Full wwPDB X-ray Structure Validation Report (i)

Sep 4, 2023 – 04:41 PM EDT

PDB ID	:	3U8P
Title	:	Cytochrome b562 integral fusion with EGFP
Authors	:	Arpino, J.; Czapinska, H.; Piasecka, A.; Edwards, W.R.; Barker, P.; Gajda, M.; Bochtler, M.; Jones, D.D.
Deposited on	:	2011-10-17
Resolution	:	2.75 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

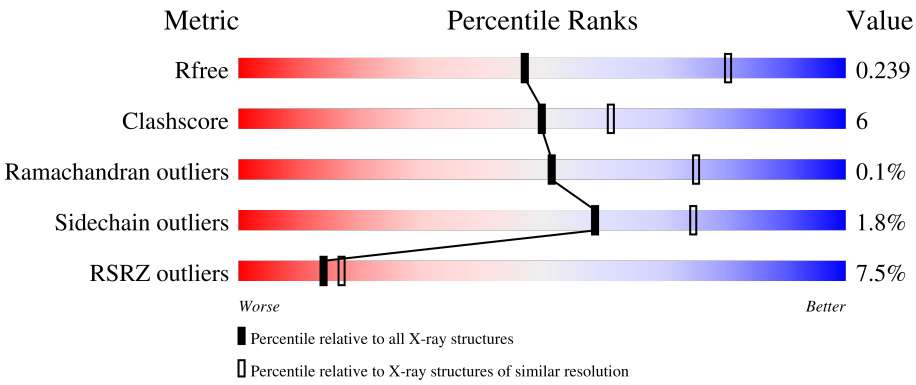
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.75 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))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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% 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	347	% 89% 8% •
1	B	347	5% 83% 13% • •
1	C	347	16% 81% 15% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8446 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 Cytochrome b562 integral fusion with enhanced green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	2669	1680	458	522	9	0	1	0
1	B	336	2652	1669	456	518	9	0	0	0
1	C	336	2652	1669	456	518	9	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P42212
A	1	VAL	-	expression tag	UNP P42212
A	39	PHE	-	linker	UNP P0ABE7
A	40	GLY	-	linker	UNP P0ABE7
A	41	GLY	-	linker	UNP P0ABE7
A	42	SER	-	linker	UNP P0ABE7
A	149	GLY	-	linker	UNP P42212
A	174	LEU	PHE	engineered mutation	UNP P42212
A	175	CRO	SER	chromophore	UNP P42212
A	175	CRO	TYR	chromophore	UNP P42212
A	175	CRO	GLY	chromophore	UNP P42212
A	339	LEU	HIS	engineered mutation	UNP P42212
B	0	MET	-	initiating methionine	UNP P42212
B	1	VAL	-	expression tag	UNP P42212
B	39	PHE	-	linker	UNP P0ABE7
B	40	GLY	-	linker	UNP P0ABE7
B	41	GLY	-	linker	UNP P0ABE7
B	42	SER	-	linker	UNP P0ABE7
B	149	GLY	-	linker	UNP P42212
B	174	LEU	PHE	engineered mutation	UNP P42212
B	175	CRO	SER	chromophore	UNP P42212
B	175	CRO	TYR	chromophore	UNP P42212

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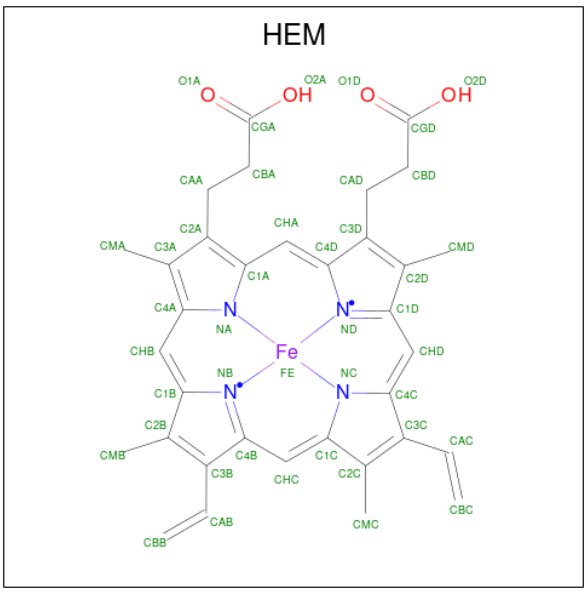
Chain	Residue	Modelled	Actual	Comment	Reference
B	175	CRO	GLY	chromophore	UNP P42212
B	339	LEU	HIS	engineered mutation	UNP P42212
C	0	MET	-	initiating methionine	UNP P42212
C	1	VAL	-	expression tag	UNP P42212
C	39	PHE	-	linker	UNP P0ABE7
C	40	GLY	-	linker	UNP P0ABE7
C	41	GLY	-	linker	UNP P0ABE7
C	42	SER	-	linker	UNP P0ABE7
C	149	GLY	-	linker	UNP P42212
C	174	LEU	PHE	engineered mutation	UNP P42212
C	175	CRO	SER	chromophore	UNP P42212
C	175	CRO	TYR	chromophore	UNP P42212
C	175	CRO	GLY	chromophore	UNP P42212
C	339	LEU	HIS	engineered mutation	UNP P42212

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is water.

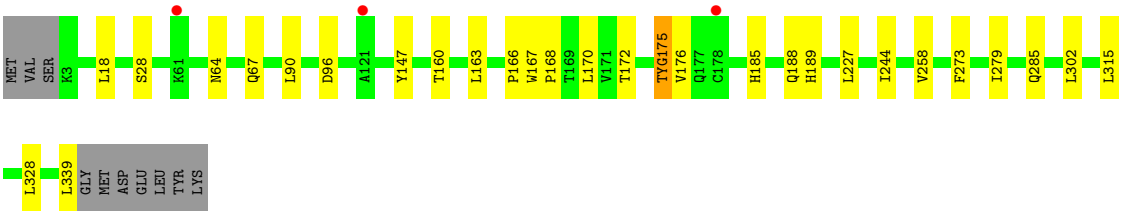
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	131	131	131	0	0
			Total	O		
3	B	126	126	126	0	0
			Total	O		
3	C	87	87	87	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

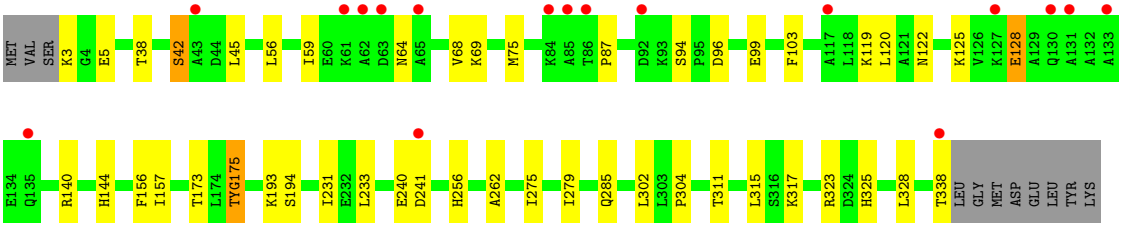
• Molecule 1: Cytochrome b562 integral fusion with enhanced green fluorescent protein

Chain A:



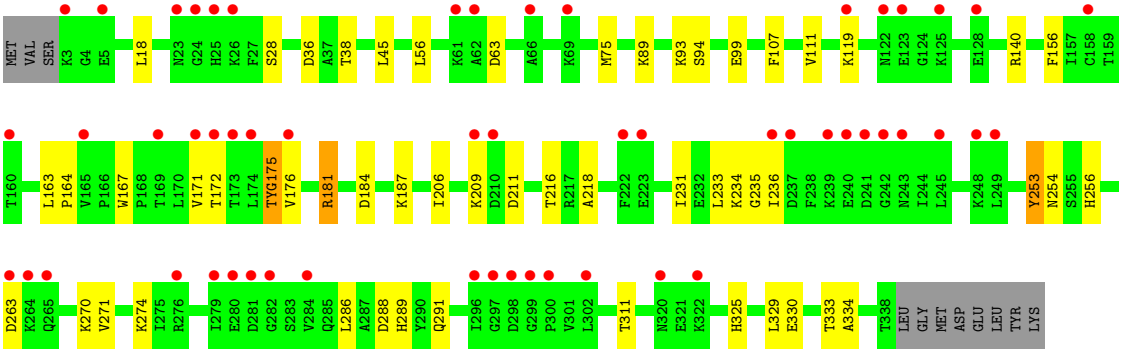
• Molecule 1: Cytochrome b562 integral fusion with enhanced green fluorescent protein

Chain B:



• Molecule 1: Cytochrome b562 integral fusion with enhanced green fluorescent protein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.75Å 125.20Å 89.25Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	28.94 – 2.75 29.52 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.94-2.75) 99.3 (29.52-2.75)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	3.36 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.242 0.197 , 0.239	Depositor DCC
R_{free} test set	1882 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	63.0	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8446	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CRO, 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	0.56	0/2697	0.66	0/3638
1	B	0.61	0/2680	0.68	0/3615
1	C	0.45	0/2680	0.59	0/3615
All	All	0.54	0/8057	0.65	0/10868

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2669	0	2613	22	0
1	B	2652	0	2597	31	0
1	C	2652	0	2597	37	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
3	A	131	0	0	1	0
3	B	126	0	0	2	0
3	C	87	0	0	2	0
All	All	8446	0	7897	93	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 (93) 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:C:333:THR:HG22	1:C:334:ALA:O	1.90	0.70
1:C:216:THR:HG22	1:C:233:LEU:HG	1.74	0.70
1:B:279:ILE:HD11	1:B:285:GLN:HB3	1.75	0.68
1:C:181:ARG:HG2	1:C:181:ARG:NH1	2.09	0.66
1:B:156:PHE:O	1:B:325:HIS:HB2	1.98	0.64
1:C:107:PHE:O	1:C:111:VAL:HG23	2.00	0.62
1:B:87:PRO:HG3	1:B:103:PHE:CE1	2.35	0.61
1:A:175:CRO:HG11	1:A:328:LEU:HD23	1.84	0.60
1:B:157:ILE:HD13	1:B:323:ARG:CZ	2.32	0.59
1:A:339:LEU:HD12	1:A:339:LEU:N	2.17	0.59
1:B:59:ILE:HG23	1:B:68:VAL:HG13	1.87	0.57
1:C:181:ARG:HG2	1:C:181:ARG:HH11	1.70	0.56
1:B:125:LYS:HB3	1:B:128:GLU:HB2	1.87	0.55
1:C:38:THR:HG21	1:C:89:LYS:HD3	1.87	0.55
1:C:163:LEU:HD12	1:C:164:PRO:HD2	1.88	0.55
2:A:347:HEM:CMB	2:A:347:HEM:HBB2	2.37	0.54
1:C:175:CRO:CE2	1:C:311:THR:HG21	2.39	0.53
1:A:315:LEU:CD2	1:A:328:LEU:HD13	2.39	0.52
1:B:175:CRO:CE2	1:B:311:THR:HG21	2.41	0.50
1:B:317:LYS:NZ	3:B:464:HOH:O	2.45	0.50
1:A:64:ASN:HD21	1:A:67:GLN:NE2	2.10	0.49
1:C:181:ARG:HH11	1:C:181:ARG:CG	2.24	0.49
1:C:274:LYS:HG2	1:C:288:ASP:OD1	2.12	0.49
1:C:56:LEU:HB2	1:C:75:MET:HE3	1.93	0.49
1:B:140:ARG:HB2	2:B:347:HEM:HAB	1.94	0.49
1:C:329:LEU:HD12	1:C:330:GLU:N	2.28	0.49
1:A:166:PRO:HD3	1:A:244:ILE:O	2.13	0.49
1:B:140:ARG:HG3	2:B:347:HEM:C4B	2.47	0.49
1:C:140:ARG:HG3	2:C:347:HEM:C4B	2.48	0.48
1:A:258:VAL:HG13	1:A:273:PHE:CD2	2.48	0.48
2:A:347:HEM:HBB2	2:A:347:HEM:HMB2	1.95	0.48
1:C:181:ARG:NH1	1:C:333:THR:HG23	2.28	0.48
1:C:333:THR:HG22	1:C:334:ALA:N	2.28	0.48
1:B:3:LYS:HG3	1:B:5:GLU:H	1.78	0.48
1:B:233:LEU:C	1:B:233:LEU:HD23	2.34	0.48
1:C:163:LEU:HD22	1:C:167:TRP:CE2	2.49	0.47
1:C:271:VAL:HB	1:C:291:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:HIS:CE1	1:B:275:ILE:CD1	2.97	0.47
1:A:163:LEU:HD21	1:A:170:LEU:HD12	1.97	0.47
1:B:99:GLU:N	1:B:99:GLU:OE2	2.47	0.47
1:A:188:GLN:N	1:A:188:GLN:OE1	2.46	0.47
1:B:56:LEU:HB2	1:B:75:MET:HE3	1.97	0.47
1:C:235:GLY:O	1:C:236:ILE:HG23	2.15	0.47
1:B:256:HIS:CE1	1:B:275:ILE:HD12	2.49	0.47
1:C:233:LEU:HD23	1:C:234:LYS:N	2.30	0.47
1:C:176:VAL:N	3:C:386:HOH:O	2.48	0.46
1:A:28:SER:HB2	1:A:160:THR:HG23	1.97	0.46
1:A:279:ILE:HD11	1:A:285:GLN:HB3	1.97	0.46
1:C:184:ASP:O	1:C:187:LYS:HG3	2.16	0.45
1:A:176:VAL:N	3:A:388:HOH:O	2.49	0.45
1:B:173:THR:CG2	1:B:231:ILE:HG21	2.46	0.45
1:B:69:LYS:HD2	1:B:122:ASN:OD1	2.17	0.44
1:C:254:ASN:O	1:C:256:HIS:CE1	2.70	0.44
1:B:42:SER:HB2	1:B:45:LEU:HB3	2.00	0.44
1:B:175:CRO:HG11	1:B:328:LEU:HD23	2.00	0.44
1:C:18:LEU:HD12	1:C:231:ILE:HD12	2.00	0.44
1:C:36:ASP:OD1	1:C:89:LYS:HE3	2.18	0.44
1:B:64:ASN:O	1:B:68:VAL:HG23	2.18	0.44
1:A:90:LEU:HD11	1:A:147:TYR:CE2	2.53	0.43
1:A:167:TRP:N	1:A:168:PRO:CD	2.80	0.43
1:A:188:GLN:HG2	1:A:189:HIS:CD2	2.54	0.43
1:C:233:LEU:HD23	1:C:233:LEU:C	2.38	0.43
1:C:218:ALA:HB2	1:C:231:ILE:HG23	2.00	0.43
1:B:193:LYS:NZ	3:B:418:HOH:O	2.50	0.43
1:B:194:SER:HB3	1:B:302:LEU:HD12	2.01	0.43
1:B:96:ASP:OD2	1:B:96:ASP:N	2.52	0.43
1:A:227:LEU:C	1:A:227:LEU:HD13	2.39	0.43
1:A:188:GLN:HA	1:A:302:LEU:HD13	2.00	0.42
1:B:262:ALA:HB2	1:B:304:PRO:O	2.19	0.42
1:C:263:ASP:HB2	1:C:270:LYS:HG3	2.01	0.42
1:B:315:LEU:CD2	1:B:328:LEU:HD13	2.49	0.42
1:B:140:ARG:HG3	2:B:347:HEM:C3B	2.54	0.42
1:C:38:THR:HG21	1:C:89:LYS:CD	2.49	0.42
1:A:96:ASP:C	1:A:96:ASP:OD2	2.58	0.42
1:B:256:HIS:CD2	1:B:275:ILE:HD13	2.55	0.41
1:C:209:LYS:HE3	1:C:286:LEU:HD13	2.02	0.41
1:A:188:GLN:CD	1:A:188:GLN:H	2.22	0.41
2:A:347:HEM:CMC	2:A:347:HEM:HBC2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:N	1:A:339:LEU:CD1	2.82	0.41
1:C:163:LEU:HD22	1:C:167:TRP:CD2	2.54	0.41
1:A:172:THR:O	1:A:175:CRO:C2	2.68	0.41
1:C:172:THR:HG23	3:C:416:HOH:O	2.21	0.41
1:C:119:LYS:HB2	1:C:119:LYS:HE2	1.80	0.41
1:A:185:HIS:O	1:A:188:GLN:NE2	2.52	0.41
1:B:256:HIS:CG	1:B:275:ILE:HD13	2.55	0.41
1:C:140:ARG:HB2	2:C:347:HEM:HAB	2.03	0.41
1:C:206:ILE:HD13	1:C:289:HIS:NE2	2.36	0.41
1:C:171:VAL:HB	1:C:253:TYR:CE1	2.56	0.41
1:B:56:LEU:HB2	1:B:75:MET:CE	2.51	0.40
1:A:18:LEU:C	1:A:18:LEU:HD23	2.41	0.40
1:C:156:PHE:O	1:C:325:HIS:HB2	2.22	0.40
1:C:93:LYS:HE3	1:C:99:GLU:OE1	2.21	0.40
1:B:140:ARG:CG	1:B:144:HIS:CE1	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/347 (96%)	328 (98%)	5 (2%)	0	100	100
1	B	331/347 (95%)	324 (98%)	6 (2%)	1 (0%)	41	60
1	C	331/347 (95%)	319 (96%)	12 (4%)	0	100	100
All	All	995/1041 (96%)	971 (98%)	23 (2%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	SER

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	286/294 (97%)	286 (100%)	0	100	100
1	B	284/294 (97%)	276 (97%)	8 (3%)	43	63
1	C	284/294 (97%)	277 (98%)	7 (2%)	47	67
All	All	854/882 (97%)	839 (98%)	15 (2%)	59	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	THR
1	B	94	SER
1	B	119	LYS
1	B	120	LEU
1	B	128	GLU
1	B	240	GLU
1	B	241	ASP
1	B	338	THR
1	C	28	SER
1	C	45	LEU
1	C	63	ASP
1	C	94	SER
1	C	181	ARG
1	C	211	ASP
1	C	253	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	267	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CRO	A	175	1	23,23,24	2.45	6 (26%)	30,32,34	2.87	8 (26%)
1	CRO	C	175	1	23,23,24	2.71	6 (26%)	30,32,34	3.26	7 (23%)
1	CRO	B	175	1	23,23,24	2.45	4 (17%)	30,32,34	2.84	7 (23%)

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
1	CRO	A	175	1	-	0/12/31/32	0/2/2/2
1	CRO	C	175	1	-	0/12/31/32	0/2/2/2
1	CRO	B	175	1	-	0/12/31/32	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	CRO	CA2-C2	-8.84	1.39	1.48
1	C	175	CRO	CA2-C2	-8.68	1.40	1.48
1	B	175	CRO	CB2-CA2	8.35	1.42	1.35
1	C	175	CRO	CB2-CA2	7.65	1.41	1.35
1	B	175	CRO	CA2-C2	-6.68	1.42	1.48
1	A	175	CRO	CB2-CA2	5.13	1.39	1.35
1	B	175	CRO	C2-N3	-3.32	1.32	1.39
1	A	175	CRO	CG2-CB2	-2.92	1.41	1.46
1	A	175	CRO	C2-N3	-2.85	1.33	1.39
1	C	175	CRO	CG2-CB2	-2.81	1.41	1.46
1	C	175	CRO	C2-N3	-2.66	1.33	1.39
1	A	175	CRO	CA2-N2	-2.51	1.33	1.38
1	B	175	CRO	CG2-CB2	-2.36	1.42	1.46
1	C	175	CRO	CA1-C1	2.30	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	CRO	C1-N3	-2.27	1.33	1.37
1	C	175	CRO	C1-N3	-2.25	1.33	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	175	CRO	CA2-C2-N3	11.75	108.93	103.37
1	A	175	CRO	CA2-C2-N3	11.21	108.67	103.37
1	B	175	CRO	CA2-C2-N3	10.99	108.57	103.37
1	C	175	CRO	O2-C2-CA2	-8.33	126.28	130.96
1	B	175	CRO	C2-CA2-N2	-6.34	104.49	108.93
1	C	175	CRO	C2-CA2-N2	-6.07	104.68	108.93
1	A	175	CRO	O2-C2-CA2	-5.38	127.94	130.96
1	C	175	CRO	CA2-N2-C1	5.35	109.71	105.77
1	A	175	CRO	C2-CA2-N2	-5.05	105.40	108.93
1	B	175	CRO	CA2-N2-C1	4.87	109.36	105.77
1	A	175	CRO	CA2-N2-C1	4.64	109.19	105.77
1	C	175	CRO	N3-C1-N2	-3.68	108.90	111.45
1	C	175	CRO	CB2-CA2-N2	3.58	133.80	128.83
1	B	175	CRO	C1-CA1-N1	-3.55	104.20	109.96
1	B	175	CRO	CB2-CA2-N2	3.22	133.29	128.83
1	B	175	CRO	N3-C1-N2	-3.09	109.31	111.45
1	A	175	CRO	N3-C1-N2	-2.88	109.46	111.45
1	A	175	CRO	CB2-CA2-N2	2.80	132.72	128.83
1	B	175	CRO	O2-C2-CA2	-2.80	129.39	130.96
1	C	175	CRO	CG2-CB2-CA2	-2.53	126.84	129.94
1	A	175	CRO	C1-CA1-N1	-2.28	106.26	109.96
1	A	175	CRO	O3-C3-CA3	-2.06	120.16	126.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	175	CRO	2	0
1	C	175	CRO	1	0
1	B	175	CRO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
2	HEM	A	347	1	41,50,50	1.87	10 (24%)	45,82,82	1.47	6 (13%)
2	HEM	B	347	1	41,50,50	1.80	13 (31%)	45,82,82	1.70	6 (13%)
2	HEM	C	347	1	41,50,50	1.89	11 (26%)	45,82,82	1.50	7 (15%)

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
2	HEM	A	347	1	-	3/12/54/54	-
2	HEM	B	347	1	-	4/12/54/54	-
2	HEM	C	347	1	-	9/12/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	347	HEM	C4D-C3D	-3.89	1.38	1.45
2	A	347	HEM	C4D-C3D	-3.84	1.38	1.45
2	A	347	HEM	C3C-CAC	-3.83	1.39	1.47
2	C	347	HEM	C3C-CAC	-3.73	1.40	1.47
2	A	347	HEM	C4D-ND	-3.49	1.34	1.40
2	C	347	HEM	C3B-C4B	-3.43	1.38	1.44
2	B	347	HEM	C4D-ND	-3.42	1.34	1.40
2	B	347	HEM	C1D-C2D	-3.40	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	347	HEM	C1D-C2D	-3.36	1.38	1.44
2	A	347	HEM	C1B-NB	-3.31	1.34	1.40
2	C	347	HEM	C1D-C2D	-3.29	1.38	1.44
2	C	347	HEM	C1B-C2B	-3.28	1.38	1.44
2	A	347	HEM	C3C-C2C	-3.19	1.35	1.40
2	C	347	HEM	CAA-C2A	3.16	1.56	1.52
2	A	347	HEM	C1B-C2B	-3.13	1.38	1.44
2	C	347	HEM	C4D-C3D	-3.01	1.39	1.45
2	B	347	HEM	C1B-C2B	-2.93	1.38	1.44
2	C	347	HEM	C1B-NB	-2.91	1.35	1.40
2	C	347	HEM	C4D-ND	-2.83	1.35	1.40
2	C	347	HEM	CAB-C3B	-2.74	1.40	1.47
2	A	347	HEM	C3B-C4B	-2.74	1.39	1.44
2	A	347	HEM	CAB-C3B	-2.67	1.40	1.47
2	B	347	HEM	C3C-CAC	-2.65	1.42	1.47
2	B	347	HEM	C1B-NB	-2.58	1.35	1.40
2	B	347	HEM	CAB-C3B	-2.50	1.40	1.47
2	B	347	HEM	C4B-NB	-2.48	1.33	1.38
2	B	347	HEM	FE-ND	2.47	2.09	1.96
2	B	347	HEM	C3B-C4B	-2.38	1.40	1.44
2	C	347	HEM	C3C-C2C	-2.37	1.37	1.40
2	C	347	HEM	C4B-NB	-2.27	1.34	1.38
2	B	347	HEM	C1D-ND	-2.11	1.34	1.38
2	B	347	HEM	CBB-CAB	2.10	1.40	1.30
2	A	347	HEM	C1D-ND	-2.05	1.34	1.38
2	B	347	HEM	CBD-CGD	2.00	1.55	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	347	HEM	C4C-CHD-C1D	5.39	129.67	122.56
2	C	347	HEM	C4B-CHC-C1C	4.89	129.01	122.56
2	A	347	HEM	C4B-CHC-C1C	4.66	128.71	122.56
2	B	347	HEM	C4B-CHC-C1C	4.66	128.71	122.56
2	C	347	HEM	C4C-CHD-C1D	3.97	127.80	122.56
2	A	347	HEM	C4C-CHD-C1D	3.53	127.22	122.56
2	B	347	HEM	C1B-NB-C4B	3.21	108.39	105.07
2	B	347	HEM	CBD-CAD-C3D	-3.17	103.83	112.63
2	C	347	HEM	C1B-NB-C4B	3.00	108.17	105.07
2	A	347	HEM	C1B-NB-C4B	2.95	108.12	105.07
2	B	347	HEM	O1D-CGD-CBD	-2.70	114.42	123.08
2	B	347	HEM	C4D-ND-C1D	2.64	107.81	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	347	HEM	CAD-C3D-C4D	2.62	129.24	124.66
2	A	347	HEM	C4D-ND-C1D	2.60	107.76	105.07
2	C	347	HEM	C4A-C3A-C2A	2.45	108.70	107.00
2	A	347	HEM	CBD-CAD-C3D	-2.22	106.46	112.63
2	A	347	HEM	CHA-C4D-ND	2.18	127.08	124.38
2	C	347	HEM	C4D-ND-C1D	2.14	107.28	105.07
2	C	347	HEM	O1A-CGA-CBA	-2.05	116.50	123.08

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	347	HEM	C2B-C3B-CAB-CBB
2	C	347	HEM	C4B-C3B-CAB-CBB
2	C	347	HEM	C2A-CAA-CBA-CGA
2	B	347	HEM	C2B-C3B-CAB-CBB
2	C	347	HEM	C1A-C2A-CAA-CBA
2	C	347	HEM	C3A-C2A-CAA-CBA
2	B	347	HEM	CAA-CBA-CGA-O1A
2	B	347	HEM	CAA-CBA-CGA-O2A
2	C	347	HEM	CAA-CBA-CGA-O2A
2	C	347	HEM	CAA-CBA-CGA-O1A
2	C	347	HEM	CAD-CBD-CGD-O2D
2	C	347	HEM	CAD-CBD-CGD-O1D
2	A	347	HEM	CAA-CBA-CGA-O1A
2	B	347	HEM	C4B-C3B-CAB-CBB
2	A	347	HEM	CAA-CBA-CGA-O2A
2	A	347	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

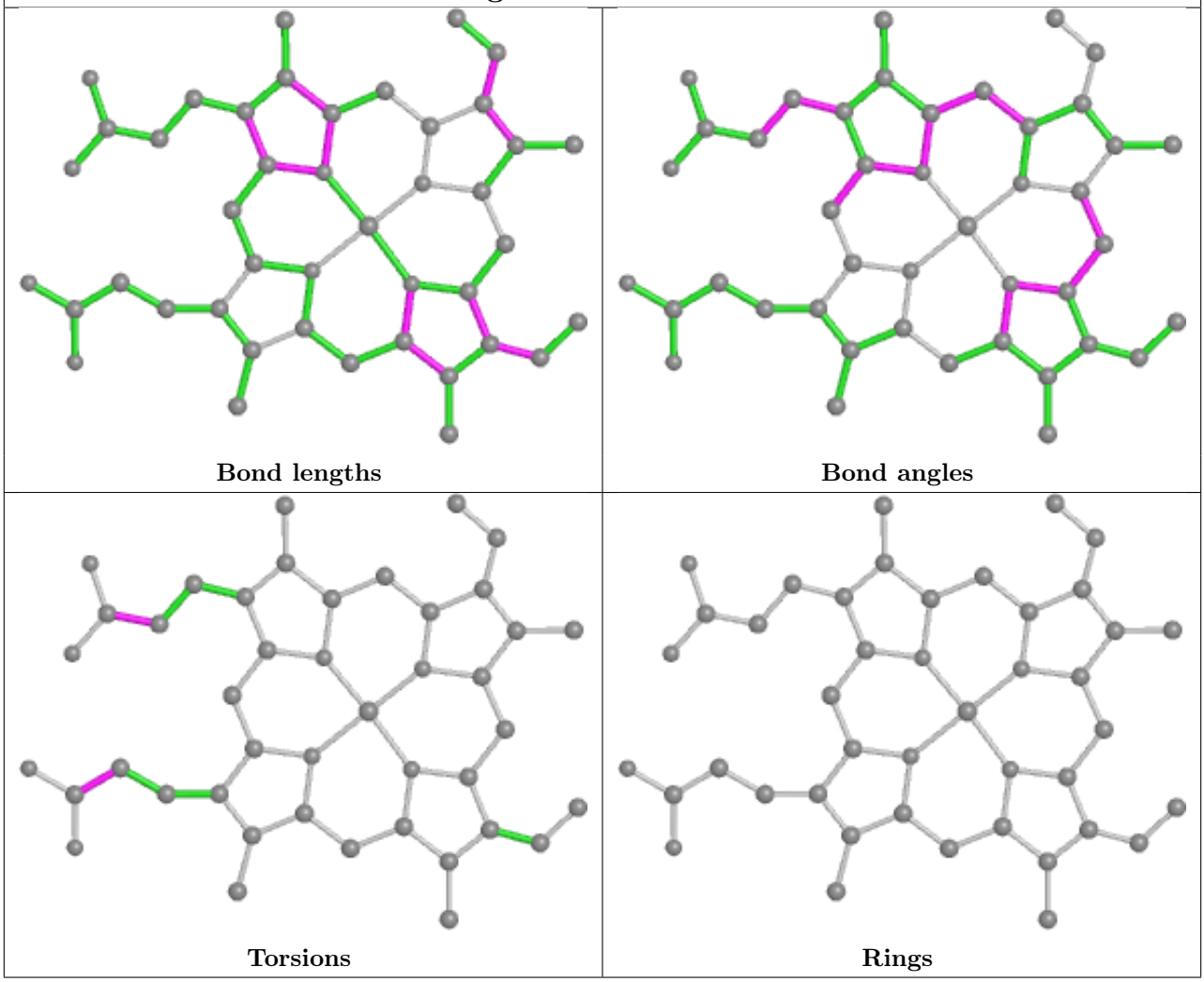
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	347	HEM	3	0
2	B	347	HEM	3	0
2	C	347	HEM	2	0

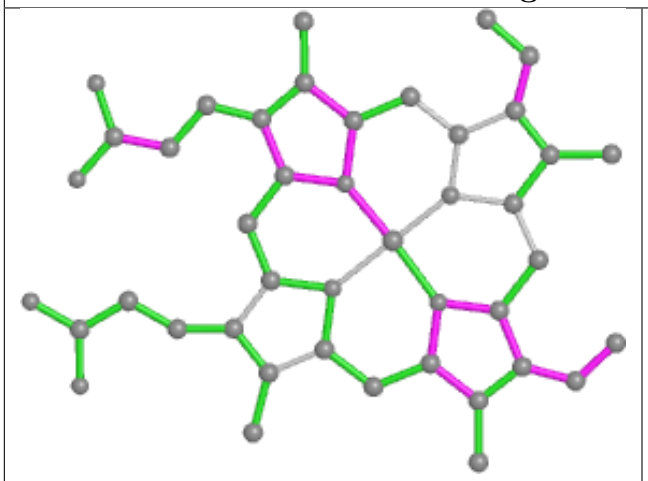
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

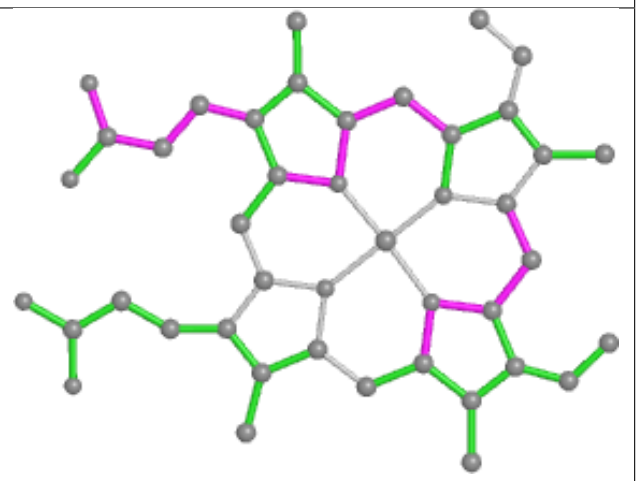
Ligand HEM A 347



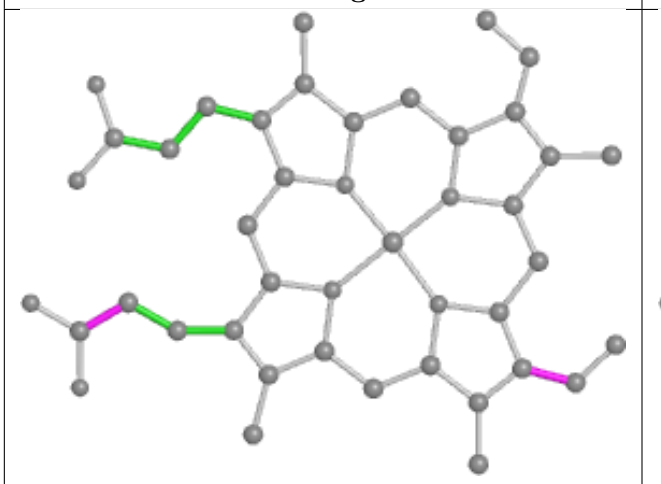
Ligand HEM B 347



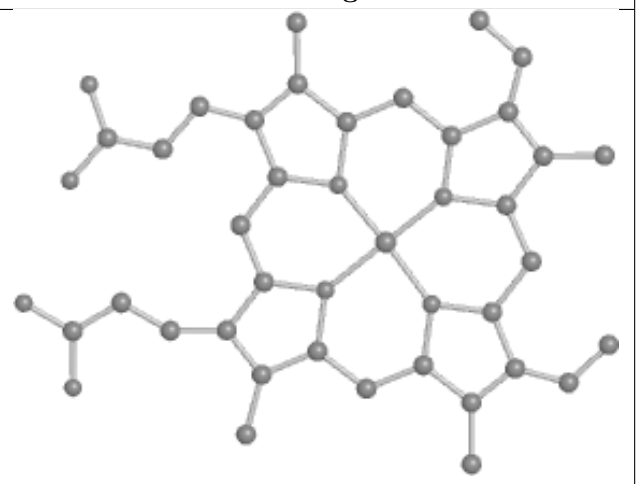
Bond lengths



Bond angles

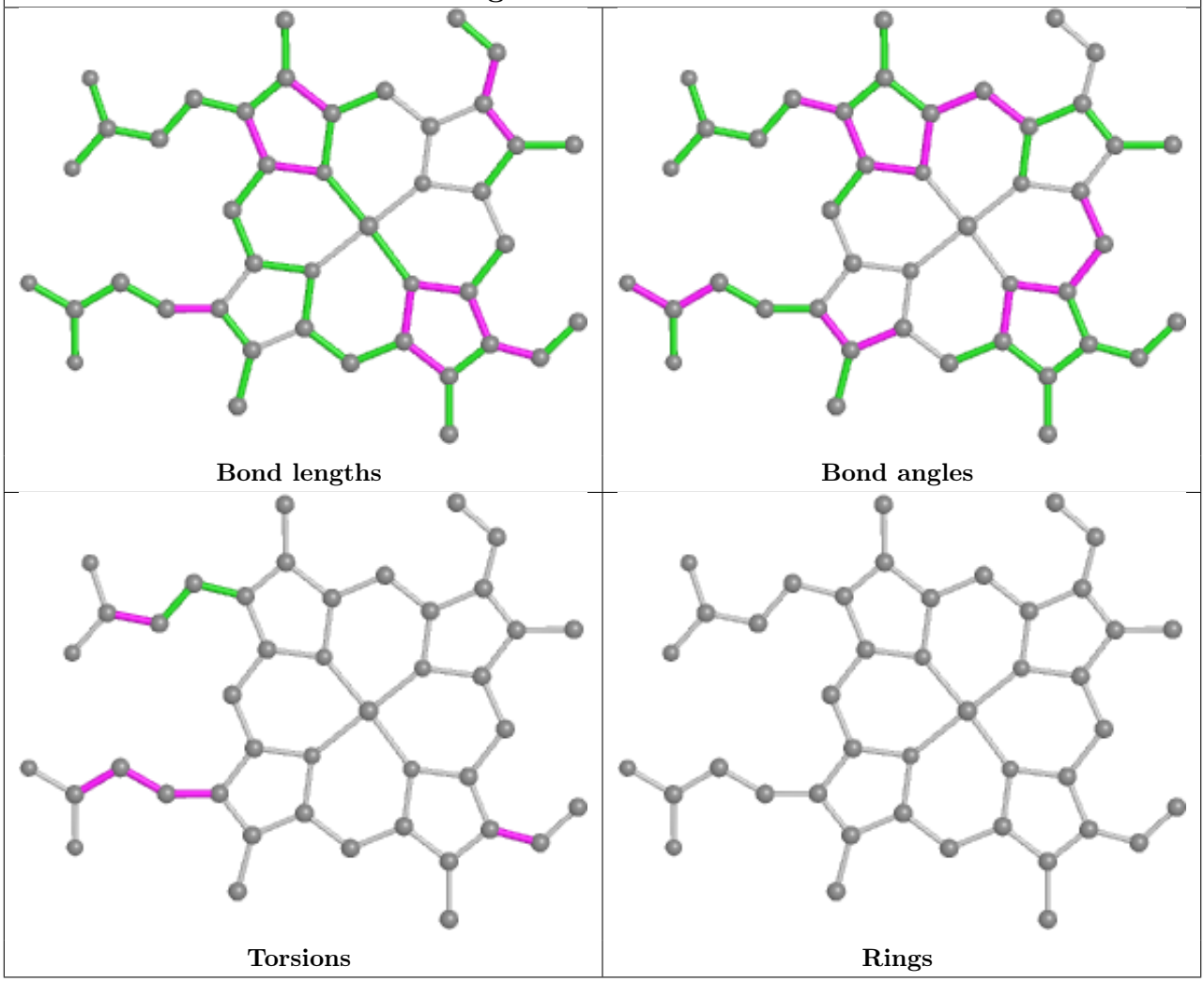


Torsions



Rings

Ligand HEM C 347



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	336/347 (96%)	-0.09	3 (0%)	84	89	35, 57, 98, 117	0
1	B	335/347 (96%)	0.20	17 (5%)	28	34	34, 59, 94, 123	0
1	C	335/347 (96%)	0.74	55 (16%)	1	1	46, 105, 180, 235	0
All	All	1006/1041 (96%)	0.28	75 (7%)	14	17	34, 66, 153, 235	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	298	ASP	7.4
1	C	241	ASP	5.4
1	C	281	ASP	5.3
1	C	265	GLN	4.8
1	C	119	LYS	4.5
1	C	280	GLU	4.5
1	C	173	THR	4.5
1	C	24	GLY	4.3
1	C	264	LYS	4.2
1	B	92	ASP	4.2
1	B	61	LYS	4.2
1	B	85	ALA	4.2
1	C	209	LYS	4.2
1	C	26	LYS	4.1
1	C	174	LEU	4.0
1	C	223	GLU	4.0
1	C	69	LYS	3.9
1	C	3	LYS	3.9
1	B	86	THR	3.8
1	C	279	ILE	3.8
1	C	176	VAL	3.6
1	C	282	GLY	3.5
1	C	248	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	222	PHE	3.4
1	C	249	LEU	3.4
1	C	123	GLU	3.3
1	C	320	ASN	3.2
1	B	131	ALA	3.2
1	C	125	LYS	3.2
1	C	240	GLU	3.2
1	C	242	GLY	3.2
1	C	276	ARG	3.1
1	C	299	GLY	3.1
1	C	284	VAL	3.0
1	C	171	VAL	3.0
1	C	172	THR	2.9
1	C	300	PRO	2.9
1	B	84	LYS	2.8
1	B	117	ALA	2.8
1	B	127	LYS	2.8
1	C	66	ALA	2.8
1	C	122	ASN	2.8
1	C	169	THR	2.7
1	B	130	GLN	2.7
1	C	302	LEU	2.6
1	C	160	THR	2.6
1	B	43	ALA	2.6
1	A	61	LYS	2.6
1	C	296	ILE	2.6
1	B	241	ASP	2.6
1	C	239	LYS	2.5
1	A	121	ALA	2.5
1	C	236	ILE	2.5
1	C	5	GLU	2.5
1	B	135	GLN	2.5
1	C	297	GLY	2.4
1	C	23	ASN	2.4
1	C	322	LYS	2.4
1	B	62	ALA	2.3
1	C	237	ASP	2.3
1	C	25	HIS	2.3
1	C	245	LEU	2.2
1	C	61	LYS	2.2
1	C	128	GLU	2.2
1	B	63	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	243	ASN	2.2
1	C	263	ASP	2.2
1	C	158	CYS	2.1
1	C	62	ALA	2.1
1	B	65	ALA	2.1
1	B	133	ALA	2.1
1	C	210	ASP	2.1
1	C	165	VAL	2.0
1	B	338	THR	2.0
1	A	178	CYS	2.0

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

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
1	CRO	C	175	22/23	0.95	0.37	83,86,92,94	0
1	CRO	B	175	22/23	0.97	0.25	37,39,40,41	0
1	CRO	A	175	22/23	0.98	0.29	38,41,42,42	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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.

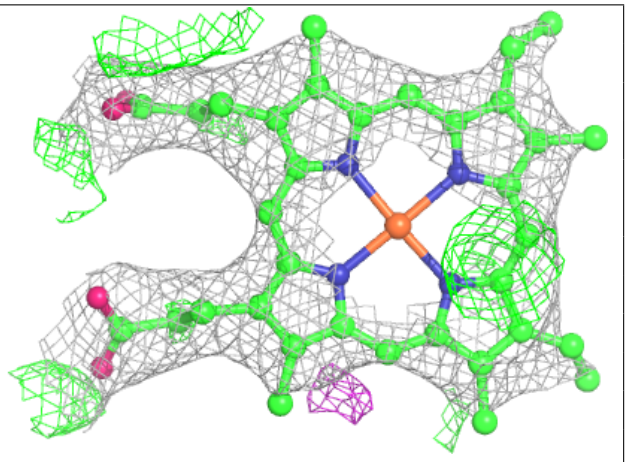
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	347	43/43	0.93	0.22	61,63,74,77	0
2	HEM	C	347	43/43	0.97	0.18	45,52,63,68	0
2	HEM	A	347	43/43	0.98	0.17	32,38,45,55	0

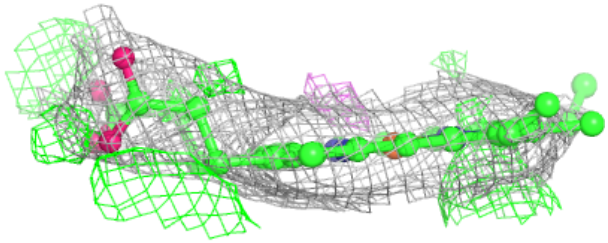
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

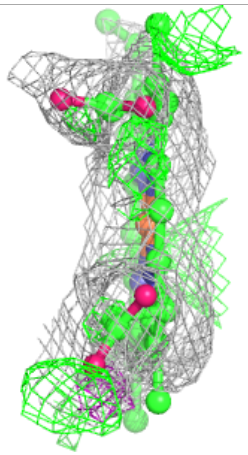
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM B 347:

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

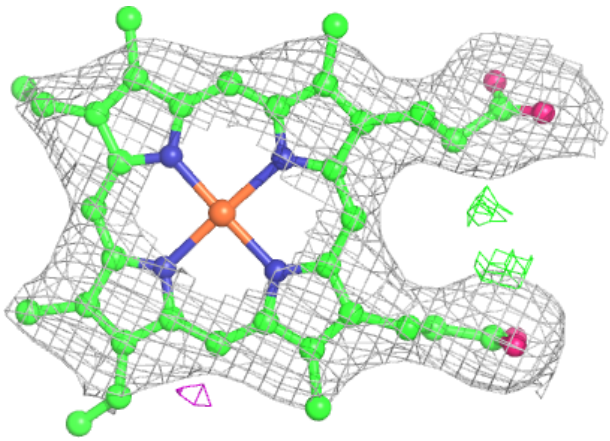


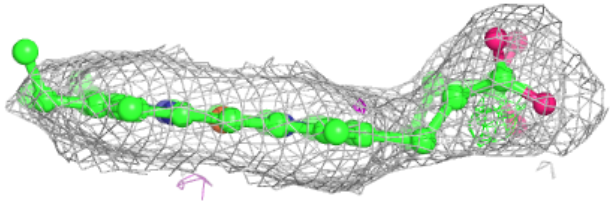


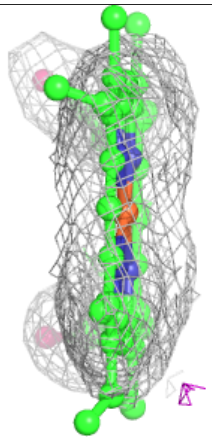


Electron density around HEM C 347:

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

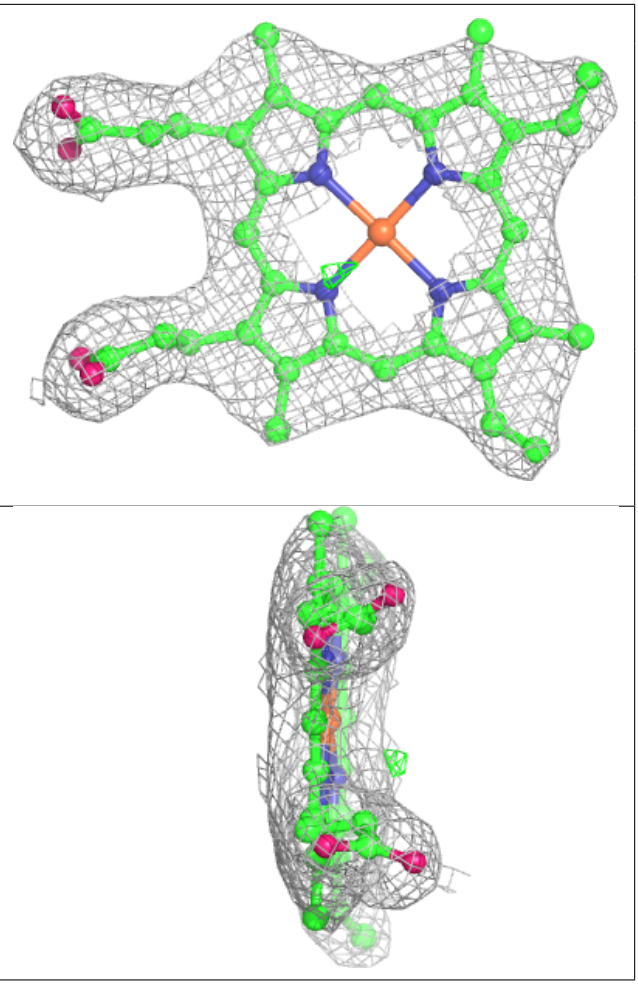






Electron density around HEM A 347:

$2mF_o$-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.