



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:55 pm BST

PDB ID : 2IAG  
Title : Crystal structure of human prostacyclin synthase  
Authors : Chiang, C.-W.; Yeh, H.-C.; Wang, L.-H.; Chan, N.-L.  
Deposited on : 2006-09-08  
Resolution : 2.15 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

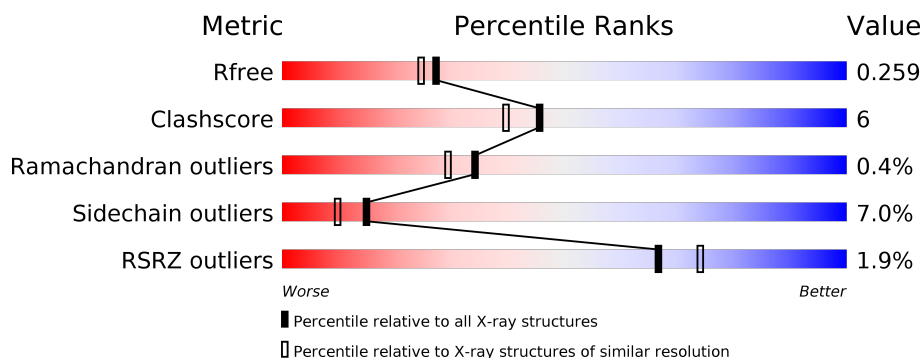
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	482	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	482	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8133 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 Prostacyclin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3816	2454	670	677	15			
1	B	468	Total	C	N	O	S	0	0	0
			3795	2441	668	671	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	HIS	-	EXPRESSION TAG	UNP Q16647
A	502	HIS	-	EXPRESSION TAG	UNP Q16647
A	503	HIS	-	EXPRESSION TAG	UNP Q16647
A	504	HIS	-	EXPRESSION TAG	UNP Q16647
B	501	HIS	-	EXPRESSION TAG	UNP Q16647
B	502	HIS	-	EXPRESSION TAG	UNP Q16647
B	503	HIS	-	EXPRESSION TAG	UNP Q16647
B	504	HIS	-	EXPRESSION TAG	UNP Q16647

- 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
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0

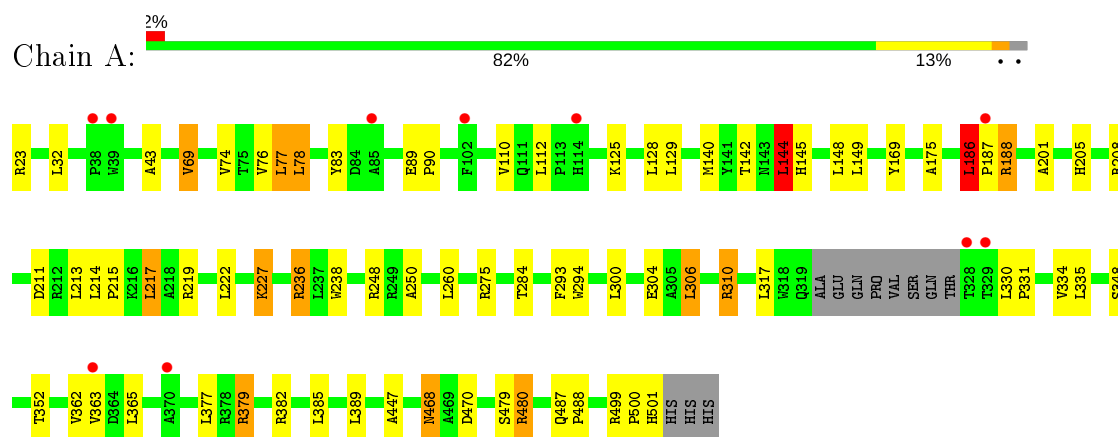
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	212	Total O 212 212	0	0
4	B	223	Total O 223 223	0	0

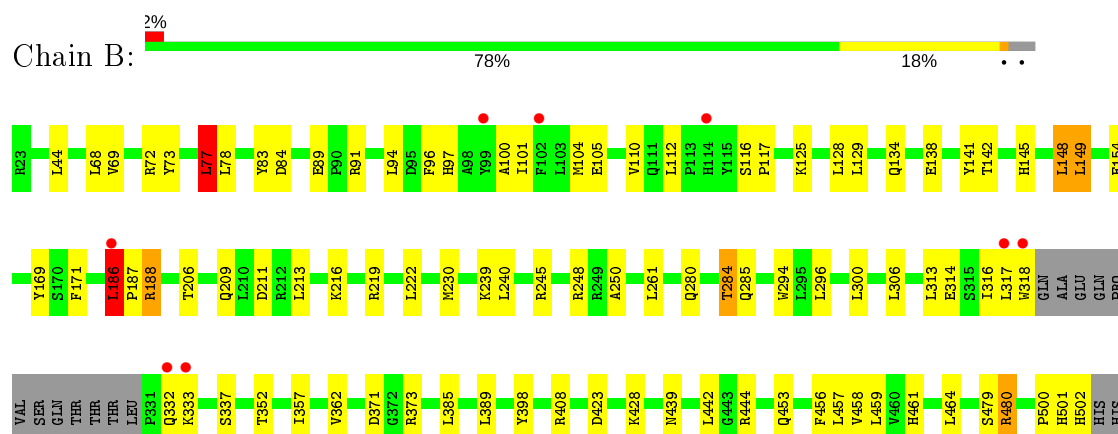
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Prostacyclin synthase



#### • Molecule 1: Prostacyclin synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.73Å 105.60Å 73.95Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	20.15 – 2.15 20.15 – 2.15	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.15-2.15) 90.9 (20.15-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.263 0.201 , 0.259	Depositor DCC
$R_{free}$ test set	2601 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8133	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NA

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	0.54	0/3917	0.69	3/5311 (0.1%)
1	B	0.53	0/3897	0.66	2/5282 (0.0%)
All	All	0.53	0/7814	0.68	5/10593 (0.0%)

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	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	144	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	310	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	480	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	77	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	186	LEU	Peptide

## 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	3816	0	3800	51	0
1	B	3795	0	3775	46	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	B	1	0	0	0	0
4	A	212	0	0	2	0
4	B	223	0	0	5	0
All	All	8133	0	7635	98	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 (98) 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:236:ARG:HG3	1:A:236:ARG:HH11	1.30	0.96
1:B:100:ALA:O	1:B:104:MET:HG3	1.71	0.90
1:A:140:MET:CE	1:A:175:ALA:HB1	2.03	0.88
1:B:284:THR:HG23	1:B:285:GLN:HE21	1.38	0.87
1:A:140:MET:HE3	1:A:175:ALA:HB1	1.57	0.86
1:B:423:ASP:CB	4:B:881:HOH:O	2.25	0.85
1:A:236:ARG:CG	1:A:236:ARG:HH11	1.89	0.85
1:B:423:ASP:HB2	4:B:881:HOH:O	1.79	0.83
1:B:316:ILE:HD11	1:B:337:SER:O	1.84	0.78
1:A:77:LEU:HB3	1:A:385:LEU:HD22	1.64	0.77
1:B:125:LYS:HD2	1:B:129:LEU:HD11	1.67	0.76
1:B:284:THR:HG23	1:B:285:GLN:NE2	2.01	0.75
1:A:140:MET:HE1	1:A:175:ALA:CB	2.16	0.74
1:A:365:LEU:HD11	1:A:377:LEU:HD12	1.69	0.73
1:A:330:LEU:HD11	1:A:334:VAL:HB	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HD13	1:A:222:LEU:HD11	1.73	0.69
1:A:211:ASP:O	1:A:480:ARG:NH2	2.25	0.67
1:B:423:ASP:HB3	4:B:881:HOH:O	1.91	0.66
1:B:371:ASP:OD1	1:B:373:ARG:HD3	1.96	0.66
1:A:187:PRO:HD2	1:A:188:ARG:H	1.60	0.65
1:A:208:ARG:HH12	1:A:487:GLN:HE22	1.44	0.64
1:B:280:GLN:O	1:B:284:THR:HB	1.98	0.64
1:A:125:LYS:HE2	1:A:129:LEU:HD11	1.81	0.63
1:A:140:MET:HE1	1:A:175:ALA:HB3	1.80	0.62
1:A:140:MET:HE1	1:A:175:ALA:HB1	1.78	0.62
1:B:211:ASP:O	1:B:480:ARG:NH2	2.23	0.62
1:A:140:MET:CE	1:A:175:ALA:CB	2.74	0.61
1:A:187:PRO:CD	1:A:188:ARG:H	2.13	0.61
1:A:236:ARG:HG3	1:A:236:ARG:NH1	2.10	0.59
1:A:362:VAL:O	1:A:379:ARG:HD3	2.02	0.58
1:A:219:ARG:NH2	1:A:479:SER:O	2.35	0.58
1:B:216:LYS:HB3	1:B:222:LEU:CD2	2.34	0.58
1:A:306:LEU:O	1:A:310:ARG:HG3	2.04	0.57
1:B:458:VAL:HG11	1:B:464:LEU:HD22	1.88	0.56
1:B:125:LYS:HD2	1:B:129:LEU:CD1	2.36	0.56
1:B:219:ARG:HH12	1:B:479:SER:HB2	1.70	0.55
1:B:145:HIS:O	1:B:149:LEU:HB2	2.07	0.54
1:A:447:ALA:HB2	2:A:600:HEM:HMC2	1.89	0.54
1:B:500:PRO:O	1:B:502:HIS:N	2.41	0.54
1:B:284:THR:HG22	1:B:285:GLN:HG2	1.90	0.54
1:A:76:VAL:HG12	1:A:78:LEU:HD13	1.89	0.53
1:A:236:ARG:CG	1:A:236:ARG:NH1	2.60	0.53
1:A:145:HIS:NE2	1:A:149:LEU:HD12	2.24	0.52
1:A:330:LEU:CD1	1:A:334:VAL:HB	2.37	0.52
1:A:201:ALA:O	1:A:205:HIS:CD2	2.63	0.51
1:A:487:GLN:NE2	4:A:777:HOH:O	2.43	0.51
1:B:97:HIS:CD2	1:B:101:ILE:HD11	2.45	0.51
1:A:186:LEU:HB2	1:A:250:ALA:HB1	1.93	0.51
1:B:68:LEU:HD13	1:B:73:TYR:CE1	2.46	0.50
1:B:284:THR:CG2	1:B:285:GLN:HE21	2.15	0.50
1:A:145:HIS:CE1	1:A:149:LEU:HD12	2.46	0.49
1:B:84:ASP:OD2	1:B:428:LYS:HD2	2.11	0.49
1:A:330:LEU:HD22	1:A:331:PRO:HD2	1.94	0.49
1:B:89:GLU:HG3	1:B:94:LEU:HD12	1.94	0.49
1:A:83:TYR:CD1	1:A:385:LEU:HD13	2.48	0.49
1:B:96:PHE:HB2	1:B:439:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:HB3	1:A:215:PRO:HD3	1.94	0.49
1:B:77:LEU:HB3	1:B:385:LEU:HD22	1.95	0.48
1:B:91:ARG:O	1:B:362:VAL:HG21	2.14	0.48
1:A:201:ALA:O	1:A:205:HIS:HD2	1.97	0.48
1:B:206:THR:HA	1:B:209:GLN:HE21	1.79	0.47
1:B:357:ILE:HB	1:B:385:LEU:HB2	1.96	0.47
1:B:245:ARG:NH2	4:B:796:HOH:O	2.47	0.47
1:B:294:TRP:CG	1:B:352:THR:HG21	2.50	0.46
1:B:83:TYR:CD1	1:B:385:LEU:HD13	2.51	0.46
1:A:187:PRO:CD	1:A:188:ARG:N	2.76	0.46
1:B:219:ARG:NH1	1:B:479:SER:HB2	2.31	0.46
1:A:227:LYS:HB2	1:A:227:LYS:HE2	1.74	0.46
1:B:154:GLU:HG3	4:B:869:HOH:O	2.16	0.45
1:A:43:ALA:HA	1:A:69:VAL:HG23	1.99	0.45
2:B:600:HEM:HHC	2:B:600:HEM:HBB2	1.98	0.45
1:A:140:MET:HE2	1:A:144:LEU:HD22	1.98	0.44
1:A:499:ARG:HA	1:A:500:PRO:HD3	1.79	0.44
1:B:148:LEU:HD22	1:B:171:PHE:CG	2.53	0.44
1:B:284:THR:CG2	1:B:285:GLN:HG2	2.47	0.44
1:B:116:SER:HA	1:B:117:PRO:HD3	1.88	0.44
1:B:239:LYS:HD2	1:B:239:LYS:HA	1.73	0.42
1:A:187:PRO:HD2	1:A:188:ARG:N	2.33	0.42
1:B:316:ILE:CG2	1:B:333:LYS:HB2	2.50	0.42
1:B:457:LEU:O	1:B:461:HIS:HB2	2.18	0.42
1:A:23:ARG:HG3	1:A:32:LEU:HD21	2.00	0.42
1:B:97:HIS:CD2	1:B:117:PRO:HG3	2.54	0.42
1:B:186:LEU:HB2	1:B:250:ALA:HB1	2.01	0.42
1:A:74:VAL:HA	1:A:382:ARG:O	2.19	0.42
1:A:89:GLU:HA	1:A:90:PRO:HD3	1.86	0.42
1:B:134:GLN:O	1:B:138:GLU:HG3	2.19	0.42
1:A:238:TRP:CE2	1:A:275:ARG:HG2	2.54	0.42
1:A:501:HIS:HB3	1:B:444:ARG:HD3	2.02	0.41
1:B:141:TYR:HB2	1:B:453:GLN:NE2	2.35	0.41
1:A:293:PHE:CE2	1:A:488:PRO:HG3	2.55	0.41
1:A:125:LYS:HE3	4:A:657:HOH:O	2.21	0.41
1:A:284:THR:HB	2:A:600:HEM:CBC	2.51	0.41
1:A:389:LEU:HD12	1:A:389:LEU:HA	1.89	0.40
1:A:468:ASN:ND2	1:A:470:ASP:H	2.19	0.40
1:B:313:LEU:HD22	1:B:456:PHE:HD1	1.85	0.40
1:B:398:TYR:CD2	1:B:408:ARG:HD3	2.56	0.40
1:A:294:TRP:CG	1:A:352:THR:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:600:HEM:HBB2	2:A:600:HEM:HMB2	2.03	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	467/482 (97%)	458 (98%)	9 (2%)	0	100	100
1	B	464/482 (96%)	447 (96%)	13 (3%)	4 (1%)	17	11
All	All	931/964 (97%)	905 (97%)	22 (2%)	4 (0%)	34	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	501	HIS
1	B	188	ARG
1	B	332	GLN
1	B	187	PRO

### 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	408/418 (98%)	381 (93%)	27 (7%)	16	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	405/418 (97%)	375 (93%)	30 (7%)	13	9
All	All	813/836 (97%)	756 (93%)	57 (7%)	15	10

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	VAL
1	A	77	LEU
1	A	78	LEU
1	A	110	VAL
1	A	112	LEU
1	A	128	LEU
1	A	142	THR
1	A	144	LEU
1	A	148	LEU
1	A	169	TYR
1	A	186	LEU
1	A	188	ARG
1	A	213	LEU
1	A	217	LEU
1	A	227	LYS
1	A	236	ARG
1	A	248	ARG
1	A	260	LEU
1	A	300	LEU
1	A	304	GLU
1	A	306	LEU
1	A	317	LEU
1	A	335	LEU
1	A	348	SER
1	A	363	VAL
1	A	379	ARG
1	A	468	ASN
1	B	44	LEU
1	B	69	VAL
1	B	72	ARG
1	B	77	LEU
1	B	78	LEU
1	B	105	GLU
1	B	110	VAL
1	B	112	LEU
1	B	128	LEU

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Mol	Chain	Res	Type
1	B	142	THR
1	B	148	LEU
1	B	149	LEU
1	B	169	TYR
1	B	186	LEU
1	B	188	ARG
1	B	213	LEU
1	B	230	MET
1	B	240	LEU
1	B	248	ARG
1	B	261	LEU
1	B	284	THR
1	B	296	LEU
1	B	300	LEU
1	B	306	LEU
1	B	314	GLU
1	B	317	LEU
1	B	318	TRP
1	B	389	LEU
1	B	442	LEU
1	B	459	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	160	HIS
1	A	205	HIS
1	A	449	ASN
1	A	453	GLN
1	A	468	ASN
1	A	487	GLN
1	A	490	HIS
1	B	195	GLN
1	B	209	GLN
1	B	285	GLN
1	B	332	GLN
1	B	449	ASN
1	B	468	ASN
1	B	490	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	B	600	1	27,50,50	2.31	8 (29%)	17,82,82	1.29	2 (11%)
2	HEM	A	600	1	27,50,50	2.23	7 (25%)	17,82,82	1.75	5 (29%)

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	B	600	1	-	3/6/54/54	-
2	HEM	A	600	1	-	4/6/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3D-C2D	5.87	1.55	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HEM	C3D-C2D	5.60	1.54	1.37
2	B	600	HEM	C3C-C2C	-4.68	1.33	1.40
2	B	600	HEM	C3B-C2B	-4.63	1.33	1.40
2	B	600	HEM	C3C-CAC	4.34	1.56	1.47
2	A	600	HEM	C3C-C2C	-4.15	1.34	1.40
2	A	600	HEM	C3B-CAB	3.85	1.55	1.47
2	A	600	HEM	C3B-C2B	-3.80	1.35	1.40
2	A	600	HEM	C3C-CAC	3.77	1.55	1.47
2	B	600	HEM	C3B-CAB	3.56	1.55	1.47
2	B	600	HEM	CAA-C2A	2.56	1.55	1.52
2	A	600	HEM	CAA-C2A	2.25	1.55	1.52
2	A	600	HEM	CAD-C3D	2.09	1.55	1.52
2	B	600	HEM	C1D-ND	2.07	1.40	1.36
2	B	600	HEM	CAD-C3D	2.04	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	CMA-C3A-C4A	-2.78	124.19	128.46
2	B	600	HEM	CMA-C3A-C4A	-2.70	124.32	128.46
2	A	600	HEM	CMD-C2D-C3D	2.48	129.62	124.94
2	A	600	HEM	CMD-C2D-C1D	-2.43	124.72	128.46
2	A	600	HEM	CAA-CBA-CGA	-2.34	108.74	112.67
2	A	600	HEM	CMB-C2B-C3B	2.27	128.93	124.68
2	B	600	HEM	CBA-CAA-C2A	-2.09	108.64	112.49

There are no chirality outliers.

All (7) torsion outliers are listed below:

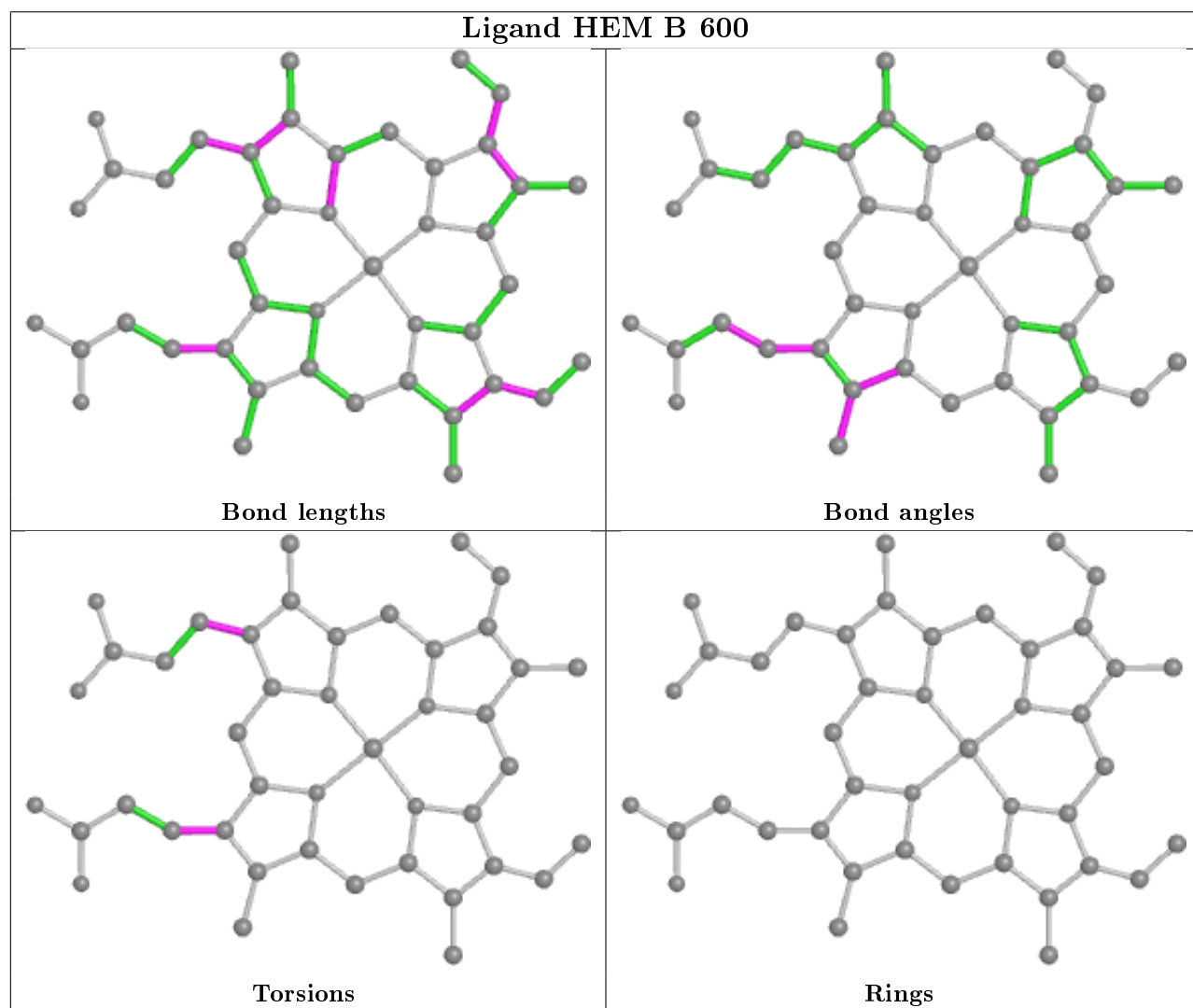
Mol	Chain	Res	Type	Atoms
2	B	600	HEM	C2D-C3D-CAD-CBD
2	A	600	HEM	C2A-CAA-CBA-CGA
2	A	600	HEM	C2D-C3D-CAD-CBD
2	A	600	HEM	C4D-C3D-CAD-CBD
2	A	600	HEM	C3D-CAD-CBD-CGD
2	B	600	HEM	C1A-C2A-CAA-CBA
2	B	600	HEM	C4D-C3D-CAD-CBD

There are no ring outliers.

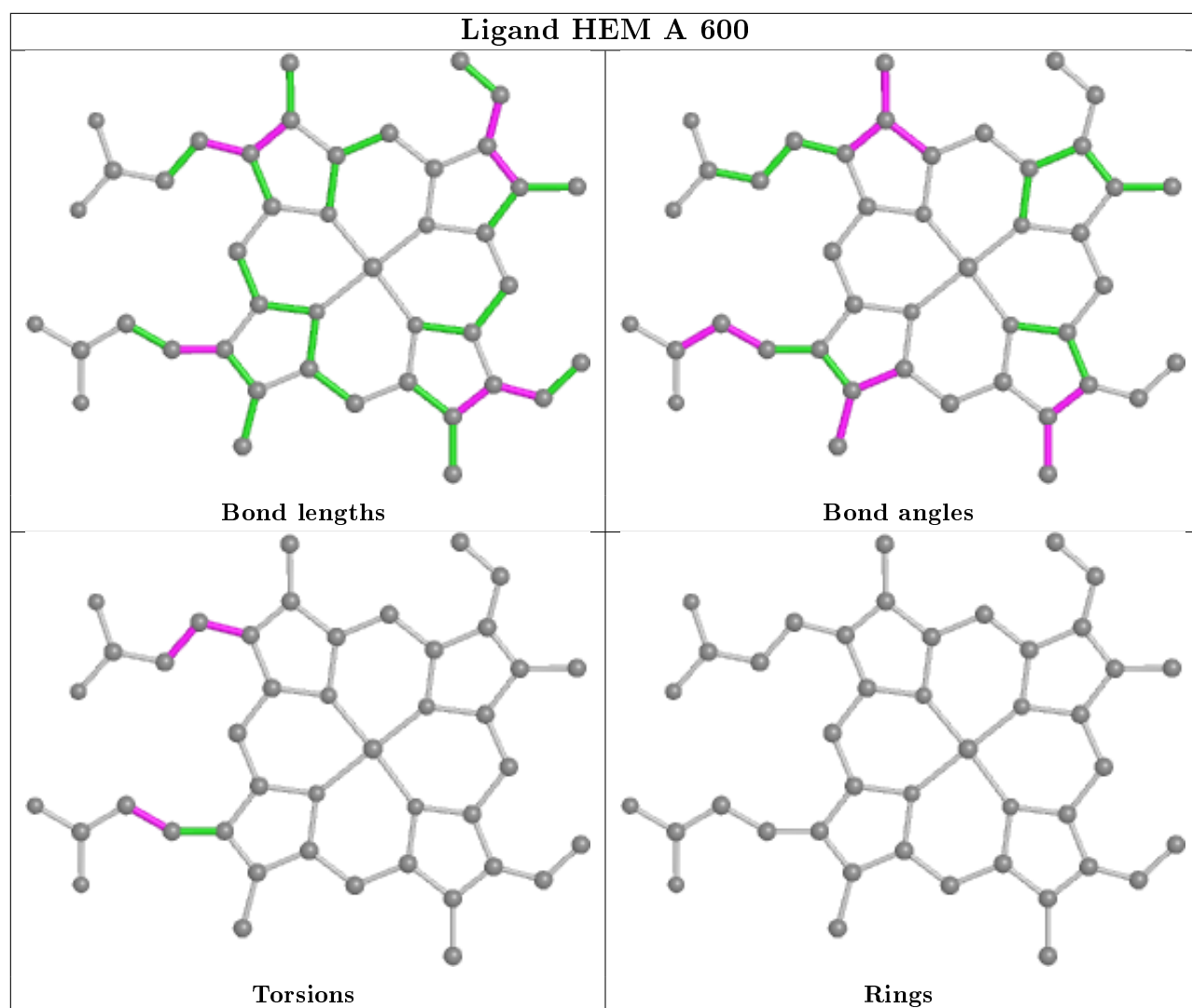
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	HEM	1	0
2	A	600	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	471/482 (97%)	0.02	10 (2%) 63 71	10, 26, 45, 53	0
1	B	468/482 (97%)	-0.09	8 (1%) 70 76	13, 25, 38, 55	0
All	All	939/964 (97%)	-0.04	18 (1%) 66 74	10, 25, 42, 55	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	TRP	5.1
1	A	328	THR	4.3
1	A	38	PRO	3.8
1	A	39	TRP	3.5
1	A	363	VAL	3.4
1	A	114	HIS	3.3
1	A	370	ALA	3.3
1	A	187	PRO	3.3
1	B	102	PHE	3.2
1	B	186	LEU	3.1
1	B	114	HIS	2.8
1	B	317	LEU	2.5
1	B	333	LYS	2.4
1	A	329	THR	2.4
1	A	102	PHE	2.4
1	A	85	ALA	2.3
1	B	99	TYR	2.1
1	B	332	GLN	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

There are no carbohydrates in this entry.

### 6.4 Ligands

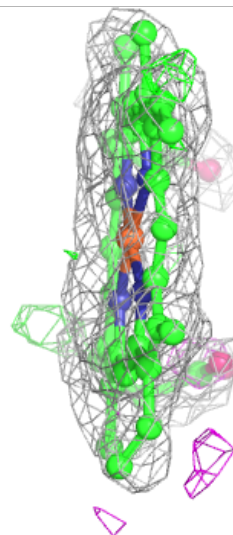
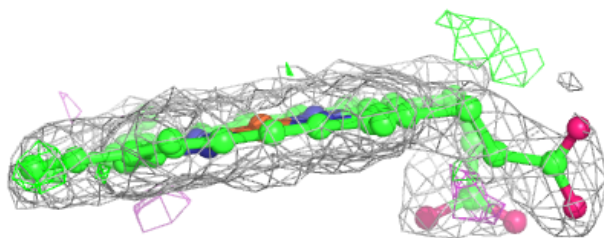
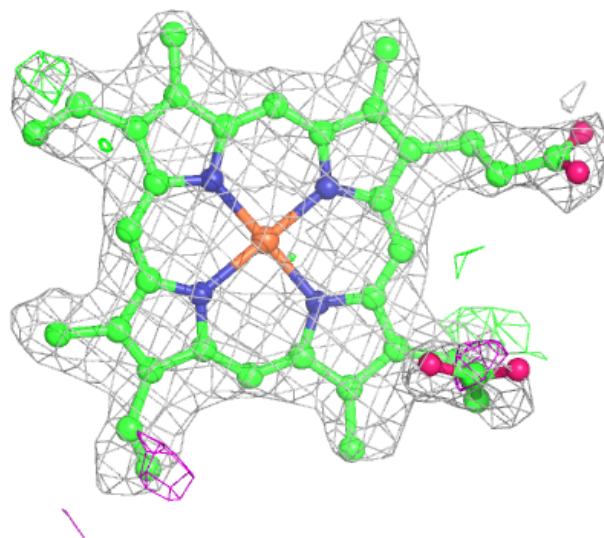
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	B	600	43/43	0.95	0.13	19,23,40,44	0
2	HEM	A	600	43/43	0.96	0.12	20,23,38,40	0
3	NA	B	701	1/1	0.99	0.08	15,15,15,15	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.

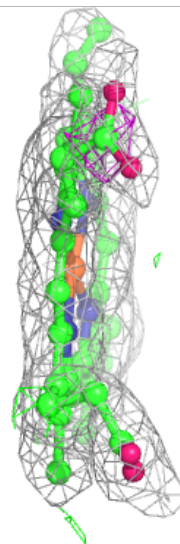
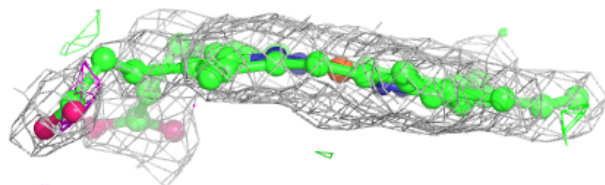
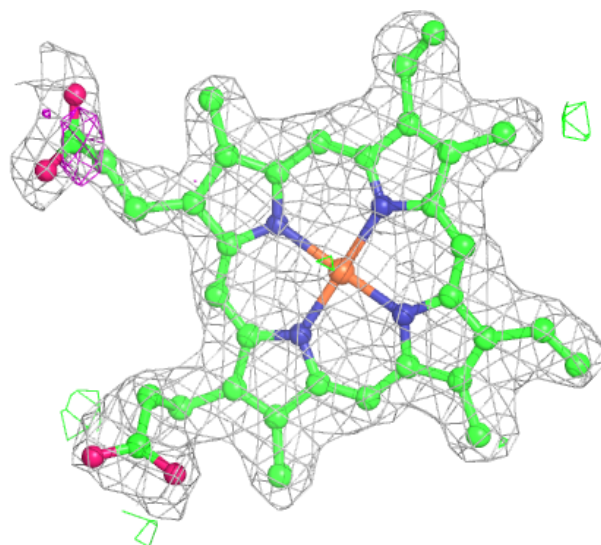
**Electron density around HEM B 600:**

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



**Electron density around HEM A 600:**

$2mF_o-DF_c$  (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.