

wwPDB X-ray Structure Validation Summary Report (i)

Dec 19, 2023 – 03:04 PM EST

PDB ID : 1J40

Title : Direct observation of photolysis-induced tertiary structural changes in human

haemoglobin; Crystal structure of alpha(Ni)-beta(Fe-CO) hemoglobin (laser

unphotolysed)

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Structural Genomics/Proteomics Initiative (RSGI)

Deposited on : 2003-02-21

Resolution : 1.45 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

MolProbity: 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

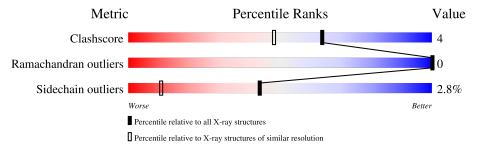
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$		
Clashscore	141614	1202 (1.46-1.46)		
Ramachandran outliers	138981	1178 (1.46-1.46)		
Sidechain outliers	138945	1178 (1.46-1.46)		

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	A	141	96%	
1	С	141	94%	5%•
1	E	141	91%	9%
1	G	141	94%	6%
2	В	146	86%	12% •
2	D	146	88%	12% •
2	F	146	87%	12% •
2	Н	146	90%	9% •



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HNI	A	142	X	-	-	-
3	HNI	С	142	X	-	-	-
3	HNI	Е	142	X	-	-	-
3	HNI	G	142	X	-	-	-
5	CMO	D	148	-	-	X	-



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11364 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 Hemoglobin alpha Chain.

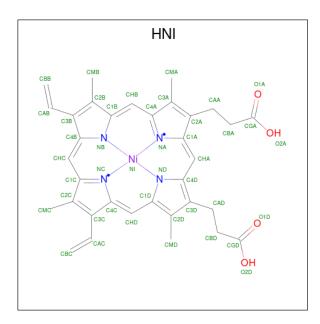
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	141	Total	С	N	О	S	0	0	0
1	A	141	1069	685	187	194	3	0	U	U
1	С	141	Total	С	N	О	S	0	0	0
1		141	1069	685	187	194	3	0		
1	E	141	Total	С	N	О	S	0	0	0
1	12	141	1069	685	187	194	3	0	0	U
1	С	141	Total	С	N	О	S	0	0	0
1	1 G	141	1069	685	187	194	3			

• Molecule 2 is a protein called Hemoglobin beta Chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	146	Total	С	N	О	S	0	0	0
2	Б	140	1123	724	195	201	3	0	U	U
2	D	146	Total	С	N	О	S	0	0	0
2	ט	140	1123	724	195	201	3	U		
2	F	146	Total	С	N	О	S	0	0	0
2	I'	140	1123	724	195	201	3	0	0	
2	Н	H 146	Total	С	N	О	S	0	0	0
	11	140	1123	724	195	201	3	U	U	U

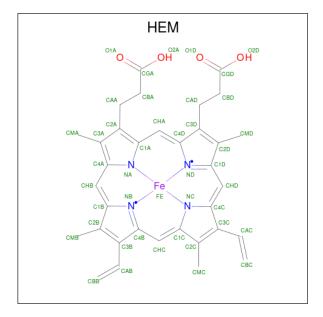
• Molecule 3 is PROTOPORPHYRIN IX CONTAINING NI(II) (three-letter code: HNI) (formula: $C_{34}H_{32}N_4NiO_4$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	٨	1	Total	С	N	Ni	О	0	0
3	A	1	43	34	4	1	4	0	
3	С	1	Total	С	N	Ni	О	0	0
3	3 0	1	43	34	4	1	4		
3	E	1	Total	С	N	Ni	О	0	0
3	9 E	1	43	34	4	1	4	0	
2	С	1	Total	С	N	Ni	О	0	0
3	G		43	34	4	1	4	U	U

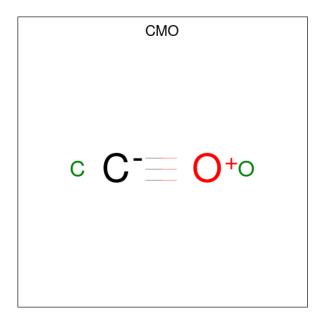
 \bullet Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\rm C_{34}H_{32}FeN_4O_4).$





Mol	Chain	Residues	${f Atoms}$					ZeroOcc	AltConf
4	В	1	Total	С	Fe	N	О	0	0
4	Б	1	43	34	1	4	4	0	U
1	D	1	Total	С	Fe	N	О	0	0
4		1	43	34	1	4	4		
1	F	1	Total	С	Fe	N	О	0	0
4	Г	1	43	34	1	4	4	0	U
1	Н	1	Total	С	Fe	N	О	0	0
4	11	1	43	34	1	4	4	U	U

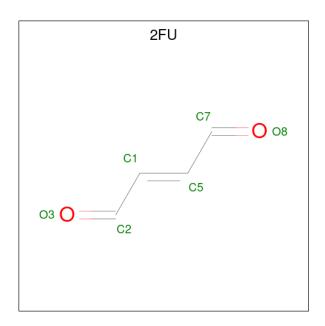
 \bullet Molecule 5 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total C O 2 1 1	0	0
5	D	1	Total C O 2 1 1	0	0
5	F	1	Total C O 2 1 1	0	0
5	Н	1	Total C O 2 1 1	0	0

 \bullet Molecule 6 is BUT-2-ENEDIAL (three-letter code: 2FU) (formula: $\mathrm{C_4H_4O_2}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 6 4 2	0	0
6	F	1	Total C O 6 4 2	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	350	Total O 350 350	0	0
7	В	284	Total O 284 284	0	0
7	С	281	Total O 281 281	0	0
7	D	310	Total O 310 310	0	0
7	E	248	Total O 248 248	0	0
7	F	278	Total O 278 278	0	0
7	G	249	Total O 249 249	0	0
7	Н	232	Total O 232 232	0	0

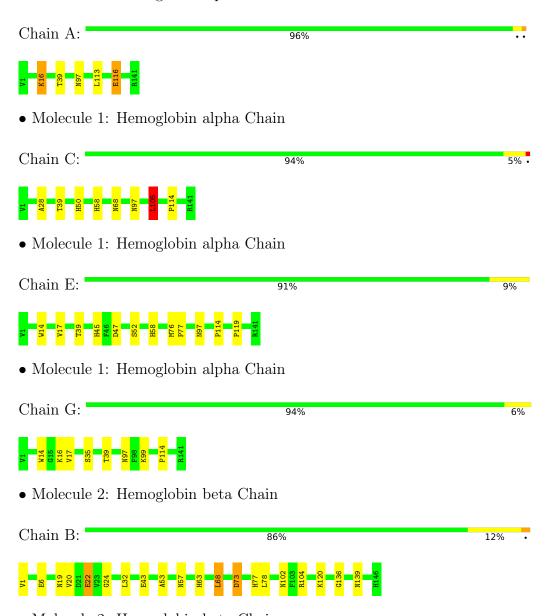


3 Residue-property plots (i)

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.

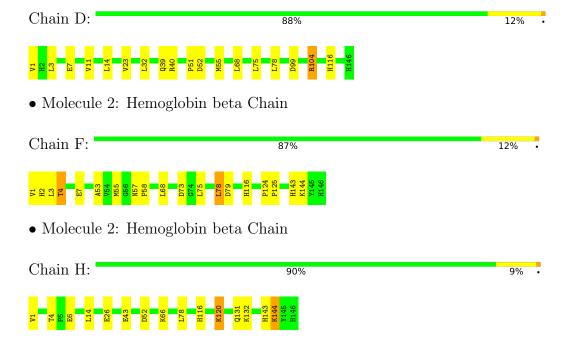
Note EDS was not executed.

• Molecule 1: Hemoglobin alpha Chain



• Molecule 2: Hemoglobin beta Chain







4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	64.71Å 94.86Å 99.73Å	Depositor	
a, b, c, α , β , γ	90.00° 101.97° 90.00°	Depositor	
Resolution (Å)	20.00 - 1.45	Depositor	
% Data completeness	95.9 (20.00-1.45)	Depositor	
(in resolution range)	39.3 (20.00-1.49)		
R_{merge}	0.06	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	REFMAC 5.1.22	Depositor	
R, R_{free}	0.165 , 0.197	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	11364	wwPDB-VP	
Average B, all atoms (Å ²)	16.0	wwPDB-VP	



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: HNI, 2FU, HEM, CMO

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	Bo	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	A	0.44	0/1097	0.68	0/1491		
1	С	0.44	0/1097	0.68	1/1491 (0.1%)		
1	Е	0.41	0/1097	0.66	0/1491		
1	G	0.44	0/1097	0.64	0/1491		
2	В	0.49	0/1153	0.70	$2/1566 \ (0.1\%)$		
2	D	0.43	0/1153	0.69	$2/1566 \ (0.1\%)$		
2	F	0.44	0/1153	0.71	$2/1566 \ (0.1\%)$		
2	Н	0.45	0/1153	0.68	1/1566 (0.1%)		
All	All	0.44	0/9000	0.68	8/12228 (0.1%)		

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	F	79	ASP	CB-CG-OD2	6.90	124.51	118.30
2	Н	52	ASP	CB-CG-OD2	6.40	124.06	118.30
2	D	52	ASP	CB-CG-OD2	6.07	123.76	118.30
2	В	73	ASP	CB-CG-OD2	5.56	123.30	118.30
2	D	99	ASP	CB-CG-OD1	5.49	123.24	118.30

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	1069	0	1073	3	0
1	С	1069	0	1073	7	0
1	Е	1069	0	1073	7	0
1	G	1069	0	1073	6	0
2	В	1123	0	1116	16	0
2	D	1123	0	1116	10	0
2	F	1123	0	1116	11	0
2	Н	1123	0	1116	12	0
3	A	43	0	30	0	0
3	С	43	0	30	1	0
3	Е	43	0	30	1	0
3	G	43	0	30	0	0
4	В	43	0	30	2	0
4	D	43	0	30	5	0
4	F	43	0	30	2	0
4	Н	43	0	30	1	0
5	В	2	0	0	0	0
5	D	2	0	0	4	0
5	F	2	0	0	0	0
5	Н	2	0	0	0	0
6	D	6	0	2	0	0
6	F	6	0	2	0	0
7	A	350	0	0	2	0
7	В	284	0	0	6	0
7	С	281	0	0	3	0
7	D	310	0	0	2	0
7	Е	248	0	0	1	0
7	F	278	0	0	2	0
7	G	249	0	0	5	0
7	Н	232	0	0	5	0
All	All	11364	0	9000	75	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 4.

The worst 5 of 75 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
2:H:26:GLU:HG2	7:H:237:HOH:O	1.55	1.05
1:G:99:LYS:HG3	7:G:360:HOH:O	1.59	1.02
2:B:139:ASN:HB3	7:B:309:HOH:O	1.60	0.99
4:D:147:HEM:NC	5:D:148:CMO:C	2.35	0.89

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Atom-1	Atom-1 Atom-2		$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
7:A:268:HOH:O	2:D:40:ARG:HD3	1.72	0.89	

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	Perce	ntiles
1	A	139/141~(99%)	137 (99%)	2 (1%)	0	100	100
1	\mathbf{C}	$139/141\ (99\%)$	136 (98%)	3 (2%)	0	100	100
1	E	$139/141\ (99\%)$	137 (99%)	2 (1%)	0	100	100
1	G	139/141~(99%)	135 (97%)	4 (3%)	0	100	100
2	В	144/146~(99%)	142 (99%)	2 (1%)	0	100	100
2	D	144/146~(99%)	140 (97%)	4 (3%)	0	100	100
2	F	144/146~(99%)	140 (97%)	4 (3%)	0	100	100
2	Н	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
All	All	1132/1148 (99%)	1108 (98%)	24 (2%)	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 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	Perce	ntiles
1	A	113/113 (100%)	111 (98%)	2 (2%)	59	26
1	C	113/113 (100%)	112 (99%)	1 (1%)	78	57
1	\mathbf{E}	113/113 (100%)	111 (98%)	2 (2%)	59	26
1	G	113/113 (100%)	113 (100%)	0	100	100
2	В	118/118 (100%)	113 (96%)	5 (4%)	30	4
2	D	118/118 (100%)	114 (97%)	4 (3%)	37	6
2	F	118/118 (100%)	112 (95%)	6 (5%)	24	2
2	Н	118/118 (100%)	112 (95%)	6 (5%)	24	2
All	All	924/924 (100%)	898 (97%)	26 (3%)	43	11

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	2	HIS
2	F	58	PRO
2	Н	120	LYS
2	F	4	THR
2	F	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	102	ASN
1	G	58	HIS
2	Н	116	HIS
1	G	97	ASN
1	С	58	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)

14 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).

λ π - 1	Ф	Cl :	D	T : 1-	Во	ond leng	ths	В	ond ang	gles
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	2FU	D	3001	2	5,5,5	0.62	0	4,4,4	1.63	0
3	HNI	Е	142	-	47,50,50	1.29	7 (14%)	56,82,82	1.29	5 (8%)
6	2FU	F	3002	2	5,5,5	0.80	0	4,4,4	4.05	2 (50%)
5	CMO	D	148	4	0,1,1	-	-	-		
4	HEM	Н	147	5,2	41,50,50	1.70	4 (9%)	45,82,82	1.79	10 (22%)
4	HEM	F	147	5,2	41,50,50	1.73	4 (9%)	45,82,82	1.73	11 (24%)
3	HNI	G	142	-	47,50,50	1.15	3 (6%)	56,82,82	1.23	5 (8%)
3	HNI	A	142	-	47,50,50	1.30	7 (14%)	56,82,82	0.88	2 (3%)
5	CMO	В	148	4	0,1,1	-	-	-		
5	CMO	F	148	4	0,1,1	-	-	-		
5	CMO	Н	148	4	0,1,1	-	-	-		
4	HEM	В	147	5,2	41,50,50	1.76	5 (12%)	45,82,82	1.71	11 (24%)
3	HNI	С	142	-	47,50,50	1.36	6 (12%)	56,82,82	1.06	4 (7%)
4	HEM	D	147	5,2	41,50,50	1.86	5 (12%)	45,82,82	1.62	10 (22%)

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
6	2FU	D	3001	2	-	2/3/3/3	-
3	HNI	Е	142	-	1/1/3/9	4/14/54/54	-
6	2FU	F	3002	2	-	2/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	Н	147	5,2	-	4/12/54/54	-
4	HEM	F	147	5,2	-	4/12/54/54	-
3	HNI	G	142	-	1/1/3/9	4/14/54/54	-
3	HNI	A	142	-	1/1/3/9	4/14/54/54	-
4	HEM	В	147	5,2	-	4/12/54/54	-
3	HNI	С	142	-	1/1/3/9	4/14/54/54	-
4	HEM	D	147	5,2	-	4/12/54/54	-

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(Å)
4	D	147	HEM	C3D-C2D	7.05	1.51	1.36
4	В	147	HEM	C3D-C2D	6.87	1.51	1.36
4	Н	147	HEM	C3D-C2D	6.83	1.51	1.36
4	F	147	HEM	C3D-C2D	6.33	1.50	1.36
4	D	147	HEM	C3C-C2C	-4.46	1.34	1.40

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
6	F	3002	2FU	C5-C1-C2	7.15	131.68	121.70
4	F	147	HEM	C4D-ND-C1D	5.31	110.56	105.07
4	Н	147	HEM	C4D-ND-C1D	5.29	110.54	105.07
4	В	147	HEM	CBA-CAA-C2A	-4.44	105.05	112.62
4	Н	147	HEM	CBA-CAA-C2A	-4.43	105.06	112.62

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	142	HNI	NB
3	С	142	HNI	NB
3	Е	142	HNI	NB
3	G	142	HNI	NB

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	3001	2FU	C5-C1-C2-O3
6	D	3001	2FU	C1-C5-C7-O8
6	F	3002	2FU	C5-C1-C2-O3

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Mol	Chain	Res	Type	Atoms
6	F	3002	2FU	C1-C5-C7-O8
3	A	142	HNI	CAD-CBD-CGD-O1D

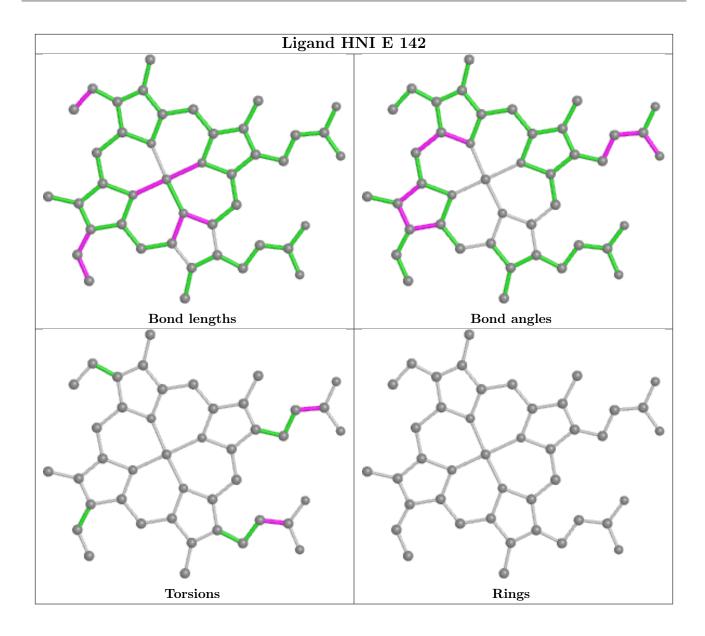
There are no ring outliers.

7 monomers are involved in 12 short contacts:

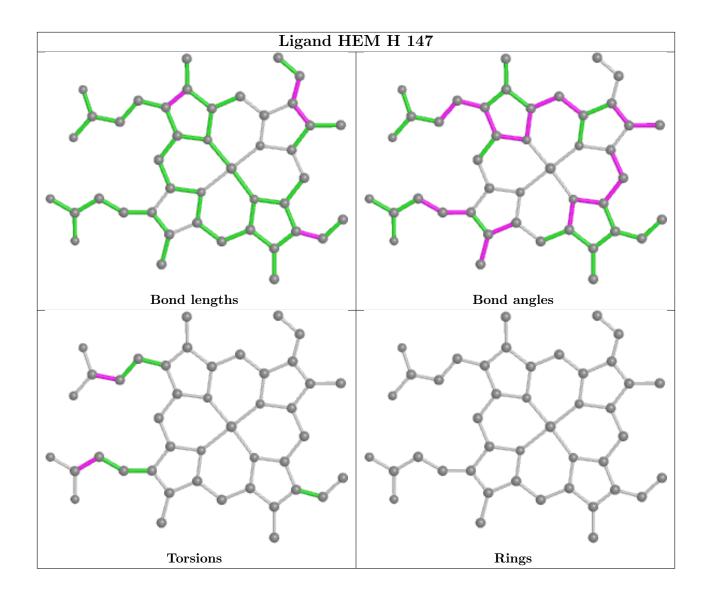
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Е	142	HNI	1	0
5	D	148	CMO	4	0
4	Н	147	HEM	1	0
4	F	147	HEM	2	0
4	В	147	HEM	2	0
3	С	142	HNI	1	0
4	D	147	HEM	5	0

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.

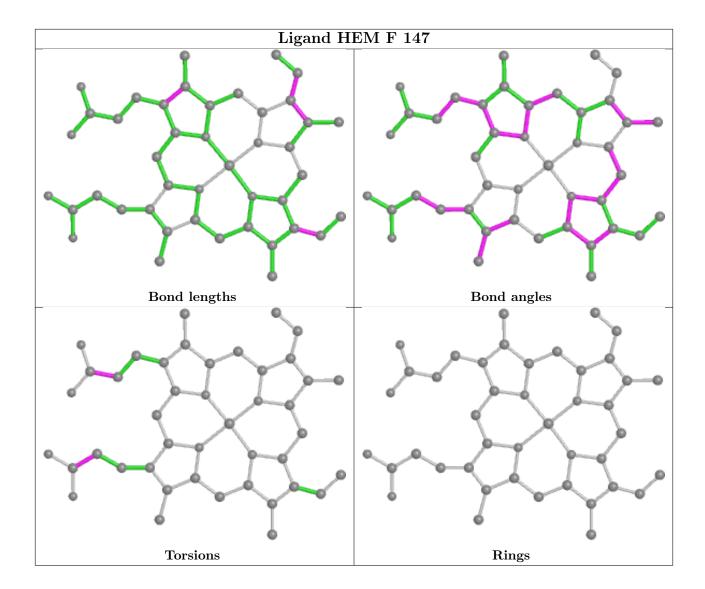




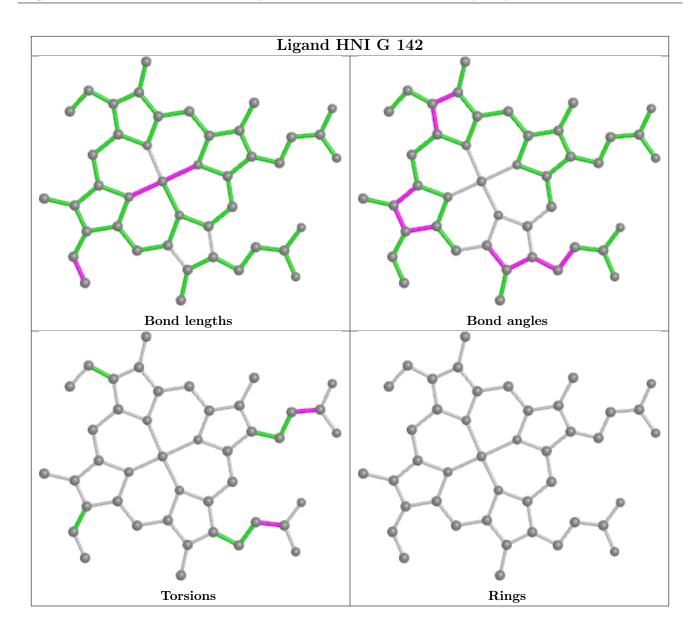




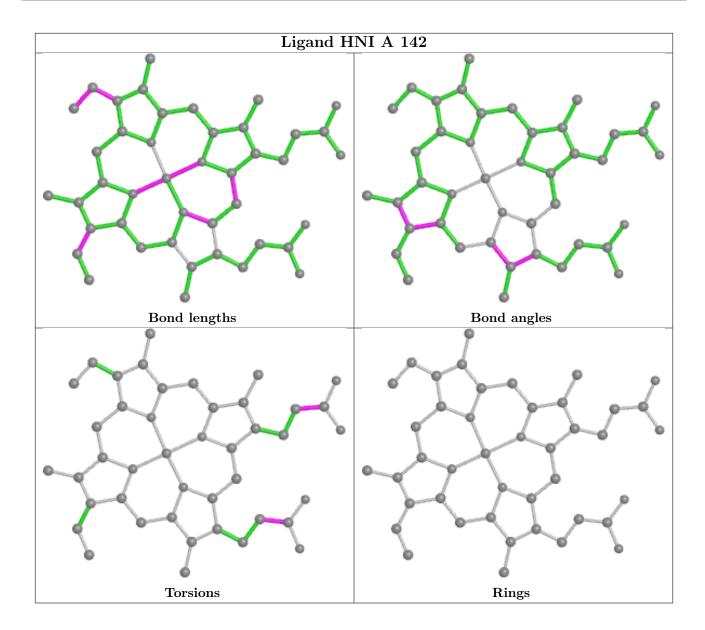




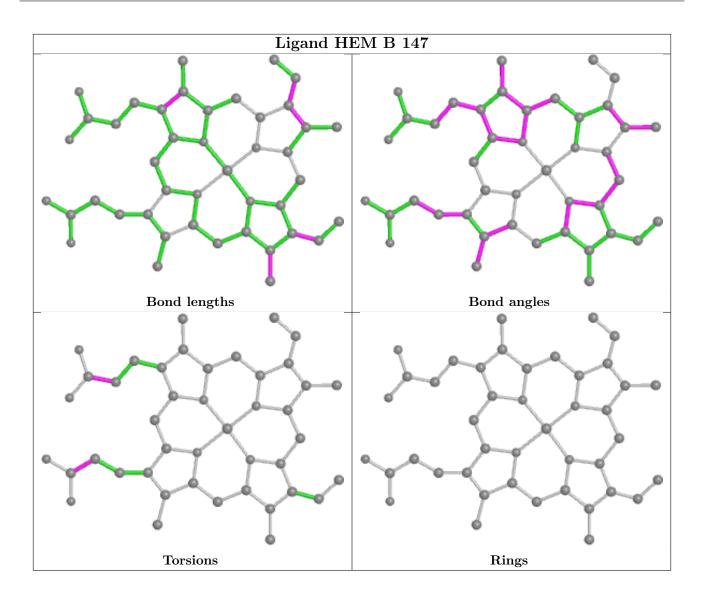




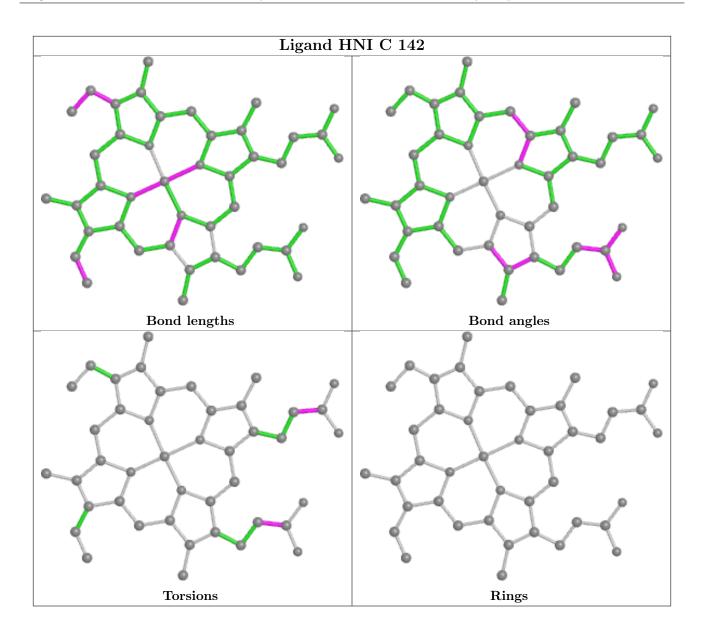




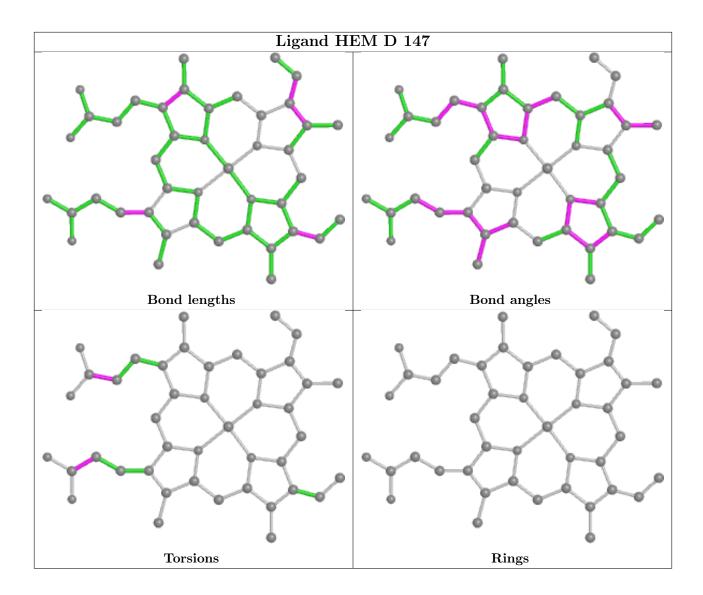












5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

