



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 03:51 AM UTC

PDB ID : 1HDS / pdb_00001hds
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 ⓘ 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

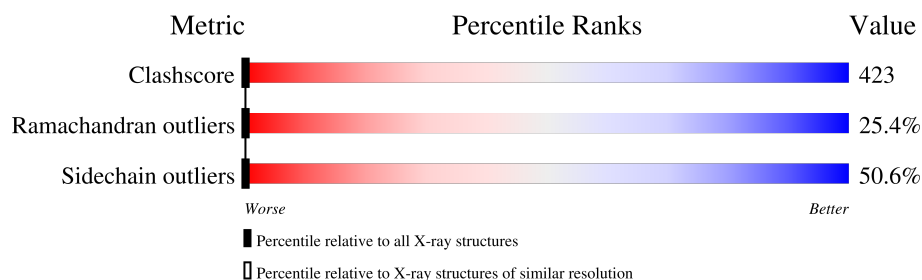
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (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 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	141	
1	C	141	
2	B	145	
2	D	145	

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	X	-
3	HEM	B	146	-	X	X	-
3	HEM	C	142	-	X	X	-
3	HEM	D	146	-	X	X	-

2 Entry composition

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:

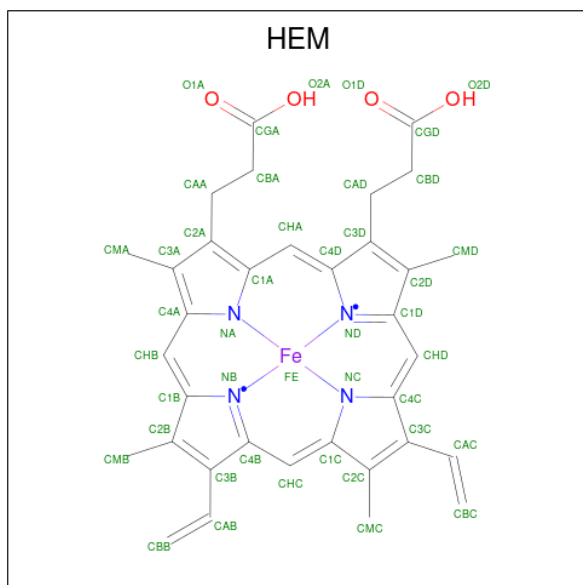
Chain	Residue	Modelled	Actual	Comment	Reference
B	18	ASP	ASN	conflict	UNP P02074
B	25	GLN	GLU	conflict	UNP P02074
B	42	GLN	GLU	conflict	UNP P02074
B	46	ASN	ASP	conflict	UNP P02074
B	55	ASN	GLY	conflict	UNP P02074
B	71	THR	SER	conflict	UNP P02074
B	72	GLN	GLU	conflict	UNP P02074
B	86	GLN	GLU	conflict	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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



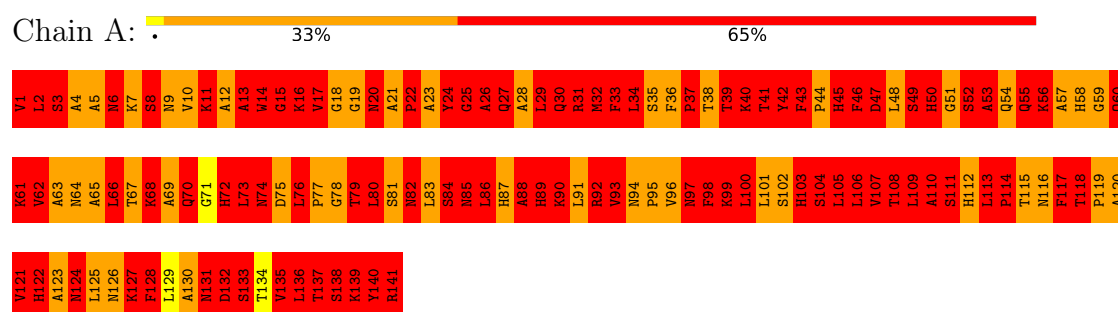
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

3 Residue-property plots

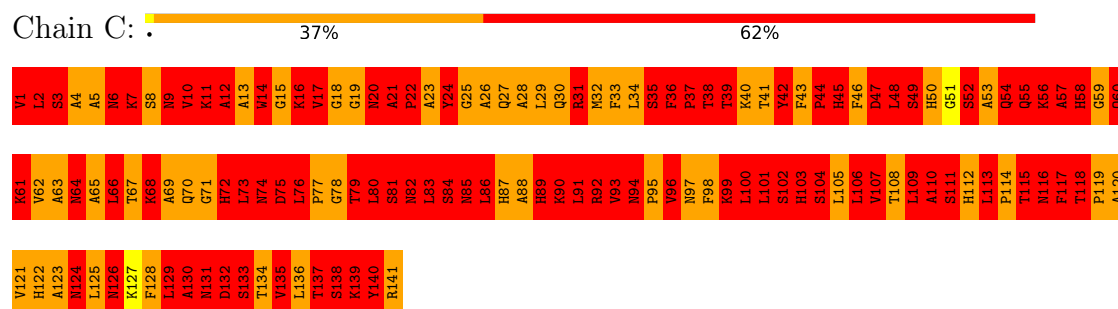
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

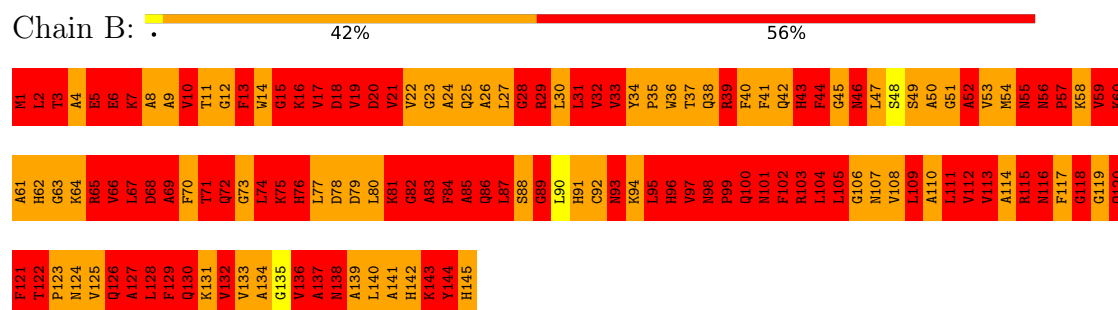
• Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)



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



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



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

Chain D: . 27% 72%

M1	A81	F121
L2	H62	T122
T3	G83	P123
A4	K64	N124
E5	R65	V125
E6	V66	Q126
K7	L67	A127
A8	D68	L128
A9	A69	F129
V10	F70	Q130
T11	T71	K131
G12	Q72	V132
F13	G73	V133
M14	L74	A134
G15	K75	G135
K16	H76	V136
V17	L77	A137
D18	D78	N138
V19	D79	A139
D20	L80	L140
V21	K81	A141
V22	G82	H142
G23	A83	K143
A24	F84	Y144
Q25	A85	H145
A26	Q86	
L27	L87	
G28	S88	
R29	G89	
L30	L90	
L31	H91	
V32	G92	
V33	N93	
Y34	K94	
P35	L95	
W36	H96	
T37	V97	
Q38	N98	
R39	P99	
F40	Q100	
F41	N101	
Q42	F102	
H43	R103	
F44	L104	
G45	L105	
R46	G106	
L47	N107	
S48	V108	
S49	L109	
A50	A110	
G51	L111	
A52	V112	
V53	V113	
M54	A114	
N55	R115	
N56	N116	
P57	F117	
K58	G118	
V59	G119	
K60	Q120	

4 Data and refinement statistics

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 [i](#)

5.1 Standard geometry [i](#)

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	14.76	785/1103 (71.2%)	11.56	941/1498 (62.8%)
1	C	13.93	776/1103 (70.4%)	11.39	970/1498 (64.8%)
2	B	14.29	782/1142 (68.5%)	11.25	964/1545 (62.4%)
2	D	14.94	798/1142 (69.9%)	12.74	1002/1545 (64.9%)
All	All	14.49	3141/4490 (70.0%)	11.75	3877/6086 (63.7%)

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 3141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	145	HIS	CD2-NE2	81.18	2.27	1.37
1	A	72	HIS	CE1-NE2	62.40	1.95	1.32
2	D	145	HIS	CG-ND1	61.95	2.06	1.38
2	D	70	PHE	C-O	60.24	1.98	1.23
2	B	43	HIS	ND1-CE1	59.63	1.92	1.32

The worst 5 of 3877 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	LYS	O-C-N	-56.69	47.19	122.59
1	C	122	HIS	CA-CB-CG	55.70	169.50	113.80
2	D	100	GLN	OE1-CD-NE2	-51.06	71.54	122.60
2	D	11	THR	CB-CA-C	45.62	174.25	111.74
1	A	131	ASN	OD1-CG-ND2	-45.33	77.27	122.60

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	Peptide,Mainchain
1	A	15	GLY	Peptide
1	A	22	PRO	Mainchain
1	A	3	SER	Mainchain
1	A	8	SER	Peptide,Mainchain

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	1076	0	1041	839	80
1	C	1076	0	1038	826	3
2	B	1116	0	1081	1146	0
2	D	1116	0	1079	947	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	4359	3772	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 423.

The worst 5 of 3772 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:CD2	2:B:144:TYR:CG	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:CE3	2:D:14:TRP:CZ3	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 ⓘ

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%)	54 (47%)	61 (53%)	0	0
1	C	115/115 (100%)	63 (55%)	52 (45%)	0	0
2	B	56/113 (50%)	30 (54%)	26 (46%)	0	0
2	D	113/113 (100%)	50 (44%)	63 (56%)	0	0
All	All	399/456 (88%)	197 (49%)	202 (51%)	0	0

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	79	THR
2	D	10	VAL
2	D	142	HIS
1	C	90	LYS
1	C	116	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	55	GLN
2	D	130	GLN
1	C	70	GLN
2	D	56	ASN
1	C	64	ASN

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 oligosaccharides 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	A	142	1	50,50,50	10.75	43 (86%)	67,82,82	9.98	59 (88%)
3	HEM	B	146	2	50,50,50	9.11	43 (86%)	67,82,82	8.11	49 (73%)
3	HEM	C	142	1	50,50,50	9.37	42 (84%)	67,82,82	6.08	46 (68%)
3	HEM	D	146	-	50,50,50	11.42	41 (82%)	67,82,82	7.42	54 (80%)

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	A	142	1	-	5/14/54/54	-
3	HEM	B	146	2	-	4/14/54/54	-
3	HEM	C	142	1	-	7/14/54/54	-
3	HEM	D	146	-	-	7/14/54/54	-

The worst 5 of 169 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	146	HEM	C4D-C3D	30.43	1.96	1.45
3	A	142	HEM	CBD-CGD	26.54	2.12	1.50
3	D	146	HEM	C1B-NB	26.42	1.85	1.40
3	D	146	HEM	CBD-CGD	25.73	2.10	1.50
3	A	142	HEM	CHA-C4D	25.59	1.89	1.38

The worst 5 of 208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	C2B-C1B-NB	27.85	141.86	109.84
3	B	146	HEM	CHA-C4D-ND	27.54	158.43	124.37
3	A	142	HEM	C3D-C4D-ND	25.35	137.98	110.17
3	A	142	HEM	C4D-ND-C1D	-22.73	78.29	105.21
3	D	146	HEM	C3B-C2B-C1B	22.51	123.31	106.41

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	142	HEM	C3A-C2A-CAA-CBA
3	B	146	HEM	C2D-C3D-CAD-CBD
3	D	146	HEM	C3A-C2A-CAA-CBA
3	D	146	HEM	C2C-C3C-CAC-CBC
3	D	146	HEM	C4C-C3C-CAC-CBC

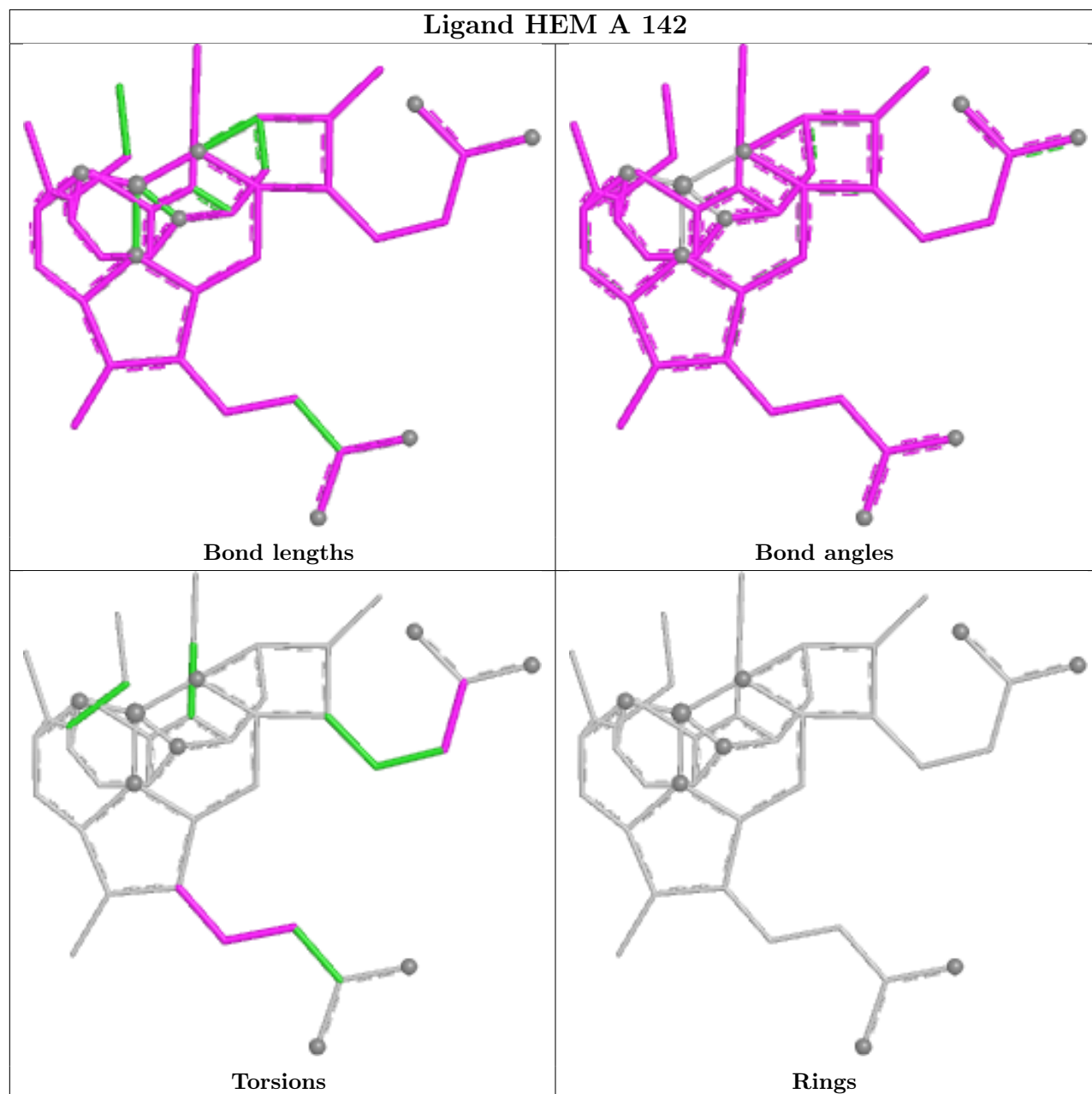
There are no ring outliers.

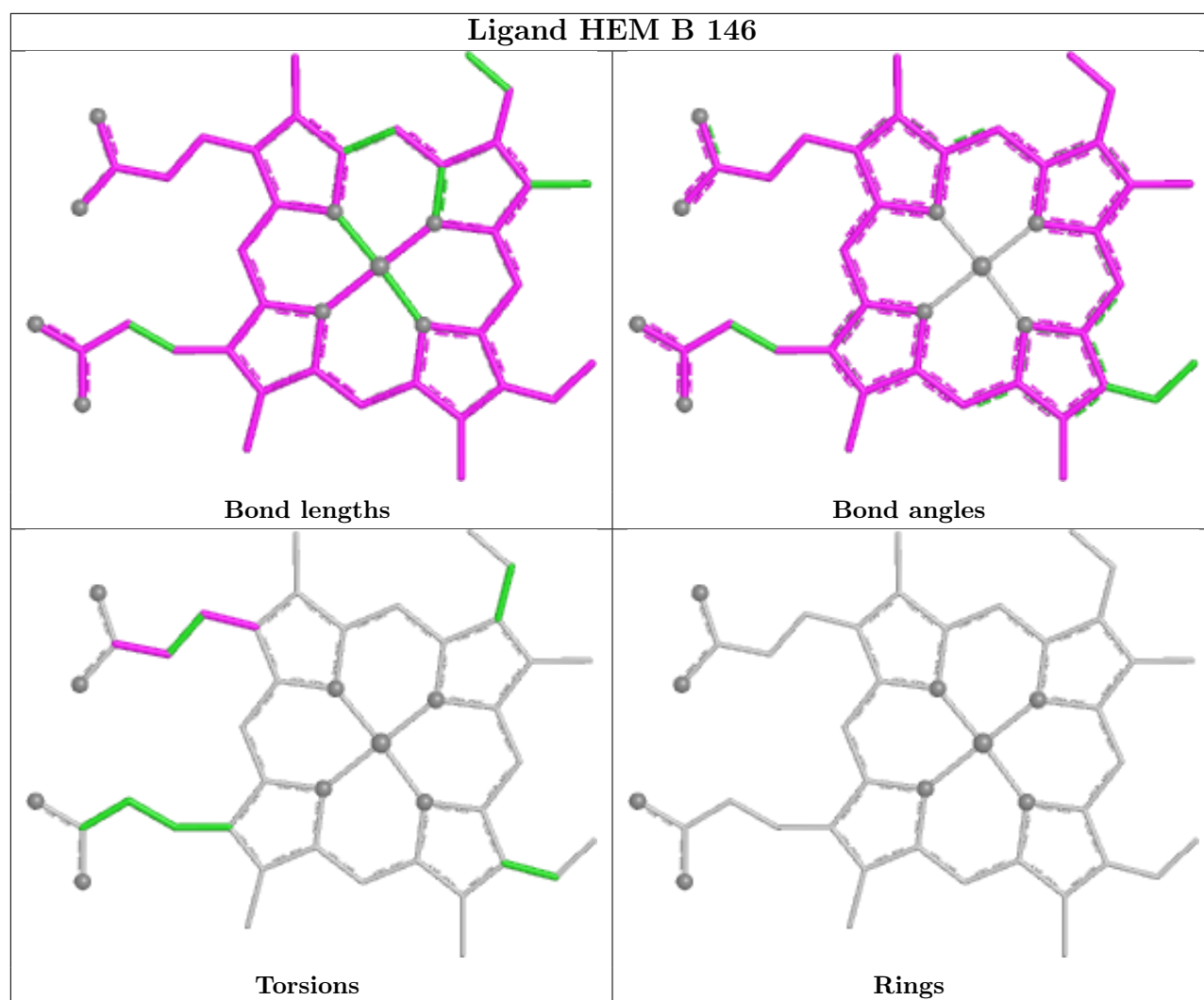
4 monomers are involved in 176 short contacts:

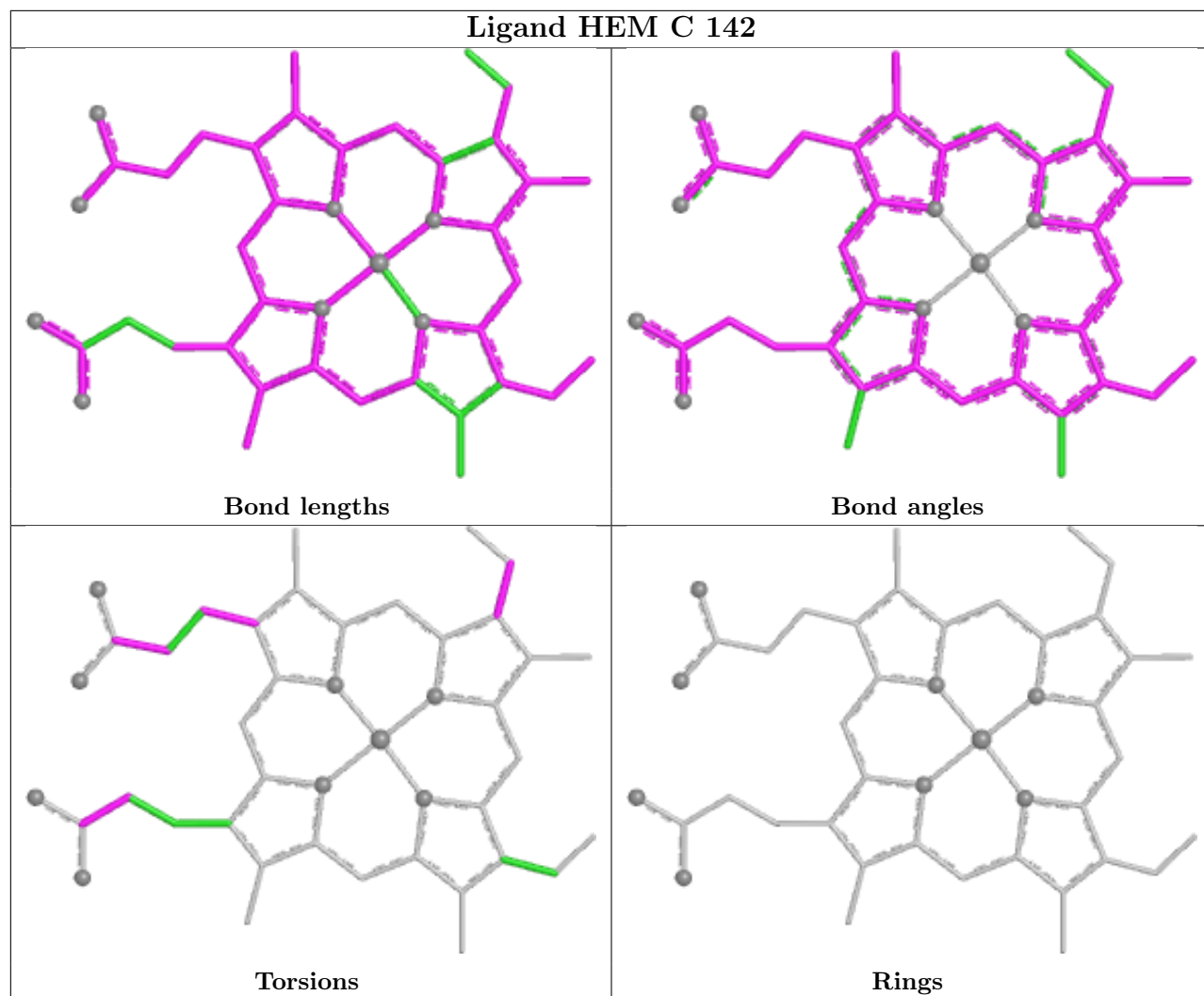
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	142	HEM	49	0
3	B	146	HEM	56	0
3	C	142	HEM	42	0
3	D	146	HEM	29	0

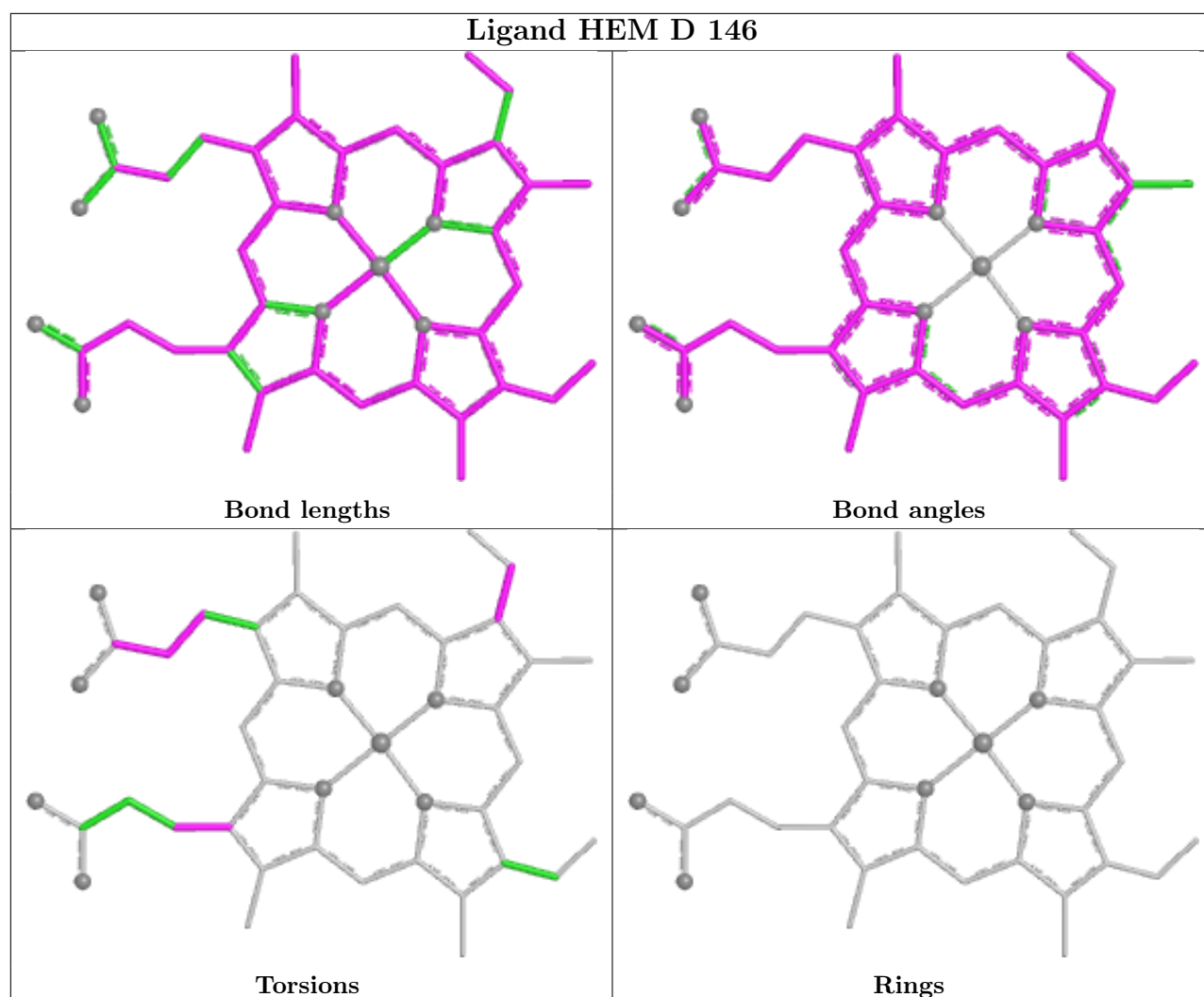
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The following chains have linkage breaks:

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