Full wwPDB X-ray Structure Validation Report (i)

Sep 4, 2023 – 07:07 PM EDT

PDB ID	:	3UOY
Title	:	Crystal Structure of OTEMO complex with FAD and NADP (form 1)
Authors	:	Shi, R.; Matte, A.; Cygler, M.; Lau, P.
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 (i) 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 (i)) were used in the production of this report:

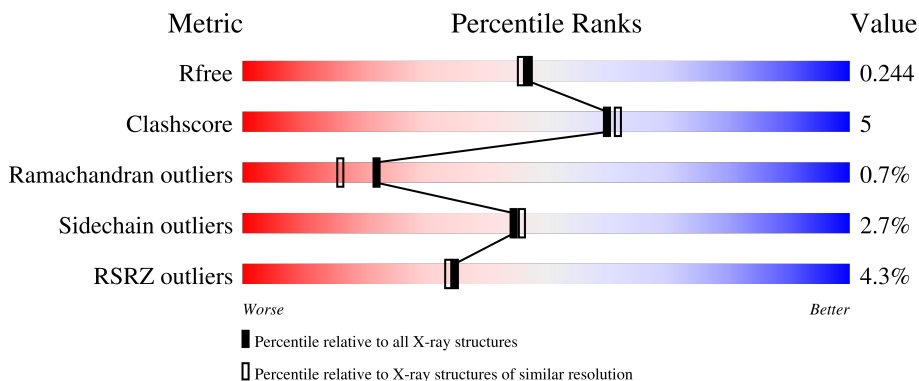|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1　Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
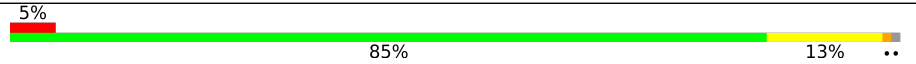*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Rfree		0.244
Clashscore		5
Ramachandran outliers		0.7%
Sidechain outliers		2.7%
RSRZ outliers		4.3%

Worse　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	3%　　87%　　11%　・
1	B	545	5%　　85%　　13%　‥

2 Entry composition ⓘ

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 4269	C 2712	N 736	O 807	S 14	0	1	0
1	B	537	Total 4264	C 2707	N 738	O 804	S 15	0	2	0

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

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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

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

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

Chain A:

• Molecule 1: OTEMO

Chain B:
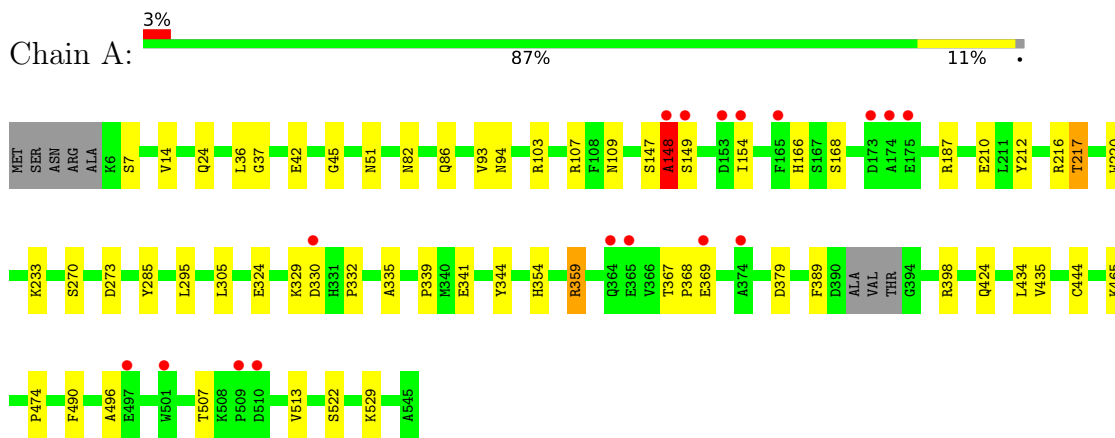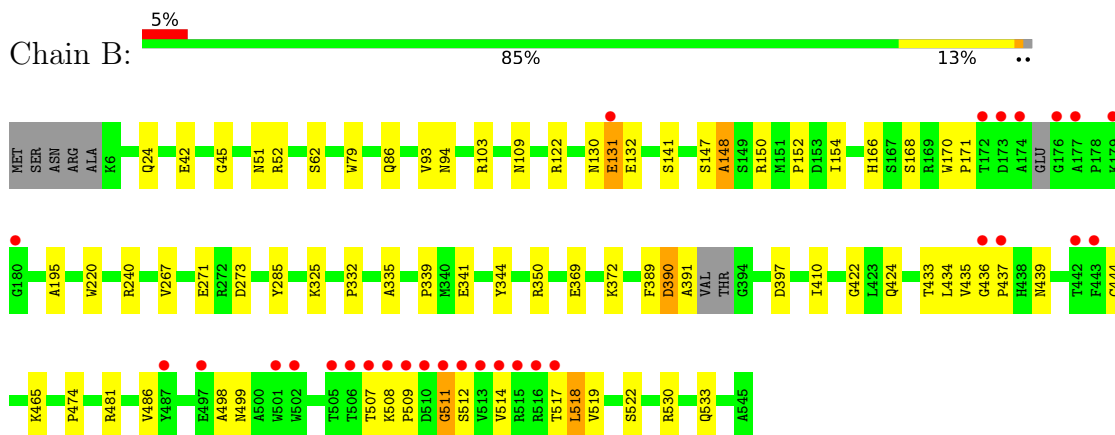
4 Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [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 , 44.0	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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	0.49	0/4382	0.59	0/5953
1	B	0.53	0/4377	0.61	0/5942
All	All	0.51	0/8759	0.60	0/11895

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

There are no bond length outliers.

There are no bond angle outliers.

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4269	0	4113	32	0
1	B	4264	0	4122	43	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	48	0	25	2	0
3	B	48	0	25	1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:367:THR:HG23	1:A:368:PRO:HD2	1.97	0.46
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
2:A:551:FAD:HM73	3:A:552:NAP:C5N	2.47	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
2:B:551:FAD:HM73	3:B:552:NAP:C5N	2.48	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:148:ALA:HB2	1:A:398:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:436:GLY:O	1:B:437:PRO:C	2.58	0.41
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%)	34	30
1	B	533/545 (98%)	514 (96%)	14 (3%)	5 (1%)	17	11
All	All	1067/1090 (98%)	1035 (97%)	25 (2%)	7 (1%)	22	16

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

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Mol	Chain	Res	Type
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%)	435 (98%)	11 (2%)	47	49
1	B	446/454 (98%)	432 (97%)	14 (3%)	40	40
All	All	892/908 (98%)	867 (97%)	25 (3%)	44	44

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	149	SER
1	A	216	ARG
1	A	217	THR
1	A	270	SER
1	A	273	ASP
1	A	285	TYR
1	A	330	ASP
1	A	359	ARG
1	A	444	CYS
1	A	465	LYS
1	B	130[A]	ASN
1	B	130[B]	ASN
1	B	131	GLU
1	B	150	ARG
1	B	273	ASP
1	B	285	TYR
1	B	325	LYS
1	B	369	GLU
1	B	372	LYS
1	B	444	CYS

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Mol	Chain	Res	Type
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 (23) 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	B	24	GLN
1	B	82	ASN
1	B	94	ASN
1	B	105	HIS
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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
2	FAD	B	551	-	53,58,58	1.17	4 (7%)	68,89,89	1.54	10 (14%)
3	NAP	B	552	-	45,52,52	1.69	5 (11%)	56,80,80	1.04	1 (1%)
2	FAD	A	551	-	53,58,58	1.24	4 (7%)	68,89,89	1.39	9 (13%)
3	NAP	A	552	-	45,52,52	1.78	3 (6%)	56,80,80	1.04	2 (3%)

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	FAD	B	551	-	-	5/30/50/50	0/6/6/6
3	NAP	B	552	-	-	3/31/67/67	0/5/5/5
2	FAD	A	551	-	-	4/30/50/50	0/6/6/6
3	NAP	A	552	-	-	6/31/67/67	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	552	NAP	O7N-C7N	9.30	1.42	1.24
3	B	552	NAP	O7N-C7N	8.63	1.40	1.24
3	A	552	NAP	C2A-N3A	4.46	1.39	1.32
2	A	551	FAD	C4X-N5	4.38	1.39	1.30
2	B	551	FAD	C4X-N5	4.18	1.38	1.30
2	A	551	FAD	C2A-N3A	4.11	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	552	NAP	C2A-N3A	3.99	1.38	1.32
2	B	551	FAD	C2A-N3A	3.60	1.37	1.32
2	A	551	FAD	C10-N1	3.13	1.39	1.33
3	A	552	NAP	C2A-N1A	3.01	1.39	1.33
2	A	551	FAD	C2A-N1A	2.98	1.39	1.33
2	B	551	FAD	C2A-N1A	2.83	1.39	1.33
3	B	552	NAP	C2A-N1A	2.51	1.38	1.33
2	B	551	FAD	C10-N1	2.30	1.37	1.33
3	B	552	NAP	C2N-N1N	2.22	1.37	1.35
3	B	552	NAP	P2B-O2B	2.01	1.63	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	551	FAD	N3A-C2A-N1A	-6.29	118.85	128.68
2	A	551	FAD	N3A-C2A-N1A	-6.09	119.16	128.68
3	B	552	NAP	N3A-C2A-N1A	-5.55	120.01	128.68
3	A	552	NAP	N3A-C2A-N1A	-4.99	120.87	128.68
2	B	551	FAD	C4-N3-C2	-3.64	118.92	125.64
2	B	551	FAD	C4X-C10-N10	3.37	121.42	116.48
2	B	551	FAD	C10-C4X-N5	-3.12	118.23	124.86
3	A	552	NAP	C3D-C2D-C1D	3.11	105.66	100.98
2	B	551	FAD	C4X-C4-N3	2.97	120.74	113.19
2	B	551	FAD	C4-C4X-N5	2.86	122.30	118.23
2	A	551	FAD	C4-N3-C2	-2.77	120.52	125.64
2	A	551	FAD	C9A-C5X-N5	-2.68	119.52	122.43
2	B	551	FAD	P-O3P-PA	-2.61	123.87	132.83
2	A	551	FAD	C4X-C4-N3	2.58	119.74	113.19
2	B	551	FAD	C10-N1-C2	2.52	121.93	116.90
2	B	551	FAD	C4X-C10-N1	-2.47	119.01	124.73
2	A	551	FAD	O4-C4-C4X	-2.35	120.37	126.60
2	A	551	FAD	C4X-C10-N10	2.34	119.90	116.48
2	A	551	FAD	C10-C4X-N5	-2.32	119.93	124.86
2	A	551	FAD	C5X-C9A-N10	2.24	120.27	117.95
2	B	551	FAD	O4-C4-C4X	-2.17	120.84	126.60
2	A	551	FAD	C4X-C10-N1	-2.06	119.94	124.73

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	551	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
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'
3	A	552	NAP	O4B-C4B-C5B-O5B
3	A	552	NAP	C2B-O2B-P2B-O2X
2	B	551	FAD	P-O3P-PA-O1A
2	A	551	FAD	O4B-C4B-C5B-O5B
2	B	551	FAD	O4B-C4B-C5B-O5B
3	B	552	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.
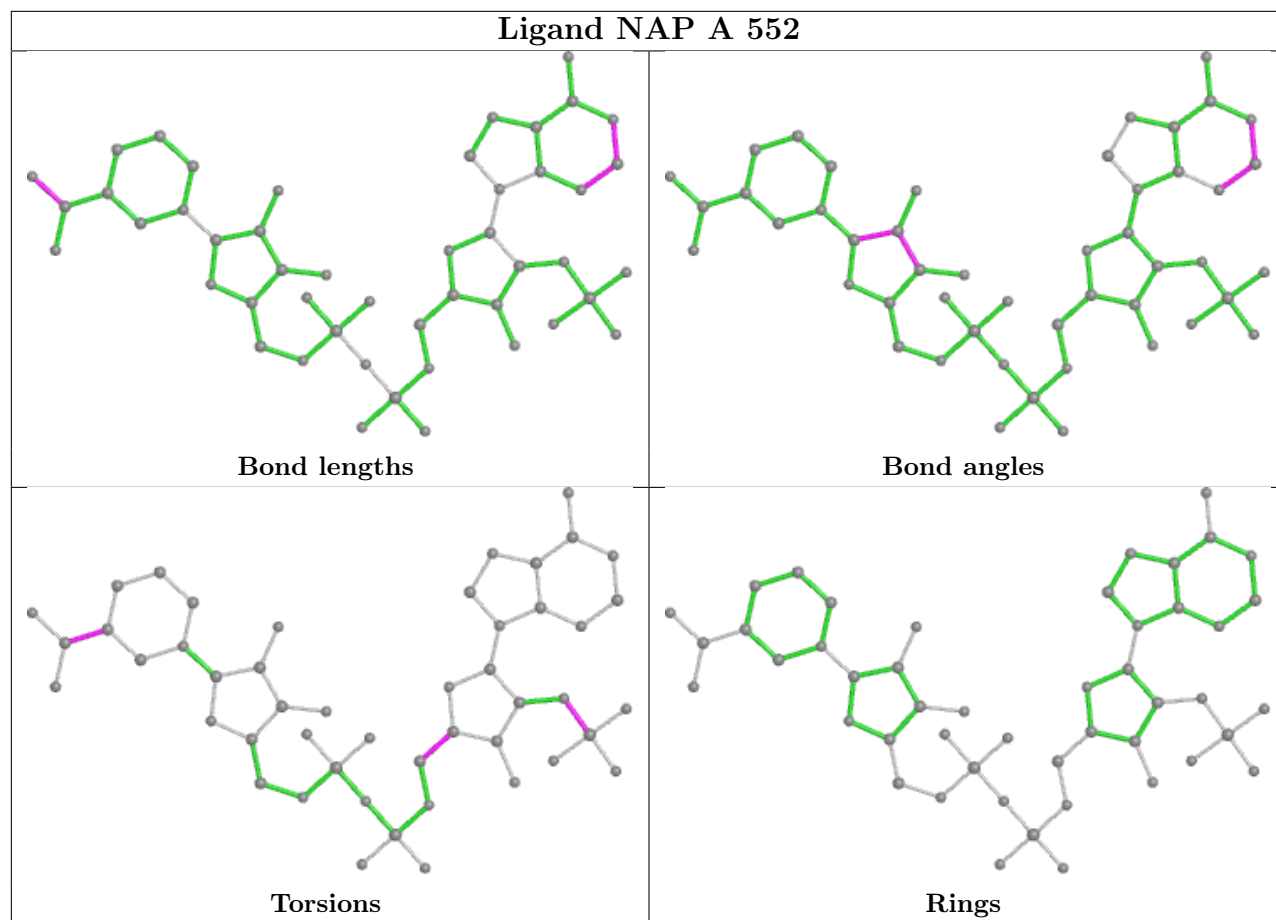
4 monomers are involved in 3 short contacts:

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

Ligand FAD B 551

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 552

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 551

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 552

Bond lengths

Bond angles

Torsions

Rings
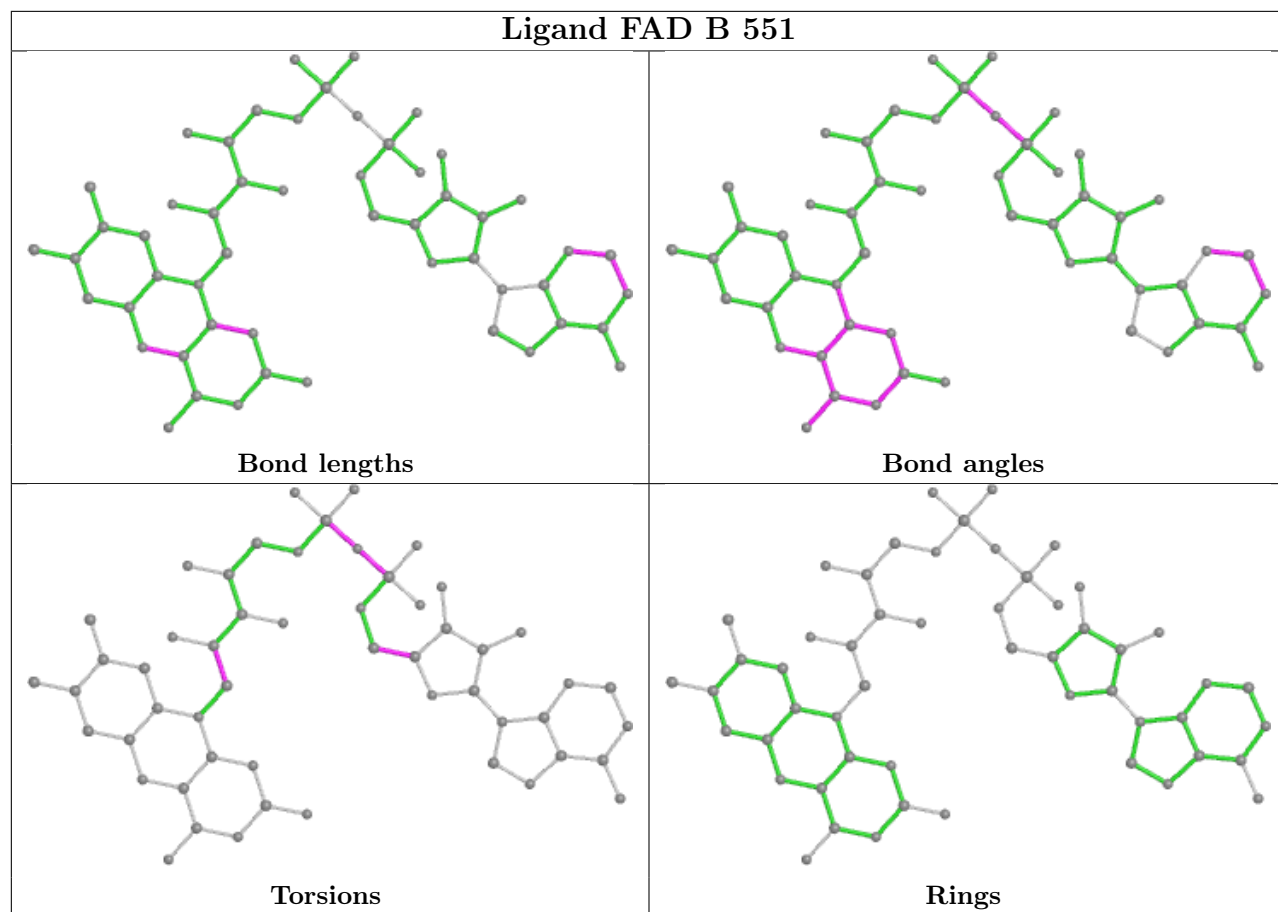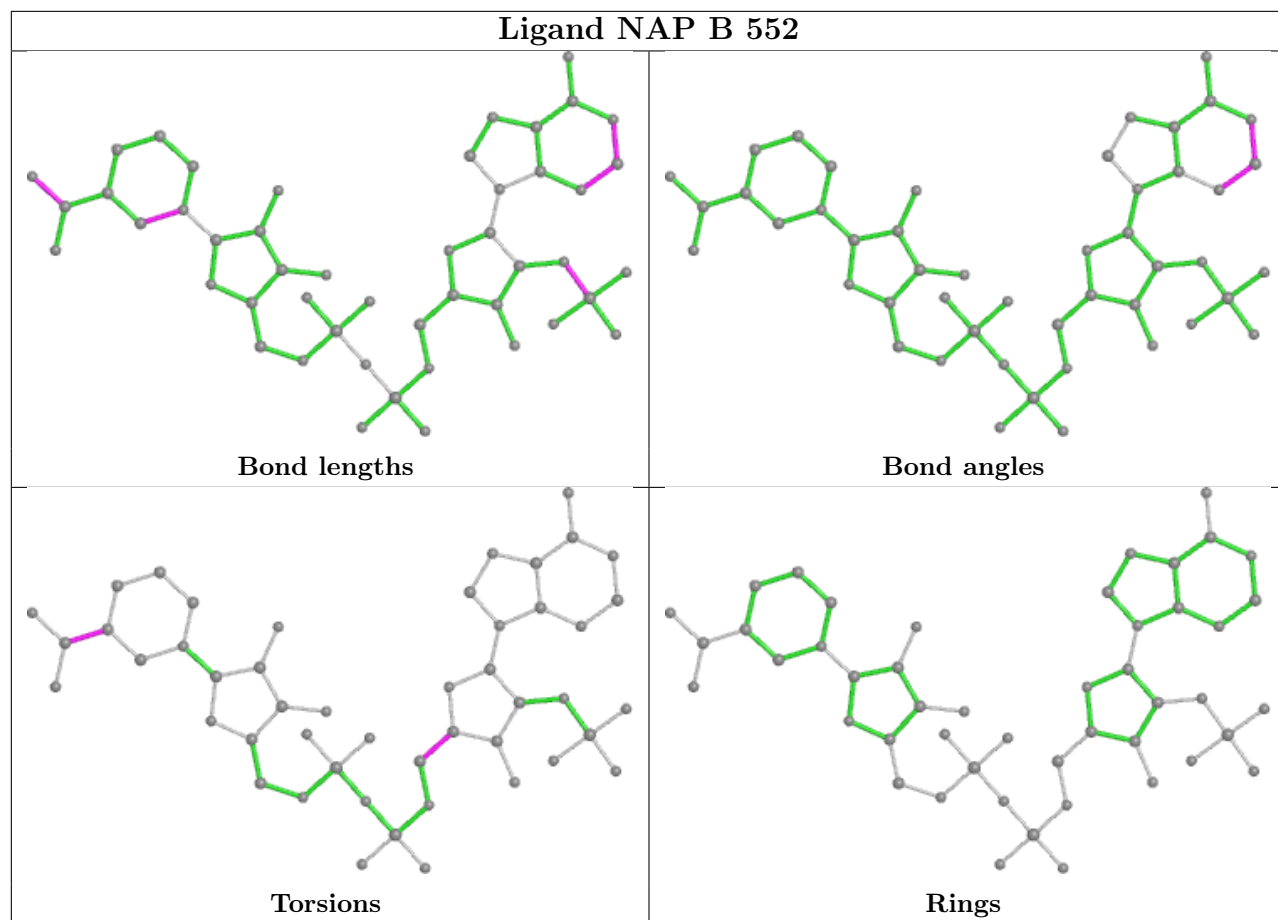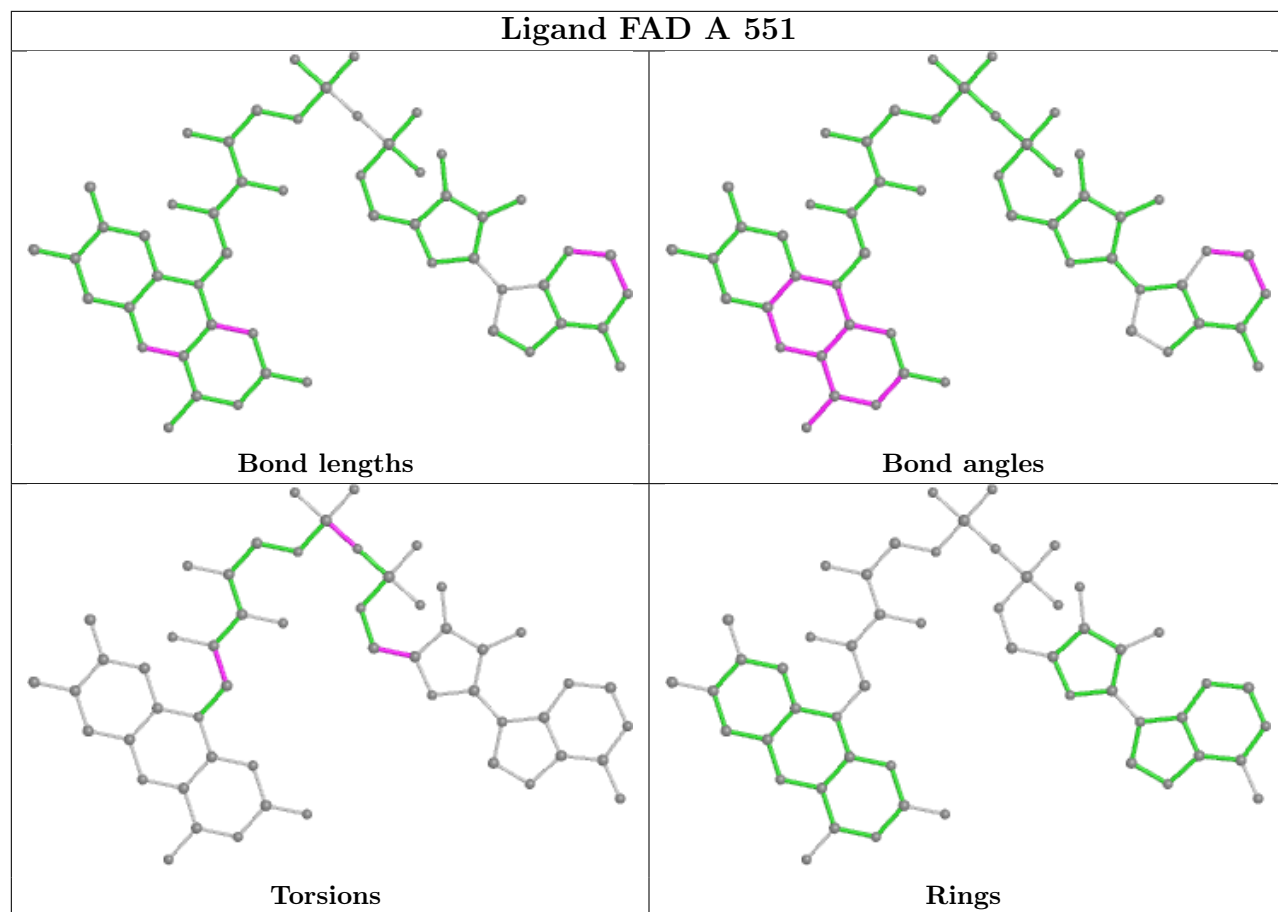
5.7 Other polymers (i)

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%)	-0.05	17 (3%)	47	46	13, 25, 43, 50	0
1	B	537/545 (98%)	-0.13	29 (5%)	25	24	12, 20, 44, 71	0
All	All	1074/1090 (98%)	-0.09	46 (4%)	35	34	12, 23, 43, 71	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	513	VAL	7.6
1	B	507	THR	7.1
1	B	509	PRO	6.1
1	B	512	SER	5.9
1	B	510	ASP	5.4
1	B	511	GLY	4.8
1	B	506	THR	4.3
1	B	505	THR	4.2
1	A	149	SER	4.1
1	B	177	ALA	4.1
1	A	154	ILE	3.9
1	B	501	TRP	3.9
1	A	364	GLN	3.8
1	A	374	ALA	3.7
1	B	180	GLY	3.7
1	B	437	PRO	3.7
1	B	515	ARG	3.7
1	B	179	LYS	3.6
1	B	514	VAL	3.6
1	B	508	LYS	3.5
1	A	330	ASP	3.5
1	B	502	TRP	3.4
1	B	176	GLY	3.4
1	B	174	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	509	PRO	3.0
1	B	497	GLU	2.9
1	A	510	ASP	2.7
1	A	175	GLU	2.6
1	A	148	ALA	2.6
1	B	487	TYR	2.5
1	A	173	ASP	2.5
1	A	165	PHE	2.5
1	B	443	PHE	2.5
1	B	442	THR	2.4
1	A	497	GLU	2.4
1	B	516	ARG	2.4
1	A	174	ALA	2.4
1	A	501	TRP	2.3
1	B	172	THR	2.3
1	B	517	THR	2.3
1	B	131	GLU	2.1
1	B	173	ASP	2.1
1	A	369	GLU	2.1
1	A	365	GLU	2.1
1	B	436	GLY	2.1
1	A	153	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.
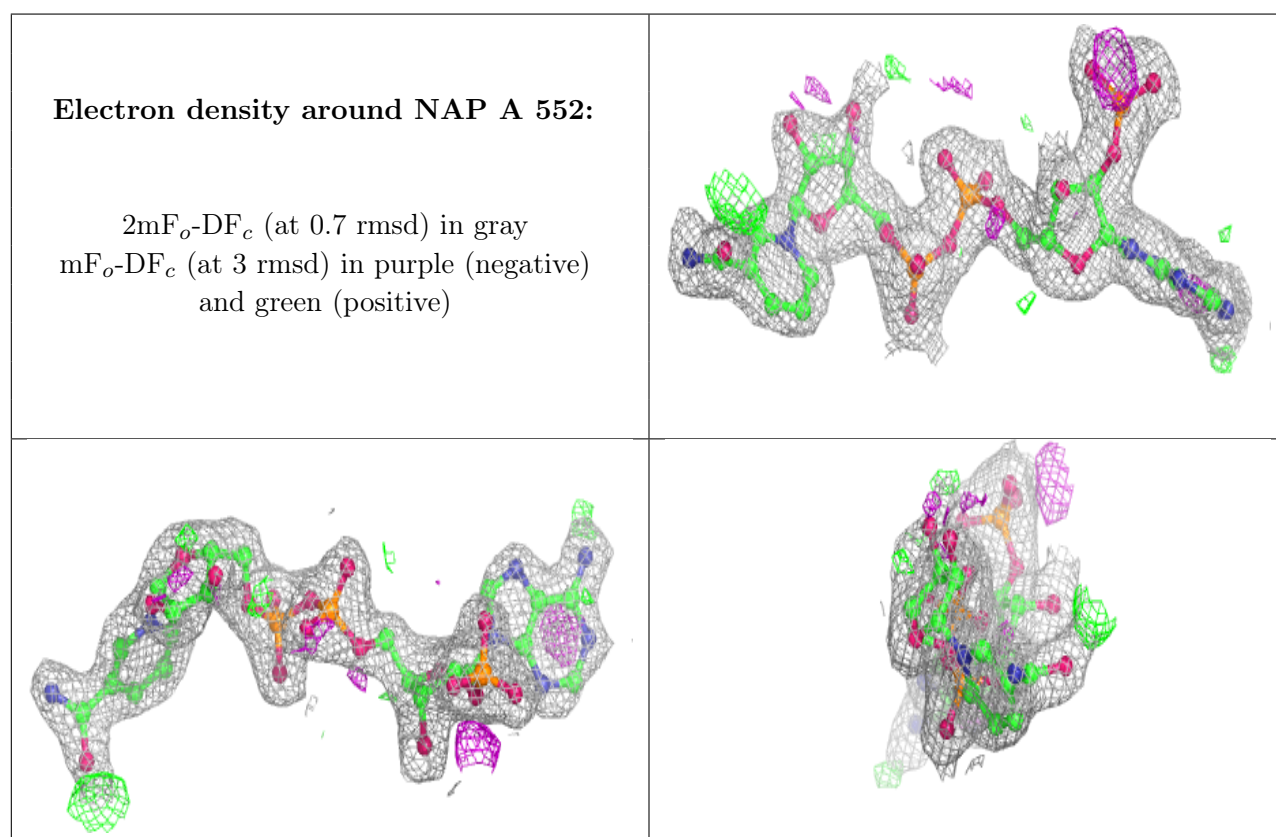
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAP	A	552	48/48	0.93	0.12	23,29,32,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	NA	A	546	1/1	0.94	0.09	23,23,23,23	0
3	NAP	B	552	48/48	0.97	0.10	13,17,27,30	0
2	FAD	B	551	53/53	0.98	0.10	11,14,16,18	0
2	FAD	A	551	53/53	0.98	0.09	13,17,19,20	0
4	NA	B	546	1/1	0.99	0.12	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 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:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.