



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 10, 2020 – 02:17 PM EST

PDB ID : 6PW9  
EMDB ID: : EMD-20501  
Title : Cryo-EM structure of human NatE/HYPK complex  
Authors : Deng, S.; Marmorstein, R.  
Deposited on : 2019-07-22  
Resolution : 4.03 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

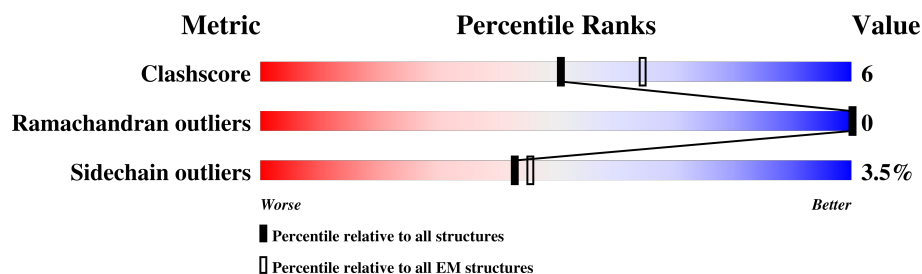
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.03 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	169	62% 27% • 8%
2	B	866	68% 8% • 23%
3	C	236	55% 12% • 32%
4	D	129	66% 6% • 26%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8836 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 N-alpha-acetyltransferase 50.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	155	Total	C	N	O	S	0	0
			1260	808	221	225	6		

- Molecule 2 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	665	Total	C	N	O	S	0	0
			5470	3507	922	1007	34		

- Molecule 3 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	161	Total	C	N	O	S	0	0
			1287	811	227	238	11		

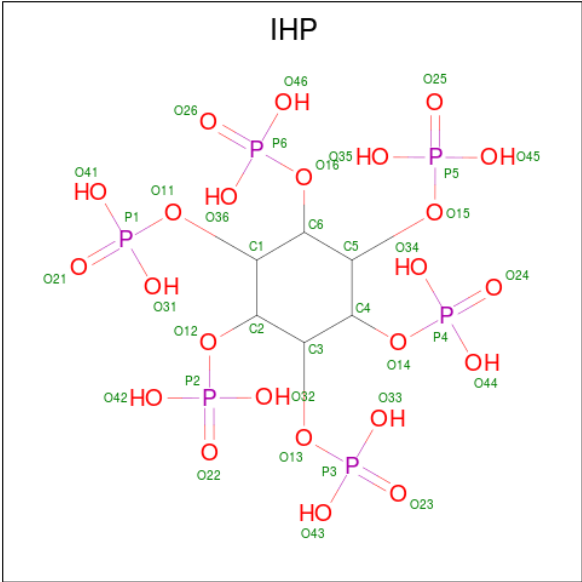
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ACE	-	acetylation	UNP P41227

- Molecule 4 is a protein called Huntingtin-interacting protein K.

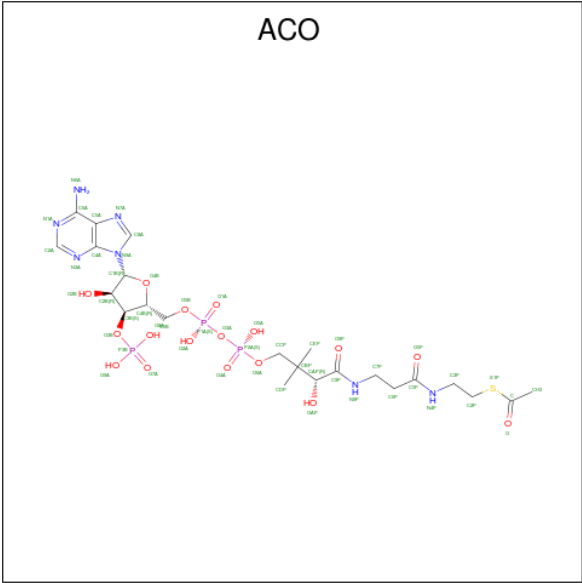
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	95	Total	C	N	O	S	0	0
			732	442	131	155	4		

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ).



Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 6 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						AltConf
6	C	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	



SER
SER
GLU
ALA
SER
ASP
SER
ALA
SER

● Molecule 4: Huntingtin-interacting protein K



MET	ARG	ARG	ARG	GLY	GLY	ILE	ASP	MET	MET	ALA	THR	GLY	GLY	ASP	VAL	GLU	LEU	GLU	LEU	GLU	THR	THR	THR	SER	GLY	PRO	GLU	ARG	ARG	PRO	PRO	GLU	LYS	PRO	PRO	ARG	K35	R45	D48	E61	M64	I67	K91	K92	E93	M102	R106	L124	W129
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	168536	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.6	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, ACO, ACE

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.35	1/1284 (0.1%)	0.66	1/1728 (0.1%)
2	B	0.29	0/5586	0.62	2/7535 (0.0%)
3	C	0.28	0/1313	0.63	2/1773 (0.1%)
4	D	0.27	0/734	0.59	0/983
All	All	0.30	1/8917 (0.0%)	0.63	5/12019 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	PRO	N-CD	5.27	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	140	LEU	CA-CB-CG	5.68	128.37	115.30
2	B	544	LEU	CA-CB-CG	5.55	128.06	115.30
3	C	11	LEU	CA-CB-CG	5.12	127.08	115.30
3	C	75	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	22	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1260	0	1282	39	0
2	B	5470	0	5497	57	0
3	C	1287	0	1244	17	0
4	D	732	0	718	7	0
5	C	36	0	6	0	0
6	C	51	0	34	1	0
All	All	8836	0	8781	112	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 6.

All (112) 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:13:PRO:O	1:A:16:ILE:CD1	1.78	1.29
6:C:902:ACO:C1B	6:C:902:ACO:O4B	1.66	1.28
2:B:528:TYR:CE2	2:B:532:LYS:CE	2.18	1.27
1:A:143:GLU:HB3	1:A:144:PRO:HD3	1.23	1.14
1:A:13:PRO:O	1:A:16:ILE:HD11	1.45	1.10
2:B:528:TYR:CE2	2:B:532:LYS:HE2	1.91	0.99
2:B:191:GLU:OE2	2:B:533:ILE:HG22	1.62	0.99
2:B:528:TYR:CE2	2:B:532:LYS:HE3	1.95	0.99
2:B:528:TYR:CZ	2:B:532:LYS:HE2	1.98	0.98
2:B:528:TYR:HE2	2:B:532:LYS:CE	1.74	0.96
1:A:13:PRO:O	1:A:16:ILE:HD12	1.61	0.95
2:B:528:TYR:HE2	2:B:532:LYS:NZ	1.67	0.91
1:A:142:ILE:HD13	1:A:144:PRO:HD2	1.51	0.91
1:A:137:ASN:HA	1:A:145:ALA:O	1.72	0.89
1:A:143:GLU:OE2	1:A:143:GLU:O	1.92	0.88
2:B:191:GLU:OE2	2:B:533:ILE:O	1.91	0.87
1:A:143:GLU:HB3	1:A:144:PRO:CD	2.04	0.86
3:C:2:ASN:O	3:C:45:ALA:HA	1.78	0.84
1:A:12:THR:OG1	1:A:13:PRO:CD	2.31	0.79
3:C:13:ASN:O	3:C:16:HIS:HB3	1.87	0.75
2:B:528:TYR:OH	2:B:532:LYS:HE2	1.90	0.71
2:B:528:TYR:HD1	2:B:531:ARG:HE	1.42	0.67
1:A:12:THR:OG1	1:A:13:PRO:HD2	1.95	0.67
1:A:13:PRO:C	1:A:16:ILE:HD11	2.17	0.63
1:A:62:ARG:HE	1:A:75:MET:HG2	1.64	0.63
1:A:137:ASN:CA	1:A:145:ALA:O	2.47	0.62
2:B:188:GLU:CG	2:B:533:ILE:HB	2.30	0.60
1:A:12:THR:OG1	1:A:13:PRO:HD3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:TYR:HE2	2:B:532:LYS:HZ1	1.48	0.60
1:A:129:PHE:HB3	1:A:150:LEU:HB3	1.83	0.59
1:A:143:GLU:CD	1:A:143:GLU:O	2.41	0.58
2:B:531:ARG:NH2	4:D:48:ASP:OD1	2.34	0.58
2:B:532:LYS:HZ2	3:C:37:SER:HA	1.70	0.57
2:B:188:GLU:HG3	2:B:533:ILE:HB	1.85	0.57
2:B:137:ARG:HH12	2:B:154:TYR:HD1	1.53	0.56
2:B:780:GLN:NE2	2:B:817:CYS:SG	2.79	0.56
2:B:689:LEU:HD11	4:D:102:MET:HB3	1.87	0.56
1:A:122:ASP:OD1	1:A:125:ARG:NH1	2.39	0.55
2:B:528:TYR:CE2	2:B:532:LYS:NZ	2.55	0.54
1:A:115:ILE:HD13	1:A:146:ASP:HB2	1.90	0.53
2:B:765:ARG:NH2	2:B:789:THR:OG1	2.41	0.52
1:A:12:THR:HG23	1:A:14:HIS:H	1.74	0.52
2:B:651:GLU:HG2	2:B:652:THR:HG22	1.91	0.52
1:A:69:GLN:OE1	1:A:108:ASN:ND2	2.43	0.51
1:A:133:GLU:HB2	1:A:149:VAL:HB	1.93	0.51
2:B:450:LYS:HB2	2:B:486:TRP:HZ2	1.76	0.50
2:B:188:GLU:HG2	2:B:533:ILE:CG1	2.42	0.50
2:B:532:LYS:NZ	3:C:37:SER:HA	2.26	0.50
1:A:57:GLY:HA2	1:A:78:GLY:O	2.12	0.49
3:C:18:ASN:OD1	3:C:31:TYR:OH	2.30	0.49
2:B:528:TYR:CZ	2:B:532:LYS:CE	2.73	0.49
3:C:45:ALA:HB2	3:C:90:LEU:HD11	1.95	0.49
2:B:292:VAL:HG22	2:B:296:LEU:HG	1.95	0.49
2:B:200:LEU:HB3	2:B:209:ALA:HB2	1.94	0.49
2:B:759:SER:O	2:B:765:ARG:NH1	2.46	0.49
2:B:432:ASP:OD1	2:B:435:GLN:NE2	2.40	0.48
3:C:57:LEU:O	3:C:73:THR:OG1	2.30	0.48
3:C:4:ARG:NH2	3:C:46:GLU:OE2	2.45	0.48
2:B:642:LEU:HD22	2:B:647:LEU:HG	1.95	0.48
1:A:61:CYS:HA	1:A:75:MET:H	1.78	0.48
1:A:26:ILE:HD12	1:A:27:PHE:HB2	1.97	0.47
2:B:234:LEU:HB3	2:B:243:ALA:HB2	1.95	0.47
2:B:394:LEU:HA	2:B:397:ILE:HG22	1.96	0.47
2:B:536:ARG:HH12	3:C:40:GLN:HE21	1.62	0.46
2:B:191:GLU:CD	2:B:533:ILE:O	2.53	0.46
3:C:96:ARG:HA	3:C:99:ILE:HG22	1.96	0.46
1:A:48:LEU:HA	1:A:58:ALA:HA	1.97	0.46
1:A:90:THR:HG23	1:A:127:PHE:HZ	1.81	0.45
1:A:74:ILE:HB	1:A:111:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:ASN:OD1	3:C:102:PHE:N	2.50	0.45
1:A:143:GLU:CB	1:A:144:PRO:HD3	2.15	0.45
1:A:79:CYS:HB3	1:A:88:ILE:HG21	1.98	0.45
1:A:8:LEU:HD11	1:A:92:MET:HB3	1.99	0.45
2:B:776:ASP:OD1	2:B:776:ASP:N	2.50	0.45
2:B:137:ARG:HD3	2:B:150:SER:HA	1.99	0.44
2:B:550:GLN:NE2	3:C:9:GLU:OE2	2.51	0.44
3:C:28:MET:HA	3:C:31:TYR:HD2	1.83	0.44
1:A:84:ARG:HE	1:A:85:ARG:H	1.66	0.43
1:A:91:LYS:HB3	1:A:91:LYS:HE3	1.82	0.43
2:B:188:GLU:HB3	2:B:533:ILE:HG21	2.00	0.43
1:A:26:ILE:HD13	1:A:78:GLY:HA2	1.99	0.43
2:B:733:VAL:HG21	4:D:124:LEU:HD22	2.01	0.43
2:B:738:MET:O	2:B:742:PHE:HB3	2.18	0.43
2:B:531:ARG:NH1	4:D:48:ASP:OD1	2.51	0.43
2:B:569:HIS:HD2	2:B:684:ARG:HD3	1.83	0.43
1:A:65:HIS:HE1	1:A:70:LYS:HE3	1.83	0.43
1:A:99:ILE:HA	1:A:102:LYS:HG2	2.00	0.43
3:C:59:LYS:O	3:C:71:HIS:N	2.50	0.43
2:B:170:ILE:HG12	4:D:67:ILE:HD11	2.00	0.43
4:D:91:LYS:HD3	4:D:93:GLU:H	1.84	0.43
2:B:307:LYS:HE2	2:B:345:LEU:HD12	2.01	0.42
2:B:137:ARG:HA	2:B:140:LEU:HD13	2.01	0.42
1:A:60:CYS:O	1:A:75:MET:N	2.53	0.42
2:B:547:VAL:HG23	2:B:667:LEU:HD12	2.00	0.42
2:B:559:ARG:HD3	2:B:560:ILE:HG23	2.00	0.42
4:D:61:GLU:HA	4:D:64:MET:HG3	2.02	0.42
2:B:733:VAL:HA	2:B:736:GLN:HG2	2.02	0.42
2:B:784:ILE:O	2:B:788:THR:OG1	2.26	0.42
2:B:324:PRO:O	2:B:327:ASN:HB2	2.19	0.41
3:C:32:PHE:HD1	3:C:32:PHE:HA	1.74	0.41
2:B:188:GLU:HG2	2:B:533:ILE:HG13	2.03	0.41
2:B:353:LEU:HD22	2:B:373:LEU:HD13	2.02	0.41
2:B:400:ALA:HB1	2:B:410:LEU:HD11	2.02	0.41
2:B:134:ARG:HH11	2:B:138:TYR:HE2	1.68	0.41
2:B:327:ASN:O	2:B:330:ARG:HG3	2.20	0.41
2:B:194:LEU:HA	2:B:194:LEU:HD23	1.84	0.41
3:C:41:LEU:HG	3:C:58:ALA:HB3	2.03	0.40
2:B:274:LEU:HD13	2:B:277:LEU:HD21	2.03	0.40
1:A:85:ARG:HH21	1:A:123:PHE:HE1	1.68	0.40
1:A:143:GLU:CB	1:A:144:PRO:CD	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD11	1:A:106:PHE:HD2	1.86	0.40
3:C:60:MET:HA	3:C:70:GLY:HA2	2.04	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 PDB entries followed by that with respect to all EM entries.

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	153/169 (90%)	141 (92%)	12 (8%)	0	100	100
2	B	661/866 (76%)	638 (96%)	23 (4%)	0	100	100
3	C	159/236 (67%)	151 (95%)	8 (5%)	0	100	100
4	D	93/129 (72%)	89 (96%)	4 (4%)	0	100	100
All	All	1066/1400 (76%)	1019 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	137/150 (91%)	130 (95%)	7 (5%)	26	59
2	B	593/769 (77%)	576 (97%)	17 (3%)	45	71
3	C	134/202 (66%)	129 (96%)	5 (4%)	37	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	77/111 (69%)	73 (95%)	4 (5%)	25	59
All	All	941/1232 (76%)	908 (96%)	33 (4%)	43	68

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

Mol	Chain	Res	Type
1	A	2	LYS
1	A	34	LYS
1	A	91	LYS
1	A	92	MET
1	A	141	ARG
1	A	142	ILE
1	A	143	GLU
2	B	169	LYS
2	B	213	LEU
2	B	266	LYS
2	B	286	LYS
2	B	330	ARG
2	B	366	LYS
2	B	429	ARG
2	B	498	MET
2	B	500	LYS
2	B	531	ARG
2	B	536	ARG
2	B	541	LEU
2	B	559	ARG
2	B	714	ARG
2	B	724	LYS
2	B	757	ARG
2	B	827	ASN
3	C	1	MET
3	C	5	ASN
3	C	18	ASN
3	C	32	PHE
3	C	126	LEU
4	D	45	ARG
4	D	64	MET
4	D	67	ILE
4	D	106	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	151	GLN
2	B	299	ASN
2	B	509	HIS
2	B	569	HIS
2	B	749	ASN
2	B	827	ASN
3	C	5	ASN
3	C	18	ASN
4	D	36	HIS

### 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	$\# Z  > 2$
5	IHP	C	901	-	36,36,36	1.45	6 (16%)	54,60,60	0.52	0
6	ACO	C	902	-	44,53,53	3.61	15 (34%)	56,79,79	2.11	9 (16%)

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
5	IHP	C	901	-	-	2/30/54/54	0/1/1/1
6	ACO	C	902	-	-	19/47/67/67	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	902	ACO	O4B-C1B	18.07	1.66	1.41
6	C	902	ACO	C5P-N4P	7.40	1.50	1.33
6	C	902	ACO	O4B-C4B	-6.53	1.30	1.45
6	C	902	ACO	C9P-N8P	5.77	1.46	1.33
6	C	902	ACO	C6P-C5P	3.36	1.57	1.51
6	C	902	ACO	C6A-N6A	3.36	1.46	1.34
6	C	902	ACO	O3B-C3B	-3.26	1.32	1.44
5	C	901	IHP	P6-O16	3.12	1.65	1.59
5	C	901	IHP	P2-O12	3.12	1.65	1.59
5	C	901	IHP	P3-O13	3.11	1.65	1.59
5	C	901	IHP	P4-O14	3.11	1.65	1.59
5	C	901	IHP	P5-O15	3.11	1.65	1.59
6	C	902	ACO	P2A-O6A	3.00	1.71	1.59
5	C	901	IHP	P1-O11	2.99	1.65	1.59
6	C	902	ACO	P3B-O3B	2.99	1.65	1.59
6	C	902	ACO	O5P-C5P	-2.86	1.17	1.23
6	C	902	ACO	C3B-C4B	2.61	1.59	1.52
6	C	902	ACO	P1A-O5B	2.36	1.68	1.59
6	C	902	ACO	OAP-CAP	-2.29	1.38	1.42
6	C	902	ACO	C5A-C4A	-2.26	1.35	1.40
6	C	902	ACO	O2B-C2B	2.07	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	902	ACO	C5A-C6A-N6A	9.29	134.97	120.38
6	C	902	ACO	N6A-C6A-N1A	-6.78	104.50	118.57
6	C	902	ACO	N3A-C2A-N1A	-5.80	119.33	128.68
6	C	902	ACO	C4B-O4B-C1B	-3.49	106.19	109.83
6	C	902	ACO	P2A-O3A-P1A	-3.43	121.67	132.57
6	C	902	ACO	C7P-C6P-C5P	-2.82	107.66	112.36
6	C	902	ACO	O9P-C9P-N8P	-2.22	118.13	122.98
6	C	902	ACO	C1B-N9A-C4A	2.19	130.42	126.64

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	902	ACO	CEP-CBP-CAP	2.14	112.53	108.82

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	902	ACO	C3B-C4B-C5B-O5B
6	C	902	ACO	O4B-C4B-C5B-O5B
6	C	902	ACO	C5B-O5B-P1A-O1A
6	C	902	ACO	CCP-O6A-P2A-O4A
6	C	902	ACO	CCP-O6A-P2A-O5A
6	C	902	ACO	CAP-C9P-N8P-C7P
6	C	902	ACO	O-C-S1P-C2P
6	C	902	ACO	CH3-C-S1P-C2P
6	C	902	ACO	O9P-C9P-N8P-C7P
6	C	902	ACO	S1P-C2P-C3P-N4P
6	C	902	ACO	O9P-C9P-CAP-OAP
6	C	902	ACO	C4B-C5B-O5B-P1A
6	C	902	ACO	C3B-O3B-P3B-O9A
5	C	901	IHP	C6-O16-P6-O46
6	C	902	ACO	CCP-O6A-P2A-O3A
6	C	902	ACO	C2P-C3P-N4P-C5P
6	C	902	ACO	O9P-C9P-CAP-CBP
6	C	902	ACO	N8P-C9P-CAP-CBP
6	C	902	ACO	C3B-O3B-P3B-O8A
5	C	901	IHP	C6-O16-P6-O36
6	C	902	ACO	C5B-O5B-P1A-O3A

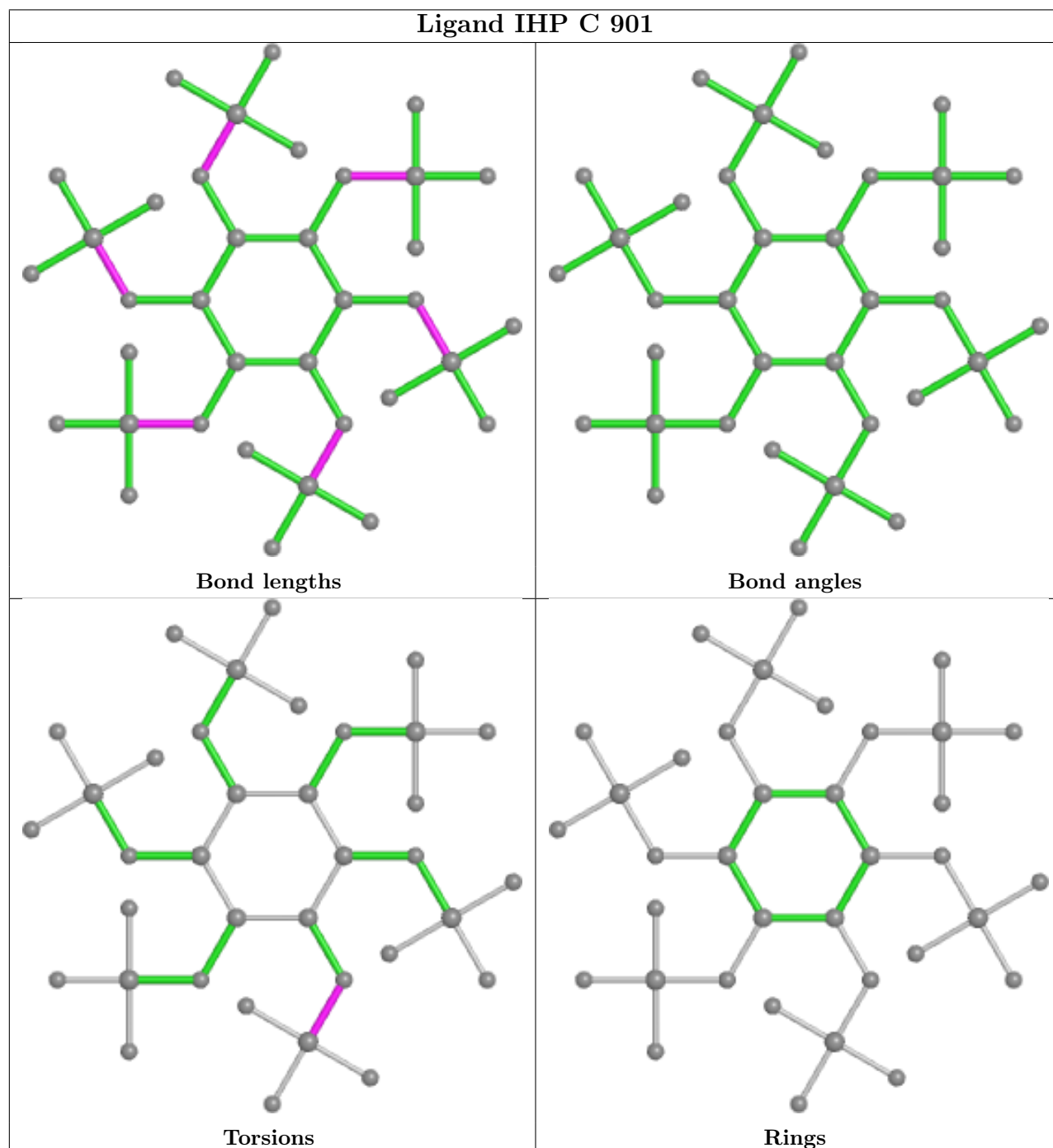
There are no ring outliers.

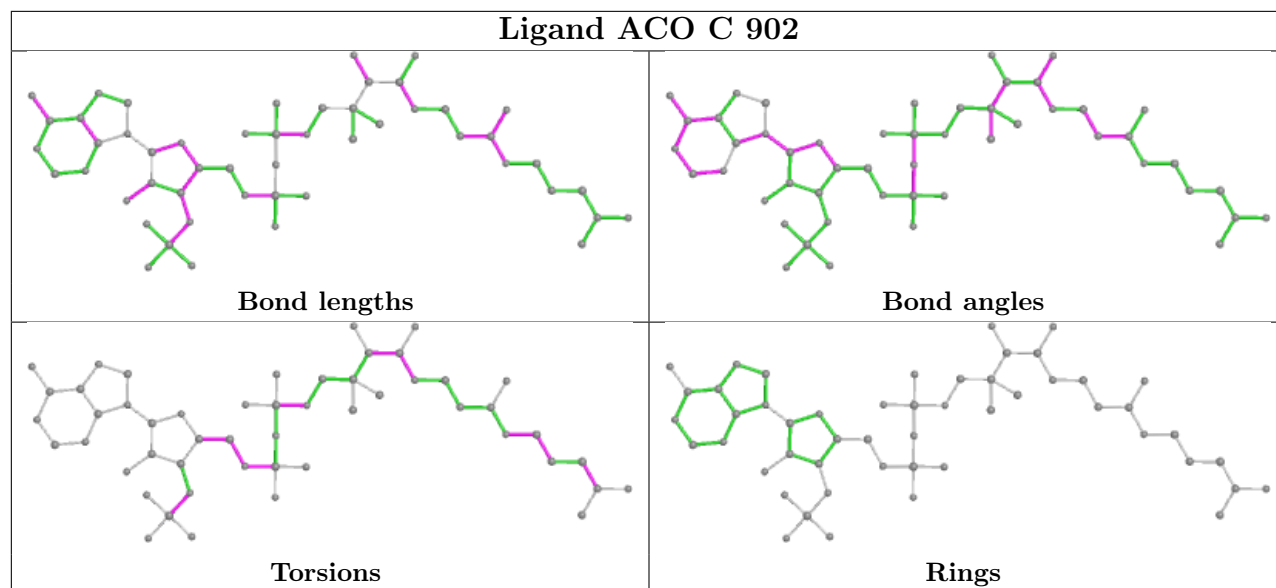
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	902	ACO	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.