



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:44 AM UTC

PDB ID : 1PBE / pdb_00001pbe
Title : CRYSTAL STRUCTURE OF THE P-HYDROXYBENZOATE HYDROXYLASE-SUBSTRATE COMPLEX REFINED AT 1.9 ANGSTROMS RESOLUTION. ANALYSIS OF THE ENZYME-SUBSTRATE AND ENZYME-PRODUCT COMPLEXES
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Deposited on : 1994-07-06
Resolution : 1.90 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)	:	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

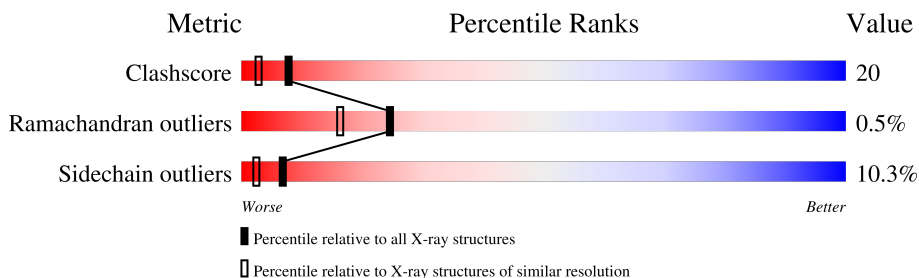
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	 51% 34% 12% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3491 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	391	3098	1960	560	567	11	0	0	0

- 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
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is P-HYDROXYBENZOIC ACID (CCD ID: PHB) (formula: $C_7H_6O_3$).



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	330	Total	O	0	0
			330	330		

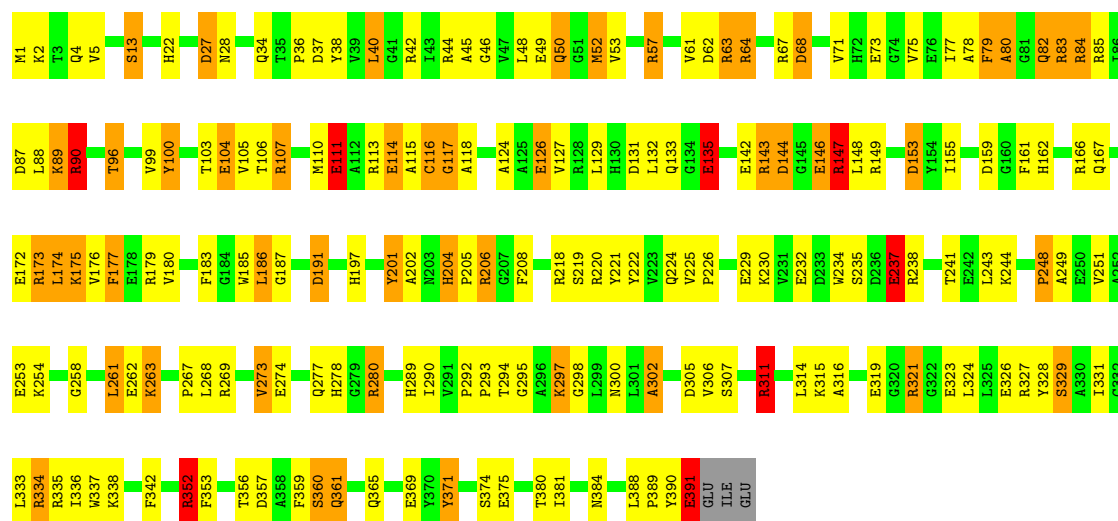
3 Residue-property plots [i](#)

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. 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	71.50 Å 145.80 Å 88.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3491	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: FAD, PHB

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	1.32	1/3163 (0.0%)	2.23	152/4282 (3.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	VAL	N-CA	5.79	1.53	1.46

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ARG	NE-CZ-NH2	-10.88	109.41	119.20
1	A	254	LYS	CA-CB-CG	10.69	135.48	114.10
1	A	334	ARG	CD-NE-CZ	9.76	138.06	124.40
1	A	269	ARG	CA-C-N	9.10	135.82	122.99
1	A	269	ARG	C-N-CA	9.10	135.82	122.99
1	A	342	PHE	CA-C-N	9.03	132.37	120.28
1	A	342	PHE	C-N-CA	9.03	132.37	120.28
1	A	180	VAL	CA-C-O	-8.83	111.08	120.53
1	A	262	GLU	CB-CG-CD	8.68	127.35	112.60
1	A	87	ASP	CA-CB-CG	-8.65	103.94	112.60
1	A	238	ARG	CD-NE-CZ	-8.61	112.34	124.40
1	A	374	SER	CA-C-O	-8.60	111.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	CD-NE-CZ	8.58	136.42	124.40
1	A	174	LEU	O-C-N	8.56	133.21	123.19
1	A	166	ARG	CD-NE-CZ	8.38	136.13	124.40
1	A	111	GLU	CA-CB-CG	8.36	130.81	114.10
1	A	131	ASP	CA-CB-CG	8.17	120.77	112.60
1	A	369	GLU	CA-C-O	-8.14	111.92	120.55
1	A	359	PHE	CA-C-N	8.11	131.49	120.38
1	A	359	PHE	C-N-CA	8.11	131.49	120.38
1	A	111	GLU	N-CA-CB	7.98	121.64	110.07
1	A	384	ASN	OD1-CG-ND2	7.74	130.34	122.60
1	A	107	ARG	CD-NE-CZ	7.53	134.94	124.40
1	A	220	ARG	CB-CA-C	7.47	121.64	110.14
1	A	201	TYR	O-C-N	-7.46	114.83	123.27
1	A	262	GLU	CA-CB-CG	7.33	128.77	114.10
1	A	57	ARG	CD-NE-CZ	7.21	134.50	124.40
1	A	183	PHE	CA-C-N	7.15	127.83	121.82
1	A	183	PHE	C-N-CA	7.15	127.83	121.82
1	A	369	GLU	O-C-N	7.11	129.66	122.12
1	A	44	ARG	N-CA-C	7.06	119.03	108.31
1	A	83	ARG	CD-NE-CZ	-7.05	114.53	124.40
1	A	105	VAL	O-C-N	7.02	128.79	121.91
1	A	114	GLU	CA-CB-CG	7.02	128.13	114.10
1	A	316	ALA	CA-C-O	-6.98	113.02	120.42
1	A	237	GLU	CA-C-N	6.87	129.37	120.44
1	A	237	GLU	C-N-CA	6.87	129.37	120.44
1	A	202	ALA	CA-C-O	6.79	127.85	120.32
1	A	241	THR	CA-CB-OG1	-6.66	99.61	109.60
1	A	13	SER	O-C-N	6.63	128.93	122.03
1	A	68	ASP	N-CA-C	6.58	121.60	113.50
1	A	146	GLU	CA-CB-CG	6.55	127.21	114.10
1	A	40	LEU	N-CA-CB	-6.52	98.97	110.39
1	A	45	ALA	N-CA-C	6.48	119.62	110.23
1	A	380	THR	O-C-N	6.46	129.51	122.15
1	A	82	GLN	N-CA-C	6.42	119.64	109.81
1	A	13	SER	CA-C-O	-6.37	114.31	121.00
1	A	159	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	267	PRO	CB-CA-C	6.29	119.62	110.63
1	A	206	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	A	103	THR	O-C-N	6.22	128.72	122.12
1	A	261	LEU	N-CA-C	-6.16	103.89	112.45
1	A	50	GLN	CA-C-N	6.13	126.79	119.98
1	A	50	GLN	C-N-CA	6.13	126.79	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ARG	CD-NE-CZ	6.12	132.97	124.40
1	A	374	SER	N-CA-CB	-6.11	100.44	110.52
1	A	333	LEU	CA-C-O	-6.10	113.21	120.10
1	A	135	GLU	CB-CG-CD	6.08	122.93	112.60
1	A	27	ASP	CB-CA-C	6.07	120.70	109.54
1	A	133	GLN	OE1-CD-NE2	6.06	128.66	122.60
1	A	161	PHE	N-CA-C	6.04	118.36	111.11
1	A	100	TYR	CB-CA-C	6.03	119.04	110.24
1	A	235	SER	N-CA-C	-5.99	103.05	110.41
1	A	106	THR	CA-C-N	5.99	128.62	120.54
1	A	106	THR	C-N-CA	5.99	128.62	120.54
1	A	328	TYR	CA-C-O	-5.97	114.50	121.07
1	A	22	HIS	O-C-N	5.96	128.21	122.07
1	A	113	ARG	CA-C-N	5.91	128.52	120.54
1	A	113	ARG	C-N-CA	5.91	128.52	120.54
1	A	280	ARG	CA-CB-CG	-5.91	102.28	114.10
1	A	380	THR	N-CA-CB	5.89	118.88	110.16
1	A	116	CYS	CA-C-N	5.89	131.41	120.87
1	A	116	CYS	C-N-CA	5.89	131.41	120.87
1	A	142	GLU	CB-CG-CD	5.85	122.55	112.60
1	A	85	ARG	O-C-N	-5.84	116.35	123.19
1	A	68	ASP	N-CA-CB	-5.84	101.94	110.53
1	A	177	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	248	PRO	CA-C-N	5.83	128.37	120.38
1	A	248	PRO	C-N-CA	5.83	128.37	120.38
1	A	52	MET	CB-CA-C	5.82	120.74	110.85
1	A	353	PHE	CA-C-O	-5.81	114.79	120.19
1	A	124	ALA	CA-C-O	-5.73	114.13	120.60
1	A	118	ALA	CB-CA-C	5.69	120.01	109.54
1	A	258	GLY	O-C-N	5.69	127.46	121.77
1	A	147	ARG	N-CA-CB	5.68	119.68	110.42
1	A	79	PHE	O-C-N	5.67	130.19	123.33
1	A	167	GLN	CB-CG-CD	-5.65	103.00	112.60
1	A	153	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	75	VAL	CA-C-O	-5.64	116.05	121.63
1	A	338	LYS	CA-CB-CG	5.63	125.37	114.10
1	A	206	ARG	N-CA-C	-5.63	106.36	113.18
1	A	273	VAL	CB-CA-C	5.62	119.00	110.62
1	A	237	GLU	CB-CA-C	-5.58	101.88	110.81
1	A	27	ASP	CA-CB-CG	-5.56	107.04	112.60
1	A	263	LYS	N-CA-CB	5.56	120.15	110.81
1	A	27	ASP	O-C-N	5.54	129.40	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	241	THR	CA-C-N	5.48	127.57	120.44
1	A	241	THR	C-N-CA	5.48	127.57	120.44
1	A	371	TYR	CA-C-O	-5.48	113.91	120.10
1	A	391	GLU	CA-C-O	-5.46	111.52	120.80
1	A	329	SER	CA-C-O	-5.46	114.77	120.55
1	A	204	HIS	O-C-N	5.42	126.46	121.80
1	A	334	ARG	CA-C-O	5.42	126.51	120.82
1	A	302	ALA	N-CA-C	-5.39	105.30	111.07
1	A	44	ARG	CA-C-N	5.38	128.35	120.71
1	A	44	ARG	C-N-CA	5.38	128.35	120.71
1	A	278	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	243	LEU	CA-C-N	5.36	127.72	120.38
1	A	243	LEU	C-N-CA	5.36	127.72	120.38
1	A	365	GLN	CA-C-N	5.36	127.46	120.28
1	A	365	GLN	C-N-CA	5.36	127.46	120.28
1	A	40	LEU	CB-CA-C	5.35	121.09	110.17
1	A	292	PRO	N-CA-C	-5.35	105.34	110.47
1	A	71	VAL	CA-C-O	5.35	126.75	120.71
1	A	174	LEU	N-CA-C	5.33	118.50	109.76
1	A	290	ILE	CA-C-O	-5.32	114.72	120.36
1	A	336	ILE	CA-CB-CG2	5.31	119.53	110.50
1	A	369	GLU	N-CA-CB	5.31	117.93	110.12
1	A	104	GLU	N-CA-CB	5.30	117.76	110.07
1	A	96	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	159	ASP	N-CA-C	5.30	118.76	112.72
1	A	311	ARG	CG-CD-NE	-5.30	100.34	112.00
1	A	337	TRP	CA-C-O	-5.29	114.94	120.55
1	A	390	TYR	CA-CB-CG	5.28	123.41	113.90
1	A	253	GLU	CA-C-N	5.28	131.88	122.06
1	A	253	GLU	C-N-CA	5.28	131.88	122.06
1	A	117	GLY	O-C-N	5.25	128.08	122.41
1	A	390	TYR	N-CA-C	-5.25	101.98	110.32
1	A	249	ALA	O-C-N	5.23	127.67	122.12
1	A	53	VAL	CB-CA-C	5.22	118.65	111.97
1	A	316	ALA	O-C-N	5.22	128.10	122.15
1	A	115	ALA	CA-C-N	5.21	128.94	120.60
1	A	115	ALA	C-N-CA	5.21	128.94	120.60
1	A	129	LEU	CA-C-O	-5.20	114.72	120.38
1	A	389	PRO	N-CD-CG	-5.19	95.42	103.20
1	A	186	LEU	CA-C-O	5.19	126.24	120.43
1	A	186	LEU	CB-CA-C	5.18	118.87	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLY	CA-C-O	-5.18	115.64	121.23
1	A	162	HIS	CA-C-O	-5.15	113.66	119.78
1	A	143	ARG	CB-CA-C	5.13	119.85	111.23
1	A	335	ARG	CA-C-N	5.13	127.48	120.77
1	A	335	ARG	C-N-CA	5.13	127.48	120.77
1	A	63	ARG	CA-C-N	5.12	127.44	120.54
1	A	63	ARG	C-N-CA	5.12	127.44	120.54
1	A	27	ASP	CB-CG-OD2	-5.11	106.65	118.40
1	A	126	GLU	CA-C-O	-5.10	115.21	121.28
1	A	22	HIS	CA-CB-CG	-5.09	108.71	113.80
1	A	311	ARG	CA-CB-CG	-5.09	103.93	114.10
1	A	90	ARG	N-CA-CB	5.08	117.69	110.16
1	A	371	TYR	O-C-N	5.08	128.16	122.22
1	A	278	HIS	CB-CA-C	-5.05	104.48	110.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	ARG	Sidechain

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	3098	0	3099	125	1
2	A	53	0	31	1	0
3	A	10	0	4	1	0
4	A	330	0	0	28	3
All	All	3491	0	3134	125	4

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 20.

All (125) 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:146:GLU:HG3	1:A:148:LEU:HD21	1.36	1.06
1:A:132:LEU:HD22	4:A:581:HOH:O	1.58	1.02
1:A:64:ARG:HE	1:A:107:ARG:HH21	1.02	0.97
1:A:356:THR:HG23	1:A:360:SER:OG	1.75	0.87
1:A:64:ARG:NE	1:A:107:ARG:HH21	1.72	0.86
1:A:204:HIS:HD2	1:A:206:ARG:H	1.23	0.86
1:A:197:HIS:HB3	4:A:598:HOH:O	1.77	0.83
1:A:319:GLU:OE1	1:A:321:ARG:NH1	2.14	0.80
1:A:174:LEU:HD13	1:A:273:VAL:CG2	2.12	0.80
1:A:104:GLU:HG3	1:A:107:ARG:HH12	1.47	0.79
1:A:352:ARG:HH11	1:A:352:ARG:HG2	1.47	0.78
1:A:116:CYS:SG	4:A:505:HOH:O	2.42	0.75
1:A:63:ARG:HH21	1:A:67:ARG:NH1	1.84	0.75
1:A:307:SER:OG	1:A:311:ARG:NH1	2.20	0.74
1:A:146:GLU:HG3	1:A:148:LEU:CD2	2.18	0.73
1:A:327:ARG:HG3	1:A:331:ILE:CD1	2.18	0.73
1:A:327:ARG:HG3	1:A:331:ILE:HD11	1.74	0.70
1:A:204:HIS:CG	1:A:205:PRO:HD2	2.26	0.70
1:A:204:HIS:CD2	1:A:205:PRO:HD2	2.26	0.69
1:A:155:ILE:HD12	4:A:581:HOH:O	1.93	0.69
1:A:174:LEU:HD13	1:A:273:VAL:HG21	1.75	0.69
1:A:135:GLU:HG2	4:A:484:HOH:O	1.93	0.68
1:A:96:THR:HA	4:A:679:HOH:O	1.93	0.68
1:A:63:ARG:NH2	1:A:67:ARG:NH1	2.42	0.68
1:A:64:ARG:NE	1:A:107:ARG:NH2	2.40	0.67
1:A:237:GLU:HG3	4:A:635:HOH:O	1.93	0.67
1:A:225:VAL:HG23	4:A:592:HOH:O	1.95	0.67
1:A:174:LEU:HD13	1:A:273:VAL:HG22	1.76	0.66
1:A:356:THR:HG22	1:A:361:GLN:HG2	1.76	0.65
1:A:5:VAL:O	1:A:28:ASN:HA	1.96	0.65
1:A:204:HIS:CD2	1:A:206:ARG:H	2.09	0.65
1:A:218:ARG:HH21	1:A:261:LEU:CD1	2.09	0.65
1:A:64:ARG:HE	1:A:107:ARG:NH2	1.84	0.65
1:A:352:ARG:HG2	1:A:352:ARG:NH1	2.11	0.64
1:A:315:LYS:HD3	1:A:324:LEU:CD1	2.29	0.61
1:A:64:ARG:NH2	4:A:640:HOH:O	2.32	0.60
1:A:88:LEU:HB2	4:A:679:HOH:O	2.02	0.60
1:A:315:LYS:HD3	1:A:324:LEU:HD12	1.84	0.59
1:A:114:GLU:HG3	4:A:655:HOH:O	2.01	0.59
1:A:147:ARG:O	1:A:147:ARG:HD3	2.03	0.58
1:A:175:LYS:HG2	4:A:660:HOH:O	2.03	0.58
1:A:277:GLN:NE2	1:A:329:SER:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:HB2	1:A:391:GLU:OE2	2.05	0.57
1:A:61:VAL:HG12	1:A:61:VAL:O	2.04	0.57
1:A:327:ARG:HG3	1:A:331:ILE:HD12	1.87	0.55
1:A:63:ARG:HA	4:A:444:HOH:O	2.07	0.55
1:A:175:LYS:HE2	1:A:274:GLU:OE1	2.07	0.55
1:A:73:GLU:HA	4:A:679:HOH:O	2.06	0.55
1:A:77:ILE:HD13	1:A:201:TYR:HB2	1.89	0.55
1:A:321:ARG:NH1	1:A:321:ARG:HG3	2.23	0.53
1:A:13:SER:OG	1:A:302:ALA:HB1	2.08	0.53
1:A:357:ASP:O	1:A:361:GLN:HG3	2.09	0.53
1:A:40:LEU:HD22	1:A:110:MET:HE1	1.90	0.52
1:A:219:SER:HB3	1:A:221:TYR:CE2	2.45	0.52
1:A:277:GLN:HE22	1:A:329:SER:H	1.58	0.52
1:A:135:GLU:HG3	4:A:675:HOH:O	2.09	0.52
1:A:295:GLY:O	1:A:297:LYS:HD3	2.09	0.52
1:A:356:THR:CG2	1:A:361:GLN:HG2	2.40	0.51
1:A:63:ARG:NH2	1:A:67:ARG:HH12	2.08	0.51
1:A:4:GLN:HB2	1:A:27:ASP:O	2.10	0.51
1:A:63:ARG:HG3	4:A:444:HOH:O	2.09	0.51
1:A:237:GLU:CG	4:A:635:HOH:O	2.55	0.51
1:A:67:ARG:NH1	4:A:512:HOH:O	2.41	0.50
1:A:356:THR:HG22	1:A:361:GLN:CG	2.42	0.50
1:A:104:GLU:OE2	1:A:107:ARG:NH1	2.44	0.50
1:A:173:ARG:NH2	4:A:429:HOH:O	2.44	0.50
1:A:234:TRP:O	1:A:263:LYS:NZ	2.30	0.50
1:A:391:GLU:HG2	4:A:549:HOH:O	2.12	0.50
1:A:147:ARG:HH12	1:A:149:ARG:HB2	1.76	0.50
1:A:172:GLU:HB2	4:A:543:HOH:O	2.12	0.49
1:A:34:GLN:NE2	1:A:38:TYR:CD2	2.80	0.49
1:A:324:LEU:CD2	1:A:327:ARG:HH11	2.25	0.49
1:A:289:HIS:NE2	1:A:305:ASP:OD2	2.44	0.49
1:A:321:ARG:HG3	1:A:321:ARG:HH11	1.78	0.49
1:A:143:ARG:HH11	1:A:143:ARG:HG3	1.78	0.48
1:A:78:ALA:HA	1:A:82:GLN:O	2.14	0.48
1:A:185:TRP:CZ3	1:A:293:PRO:HB2	2.49	0.47
1:A:186:LEU:O	1:A:222:TYR:HA	2.13	0.47
1:A:371:TYR:HB3	1:A:381:ILE:HD11	1.97	0.47
1:A:204:HIS:CG	1:A:205:PRO:CD	2.96	0.47
1:A:107:ARG:O	1:A:111:GLU:HG2	2.14	0.46
1:A:104:GLU:HG3	1:A:107:ARG:NH1	2.23	0.46
1:A:153:ASP:O	1:A:280:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLN:NE2	1:A:38:TYR:CE2	2.85	0.45
1:A:89:LYS:HG3	1:A:96:THR:HG22	1.97	0.45
1:A:268:LEU:HG	1:A:293:PRO:HD2	1.99	0.45
1:A:352:ARG:NH1	4:A:715:HOH:O	2.50	0.45
1:A:143:ARG:O	1:A:144:ASP:HB3	2.17	0.45
1:A:143:ARG:HG3	1:A:143:ARG:NH1	2.32	0.44
1:A:49:GLU:HG3	1:A:300:ASN:CG	2.43	0.44
1:A:298:GLY:HA3	2:A:395:FAD:H1'2	2.00	0.44
1:A:334:ARG:HD2	1:A:391:GLU:OE1	2.17	0.44
1:A:67:ARG:HD3	4:A:512:HOH:O	2.18	0.44
1:A:146:GLU:HG2	1:A:146:GLU:O	2.17	0.44
1:A:321:ARG:HH11	1:A:321:ARG:CG	2.31	0.44
1:A:226:PRO:O	4:A:592:HOH:O	2.20	0.43
1:A:352:ARG:HH11	1:A:352:ARG:CG	2.25	0.43
1:A:62:ASP:N	1:A:62:ASP:OD1	2.52	0.43
1:A:100:TYR:CZ	1:A:104:GLU:HB3	2.53	0.43
1:A:36:PRO:O	1:A:40:LEU:HB2	2.17	0.43
1:A:89:LYS:HG3	1:A:96:THR:CG2	2.49	0.43
1:A:248:PRO:HB2	1:A:251:VAL:HG23	1.99	0.43
1:A:204:HIS:CD2	1:A:206:ARG:HG3	2.53	0.43
1:A:79:PHE:O	1:A:80:ALA:C	2.60	0.43
1:A:176:VAL:HG22	1:A:273:VAL:HG23	2.01	0.42
1:A:226:PRO:HD2	1:A:229:GLU:CG	2.49	0.42
1:A:46:GLY:O	1:A:99:VAL:HA	2.19	0.42
1:A:64:ARG:O	1:A:68:ASP:HB2	2.19	0.42
1:A:50:GLN:O	1:A:50:GLN:HG3	2.19	0.42
1:A:57:ARG:HG3	1:A:62:ASP:OD2	2.19	0.42
1:A:226:PRO:HD2	1:A:229:GLU:HG3	2.02	0.42
1:A:64:ARG:HG2	1:A:67:ARG:NH2	2.34	0.42
1:A:90:ARG:HH22	1:A:375:GLU:CD	2.27	0.42
1:A:175:LYS:HG3	1:A:274:GLU:HB2	2.02	0.42
1:A:324:LEU:HD23	1:A:327:ARG:HH11	1.85	0.42
1:A:222:TYR:OH	3:A:396:PHB:O2'	2.33	0.42
1:A:84:ARG:NH1	4:A:452:HOH:O	2.53	0.41
1:A:315:LYS:CE	1:A:321:ARG:NH2	2.83	0.41
1:A:307:SER:HG	1:A:311:ARG:NH1	2.16	0.41
1:A:117:GLY:HA2	4:A:428:HOH:O	2.20	0.41
1:A:208:PHE:HB3	1:A:224:GLN:HB2	2.02	0.41
1:A:324:LEU:HB2	4:A:554:HOH:O	2.20	0.41
1:A:352:ARG:HB2	4:A:470:HOH:O	2.19	0.41
1:A:83:ARG:HD2	1:A:248:PRO:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TRP:CH2	1:A:293:PRO:HB2	2.56	0.40

All (4) 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:712:HOH:O	4:A:712:HOH:O[3_656]	1.52	0.68
4:A:692:HOH:O	4:A:692:HOH:O[3_556]	1.57	0.63
4:A:728:HOH:O	4:A:728:HOH:O[4_566]	1.80	0.40
1:A:114:GLU:OE2	1:A:244:LYS:NZ[6_565]	2.06	0.14

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	389/394 (99%)	373 (96%)	14 (4%)	2 (0%)	24 16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ALA
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	321/324 (99%)	288 (90%)	33 (10%)	7 2

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	37	ASP
1	A	48	LEU
1	A	52	MET
1	A	64	ARG
1	A	84	ARG
1	A	89	LYS
1	A	90	ARG
1	A	111	GLU
1	A	126	GLU
1	A	135	GLU
1	A	147	ARG
1	A	173	ARG
1	A	175	LYS
1	A	177	PHE
1	A	179	ARG
1	A	191	ASP
1	A	230	LYS
1	A	232	GLU
1	A	237	GLU
1	A	294	THR
1	A	297	LYS
1	A	306	VAL
1	A	314	LEU
1	A	321	ARG
1	A	323	GLU
1	A	326	GLU
1	A	352	ARG
1	A	360	SER
1	A	361	GLN
1	A	388	LEU
1	A	391	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	204	HIS
1	A	277	GLN
1	A	361	GLN
1	A	365	GLN

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](#)

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	$\# Z > 2$
2	FAD	A	395	-	58,58,58	1.32	8 (13%)	85,89,89	1.51	14 (16%)
3	PHB	A	396	-	10,10,10	0.65	0	13,13,13	0.56	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	A	395	-	-	3/34/50/50	0/6/6/6
3	PHB	A	396	-	-	0/4/4/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	FAD	C9-C8	-4.27	1.33	1.39
2	A	395	FAD	O2-C2	-2.96	1.18	1.24
2	A	395	FAD	C5'-C4'	2.50	1.55	1.51
2	A	395	FAD	C5A-C4A	2.47	1.43	1.39
2	A	395	FAD	C4-N3	2.44	1.43	1.38
2	A	395	FAD	C5X-N5	-2.25	1.35	1.39
2	A	395	FAD	C6-C7	-2.16	1.36	1.39
2	A	395	FAD	PA-O3P	-2.15	1.57	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	FAD	O2-C2-N1	-5.20	113.16	121.80
2	A	395	FAD	O4'-C4'-C5'	-3.41	102.46	109.99
2	A	395	FAD	O2-C2-N3	3.22	124.75	118.58
2	A	395	FAD	C4-N3-C2	-3.21	119.94	125.64
2	A	395	FAD	C4X-C10-N10	3.07	120.87	116.48
2	A	395	FAD	C10-N1-C2	2.94	123.22	116.85
2	A	395	FAD	O2A-PA-O1A	2.54	124.25	112.44
2	A	395	FAD	C4X-C10-N1	-2.53	118.39	124.59
2	A	395	FAD	C9A-N10-C10	-2.50	116.94	120.75
2	A	395	FAD	O4B-C1B-N9A	2.45	112.79	108.09
2	A	395	FAD	N3A-C2A-N1A	-2.44	124.88	128.58
2	A	395	FAD	C5A-N7A-C8A	2.40	107.22	103.45
2	A	395	FAD	C8M-C8-C9	-2.34	115.46	119.57
2	A	395	FAD	C9-C8-C7	2.32	123.09	119.69

There are no chirality outliers.

All (3) torsion outliers are listed below:

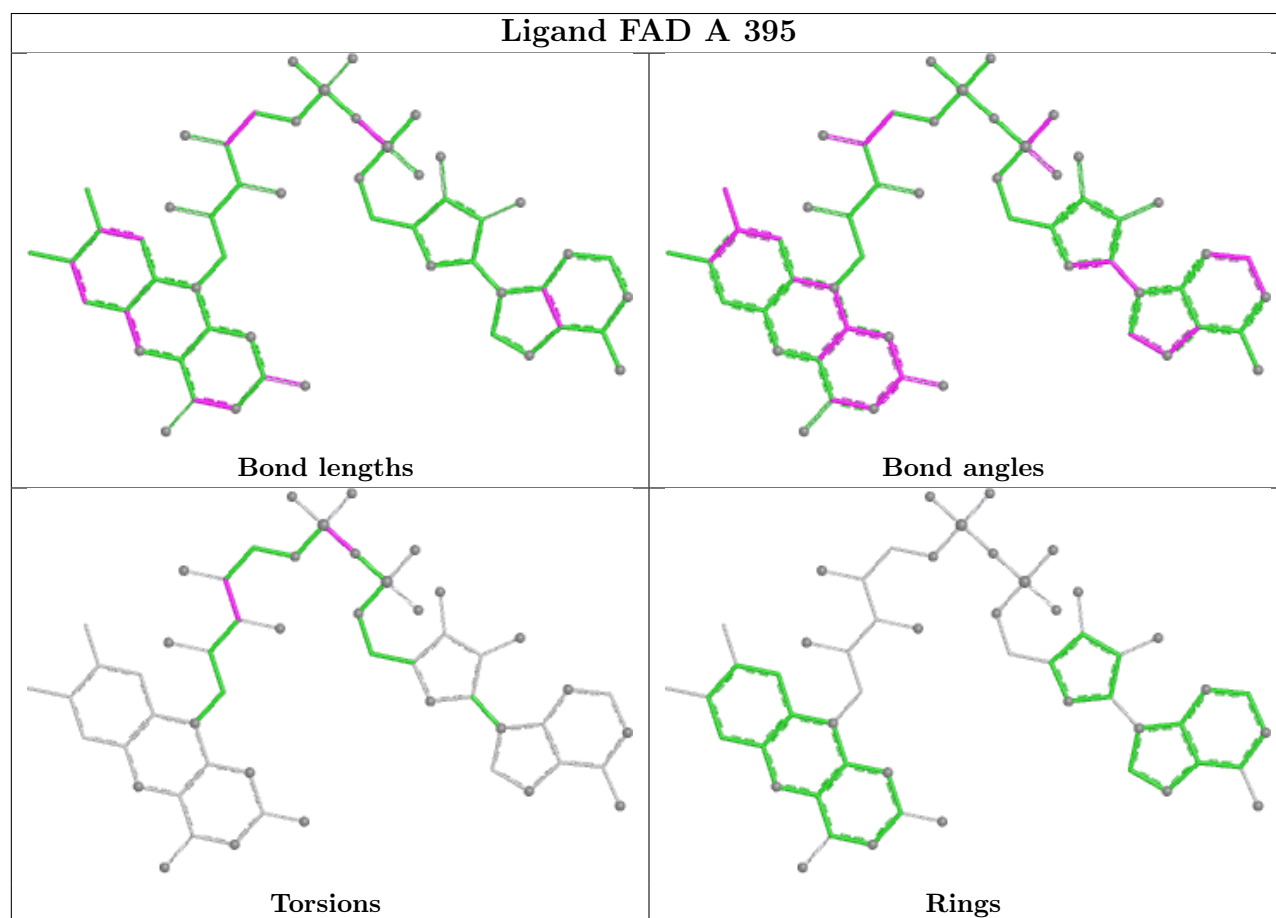
Mol	Chain	Res	Type	Atoms
2	A	395	FAD	O3'-C3'-C4'-O4'
2	A	395	FAD	C2'-C3'-C4'-O4'
2	A	395	FAD	PA-O3P-P-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	395	FAD	1	0
3	A	396	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.



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.