



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:35 PM UTC

PDB ID : 2RGZ / pdb_00002rgz
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

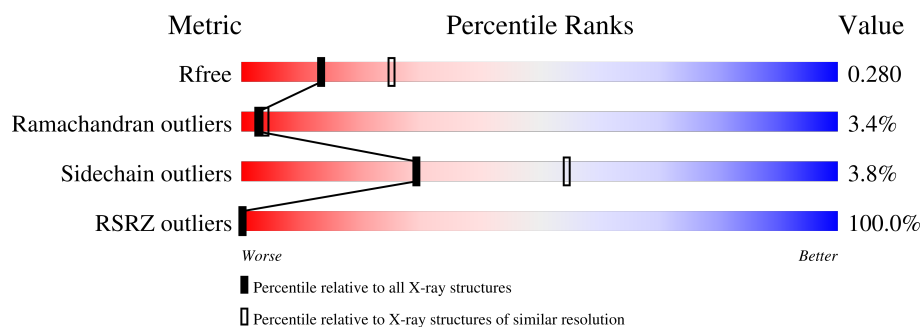
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	180053	4951 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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 $\leq 5\%$. 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	1-A	264	81% 77% 19%
1	1-B	264	83% 77% 6% 17%
1	10-A	264	78% 19%
1	10-B	264	77% 6% 17%
1	11-A	264	77% 19%
1	11-B	264	78% 5% 17%

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Mol	Chain	Length	Quality of chain
1	12-A	264	 78% 1% 19%
1	12-B	264	 77% 6% 17%
1	13-A	264	 77% 5% 19%
1	13-B	264	 77% 6% 17%
1	14-A	264	 76% 5% 19%
1	14-B	264	 74% 9% 17%
1	15-A	264	 75% 6% 19%
1	15-B	264	 77% 6% 17%
1	16-A	264	 77% 1% 19%
1	16-B	264	 74% 8% 17%
1	2-A	264	 77% 5% 19%
1	2-B	264	 79% 1% 17%
1	3-A	264	 77% 1% 19%
1	3-B	264	 77% 6% 17%
1	4-A	264	 76% 5% 19%
1	4-B	264	 78% 5% 17%
1	5-A	264	 77% 5% 19%
1	5-B	264	 77% 6% 17%
1	6-A	264	 76% 5% 19%
1	6-B	264	 76% 7% 17%
1	7-A	264	 77% 1% 19%
1	7-B	264	 78% 5% 17%
1	8-A	264	 77% 1% 19%
1	8-B	264	 76% 7% 17%
1	9-A	264	 75% 6% 19%

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Mol	Chain	Length	Quality of chain
1	9-B	264	 77% 6% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEM	1-A	300	-	-	-	X
2	HEM	1-B	265	-	-	-	X

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

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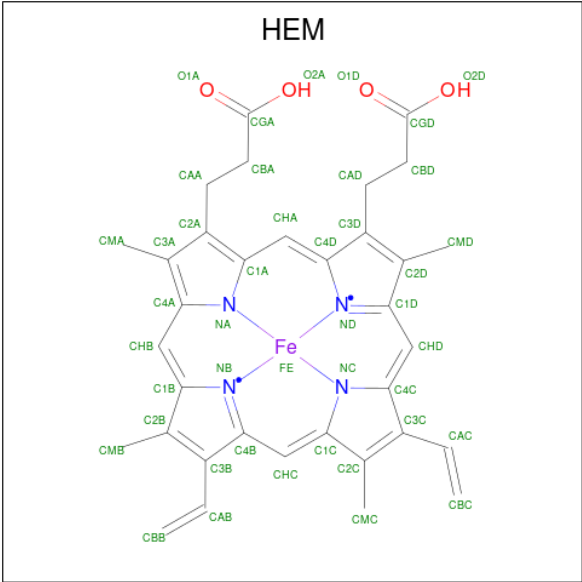
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	2-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	3-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	4-B	219	Total	C	N	O	S	0	0	0
			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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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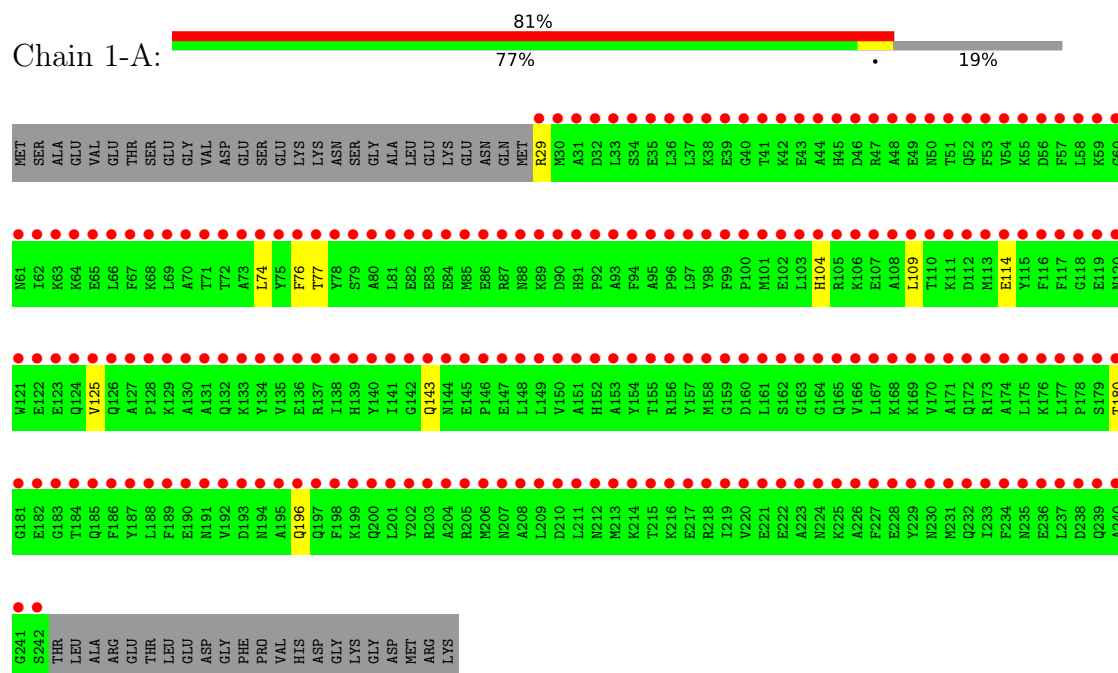
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-B	34	Total	O	0	0
			34	34		

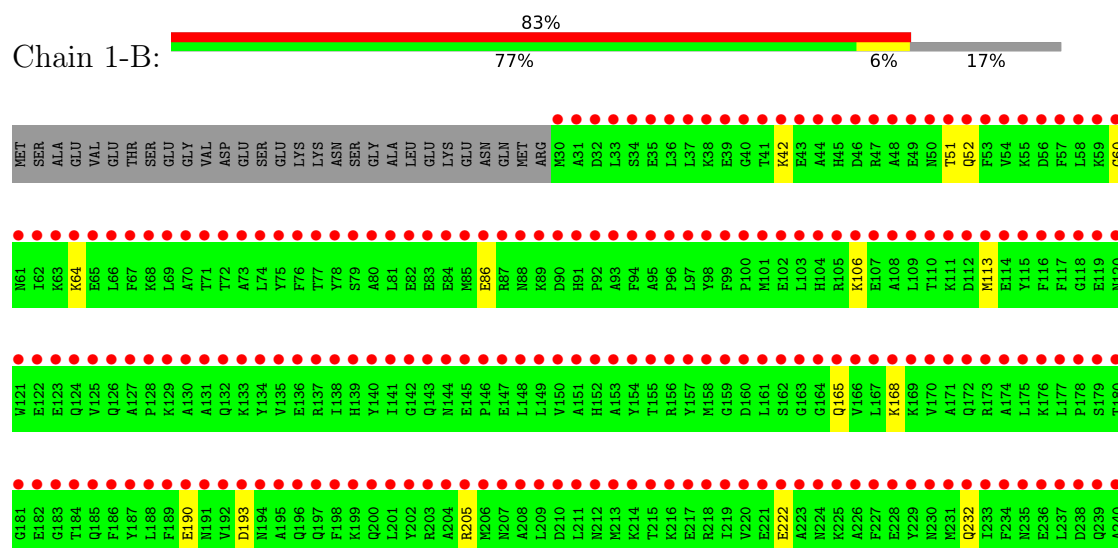
3 Residue-property plots [i](#)

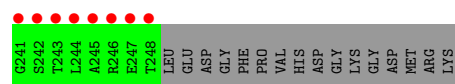
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Heme oxygenase 2

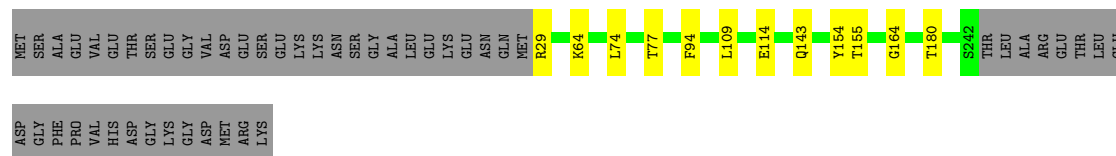
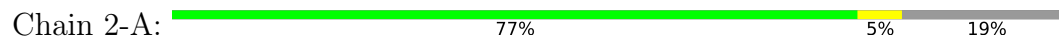


• Molecule 1: Heme oxygenase 2

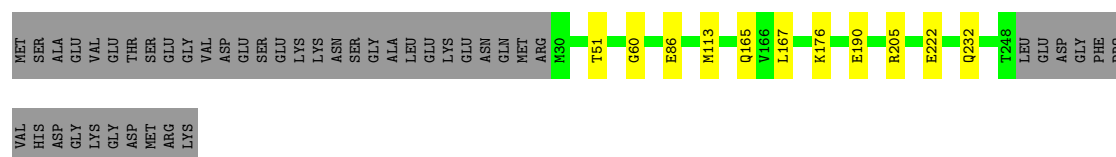
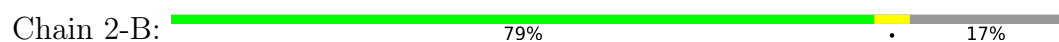




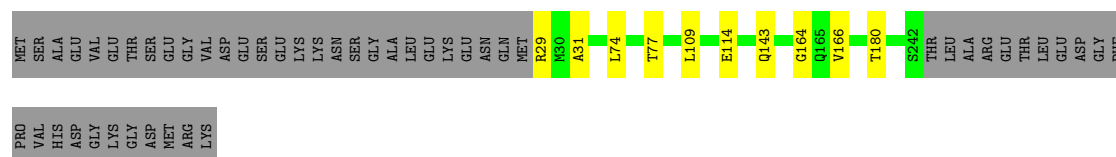
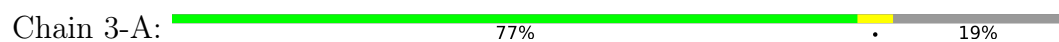
- Molecule 1: Heme oxygenase 2



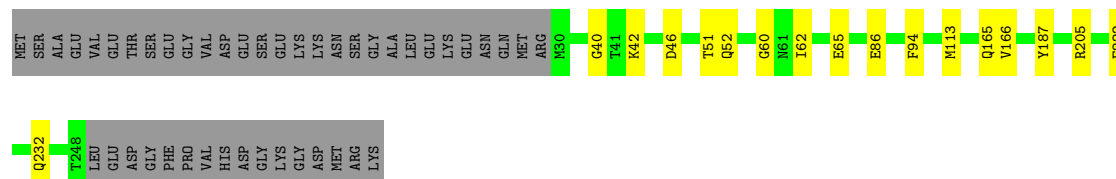
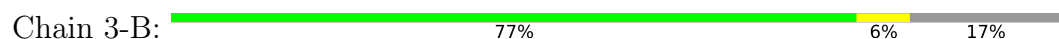
- Molecule 1: Heme oxygenase 2



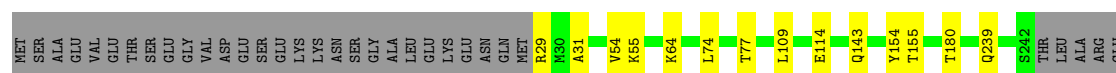
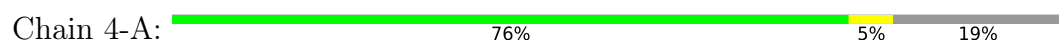
- Molecule 1: Heme oxygenase 2



- Molecule 1: Heme oxygenase 2



- Molecule 1: Heme oxygenase 2



THR
LEU
GLU
ASP
GLY
PHE
PRO
VAL
HIS
GLY
ASP
GLY
LYS
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

Chain 4-B:  78% 5% 17%

MET SER ALA GLU VAL THR SER GLY VAL ASP GLU SER GLU LYS ASN SER GLY ALA LEU LEU LYS ASN GLN MET MET ARG K30 A44 T51 V54 K63 K64 E86 M113 Q165 V170 P178 R205 E222 Q232 E247 T248 LEU

ASP
GLY
PHE
PRO
VAL
HIS
ASP
GLY
LYS
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

Chain 5-A:  77% 5% 19%

MET SER ALA GLU VAL THR SER GLY VAL ASP GLU SER GLU LYS ASN SER GLY ALA LEU LEU LYS ASN GLN MET MET ARG R29 L74 T77 F94 L109 E114 I138 Q143 T180 E190 N191 G241 S242 THR LEU ALA ARG GLU THR LEU ASP

GLY
PHE
PRO
VAL
HIS
ASP
GLY
LYS
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

Chain 5-B:  77% 6% 17%

MET SER ALA GLU VAL THR SER GLY VAL ASP GLU SER GLU LYS ASN SER GLY ALA LEU LEU LYS ASN GLN MET MET ARG K30 G40 T51 I62 K63 K64 E86 M113 E119 G164 Q165 P178 S179 E182 R205 E222 Q232 T243

T248
LEU
GLU
PHE
PRO
VAL
HIS
ASP
GLY
LYS
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

Chain 6-A:  76% 5% 19%

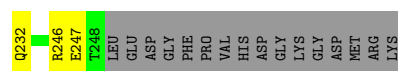
MET SER ALA GLU VAL THR SER GLY VAL ASP GLU SER GLU LYS ASN SER GLY ALA LEU LEU LYS ASN GLN MET MET ARG R29 K30 A31 L74 T77 P100 M101 L109 E114 Q143 S162 G163 K176 T180 S242 THR LEU ALA ARG GLU THR LEU

GLU
ASP
GLY
PHE
PRO
VAL
HIS
ASP
GLY
LYS
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

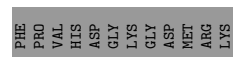
Chain 6-B:  76% 7% 17%

MET SER ALA GLU VAL THR SER GLY VAL ASP GLU SER GLU LYS ASN SER GLY ALA LEU LEU LYS ASN GLN MET MET ARG K30 T51 Q52 K64 E86 F99 H104 R105 M113 Q165 L175 P178 S179 V192 R205 N212 E222



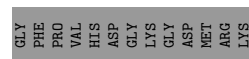
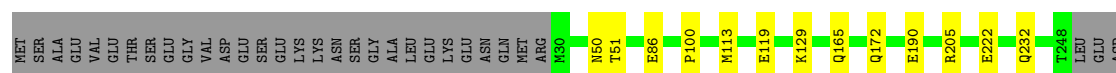
- Molecule 1: Heme oxygenase 2

Chain 7-A: 77% 19%



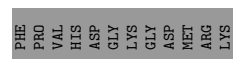
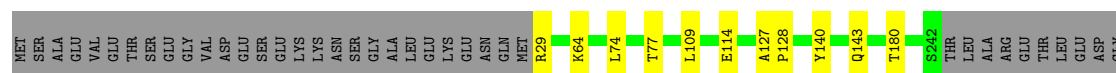
- Molecule 1: Heme oxygenase 2

Chain 7-B: 78% 5% 17%



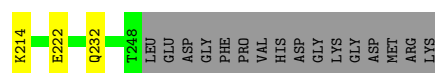
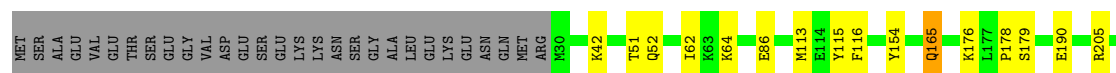
- Molecule 1: Heme oxygenase 2

Chain 8-A: 77% 19%



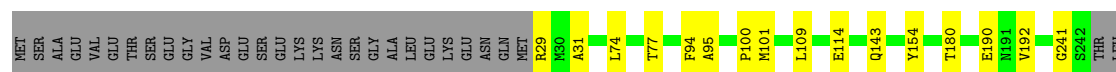
- Molecule 1: Heme oxygenase 2

Chain 8-B: 76% 7% 17%



- Molecule 1: Heme oxygenase 2

Chain 9-A: 75% 6% 19%



ALA
ARG
GLU
THR
LEU
GLU
ASP
GLY
PHE
PRO
VAL
GLY
HIS
ASP
GLY
LYS
GLY
ASP
MET
ARG
LYS

- Molecule 1: Heme oxygenase 2

Chain 9-B:  77% 6% 17%

MET SER ALA VAL THR SER GLY VAL ASP HIS ASP GLY LYS LYS ASP MET ARG LYS
K30 T51 L58 K59 G80 K64 E85 E86 M113 Y154 G164 Q165 V166 P178 Q196 R205 E222 Q232
N235 T248 LEU ASP GLY PHE VAL HIS ASP GLY LYS LYS ASP MET ARG LYS

- Molecule 1: Heme oxygenase 2

Chain 10-A:  78% 19%

MET SER ALA VAL THR SER GLY VAL ASP HIS ASP GLY LYS LYS ASP MET ARG LYS
R29 K64 L74 Y75 F76 T77 L109 E114 Q143 T180 S242 THR LEU ALA ARG GLU THR LEU GLU ASP PHE PRO VAL HIS
ASP GLY LYS ASP MET ARG LYS

- Molecule 1: Heme oxygenase 2

Chain 10-B:  77% 6% 17%

MET SER ALA VAL THR SER GLY VAL ASP HIS ASP GLY LYS LYS ASP MET ARG LYS
K30 T51 K68 E86 E102 M113 G163 G164 Q165 K169 V170 P178 S179 D193 Q196 R205 E222 Q232
T248 LEU ASP GLY PHE VAL HIS ASP GLY LYS LYS ASP MET ARG LYS

- Molecule 1: Heme oxygenase 2

Chain 11-A:  77% 19%

MET SER ALA VAL THR SER GLY VAL ASP HIS ASP GLY LYS LYS ASP MET ARG LYS
R29 L74 T77 L109 E114 Q143 Y154 T180 M194 L209 S242 THR LEU ALA ARG GLU THR LEU GLU ASP PHE
PRO VAL HIS ASP MET ARG LYS

- Molecule 1: Heme oxygenase 2

Chain 11-B:  78% 5% 17%

MET SER ALA VAL THR SER GLY VAL ASP HIS ASP GLY LYS LYS ASP MET ARG LYS
K30 T51 E86 P100 M113 Q165 V166 L167 K168 R205 E222 Q232 N235 E247 T248 LEU GLU ASP GLY PHE PRO

VAL
HIS
ASP
GLY
LYS
GLY
ASP
MET
ARG
LYS

● Molecule 1: Heme oxygenase 2

Chain 12-A: 78% 19%

MET SER ALA VAL THR SER GLY VAL ASP GLU SER GLU LYS ASN GLN MET R29 L74 T77 H104 L109 E114 Q143 T180 Q196 S242 THR LEU ALA ARG GLU THR LEU GLU ASP GLY PHE PRO VAL

HIS
ASP
GLY
LYS
GLY
ASP
MET
ARG
LYS

● Molecule 1: Heme oxygenase 2

Chain 12-B: 77% 6% 17%

MET SER ALA VAL THR SER GLY VAL ASP GLU SER GLU LYS ASN GLN MET M30 T51 K64 E86 M113 E119 N120 W121 E122 V125 S162 Q165 V166 T180 R205 E222 Q232 T248

LEU
GLU
ASP
GLY
PHE
PRO
VAL
HIS
ASP
GLY
LYS
GLY
ASP
MET
ARG
LYS

● Molecule 1: Heme oxygenase 2

Chain 13-A: 77% 5% 19%

MET SER ALA VAL THR SER GLY VAL ASP GLU SER GLU LYS ASN GLN MET R29 L74 T77 A95 H104 L109 E114 Q143 G163 T180 Q185 G241 S242 THR LEU ALA ARG GLU THR LEU GLU

ASP
GLY
PHE
PRO
VAL
HIS
ASP
GLY
LYS
GLY
ASP
MET
ARG
LYS

● Molecule 1: Heme oxygenase 2

Chain 13-B: 77% 6% 17%

MET SER ALA VAL THR SER GLY VAL ASP GLU SER GLU LYS ASN GLN MET M30 T51 G60 E86 K106 M113 Y164 T155 G163 G164 Q165 T180 E190 R205 E222 Q232 E247 T248

LEU
GLU
ASP
GLY
PHE
PRO
VAL
HIS
ASP
GLY
LYS
GLY
ASP
MET
ARG
LYS

● Molecule 1: Heme oxygenase 2

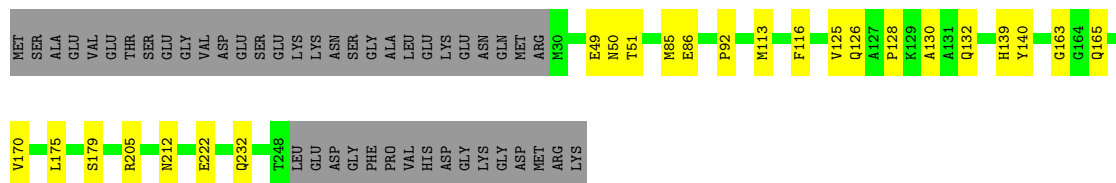
Chain 14-A: 76% 5% 19%

MET SER ALA VAL THR SER GLY VAL ASP GLU SER GLU LYS ASN GLN MET R29 L74 T77 F94 L109 E114 E136 Q143 V166 L177 T180 G181 E182 G241 S242 THR LEU ALA ARG GLU THR

LEU
GLU
ASP
GLY
PHE
PRO
VAL
HIS
ASP
GLY
LYS
GLY
ASP
MET
ARG
LYS

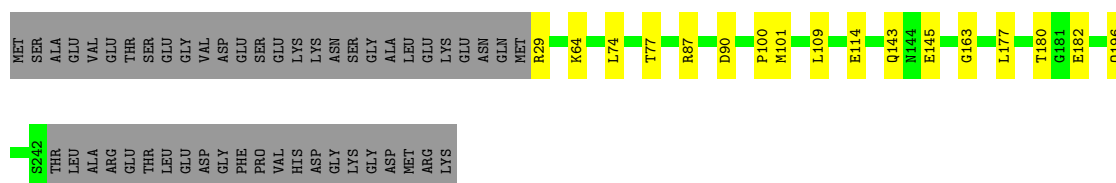
- Molecule 1: Heme oxygenase 2

Chain 14-B:  74% 9% 17%



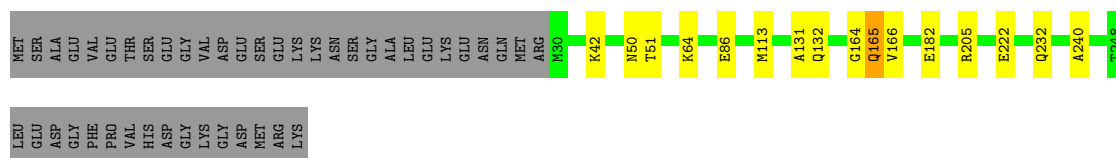
- Molecule 1: Heme oxygenase 2

Chain 15-A:  75% 6% 19%



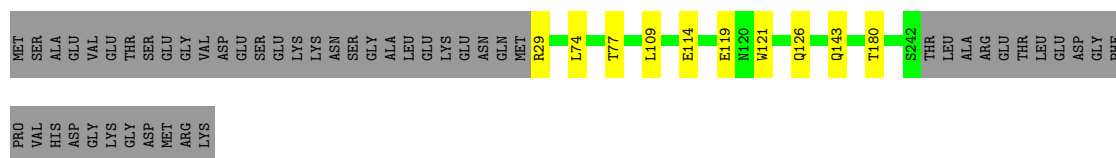
- Molecule 1: Heme oxygenase 2

Chain 15-B:  77% 6% 17%



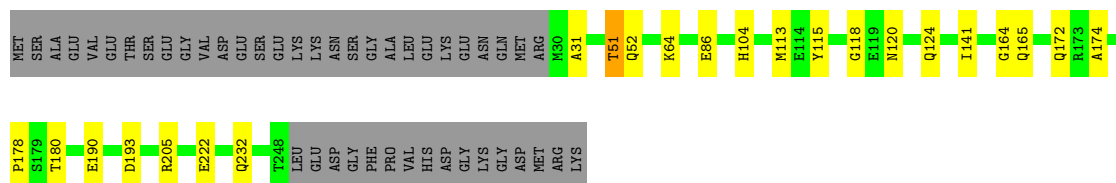
- Molecule 1: Heme oxygenase 2

Chain 16-A:  77% 6% 19%



- Molecule 1: Heme oxygenase 2

Chain 16-B:  74% 8% 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) 99.3 (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)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.161 , 0.249 0.209 , 0.280	Depositor DCC
R_{free} test set	1005 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.52	EDS
Total number of atoms	58291	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1-A	0.19	0/1794	0.32	0/2410
1	1-B	0.18	0/1830	0.29	0/2460
1	2-A	0.19	0/1794	0.32	0/2410
1	2-B	0.18	0/1830	0.29	0/2460
1	3-A	0.19	0/1794	0.32	0/2410
1	3-B	0.18	0/1830	0.29	0/2460
1	4-A	0.19	0/1794	0.32	0/2410
1	4-B	0.18	0/1830	0.29	0/2460
1	5-A	0.19	0/1794	0.32	0/2410
1	5-B	0.18	0/1830	0.29	0/2460
1	6-A	0.19	0/1794	0.32	0/2410
1	6-B	0.18	0/1830	0.29	0/2460
1	7-A	0.19	0/1794	0.32	0/2410
1	7-B	0.18	0/1830	0.29	0/2460
1	8-A	0.19	0/1794	0.32	0/2410
1	8-B	0.18	0/1830	0.29	0/2460
1	9-A	0.19	0/1794	0.32	0/2410
1	9-B	0.18	0/1830	0.29	0/2460
1	10-A	0.19	0/1794	0.32	0/2410
1	10-B	0.18	0/1830	0.29	0/2460
1	11-A	0.19	0/1794	0.32	0/2410
1	11-B	0.18	0/1830	0.29	0/2460
1	12-A	0.19	0/1794	0.32	0/2410
1	12-B	0.18	0/1830	0.29	0/2460
1	13-A	0.19	0/1794	0.32	0/2410
1	13-B	0.18	0/1830	0.29	0/2460
1	14-A	0.19	0/1794	0.32	0/2410
1	14-B	0.18	0/1830	0.29	0/2460
1	15-A	0.19	0/1794	0.32	0/2410
1	15-B	0.18	0/1830	0.29	0/2460
1	16-A	0.19	0/1794	0.32	0/2410
1	16-B	0.18	0/1830	0.29	0/2460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.19	0/57984	0.31	0/77920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	212/264 (80%)	185 (87%)	23 (11%)	4 (2%)	6	12
1	1-B	217/264 (82%)	190 (88%)	19 (9%)	8 (4%)	2	3
1	2-A	212/264 (80%)	184 (87%)	23 (11%)	5 (2%)	4	8
1	2-B	217/264 (82%)	183 (84%)	30 (14%)	4 (2%)	6	13
1	3-A	212/264 (80%)	192 (91%)	17 (8%)	3 (1%)	9	17
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%)	3	4
1	4-B	217/264 (82%)	175 (81%)	35 (16%)	7 (3%)	3	4
1	5-A	212/264 (80%)	189 (89%)	18 (8%)	5 (2%)	4	8
1	5-B	217/264 (82%)	186 (86%)	22 (10%)	9 (4%)	2	2
1	6-A	212/264 (80%)	181 (85%)	25 (12%)	6 (3%)	4	6
1	6-B	217/264 (82%)	167 (77%)	38 (18%)	12 (6%)	1	1
1	7-A	212/264 (80%)	182 (86%)	26 (12%)	4 (2%)	6	12
1	7-B	217/264 (82%)	183 (84%)	28 (13%)	6 (3%)	4	6
1	8-A	212/264 (80%)	187 (88%)	21 (10%)	4 (2%)	6	12
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%)	2	2
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%)	9	17
1	10-B	217/264 (82%)	185 (85%)	23 (11%)	9 (4%)	2	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	11-A	212/264 (80%)	185 (87%)	24 (11%)	3 (1%)	9	17
1	11-B	217/264 (82%)	184 (85%)	28 (13%)	5 (2%)	5	8
1	12-A	212/264 (80%)	198 (93%)	12 (6%)	2 (1%)	14	28
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%)	4	8
1	13-B	217/264 (82%)	182 (84%)	26 (12%)	9 (4%)	2	2
1	14-A	212/264 (80%)	176 (83%)	30 (14%)	6 (3%)	4	6
1	14-B	217/264 (82%)	165 (76%)	35 (16%)	17 (8%)	1	0
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%)	9	17
1	16-B	217/264 (82%)	172 (79%)	28 (13%)	17 (8%)	1	0
All	All	6864/8448 (81%)	5812 (85%)	817 (12%)	235 (3%)	3	4

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	175 (96%)	7 (4%)	29	54
1	1-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	2-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	2-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	3-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	3-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	4-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	4-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	5-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	5-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	6-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	6-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	7-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	7-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	8-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	8-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	9-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	9-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	10-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	10-B	186/224 (83%)	179 (96%)	7 (4%)	29	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	11-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	11-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	12-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	12-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	13-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	13-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	14-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	14-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	15-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	15-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
1	16-A	182/224 (81%)	175 (96%)	7 (4%)	29	54
1	16-B	186/224 (83%)	179 (96%)	7 (4%)	29	54
All	All	5888/7168 (82%)	5664 (96%)	224 (4%)	29	54

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	29	ARG
1	1-A	74	LEU
1	1-A	77	THR
1	1-A	109	LEU
1	1-A	114	GLU
1	1-A	143	GLN
1	1-A	180	THR
1	1-B	51	THR
1	1-B	86	GLU
1	1-B	113	MET
1	1-B	165	GLN
1	1-B	205	ARG
1	1-B	222	GLU
1	1-B	232	GLN
1	2-A	29	ARG
1	2-A	74	LEU
1	2-A	77	THR
1	2-A	109	LEU
1	2-A	114	GLU
1	2-A	143	GLN
1	2-A	180	THR

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Mol	Chain	Res	Type
1	2-B	51	THR
1	2-B	86	GLU
1	2-B	113	MET
1	2-B	165	GLN
1	2-B	205	ARG
1	2-B	222	GLU
1	2-B	232	GLN
1	3-A	29	ARG
1	3-A	74	LEU
1	3-A	77	THR
1	3-A	109	LEU
1	3-A	114	GLU
1	3-A	143	GLN
1	3-A	180	THR
1	3-B	51	THR
1	3-B	86	GLU
1	3-B	113	MET
1	3-B	165	GLN
1	3-B	205	ARG
1	3-B	222	GLU
1	3-B	232	GLN
1	4-A	29	ARG
1	4-A	74	LEU
1	4-A	77	THR
1	4-A	109	LEU
1	4-A	114	GLU
1	4-A	143	GLN
1	4-A	180	THR
1	4-B	51	THR
1	4-B	86	GLU
1	4-B	113	MET
1	4-B	165	GLN
1	4-B	205	ARG
1	4-B	222	GLU
1	4-B	232	GLN
1	5-A	29	ARG
1	5-A	74	LEU
1	5-A	77	THR
1	5-A	109	LEU
1	5-A	114	GLU
1	5-A	143	GLN
1	5-A	180	THR

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Mol	Chain	Res	Type
1	5-B	51	THR
1	5-B	86	GLU
1	5-B	113	MET
1	5-B	165	GLN
1	5-B	205	ARG
1	5-B	222	GLU
1	5-B	232	GLN
1	6-A	29	ARG
1	6-A	74	LEU
1	6-A	77	THR
1	6-A	109	LEU
1	6-A	114	GLU
1	6-A	143	GLN
1	6-A	180	THR
1	6-B	51	THR
1	6-B	86	GLU
1	6-B	113	MET
1	6-B	165	GLN
1	6-B	205	ARG
1	6-B	222	GLU
1	6-B	232	GLN
1	7-A	29	ARG
1	7-A	74	LEU
1	7-A	77	THR
1	7-A	109	LEU
1	7-A	114	GLU
1	7-A	143	GLN
1	7-A	180	THR
1	7-B	51	THR
1	7-B	86	GLU
1	7-B	113	MET
1	7-B	165	GLN
1	7-B	205	ARG
1	7-B	222	GLU
1	7-B	232	GLN
1	8-A	29	ARG
1	8-A	74	LEU
1	8-A	77	THR
1	8-A	109	LEU
1	8-A	114	GLU
1	8-A	143	GLN
1	8-A	180	THR

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Mol	Chain	Res	Type
1	8-B	51	THR
1	8-B	86	GLU
1	8-B	113	MET
1	8-B	165	GLN
1	8-B	205	ARG
1	8-B	222	GLU
1	8-B	232	GLN
1	9-A	29	ARG
1	9-A	74	LEU
1	9-A	77	THR
1	9-A	109	LEU
1	9-A	114	GLU
1	9-A	143	GLN
1	9-A	180	THR
1	9-B	51	THR
1	9-B	86	GLU
1	9-B	113	MET
1	9-B	165	GLN
1	9-B	205	ARG
1	9-B	222	GLU
1	9-B	232	GLN
1	10-A	29	ARG
1	10-A	74	LEU
1	10-A	77	THR
1	10-A	109	LEU
1	10-A	114	GLU
1	10-A	143	GLN
1	10-A	180	THR
1	10-B	51	THR
1	10-B	86	GLU
1	10-B	113	MET
1	10-B	165	GLN
1	10-B	205	ARG
1	10-B	222	GLU
1	10-B	232	GLN
1	11-A	29	ARG
1	11-A	74	LEU
1	11-A	77	THR
1	11-A	109	LEU
1	11-A	114	GLU
1	11-A	143	GLN
1	11-A	180	THR

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Mol	Chain	Res	Type
1	11-B	51	THR
1	11-B	86	GLU
1	11-B	113	MET
1	11-B	165	GLN
1	11-B	205	ARG
1	11-B	222	GLU
1	11-B	232	GLN
1	12-A	29	ARG
1	12-A	74	LEU
1	12-A	77	THR
1	12-A	109	LEU
1	12-A	114	GLU
1	12-A	143	GLN
1	12-A	180	THR
1	12-B	51	THR
1	12-B	86	GLU
1	12-B	113	MET
1	12-B	165	GLN
1	12-B	205	ARG
1	12-B	222	GLU
1	12-B	232	GLN
1	13-A	29	ARG
1	13-A	74	LEU
1	13-A	77	THR
1	13-A	109	LEU
1	13-A	114	GLU
1	13-A	143	GLN
1	13-A	180	THR
1	13-B	51	THR
1	13-B	86	GLU
1	13-B	113	MET
1	13-B	165	GLN
1	13-B	205	ARG
1	13-B	222	GLU
1	13-B	232	GLN
1	14-A	29	ARG
1	14-A	74	LEU
1	14-A	77	THR
1	14-A	109	LEU
1	14-A	114	GLU
1	14-A	143	GLN
1	14-A	180	THR

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Mol	Chain	Res	Type
1	14-B	51	THR
1	14-B	86	GLU
1	14-B	113	MET
1	14-B	165	GLN
1	14-B	205	ARG
1	14-B	222	GLU
1	14-B	232	GLN
1	15-A	29	ARG
1	15-A	74	LEU
1	15-A	77	THR
1	15-A	109	LEU
1	15-A	114	GLU
1	15-A	143	GLN
1	15-A	180	THR
1	15-B	51	THR
1	15-B	86	GLU
1	15-B	113	MET
1	15-B	165	GLN
1	15-B	205	ARG
1	15-B	222	GLU
1	15-B	232	GLN
1	16-A	29	ARG
1	16-A	74	LEU
1	16-A	77	THR
1	16-A	109	LEU
1	16-A	114	GLU
1	16-A	143	GLN
1	16-A	180	THR
1	16-B	51	THR
1	16-B	86	GLU
1	16-B	113	MET
1	16-B	165	GLN
1	16-B	205	ARG
1	16-B	222	GLU
1	16-B	232	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (203) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	52	GLN
1	1-A	61	ASN
1	1-A	104	HIS

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Mol	Chain	Res	Type
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-A	239	GLN
1	1-B	124	GLN
1	1-B	143	GLN
1	1-B	165	GLN
1	1-B	172	GLN
1	1-B	196	GLN
1	1-B	230	ASN
1	2-A	52	GLN
1	2-A	104	HIS
1	2-A	165	GLN
1	2-A	194	ASN
1	2-A	196	GLN
1	2-A	197	GLN
1	2-B	50	ASN
1	2-B	104	HIS
1	2-B	124	GLN
1	2-B	165	GLN
1	2-B	185	GLN
1	2-B	191	ASN
1	2-B	196	GLN
1	2-B	197	GLN
1	2-B	224	ASN
1	2-B	230	ASN
1	3-A	52	GLN
1	3-A	61	ASN
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

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Mol	Chain	Res	Type
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	4-B	232	GLN
1	5-A	61	ASN
1	5-A	104	HIS
1	5-A	143	GLN
1	5-A	165	GLN
1	5-A	185	GLN
1	5-A	196	GLN
1	5-A	239	GLN
1	5-B	61	ASN
1	5-B	104	HIS
1	5-B	124	GLN
1	5-B	185	GLN
1	5-B	230	ASN
1	6-A	50	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	165	GLN
1	6-A	172	GLN
1	6-A	197	GLN
1	6-A	200	GLN
1	6-B	61	ASN
1	6-B	144	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	143	GLN
1	7-A	152	HIS
1	7-A	165	GLN

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Mol	Chain	Res	Type
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	88	ASN
1	8-A	104	HIS
1	8-A	120	ASN
1	8-A	143	GLN
1	8-A	144	ASN
1	8-A	185	GLN
1	8-B	124	GLN
1	8-B	126	GLN
1	8-B	144	ASN
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	124	GLN
1	9-A	143	GLN
1	9-A	172	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	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

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Mol	Chain	Res	Type
1	10-B	165	GLN
1	10-B	172	GLN
1	10-B	185	GLN
1	10-B	194	ASN
1	10-B	212	ASN
1	10-B	230	ASN
1	11-A	61	ASN
1	11-A	104	HIS
1	11-A	143	GLN
1	11-A	165	GLN
1	11-A	191	ASN
1	11-A	194	ASN
1	11-B	50	ASN
1	11-B	124	GLN
1	11-B	152	HIS
1	11-B	165	GLN
1	11-B	172	GLN
1	11-B	235	ASN
1	12-A	52	GLN
1	12-A	143	GLN
1	12-A	239	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
1	12-B	224	ASN
1	12-B	230	ASN
1	13-A	88	ASN
1	13-B	61	ASN
1	13-B	124	GLN
1	13-B	165	GLN
1	13-B	191	ASN
1	13-B	197	GLN
1	13-B	230	ASN
1	13-B	232	GLN
1	14-A	88	ASN
1	14-A	104	HIS
1	14-A	152	HIS
1	14-A	197	GLN
1	14-A	232	GLN
1	14-B	120	ASN

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Mol	Chain	Res	Type
1	14-B	143	GLN
1	14-B	165	GLN
1	14-B	172	GLN
1	15-A	61	ASN
1	15-A	144	ASN
1	15-A	191	ASN
1	15-A	197	GLN
1	15-A	235	ASN
1	15-B	61	ASN
1	15-B	104	HIS
1	15-B	144	ASN
1	15-B	172	GLN
1	15-B	230	ASN
1	15-B	232	GLN
1	16-A	50	ASN
1	16-A	88	ASN
1	16-A	104	HIS
1	16-A	126	GLN
1	16-A	143	GLN
1	16-A	165	GLN
1	16-A	194	ASN
1	16-A	196	GLN
1	16-A	235	ASN
1	16-B	104	HIS
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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	5-A	300	1	50,50,50	1.11	4 (8%)	67,82,82	0.94	2 (2%)
2	HEM	13-B	265	1	50,50,50	1.19	4 (8%)	67,82,82	0.92	1 (1%)
2	HEM	4-B	265	1	50,50,50	1.19	4 (8%)	67,82,82	0.94	2 (2%)
2	HEM	3-B	265	1	50,50,50	1.19	4 (8%)	67,82,82	0.93	1 (1%)
2	HEM	12-B	265	1	50,50,50	1.21	4 (8%)	67,82,82	0.89	1 (1%)
2	HEM	5-B	265	1	50,50,50	1.17	4 (8%)	67,82,82	0.89	1 (1%)
2	HEM	11-B	265	1	50,50,50	1.16	4 (8%)	67,82,82	0.93	1 (1%)
2	HEM	7-B	265	1	50,50,50	1.19	4 (8%)	67,82,82	0.90	1 (1%)
2	HEM	15-B	265	1	50,50,50	1.20	4 (8%)	67,82,82	0.94	1 (1%)
2	HEM	9-B	265	1	50,50,50	1.20	4 (8%)	67,82,82	0.92	1 (1%)
2	HEM	6-A	300	1	50,50,50	1.13	4 (8%)	67,82,82	0.97	1 (1%)
2	HEM	14-A	300	1	50,50,50	1.18	5 (10%)	67,82,82	0.98	1 (1%)
2	HEM	13-A	300	1	50,50,50	1.20	4 (8%)	67,82,82	0.94	1 (1%)
2	HEM	16-A	300	1	50,50,50	1.10	4 (8%)	67,82,82	0.98	1 (1%)
2	HEM	6-B	265	1	50,50,50	1.16	4 (8%)	67,82,82	0.89	2 (2%)
2	HEM	1-B	265	1	50,50,50	1.19	4 (8%)	67,82,82	0.91	1 (1%)
2	HEM	10-B	265	1	50,50,50	1.20	4 (8%)	67,82,82	0.92	1 (1%)
2	HEM	8-A	300	1	50,50,50	1.13	4 (8%)	67,82,82	0.98	1 (1%)
2	HEM	11-A	300	1	50,50,50	1.13	4 (8%)	67,82,82	0.97	1 (1%)
2	HEM	3-A	300	1	50,50,50	1.14	4 (8%)	67,82,82	0.96	1 (1%)
2	HEM	9-A	300	1	50,50,50	1.21	4 (8%)	67,82,82	0.95	1 (1%)
2	HEM	8-B	265	1	50,50,50	1.17	4 (8%)	67,82,82	0.89	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	10-A	300	1	50,50,50	1.10	4 (8%)	67,82,82	0.95	1 (1%)
2	HEM	12-A	300	1	50,50,50	1.14	4 (8%)	67,82,82	0.97	1 (1%)
2	HEM	16-B	265	1	50,50,50	1.23	4 (8%)	67,82,82	0.96	1 (1%)
2	HEM	14-B	265	1	50,50,50	1.25	5 (10%)	67,82,82	1.06	3 (4%)
2	HEM	15-A	300	1	50,50,50	1.13	4 (8%)	67,82,82	0.97	3 (4%)
2	HEM	2-A	300	1	50,50,50	1.11	4 (8%)	67,82,82	0.96	1 (1%)
2	HEM	1-A	300	1	50,50,50	1.10	4 (8%)	67,82,82	0.95	1 (1%)
2	HEM	2-B	265	1	50,50,50	1.20	4 (8%)	67,82,82	0.92	1 (1%)
2	HEM	7-A	300	1	50,50,50	1.12	4 (8%)	67,82,82	0.97	1 (1%)
2	HEM	4-A	300	1	50,50,50	1.21	4 (8%)	67,82,82	0.94	1 (1%)

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	5-A	300	1	-	2/14/54/54	-
2	HEM	13-B	265	1	-	6/14/54/54	-
2	HEM	4-B	265	1	-	10/14/54/54	-
2	HEM	3-B	265	1	-	11/14/54/54	-
2	HEM	12-B	265	1	-	11/14/54/54	-
2	HEM	5-B	265	1	-	8/14/54/54	-
2	HEM	11-B	265	1	-	6/14/54/54	-
2	HEM	7-B	265	1	-	8/14/54/54	-
2	HEM	15-B	265	1	-	8/14/54/54	-
2	HEM	9-B	265	1	-	7/14/54/54	-
2	HEM	6-A	300	1	-	6/14/54/54	-
2	HEM	14-A	300	1	-	4/14/54/54	-
2	HEM	13-A	300	1	-	5/14/54/54	-
2	HEM	16-A	300	1	-	5/14/54/54	-
2	HEM	6-B	265	1	-	6/14/54/54	-
2	HEM	1-B	265	1	-	9/14/54/54	-
2	HEM	10-B	265	1	-	9/14/54/54	-
2	HEM	8-A	300	1	-	2/14/54/54	-
2	HEM	11-A	300	1	-	6/14/54/54	-

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

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	12-B	265	HEM	CAB-C3B	-3.50	1.38	1.47
2	14-B	265	HEM	CBB-CAB	3.44	1.46	1.30
2	12-B	265	HEM	CBC-CAC	3.44	1.46	1.30
2	1-B	265	HEM	CAB-C3B	-3.36	1.38	1.47
2	9-B	265	HEM	CAB-C3B	-3.36	1.38	1.47
2	4-B	265	HEM	CBB-CAB	3.33	1.46	1.30
2	3-A	300	HEM	CBC-CAC	3.33	1.46	1.30
2	11-B	265	HEM	CAB-C3B	-3.30	1.38	1.47
2	13-B	265	HEM	CBB-CAB	3.30	1.46	1.30
2	3-B	265	HEM	CBC-CAC	3.30	1.46	1.30
2	9-A	300	HEM	CAC-C3C	-3.29	1.38	1.47
2	15-B	265	HEM	CAB-C3B	-3.28	1.38	1.47
2	10-B	265	HEM	CBB-CAB	3.28	1.46	1.30
2	7-B	265	HEM	CAB-C3B	-3.28	1.38	1.47
2	13-B	265	HEM	CAB-C3B	-3.27	1.38	1.47
2	9-B	265	HEM	CBB-CAB	3.26	1.46	1.30
2	10-B	265	HEM	CAB-C3B	-3.25	1.38	1.47
2	16-B	265	HEM	CBB-CAB	3.25	1.46	1.30
2	15-A	300	HEM	CBC-CAC	3.24	1.46	1.30
2	14-B	265	HEM	CAC-C3C	-3.24	1.38	1.47
2	3-A	300	HEM	CAB-C3B	-3.24	1.38	1.47
2	1-B	265	HEM	CBB-CAB	3.24	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-A	300	HEM	CAC-C3C	-3.23	1.38	1.47
2	5-B	265	HEM	CBB-CAB	3.23	1.45	1.30
2	11-A	300	HEM	CAC-C3C	-3.22	1.38	1.47
2	4-A	300	HEM	CAC-C3C	-3.20	1.38	1.47
2	8-B	265	HEM	CBB-CAB	3.20	1.45	1.30
2	7-B	265	HEM	CBB-CAB	3.20	1.45	1.30
2	12-A	300	HEM	CAC-C3C	-3.19	1.38	1.47
2	6-B	265	HEM	CBB-CAB	3.19	1.45	1.30
2	2-B	265	HEM	CBB-CAB	3.18	1.45	1.30
2	7-A	300	HEM	CBB-CAB	3.17	1.45	1.30
2	9-A	300	HEM	CBC-CAC	3.17	1.45	1.30
2	8-A	300	HEM	CBB-CAB	3.16	1.45	1.30
2	5-A	300	HEM	CBC-CAC	3.16	1.45	1.30
2	2-B	265	HEM	CAB-C3B	-3.16	1.38	1.47
2	15-A	300	HEM	CAB-C3B	-3.16	1.39	1.47
2	12-A	300	HEM	CBB-CAB	3.15	1.45	1.30
2	4-A	300	HEM	CBC-CAC	3.15	1.45	1.30
2	16-B	265	HEM	CAC-C3C	-3.14	1.39	1.47
2	10-B	265	HEM	CAC-C3C	-3.14	1.39	1.47
2	10-A	300	HEM	CBB-CAB	3.14	1.45	1.30
2	13-A	300	HEM	CAC-C3C	-3.14	1.39	1.47
2	13-A	300	HEM	CBC-CAC	3.14	1.45	1.30
2	4-B	265	HEM	CAC-C3C	-3.13	1.39	1.47
2	1-A	300	HEM	CBB-CAB	3.13	1.45	1.30
2	2-A	300	HEM	CBB-CAB	3.13	1.45	1.30
2	3-B	265	HEM	CBB-CAB	3.13	1.45	1.30
2	15-B	265	HEM	CBB-CAB	3.13	1.45	1.30
2	6-B	265	HEM	CAC-C3C	-3.13	1.39	1.47
2	6-A	300	HEM	CBB-CAB	3.13	1.45	1.30
2	11-A	300	HEM	CBB-CAB	3.12	1.45	1.30
2	11-B	265	HEM	CBB-CAB	3.12	1.45	1.30
2	8-A	300	HEM	CBC-CAC	3.11	1.45	1.30
2	4-B	265	HEM	CBC-CAC	3.11	1.45	1.30
2	13-B	265	HEM	CBC-CAC	3.11	1.45	1.30
2	2-B	265	HEM	CBC-CAC	3.11	1.45	1.30
2	1-A	300	HEM	CBC-CAC	3.10	1.45	1.30
2	10-A	300	HEM	CBC-CAC	3.10	1.45	1.30
2	5-B	265	HEM	CBC-CAC	3.09	1.45	1.30
2	7-B	265	HEM	CAC-C3C	-3.08	1.39	1.47
2	9-B	265	HEM	CAC-C3C	-3.08	1.39	1.47
2	9-B	265	HEM	CBC-CAC	3.08	1.45	1.30
2	15-B	265	HEM	CBC-CAC	3.08	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8-B	265	HEM	CBC-CAC	3.07	1.45	1.30
2	1-B	265	HEM	CAC-C3C	-3.07	1.39	1.47
2	14-B	265	HEM	CBC-CAC	3.07	1.45	1.30
2	8-B	265	HEM	CAC-C3C	-3.07	1.39	1.47
2	5-A	300	HEM	CBB-CAB	3.07	1.45	1.30
2	16-A	300	HEM	CBB-CAB	3.06	1.45	1.30
2	11-B	265	HEM	CBC-CAC	3.06	1.45	1.30
2	3-B	265	HEM	CAB-C3B	-3.06	1.39	1.47
2	16-B	265	HEM	CBC-CAC	3.06	1.45	1.30
2	2-B	265	HEM	CAC-C3C	-3.05	1.39	1.47
2	5-B	265	HEM	CAC-C3C	-3.05	1.39	1.47
2	7-A	300	HEM	CAC-C3C	-3.05	1.39	1.47
2	6-B	265	HEM	CBC-CAC	3.05	1.45	1.30
2	10-B	265	HEM	CBC-CAC	3.04	1.45	1.30
2	9-A	300	HEM	CBB-CAB	3.04	1.45	1.30
2	7-B	265	HEM	CBC-CAC	3.03	1.44	1.30
2	5-A	300	HEM	CAB-C3B	-3.02	1.39	1.47
2	14-A	300	HEM	CBC-CAC	3.02	1.44	1.30
2	12-A	300	HEM	CBC-CAC	3.02	1.44	1.30
2	11-B	265	HEM	CAC-C3C	-3.02	1.39	1.47
2	15-B	265	HEM	CAC-C3C	-3.02	1.39	1.47
2	1-B	265	HEM	CBC-CAC	3.02	1.44	1.30
2	2-A	300	HEM	CBC-CAC	3.02	1.44	1.30
2	4-A	300	HEM	CBB-CAB	3.02	1.44	1.30
2	14-A	300	HEM	CAC-C3C	-3.01	1.39	1.47
2	7-A	300	HEM	CBC-CAC	3.01	1.44	1.30
2	12-B	265	HEM	CBB-CAB	3.01	1.44	1.30
2	16-A	300	HEM	CBC-CAC	3.00	1.44	1.30
2	11-A	300	HEM	CBC-CAC	3.00	1.44	1.30
2	14-A	300	HEM	CBB-CAB	3.00	1.44	1.30
2	15-A	300	HEM	CBB-CAB	3.00	1.44	1.30
2	6-A	300	HEM	CBC-CAC	2.99	1.44	1.30
2	13-A	300	HEM	CBB-CAB	2.99	1.44	1.30
2	13-B	265	HEM	CAC-C3C	-2.95	1.39	1.47
2	8-B	265	HEM	CAB-C3B	-2.95	1.39	1.47
2	16-B	265	HEM	CAB-C3B	-2.94	1.39	1.47
2	16-A	300	HEM	CAC-C3C	-2.94	1.39	1.47
2	3-A	300	HEM	CBB-CAB	2.91	1.44	1.30
2	9-A	300	HEM	CAB-C3B	-2.90	1.39	1.47
2	4-B	265	HEM	CAB-C3B	-2.89	1.39	1.47
2	1-A	300	HEM	CAC-C3C	-2.89	1.39	1.47
2	6-B	265	HEM	CAB-C3B	-2.87	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-A	300	HEM	CAC-C3C	-2.81	1.39	1.47
2	3-B	265	HEM	CAC-C3C	-2.81	1.39	1.47
2	7-A	300	HEM	CAB-C3B	-2.79	1.39	1.47
2	4-A	300	HEM	CAB-C3B	-2.79	1.39	1.47
2	10-A	300	HEM	CAC-C3C	-2.79	1.40	1.47
2	8-A	300	HEM	CAC-C3C	-2.78	1.40	1.47
2	8-A	300	HEM	CAB-C3B	-2.74	1.40	1.47
2	10-A	300	HEM	CAB-C3B	-2.74	1.40	1.47
2	11-A	300	HEM	CAB-C3B	-2.74	1.40	1.47
2	13-A	300	HEM	CAB-C3B	-2.73	1.40	1.47
2	6-A	300	HEM	CAB-C3B	-2.73	1.40	1.47
2	12-A	300	HEM	CAB-C3B	-2.72	1.40	1.47
2	16-A	300	HEM	CAB-C3B	-2.70	1.40	1.47
2	1-A	300	HEM	CAB-C3B	-2.69	1.40	1.47
2	5-B	265	HEM	CAB-C3B	-2.67	1.40	1.47
2	2-A	300	HEM	CAB-C3B	-2.66	1.40	1.47
2	14-A	300	HEM	CAB-C3B	-2.56	1.40	1.47
2	5-A	300	HEM	CAC-C3C	-2.51	1.40	1.47
2	3-A	300	HEM	CAC-C3C	-2.42	1.40	1.47
2	12-B	265	HEM	CAC-C3C	-2.41	1.41	1.47
2	15-A	300	HEM	CAC-C3C	-2.30	1.41	1.47
2	14-B	265	HEM	CAB-C3B	-2.23	1.41	1.47
2	14-A	300	HEM	CBA-CGA	2.14	1.55	1.50
2	14-B	265	HEM	FE-ND	2.02	2.01	1.94

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	14-A	300	HEM	C3B-C4B-NB	4.17	112.46	109.47
2	16-A	300	HEM	C3B-C4B-NB	3.80	112.20	109.47
2	2-A	300	HEM	C3B-C4B-NB	3.63	112.07	109.47
2	13-A	300	HEM	C3B-C4B-NB	3.61	112.06	109.47
2	12-A	300	HEM	C3B-C4B-NB	3.46	111.95	109.47
2	11-A	300	HEM	C3B-C4B-NB	3.40	111.91	109.47
2	6-A	300	HEM	C3B-C4B-NB	3.40	111.91	109.47
2	9-A	300	HEM	C3B-C4B-NB	3.39	111.90	109.47
2	1-A	300	HEM	C3B-C4B-NB	3.32	111.86	109.47
2	10-A	300	HEM	C3B-C4B-NB	3.27	111.81	109.47
2	8-A	300	HEM	C3B-C4B-NB	3.26	111.81	109.47
2	7-A	300	HEM	C3B-C4B-NB	3.15	111.73	109.47
2	14-B	265	HEM	C3B-C4B-NB	3.09	111.69	109.47
2	4-A	300	HEM	C3B-C4B-NB	3.09	111.68	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	16-B	265	HEM	C3B-C4B-NB	2.99	111.61	109.47
2	3-A	300	HEM	C3B-C4B-NB	2.85	111.51	109.47
2	5-A	300	HEM	C3B-C4B-NB	2.77	111.46	109.47
2	7-B	265	HEM	C3B-C4B-NB	2.71	111.42	109.47
2	15-A	300	HEM	C3B-C4B-NB	2.67	111.39	109.47
2	1-B	265	HEM	C3B-C4B-NB	2.66	111.38	109.47
2	9-B	265	HEM	C3B-C4B-NB	2.63	111.36	109.47
2	11-B	265	HEM	C3B-C4B-NB	2.63	111.36	109.47
2	13-B	265	HEM	C3B-C4B-NB	2.62	111.35	109.47
2	2-B	265	HEM	C3B-C4B-NB	2.61	111.34	109.47
2	10-B	265	HEM	C3B-C4B-NB	2.60	111.34	109.47
2	12-B	265	HEM	C3B-C4B-NB	2.57	111.31	109.47
2	8-B	265	HEM	C3B-C4B-NB	2.55	111.30	109.47
2	3-B	265	HEM	C3B-C4B-NB	2.50	111.26	109.47
2	4-B	265	HEM	C3B-C4B-NB	2.47	111.24	109.47
2	15-B	265	HEM	C3B-C4B-NB	2.44	111.22	109.47
2	6-B	265	HEM	C3B-C4B-NB	2.40	111.19	109.47
2	5-B	265	HEM	C3B-C4B-NB	2.39	111.18	109.47
2	4-B	265	HEM	C2B-C1B-NB	2.10	112.25	109.84
2	14-B	265	HEM	C4D-ND-C1D	-2.10	102.72	105.21
2	6-B	265	HEM	C2B-C1B-NB	2.10	112.25	109.84
2	14-B	265	HEM	C2D-C1D-ND	2.08	112.31	109.90
2	5-A	300	HEM	C2B-C1B-NB	2.06	112.21	109.84
2	15-A	300	HEM	C2B-C1B-NB	2.06	112.21	109.84
2	15-A	300	HEM	C2A-C1A-NA	2.02	112.40	110.15

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	6-A	300	HEM	C2C-C3C-CAC-CBC
2	6-A	300	HEM	C4C-C3C-CAC-CBC
2	7-A	300	HEM	C2C-C3C-CAC-CBC
2	7-A	300	HEM	C4C-C3C-CAC-CBC
2	11-A	300	HEM	C2C-C3C-CAC-CBC
2	11-A	300	HEM	C4C-C3C-CAC-CBC
2	12-A	300	HEM	C2C-C3C-CAC-CBC
2	1-B	265	HEM	C2B-C3B-CAB-CBB
2	1-B	265	HEM	C2C-C3C-CAC-CBC
2	1-B	265	HEM	C4C-C3C-CAC-CBC
2	2-B	265	HEM	C2A-CAA-CBA-CGA
2	2-B	265	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	3-B	265	HEM	C1A-C2A-CAA-CBA
2	3-B	265	HEM	C2C-C3C-CAC-CBC
2	3-B	265	HEM	C4C-C3C-CAC-CBC
2	4-B	265	HEM	C2C-C3C-CAC-CBC
2	5-B	265	HEM	C2C-C3C-CAC-CBC
2	6-B	265	HEM	C2B-C3B-CAB-CBB
2	6-B	265	HEM	C2C-C3C-CAC-CBC
2	6-B	265	HEM	C4C-C3C-CAC-CBC
2	7-B	265	HEM	C2B-C3B-CAB-CBB
2	7-B	265	HEM	C2C-C3C-CAC-CBC
2	7-B	265	HEM	C4C-C3C-CAC-CBC
2	8-B	265	HEM	C2B-C3B-CAB-CBB
2	8-B	265	HEM	C2C-C3C-CAC-CBC
2	8-B	265	HEM	C4C-C3C-CAC-CBC
2	9-B	265	HEM	C2B-C3B-CAB-CBB
2	9-B	265	HEM	C2C-C3C-CAC-CBC
2	10-B	265	HEM	C2B-C3B-CAB-CBB
2	10-B	265	HEM	C2C-C3C-CAC-CBC
2	10-B	265	HEM	C4C-C3C-CAC-CBC
2	11-B	265	HEM	C2B-C3B-CAB-CBB
2	11-B	265	HEM	C4B-C3B-CAB-CBB
2	11-B	265	HEM	C2C-C3C-CAC-CBC
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	14-B	265	HEM	C2C-C3C-CAC-CBC
2	15-B	265	HEM	C2B-C3B-CAB-CBB
2	15-B	265	HEM	C4B-C3B-CAB-CBB
2	15-B	265	HEM	C2C-C3C-CAC-CBC
2	15-B	265	HEM	C4C-C3C-CAC-CBC
2	16-B	265	HEM	C1A-C2A-CAA-CBA
2	16-B	265	HEM	C2B-C3B-CAB-CBB
2	16-B	265	HEM	C2C-C3C-CAC-CBC
2	10-B	265	HEM	C2A-CAA-CBA-CGA
2	3-B	265	HEM	C3A-C2A-CAA-CBA
2	4-B	265	HEM	C3A-C2A-CAA-CBA
2	16-B	265	HEM	C3A-C2A-CAA-CBA
2	9-A	300	HEM	C2A-CAA-CBA-CGA
2	16-B	265	HEM	C2A-CAA-CBA-CGA
2	4-B	265	HEM	C1A-C2A-CAA-CBA
2	3-A	300	HEM	C3D-CAD-CBD-CGD
2	4-B	265	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	9-B	265	HEM	C2A-CAA-CBA-CGA
2	1-B	265	HEM	C2A-CAA-CBA-CGA
2	4-A	300	HEM	C2B-C3B-CAB-CBB
2	2-B	265	HEM	C2C-C3C-CAC-CBC
2	13-B	265	HEM	C2C-C3C-CAC-CBC
2	12-B	265	HEM	C3A-C2A-CAA-CBA
2	12-A	300	HEM	C4C-C3C-CAC-CBC
2	4-B	265	HEM	C4C-C3C-CAC-CBC
2	6-B	265	HEM	C4B-C3B-CAB-CBB
2	7-B	265	HEM	C4B-C3B-CAB-CBB
2	8-B	265	HEM	C4B-C3B-CAB-CBB
2	9-B	265	HEM	C4C-C3C-CAC-CBC
2	11-B	265	HEM	C4C-C3C-CAC-CBC
2	13-B	265	HEM	C4C-C3C-CAC-CBC
2	14-B	265	HEM	C4C-C3C-CAC-CBC
2	12-B	265	HEM	C4D-C3D-CAD-CBD
2	2-A	300	HEM	C1A-C2A-CAA-CBA
2	3-B	265	HEM	C2A-CAA-CBA-CGA
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	4-A	300	HEM	C2C-C3C-CAC-CBC
2	9-A	300	HEM	C2C-C3C-CAC-CBC
2	12-B	265	HEM	C2C-C3C-CAC-CBC
2	4-A	300	HEM	C4B-C3B-CAB-CBB
2	1-B	265	HEM	C4B-C3B-CAB-CBB
2	2-B	265	HEM	C4B-C3B-CAB-CBB
2	2-B	265	HEM	C4C-C3C-CAC-CBC
2	5-B	265	HEM	C4C-C3C-CAC-CBC
2	9-B	265	HEM	C4B-C3B-CAB-CBB
2	10-B	265	HEM	C4B-C3B-CAB-CBB
2	16-B	265	HEM	C4B-C3B-CAB-CBB
2	12-B	265	HEM	C1A-C2A-CAA-CBA
2	16-A	300	HEM	CAD-CBD-CGD-O2D
2	9-B	265	HEM	CAD-CBD-CGD-O2D
2	13-B	265	HEM	C4B-C3B-CAB-CBB
2	16-B	265	HEM	C4C-C3C-CAC-CBC
2	15-A	300	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

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Mol	Chain	Res	Type	Atoms
2	16-A	300	HEM	CAD-CBD-CGD-O1D
2	4-B	265	HEM	CAD-CBD-CGD-O2D
2	12-B	265	HEM	CAD-CBD-CGD-O1D
2	2-A	300	HEM	CAD-CBD-CGD-O2D
2	5-A	300	HEM	CAD-CBD-CGD-O2D
2	16-B	265	HEM	CAD-CBD-CGD-O1D
2	10-A	300	HEM	CAD-CBD-CGD-O2D
2	2-B	265	HEM	CAD-CBD-CGD-O2D
2	12-A	300	HEM	C2A-CAA-CBA-CGA
2	12-B	265	HEM	CAD-CBD-CGD-O2D
2	9-A	300	HEM	CAD-CBD-CGD-O2D
2	13-A	300	HEM	CAD-CBD-CGD-O2D
2	15-A	300	HEM	CAD-CBD-CGD-O1D
2	5-B	265	HEM	CAA-CBA-CGA-O2A
2	16-B	265	HEM	CAD-CBD-CGD-O2D
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	11-A	300	HEM	CAD-CBD-CGD-O2D
2	12-A	300	HEM	CAD-CBD-CGD-O2D
2	6-A	300	HEM	CAD-CBD-CGD-O2D
2	2-B	265	HEM	CAD-CBD-CGD-O1D
2	1-A	300	HEM	CAD-CBD-CGD-O2D
2	2-A	300	HEM	CAD-CBD-CGD-O1D
2	14-A	300	HEM	CAD-CBD-CGD-O2D
2	8-A	300	HEM	CAD-CBD-CGD-O2D
2	10-A	300	HEM	CAD-CBD-CGD-O1D
2	7-B	265	HEM	CAA-CBA-CGA-O2A
2	14-A	300	HEM	CAA-CBA-CGA-O2A
2	11-B	265	HEM	CAD-CBD-CGD-O2D
2	15-B	265	HEM	CAA-CBA-CGA-O2A
2	9-A	300	HEM	CAA-CBA-CGA-O1A
2	4-A	300	HEM	CAA-CBA-CGA-O2A
2	9-A	300	HEM	CAD-CBD-CGD-O1D
2	8-B	265	HEM	CAA-CBA-CGA-O2A
2	2-A	300	HEM	CAA-CBA-CGA-O2A
2	5-A	300	HEM	CAD-CBD-CGD-O1D
2	5-B	265	HEM	CAD-CBD-CGD-O2D
2	7-B	265	HEM	CAD-CBD-CGD-O2D
2	1-B	265	HEM	CAD-CBD-CGD-O2D
2	4-B	265	HEM	CAA-CBA-CGA-O2A
2	4-A	300	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
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	1-B	265	HEM	CAA-CBA-CGA-O2A
2	3-B	265	HEM	CAA-CBA-CGA-O2A
2	14-B	265	HEM	CAD-CBD-CGD-O2D
2	6-A	300	HEM	CAD-CBD-CGD-O1D
2	7-B	265	HEM	CAA-CBA-CGA-O1A
2	1-B	265	HEM	CAD-CBD-CGD-O1D
2	12-B	265	HEM	CAA-CBA-CGA-O2A
2	1-A	300	HEM	CAD-CBD-CGD-O1D
2	5-B	265	HEM	CAD-CBD-CGD-O1D
2	11-B	265	HEM	CAD-CBD-CGD-O1D
2	2-A	300	HEM	CAA-CBA-CGA-O1A
2	14-B	265	HEM	C3A-C2A-CAA-CBA
2	13-A	300	HEM	CAA-CBA-CGA-O2A
2	3-B	265	HEM	CAD-CBD-CGD-O2D
2	7-B	265	HEM	CAD-CBD-CGD-O1D
2	15-B	265	HEM	CAA-CBA-CGA-O1A
2	14-A	300	HEM	CAA-CBA-CGA-O1A
2	1-B	265	HEM	CAA-CBA-CGA-O1A
2	8-B	265	HEM	CAA-CBA-CGA-O1A
2	3-B	265	HEM	CAD-CBD-CGD-O1D
2	3-A	300	HEM	CAD-CBD-CGD-O2D
2	4-A	300	HEM	CAA-CBA-CGA-O1A
2	4-B	265	HEM	CAA-CBA-CGA-O1A
2	3-A	300	HEM	C4B-C3B-CAB-CBB
2	4-A	300	HEM	C4C-C3C-CAC-CBC
2	9-A	300	HEM	C4C-C3C-CAC-CBC
2	3-B	265	HEM	C4B-C3B-CAB-CBB
2	12-B	265	HEM	C4C-C3C-CAC-CBC
2	11-A	300	HEM	C2A-CAA-CBA-CGA
2	3-B	265	HEM	CAA-CBA-CGA-O1A
2	3-A	300	HEM	CAA-CBA-CGA-O1A
2	12-B	265	HEM	CAA-CBA-CGA-O1A
2	13-A	300	HEM	CAA-CBA-CGA-O1A
2	6-B	265	HEM	CAD-CBD-CGD-O2D
2	10-B	265	HEM	CAD-CBD-CGD-O2D
2	3-A	300	HEM	CAD-CBD-CGD-O1D

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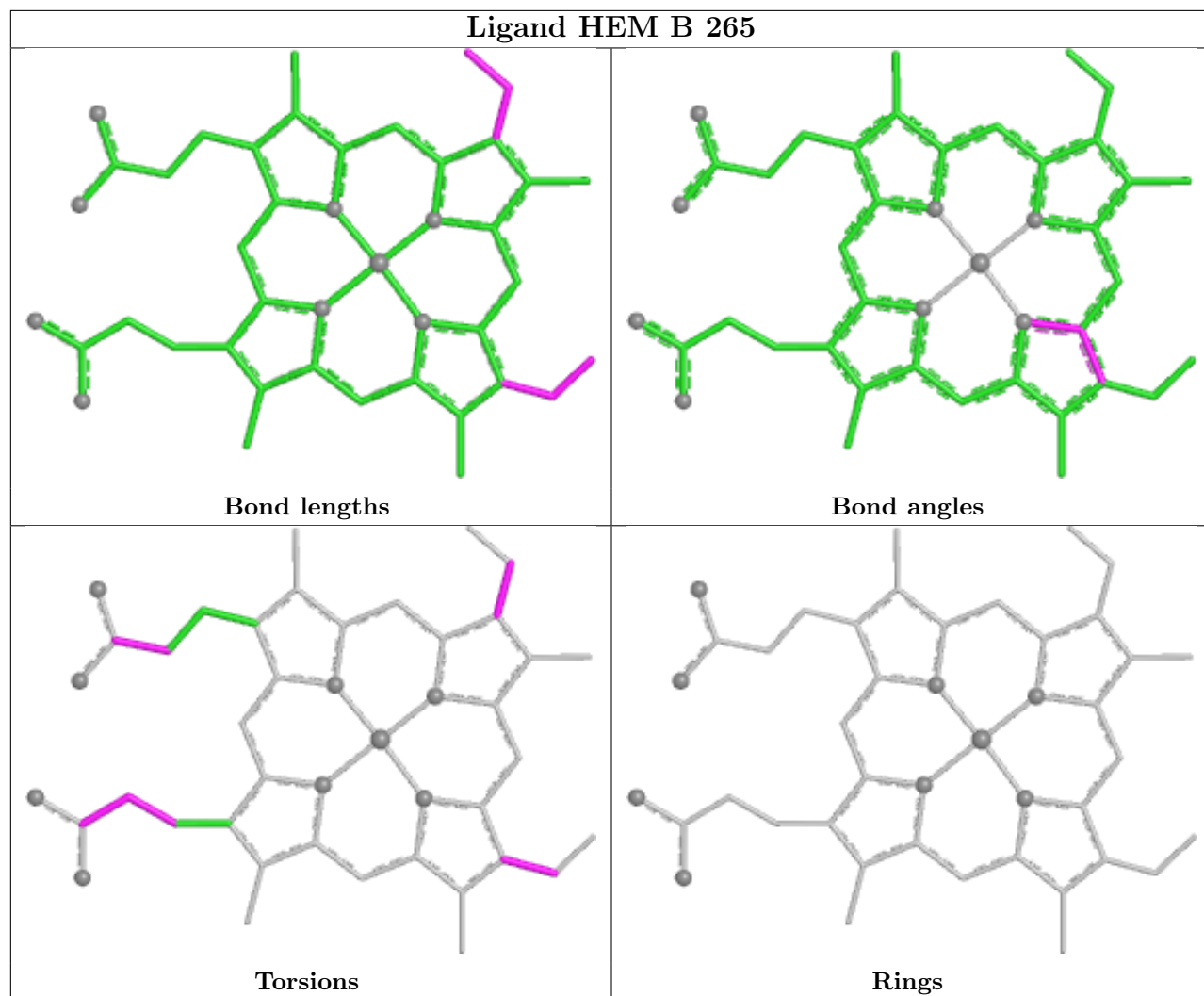
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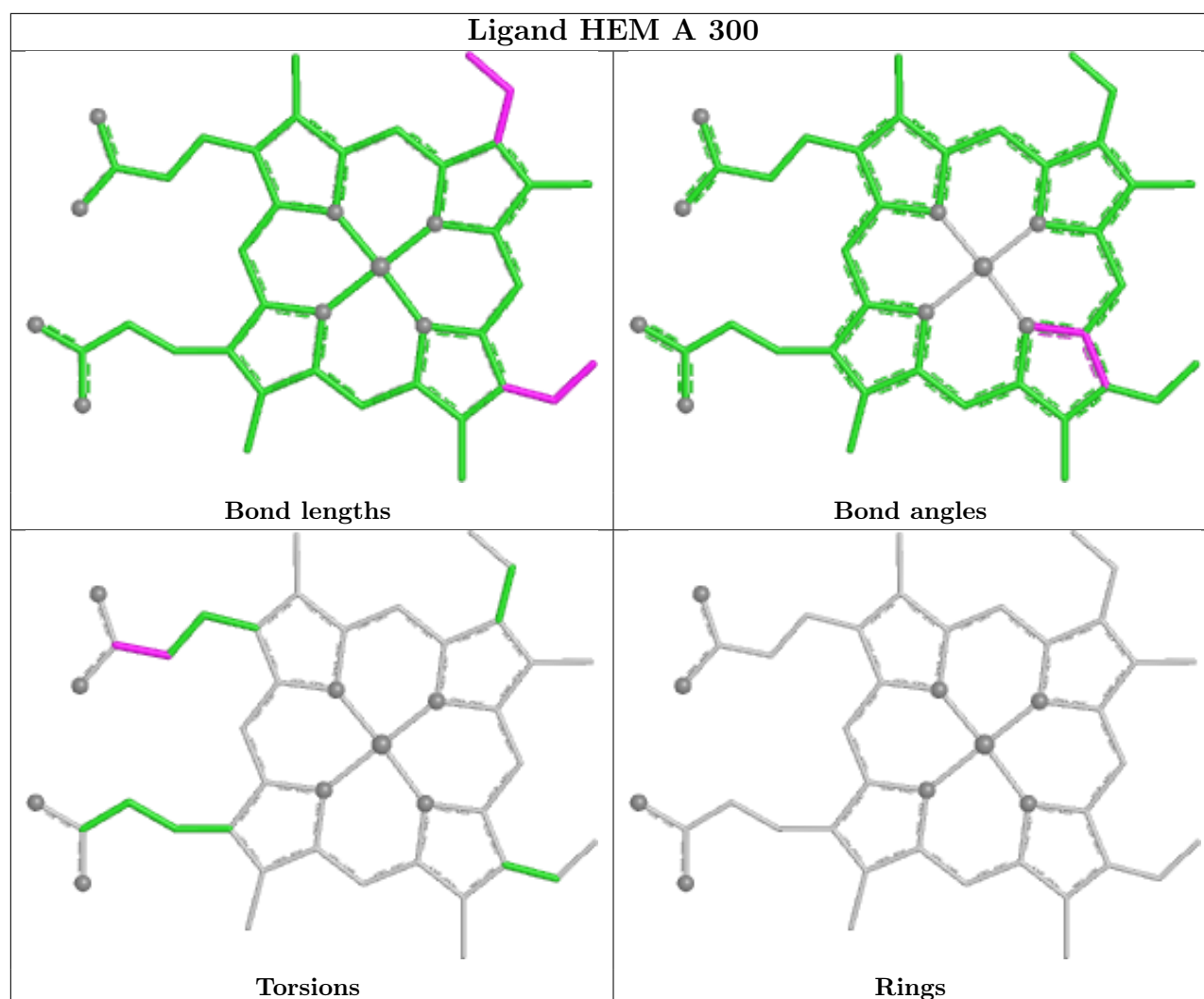
Mol	Chain	Res	Type	Atoms
2	10-B	265	HEM	CAD-CBD-CGD-O1D
2	14-B	265	HEM	CAD-CBD-CGD-O1D
2	6-B	265	HEM	CAD-CBD-CGD-O1D
2	16-A	300	HEM	C1A-C2A-CAA-CBA
2	15-B	265	HEM	CAD-CBD-CGD-O2D
2	16-B	265	HEM	CAA-CBA-CGA-O2A
2	8-B	265	HEM	CAD-CBD-CGD-O1D
2	13-B	265	HEM	CAA-CBA-CGA-O2A
2	10-B	265	HEM	CAA-CBA-CGA-O2A
2	16-A	300	HEM	CAA-CBA-CGA-O2A
2	15-B	265	HEM	CAD-CBD-CGD-O1D
2	16-B	265	HEM	CAA-CBA-CGA-O1A
2	3-A	300	HEM	CAA-CBA-CGA-O2A
2	10-B	265	HEM	CAA-CBA-CGA-O1A
2	16-A	300	HEM	CAA-CBA-CGA-O1A
2	13-B	265	HEM	CAA-CBA-CGA-O1A
2	8-B	265	HEM	CAD-CBD-CGD-O2D
2	13-A	300	HEM	C2C-C3C-CAC-CBC
2	3-B	265	HEM	C2B-C3B-CAB-CBB
2	12-A	300	HEM	CAA-CBA-CGA-O2A
2	6-A	300	HEM	CAA-CBA-CGA-O2A
2	6-A	300	HEM	CAA-CBA-CGA-O1A
2	11-A	300	HEM	CAA-CBA-CGA-O2A
2	12-A	300	HEM	CAA-CBA-CGA-O1A

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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	214/264 (81%)	13.20	214 (100%) 0 0	2, 3, 4, 4	214 (100%)
1	1-B	219/264 (82%)	13.05	219 (100%) 0 0	3, 4, 5, 5	219 (100%)
1	2-A	0/264	-	-	-	-
1	2-B	0/264	-	-	-	-
1	3-A	0/264	-	-	-	-
1	3-B	0/264	-	-	-	-
1	4-A	0/264	-	-	-	-
1	4-B	0/264	-	-	-	-
1	5-A	0/264	-	-	-	-
1	5-B	0/264	-	-	-	-
1	6-A	0/264	-	-	-	-
1	6-B	0/264	-	-	-	-
1	7-A	0/264	-	-	-	-
1	7-B	0/264	-	-	-	-
1	8-A	0/264	-	-	-	-
1	8-B	0/264	-	-	-	-
1	9-A	0/264	-	-	-	-
1	9-B	0/264	-	-	-	-
1	10-A	0/264	-	-	-	-
1	10-B	0/264	-	-	-	-
1	11-A	0/264	-	-	-	-
1	11-B	0/264	-	-	-	-
1	12-A	0/264	-	-	-	-
1	12-B	0/264	-	-	-	-
1	13-A	0/264	-	-	-	-
1	13-B	0/264	-	-	-	-
1	14-A	0/264	-	-	-	-
1	14-B	0/264	-	-	-	-
1	15-A	0/264	-	-	-	-
1	15-B	0/264	-	-	-	-
1	16-A	0/264	-	-	-	-
1	16-B	0/264	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	433/8448 (5%)	13.13	433 (100%) 0 0	2, 3, 5, 5	433 (100%)

All (433) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	229	TYR	35.3
1	1-A	172	GLN	30.2
1	1-B	48	ALA	29.8
1	1-B	219	ILE	29.6
1	1-B	227	PHE	29.3
1	1-A	210	ASP	28.0
1	1-B	161	LEU	27.3
1	1-A	214	LYS	26.5
1	1-B	116	PHE	26.2
1	1-B	98	TYR	26.0
1	1-A	109	LEU	25.3
1	1-B	125	VAL	24.9
1	1-A	209	LEU	24.5
1	1-A	94	PHE	24.5
1	1-A	223	ALA	24.5
1	1-A	61	ASN	24.2
1	1-A	39	GLU	24.1
1	1-A	81	LEU	24.0
1	1-B	154	TYR	24.0
1	1-A	129	LYS	23.1
1	1-A	185	GLN	23.0
1	1-B	67	PHE	23.0
1	1-B	117	PHE	22.4
1	1-B	113	MET	22.2
1	1-A	67	PHE	22.2
1	1-A	191	ASN	22.1
1	1-B	49	GLU	22.0
1	1-A	177	LEU	21.8
1	1-A	59	LYS	21.6
1	1-A	219	ILE	21.4
1	1-A	238	ASP	21.4
1	1-B	75	TYR	21.4
1	1-A	224	ASN	21.3
1	1-A	175	LEU	21.3
1	1-A	88	ASN	21.2
1	1-A	113	MET	21.2
1	1-A	50	ASN	21.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	124	GLN	21.1
1	1-B	42	LYS	20.7
1	1-B	109	LEU	20.6
1	1-A	197	GLN	20.4
1	1-B	176	LYS	20.3
1	1-B	57	PHE	20.3
1	1-A	117	PHE	20.0
1	1-B	53	PHE	19.6
1	1-B	150	VAL	19.6
1	1-B	66	LEU	19.6
1	1-A	77	THR	19.4
1	1-B	81	LEU	19.4
1	1-B	244	LEU	19.2
1	1-B	97	LEU	19.1
1	1-B	31	ALA	19.0
1	1-A	73	ALA	18.9
1	1-B	247	GLU	18.8
1	1-B	174	ALA	18.3
1	1-A	123	GLU	18.3
1	1-B	162	SER	18.2
1	1-B	54	VAL	18.2
1	1-B	58	LEU	18.2
1	1-A	171	ALA	17.9
1	1-B	60	GLY	17.8
1	1-A	31	ALA	17.8
1	1-A	227	PHE	17.6
1	1-A	188	LEU	17.6
1	1-A	154	TYR	17.4
1	1-B	232	GLN	17.3
1	1-A	47	ARG	17.1
1	1-B	190	GLU	17.1
1	1-B	239	GLN	17.0
1	1-A	222	GLU	17.0
1	1-B	77	THR	17.0
1	1-B	225	LYS	16.9
1	1-B	103	LEU	16.9
1	1-A	85	MET	16.9
1	1-A	33	LEU	16.9
1	1-A	200	GLN	16.9
1	1-B	171	ALA	16.8
1	1-B	140	TYR	16.8
1	1-A	213	MET	16.7

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Mol	Chain	Res	Type	RSRZ
1	1-A	157	TYR	16.7
1	1-A	126	GLN	16.5
1	1-B	145	GLU	16.4
1	1-A	66	LEU	16.3
1	1-B	168	LYS	16.2
1	1-B	157	TYR	16.2
1	1-B	78	TYR	16.2
1	1-B	114	GLU	16.0
1	1-A	153	ALA	16.0
1	1-B	134	TYR	16.0
1	1-A	56	ASP	15.9
1	1-B	223	ALA	15.8
1	1-A	232	GLN	15.8
1	1-B	175	LEU	15.6
1	1-A	150	VAL	15.6
1	1-A	141	ILE	15.5
1	1-B	138	ILE	15.5
1	1-A	101	MET	15.4
1	1-B	47	ARG	15.3
1	1-B	211	LEU	15.3
1	1-B	50	ASN	15.2
1	1-A	58	LEU	15.2
1	1-B	163	GLY	15.2
1	1-A	137	ARG	15.1
1	1-B	133	LYS	15.1
1	1-B	128	PRO	15.0
1	1-A	70	ALA	15.0
1	1-B	200	GLN	14.9
1	1-A	63	LYS	14.9
1	1-A	204	ALA	14.9
1	1-B	73	ALA	14.8
1	1-B	95	ALA	14.7
1	1-A	86	GLU	14.6
1	1-A	53	PHE	14.6
1	1-B	136	GLU	14.6
1	1-A	179	SER	14.6
1	1-A	83	GLU	14.6
1	1-B	234	PHE	14.6
1	1-A	49	GLU	14.5
1	1-B	177	LEU	14.5
1	1-A	48	ALA	14.4
1	1-A	235	ASN	14.4

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Mol	Chain	Res	Type	RSRZ
1	1-B	55	LYS	14.4
1	1-B	185	GLN	14.4
1	1-A	239	GLN	14.3
1	1-A	124	GLN	14.2
1	1-A	149	LEU	14.2
1	1-A	103	LEU	14.1
1	1-A	161	LEU	14.1
1	1-A	166	VAL	14.1
1	1-A	116	PHE	14.1
1	1-A	78	TYR	14.0
1	1-A	236	GLU	13.9
1	1-A	186	PHE	13.9
1	1-A	41	THR	13.8
1	1-B	118	GLY	13.8
1	1-B	215	THR	13.8
1	1-A	60	GLY	13.8
1	1-B	144	ASN	13.8
1	1-B	130	ALA	13.8
1	1-A	198	PHE	13.8
1	1-A	217	GLU	13.7
1	1-A	138	ILE	13.7
1	1-A	128	PRO	13.7
1	1-B	198	PHE	13.7
1	1-A	76	PHE	13.6
1	1-A	230	ASN	13.5
1	1-A	37	LEU	13.5
1	1-B	32	ASP	13.5
1	1-A	142	GLY	13.5
1	1-B	70	ALA	13.5
1	1-A	54	VAL	13.5
1	1-B	64	LYS	13.4
1	1-A	99	PHE	13.4
1	1-A	189	PHE	13.4
1	1-B	89	LYS	13.3
1	1-B	56	ASP	13.3
1	1-B	233	ILE	13.3
1	1-A	79	SER	13.3
1	1-A	136	GLU	13.2
1	1-A	187	TYR	13.2
1	1-A	102	GLU	13.2
1	1-B	195	ALA	13.2
1	1-B	167	LEU	13.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	230	ASN	13.1
1	1-B	72	THR	13.1
1	1-B	166	VAL	13.1
1	1-A	98	TYR	13.0
1	1-A	143	GLN	13.0
1	1-B	68	LYS	13.0
1	1-B	193	ASP	12.9
1	1-B	151	ALA	12.9
1	1-B	99	PHE	12.9
1	1-A	112	ASP	12.9
1	1-B	36	LEU	12.9
1	1-B	45	HIS	12.9
1	1-A	147	GLU	12.9
1	1-B	208	ALA	12.9
1	1-B	216	LYS	12.8
1	1-A	233	ILE	12.8
1	1-B	201	LEU	12.8
1	1-A	35	GLU	12.8
1	1-A	95	ALA	12.8
1	1-A	240	ALA	12.7
1	1-B	62	ILE	12.7
1	1-A	237	LEU	12.7
1	1-A	46	ASP	12.7
1	1-A	234	PHE	12.7
1	1-A	202	TYR	12.6
1	1-B	106	LYS	12.6
1	1-B	132	GLN	12.6
1	1-A	192	VAL	12.6
1	1-B	59	LYS	12.5
1	1-B	169	LYS	12.5
1	1-A	134	TYR	12.5
1	1-A	125	VAL	12.5
1	1-B	94	PHE	12.5
1	1-A	51	THR	12.5
1	1-A	93	ALA	12.5
1	1-B	76	PHE	12.5
1	1-B	206	MET	12.5
1	1-A	69	LEU	12.4
1	1-B	184	THR	12.4
1	1-B	148	LEU	12.4
1	1-A	45	HIS	12.4
1	1-B	123	GLU	12.4

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Mol	Chain	Res	Type	RSRZ
1	1-B	71	THR	12.4
1	1-A	133	LYS	12.3
1	1-A	105	ARG	12.3
1	1-B	111	LYS	12.3
1	1-A	96	PRO	12.3
1	1-B	188	LEU	12.3
1	1-A	75	TYR	12.2
1	1-A	74	LEU	12.2
1	1-A	220	VAL	12.2
1	1-A	205	ARG	12.1
1	1-B	235	ASN	12.1
1	1-B	135	VAL	12.1
1	1-A	203	ARG	12.0
1	1-A	242	SER	12.0
1	1-B	209	LEU	12.0
1	1-B	129	LYS	12.0
1	1-A	108	ALA	12.0
1	1-A	34	SER	11.9
1	1-B	155	THR	11.9
1	1-A	159	GLY	11.9
1	1-A	65	GLU	11.9
1	1-B	86	GLU	11.9
1	1-A	158	MET	11.9
1	1-A	195	ALA	11.9
1	1-B	189	PHE	11.9
1	1-A	211	LEU	11.8
1	1-A	90	ASP	11.8
1	1-A	196	GLN	11.8
1	1-A	80	ALA	11.8
1	1-A	201	LEU	11.8
1	1-B	65	GLU	11.7
1	1-B	196	GLN	11.7
1	1-A	155	THR	11.7
1	1-B	115	TYR	11.6
1	1-B	127	ALA	11.6
1	1-A	151	ALA	11.6
1	1-A	62	ILE	11.6
1	1-A	97	LEU	11.6
1	1-B	241	GLY	11.6
1	1-A	111	LYS	11.6
1	1-A	57	PHE	11.5
1	1-B	237	LEU	11.5

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Mol	Chain	Res	Type	RSRZ
1	1-B	207	ASN	11.4
1	1-B	218	ARG	11.4
1	1-B	110	THR	11.4
1	1-B	204	ALA	11.4
1	1-A	152	HIS	11.4
1	1-B	152	HIS	11.4
1	1-A	110	THR	11.4
1	1-B	84	GLU	11.3
1	1-B	238	ASP	11.3
1	1-A	104	HIS	11.3
1	1-A	43	GLU	11.3
1	1-B	242	SER	11.3
1	1-A	44	ALA	11.3
1	1-B	194	ASN	11.3
1	1-B	236	GLU	11.3
1	1-B	187	TYR	11.2
1	1-B	181	GLY	11.2
1	1-A	72	THR	11.2
1	1-B	52	GLN	11.2
1	1-B	43	GLU	11.2
1	1-B	112	ASP	11.2
1	1-A	40	GLY	11.2
1	1-B	69	LEU	11.1
1	1-A	206	MET	11.1
1	1-B	39	GLU	11.1
1	1-B	141	ILE	11.1
1	1-A	162	SER	11.1
1	1-A	82	GLU	11.1
1	1-B	131	ALA	11.1
1	1-B	202	TYR	11.0
1	1-B	210	ASP	11.0
1	1-B	37	LEU	11.0
1	1-A	218	ARG	11.0
1	1-A	132	GLN	11.0
1	1-B	186	PHE	11.0
1	1-A	115	TYR	11.0
1	1-B	74	LEU	11.0
1	1-A	135	VAL	11.0
1	1-A	71	THR	10.9
1	1-A	100	PRO	10.9
1	1-B	93	ALA	10.9
1	1-B	122	GLU	10.9

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Mol	Chain	Res	Type	RSRZ
1	1-B	30	MET	10.8
1	1-A	156	ARG	10.8
1	1-B	182	GLU	10.8
1	1-B	61	ASN	10.8
1	1-B	173	ARG	10.8
1	1-B	88	ASN	10.8
1	1-B	240	ALA	10.7
1	1-B	63	LYS	10.7
1	1-A	64	LYS	10.7
1	1-A	52	GLN	10.6
1	1-B	179	SER	10.6
1	1-A	92	PRO	10.6
1	1-B	165	GLN	10.6
1	1-B	160	ASP	10.6
1	1-B	149	LEU	10.6
1	1-A	160	ASP	10.5
1	1-B	96	PRO	10.5
1	1-A	68	LYS	10.4
1	1-A	89	LYS	10.4
1	1-B	105	ARG	10.4
1	1-B	180	THR	10.4
1	1-A	36	LEU	10.4
1	1-A	119	GLU	10.3
1	1-A	55	LYS	10.3
1	1-B	108	ALA	10.3
1	1-B	79	SER	10.3
1	1-B	212	ASN	10.3
1	1-B	38	LYS	10.2
1	1-B	224	ASN	10.2
1	1-A	182	GLU	10.1
1	1-B	121	TRP	10.1
1	1-A	174	ALA	10.1
1	1-B	205	ARG	10.0
1	1-B	226	ALA	10.0
1	1-A	194	ASN	10.0
1	1-B	203	ARG	10.0
1	1-B	119	GLU	10.0
1	1-B	222	GLU	10.0
1	1-B	104	HIS	10.0
1	1-A	208	ALA	10.0
1	1-B	41	THR	9.9
1	1-B	220	VAL	9.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	144	ASN	9.9
1	1-B	34	SER	9.9
1	1-A	140	TYR	9.8
1	1-A	170	VAL	9.8
1	1-B	243	THR	9.8
1	1-A	30	MET	9.8
1	1-A	229	TYR	9.8
1	1-B	153	ALA	9.8
1	1-A	120	ASN	9.7
1	1-B	51	THR	9.7
1	1-B	228	GLU	9.7
1	1-B	126	GLN	9.7
1	1-B	221	GLU	9.6
1	1-B	91	HIS	9.6
1	1-A	84	GLU	9.6
1	1-B	217	GLU	9.6
1	1-B	197	GLN	9.5
1	1-A	226	ALA	9.5
1	1-B	172	GLN	9.5
1	1-B	170	VAL	9.5
1	1-A	114	GLU	9.5
1	1-A	145	GLU	9.5
1	1-A	32	ASP	9.4
1	1-B	146	PRO	9.3
1	1-A	38	LYS	9.3
1	1-A	148	LEU	9.3
1	1-A	122	GLU	9.3
1	1-B	85	MET	9.3
1	1-B	137	ARG	9.3
1	1-A	87	ARG	9.3
1	1-A	241	GLY	9.2
1	1-A	139	HIS	9.2
1	1-A	207	ASN	9.1
1	1-B	92	PRO	9.1
1	1-B	192	VAL	9.1
1	1-A	107	GLU	9.1
1	1-B	199	LYS	9.1
1	1-A	91	HIS	9.0
1	1-B	82	GLU	9.0
1	1-B	156	ARG	9.0
1	1-B	143	GLN	9.0
1	1-B	246	ARG	8.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	106	LYS	8.9
1	1-B	107	GLU	8.8
1	1-B	100	PRO	8.8
1	1-B	214	LYS	8.8
1	1-A	231	MET	8.8
1	1-A	225	LYS	8.7
1	1-A	221	GLU	8.7
1	1-B	44	ALA	8.7
1	1-A	167	LEU	8.7
1	1-B	158	MET	8.7
1	1-B	191	ASN	8.6
1	1-A	199	LYS	8.6
1	1-B	147	GLU	8.6
1	1-B	120	ASN	8.5
1	1-B	90	ASP	8.4
1	1-B	164	GLY	8.4
1	1-A	121	TRP	8.4
1	1-A	184	THR	8.4
1	1-A	216	LYS	8.3
1	1-B	159	GLY	8.2
1	1-A	118	GLY	8.2
1	1-A	163	GLY	8.1
1	1-A	176	LYS	8.0
1	1-B	178	PRO	8.0
1	1-A	212	ASN	8.0
1	1-A	169	LYS	8.0
1	1-A	131	ALA	8.0
1	1-B	33	LEU	7.9
1	1-A	127	ALA	7.9
1	1-A	173	ARG	7.9
1	1-A	165	GLN	7.9
1	1-B	35	GLU	7.8
1	1-A	168	LYS	7.8
1	1-A	130	ALA	7.7
1	1-B	139	HIS	7.7
1	1-B	142	GLY	7.7
1	1-A	42	LYS	7.7
1	1-A	193	ASP	7.5
1	1-B	46	ASP	7.5
1	1-B	231	MET	7.4
1	1-A	146	PRO	7.4
1	1-B	101	MET	7.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	178	PRO	7.2
1	1-B	245	ALA	7.2
1	1-A	183	GLY	7.0
1	1-A	215	THR	7.0
1	1-A	228	GLU	6.9
1	1-B	80	ALA	6.8
1	1-B	248	THR	6.8
1	1-B	40	GLY	6.7
1	1-A	29	ARG	6.7
1	1-B	183	GLY	6.5
1	1-A	190	GLU	6.2
1	1-B	83	GLU	6.2
1	1-B	213	MET	5.9
1	1-A	180	THR	5.8
1	1-A	164	GLY	5.6
1	1-B	87	ARG	5.5
1	1-A	181	GLY	5.2
1	1-B	102	GLU	5.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	1-B	265	43/43	0.60	0.61	57,64,65,65	43
2	HEM	2-A	300	43/43	-	-	47,52,56,56	43
2	HEM	3-A	300	43/43	-	-	42,51,53,54	43
2	HEM	4-A	300	43/43	-	-	43,49,53,57	43
2	HEM	5-A	300	43/43	-	-	47,53,60,61	43

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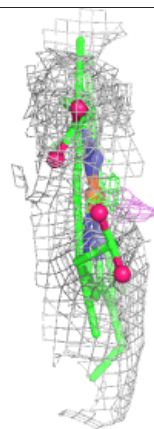
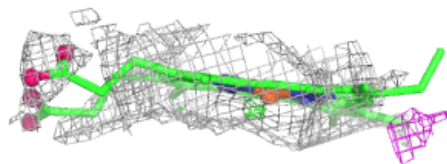
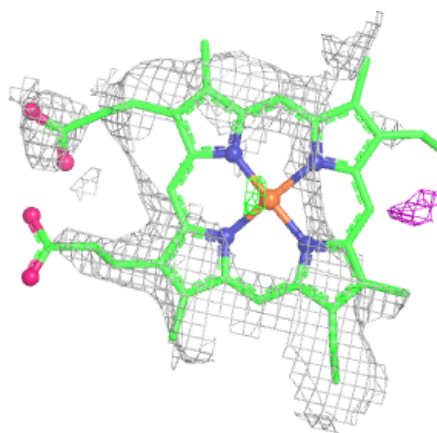
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	6-A	300	43/43	-	-	47,53,59,60	43
2	HEM	7-A	300	43/43	-	-	48,53,59,60	43
2	HEM	8-A	300	43/43	-	-	47,52,55,56	43
2	HEM	9-A	300	43/43	-	-	45,50,52,53	43
2	HEM	10-A	300	43/43	-	-	47,53,59,60	43
2	HEM	11-A	300	43/43	-	-	47,53,58,60	43
2	HEM	12-A	300	43/43	-	-	47,53,59,60	43
2	HEM	13-A	300	43/43	-	-	44,49,53,55	43
2	HEM	14-A	300	43/43	-	-	44,50,53,56	43
2	HEM	15-A	300	43/43	-	-	41,51,59,62	43
2	HEM	16-A	300	43/43	-	-	44,51,55,56	43
2	HEM	1-A	300	43/43	0.62	0.61	47,53,59,60	43
2	HEM	2-B	265	43/43	-	-	57,62,64,64	43
2	HEM	3-B	265	43/43	-	-	44,62,64,65	43
2	HEM	4-B	265	43/43	-	-	59,63,65,66	43
2	HEM	5-B	265	43/43	-	-	56,64,66,67	43
2	HEM	6-B	265	43/43	-	-	57,64,66,68	43
2	HEM	7-B	265	43/43	-	-	58,64,65,66	43
2	HEM	8-B	265	43/43	-	-	55,64,65,66	43
2	HEM	9-B	265	43/43	-	-	54,63,65,65	43
2	HEM	10-B	265	43/43	-	-	59,64,66,67	43
2	HEM	11-B	265	43/43	-	-	57,62,64,65	43
2	HEM	12-B	265	43/43	-	-	56,62,65,65	43
2	HEM	13-B	265	43/43	-	-	56,63,65,67	43
2	HEM	14-B	265	43/43	-	-	50,60,64,66	43
2	HEM	15-B	265	43/43	-	-	54,63,65,66	43
2	HEM	16-B	265	43/43	-	-	54,61,63,64	43

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.

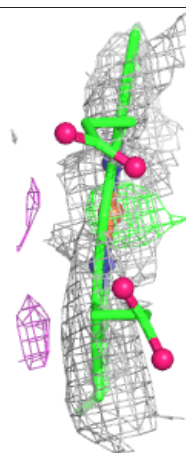
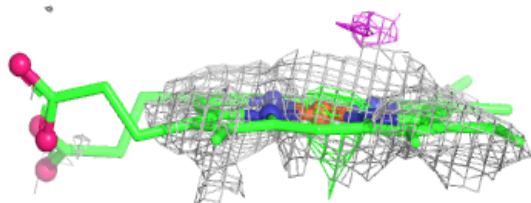
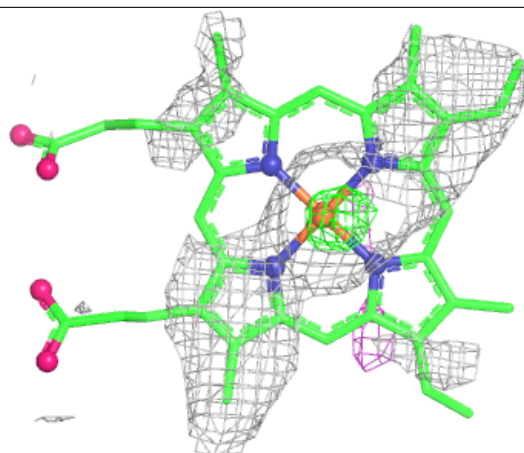
Electron density around HEM B 265:

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



Electron density around HEM A 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](#)

There are no such residues in this entry.