



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:52 am BST

PDB ID : 2PHH
Title : THE COENZYME ANALOGUE ADENOSINE 5-DIPHOSPHORIBOSE DIS-
PLACES FAD IN THE ACTIVE SITE OF P-HYDROXYBENZOATE HY-
DROXYLASE. AN X-RAY CRYSTALLOGRAPHIC INVESTIGATION
Authors : Van Derlaan, J.M.; Drenth, J.; Hol, W.G.J.
Deposited on : 1989-06-19
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

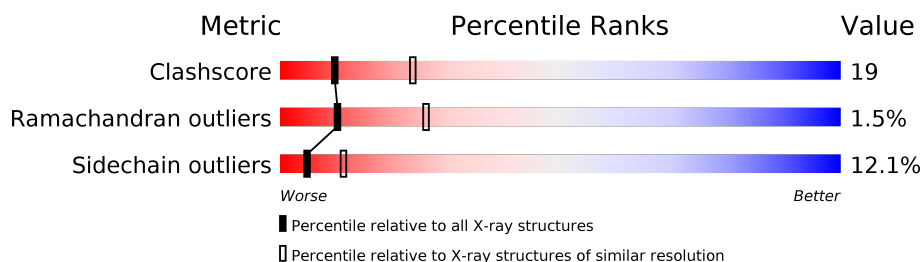
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 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	

2 Entry composition [i](#)

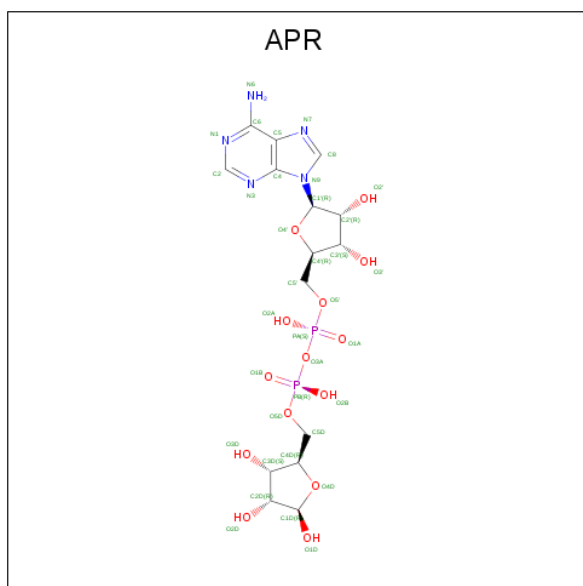
There are 4 unique types of molecules in this entry. The entry contains 3201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

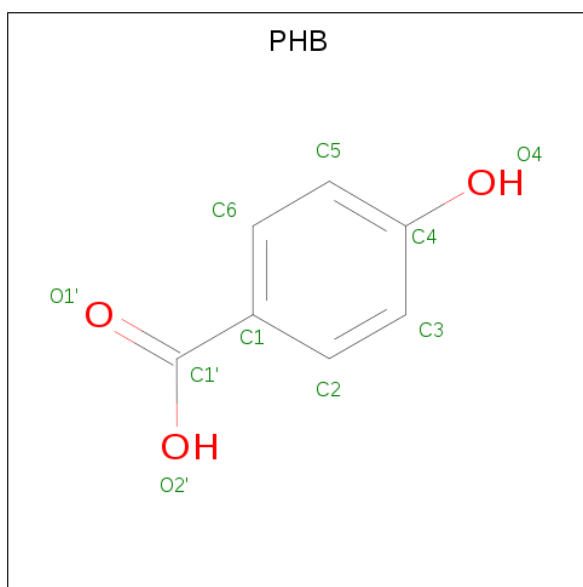
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	3098	1960	560	567	11	0	0	0

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	36	15	5	14	2	0	0

- 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	0	0
			10	7	3		

- Molecule 4 is water.

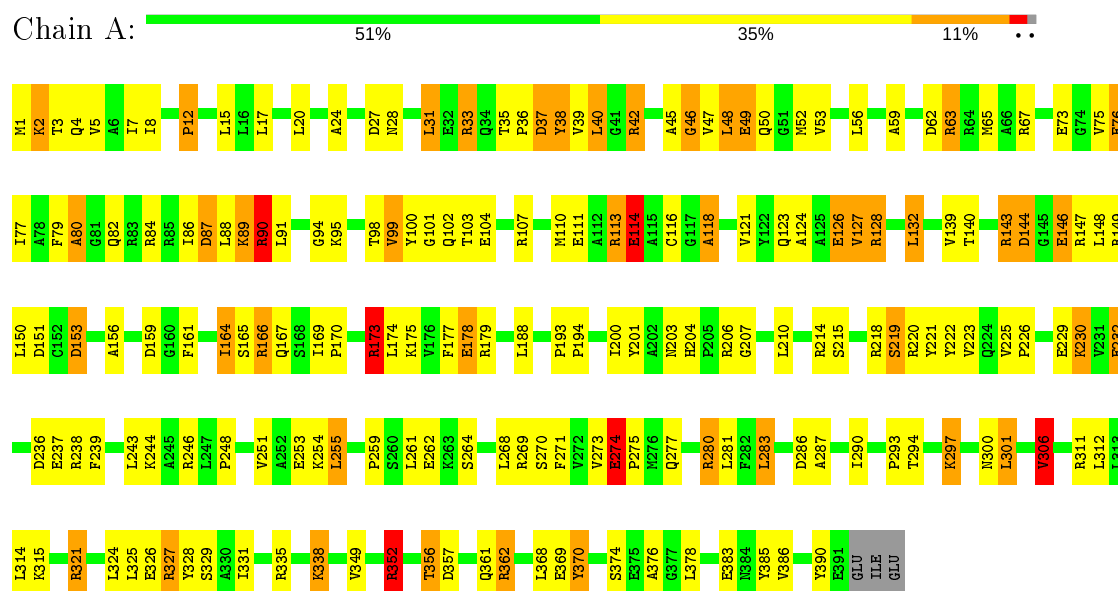
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		

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 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



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	71.70Å 146.40Å 89.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3201	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: APR, 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	0.91	0/3163	1.83	79/4282 (1.8%)

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	A	352	ARG	CD-NE-CZ	13.07	141.90	123.60
1	A	153	ASP	CB-CG-OD1	12.29	129.37	118.30
1	A	238	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	A	42	ARG	NE-CZ-NH2	-10.71	114.94	120.30
1	A	90	ARG	NE-CZ-NH1	10.11	125.36	120.30
1	A	63	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	A	90	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	A	220	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	A	63	ARG	CD-NE-CZ	9.21	136.49	123.60
1	A	153	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	A	269	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	A	280	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	A	113	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	A	38	TYR	CB-CG-CD1	8.57	126.14	121.00
1	A	143	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	166	ARG	NE-CZ-NH2	8.47	124.53	120.30
1	A	140	THR	N-CA-CB	8.46	126.37	110.30
1	A	63	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	A	335	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	56	LEU	CB-CA-C	8.11	125.62	110.20
1	A	42	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	A	111	GLU	CA-CB-CG	8.01	131.03	113.40
1	A	166	ARG	CD-NE-CZ	7.61	134.25	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	A	146	GLU	CB-CG-CD	7.50	134.44	114.20
1	A	173	ARG	CD-NE-CZ	7.31	133.84	123.60
1	A	173	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	311	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	153	ASP	CA-CB-CG	7.17	129.17	113.40
1	A	87	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	A	62	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	A	33	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	269	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	352	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	253	GLU	CA-CB-CG	6.75	128.24	113.40
1	A	146	GLU	CA-CB-CG	6.68	128.10	113.40
1	A	220	ARG	CD-NE-CZ	6.63	132.88	123.60
1	A	114	GLU	CA-CB-CG	6.57	127.86	113.40
1	A	321	ARG	CD-NE-CZ	6.47	132.66	123.60
1	A	113	ARG	CD-NE-CZ	6.40	132.56	123.60
1	A	376	ALA	N-CA-CB	6.28	118.89	110.10
1	A	274	GLU	CA-CB-CG	6.28	127.22	113.40
1	A	356	THR	N-CA-CB	6.19	122.06	110.30
1	A	352	ARG	CG-CD-NE	6.08	124.57	111.80
1	A	76	GLU	CG-CD-OE1	6.08	130.45	118.30
1	A	338	LYS	N-CA-CB	5.98	121.36	110.60
1	A	338	LYS	CA-CB-CG	5.97	126.54	113.40
1	A	390	TYR	CA-CB-CG	5.96	124.73	113.40
1	A	38	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	A	116	CYS	C-N-CA	5.89	134.68	122.30
1	A	254	LYS	CA-CB-CG	5.85	126.28	113.40
1	A	37	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	143	ARG	CB-CA-C	5.82	122.04	110.40
1	A	76	GLU	CB-CA-C	-5.81	98.78	110.40
1	A	33	ARG	CD-NE-CZ	5.78	131.70	123.60
1	A	94	GLY	N-CA-C	5.78	127.54	113.10
1	A	40	LEU	CB-CA-C	5.77	121.16	110.20
1	A	262	GLU	CG-CD-OE1	5.73	129.75	118.30
1	A	132	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	274	GLU	N-CA-CB	5.64	120.75	110.60
1	A	311	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	262	GLU	CG-CD-OE2	-5.60	107.10	118.30
1	A	178	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	370	TYR	N-CA-CB	5.51	120.53	110.60
1	A	99	VAL	CA-CB-CG1	5.51	119.16	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	327	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	201	TYR	CA-CB-CG	5.46	123.78	113.40
1	A	362	ARG	NH1-CZ-NH2	5.42	125.37	119.40
1	A	149	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	A	306	VAL	CB-CA-C	5.34	121.55	111.40
1	A	111	GLU	N-CA-CB	5.29	120.12	110.60
1	A	369	GLU	CA-CB-CG	5.24	124.92	113.40
1	A	238	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	127	VAL	CB-CA-C	5.15	121.18	111.40
1	A	84	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	118	ALA	CB-CA-C	5.05	117.67	110.10
1	A	301	LEU	CB-CA-C	5.03	119.77	110.20

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	3098	0	3099	121	3
2	A	36	0	21	4	0
3	A	10	0	5	0	0
4	A	57	0	0	8	0
All	All	3201	0	3125	121	3

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 (121) 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:47:VAL:HG22	1:A:99:VAL:HG22	1.51	0.91
1:A:63:ARG:HH22	1:A:67:ARG:HH11	1.19	0.85
1:A:169:ILE:HD11	1:A:283:LEU:HD21	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HH22	1:A:67:ARG:NH1	1.80	0.79
1:A:45:ALA:HB3	1:A:102:GLN:HB2	1.65	0.79
1:A:218:ARG:HH21	1:A:261:LEU:HD13	1.48	0.78
1:A:146:GLU:HG3	1:A:148:LEU:HD21	1.67	0.77
1:A:118:ALA:HA	4:A:434:HOH:O	1.86	0.75
1:A:24:ALA:HB1	1:A:314:LEU:HD21	1.69	0.74
1:A:15:LEU:HD11	1:A:110:MET:HG3	1.72	0.71
1:A:121:VAL:HG12	1:A:124:ALA:HB2	1.72	0.71
1:A:214:ARG:HB2	1:A:218:ARG:HB3	1.76	0.67
1:A:46:GLY:O	1:A:99:VAL:HA	1.96	0.65
1:A:20:LEU:HG	1:A:59:ALA:HB2	1.77	0.65
1:A:312:LEU:HB3	1:A:325:LEU:HD23	1.78	0.65
1:A:204:HIS:CD2	1:A:206:ARG:H	2.16	0.64
1:A:39:VAL:HG13	1:A:42:ARG:NH2	2.13	0.64
1:A:226:PRO:HG2	1:A:229:GLU:HG2	1.81	0.63
1:A:173:ARG:HH11	1:A:173:ARG:HB2	1.64	0.62
1:A:126:GLU:HG3	4:A:402:HOH:O	2.00	0.61
1:A:31:LEU:HD12	1:A:121:VAL:HB	1.81	0.61
1:A:286:ASP:OD1	2:A:395:APR:HR'2	2.00	0.61
1:A:225:VAL:HB	1:A:226:PRO:HD2	1.84	0.60
1:A:36:PRO:O	1:A:40:LEU:HB2	2.02	0.59
1:A:223:VAL:HB	1:A:246:ARG:NH1	2.19	0.58
1:A:277:GLN:NE2	1:A:329:SER:H	2.02	0.57
1:A:161:PHE:HB2	1:A:290:ILE:HD11	1.86	0.56
1:A:244:LYS:HG2	1:A:255:LEU:HD22	1.88	0.56
1:A:277:GLN:HE22	1:A:328:TYR:HB3	1.70	0.55
1:A:203:ASN:ND2	1:A:349:VAL:O	2.40	0.55
1:A:204:HIS:HD2	1:A:206:ARG:H	1.52	0.55
1:A:63:ARG:NH2	1:A:67:ARG:HH11	1.98	0.55
1:A:76:GLU:HB2	1:A:200:ILE:HA	1.89	0.54
1:A:264:SER:HB2	4:A:433:HOH:O	2.10	0.52
1:A:277:GLN:HE21	1:A:329:SER:H	1.57	0.52
1:A:277:GLN:NE2	1:A:328:TYR:HB3	2.25	0.52
1:A:357:ASP:O	1:A:361:GLN:HG3	2.10	0.51
1:A:219:SER:HB2	1:A:221:TYR:CE2	2.45	0.51
1:A:104:GLU:HG3	1:A:107:ARG:HH22	1.75	0.51
1:A:17:LEU:HB2	1:A:306:VAL:HG22	1.93	0.50
1:A:173:ARG:NH1	1:A:173:ARG:HB2	2.26	0.50
1:A:87:ASP:HB3	1:A:90:ARG:HG2	1.92	0.50
1:A:169:ILE:HD12	1:A:283:LEU:HD11	1.94	0.50
1:A:239:PHE:HE2	1:A:243:LEU:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLN:NE2	2:A:395:APR:HR'4	2.27	0.49
1:A:102:GLN:HE22	2:A:395:APR:C4D	2.26	0.48
1:A:47:VAL:HA	1:A:98:THR:O	2.13	0.48
1:A:327:ARG:HG3	1:A:331:ILE:CD1	2.44	0.48
1:A:100:TYR:CZ	1:A:104:GLU:HB3	2.48	0.47
1:A:204:HIS:NE2	1:A:206:ARG:HG3	2.30	0.47
1:A:33:ARG:HB3	1:A:33:ARG:HE	1.58	0.47
1:A:104:GLU:HG3	1:A:107:ARG:NH2	2.31	0.46
1:A:315:LYS:HD3	1:A:324:LEU:HD12	1.95	0.46
1:A:77:ILE:HG12	1:A:86:ILE:HD11	1.96	0.46
1:A:324:LEU:O	1:A:327:ARG:HG2	2.15	0.46
1:A:8:ILE:HG22	1:A:159:ASP:HB3	1.96	0.46
1:A:49:GLU:HG2	1:A:300:ASN:CG	2.36	0.46
1:A:164:ILE:HA	1:A:167:GLN:NE2	2.29	0.46
1:A:297:LYS:O	1:A:301:LEU:HG	2.15	0.46
1:A:164:ILE:HG13	1:A:164:ILE:O	2.15	0.46
1:A:218:ARG:HH21	1:A:261:LEU:CD1	2.24	0.46
1:A:5:VAL:O	1:A:28:ASN:HA	2.16	0.46
1:A:2:LYS:HB2	1:A:151:ASP:HB2	1.97	0.46
1:A:178:GLU:HB2	1:A:271:PHE:CD2	2.51	0.46
1:A:4:GLN:HB2	1:A:27:ASP:O	2.15	0.46
1:A:210:LEU:HB3	1:A:222:TYR:HB2	1.99	0.45
1:A:207:GLY:HA2	1:A:352:ARG:HB3	1.99	0.45
1:A:169:ILE:HG21	1:A:174:LEU:HG	1.97	0.45
1:A:45:ALA:HA	4:A:456:HOH:O	2.15	0.45
1:A:91:LEU:CD1	1:A:378:LEU:HB3	2.47	0.45
1:A:3:THR:HG22	1:A:150:LEU:HD11	1.99	0.45
1:A:127:VAL:O	1:A:128:ARG:HG2	2.17	0.45
1:A:95:LYS:HB2	1:A:386:VAL:HG21	1.99	0.45
1:A:315:LYS:HD3	1:A:324:LEU:CD1	2.47	0.44
1:A:12:PRO:HG2	1:A:102:GLN:NE2	2.33	0.44
1:A:248:PRO:HB2	1:A:251:VAL:HG23	1.98	0.44
1:A:236:ASP:OD2	1:A:259:PRO:HA	2.18	0.44
1:A:89:LYS:HA	1:A:95:LYS:O	2.18	0.44
1:A:73:GLU:HB3	1:A:89:LYS:HB2	1.99	0.44
1:A:327:ARG:O	1:A:331:ILE:HG13	2.18	0.44
1:A:53:VAL:HG13	1:A:65:MET:CE	2.47	0.44
1:A:230:LYS:HB2	1:A:232:GLU:HG2	2.00	0.43
1:A:174:LEU:HD23	1:A:275:PRO:HD2	1.99	0.43
1:A:169:ILE:CD1	1:A:283:LEU:HD11	2.49	0.43
1:A:118:ALA:CA	4:A:434:HOH:O	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:HG3	1:A:331:ILE:HD11	2.00	0.43
1:A:45:ALA:HB3	1:A:102:GLN:CB	2.44	0.43
1:A:17:LEU:HD13	1:A:306:VAL:HG22	2.01	0.43
1:A:268:LEU:HG	1:A:293:PRO:HD2	2.00	0.43
1:A:35:THR:HB	1:A:36:PRO:HD2	2.01	0.43
1:A:88:LEU:HD22	1:A:385:TYR:HB3	2.01	0.42
1:A:2:LYS:HD2	1:A:3:THR:N	2.34	0.42
1:A:4:GLN:OE1	1:A:27:ASP:N	2.42	0.42
1:A:127:VAL:O	1:A:128:ARG:NH1	2.50	0.42
1:A:132:LEU:HD22	1:A:281:LEU:HB2	2.00	0.42
1:A:79:PHE:CB	1:A:368:LEU:HD13	2.50	0.42
1:A:63:ARG:NH2	1:A:67:ARG:NH1	2.57	0.42
1:A:169:ILE:HA	1:A:170:PRO:HD3	1.92	0.42
1:A:2:LYS:HD2	1:A:3:THR:H	1.84	0.42
1:A:143:ARG:HB3	1:A:146:GLU:OE1	2.19	0.42
1:A:153:ASP:O	1:A:280:ARG:HD3	2.20	0.42
1:A:161:PHE:H	1:A:286:ASP:HB3	1.85	0.42
1:A:193:PRO:HA	1:A:194:PRO:HD3	1.76	0.42
1:A:161:PHE:N	1:A:286:ASP:HB3	2.35	0.42
1:A:102:GLN:HE22	2:A:395:APR:HR'4	1.83	0.42
1:A:178:GLU:HB2	1:A:271:PHE:HD2	1.85	0.41
1:A:143:ARG:O	1:A:144:ASP:HB3	2.20	0.41
1:A:48:LEU:HA	1:A:300:ASN:OD1	2.21	0.41
1:A:352:ARG:HG2	1:A:352:ARG:HH11	1.84	0.41
1:A:128:ARG:O	1:A:139:VAL:HA	2.20	0.41
1:A:31:LEU:HD23	1:A:139:VAL:HG11	2.03	0.41
1:A:103:THR:HG22	4:A:436:HOH:O	2.20	0.41
1:A:40:LEU:HD13	1:A:110:MET:SD	2.61	0.41
1:A:45:ALA:CB	1:A:102:GLN:HB2	2.43	0.41
1:A:33:ARG:O	1:A:123:GLN:HA	2.21	0.41
1:A:50:GLN:HB3	4:A:431:HOH:O	2.21	0.41
1:A:166:ARG:HD3	1:A:287:ALA:O	2.22	0.40
1:A:7:ILE:HG12	1:A:156:ALA:HB3	2.04	0.40
1:A:82:GLN:HB3	4:A:454:HOH:O	2.21	0.40
1:A:113:ARG:HG2	1:A:118:ALA:HB3	2.03	0.40
1:A:79:PHE:O	1:A:80:ALA:C	2.59	0.40

All (3) 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)
1:A:370:TYR:OH	1:A:383:GLU:OE1[4_566]	1.77	0.43
1:A:114:GLU:OE1	1:A:244:LYS:NZ[6_565]	2.06	0.14
1:A:274:GLU:OE1	1:A:362:ARG:NH2[4_566]	2.19	0.01

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%)	355 (91%)	28 (7%)	6 (2%)	10	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ALA
1	A	101	GLY
1	A	144	ASP
1	A	165	SER
1	A	12	PRO
1	A	46	GLY

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%)	282 (88%)	39 (12%)	5	11

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	31	LEU
1	A	37	ASP
1	A	38	TYR
1	A	48	LEU
1	A	49	GLU
1	A	52	MET
1	A	75	VAL
1	A	89	LYS
1	A	90	ARG
1	A	114	GLU
1	A	126	GLU
1	A	147	ARG
1	A	164	ILE
1	A	173	ARG
1	A	175	LYS
1	A	177	PHE
1	A	179	ARG
1	A	188	LEU
1	A	215	SER
1	A	219	SER
1	A	230	LYS
1	A	232	GLU
1	A	237	GLU
1	A	255	LEU
1	A	270	SER
1	A	273	VAL
1	A	274	GLU
1	A	283	LEU
1	A	294	THR
1	A	297	LYS
1	A	306	VAL
1	A	321	ARG
1	A	326	GLU
1	A	338	LYS
1	A	352	ARG
1	A	356	THR
1	A	374	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	204	HIS
1	A	277	GLN
1	A	278	HIS
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 carbohydrates 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	-	8,10,10	0.60	0	10,13,13	1.15	1 (10%)
2	APR	A	395	-	34,39,39	1.04	2 (5%)	40,60,60	1.74	7 (17%)

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	-	-	0/0/4/4	0/1/1/1
2	APR	A	395	-	-	3/18/54/54	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	APR	C2-N1	3.30	1.40	1.33
2	A	395	APR	O5D-C5D	-2.32	1.35	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	APR	PB-O3A-PA	6.41	154.82	132.83
2	A	395	APR	O5D-C5D-C4D	4.23	123.53	108.99
2	A	395	APR	N3-C2-N1	-3.05	123.91	128.68
2	A	395	APR	O5'-PA-O1A	2.95	120.60	109.07
3	A	396	PHB	C6-C1-C1'	2.67	123.97	120.37
2	A	395	APR	PB-O5D-C5D	2.53	136.54	121.68
2	A	395	APR	C5-C6-N6	2.38	123.97	120.35
2	A	395	APR	C1'-N9-C4	-2.02	123.09	126.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	395	APR	PA-O3A-PB-O5D
2	A	395	APR	PA-O3A-PB-O1B
2	A	395	APR	O4'-C4'-C5'-O5'

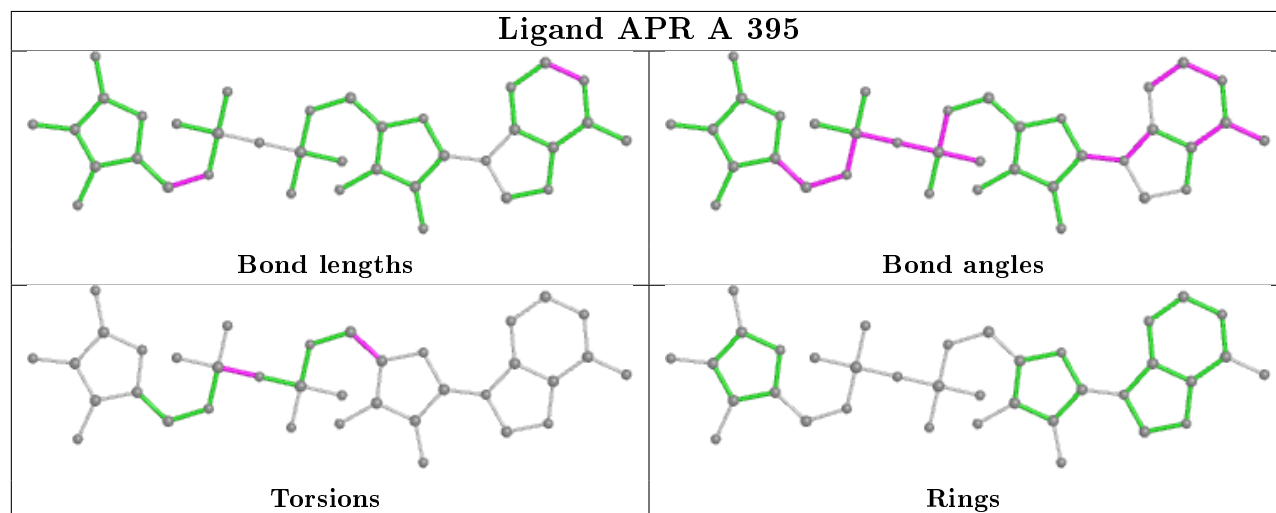
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	395	APR	4	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.