Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:30 PM GMT

PDB ID	:	1PBE
Title	:	CRYSTAL STRUCTURE OF THE P-HYDROXYBENZOATE HYDROXY LASE-SUBSTRATE COMPLEX REFINED AT 1.9 ANGSTROMS RES-OLUTION. 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

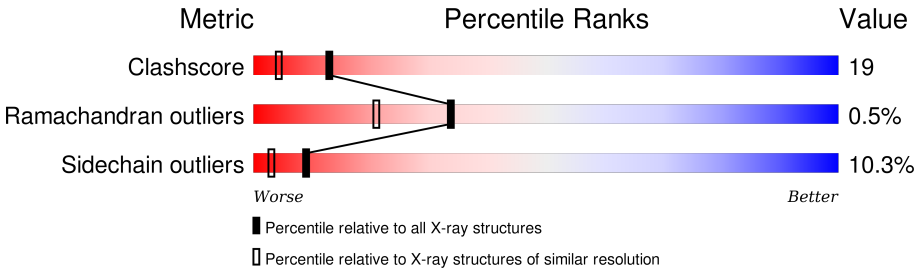
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	394	62% 25% 10%

2 Entry composition

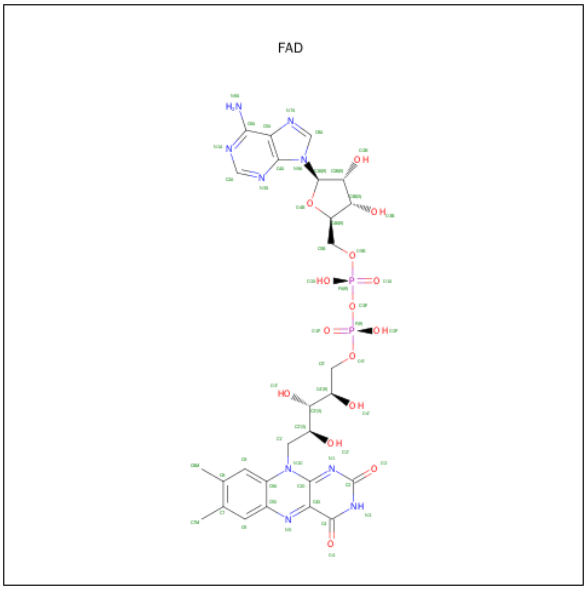
There are 4 unique types of molecules in this entry. The entry contains 3491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

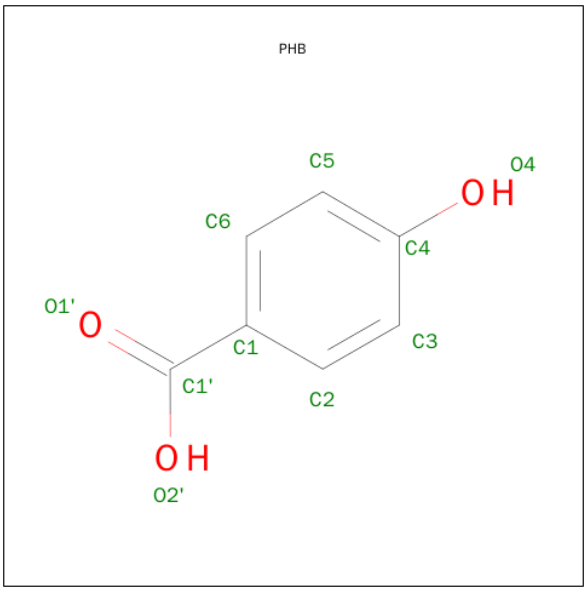
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3098	1960	560	567	11			

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



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

- Molecule 3 is P-HYDROXYBENZOIC ACID (three-letter code: PHB) (formula: $C_7H_6O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	330	Total O 330 330	0	0

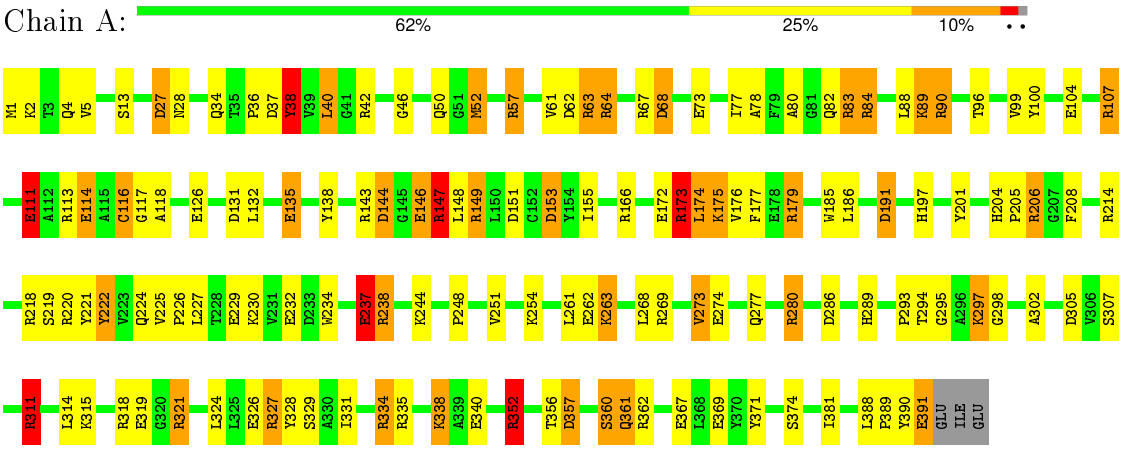
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: P-HYDROXYBENZOATE HYDROXYLASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	71.50Å 145.80Å 88.20Å 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: 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	1.05	2/3163 (0.1%)	1.90	79/4282 (1.8%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	GLU	CD-OE2	-6.45	1.18	1.25
1	A	340	GLU	CD-OE1	-5.02	1.20	1.25

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	42	ARG	NE-CZ-NH2	-21.78	109.41	120.30
1	A	27	ASP	CB-CG-OD2	-12.95	106.65	118.30
1	A	151	ASP	CB-CG-OD1	12.67	129.70	118.30
1	A	214	ARG	NE-CZ-NH1	11.83	126.22	120.30
1	A	42	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	166	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	A	334	ARG	CD-NE-CZ	10.33	138.06	123.60
1	A	254	LYS	CA-CB-CG	10.04	135.48	113.40
1	A	220	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	A	318	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	A	362	ARG	NE-CZ-NH1	9.26	124.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	A	173	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	A	269	ARG	CD-NE-CZ	9.15	136.42	123.60
1	A	206	ARG	NE-CZ-NH2	9.03	124.82	120.30
1	A	166	ARG	CD-NE-CZ	8.95	136.13	123.60
1	A	191	ASP	CB-CG-OD1	8.57	126.02	118.30
1	A	220	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	A	63	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	A	107	ARG	CD-NE-CZ	8.10	134.94	123.60
1	A	238	ARG	CD-NE-CZ	-8.04	112.34	123.60
1	A	335	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	A	111	GLU	CA-CB-CG	7.92	130.81	113.40
1	A	57	ARG	CD-NE-CZ	7.79	134.50	123.60
1	A	286	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	318	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	280	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	352	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	131	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	262	GLU	CA-CB-CG	6.99	128.77	113.40
1	A	179	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	374	SER	N-CA-CB	-6.71	100.44	110.50
1	A	114	GLU	CA-CB-CG	6.70	128.13	113.40
1	A	352	ARG	CD-NE-CZ	6.70	132.97	123.60
1	A	118	ALA	CB-CA-C	6.61	120.01	110.10
1	A	68	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	174	LEU	O-C-N	6.57	133.21	122.70
1	A	107	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	A	83	ARG	CD-NE-CZ	-6.48	114.53	123.60
1	A	369	GLU	OE1-CD-OE2	6.46	131.05	123.30
1	A	237	GLU	OE1-CD-OE2	6.41	130.99	123.30
1	A	146	GLU	CA-CB-CG	6.28	127.21	113.40
1	A	138	TYR	CB-CG-CD2	6.15	124.69	121.00
1	A	111	GLU	N-CA-CB	6.14	121.64	110.60
1	A	151	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	153	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	328	TYR	CB-CG-CD2	-5.96	117.43	121.00
1	A	63	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	40	LEU	CB-CA-C	5.73	121.09	110.20
1	A	286	ASP	CB-CG-OD2	-5.73	113.15	118.30
1	A	335	ARG	NH1-CZ-NH2	-5.72	113.10	119.40
1	A	40	LEU	N-CA-CB	-5.71	98.97	110.40
1	A	269	ARG	C-N-CA	5.65	135.82	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	ARG	CB-CA-C	5.62	121.64	110.40
1	A	116	CYS	CA-CB-SG	-5.52	104.07	114.00
1	A	311	ARG	CG-CD-NE	-5.46	100.34	111.80
1	A	338	LYS	CA-CB-CG	5.44	125.37	113.40
1	A	262	GLU	CG-CD-OE1	5.43	129.16	118.30
1	A	114	GLU	CG-CD-OE1	-5.37	107.57	118.30
1	A	280	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	57	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	263	LYS	N-CA-CB	5.31	120.15	110.60
1	A	114	GLU	OE1-CD-OE2	5.29	129.65	123.30
1	A	390	TYR	CA-CB-CG	5.27	123.41	113.40
1	A	327	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	149	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	227	LEU	CB-CA-C	5.23	120.14	110.20
1	A	273	VAL	CG1-CB-CG2	5.22	119.25	110.90
1	A	334	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	389	PRO	N-CD-CG	-5.19	95.42	103.20
1	A	222	TYR	CZ-CE2-CD2	-5.18	115.13	119.80
1	A	52	MET	CB-CA-C	5.17	120.74	110.40
1	A	27	ASP	CB-CA-C	5.15	120.70	110.40
1	A	38	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	280	ARG	CA-CB-CG	-5.05	102.28	113.40
1	A	147	ARG	N-CA-CB	5.04	119.68	110.60
1	A	111	GLU	OE1-CD-OE2	5.03	129.34	123.30
1	A	90	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	357	ASP	CB-CG-OD1	5.01	122.81	118.30

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 (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	3098	0	3099	120	1
2	A	53	0	31	1	0
3	A	10	0	4	0	0
4	A	330	0	0	28	3
All	All	3491	0	3134	120	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 19.

All (120) 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:HG2	1:A:352:ARG:HH11	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:204:HIS:CD2	1:A:206:ARG:H	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:O	1:A:28:ASN:HA	1.96	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:HD3	1:A:147:ARG:O	2.03	0.58
1:A:277:GLN:NE2	1:A:329:SER:H	2.01	0.58
1:A:175:LYS:HG2	4:A:660:HOH:O	2.03	0.58
1:A:234:TRP:O	1:A:263:LYS:NZ	2.30	0.58
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:HG3	1:A:321:ARG:NH1	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:277:GLN:HE22	1:A:329:SER:H	1.58	0.52
1:A:219:SER:HB3	1:A:221:TYR:CE2	2.45	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:63:ARG:HG3	4:A:444:HOH:O	2.09	0.51
1:A:4:GLN:HB2	1:A:27:ASP:O	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:A:143:ARG:HH11	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
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: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:146:GLU:O	1:A:146:GLU:HG2	2.17	0.44
1:A:67:ARG:HD3	4:A:512:HOH:O	2.18	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:CG	1:A:352:ARG:HH11	2.25	0.43
1:A:100:TYR:CZ	1:A:104:GLU:HB3	2.53	0.43
1:A:62:ASP:N	1:A:62:ASP:OD1	2.52	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:36:PRO:O	1:A:40:LEU:HB2	2.17	0.43
1:A:204:HIS:CD2	1:A:206:ARG:HG3	2.53	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:64:ARG:O	1:A:68:ASP:HB2	2.19	0.42
1:A:46:GLY:O	1:A:99:VAL:HA	2.19	0.42
1:A:57:ARG:HG3	1:A:62:ASP:OD2	2.19	0.42
1:A:50:GLN:HG3	1:A:50:GLN:O	2.19	0.42
1:A:226:PRO:HD2	1:A:229:GLU:HG3	2.02	0.42
1:A:307:SER:HG	1:A:311:ARG:NH1	2.16	0.42
1:A:64:ARG:HG2	1:A:67:ARG:NH2	2.34	0.42
1:A:324:LEU:HD23	1:A:327:ARG:HH11	1.85	0.42
1:A:175:LYS:HG3	1:A:274:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:117:GLY:HA2	4:A:428:HOH:O	2.20	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:208:PHE:HB3	1:A:224:GLN:HB2	2.02	0.41
1:A:83:ARG:HD2	1:A:248:PRO:HG2	2.01	0.41
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%)	34 21

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%)	9 3

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	38	TYR
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	238	ARG
1	A	294	THR
1	A	297	LYS
1	A	314	LEU
1	A	321	ARG
1	A	326	GLU
1	A	338	LYS
1	A	352	ARG
1	A	360	SER

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Mol	Chain	Res	Type
1	A	361	GLN
1	A	388	LEU
1	A	391	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	277	GLN
1	A	361	GLN
1	A	365	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 carbohydrates in this entry.

5.6 Ligand geometry

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	-	48,58,58	1.62	8 (16%)	54,89,89	1.73	8 (14%)
3	PHB	A	396	-	7,10,10	0.71	0	10,13,13	0.65	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	-	-	0/30/50/50	0/6/6/6
3	PHB	A	396	-	-	0/0/4/4	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	C10-N10	-3.15	1.35	1.39
2	A	395	FAD	C4X-N5	-2.40	1.29	1.33
2	A	395	FAD	C4A-N3A	-2.24	1.32	1.35
2	A	395	FAD	C5'-C4'	2.31	1.55	1.51
2	A	395	FAD	C1'-N10	2.37	1.50	1.48
2	A	395	FAD	C9A-N10	2.41	1.42	1.38
2	A	395	FAD	C4-C4X	4.59	1.50	1.41
2	A	395	FAD	C4-N3	5.55	1.43	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	395	FAD	C4X-C4-N3	-5.61	115.92	123.59
2	A	395	FAD	N3A-C2A-N1A	-5.24	124.88	128.89
2	A	395	FAD	O4'-C4'-C5'	-3.55	102.46	110.19
2	A	395	FAD	C1B-N9A-C4A	-2.79	122.72	126.94
2	A	395	FAD	P-O3P-PA	2.01	138.37	132.73
2	A	395	FAD	O2A-PA-O1A	2.16	124.25	112.53
2	A	395	FAD	O4B-C1B-N9A	2.24	112.79	108.10
2	A	395	FAD	C4-N3-C2	5.43	119.94	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.