



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:20 PM UTC

PDB ID : 2PHH / pdb_00002phh
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 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

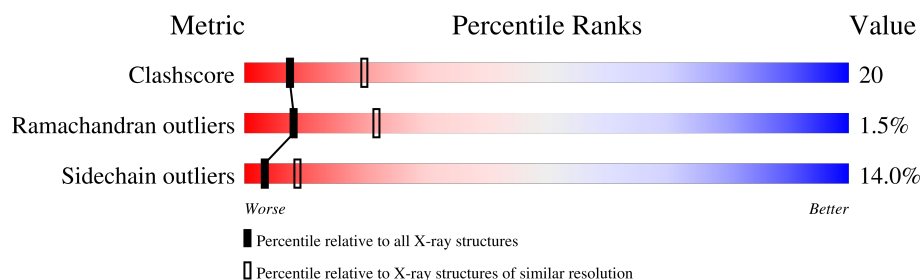
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 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	

2 Entry composition [i](#)

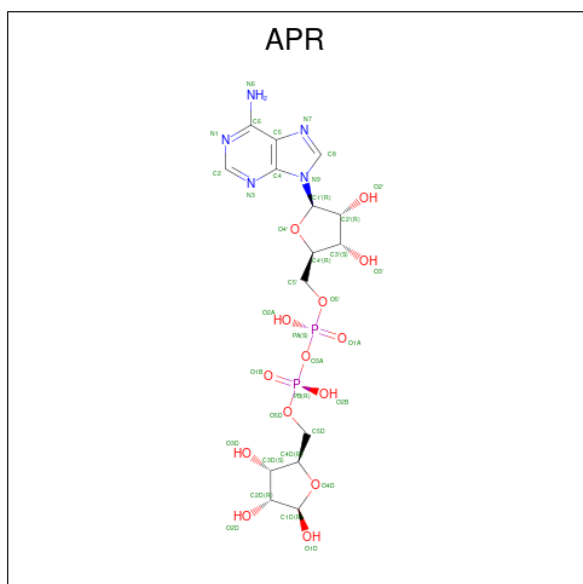
There are 4 unique types of molecules in this entry. The entry contains 3201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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 (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.

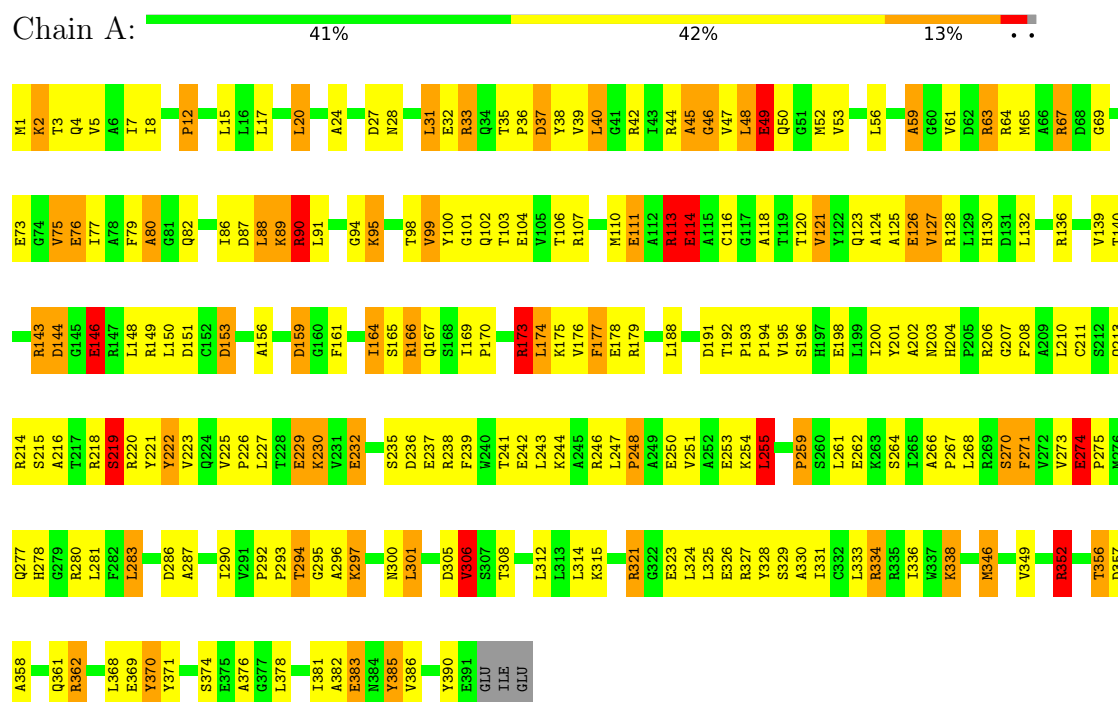
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		

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



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	1.13	2/3163 (0.1%)	2.17	129/4282 (3.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	THR	CA-CB	5.47	1.60	1.53
1	A	153	ASP	CA-CB	-5.03	1.46	1.53

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ASP	CA-CB-CG	16.57	129.17	112.60
1	A	146	GLU	CB-CG-CD	12.85	134.44	112.60
1	A	352	ARG	CD-NE-CZ	12.50	141.90	124.40
1	A	191	ASP	CA-CB-CG	9.99	122.59	112.60
1	A	94	GLY	N-CA-C	9.71	127.54	114.92
1	A	271	PHE	CA-CB-CG	9.69	123.48	113.80
1	A	56	LEU	CB-CA-C	9.26	125.62	110.81
1	A	140	THR	N-CA-CB	8.93	126.37	110.83
1	A	63	ARG	CD-NE-CZ	8.63	136.49	124.40
1	A	44	ARG	CA-C-N	8.56	133.40	120.82
1	A	44	ARG	C-N-CA	8.56	133.40	120.82
1	A	177	PHE	CA-CB-CG	8.50	122.30	113.80
1	A	176	VAL	N-CA-C	8.49	120.50	108.36
1	A	111	GLU	CA-CB-CG	8.46	131.03	114.10
1	A	247	LEU	N-CA-C	8.33	119.71	110.13
1	A	37	ASP	CA-CB-CG	7.72	120.32	112.60
1	A	116	CYS	CA-C-N	7.71	134.68	120.87
1	A	116	CYS	C-N-CA	7.71	134.68	120.87
1	A	383	GLU	CB-CG-CD	7.56	125.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ALA	N-CA-C	7.42	121.00	108.02
1	A	294	THR	CA-C-O	-7.34	113.14	120.70
1	A	229	GLU	CB-CG-CD	7.25	124.92	112.60
1	A	381	ILE	CA-C-N	7.19	130.50	120.29
1	A	381	ILE	C-N-CA	7.19	130.50	120.29
1	A	213	GLN	N-CA-C	7.14	119.61	108.96
1	A	370	TYR	N-CA-CB	7.11	120.53	110.07
1	A	253	GLU	CA-CB-CG	7.07	128.24	114.10
1	A	166	ARG	CD-NE-CZ	7.04	134.25	124.40
1	A	376	ALA	N-CA-C	-7.04	103.69	111.36
1	A	136	ARG	O-C-N	7.02	125.48	121.27
1	A	146	GLU	CA-CB-CG	7.00	128.10	114.10
1	A	255	LEU	N-CA-C	6.99	119.87	109.59
1	A	111	GLU	N-CA-CB	6.93	120.12	110.07
1	A	242	GLU	CB-CG-CD	6.92	124.37	112.60
1	A	45	ALA	N-CA-C	6.88	119.18	110.24
1	A	114	GLU	CA-CB-CG	6.88	127.86	114.10
1	A	250	GLU	CB-CG-CD	6.82	124.19	112.60
1	A	306	VAL	CB-CA-C	6.76	121.55	112.22
1	A	49	GLU	CB-CG-CD	6.75	124.07	112.60
1	A	173	ARG	CD-NE-CZ	6.74	133.84	124.40
1	A	75	VAL	CA-C-N	6.69	133.04	122.74
1	A	75	VAL	C-N-CA	6.69	133.04	122.74
1	A	336	ILE	CB-CA-C	6.57	120.11	111.70
1	A	274	GLU	CA-CB-CG	6.56	127.22	114.10
1	A	69	GLY	N-CA-C	-6.56	104.15	112.54
1	A	111	GLU	CB-CA-C	-6.53	100.58	110.90
1	A	127	VAL	CB-CA-C	6.53	121.18	111.26
1	A	247	LEU	N-CA-CB	-6.53	102.12	109.49
1	A	323	GLU	N-CA-C	6.52	118.39	111.28
1	A	356	THR	N-CA-CB	6.51	122.06	110.80
1	A	338	LYS	N-CA-CB	6.50	121.36	110.32
1	A	143	ARG	CB-CA-C	6.43	122.04	111.23
1	A	278	HIS	CA-CB-CG	-6.30	107.50	113.80
1	A	362	ARG	NE-CZ-NH2	-6.25	113.58	119.20
1	A	338	LYS	CA-CB-CG	6.22	126.54	114.10
1	A	333	LEU	N-CA-C	6.21	118.85	111.71
1	A	294	THR	N-CA-C	6.14	117.77	111.14
1	A	67	ARG	N-CA-C	6.13	119.23	111.69
1	A	266	ALA	O-C-N	6.13	126.85	121.39
1	A	254	LYS	CA-CB-CG	6.09	126.28	114.10
1	A	153	ASP	N-CA-C	-6.07	106.01	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ARG	CD-NE-CZ	6.06	132.88	124.40
1	A	76	GLU	CB-CA-C	-6.03	98.78	109.70
1	A	390	TYR	CA-CB-CG	6.02	124.73	113.90
1	A	99	VAL	CB-CA-C	5.98	119.68	111.31
1	A	196	SER	N-CA-C	5.97	118.19	108.76
1	A	292	PRO	N-CA-C	-5.96	103.43	110.70
1	A	346	MET	CA-C-N	5.95	129.06	120.79
1	A	346	MET	C-N-CA	5.95	129.06	120.79
1	A	166	ARG	NE-CZ-NH2	5.93	124.53	119.20
1	A	20	LEU	O-C-N	5.92	128.92	122.11
1	A	371	TYR	N-CA-C	5.92	118.51	111.71
1	A	321	ARG	CD-NE-CZ	5.90	132.66	124.40
1	A	376	ALA	N-CA-CB	5.90	118.89	110.16
1	A	242	GLU	N-CA-CB	5.87	118.85	110.16
1	A	274	GLU	N-CA-CB	5.83	120.75	110.37
1	A	113	ARG	CD-NE-CZ	5.83	132.56	124.40
1	A	76	GLU	CB-CG-CD	5.83	122.51	112.60
1	A	37	ASP	N-CA-CB	5.81	119.04	110.33
1	A	95	LYS	N-CA-C	5.81	118.03	110.53
1	A	88	LEU	N-CA-C	-5.80	104.86	111.07
1	A	358	ALA	N-CA-C	5.79	118.37	111.71
1	A	222	TYR	N-CA-C	5.78	118.19	109.23
1	A	38	TYR	N-CA-C	-5.75	104.91	111.07
1	A	352	ARG	CG-CD-NE	5.71	124.57	112.00
1	A	120	THR	N-CA-CB	5.69	118.68	110.37
1	A	385	TYR	O-C-N	5.67	128.13	122.12
1	A	262	GLU	CB-CG-CD	5.61	122.14	112.60
1	A	130	HIS	N-CA-C	5.58	118.32	109.50
1	A	121	VAL	CB-CA-C	5.57	119.06	111.88
1	A	159	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	211	CYS	CA-C-O	-5.50	114.63	120.40
1	A	201	TYR	CA-CB-CG	5.49	123.78	113.90
1	A	216	ALA	N-CA-C	-5.46	105.48	111.82
1	A	235	SER	O-C-N	5.42	129.03	122.85
1	A	369	GLU	CA-CB-CG	5.41	124.92	114.10
1	A	390	TYR	N-CA-C	-5.39	102.54	110.52
1	A	219	SER	CA-CB-OG	5.39	121.88	111.10
1	A	308	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	90	ARG	N-CA-CB	5.29	117.96	110.13
1	A	174	LEU	N-CA-C	5.28	118.42	109.76
1	A	235	SER	N-CA-C	-5.28	103.42	110.55
1	A	208	PHE	CA-CB-CG	5.27	119.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	PRO	CA-C-O	-5.26	115.51	121.98
1	A	76	GLU	CG-CD-OE1	5.24	130.45	118.40
1	A	121	VAL	O-C-N	5.24	128.75	122.62
1	A	61	VAL	CA-C-N	-5.23	114.31	122.37
1	A	61	VAL	C-N-CA	-5.23	114.31	122.37
1	A	213	GLN	CA-C-O	5.22	127.04	121.45
1	A	140	THR	CA-CB-CG2	5.21	119.37	110.50
1	A	33	ARG	CD-NE-CZ	5.21	131.70	124.40
1	A	241	THR	N-CA-CB	5.20	117.95	110.20
1	A	40	LEU	CB-CA-C	5.19	121.16	110.31
1	A	59	ALA	N-CA-C	-5.17	106.82	113.02
1	A	99	VAL	CA-CB-CG1	5.15	119.16	110.40
1	A	198	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	305	ASP	O-C-N	5.11	127.98	122.15
1	A	32	GLU	CB-CG-CD	5.11	121.29	112.60
1	A	106	THR	N-CA-CB	5.09	117.53	109.94
1	A	305	ASP	CA-CB-CG	-5.09	107.51	112.60
1	A	371	TYR	CA-C-O	-5.09	114.35	120.10
1	A	248	PRO	CA-C-N	5.08	128.45	120.82
1	A	248	PRO	C-N-CA	5.08	128.45	120.82
1	A	238	ARG	O-C-N	5.08	127.30	122.07
1	A	259	PRO	CA-C-O	-5.05	115.70	121.56
1	A	382	ALA	N-CA-C	5.04	116.86	111.36
1	A	270	SER	CA-C-O	-5.03	114.92	120.30
1	A	301	LEU	CB-CA-C	5.02	119.77	109.67
1	A	125	ALA	O-C-N	5.02	128.66	122.84

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	127	3
2	A	36	0	21	4	0
3	A	10	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	57	0	0	8	0
All	All	3201	0	3125	127	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 20.

All (127) 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
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:HB2	1:A:173:ARG:HH11	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:53:VAL:HG13	1:A:65:MET:HE1	1.86	0.58
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:203:ASN:ND2	1:A:349:VAL:O	2.40	0.55
1:A:277:GLN:HE22	1:A:328:TYR:HB3	1.70	0.55
1:A:204:HIS:HD2	1:A:206:ARG:H	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:40:LEU:HD22	1:A:110:MET:HE1	1.90	0.53
1:A:264:SER:HB2	4:A:433:HOH:O	2.10	0.52
1:A:277:GLN:NE2	1:A:328:TYR:HB3	2.25	0.52
1:A:277:GLN:HE21	1:A:329:SER:H	1.57	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:HB2	1:A:173:ARG:NH1	2.26	0.50
1:A:49:GLU:HG2	1:A:300:ASN:CG	2.36	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
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:HE	1:A:33:ARG:HB3	1.58	0.47
1:A:77:ILE:HG12	1:A:86:ILE:HD11	1.96	0.46
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: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: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:5:VAL:O	1:A:28:ASN:HA	2.16	0.46
1:A:164:ILE:O	1:A:164:ILE:HG13	2.15	0.46
1:A:218:ARG:HH21	1:A:261:LEU:CD1	2.24	0.46
1:A:2:LYS:HB2	1:A:151:ASP:HB2	1.97	0.46
1:A:4:GLN:HB2	1:A:27:ASP:O	2.15	0.46
1:A:178:GLU:HB2	1:A:271:PHE:CD2	2.51	0.46
1:A:207:GLY:HA2	1:A:352:ARG:HB3	1.99	0.45
1:A:210:LEU:HB3	1:A:222:TYR:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:O	1:A:80:ALA:C	2.59	0.45
1:A:95:LYS:HB2	1:A:386:VAL:HG21	1.99	0.45
1:A:127:VAL:O	1:A:128:ARG:HG2	2.17	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:53:VAL:HG13	1:A:65:MET:CE	2.47	0.44
1:A:327:ARG:O	1:A:331:ILE:HG13	2.18	0.44
1:A:174:LEU:HD23	1:A:275:PRO:HD2	1.99	0.43
1:A:230:LYS:HB2	1:A:232:GLU:HG2	2.00	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
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:2:LYS:HD2	1:A:3:THR:N	2.34	0.42
1:A:88:LEU:HD22	1:A:385:TYR:HB3	2.01	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:127:VAL:C	1:A:128:ARG:HG2	2.45	0.42
1:A:132:LEU:HD22	1:A:281:LEU:HB2	2.00	0.42
1:A:63:ARG:NH2	1:A:67:ARG:NH1	2.57	0.42
1:A:79:PHE:CB	1:A:368:LEU:HD13	2.50	0.42
1:A:2:LYS:HD2	1:A:3:THR:H	1.84	0.42
1:A:169:ILE:HA	1:A:170:PRO:HD3	1.92	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:330:ALA:C	1:A:334:ARG:HH11	2.27	0.42
1:A:161:PHE:N	1:A:286:ASP:HB3	2.35	0.42
1:A:193:PRO:HA	1:A:194:PRO:HD3	1.76	0.42
1:A:102:GLN:HE22	2:A:395:APR:HR'4	1.83	0.42
1:A:295:GLY:O	1:A:296:ALA:C	2.62	0.42
1:A:178:GLU:HB2	1:A:271:PHE:HD2	1.85	0.41
1:A:48:LEU:HA	1:A:300:ASN:OD1	2.21	0.41
1:A:143:ARG:O	1:A:144:ASP:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:HH11	1:A:352:ARG:HG2	1.84	0.41
1:A:128:ARG:O	1:A:139:VAL:HA	2.20	0.41
1:A:149:ARG:HE	1:A:151:ASP:CG	2.27	0.41
1:A:31:LEU:HD23	1:A:139:VAL:HG11	2.03	0.41
1:A:33:ARG:O	1:A:123:GLN:HA	2.21	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:50:GLN:HB3	4:A:431:HOH:O	2.21	0.41
1:A:103:THR:HG22	4:A:436:HOH:O	2.20	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

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%)	8 22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ALA

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Mol	Chain	Res	Type
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 ⓘ

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%)	276 (86%)	45 (14%)	3 9

All (45) 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	48	LEU
1	A	49	GLU
1	A	52	MET
1	A	64	ARG
1	A	75	VAL
1	A	89	LYS
1	A	90	ARG
1	A	111	GLU
1	A	113	ARG
1	A	114	GLU
1	A	126	GLU
1	A	146	GLU
1	A	164	ILE
1	A	173	ARG
1	A	175	LYS
1	A	177	PHE
1	A	179	ARG

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Mol	Chain	Res	Type
1	A	188	LEU
1	A	195	VAL
1	A	215	SER
1	A	219	SER
1	A	227	LEU
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	334	ARG
1	A	338	LYS
1	A	346	MET
1	A	352	ARG
1	A	356	THR
1	A	374	SER

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	50	GLN
1	A	72	HIS
1	A	123	GLN
1	A	204	HIS
1	A	277	GLN
1	A	278	HIS
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 [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	APR	A	395	-	39,39,39	1.52	6 (15%)	56,60,60	1.29	5 (8%)
3	PHB	A	396	-	10,10,10	1.36	2 (20%)	13,13,13	1.39	2 (15%)

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	APR	A	395	-	-	5/22/54/54	0/4/4/4
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	APR	PB-O3A	4.51	1.64	1.59
2	A	395	APR	PA-O3A	4.41	1.64	1.59
2	A	395	APR	C2-N1	3.45	1.40	1.33
3	A	396	PHB	O1'-C1'	3.07	1.31	1.22
2	A	395	APR	C5-C4	2.72	1.43	1.39
2	A	395	APR	C2-N3	-2.46	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	APR	O5D-C5D	-2.31	1.35	1.44
3	A	396	PHB	O2'-C1'	-2.20	1.24	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	APR	O5D-C5D-C4D	4.27	123.53	108.99
2	A	395	APR	N3-C2-N1	-3.09	123.91	128.58
3	A	396	PHB	O2'-C1'-O1'	-3.04	116.81	123.35
2	A	395	APR	O5'-PA-O1A	2.94	120.60	108.94
3	A	396	PHB	O2'-C1'-C1	2.83	122.11	114.84
2	A	395	APR	PB-O5D-C5D	2.65	136.54	121.35
2	A	395	APR	C2-N1-C6	2.04	122.08	118.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	395	APR	PA-O3A-PB-O5D
2	A	395	APR	C2'-C1'-N9-C8
2	A	395	APR	O4'-C1'-N9-C8
2	A	395	APR	PA-O3A-PB-O1B
2	A	395	APR	PA-O3A-PB-O2B

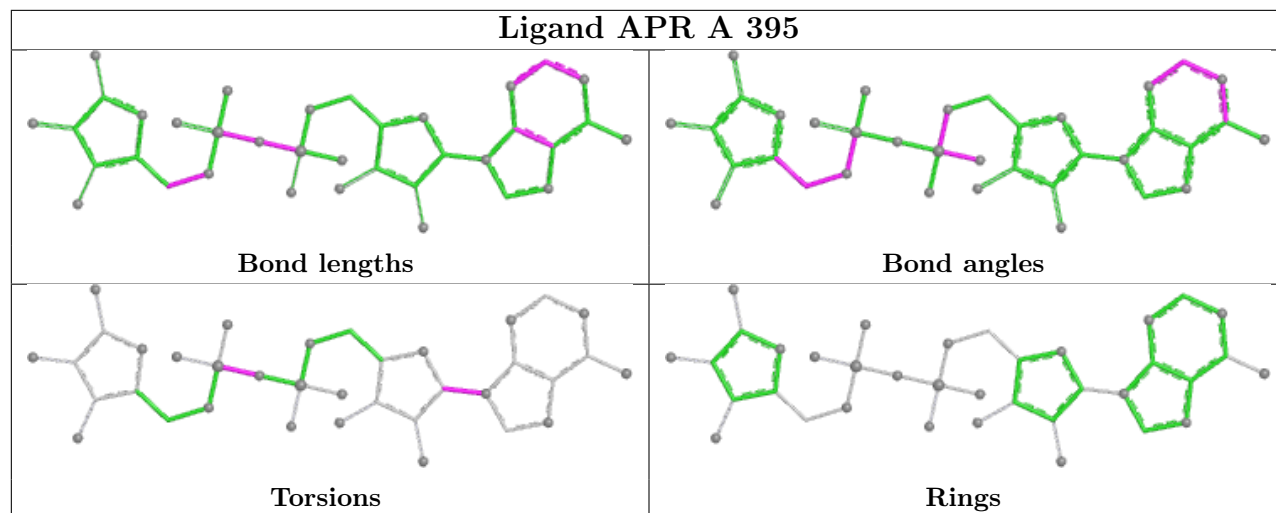
There are no ring outliers.

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.