



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:08 PM UTC

PDB ID : 9DL4 / pdb_00009dl4
Title : Structure of proline utilization A complexed with 2-pyridinethiol
Authors : Tanner, J.J.; Meeks, K.R.
Deposited on : 2024-09-10
Resolution : 1.80 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

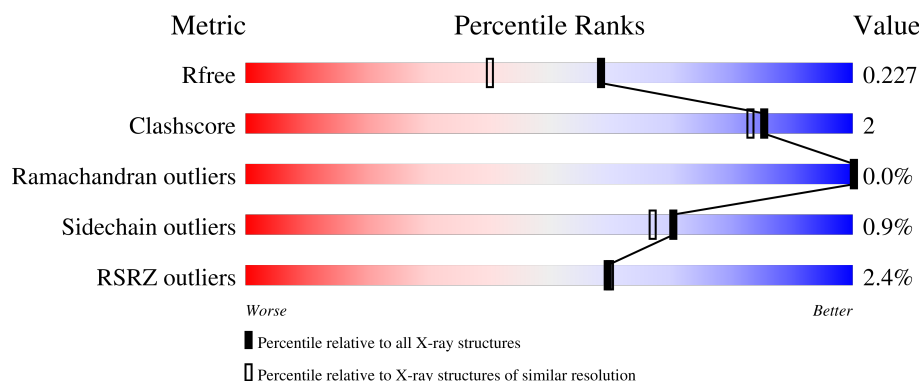
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	1235	
1	B	1235	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FMT	B	1307	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19251 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.

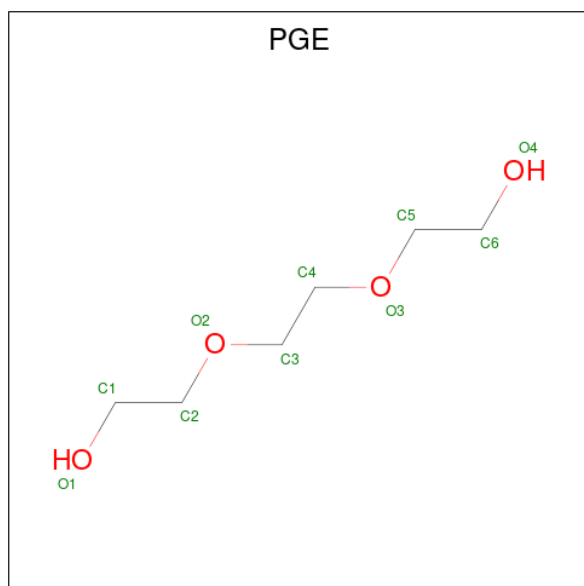
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1205	Total	C	N	O	S	0	12	0
			8938	5631	1605	1669	33			
1	B	1199	Total	C	N	O	S	0	4	0
			8685	5467	1563	1622	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



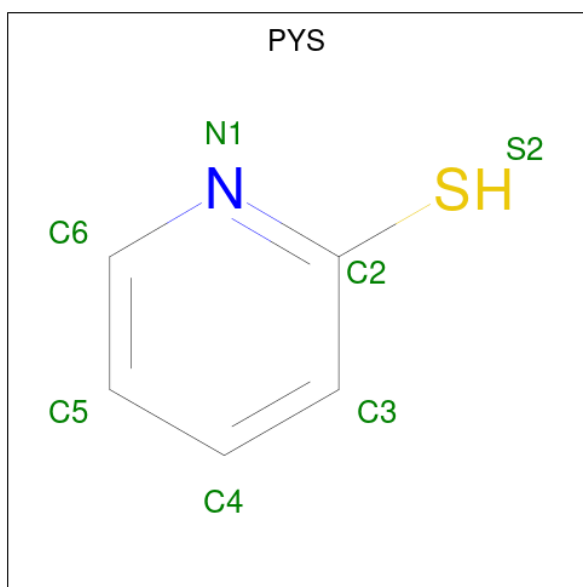
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



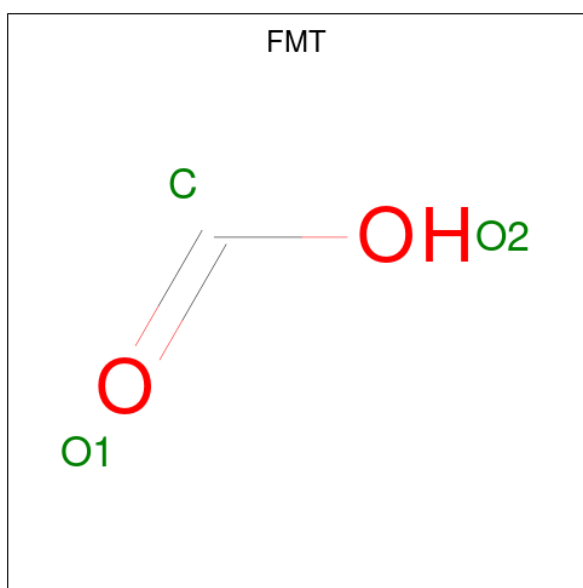
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 2-PYRIDINETHIOL (CCD ID: PYS) (formula: C_5H_5NS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			7	5	1	1		
4	B	1	Total	C	N	S	0	0
			7	5	1	1		

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

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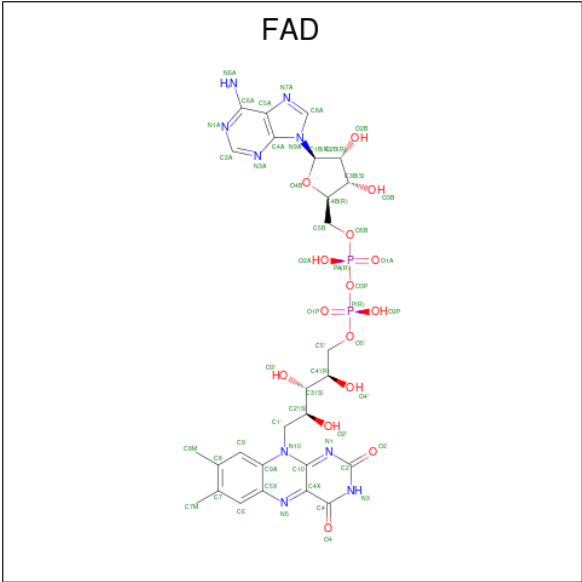
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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

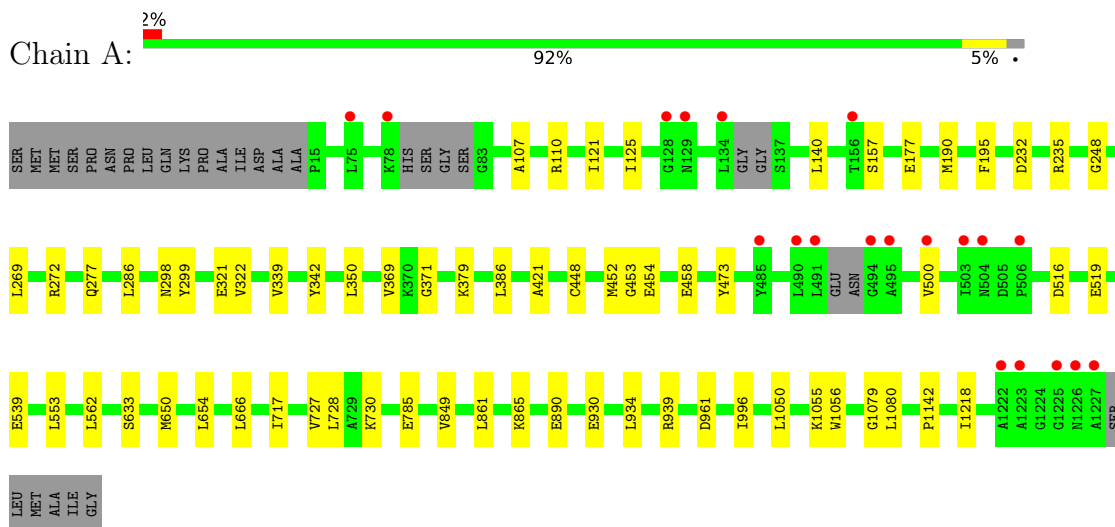
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	748	Total	O	0	0
			748	748		
8	B	645	Total	O	0	0
			645	645		

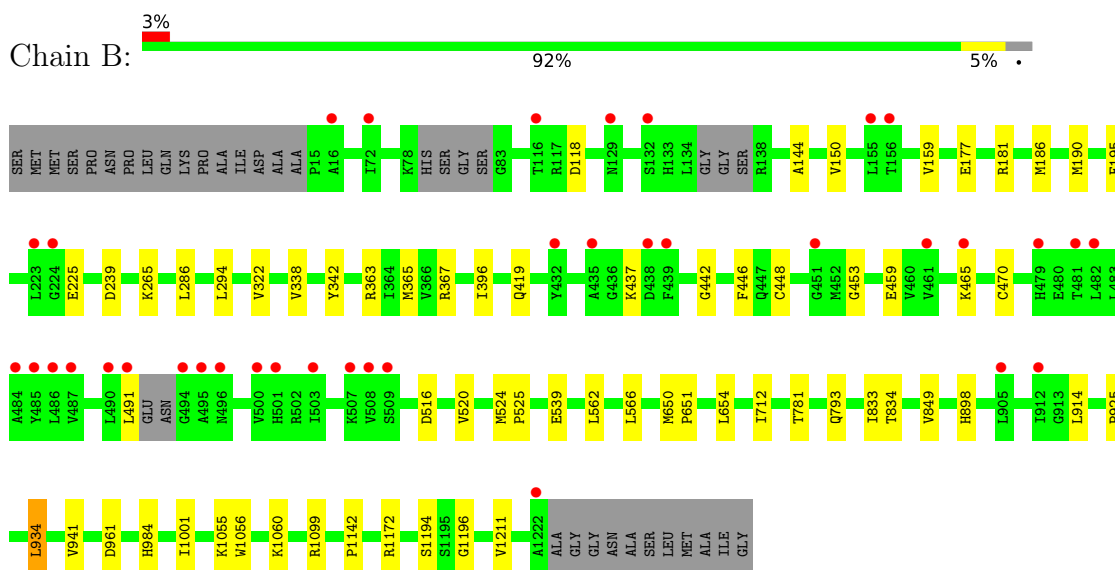
3 Residue-property plots [i](#)

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: Bifunctional protein PutA



- Molecule 1: Bifunctional protein PutA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.16Å 102.37Å 127.50Å 90.00° 106.29° 90.00°	Depositor
Resolution (Å)	40.77 – 1.80 40.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (40.77-1.80) 95.6 (40.77-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.224 0.196 , 0.227	Depositor DCC
R_{free} test set	11292 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19251	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: FAD, PYS, PGE, FMT, PEG, SO4

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	0.27	0/9132	0.45	0/12433
1	B	0.27	0/8849	0.46	0/12070
All	All	0.27	0/17981	0.46	0/24503

There are no bond length outliers.

There are no bond angle outliers.

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	8938	0	8921	37	0
1	B	8685	0	8525	38	0
2	A	10	0	14	1	0
2	B	10	0	14	0	0
3	A	35	0	50	3	0
3	B	21	0	30	2	0
4	A	7	0	5	0	0
4	B	7	0	5	1	0
5	A	3	0	1	1	0
5	B	6	0	2	3	0
6	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	10	0	0	0	0
7	A	53	0	31	4	0
7	B	53	0	31	2	0
8	A	748	0	0	2	1
8	B	645	0	0	2	1
All	All	19251	0	17629	78	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 (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:539:GLU:OE1	8:A:1401:HOH:O	2.05	0.75
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.21	0.73
3:A:1304:PEG:H32	3:A:1305:PEG:H41	1.75	0.68
1:B:539:GLU:OE1	8:B:1401:HOH:O	2.12	0.66
7:A:1313:FAD:HO3'	7:A:1313:FAD:HO3A	1.47	0.61
1:B:118:ASP:OD1	1:B:181:ARG:NH2	2.34	0.61
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.82	0.61
1:B:914:LEU:HD11	1:B:925:PRO:HD3	1.82	0.60
1:B:650:MET:O	1:B:654:LEU:HG	2.03	0.59
1:B:1172:ARG:HH12	5:B:1307:FMT:H	1.68	0.58
1:A:473:TYR:HB2	7:A:1313:FAD:HM71	1.85	0.58
1:B:849:VAL:HG21	1:B:934:LEU:HD11	1.85	0.57
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.86	0.57
1:B:1196:GLY:HA3	3:B:1305:PEG:H22	1.85	0.57
1:A:996[A]:ILE:HD12	1:A:1218:ILE:HG12	1.86	0.56
1:A:650:MET:O	1:A:654:LEU:HG	2.07	0.54
1:A:861[A]:LEU:HG	1:A:865:LYS:HE3	1.89	0.54
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.43	0.53
1:A:849:VAL:HG11	1:A:934:LEU:HD13	1.90	0.53
1:A:562:LEU:HD11	1:A:654:LEU:HD12	1.91	0.53
1:B:365:MET:HE2	1:B:419:GLN:NE2	2.25	0.52
1:A:1079:GLY:HA2	2:A:1301:PGE:H32	1.92	0.52
1:B:898:HIS:CD2	1:B:941:VAL:HG21	2.45	0.52
1:B:712:ILE:HD13	1:B:781:THR:HG21	1.92	0.51
1:A:371:GLY:N	7:A:1313:FAD:O2'	2.43	0.51
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.93	0.51
1:B:834:THR:HG22	1:B:1001:ILE:HD11	1.92	0.51
1:A:386:LEU:HD22	5:A:1307:FMT:H	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:CYS:HB2	1:B:453:GLY:HA3	1.94	0.50
1:B:524[B]:MET:HE3	1:B:525:PRO:HD2	1.93	0.50
1:A:232:ASP:OD1	1:A:235:ARG:NH2	2.46	0.49
1:B:1172:ARG:NH1	5:B:1307:FMT:H	2.27	0.48
1:B:651:PRO:HG3	5:B:1306:FMT:H	1.95	0.48
1:B:1194:SER:OG	3:B:1305:PEG:H32	2.13	0.47
1:B:225:GLU:HB3	1:B:265:LYS:HD2	1.96	0.47
1:B:459:GLU:HA	1:B:465:LYS:HD2	1.96	0.46
1:B:239:ASP:OD2	8:B:1402:HOH:O	2.21	0.46
1:A:107:ALA:HA	1:A:110:ARG:HD3	1.98	0.46
1:B:338:VAL:HG22	1:B:367:ARG:HB3	1.97	0.46
1:B:396:ILE:HD11	1:B:520:VAL:HB	1.98	0.45
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.50	0.45
1:A:785:GLU:H	1:A:785:GLU:HG3	1.59	0.44
7:B:1310:FAD:H9	7:B:1310:FAD:H1'1	1.79	0.44
1:A:1055:LYS:NZ	1:B:961:ASP:OD2	2.39	0.43
1:A:1080:LEU:C	1:A:1080:LEU:HD23	2.43	0.43
1:A:448:CYS:HB2	1:A:453:GLY:HA3	1.99	0.43
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.43	0.43
1:B:1056:TRP:CZ2	1:B:1060:LYS:HD2	2.53	0.43
1:B:363:ARG:NH1	1:B:442:GLY:O	2.48	0.43
1:A:666:LEU:HD12	1:A:666:LEU:HA	1.85	0.43
1:A:379:LYS:HE2	3:A:1304:PEG:H21	2.01	0.43
1:B:793:GLN:HE22	4:B:1303:PYS:H4	1.84	0.43
1:A:454:GLU:O	1:A:458:GLU:HG3	2.18	0.42
1:A:190:MET:HE2	1:A:195:PHE:CZ	2.55	0.42
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.86	0.42
1:A:121:ILE:HA	1:A:125:ILE:HB	2.01	0.42
1:B:150:VAL:CG1	1:B:190:MET:HE1	2.49	0.42
1:A:717:ILE:HG12	1:A:727:VAL:HG11	2.01	0.42
1:A:379:LYS:HE2	3:A:1304:PEG:H31	2.02	0.42
1:B:190:MET:HE2	1:B:195:PHE:CZ	2.54	0.42
7:A:1313:FAD:HM81	7:A:1313:FAD:HM73	1.72	0.41
1:A:298:ASN:ND2	8:A:1406:HOH:O	2.37	0.41
1:B:491:LEU:HD23	1:B:491:LEU:HA	1.86	0.41
1:A:553:LEU:HD12	1:A:666:LEU:HD13	2.01	0.41
1:B:446:PHE:O	1:B:470:CYS:HA	2.21	0.41
1:B:186:MET:O	1:B:190:MET:HG3	2.20	0.41
1:B:1099:ARG:HG3	1:B:1211:VAL:C	2.46	0.41
7:B:1310:FAD:H1'1	7:B:1310:FAD:H4'	1.84	0.41
1:A:272:ARG:HB3	1:A:277:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861[A]:LEU:HD21	1:A:930:GLU:CD	2.46	0.41
1:B:562:LEU:O	1:B:566:LEU:HG	2.21	0.41
1:B:984:HIS:CD2	1:B:984:HIS:C	2.98	0.41
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.55	0.41
1:A:369:VAL:HG12	1:A:421:ALA:HB3	2.03	0.40
1:B:516:ASP:O	1:B:520:VAL:HG23	2.21	0.40
1:A:516:ASP:OD2	1:A:519:GLU:HG2	2.21	0.40
1:A:890:GLU:OE1	1:A:890:GLU:N	2.52	0.40
1:B:144:ALA:HB3	1:B:159:VAL:CG2	2.52	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)
8:A:1611:HOH:O	8:B:1984:HOH:O[1_565]	2.19	0.01

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	1210/1235 (98%)	1189 (98%)	20 (2%)	1 (0%)	48	34
1	B	1195/1235 (97%)	1170 (98%)	25 (2%)	0	100	100
All	All	2405/2470 (97%)	2359 (98%)	45 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	452	MET

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	890/951 (94%)	880 (99%)	10 (1%)	65	60
1	B	835/951 (88%)	829 (99%)	6 (1%)	76	73
All	All	1725/1902 (91%)	1709 (99%)	16 (1%)	70	67

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	157	SER
1	A	177	GLU
1	A	321	GLU
1	A	342	TYR
1	A	500	VAL
1	A	633	SER
1	A	728	LEU
1	A	730	LYS
1	A	939	ARG
1	B	177	GLU
1	B	294	LEU
1	B	342	TYR
1	B	437	LYS
1	B	833	ILE
1	B	934	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	A	479	HIS
1	A	579	GLN
1	A	685	GLN
1	A	975	HIS
1	A	1040	GLN

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Mol	Chain	Res	Type
1	B	419	GLN
1	B	685	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 ⓘ

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PEG	B	1305	-	6,6,6	0.13	0	5,5,5	0.10	0
7	FAD	A	1313	-	58,58,58	2.32	14 (24%)	85,89,89	1.84	20 (23%)
3	PEG	A	1306	-	6,6,6	0.14	0	5,5,5	0.06	0
4	PYS	A	1303	-	6,7,7	0.48	0	6,8,8	0.54	0
7	FAD	B	1310	-	58,58,58	2.17	15 (25%)	85,89,89	1.80	19 (22%)
6	SO4	B	1308	-	4,4,4	0.33	0	6,6,6	0.20	0
3	PEG	B	1302	-	6,6,6	0.21	0	5,5,5	0.11	0
5	FMT	B	1307	-	2,2,2	0.72	0	1,1,1	0.30	0
3	PEG	A	1302	-	6,6,6	0.13	0	5,5,5	0.16	0
3	PEG	A	1304	-	6,6,6	0.19	0	5,5,5	0.07	0
3	PEG	B	1304	-	6,6,6	0.14	0	5,5,5	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	1309	-	4,4,4	0.18	0	6,6,6	0.49	0
2	PGE	A	1301	-	9,9,9	0.35	0	8,8,8	0.33	0
6	SO4	A	1311	-	4,4,4	0.23	0	6,6,6	0.25	0
6	SO4	B	1309	-	4,4,4	0.19	0	6,6,6	0.16	0
3	PEG	A	1305	-	6,6,6	0.20	0	5,5,5	0.13	0
2	PGE	B	1301	-	9,9,9	0.36	0	8,8,8	0.35	0
5	FMT	B	1306	-	2,2,2	0.69	0	1,1,1	0.18	0
4	PYS	B	1303	-	6,7,7	0.43	0	6,8,8	0.67	0
6	SO4	A	1312	-	4,4,4	0.22	0	6,6,6	0.19	0
3	PEG	A	1308	-	6,6,6	0.10	0	5,5,5	0.13	0
6	SO4	A	1310	-	4,4,4	0.20	0	6,6,6	0.27	0
5	FMT	A	1307	-	2,2,2	0.72	0	1,1,1	0.23	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
3	PEG	B	1305	-	-	1/4/4/4	-
7	FAD	A	1313	-	-	9/34/50/50	0/6/6/6
3	PEG	A	1305	-	-	1/4/4/4	-
2	PGE	B	1301	-	-	1/7/7/7	-
3	PEG	A	1306	-	-	1/4/4/4	-
2	PGE	A	1301	-	-	4/7/7/7	-
4	PYS	A	1303	-	-	-	0/1/1/1
4	PYS	B	1303	-	-	-	0/1/1/1
3	PEG	A	1302	-	-	3/4/4/4	-
7	FAD	B	1310	-	-	7/34/50/50	0/6/6/6
3	PEG	A	1304	-	-	4/4/4/4	-
3	PEG	B	1302	-	-	4/4/4/4	-
3	PEG	A	1308	-	-	3/4/4/4	-
3	PEG	B	1304	-	-	2/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1313	FAD	PA-O3P	-8.79	1.50	1.59
7	B	1310	FAD	PA-O3P	-8.09	1.50	1.59
7	A	1313	FAD	O4-C4	7.35	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1310	FAD	O4-C4	6.77	1.36	1.23
7	B	1310	FAD	O2-C2	5.74	1.35	1.24
7	A	1313	FAD	O2-C2	5.06	1.34	1.24
7	B	1310	FAD	C4X-N5	4.36	1.40	1.30
7	A	1313	FAD	C6A-N6A	4.26	1.45	1.34
7	A	1313	FAD	C4X-N5	4.26	1.39	1.30
7	B	1310	FAD	C6A-N6A	3.66	1.43	1.34
7	A	1313	FAD	C2-N1	3.47	1.44	1.36
7	A	1313	FAD	P-O3P	3.11	1.62	1.59
7	A	1313	FAD	O2'-C2'	-3.05	1.36	1.43
7	B	1310	FAD	C2-N1	2.85	1.43	1.36
7	A	1313	FAD	C10-N1	2.77	1.38	1.33
7	A	1313	FAD	PA-O5B	-2.70	1.48	1.59
7	B	1310	FAD	C10-N1	2.69	1.38	1.33
7	A	1313	FAD	O4'-C4'	-2.53	1.38	1.43
7	B	1310	FAD	O2'-C2'	-2.46	1.38	1.43
7	B	1310	FAD	PA-O5B	-2.33	1.50	1.59
7	B	1310	FAD	O4B-C4B	-2.21	1.40	1.45
7	B	1310	FAD	P-O1P	2.21	1.58	1.50
7	A	1313	FAD	PA-O2A	-2.21	1.45	1.55
7	A	1313	FAD	C5A-C4A	2.16	1.42	1.39
7	B	1310	FAD	P-O3P	2.16	1.61	1.59
7	B	1310	FAD	O2B-C2B	-2.14	1.37	1.43
7	B	1310	FAD	PA-O2A	-2.13	1.45	1.55
7	B	1310	FAD	O4'-C4'	-2.08	1.39	1.43
7	A	1313	FAD	P-O1P	2.07	1.58	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1310	FAD	N3A-C2A-N1A	-5.90	119.65	128.58
7	A	1313	FAD	N3A-C2A-N1A	-5.78	119.83	128.58
7	A	1313	FAD	C5A-C4A-N3A	-5.07	119.74	126.72
7	B	1310	FAD	C5A-C4A-N3A	-4.53	120.48	126.72
7	B	1310	FAD	O2P-P-O3P	-4.18	95.98	107.27
7	A	1313	FAD	N3A-C4A-N9A	4.01	134.00	127.17
7	A	1313	FAD	O2P-P-O3P	-4.00	96.47	107.27
7	B	1310	FAD	C5A-N7A-C8A	3.81	109.43	103.45
7	A	1313	FAD	C5A-N7A-C8A	3.77	109.37	103.45
7	A	1313	FAD	C2A-N3A-C4A	3.63	120.69	111.83
7	B	1310	FAD	N3A-C4A-N9A	3.62	133.33	127.17
7	B	1310	FAD	C2A-N3A-C4A	3.47	120.31	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1313	FAD	C4-C4X-N5	3.34	122.82	118.21
7	B	1310	FAD	C4X-C4-N3	3.13	121.21	113.25
7	B	1310	FAD	N9A-C8A-N7A	-3.13	109.50	113.94
7	A	1313	FAD	O3P-P-O1P	3.08	119.98	110.70
7	A	1313	FAD	O2A-PA-O3P	-3.08	98.96	107.27
7	A	1313	FAD	N9A-C8A-N7A	-3.07	109.58	113.94
7	B	1310	FAD	O3P-P-O1P	3.05	119.86	110.70
7	B	1310	FAD	C4-N3-C2	-3.02	120.27	125.64
7	A	1313	FAD	C4A-C5A-N7A	-2.99	107.16	110.58
7	B	1310	FAD	C5X-C9A-N10	2.97	120.66	117.97
7	B	1310	FAD	C4A-C5A-N7A	-2.96	107.20	110.58
7	A	1313	FAD	C4'-C3'-C2'	2.96	118.49	113.57
7	A	1313	FAD	C4-N3-C2	-2.95	120.41	125.64
7	B	1310	FAD	O2A-PA-O3P	-2.91	99.40	107.27
7	B	1310	FAD	O4-C4-C4X	-2.86	118.99	126.53
7	B	1310	FAD	C4-C4X-N5	2.83	122.11	118.21
7	A	1313	FAD	C4X-C4-N3	2.76	120.29	113.25
7	A	1313	FAD	O5'-P-O1P	2.47	118.72	108.94
7	A	1313	FAD	C5X-C9A-N10	2.40	120.14	117.97
7	B	1310	FAD	C9-C9A-N10	-2.36	118.67	121.85
7	A	1313	FAD	C10-C4X-N5	-2.24	120.24	124.81
7	B	1310	FAD	C2A-N1A-C6A	2.15	122.27	118.73
7	B	1310	FAD	O2-C2-N1	-2.15	118.24	121.80
7	A	1313	FAD	C1'-C2'-C3'	2.14	115.45	109.66
7	A	1313	FAD	O2P-P-O5'	-2.04	98.34	107.57
7	B	1310	FAD	O5'-P-O1P	2.03	116.99	108.94
7	A	1313	FAD	C4X-C10-N10	2.02	119.38	116.48

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1310	FAD	N10-C1'-C2'-O2'
7	B	1310	FAD	N10-C1'-C2'-C3'
7	B	1310	FAD	C5'-O5'-P-O2P
7	A	1313	FAD	C2'-C3'-C4'-O4'
7	A	1313	FAD	O3'-C3'-C4'-O4'
3	B	1302	PEG	O1-C1-C2-O2
7	A	1313	FAD	O3'-C3'-C4'-C5'
7	A	1313	FAD	C2'-C3'-C4'-C5'
3	A	1304	PEG	O1-C1-C2-O2
3	A	1308	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	B	1302	PEG	O2-C3-C4-O4
7	A	1313	FAD	C3B-C4B-C5B-O5B
2	B	1301	PGE	O1-C1-C2-O2
2	A	1301	PGE	O1-C1-C2-O2
3	A	1304	PEG	O2-C3-C4-O4
3	A	1308	PEG	O1-C1-C2-O2
3	A	1306	PEG	O1-C1-C2-O2
3	A	1308	PEG	C1-C2-O2-C3
7	A	1313	FAD	P-O3P-PA-O5B
7	B	1310	FAD	P-O3P-PA-O5B
3	A	1304	PEG	C1-C2-O2-C3
3	B	1302	PEG	C1-C2-O2-C3
3	B	1304	PEG	C1-C2-O2-C3
2	A	1301	PGE	C1-C2-O2-C3
3	A	1304	PEG	C4-C3-O2-C2
3	A	1302	PEG	C4-C3-O2-C2
3	B	1304	PEG	C4-C3-O2-C2
2	A	1301	PGE	O3-C5-C6-O4
2	A	1301	PGE	C4-C3-O2-C2
3	B	1302	PEG	C4-C3-O2-C2
7	A	1313	FAD	C5B-O5B-PA-O3P
7	B	1310	FAD	C5B-O5B-PA-O3P
7	B	1310	FAD	C5'-O5'-P-O1P
3	A	1302	PEG	O2-C3-C4-O4
3	A	1305	PEG	O2-C3-C4-O4
7	B	1310	FAD	C3B-C4B-C5B-O5B
3	B	1305	PEG	C1-C2-O2-C3
3	A	1302	PEG	C1-C2-O2-C3
7	A	1313	FAD	O4'-C4'-C5'-O5'
7	A	1313	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

10 monomers are involved in 17 short contacts:

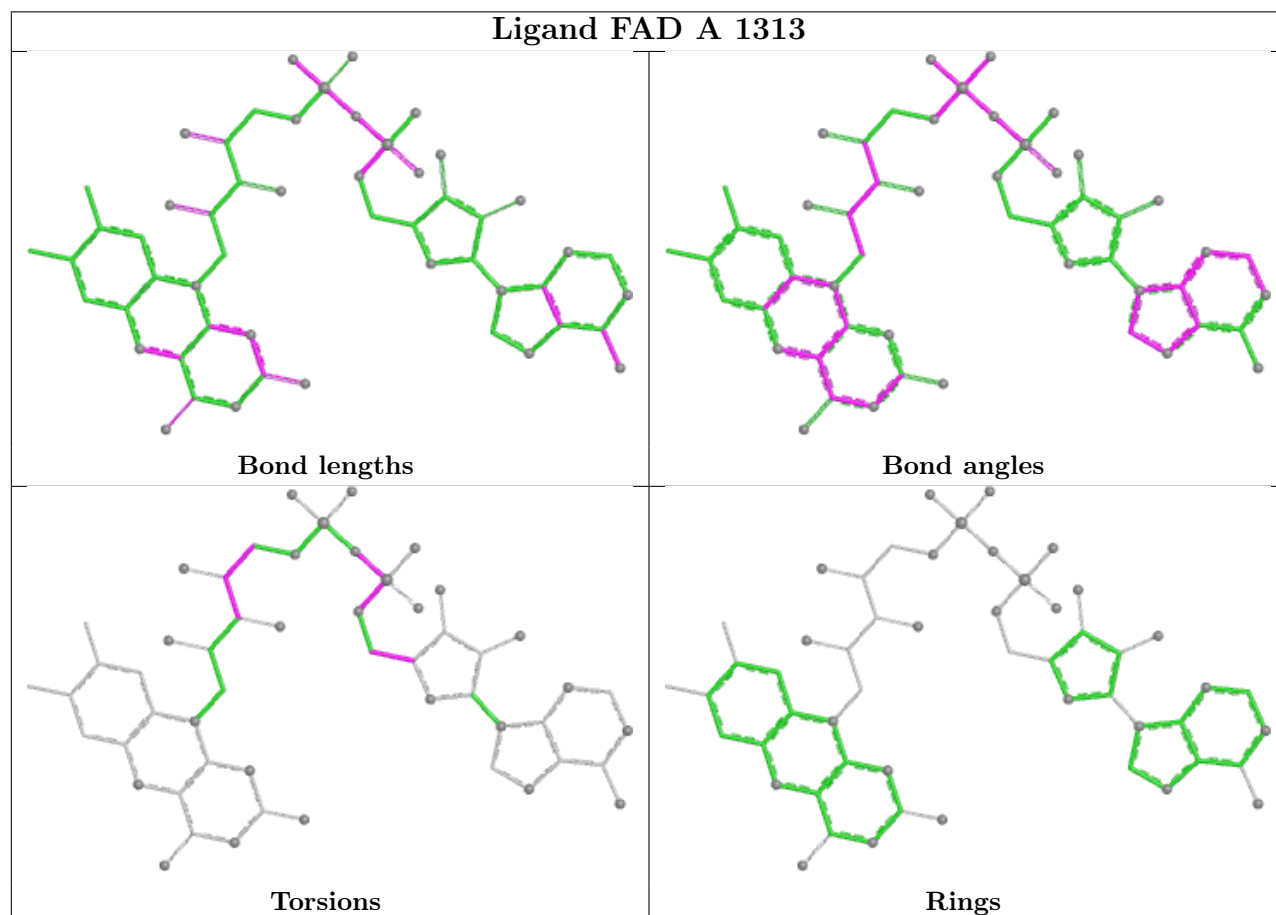
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1305	PEG	2	0
7	A	1313	FAD	4	0
7	B	1310	FAD	2	0
5	B	1307	FMT	2	0
3	A	1304	PEG	3	0
2	A	1301	PGE	1	0
3	A	1305	PEG	1	0

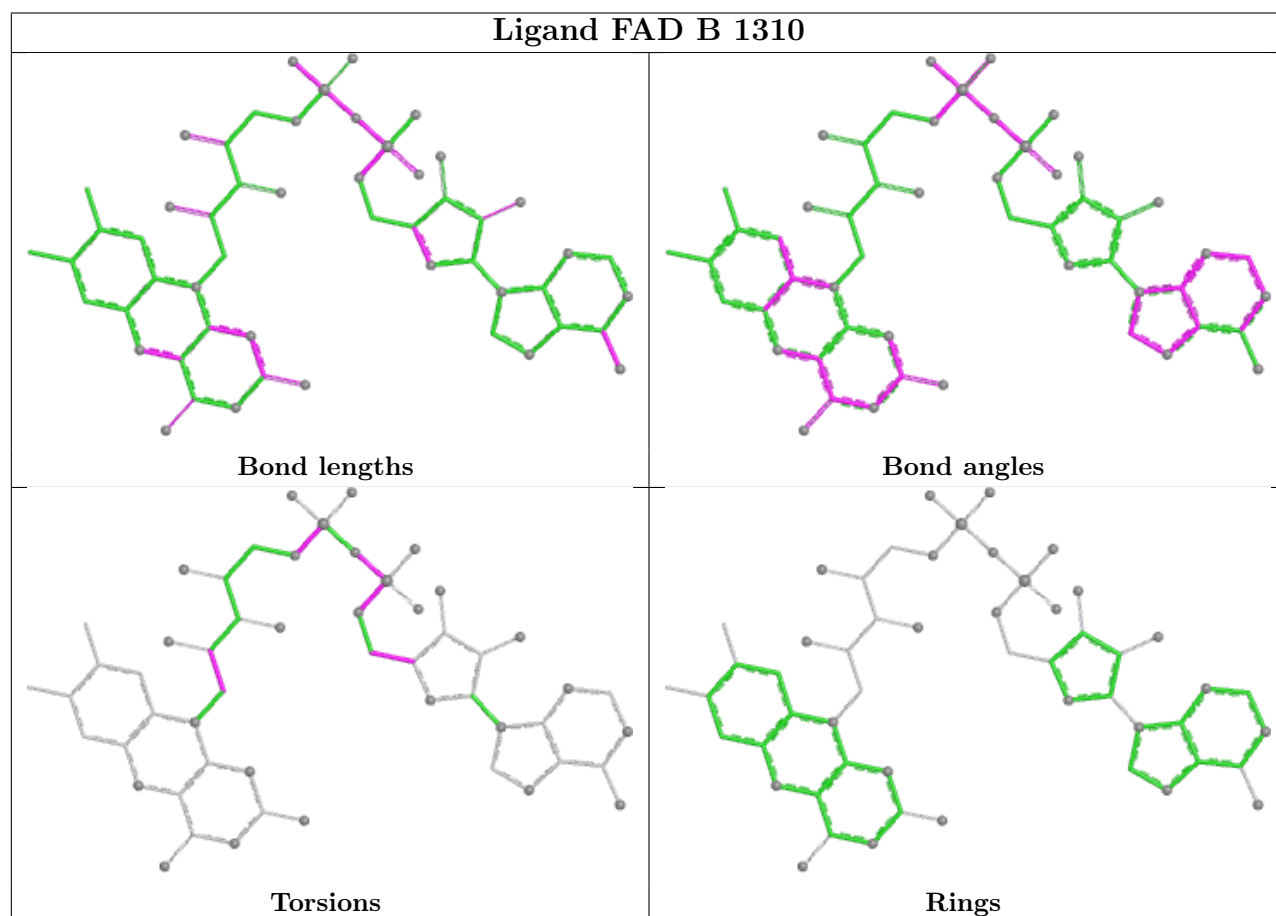
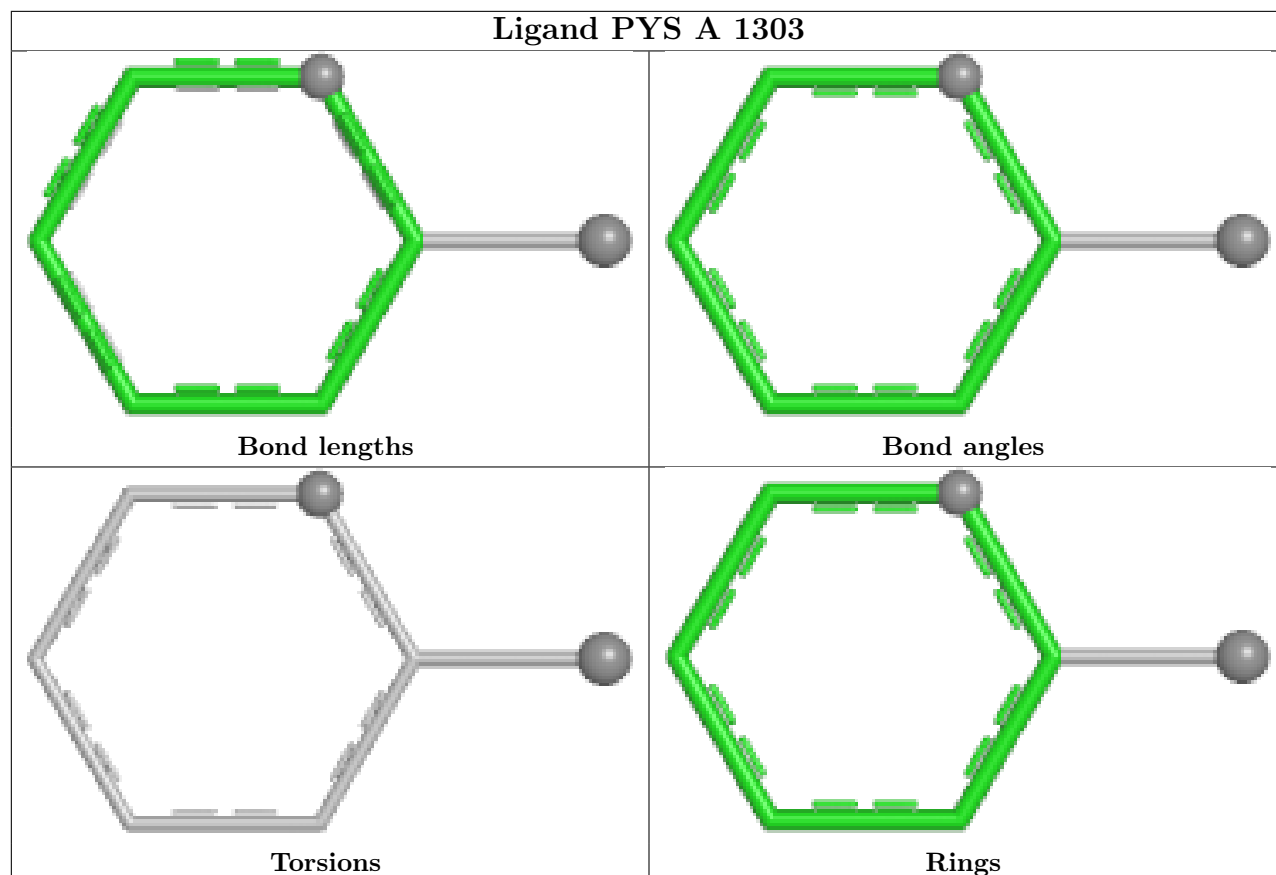
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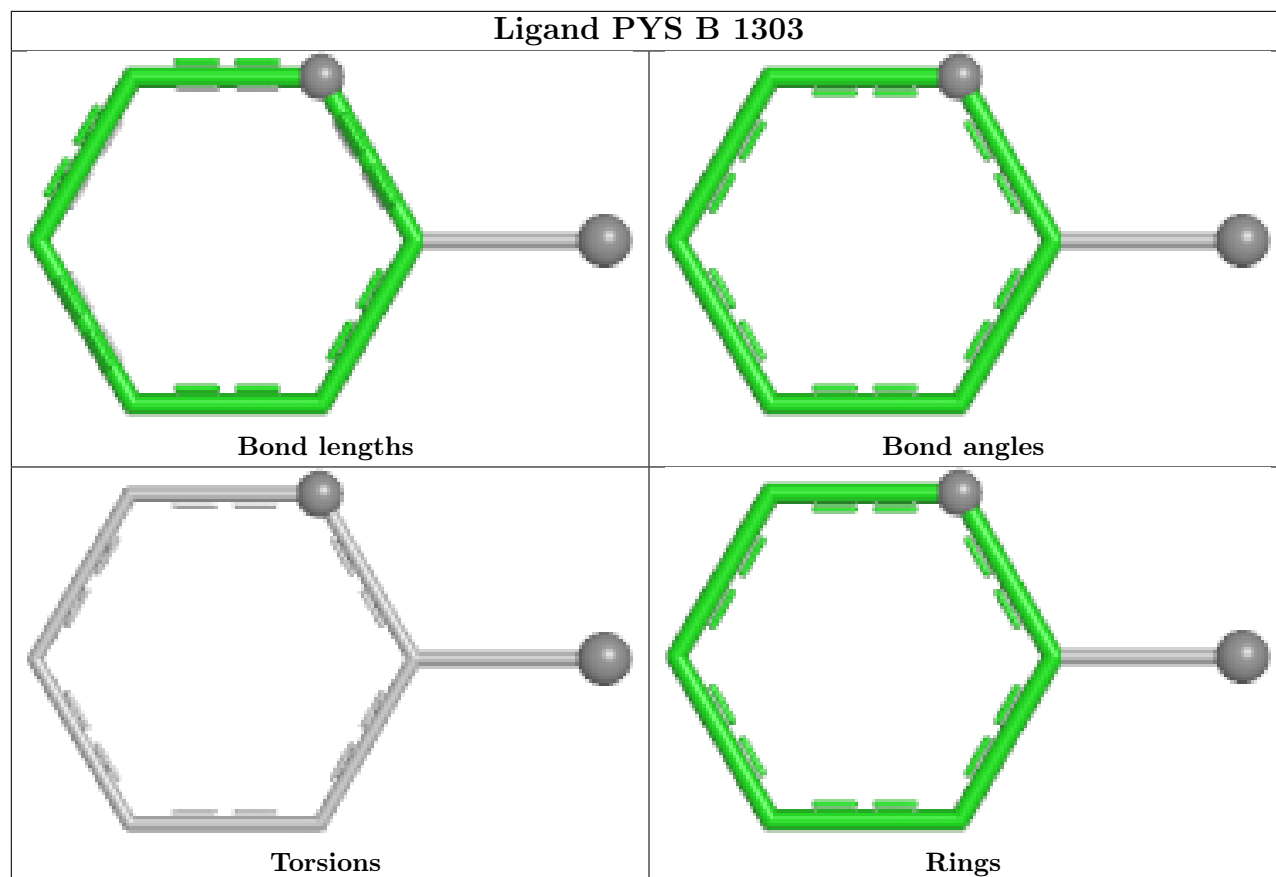
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1306	FMT	1	0
4	B	1303	PYS	1	0
5	A	1307	FMT	1	0

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	1205/1235 (97%)	-0.03	20 (1%) 69 69	11, 30, 50, 63	12 (0%)
1	B	1199/1235 (97%)	0.10	37 (3%) 51 51	14, 32, 54, 66	4 (0%)
All	All	2404/2470 (97%)	0.04	57 (2%) 59 60	11, 31, 52, 66	16 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	494	GLY	6.0
1	B	491	LEU	5.5
1	B	487	VAL	4.8
1	B	495	ALA	4.3
1	A	495	ALA	4.0
1	B	1222	ALA	3.8
1	A	1223	ALA	3.6
1	B	486	LEU	3.4
1	B	490	LEU	3.4
1	B	485	TYR	3.3
1	B	439	PHE	3.3
1	A	1222	ALA	3.2
1	A	503	ILE	3.2
1	A	156	THR	3.1
1	A	1226	ASN	3.1
1	B	507	LYS	3.0
1	A	1225	GLY	2.9
1	A	506	PRO	2.8
1	B	223	LEU	2.8
1	A	75	LEU	2.8
1	B	438	ASP	2.7
1	B	912	ILE	2.7
1	B	16	ALA	2.7
1	B	129	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	482	LEU	2.6
1	A	485	TYR	2.6
1	B	116	THR	2.6
1	B	465	LYS	2.5
1	B	508	VAL	2.5
1	A	494	GLY	2.5
1	B	224	GLY	2.5
1	B	479	HIS	2.4
1	B	72	ILE	2.4
1	A	504	ASN	2.4
1	B	155	LEU	2.4
1	B	500	VAL	2.4
1	A	491	LEU	2.3
1	A	134	LEU	2.3
1	B	509	SER	2.3
1	B	481	THR	2.3
1	B	432	TYR	2.2
1	B	435	ALA	2.2
1	A	490	LEU	2.2
1	B	503	ILE	2.2
1	B	501	HIS	2.2
1	B	905	LEU	2.2
1	B	484	ALA	2.2
1	A	500	VAL	2.1
1	B	461	VAL	2.1
1	A	128	GLY	2.1
1	A	78	LYS	2.1
1	A	1227	ALA	2.1
1	B	496	ASN	2.0
1	B	132	SER	2.0
1	B	156	THR	2.0
1	A	129	ASN	2.0
1	B	451	GLY	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 ⓘ

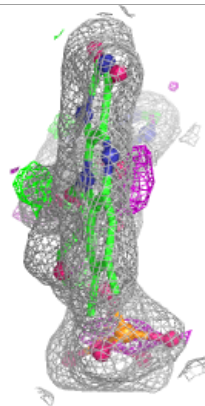
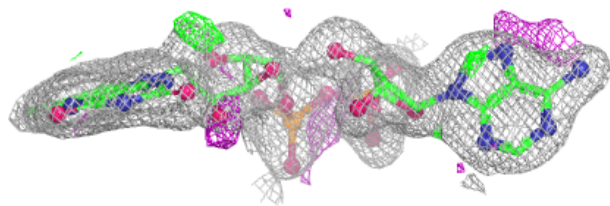
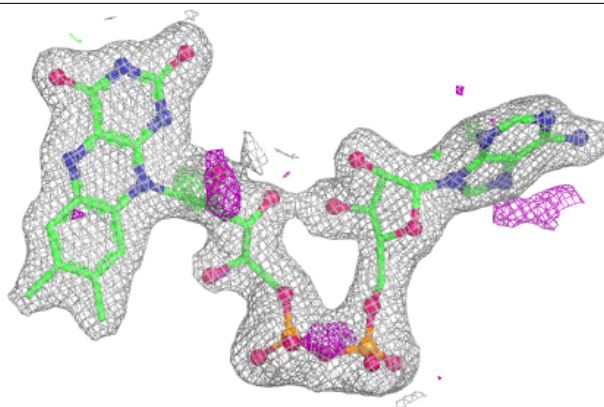
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PEG	A	1305	7/7	0.79	0.13	32,36,43,44	0
3	PEG	B	1305	7/7	0.80	0.12	46,46,48,50	0
3	PEG	A	1308	7/7	0.84	0.11	41,43,49,50	0
5	FMT	B	1306	3/3	0.84	0.13	38,38,38,40	3
5	FMT	B	1307	3/3	0.85	0.12	48,48,49,53	0
2	PGE	A	1301	10/10	0.86	0.10	28,36,46,48	0
3	PEG	A	1304	7/7	0.88	0.11	26,31,36,45	0
6	SO4	A	1312	5/5	0.89	0.07	56,57,60,60	0
6	SO4	B	1309	5/5	0.89	0.11	31,33,36,40	5
3	PEG	B	1302	7/7	0.90	0.11	26,33,36,46	0
3	PEG	B	1304	7/7	0.91	0.08	33,34,42,43	0
3	PEG	A	1306	7/7	0.92	0.09	35,38,43,44	0
6	SO4	A	1311	5/5	0.92	0.08	42,43,44,53	5
5	FMT	A	1307	3/3	0.93	0.08	23,23,33,34	3
3	PEG	A	1302	7/7	0.93	0.09	36,37,42,44	0
7	FAD	A	1313	53/53	0.93	0.08	23,33,39,44	0
4	PYS	A	1303	7/7	0.94	0.09	35,38,41,42	0
2	PGE	B	1301	10/10	0.94	0.07	31,35,39,39	0
7	FAD	B	1310	53/53	0.94	0.08	23,30,35,39	0
6	SO4	A	1310	5/5	0.95	0.08	32,36,42,43	5
4	PYS	B	1303	7/7	0.95	0.08	30,33,34,39	0
6	SO4	A	1309	5/5	0.98	0.05	27,28,29,31	0
6	SO4	B	1308	5/5	0.99	0.05	23,25,26,28	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.

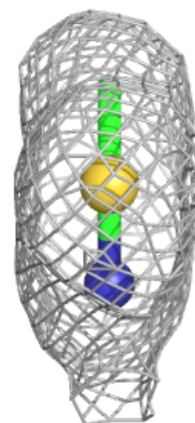
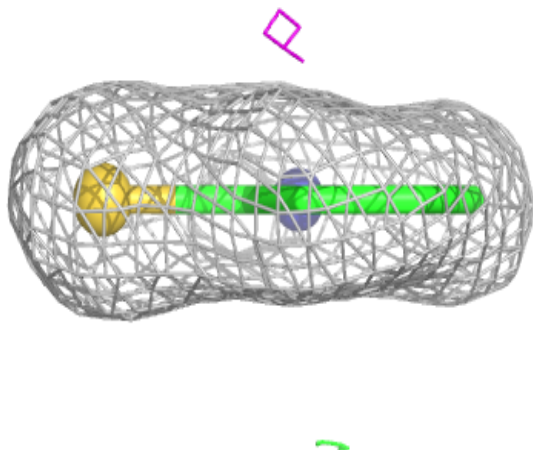
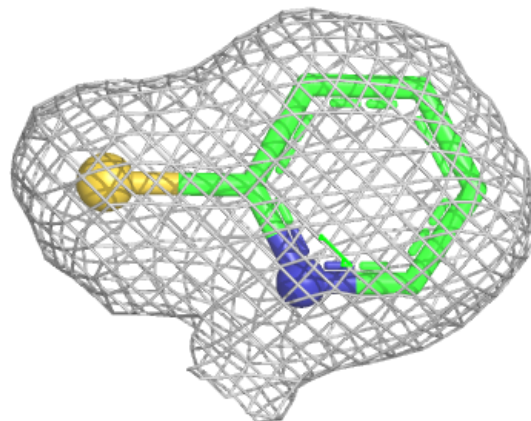
Electron density around FAD A 1313:

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



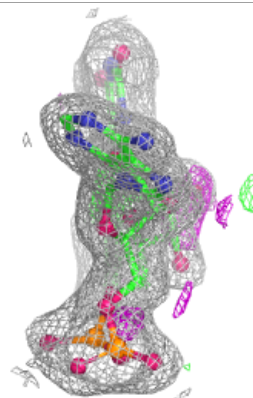
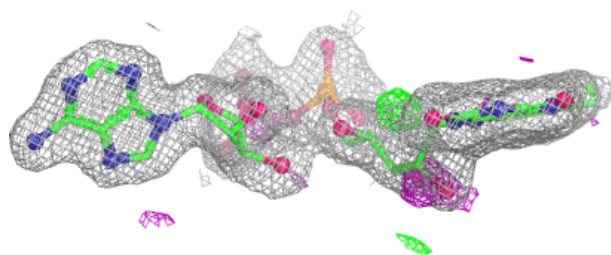
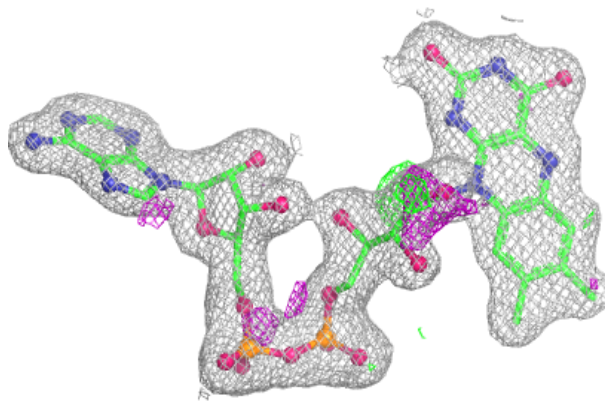
Electron density around PYS A 1303:

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

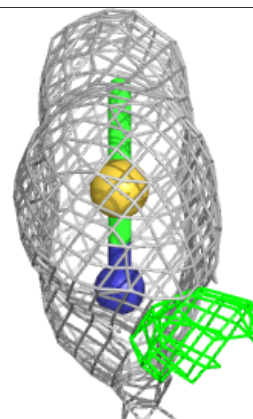
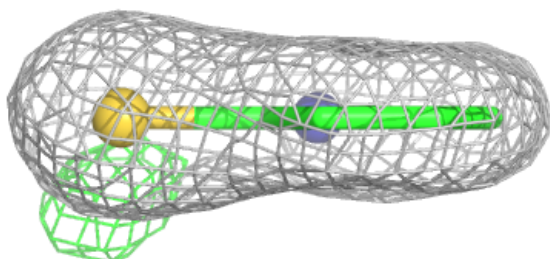
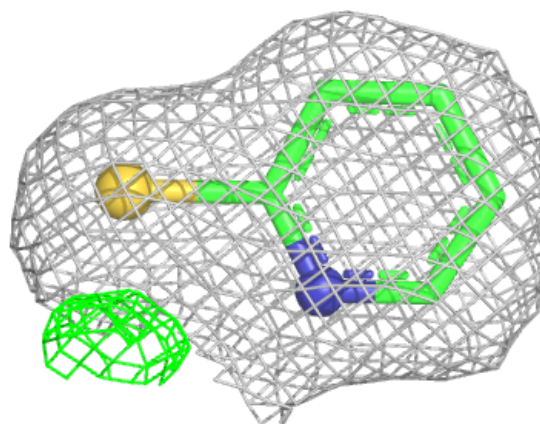


Electron density around FAD B 1310:

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

**Electron density around PYS B 1303:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.