



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 05:07 PM UTC

PDB ID : 2BRY / pdb_00002bry
Title : Crystal structure of the native monooxygenase domain of MICAL at 1.45 Å resolution
Authors : Siebold, C.; Berrow, N.; Walter, T.S.; Harlos, K.; Owens, R.J.; Terman, J.R.; Stuart, D.I.; Kolodkin, A.L.; Pasterkamp, R.J.; Jones, E.Y.
Deposited on : 2005-05-13
Resolution : 1.45 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

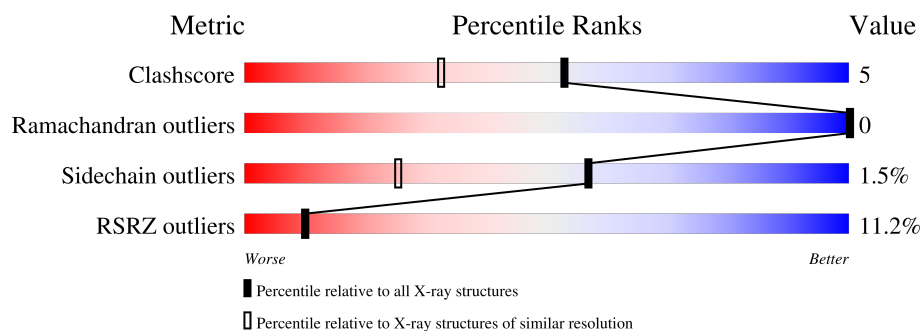
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	497	18% 86% 10% ..
1	B	497	4% 86% 10% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9235 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 NEDD9 INTERACTING PROTEIN WITH CALPONIN HO- MOLOGY AND LIM DOMAINS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	9	0
			3765	2406	669	673	17			
1	B	479	Total	C	N	O	S	0	8	0
			3763	2403	669	674	17			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

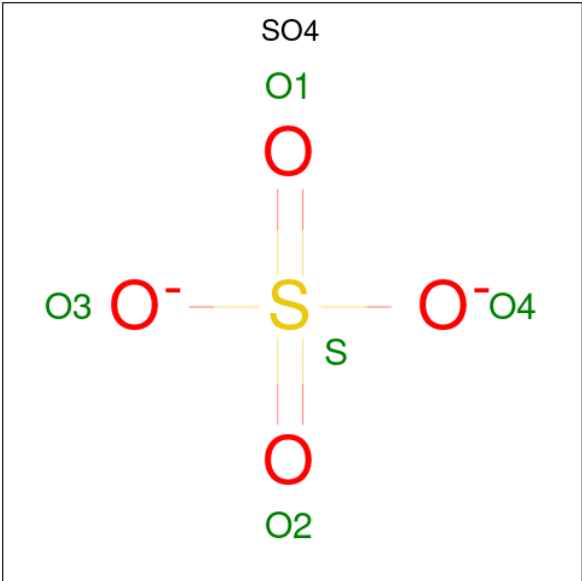
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



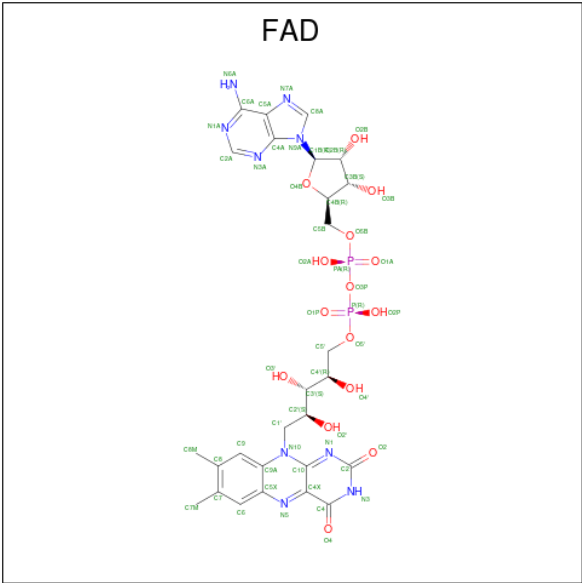
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

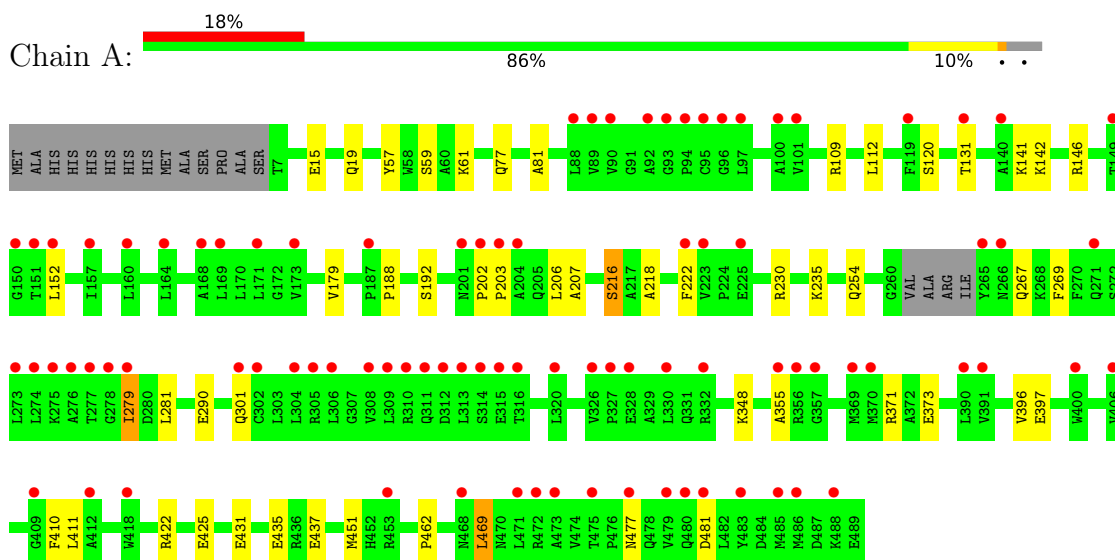
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	757	Total	O	0	0
			757	757		
6	B	826	Total	O	0	0
			826	826		

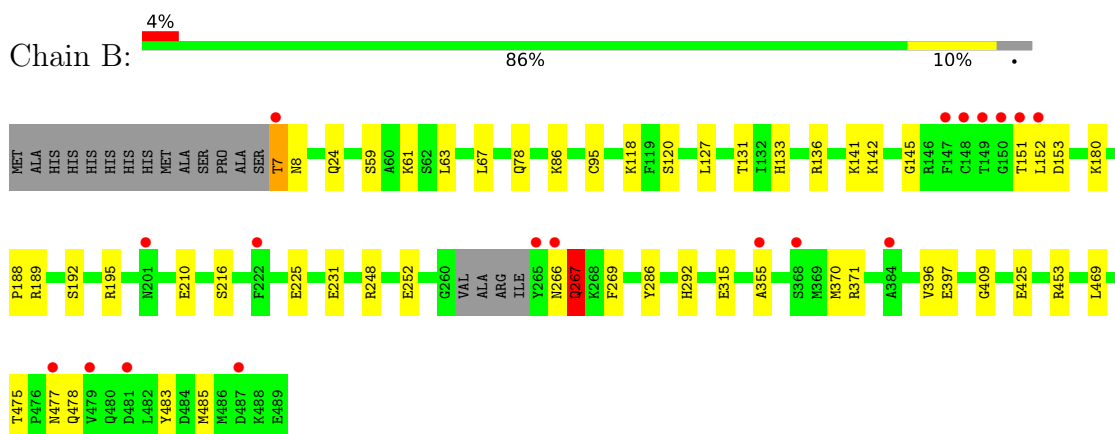
3 Residue-property plots

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: NEDD9 INTERACTING PROTEIN WITH CALPONIN HOMOLGY AND LIM DOMAINS



• Molecule 1: NEDD9 INTERACTING PROTEIN WITH CALPONIN HOMOLGY AND LIM DOMAINS



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.59Å 89.55Å 83.46Å 90.00° 114.35° 90.00°	Depositor
Resolution (Å)	76.03 – 1.45 76.03 – 1.45	Depositor EDS
% Data completeness (in resolution range)	88.3 (76.03-1.45) 88.4 (76.03-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.180 , 0.222 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9235	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, GOL, 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	0.73	0/3883	0.86	0/5258
1	B	0.65	0/3881	0.80	1/5255 (0.0%)
All	All	0.69	0/7764	0.83	1/10513 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	GLN	N-CA-C	7.68	121.58	107.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3765	0	3791	38	1
1	B	3763	0	3787	40	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	8	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	53	0	31	0	0
6	A	757	0	0	14	0
6	B	826	0	0	21	1
All	All	9235	0	7648	77	2

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 (77) 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:131[B]:THR:HG21	6:B:2318:HOH:O	1.54	1.08
1:B:267:GLN:HG3	1:B:269:PHE:HB3	1.53	0.89
1:A:152:LEU:HG	6:A:2338:HOH:O	1.80	0.81
1:A:254:GLN:HG3	6:A:2463:HOH:O	1.83	0.78
1:B:371:ARG:HB2	1:B:396[B]:VAL:HG12	1.73	0.70
1:A:422:ARG:NH1	1:A:435:GLU:OE1	2.24	0.70
1:B:478:GLN:HG3	6:B:2792:HOH:O	1.99	0.62
1:A:371:ARG:HB2	1:A:396[B]:VAL:HG12	1.81	0.60
1:B:78:GLN:NE2	6:B:2204:HOH:O	2.34	0.58
1:B:152:LEU:HD21	6:B:2508:HOH:O	2.02	0.57
1:B:131[A]:THR:HG21	6:B:2318:HOH:O	2.04	0.57
1:A:216[B]:SER:HB3	6:A:2425:HOH:O	2.06	0.55
1:B:63:LEU:HD12	6:B:2163:HOH:O	2.06	0.54
1:B:231:GLU:OE2	1:B:370:MET:HG3	2.07	0.54
1:B:118:LYS:HE2	6:B:2286:HOH:O	2.07	0.53
1:A:431:GLU:HG2	6:A:2357:HOH:O	2.09	0.53
1:A:59:SER:O	1:A:142:LYS:HE2	2.08	0.52
1:B:188:PRO:HD2	1:B:192:SER:HB3	1.91	0.52
1:A:19:GLN:HG3	6:A:2034:HOH:O	2.09	0.52
1:B:86:LYS:HE2	1:B:210:GLU:O	2.10	0.52
1:B:216[B]:SER:HB3	6:B:2461:HOH:O	2.10	0.52
1:A:371:ARG:CB	1:A:396[B]:VAL:HG12	2.40	0.51
1:A:230:ARG:HD2	1:A:373:GLU:HG3	1.92	0.51
1:A:348:LYS:HD2	6:A:2302:HOH:O	2.09	0.51
1:B:59:SER:O	1:B:142:LYS:HE2	2.10	0.51
1:A:235:LYS:HD2	1:B:225:GLU:OE1	2.11	0.51
1:A:203:PRO:HB2	6:A:2414:HOH:O	2.10	0.50
1:B:67:LEU:HG	6:B:2163:HOH:O	2.12	0.50
1:A:141:LYS:HD3	6:A:2337:HOH:O	2.12	0.50
1:A:146:ARG:HD2	1:A:290:GLU:OE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ASN:HB2	6:B:2792:HOH:O	2.11	0.49
1:A:279:ILE:HG22	1:A:281:LEU:HG	1.96	0.48
1:A:267:GLN:HB3	1:A:269:PHE:H	1.78	0.48
1:A:218:ALA:HB3	1:A:222:PHE:CG	2.49	0.48
1:B:133:HIS:HB2	6:B:2125:HOH:O	2.12	0.48
1:A:61:LYS:HE2	1:A:61:LYS:HB2	1.64	0.47
1:B:141:LYS:HE2	1:B:145:GLY:O	2.14	0.47
1:B:141:LYS:HD3	6:B:2335:HOH:O	2.15	0.47
1:A:188:PRO:HD2	1:A:192:SER:CB	2.45	0.46
1:B:397:GLU:HG3	6:B:2687:HOH:O	2.14	0.46
1:B:188:PRO:HD2	1:B:192:SER:CB	2.45	0.46
1:B:315:GLU:HG3	6:B:2595:HOH:O	2.16	0.46
1:A:425:GLU:HG3	6:A:2647:HOH:O	2.16	0.45
1:B:127:LEU:HB3	1:B:131[B]:THR:HG23	1.99	0.45
1:B:189:ARG:O	1:B:192:SER:HB2	2.17	0.45
1:B:370:MET:HB3	6:B:2665:HOH:O	2.16	0.45
1:A:437:GLU:HG2	6:A:2663:HOH:O	2.16	0.45
1:B:24:GLN:NE2	6:B:2039:HOH:O	2.41	0.45
1:A:142:LYS:HD3	6:A:2174:HOH:O	2.17	0.44
1:B:136:ARG:NH1	6:B:2333:HOH:O	2.51	0.44
1:A:77:GLN:HE21	1:A:81:ALA:HA	1.83	0.43
1:A:202:PRO:HB2	1:A:206:LEU:HB3	1.99	0.43
1:B:180:LYS:HE2	6:B:2406:HOH:O	2.18	0.43
1:B:195:ARG:HD3	6:B:2426:HOH:O	2.17	0.43
1:B:151:THR:HB	6:B:2363:HOH:O	2.18	0.43
1:A:112:LEU:C	1:A:112:LEU:HD23	2.44	0.43
1:B:483:TYR:CE2	1:B:485:MET:HE2	2.53	0.43
1:A:188:PRO:HD2	1:A:192:SER:HB3	2.01	0.43
1:B:286:TYR:OH	1:B:292:HIS:CD2	2.72	0.43
1:B:425:GLU:HG3	6:B:2715:HOH:O	2.19	0.42
1:B:95:CYS:SG	1:B:409:GLY:HA3	2.60	0.42
1:B:120[B]:SER:HB2	1:B:355:ALA:HB2	2.01	0.42
1:B:252:GLU:OE2	1:B:292:HIS:HE1	2.02	0.42
1:A:462:PRO:HB2	1:A:469:LEU:HD11	2.00	0.42
1:B:7:THR:HB	1:B:8:ASN:H	1.72	0.42
1:A:15:GLU:O	1:A:19:GLN:HG2	2.19	0.42
1:A:57:TYR:CZ	1:A:59:SER:HB3	2.54	0.42
1:A:397:GLU:HB2	6:A:2618:HOH:O	2.20	0.41
1:A:120:SER:HB2	1:A:355:ALA:HB2	2.01	0.41
1:A:109:ARG:NH1	6:A:2251:HOH:O	2.43	0.41
1:A:131[B]:THR:HG23	1:A:410:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:TYR:OH	1:B:292:HIS:HD2	2.04	0.40
1:A:202:PRO:HG2	1:A:207:ALA:HB2	2.02	0.40
1:A:301:GLN:HG2	6:A:2515:HOH:O	2.20	0.40
1:A:411:LEU:HD21	1:A:451:MET:HE1	2.03	0.40
1:B:153:ASP:OD1	1:B:153:ASP:N	2.53	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:NH2	1:B:248:ARG:O[1_556]	2.03	0.17
6:B:2039:HOH:O	6:B:2786:HOH:O[2_655]	2.15	0.05

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	484/497 (97%)	481 (99%)	3 (1%)	0	100	100
1	B	484/497 (97%)	477 (99%)	7 (1%)	0	100	100
All	All	968/994 (97%)	958 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/403 (98%)	391 (98%)	6 (2%)	57	25
1	B	397/403 (98%)	390 (98%)	7 (2%)	51	19
All	All	794/806 (98%)	781 (98%)	13 (2%)	57	23

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216[A]	SER
1	A	216[B]	SER
1	A	279	ILE
1	A	469	LEU
1	A	477	ASN
1	A	481	ASP
1	B	7	THR
1	B	61	LYS
1	B	266	ASN
1	B	267	GLN
1	B	453	ARG
1	B	469	LEU
1	B	475	THR

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	77	GLN
1	A	78	GLN
1	A	84	ASN
1	A	133	HIS
1	A	159	GLN
1	A	267	GLN
1	A	283	ASN
1	A	301	GLN
1	A	311	GLN
1	A	331	GLN
1	A	353	GLN
1	A	445	GLN
1	A	457	GLN
1	A	480	GLN
1	B	19	GLN
1	B	78	GLN
1	B	84	ASN

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Mol	Chain	Res	Type
1	B	159	GLN
1	B	185	GLN
1	B	266	ASN
1	B	267	GLN
1	B	292	HIS
1	B	382	HIS

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	GOL	A	1491	-	5,5,5	0.75	0	5,5,5	0.69	0
4	SO4	B	1491	-	4,4,4	0.22	0	6,6,6	0.45	0
4	SO4	A	1492	-	4,4,4	0.35	0	6,6,6	0.46	0
5	FAD	B	1492	-	58,58,58	1.13	5 (8%)	85,89,89	1.37	12 (14%)
5	FAD	A	1493	-	58,58,58	1.16	6 (10%)	85,89,89	1.57	14 (16%)

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	GOL	A	1491	-	-	2/4/4/4	-
5	FAD	A	1493	-	-	2/34/50/50	0/6/6/6
5	FAD	B	1492	-	-	3/34/50/50	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1492	FAD	C4X-N5	3.22	1.37	1.30
5	A	1493	FAD	C4X-N5	3.19	1.37	1.30
5	A	1493	FAD	C2A-N3A	3.16	1.39	1.33
5	B	1492	FAD	C8A-N7A	3.06	1.37	1.31
5	B	1492	FAD	C2A-N3A	3.03	1.39	1.33
5	B	1492	FAD	C10-N1	2.69	1.38	1.33
5	B	1492	FAD	C2A-N1A	2.69	1.38	1.33
5	A	1493	FAD	P-O3P	2.39	1.62	1.59
5	A	1493	FAD	C8A-N7A	2.37	1.36	1.31
5	A	1493	FAD	C2A-N1A	2.20	1.37	1.33
5	A	1493	FAD	PA-O3P	2.04	1.61	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1492	FAD	N3A-C2A-N1A	-5.93	119.61	128.58
5	A	1493	FAD	N3A-C2A-N1A	-4.81	121.30	128.58
5	A	1493	FAD	N9A-C8A-N7A	-4.12	108.09	113.94
5	A	1493	FAD	C5A-C4A-N3A	-4.09	121.09	126.72
5	A	1493	FAD	C4X-C10-N10	3.80	121.92	116.48
5	A	1493	FAD	C5A-N7A-C8A	3.79	109.41	103.45
5	B	1492	FAD	C4X-C10-N10	3.78	121.89	116.48
5	A	1493	FAD	C4A-C5A-N7A	-3.40	106.70	110.58
5	B	1492	FAD	N9A-C8A-N7A	-3.13	109.50	113.94
5	A	1493	FAD	C4-N3-C2	-2.98	120.34	125.64
5	A	1493	FAD	C2A-N3A-C4A	2.97	119.08	111.83
5	A	1493	FAD	C10-C4X-N5	-2.86	118.97	124.81
5	B	1492	FAD	C5A-C4A-N3A	-2.79	122.87	126.72
5	B	1492	FAD	C2A-N3A-C4A	2.72	118.48	111.83
5	A	1493	FAD	N3A-C4A-N9A	2.55	131.50	127.17
5	B	1492	FAD	C10-C4X-N5	-2.53	119.63	124.81
5	A	1493	FAD	C4A-N9A-C8A	2.51	108.38	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1492	FAD	C4-N3-C2	-2.49	121.22	125.64
5	B	1492	FAD	C2A-N1A-C6A	2.30	122.51	118.73
5	B	1492	FAD	C4A-N9A-C8A	2.24	108.09	105.74
5	A	1493	FAD	C4X-C4-N3	2.19	118.83	113.25
5	A	1493	FAD	C4-C4X-N5	2.18	121.22	118.21
5	B	1492	FAD	C5A-N7A-C8A	2.11	106.77	103.45
5	B	1492	FAD	N3A-C4A-N9A	2.09	130.72	127.17
5	A	1493	FAD	C6A-C5A-C4A	2.08	120.02	117.18
5	B	1492	FAD	C4X-C4-N3	2.01	118.36	113.25

There are no chirality outliers.

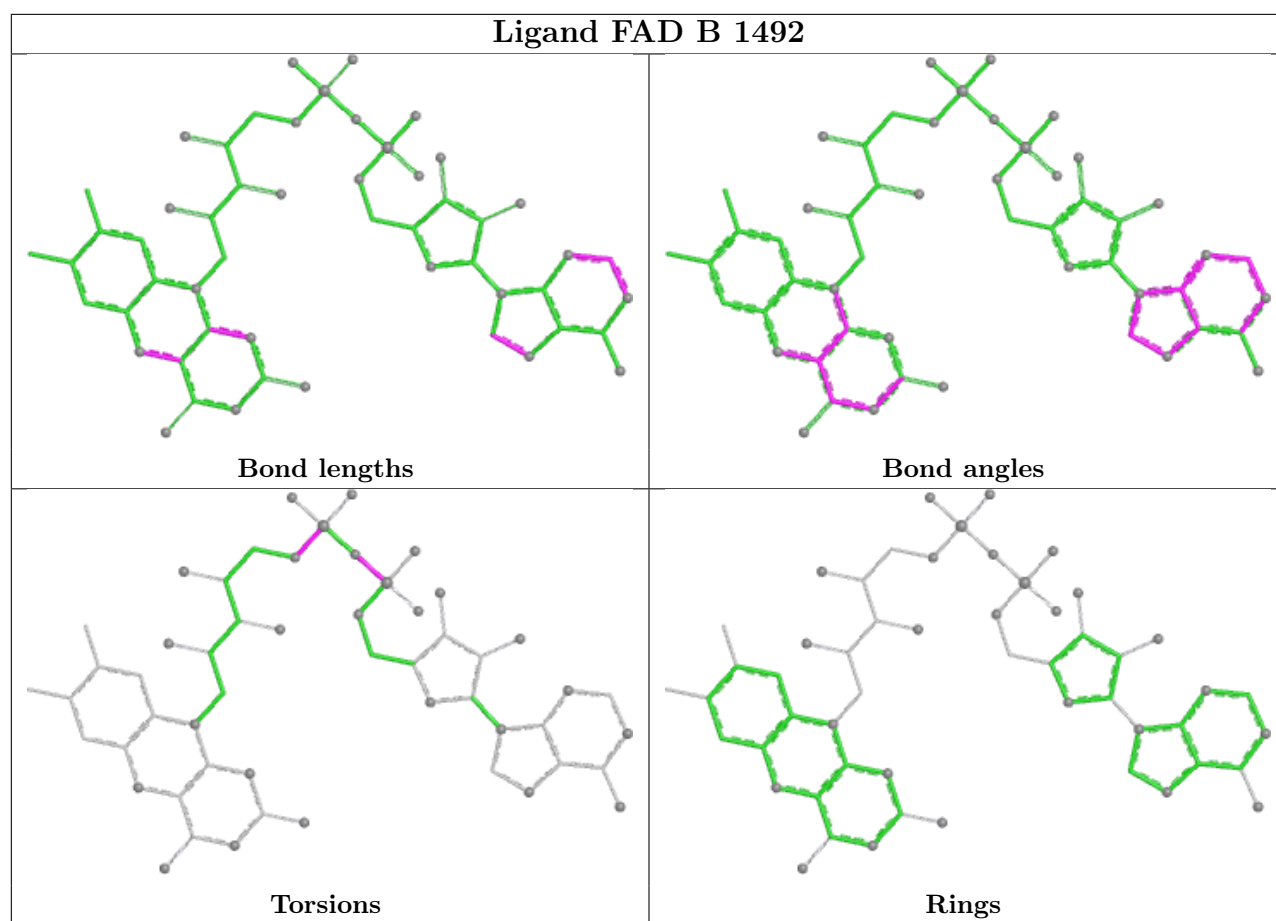
All (7) torsion outliers are listed below:

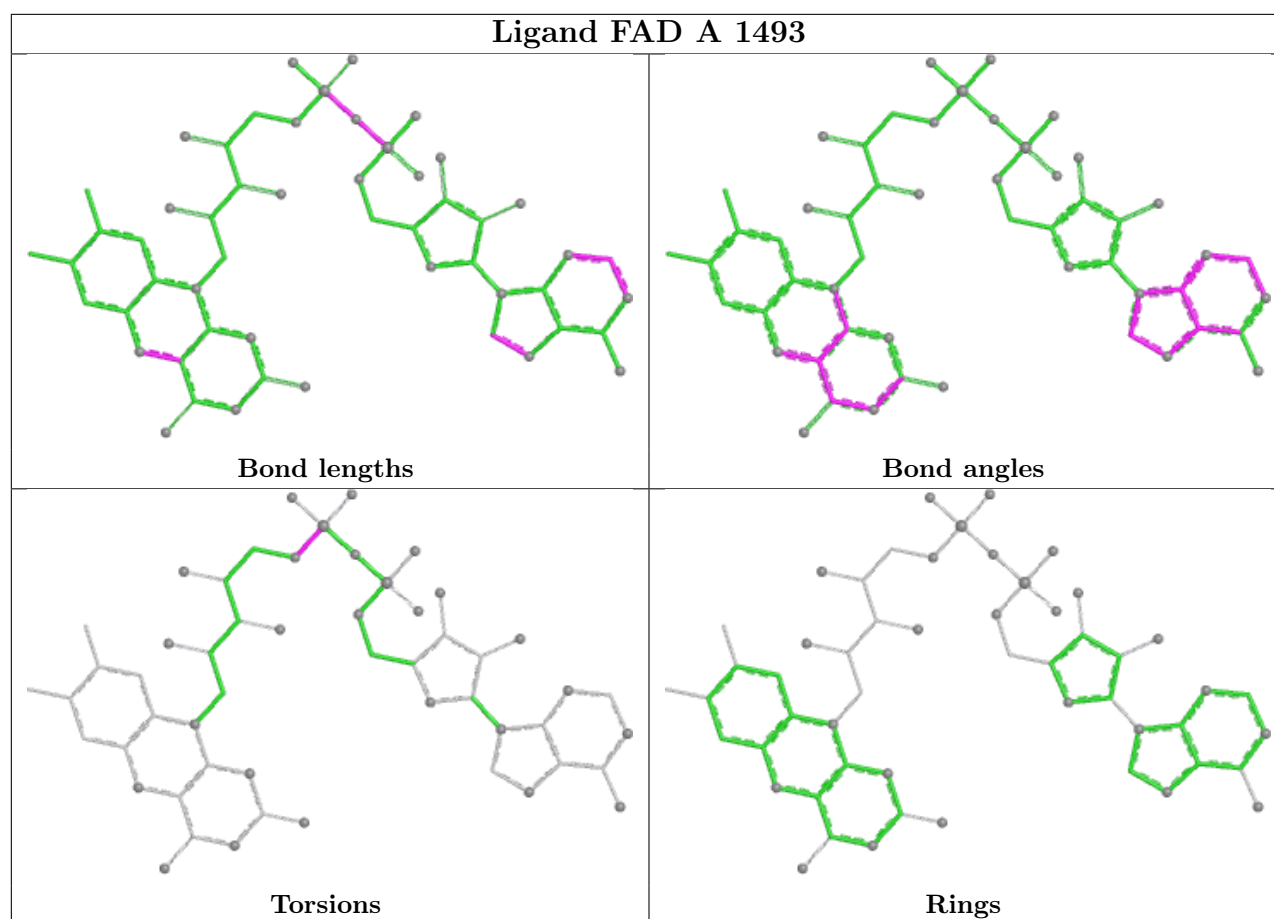
Mol	Chain	Res	Type	Atoms
5	A	1493	FAD	C5'-O5'-P-O2P
5	A	1493	FAD	C5'-O5'-P-O3P
5	B	1492	FAD	C5'-O5'-P-O2P
5	B	1492	FAD	C5'-O5'-P-O3P
3	A	1491	GOL	O2-C2-C3-O3
3	A	1491	GOL	C1-C2-C3-O3
5	B	1492	FAD	P-O3P-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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	479/497 (96%)	1.25	89 (18%) 3 3	11, 20, 31, 45	9 (1%)
1	B	479/497 (96%)	0.31	18 (3%) 44 47	6, 15, 28, 46	8 (1%)
All	All	958/994 (96%)	0.78	107 (11%) 10 10	6, 19, 30, 46	17 (1%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	THR	7.3
1	A	265	TYR	5.9
1	B	265	TYR	4.5
1	A	355	ALA	4.5
1	A	473	ALA	4.2
1	A	222	PHE	4.2
1	A	468	ASN	4.0
1	B	151	THR	4.0
1	A	302	CYS	4.0
1	A	488	LYS	3.8
1	A	149	THR	3.6
1	A	274	LEU	3.5
1	A	311	GLN	3.5
1	A	204	ALA	3.5
1	A	203	PRO	3.5
1	A	301	GLN	3.5
1	A	152	LEU	3.4
1	A	304	LEU	3.4
1	B	222	PHE	3.3
1	A	150	GLY	3.3
1	A	309	LEU	3.3
1	B	149	THR	3.3
1	A	475	THR	3.2
1	A	477	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	279	ILE	3.1
1	A	320	LEU	3.1
1	A	312	ASP	3.1
1	A	278	GLY	3.0
1	A	306	LEU	3.0
1	A	275	LYS	2.9
1	A	328	GLU	2.9
1	A	472	ARG	2.9
1	A	92	ALA	2.9
1	A	225	GLU	2.9
1	A	326	VAL	2.9
1	B	7	THR	2.8
1	A	266	ASN	2.8
1	B	487	ASP	2.8
1	A	97	LEU	2.8
1	A	169	LEU	2.8
1	A	314	SER	2.7
1	A	409	GLY	2.7
1	A	471	LEU	2.6
1	A	406	VAL	2.6
1	A	173	VAL	2.6
1	A	201	ASN	2.6
1	B	384	ALA	2.6
1	A	315	GLU	2.6
1	B	152	LEU	2.5
1	A	453	ARG	2.5
1	A	481	ASP	2.5
1	A	486	MET	2.5
1	A	313	LEU	2.5
1	A	271	GLN	2.5
1	A	223	VAL	2.5
1	A	479	VAL	2.5
1	B	148	CYS	2.4
1	A	93	GLY	2.4
1	A	480	GLN	2.4
1	A	160	LEU	2.4
1	B	481	ASP	2.4
1	A	316	THR	2.4
1	A	90	VAL	2.4
1	A	276	ALA	2.4
1	A	96	GLY	2.4
1	A	171	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	356	ARG	2.4
1	A	157	ILE	2.4
1	B	201	ASN	2.4
1	A	95	CYS	2.3
1	A	101	VAL	2.3
1	A	308	VAL	2.3
1	A	483	TYR	2.3
1	B	266	ASN	2.3
1	B	477	ASN	2.3
1	A	369	MET	2.3
1	A	485	MET	2.3
1	A	202	PRO	2.3
1	A	88	LEU	2.3
1	A	305	ARG	2.3
1	B	355	ALA	2.3
1	A	418	TRP	2.3
1	A	370	MET	2.3
1	A	168	ALA	2.2
1	A	412	ALA	2.2
1	A	164	LEU	2.2
1	A	140	ALA	2.2
1	A	310	ARG	2.2
1	A	332	ARG	2.2
1	A	273	LEU	2.2
1	A	94	PRO	2.2
1	B	150	GLY	2.2
1	A	390	LEU	2.1
1	A	327	PRO	2.1
1	A	119	PHE	2.1
1	A	100	ALA	2.1
1	A	187	PRO	2.1
1	A	330	LEU	2.1
1	A	89	VAL	2.1
1	B	479	VAL	2.1
1	A	400	TRP	2.1
1	A	357	GLY	2.1
1	A	131[A]	THR	2.0
1	A	277	THR	2.0
1	A	391	VAL	2.0
1	B	147	PHE	2.0
1	B	368	SER	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](#)

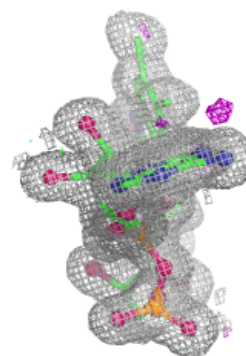
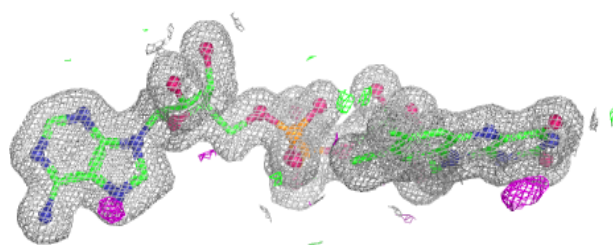
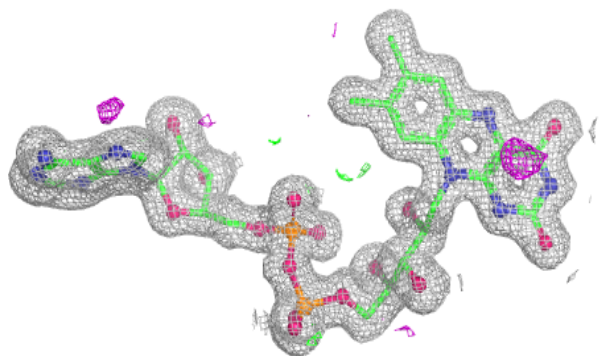
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1491	6/6	0.78	0.15	18,21,22,22	0
4	SO4	A	1492	5/5	0.92	0.10	30,30,32,32	0
4	SO4	B	1491	5/5	0.96	0.12	22,22,26,27	0
5	FAD	A	1493	53/53	0.98	0.04	6,9,10,12	0
5	FAD	B	1492	53/53	0.98	0.04	5,8,12,13	0
2	CL	B	1490	1/1	0.99	0.04	16,16,16,16	0
2	CL	A	1490	1/1	0.99	0.02	12,12,12,12	0

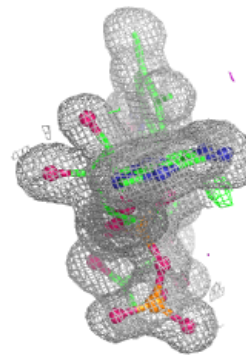
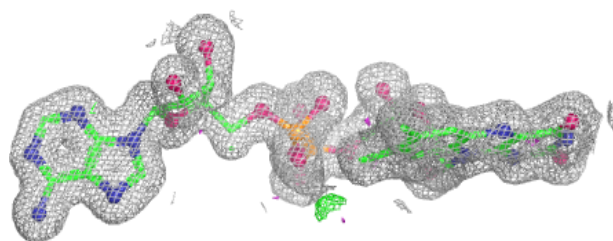
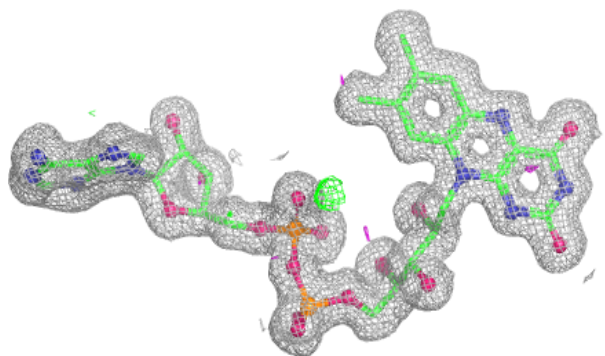
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 1493:

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

**Electron density around FAD B 1492:**

$2mF_o-DF_c$ (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.