WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2024 – 05:51 PM EST

PDB ID	:	1HBS
Title	:	REFINED CRYSTAL STRUCTURE OF DEOXYHEMOGLOBIN S. I. RE-STRAINED LEAST-SQUARES REFINEMENT AT 3.0-ANGSTROMS RESOLUTION
Authors	:	Padlan, E.A.; Love, W.E.
Deposited on	:	1982-06-02
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

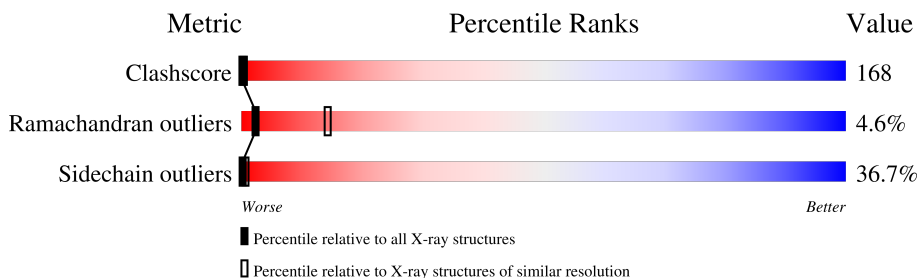|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Clashscore		168
Ramachandran outliers		4.6%
Sidechain outliers		36.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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	· 15% 62% 21%
1	C	141	9% 55% 36%
1	E	141	· 16% 52% 31%
1	G	141	15% 50% 35%
2	B	146	12% 62% 26%
2	D	146	10% 66% 24%
2	F	146	· 12% 63% 24%
2	H	146	· 12% 51% 36%

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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	-
3	HEM	D	147	-	-	X	-
3	HEM	E	142	-	-	X	-
3	HEM	G	142	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9104 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
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	E	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	G	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			
2	D	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			
2	F	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			
2	H	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	VAL	GLU	conflict	UNP P68871
D	6	VAL	GLU	conflict	UNP P68871
F	6	VAL	GLU	conflict	UNP P68871
H	6	VAL	GLU	conflict	UNP P68871

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

HEM

| 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	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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.
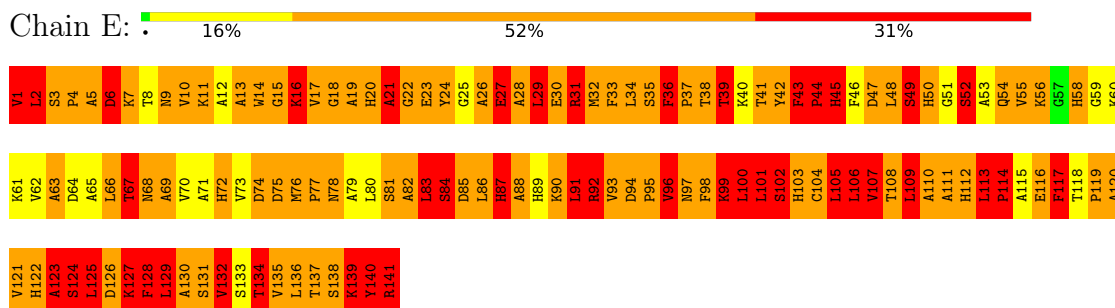
Note EDS was not executed.

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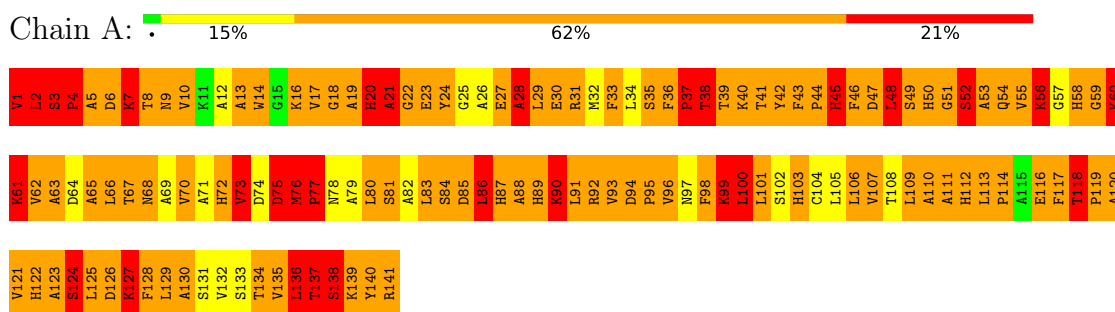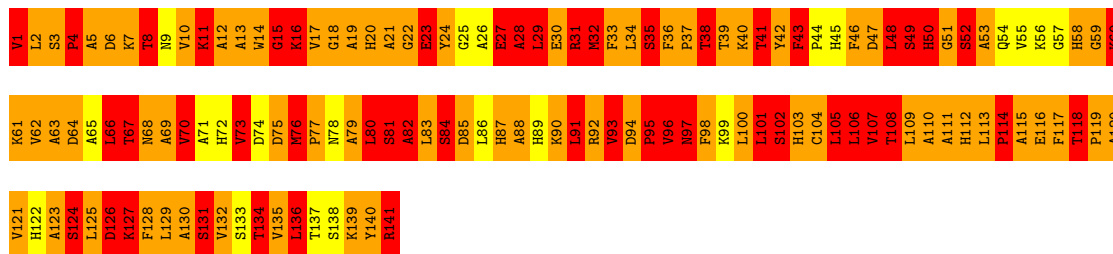
Chain A:

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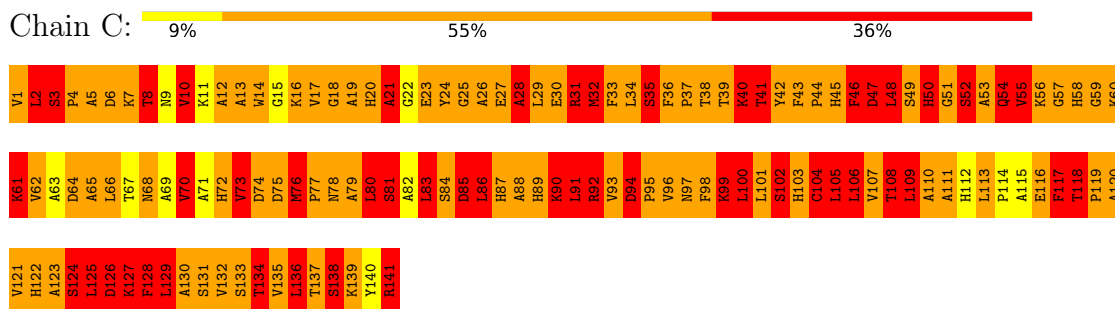
Chain C:
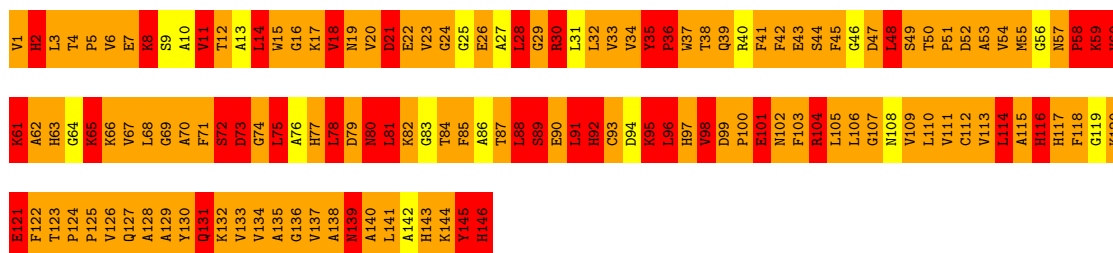

• Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)

Chain E:

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

Chain G:　15%　　　　　50%　　　　　35%

V1 L2 S3 P4 A5 D6 K7 T8 N9 V10 K11 A12 A13 W14 G15 K16 V17 G18 A19 H20 A21 G22 E23 Y24 G25 A26 E27 A28 L29 E30 R31 M32 F33 L34 S35 F36 P37 T38 T39 K40 T41 Y42 F43 P44 H45 F46 D47 L48 S49 H50 G51 S52 A53 Q54 V55 K56 G57 H58 G59 K60

K61 V62 A63 D64 A65 L66 T67 N68 A69 V70 A71 H72 V73 D74 D75 M76 P77 N78 A79 L80 S81 A82 L83 S84 D85 L86 H87 A88 H89 K90 L91 R92 V93 D94 P95 V96 N97 F98 K99 L100 L101 S102 H103 C104 L105 L106 V107 T108 L109 A110 A111 H112 L113 P114 A115 E116 F117 T118 P119 A120

V121 H122 A123 S124 L125 D126 K127 F128 L129 A130 S131 V132 S133 T134 V135 L136 T137 S138 K139 Y140 R141

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

Chain B:　12%　　　　　62%　　　　　26%

V1 H2 L3 T4 P5 V6 E7 K8 S9 A10 V11 T12 A13 L14 W15 G16 K17 V18 N19 V20 D21 E22 V23 G24 G25 E26 A27 L28 G29 R30 L31 L32 V33 V34 Y35 P36 W37 T38 Q39 R40 F41 F42 E43 S44 F45 G46 D47 L48 S49 T50 P51 D52 A53 V54 M55 G56 N57 P58 K59 V60

K61 A62 H63 G64 K65 K66 V67 L68 G69 A70 F71 S72 D73 G74 L75 A76 H77 L78 D79 N80 L81 K82 G83 T84 A86 T87 L88 S89 E90 L91 H92 C93 D94 K95 L96 H97 V98 D99 P100 E101 N102 F103 R104 L105 L106 G107 N108 V109 L110 V111 C112 V113 L114 A115 H116 H117 F118 G119 K120

E121 F122 T123 P124 P125 V126 Q127 A128 A129 Y130 Q131 K132 V133 V134 A135 G136 V137 A138 N139 A140 L141 A142 H143 K144 Y145 H146

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

Chain D:　10%　　　　　66%　　　　　24%

V1 H2 L3 T4 P5 V6 E7 K8 S9 A10 V11 T12 A13 L14 W15 G16 K17 V18 N19 V20 D21 E22 V23 G24 G25 E26 A27 L28 G29 R30 L31 L32 V33 V34 Y35 P36 W37 T38 Q39 R40 F41 F42 E43 S44 F45 G46 D47 L48 S49 T50 P51 D52 A53 V54 M55 G56 N57 P58 K59 V60

K61 A62 H63 G64 K65 K66 V67 L68 G69 A70 F71 S72 D73 G74 L75 A76 H77 L78 D79 N80 L81 K82 G83 T84 F85 A86 T87 L88 S89 E90 L91 H92 C93 D94 K95 L96 H97 V98 D99 P100 E101 N102 F103 R104 L105 L106 G107 N108 V109 L110 V111 C112 V113 L114 A115 H116 H117 F118 G119 K120

E121 F122 T123 P124 P125 V126 Q127 A128 A129 Y130 Q131 K132 V133 V134 A135 G136 V137 A138 N139 A140 L141 A142 H143 K144 Y145 H146

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

Chain F: •　12%　　　　　63%　　　　　24%

V1 H2 L3 T4 P5 V6 E7 K8 S9 A10 V11 T12 A13 L14 W15 G16 K17 V18 N19 V20 D21 E22 V23 G24 G25 E26 A27 L28 G29 R30 L31 L32 V33 V34 Y35 P36 W37 T38 Q39 R40 F41 F42 E43 S44 F45 G46 D47 L48 S49 T50 P51 D52 A53 V54 M55 G56 N57 P58 K59 V60

K61 A62 H63 G64 K65 K66 V67 L68 G69 A70 F71 S72 D73 G74 L75 A76 H77 L78 D79 N80 L81 K82 G83 T84 F85 A86 T87 L88 S89 E90 L91 H92 C93 D94 K95 L96 H97 V98 D99 P100 E101 N102 F103 R104 L105 L106 G107 N108 V109 L110 V111 C112 V113 L114 A115 H116 H117 F118 G119 K120

E121 F122 T123 P124 P125 V126 Q127 A128 A129 Y130 Q131 K132 V133 V134 A135 G136 V137 A138 N139 A140 L141 A142 H143 K144 Y145 H146

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

Chain H: •　12%　　　　　51%　　　　　36%

V1 H2 L3 T4 P5 V6 E7 K8 S9 A10 V11 T12 A13 L14 W15 G16 K17 V18 N19 V20 D21 E22 V23 G24 G25 E26 A27 L28 G29 R30 L31 L32 V33 V34 Y35 P36 W37 T38 Q39 R40 F41 F42 E43 S44 F45 G46 D47 L48 S49 T50 P51 D52 A53 V54 M55 G56 N57 P58 K59 V60

K61 A62 H63 G64 K65 K66 V67 L68 G69 A70 F71 S72 D73 G74 L75 A76 H77 L78 D79 N80 L81 K82 G83 T84 F85 A86 T87 L88 S89 E90 L91 H92 C93 D94 K95 L96 H97 V98 D99 P100 E101 N102 F103 R104 L105 L106 G107 N108 V109 L110 V111 C112 V113 L114 A115 H116 H117 F118 G119 K120

E121 F122 T123 P124 P125 V126 Q127 A128 A129 Y130 Q131 K132 V133 V134 A135 G136 V137 A138 N139 A140 L141 A142 H143 K144 Y145 H146

4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.33Å 185.66Å 52.97Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.254 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9104	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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	4.15	213/1097 (19.4%)	5.92	486/1491 (32.6%)
1	C	4.30	232/1097 (21.1%)	6.41	521/1491 (34.9%)
1	E	3.93	195/1097 (17.8%)	7.24	524/1491 (35.1%)
1	G	4.08	213/1097 (19.4%)	6.34	533/1491 (35.7%)
2	B	4.12	214/1151 (18.6%)	6.08	512/1564 (32.7%)
2	D	4.35	252/1151 (21.9%)	5.80	499/1564 (31.9%)
2	F	4.23	224/1151 (19.5%)	6.33	516/1564 (33.0%)
2	H	3.98	200/1151 (17.4%)	6.16	548/1564 (35.0%)
All	All	4.14	1743/8992 (19.4%)	6.29	4139/12220 (33.9%)

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	1	0
1	C	0	1
2	F	0	2
All	All	1	3

The worst 5 of 1743 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	GLU	CD-OE2	32.40	1.61	1.25
2	D	26	GLU	CD-OE2	25.33	1.53	1.25
2	B	38	THR	C-O	21.93	1.65	1.23
2	D	90	GLU	CD-OE2	21.93	1.49	1.25
2	D	26	GLU	CD-OE1	-21.33	1.02	1.25

The worst 5 of 4139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	31	ARG	NE-CZ-NH1	103.78	172.19	120.30
1	E	31	ARG	NE-CZ-NH2	-80.58	80.01	120.30
1	G	141	ARG	NE-CZ-NH2	-63.78	88.41	120.30
1	E	42	TYR	CB-CG-CD2	60.94	157.56	121.00
2	F	30	ARG	NE-CZ-NH1	-54.59	93.01	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	20	HIS	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	141	ARG	Sidechain
2	F	23	VAL	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	1069	0	1048	329	0
1	C	1069	0	1035	398	3
1	E	1069	0	1048	334	0
1	G	1069	0	1044	405	0
2	B	1121	0	1100	378	0
2	D	1121	0	1091	467	3
2	F	1121	0	1094	354	3
2	H	1121	0	1091	438	0
3	A	43	0	30	23	0
3	B	43	0	30	14	0
3	C	43	0	30	15	0
3	D	43	0	30	25	0
3	E	43	0	30	24	0
3	F	43	0	30	16	1
3	G	43	0	30	21	0
3	H	43	0	30	7	0
All	All	9104	0	8791	3010	5

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 168.

The worst 5 of 3010 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:CA	1:A:76:MET:CB	1.76	1.64
2:D:104:ARG:CB	2:D:104:ARG:CG	1.74	1.64
2:F:29:GLY:HA3	2:F:55:MET:SD	1.32	1.64
2:H:14:LEU:CD2	2:H:14:LEU:CG	1.76	1.63
1:G:32:MET:CA	1:G:32:MET:CB	1.75	1.62

All (5) 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:C:53:ALA:CB	2:F:43:GLU:O[1_454]	1.28	0.92
2:D:6:VAL:CG2	2:F:73:ASP:OD2[1_455]	1.92	0.28
1:C:54:GLN:OE1	2:F:46:GLY:CA[1_454]	1.94	0.26
1:C:85:ASP:OD2	2:D:83:GLY:O[1_554]	2.00	0.20
2:D:9:SER:OG	3:F:147:HEM:O2A[1_455]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	121 (87%)	15 (11%)	3 (2%)	6	31
1	C	139/141 (99%)	116 (84%)	13 (9%)	10 (7%)	1	5
1	E	139/141 (99%)	113 (81%)	20 (14%)	6 (4%)	2	15
1	G	139/141 (99%)	105 (76%)	24 (17%)	10 (7%)	1	5
2	B	144/146 (99%)	120 (83%)	23 (16%)	1 (1%)	22	60
2	D	144/146 (99%)	120 (83%)	17 (12%)	7 (5%)	2	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	144/146 (99%)	123 (85%)	14 (10%)	7 (5%)	2	13
2	H	144/146 (99%)	114 (79%)	22 (15%)	8 (6%)	2	10
All	All	1132/1148 (99%)	932 (82%)	148 (13%)	52 (5%)	2	14

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	C	73	VAL
2	D	11	VAL
2	D	40	ARG
2	D	54	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	113/113 (100%)	84 (74%)	29 (26%)	0	3
1	C	113/113 (100%)	66 (58%)	47 (42%)	0	0
1	E	113/113 (100%)	69 (61%)	44 (39%)	0	0
1	G	113/113 (100%)	67 (59%)	46 (41%)	0	0
2	B	118/118 (100%)	73 (62%)	45 (38%)	0	0
2	D	118/118 (100%)	82 (70%)	36 (30%)	0	1
2	F	118/118 (100%)	81 (69%)	37 (31%)	0	1
2	H	118/118 (100%)	63 (53%)	55 (47%)	0	0
All	All	924/924 (100%)	585 (63%)	339 (37%)	0	1

5 of 339 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	112	CYS
2	H	8	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	1	VAL
1	G	76	MET
2	H	44	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	72	HIS
2	H	139	ASN
1	G	97	ASN
2	H	63	HIS
1	C	72	HIS

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 ⓘ

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	$\#|Z| > 2$
3	HEM	H	147	-	41,50,50	3.40	21 (51%)	45,82,82	5.18	30 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	HEM	A	142	1	41,50,50	3.35	16 (39%)	45,82,82	5.57	27 (60%)
3	HEM	G	142	-	41,50,50	3.74	22 (53%)	45,82,82	4.21	27 (60%)
3	HEM	C	142	1	41,50,50	3.08	22 (53%)	45,82,82	4.51	30 (66%)
3	HEM	E	142	1	41,50,50	3.48	21 (51%)	45,82,82	4.80	33 (73%)
3	HEM	B	147	2	41,50,50	4.37	32 (78%)	45,82,82	5.08	31 (68%)
3	HEM	F	147	2	41,50,50	3.52	20 (48%)	45,82,82	4.63	32 (71%)
3	HEM	D	147	2	41,50,50	2.73	20 (48%)	45,82,82	4.36	29 (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	H	147	-	-	8/12/54/54	-
3	HEM	A	142	1	-	4/12/54/54	-
3	HEM	G	142	-	-	3/12/54/54	-
3	HEM	C	142	1	-	4/12/54/54	-
3	HEM	E	142	1	-	3/12/54/54	-
3	HEM	B	147	2	-	5/12/54/54	-
3	HEM	F	147	2	-	5/12/54/54	-
3	HEM	D	147	2	-	5/12/54/54	-

The worst 5 of 174 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	C3C-C2C	-15.51	1.18	1.40
3	G	142	HEM	C3C-C2C	14.14	1.60	1.40
3	F	147	HEM	CBD-CGD	10.07	1.74	1.50
3	D	147	HEM	C4D-C3D	9.94	1.62	1.45
3	B	147	HEM	CAA-C2A	9.35	1.65	1.52

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	147	HEM	CHA-C4D-ND	15.22	143.19	124.38
3	A	142	HEM	CBA-CAA-C2A	15.06	138.31	112.62
3	H	147	HEM	O2A-CGA-O1A	14.68	159.90	123.30
3	F	147	HEM	CHC-C4B-NB	14.59	140.28	124.43

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	142	HEM	CMA-C3A-C4A	14.45	150.68	128.46

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	147	HEM	C1A-C2A-CAA-CBA
3	B	147	HEM	C3A-C2A-CAA-CBA
3	D	147	HEM	C3A-C2A-CAA-CBA
3	F	147	HEM	C2B-C3B-CAB-CBB
3	F	147	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

8 monomers are involved in 146 short contacts:

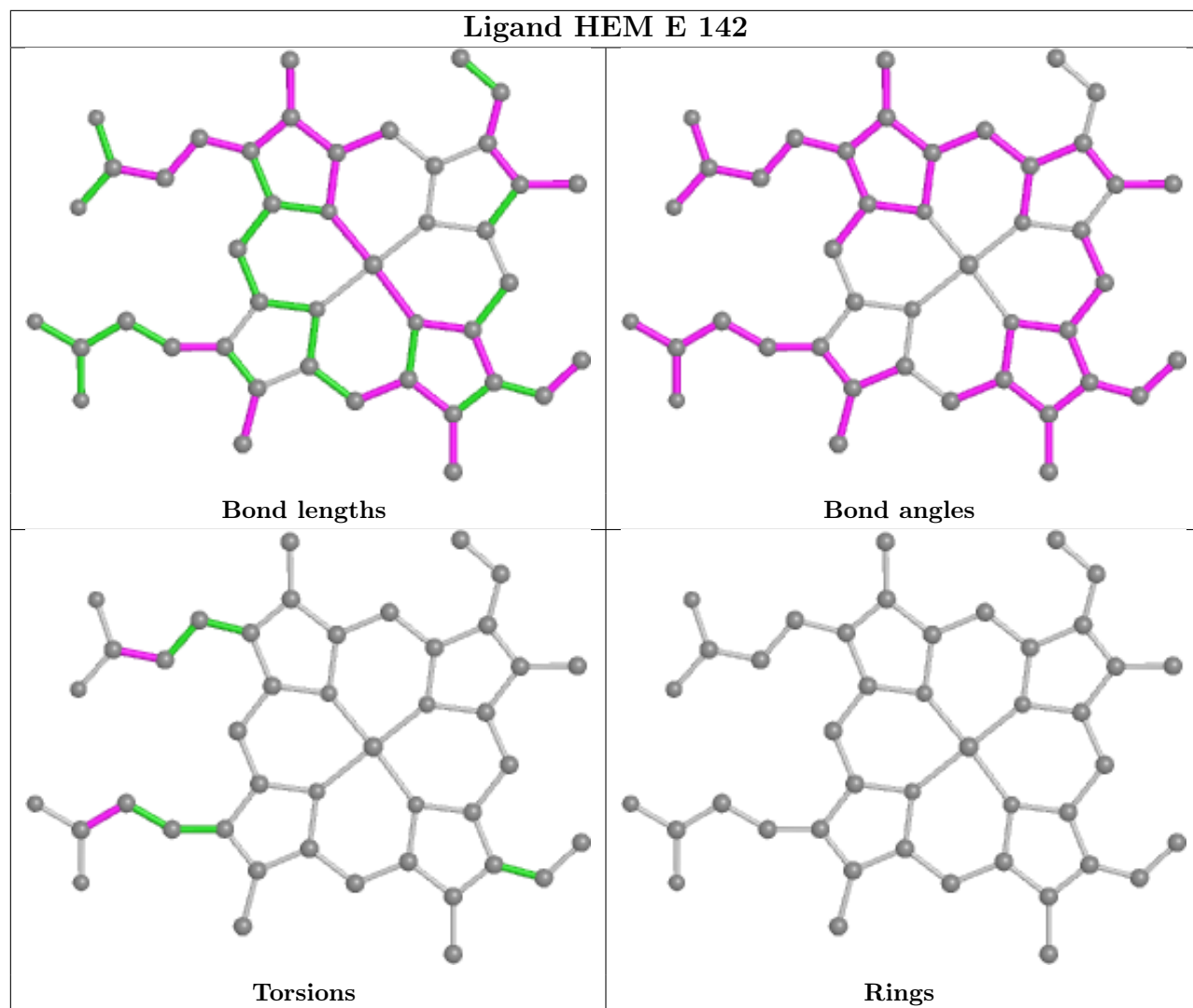| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	147	HEM	7	0
3	A	142	HEM	23	0
3	G	142	HEM	21	0
3	C	142	HEM	15	0
3	E	142	HEM	24	0
3	B	147	HEM	14	0
3	F	147	HEM	16	1
3	D	147	HEM	25	0

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.
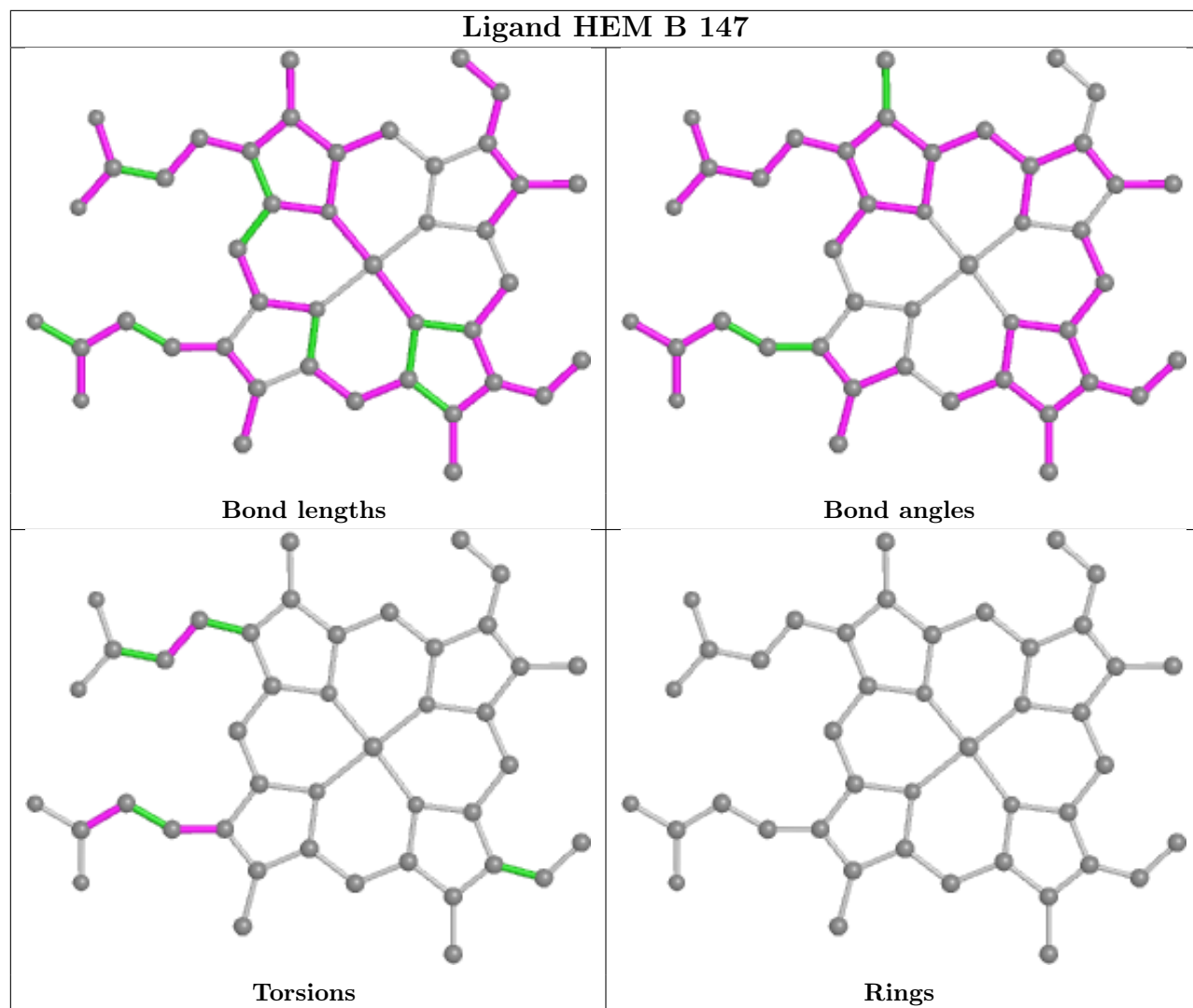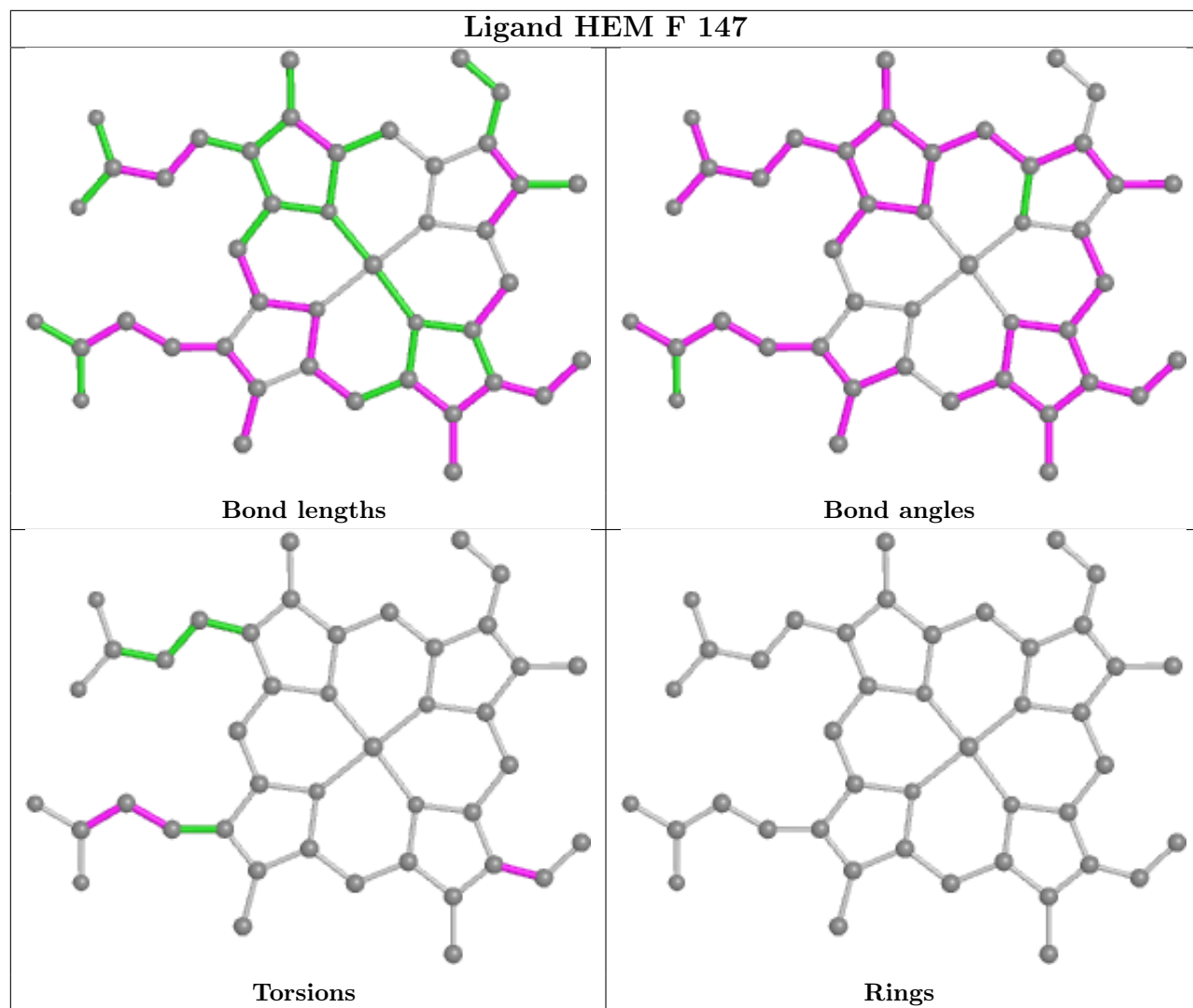
Ligand HEM H 147

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 142

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM G 142

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 142

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 142

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 147

Bond lengths

Bond angles

Torsions

Rings

wwPDB X-ray Structure Validation Summary Report

Ligand HEM F 147

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 147
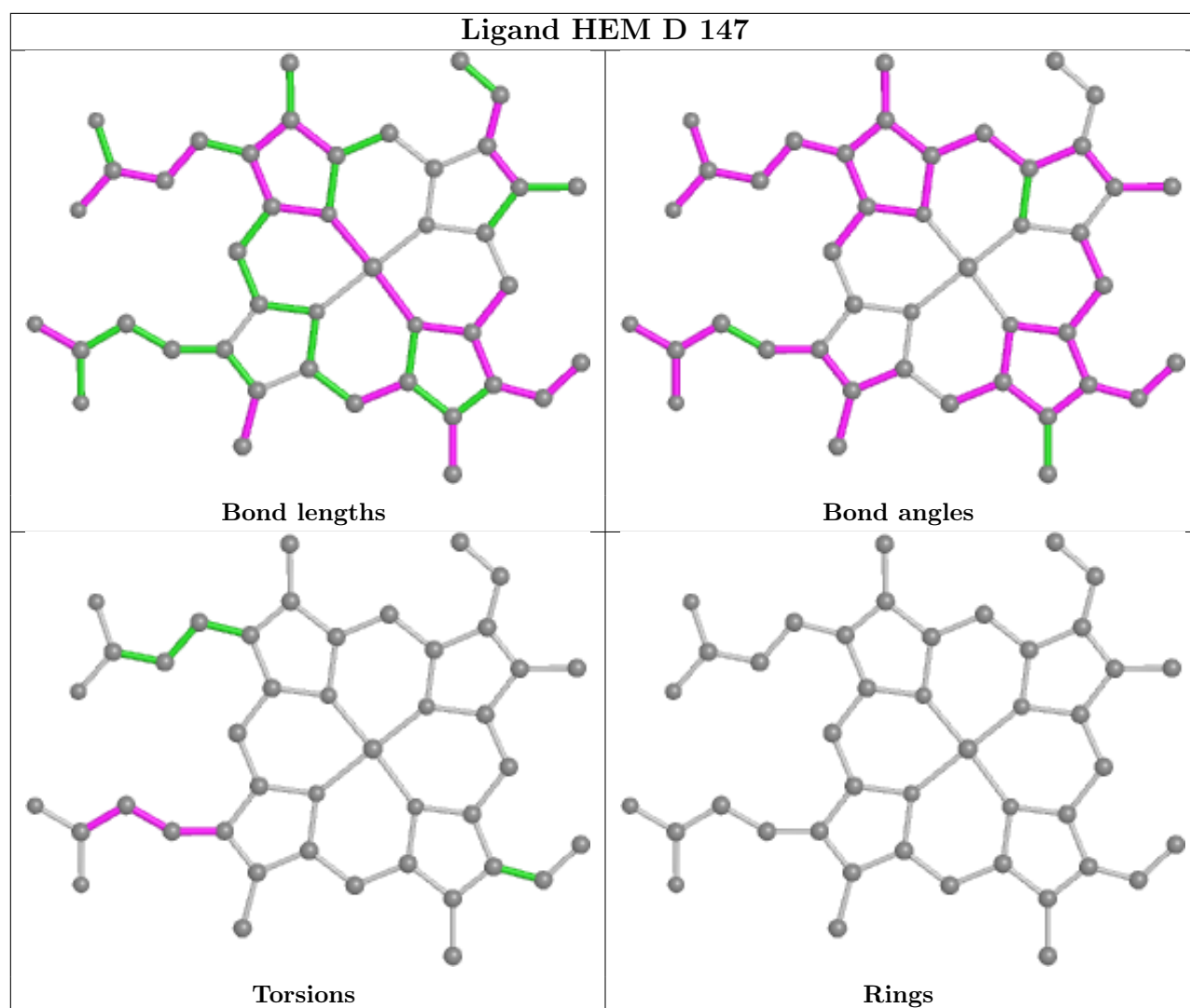
Bond lengths

Bond angles

Torsions

Rings

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
1	A	12
2	D	12
1	C	12
2	F	11
1	G	11
1	E	10

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
2	H	10
2	B	2

The worst 5 of 80 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	125:LEU	C	126:ASP	N	1.62
1	F	145:TYR	C	146:HIS	N	1.62
1	D	129:ALA	C	130:TYR	N	1.61
1	C	37:PRO	C	38:THR	N	1.20
1	C	135:VAL	C	136:LEU	N	1.20

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.