



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:41 AM UTC

PDB ID : 1A00 / pdb_00001a00
Title : HEMOGLOBIN (VAL BETA1 MET, TRP BETA37 TYR) MUTANT
Authors : Kavanaugh, J.S.; Arnone, A.
Deposited on : 1997-12-08
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

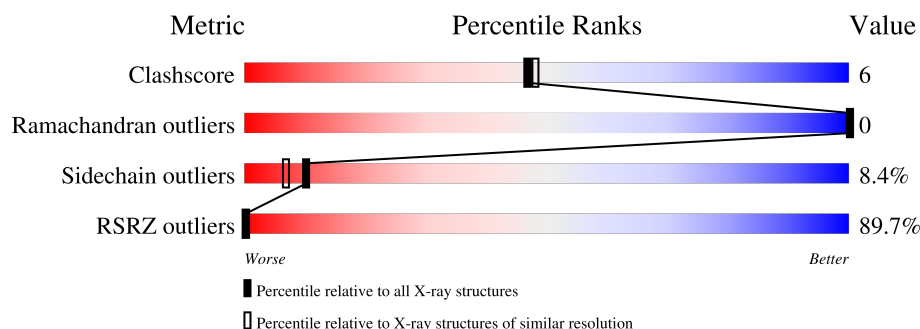
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	141	94% 74% 22% .
1	C	141	83% 82% 14% ..
2	B	146	88% 75% 20% ..
2	D	146	95% 73% 22% 5%.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4770 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	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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1122	722	194	202	4			
2	D	146	Total	C	N	O	S	0	0	0
			1122	722	194	202	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	TYR	TRP	engineered mutation	UNP P68871
D	37	TYR	TRP	engineered mutation	UNP P68871

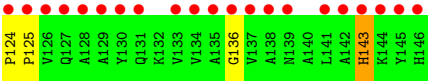
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



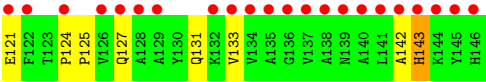
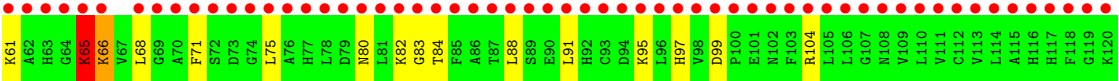
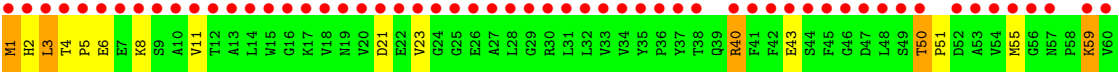
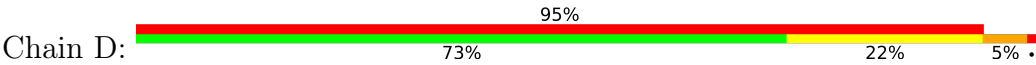
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	52	Total O 52 52	0	0
4	B	52	Total O 52 52	0	0
4	C	66	Total O 66 66	0	0
4	D	46	Total O 46 46	0	0



● Molecule 2: HEMOGLOBIN (BETA CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.10Å 112.00Å 63.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (8.00-2.00) 90.7 (8.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.73Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , 0.223 0.531 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.955	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 177.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.37	EDS
Total number of atoms	4770	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.05	0/1097	1.82	21/1491 (1.4%)
1	C	1.06	0/1097	1.81	14/1491 (0.9%)
2	B	1.04	0/1151	1.84	19/1561 (1.2%)
2	D	1.04	0/1151	1.86	22/1561 (1.4%)
All	All	1.05	0/4496	1.83	76/6104 (1.2%)

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
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	HIS	CA-CB-CG	-10.54	103.25	113.80
1	C	92	ARG	NE-CZ-NH2	-10.31	109.92	119.20
1	C	78	ASN	CA-CB-CG	-9.21	103.39	112.60
2	B	143	HIS	CA-CB-CG	-8.73	105.07	113.80
2	D	66	LYS	CA-CB-CG	8.09	130.29	114.10
1	A	6	ASP	O-C-N	7.66	129.96	122.07
2	B	77	HIS	CA-CB-CG	-7.62	106.18	113.80
1	A	72	HIS	CA-CB-CG	-7.43	106.37	113.80
2	B	92	HIS	CA-CB-CG	-7.29	106.51	113.80
1	C	99	LYS	CB-CA-C	7.29	124.67	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	97	HIS	CA-CB-CG	-7.20	106.60	113.80
2	B	43	GLU	CB-CG-CD	7.03	124.54	112.60
2	D	65	LYS	CA-C-N	6.93	129.79	120.65
2	D	65	LYS	C-N-CA	6.93	129.79	120.65
1	A	20	HIS	CA-CB-CG	-6.76	107.04	113.80
1	C	72	HIS	CA-CB-CG	-6.74	107.06	113.80
1	C	47	ASP	O-C-N	6.67	130.94	122.93
1	A	47	ASP	N-CA-C	-6.62	98.40	108.67
1	A	14	TRP	CA-C-N	6.61	127.28	119.94
1	A	14	TRP	C-N-CA	6.61	127.28	119.94
2	B	117	HIS	N-CA-C	6.59	118.26	111.14
1	A	107	VAL	O-C-N	6.52	128.30	121.91
2	D	40	ARG	CD-NE-CZ	6.51	133.51	124.40
2	B	20	VAL	CA-C-O	6.50	128.03	121.27
1	A	21	ALA	CA-C-N	6.49	128.25	120.14
1	A	21	ALA	C-N-CA	6.49	128.25	120.14
2	B	12	THR	CA-CB-OG1	-6.27	100.19	109.60
1	C	99	LYS	CA-CB-CG	6.27	126.64	114.10
2	B	6	GLU	CA-CB-CG	6.25	126.59	114.10
1	A	108	THR	CA-C-N	6.14	128.43	120.44
1	A	108	THR	C-N-CA	6.14	128.43	120.44
1	A	89	HIS	CA-CB-CG	-6.06	107.74	113.80
1	C	122	HIS	CA-CB-CG	6.06	119.86	113.80
2	B	143	HIS	N-CA-C	6.04	118.63	111.33
1	C	47	ASP	CA-C-O	-5.89	114.28	120.58
1	A	47	ASP	CA-C-O	-5.85	113.99	120.60
1	C	117	PHE	CA-CB-CG	5.72	119.52	113.80
1	A	23	GLU	CA-CB-CG	5.71	125.52	114.10
1	A	83	LEU	O-C-N	5.69	128.64	122.15
1	C	47	ASP	N-CA-C	-5.66	99.29	108.41
2	B	19	ASN	CA-CB-CG	5.66	118.26	112.60
2	B	22	GLU	CB-CG-CD	5.66	122.22	112.60
2	D	142	ALA	CA-C-N	5.64	128.11	120.38
2	D	142	ALA	C-N-CA	5.64	128.11	120.38
2	D	2	HIS	N-CA-CB	5.56	119.88	110.49
2	D	99	ASP	CA-C-N	5.56	125.27	119.82
2	D	99	ASP	C-N-CA	5.56	125.27	119.82
2	D	143	HIS	CA-CB-CG	-5.55	108.25	113.80
2	D	71	PHE	CA-C-N	5.53	128.00	120.54
2	D	71	PHE	C-N-CA	5.53	128.00	120.54
1	A	83	LEU	CA-C-O	-5.51	114.57	120.42
1	C	92	ARG	NH1-CZ-NH2	5.47	126.41	119.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	HIS	CA-C-O	-5.42	112.94	118.90
1	A	75	ASP	CA-CB-CG	-5.42	107.18	112.60
2	B	42	PHE	N-CA-CB	-5.37	103.56	111.51
1	A	108	THR	CA-CB-OG1	-5.36	101.55	109.60
2	D	121	GLU	CB-CG-CD	5.28	121.58	112.60
2	D	143	HIS	N-CA-C	5.26	117.69	111.33
1	C	58	HIS	CA-CB-CG	-5.24	108.56	113.80
2	B	116	HIS	CA-C-N	5.21	127.53	120.44
2	B	116	HIS	C-N-CA	5.21	127.53	120.44
2	D	23	VAL	N-CA-C	5.19	115.96	110.72
2	D	40	ARG	NE-CZ-NH1	5.19	126.69	121.50
2	B	89	SER	N-CA-CB	5.18	117.53	110.01
2	B	115	ALA	CA-C-N	5.18	127.53	120.54
2	B	115	ALA	C-N-CA	5.18	127.53	120.54
2	B	99	ASP	CA-CB-CG	5.17	117.77	112.60
1	C	3	SER	N-CA-C	-5.17	104.19	110.13
1	C	1	VAL	CG1-CB-CG2	5.13	122.10	110.80
2	D	84	THR	CA-CB-CG2	5.10	119.18	110.50
2	D	50	THR	O-C-N	5.09	127.17	121.32
1	A	131	SER	O-C-N	5.09	127.95	122.15
1	A	36	PHE	O-C-N	5.09	125.95	121.37
2	D	11	VAL	CA-C-O	5.08	126.56	121.17
2	D	59	LYS	N-CA-C	-5.02	105.89	111.36
2	B	6	GLU	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	104	ARG	Sidechain
2	D	40	ARG	Sidechain

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	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1069	0	1073	10	0
2	B	1122	0	1117	12	0
2	D	1122	0	1117	15	0
3	A	43	0	30	0	0
3	B	43	0	30	3	0
3	C	43	0	30	0	0
3	D	43	0	30	2	0
4	A	52	0	0	1	0
4	B	52	0	0	0	0
4	C	66	0	0	0	0
4	D	46	0	0	1	0
All	All	4770	0	4500	52	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 6.

All (52) 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)
3:B:147:HEM:HMC2	3:B:147:HEM:HBC2	1.42	1.01
2:D:1:MET:HE1	2:D:133:VAL:HA	1.63	0.80
3:D:147:HEM:HBC2	3:D:147:HEM:HMC2	1.69	0.73
3:B:147:HEM:HBC2	3:B:147:HEM:CMC	2.20	0.66
1:A:96:VAL:O	1:A:99:LYS:HG2	1.96	0.66
2:D:124:PRO:HB2	2:D:125:PRO:HD3	1.80	0.63
1:C:49:SER:O	1:C:52:SER:HB3	2.03	0.58
1:A:96:VAL:HB	1:A:99:LYS:NZ	2.18	0.57
2:B:51:PRO:O	2:B:55:MET:HG2	2.07	0.55
2:B:6:GLU:H	2:B:6:GLU:CD	2.15	0.55
2:B:1:MET:HG3	2:B:136:GLY:HA3	1.88	0.55
1:A:75:ASP:OD2	1:A:78:ASN:HB2	2.07	0.54
2:D:80:ASN:ND2	2:D:83:GLY:HA3	2.22	0.54
1:C:35:SER:HB3	2:D:131:GLN:HG3	1.89	0.54
2:D:143:HIS:HB3	4:D:414:HOH:O	2.07	0.53
2:B:124:PRO:HB2	2:B:125:PRO:HD3	1.89	0.53
1:A:51:GLY:O	1:A:52:SER:C	2.51	0.52
1:A:13:ALA:O	1:A:17:VAL:HG23	2.10	0.51
1:C:90:LYS:NZ	1:C:90:LYS:HB3	2.26	0.50
1:A:76:MET:N	1:A:77:PRO:CD	2.75	0.50
2:D:91:LEU:HD12	2:D:95:LYS:HB2	1.94	0.49
1:C:3:SER:HB2	1:C:4:PRO:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LYS:O	1:C:92:ARG:HD3	2.13	0.49
1:A:3:SER:O	1:A:7:LYS:HG3	2.13	0.48
1:C:3:SER:HB2	1:C:4:PRO:CD	2.44	0.47
2:B:86:ALA:O	2:B:90:GLU:HG3	2.14	0.47
2:B:82:LYS:HE3	2:B:143:HIS:CD2	2.50	0.46
2:D:50:THR:HB	2:D:51:PRO:HD2	1.98	0.46
1:A:16:LYS:HG3	1:A:116:GLU:HG2	1.97	0.45
2:D:88:LEU:HD21	3:D:147:HEM:HMA3	1.97	0.45
2:D:1:MET:HE3	2:D:3:LEU:HD21	1.99	0.44
1:A:113:LEU:HB3	1:A:116:GLU:HB2	1.99	0.44
2:D:51:PRO:O	2:D:55:MET:HG2	2.18	0.44
2:B:3:LEU:HA	2:B:7:GLU:OE1	2.18	0.44
2:D:88:LEU:HD23	2:D:91:LEU:HD23	2.00	0.43
2:D:3:LEU:HD23	2:D:3:LEU:N	2.33	0.43
2:B:18:VAL:HG13	2:B:23:VAL:HG21	2.00	0.43
2:B:95:LYS:HA	2:B:95:LYS:HD3	1.72	0.43
1:A:21:ALA:HB1	1:A:63:ALA:HB1	2.01	0.43
1:C:31:ARG:HD3	2:D:127:GLN:OE1	2.19	0.43
2:B:1:MET:HE3	2:B:1:MET:HB3	1.87	0.42
2:D:21:ASP:HA	2:D:65:LYS:HG3	2.00	0.42
1:C:20:HIS:HB3	1:C:24:TYR:CE1	2.55	0.42
1:C:17:VAL:HG13	1:C:24:TYR:CD2	2.55	0.42
2:D:4:THR:HB	2:D:5:PRO:HD2	2.02	0.41
1:C:43:PHE:N	1:C:44:PRO:CD	2.84	0.41
1:A:49:SER:O	1:A:52:SER:HB3	2.21	0.41
1:A:76:MET:HB2	1:A:77:PRO:HD3	2.03	0.41
1:A:96:VAL:HB	1:A:99:LYS:HZ3	1.85	0.41
1:A:4:PRO:HD2	4:A:308:HOH:O	2.21	0.40
2:B:96:LEU:HD13	3:B:147:HEM:C3D	2.57	0.40
2:B:57:ASN:HA	2:B:58:PRO:HD3	1.75	0.40

There are no symmetry-related clashes.

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%)	135 (97%)	4 (3%)	0	100	100
1	C	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
2	B	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
All	All	566/574 (99%)	554 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	106 (94%)	7 (6%)	16	13
1	C	113/113 (100%)	103 (91%)	10 (9%)	9	6
2	B	118/118 (100%)	109 (92%)	9 (8%)	12	9
2	D	118/118 (100%)	105 (89%)	13 (11%)	6	3
All	All	462/462 (100%)	423 (92%)	39 (8%)	10	7

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	7	LYS
1	A	16	LYS
1	A	52	SER
1	A	56	LYS
1	A	90	LYS
1	A	109	LEU
2	B	1	MET
2	B	6	GLU
2	B	12	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	20	VAL
2	B	22	GLU
2	B	26	GLU
2	B	32	LEU
2	B	68	LEU
2	B	104	ARG
1	C	1	VAL
1	C	16	LYS
1	C	52	SER
1	C	56	LYS
1	C	61	LYS
1	C	85	ASP
1	C	90	LYS
1	C	92	ARG
1	C	99	LYS
1	C	105	LEU
2	D	1	MET
2	D	3	LEU
2	D	6	GLU
2	D	8	LYS
2	D	43	GLU
2	D	59	LYS
2	D	61	LYS
2	D	65	LYS
2	D	66	LYS
2	D	68	LEU
2	D	75	LEU
2	D	82	LYS
2	D	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	68	ASN
2	B	63	HIS
2	B	139	ASN
2	D	77	HIS
2	D	80	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	D	147	2	50,50,50	1.47	11 (22%)	67,82,82	0.97	3 (4%)
3	HEM	B	147	2	50,50,50	1.50	12 (24%)	67,82,82	1.20	7 (10%)
3	HEM	A	142	1	50,50,50	1.43	9 (18%)	67,82,82	1.25	5 (7%)
3	HEM	C	142	1	50,50,50	1.35	7 (14%)	67,82,82	1.17	7 (10%)

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	D	147	2	-	4/14/54/54	-
3	HEM	B	147	2	-	4/14/54/54	-
3	HEM	A	142	1	-	3/14/54/54	-
3	HEM	C	142	1	-	6/14/54/54	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	FE-NB	3.82	2.06	1.94
3	A	142	HEM	FE-NA	3.79	2.07	1.95
3	A	142	HEM	FE-NC	3.55	2.06	1.95
3	D	147	HEM	FE-NC	3.44	2.06	1.95
3	C	142	HEM	FE-NA	3.24	2.05	1.95
3	A	142	HEM	FE-ND	3.21	2.04	1.94
3	B	147	HEM	FE-NC	3.16	2.05	1.95
3	B	147	HEM	CAC-C3C	3.11	1.55	1.47
3	D	147	HEM	CAB-C3B	3.10	1.55	1.47
3	C	142	HEM	CAC-C3C	3.00	1.55	1.47
3	C	142	HEM	FE-ND	2.95	2.04	1.94
3	D	147	HEM	CMA-C3A	2.86	1.56	1.50
3	D	147	HEM	FE-NB	2.84	2.03	1.94
3	B	147	HEM	CMC-C2C	2.80	1.56	1.50
3	D	147	HEM	CAC-C3C	2.78	1.54	1.47
3	D	147	HEM	CMB-C2B	2.76	1.56	1.50
3	A	142	HEM	FE-NB	2.69	2.03	1.94
3	C	142	HEM	CAB-C3B	2.65	1.54	1.47
3	C	142	HEM	FE-NC	2.56	2.03	1.95
3	B	147	HEM	CMA-C3A	2.49	1.55	1.50
3	B	147	HEM	FE-NA	2.47	2.03	1.95
3	A	142	HEM	CAB-C3B	2.47	1.54	1.47
3	C	142	HEM	FE-NB	2.42	2.02	1.94
3	A	142	HEM	CAC-C3C	2.41	1.53	1.47
3	D	147	HEM	FE-ND	2.34	2.02	1.94
3	B	147	HEM	FE-ND	2.24	2.01	1.94
3	B	147	HEM	CAB-C3B	2.21	1.53	1.47
3	A	142	HEM	CMB-C2B	2.21	1.55	1.50
3	B	147	HEM	CMB-C2B	2.19	1.55	1.50
3	A	142	HEM	C2A-C3A	-2.16	1.33	1.38
3	B	147	HEM	CAA-C2A	2.15	1.56	1.51
3	D	147	HEM	CMD-C2D	2.13	1.55	1.50
3	B	147	HEM	C2A-C3A	-2.13	1.33	1.38
3	D	147	HEM	C3D-C2D	-2.07	1.32	1.36
3	A	142	HEM	CMA-C3A	2.06	1.55	1.50
3	C	142	HEM	O2D-CGD	-2.04	1.24	1.30
3	D	147	HEM	C2A-C3A	-2.02	1.33	1.38
3	D	147	HEM	FE-NA	2.02	2.01	1.95
3	B	147	HEM	CMD-C2D	2.01	1.54	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	CHB-C1B-NB	3.34	128.49	124.37
3	A	142	HEM	CHD-C1D-ND	2.93	127.57	124.42
3	A	142	HEM	CBA-CAA-C2A	2.90	120.56	112.53
3	B	147	HEM	O1D-CGD-CBD	-2.77	114.30	123.09
3	C	142	HEM	CHD-C4C-NC	2.69	127.38	124.45
3	A	142	HEM	C4A-CHB-C1B	-2.45	120.48	126.25
3	C	142	HEM	CMA-C3A-C2A	2.43	130.78	125.62
3	D	147	HEM	O2D-CGD-O1D	2.43	129.59	123.33
3	B	147	HEM	C3D-C4D-ND	-2.37	107.57	110.17
3	D	147	HEM	O1D-CGD-CBD	-2.35	115.62	123.09
3	C	142	HEM	O1A-CGA-CBA	-2.35	115.64	123.09
3	B	147	HEM	CHD-C1D-ND	2.30	126.90	124.42
3	B	147	HEM	CBC-CAC-C3C	-2.27	116.17	127.53
3	C	142	HEM	O1D-CGD-CBD	-2.27	115.89	123.09
3	A	142	HEM	CHB-C4A-NA	2.27	127.97	123.86
3	B	147	HEM	CHB-C4A-NA	2.26	127.96	123.86
3	B	147	HEM	O1A-CGA-CBA	-2.25	115.97	123.09
3	C	142	HEM	O2A-CGA-O1A	2.23	129.06	123.33
3	B	147	HEM	C4C-C3C-C2C	2.16	108.68	106.81
3	C	142	HEM	CHD-C1D-ND	2.13	126.71	124.42
3	C	142	HEM	CMA-C3A-C4A	-2.12	122.20	125.42
3	D	147	HEM	CBB-CAB-C3B	-2.10	117.03	127.53

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	142	HEM	C2B-C3B-CAB-CBB
3	C	142	HEM	C4B-C3B-CAB-CBB
3	B	147	HEM	CAA-CBA-CGA-O1A
3	D	147	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAA-CBA-CGA-O1A
3	B	147	HEM	CAA-CBA-CGA-O2A
3	D	147	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAD-CBD-CGD-O2D
3	D	147	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAD-CBD-CGD-O2D
3	D	147	HEM	CAA-CBA-CGA-O2A
3	C	142	HEM	CAA-CBA-CGA-O2A
3	B	147	HEM	C4B-C3B-CAB-CBB
3	A	142	HEM	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

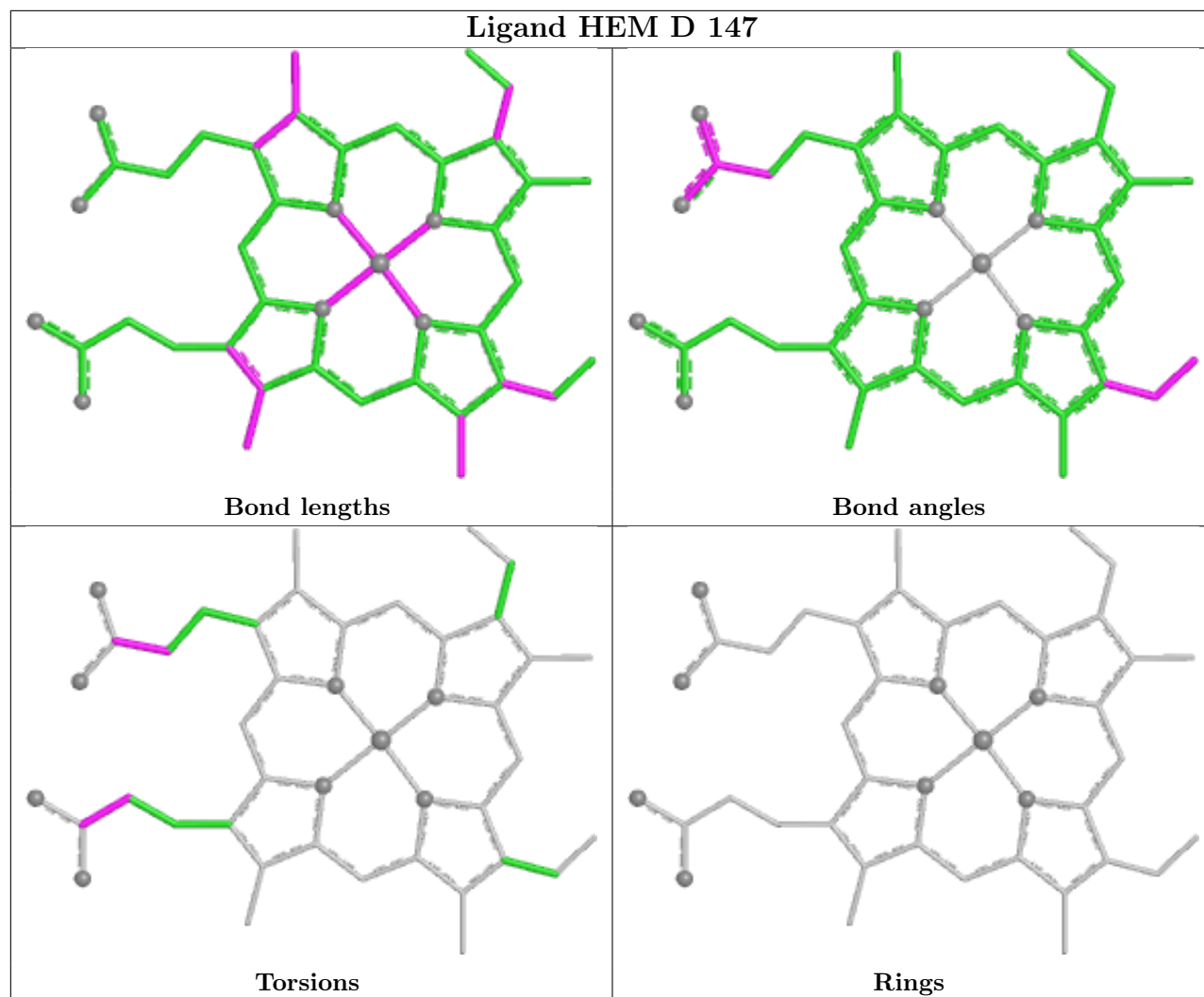
Mol	Chain	Res	Type	Atoms
3	B	147	HEM	C2B-C3B-CAB-CBB

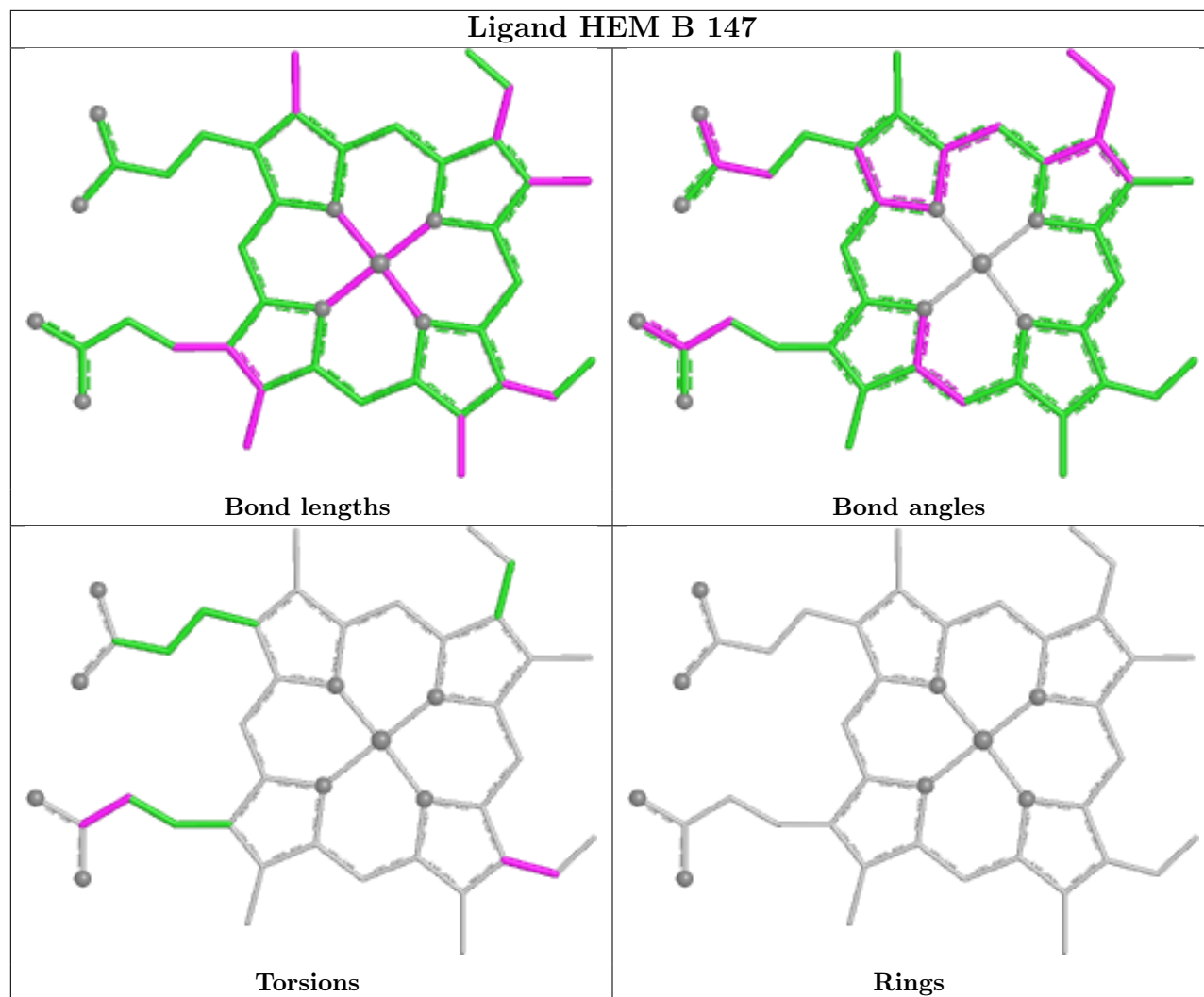
There are no ring outliers.

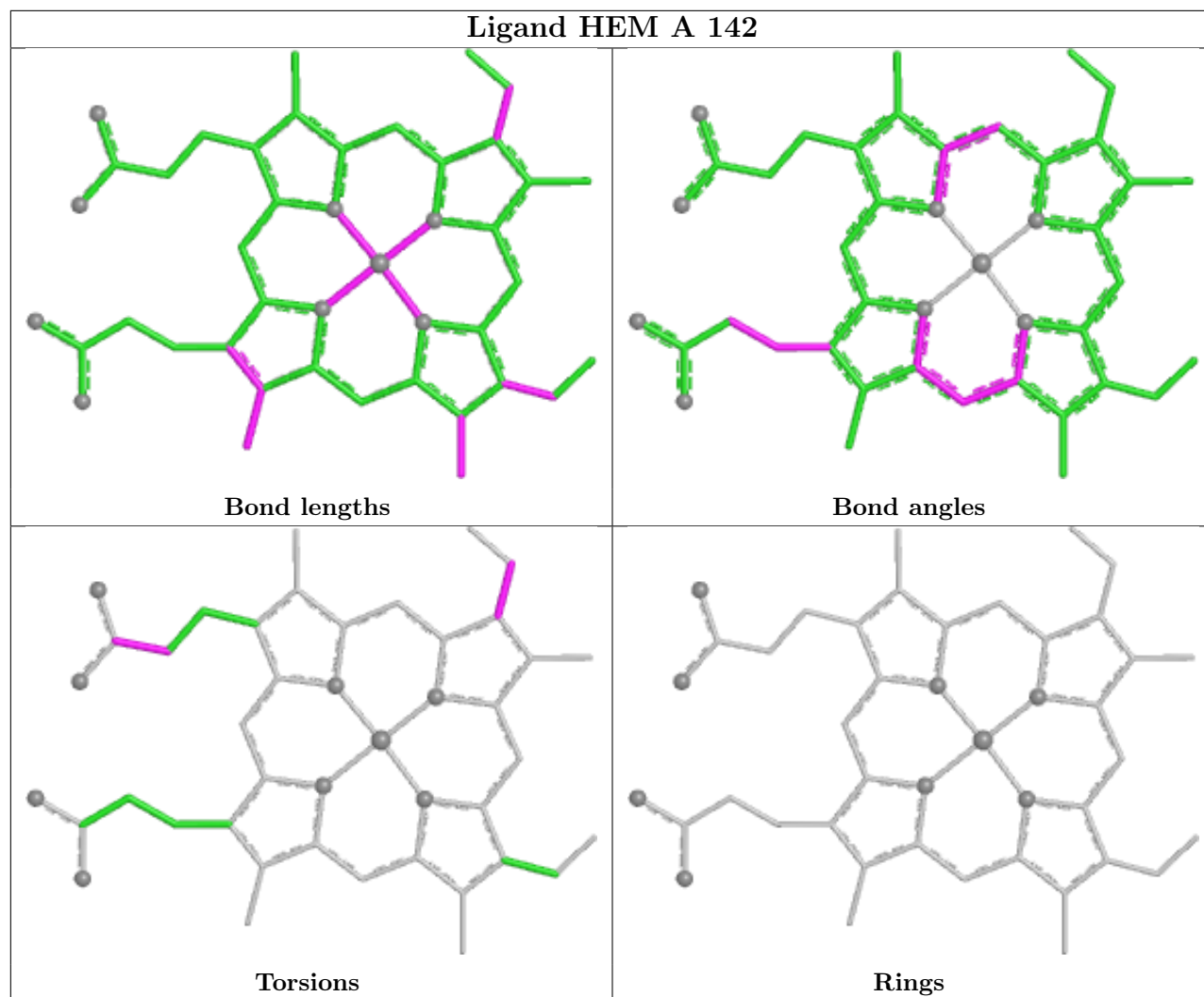
2 monomers are involved in 5 short contacts:

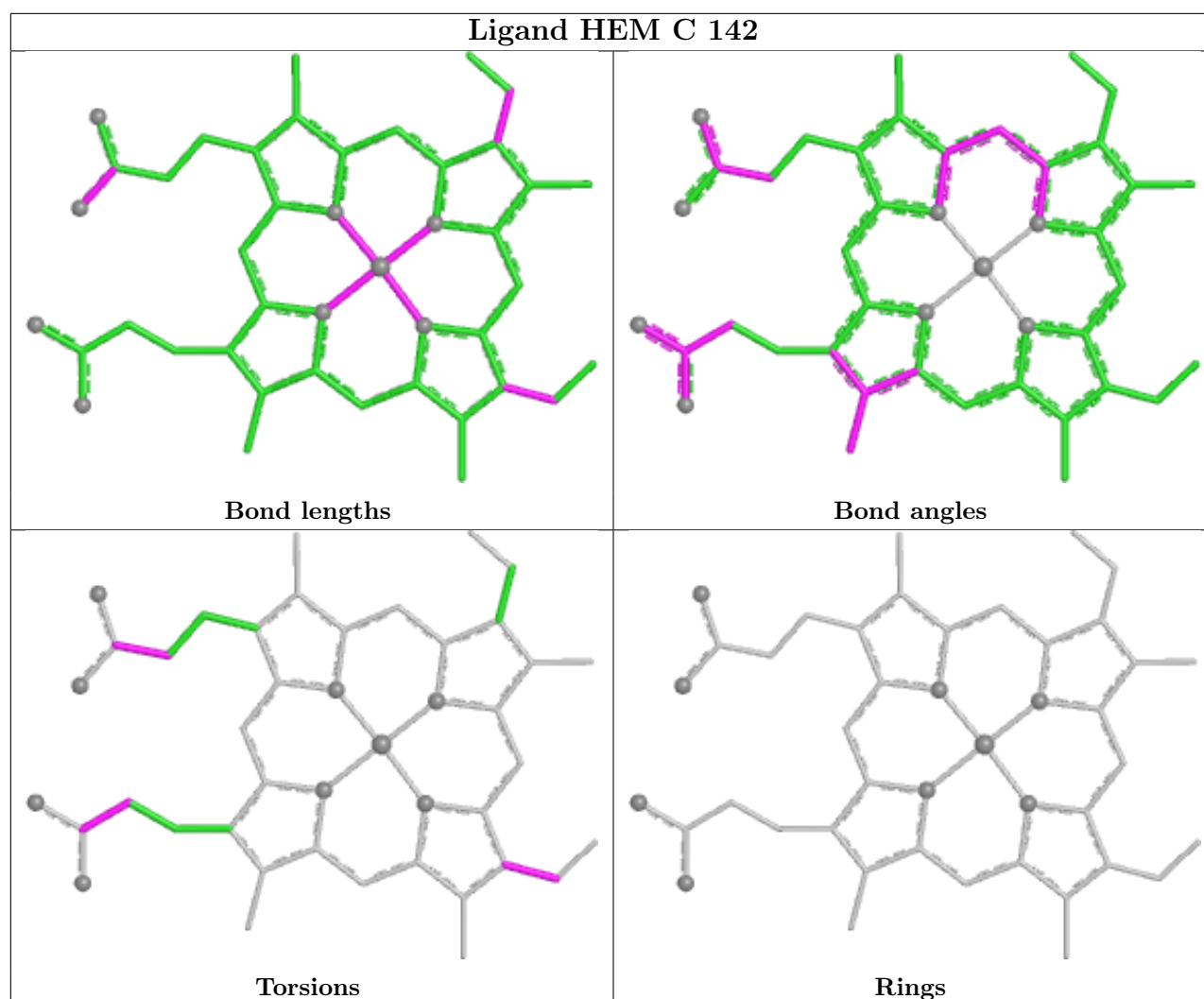
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	147	HEM	2	0
3	B	147	HEM	3	0

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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	141/141 (100%)	3.91	132 (93%) 0 0	8, 18, 45, 58	0
1	C	141/141 (100%)	3.23	117 (82%) 0 0	6, 13, 33, 46	0
2	B	146/146 (100%)	3.61	128 (87%) 0 0	7, 16, 49, 64	0
2	D	146/146 (100%)	4.10	138 (94%) 0 0	8, 19, 48, 103	0
All	All	574/574 (100%)	3.72	515 (89%) 0 0	6, 17, 45, 103	0

All (515) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	37	TYR	10.3
2	D	44	SER	10.2
2	D	93	CYS	9.0
2	D	61	LYS	8.9
2	D	142	ALA	8.9
2	B	69	GLY	8.5
2	B	58	PRO	8.0
1	A	10	VAL	7.7
1	A	47	ASP	7.7
1	A	79	ALA	7.6
1	A	135	VAL	7.5
2	D	9	SER	7.5
1	A	5	ALA	7.4
1	A	19	ALA	7.3
1	A	128	PHE	7.3
2	B	19	ASN	7.3
2	B	2	HIS	7.2
1	C	93	VAL	7.2
1	A	136	LEU	7.1
1	A	96	VAL	7.0
2	D	5	PRO	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	73	VAL	6.8
1	A	51	GLY	6.8
2	D	53	ALA	6.8
2	B	1	MET	6.8
2	D	19	ASN	6.6
2	D	76	ALA	6.6
1	A	46	PHE	6.4
1	C	51	GLY	6.4
2	D	33	VAL	6.4
1	A	50	HIS	6.4
1	C	73	VAL	6.3
1	C	96	VAL	6.3
1	A	52	SER	6.3
2	B	44	SER	6.3
1	A	81	SER	6.3
1	C	140	TYR	6.3
2	B	4	THR	6.2
2	B	125	PRO	6.2
1	A	4	PRO	6.1
2	B	9	SER	6.1
1	A	25	GLY	6.1
1	C	18	GLY	6.1
1	A	117	PHE	6.1
2	B	60	VAL	6.0
1	A	75	ASP	6.0
1	A	78	ASN	6.0
2	D	63	HIS	5.9
2	D	7	GLU	5.9
2	D	84	THR	5.9
2	D	77	HIS	5.9
2	B	137	VAL	5.9
1	A	13	ALA	5.9
1	C	108	THR	5.9
1	A	53	ALA	5.8
2	B	18	VAL	5.8
1	A	105	LEU	5.8
2	B	12	THR	5.8
2	B	33	VAL	5.8
2	D	24	GLY	5.8
1	A	140	TYR	5.7
2	D	50	THR	5.7
2	B	54	VAL	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	113	VAL	5.6
2	D	133	VAL	5.6
2	B	11	VAL	5.5
2	B	15	TRP	5.5
2	D	56	GLY	5.5
2	D	2	HIS	5.5
1	C	135	VAL	5.5
2	D	18	VAL	5.5
1	A	84	SER	5.4
1	A	113	LEU	5.4
2	B	10	ALA	5.3
1	C	48	LEU	5.3
2	B	47	ASP	5.3
2	D	100	PRO	5.3
1	A	115	ALA	5.3
2	B	70	ALA	5.3
2	D	31	LEU	5.3
2	D	109	VAL	5.3
2	D	72	SER	5.3
2	D	141	LEU	5.3
1	A	17	VAL	5.3
2	D	1	MET	5.3
2	D	122	PHE	5.3
2	D	6	GLU	5.2
2	D	71	PHE	5.2
1	A	111	ALA	5.2
1	C	3	SER	5.2
2	D	140	ALA	5.2
2	D	92	HIS	5.2
1	C	117	PHE	5.2
1	A	131	SER	5.2
1	A	120	ALA	5.2
1	A	132	VAL	5.2
1	C	132	VAL	5.2
2	D	22	GLU	5.1
1	A	103	HIS	5.1
2	B	48	LEU	5.1
2	D	136	GLY	5.1
1	C	12	ALA	5.1
1	A	18	GLY	5.1
1	A	34	LEU	5.0
1	C	50	HIS	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	83	GLY	5.0
1	C	115	ALA	5.0
2	B	45	PHE	5.0
2	D	41	PHE	5.0
2	D	42	PHE	5.0
2	D	104	ARG	5.0
2	D	21	ASP	4.9
1	C	23	GLU	4.9
1	A	61	LYS	4.9
2	B	62	ALA	4.9
2	B	31	LEU	4.9
1	A	63	ALA	4.9
1	A	137	THR	4.8
2	B	41	PHE	4.8
2	B	74	GLY	4.8
2	B	87	THR	4.8
2	D	25	GLY	4.8
1	C	63	ALA	4.8
2	B	49	SER	4.8
1	A	129	LEU	4.8
2	B	95	LYS	4.8
2	B	53	ALA	4.8
2	D	12	THR	4.8
2	D	57	ASN	4.7
2	D	81	LEU	4.7
2	B	6	GLU	4.7
1	A	97	ASN	4.7
1	C	60	LYS	4.7
2	D	107	GLY	4.7
2	D	4	THR	4.6
1	C	127	LYS	4.6
1	A	15	GLY	4.6
1	C	113	LEU	4.6
2	B	100	PRO	4.6
1	C	47	ASP	4.6
2	D	115	ALA	4.6
2	B	75	LEU	4.6
1	A	122	HIS	4.6
1	C	38	THR	4.5
2	B	52	ASP	4.5
2	D	27	ALA	4.5
1	A	42	TYR	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	85	PHE	4.5
2	B	20	VAL	4.5
2	D	62	ALA	4.5
2	B	102	ASN	4.5
2	D	45	PHE	4.5
2	D	49	SER	4.5
1	A	121	VAL	4.5
2	B	138	ALA	4.5
2	D	108	ASN	4.5
2	B	144	LYS	4.4
2	D	15	TRP	4.4
1	C	79	ALA	4.4
2	B	43	GLU	4.4
1	C	55	VAL	4.3
2	D	126	VAL	4.3
1	A	56	LYS	4.3
2	B	73	ASP	4.3
2	B	93	CYS	4.3
2	B	78	LEU	4.3
2	D	106	LEU	4.3
1	C	75	ASP	4.3
2	D	23	VAL	4.3
1	C	98	PHE	4.2
1	A	107	VAL	4.2
1	C	17	VAL	4.2
1	A	9	ASN	4.2
2	B	61	LYS	4.2
1	C	64	ASP	4.2
2	D	13	ALA	4.2
2	B	81	LEU	4.2
2	D	105	LEU	4.2
2	D	8	LYS	4.2
2	D	20	VAL	4.2
1	C	136	LEU	4.2
2	B	63	HIS	4.1
2	B	96	LEU	4.1
2	B	71	PHE	4.1
1	A	55	VAL	4.1
2	D	117	HIS	4.1
2	D	146	HIS	4.1
2	D	17	LYS	4.1
2	D	29	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	121	VAL	4.1
1	A	49	SER	4.1
1	C	49	SER	4.1
2	B	121	GLU	4.1
2	D	86	ALA	4.1
1	C	2	LEU	4.1
2	D	3	LEU	4.1
2	B	72	SER	4.1
1	A	68	ASN	4.0
1	A	29	LEU	4.0
1	A	54	GLN	4.0
2	D	82	LYS	4.0
1	A	36	PHE	4.0
1	A	45	HIS	4.0
1	A	77	PRO	4.0
2	B	86	ALA	4.0
1	A	83	LEU	4.0
2	B	21	ASP	4.0
1	A	24	TYR	4.0
1	A	98	PHE	4.0
1	C	46	PHE	4.0
1	C	62	VAL	4.0
2	B	56	GLY	4.0
1	A	92	ARG	4.0
1	C	128	PHE	4.0
2	D	94	ASP	4.0
1	C	28	ALA	3.9
1	C	14	TRP	3.9
1	A	60	LYS	3.9
2	B	127	GLN	3.9
2	D	11	VAL	3.9
2	D	134	VAL	3.9
1	C	43	PHE	3.9
1	A	26	ALA	3.9
1	C	52	SER	3.9
2	D	14	LEU	3.9
2	D	68	LEU	3.9
2	B	37	TYR	3.9
2	B	128	ALA	3.9
2	D	135	ALA	3.9
2	B	28	LEU	3.9
2	D	28	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	90	GLU	3.9
2	B	35	TYR	3.8
1	C	99	LYS	3.8
2	D	59	LYS	3.8
2	B	38	THR	3.8
2	D	60	VAL	3.8
1	C	45	HIS	3.8
1	C	103	HIS	3.8
1	C	74	ASP	3.8
1	C	33	PHE	3.8
2	B	42	PHE	3.8
2	D	88	LEU	3.8
2	D	97	HIS	3.8
1	A	59	GLY	3.8
1	C	41	THR	3.7
2	B	3	LEU	3.7
2	D	38	THR	3.7
1	A	86	LEU	3.7
1	A	109	LEU	3.7
2	B	110	LEU	3.7
2	D	52	ASP	3.7
1	A	23	GLU	3.7
1	A	99	LYS	3.7
2	D	121	GLU	3.7
2	B	124	PRO	3.7
2	D	36	PRO	3.7
1	A	12	ALA	3.7
2	D	48	LEU	3.6
2	D	114	LEU	3.6
1	C	68	ASN	3.6
1	A	102	SER	3.6
2	B	22	GLU	3.6
2	D	40	ARG	3.6
1	C	36	PHE	3.6
2	B	115	ALA	3.6
1	A	91	LEU	3.6
2	B	5	PRO	3.6
2	B	40	ARG	3.6
1	A	43	PHE	3.6
2	B	122	PHE	3.6
1	C	5	ALA	3.6
1	C	26	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	10	ALA	3.6
2	D	78	LEU	3.6
2	B	57	ASN	3.6
2	D	145	TYR	3.6
1	A	74	ASP	3.6
2	D	79	ASP	3.6
1	C	119	PRO	3.6
1	C	34	LEU	3.6
2	D	143	HIS	3.6
2	D	120	LYS	3.6
2	D	55	MET	3.5
2	B	85	PHE	3.5
1	A	21	ALA	3.5
1	C	65	ALA	3.5
2	B	36	PRO	3.5
2	D	138	ALA	3.5
2	D	137	VAL	3.5
1	C	39	THR	3.5
2	B	143	HIS	3.5
1	A	114	PRO	3.5
1	C	21	ALA	3.5
1	C	69	ALA	3.5
2	D	46	GLY	3.5
2	B	116	HIS	3.5
2	D	118	PHE	3.4
1	C	84	SER	3.4
1	C	106	LEU	3.4
1	C	90	LYS	3.4
1	A	41	THR	3.4
2	B	109	VAL	3.4
1	A	119	PRO	3.4
2	D	103	PHE	3.4
1	C	83	LEU	3.4
1	C	40	LYS	3.4
1	C	61	LYS	3.4
1	C	20	HIS	3.4
2	D	34	VAL	3.4
2	B	27	ALA	3.4
2	B	103	PHE	3.4
1	C	30	GLU	3.4
1	A	44	PRO	3.4
2	B	14	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	106	LEU	3.4
1	A	27	GLU	3.3
1	C	8	THR	3.3
1	C	118	THR	3.3
2	D	35	TYR	3.3
1	A	3	SER	3.3
1	A	14	TRP	3.3
2	B	139	ASN	3.3
1	C	56	LYS	3.3
1	C	134	THR	3.3
1	C	125	LEU	3.3
1	A	7	LYS	3.3
1	A	57	GLY	3.3
1	A	95	PRO	3.3
2	B	111	VAL	3.3
2	D	66	LYS	3.3
1	A	67	THR	3.2
2	B	30	ARG	3.2
1	A	16	LYS	3.2
1	C	15	GLY	3.2
1	A	28	ALA	3.2
2	B	68	LEU	3.2
2	B	114	LEU	3.2
1	A	112	HIS	3.2
1	C	133	SER	3.2
1	C	67	THR	3.2
1	C	37	PRO	3.2
2	D	80	ASN	3.2
2	B	126	VAL	3.2
2	D	75	LEU	3.2
2	B	92	HIS	3.2
1	A	110	ALA	3.1
1	C	110	ALA	3.1
2	B	91	LEU	3.1
1	C	89	HIS	3.1
2	B	76	ALA	3.1
1	A	116	GLU	3.1
2	D	26	GLU	3.1
2	D	16	GLY	3.1
1	C	19	ALA	3.1
2	B	142	ALA	3.1
1	A	87	HIS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	37	PRO	3.1
2	B	79	ASP	3.1
1	A	71	ALA	3.1
1	A	1	VAL	3.1
2	B	23	VAL	3.1
1	A	48	LEU	3.1
1	C	109	LEU	3.1
1	A	124	SER	3.1
2	B	107	GLY	3.0
2	D	69	GLY	3.0
2	D	102	ASN	3.0
2	B	90	GLU	3.0
2	D	70	ALA	3.0
2	D	128	ALA	3.0
1	A	2	LEU	3.0
1	A	100	LEU	3.0
1	C	1	VAL	3.0
2	B	113	VAL	3.0
2	D	98	VAL	3.0
2	B	94	ASP	3.0
1	A	127	LYS	3.0
2	B	17	LYS	3.0
1	A	66	LEU	3.0
1	C	80	LEU	3.0
1	A	8	THR	3.0
1	A	108	THR	3.0
2	B	145	TYR	3.0
1	C	53	ALA	3.0
1	C	141	ARG	3.0
1	A	70	VAL	3.0
1	C	70	VAL	3.0
2	D	110	LEU	3.0
1	C	24	TYR	3.0
2	B	104	ARG	2.9
1	A	130	ALA	2.9
1	C	71	ALA	2.9
2	D	112	CYS	2.9
1	A	20	HIS	2.9
2	D	89	SER	2.9
1	A	93	VAL	2.9
2	B	26	GLU	2.9
1	A	90	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	65	LYS	2.9
1	C	10	VAL	2.9
1	C	54	GLN	2.9
1	A	141	ARG	2.9
2	B	7	GLU	2.9
1	C	124	SER	2.9
1	A	22	GLY	2.9
2	B	99	ASP	2.8
2	D	119	GLY	2.8
2	D	54	VAL	2.8
2	B	66	LYS	2.8
2	B	120	LYS	2.8
1	C	122	HIS	2.8
1	A	126	ASP	2.8
1	C	78	ASN	2.8
1	C	85	ASP	2.8
1	A	33	PHE	2.8
2	D	43	GLU	2.7
1	C	66	LEU	2.7
2	B	141	LEU	2.7
2	D	73	ASP	2.7
2	B	16	GLY	2.7
2	B	82	LYS	2.7
1	C	29	LEU	2.7
2	B	117	HIS	2.7
2	D	116	HIS	2.7
1	C	92	ARG	2.7
2	D	127	GLN	2.7
2	B	101	GLU	2.7
1	C	58	HIS	2.7
2	D	111	VAL	2.7
2	D	65	LYS	2.7
2	B	13	ALA	2.6
1	A	32	MET	2.6
2	D	99	ASP	2.6
2	D	144	LYS	2.6
2	B	131	GLN	2.6
2	D	101	GLU	2.6
2	D	96	LEU	2.6
1	A	94	ASP	2.6
1	A	138	SER	2.6
1	A	72	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	118	THR	2.6
1	C	139	LYS	2.6
1	A	64	ASP	2.6
2	D	32	LEU	2.6
1	A	39	THR	2.6
2	D	124	PRO	2.6
1	C	105	LEU	2.6
1	C	76	MET	2.5
2	B	64	GLY	2.5
1	C	72	HIS	2.5
1	C	82	ALA	2.5
2	B	77	HIS	2.5
2	B	130	TYR	2.5
1	A	82	ALA	2.5
1	C	4	PRO	2.5
1	C	116	GLU	2.5
1	C	59	GLY	2.5
2	B	29	GLY	2.5
2	B	133	VAL	2.5
2	D	30	ARG	2.5
1	C	9	ASN	2.5
1	C	81	SER	2.4
2	D	139	ASN	2.4
1	A	31	ARG	2.4
1	C	91	LEU	2.4
1	C	7	LYS	2.4
1	C	95	PRO	2.4
1	C	87	HIS	2.4
2	B	146	HIS	2.4
2	B	129	ALA	2.4
2	B	34	VAL	2.4
2	D	87	THR	2.4
1	C	42	TYR	2.3
2	B	46	GLY	2.3
2	D	95	LYS	2.3
1	A	104	CYS	2.3
1	A	101	LEU	2.3
1	A	30	GLU	2.3
1	A	62	VAL	2.3
2	B	134	VAL	2.3
1	C	129	LEU	2.3
1	C	97	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	91	LEU	2.2
2	D	64	GLY	2.2
1	A	69	ALA	2.2
2	D	129	ALA	2.2
2	B	32	LEU	2.2
1	A	133	SER	2.2
1	A	134	THR	2.2
2	B	136	GLY	2.2
2	D	74	GLY	2.2
1	A	123	ALA	2.2
1	A	35	SER	2.2
2	B	88	LEU	2.1
1	C	138	SER	2.1
1	A	76	MET	2.1
2	B	84	THR	2.1
1	C	112	HIS	2.1
1	C	13	ALA	2.1
1	C	120	ALA	2.1
2	B	135	ALA	2.1
1	A	11	LYS	2.1
1	A	38	THR	2.1
1	A	58	HIS	2.1
2	B	51	PRO	2.1
1	C	86	LEU	2.0
1	C	104	CYS	2.0
2	B	112	CYS	2.0
2	D	132	LYS	2.0
1	A	80	LEU	2.0
1	C	100	LEU	2.0
2	D	47	ASP	2.0
2	B	50	THR	2.0
2	B	83	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

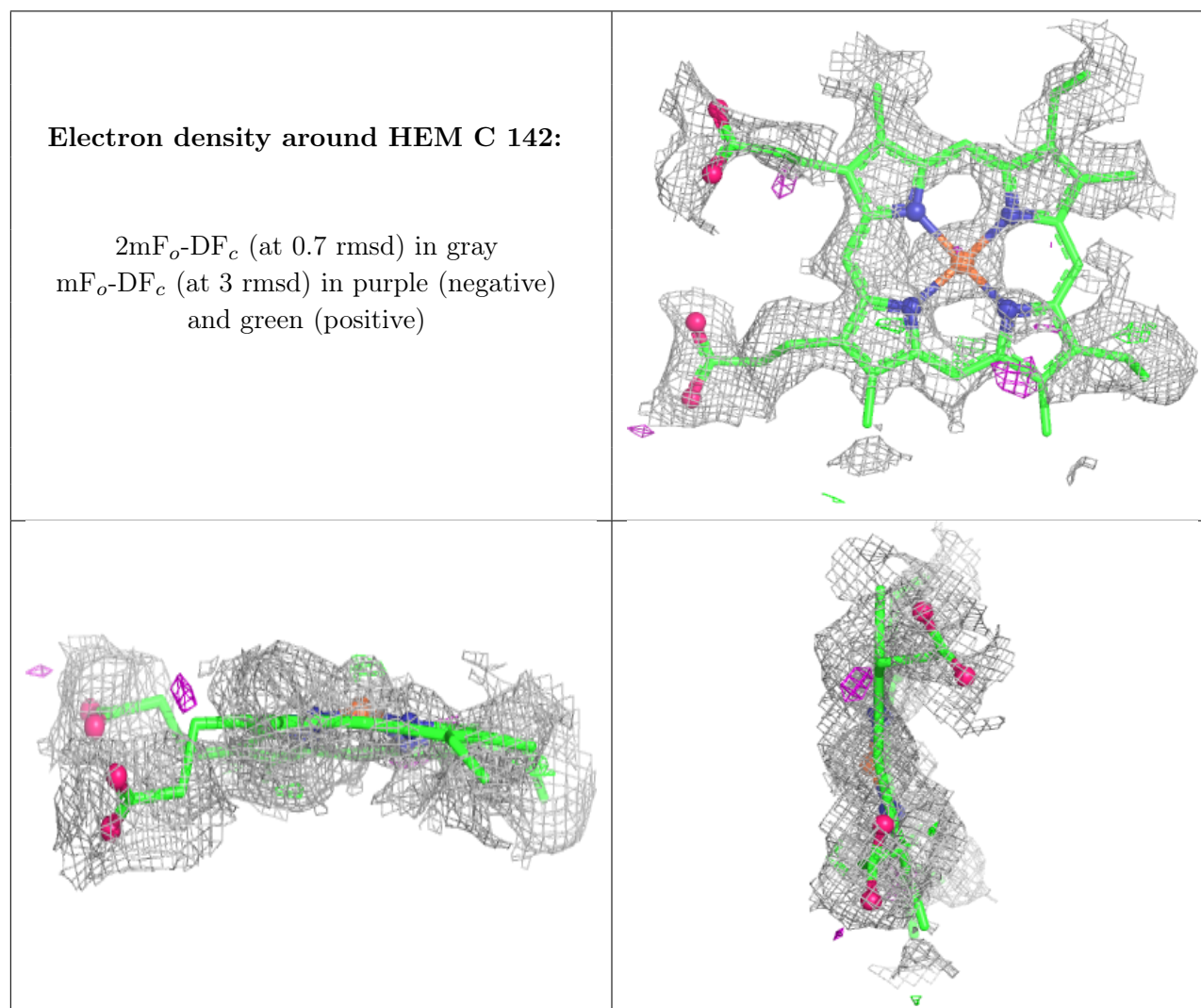
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

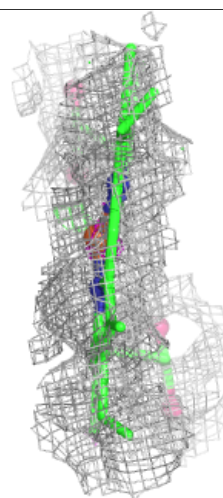
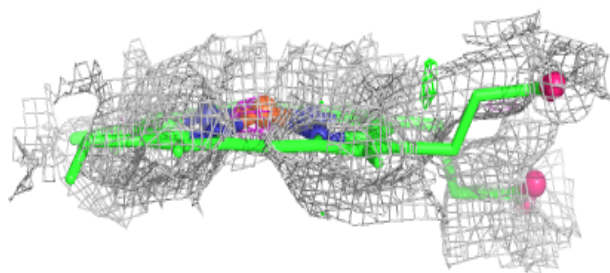
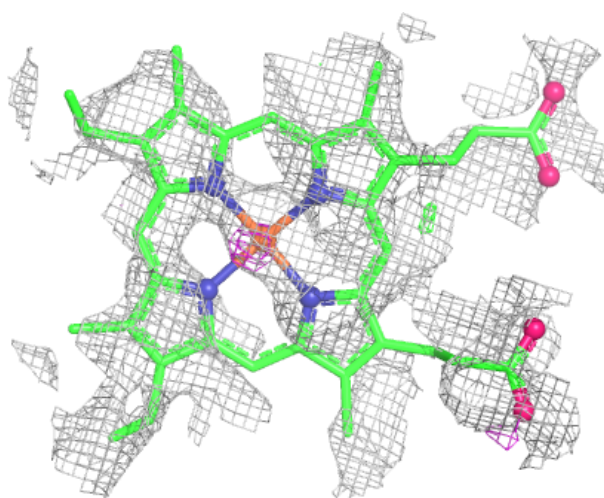
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HEM	C	142	43/43	0.43	0.21	6,9,24,42	0
3	HEM	D	147	43/43	0.49	0.21	10,18,51,54	0
3	HEM	A	142	43/43	0.59	0.16	9,14,30,49	0
3	HEM	B	147	43/43	0.59	0.19	2,10,37,46	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



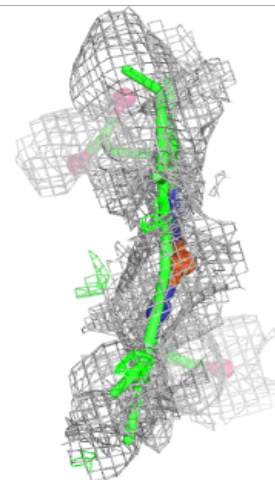
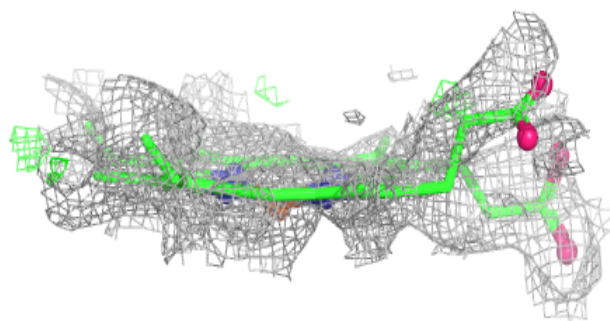
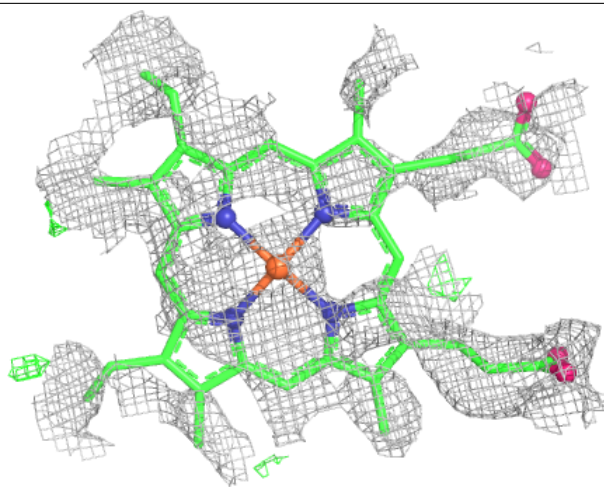
Electron density around HEM D 147:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



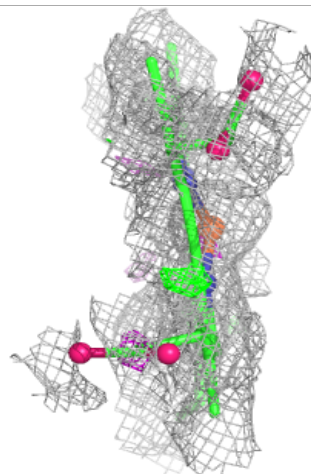
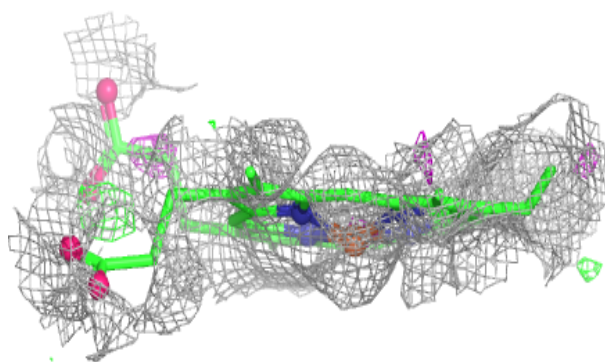
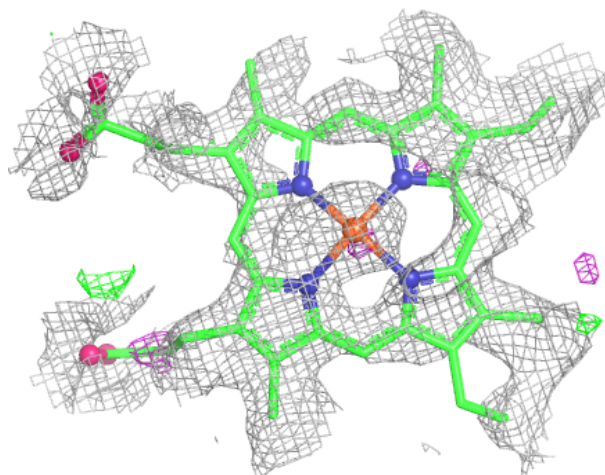
Electron density around HEM A 142:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 147:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.