



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:57 pm BST

PDB ID : 3UOZ  
Title : Crystal Structure of OTEMO complex with FAD and NADP (form 2)  
Authors : Shi, R.; Matte, A.; Cygler, M.; Lau, P.  
Deposited on : 2011-11-17  
Resolution : 2.41 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) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

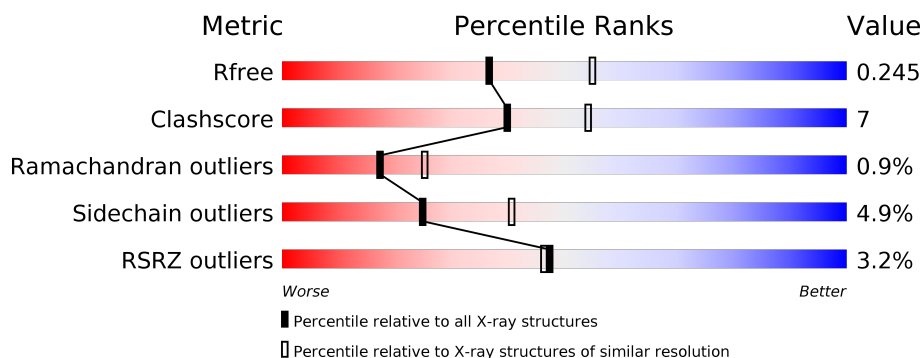
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	545	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>...</div> </div> </div>
1	B	545	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

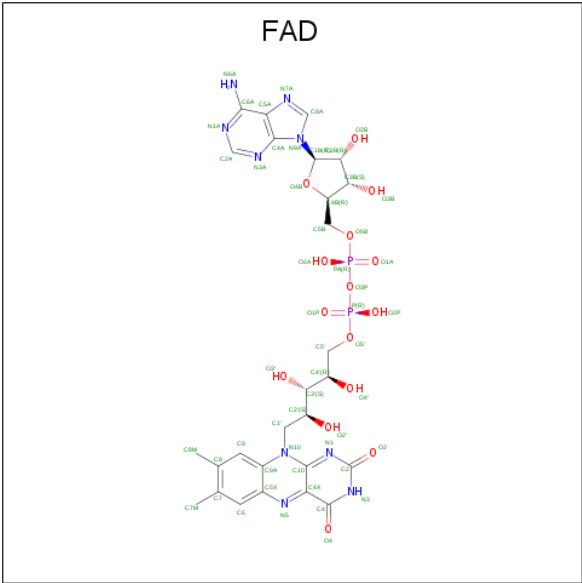
There are 4 unique types of molecules in this entry. The entry contains 9041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OTEMO.

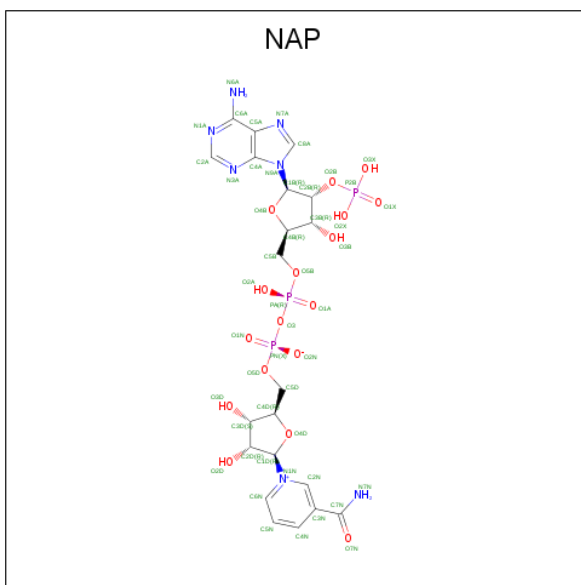
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	1	0
			4297	2729	742	811	15			
1	B	540	Total	C	N	O	S	0	3	0
			4299	2727	743	814	15			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

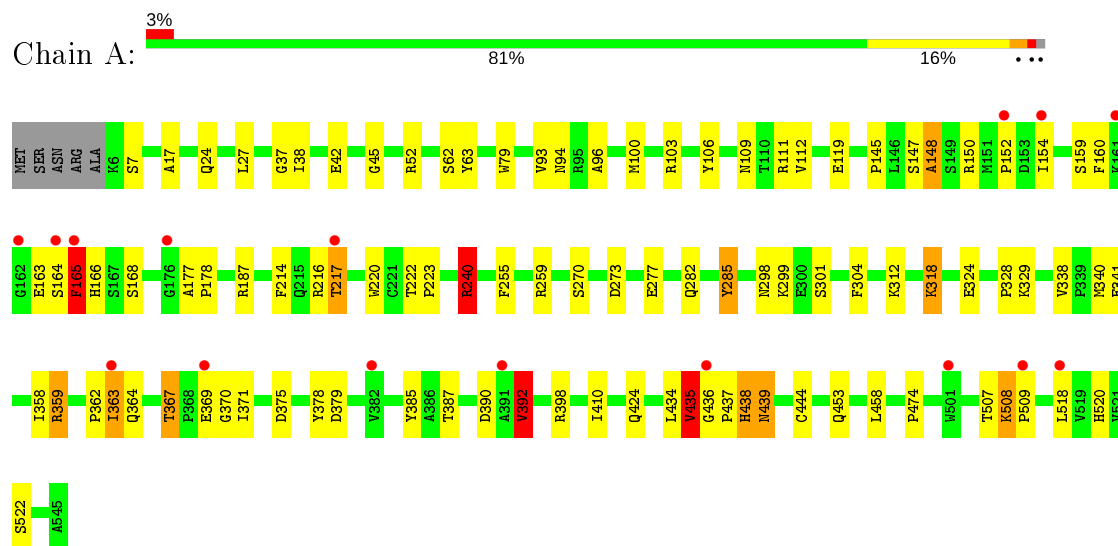
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	102	Total O 102 102	0	0
4	B	141	Total O 141 141	0	0

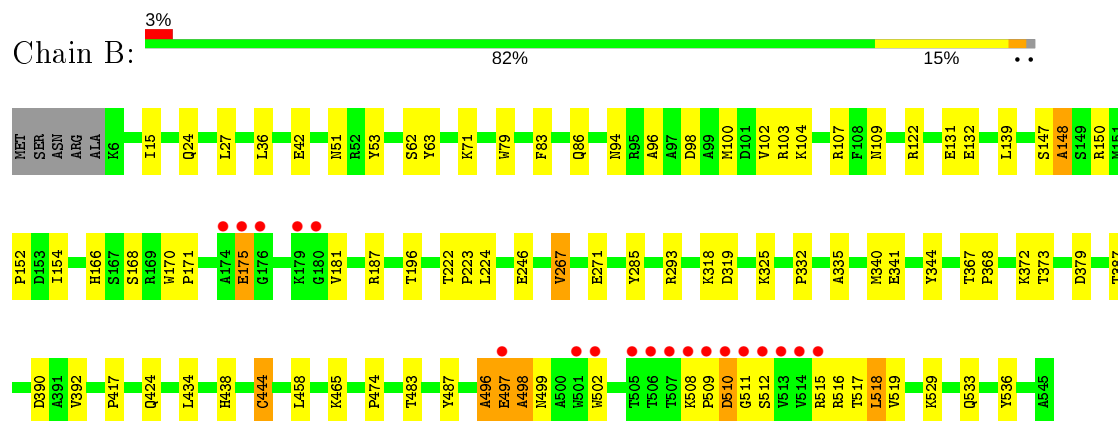
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

#### • Molecule 1: OTEMO



#### • Molecule 1: OTEMO



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.76Å 95.18Å 93.13Å 90.00° 101.82° 90.00°	Depositor
Resolution (Å)	48.61 – 2.41 48.60 – 2.41	Depositor EDS
% Data completeness (in resolution range)	95.0 (48.61-2.41) 95.0 (48.60-2.41)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.196 , 0.247 0.196 , 0.245	Depositor DCC
$R_{free}$ test set	2122 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9041	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, 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	0.68	0/4411	0.74	4/5993 (0.1%)
1	B	0.76	0/4414	0.77	0/5996
All	All	0.72	0/8825	0.75	4/11989 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	VAL	CB-CA-C	6.10	122.99	111.40
1	A	240	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	240	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	165	PHE	CB-CA-C	-5.58	99.25	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	PHE	Peptide
1	B	444	CYS	Peptide

## 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	4297	0	4153	76	0
1	B	4299	0	4155	47	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	48	0	25	3	0
3	B	48	0	25	1	0
4	A	102	0	0	20	0
4	B	141	0	0	3	0
All	All	9041	0	8420	125	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 (125) 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:367:THR:HG22	1:A:369:GLU:H	1.39	0.86
1:B:166:HIS:HD2	1:B:168:SER:H	1.24	0.82
1:B:187:ARG:NH1	1:B:379:ASP:O	2.14	0.80
1:B:42:GLU:HG3	1:B:109:ASN:HD21	1.48	0.79
1:B:27:LEU:HB3	1:B:458:LEU:HD22	1.66	0.77
1:B:424:GLN:HE21	1:B:474:PRO:HD3	1.50	0.77
1:A:318:LYS:HE2	4:A:623:HOH:O	1.85	0.75
1:B:94:ASN:HD22	1:B:103:ARG:HH21	1.35	0.73
1:B:166:HIS:CD2	1:B:168:SER:H	2.06	0.73
1:A:520:HIS:HE2	1:A:522:SER:HG	1.34	0.72
1:A:438:HIS:HE1	4:A:557:HOH:O	1.73	0.72
2:B:551:FAD:HM73	3:B:552:NAP:C5N	2.20	0.72
1:B:24:GLN:HE21	1:B:434:LEU:HD11	1.57	0.69
1:A:410:ILE:HG23	4:A:643:HOH:O	1.93	0.69
1:A:424:GLN:HE21	1:A:474:PRO:HD3	1.57	0.69
1:A:147:SER:O	1:A:148:ALA:HB3	1.92	0.68
1:A:438:HIS:HA	1:A:520:HIS:HB2	1.75	0.68
1:A:437:PRO:O	1:A:439:ASN:N	2.26	0.68
1:A:358:ILE:HD12	1:A:363:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLN:HE21	1:A:434:LEU:HD11	1.59	0.66
1:A:111:ARG:HD3	4:A:555:HOH:O	1.94	0.66
1:B:150:ARG:NH1	1:B:387:THR:O	2.29	0.66
1:A:508:LYS:HB3	1:A:509:PRO:CD	2.26	0.66
1:A:220:TRP:CE2	1:A:328:PRO:HG2	2.31	0.65
1:A:145:PRO:HD3	1:A:435:VAL:HG22	1.77	0.64
1:A:94:ASN:HD22	1:A:103:ARG:HH21	1.45	0.64
1:A:370:GLY:HA3	1:A:378:TYR:O	1.97	0.64
1:A:507:THR:HG23	4:A:582:HOH:O	1.98	0.63
1:A:410:ILE:HG12	4:A:643:HOH:O	1.98	0.63
1:B:147:SER:O	1:B:148:ALA:HB3	1.99	0.63
1:A:508:LYS:HB3	1:A:509:PRO:HD2	1.80	0.63
1:A:439:ASN:HB2	1:A:453:GLN:HE22	1.65	0.62
1:A:166:HIS:HD2	1:A:168:SER:H	1.46	0.62
1:A:214:PHE:HB3	1:A:358:ILE:HD13	1.83	0.60
1:A:520:HIS:CE1	1:A:522:SER:HG	2.20	0.59
1:A:166:HIS:CD2	1:A:168:SER:H	2.20	0.59
1:A:520:HIS:NE2	1:A:522:SER:OG	2.32	0.59
1:B:519:VAL:HG23	4:B:580:HOH:O	2.04	0.58
1:B:332:PRO:HG2	1:B:335:ALA:HB2	1.86	0.57
1:B:529:LYS:O	1:B:533:GLN:HG3	2.04	0.57
1:A:217:THR:CG2	1:A:359:ARG:HH22	2.18	0.57
1:A:152:PRO:HB2	1:A:154:ILE:HG12	1.86	0.56
1:B:170:TRP:CD1	1:B:171:PRO:HD2	2.41	0.56
1:A:166:HIS:HA	1:A:385:TYR:HB2	1.87	0.55
1:B:222:THR:HB	1:B:223:PRO:HD2	1.89	0.55
1:A:436:GLY:O	1:A:439:ASN:ND2	2.39	0.54
2:A:551:FAD:HM73	3:A:552:NAP:C5N	2.38	0.54
1:A:27:LEU:HB3	1:A:458:LEU:HG	1.90	0.53
1:A:439:ASN:HB3	4:A:595:HOH:O	2.08	0.52
1:A:324:GLU:O	1:A:329:LYS:NZ	2.43	0.51
1:A:163:GLU:HB3	4:A:592:HOH:O	2.09	0.51
1:B:367:THR:HB	1:B:368:PRO:HD2	1.93	0.51
1:A:438:HIS:CE1	4:A:557:HOH:O	2.57	0.50
1:A:45:GLY:HA2	1:A:93:VAL:HG11	1.92	0.50
1:A:147:SER:O	1:A:148:ALA:CB	2.56	0.50
1:A:148:ALA:HB1	1:A:398:ARG:HE	1.76	0.50
1:A:410:ILE:CG2	4:A:643:HOH:O	2.57	0.50
1:A:63:TYR:HA	4:A:569:HOH:O	2.11	0.50
1:A:164:SER:HB2	4:A:621:HOH:O	2.10	0.50
1:A:217:THR:OG1	3:A:552:NAP:O2X	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:SER:CB	4:A:621:HOH:O	2.59	0.49
1:B:246:GLU:HG2	4:B:629:HOH:O	2.12	0.49
1:B:147:SER:O	1:B:148:ALA:CB	2.61	0.49
1:A:438:HIS:CA	1:A:520:HIS:HB2	2.42	0.49
1:B:508:LYS:HB3	1:B:509:PRO:HD2	1.94	0.49
1:A:152:PRO:HB2	1:A:154:ILE:CG1	2.41	0.49
1:B:496:ALA:O	1:B:498:ALA:N	2.46	0.49
1:B:319:ASP:OD1	1:B:319:ASP:C	2.51	0.48
1:A:145:PRO:O	1:A:392:VAL:N	2.46	0.48
1:A:240:ARG:NH2	1:B:536:TYR:O	2.47	0.48
1:B:152:PRO:HB2	1:B:154:ILE:HG12	1.95	0.48
1:A:145:PRO:HD2	4:A:604:HOH:O	2.14	0.47
1:B:372:LYS:HD3	1:B:373:THR:O	2.14	0.47
1:A:38:ILE:HG21	1:A:112:VAL:HG23	1.96	0.47
1:A:439:ASN:CB	4:A:595:HOH:O	2.62	0.47
1:B:510:ASP:CG	1:B:511:GLY:H	2.18	0.47
1:B:24:GLN:NE2	1:B:434:LEU:HD11	2.26	0.46
3:A:552:NAP:H2N	4:A:570:HOH:O	2.14	0.46
1:B:417:PRO:HD3	1:B:518:LEU:HD22	1.96	0.46
1:A:410:ILE:HG13	4:A:550:HOH:O	2.15	0.46
1:B:94:ASN:ND2	1:B:103:ARG:HH21	2.08	0.45
1:A:37:GLY:O	1:A:106:TYR:HA	2.16	0.45
1:A:159:SER:O	1:A:160:PHE:C	2.55	0.45
1:B:175:GLU:CD	1:B:175:GLU:H	2.20	0.45
1:B:267:VAL:HG13	1:B:271:GLU:HB2	1.98	0.45
1:B:71:LYS:HA	1:B:71:LYS:HD2	1.78	0.44
1:A:222:THR:O	1:A:340:MET:HA	2.17	0.44
1:B:107:ARG:NH2	1:B:132:GLU:OE1	2.51	0.44
1:B:53:TYR:CZ	1:B:196:THR:HG23	2.53	0.44
1:B:98:ASP:OD1	1:B:103:ARG:NH1	2.42	0.44
1:A:282:GLN:HG3	4:A:619:HOH:O	2.18	0.43
1:A:119:GLU:HG3	4:A:549:HOH:O	2.18	0.43
1:A:62:SER:HB3	1:A:79:TRP:CD2	2.54	0.43
1:B:487:TYR:OH	1:B:515:ARG:HD3	2.19	0.43
1:A:220:TRP:O	1:A:338:VAL:HG13	2.19	0.43
1:B:83:PHE:CG	1:B:224:LEU:HD11	2.54	0.43
1:B:96:ALA:HB1	1:B:100:MET:HE3	2.01	0.43
1:A:187:ARG:NH1	1:A:379:ASP:O	2.44	0.43
1:A:152:PRO:HD3	1:A:387:THR:OG1	2.19	0.42
1:B:62:SER:HB3	1:B:79:TRP:CD2	2.55	0.42
1:B:51:ASN:O	1:B:86:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLU:OE1	1:A:312:LYS:NZ	2.37	0.42
1:A:96:ALA:O	1:A:100:MET:HG3	2.19	0.42
1:B:63:TYR:HA	4:B:566:HOH:O	2.18	0.42
1:A:363:ILE:HG23	1:A:371:ILE:HG23	2.02	0.42
1:B:15:ILE:HD11	1:B:139:LEU:HD11	2.01	0.42
1:A:358:ILE:O	1:A:362:PRO:HA	2.20	0.42
1:A:298:ASN:HB3	1:A:301:SER:HB3	2.02	0.41
1:B:36:LEU:HD11	1:B:107:ARG:HD3	2.02	0.41
1:A:255:PHE:CE1	1:A:285:TYR:HD2	2.39	0.41
1:A:301:SER:HA	1:A:304:PHE:CD2	2.56	0.41
1:A:42:GLU:HG2	1:A:109:ASN:HD21	1.86	0.41
1:B:341:GLU:HB2	1:B:344:TYR:HB2	2.01	0.41
1:B:152:PRO:HG3	1:B:387:THR:HG21	2.00	0.41
1:B:483:THR:CG2	1:B:516:ARG:HG2	2.51	0.41
1:A:369:GLU:HG3	4:A:558:HOH:O	2.20	0.41
1:A:437:PRO:C	1:A:439:ASN:N	2.75	0.41
1:A:424:GLN:NE2	1:A:474:PRO:HD3	2.30	0.41
1:A:437:PRO:O	1:A:438:HIS:C	2.59	0.40
1:A:177:ALA:HA	1:A:178:PRO:HD2	1.86	0.40
1:A:520:HIS:CE1	1:A:522:SER:OG	2.73	0.40
1:B:222:THR:O	1:B:340:MET:HA	2.22	0.40
1:A:222:THR:HB	1:A:223:PRO:HD2	2.02	0.40
1:B:438:HIS:NE2	1:B:517:THR:O	2.43	0.40
1:A:17:ALA:HB2	1:A:106:TYR:CE2	2.57	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	539/545 (99%)	513 (95%)	22 (4%)	4 (1%)	22 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	541/545 (99%)	503 (93%)	32 (6%)	6 (1%)	14	20
All	All	1080/1090 (99%)	1016 (94%)	54 (5%)	10 (1%)	17	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	HIS
1	B	497	GLU
1	B	498	ALA
1	A	392	VAL
1	A	508	LYS
1	B	496	ALA
1	B	148	ALA
1	B	104	LYS
1	A	148	ALA
1	B	510	ASP

### 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	450/454 (99%)	425 (94%)	25 (6%)	21	34
1	B	451/454 (99%)	432 (96%)	19 (4%)	30	47
All	All	901/908 (99%)	857 (95%)	44 (5%)	25	40

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	52	ARG
1	A	150	ARG
1	A	165	PHE
1	A	216	ARG
1	A	217	THR

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Mol	Chain	Res	Type
1	A	240	ARG
1	A	259	ARG
1	A	270	SER
1	A	273	ASP
1	A	285	TYR
1	A	299	LYS
1	A	318	LYS
1	A	341	GLU
1	A	359	ARG
1	A	363	ILE
1	A	364	GLN
1	A	367	THR
1	A	375	ASP
1	A	390	ASP
1	A	392	VAL
1	A	435	VAL
1	A	439	ASN
1	A	444	CYS
1	A	518	LEU
1	B	102	VAL
1	B	122	ARG
1	B	131	GLU
1	B	175	GLU
1	B	181	VAL
1	B	267	VAL
1	B	285	TYR
1	B	293	ARG
1	B	318	LYS
1	B	325	LYS
1	B	390	ASP
1	B	392	VAL
1	B	444	CYS
1	B	465	LYS
1	B	497	GLU
1	B	499	ASN
1	B	502	TRP
1	B	512	SER
1	B	518	LEU

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

Mol	Chain	Res	Type
1	A	24	GLN
1	A	82	ASN
1	A	94	ASN
1	A	109	ASN
1	A	166	HIS
1	A	215	GLN
1	A	315	GLN
1	A	406	ASN
1	A	424	GLN
1	A	438	HIS
1	A	499	ASN
1	B	24	GLN
1	B	51	ASN
1	B	82	ASN
1	B	94	ASN
1	B	109	ASN
1	B	166	HIS
1	B	215	GLN
1	B	315	GLN
1	B	406	ASN
1	B	424	GLN
1	B	467	ASN
1	B	499	ASN
1	B	520	HIS

### 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 ⓘ

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
3	NAP	A	552	-	45,52,52	1.73	4 (8%)	56,80,80	1.23	3 (5%)
3	NAP	B	552	-	45,52,52	1.84	5 (11%)	56,80,80	1.27	5 (8%)
2	FAD	B	551	-	51,58,58	1.52	6 (11%)	60,89,89	1.92	12 (20%)
2	FAD	A	551	-	51,58,58	1.43	5 (9%)	60,89,89	1.75	7 (11%)

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
3	NAP	A	552	-	-	10/31/67/67	0/5/5/5
3	NAP	B	552	-	-	7/31/67/67	0/5/5/5
2	FAD	B	551	-	-	5/30/50/50	0/6/6/6
2	FAD	A	551	-	-	3/30/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	552	NAP	O7N-C7N	9.36	1.42	1.24
3	A	552	NAP	O7N-C7N	8.86	1.41	1.24
3	A	552	NAP	C2A-N3A	4.64	1.39	1.32
2	A	551	FAD	C4X-N5	4.49	1.39	1.33
2	B	551	FAD	C4X-N5	4.30	1.39	1.33
2	B	551	FAD	C4-N3	4.08	1.40	1.33
2	A	551	FAD	C2A-N3A	3.95	1.38	1.32
2	B	551	FAD	C1'-N10	3.89	1.52	1.48
3	B	552	NAP	C2A-N3A	3.76	1.38	1.32
2	B	551	FAD	C2A-N3A	3.75	1.38	1.32
2	A	551	FAD	C4-N3	3.52	1.39	1.33
2	A	551	FAD	C10-N1	3.48	1.37	1.33
2	B	551	FAD	C10-N1	3.46	1.37	1.33
2	B	551	FAD	C2A-N1A	3.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	552	NAP	C2N-N1N	3.08	1.38	1.35
2	A	551	FAD	C2A-N1A	2.95	1.39	1.33
3	A	552	NAP	C2A-N1A	2.88	1.39	1.33
3	A	552	NAP	C2N-N1N	2.54	1.38	1.35
3	B	552	NAP	C2A-N1A	2.41	1.38	1.33
3	B	552	NAP	PA-O2A	-2.30	1.44	1.55

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	551	FAD	C4-N3-C2	6.23	120.40	115.14
2	A	551	FAD	C4-N3-C2	6.00	120.21	115.14
2	A	551	FAD	N3A-C2A-N1A	-5.74	119.70	128.68
3	A	552	NAP	N3A-C2A-N1A	-5.51	120.07	128.68
2	B	551	FAD	N3A-C2A-N1A	-5.49	120.09	128.68
3	B	552	NAP	N3A-C2A-N1A	-5.25	120.47	128.68
2	A	551	FAD	C5X-C9A-N10	4.46	120.94	117.72
2	B	551	FAD	C1'-N10-C9A	4.31	121.68	118.29
2	B	551	FAD	C4X-N5-C5X	4.14	120.91	116.77
2	B	551	FAD	C10-C4X-N5	-3.85	118.60	121.26
2	A	551	FAD	C4X-N5-C5X	3.80	120.57	116.77
3	B	552	NAP	C3D-C2D-C1D	3.51	106.26	100.98
2	B	551	FAD	C4-C4X-N5	3.43	122.52	118.60
2	A	551	FAD	O5'-C5'-C4'	-3.02	101.31	109.36
2	A	551	FAD	C4X-C4-N3	-2.99	119.34	123.43
2	B	551	FAD	C5X-C9A-N10	2.93	119.84	117.72
3	A	552	NAP	C3D-C2D-C1D	2.89	105.33	100.98
2	A	551	FAD	C1'-N10-C9A	2.82	120.51	118.29
3	A	552	NAP	C3N-C7N-N7N	2.78	121.09	117.75
2	B	551	FAD	C4X-C4-N3	-2.66	119.80	123.43
2	B	551	FAD	C4'-C3'-C2'	2.56	118.68	113.36
2	B	551	FAD	O3'-C3'-C4'	-2.56	102.64	108.81
2	B	551	FAD	O4B-C1B-C2B	-2.45	103.35	106.93
2	B	551	FAD	C1'-C2'-C3'	2.35	116.36	109.79
3	B	552	NAP	C6N-N1N-C2N	-2.24	119.93	121.97
3	B	552	NAP	C5N-C4N-C3N	-2.08	117.89	120.34
3	B	552	NAP	O4B-C4B-C3B	2.05	109.17	105.11

There are no chirality outliers.

All (25) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	A	552	NAP	O4D-C1D-N1N-C2N
3	B	552	NAP	O4D-C1D-N1N-C6N
2	B	551	FAD	N10-C1'-C2'-O2'
2	A	551	FAD	N10-C1'-C2'-O2'
3	B	552	NAP	C4N-C3N-C7N-O7N
3	B	552	NAP	C4N-C3N-C7N-N7N
3	A	552	NAP	C4N-C3N-C7N-N7N
3	A	552	NAP	C4N-C3N-C7N-O7N
3	A	552	NAP	PN-O3-PA-O1A
3	A	552	NAP	C2N-C3N-C7N-N7N
3	A	552	NAP	C2N-C3N-C7N-O7N
3	A	552	NAP	PA-O3-PN-O5D
2	B	551	FAD	PA-O3P-P-O5'
2	B	551	FAD	N10-C1'-C2'-C3'
2	A	551	FAD	N10-C1'-C2'-C3'
3	B	552	NAP	C2N-C3N-C7N-O7N
3	B	552	NAP	O4B-C4B-C5B-O5B
2	B	551	FAD	P-O3P-PA-O1A
2	B	551	FAD	O4B-C4B-C5B-O5B
3	B	552	NAP	C2N-C3N-C7N-N7N
3	A	552	NAP	C2B-O2B-P2B-O2X
3	B	552	NAP	C2B-O2B-P2B-O2X
3	A	552	NAP	C5B-O5B-PA-O1A
3	A	552	NAP	O4B-C4B-C5B-O5B
2	A	551	FAD	O4B-C4B-C5B-O5B

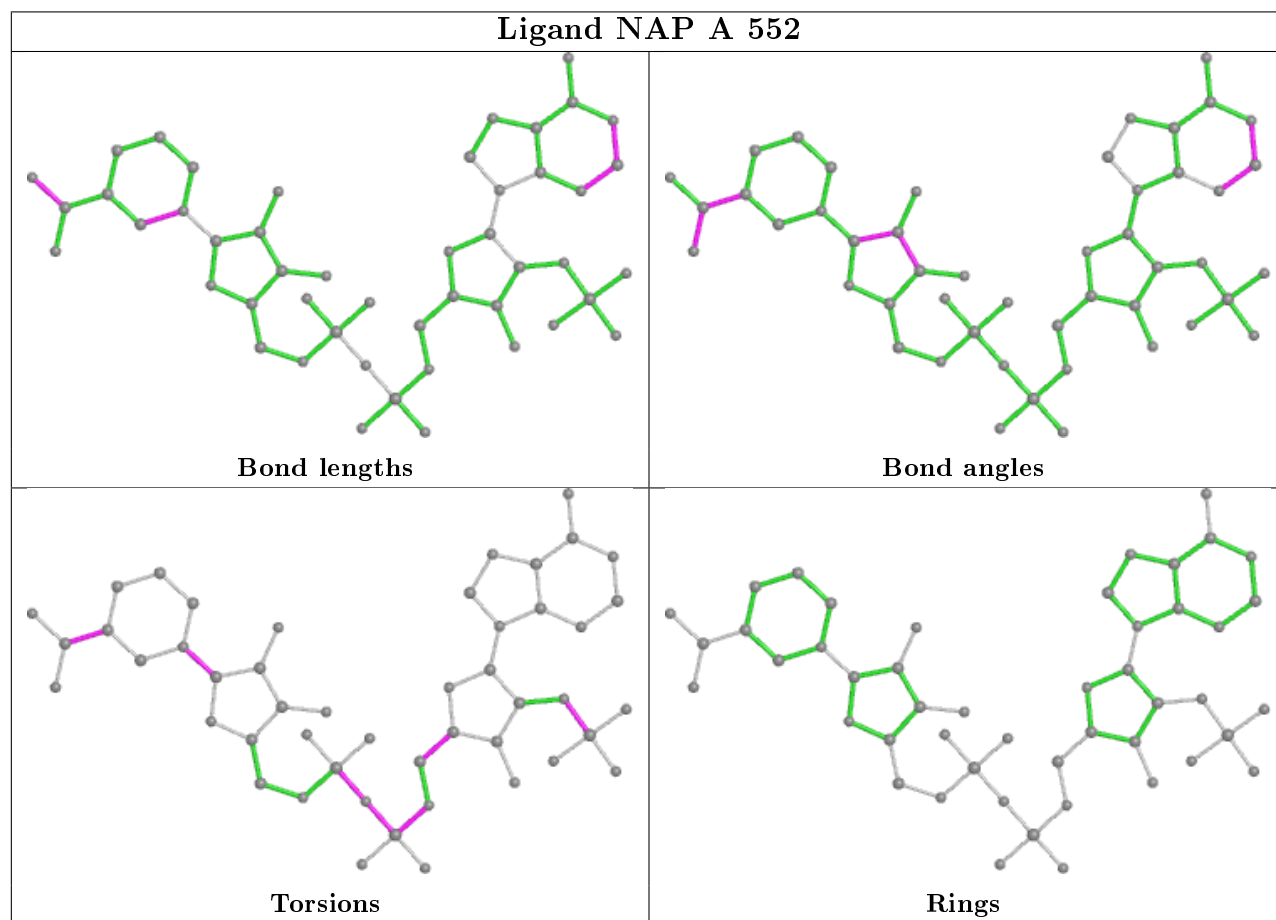
There are no ring outliers.

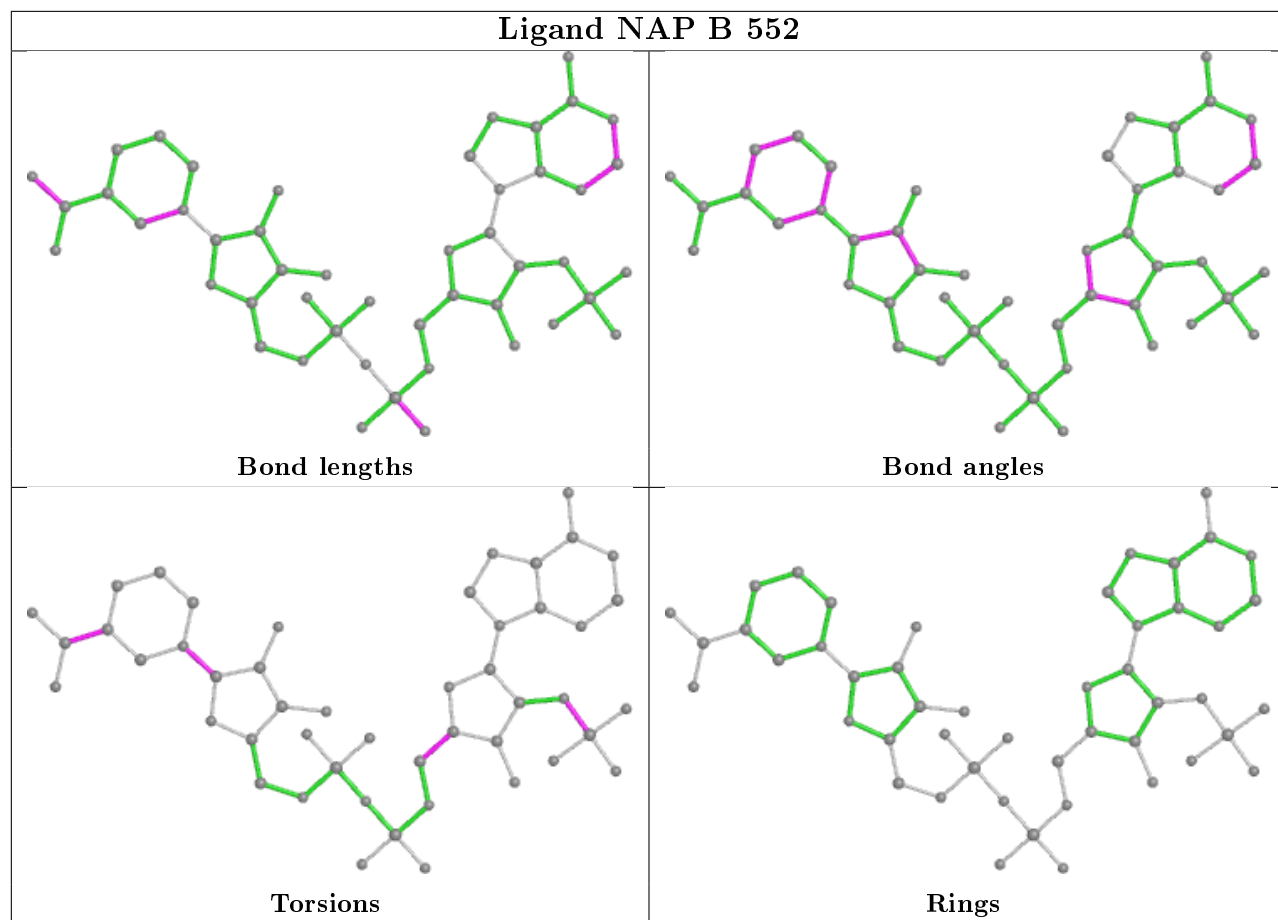
4 monomers are involved in 4 short contacts:

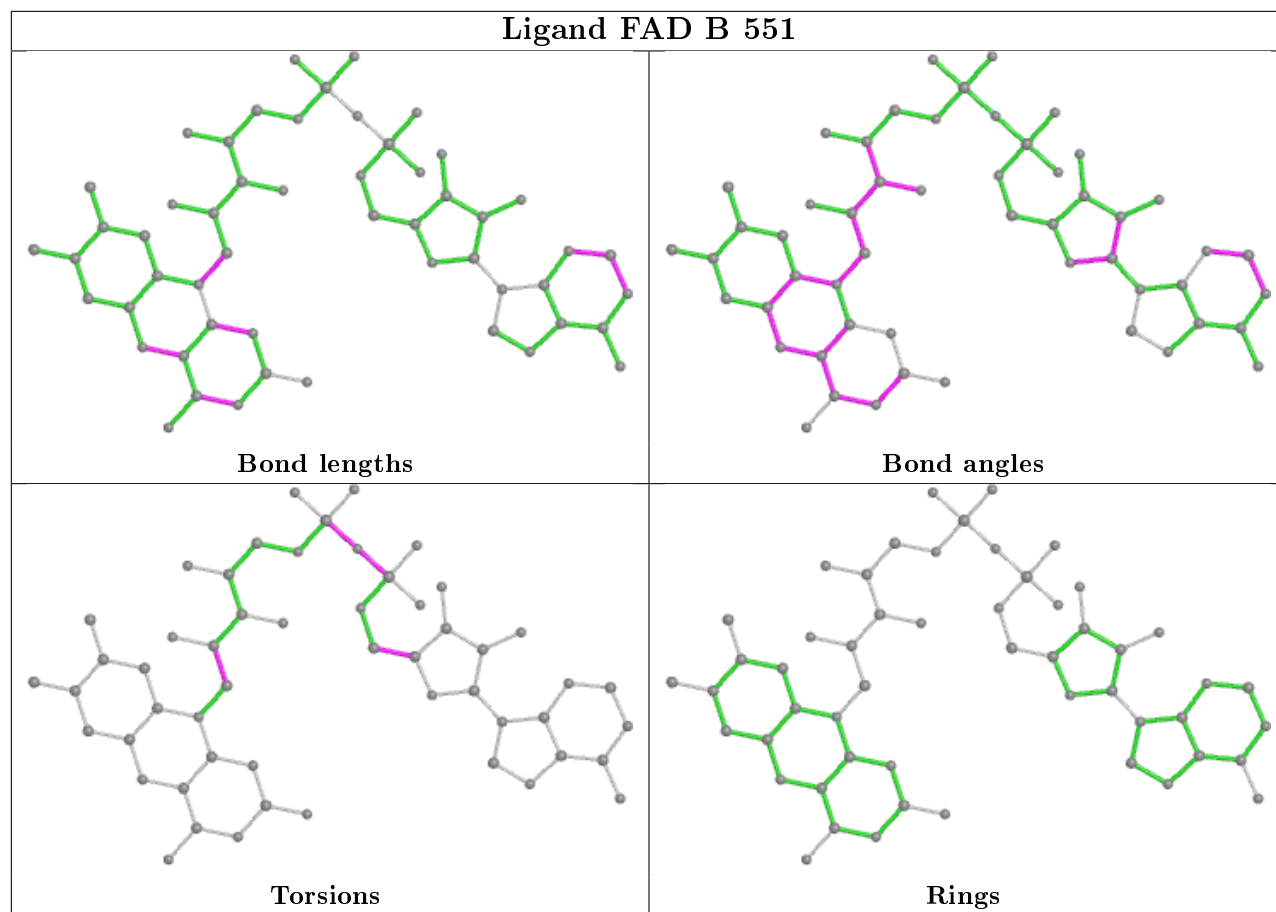
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	552	NAP	3	0
3	B	552	NAP	1	0
2	B	551	FAD	1	0
2	A	551	FAD	1	0

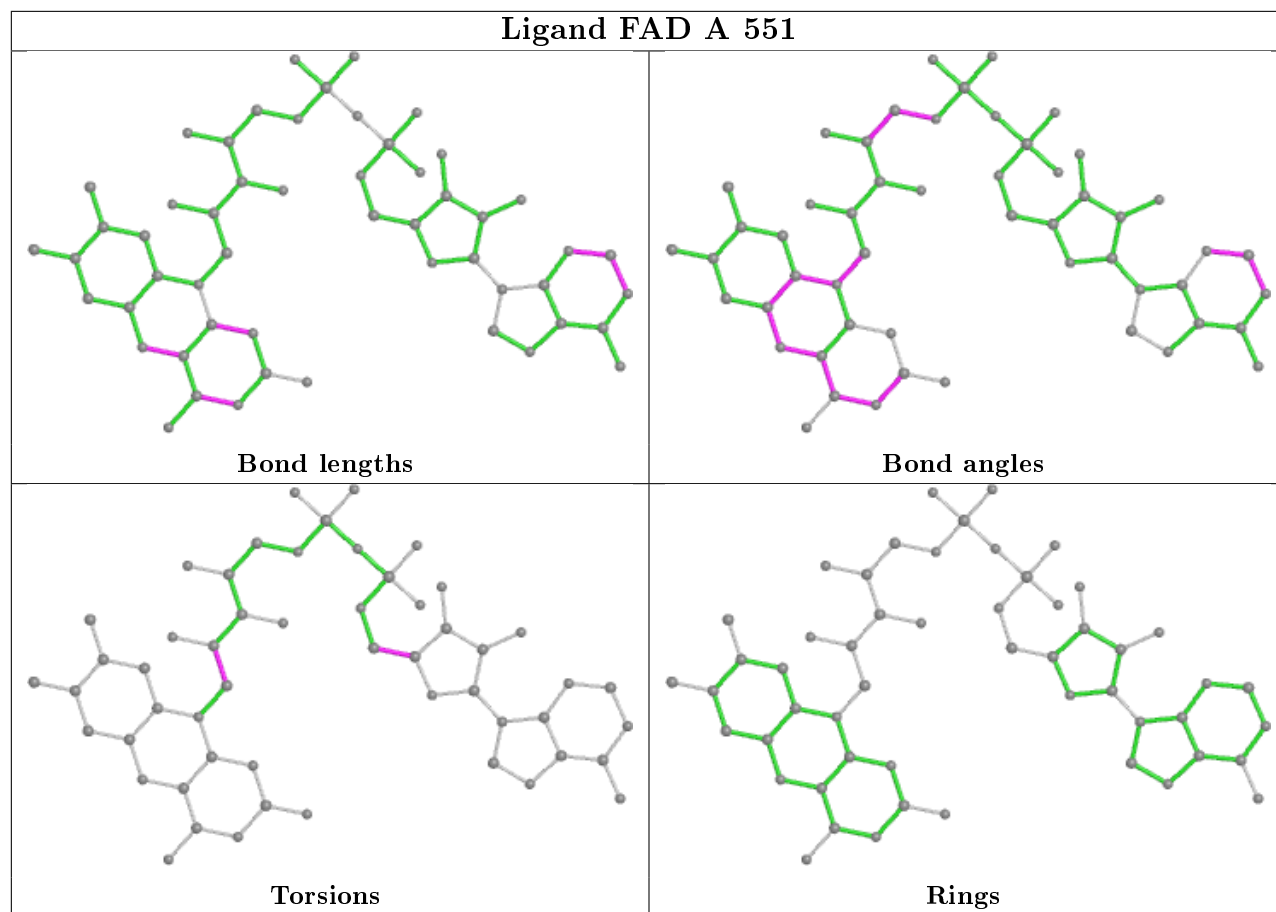
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	540/545 (99%)	-0.03	16 (2%)	50 49	14, 27, 53, 62	0
1	B	540/545 (99%)	-0.15	19 (3%)	44 43	11, 21, 42, 73	0
All	All	1080/1090 (99%)	-0.09	35 (3%)	47 46	11, 24, 50, 73	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	507	THR	5.3
1	B	509	PRO	4.6
1	B	513	VAL	4.6
1	B	176	GLY	3.6
1	B	505	THR	3.6
1	B	511	GLY	3.3
1	A	501	TRP	3.3
1	B	515	ARG	3.2
1	A	382	VAL	3.1
1	A	176	GLY	3.1
1	A	154	ILE	3.0
1	B	508	LYS	3.0
1	A	369	GLU	2.9
1	B	512	SER	2.8
1	B	174	ALA	2.8
1	B	180	GLY	2.8
1	B	175	GLU	2.7
1	B	506	THR	2.7
1	A	217	THR	2.6
1	A	165	PHE	2.6
1	B	501	TRP	2.5
1	B	179	LYS	2.4
1	B	514	VAL	2.4
1	A	152	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	162	GLY	2.4
1	A	161	LYS	2.3
1	A	363	ILE	2.3
1	A	391	ALA	2.2
1	A	436	GLY	2.2
1	B	497	GLU	2.1
1	B	502	TRP	2.1
1	A	518	LEU	2.1
1	A	509	PRO	2.0
1	A	164	SER	2.0
1	B	510	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

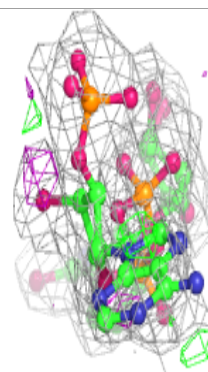
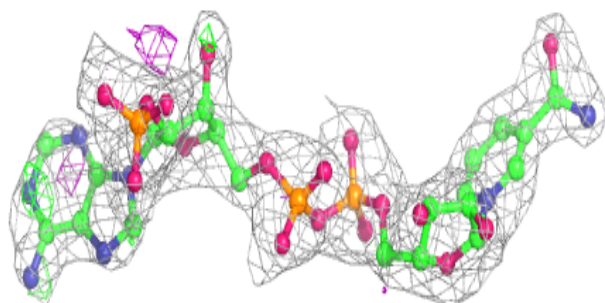
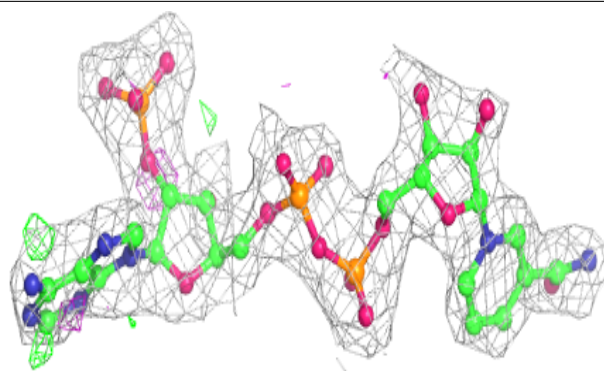
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAP	A	552	48/48	0.96	0.15	22,28,40,42	0
3	NAP	B	552	48/48	0.98	0.13	16,19,24,28	0
2	FAD	B	551	53/53	0.98	0.12	11,15,18,19	0
2	FAD	A	551	53/53	0.98	0.12	13,17,22,23	0

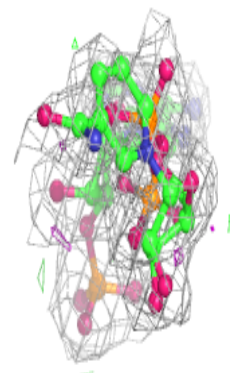
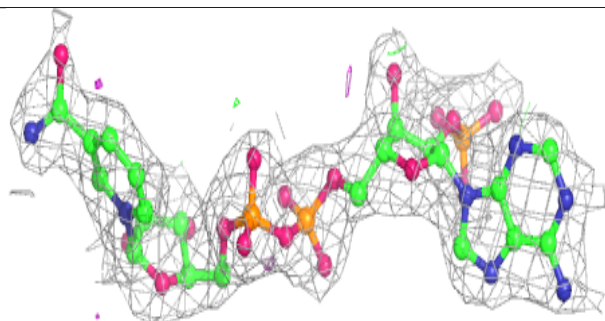
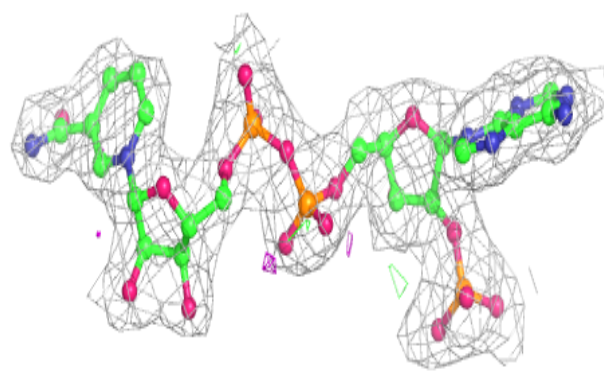
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NAP A 552:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAP B 552:**

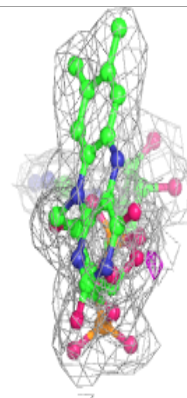
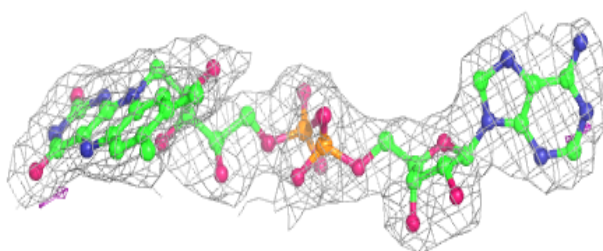
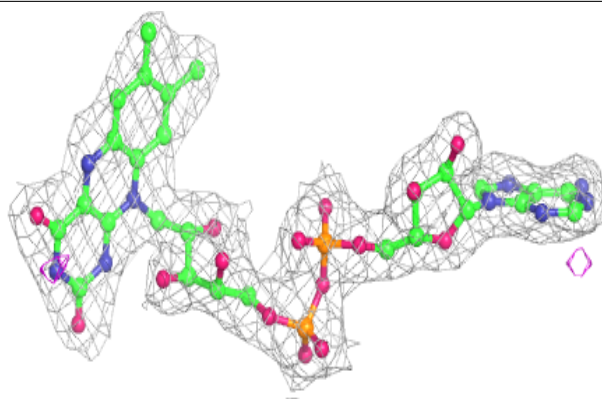
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



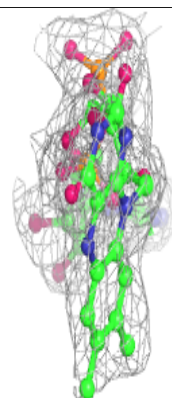
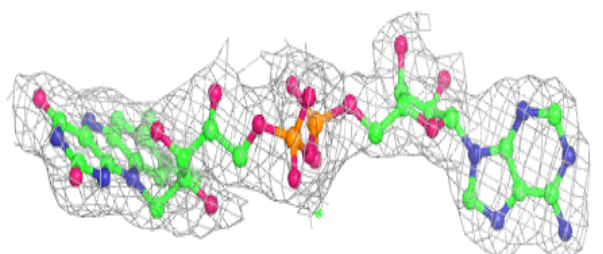
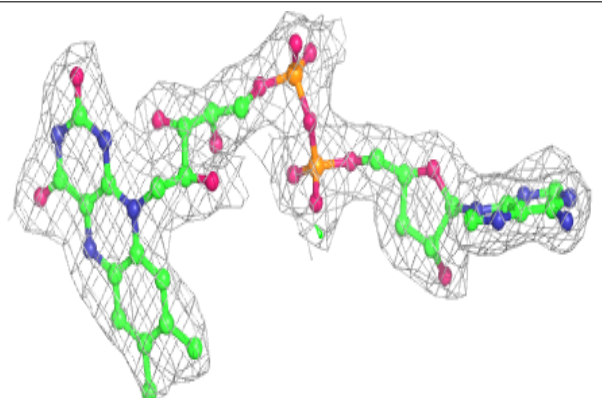


**Electron density around FAD B 551:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FAD A 551:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.