



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 10:31 AM EDT

PDB ID : 2RGZ
Title : Ensemble refinement of the protein crystal structure of human heme oxygenase-2 C127A (HO-2) with bound heme
Authors : Bianchetti, C.M.; Bingman, C.A.; Bitto, E.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-10-05
Resolution : 2.61 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 : 4.02b-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

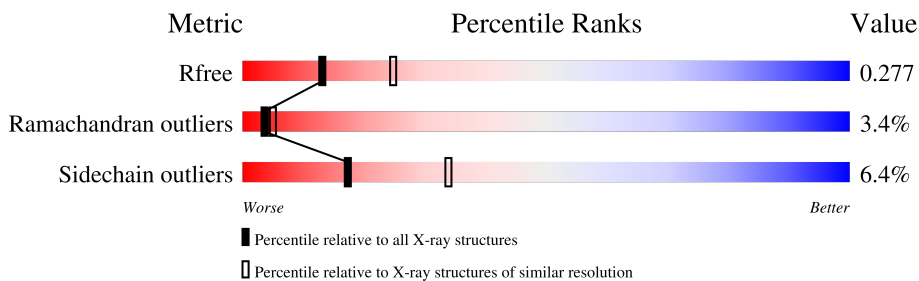
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1-A	264	
1	1-B	264	
1	10-A	264	
1	10-B	264	
1	11-A	264	
1	11-B	264	
1	12-A	264	
1	12-B	264	

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Mol	Chain	Length	Quality of chain		
1	13-A	264	72%	9%	19%
1	13-B	264	76%	7%	17%
1	14-A	264	72%	9%	19%
1	14-B	264	72%	11%	17%
1	15-A	264	72%	9%	19%
1	15-B	264	73%	9%	17%
1	16-A	264	73%	7%	19%
1	16-B	264	71%	12%	17%
1	2-A	264	76%	5%	19%
1	2-B	264	79%	.	17%
1	3-A	264	75%	6%	19%
1	3-B	264	73%	9%	17%
1	4-A	264	73%	8%	19%
1	4-B	264	77%	6%	17%
1	5-A	264	75%	6%	19%
1	5-B	264	76%	7%	17%
1	6-A	264	76%	5%	19%
1	6-B	264	74%	9%	17%
1	7-A	264	75%	6%	19%
1	7-B	264	77%	6%	17%
1	8-A	264	77%	.	19%
1	8-B	264	74%	8%	17%
1	9-A	264	74%	7%	19%
1	9-B	264	77%	6%	17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 58291 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 Heme oxygenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	2-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	3-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	4-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	5-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	6-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	7-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	8-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	9-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	10-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	11-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	12-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	13-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	14-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	15-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0
1	16-A	214	Total 1758	C 1118	N 299	O 333	S 8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	2-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	3-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	4-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	5-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	6-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	7-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	8-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	9-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	10-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	11-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	12-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	13-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	14-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	15-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	16-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	CYS	engineered mutation	UNP P30519
B	127	ALA	CYS	engineered mutation	UNP P30519

- 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	1-A	1	43	34	1	4	4	0	0
2	2-A	1	43	34	1	4	4	0	0
2	3-A	1	43	34	1	4	4	0	0
2	4-A	1	43	34	1	4	4	0	0
2	5-A	1	43	34	1	4	4	0	0
2	6-A	1	43	34	1	4	4	0	0
2	7-A	1	43	34	1	4	4	0	0
2	8-A	1	43	34	1	4	4	0	0
2	9-A	1	43	34	1	4	4	0	0
2	10-A	1	43	34	1	4	4	0	0
2	11-A	1	43	34	1	4	4	0	0
2	12-A	1	43	34	1	4	4	0	0
2	13-A	1	43	34	1	4	4	0	0
2	14-A	1	43	34	1	4	4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	15-A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	16-A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	1-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	2-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	3-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	4-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	5-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	6-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	7-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	8-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	9-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	10-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	11-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	12-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	13-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	14-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	15-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	16-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	49	Total	O	0	0
			49	49		

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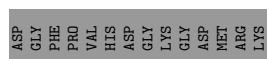
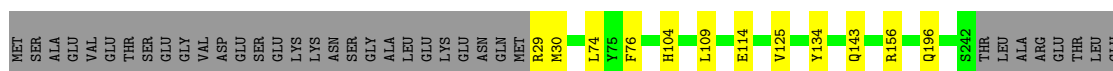
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-B	34	Total	O	0	0
			34	34		

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

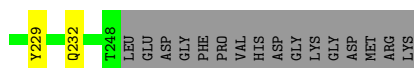
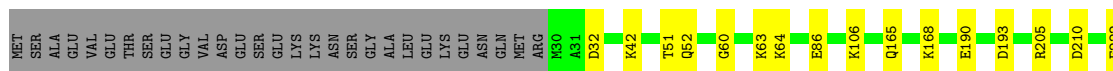
- Molecule 1: Heme oxygenase 2

Chain 1-A:  77% 5% 19%




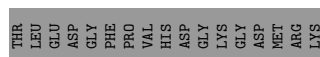
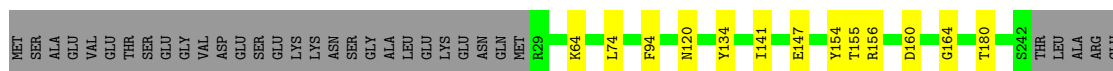
- Molecule 1: Heme oxygenase 2

Chain 1-B:  76% 7% 17%




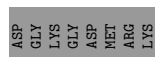
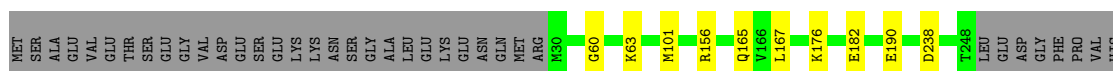
- Molecule 1: Heme oxygenase 2

Chain 2-A:  76% 5% 19%

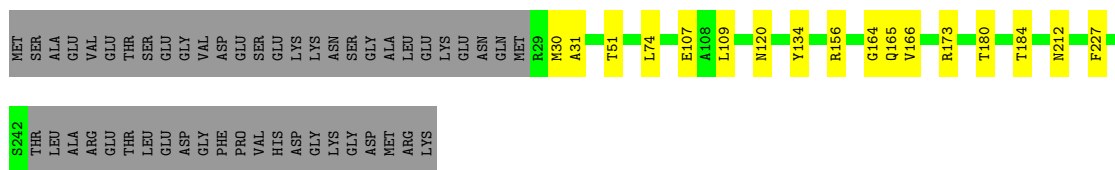
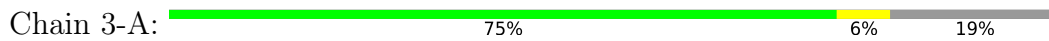


- Molecule 1: Heme oxygenase 2

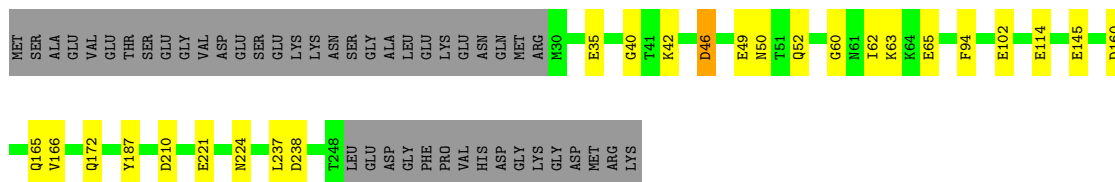
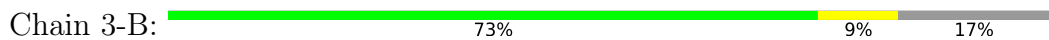
Chain 2-B:  79% 1% 17%



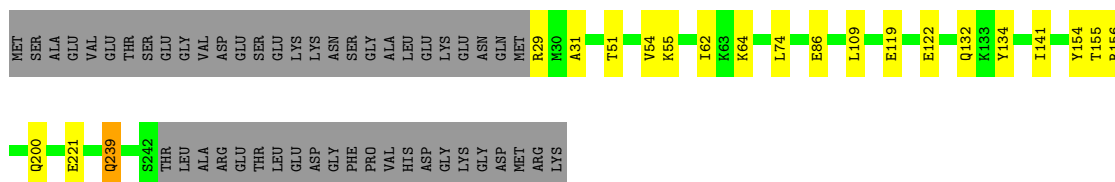
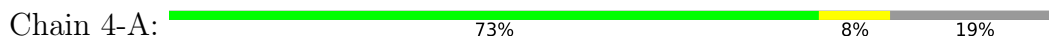
- Molecule 1: Heme oxygenase 2



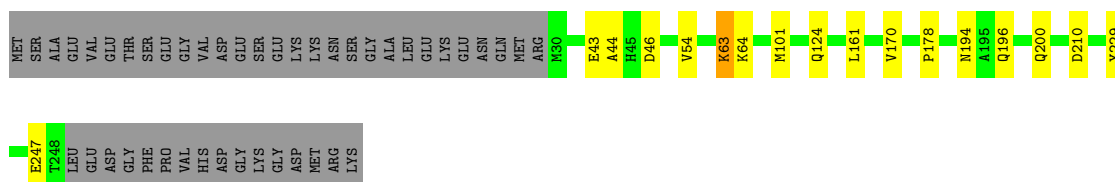
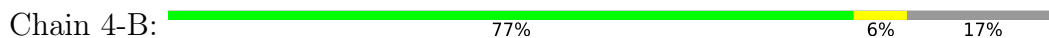
- Molecule 1: Heme oxygenase 2



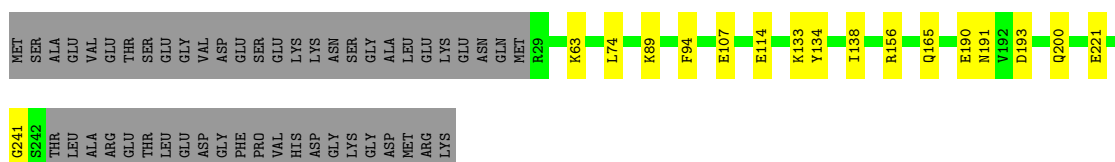
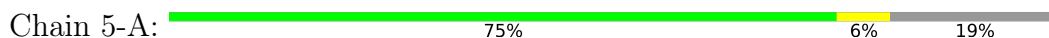
- Molecule 1: Heme oxygenase 2




- Molecule 1: Heme oxygenase 2

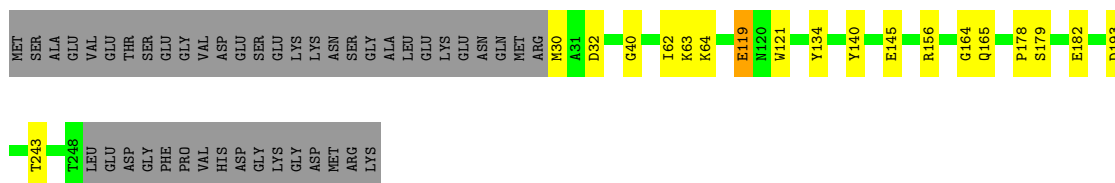


- Molecule 1: Heme oxygenase 2




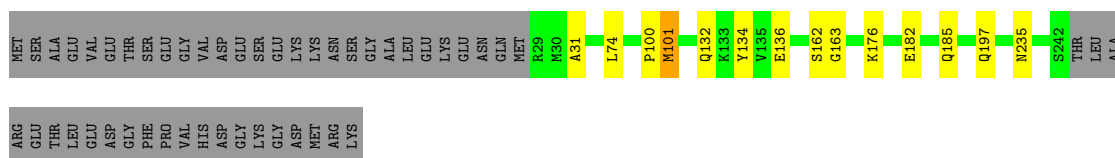
- Molecule 1: Heme oxygenase 2

Chain 5-B:  76% 7% 17%




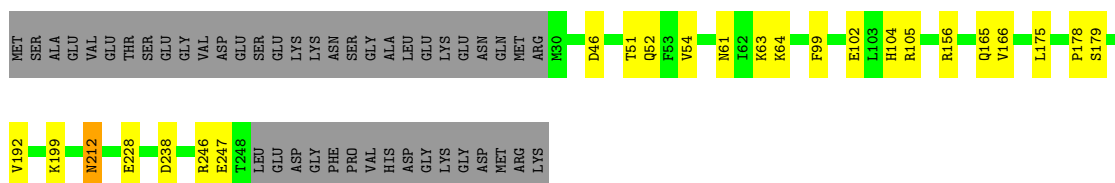
- Molecule 1: Heme oxygenase 2

Chain 6-A:  76% 5% 19%




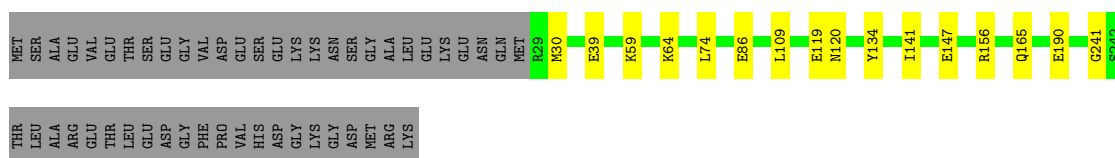
- Molecule 1: Heme oxygenase 2

Chain 6-B:  74% 9% 17%




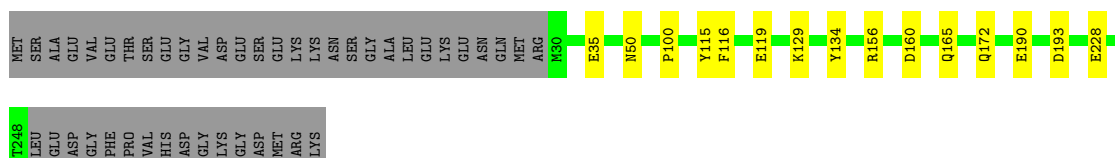
- Molecule 1: Heme oxygenase 2

Chain 7-A:  75% 6% 19%




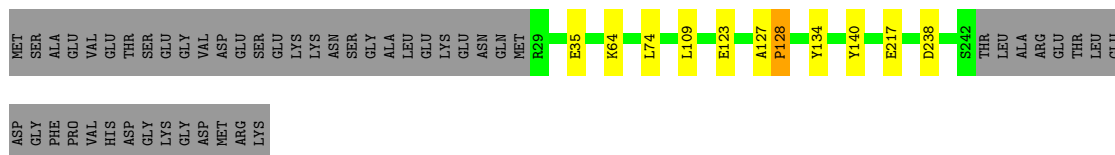
- Molecule 1: Heme oxygenase 2

Chain 7-B:  77% 6% 17%



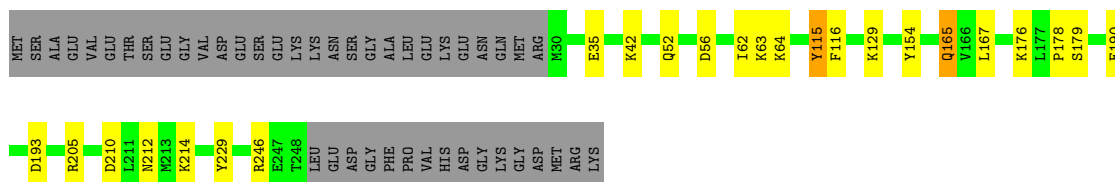
- Molecule 1: Heme oxygenase 2

Chain 8-A:  77% 19%



• Molecule 1: Heme oxygenase 2

Chain 8-B: 74% 8% 17%



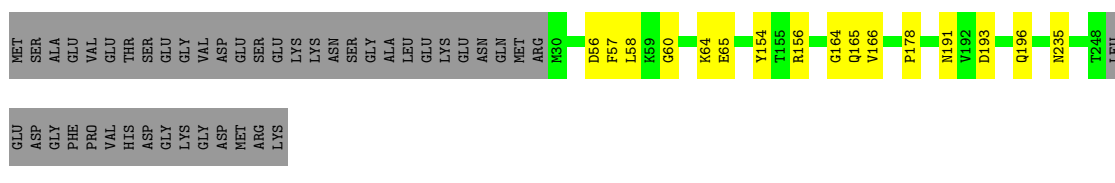
• Molecule 1: Heme oxygenase 2

Chain 9-A: 74% 7% 19%



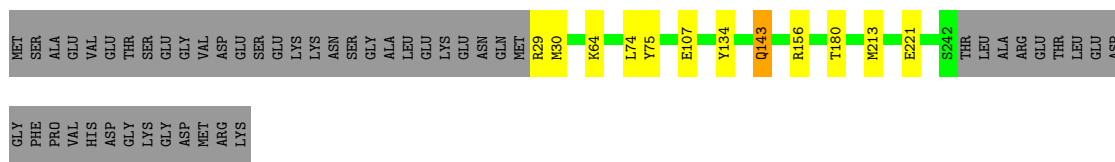
• Molecule 1: Heme oxygenase 2

Chain 9-B: 77% 6% 17%



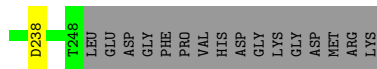
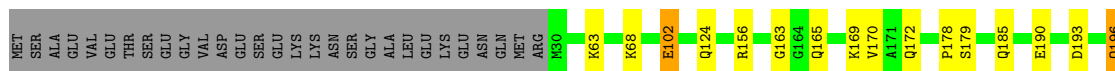
• Molecule 1: Heme oxygenase 2

Chain 10-A: 77% 6% 19%



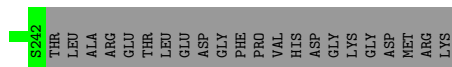
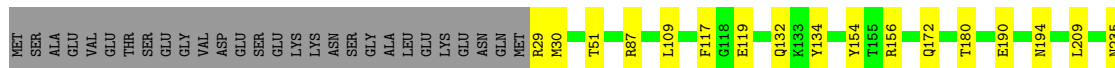
• Molecule 1: Heme oxygenase 2

Chain 10-B: 77% 6% 17%



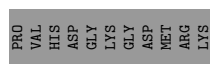
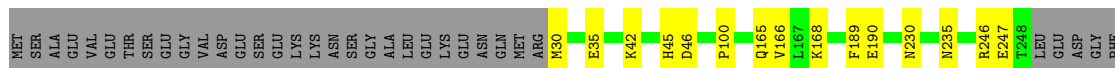
- Molecule 1: Heme oxygenase 2

Chain 11-A: 75% 6% 19%



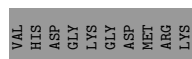
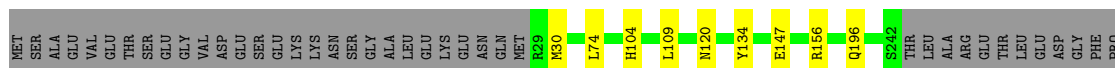
- Molecule 1: Heme oxygenase 2

Chain 11-B: 77% 6% 17%



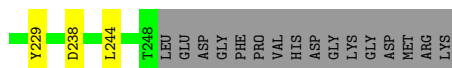
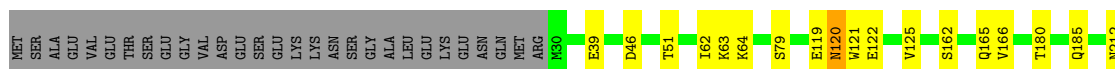
- Molecule 1: Heme oxygenase 2

Chain 12-A: 78% 0% 19%



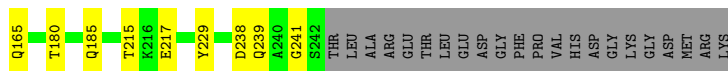
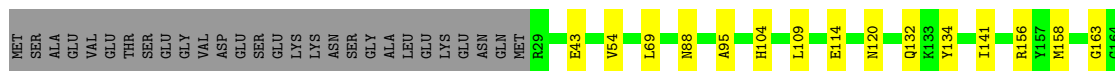
- Molecule 1: Heme oxygenase 2

Chain 12-B: 75% 8% 17%



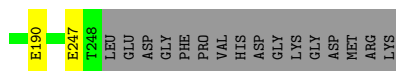
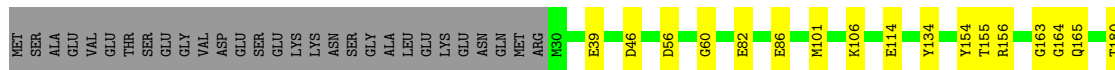
- Molecule 1: Heme oxygenase 2

Chain 13-A: 72% 9% 19%



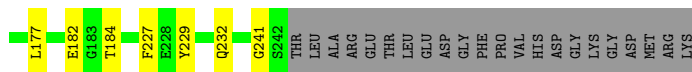
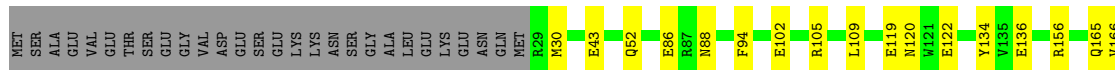
- Molecule 1: Heme oxygenase 2

Chain 13-B: 76% 7% 17%



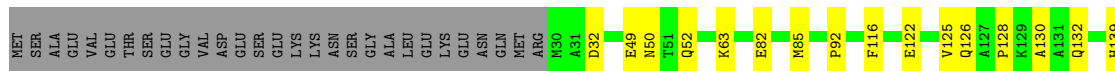
- Molecule 1: Heme oxygenase 2

Chain 14-A: 72% 9% 19%



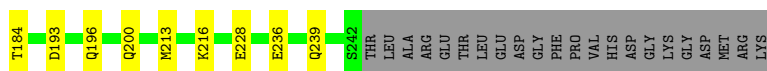
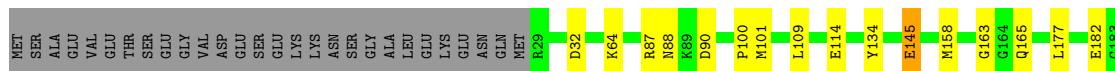
- Molecule 1: Heme oxygenase 2

Chain 14-B: 72% 11% 17%



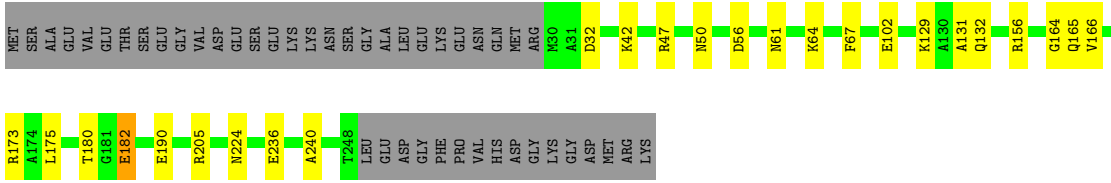
- Molecule 1: Heme oxygenase 2

Chain 15-A: 72% 9% 19%



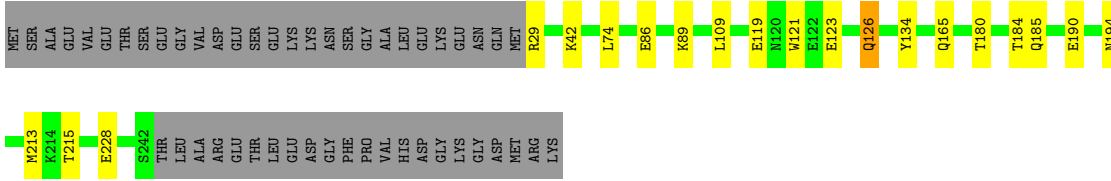
- Molecule 1: Heme oxygenase 2

Chain 15-B: 73% 9% 17%



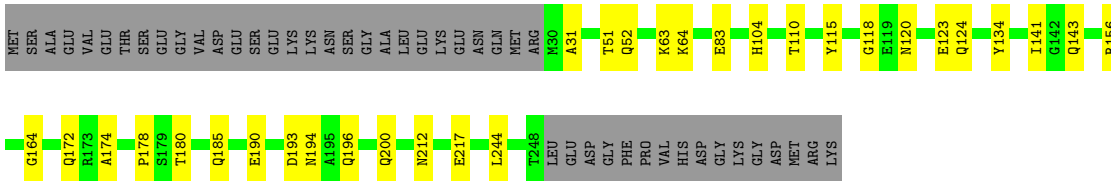
- Molecule 1: Heme oxygenase 2

Chain 16-A: 73% 7% 19%



- Molecule 1: Heme oxygenase 2

Chain 16-B: 71% 12% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.98Å 85.09Å 97.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.02 – 2.61 39.02 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.02-2.61) 99.4 (39.02-2.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.61Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.161 , 0.249 0.205 , 0.277	Depositor DCC
R_{free} test set	1005 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 158.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	58291	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1-A	0.43	0/1794	0.57	0/2410
1	1-B	0.39	0/1830	0.54	0/2460
1	2-A	0.43	0/1794	0.56	0/2410
1	2-B	0.40	0/1830	0.54	0/2460
1	3-A	0.43	0/1794	0.57	0/2410
1	3-B	0.39	0/1830	0.56	0/2460
1	4-A	0.44	0/1794	0.58	0/2410
1	4-B	0.39	0/1830	0.56	0/2460
1	5-A	0.43	0/1794	0.58	1/2410 (0.0%)
1	5-B	0.39	0/1830	0.54	0/2460
1	6-A	0.42	0/1794	0.56	0/2410
1	6-B	0.40	0/1830	0.55	0/2460
1	7-A	0.42	0/1794	0.57	0/2410
1	7-B	0.39	0/1830	0.54	0/2460
1	8-A	0.44	0/1794	0.57	0/2410
1	8-B	0.39	0/1830	0.55	0/2460
1	9-A	0.43	0/1794	0.57	0/2410
1	9-B	0.39	0/1830	0.54	0/2460
1	10-A	0.43	0/1794	0.57	0/2410
1	10-B	0.40	0/1830	0.55	0/2460
1	11-A	0.43	0/1794	0.56	0/2410
1	11-B	0.40	0/1830	0.55	0/2460
1	12-A	0.43	0/1794	0.55	0/2410
1	12-B	0.40	0/1830	0.55	0/2460
1	13-A	0.47	0/1794	0.63	0/2410
1	13-B	0.43	0/1830	0.55	0/2460
1	14-A	0.48	0/1794	0.61	0/2410
1	14-B	0.44	0/1830	0.58	0/2460
1	15-A	0.50	0/1794	0.64	0/2410
1	15-B	0.43	0/1830	0.60	0/2460
1	16-A	0.49	0/1794	0.64	0/2410
1	16-B	0.42	0/1830	0.57	0/2460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.42	0/57984	0.57	1/77920 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	5-A	156	ARG	NE-CZ-NH2	-5.48	117.56	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1-A	1758	0	1717	0	0
1	1-B	1794	0	1753	0	0
1	2-A	1758	0	1717	0	0
1	2-B	1794	0	1753	0	0
1	3-A	1758	0	1717	0	0
1	3-B	1794	0	1753	0	0
1	4-A	1758	0	1717	0	0
1	4-B	1794	0	1753	0	0
1	5-A	1758	0	1717	0	0
1	5-B	1794	0	1753	0	0
1	6-A	1758	0	1717	0	0
1	6-B	1794	0	1753	0	0
1	7-A	1758	0	1717	0	0
1	7-B	1794	0	1753	0	0
1	8-A	1758	0	1717	0	0
1	8-B	1794	0	1753	0	0
1	9-A	1758	0	1717	0	0
1	9-B	1794	0	1753	0	0
1	10-A	1758	0	1717	0	0
1	10-B	1794	0	1753	0	0
1	11-A	1758	0	1717	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	11-B	1794	0	1753	0	0
1	12-A	1758	0	1717	0	0
1	12-B	1794	0	1753	0	0
1	13-A	1758	0	1717	0	0
1	13-B	1794	0	1753	0	0
1	14-A	1758	0	1717	0	0
1	14-B	1794	0	1753	0	0
1	15-A	1758	0	1717	0	0
1	15-B	1794	0	1753	0	0
1	16-A	1758	0	1717	0	0
1	16-B	1794	0	1753	0	0
2	1-A	43	0	30	0	0
2	1-B	43	0	30	0	0
2	2-A	43	0	30	0	0
2	2-B	43	0	30	0	0
2	3-A	43	0	30	0	0
2	3-B	43	0	30	0	0
2	4-A	43	0	30	0	0
2	4-B	43	0	30	0	0
2	5-A	43	0	30	0	0
2	5-B	43	0	30	0	0
2	6-A	43	0	30	0	0
2	6-B	43	0	30	0	0
2	7-A	43	0	30	0	0
2	7-B	43	0	30	0	0
2	8-A	43	0	30	0	0
2	8-B	43	0	30	0	0
2	9-A	43	0	30	0	0
2	9-B	43	0	30	0	0
2	10-A	43	0	30	0	0
2	10-B	43	0	30	0	0
2	11-A	43	0	30	0	0
2	11-B	43	0	30	0	0
2	12-A	43	0	30	0	0
2	12-B	43	0	30	0	0
2	13-A	43	0	30	0	0
2	13-B	43	0	30	0	0
2	14-A	43	0	30	0	0
2	14-B	43	0	30	0	0
2	15-A	43	0	30	0	0
2	15-B	43	0	30	0	0
2	16-A	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	16-B	43	0	30	0	0
3	1-A	49	0	0	0	0
3	1-B	34	0	0	0	0
All	All	58291	0	56480	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	212/264 (80%)	185 (87%)	23 (11%)	4 (2%)	8	14
1	1-B	217/264 (82%)	190 (88%)	19 (9%)	8 (4%)	3	4
1	2-A	212/264 (80%)	184 (87%)	23 (11%)	5 (2%)	6	9
1	2-B	217/264 (82%)	183 (84%)	30 (14%)	4 (2%)	8	15
1	3-A	212/264 (80%)	192 (91%)	17 (8%)	3 (1%)	11	21
1	3-B	217/264 (82%)	174 (80%)	33 (15%)	10 (5%)	2	2
1	4-A	212/264 (80%)	188 (89%)	17 (8%)	7 (3%)	4	5
1	4-B	217/264 (82%)	175 (81%)	35 (16%)	7 (3%)	4	5
1	5-A	212/264 (80%)	189 (89%)	18 (8%)	5 (2%)	6	9
1	5-B	217/264 (82%)	186 (86%)	22 (10%)	9 (4%)	3	3
1	6-A	212/264 (80%)	181 (85%)	25 (12%)	6 (3%)	5	7
1	6-B	217/264 (82%)	167 (77%)	38 (18%)	12 (6%)	2	1
1	7-A	212/264 (80%)	182 (86%)	26 (12%)	4 (2%)	8	14
1	7-B	217/264 (82%)	183 (84%)	28 (13%)	6 (3%)	5	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-A	212/264 (80%)	187 (88%)	21 (10%)	4 (2%)	8	14
1	8-B	217/264 (82%)	183 (84%)	21 (10%)	13 (6%)	1	1
1	9-A	212/264 (80%)	179 (84%)	24 (11%)	9 (4%)	3	3
1	9-B	217/264 (82%)	184 (85%)	23 (11%)	10 (5%)	2	2
1	10-A	212/264 (80%)	189 (89%)	20 (9%)	3 (1%)	11	21
1	10-B	217/264 (82%)	185 (85%)	23 (11%)	9 (4%)	3	3
1	11-A	212/264 (80%)	185 (87%)	24 (11%)	3 (1%)	11	21
1	11-B	217/264 (82%)	184 (85%)	28 (13%)	5 (2%)	6	10
1	12-A	212/264 (80%)	198 (93%)	12 (6%)	2 (1%)	17	33
1	12-B	217/264 (82%)	174 (80%)	33 (15%)	10 (5%)	2	2
1	13-A	212/264 (80%)	186 (88%)	21 (10%)	5 (2%)	6	9
1	13-B	217/264 (82%)	182 (84%)	26 (12%)	9 (4%)	3	3
1	14-A	212/264 (80%)	176 (83%)	30 (14%)	6 (3%)	5	7
1	14-B	217/264 (82%)	165 (76%)	35 (16%)	17 (8%)	1	1
1	15-A	212/264 (80%)	176 (83%)	26 (12%)	10 (5%)	2	2
1	15-B	217/264 (82%)	171 (79%)	36 (17%)	10 (5%)	2	2
1	16-A	212/264 (80%)	177 (84%)	32 (15%)	3 (1%)	11	21
1	16-B	217/264 (82%)	172 (79%)	28 (13%)	17 (8%)	1	1
All	All	6864/8448 (81%)	5812 (85%)	817 (12%)	235 (3%)	3	5

All (235) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-B	64	LYS
1	2-A	64	LYS
1	3-B	46	ASP
1	3-B	52	GLN
1	3-B	65	GLU
1	4-A	154	TYR
1	4-A	239	GLN
1	4-B	44	ALA
1	5-B	62	ILE
1	5-B	64	LYS
1	5-B	119	GLU
1	6-A	31	ALA
1	6-A	100	PRO

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Mol	Chain	Res	Type
1	6-A	101	MET
1	6-B	247	GLU
1	7-A	64	LYS
1	8-A	64	LYS
1	8-A	127	ALA
1	8-A	128	PRO
1	8-B	62	ILE
1	8-B	64	LYS
1	8-B	154	TYR
1	9-A	31	ALA
1	9-A	100	PRO
1	9-A	101	MET
1	9-B	166	VAL
1	10-A	64	LYS
1	12-B	51	THR
1	12-B	64	LYS
1	12-B	120	ASN
1	12-B	166	VAL
1	14-B	50	ASN
1	15-A	100	PRO
1	15-B	164	GLY
1	15-B	182	GLU
1	16-A	121	TRP
1	16-B	31	ALA
1	16-B	64	LYS
1	16-B	120	ASN
1	16-B	124	GLN
1	16-B	193	ASP
1	1-A	125	VAL
1	1-B	52	GLN
1	1-B	193	ASP
1	2-A	94	PHE
1	2-A	155	THR
1	2-B	176	LYS
1	2-B	190	GLU
1	3-A	31	ALA
1	3-A	164	GLY
1	3-A	166	VAL
1	3-B	42	LYS
1	4-A	31	ALA
1	4-A	155	THR
1	5-A	94	PHE

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Mol	Chain	Res	Type
1	5-A	191	ASN
1	5-B	179	SER
1	6-A	162	SER
1	6-B	64	LYS
1	6-B	104	HIS
1	6-B	105	ARG
1	6-B	175	LEU
1	6-B	212	ASN
1	7-A	59	LYS
1	7-A	241	GLY
1	8-B	52	GLN
1	8-B	165	GLN
1	9-A	190	GLU
1	9-A	241	GLY
1	9-B	154	TYR
1	10-A	143	GLN
1	10-B	68	LYS
1	10-B	179	SER
1	11-B	166	VAL
1	11-B	247	GLU
1	12-B	119	GLU
1	12-B	122	GLU
1	13-A	104	HIS
1	13-B	154	TYR
1	13-B	164	GLY
1	13-B	190	GLU
1	13-B	247	GLU
1	14-A	182	GLU
1	14-B	132	GLN
1	15-A	64	LYS
1	15-B	50	ASN
1	15-B	64	LYS
1	15-B	131	ALA
1	15-B	165	GLN
1	16-B	104	HIS
1	16-B	115	TYR
1	16-B	141	ILE
1	16-B	164	GLY
1	16-B	172	GLN
1	1-A	76	PHE
1	1-A	104	HIS
1	1-A	196	GLN

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Mol	Chain	Res	Type
1	1-B	60	GLY
1	2-A	154	TYR
1	2-B	167	LEU
1	3-B	60	GLY
1	3-B	62	ILE
1	5-A	190	GLU
1	5-B	182	GLU
1	6-B	179	SER
1	7-B	172	GLN
1	8-B	42	LYS
1	8-B	179	SER
1	8-B	190	GLU
1	9-A	94	PHE
1	9-B	58	LEU
1	9-B	64	LYS
1	9-B	65	GLU
1	10-B	163	GLY
1	10-B	178	PRO
1	10-B	196	GLN
1	11-B	100	PRO
1	12-B	121	TRP
1	12-B	162	SER
1	13-A	163	GLY
1	13-A	185	GLN
1	13-B	60	GLY
1	14-B	116	PHE
1	14-B	139	HIS
1	14-B	175	LEU
1	15-A	101	MET
1	15-B	42	LYS
1	15-B	132	GLN
1	15-B	240	ALA
1	16-B	51	THR
1	16-B	118	GLY
1	16-B	174	ALA
1	16-B	180	THR
1	16-B	190	GLU
1	1-B	168	LYS
1	1-B	190	GLU
1	3-B	187	TYR
1	4-A	54	VAL
1	4-B	63	LYS

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Mol	Chain	Res	Type
1	4-B	247	GLU
1	6-B	52	GLN
1	7-A	190	GLU
1	7-B	119	GLU
1	8-B	115	TYR
1	8-B	214	LYS
1	9-A	154	TYR
1	9-B	60	GLY
1	9-B	196	GLN
1	9-B	235	ASN
1	10-B	169	LYS
1	11-A	194	ASN
1	11-B	235	ASN
1	12-A	104	HIS
1	12-A	196	GLN
1	12-B	180	THR
1	13-A	95	ALA
1	13-B	155	THR
1	13-B	180	THR
1	14-A	94	PHE
1	14-A	177	LEU
1	14-B	49	GLU
1	14-B	179	SER
1	14-B	212	ASN
1	15-A	90	ASP
1	15-A	163	GLY
1	15-A	182	GLU
1	16-A	119	GLU
1	16-B	52	GLN
1	1-B	42	LYS
1	1-B	106	LYS
1	2-A	164	GLY
1	3-B	40	GLY
1	4-A	55	LYS
1	4-A	64	LYS
1	5-A	138	ILE
1	5-B	178	PRO
1	5-B	243	THR
1	6-A	176	LYS
1	7-B	50	ASN
1	7-B	129	LYS
1	7-B	190	GLU

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Mol	Chain	Res	Type
1	8-A	140	TYR
1	8-B	116	PHE
1	8-B	176	LYS
1	10-B	170	VAL
1	11-A	209	LEU
1	11-B	168	LYS
1	14-A	136	GLU
1	14-B	85	MET
1	14-B	130	ALA
1	14-B	163	GLY
1	15-A	145	GLU
1	15-A	196	GLN
1	16-A	126	GLN
1	3-B	94	PHE
1	4-B	54	VAL
1	4-B	64	LYS
1	4-B	178	PRO
1	6-B	99	PHE
1	6-B	246	ARG
1	8-B	178	PRO
1	9-A	192	VAL
1	9-B	164	GLY
1	9-B	178	PRO
1	10-A	75	TYR
1	10-B	102	GLU
1	10-B	193	ASP
1	11-A	154	TYR
1	13-B	106	LYS
1	13-B	163	GLY
1	14-A	241	GLY
1	14-B	125	VAL
1	14-B	126	GLN
1	14-B	140	TYR
1	14-B	170	VAL
1	15-A	87	ARG
1	16-B	178	PRO
1	5-A	241	GLY
1	5-B	40	GLY
1	6-B	178	PRO
1	13-A	241	GLY
1	14-B	92	PRO
1	15-B	166	VAL

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Mol	Chain	Res	Type
1	5-B	164	GLY
1	9-A	95	ALA
1	14-B	128	PRO
1	2-B	60	GLY
1	4-B	170	VAL
1	6-B	192	VAL
1	3-B	166	VAL
1	6-A	163	GLY
1	12-B	125	VAL
1	14-A	166	VAL
1	15-A	177	LEU
1	7-B	100	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	1-A	182/224 (81%)	174 (96%)	8 (4%)	28	52
1	1-B	186/224 (83%)	176 (95%)	10 (5%)	22	42
1	2-A	182/224 (81%)	174 (96%)	8 (4%)	28	52
1	2-B	186/224 (83%)	180 (97%)	6 (3%)	39	63
1	3-A	182/224 (81%)	168 (92%)	14 (8%)	13	24
1	3-B	186/224 (83%)	170 (91%)	16 (9%)	10	19
1	4-A	182/224 (81%)	167 (92%)	15 (8%)	11	21
1	4-B	186/224 (83%)	175 (94%)	11 (6%)	19	37
1	5-A	182/224 (81%)	171 (94%)	11 (6%)	19	37
1	5-B	186/224 (83%)	175 (94%)	11 (6%)	19	37
1	6-A	182/224 (81%)	173 (95%)	9 (5%)	25	46
1	6-B	186/224 (83%)	173 (93%)	13 (7%)	15	29
1	7-A	182/224 (81%)	170 (93%)	12 (7%)	16	32
1	7-B	186/224 (83%)	177 (95%)	9 (5%)	25	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-A	182/224 (81%)	174 (96%)	8 (4%)	28	52
1	8-B	186/224 (83%)	173 (93%)	13 (7%)	15	29
1	9-A	182/224 (81%)	173 (95%)	9 (5%)	25	46
1	9-B	186/224 (83%)	180 (97%)	6 (3%)	39	63
1	10-A	182/224 (81%)	172 (94%)	10 (6%)	21	41
1	10-B	186/224 (83%)	176 (95%)	10 (5%)	22	42
1	11-A	182/224 (81%)	168 (92%)	14 (8%)	13	24
1	11-B	186/224 (83%)	176 (95%)	10 (5%)	22	42
1	12-A	182/224 (81%)	175 (96%)	7 (4%)	33	57
1	12-B	186/224 (83%)	174 (94%)	12 (6%)	17	33
1	13-A	182/224 (81%)	163 (90%)	19 (10%)	7	12
1	13-B	186/224 (83%)	176 (95%)	10 (5%)	22	42
1	14-A	182/224 (81%)	164 (90%)	18 (10%)	8	14
1	14-B	186/224 (83%)	175 (94%)	11 (6%)	19	37
1	15-A	182/224 (81%)	166 (91%)	16 (9%)	10	18
1	15-B	186/224 (83%)	170 (91%)	16 (9%)	10	19
1	16-A	182/224 (81%)	164 (90%)	18 (10%)	8	14
1	16-B	186/224 (83%)	172 (92%)	14 (8%)	13	25
All	All	5888/7168 (82%)	5514 (94%)	374 (6%)	17	34

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	29	ARG
1	1-A	30	MET
1	1-A	74	LEU
1	1-A	109	LEU
1	1-A	114	GLU
1	1-A	134	TYR
1	1-A	143	GLN
1	1-A	156	ARG
1	1-B	32	ASP
1	1-B	51	THR
1	1-B	63	LYS
1	1-B	86	GLU
1	1-B	165	GLN

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Mol	Chain	Res	Type
1	1-B	205	ARG
1	1-B	210	ASP
1	1-B	222	GLU
1	1-B	229	TYR
1	1-B	232	GLN
1	2-A	74	LEU
1	2-A	120	ASN
1	2-A	134	TYR
1	2-A	141	ILE
1	2-A	147	GLU
1	2-A	156	ARG
1	2-A	160	ASP
1	2-A	180	THR
1	2-B	63	LYS
1	2-B	101	MET
1	2-B	156	ARG
1	2-B	165	GLN
1	2-B	182	GLU
1	2-B	238	ASP
1	3-A	30	MET
1	3-A	51	THR
1	3-A	74	LEU
1	3-A	107	GLU
1	3-A	109	LEU
1	3-A	120	ASN
1	3-A	134	TYR
1	3-A	156	ARG
1	3-A	165	GLN
1	3-A	173	ARG
1	3-A	180	THR
1	3-A	184	THR
1	3-A	212	ASN
1	3-A	227	PHE
1	3-B	35	GLU
1	3-B	46	ASP
1	3-B	49	GLU
1	3-B	50	ASN
1	3-B	63	LYS
1	3-B	102	GLU
1	3-B	114	GLU
1	3-B	145	GLU
1	3-B	160	ASP

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Mol	Chain	Res	Type
1	3-B	165	GLN
1	3-B	172	GLN
1	3-B	210	ASP
1	3-B	221	GLU
1	3-B	224	ASN
1	3-B	237	LEU
1	3-B	238	ASP
1	4-A	29	ARG
1	4-A	51	THR
1	4-A	62	ILE
1	4-A	74	LEU
1	4-A	86	GLU
1	4-A	109	LEU
1	4-A	119	GLU
1	4-A	122	GLU
1	4-A	132	GLN
1	4-A	134	TYR
1	4-A	141	ILE
1	4-A	156	ARG
1	4-A	200	GLN
1	4-A	221	GLU
1	4-A	239	GLN
1	4-B	43	GLU
1	4-B	46	ASP
1	4-B	63	LYS
1	4-B	101	MET
1	4-B	124	GLN
1	4-B	161	LEU
1	4-B	194	ASN
1	4-B	196	GLN
1	4-B	200	GLN
1	4-B	210	ASP
1	4-B	229	TYR
1	5-A	63	LYS
1	5-A	74	LEU
1	5-A	89	LYS
1	5-A	107	GLU
1	5-A	114	GLU
1	5-A	133	LYS
1	5-A	134	TYR
1	5-A	165	GLN
1	5-A	193	ASP

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Mol	Chain	Res	Type
1	5-A	200	GLN
1	5-A	221	GLU
1	5-B	30	MET
1	5-B	32	ASP
1	5-B	63	LYS
1	5-B	119	GLU
1	5-B	121	TRP
1	5-B	134	TYR
1	5-B	140	TYR
1	5-B	145	GLU
1	5-B	156	ARG
1	5-B	165	GLN
1	5-B	193	ASP
1	6-A	74	LEU
1	6-A	101	MET
1	6-A	132	GLN
1	6-A	134	TYR
1	6-A	136	GLU
1	6-A	182	GLU
1	6-A	185	GLN
1	6-A	197	GLN
1	6-A	235	ASN
1	6-B	46	ASP
1	6-B	51	THR
1	6-B	54	VAL
1	6-B	61	ASN
1	6-B	63	LYS
1	6-B	102	GLU
1	6-B	156	ARG
1	6-B	165	GLN
1	6-B	166	VAL
1	6-B	199	LYS
1	6-B	212	ASN
1	6-B	228	GLU
1	6-B	238	ASP
1	7-A	30	MET
1	7-A	39	GLU
1	7-A	74	LEU
1	7-A	86	GLU
1	7-A	109	LEU
1	7-A	119	GLU
1	7-A	120	ASN

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Mol	Chain	Res	Type
1	7-A	134	TYR
1	7-A	141	ILE
1	7-A	147	GLU
1	7-A	156	ARG
1	7-A	165	GLN
1	7-B	35	GLU
1	7-B	115	TYR
1	7-B	116	PHE
1	7-B	134	TYR
1	7-B	156	ARG
1	7-B	160	ASP
1	7-B	165	GLN
1	7-B	193	ASP
1	7-B	228	GLU
1	8-A	35	GLU
1	8-A	74	LEU
1	8-A	109	LEU
1	8-A	123	GLU
1	8-A	128	PRO
1	8-A	134	TYR
1	8-A	217	GLU
1	8-A	238	ASP
1	8-B	35	GLU
1	8-B	56	ASP
1	8-B	63	LYS
1	8-B	115	TYR
1	8-B	129	LYS
1	8-B	165	GLN
1	8-B	167	LEU
1	8-B	193	ASP
1	8-B	205	ARG
1	8-B	210	ASP
1	8-B	212	ASN
1	8-B	229	TYR
1	8-B	246	ARG
1	9-A	39	GLU
1	9-A	52	GLN
1	9-A	74	LEU
1	9-A	109	LEU
1	9-A	134	TYR
1	9-A	156	ARG
1	9-A	180	THR

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Mol	Chain	Res	Type
1	9-A	217	GLU
1	9-A	221	GLU
1	9-B	56	ASP
1	9-B	57	PHE
1	9-B	156	ARG
1	9-B	165	GLN
1	9-B	191	ASN
1	9-B	193	ASP
1	10-A	29	ARG
1	10-A	30	MET
1	10-A	74	LEU
1	10-A	107	GLU
1	10-A	134	TYR
1	10-A	143	GLN
1	10-A	156	ARG
1	10-A	180	THR
1	10-A	213	MET
1	10-A	221	GLU
1	10-B	63	LYS
1	10-B	102	GLU
1	10-B	124	GLN
1	10-B	156	ARG
1	10-B	165	GLN
1	10-B	172	GLN
1	10-B	185	GLN
1	10-B	190	GLU
1	10-B	196	GLN
1	10-B	238	ASP
1	11-A	29	ARG
1	11-A	30	MET
1	11-A	51	THR
1	11-A	87	ARG
1	11-A	109	LEU
1	11-A	117	PHE
1	11-A	119	GLU
1	11-A	132	GLN
1	11-A	134	TYR
1	11-A	156	ARG
1	11-A	172	GLN
1	11-A	180	THR
1	11-A	190	GLU
1	11-A	235	ASN

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Mol	Chain	Res	Type
1	11-B	30	MET
1	11-B	35	GLU
1	11-B	42	LYS
1	11-B	45	HIS
1	11-B	46	ASP
1	11-B	165	GLN
1	11-B	189	PHE
1	11-B	190	GLU
1	11-B	230	ASN
1	11-B	246	ARG
1	12-A	30	MET
1	12-A	74	LEU
1	12-A	109	LEU
1	12-A	120	ASN
1	12-A	134	TYR
1	12-A	147	GLU
1	12-A	156	ARG
1	12-B	39	GLU
1	12-B	46	ASP
1	12-B	62	ILE
1	12-B	63	LYS
1	12-B	79	SER
1	12-B	120	ASN
1	12-B	165	GLN
1	12-B	185	GLN
1	12-B	212	ASN
1	12-B	229	TYR
1	12-B	238	ASP
1	12-B	244	LEU
1	13-A	43	GLU
1	13-A	54	VAL
1	13-A	69	LEU
1	13-A	88	ASN
1	13-A	109	LEU
1	13-A	114	GLU
1	13-A	120	ASN
1	13-A	132	GLN
1	13-A	134	TYR
1	13-A	141	ILE
1	13-A	156	ARG
1	13-A	158	MET
1	13-A	165	GLN

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Mol	Chain	Res	Type
1	13-A	180	THR
1	13-A	215	THR
1	13-A	217	GLU
1	13-A	229	TYR
1	13-A	238	ASP
1	13-A	239	GLN
1	13-B	39	GLU
1	13-B	46	ASP
1	13-B	56	ASP
1	13-B	82	GLU
1	13-B	86	GLU
1	13-B	101	MET
1	13-B	114	GLU
1	13-B	134	TYR
1	13-B	156	ARG
1	13-B	165	GLN
1	14-A	30	MET
1	14-A	43	GLU
1	14-A	52	GLN
1	14-A	86	GLU
1	14-A	88	ASN
1	14-A	102	GLU
1	14-A	105	ARG
1	14-A	109	LEU
1	14-A	119	GLU
1	14-A	120	ASN
1	14-A	122	GLU
1	14-A	134	TYR
1	14-A	156	ARG
1	14-A	165	GLN
1	14-A	184	THR
1	14-A	227	PHE
1	14-A	229	TYR
1	14-A	232	GLN
1	14-B	32	ASP
1	14-B	52	GLN
1	14-B	63	LYS
1	14-B	82	GLU
1	14-B	122	GLU
1	14-B	147	GLU
1	14-B	156	ARG
1	14-B	165	GLN

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Mol	Chain	Res	Type
1	14-B	184	THR
1	14-B	189	PHE
1	14-B	210	ASP
1	15-A	32	ASP
1	15-A	88	ASN
1	15-A	109	LEU
1	15-A	114	GLU
1	15-A	134	TYR
1	15-A	145	GLU
1	15-A	158	MET
1	15-A	165	GLN
1	15-A	184	THR
1	15-A	193	ASP
1	15-A	200	GLN
1	15-A	213	MET
1	15-A	216	LYS
1	15-A	228	GLU
1	15-A	236	GLU
1	15-A	239	GLN
1	15-B	32	ASP
1	15-B	47	ARG
1	15-B	56	ASP
1	15-B	61	ASN
1	15-B	67	PHE
1	15-B	102	GLU
1	15-B	129	LYS
1	15-B	156	ARG
1	15-B	173	ARG
1	15-B	175	LEU
1	15-B	180	THR
1	15-B	182	GLU
1	15-B	190	GLU
1	15-B	205	ARG
1	15-B	224	ASN
1	15-B	236	GLU
1	16-A	29	ARG
1	16-A	42	LYS
1	16-A	74	LEU
1	16-A	86	GLU
1	16-A	89	LYS
1	16-A	109	LEU
1	16-A	123	GLU

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Mol	Chain	Res	Type
1	16-A	126	GLN
1	16-A	134	TYR
1	16-A	165	GLN
1	16-A	180	THR
1	16-A	184	THR
1	16-A	185	GLN
1	16-A	190	GLU
1	16-A	194	ASN
1	16-A	213	MET
1	16-A	215	THR
1	16-A	228	GLU
1	16-B	63	LYS
1	16-B	83	GLU
1	16-B	110	THR
1	16-B	123	GLU
1	16-B	134	TYR
1	16-B	143	GLN
1	16-B	156	ARG
1	16-B	185	GLN
1	16-B	194	ASN
1	16-B	196	GLN
1	16-B	200	GLN
1	16-B	212	ASN
1	16-B	217	GLU
1	16-B	244	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	52	GLN
1	1-A	61	ASN
1	1-A	104	HIS
1	1-A	120	ASN
1	1-A	124	GLN
1	1-A	126	GLN
1	1-A	143	GLN
1	1-A	165	GLN
1	1-A	200	GLN
1	1-B	124	GLN
1	1-B	165	GLN
1	1-B	172	GLN
1	1-B	196	GLN

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Mol	Chain	Res	Type
1	1-B	230	ASN
1	2-A	52	GLN
1	2-A	104	HIS
1	2-A	165	GLN
1	2-B	104	HIS
1	2-B	124	GLN
1	2-B	165	GLN
1	2-B	172	GLN
1	2-B	185	GLN
1	2-B	191	ASN
1	2-B	196	GLN
1	2-B	230	ASN
1	3-A	52	GLN
1	3-A	61	ASN
1	3-A	124	GLN
1	3-A	165	GLN
1	3-A	200	GLN
1	3-A	212	ASN
1	3-A	239	GLN
1	3-B	50	ASN
1	3-B	104	HIS
1	3-B	143	GLN
1	3-B	165	GLN
1	3-B	172	GLN
1	3-B	196	GLN
1	3-B	200	GLN
1	3-B	235	ASN
1	4-A	139	HIS
1	4-A	185	GLN
1	4-B	61	ASN
1	4-B	124	GLN
1	4-B	165	GLN
1	4-B	172	GLN
1	4-B	185	GLN
1	4-B	194	ASN
1	4-B	196	GLN
1	4-B	230	ASN
1	5-A	88	ASN
1	5-A	104	HIS
1	5-A	120	ASN
1	5-A	143	GLN
1	5-A	165	GLN

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Mol	Chain	Res	Type
1	5-B	104	HIS
1	5-B	124	GLN
1	5-B	172	GLN
1	5-B	185	GLN
1	5-B	230	ASN
1	6-A	52	GLN
1	6-A	61	ASN
1	6-A	88	ASN
1	6-A	104	HIS
1	6-A	124	GLN
1	6-A	197	GLN
1	6-A	200	GLN
1	6-B	61	ASN
1	6-B	165	GLN
1	6-B	172	GLN
1	6-B	185	GLN
1	6-B	230	ASN
1	7-A	88	ASN
1	7-A	104	HIS
1	7-A	165	GLN
1	7-A	200	GLN
1	7-B	104	HIS
1	7-B	124	GLN
1	7-B	165	GLN
1	7-B	185	GLN
1	7-B	230	ASN
1	7-B	232	GLN
1	8-A	104	HIS
1	8-A	143	GLN
1	8-A	144	ASN
1	8-A	185	GLN
1	8-A	200	GLN
1	8-A	230	ASN
1	8-B	124	GLN
1	8-B	126	GLN
1	8-B	165	GLN
1	8-B	172	GLN
1	8-B	185	GLN
1	8-B	224	ASN
1	9-A	104	HIS
1	9-A	120	ASN
1	9-A	124	GLN

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Mol	Chain	Res	Type
1	9-A	143	GLN
1	9-A	196	GLN
1	9-A	200	GLN
1	9-A	235	ASN
1	9-A	239	GLN
1	9-B	104	HIS
1	9-B	124	GLN
1	9-B	165	GLN
1	9-B	172	GLN
1	9-B	191	ASN
1	9-B	194	ASN
1	9-B	200	GLN
1	9-B	230	ASN
1	10-A	52	GLN
1	10-A	104	HIS
1	10-A	143	GLN
1	10-A	165	GLN
1	10-B	120	ASN
1	10-B	124	GLN
1	10-B	143	GLN
1	10-B	165	GLN
1	10-B	172	GLN
1	10-B	185	GLN
1	10-B	194	ASN
1	10-B	230	ASN
1	10-B	232	GLN
1	11-A	61	ASN
1	11-A	104	HIS
1	11-A	143	GLN
1	11-B	50	ASN
1	11-B	124	GLN
1	11-B	165	GLN
1	11-B	172	GLN
1	11-B	196	GLN
1	11-B	224	ASN
1	12-A	52	GLN
1	12-A	143	GLN
1	12-B	61	ASN
1	12-B	120	ASN
1	12-B	165	GLN
1	12-B	172	GLN
1	12-B	185	GLN

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Mol	Chain	Res	Type
1	12-B	224	ASN
1	12-B	230	ASN
1	13-A	88	ASN
1	13-A	124	GLN
1	13-A	144	ASN
1	13-B	124	GLN
1	13-B	165	GLN
1	13-B	191	ASN
1	13-B	230	ASN
1	14-A	88	ASN
1	14-A	104	HIS
1	14-A	197	GLN
1	14-B	120	ASN
1	14-B	143	GLN
1	14-B	144	ASN
1	14-B	165	GLN
1	15-A	61	ASN
1	15-A	144	ASN
1	15-B	61	ASN
1	15-B	104	HIS
1	15-B	172	GLN
1	15-B	230	ASN
1	15-B	232	GLN
1	16-A	88	ASN
1	16-A	165	GLN
1	16-A	194	ASN
1	16-A	196	GLN
1	16-A	235	ASN
1	16-B	120	ASN
1	16-B	124	GLN
1	16-B	143	GLN
1	16-B	165	GLN
1	16-B	172	GLN
1	16-B	185	GLN
1	16-B	194	ASN
1	16-B	230	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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	12-A	300	1	41,50,50	1.38	5 (12%)	45,82,82	1.00	1 (2%)
2	HEM	12-B	265	1	41,50,50	1.41	5 (12%)	45,82,82	1.01	2 (4%)
2	HEM	2-A	300	1	41,50,50	1.34	5 (12%)	45,82,82	0.99	0
2	HEM	9-A	300	1	41,50,50	1.43	5 (12%)	45,82,82	0.95	0
2	HEM	5-A	300	1	41,50,50	1.29	5 (12%)	45,82,82	1.04	2 (4%)
2	HEM	2-B	265	1	41,50,50	1.48	5 (12%)	45,82,82	0.98	2 (4%)
2	HEM	1-B	265	1	41,50,50	1.47	5 (12%)	45,82,82	0.95	1 (2%)
2	HEM	5-B	265	1	41,50,50	1.43	5 (12%)	45,82,82	0.97	2 (4%)
2	HEM	16-A	300	1	41,50,50	1.33	5 (12%)	45,82,82	1.01	1 (2%)
2	HEM	3-A	300	1	41,50,50	1.35	5 (12%)	45,82,82	1.03	1 (2%)
2	HEM	8-B	265	1	41,50,50	1.43	5 (12%)	45,82,82	0.97	1 (2%)
2	HEM	15-B	265	1	41,50,50	1.44	5 (12%)	45,82,82	1.02	2 (4%)
2	HEM	7-B	265	1	41,50,50	1.45	5 (12%)	45,82,82	0.95	2 (4%)
2	HEM	3-B	265	1	41,50,50	1.39	5 (12%)	45,82,82	1.03	1 (2%)
2	HEM	6-B	265	1	41,50,50	1.42	5 (12%)	45,82,82	0.96	3 (6%)
2	HEM	4-A	300	1	41,50,50	1.44	5 (12%)	45,82,82	0.97	2 (4%)
2	HEM	11-A	300	1	41,50,50	1.38	5 (12%)	45,82,82	0.99	1 (2%)
2	HEM	13-A	300	1	41,50,50	1.44	5 (12%)	45,82,82	0.92	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	7-A	300	1	41,50,50	1.35	5 (12%)	45,82,82	1.01	0
2	HEM	9-B	265	1	41,50,50	1.48	5 (12%)	45,82,82	0.99	2 (4%)
2	HEM	13-B	265	1	41,50,50	1.45	5 (12%)	45,82,82	0.96	2 (4%)
2	HEM	6-A	300	1	41,50,50	1.38	5 (12%)	45,82,82	1.00	1 (2%)
2	HEM	10-A	300	1	41,50,50	1.29	5 (12%)	45,82,82	1.01	1 (2%)
2	HEM	14-A	300	1	41,50,50	1.44	7 (17%)	45,82,82	0.95	1 (2%)
2	HEM	4-B	265	1	41,50,50	1.42	5 (12%)	45,82,82	1.00	2 (4%)
2	HEM	16-B	265	1	41,50,50	1.52	5 (12%)	45,82,82	1.01	2 (4%)
2	HEM	15-A	300	1	41,50,50	1.28	5 (12%)	45,82,82	1.07	1 (2%)
2	HEM	11-B	265	1	41,50,50	1.43	5 (12%)	45,82,82	0.99	2 (4%)
2	HEM	10-B	265	1	41,50,50	1.48	5 (12%)	45,82,82	0.97	2 (4%)
2	HEM	1-A	300	1	41,50,50	1.31	5 (12%)	45,82,82	1.00	1 (2%)
2	HEM	8-A	300	1	41,50,50	1.33	5 (12%)	45,82,82	1.04	1 (2%)
2	HEM	14-B	265	1	41,50,50	1.52	5 (12%)	45,82,82	1.10	3 (6%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	12-A	300	1	-	5/12/54/54	-
2	HEM	12-B	265	1	-	8/12/54/54	-
2	HEM	2-A	300	1	-	5/12/54/54	-
2	HEM	9-A	300	1	-	5/12/54/54	-
2	HEM	5-A	300	1	-	2/12/54/54	-
2	HEM	2-B	265	1	-	5/12/54/54	-
2	HEM	1-B	265	1	-	7/12/54/54	-
2	HEM	5-B	265	1	-	6/12/54/54	-
2	HEM	16-A	300	1	-	5/12/54/54	-
2	HEM	3-A	300	1	-	7/12/54/54	-
2	HEM	8-B	265	1	-	6/12/54/54	-
2	HEM	15-B	265	1	-	6/12/54/54	-
2	HEM	7-B	265	1	-	6/12/54/54	-
2	HEM	3-B	265	1	-	8/12/54/54	-
2	HEM	6-B	265	1	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	4-A	300	1	-	6/12/54/54	-
2	HEM	11-A	300	1	-	4/12/54/54	-
2	HEM	13-A	300	1	-	4/12/54/54	-
2	HEM	7-A	300	1	-	3/12/54/54	-
2	HEM	9-B	265	1	-	5/12/54/54	-
2	HEM	13-B	265	1	-	4/12/54/54	-
2	HEM	6-A	300	1	-	5/12/54/54	-
2	HEM	10-A	300	1	-	2/12/54/54	-
2	HEM	14-A	300	1	-	4/12/54/54	-
2	HEM	4-B	265	1	-	8/12/54/54	-
2	HEM	16-B	265	1	-	9/12/54/54	-
2	HEM	15-A	300	1	-	2/12/54/54	-
2	HEM	11-B	265	1	-	4/12/54/54	-
2	HEM	10-B	265	1	-	7/12/54/54	-
2	HEM	1-A	300	1	-	3/12/54/54	-
2	HEM	8-A	300	1	-	2/12/54/54	-
2	HEM	14-B	265	1	-	3/12/54/54	-

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9-A	300	HEM	C3C-CAC	-4.49	1.38	1.47
2	14-B	265	HEM	C3C-CAC	-4.42	1.38	1.47
2	6-A	300	HEM	C3C-CAC	-4.41	1.38	1.47
2	11-A	300	HEM	C3C-CAC	-4.40	1.38	1.47
2	4-A	300	HEM	C3C-CAC	-4.37	1.38	1.47
2	14-B	265	HEM	C3C-C2C	-4.37	1.34	1.40
2	12-A	300	HEM	C3C-CAC	-4.36	1.38	1.47
2	16-B	265	HEM	C3C-CAC	-4.29	1.39	1.47
2	10-B	265	HEM	C3C-CAC	-4.29	1.39	1.47
2	13-A	300	HEM	C3C-CAC	-4.29	1.39	1.47
2	4-B	265	HEM	C3C-CAC	-4.28	1.39	1.47
2	6-B	265	HEM	C3C-CAC	-4.27	1.39	1.47
2	7-B	265	HEM	C3C-CAC	-4.21	1.39	1.47
2	9-B	265	HEM	C3C-CAC	-4.21	1.39	1.47
2	1-B	265	HEM	C3C-CAC	-4.20	1.39	1.47
2	8-B	265	HEM	C3C-CAC	-4.20	1.39	1.47
2	2-B	265	HEM	C3C-CAC	-4.18	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-B	265	HEM	C3C-CAC	-4.17	1.39	1.47
2	7-A	300	HEM	C3C-CAC	-4.17	1.39	1.47
2	11-B	265	HEM	C3C-CAC	-4.13	1.39	1.47
2	15-B	265	HEM	C3C-CAC	-4.13	1.39	1.47
2	14-A	300	HEM	C3C-CAC	-4.13	1.39	1.47
2	13-B	265	HEM	C3C-CAC	-4.05	1.39	1.47
2	16-A	300	HEM	C3C-CAC	-4.02	1.39	1.47
2	1-A	300	HEM	C3C-CAC	-3.96	1.39	1.47
2	2-A	300	HEM	C3C-CAC	-3.86	1.39	1.47
2	3-B	265	HEM	C3C-CAC	-3.86	1.39	1.47
2	10-A	300	HEM	C3C-CAC	-3.83	1.40	1.47
2	8-A	300	HEM	C3C-CAC	-3.82	1.40	1.47
2	8-B	265	HEM	C3C-C2C	-3.82	1.35	1.40
2	5-B	265	HEM	C3C-C2C	-3.75	1.35	1.40
2	6-B	265	HEM	C3C-C2C	-3.59	1.35	1.40
2	16-B	265	HEM	C3C-C2C	-3.57	1.35	1.40
2	1-B	265	HEM	C3C-C2C	-3.55	1.35	1.40
2	7-B	265	HEM	C3C-C2C	-3.50	1.35	1.40
2	15-B	265	HEM	C3C-C2C	-3.48	1.35	1.40
2	5-A	300	HEM	C3C-CAC	-3.47	1.40	1.47
2	2-B	265	HEM	C3C-C2C	-3.47	1.35	1.40
2	10-B	265	HEM	C3C-C2C	-3.46	1.35	1.40
2	12-B	265	HEM	CAB-C3B	-3.44	1.38	1.47
2	13-B	265	HEM	C3C-C2C	-3.42	1.35	1.40
2	9-B	265	HEM	C3C-C2C	-3.39	1.35	1.40
2	11-B	265	HEM	C3C-C2C	-3.38	1.35	1.40
2	14-B	265	HEM	CBB-CAB	3.36	1.46	1.30
2	3-A	300	HEM	C3C-CAC	-3.35	1.40	1.47
2	12-B	265	HEM	C3C-CAC	-3.33	1.41	1.47
2	1-B	265	HEM	CAB-C3B	-3.31	1.38	1.47
2	9-B	265	HEM	CAB-C3B	-3.31	1.38	1.47
2	11-B	265	HEM	CAB-C3B	-3.25	1.38	1.47
2	4-B	265	HEM	CBB-CAB	3.24	1.46	1.30
2	15-B	265	HEM	CAB-C3B	-3.23	1.38	1.47
2	7-B	265	HEM	CAB-C3B	-3.23	1.38	1.47
2	13-B	265	HEM	CBB-CAB	3.22	1.46	1.30
2	13-B	265	HEM	CAB-C3B	-3.22	1.38	1.47
2	10-B	265	HEM	CBB-CAB	3.20	1.46	1.30
2	15-A	300	HEM	C3C-CAC	-3.20	1.41	1.47
2	12-B	265	HEM	C3C-C2C	-3.20	1.35	1.40
2	10-B	265	HEM	CAB-C3B	-3.20	1.38	1.47
2	3-A	300	HEM	CAB-C3B	-3.19	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4-B	265	HEM	C3C-C2C	-3.19	1.35	1.40
2	9-B	265	HEM	CBB-CAB	3.18	1.46	1.30
2	16-B	265	HEM	CBB-CAB	3.17	1.46	1.30
2	1-B	265	HEM	CBB-CAB	3.16	1.45	1.30
2	5-B	265	HEM	CBB-CAB	3.15	1.45	1.30
2	8-B	265	HEM	CBB-CAB	3.12	1.45	1.30
2	7-B	265	HEM	CBB-CAB	3.12	1.45	1.30
2	2-B	265	HEM	CAB-C3B	-3.12	1.38	1.47
2	15-A	300	HEM	CAB-C3B	-3.11	1.39	1.47
2	11-A	300	HEM	C3C-C2C	-3.11	1.36	1.40
2	6-B	265	HEM	CBB-CAB	3.11	1.45	1.30
2	2-B	265	HEM	CBB-CAB	3.11	1.45	1.30
2	6-A	300	HEM	C3C-C2C	-3.10	1.36	1.40
2	7-A	300	HEM	CBB-CAB	3.09	1.45	1.30
2	8-A	300	HEM	CBB-CAB	3.09	1.45	1.30
2	12-A	300	HEM	CBB-CAB	3.08	1.45	1.30
2	10-A	300	HEM	CBB-CAB	3.07	1.45	1.30
2	12-A	300	HEM	C3C-C2C	-3.06	1.36	1.40
2	1-A	300	HEM	CBB-CAB	3.06	1.45	1.30
2	2-A	300	HEM	CBB-CAB	3.06	1.45	1.30
2	3-B	265	HEM	CBB-CAB	3.05	1.45	1.30
2	15-B	265	HEM	CBB-CAB	3.05	1.45	1.30
2	6-A	300	HEM	CBB-CAB	3.05	1.45	1.30
2	11-A	300	HEM	CBB-CAB	3.05	1.45	1.30
2	11-B	265	HEM	CBB-CAB	3.05	1.45	1.30
2	3-B	265	HEM	CAB-C3B	-3.01	1.39	1.47
2	5-A	300	HEM	CBB-CAB	2.99	1.45	1.30
2	16-A	300	HEM	CBB-CAB	2.99	1.45	1.30
2	7-A	300	HEM	C3C-C2C	-2.99	1.36	1.40
2	5-A	300	HEM	CAB-C3B	-2.98	1.39	1.47
2	9-A	300	HEM	CBB-CAB	2.97	1.45	1.30
2	4-A	300	HEM	CBB-CAB	2.94	1.44	1.30
2	12-B	265	HEM	CBB-CAB	2.94	1.44	1.30
2	9-A	300	HEM	C3C-C2C	-2.94	1.36	1.40
2	4-A	300	HEM	C3C-C2C	-2.94	1.36	1.40
2	14-A	300	HEM	C3C-C2C	-2.93	1.36	1.40
2	14-A	300	HEM	CBB-CAB	2.93	1.44	1.30
2	15-A	300	HEM	CBB-CAB	2.93	1.44	1.30
2	13-A	300	HEM	CBB-CAB	2.92	1.44	1.30
2	8-B	265	HEM	CAB-C3B	-2.90	1.39	1.47
2	16-B	265	HEM	CAB-C3B	-2.90	1.39	1.47
2	3-A	300	HEM	C3C-C2C	-2.89	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-A	300	HEM	C3C-C2C	-2.88	1.36	1.40
2	9-A	300	HEM	CAB-C3B	-2.85	1.39	1.47
2	4-B	265	HEM	CAB-C3B	-2.85	1.39	1.47
2	3-A	300	HEM	CBB-CAB	2.84	1.44	1.30
2	6-B	265	HEM	CAB-C3B	-2.82	1.39	1.47
2	7-A	300	HEM	CAB-C3B	-2.75	1.39	1.47
2	4-A	300	HEM	CAB-C3B	-2.75	1.39	1.47
2	8-A	300	HEM	CAB-C3B	-2.70	1.40	1.47
2	10-A	300	HEM	CAB-C3B	-2.70	1.40	1.47
2	11-A	300	HEM	CAB-C3B	-2.70	1.40	1.47
2	13-A	300	HEM	CAB-C3B	-2.69	1.40	1.47
2	6-A	300	HEM	CAB-C3B	-2.69	1.40	1.47
2	12-A	300	HEM	CAB-C3B	-2.68	1.40	1.47
2	16-A	300	HEM	CAB-C3B	-2.66	1.40	1.47
2	12-B	265	HEM	CBC-CAC	2.66	1.46	1.29
2	1-A	300	HEM	CAB-C3B	-2.65	1.40	1.47
2	3-B	265	HEM	C3C-C2C	-2.65	1.36	1.40
2	5-B	265	HEM	CAB-C3B	-2.63	1.40	1.47
2	2-A	300	HEM	CAB-C3B	-2.62	1.40	1.47
2	3-A	300	HEM	CBC-CAC	2.58	1.46	1.29
2	3-B	265	HEM	CBC-CAC	2.56	1.46	1.29
2	16-A	300	HEM	C3C-C2C	-2.55	1.36	1.40
2	14-A	300	HEM	CAB-C3B	-2.52	1.40	1.47
2	15-A	300	HEM	CBC-CAC	2.52	1.46	1.29
2	2-A	300	HEM	C3C-C2C	-2.50	1.36	1.40
2	9-A	300	HEM	CBC-CAC	2.46	1.45	1.29
2	5-A	300	HEM	CBC-CAC	2.46	1.45	1.29
2	1-A	300	HEM	C3C-C2C	-2.46	1.37	1.40
2	4-A	300	HEM	CBC-CAC	2.45	1.45	1.29
2	13-A	300	HEM	CBC-CAC	2.44	1.45	1.29
2	8-A	300	HEM	CBC-CAC	2.43	1.45	1.29
2	4-B	265	HEM	CBC-CAC	2.42	1.45	1.29
2	13-B	265	HEM	CBC-CAC	2.42	1.45	1.29
2	2-B	265	HEM	CBC-CAC	2.42	1.45	1.29
2	8-A	300	HEM	C3C-C2C	-2.42	1.37	1.40
2	1-A	300	HEM	CBC-CAC	2.42	1.45	1.29
2	10-A	300	HEM	CBC-CAC	2.41	1.45	1.29
2	5-B	265	HEM	CBC-CAC	2.41	1.45	1.29
2	9-B	265	HEM	CBC-CAC	2.40	1.45	1.29
2	15-B	265	HEM	CBC-CAC	2.40	1.45	1.29
2	8-B	265	HEM	CBC-CAC	2.40	1.45	1.29
2	14-B	265	HEM	CBC-CAC	2.39	1.45	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-A	300	HEM	C3C-C2C	-2.39	1.37	1.40
2	11-B	265	HEM	CBC-CAC	2.39	1.45	1.29
2	16-B	265	HEM	CBC-CAC	2.39	1.45	1.29
2	6-B	265	HEM	CBC-CAC	2.38	1.45	1.29
2	10-B	265	HEM	CBC-CAC	2.38	1.45	1.29
2	7-B	265	HEM	CBC-CAC	2.37	1.44	1.29
2	14-A	300	HEM	CBC-CAC	2.36	1.44	1.29
2	12-A	300	HEM	CBC-CAC	2.36	1.44	1.29
2	1-B	265	HEM	CBC-CAC	2.36	1.44	1.29
2	2-A	300	HEM	CBC-CAC	2.36	1.44	1.29
2	7-A	300	HEM	CBC-CAC	2.36	1.44	1.29
2	16-A	300	HEM	CBC-CAC	2.35	1.44	1.29
2	11-A	300	HEM	CBC-CAC	2.35	1.44	1.29
2	6-A	300	HEM	CBC-CAC	2.34	1.44	1.29
2	5-A	300	HEM	C3C-C2C	-2.31	1.37	1.40
2	15-A	300	HEM	C3C-C2C	-2.22	1.37	1.40
2	14-B	265	HEM	CAB-C3B	-2.20	1.41	1.47
2	14-A	300	HEM	CBA-CGA	2.13	1.55	1.50
2	14-A	300	HEM	CAA-C2A	2.11	1.55	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-B	265	HEM	C4B-CHC-C1C	2.44	125.78	122.56
2	12-B	265	HEM	C4C-CHD-C1D	2.33	125.64	122.56
2	16-B	265	HEM	C4C-CHD-C1D	2.30	125.59	122.56
2	2-B	265	HEM	C4C-CHD-C1D	2.29	125.58	122.56
2	13-A	300	HEM	C4C-CHD-C1D	2.29	125.58	122.56
2	12-B	265	HEM	C4B-CHC-C1C	2.28	125.57	122.56
2	11-B	265	HEM	C4B-CHC-C1C	2.28	125.57	122.56
2	14-B	265	HEM	C4D-ND-C1D	-2.28	102.72	105.07
2	9-B	265	HEM	C4B-CHC-C1C	2.27	125.55	122.56
2	13-B	265	HEM	C4B-CHC-C1C	2.25	125.53	122.56
2	3-B	265	HEM	C4B-CHC-C1C	2.23	125.50	122.56
2	10-B	265	HEM	C4B-CHC-C1C	2.23	125.50	122.56
2	6-B	265	HEM	C4B-CHC-C1C	2.23	125.50	122.56
2	5-B	265	HEM	C4B-CHC-C1C	2.20	125.47	122.56
2	2-B	265	HEM	C4B-CHC-C1C	2.19	125.45	122.56
2	4-B	265	HEM	C4C-CHD-C1D	2.17	125.42	122.56
2	10-A	300	HEM	C4B-CHC-C1C	2.11	125.35	122.56
2	5-B	265	HEM	C4C-CHD-C1D	2.11	125.35	122.56
2	1-B	265	HEM	C4B-CHC-C1C	2.11	125.34	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	11-B	265	HEM	C4C-CHD-C1D	2.11	125.34	122.56
2	3-A	300	HEM	C4B-CHC-C1C	2.10	125.33	122.56
2	10-B	265	HEM	C4C-CHD-C1D	2.10	125.33	122.56
2	12-A	300	HEM	C4C-CHD-C1D	2.10	125.33	122.56
2	4-A	300	HEM	C4B-CHC-C1C	2.10	125.33	122.56
2	1-A	300	HEM	C4B-CHC-C1C	2.09	125.32	122.56
2	15-B	265	HEM	C4C-CHD-C1D	2.09	125.32	122.56
2	14-A	300	HEM	C4C-CHD-C1D	2.09	125.32	122.56
2	14-B	265	HEM	C4B-CHC-C1C	2.09	125.32	122.56
2	7-B	265	HEM	C4B-CHC-C1C	2.09	125.31	122.56
2	9-B	265	HEM	C4C-CHD-C1D	2.09	125.31	122.56
2	6-B	265	HEM	C4C-CHD-C1D	2.08	125.31	122.56
2	15-A	300	HEM	C4B-CHC-C1C	2.08	125.31	122.56
2	6-A	300	HEM	C4C-CHD-C1D	2.06	125.28	122.56
2	16-B	265	HEM	C4B-CHC-C1C	2.06	125.27	122.56
2	4-B	265	HEM	C2B-C1B-NB	2.04	112.25	109.84
2	6-B	265	HEM	C2B-C1B-NB	2.03	112.25	109.84
2	15-B	265	HEM	C4B-CHC-C1C	2.03	125.24	122.56
2	4-A	300	HEM	C4C-CHD-C1D	2.03	125.24	122.56
2	7-B	265	HEM	C4C-CHD-C1D	2.03	125.24	122.56
2	5-A	300	HEM	C4B-CHC-C1C	2.03	125.23	122.56
2	14-B	265	HEM	C2D-C1D-ND	2.03	112.31	109.88
2	13-B	265	HEM	C4C-CHD-C1D	2.03	125.23	122.56
2	16-A	300	HEM	C4C-CHD-C1D	2.01	125.20	122.56
2	8-A	300	HEM	C4B-CHC-C1C	2.00	125.20	122.56
2	5-A	300	HEM	C2B-C1B-NB	2.00	112.21	109.84
2	11-A	300	HEM	C4B-CHC-C1C	2.00	125.20	122.56

There are no chirality outliers.

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2-A	300	HEM	C1A-C2A-CAA-CBA
2	4-A	300	HEM	C4B-C3B-CAB-CBB
2	16-A	300	HEM	C1A-C2A-CAA-CBA
2	1-B	265	HEM	C2B-C3B-CAB-CBB
2	1-B	265	HEM	C4B-C3B-CAB-CBB
2	2-B	265	HEM	C2A-CAA-CBA-CGA
2	2-B	265	HEM	C2B-C3B-CAB-CBB
2	2-B	265	HEM	C4B-C3B-CAB-CBB
2	3-B	265	HEM	C1A-C2A-CAA-CBA
2	3-B	265	HEM	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	4-B	265	HEM	C1A-C2A-CAA-CBA
2	4-B	265	HEM	C3A-C2A-CAA-CBA
2	6-B	265	HEM	C2B-C3B-CAB-CBB
2	7-B	265	HEM	C2B-C3B-CAB-CBB
2	7-B	265	HEM	C4B-C3B-CAB-CBB
2	8-B	265	HEM	C2B-C3B-CAB-CBB
2	9-B	265	HEM	C2B-C3B-CAB-CBB
2	9-B	265	HEM	C4B-C3B-CAB-CBB
2	10-B	265	HEM	C2A-CAA-CBA-CGA
2	10-B	265	HEM	C2B-C3B-CAB-CBB
2	10-B	265	HEM	C4B-C3B-CAB-CBB
2	11-B	265	HEM	C2B-C3B-CAB-CBB
2	11-B	265	HEM	C4B-C3B-CAB-CBB
2	12-B	265	HEM	C3A-C2A-CAA-CBA
2	12-B	265	HEM	C2B-C3B-CAB-CBB
2	12-B	265	HEM	C4B-C3B-CAB-CBB
2	13-B	265	HEM	C2B-C3B-CAB-CBB
2	15-B	265	HEM	C2B-C3B-CAB-CBB
2	15-B	265	HEM	C4B-C3B-CAB-CBB
2	16-B	265	HEM	C1A-C2A-CAA-CBA
2	16-B	265	HEM	C3A-C2A-CAA-CBA
2	16-B	265	HEM	C2B-C3B-CAB-CBB
2	9-A	300	HEM	C2A-CAA-CBA-CGA
2	1-B	265	HEM	C2A-CAA-CBA-CGA
2	4-B	265	HEM	C2A-CAA-CBA-CGA
2	9-B	265	HEM	C2A-CAA-CBA-CGA
2	16-B	265	HEM	C2A-CAA-CBA-CGA
2	3-A	300	HEM	C3D-CAD-CBD-CGD
2	3-B	265	HEM	C2A-CAA-CBA-CGA
2	12-B	265	HEM	C4D-C3D-CAD-CBD
2	4-A	300	HEM	C2B-C3B-CAB-CBB
2	6-B	265	HEM	C4B-C3B-CAB-CBB
2	8-B	265	HEM	C4B-C3B-CAB-CBB
2	13-B	265	HEM	C4B-C3B-CAB-CBB
2	16-B	265	HEM	C4B-C3B-CAB-CBB
2	5-B	265	HEM	C2D-C3D-CAD-CBD
2	4-B	265	HEM	C4D-C3D-CAD-CBD
2	5-B	265	HEM	C4D-C3D-CAD-CBD
2	3-A	300	HEM	C2B-C3B-CAB-CBB
2	12-A	300	HEM	C2A-CAA-CBA-CGA
2	14-B	265	HEM	C3A-C2A-CAA-CBA
2	11-A	300	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	16-A	300	HEM	CAD-CBD-CGD-O2D
2	9-B	265	HEM	CAD-CBD-CGD-O2D
2	4-B	265	HEM	CAD-CBD-CGD-O1D
2	5-B	265	HEM	CAA-CBA-CGA-O1A
2	9-B	265	HEM	CAD-CBD-CGD-O1D
2	16-A	300	HEM	CAD-CBD-CGD-O1D
2	15-A	300	HEM	CAD-CBD-CGD-O2D
2	11-B	265	HEM	CAD-CBD-CGD-O2D
2	12-B	265	HEM	CAD-CBD-CGD-O1D
2	15-B	265	HEM	CAA-CBA-CGA-O2A
2	16-B	265	HEM	CAD-CBD-CGD-O1D
2	4-B	265	HEM	CAD-CBD-CGD-O2D
2	12-B	265	HEM	CAD-CBD-CGD-O2D
2	4-B	265	HEM	CAA-CBA-CGA-O2A
2	7-B	265	HEM	CAD-CBD-CGD-O2D
2	16-B	265	HEM	CAD-CBD-CGD-O2D
2	5-A	300	HEM	CAD-CBD-CGD-O2D
2	15-A	300	HEM	CAD-CBD-CGD-O1D
2	3-B	265	HEM	CAA-CBA-CGA-O2A
2	14-B	265	HEM	CAD-CBD-CGD-O2D
2	2-A	300	HEM	CAD-CBD-CGD-O2D
2	10-A	300	HEM	CAD-CBD-CGD-O2D
2	2-B	265	HEM	CAD-CBD-CGD-O1D
2	5-B	265	HEM	CAA-CBA-CGA-O2A
2	2-A	300	HEM	CAD-CBD-CGD-O1D
2	2-B	265	HEM	CAD-CBD-CGD-O2D
2	3-A	300	HEM	CAA-CBA-CGA-O1A
2	9-A	300	HEM	CAD-CBD-CGD-O2D
2	13-A	300	HEM	CAD-CBD-CGD-O2D
2	14-A	300	HEM	CAA-CBA-CGA-O2A
2	11-B	265	HEM	CAD-CBD-CGD-O1D
2	4-A	300	HEM	CAD-CBD-CGD-O2D
2	7-A	300	HEM	CAD-CBD-CGD-O2D
2	9-A	300	HEM	CAA-CBA-CGA-O2A
2	10-A	300	HEM	CAD-CBD-CGD-O1D
2	11-A	300	HEM	CAD-CBD-CGD-O2D
2	12-A	300	HEM	CAD-CBD-CGD-O2D
2	5-B	265	HEM	CAD-CBD-CGD-O2D
2	4-A	300	HEM	CAA-CBA-CGA-O2A
2	6-A	300	HEM	CAD-CBD-CGD-O2D
2	1-B	265	HEM	CAD-CBD-CGD-O2D
2	1-A	300	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	14-A	300	HEM	CAD-CBD-CGD-O2D
2	8-B	265	HEM	CAA-CBA-CGA-O2A
2	15-B	265	HEM	CAA-CBA-CGA-O1A
2	8-A	300	HEM	CAD-CBD-CGD-O2D
2	7-B	265	HEM	CAA-CBA-CGA-O2A
2	9-A	300	HEM	CAA-CBA-CGA-O1A
2	9-A	300	HEM	CAD-CBD-CGD-O1D
2	1-B	265	HEM	CAD-CBD-CGD-O1D
2	4-B	265	HEM	CAA-CBA-CGA-O1A
2	5-A	300	HEM	CAD-CBD-CGD-O1D
2	5-B	265	HEM	CAD-CBD-CGD-O1D
2	2-A	300	HEM	CAA-CBA-CGA-O2A
2	3-B	265	HEM	CAA-CBA-CGA-O1A
2	8-B	265	HEM	CAD-CBD-CGD-O1D
2	4-A	300	HEM	CAD-CBD-CGD-O1D
2	7-A	300	HEM	CAD-CBD-CGD-O1D
2	8-A	300	HEM	CAD-CBD-CGD-O1D
2	11-A	300	HEM	CAD-CBD-CGD-O1D
2	12-A	300	HEM	CAD-CBD-CGD-O1D
2	13-A	300	HEM	CAD-CBD-CGD-O1D
2	14-A	300	HEM	CAD-CBD-CGD-O1D
2	7-B	265	HEM	CAD-CBD-CGD-O1D
2	6-A	300	HEM	CAD-CBD-CGD-O1D
2	13-A	300	HEM	CAA-CBA-CGA-O2A
2	1-B	265	HEM	CAA-CBA-CGA-O2A
2	7-B	265	HEM	CAA-CBA-CGA-O1A
2	12-B	265	HEM	CAA-CBA-CGA-O2A
2	1-A	300	HEM	CAD-CBD-CGD-O1D
2	3-B	265	HEM	CAD-CBD-CGD-O2D
2	14-B	265	HEM	CAD-CBD-CGD-O1D
2	4-A	300	HEM	CAA-CBA-CGA-O1A
2	3-A	300	HEM	CAD-CBD-CGD-O2D
2	3-B	265	HEM	CAD-CBD-CGD-O1D
2	6-B	265	HEM	CAD-CBD-CGD-O2D
2	3-A	300	HEM	C4B-C3B-CAB-CBB
2	3-B	265	HEM	C4B-C3B-CAB-CBB
2	2-A	300	HEM	CAA-CBA-CGA-O1A
2	13-A	300	HEM	CAA-CBA-CGA-O1A
2	14-A	300	HEM	CAA-CBA-CGA-O1A
2	8-B	265	HEM	CAA-CBA-CGA-O1A
2	15-B	265	HEM	CAD-CBD-CGD-O2D
2	1-B	265	HEM	CAA-CBA-CGA-O1A

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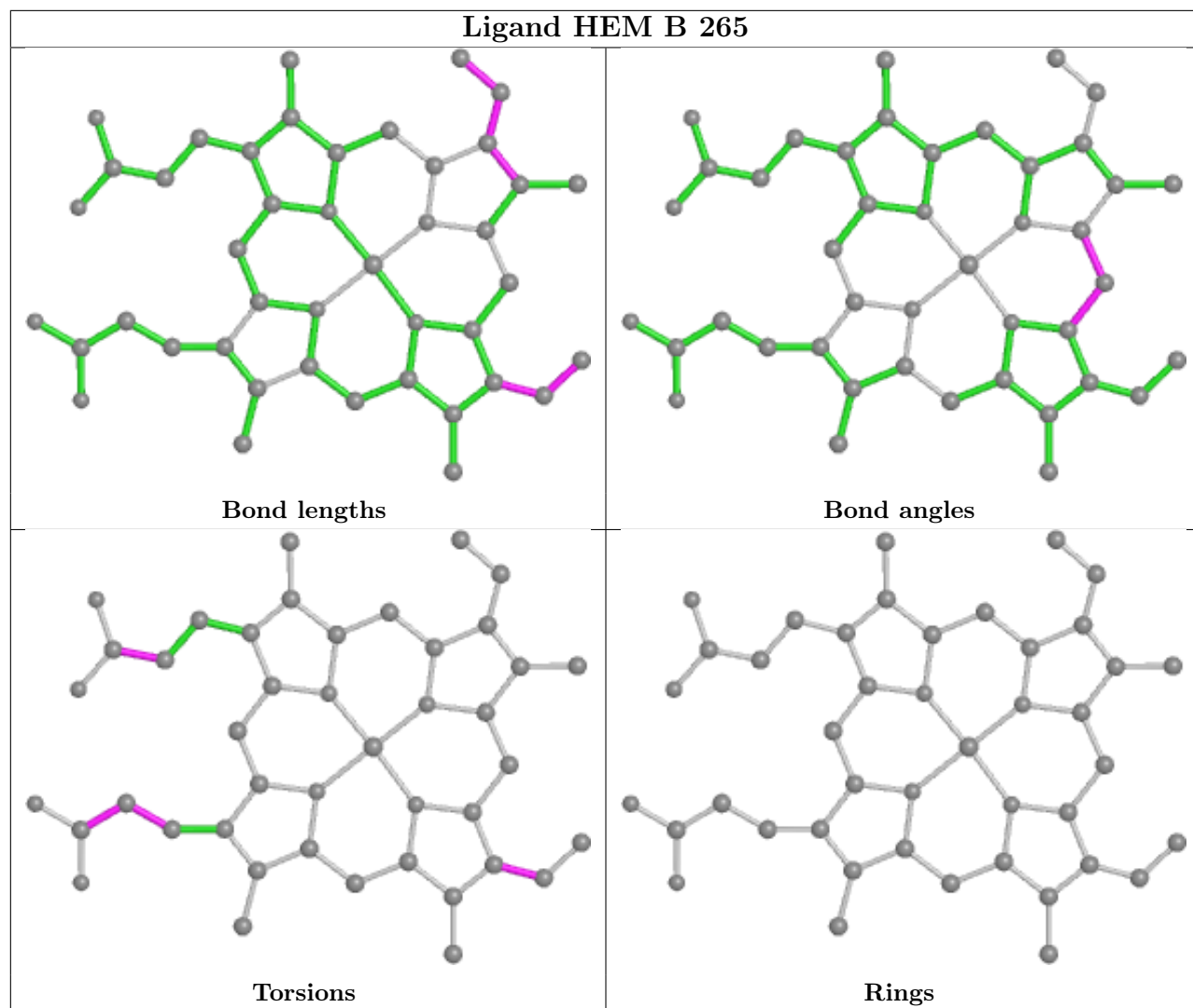
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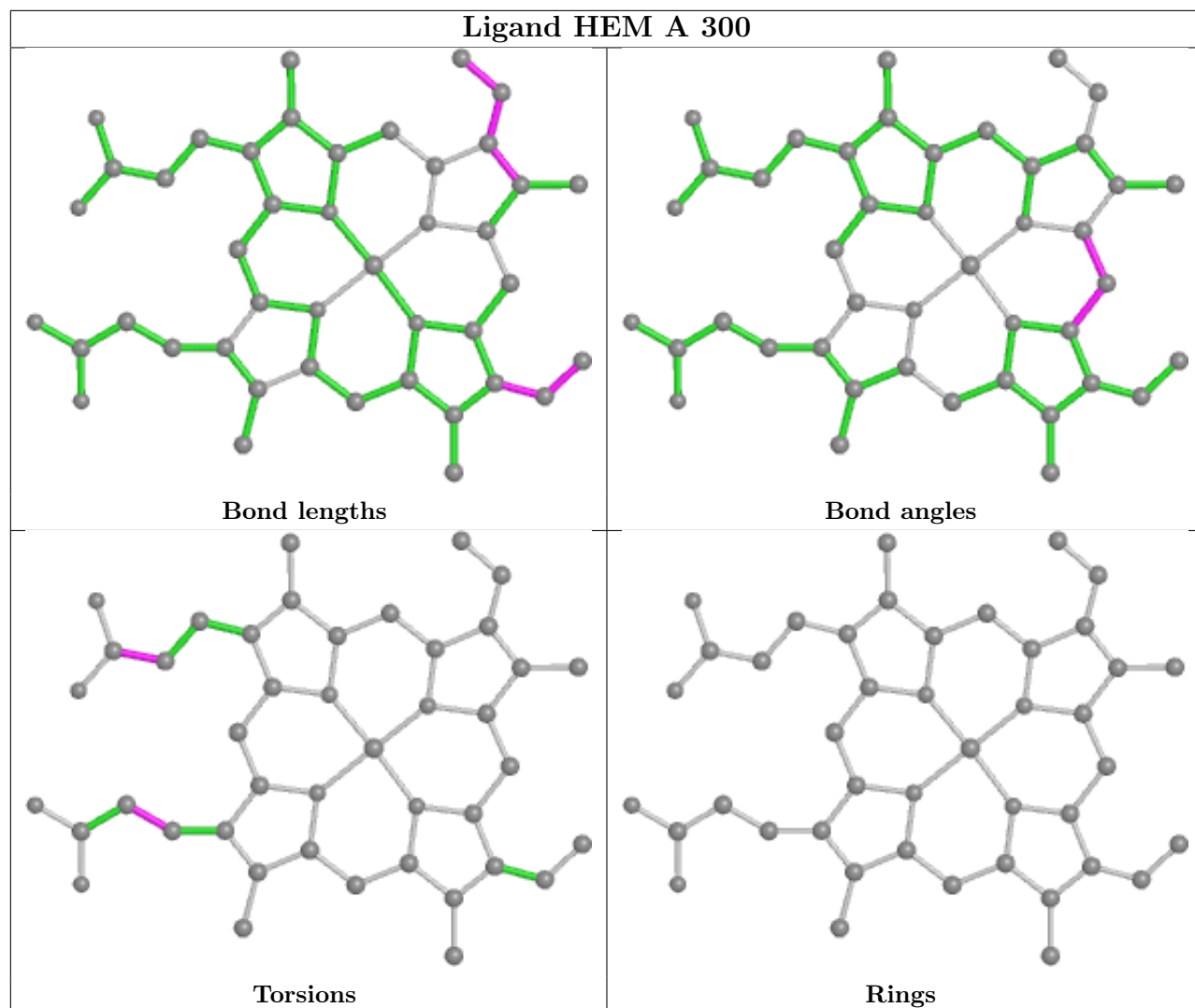
Mol	Chain	Res	Type	Atoms
2	10-B	265	HEM	CAD-CBD-CGD-O1D
2	10-B	265	HEM	CAD-CBD-CGD-O2D
2	12-B	265	HEM	CAA-CBA-CGA-O1A
2	16-B	265	HEM	CAA-CBA-CGA-O2A
2	3-A	300	HEM	CAD-CBD-CGD-O1D
2	6-B	265	HEM	CAD-CBD-CGD-O1D
2	13-B	265	HEM	CAA-CBA-CGA-O2A
2	10-B	265	HEM	CAA-CBA-CGA-O2A
2	16-A	300	HEM	CAA-CBA-CGA-O2A
2	3-A	300	HEM	CAA-CBA-CGA-O2A
2	1-A	300	HEM	C2A-CAA-CBA-CGA
2	15-B	265	HEM	CAD-CBD-CGD-O1D
2	16-B	265	HEM	CAA-CBA-CGA-O1A
2	8-B	265	HEM	CAD-CBD-CGD-O2D
2	10-B	265	HEM	CAA-CBA-CGA-O1A
2	6-A	300	HEM	CAA-CBA-CGA-O2A
2	12-A	300	HEM	CAA-CBA-CGA-O2A
2	16-A	300	HEM	CAA-CBA-CGA-O1A
2	13-B	265	HEM	CAA-CBA-CGA-O1A
2	6-A	300	HEM	CAA-CBA-CGA-O1A
2	12-A	300	HEM	CAA-CBA-CGA-O1A
2	6-A	300	HEM	C2A-CAA-CBA-CGA
2	11-A	300	HEM	CAA-CBA-CGA-O2A
2	7-A	300	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

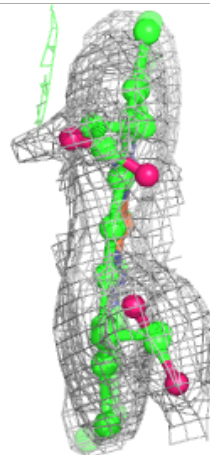
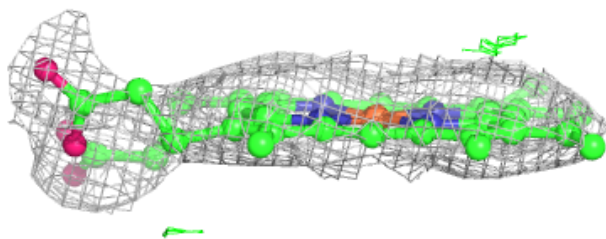
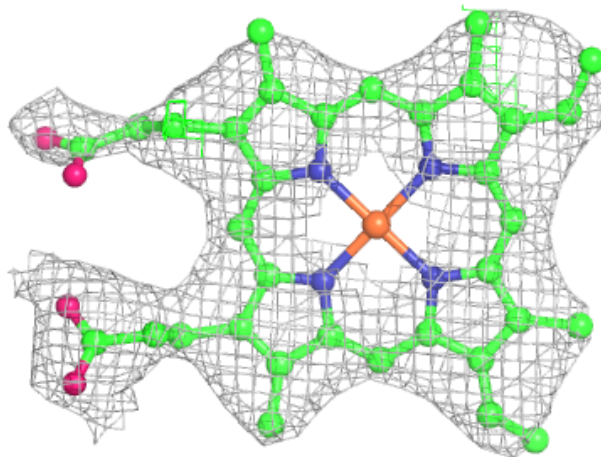
6.4 Ligands

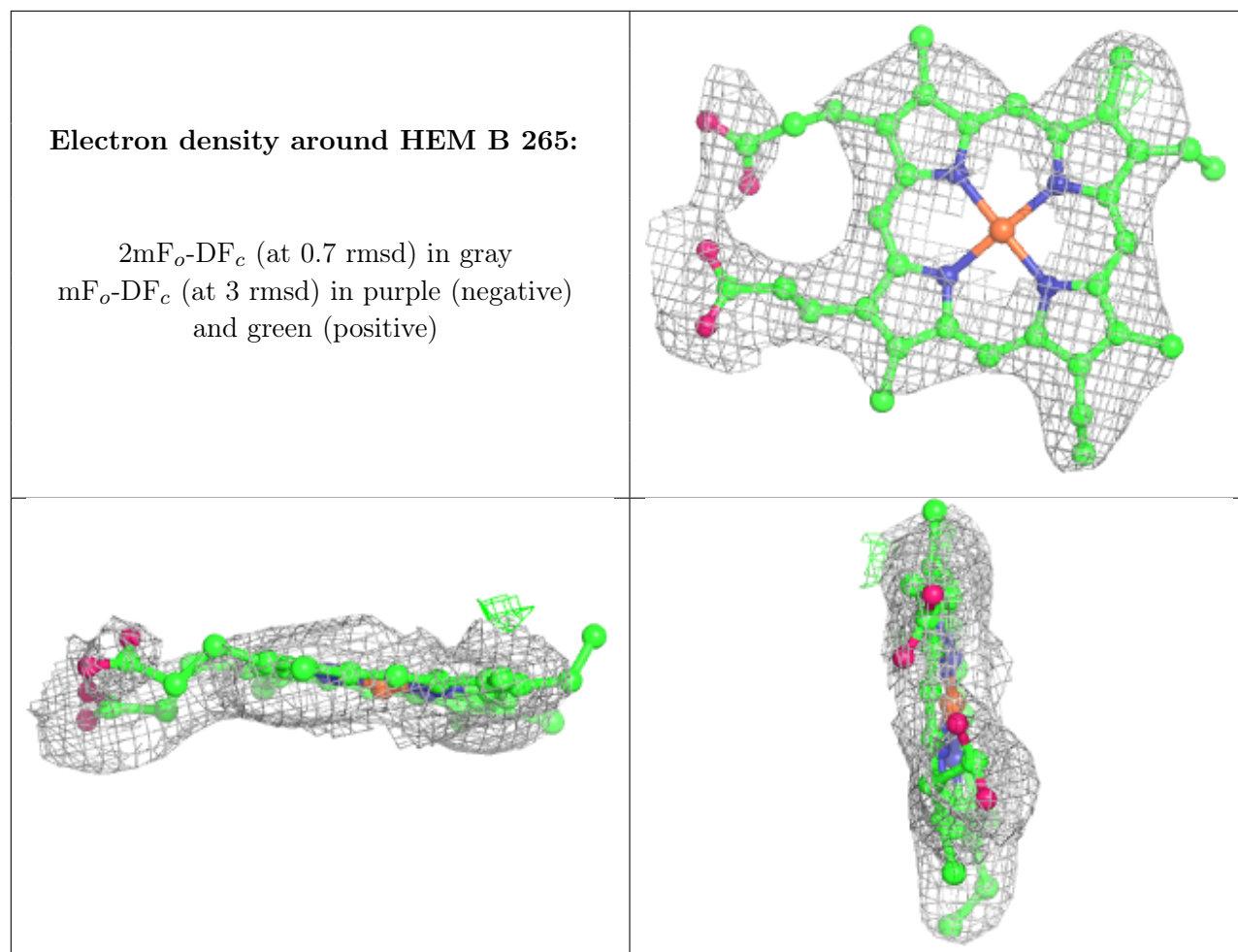
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The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also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

Electron density around HEM A 300:

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





6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.