wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 – 02:58 AM BST

PDB ID	:	1HDS
Title	:	MACROMOLECULAR STRUCTURE REFINEMENT BY RESTRAINED LEAST-SQUARES AND INTERACTIVE GRAPHICS AS APPLIED TO SICKLING DEER TYPE III HEMOGLOBIN
Authors	:	Amma, E.L.; Girling, R.L.
Deposited on	:	1979-10-01
Resolution	:	1.98 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 following versions of software and data (see references (1)) were used in the production of this report:

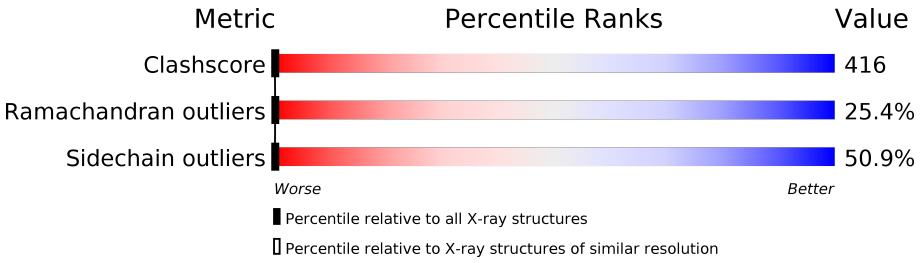
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.98 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	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)

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 on 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	35% 63%
1	C	141	38% 61%
2	B	145	28% 70%
2	D	145	28% 70%

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	HEM	A	142	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEM	B	146	-	-	X	-
3	HEM	C	142	-	-	X	-
3	HEM	D	146	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4556 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 S (DEOXY) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1076	684	199	192	1			
1	C	141	Total	C	N	O	S	0	0	0
			1076	684	199	192	1			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ASN	ASP	conflict	UNP P01972
A	27	GLN	GLU	conflict	UNP P01972
A	30	GLN	GLU	conflict	UNP P01972
A	55	GLN	VAL	conflict	UNP P01972
A	60	GLN	GLU	conflict	UNP P01972
A	70	GLN	VAL	conflict	UNP P01972
A	74	ASN	ASP	conflict	UNP P01972
A	82	ASN	ASP	conflict	UNP P01972
A	85	ASN	ASP	conflict	UNP P01972
A	94	ASN	ASP	conflict	UNP P01972
A	104	SER	THR	conflict	UNP P01972
A	115	THR	SER	conflict	UNP P01972
A	116	ASN	ASP	conflict	UNP P01972
A	124	ASN	SER	conflict	UNP P01972
A	126	ASN	ASP	conflict	UNP P01972
A	132	ASP	VAL	conflict	UNP P01972
C	6	ASN	ASP	conflict	UNP P01972
C	27	GLN	GLU	conflict	UNP P01972
C	30	GLN	GLU	conflict	UNP P01972
C	55	GLN	VAL	conflict	UNP P01972
C	60	GLN	GLU	conflict	UNP P01972
C	70	GLN	VAL	conflict	UNP P01972
C	74	ASN	ASP	conflict	UNP P01972
C	82	ASN	ASP	conflict	UNP P01972
C	85	ASN	ASP	conflict	UNP P01972

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Chain	Residue	Modelled	Actual	Comment	Reference
C	94	ASN	ASP	conflict	UNP P01972
C	104	SER	THR	conflict	UNP P01972
C	115	THR	SER	conflict	UNP P01972
C	116	ASN	ASP	conflict	UNP P01972
C	124	ASN	SER	conflict	UNP P01972
C	126	ASN	ASP	conflict	UNP P01972
C	132	ASP	VAL	conflict	UNP P01972

- Molecule 2 is a protein called HEMOGLOBIN S (DEOXY) (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1116	719	205	189	3			
2	D	145	Total	C	N	O	S	0	0	0
			1116	719	205	189	3			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	ASP	ASN	conflict	UNP P02074
B	25	GLN	GLU	conflict	UNP P02074
B	42	GLN	GLU	conflict	UNP P02074
B	46	ASN	ASP	conflict	UNP P02074
B	55	ASN	GLY	conflict	UNP P02074
B	71	THR	SER	conflict	UNP P02074
B	72	GLN	GLU	conflict	UNP P02074
B	86	GLN	GLU	conflict	UNP P02074
B	89	GLY	GLU	conflict	UNP P02074
B	98	ASN	ASP	conflict	UNP P02074
B	100	GLN	GLU	conflict	UNP P02074
B	110	ALA	VAL	conflict	UNP P02074
B	111	LEU	VAL	conflict	UNP P02074
B	113	VAL	LEU	conflict	UNP P02074
B	120	GLN	GLU	conflict	UNP P02074
B	124	ASN	LEU	conflict	UNP P02074
B	128	LEU	ASP	conflict	UNP P02074
B	143	LYS	ARG	conflict	UNP P02074
D	18	ASP	ASN	conflict	UNP P02074
D	25	GLN	GLU	conflict	UNP P02074
D	42	GLN	GLU	conflict	UNP P02074
D	46	ASN	ASP	conflict	UNP P02074
D	55	ASN	GLY	conflict	UNP P02074

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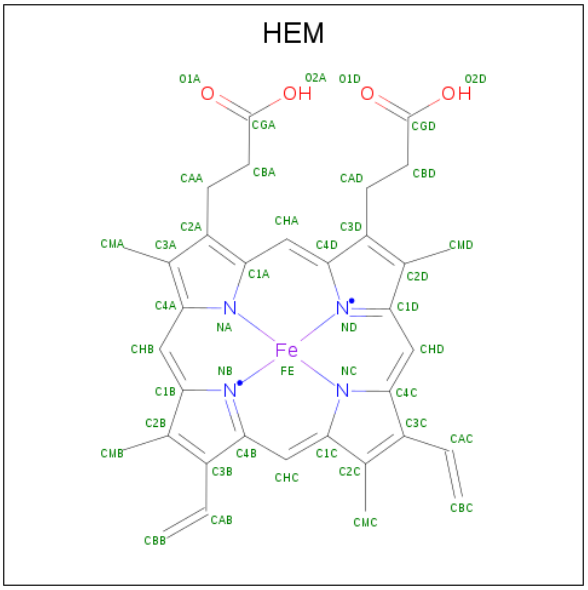
Chain	Residue	Modelled	Actual	Comment	Reference
D	71	THR	SER	conflict	UNP P02074
D	72	GLN	GLU	conflict	UNP P02074
D	86	GLN	GLU	conflict	UNP P02074
D	89	GLY	GLU	conflict	UNP P02074
D	98	ASN	ASP	conflict	UNP P02074
D	100	GLN	GLU	conflict	UNP P02074
D	110	ALA	VAL	conflict	UNP P02074
D	111	LEU	VAL	conflict	UNP P02074
D	113	VAL	LEU	conflict	UNP P02074
D	120	GLN	GLU	conflict	UNP P02074
D	124	ASN	LEU	conflict	UNP P02074
D	128	LEU	ASP	conflict	UNP P02074
D	143	LYS	ARG	conflict	UNP P02074

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

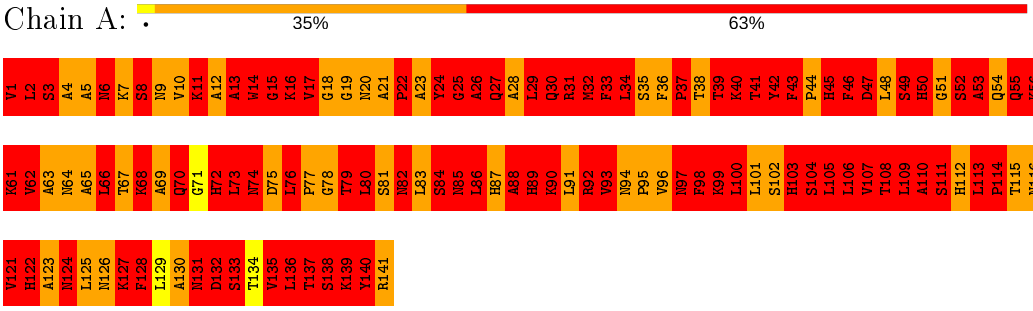
3 Residue-property plots (i)

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.

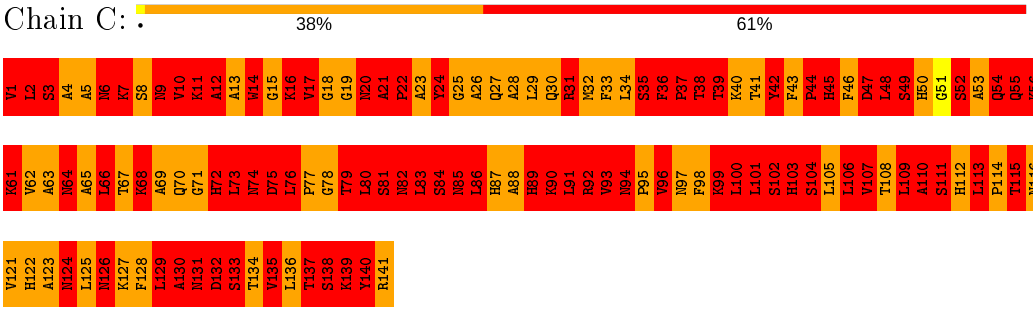
- Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)

Chain A:



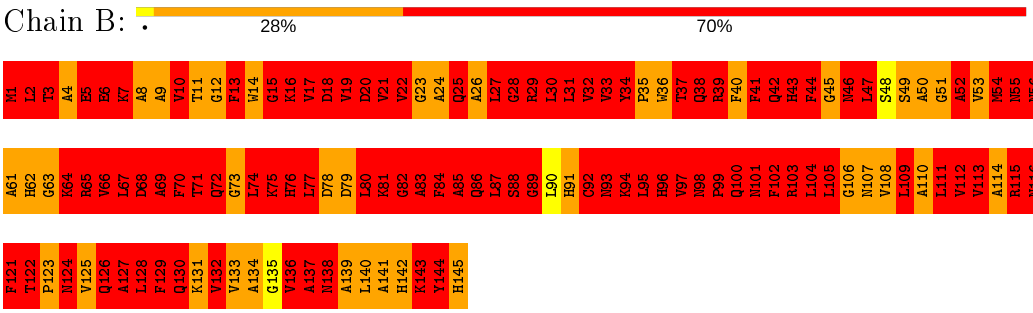
- Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)

Chain C:



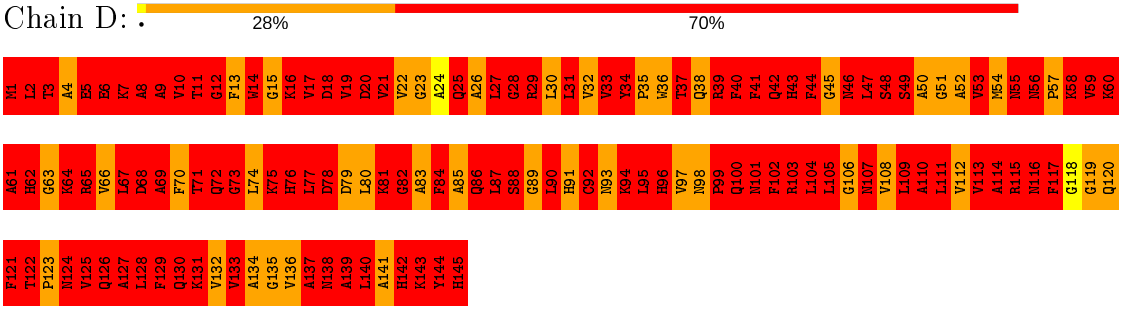
- Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain B:



- Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain D: .


28%
70%
M1 L2 T3 A4 E5 E6 K7 A8 A9 V10 T11 G12 F13 W14 G15 K16 V17 D18 V19 D20 V21 V22 G23 A24 Q25 A26 L27 G28 R29 L30 L31 V32 V33 Y34 P35 W36 T37 Q38 R39 F40 F41 Q42 H43 F44 G45 N46 L47 S48 S49 A50 G51 A52 V53 M54 N55 N56 P57 K58 V59 K60
A61 H62 G63 K64 R65 V66 L67 D68 A69 F70 T71 Q72 G73 L74 K75 H76 L77 D78 D79 L80 K81 G82 A83 F84 A85 Q86 L87 S88 G89 L90 H91 G92 N93 A94 L95 H96 V97 N98 P99 Q100 N101 F102 R103 L104 L105 G106 N107 V108 L109 A110 L111 V112 V113 A114 R115 N116 F117 G118 G119 Q120
F121 T122 P123 N124 V125 Q126 A127 L128 F129 Q130 K131 V132 V133 A134 G135 V136 A137 N138 A139 L140 A141 H142 K143 Y144 R145

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.50Å 70.83Å 65.95Å 90.00° 94.15° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.98	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.98)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4556	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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: HEM

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	10.87	704/1103 (63.8%)	9.83	796/1498 (53.1%)
1	C	10.65	668/1103 (60.6%)	9.48	847/1498 (56.5%)
2	B	11.08	695/1142 (60.9%)	10.07	841/1545 (54.4%)
2	D	11.22	702/1142 (61.5%)	11.17	890/1545 (57.6%)
All	All	10.96	2769/4490 (61.7%)	10.16	3374/6086 (55.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	9	52
1	C	2	41
2	B	2	40
2	D	6	51
All	All	19	184

The worst 5 of 2769 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	SER	CB-OG	64.78	2.26	1.42
2	B	144	TYR	CE2-CZ	55.70	2.10	1.38
2	D	123	PRO	N-CD	53.15	2.22	1.47
2	B	32	VAL	CB-CG2	50.79	2.59	1.52
1	C	84	SER	CB-OG	49.53	2.06	1.42

The worst 5 of 3374 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	70	PHE	CB-CG-CD2	71.93	171.15	120.80
1	A	92	ARG	NE-CZ-NH2	-65.06	87.77	120.30
1	A	141	ARG	NE-CZ-NH1	61.72	151.16	120.30
2	D	44	PHE	CB-CG-CD2	60.92	163.44	120.80
2	D	84	PHE	CB-CG-CD1	-60.50	78.45	120.80

5 of 19 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2	LEU	CA
1	A	31	ARG	CA
1	A	33	PHE	CA
1	A	93	VAL	CA
1	A	100	LEU	CA

5 of 184 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Mainchain,Peptide
1	A	15	GLY	Peptide
1	A	22	PRO	Mainchain
1	A	3	SER	Mainchain
1	A	8	SER	Mainchain,Peptide

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	1076	0	1032	834	80
1	C	1076	0	1034	805	3
2	B	1116	0	1070	1126	0
2	D	1116	0	1068	917	77
3	A	43	0	30	49	0
3	B	43	0	30	56	0
3	C	43	0	30	42	0
3	D	43	0	30	29	0
All	All	4556	0	4324	3698	80

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 416.

The worst 5 of 3698 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)
2:B:34:TYR:CZ	2:B:34:TYR:CE2	1.79	1.70
2:B:144:TYR:CG	2:B:144:TYR:CD2	1.76	1.69
3:A:142:HEM:CMA	3:A:142:HEM:C3A	1.75	1.67
1:C:140:TYR:CB	1:C:140:TYR:CG	1.77	1.67
2:D:14:TRP:CZ3	2:D:14:TRP:CE3	1.76	1.66

The worst 5 of 80 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:2:LEU:O	2:D:49:SER:CB[4_555]	0.51	1.69
1:A:75:ASP:C	2:D:55:ASN:CG[4_555]	0.81	1.39
1:A:74:ASN:CG	2:D:54:MET:CA[4_555]	0.92	1.28
1:A:2:LEU:O	2:D:49:SER:CA[4_555]	1.05	1.15
1:A:7:LYS:NZ	2:D:51:GLY:N[4_555]	1.06	1.14

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	139/141 (99%)	74 (53%)	34 (24%)	31 (22%)	0	0
1	C	139/141 (99%)	78 (56%)	28 (20%)	33 (24%)	0	0
2	B	143/145 (99%)	75 (52%)	28 (20%)	40 (28%)	0	0
2	D	143/145 (99%)	78 (54%)	26 (18%)	39 (27%)	0	0
All	All	564/572 (99%)	305 (54%)	116 (21%)	143 (25%)	0	0

5 of 143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	6	ASN
1	A	13	ALA
1	A	15	GLY
1	A	17	VAL

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	115/115 (100%)	57 (50%)	58 (50%)	0	0
1	C	115/115 (100%)	64 (56%)	51 (44%)	0	0
2	B	113/113 (100%)	50 (44%)	63 (56%)	0	0
2	D	113/113 (100%)	53 (47%)	60 (53%)	0	0
All	All	456/456 (100%)	224 (49%)	232 (51%)	0	0

5 of 232 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	104	LEU
1	C	20	ASN
2	D	109	LEU
2	B	112	VAL
2	B	129	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	145	HIS
1	C	60	GLN
2	D	76	HIS
1	C	45	HIS
1	C	70	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
3	HEM	B	146	2	27,50,50	10.55	22 (81%)	17,82,82	8.98	10 (58%)
3	HEM	D	146	-	27,50,50	10.88	23 (85%)	17,82,82	9.27	15 (88%)
3	HEM	A	142	1	27,50,50	9.67	21 (77%)	17,82,82	11.88	15 (88%)
3	HEM	C	142	1	27,50,50	8.96	20 (74%)	17,82,82	6.87	11 (64%)

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	HEM	B	146	2	-	2/6/54/54	-
3	HEM	D	146	-	-	3/6/54/54	-
3	HEM	A	142	1	-	2/6/54/54	-
3	HEM	C	142	1	-	1/6/54/54	-

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	146	HEM	CAD-C3D	-27.74	1.03	1.52
3	B	146	HEM	C4D-C3D	23.91	1.96	1.42
3	B	146	HEM	C3B-C2B	-23.74	1.07	1.40
3	D	146	HEM	CMD-C2D	-23.16	1.03	1.51
3	B	146	HEM	CMA-C3A	20.85	1.95	1.51

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	142	HEM	CBD-CAD-C3D	27.20	162.59	112.48
3	D	146	HEM	C4A-C3A-C2A	25.96	125.06	107.00
3	A	142	HEM	C4C-C3C-C2C	-24.18	90.01	106.90
3	B	146	HEM	CMA-C3A-C4A	-20.36	97.18	128.46
3	B	146	HEM	CMC-C2C-C3C	17.94	158.24	124.68

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	146	HEM	C2D-C3D-CAD-CBD
3	B	146	HEM	C4D-C3D-CAD-CBD
3	D	146	HEM	C1A-C2A-CAA-CBA
3	D	146	HEM	C3A-C2A-CAA-CBA
3	D	146	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.

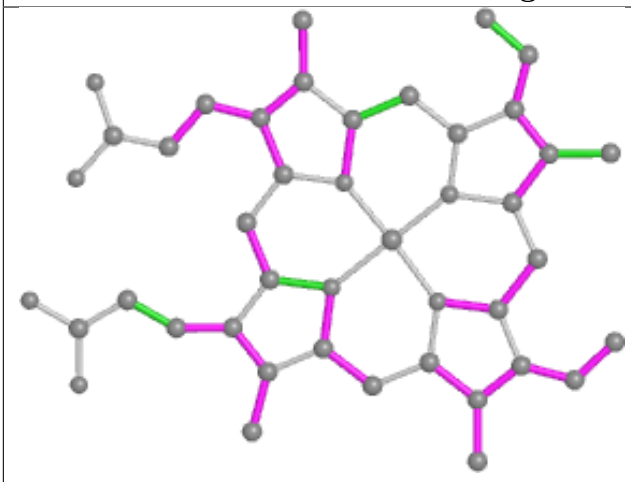
4 monomers are involved in 176 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	146	HEM	56	0
3	D	146	HEM	29	0
3	A	142	HEM	49	0
3	C	142	HEM	42	0

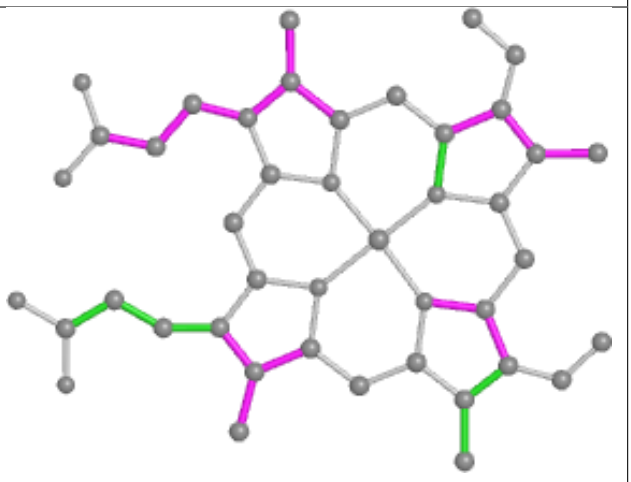
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

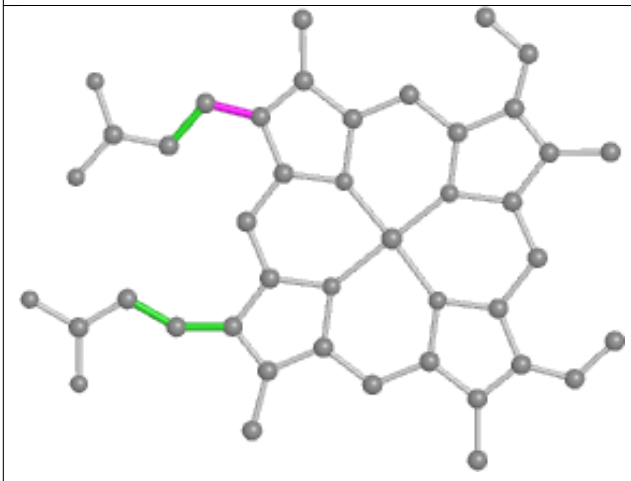
Ligand HEM B 146



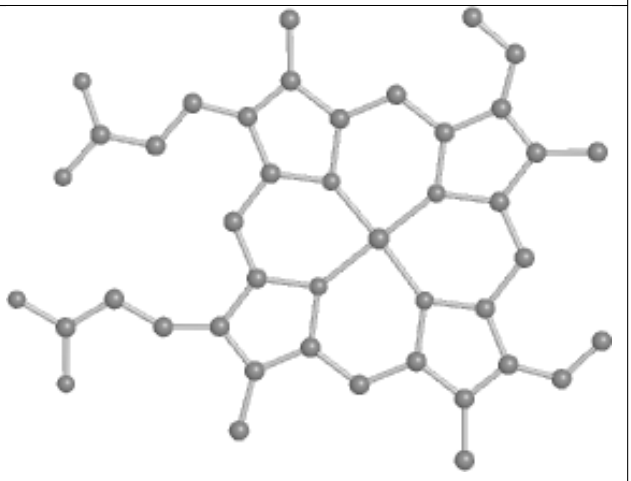
Bond lengths



Bond angles

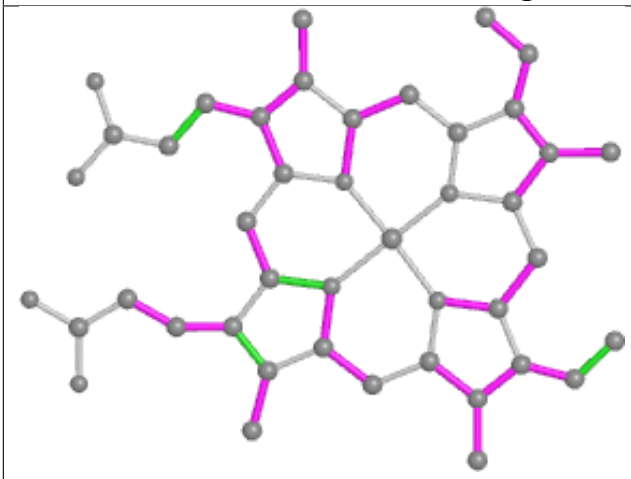


Torsions

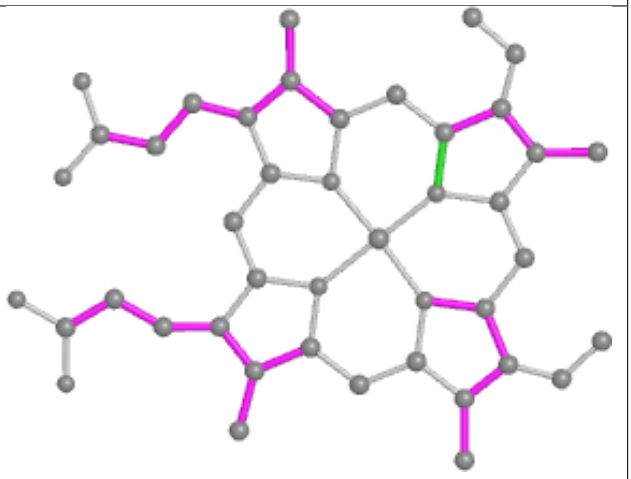


Rings

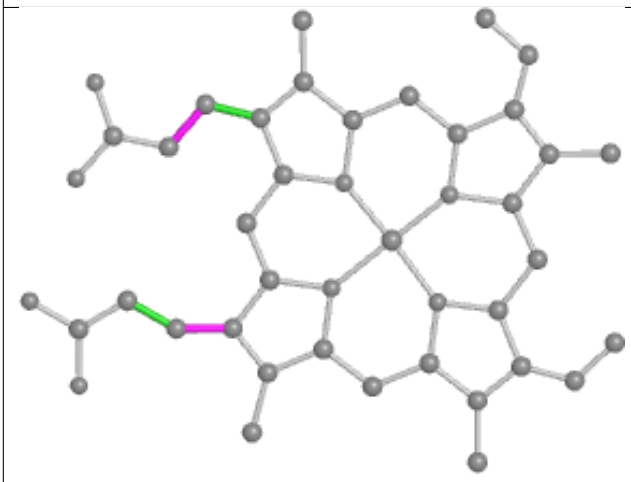
Ligand HEM D 146



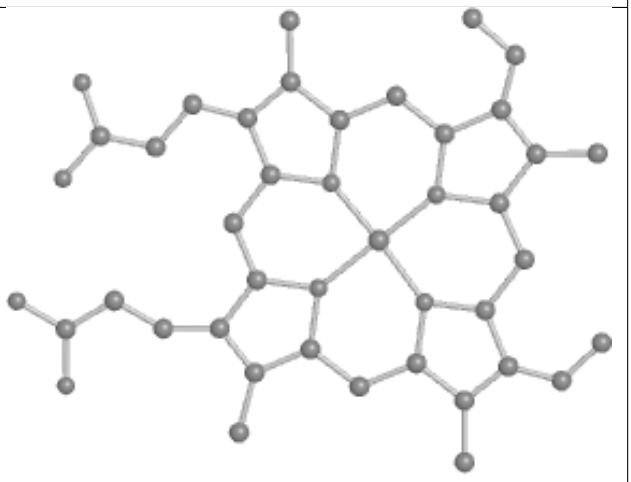
Bond lengths



Bond angles

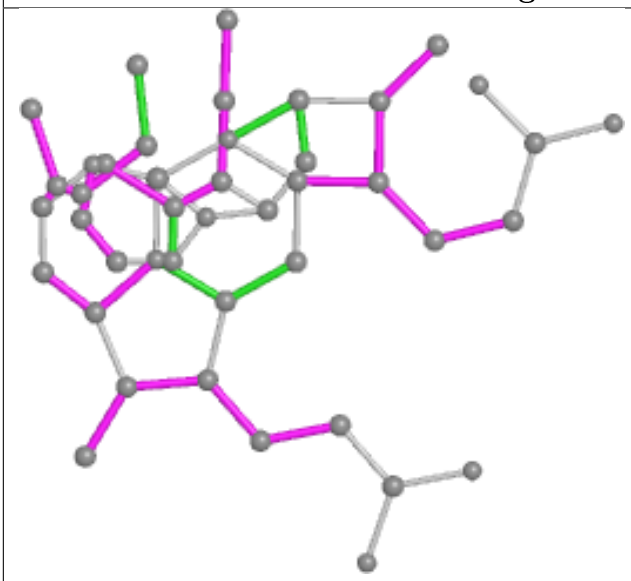


Torsions

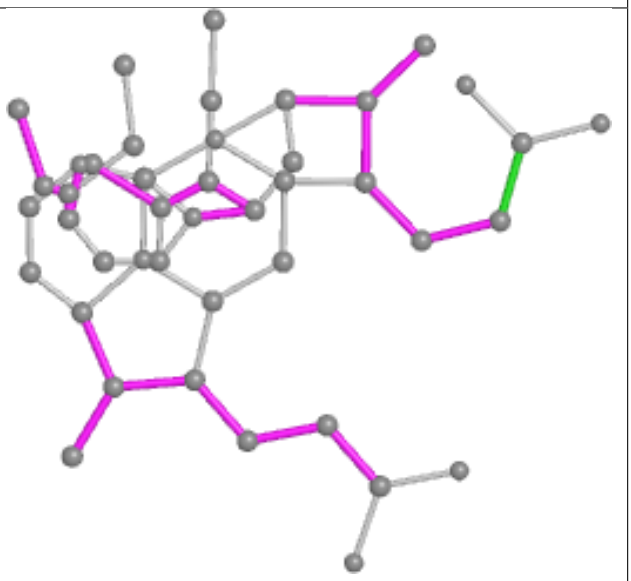


Rings

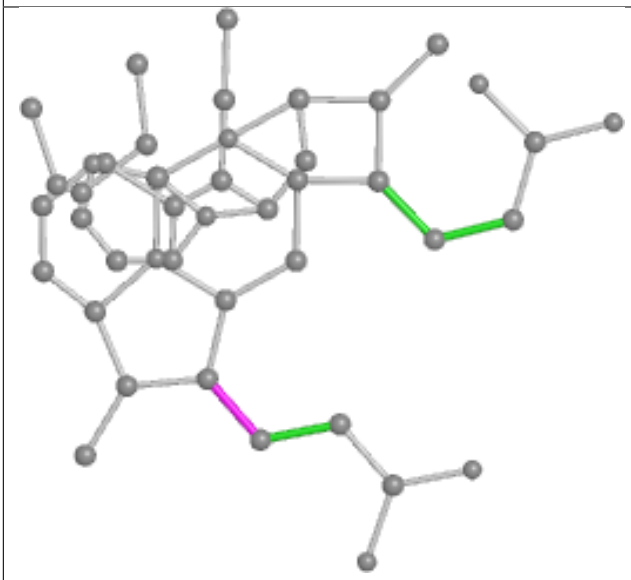
Ligand HEM A 142



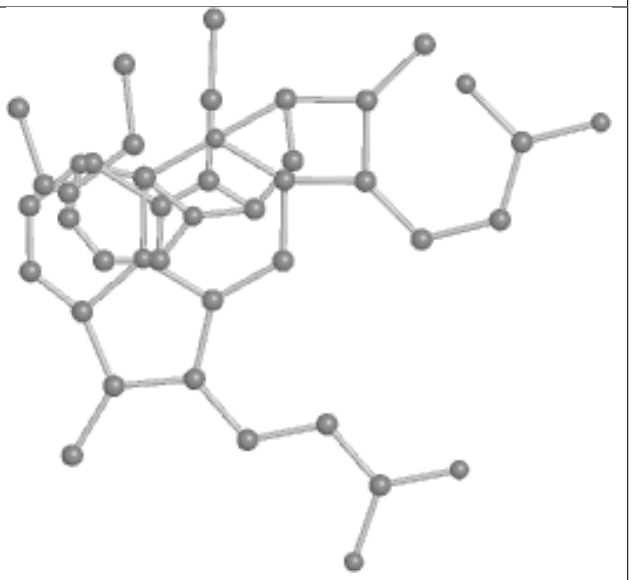
Bond lengths



Bond angles

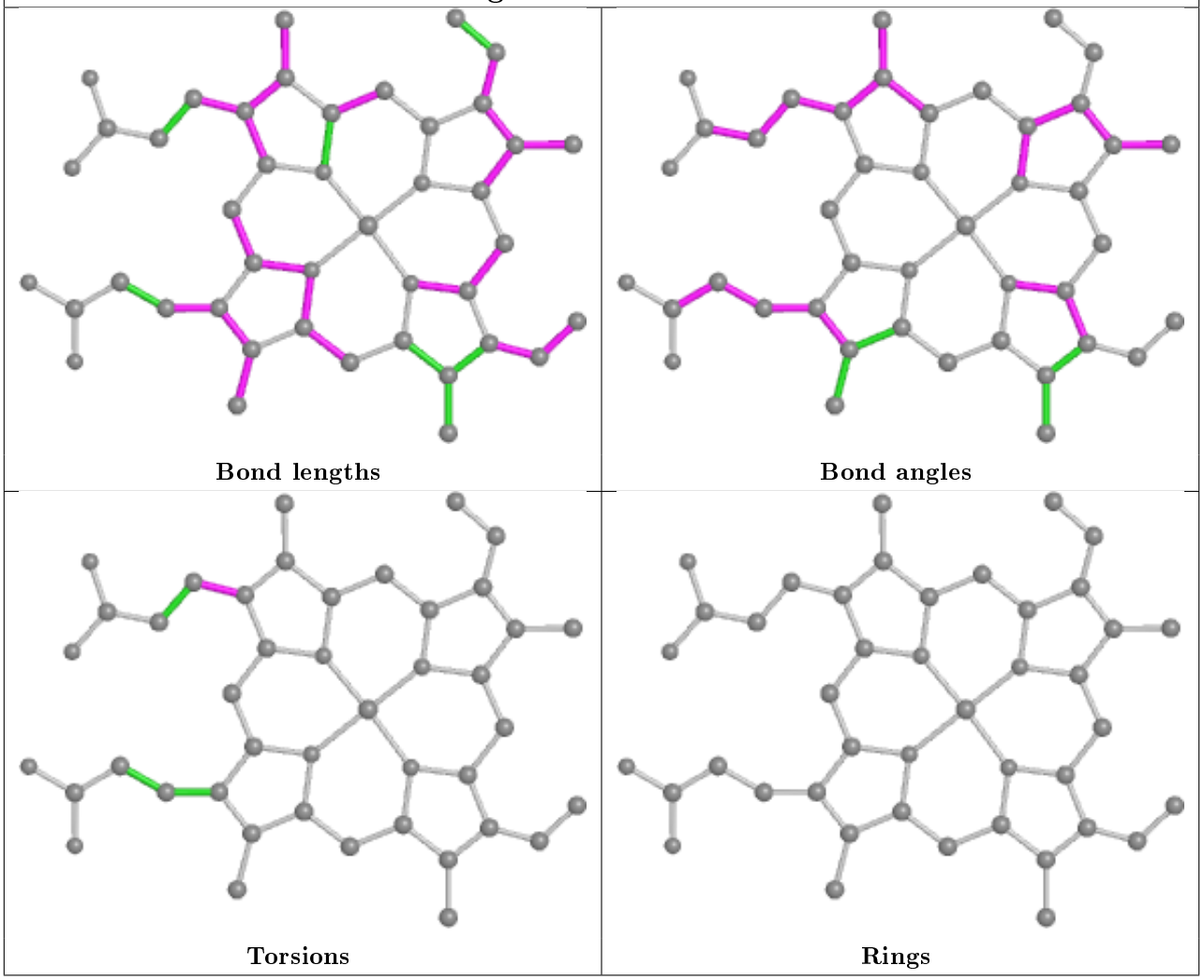


Torsions



Rings

Ligand HEM C 142



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	53
1	A	51
2	B	47
1	C	47

The worst 5 of 198 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	98:PHE	C	99:LYS	N	1.99
1	B	42:GLN	C	43:HIS	N	1.93
1	D	51:GLY	C	52:ALA	N	1.87
1	B	41:PHE	C	42:GLN	N	1.85
1	C	74:ASN	C	75:ASP	N	1.84

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.