



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:10 AM UTC

PDB ID : 3UOY / pdb_00003uoy
Title : Crystal Structure of OTEMO complex with FAD and NADP (form 1)
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Deposited on : 2011-11-17
Resolution : 2.00 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

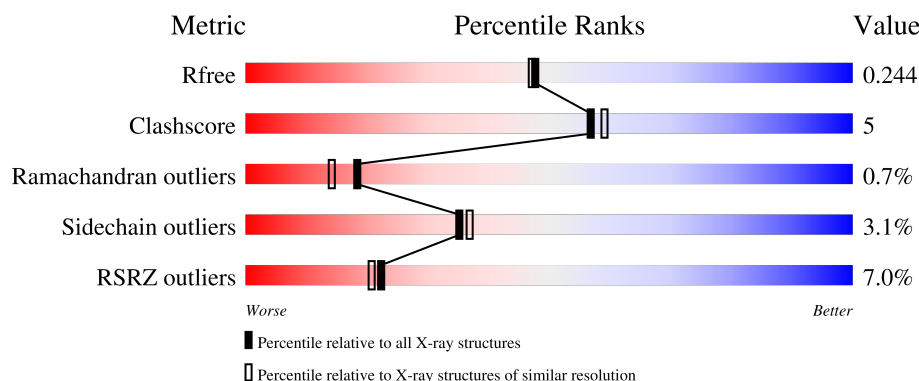
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	5% 87% 10% ..
1	B	545	9% 84% 13% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9485 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	537	Total	C	N	O	S	0	1	0
			4269	2712	736	807	14			
1	B	537	Total	C	N	O	S	0	2	0
			4264	2707	738	804	15			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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 (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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 SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0

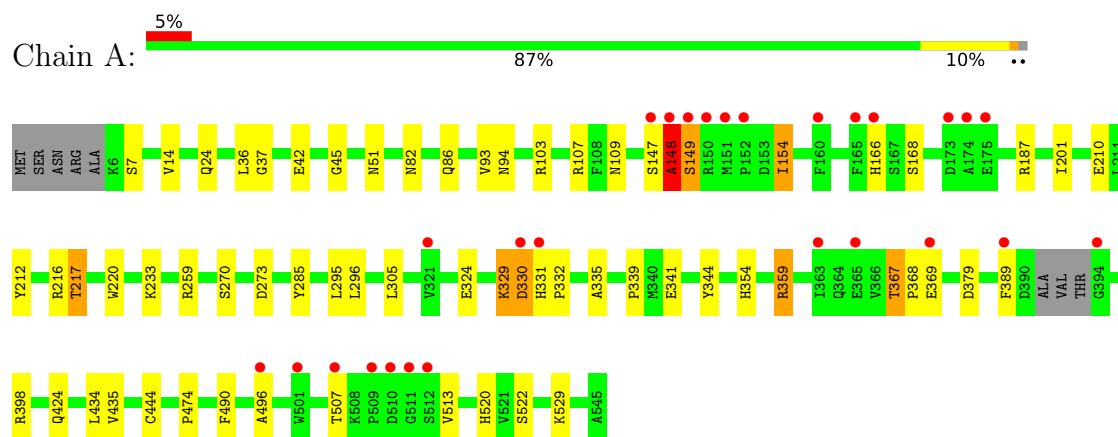
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	327	Total O 327 327	0	0
5	B	421	Total O 421 421	0	0

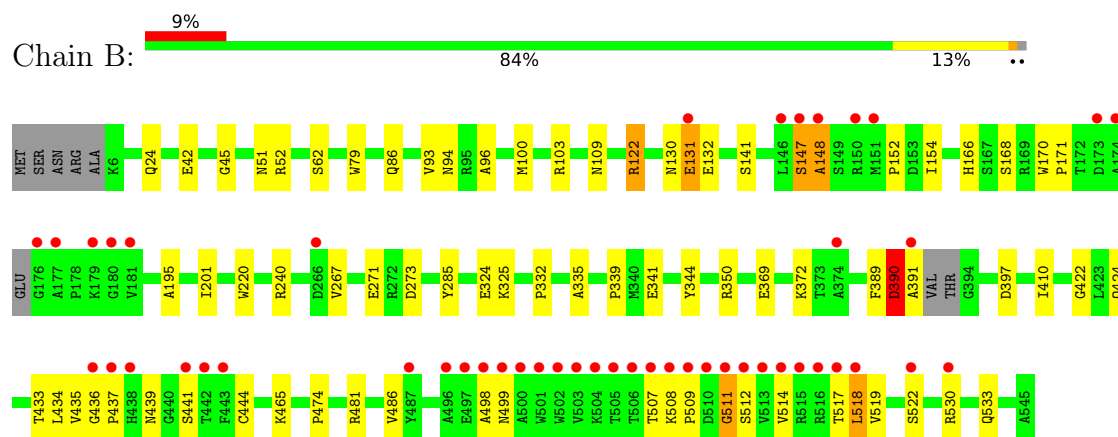
3 Residue-property plots

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 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, α , β , γ	66.75Å 94.99Å 93.09Å 90.00° 102.25° 90.00°	Depositor
Resolution (Å)	43.11 – 2.00 43.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.11-2.00) 99.6 (43.11-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.245 0.197 , 0.244	Depositor DCC
R_{free} test set	3840 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9485	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: FAD, NAP, NA

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	0.59	1/4382 (0.0%)	0.83	5/5953 (0.1%)
1	B	0.65	1/4377 (0.0%)	0.84	3/5942 (0.1%)
All	All	0.62	2/8759 (0.0%)	0.83	8/11895 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	ILE	CA-CB	5.61	1.57	1.54
1	A	201	ILE	CA-CB	5.09	1.56	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	SER	N-CA-C	-7.22	98.05	109.23
1	A	330	ASP	N-CA-C	6.11	118.73	111.33
1	A	331	HIS	N-CA-C	5.74	115.52	108.11
1	B	390	ASP	N-CA-C	5.61	122.75	110.80
1	B	441	SER	N-CA-C	5.48	117.68	111.11
1	A	329	LYS	CA-C-N	5.37	127.73	120.38
1	A	329	LYS	C-N-CA	5.37	127.73	120.38
1	A	149	SER	N-CA-C	-5.05	102.39	109.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ALA	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	4269	0	4113	33	0
1	B	4264	0	4122	44	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	48	0	25	1	0
3	B	48	0	25	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	327	0	0	5	0
5	B	421	0	0	10	0
All	All	9485	0	8347	78	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 5.

All (78) 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	1.37	0.87
1:B:389:PHE:O	1:B:390:ASP:HB2	1.83	0.78
1:B:131:GLU:HG2	1:B:132:GLU:N	2.02	0.75
1:B:166:HIS:HD2	1:B:168:SER:H	1.37	0.72
1:B:391:ALA:HB2	5:B:922:HOH:O	1.89	0.71
1:B:530:ARG:HH11	1:B:533:GLN:HE22	1.38	0.70
1:B:437:PRO:O	1:B:519:VAL:HG23	1.92	0.69
1:B:508:LYS:HE3	1:B:514:VAL:HG21	1.74	0.69
1:B:42:GLU:HG2	1:B:109:ASN:HD21	1.57	0.67
1:A:424:GLN:HE21	1:A:474:PRO:HD3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:THR:HG22	1:A:513:VAL:HG22	1.77	0.66
1:A:324:GLU:O	1:A:329:LYS:NZ	2.29	0.65
1:B:24:GLN:HE21	1:B:434:LEU:HD11	1.62	0.65
1:A:24:GLN:HE21	1:A:434:LEU:HD11	1.62	0.65
1:B:519:VAL:HG12	5:B:799:HOH:O	1.98	0.64
1:B:131:GLU:HG2	1:B:132:GLU:H	1.64	0.62
1:B:152:PRO:HB2	1:B:154:ILE:HG12	1.82	0.61
1:A:94:ASN:HD22	1:A:103:ARG:HH21	1.49	0.60
1:B:481:ARG:HG2	5:B:863:HOH:O	2.01	0.60
1:B:94:ASN:HD22	1:B:103:ARG:HH21	1.51	0.59
1:B:508:LYS:HB3	1:B:509:PRO:HD2	1.85	0.57
1:B:147:SER:O	1:B:148:ALA:HB3	2.05	0.57
1:A:166:HIS:CD2	1:A:168:SER:H	2.22	0.56
1:A:166:HIS:HD2	1:A:168:SER:H	1.51	0.56
1:B:45:GLY:HA2	1:B:93:VAL:HG11	1.89	0.54
1:B:512:SER:HB3	5:B:661:HOH:O	2.07	0.54
1:B:122:ARG:HD3	5:B:885:HOH:O	2.08	0.53
1:B:486:VAL:HG12	1:B:517:THR:CG2	2.38	0.53
1:B:51:ASN:O	1:B:86:GLN:HG3	2.11	0.51
1:A:217:THR:HG23	1:A:359:ARG:HH12	1.75	0.51
1:B:154:ILE:HD11	5:B:803:HOH:O	2.12	0.50
1:B:62:SER:HB3	1:B:79:TRP:CD2	2.47	0.50
1:B:350:ARG:NH1	5:B:783:HOH:O	2.44	0.50
1:A:187:ARG:NH1	1:A:379:ASP:O	2.44	0.50
1:B:166:HIS:CD2	1:B:168:SER:H	2.24	0.49
1:A:51:ASN:O	1:A:86:GLN:HG3	2.13	0.49
1:A:36:LEU:HD11	1:A:107:ARG:HG2	1.95	0.49
1:B:52:ARG:NH1	5:B:895:HOH:O	2.46	0.49
1:B:424:GLN:HE21	1:B:474:PRO:HD3	1.78	0.48
1:A:217:THR:HG22	1:A:359:ARG:HH22	1.78	0.48
1:A:529:LYS:HD3	5:B:666:HOH:O	2.14	0.48
1:A:187:ARG:NH2	1:A:212:TYR:OH	2.47	0.47
1:A:154:ILE:HD11	5:A:678:HOH:O	2.14	0.47
1:B:389:PHE:O	1:B:390:ASP:CB	2.57	0.47
1:B:220:TRP:O	1:B:339:PRO:HD2	2.15	0.47
1:B:518:LEU:HB3	5:B:706:HOH:O	2.14	0.47
1:B:422:GLY:HA3	1:B:439:ASN:HB3	1.96	0.47
1:B:332:PRO:HG2	1:B:335:ALA:HB2	1.98	0.46
1:A:210:GLU:OE2	1:A:354:HIS:HE1	1.97	0.46
1:B:436:GLY:O	1:B:437:PRO:C	2.58	0.46
1:A:367:THR:HG23	1:A:368:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PHE:CE2	1:A:496:ALA:HA	2.51	0.46
1:A:295:LEU:HD11	1:A:305:LEU:HD23	1.98	0.46
1:B:96:ALA:HB1	1:B:100:MET:HE3	1.99	0.45
1:A:522:SER:HB3	5:A:750:HOH:O	2.18	0.44
1:B:147:SER:O	1:B:148:ALA:CB	2.66	0.44
1:B:507:THR:HG22	1:B:511:GLY:HA2	2.00	0.44
1:A:367:THR:HG22	1:A:369:GLU:N	2.20	0.43
1:B:341:GLU:HB2	1:B:344:TYR:HB2	2.00	0.43
1:B:397:ASP:O	1:B:410:ILE:HD11	2.18	0.43
5:A:593:HOH:O	1:B:240:ARG:HD2	2.17	0.43
1:A:42:GLU:HG2	1:A:109:ASN:HD21	1.83	0.43
1:A:332:PRO:HG2	1:A:335:ALA:HB2	2.01	0.43
1:A:45:GLY:HA2	1:A:93:VAL:HG11	2.00	0.43
1:A:520:HIS:CD2	1:A:520:HIS:C	2.97	0.43
1:A:148:ALA:HB2	1:A:398:ARG:HE	1.84	0.42
1:A:82:ASN:HD21	1:A:233:LYS:NZ	2.18	0.42
1:A:341:GLU:HB2	1:A:344:TYR:HB2	2.02	0.42
1:A:367:THR:CG2	5:A:631:HOH:O	2.68	0.42
1:B:170:TRP:CD1	1:B:171:PRO:HD2	2.55	0.42
1:B:267:VAL:CG1	1:B:271:GLU:HB3	2.50	0.41
1:B:141[A]:SER:OG	1:B:433:THR:HA	2.21	0.41
1:A:220:TRP:O	1:A:339:PRO:HD2	2.21	0.41
1:B:195:ALA:HA	1:B:339:PRO:HB3	2.02	0.41
1:A:14:VAL:O	1:A:37:GLY:HA2	2.21	0.40
1:A:147:SER:O	1:A:389:PHE:HB3	2.21	0.40
3:A:552:NAP:H2N	5:A:716:HOH:O	2.19	0.40
1:B:437:PRO:O	1:B:519:VAL:HA	2.21	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	534/545 (98%)	521 (98%)	11 (2%)	2 (0%)	30	27
1	B	533/545 (98%)	514 (96%)	14 (3%)	5 (1%)	14	9
All	All	1067/1090 (98%)	1035 (97%)	25 (2%)	7 (1%)	18	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	390	ASP
1	B	498	ALA
1	B	148	ALA
1	A	148	ALA
1	A	435	VAL
1	B	511	GLY
1	B	435	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	446/454 (98%)	432 (97%)	14 (3%)	35	37
1	B	446/454 (98%)	431 (97%)	15 (3%)	32	33
All	All	892/908 (98%)	863 (97%)	29 (3%)	35	34

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	149	SER
1	A	154	ILE
1	A	216	ARG
1	A	217	THR
1	A	259	ARG
1	A	270	SER
1	A	273	ASP
1	A	285	TYR

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Mol	Chain	Res	Type
1	A	296	LEU
1	A	330	ASP
1	A	359	ARG
1	A	367	THR
1	A	444	CYS
1	B	122	ARG
1	B	130[A]	ASN
1	B	130[B]	ASN
1	B	131	GLU
1	B	273	ASP
1	B	285	TYR
1	B	324	GLU
1	B	325	LYS
1	B	369	GLU
1	B	372	LYS
1	B	444	CYS
1	B	465	LYS
1	B	499	ASN
1	B	518	LEU
1	B	522	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) 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	219	ASN
1	A	315	GLN
1	A	354	HIS
1	A	424	GLN
1	A	467	ASN
1	A	476	GLN
1	A	499	ASN
1	B	24	GLN
1	B	29	ASN
1	B	82	ASN
1	B	94	ASN
1	B	105	HIS

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Mol	Chain	Res	Type
1	B	109	ASN
1	B	166	HIS
1	B	215	GLN
1	B	282	GLN
1	B	406	ASN
1	B	424	GLN
1	B	499	ASN
1	B	520	HIS
1	B	538	ASN

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	B	552	-	50,52,52	1.64	6 (12%)	71,80,80	1.49	10 (14%)
2	FAD	A	551	-	58,58,58	1.20	6 (10%)	85,89,89	1.62	15 (17%)
3	NAP	A	552	-	50,52,52	1.76	5 (10%)	71,80,80	1.42	11 (15%)
2	FAD	B	551	-	58,58,58	1.17	7 (12%)	85,89,89	1.74	16 (18%)

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	B	552	-	-	2/35/67/67	0/5/5/5
2	FAD	A	551	-	-	3/34/50/50	0/6/6/6
3	NAP	A	552	-	-	4/35/67/67	0/5/5/5
2	FAD	B	551	-	-	4/34/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	552	NAP	O7N-C7N	9.58	1.42	1.24
3	B	552	NAP	O7N-C7N	8.88	1.40	1.24
2	A	551	FAD	C4X-N5	3.94	1.39	1.30
2	B	551	FAD	C4X-N5	3.76	1.38	1.30
2	A	551	FAD	C10-N1	3.17	1.39	1.33
3	A	552	NAP	C2A-N1A	3.14	1.39	1.33
2	A	551	FAD	C2A-N1A	3.11	1.39	1.33
3	A	552	NAP	C2A-N3A	3.02	1.39	1.33
2	B	551	FAD	C2A-N1A	2.95	1.39	1.33
2	A	551	FAD	PA-O3P	2.83	1.62	1.59
2	B	551	FAD	P-O3P	2.75	1.62	1.59
2	A	551	FAD	C2A-N3A	2.70	1.38	1.33
3	B	552	NAP	C2A-N1A	2.61	1.38	1.33
3	B	552	NAP	C2A-N3A	2.59	1.38	1.33
3	B	552	NAP	C2N-N1N	2.43	1.37	1.35
2	B	551	FAD	PA-O3P	2.42	1.62	1.59
3	A	552	NAP	C8A-N7A	2.36	1.36	1.31
2	B	551	FAD	C10-N1	2.32	1.37	1.33
2	A	551	FAD	C8A-N7A	2.29	1.36	1.31
2	B	551	FAD	C2A-N3A	2.24	1.37	1.33
2	B	551	FAD	C8A-N7A	2.22	1.36	1.31
3	B	552	NAP	C8A-N7A	2.21	1.35	1.31
3	A	552	NAP	PN-O3	2.09	1.61	1.59
3	B	552	NAP	P2B-O2B	2.04	1.63	1.59

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	551	FAD	N3A-C2A-N1A	-6.43	118.85	128.58
2	A	551	FAD	N3A-C2A-N1A	-6.23	119.16	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	552	NAP	N3A-C2A-N1A	-5.66	120.01	128.58
3	A	552	NAP	N3A-C2A-N1A	-5.09	120.87	128.58
2	B	551	FAD	N9A-C8A-N7A	-5.09	106.71	113.94
3	A	552	NAP	C5A-C4A-N3A	-4.65	120.31	126.72
2	A	551	FAD	N9A-C8A-N7A	-4.33	107.79	113.94
3	B	552	NAP	C5A-C4A-N3A	-4.26	120.85	126.72
2	A	551	FAD	C5A-C4A-N3A	-4.14	121.02	126.72
3	B	552	NAP	N9A-C8A-N7A	-3.82	108.52	113.94
2	B	551	FAD	C4-N3-C2	-3.78	118.92	125.64
2	B	551	FAD	C4A-N9A-C8A	3.75	109.67	105.74
2	B	551	FAD	C5A-N7A-C8A	3.65	109.19	103.45
2	B	551	FAD	C5A-C4A-N3A	-3.59	121.77	126.72
2	A	551	FAD	C2A-N3A-C4A	3.57	120.54	111.83
2	B	551	FAD	C4X-C10-N10	3.45	121.42	116.48
2	A	551	FAD	C5A-N7A-C8A	3.38	108.77	103.45
3	B	552	NAP	C2A-N3A-C4A	3.35	120.00	111.83
2	B	551	FAD	C2A-N3A-C4A	3.32	119.94	111.83
3	A	552	NAP	C2A-N3A-C4A	3.28	119.84	111.83
2	B	551	FAD	C10-C4X-N5	-3.22	118.23	124.81
3	A	552	NAP	C5A-N7A-C8A	3.20	108.47	103.45
3	B	552	NAP	C5A-N7A-C8A	3.15	108.41	103.45
3	A	552	NAP	N9A-C8A-N7A	-3.14	109.49	113.94
2	B	551	FAD	N3A-C4A-N9A	2.98	132.24	127.17
2	B	551	FAD	C4-C4X-N5	2.96	122.30	118.21
2	A	551	FAD	N3A-C4A-N9A	2.94	132.17	127.17
2	B	551	FAD	C4X-C4-N3	2.94	120.74	113.25
2	A	551	FAD	C4-N3-C2	-2.88	120.52	125.64
2	A	551	FAD	C4A-N9A-C8A	2.78	108.66	105.74
2	A	551	FAD	C9A-C5X-N5	-2.77	119.52	122.45
3	B	552	NAP	N3A-C4A-N9A	2.73	131.81	127.17
3	A	552	NAP	N3A-C4A-N9A	2.71	131.77	127.17
3	A	552	NAP	C4A-C5A-N7A	-2.66	107.55	110.58
2	A	551	FAD	C4X-C4-N3	2.55	119.74	113.25
2	A	551	FAD	C5X-C9A-N10	2.54	120.27	117.97
3	A	552	NAP	C4D-O4D-C1D	2.49	112.21	109.92
3	B	552	NAP	O2A-PA-O3	2.43	113.85	107.27
3	B	552	NAP	O4B-C1B-N9A	2.42	112.74	108.09
2	A	551	FAD	C10-C4X-N5	-2.39	119.93	124.81
2	A	551	FAD	C4X-C10-N10	2.39	119.90	116.48
3	B	552	NAP	C2B-C1B-N9A	-2.37	109.85	113.75
2	B	551	FAD	C10-N1-C2	2.35	121.93	116.85
2	A	551	FAD	O4-C4-C4X	-2.33	120.37	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	551	FAD	O2A-PA-O3P	2.31	113.52	107.27
2	B	551	FAD	C4X-C10-N1	-2.28	119.01	124.59
2	A	551	FAD	C4A-C5A-N7A	-2.27	107.98	110.58
2	B	551	FAD	O4-C4-C4X	-2.16	120.84	126.53
3	B	552	NAP	C4A-C5A-N7A	-2.14	108.13	110.58
3	A	552	NAP	C6A-C5A-C4A	2.12	120.07	117.18
3	A	552	NAP	C2B-C1B-N9A	2.02	117.07	113.75
3	A	552	NAP	O2A-PA-O3	2.01	112.71	107.27

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	551	FAD	N10-C1'-C2'-O2'
2	A	551	FAD	N10-C1'-C2'-C3'
2	B	551	FAD	N10-C1'-C2'-O2'
2	B	551	FAD	N10-C1'-C2'-C3'
2	B	551	FAD	PA-O3P-P-O5'
3	A	552	NAP	C2N-C3N-C7N-O7N
3	A	552	NAP	C2N-C3N-C7N-N7N
3	A	552	NAP	C4N-C3N-C7N-O7N
3	A	552	NAP	C4N-C3N-C7N-N7N
3	B	552	NAP	C4N-C3N-C7N-O7N
3	B	552	NAP	C4N-C3N-C7N-N7N
2	A	551	FAD	PA-O3P-P-O5'
2	B	551	FAD	P-O3P-PA-O1A

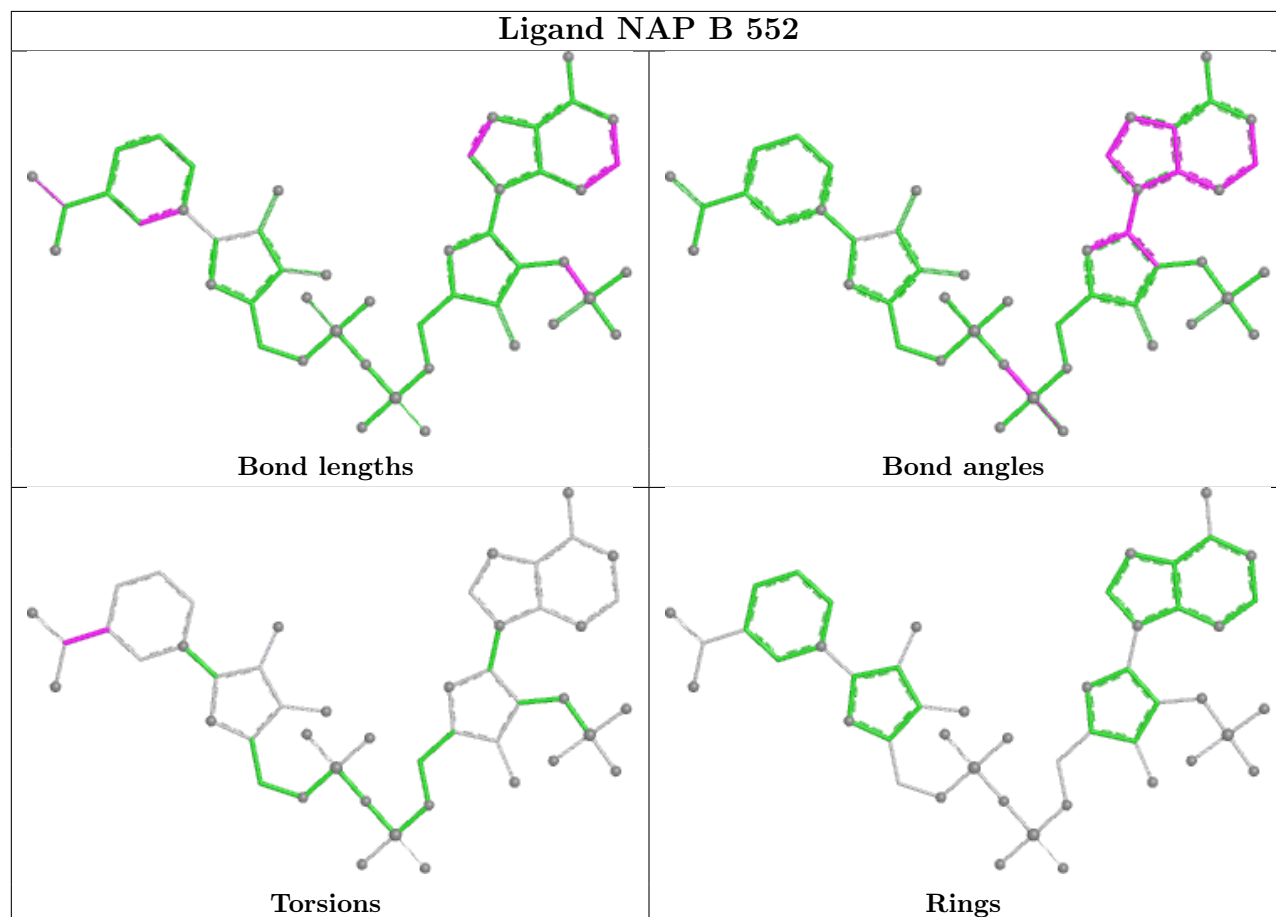
There are no ring outliers.

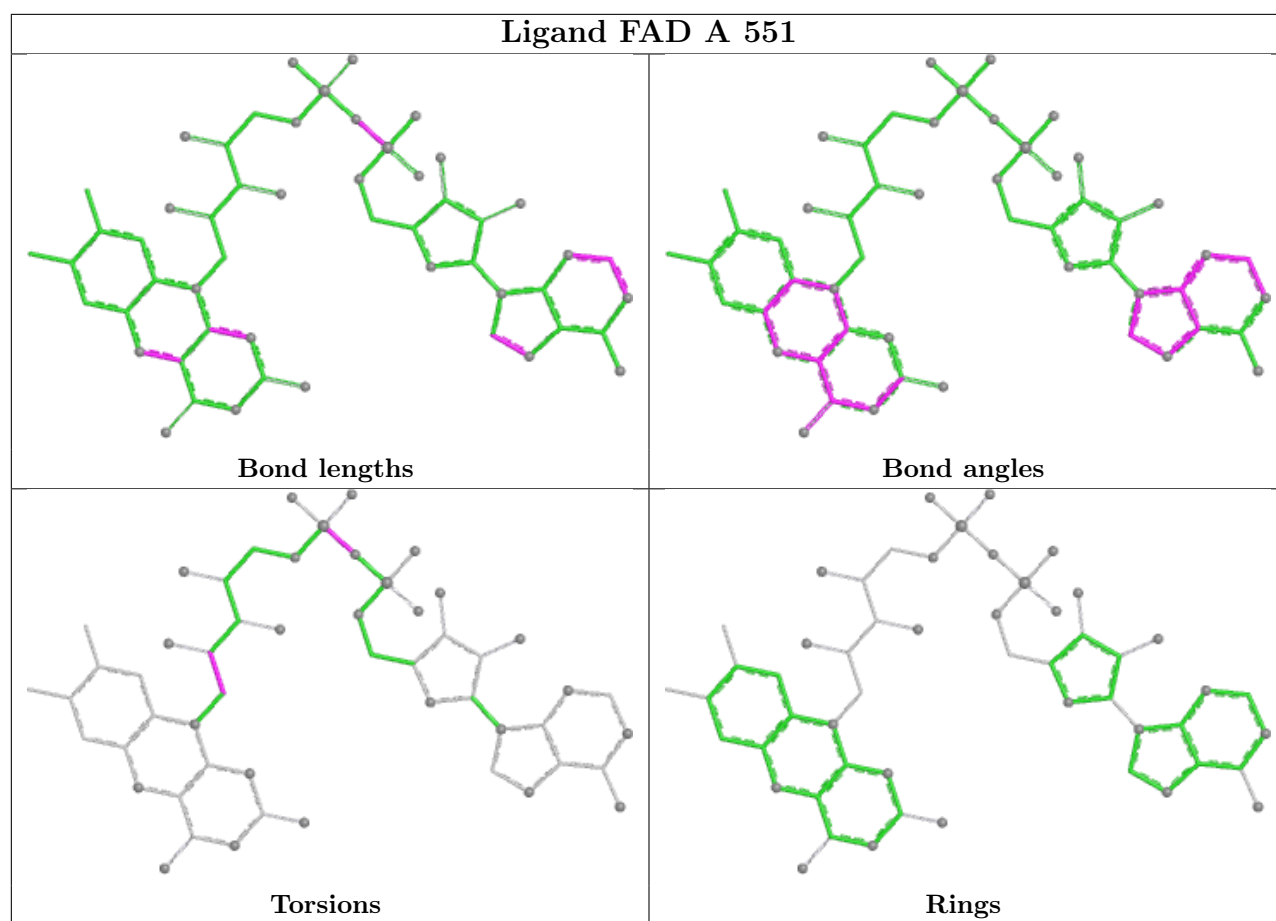
1 monomer is involved in 1 short contact:

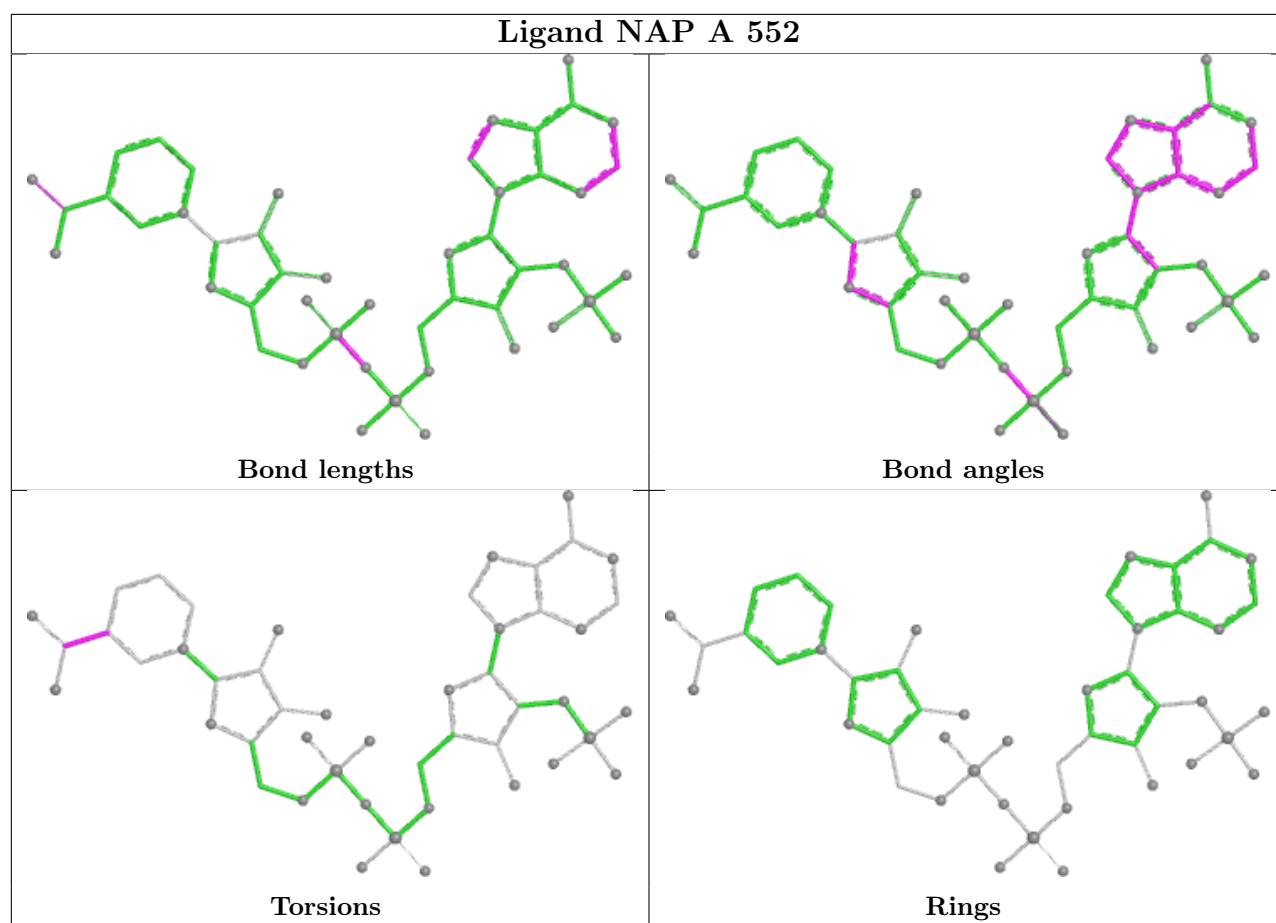
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	552	NAP	1	0

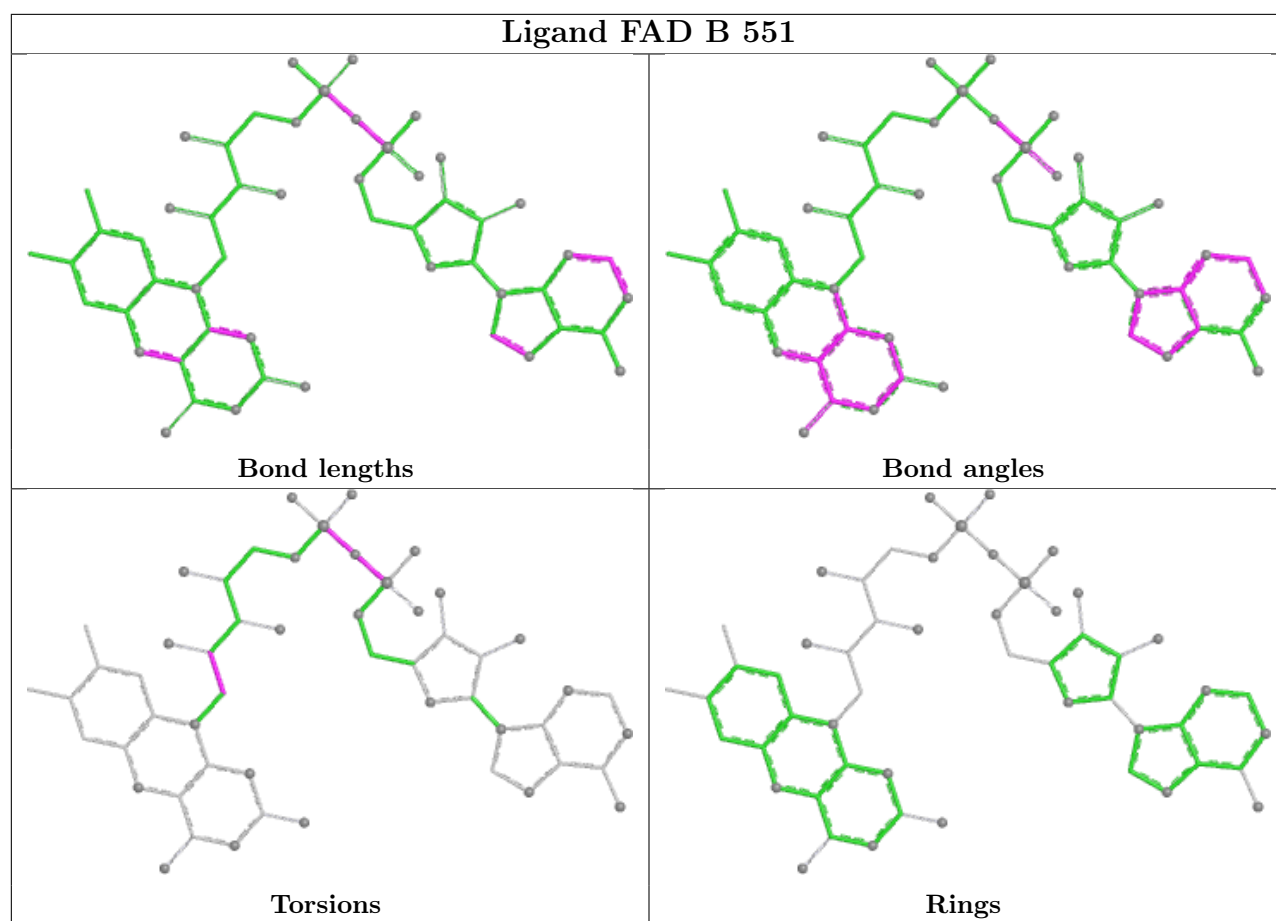
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95th 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 ²)	Q<0.9
1	A	537/545 (98%)	0.24	27 (5%) 34 33	12, 25, 43, 50	1 (0%)
1	B	537/545 (98%)	0.12	48 (8%) 15 14	10, 20, 44, 71	2 (0%)
All	All	1074/1090 (98%)	0.18	75 (6%) 22 21	10, 23, 43, 71	3 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	TRP	7.3
1	B	502	TRP	5.9
1	B	437	PRO	5.4
1	B	511	GLY	5.2
1	B	436	GLY	4.7
1	B	503	VAL	4.2
1	B	507	THR	4.1
1	B	177	ALA	4.1
1	A	330	ASP	4.1
1	A	165	PHE	3.9
1	B	513	VAL	3.9
1	B	500	ALA	3.9
1	B	516	ARG	3.9
1	B	515	ARG	3.8
1	B	442	THR	3.7
1	B	497	GLU	3.7
1	B	517	THR	3.7
1	B	512	SER	3.7
1	A	148	ALA	3.6
1	B	176	GLY	3.6
1	B	443	PHE	3.4
1	B	518	LEU	3.4
1	A	175	GLU	3.4
1	B	506	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	180	GLY	3.4
1	B	505	THR	3.2
1	A	149	SER	3.2
1	A	501	TRP	3.2
1	A	512	SER	3.2
1	B	179	LYS	3.1
1	A	173	ASP	3.1
1	B	522	SER	3.1
1	B	514	VAL	3.0
1	B	148	ALA	3.0
1	B	150	ARG	2.9
1	B	147	SER	2.9
1	B	151	MET	2.9
1	A	150	ARG	2.8
1	B	508	LYS	2.8
1	A	511	GLY	2.7
1	B	391	ALA	2.7
1	A	174	ALA	2.7
1	B	509	PRO	2.7
1	A	510	ASP	2.7
1	B	487	TYR	2.6
1	B	174	ALA	2.5
1	B	498	ALA	2.5
1	B	530	ARG	2.5
1	A	389	PHE	2.5
1	A	363	ILE	2.5
1	B	173	ASP	2.4
1	A	507	THR	2.4
1	B	496	ALA	2.4
1	A	152	PRO	2.4
1	B	438	HIS	2.3
1	B	499	ASN	2.3
1	B	266	ASP	2.3
1	A	166	HIS	2.3
1	A	160	PHE	2.3
1	A	394	GLY	2.3
1	B	131	GLU	2.2
1	B	510	ASP	2.2
1	B	374	ALA	2.2
1	B	146	LEU	2.2
1	A	147	SER	2.2
1	A	509	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	321	VAL	2.1
1	B	441	SER	2.1
1	A	151	MET	2.1
1	A	365	GLU	2.1
1	A	331	HIS	2.1
1	A	369	GLU	2.1
1	B	181	VAL	2.0
1	A	496	ALA	2.0
1	B	504	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

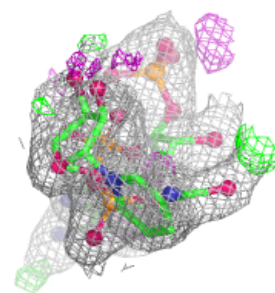
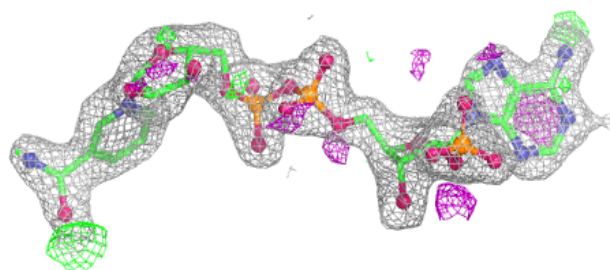
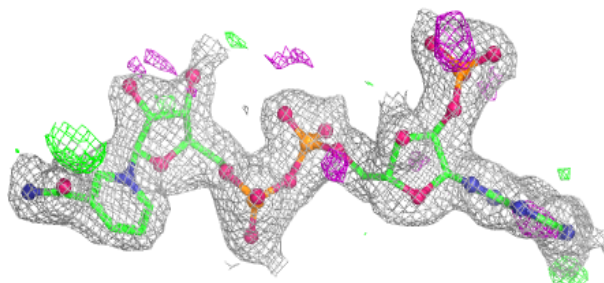
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	A	546	1/1	0.91	0.08	23,23,23,23	0
3	NAP	A	552	48/48	0.94	0.09	23,29,32,35	0
3	NAP	B	552	48/48	0.96	0.07	13,17,27,30	0
2	FAD	A	551	53/53	0.97	0.05	13,17,19,20	0
2	FAD	B	551	53/53	0.98	0.05	11,14,16,18	0
4	NA	B	546	1/1	0.99	0.07	12,12,12,12	0

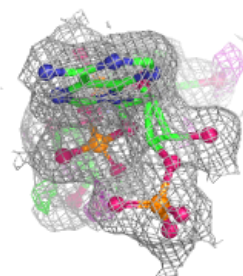
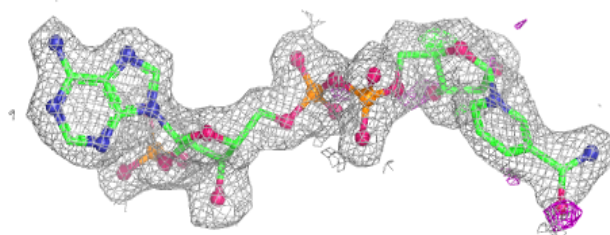
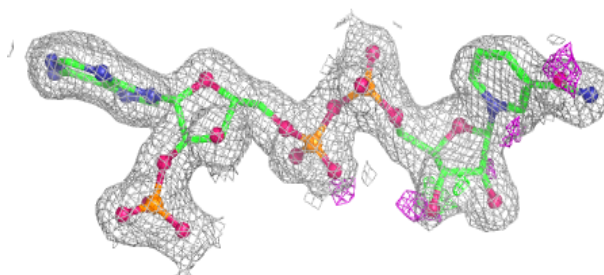
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

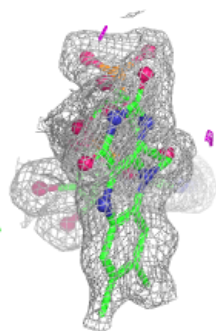
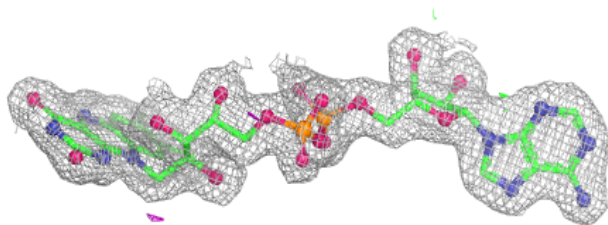
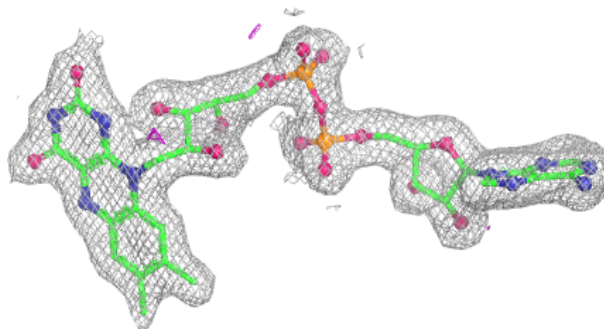
**Electron density around NAP B 552:**

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

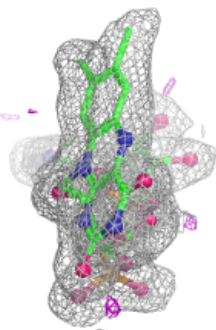
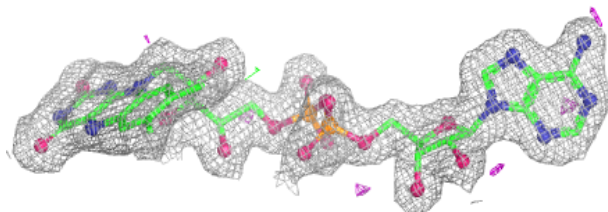
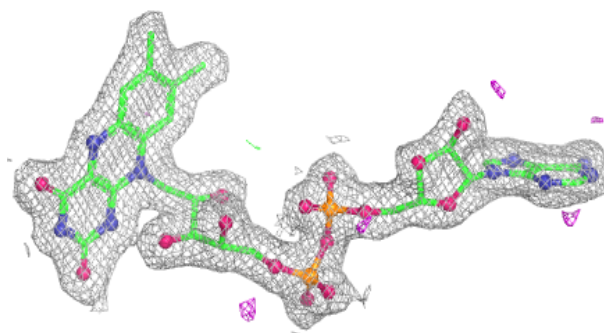


Electron density around FAD A 551:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.