



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:45 AM UTC

PDB ID : 7ON9 / pdb_00007on9
Title : Crystal structure of para-hydroxybenzoate-3-hydroxylase PraI
Authors : Zahn, M.; McGeehan, J.E.
Deposited on : 2021-05-25
Resolution : 1.63 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

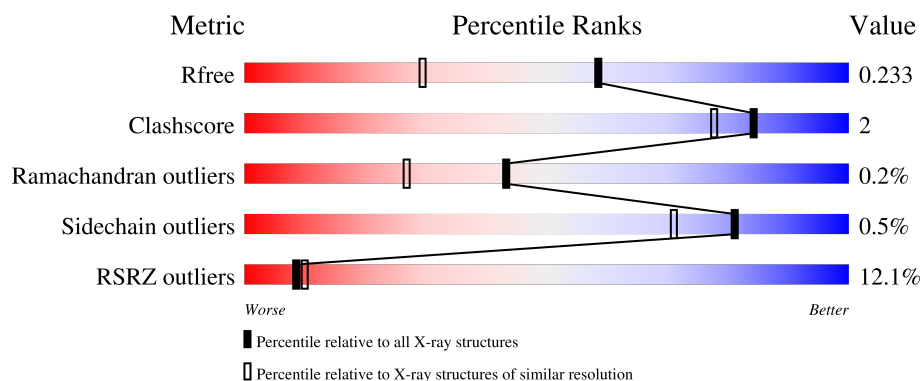
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	402	6% 92% 5% .
1	B	402	8% 92% 5% .
1	C	402	13% 90% 7% .
1	D	402	20% 92% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13837 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 4-hydroxybenzoate 3-monooxygenase (NAD(P)H).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	2	0
			3116	1966	566	568	16			
1	B	392	Total	C	N	O	S	0	2	0
			3108	1963	564	565	16			
1	C	391	Total	C	N	O	S	0	3	0
			3103	1959	563	566	15			
1	D	390	Total	C	N	O	S	0	1	0
			3084	1946	560	563	15			

There are 32 discrepancies between the modelled and reference sequences:

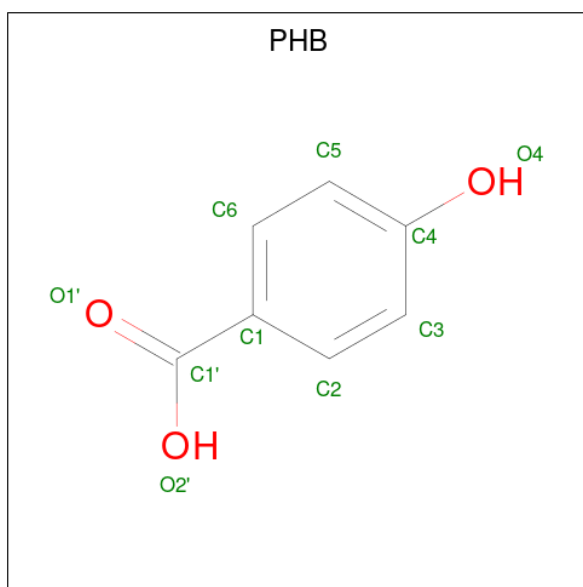
Chain	Residue	Modelled	Actual	Comment	Reference
A	395	LEU	-	expression tag	UNP C4TP09
A	396	GLU	-	expression tag	UNP C4TP09
A	397	HIS	-	expression tag	UNP C4TP09
A	398	HIS	-	expression tag	UNP C4TP09
A	399	HIS	-	expression tag	UNP C4TP09
A	400	HIS	-	expression tag	UNP C4TP09
A	401	HIS	-	expression tag	UNP C4TP09
A	402	HIS	-	expression tag	UNP C4TP09
B	395	LEU	-	expression tag	UNP C4TP09
B	396	GLU	-	expression tag	UNP C4TP09
B	397	HIS	-	expression tag	UNP C4TP09
B	398	HIS	-	expression tag	UNP C4TP09
B	399	HIS	-	expression tag	UNP C4TP09
B	400	HIS	-	expression tag	UNP C4TP09
B	401	HIS	-	expression tag	UNP C4TP09
B	402	HIS	-	expression tag	UNP C4TP09
C	395	LEU	-	expression tag	UNP C4TP09
C	396	GLU	-	expression tag	UNP C4TP09
C	397	HIS	-	expression tag	UNP C4TP09
C	398	HIS	-	expression tag	UNP C4TP09
C	399	HIS	-	expression tag	UNP C4TP09

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Chain	Residue	Modelled	Actual	Comment	Reference
C	400	HIS	-	expression tag	UNP C4TP09
C	401	HIS	-	expression tag	UNP C4TP09
C	402	HIS	-	expression tag	UNP C4TP09
D	395	LEU	-	expression tag	UNP C4TP09
D	396	GLU	-	expression tag	UNP C4TP09
D	397	HIS	-	expression tag	UNP C4TP09
D	398	HIS	-	expression tag	UNP C4TP09
D	399	HIS	-	expression tag	UNP C4TP09
D	400	HIS	-	expression tag	UNP C4TP09
D	401	HIS	-	expression tag	UNP C4TP09
D	402	HIS	-	expression tag	UNP C4TP09

- # FAD

- Molecule 3 is P-HYDROXYBENZOIC ACID (CCD ID: PHB) (formula: $C_7H_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	7	3		
3	B	1	Total	C	O	0	0
			10	7	3		
3	C	1	Total	C	O	0	0
			10	7	3		
3	D	1	Total	C	O	0	0
			10	7	3		

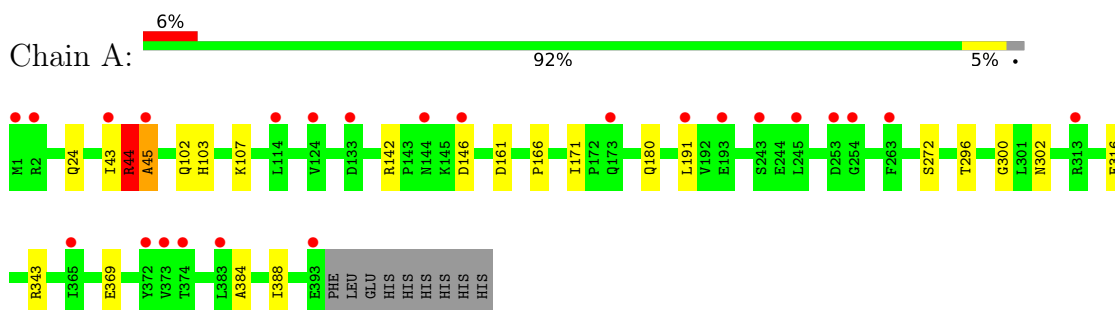
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	361	Total	O	0	0
			361	361		
4	B	330	Total	O	0	0
			330	330		
4	C	261	Total	O	0	0
			261	261		
4	D	222	Total	O	0	0
			222	222		

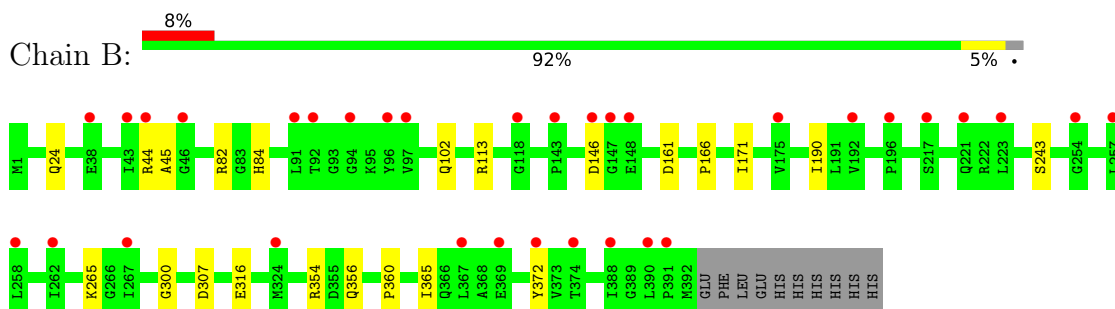
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

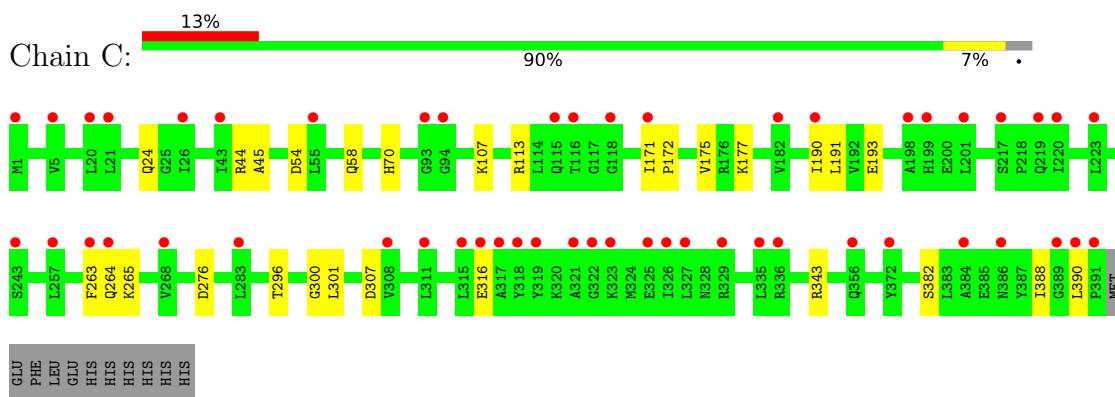
- Molecule 1: 4-hydroxybenzoate 3-monooxygenase (NAD(P)H)



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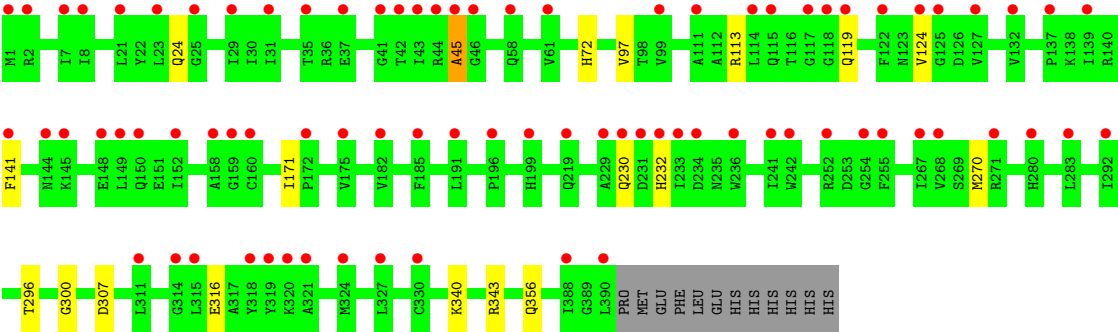


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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.11Å 101.51Å 106.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.85 – 1.63 106.85 – 1.63	Depositor EDS
% Data completeness (in resolution range)	80.5 (106.85-1.63) 80.5 (106.85-1.63)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.63Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.203 , 0.222 0.212 , 0.233	Depositor DCC
R_{free} test set	8351 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13837	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.48% 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: PHB, 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	1/3190 (0.0%)	0.96	4/4309 (0.1%)
1	B	0.70	0/3182	0.97	3/4298 (0.1%)
1	C	0.69	0/3180	0.95	3/4297 (0.1%)
1	D	0.68	0/3154	0.95	2/4261 (0.0%)
All	All	0.70	1/12706 (0.0%)	0.96	12/17165 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ARG	CA-C	5.25	1.59	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	ILE	N-CA-C	-6.08	101.62	107.76
1	D	171	ILE	N-CA-C	-5.88	102.21	107.56
1	B	307	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	171	ILE	N-CA-C	-5.68	102.03	107.76
1	D	307	ASP	CA-CB-CG	5.62	118.22	112.60
1	C	307	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	70	HIS	CA-CB-CG	-5.49	108.31	113.80
1	B	354	ARG	CB-CG-CD	-5.45	98.77	111.30
1	A	171	ILE	N-CA-C	-5.37	102.34	107.76
1	A	45	ALA	N-CA-C	5.31	117.14	110.24
1	A	44	ARG	N-CA-C	5.23	121.94	110.80
1	A	302	ASN	CA-CB-CG	-5.12	107.48	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3116	0	3090	14	0
1	B	3108	0	3087	17	0
1	C	3103	0	3078	17	0
1	D	3084	0	3055	18	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	4	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	1	0
3	D	10	0	5	0	0
4	A	361	0	0	5	1
4	B	330	0	0	0	1
4	C	261	0	0	1	0
4	D	222	0	0	0	0
All	All	13837	0	12451	58	1

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 2.

All (58) 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:D:72:HIS:HB2	1:D:97:VAL:CG2	2.13	0.78
1:C:191:LEU:HD12	1:C:264[B]:GLN:HG2	1.67	0.77
1:D:72:HIS:HB2	1:D:97:VAL:HG23	1.68	0.76
1:A:45:ALA:HB3	1:A:102:GLN:HB2	1.69	0.73
1:A:103:HIS:ND1	1:A:107:LYS:NZ	2.40	0.69
1:B:360:PRO:CG	1:D:230:GLN:HB3	2.22	0.69
1:D:124:VAL:CG1	1:D:141:PHE:HB2	2.22	0.68
1:D:124:VAL:HG11	1:D:141:PHE:HB2	1.78	0.63
1:B:45:ALA:HA	2:B:501:FAD:N5	2.16	0.61
1:A:44:ARG:HA	4:A:621:HOH:O	2.01	0.60
1:D:45:ALA:HB3	2:D:501:FAD:N5	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LYS:HD3	1:D:232:HIS:CE1	2.37	0.60
4:A:603:HOH:O	1:D:340:LYS:HG2	2.02	0.57
1:C:24:GLN:HG3	1:C:316:GLU:CD	2.30	0.56
1:B:365:ILE:HG23	1:C:343:ARG:HG2	1.87	0.55
4:A:645:HOH:O	1:D:340:LYS:HD3	2.07	0.54
1:B:161:ASP:OD2	1:B:166:PRO:HD2	2.09	0.52
1:C:107:LYS:NZ	4:C:604:HOH:O	2.42	0.52
1:C:54:ASP:O	1:C:58:GLN:HG3	2.11	0.50
1:A:180:GLN:HG3	1:A:272:SER:O	2.10	0.50
1:B:372:TYR:OH	1:C:382:SER:OG	2.29	0.50
1:A:146:ASP:OD1	4:A:601:HOH:O	2.20	0.49
1:D:300:GLY:HA3	2:D:501:FAD:H1'2	1.94	0.49
1:A:43:ILE:HD12	1:A:191:LEU:HD11	1.96	0.47
1:A:142:ARG:NH2	1:B:146:ASP:O	2.47	0.47
1:B:82:ARG:NH2	1:B:84:HIS:CE1	2.83	0.47
1:C:300:GLY:HA3	2:C:501:FAD:H1'2	1.98	0.46
1:A:384:ALA:O	1:A:388:ILE:HG13	2.15	0.46
1:B:365:ILE:HD12	1:C:343:ARG:HA	1.98	0.46
1:A:300:GLY:HA3	2:A:501:FAD:H1'2	1.98	0.46
1:A:369:GLU:OE1	1:D:343:ARG:HD3	2.16	0.45
1:A:180:GLN:HG2	4:A:842:HOH:O	2.17	0.45
1:B:300:GLY:HA3	2:B:501:FAD:H1'2	2.00	0.44
1:C:172:PRO:O	1:C:175:VAL:HG22	2.16	0.44
1:A:24:GLN:HG3	1:A:316:GLU:CD	2.43	0.44
1:C:177:LYS:HG2	1:C:276:ASP:O	2.16	0.44
1:C:190:ILE:HG22	1:C:265:LYS:HB3	2.00	0.44
1:C:193:GLU:HB2	1:C:263:PHE:CE2	2.53	0.44
1:D:24:GLN:HG3	1:D:316:GLU:CD	2.43	0.44
1:B:356:GLN:HB2	1:D:356:GLN:HE21	1.82	0.43
1:B:45:ALA:HB3	1:B:102:GLN:HB2	1.99	0.43
2:A:501:FAD:H9	2:A:501:FAD:H1'1	1.84	0.43
1:B:24:GLN:HG3	1:B:316:GLU:CD	2.44	0.43
1:B:360:PRO:HG2	1:D:230:GLN:HB3	2.00	0.42
1:D:45:ALA:CB	2:D:501:FAD:N5	2.82	0.42
1:B:360:PRO:HG3	1:D:230:GLN:HB3	1.99	0.42
1:C:45:ALA:HB2	3:C:502:PHB:C1'	2.50	0.41
1:B:82:ARG:NH2	1:B:84:HIS:HE1	2.19	0.41
1:C:113:ARG:HA	1:C:113:ARG:NE	2.36	0.41
1:A:161:ASP:OD2	1:A:166:PRO:HD2	2.21	0.41
1:C:44:ARG:HD2	2:C:501:FAD:C9	2.51	0.41
1:C:301:LEU:C	1:C:301:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ARG:HA	1:D:113:ARG:NE	2.36	0.41
1:D:270:MET:HE3	1:D:270:MET:HB3	2.00	0.40
1:B:113:ARG:HA	1:B:113:ARG:NE	2.37	0.40
1:B:190:ILE:HG22	1:B:265:LYS:HB3	2.04	0.40
2:D:501:FAD:H9	2:D:501:FAD:H1'1	1.82	0.40

All (1) 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)
4:A:855:HOH:O	4:B:706:HOH:O[3_454]	2.16	0.04

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	393/402 (98%)	385 (98%)	7 (2%)	1 (0%)	36	20
1	B	392/402 (98%)	383 (98%)	8 (2%)	1 (0%)	36	20
1	C	392/402 (98%)	383 (98%)	9 (2%)	0	100	100
1	D	389/402 (97%)	379 (97%)	9 (2%)	1 (0%)	36	20
All	All	1566/1608 (97%)	1530 (98%)	33 (2%)	3 (0%)	43	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	D	45	ALA
1	B	44	ARG

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	328/335 (98%)	327 (100%)	1 (0%)	86	79
1	B	327/335 (98%)	326 (100%)	1 (0%)	86	79
1	C	327/335 (98%)	324 (99%)	3 (1%)	70	54
1	D	324/335 (97%)	322 (99%)	2 (1%)	78	66
All	All	1306/1340 (98%)	1299 (100%)	7 (0%)	81	71

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	THR
1	B	243	SER
1	C	296	THR
1	C	388	ILE
1	C	390	LEU
1	D	119	GLN
1	D	296	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	58	GLN
1	A	89	HIS
1	A	150	GLN
1	B	33	ASN
1	B	89	HIS
1	C	89	HIS
1	C	150	GLN
1	C	366	GLN
1	C	386	ASN
1	D	119	GLN
1	D	150	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	C	501	-	58,58,58	0.54	0	85,89,89	0.69	1 (1%)
3	PHB	D	502	-	10,10,10	1.26	2 (20%)	13,13,13	0.84	1 (7%)
2	FAD	A	501	-	58,58,58	0.54	0	85,89,89	0.71	1 (1%)
3	PHB	A	502	-	10,10,10	1.18	2 (20%)	13,13,13	0.96	2 (15%)
2	FAD	B	501	-	58,58,58	0.55	0	85,89,89	0.67	1 (1%)
2	FAD	D	501	-	58,58,58	0.63	0	85,89,89	0.65	1 (1%)
3	PHB	B	502	-	10,10,10	0.22	0	13,13,13	0.18	0
3	PHB	C	502	-	10,10,10	0.25	0	13,13,13	0.48	0

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	C	501	-	-	1/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PHB	D	502	-	-	0/4/4/4	0/1/1/1
2	FAD	A	501	-	-	4/34/50/50	0/6/6/6
3	PHB	A	502	-	-	0/4/4/4	0/1/1/1
2	FAD	B	501	-	-	2/34/50/50	0/6/6/6
2	FAD	D	501	-	-	2/34/50/50	0/6/6/6
3	PHB	B	502	-	-	0/4/4/4	0/1/1/1
3	PHB	C	502	-	-	0/4/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	PHB	O2'-C1'	-2.97	1.21	1.30
3	D	502	PHB	O1'-C1'	2.88	1.31	1.22
3	D	502	PHB	O2'-C1'	-2.61	1.22	1.30
3	A	502	PHB	O1'-C1'	2.20	1.29	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	PHB	O2'-C1'-C1	2.61	121.54	114.84
2	A	501	FAD	C4-N3-C2	-2.57	121.07	125.64
2	C	501	FAD	C4-N3-C2	-2.39	121.39	125.64
2	B	501	FAD	C4-N3-C2	-2.32	121.52	125.64
3	A	502	PHB	O1'-C1'-C1	-2.25	115.55	121.46
2	D	501	FAD	C4-N3-C2	-2.24	121.67	125.64
3	D	502	PHB	O2'-C1'-C1	2.16	120.38	114.84

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	PA-O3P-P-O5'
2	A	501	FAD	O3'-C3'-C4'-C5'
2	A	501	FAD	O3'-C3'-C4'-O4'
2	D	501	FAD	C2B-C1B-N9A-C8A
2	C	501	FAD	O3'-C3'-C4'-C5'
2	B	501	FAD	O3'-C3'-C4'-C5'
2	D	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	C2B-C1B-N9A-C8A
2	A	501	FAD	O4B-C4B-C5B-O5B

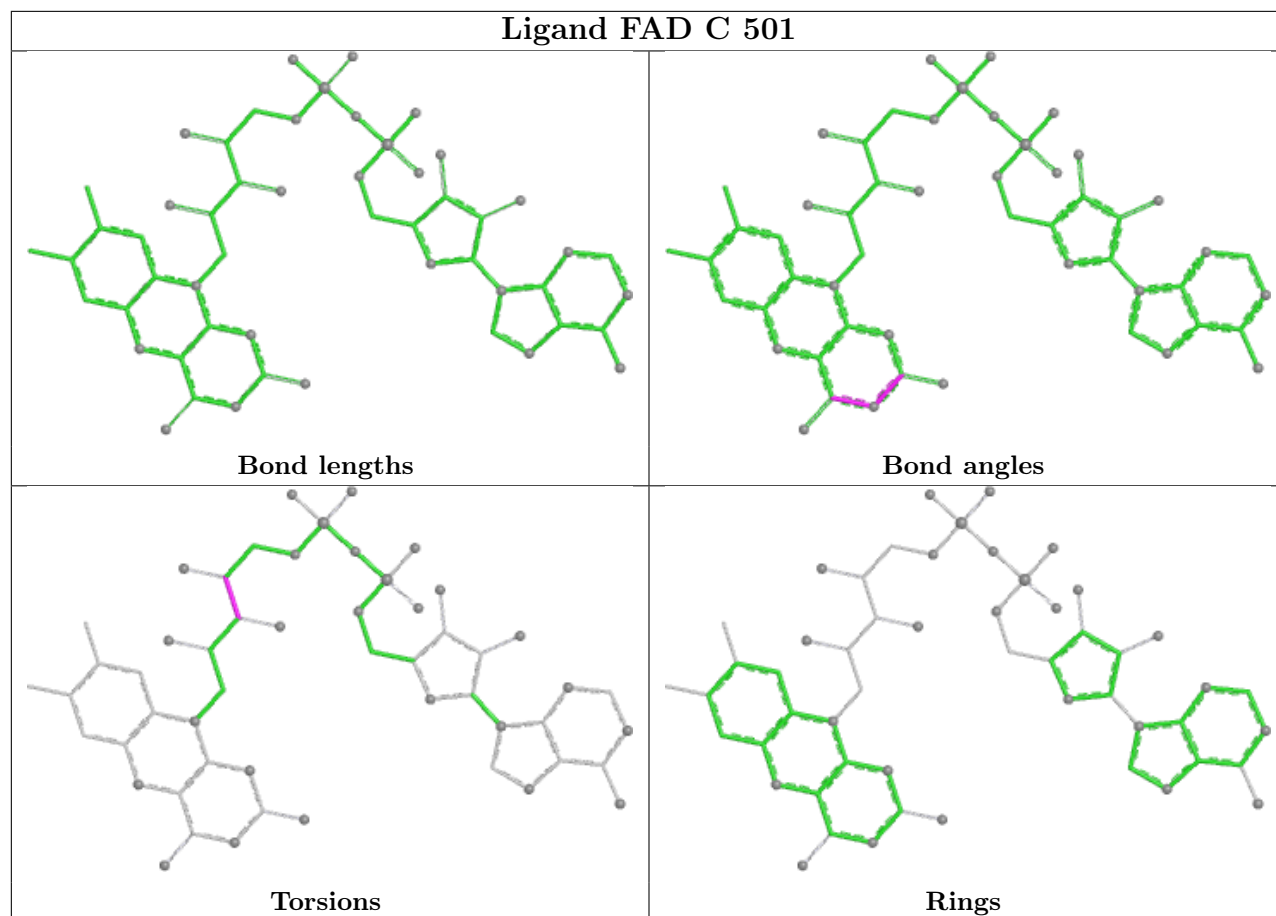
There are no ring outliers.

5 monomers are involved in 11 short contacts:

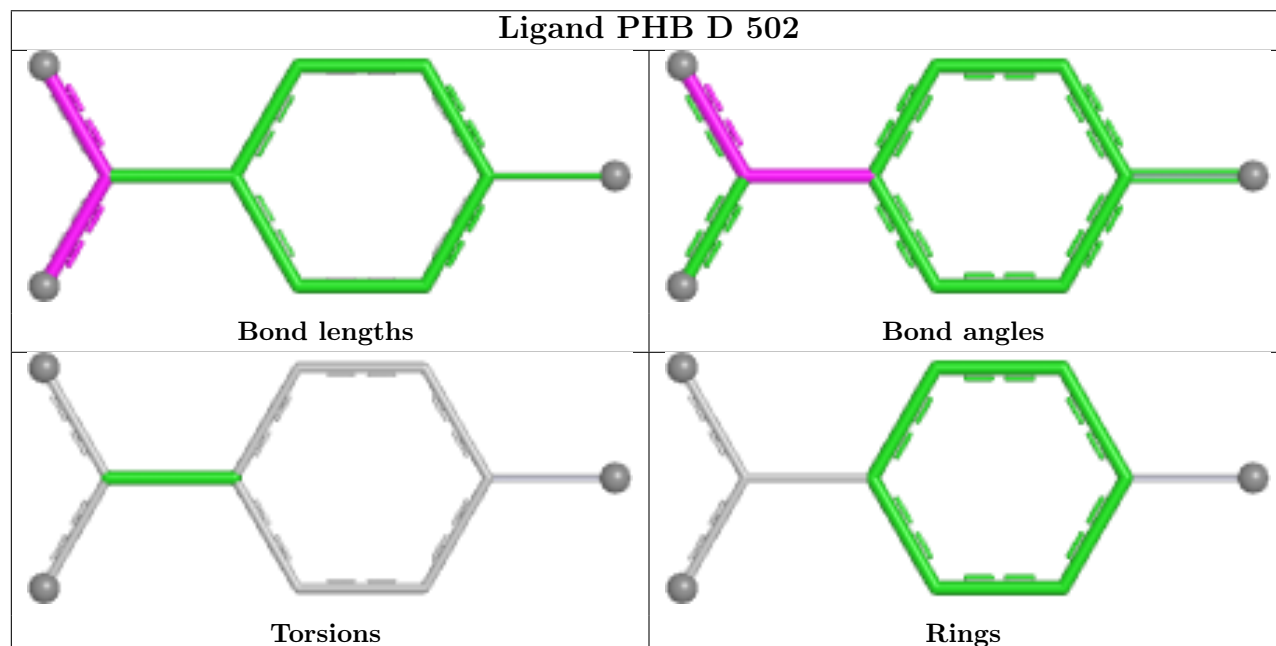
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	FAD	2	0
2	A	501	FAD	2	0
2	B	501	FAD	2	0
2	D	501	FAD	4	0
3	C	502	PHB	1	0

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.

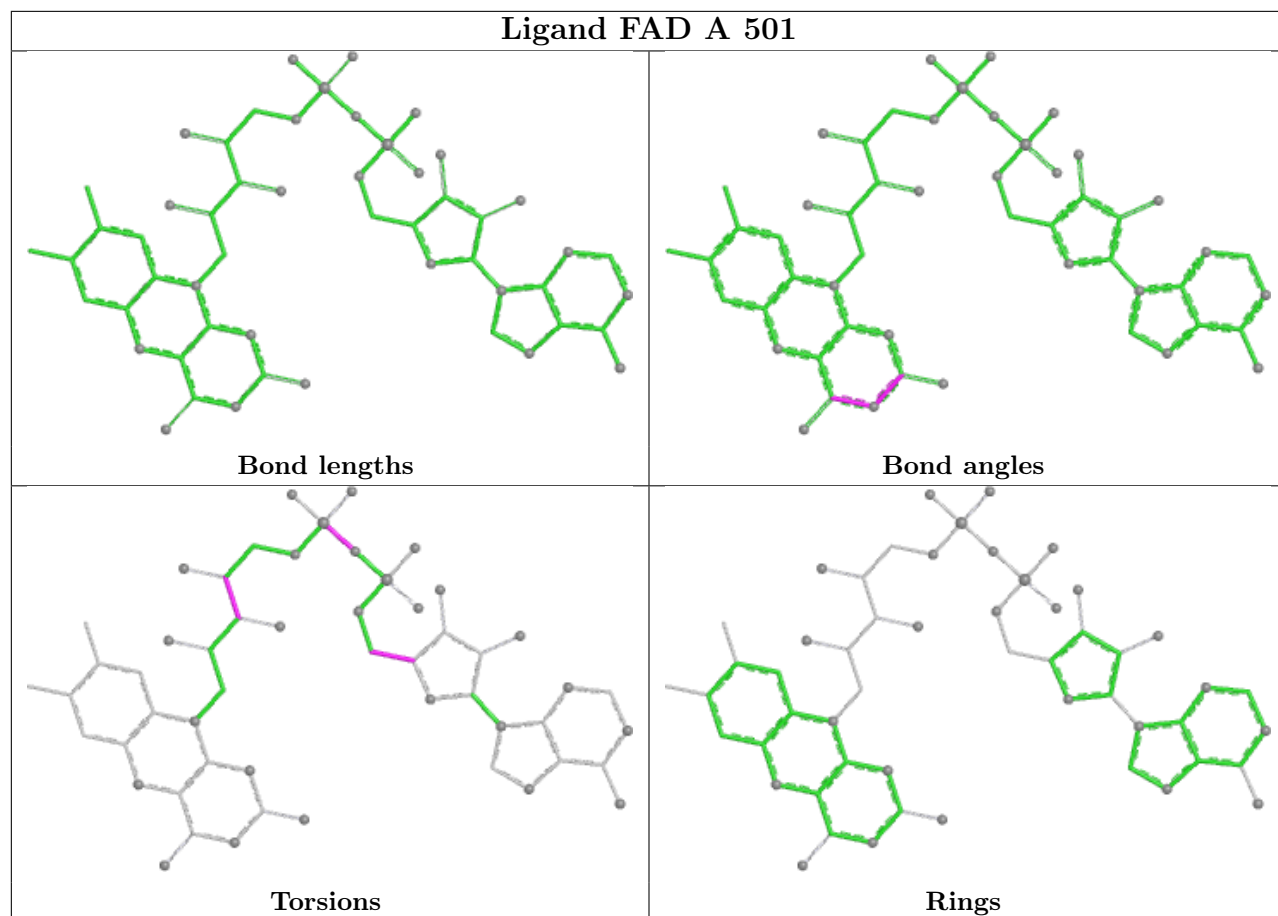
Ligand FAD C 501



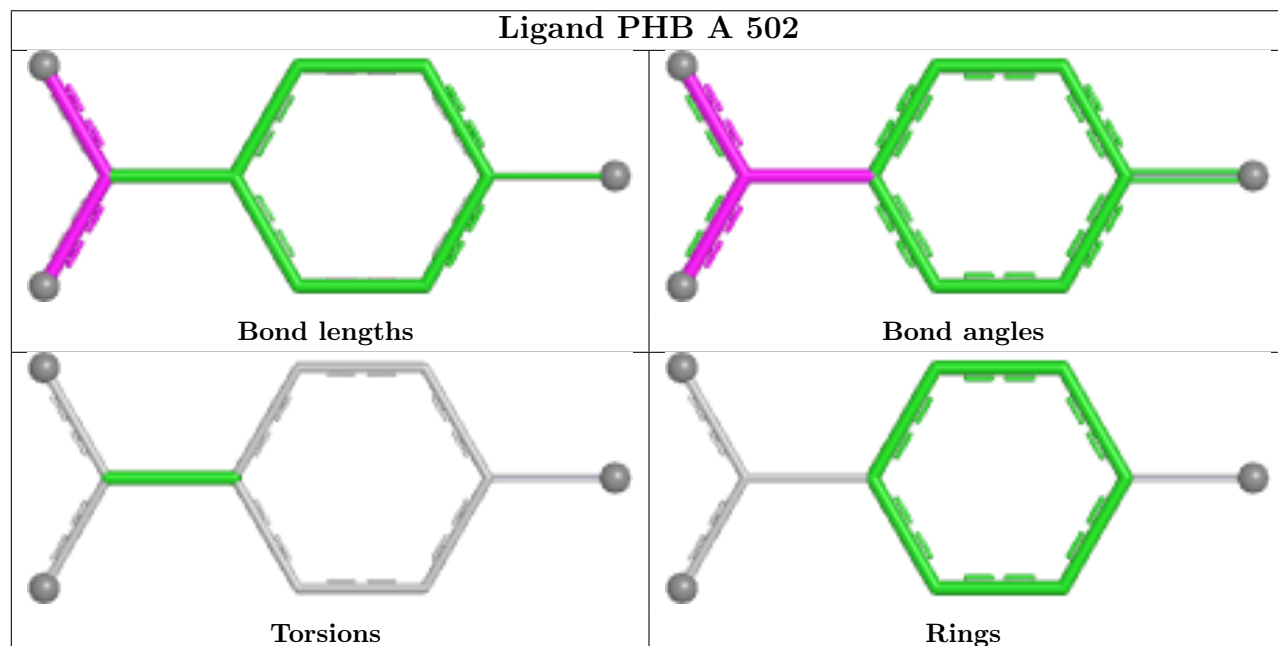
Ligand PHB D 502

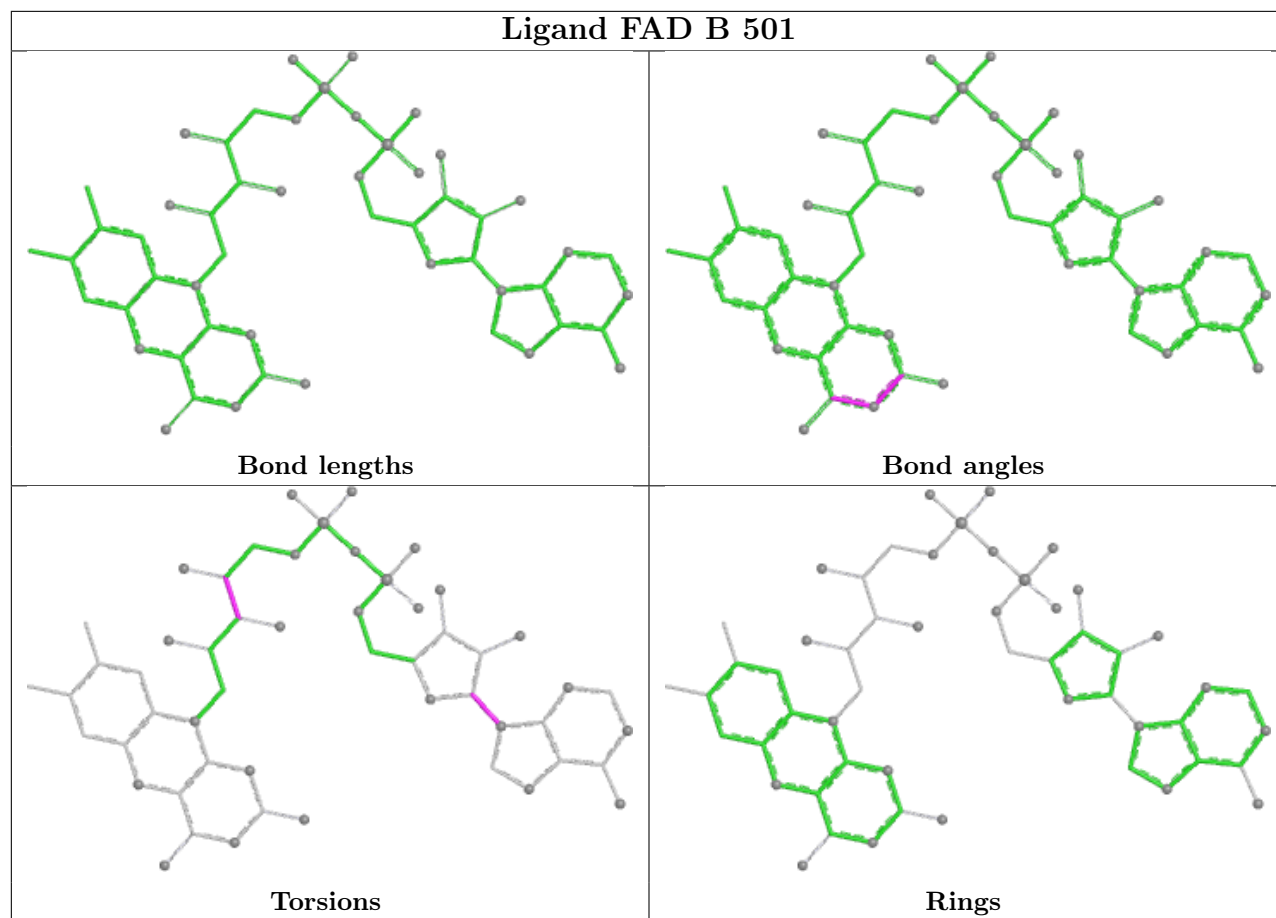


Ligand FAD A 501

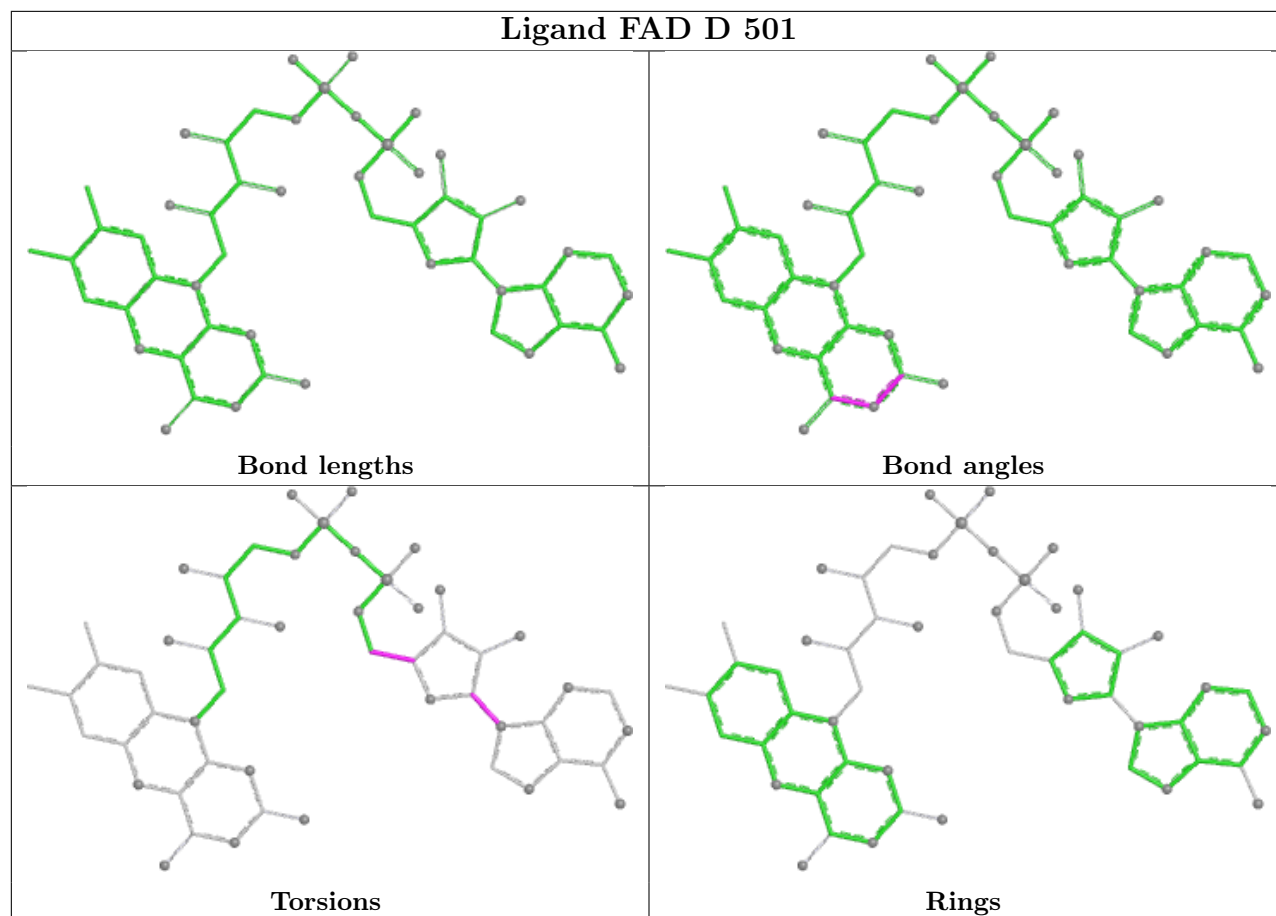


Ligand PHB A 502

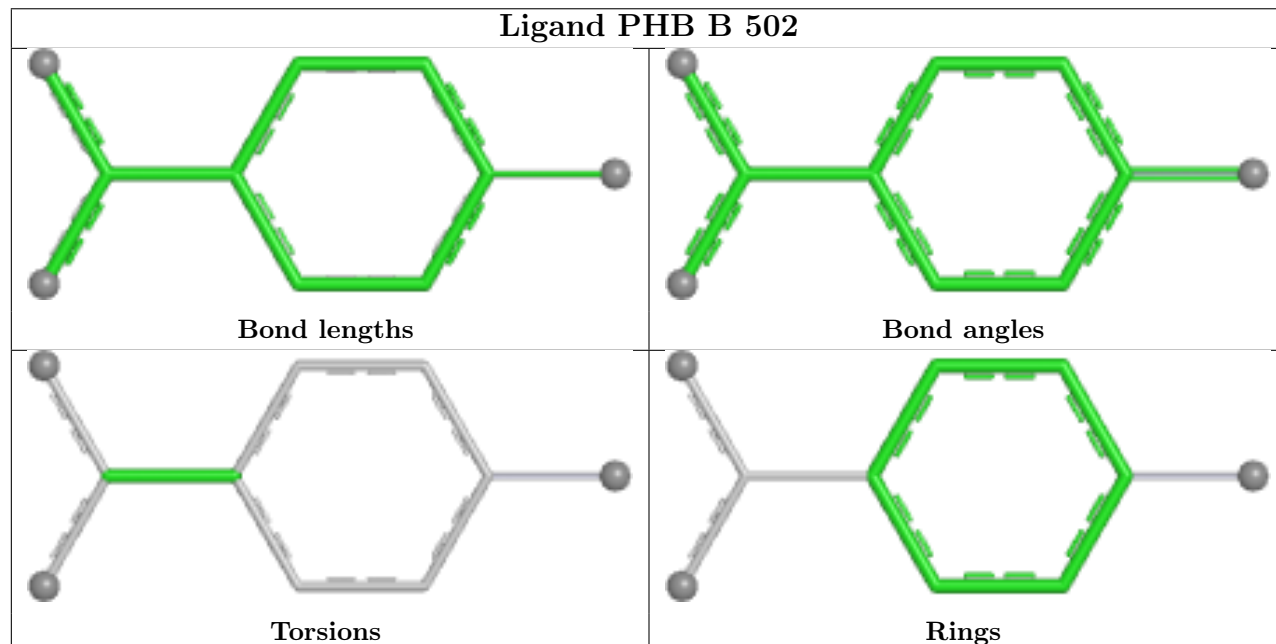


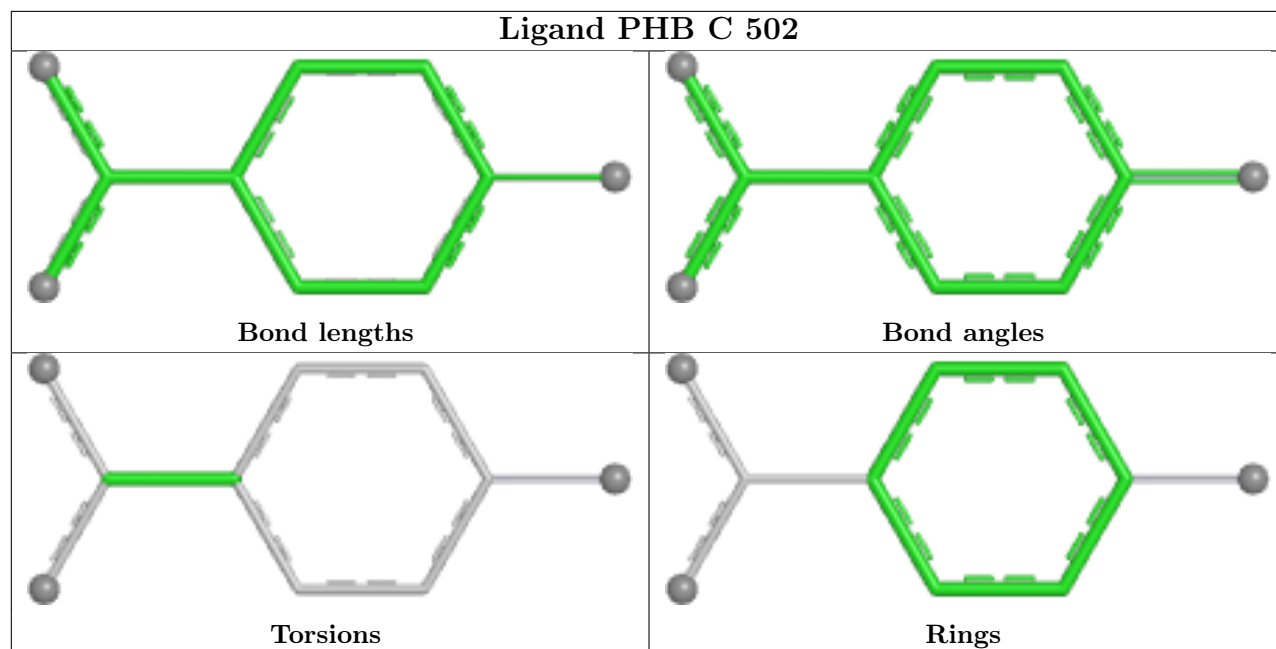


Ligand FAD D 501



Ligand PHB B 502





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	393/402 (97%)	0.45	24 (6%)	27 30	10, 20, 35, 44	2 (0%)
1	B	392/402 (97%)	0.65	33 (8%)	17 20	11, 23, 38, 46	2 (0%)
1	C	391/402 (97%)	0.98	51 (13%)	7 8	14, 26, 41, 56	3 (0%)
1	D	390/402 (97%)	1.25	81 (20%)	2 3	15, 29, 51, 61	1 (0%)
All	All	1566/1608 (97%)	0.84	189 (12%)	8 10	10, 24, 43, 61	8 (0%)

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	390	LEU	5.8
1	D	124	VAL	5.6
1	C	1	MET	5.4
1	C	390	LEU	5.3
1	C	391	PRO	5.1
1	D	315	LEU	5.0
1	C	182	VAL	4.8
1	D	132	VAL	4.5
1	D	158	ALA	4.3
1	D	230	GLN	4.3
1	C	264[A]	GLN	4.2
1	A	254	GLY	3.9
1	C	118	GLY	3.9
1	C	321	ALA	3.9
1	D	43	ILE	3.8
1	B	192	VAL	3.8
1	C	327	LEU	3.7
1	D	254	GLY	3.7
1	C	323	LYS	3.7
1	B	390	LEU	3.7
1	D	139	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	141	PHE	3.6
1	D	152	ILE	3.6
1	C	322	GLY	3.6
1	C	316	GLU	3.5
1	C	326	ILE	3.5
1	D	45	ALA	3.4
1	B	118	GLY	3.4
1	B	94	GLY	3.3
1	D	41	GLY	3.3
1	B	258	LEU	3.3
1	D	232	HIS	3.3
1	A	1	MET	3.2
1	D	46	GLY	3.2
1	D	283	LEU	3.2
1	B	267	ILE	3.2
1	D	233	ILE	3.2
1	D	182	VAL	3.2
1	D	149	LEU	3.1
1	D	137	PRO	3.1
1	A	263	PHE	3.1
1	D	114	LEU	3.1
1	D	319	TYR	3.0
1	C	311	LEU	3.0
1	D	42	THR	3.0
1	D	148	GLU	3.0
1	B	147	GLY	3.0
1	C	317	ALA	2.9
1	D	327	LEU	2.9
1	D	231	ASP	2.9
1	D	321	ALA	2.9
1	D	159	GLY	2.9
1	C	55	LEU	2.9
1	B	146	ASP	2.8
1	B	96	TYR	2.8
1	C	243	SER	2.8
1	C	257	LEU	2.8
1	D	35	THR	2.8
1	C	389	GLY	2.8
1	C	263	PHE	2.8
1	D	144	ASN	2.8
1	C	315	LEU	2.8
1	D	318	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	43	ILE	2.7
1	C	190	ILE	2.7
1	A	133	ASP	2.7
1	C	384	ALA	2.7
1	D	199	HIS	2.6
1	B	223	LEU	2.6
1	B	367	LEU	2.6
1	D	191	LEU	2.6
1	D	127	VAL	2.6
1	C	199	HIS	2.6
1	D	229	ALA	2.6
1	A	45	ALA	2.6
1	B	324	MET	2.6
1	D	25	GLY	2.6
1	D	1	MET	2.6
1	D	242	TRP	2.6
1	D	118	GLY	2.5
1	B	92	THR	2.5
1	D	150	GLN	2.5
1	A	372	TYR	2.5
1	B	175	VAL	2.5
1	D	267	ILE	2.5
1	D	37	GLU	2.5
1	D	219	GLN	2.5
1	A	243	SER	2.5
1	D	236	TRP	2.5
1	B	262	ILE	2.5
1	D	115	GLN	2.4
1	D	330	CYS	2.4
1	D	280	HIS	2.4
1	B	391	PRO	2.4
1	B	148	GLU	2.4
1	A	114	LEU	2.4
1	C	201	LEU	2.4
1	D	172	PRO	2.4
1	D	255	PHE	2.4
1	D	2	ARG	2.4
1	C	115	GLN	2.4
1	D	111	ALA	2.4
1	B	369	GLU	2.4
1	D	44	ARG	2.4
1	D	324	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	217	SER	2.3
1	B	257	LEU	2.3
1	C	319	TYR	2.3
1	C	43	ILE	2.3
1	D	292	ILE	2.3
1	D	175	VAL	2.3
1	D	268	VAL	2.3
1	B	196	PRO	2.3
1	B	374	THR	2.3
1	D	122	PHE	2.3
1	C	318	TYR	2.3
1	B	38	GLU	2.3
1	D	99	VAL	2.3
1	B	46	GLY	2.3
1	C	116	THR	2.3
1	B	91	LEU	2.3
1	C	223	LEU	2.3
1	C	94	GLY	2.3
1	D	7	ILE	2.3
1	D	58	GLN	2.2
1	D	119	GLN	2.2
1	C	325	GLU	2.2
1	D	145	LYS	2.2
1	C	171	ILE	2.2
1	B	97	VAL	2.2
1	D	196	PRO	2.2
1	A	2	ARG	2.2
1	C	198	ALA	2.2
1	C	21	LEU	2.2
1	C	283	LEU	2.2
1	C	335	LEU	2.2
1	D	23	LEU	2.2
1	D	125	GLY	2.2
1	C	26	ILE	2.2
1	D	29	ILE	2.2
1	C	386	ASN	2.2
1	A	146	ASP	2.2
1	D	234	ASP	2.2
1	B	221	GLN	2.2
1	B	44	ARG	2.2
1	D	31	ILE	2.2
1	A	124	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	268	VAL	2.1
1	D	61	VAL	2.1
1	A	393	GLU	2.1
1	A	191	LEU	2.1
1	D	21	LEU	2.1
1	A	374	THR	2.1
1	A	193	GLU	2.1
1	C	356	GLN	2.1
1	A	365	ILE	2.1
1	C	372	TYR	2.1
1	C	329	ARG	2.1
1	D	271	ARG	2.1
1	C	93	GLY	2.1
1	D	311	LEU	2.1
1	A	173	GLN	2.1
1	A	313	ARG	2.1
1	D	252	ARG	2.1
1	B	372	TYR	2.1
1	D	8	ILE	2.1
1	D	314	GLY	2.1
1	D	320	LYS	2.1
1	C	5	VAL	2.1
1	C	219[A]	GLN	2.1
1	A	245	LEU	2.1
1	A	383	LEU	2.1
1	B	143	PRO	2.1
1	D	185	PHE	2.1
1	B	388	ILE	2.1
1	D	388	ILE	2.1
1	B	254	GLY	2.0
1	A	144	ASN	2.0
1	A	253	ASP	2.0
1	C	308	VAL	2.0
1	D	160	CYS	2.0
1	C	20	LEU	2.0
1	D	117	GLY	2.0
1	A	43	ILE	2.0
1	C	220	ILE	2.0
1	C	336	ARG	2.0
1	D	241	ILE	2.0
1	B	217	SER	2.0
1	A	373	VAL	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](#)

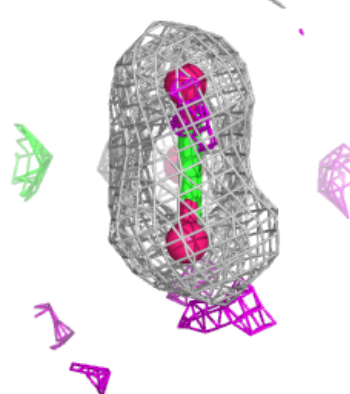
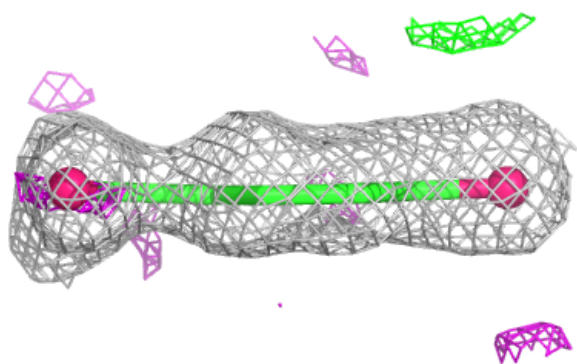
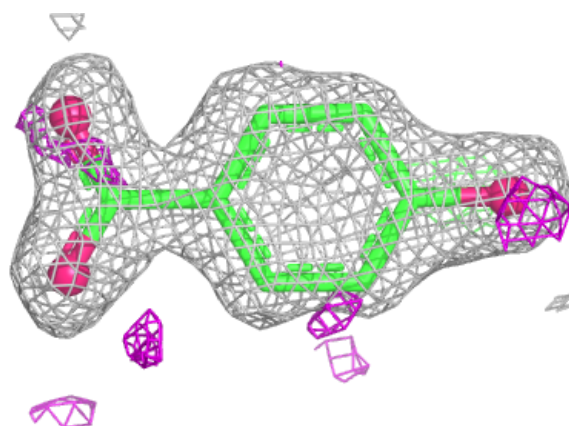
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PHB	B	502	10/10	0.92	0.08	23,24,26,26	0
3	PHB	D	502	10/10	0.93	0.08	20,21,23,23	0
2	FAD	D	501	53/53	0.94	0.08	18,22,29,30	0
3	PHB	C	502	10/10	0.94	0.07	19,20,21,21	0
3	PHB	A	502	10/10	0.94	0.08	16,17,18,19	0
2	FAD	C	501	53/53	0.96	0.07	17,19,21,21	0
2	FAD	A	501	53/53	0.96	0.06	13,15,18,19	0
2	FAD	B	501	53/53	0.97	0.06	13,17,20,22	0

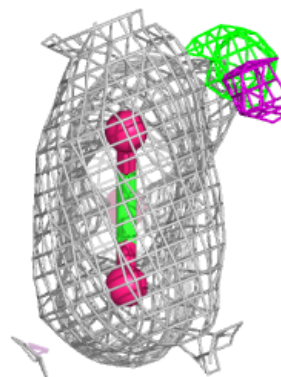
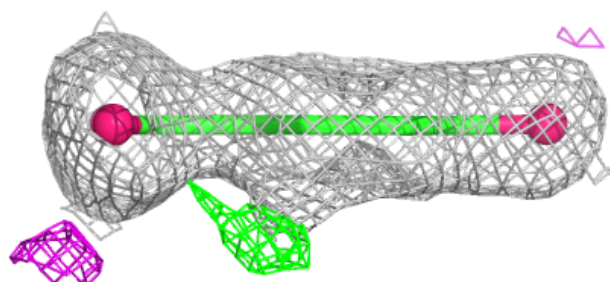
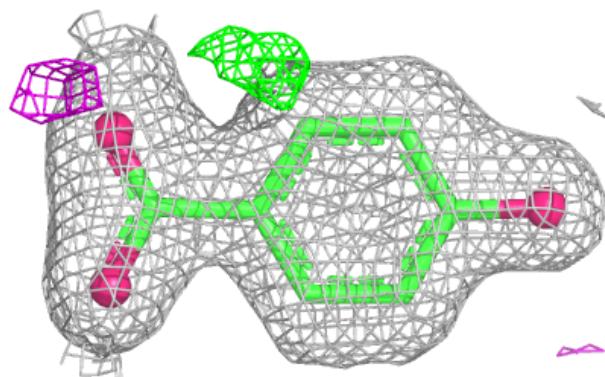
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PHB B 502:

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

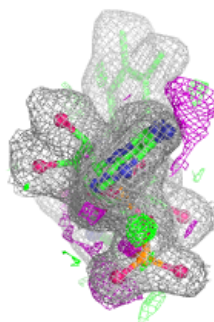
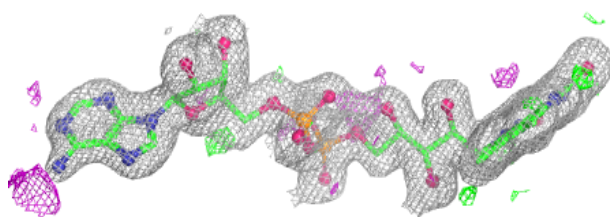
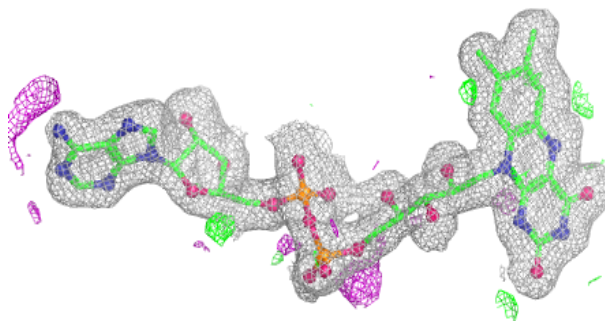
**Electron density around PHB D 502:**

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

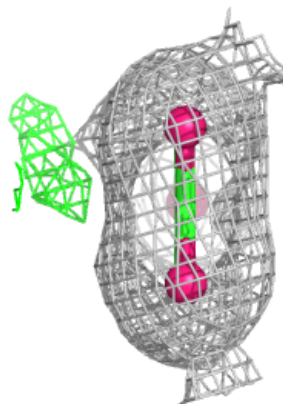
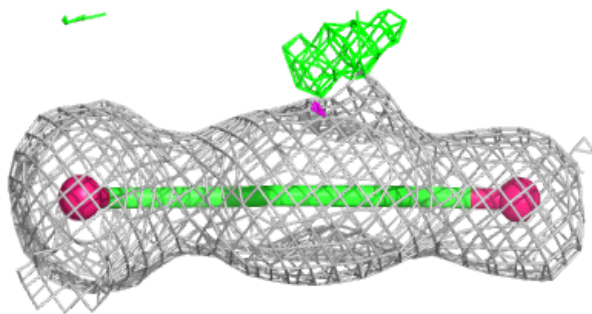
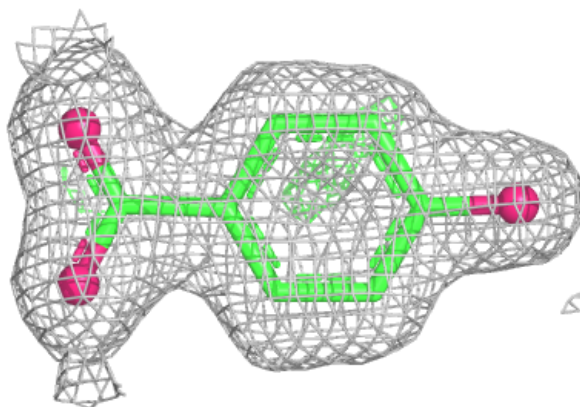


Electron density around FAD D 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

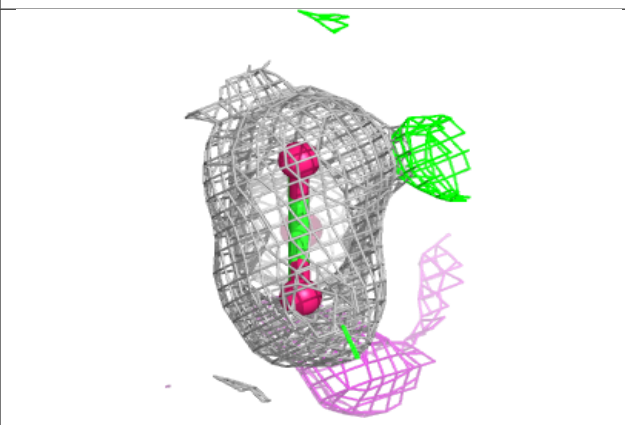
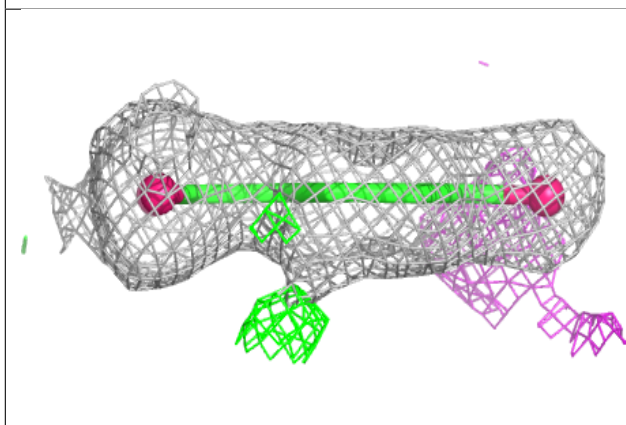
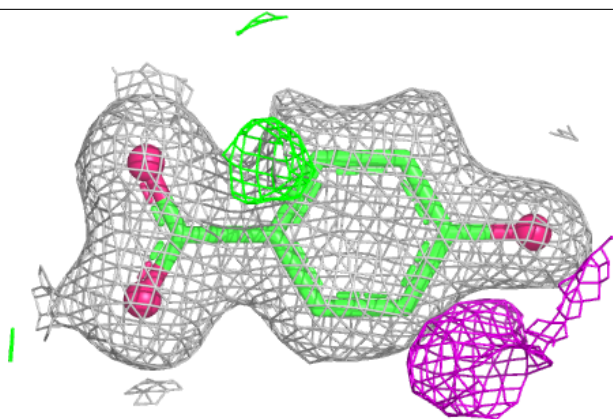
**Electron density around PHB C 502:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

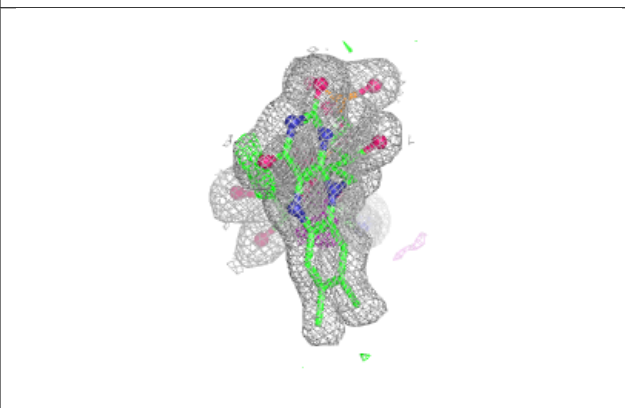
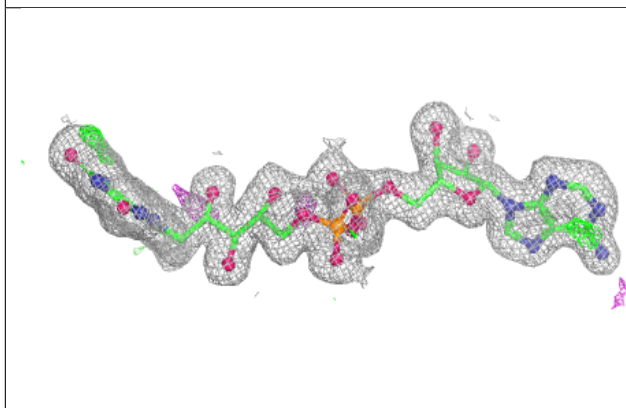
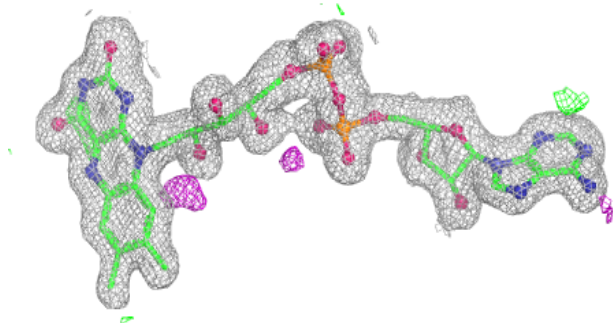


Electron density around PHB A 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

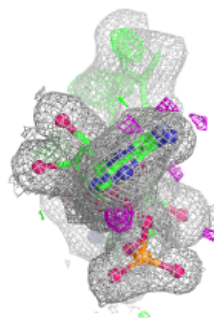
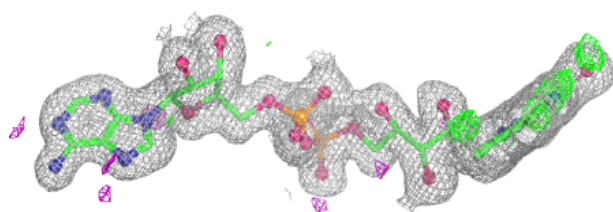
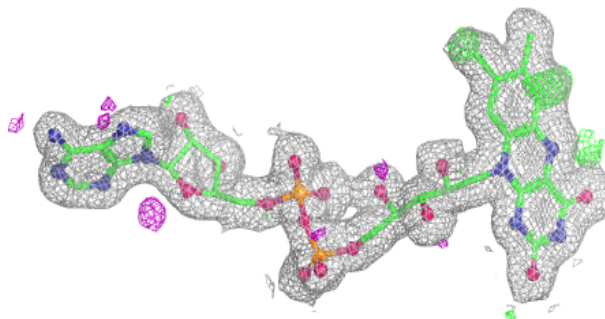
**Electron density around FAD C 501:**

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

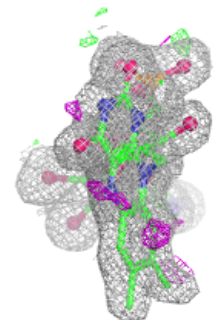
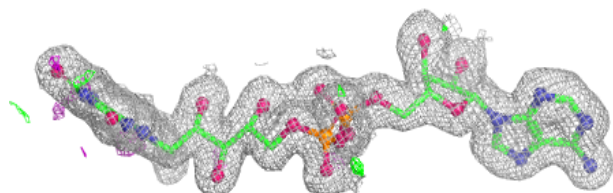
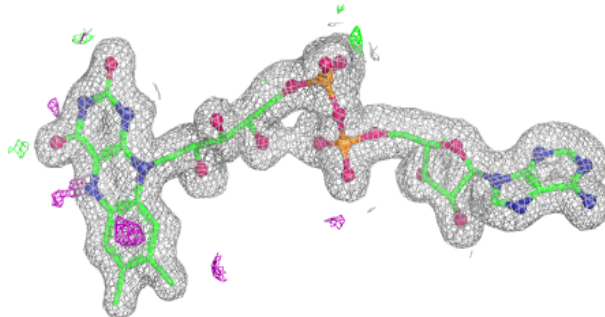


Electron density around FAD A 501:

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

**Electron density around FAD B 501:**

$2mF_o-DF_c$ (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.