



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:02 PM UTC

PDB ID : 1PU9 / pdb_00001pu9
Title : Crystal Structure of Tetrahymena GCN5 with Bound Coenzyme A and a 19-residue Histone H3 Peptide
Authors : Clements, A.; Poux, A.N.; Lo, W.S.; Pillus, L.; Berger, S.L.; Marmorstein, R.
Deposited on : 2003-06-24
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

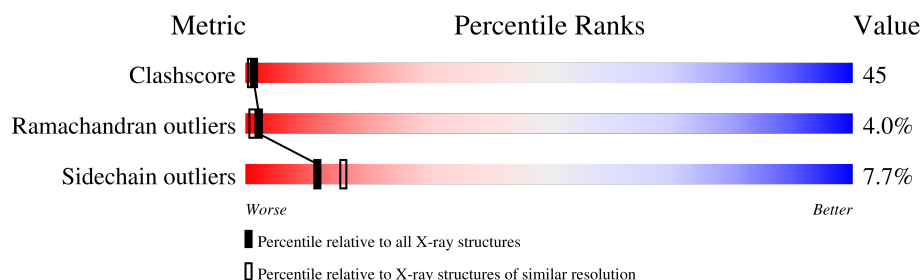
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	163	58% 36% 6%
2	B	19	26% 32% 21% 21%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1631 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 HAT A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1368	885	238	236	9			

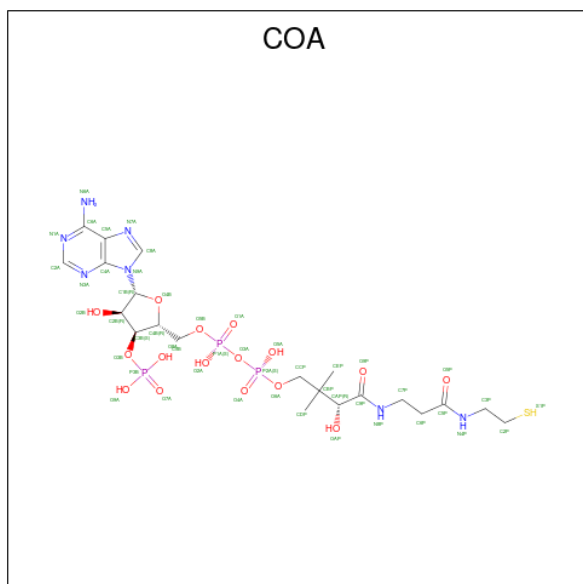
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	PHE	LEU	see remark 999	UNP Q27198
A	210	ARG	ASN	see remark 999	UNP Q27198

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	0	0	0
			109	66	25	18			

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total	O	0	0
			102	102		
4	B	4	Total	O	0	0
			4	4		

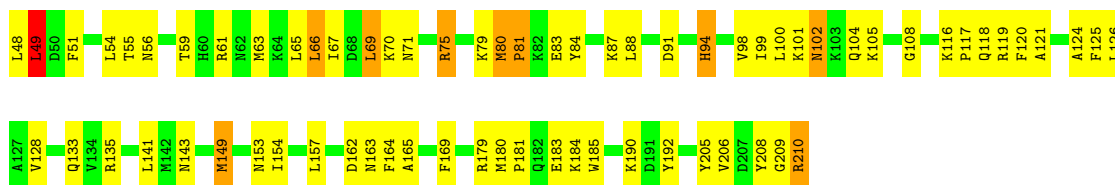
3 Residue-property plots

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: HAT A1

Chain A: 



- Molecule 2: Histone H3

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.73Å 64.73Å 96.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	21.12 – 2.30	Depositor
% Data completeness (in resolution range)	92.3 (21.12-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1631	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: COA

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	0.49	2/1401 (0.1%)	0.95	8/1878 (0.4%)
2	B	1.58	1/109 (0.9%)	2.79	13/142 (9.2%)
All	All	0.63	3/1510 (0.2%)	1.18	21/2020 (1.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	MET	SD-CE	-6.07	1.64	1.79
2	B	314	LYS	N-CA	5.64	1.53	1.46
1	A	80	MET	SD-CE	-5.31	1.66	1.79

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	308	ARG	N-CA-C	-17.00	92.98	114.56
2	B	321	ALA	N-CA-C	-9.10	85.52	111.00
2	B	313	GLY	N-CA-C	7.75	124.06	110.80
2	B	314	LYS	N-CA-C	7.39	126.55	110.80
2	B	320	LEU	N-CA-C	-6.77	96.38	110.80
1	A	49	LEU	N-CA-C	6.32	124.25	110.80
1	A	179	ARG	N-CA-C	-6.18	105.38	113.17
2	B	313	GLY	CA-C-N	5.78	132.59	121.54
2	B	313	GLY	C-N-CA	5.78	132.59	121.54
2	B	310	SER	N-CA-C	5.68	122.89	110.80
2	B	308	ARG	O-C-N	5.58	128.02	122.10
1	A	206	VAL	N-CA-C	-5.51	100.50	108.71
1	A	208	TYR	N-CA-C	-5.49	101.91	110.42
1	A	205	TYR	N-CA-C	5.46	117.43	110.61
2	B	308	ARG	CA-C-N	5.46	131.96	121.54
2	B	308	ARG	C-N-CA	5.46	131.96	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	PRO	N-CA-C	-5.35	102.72	110.80
2	B	312	GLY	N-CA-C	-5.12	101.04	113.18
1	A	105	LYS	N-CA-C	5.12	117.58	109.24
1	A	94	HIS	N-CA-C	5.11	118.39	110.17
2	B	309	LYS	N-CA-C	-5.03	100.09	110.80

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	1368	0	1376	115	0
2	B	109	0	123	68	0
3	A	48	0	32	10	0
4	A	102	0	0	8	0
4	B	4	0	0	1	0
All	All	1631	0	1531	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (137) 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:56:ASN:OD1	1:A:63:MET:HE1	1.33	1.24
4:A:467:HOH:O	2:B:318:LYS:HA	1.49	1.11
3:A:401:COA:H22	2:B:316:PRO:CG	1.82	1.09
2:B:315:ALA:H	2:B:316:PRO:HD3	1.17	1.06
3:A:401:COA:H22	2:B:316:PRO:HG2	1.08	1.04
1:A:143:ASN:HB3	1:A:209:GLY:HA2	1.45	0.99
1:A:83:GLU:OE1	2:B:309:LYS:HE2	1.65	0.97
3:A:401:COA:C2P	2:B:316:PRO:HG2	1.97	0.94
2:B:317:ARG:O	2:B:318:LYS:HG2	1.69	0.92
1:A:80:MET:HE2	1:A:125:PHE:HE2	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:ARG:C	2:B:318:LYS:HG2	1.94	0.89
1:A:56:ASN:OD1	1:A:63:MET:CE	2.18	0.89
1:A:163:ASN:OD1	2:B:318:LYS:HD2	1.71	0.88
2:B:315:ALA:H	2:B:316:PRO:CD	1.88	0.87
1:A:88:LEU:HD13	2:B:312:GLY:HA2	1.58	0.86
1:A:87:LYS:HG3	2:B:309:LYS:HB2	1.60	0.82
1:A:164:PHE:HE2	2:B:316:PRO:HB3	1.48	0.78
1:A:87:LYS:HG3	2:B:309:LYS:CB	2.14	0.77
1:A:79:LYS:HD2	2:B:317:ARG:HG3	1.69	0.75
1:A:164:PHE:HB3	4:A:467:HOH:O	1.85	0.75
2:B:315:ALA:N	2:B:316:PRO:HD3	1.96	0.75
1:A:149:MET:HE3	1:A:154:ILE:HG21	1.69	0.73
1:A:169:PHE:HZ	2:B:314:LYS:HE3	1.56	0.70
1:A:48:LEU:N	1:A:102:ASN:HA	2.06	0.70
1:A:80:MET:SD	2:B:314:LYS:O	2.49	0.70
1:A:169:PHE:CZ	2:B:314:LYS:HE3	2.28	0.69
1:A:79:LYS:HZ2	2:B:317:ARG:NE	1.90	0.69
1:A:163:ASN:HB3	4:A:467:HOH:O	1.92	0.69
2:B:319:GLN:HB3	4:B:67:HOH:O	1.93	0.69
1:A:54:LEU:HD23	1:A:66:LEU:HD13	1.75	0.69
1:A:88:LEU:HD21	2:B:310:SER:HA	1.73	0.69
1:A:80:MET:HE2	2:B:313:GLY:O	1.94	0.68
3:A:401:COA:S1P	2:B:314:LYS:NZ	2.58	0.67
2:B:309:LYS:O	2:B:310:SER:HB2	1.94	0.67
1:A:79:LYS:NZ	2:B:317:ARG:HB2	2.09	0.67
2:B:317:ARG:C	2:B:318:LYS:CG	2.68	0.67
1:A:59:THR:O	1:A:63:MET:HG2	1.95	0.66
1:A:87:LYS:CE	2:B:309:LYS:O	2.42	0.66
1:A:79:LYS:NZ	2:B:317:ARG:CB	2.59	0.66
1:A:209:GLY:O	1:A:210:ARG:HB3	1.96	0.65
1:A:162:ASP:OD1	2:B:317:ARG:HD2	1.97	0.64
1:A:83:GLU:OE1	2:B:309:LYS:CE	2.44	0.64
1:A:126:LEU:HB3	2:B:314:LYS:HZ1	1.62	0.64
1:A:99:ILE:HD11	1:A:141:LEU:HD22	1.80	0.64
1:A:143:ASN:HB3	1:A:209:GLY:CA	2.25	0.63
1:A:79:LYS:CD	2:B:317:ARG:HG3	2.30	0.62
1:A:79:LYS:NZ	2:B:317:ARG:HE	1.97	0.62
1:A:79:LYS:HZ1	2:B:317:ARG:HB2	1.64	0.62
1:A:164:PHE:CE2	2:B:319:GLN:HB2	2.36	0.61
1:A:163:ASN:OD1	2:B:318:LYS:CD	2.46	0.61
1:A:163:ASN:CG	2:B:318:LYS:HD2	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ALA:HB2	1:A:149:MET:HE1	1.83	0.60
1:A:80:MET:CE	1:A:125:PHE:HE2	2.11	0.60
1:A:164:PHE:CE2	2:B:316:PRO:HB3	2.33	0.60
1:A:133:GLN:NE2	3:A:401:COA:H62A	2.00	0.59
1:A:79:LYS:HZ1	2:B:317:ARG:CB	2.15	0.59
1:A:209:GLY:O	1:A:210:ARG:CB	2.50	0.59
1:A:209:GLY:O	1:A:210:ARG:CZ	2.51	0.58
1:A:80:MET:HE2	1:A:125:PHE:CE2	2.27	0.58
2:B:315:ALA:N	2:B:316:PRO:CD	2.62	0.58
1:A:87:LYS:HE3	2:B:309:LYS:O	2.04	0.57
1:A:121:ALA:HB3	1:A:149:MET:HE2	1.87	0.56
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.72	0.55
1:A:149:MET:CE	1:A:154:ILE:HG13	2.37	0.55
2:B:318:LYS:NZ	2:B:318:LYS:HB3	2.22	0.54
1:A:190:LYS:HD3	1:A:192:TYR:CZ	2.43	0.54
1:A:102:ASN:HD22	1:A:104:GLN:HE21	1.55	0.53
2:B:307:ALA:HA	2:B:310:SER:HB3	1.91	0.53
1:A:149:MET:CE	1:A:154:ILE:HG21	2.36	0.53
1:A:87:LYS:HG3	2:B:309:LYS:HB3	1.90	0.52
1:A:80:MET:CE	2:B:313:GLY:O	2.58	0.51
1:A:133:GLN:HE22	3:A:401:COA:H62A	1.57	0.51
1:A:164:PHE:N	4:A:467:HOH:O	2.34	0.50
1:A:87:LYS:O	1:A:87:LYS:HD3	2.11	0.50
1:A:75:ARG:HD3	4:A:483:HOH:O	2.11	0.50
1:A:149:MET:HE3	1:A:154:ILE:CG2	2.40	0.50
4:A:467:HOH:O	2:B:318:LYS:CA	2.29	0.50
1:A:55:THR:HA	4:A:447:HOH:O	2.11	0.50
1:A:79:LYS:NZ	2:B:317:ARG:NE	2.54	0.50
1:A:91:ASP:OD2	1:A:94:HIS:HB2	2.12	0.49
1:A:61:ARG:HG2	1:A:61:ARG:NH1	2.28	0.49
1:A:49:LEU:HD11	1:A:99:ILE:HG23	1.95	0.49
1:A:149:MET:HG3	1:A:157:LEU:HD21	1.95	0.49
1:A:119:ARG:HD2	1:A:153:ASN:O	2.12	0.49
1:A:125:PHE:CE2	2:B:313:GLY:O	2.66	0.49
1:A:70:LYS:NZ	1:A:71:ASN:HD21	2.11	0.49
1:A:135:ARG:HD2	4:A:493:HOH:O	2.11	0.49
1:A:88:LEU:HD13	2:B:312:GLY:CA	2.38	0.48
1:A:84:TYR:OH	2:B:311:THR:HG23	2.14	0.48
1:A:79:LYS:HZ2	2:B:317:ARG:CD	2.26	0.48
1:A:121:ALA:CB	1:A:149:MET:CE	2.92	0.48
1:A:80:MET:HE3	1:A:84:TYR:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ALA:CB	1:A:149:MET:HE1	2.44	0.47
1:A:84:TYR:HD1	2:B:309:LYS:HD3	1.79	0.47
1:A:180:MET:HE2	1:A:185:TRP:HD1	1.80	0.47
2:B:317:ARG:HE	2:B:317:ARG:HB3	1.49	0.47
1:A:87:LYS:CD	2:B:309:LYS:O	2.63	0.47
1:A:81:PRO:O	1:A:84:TYR:HB3	2.15	0.47
1:A:88:LEU:CD1	2:B:312:GLY:HA2	2.39	0.47
1:A:116:LYS:HB2	1:A:117:PRO:HD3	1.95	0.47
1:A:120:PHE:C	1:A:120:PHE:CD1	2.93	0.46
1:A:87:LYS:HD2	2:B:309:LYS:O	2.16	0.46
1:A:63:MET:O	1:A:67:ILE:HG13	2.15	0.46
1:A:164:PHE:CE2	2:B:316:PRO:CB	2.98	0.46
1:A:80:MET:HE1	1:A:84:TYR:CE2	2.50	0.46
1:A:54:LEU:HD21	1:A:65:LEU:CB	2.46	0.46
1:A:79:LYS:CE	2:B:317:ARG:HB2	2.46	0.46
3:A:401:COA:H21	2:B:314:LYS:HD3	1.99	0.45
2:B:314:LYS:HB3	2:B:316:PRO:HD3	1.99	0.45
1:A:84:TYR:HB2	2:B:309:LYS:HE3	1.99	0.44
1:A:190:LYS:HD3	1:A:192:TYR:CE2	2.52	0.44
1:A:117:PRO:HB2	1:A:118:GLN:NE2	2.33	0.44
1:A:99:ILE:HD12	1:A:108:GLY:HA3	2.00	0.44
1:A:80:MET:HE1	1:A:84:TYR:HE2	1.83	0.44
3:A:401:COA:H22	2:B:316:PRO:HG3	1.89	0.43
1:A:181:PRO:HB2	1:A:184:LYS:HG2	1.99	0.43
1:A:128:VAL:HG23	3:A:401:COA:H142	2.01	0.43
1:A:87:LYS:HD3	1:A:87:LYS:C	2.44	0.43
1:A:190:LYS:HB3	1:A:192:TYR:CE1	2.53	0.43
1:A:101:LYS:O	1:A:102:ASN:HB2	2.19	0.43
1:A:180:MET:HE3	1:A:184:LYS:HB2	2.01	0.43
1:A:163:ASN:OD1	2:B:317:ARG:HA	2.19	0.42
3:A:401:COA:O9A	3:A:401:COA:H4B	2.17	0.42
1:A:164:PHE:HE2	2:B:316:PRO:CB	2.26	0.42
1:A:80:MET:HE3	1:A:84:TYR:CD2	2.53	0.42
1:A:70:LYS:NZ	1:A:71:ASN:ND2	2.67	0.42
1:A:149:MET:HE1	1:A:154:ILE:HG13	2.01	0.42
1:A:121:ALA:HB3	1:A:149:MET:CE	2.50	0.42
1:A:124:ALA:HA	2:B:312:GLY:C	2.45	0.42
1:A:79:LYS:HB2	2:B:315:ALA:HB1	2.02	0.42
1:A:118:GLN:N	1:A:118:GLN:CD	2.77	0.41
1:A:149:MET:HE3	1:A:154:ILE:HG13	2.02	0.41
1:A:51:PHE:HA	1:A:98:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PHE:CG	1:A:165:ALA:N	2.87	0.41
1:A:70:LYS:HZ2	1:A:71:ASN:HD21	1.70	0.40
1:A:69:LEU:HG	1:A:98:VAL:HG12	2.04	0.40
1:A:164:PHE:CZ	2:B:319:GLN:OE1	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	161/163 (99%)	151 (94%)	8 (5%)	2 (1%)	10	12
2	B	13/19 (68%)	4 (31%)	4 (31%)	5 (38%)	0	0
All	All	174/182 (96%)	155 (89%)	12 (7%)	7 (4%)	2	1

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	315	ALA
1	A	49	LEU
1	A	102	ASN
2	B	314	LYS
2	B	318	LYS
2	B	309	LYS
2	B	310	SER

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	146/146 (100%)	139 (95%)	7 (5%)	23	35
2	B	10/14 (71%)	5 (50%)	5 (50%)	0	0
All	All	156/160 (98%)	144 (92%)	12 (8%)	12	16

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	66	LEU
1	A	69	LEU
1	A	75	ARG
1	A	100	LEU
1	A	183	GLU
1	A	210	ARG
2	B	308	ARG
2	B	309	LYS
2	B	311	THR
2	B	317	ARG
2	B	318	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	71	ASN
1	A	104	GLN
1	A	114	GLN
1	A	133	GLN
1	A	148	HIS
1	A	152	GLN
1	A	203	HIS
2	B	319	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](#)

1 ligand is 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	COA	A	401	-	47,50,50	2.42	17 (36%)	69,75,75	1.34	8 (11%)

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	COA	A	401	-	-	6/48/64/64	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	COA	P1A-O3A	-7.41	1.51	1.59
3	A	401	COA	O9P-C9P	6.22	1.35	1.23
3	A	401	COA	P3B-O3B	5.92	1.69	1.59
3	A	401	COA	C5A-C6A	3.83	1.51	1.41
3	A	401	COA	C2A-N1A	3.49	1.40	1.33
3	A	401	COA	P3B-O7A	3.39	1.61	1.50
3	A	401	COA	O5P-C5P	3.21	1.29	1.23
3	A	401	COA	C3P-N4P	2.97	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	COA	P2A-O3A	2.95	1.62	1.59
3	A	401	COA	C8A-N7A	2.95	1.37	1.31
3	A	401	COA	C5A-C4A	2.73	1.43	1.39
3	A	401	COA	C1B-N9A	2.67	1.53	1.46
3	A	401	COA	O4B-C4B	2.58	1.50	1.45
3	A	401	COA	CCP-CBP	2.44	1.56	1.52
3	A	401	COA	OAP-CAP	2.26	1.46	1.42
3	A	401	COA	C4A-N9A	2.19	1.42	1.37
3	A	401	COA	O4B-C1B	2.07	1.46	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	COA	CEP-CBP-CAP	4.19	115.92	108.77
3	A	401	COA	CEP-CBP-CCP	-3.70	102.11	108.22
3	A	401	COA	C3B-C2B-C1B	3.31	107.17	99.89
3	A	401	COA	O5A-P2A-O3A	3.20	115.91	107.27
3	A	401	COA	O3B-C3B-C4B	2.65	119.36	110.03
3	A	401	COA	CDP-CBP-CCP	2.55	112.44	108.22
3	A	401	COA	C3P-N4P-C5P	2.50	127.48	122.82
3	A	401	COA	C6P-C5P-N4P	-2.09	112.54	116.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	COA	C4B-C3B-O3B-P3B
3	A	401	COA	C3B-C4B-C5B-O5B
3	A	401	COA	O4B-C4B-C5B-O5B
3	A	401	COA	P2A-O3A-P1A-O1A
3	A	401	COA	C5B-O5B-P1A-O1A
3	A	401	COA	P2A-O3A-P1A-O2A

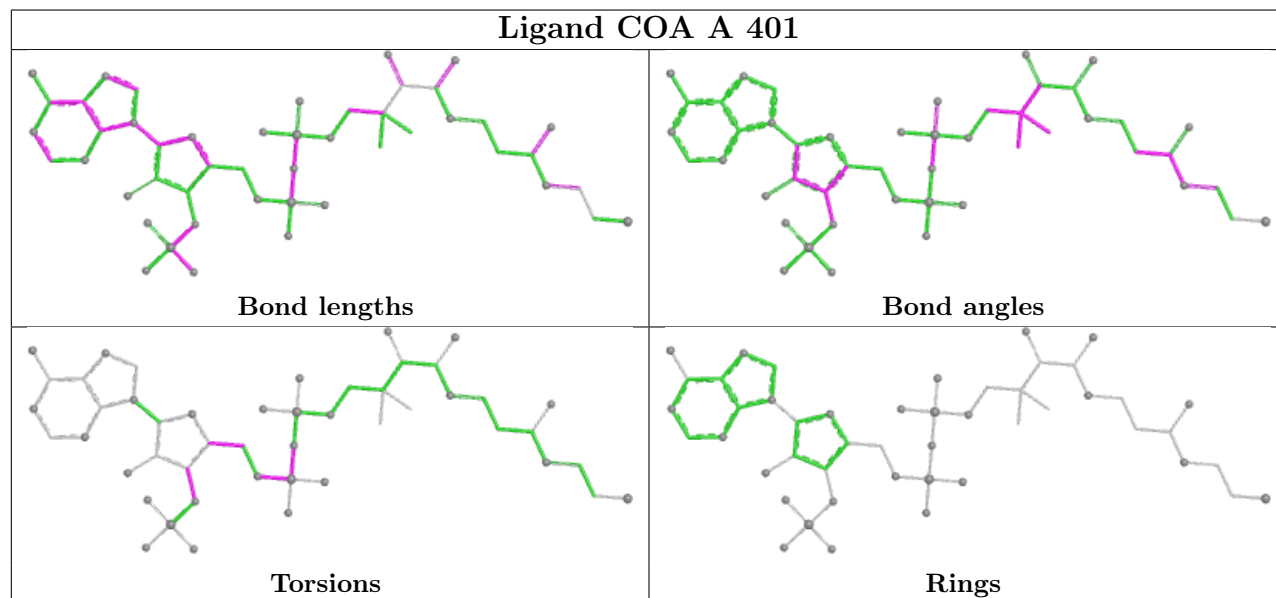
There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	COA	10	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 ⓘ

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 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.