



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:09 PM UTC

PDB ID : 1PXB / pdb_00001pxb
Title : CRYSTAL STRUCTURES OF MUTANT PSEUDOMONAS AERUGINOSA P-HYDROXYBENZOATE HYDROXYLASE: THE TYR201PHE, TYR385PHE, AND ASN300ASP VARIANTS
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Deposited on : 1994-09-27
Resolution : 2.30 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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

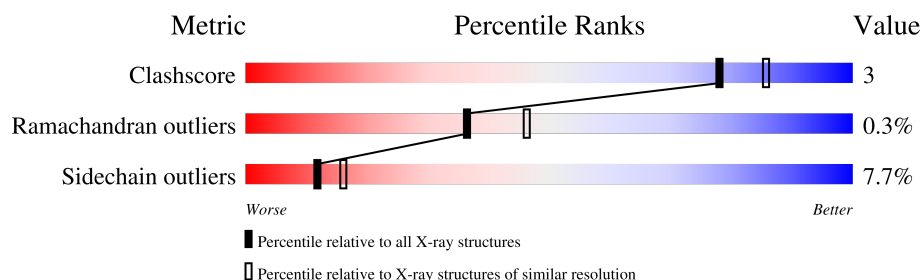
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	394	 69% 27% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3366 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.

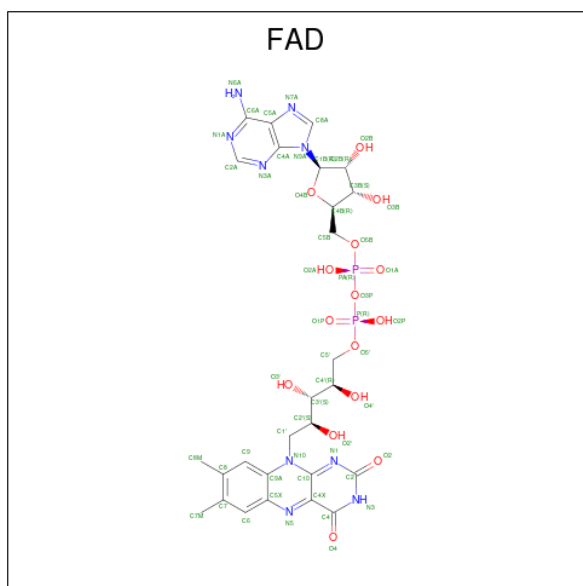
- Molecule 1 is a protein called P-HYDROXYBENZOATE HYDROXYLASE.

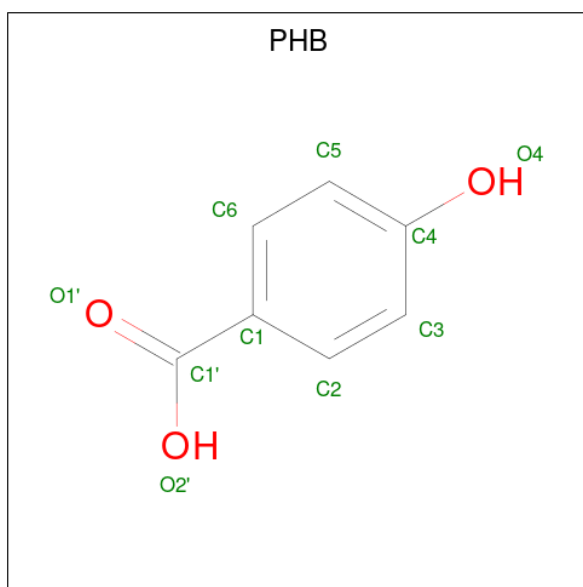
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	3124	1975	563	575	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	PHE	TYR	conflict	UNP P20586

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





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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	179	Total	O	0	0
			179	179		

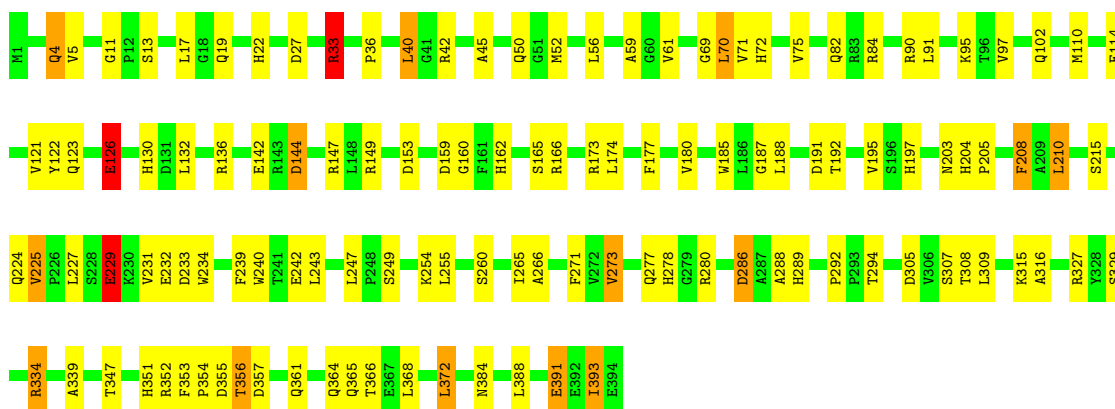
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: P-HYDROXYBENZOATE HYDROXYLASE

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.71Å 146.27Å 87.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3366	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

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	1.21	14/3189 (0.4%)	1.98	99/4314 (2.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	HIS	CD2-NE2	-7.47	1.29	1.37
1	A	289	HIS	CD2-NE2	-7.41	1.29	1.37
1	A	351	HIS	CD2-NE2	-7.39	1.29	1.37
1	A	72	HIS	CD2-NE2	-6.86	1.30	1.37
1	A	22	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	278	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	197	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	72	HIS	CG-ND1	-6.10	1.31	1.38
1	A	180	VAL	CA-CB	-5.80	1.47	1.54
1	A	351	HIS	CG-ND1	-5.78	1.31	1.38
1	A	162	HIS	CD2-NE2	-5.73	1.31	1.37
1	A	204	HIS	CG-ND1	-5.53	1.32	1.38
1	A	122	TYR	CA-CB	-5.25	1.44	1.53
1	A	130	HIS	CD2-NE2	-5.17	1.32	1.37

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	ILE	N-CA-C	11.89	124.18	111.58
1	A	45	ALA	N-CA-C	9.30	123.71	110.23
1	A	229	GLU	N-CA-C	9.26	123.84	109.96
1	A	356	THR	CA-CB-OG1	-9.00	96.10	109.60
1	A	159	ASP	N-CA-C	8.73	122.67	112.72
1	A	159	ASP	CA-CB-CG	8.34	120.94	112.60
1	A	225	VAL	N-CA-CB	-8.26	99.65	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ASN	OD1-CG-ND2	-7.96	114.64	122.60
1	A	208	PHE	N-CA-C	7.93	121.68	110.50
1	A	82	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	A	355	ASP	CA-C-O	7.71	131.05	122.03
1	A	50	GLN	OE1-CD-NE2	-7.18	115.42	122.60
1	A	354	PRO	N-CA-C	7.09	122.36	111.15
1	A	123	GLN	N-CA-C	6.94	121.06	111.90
1	A	75	VAL	CB-CA-C	-6.94	100.01	110.55
1	A	289	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	A	204	HIS	CA-C-O	-6.93	113.14	120.28
1	A	70	LEU	O-C-N	-6.91	115.34	123.22
1	A	366	THR	O-C-N	-6.88	114.31	122.15
1	A	203	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	357	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	391	GLU	N-CA-C	6.64	119.86	110.23
1	A	126	GLU	N-CA-C	6.58	120.46	111.39
1	A	254	LYS	CA-CB-CG	6.50	127.11	114.10
1	A	4	GLN	OE1-CD-NE2	-6.44	116.16	122.60
1	A	329	SER	N-CA-C	6.41	118.27	111.28
1	A	334	ARG	CG-CD-NE	-6.39	97.94	112.00
1	A	132	LEU	N-CA-C	6.36	119.02	111.71
1	A	356	THR	CA-CB-CG2	6.34	121.28	110.50
1	A	19	GLN	OE1-CD-NE2	-6.25	116.36	122.60
1	A	353	PHE	CA-C-N	6.21	126.24	119.90
1	A	353	PHE	C-N-CA	6.21	126.24	119.90
1	A	278	HIS	CB-CG-CD2	-6.19	123.15	131.20
1	A	102	GLN	OE1-CD-NE2	-6.18	116.42	122.60
1	A	204	HIS	CA-CB-CG	-6.12	107.67	113.80
1	A	277	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	A	197	HIS	CB-CG-CD2	-6.11	123.26	131.20
1	A	177	PHE	O-C-N	-6.09	116.21	123.27
1	A	355	ASP	N-CA-C	6.04	119.52	111.30
1	A	5	VAL	O-C-N	-6.03	116.05	123.10
1	A	174	LEU	N-CA-C	6.02	119.52	109.95
1	A	393	ILE	N-CA-CB	-5.97	99.35	110.40
1	A	121	VAL	CB-CA-C	-5.96	103.65	111.81
1	A	351	HIS	CB-CG-CD2	-5.95	123.46	131.20
1	A	162	HIS	CB-CG-CD2	-5.93	123.48	131.20
1	A	19	GLN	N-CA-C	5.91	117.39	111.07
1	A	185	TRP	CG-CD1-NE1	-5.90	102.53	110.20
1	A	308	THR	O-C-N	-5.89	115.05	122.17
1	A	165	SER	N-CA-C	5.85	118.60	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	247	LEU	N-CA-C	5.83	118.17	110.36
1	A	292	PRO	O-C-N	-5.77	118.66	121.31
1	A	17	LEU	CA-C-N	5.74	126.35	119.98
1	A	17	LEU	C-N-CA	5.74	126.35	119.98
1	A	22	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	A	249	SER	N-CA-C	5.62	118.14	111.33
1	A	286	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	123	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	A	149	ARG	O-C-N	-5.53	116.76	123.29
1	A	305	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	13	SER	CB-CA-C	-5.45	102.25	110.92
1	A	271	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	315	LYS	N-CA-C	-5.43	105.36	111.28
1	A	123	GLN	CA-CB-CG	-5.42	103.27	114.10
1	A	204	HIS	CB-CG-CD2	-5.41	124.16	131.20
1	A	364	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	361	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	91	LEU	N-CA-C	5.35	119.53	112.89
1	A	339	ALA	CB-CA-C	-5.28	101.87	110.85
1	A	273	VAL	CB-CA-C	-5.28	102.79	110.81
1	A	40	LEU	N-CA-CB	-5.27	101.56	110.41
1	A	95	LYS	CA-CB-CG	-5.25	103.61	114.10
1	A	42	ARG	CA-CB-CG	-5.24	103.63	114.10
1	A	231	VAL	O-C-N	-5.24	116.58	121.87
1	A	97	VAL	CB-CA-C	-5.23	103.37	110.90
1	A	192	THR	O-C-N	-5.23	116.50	121.57
1	A	52	MET	O-C-N	-5.23	116.58	122.12
1	A	289	HIS	CB-CG-ND1	5.21	130.52	122.70
1	A	233	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	144	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	307	SER	N-CA-C	-5.19	105.79	111.82
1	A	240	TRP	CG-CD2-CE3	5.15	139.05	133.90
1	A	309	LEU	N-CA-C	5.15	117.56	111.33
1	A	11	GLY	CA-C-N	5.14	124.59	119.24
1	A	11	GLY	C-N-CA	5.14	124.59	119.24
1	A	130	HIS	CB-CG-CD2	-5.14	124.51	131.20
1	A	210	LEU	O-C-N	-5.13	117.31	123.31
1	A	265	ILE	CA-C-O	5.13	126.02	120.53
1	A	187	GLY	O-C-N	-5.12	118.15	123.48
1	A	365	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	69	GLY	O-C-N	-5.12	116.62	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	CA-CB-CG	-5.11	103.88	114.10
1	A	266	ALA	CA-C-N	5.10	125.00	119.85
1	A	266	ALA	C-N-CA	5.10	125.00	119.85
1	A	71	VAL	O-C-N	-5.09	116.80	122.66
1	A	33	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	A	242	GLU	O-C-N	-5.07	116.75	122.12
1	A	316	ALA	N-CA-C	5.06	116.80	111.28
1	A	347	THR	CA-CB-CG2	5.00	119.01	110.50

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	3124	0	3120	18	0
2	A	53	0	31	0	0
3	A	10	0	5	0	0
4	A	179	0	0	2	0
All	All	3366	0	3156	18	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (18) 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:33:ARG:HG3	1:A:33:ARG:HH11	1.45	0.80
1:A:36:PRO:HB3	1:A:110:MET:HE1	1.83	0.59
1:A:142:GLU:HG3	1:A:147:ARG:HD2	1.86	0.57
1:A:188:LEU:HD13	1:A:239:PHE:CD1	2.46	0.51
1:A:160:GLY:HA2	1:A:286:ASP:HB2	1.92	0.50
1:A:166:ARG:HD2	1:A:273:VAL:HG11	1.94	0.49
1:A:327:ARG:HH22	1:A:334:ARG:HH22	1.59	0.49
1:A:70:LEU:HD21	1:A:215:SER:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLU:HG3	1:A:234:TRP:HE1	1.78	0.48
1:A:229:GLU:CG	1:A:234:TRP:HE1	2.27	0.47
1:A:368:LEU:O	1:A:372:LEU:HB2	2.14	0.46
1:A:188:LEU:HG	1:A:260:SER:HB3	1.97	0.46
1:A:126:GLU:HA	4:A:471:HOH:O	2.15	0.46
1:A:273:VAL:HG22	1:A:288:ALA:O	2.16	0.45
1:A:4:GLN:HB2	1:A:27:ASP:O	2.18	0.44
1:A:59:ALA:O	1:A:61:VAL:HG23	2.19	0.43
1:A:84:ARG:HB3	4:A:552:HOH:O	2.21	0.41
1:A:208:PHE:HB3	1:A:224:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.

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	392/394 (100%)	385 (98%)	6 (2%)	1 (0%)	36	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ASP

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	325/325 (100%)	300 (92%)	25 (8%)	12	16

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

Mol	Chain	Res	Type
1	A	33	ARG
1	A	40	LEU
1	A	56	LEU
1	A	90	ARG
1	A	114	GLU
1	A	126	GLU
1	A	136	ARG
1	A	173	ARG
1	A	191	ASP
1	A	195	VAL
1	A	205	PRO
1	A	210	LEU
1	A	225	VAL
1	A	227	LEU
1	A	229	GLU
1	A	232	GLU
1	A	243	LEU
1	A	255	LEU
1	A	294	THR
1	A	352	ARG
1	A	356	THR
1	A	372	LEU
1	A	388	LEU
1	A	391	GLU
1	A	393	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	167	GLN
1	A	361	GLN

5.3.3 RNA ⓘ

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](#)

2 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	PHB	A	396	-	10,10,10	1.75	2 (20%)	13,13,13	1.17	2 (15%)
2	FAD	A	395	-	58,58,58	1.68	14 (24%)	85,89,89	1.51	11 (12%)

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	PHB	A	396	-	-	0/4/4/4	0/1/1/1
2	FAD	A	395	-	-	3/34/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	FAD	P-O3P	-5.52	1.53	1.59
2	A	395	FAD	C6-C7	-4.61	1.33	1.39
3	A	396	PHB	C1-C1'	-4.49	1.39	1.49
2	A	395	FAD	C9-C8	-4.03	1.34	1.39
3	A	396	PHB	O2'-C1'	-2.73	1.22	1.30
2	A	395	FAD	C9A-C5X	-2.69	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	FAD	C10-N10	2.53	1.42	1.37
2	A	395	FAD	P-O1P	-2.44	1.42	1.50
2	A	395	FAD	C5'-C4'	2.38	1.55	1.51
2	A	395	FAD	C4X-N5	2.29	1.35	1.30
2	A	395	FAD	C5X-N5	-2.28	1.35	1.39
2	A	395	FAD	C9A-N10	-2.27	1.37	1.41
2	A	395	FAD	C1'-C2'	2.07	1.55	1.52
2	A	395	FAD	C4X-C10	-2.06	1.38	1.44
2	A	395	FAD	PA-O3P	-2.04	1.57	1.59
2	A	395	FAD	C5A-C4A	-2.03	1.35	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	FAD	C9A-C5X-N5	6.75	129.62	122.45
2	A	395	FAD	C5X-N5-C4X	-4.26	111.19	118.09
2	A	395	FAD	O4-C4-N3	-3.88	112.81	120.11
2	A	395	FAD	C4'-C3'-C2'	-3.23	108.20	113.57
3	A	396	PHB	O2'-C1'-O1'	-3.15	116.59	123.35
2	A	395	FAD	C6-C5X-N5	-2.60	114.13	118.44
3	A	396	PHB	O2'-C1'-C1	2.55	121.37	114.84
2	A	395	FAD	O5'-C5'-C4'	2.40	115.78	109.36
2	A	395	FAD	C5'-C4'-C3'	2.25	116.46	112.22
2	A	395	FAD	O2P-P-O1P	2.17	122.55	112.44
2	A	395	FAD	C6-C5X-C9A	-2.13	116.12	119.05
2	A	395	FAD	O4B-C1B-N9A	2.08	112.08	108.09
2	A	395	FAD	O3'-C3'-C4'	2.03	113.54	108.93

There are no chirality outliers.

All (3) torsion outliers are listed below:

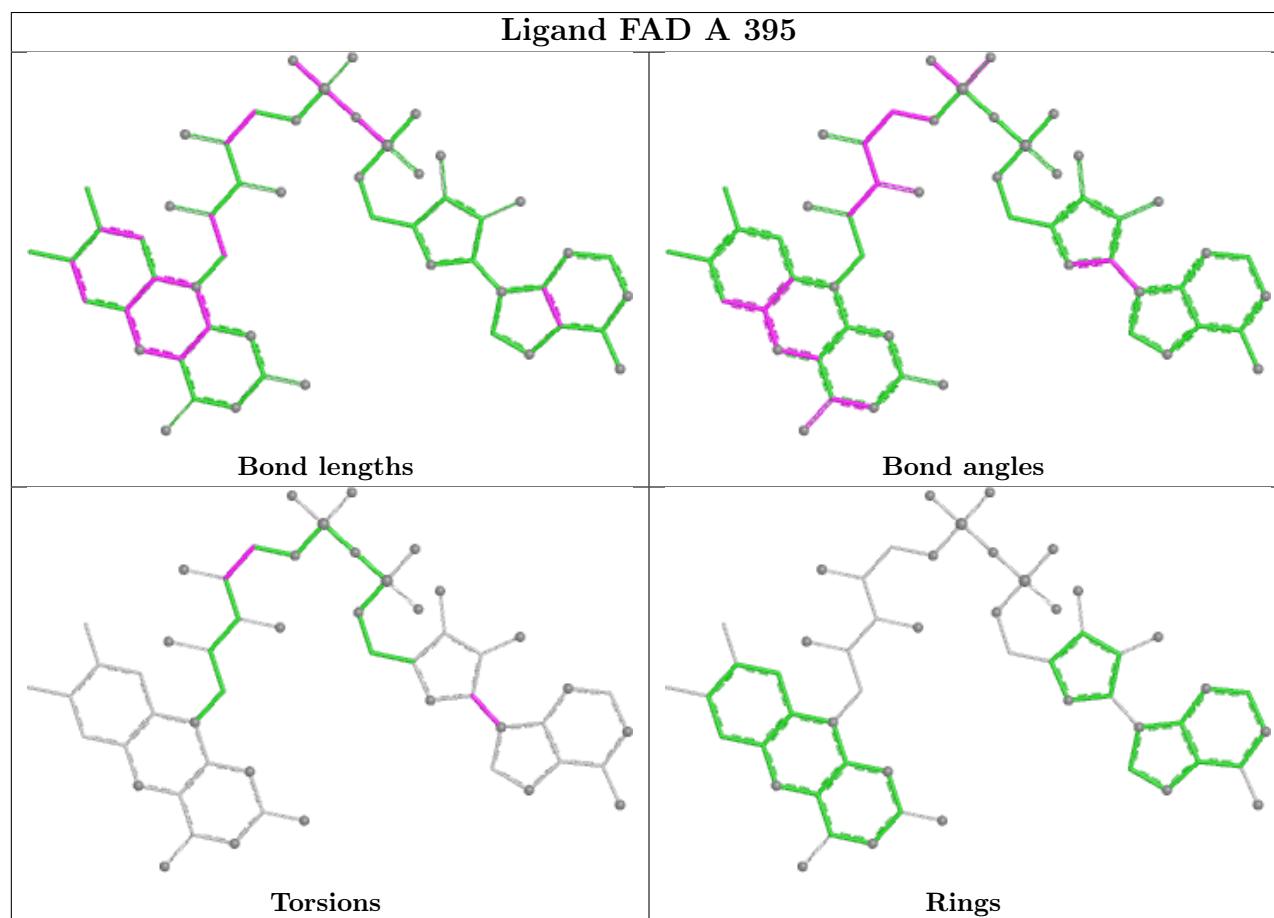
Mol	Chain	Res	Type	Atoms
2	A	395	FAD	O4'-C4'-C5'-O5'
2	A	395	FAD	C2B-C1B-N9A-C8A
2	A	395	FAD	O4B-C1B-N9A-C8A

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.