4.67	119.22	127.17
5	B	1526	NAP	N3A-C2A-N1A	-4.31	122.06	128.58
5	A	1526	NAP	N3A-C2A-N1A	-4.24	122.17	128.58
5	B	1526	NAP	C3N-C7N-N7N	3.96	122.61	117.74
5	A	1526	NAP	C3N-C7N-N7N	3.60	122.18	117.74
3	A	1524	FAD	C1'-N10-C9A	-3.40	114.03	120.63
5	B	1526	NAP	O7N-C7N-C3N	-3.33	115.52	119.60
3	A	1524	FAD	C5X-C9A-N10	-3.25	115.03	117.97
3	B	1524	FAD	C1'-N10-C9A	-3.18	114.45	120.63
3	B	1524	FAD	C5X-C9A-N10	-3.18	115.09	117.97
3	B	1524	FAD	N3A-C2A-N1A	-2.77	124.38	128.58
3	A	1524	FAD	N3A-C2A-N1A	-2.76	124.40	128.58
5	A	1526	NAP	O2A-PA-O1A	2.68	124.93	112.44
5	A	1526	NAP	O7N-C7N-C3N	-2.64	116.37	119.60
5	B	1526	NAP	O2A-PA-O1A	2.62	124.63	112.44
3	B	1524	FAD	C9-C9A-N10	2.59	125.33	121.85
3	B	1524	FAD	C1'-C2'-C3'	2.53	116.52	109.66
5	A	1526	NAP	O3X-P2B-O2X	2.52	117.26	107.80
5	B	1526	NAP	O5B-C5B-C4B	-2.51	100.43	108.99
3	A	1524	FAD	C9-C9A-N10	2.40	125.08	121.85
3	A	1524	FAD	O2B-C2B-C3B	2.29	119.17	111.82
5	B	1526	NAP	C2N-C3N-C4N	2.28	120.91	118.26
3	A	1524	FAD	C1'-C2'-C3'	2.24	115.72	109.66
5	B	1526	NAP	O4B-C4B-C5B	-2.15	102.44	109.33
5	B	1526	NAP	O3X-P2B-O2X	2.15	115.85	107.80
5	A	1526	NAP	C1B-N9A-C8A	2.14	131.83	127.09
5	A	1526	NAP	C2N-C3N-C4N	2.11	120.71	118.26
3	A	1524	FAD	O3P-PA-O1A	-2.09	104.42	110.70
3	A	1524	FAD	C5A-C4A-N3A	2.03	129.51	126.72
3	B	1524	FAD	O3P-PA-O1A	-2.03	104.61	110.70
5	B	1526	NAP	O3B-C3B-C4B	-2.02	105.28	111.08
2	A	1000	COM	O1S-S2-C2	2.02	109.78	106.73
3	B	1524	FAD	O2B-C2B-C3B	2.01	118.25	111.82
3	B	1524	FAD	C4-C4X-C10	2.00	120.36	116.93

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1526	NAP	C5B-O5B-PA-O1A

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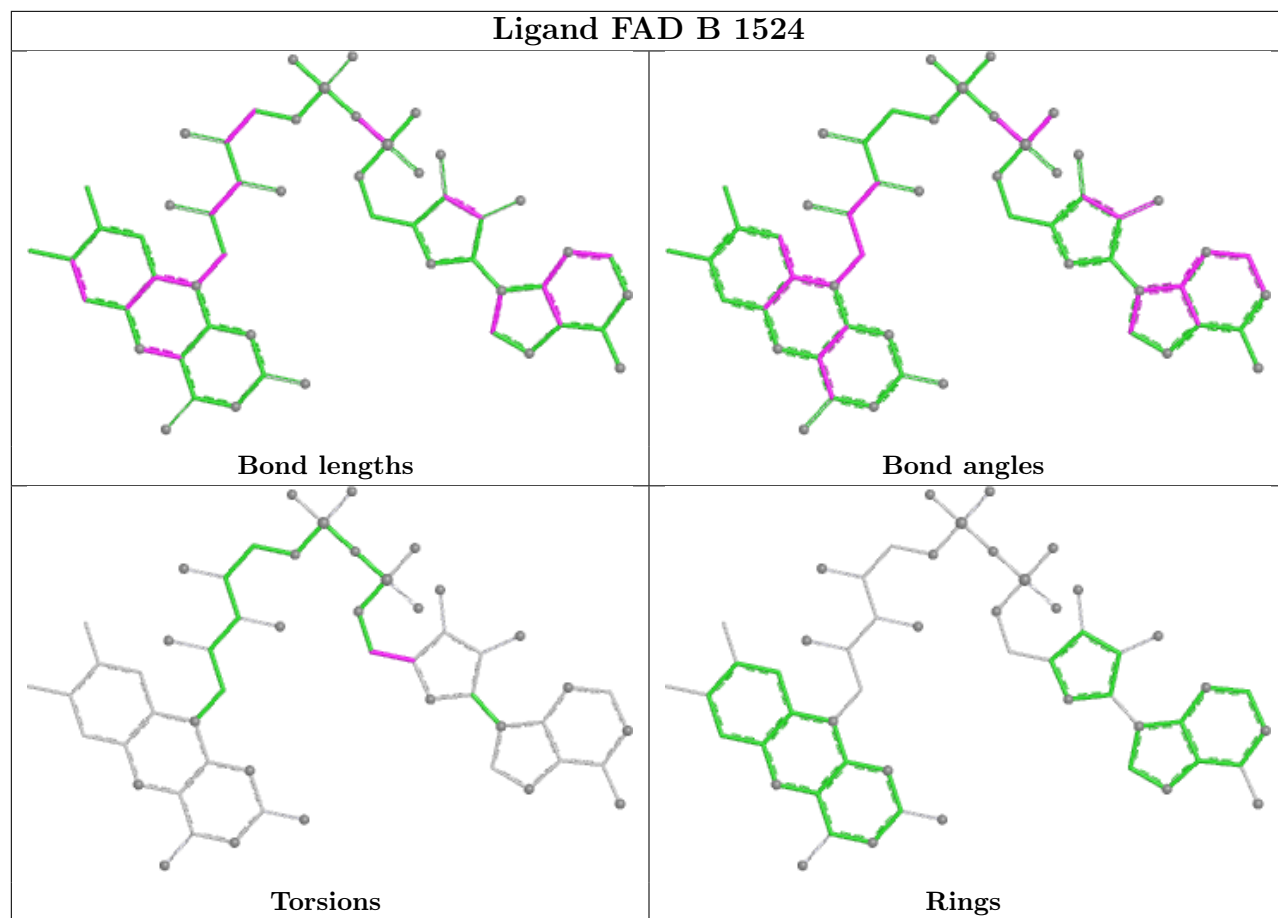
Mol	Chain	Res	Type	Atoms
5	B	1526	NAP	C5B-O5B-PA-O1A
5	A	1526	NAP	PN-O3-PA-O5B
5	B	1526	NAP	PN-O3-PA-O5B
5	A	1526	NAP	PA-O3-PN-O2N
5	B	1526	NAP	PA-O3-PN-O2N
5	B	1526	NAP	C5B-O5B-PA-O3
5	A	1526	NAP	C2B-O2B-P2B-O2X
5	B	1526	NAP	C2B-O2B-P2B-O3X
5	A	1526	NAP	PA-O3-PN-O1N
5	B	1526	NAP	PA-O3-PN-O1N
3	A	1524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

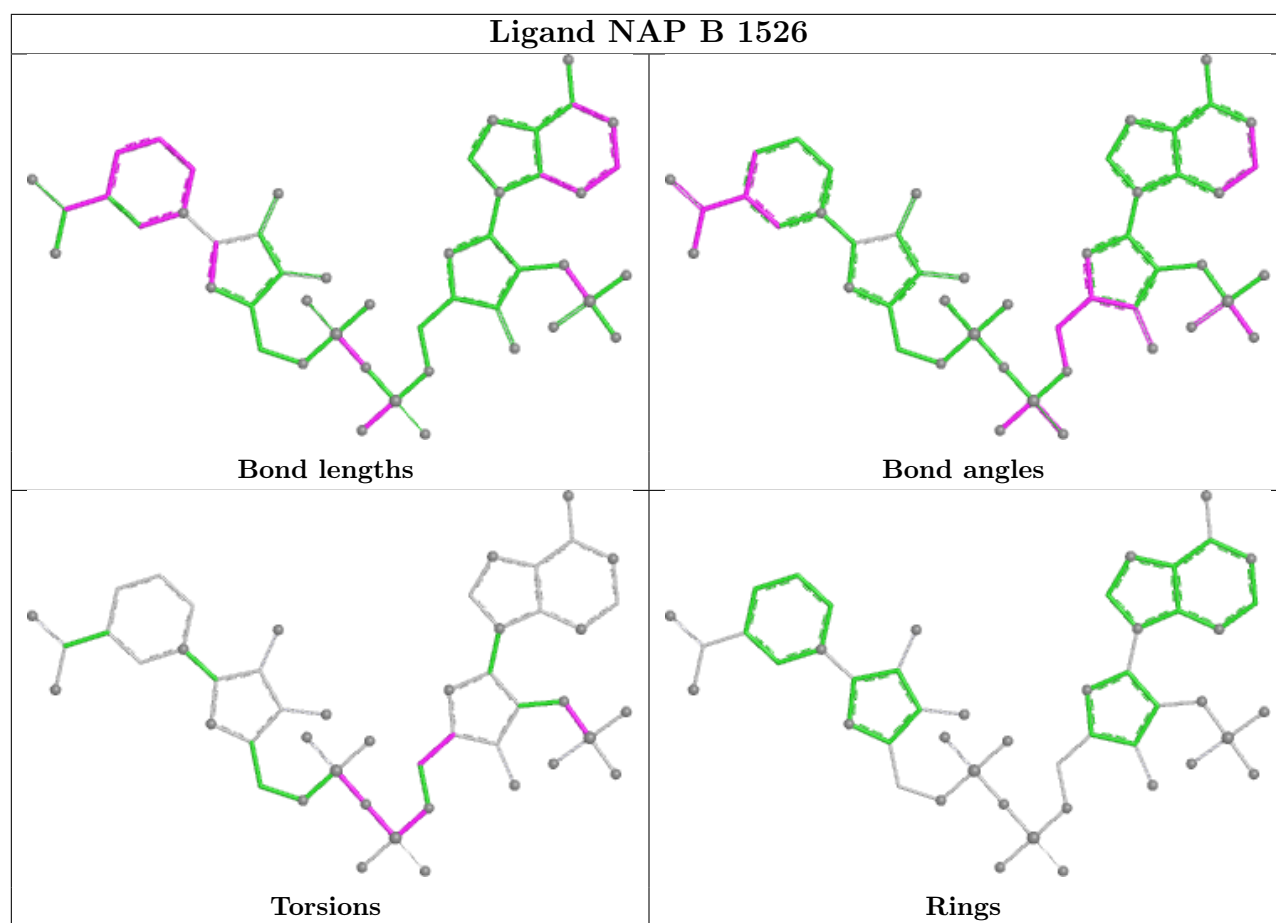
There are no ring outliers.

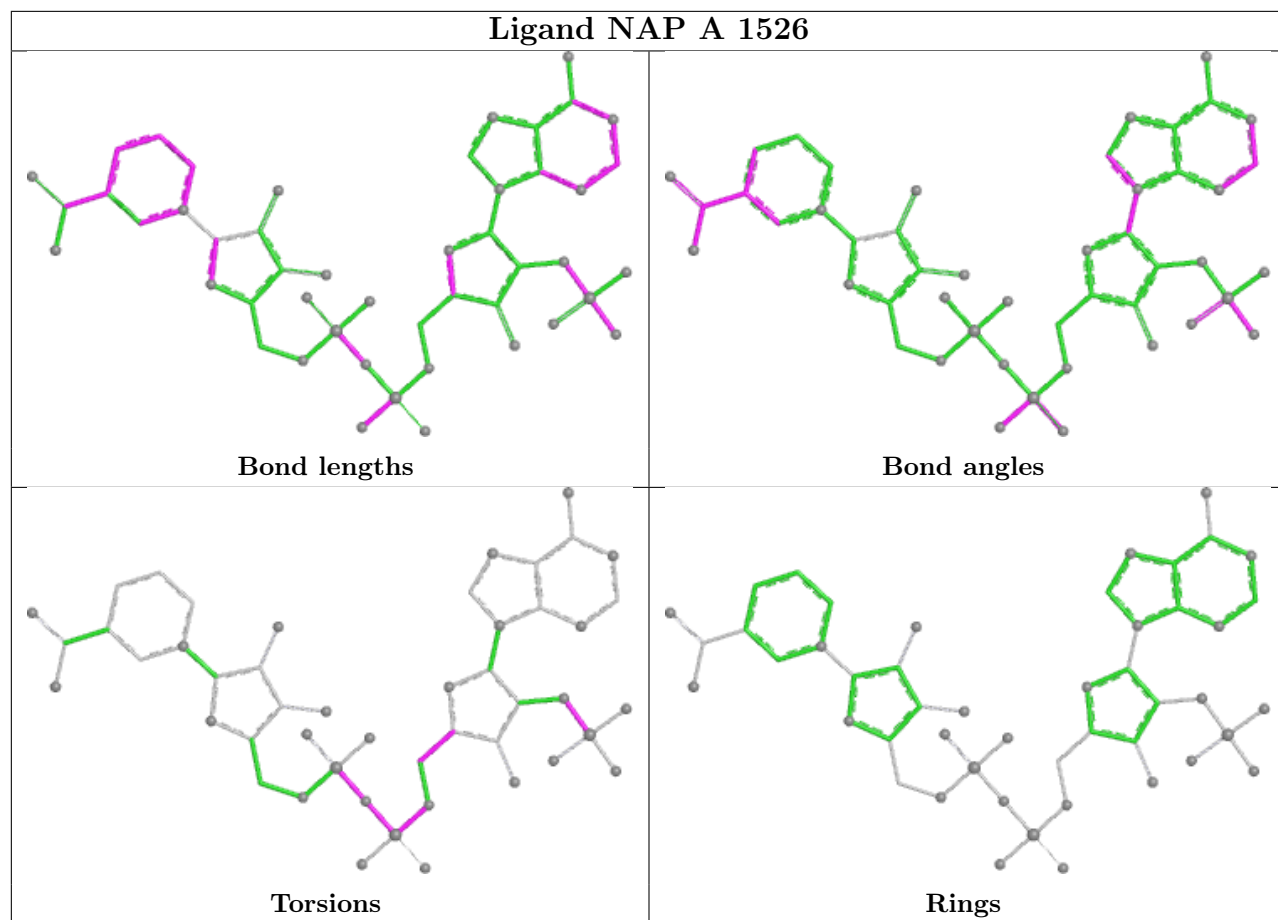
8 monomers are involved in 17 short contacts:

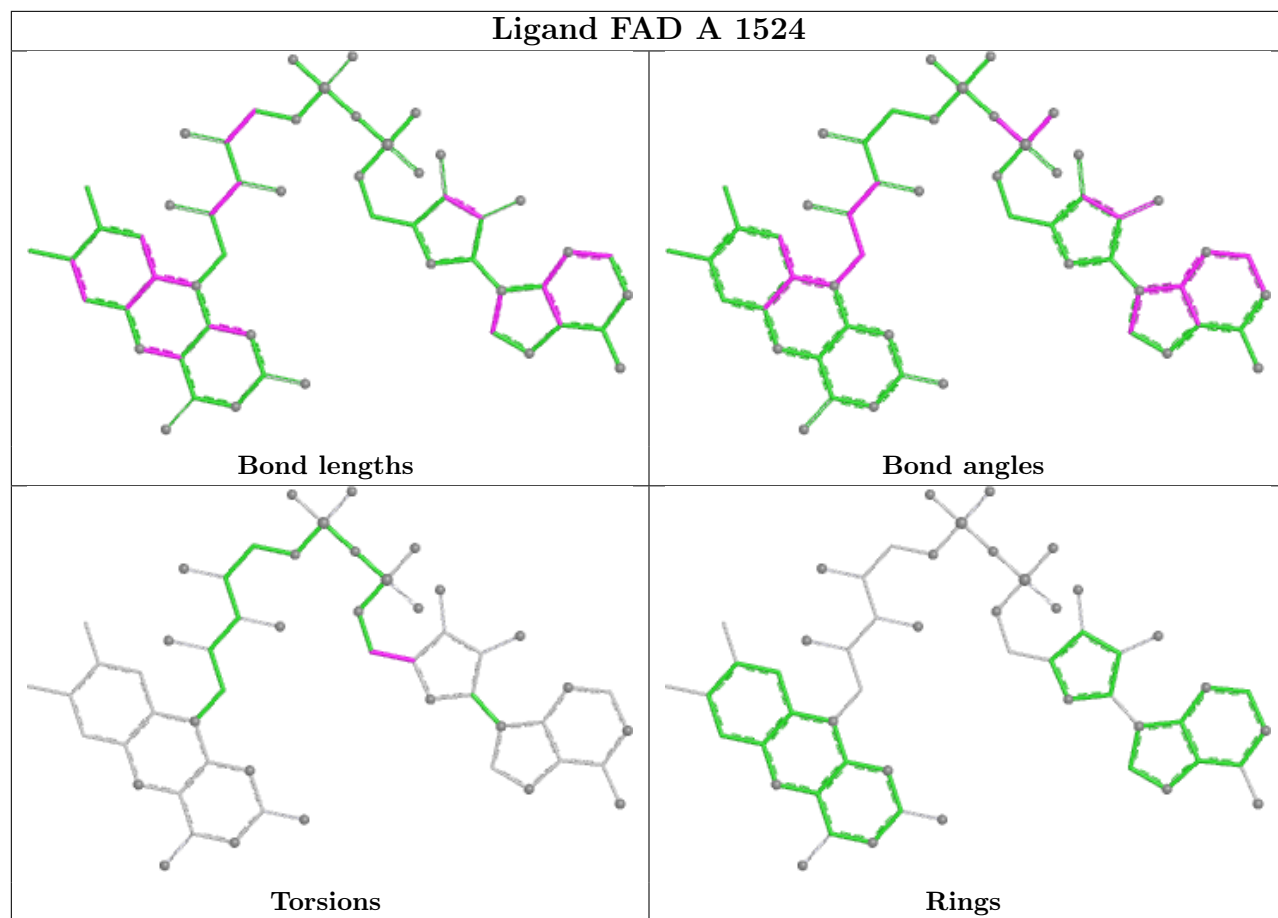
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	COM	2	0
2	A	1000	COM	2	0
3	B	1524	FAD	2	0
4	A	1525	ACN	1	0
5	B	1526	NAP	5	0
4	B	1525	ACN	1	0
5	A	1526	NAP	5	0
3	A	1524	FAD	1	0

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.