wwPDB EM Validation Summary Report (i)

Jun 13, 2024 – 02:14 PM JST

PDB ID	:	8XUQ
EMDB ID	:	EMD-38680
Title	:	Cryo-EM structure of tomato NRC2 tetramer
Authors	:	Sun, Y.; Ma, S.C.; Chai, J.J.
Deposited on	:	2024-01-14
Resolution	:	3.17 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

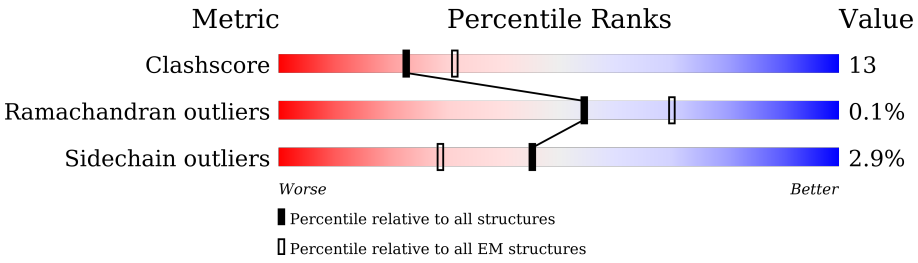
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	885	76% 24%
1	E	885	75% 24% .
1	F	885	70% 29% .
1	G	885	69% 31% .

2 Entry composition

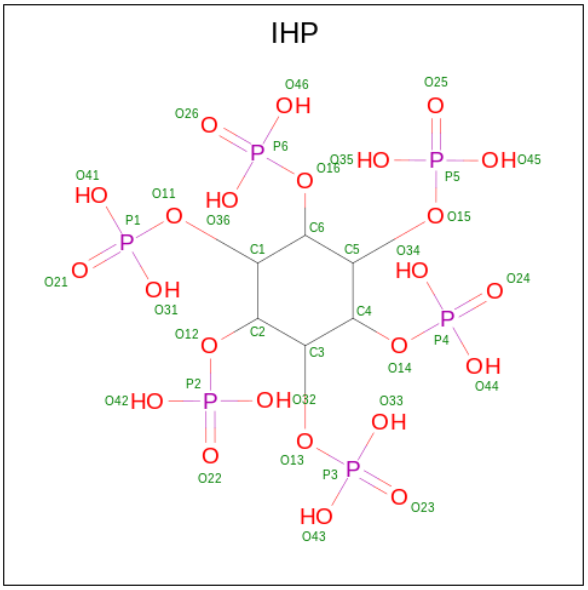
There are 3 unique types of molecules in this entry. The entry contains 28736 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NRC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	885	Total	C	N	O	S	0	0
			7121	4544	1237	1308	32		
1	E	885	Total	C	N	O	S	0	0
			7121	4544	1237	1308	32		
1	F	885	Total	C	N	O	S	0	0
			7121	4544	1237	1308	32		
1	G	885	Total	C	N	O	S	0	0
			7121	4544	1237	1308	32		

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



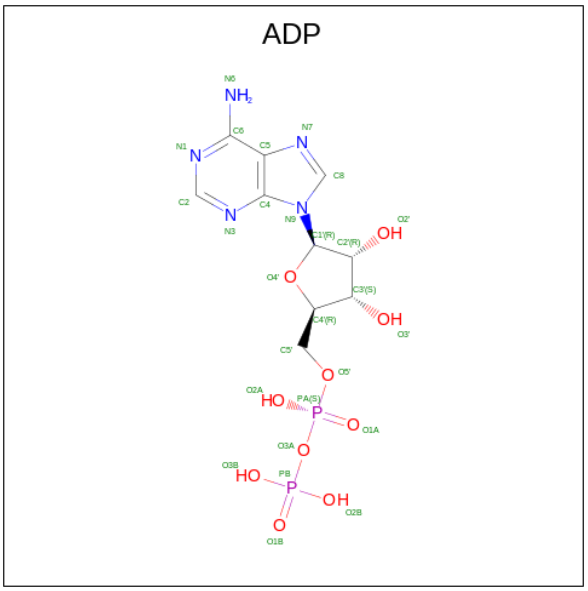
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			36	6	24	6	
2	E	1	Total	C	O	P	0
			36	6	24	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
2	F	1	Total	C	O	P	0
			36	6	24	6	
2	G	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



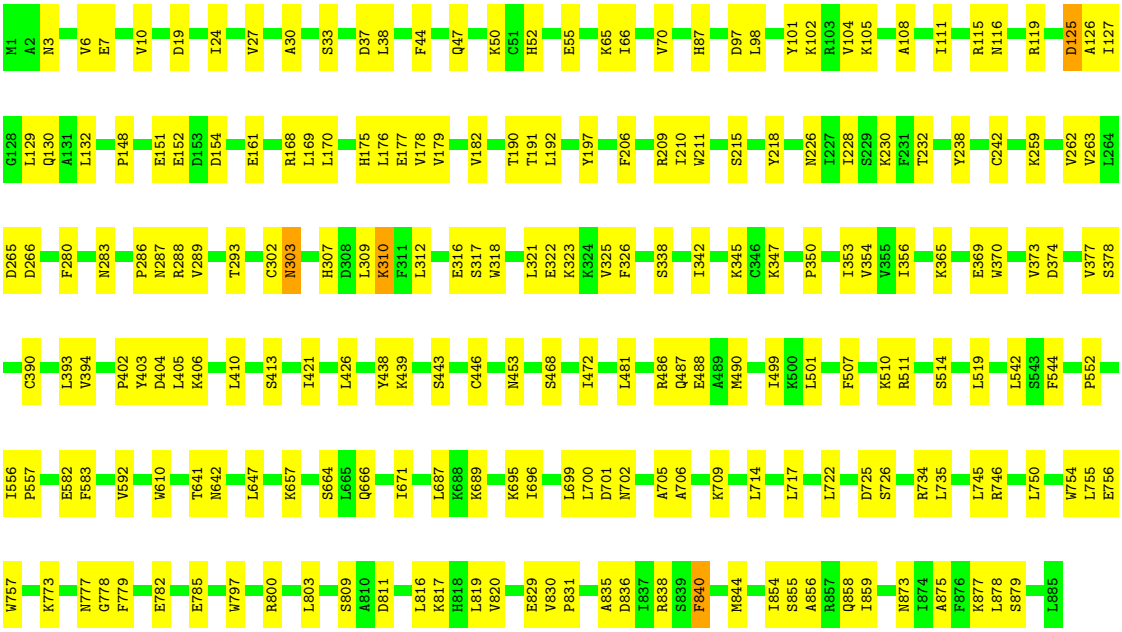
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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.

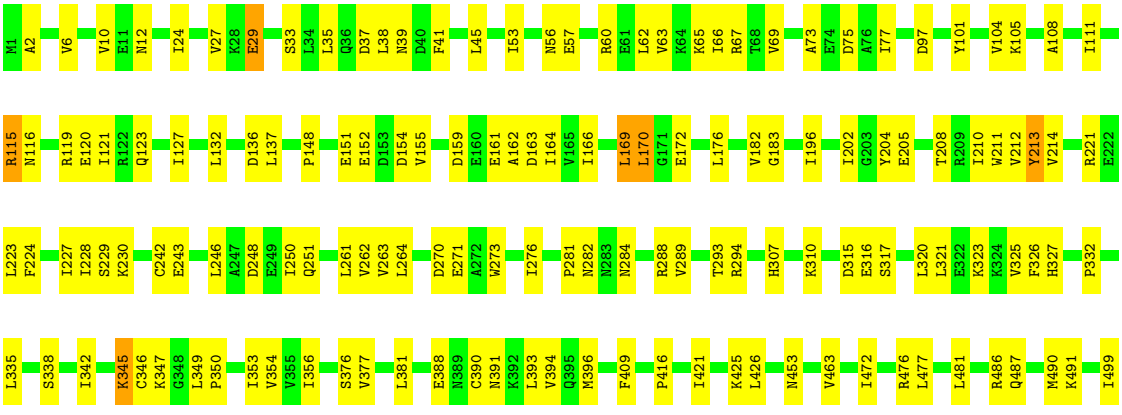
- Molecule 1: NRC2

Chain A:



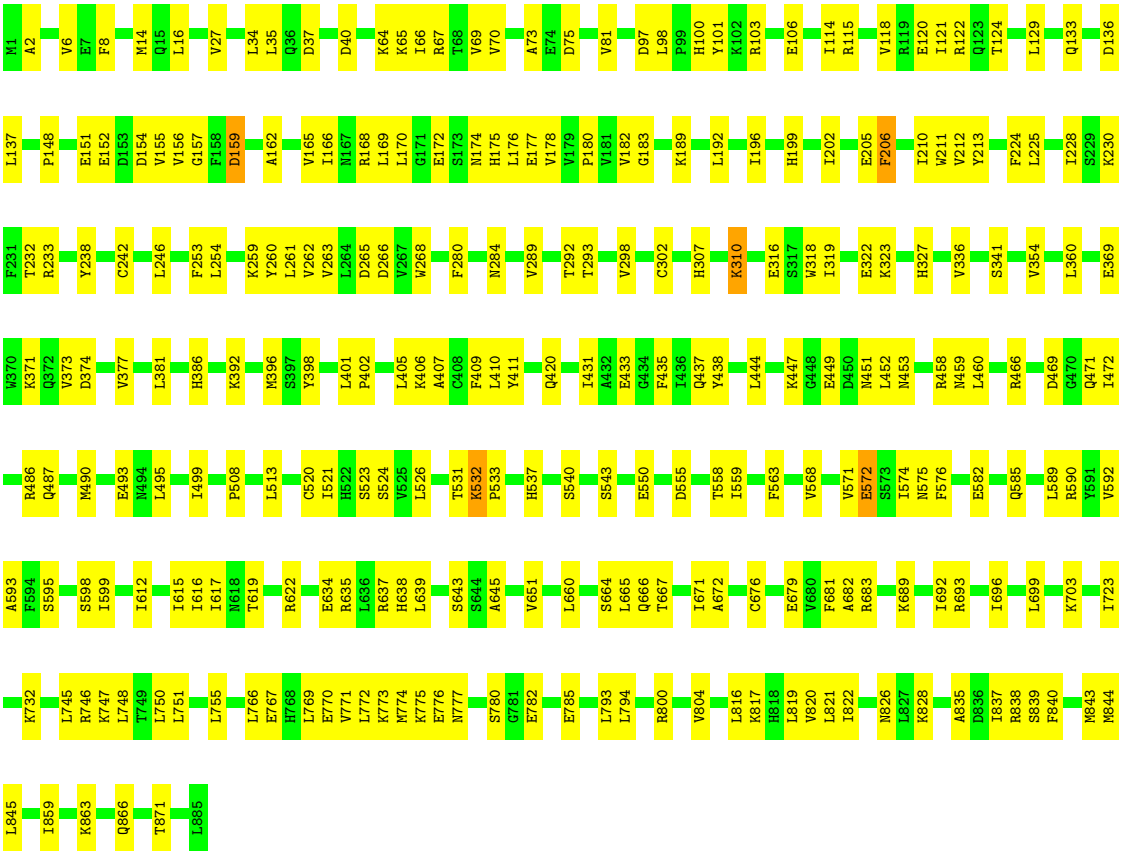
- Molecule 1: NRC2

Chain E:



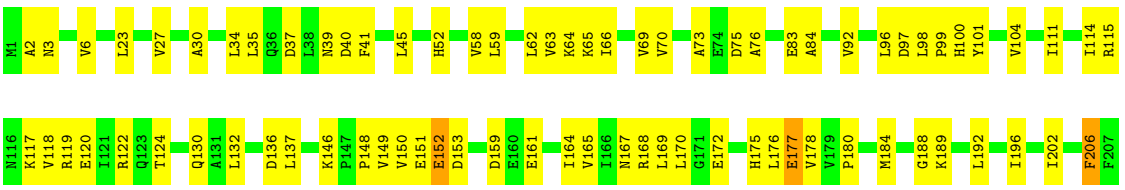
• Molecule 1: NRC2

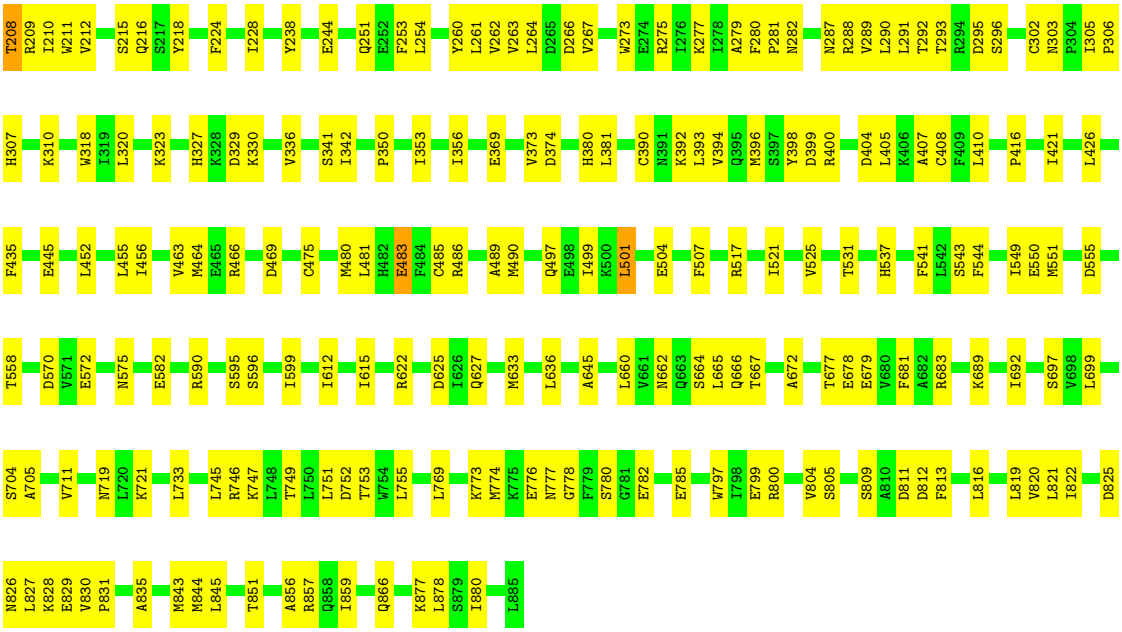
Chain F:



• Molecule 1: NRC2

Chain G:




T208 R209 I210 W211 V212 S215 Q216 S217 Y218 F224 I228 Y238 E244 Q251 E252 F253 L254 Y260 L261 V262 V263 L264 D265 D266 V267 W273 E274 R275 I276 K277 I278 A279 F280 P281 N282 N287 R288 V289 L290 L291 T292 T293 R294 D295 S296 C302 N303 P304 I305 P306
H307 K310 W318 I319 L320 K323 H327 K328 D329 K330 V336 S341 I342 P350 I353 I356 E369 V373 D374 H380 L381 C390 N391 K392 L393 V394 Q395 M396 S397 Y398 D399 R400 D404 L405 K406 A407 C408 F409 L410 P416 I421 L426
F435 E445 L452 L455 I456 V463 M464 E465 R466 D469 C475 M480 L481 H482 E483 P484 C485 R486 A489 M490 Q497 E498 I499 K500 L501 E504 F507 R517 I521 V525 T531 H537 F541 L542 S543 F544 I549 E550 M551 D555
T558 D570 V571 E572 N575 E582 R590 S595 S596 I599 I612 I615 R622 D625 I626 Q627 M633 L636 A645 L660 V661 N662 Q663 S664 L665 Q666 T667 A672 T677 E678 E679 V680 F681 A682 R683 K689 I692 S697 V698 L699
S704 A705 V711 N719 L720 K721 L733 L745 R746 K747 L748 T749 L750 L751 D752 T753 W754 L755 L769 K773 M774 K775 E776 N777 G778 F779 S780 G781 E782 E785 W797 I798 E799 R800 V804 S805 S809 A810 D811 D812 F813 L816 L819 V820 L821 I822 D825
N826 L827 K828 E829 V830 P831 A835 M843 M844 L845 T851 A856 R857 Q858 I859 Q866 K877 L878 S879 I880 L885

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154084	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.29	0/7260	0.54	0/9803
1	E	0.29	0/7260	0.53	0/9803
1	F	0.28	0/7260	0.53	0/9803
1	G	0.30	0/7260	0.53	0/9803
All	All	0.29	0/29040	0.53	0/39212

There are no bond length outliers.

There are no bond angle outliers.

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	7121	0	7283	157	0
1	E	7121	0	7283	159	0
1	F	7121	0	7283	196	0
1	G	7121	0	7283	216	0
2	A	36	0	6	1	0
2	E	36	0	6	0	0
2	F	36	0	6	1	0
2	G	36	0	6	0	0
3	A	27	0	12	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	27	0	12	1	0
3	F	27	0	12	1	0
3	G	27	0	12	3	0
All	All	28736	0	29204	725	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 13.

The worst 5 of 725 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:E:169:LEU:HD12	1:E:170:LEU:HG	1.39	1.04
1:G:169:LEU:HD12	1:G:170:LEU:HG	1.38	1.03
1:E:880:ILE:HG22	1:E:882:PRO:HD2	1.59	0.85
1:G:175:HIS:HE1	1:G:177:GLU:HG2	1.42	0.83
1:G:175:HIS:CE1	1:G:177:GLU:HG2	2.15	0.80

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	883/885 (100%)	847 (96%)	36 (4%)	0	100	100
1	E	883/885 (100%)	850 (96%)	32 (4%)	1 (0%)	51	83
1	F	883/885 (100%)	851 (96%)	32 (4%)	0	100	100
1	G	883/885 (100%)	840 (95%)	42 (5%)	1 (0%)	51	83
All	All	3532/3540 (100%)	3388 (96%)	142 (4%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	170	LEU
1	G	148	PRO

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	797/797 (100%)	780 (98%)	17 (2%)	53	79
1	E	797/797 (100%)	766 (96%)	31 (4%)	32	65
1	F	797/797 (100%)	776 (97%)	21 (3%)	46	75
1	G	797/797 (100%)	774 (97%)	23 (3%)	42	72
All	All	3188/3188 (100%)	3096 (97%)	92 (3%)	45	72

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	471	GLN
1	G	146	LYS
1	F	532	LYS
1	F	643	SER
1	G	189	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	15	GLN
1	F	174	ASN
1	G	451	ASN
1	G	175	HIS
1	A	818	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	IHP	F	901	-	36,36,36	1.52	6 (16%)	54,60,60	0.91	2 (3%)
3	ADP	E	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.37	3 (10%)
3	ADP	F	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.38	3 (10%)
2	IHP	G	901	-	36,36,36	1.48	6 (16%)	54,60,60	0.57	0
3	ADP	A	902	-	24,29,29	0.94	1 (4%)	29,45,45	1.40	5 (17%)
3	ADP	G	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.40	4 (13%)
2	IHP	A	901	-	36,36,36	1.52	6 (16%)	54,60,60	0.95	5 (9%)
2	IHP	E	901	-	36,36,36	1.52	6 (16%)	54,60,60	0.93	3 (5%)

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	IHP	F	901	-	-	10/30/54/54	0/1/1/1
3	ADP	E	902	-	-	5/12/32/32	0/3/3/3
3	ADP	F	902	-	-	2/12/32/32	0/3/3/3
2	IHP	G	901	-	-	7/30/54/54	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	902	-	-	4/12/32/32	0/3/3/3
3	ADP	G	902	-	-	6/12/32/32	0/3/3/3
2	IHP	A	901	-	-	9/30/54/54	0/1/1/1
2	IHP	E	901	-	-	11/30/54/54	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	IHP	P3-O13	3.50	1.65	1.59
2	F	901	IHP	P5-O15	3.41	1.65	1.59
2	F	901	IHP	P3-O13	3.36	1.65	1.59
2	E	901	IHP	P5-O15	3.35	1.65	1.59
2	A	901	IHP	P5-O15	3.29	1.65	1.59

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	902	ADP	PA-O3A-PB	-3.86	119.57	132.83
2	F	901	IHP	C5-C6-C1	3.78	118.68	110.41
3	G	902	ADP	N3-C2-N1	-3.60	123.05	128.68
3	E	902	ADP	N3-C2-N1	-3.59	123.06	128.68
3	A	902	ADP	N3-C2-N1	-3.57	123.09	128.68

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	IHP	C2-C1-O11-P1
2	A	901	IHP	C6-C1-O11-P1
2	A	901	IHP	C4-C3-O13-P3
2	A	901	IHP	C1-O11-P1-O21
2	A	901	IHP	C6-O16-P6-O26

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	901	IHP	1	0
3	E	902	ADP	1	0
3	F	902	ADP	1	0

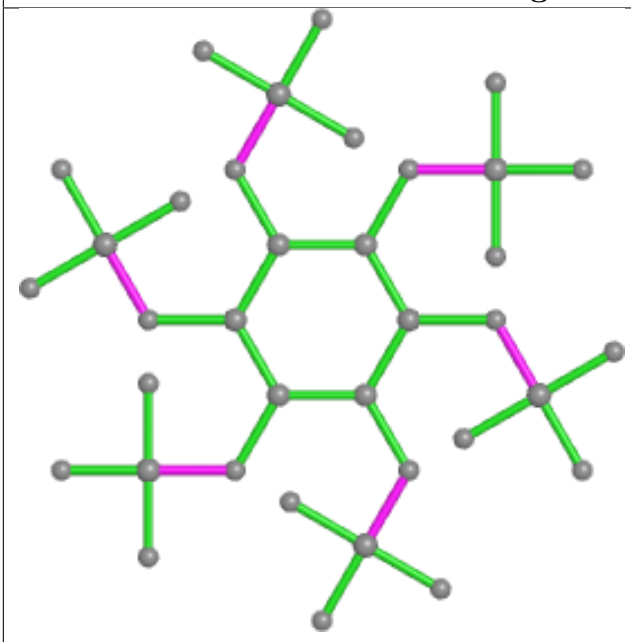
Continued on next page...

Continued from previous page...

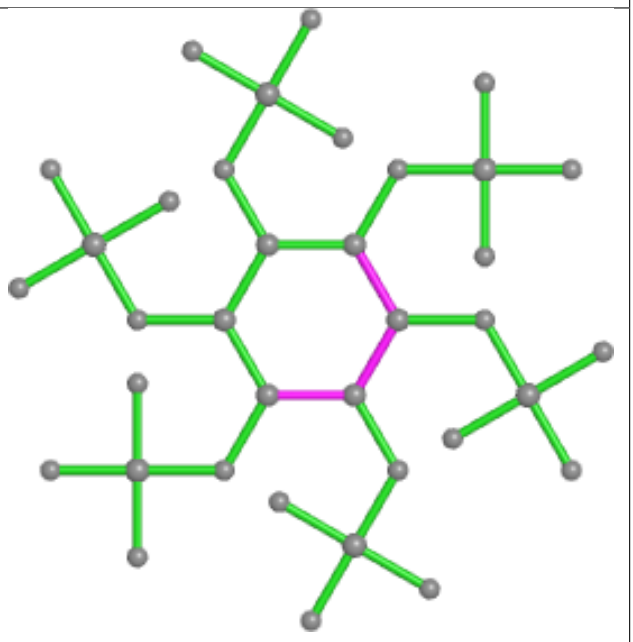
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	ADP	2	0
3	G	902	ADP	3	0
2	A	901	IHP	1	0

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 then 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.

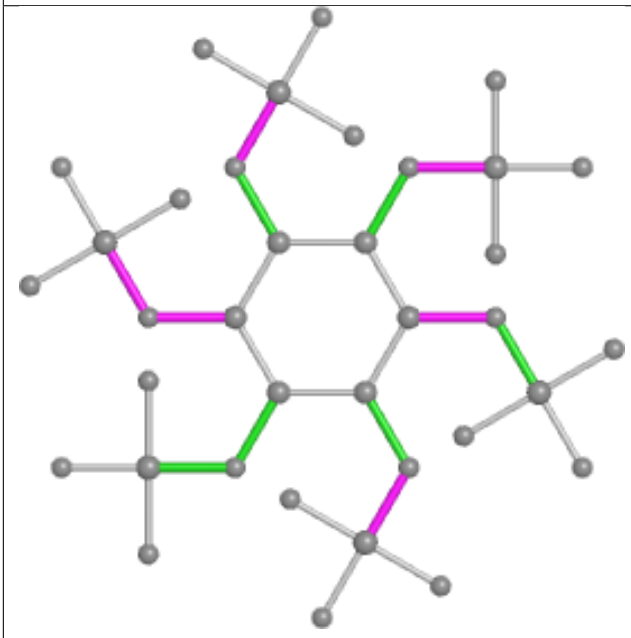
Ligand IHP F 901



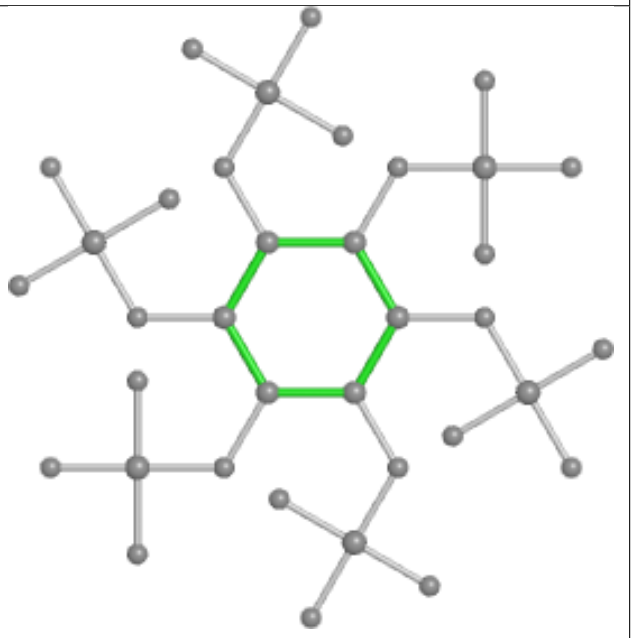
Bond lengths



Bond angles

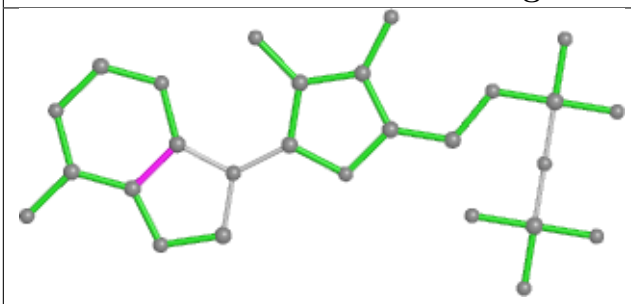


Torsions

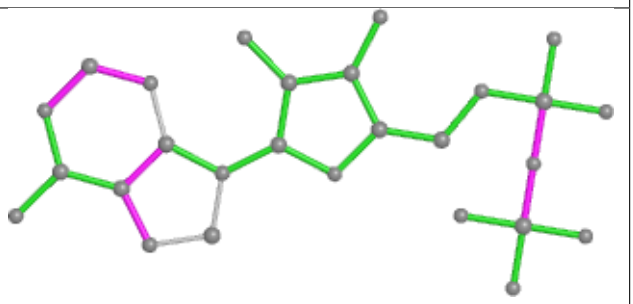


Rings

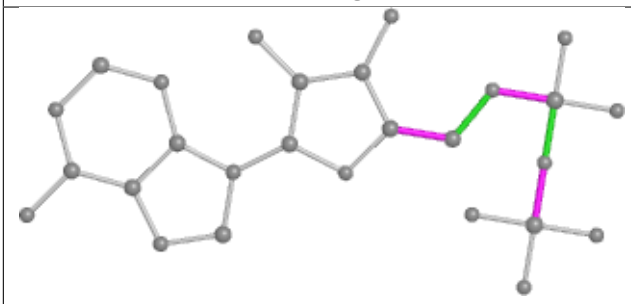
Ligand ADP E 902



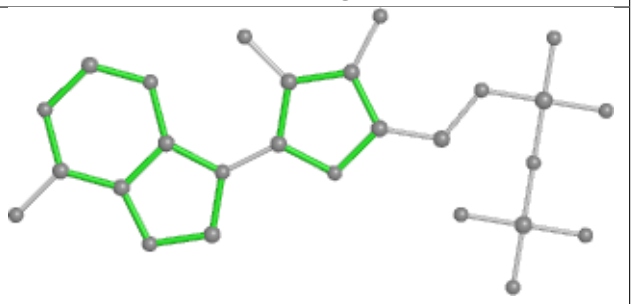
Bond lengths



Bond angles

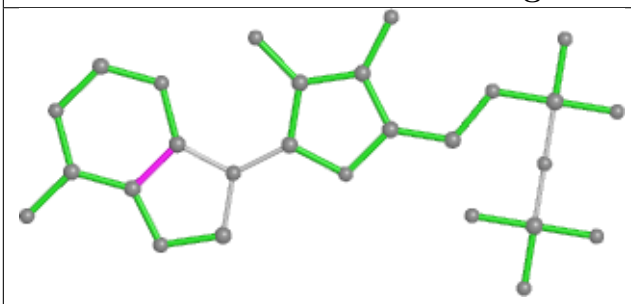


Torsions

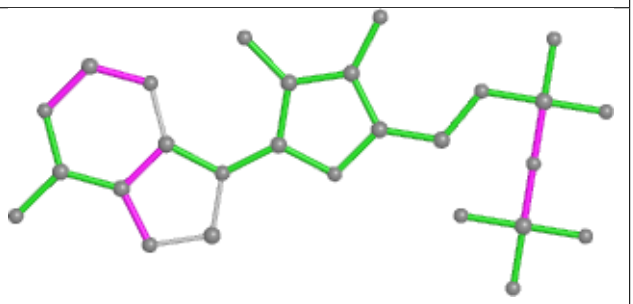


Rings

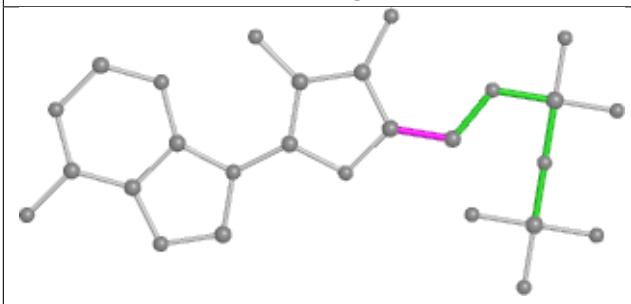
Ligand ADP F 902



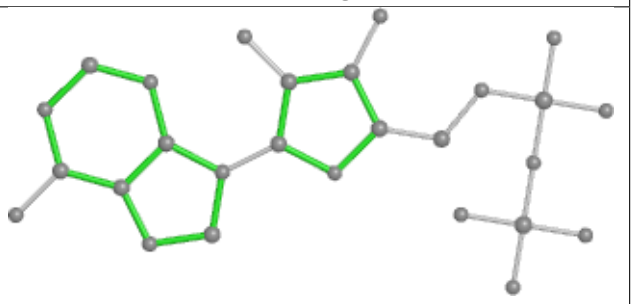
Bond lengths



Bond angles

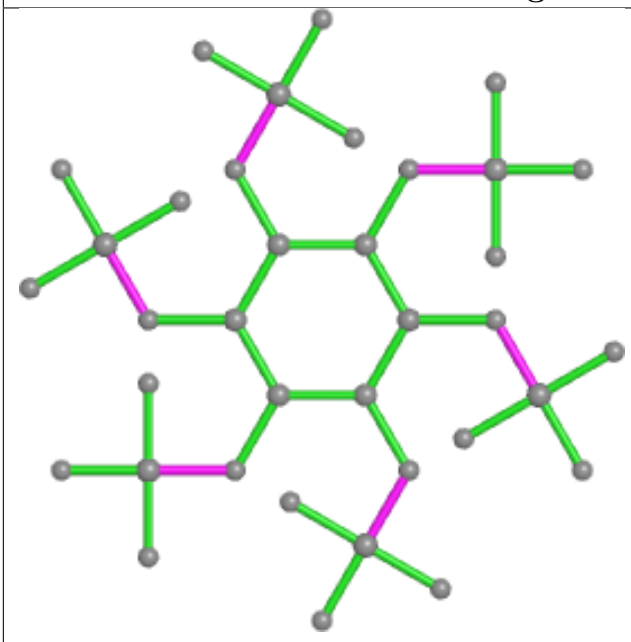


Torsions

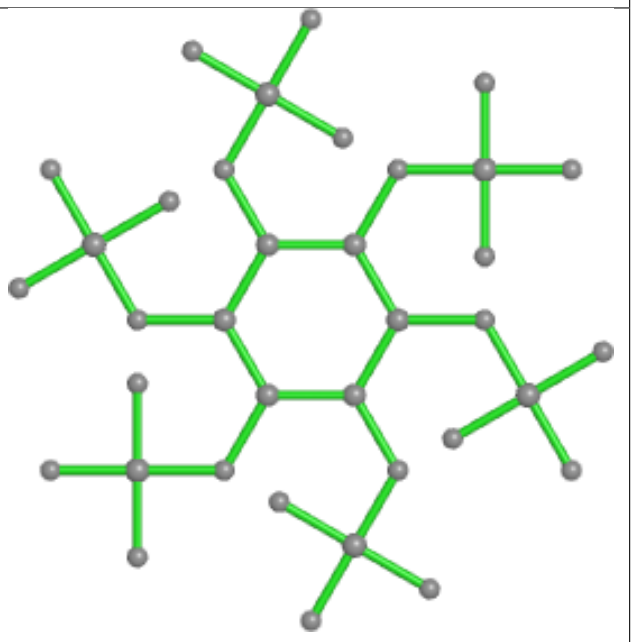


Rings

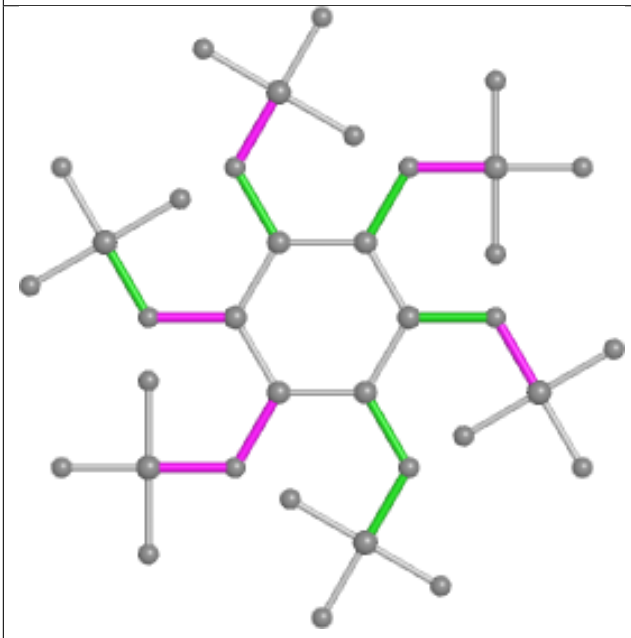
Ligand IHP G 901



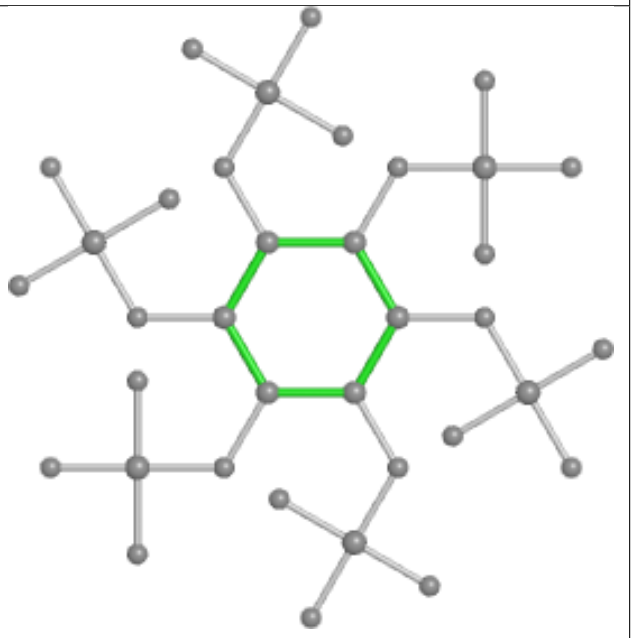
Bond lengths



Bond angles

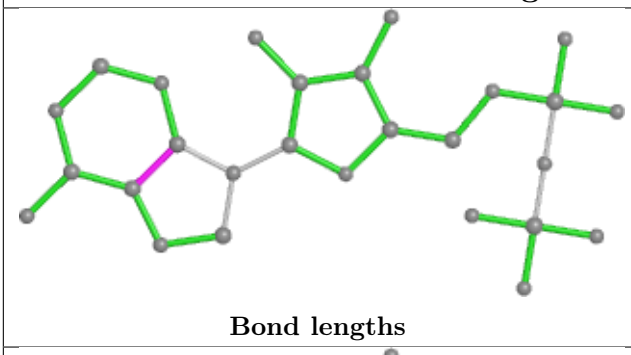


Torsions

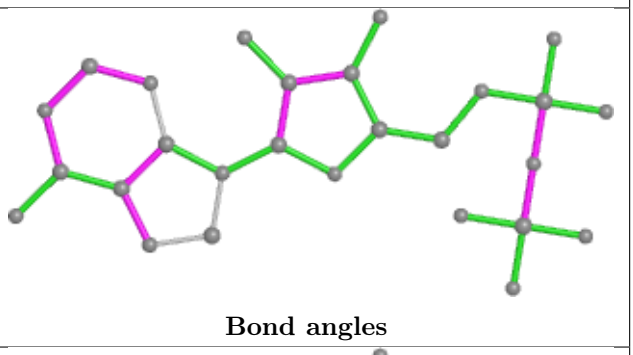


Rings

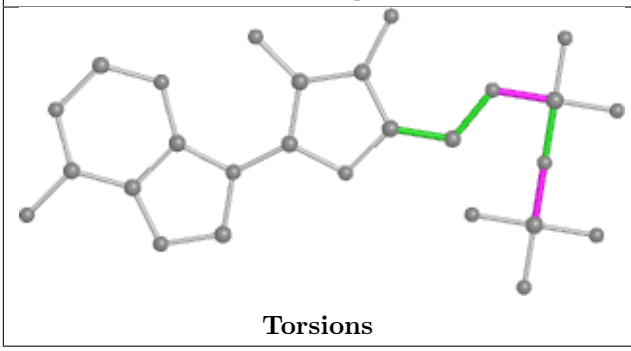
Ligand ADP A 902



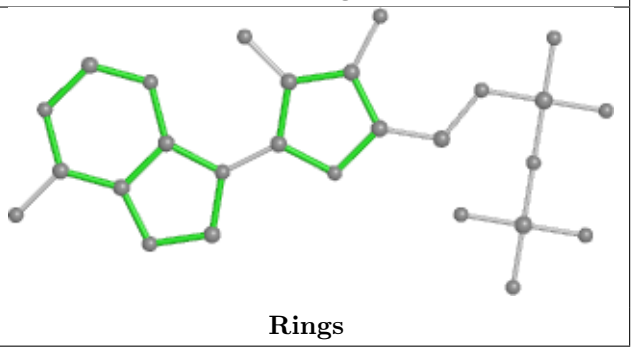
Bond lengths



Bond angles

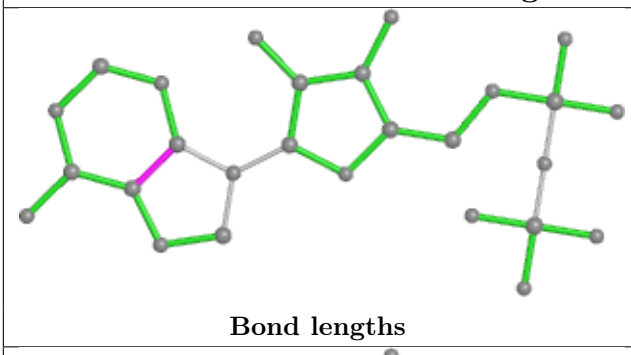


Torsions

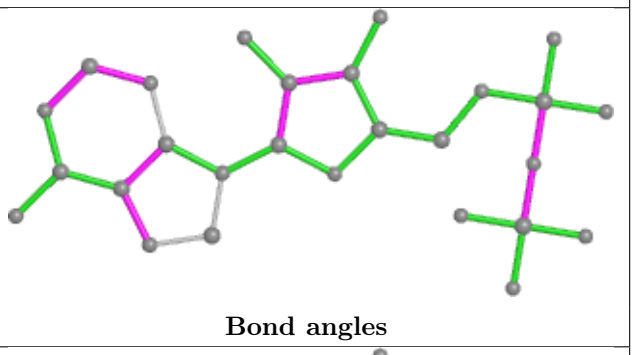


Rings

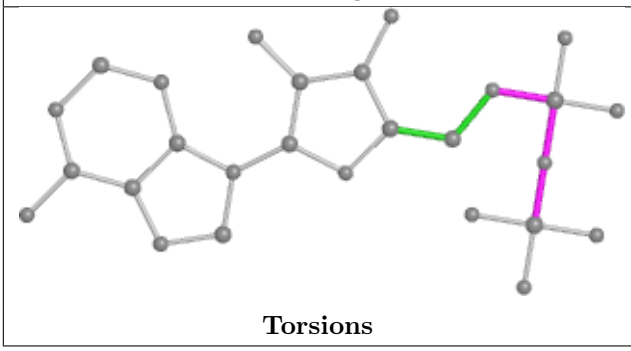
Ligand ADP G 902



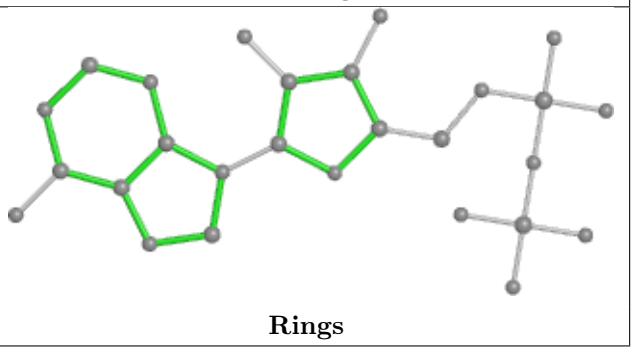
Bond lengths



Bond angles

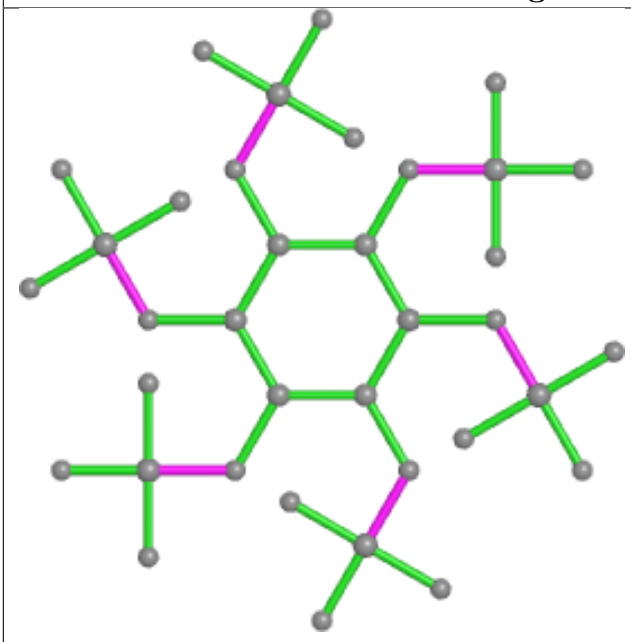


Torsions

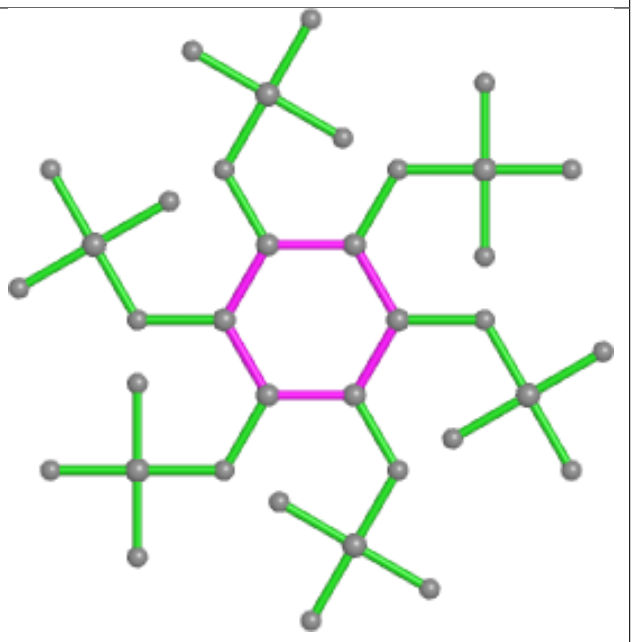


Rings

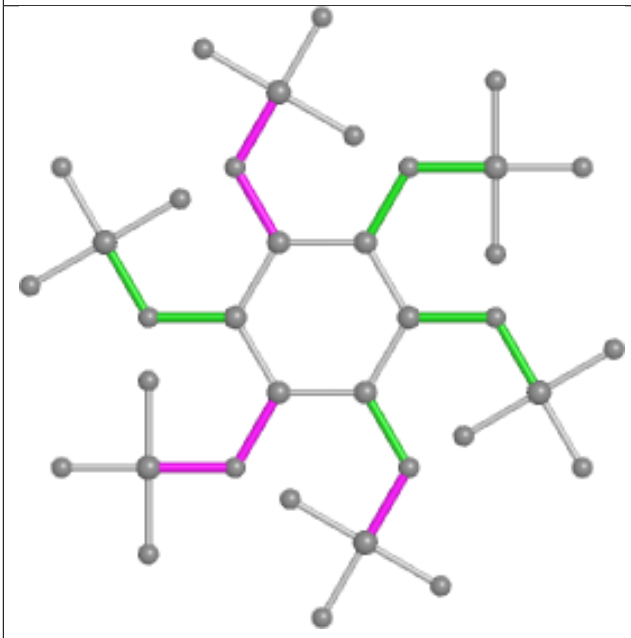
Ligand IHP A 901



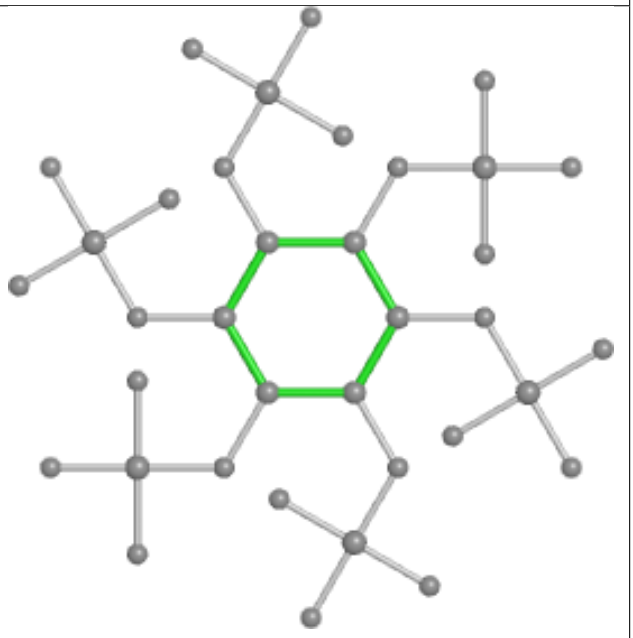
Bond lengths



Bond angles

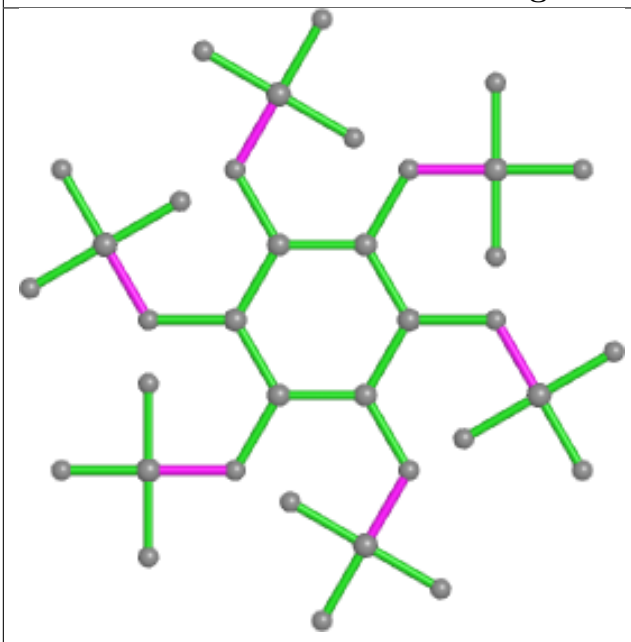


Torsions

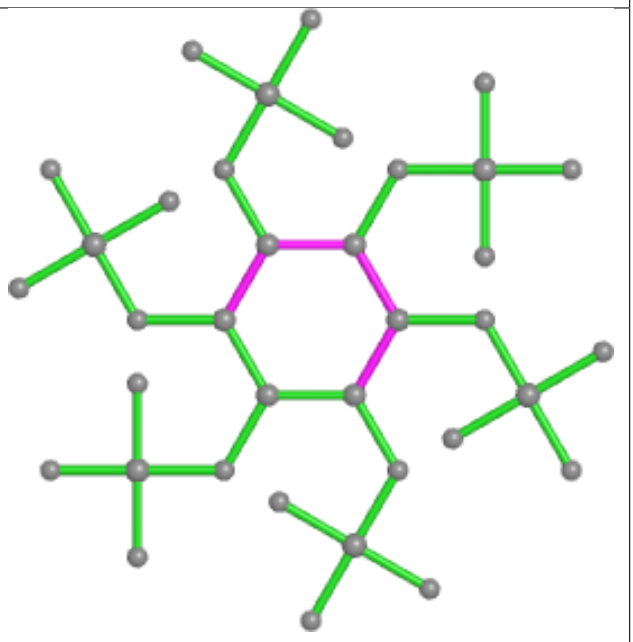


Rings

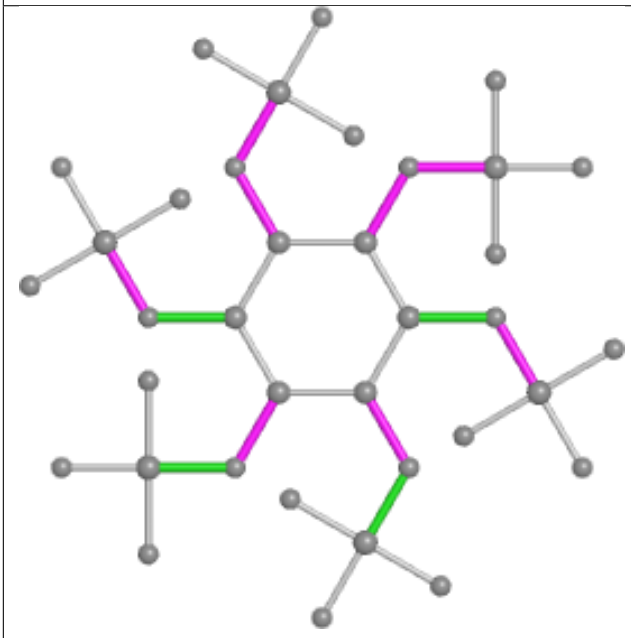
Ligand IHP E 901



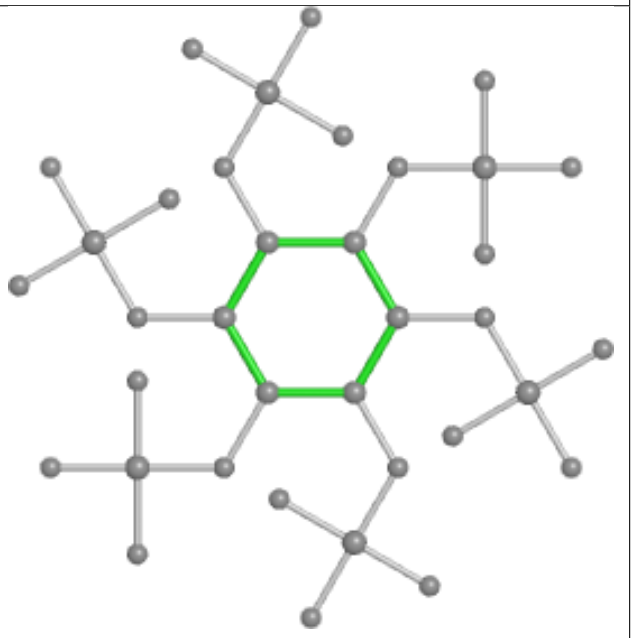
Bond lengths



Bond angles



Torsions



Rings

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.