



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:56 PM UTC

PDB ID : 3A17 / pdb_00003a17
Title : Crystal Structure of Aldoxime Dehydratase (OxdRE) in Complex with Butyraldoxime (Co-crystal)
Authors : Sawai, H.; Sugimoto, H.; Kato, Y.; Asano, Y.; Shiro, Y.; Aono, S.
Deposited on : 2009-03-26
Resolution : 2.50 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

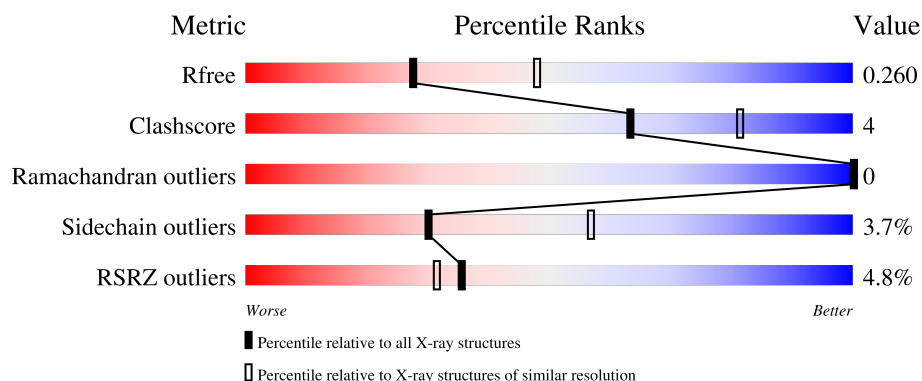
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	2% 83% 10% 6%
1	B	373	8% 86% 9% . .
1	C	373	3% 83% 11% . 6%
1	D	373	6% 84% 11% . .
1	E	373	3% 87% 7% 6%

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Mol	Chain	Length	Quality of chain
1	F	373	
1	G	373	
1	H	373	

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
3	BXO	B	355	-	X	-	-
3	BXO	D	355	-	X	-	-
3	BXO	F	355	-	X	-	-
3	BXO	H	355	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23656 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 Aldoxime dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2790	1757	492	529	12			
1	B	359	Total	C	N	O	S	0	0	0
			2853	1795	506	540	12			
1	C	352	Total	C	N	O	S	0	1	0
			2812	1770	497	533	12			
1	D	360	Total	C	N	O	S	0	1	0
			2866	1803	510	541	12			
1	E	351	Total	C	N	O	S	0	1	0
			2803	1765	496	530	12			
1	F	359	Total	C	N	O	S	0	0	0
			2853	1795	506	540	12			
1	G	353	Total	C	N	O	S	0	0	0
			2815	1771	497	535	12			
1	H	359	Total	C	N	O	S	0	0	0
			2853	1795	506	540	12			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q76K71
A	-18	GLY	-	expression tag	UNP Q76K71
A	-17	SER	-	expression tag	UNP Q76K71
A	-16	SER	-	expression tag	UNP Q76K71
A	-15	HIS	-	expression tag	UNP Q76K71
A	-14	HIS	-	expression tag	UNP Q76K71
A	-13	HIS	-	expression tag	UNP Q76K71
A	-12	HIS	-	expression tag	UNP Q76K71
A	-11	HIS	-	expression tag	UNP Q76K71
A	-10	HIS	-	expression tag	UNP Q76K71
A	-9	SER	-	expression tag	UNP Q76K71
A	-8	SER	-	expression tag	UNP Q76K71
A	-7	GLY	-	expression tag	UNP Q76K71

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q76K71
A	-5	VAL	-	expression tag	UNP Q76K71
A	-4	PRO	-	expression tag	UNP Q76K71
A	-3	ARG	-	expression tag	UNP Q76K71
A	-2	GLY	-	expression tag	UNP Q76K71
A	-1	SER	-	expression tag	UNP Q76K71
A	0	HIS	-	expression tag	UNP Q76K71
B	-19	MET	-	initiating methionine	UNP Q76K71
B	-18	GLY	-	expression tag	UNP Q76K71
B	-17	SER	-	expression tag	UNP Q76K71
B	-16	SER	-	expression tag	UNP Q76K71
B	-15	HIS	-	expression tag	UNP Q76K71
B	-14	HIS	-	expression tag	UNP Q76K71
B	-13	HIS	-	expression tag	UNP Q76K71
B	-12	HIS	-	expression tag	UNP Q76K71
B	-11	HIS	-	expression tag	UNP Q76K71
B	-10	HIS	-	expression tag	UNP Q76K71
B	-9	SER	-	expression tag	UNP Q76K71
B	-8	SER	-	expression tag	UNP Q76K71
B	-7	GLY	-	expression tag	UNP Q76K71
B	-6	LEU	-	expression tag	UNP Q76K71
B	-5	VAL	-	expression tag	UNP Q76K71
B	-4	PRO	-	expression tag	UNP Q76K71
B	-3	ARG	-	expression tag	UNP Q76K71
B	-2	GLY	-	expression tag	UNP Q76K71
B	-1	SER	-	expression tag	UNP Q76K71
B	0	HIS	-	expression tag	UNP Q76K71
C	-19	MET	-	initiating methionine	UNP Q76K71
C	-18	GLY	-	expression tag	UNP Q76K71
C	-17	SER	-	expression tag	UNP Q76K71
C	-16	SER	-	expression tag	UNP Q76K71
C	-15	HIS	-	expression tag	UNP Q76K71
C	-14	HIS	-	expression tag	UNP Q76K71
C	-13	HIS	-	expression tag	UNP Q76K71
C	-12	HIS	-	expression tag	UNP Q76K71
C	-11	HIS	-	expression tag	UNP Q76K71
C	-10	HIS	-	expression tag	UNP Q76K71
C	-9	SER	-	expression tag	UNP Q76K71
C	-8	SER	-	expression tag	UNP Q76K71
C	-7	GLY	-	expression tag	UNP Q76K71
C	-6	LEU	-	expression tag	UNP Q76K71
C	-5	VAL	-	expression tag	UNP Q76K71

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q76K71
C	-3	ARG	-	expression tag	UNP Q76K71
C	-2	GLY	-	expression tag	UNP Q76K71
C	-1	SER	-	expression tag	UNP Q76K71
C	0	HIS	-	expression tag	UNP Q76K71
D	-19	MET	-	initiating methionine	UNP Q76K71
D	-18	GLY	-	expression tag	UNP Q76K71
D	-17	SER	-	expression tag	UNP Q76K71
D	-16	SER	-	expression tag	UNP Q76K71
D	-15	HIS	-	expression tag	UNP Q76K71
D	-14	HIS	-	expression tag	UNP Q76K71
D	-13	HIS	-	expression tag	UNP Q76K71
D	-12	HIS	-	expression tag	UNP Q76K71
D	-11	HIS	-	expression tag	UNP Q76K71
D	-10	HIS	-	expression tag	UNP Q76K71
D	-9	SER	-	expression tag	UNP Q76K71
D	-8	SER	-	expression tag	UNP Q76K71
D	-7	GLY	-	expression tag	UNP Q76K71
D	-6	LEU	-	expression tag	UNP Q76K71
D	-5	VAL	-	expression tag	UNP Q76K71
D	-4	PRO	-	expression tag	UNP Q76K71
D	-3	ARG	-	expression tag	UNP Q76K71
D	-2	GLY	-	expression tag	UNP Q76K71
D	-1	SER	-	expression tag	UNP Q76K71
D	0	HIS	-	expression tag	UNP Q76K71
E	-19	MET	-	initiating methionine	UNP Q76K71
E	-18	GLY	-	expression tag	UNP Q76K71
E	-17	SER	-	expression tag	UNP Q76K71
E	-16	SER	-	expression tag	UNP Q76K71
E	-15	HIS	-	expression tag	UNP Q76K71
E	-14	HIS	-	expression tag	UNP Q76K71
E	-13	HIS	-	expression tag	UNP Q76K71
E	-12	HIS	-	expression tag	UNP Q76K71
E	-11	HIS	-	expression tag	UNP Q76K71
E	-10	HIS	-	expression tag	UNP Q76K71
E	-9	SER	-	expression tag	UNP Q76K71
E	-8	SER	-	expression tag	UNP Q76K71
E	-7	GLY	-	expression tag	UNP Q76K71
E	-6	LEU	-	expression tag	UNP Q76K71
E	-5	VAL	-	expression tag	UNP Q76K71
E	-4	PRO	-	expression tag	UNP Q76K71
E	-3	ARG	-	expression tag	UNP Q76K71

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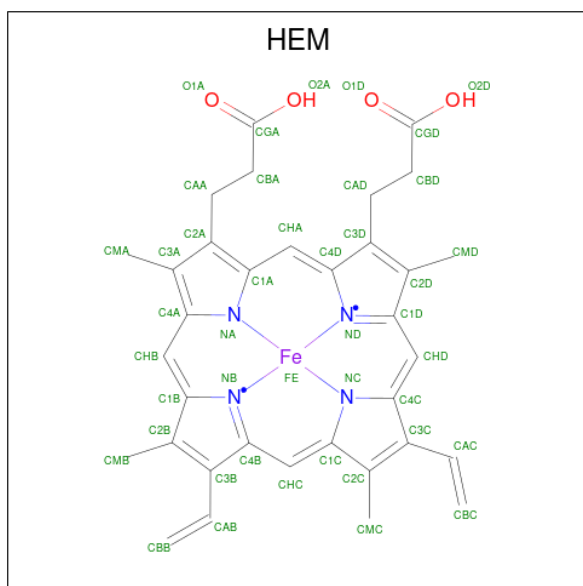
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E	-2	GLY	-	expression tag	UNP Q76K71
E	-1	SER	-	expression tag	UNP Q76K71
E	0	HIS	-	expression tag	UNP Q76K71
F	-19	MET	-	initiating methionine	UNP Q76K71
F	-18	GLY	-	expression tag	UNP Q76K71
F	-17	SER	-	expression tag	UNP Q76K71
F	-16	SER	-	expression tag	UNP Q76K71
F	-15	HIS	-	expression tag	UNP Q76K71
F	-14	HIS	-	expression tag	UNP Q76K71
F	-13	HIS	-	expression tag	UNP Q76K71
F	-12	HIS	-	expression tag	UNP Q76K71
F	-11	HIS	-	expression tag	UNP Q76K71
F	-10	HIS	-	expression tag	UNP Q76K71
F	-9	SER	-	expression tag	UNP Q76K71
F	-8	SER	-	expression tag	UNP Q76K71
F	-7	GLY	-	expression tag	UNP Q76K71
F	-6	LEU	-	expression tag	UNP Q76K71
F	-5	VAL	-	expression tag	UNP Q76K71
F	-4	PRO	-	expression tag	UNP Q76K71
F	-3	ARG	-	expression tag	UNP Q76K71
F	-2	GLY	-	expression tag	UNP Q76K71
F	-1	SER	-	expression tag	UNP Q76K71
F	0	HIS	-	expression tag	UNP Q76K71
G	-19	MET	-	initiating methionine	UNP Q76K71
G	-18	GLY	-	expression tag	UNP Q76K71
G	-17	SER	-	expression tag	UNP Q76K71
G	-16	SER	-	expression tag	UNP Q76K71
G	-15	HIS	-	expression tag	UNP Q76K71
G	-14	HIS	-	expression tag	UNP Q76K71
G	-13	HIS	-	expression tag	UNP Q76K71
G	-12	HIS	-	expression tag	UNP Q76K71
G	-11	HIS	-	expression tag	UNP Q76K71
G	-10	HIS	-	expression tag	UNP Q76K71
G	-9	SER	-	expression tag	UNP Q76K71
G	-8	SER	-	expression tag	UNP Q76K71
G	-7	GLY	-	expression tag	UNP Q76K71
G	-6	LEU	-	expression tag	UNP Q76K71
G	-5	VAL	-	expression tag	UNP Q76K71
G	-4	PRO	-	expression tag	UNP Q76K71
G	-3	ARG	-	expression tag	UNP Q76K71
G	-2	GLY	-	expression tag	UNP Q76K71
G	-1	SER	-	expression tag	UNP Q76K71

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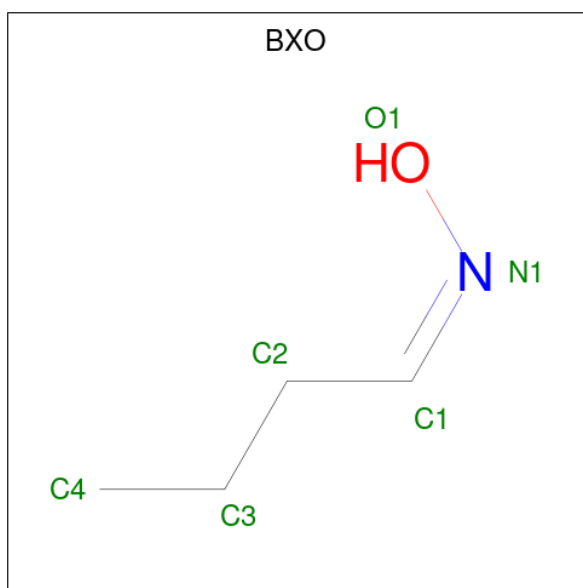
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q76K71
H	-19	MET	-	initiating methionine	UNP Q76K71
H	-18	GLY	-	expression tag	UNP Q76K71
H	-17	SER	-	expression tag	UNP Q76K71
H	-16	SER	-	expression tag	UNP Q76K71
H	-15	HIS	-	expression tag	UNP Q76K71
H	-14	HIS	-	expression tag	UNP Q76K71
H	-13	HIS	-	expression tag	UNP Q76K71
H	-12	HIS	-	expression tag	UNP Q76K71
H	-11	HIS	-	expression tag	UNP Q76K71
H	-10	HIS	-	expression tag	UNP Q76K71
H	-9	SER	-	expression tag	UNP Q76K71
H	-8	SER	-	expression tag	UNP Q76K71
H	-7	GLY	-	expression tag	UNP Q76K71
H	-6	LEU	-	expression tag	UNP Q76K71
H	-5	VAL	-	expression tag	UNP Q76K71
H	-4	PRO	-	expression tag	UNP Q76K71
H	-3	ARG	-	expression tag	UNP Q76K71
H	-2	GLY	-	expression tag	UNP Q76K71
H	-1	SER	-	expression tag	UNP Q76K71
H	0	HIS	-	expression tag	UNP Q76K71

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (1Z)-butanal oxime (CCD ID: BXO) (formula: C₄H₉NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	4	1	1		
3	B	1	Total	C	N	O	0	0
			6	4	1	1		
3	C	1	Total	C	N	O	0	0
			6	4	1	1		
3	D	1	Total	C	N	O	0	0
			6	4	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			6	4	1	1		
3	F	1	Total	C	N	O	0	0
			6	4	1	1		
3	G	1	Total	C	N	O	0	0
			6	4	1	1		
3	H	1	Total	C	N	O	0	0
			6	4	1	1		

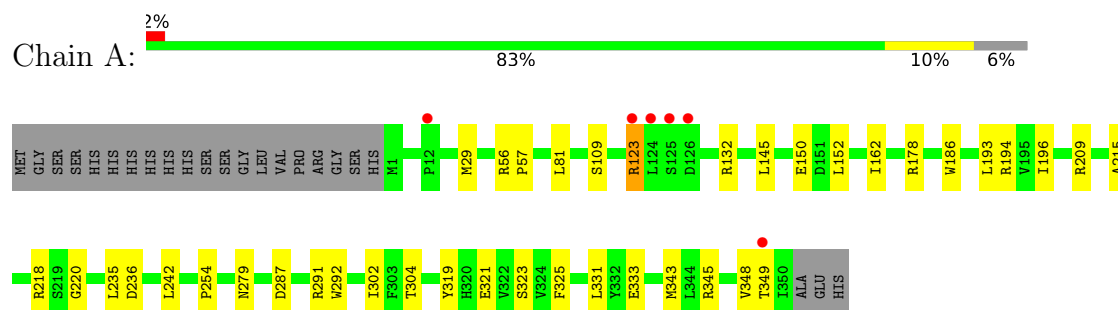
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	60	Total	O	0	0
			60	60		
4	C	93	Total	O	0	0
			93	93		
4	D	77	Total	O	0	0
			77	77		
4	E	83	Total	O	0	0
			83	83		
4	F	58	Total	O	0	0
			58	58		
4	G	84	Total	O	0	0
			84	84		
4	H	59	Total	O	0	0
			59	59		

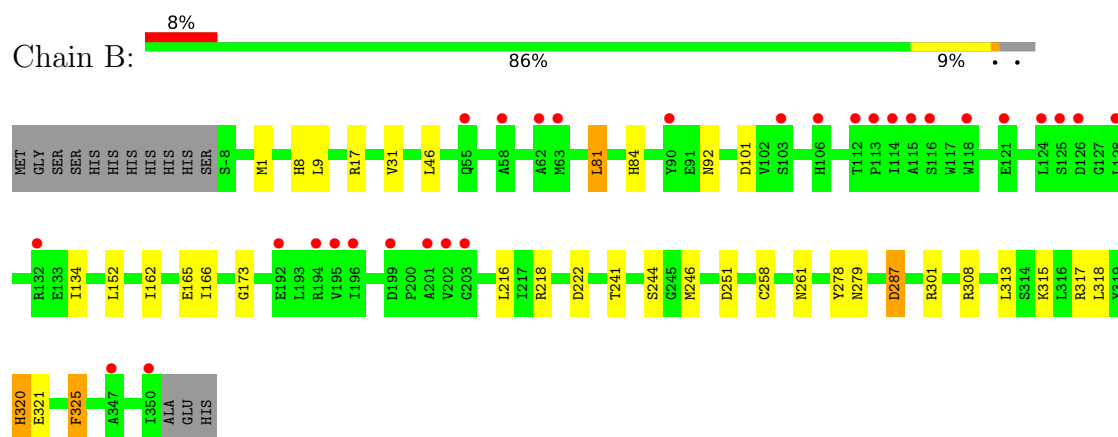
3 Residue-property plots [i](#)

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.

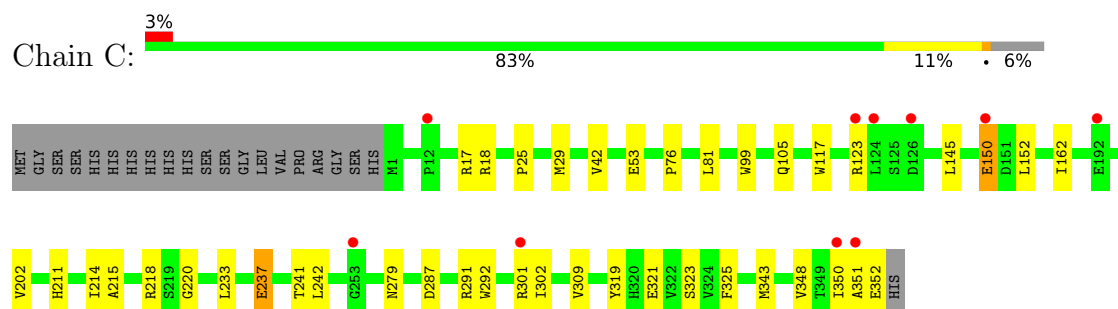
- Molecule 1: Aldoxime dehydratase



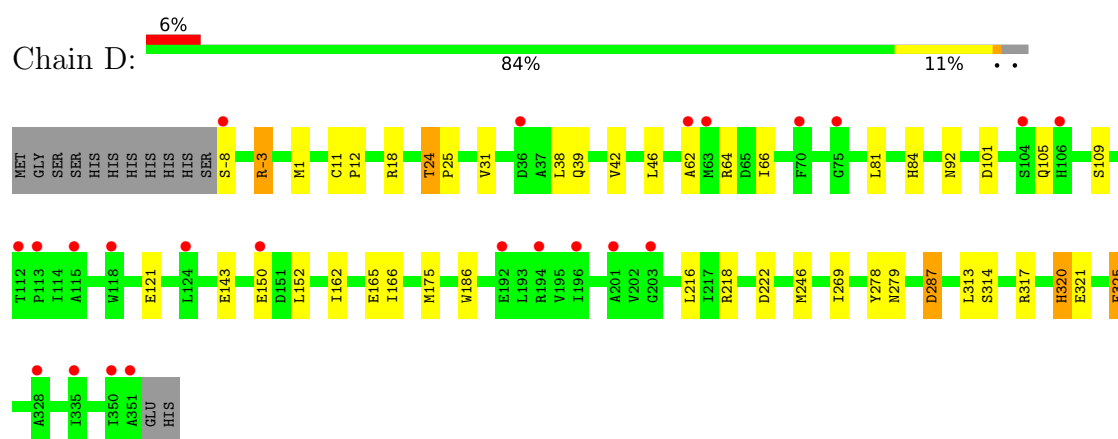
- Molecule 1: Aldoxime dehydratase



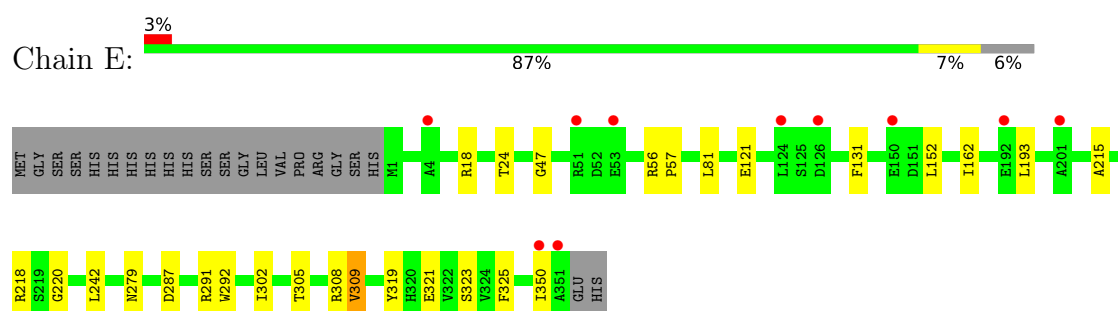
- Molecule 1: Aldoxime dehydratase



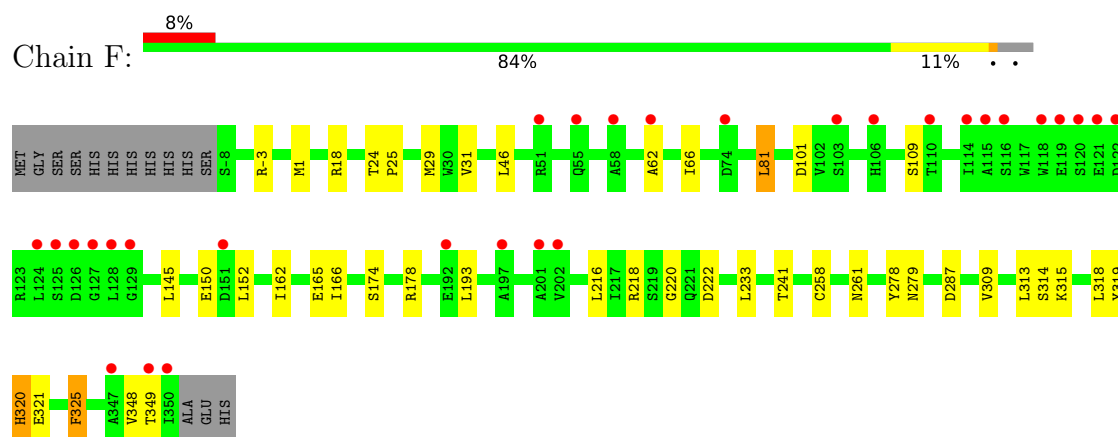
- Molecule 1: Aldoxime dehydratase



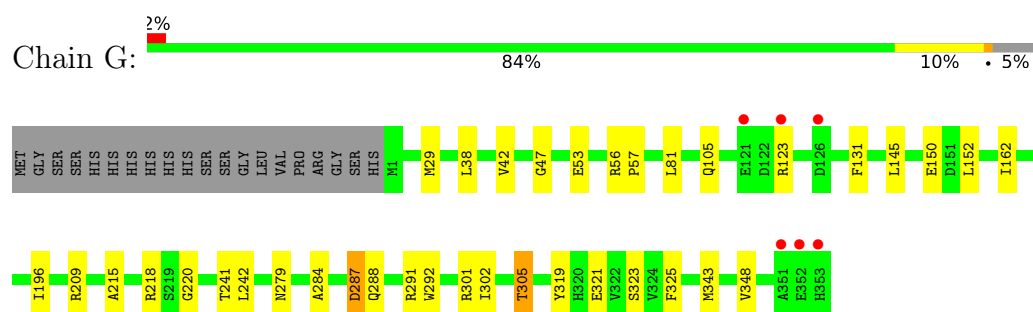
- Molecule 1: Aldoxime dehydratase



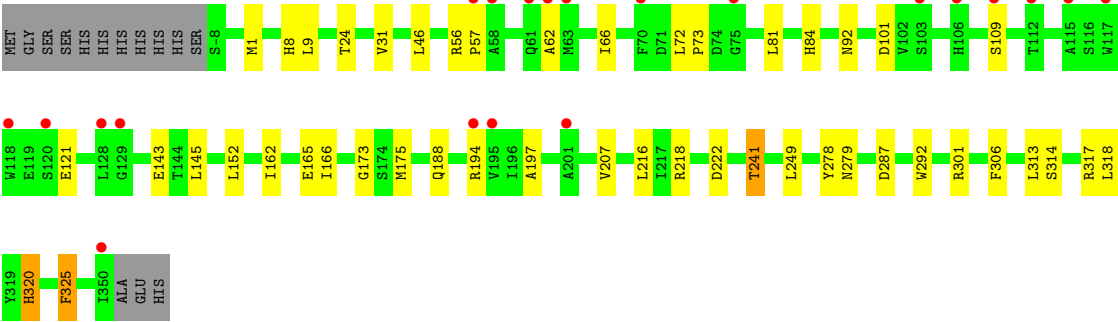
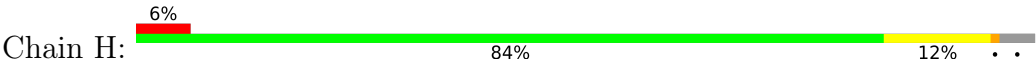
- Molecule 1: Aldoxime dehydratase



- Molecule 1: Aldoxime dehydratase



- Molecule 1: Aldoxime dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.05Å 103.93Å 114.19Å 76.50° 89.46° 87.55°	Depositor
Resolution (Å)	19.90 – 2.50 19.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.2 (19.90-2.50) 91.0 (19.90-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.50Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0019	Depositor
R, R_{free}	0.211 , 0.243 0.225 , 0.260	Depositor DCC
R_{free} test set	5656 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.098 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23656	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: BXO, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/2866	0.82	0/3900
1	B	0.52	0/2931	0.79	0/3988
1	C	0.56	1/2891 (0.0%)	0.82	0/3934
1	D	0.53	0/2947	0.78	0/4009
1	E	0.53	0/2882	0.81	2/3921 (0.1%)
1	F	0.53	0/2931	0.79	0/3988
1	G	0.55	0/2892	0.82	0/3934
1	H	0.52	0/2931	0.78	0/3988
All	All	0.54	1/23271 (0.0%)	0.80	2/31662 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	25	PRO	CA-C	5.39	1.54	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	24	THR	CA-C-N	5.10	123.39	119.66
1	E	24	THR	C-N-CA	5.10	123.39	119.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2790	0	2628	27	0
1	B	2853	0	2691	20	0
1	C	2812	0	2652	22	0
1	D	2866	0	2709	31	0
1	E	2803	0	2646	16	0
1	F	2853	0	2691	21	0
1	G	2815	0	2646	22	0
1	H	2853	0	2691	24	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	4	0
2	D	43	0	30	1	0
2	E	43	0	30	4	0
2	F	43	0	30	2	0
2	G	43	0	30	4	0
2	H	43	0	30	3	0
3	A	6	0	9	2	0
3	B	6	0	9	1	0
3	C	6	0	9	0	0
3	D	6	0	9	1	0
3	E	6	0	9	0	0
3	F	6	0	9	1	0
3	G	6	0	9	0	0
3	H	6	0	9	3	0
4	A	105	0	0	1	0
4	B	60	0	0	1	0
4	C	93	0	0	0	0
4	D	77	0	0	3	0
4	E	83	0	0	0	0
4	F	58	0	0	0	0
4	G	84	0	0	0	0
4	H	59	0	0	1	0
All	All	23656	0	21666	178	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-3[A]:ARG:HG2	1:D:-3[A]:ARG:HH11	1.41	0.84
1:G:242:LEU:HD22	2:G:354:HEM:HBB1	1.64	0.80
1:E:242:LEU:HD22	2:E:354:HEM:HBB1	1.69	0.75
1:E:305:THR:O	1:E:309:VAL:HG23	1.88	0.73
1:C:242:LEU:HD22	2:C:354:HEM:HBB1	1.70	0.73
1:D:-8:SER:HA	4:D:516:HOH:O	1.89	0.70
1:F:318:LEU:HD22	2:F:354:HEM:HBB2	1.73	0.70
1:H:1:MET:HE3	1:H:165:GLU:HB3	1.74	0.69
1:G:302:ILE:HA	1:G:305:THR:HG23	1.75	0.67
1:E:308:ARG:HE	1:E:309:VAL:HG22	1.58	0.67
1:G:292:TRP:CZ3	2:G:354:HEM:HBC2	2.29	0.67
1:D:-3[A]:ARG:HG2	1:D:-3[A]:ARG:NH1	2.09	0.64
1:B:31:VAL:HG13	1:B:166:ILE:HG12	1.78	0.64
1:A:235:LEU:HB3	1:D:-3[A]:ARG:HD2	1.79	0.63
1:H:318:LEU:HD22	2:H:354:HEM:HBB2	1.79	0.63
1:C:218:ARG:HB3	1:C:321:GLU:HG2	1.80	0.62
1:A:218:ARG:HB3	1:A:321:GLU:HG2	1.80	0.62
1:G:242:LEU:HD22	2:G:354:HEM:CBB	2.30	0.61
1:B:1:MET:HE3	1:B:165:GLU:HB3	1.81	0.61
1:F:1:MET:HE1	1:F:25:PRO:HG2	1.83	0.61
1:F:218:ARG:HG3	1:F:278:TYR:CD2	2.36	0.61
1:A:242:LEU:HD22	2:A:354:HEM:HBB1	1.82	0.60
1:H:218:ARG:HG3	1:H:278:TYR:CD2	2.37	0.59
1:A:292:TRP:CZ3	2:A:354:HEM:HBC2	2.37	0.59
1:G:301:ARG:O	1:G:305:THR:HG22	2.04	0.58
1:C:152:LEU:HD21	1:C:162:ILE:HD13	1.85	0.57
1:E:242:LEU:HD22	2:E:354:HEM:CBB	2.35	0.57
1:F:1:MET:HE3	1:F:165:GLU:HB3	1.86	0.57
1:B:318:LEU:HD22	2:B:354:HEM:HBB2	1.86	0.57
1:D:1:MET:HE3	1:D:165:GLU:HB3	1.87	0.57
1:G:218:ARG:HB3	1:G:321:GLU:HG2	1.87	0.56
1:E:218:ARG:HB3	1:E:321:GLU:HG2	1.87	0.56
1:A:235:LEU:HB3	1:D:-3[B]:ARG:HD2	1.86	0.56
1:F:31:VAL:HG13	1:F:166:ILE:HG12	1.87	0.56
1:C:150:GLU:OE1	1:C:150:GLU:N	2.37	0.55
1:B:218:ARG:HG3	1:B:278:TYR:CD2	2.42	0.55
1:C:292:TRP:CZ3	2:C:354:HEM:HBC2	2.42	0.55
1:B:81:LEU:HD23	1:B:81:LEU:N	2.22	0.54
1:G:292:TRP:HZ3	2:G:354:HEM:HBC2	1.70	0.54
1:E:292:TRP:CZ3	2:E:354:HEM:HBC2	2.42	0.54
1:H:216:LEU:HB3	1:H:325:PHE:HZ	1.73	0.54
1:H:31:VAL:HG13	1:H:166:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ASP:HB3	1:C:202:VAL:HG21	1.90	0.53
1:B:244:SER:OG	1:C:351:ALA:HB3	2.07	0.53
1:E:220:GLY:HA3	1:E:319:TYR:CE1	2.44	0.53
1:F:233:LEU:HD21	1:F:309:VAL:HG11	1.91	0.52
1:C:242:LEU:HD22	2:C:354:HEM:CBB	2.38	0.52
1:A:193:LEU:HD11	1:A:343:MET:HG3	1.92	0.52
1:H:145:LEU:HD23	3:H:355:BXO:C4	2.39	0.52
1:A:152:LEU:HD21	1:A:162:ILE:HD13	1.92	0.52
1:C:287:ASP:O	1:C:291:ARG:HG2	2.09	0.51
1:B:320:HIS:CD2	1:B:320:HIS:C	2.89	0.51
1:D:42:VAL:HG11	1:D:105:GLN:HG3	1.91	0.51
1:F:220:GLY:HA3	1:F:319:TYR:CE1	2.46	0.51
1:H:320:HIS:CD2	1:H:320:HIS:C	2.88	0.50
1:G:287:ASP:O	1:G:291:ARG:HG2	2.12	0.50
1:D:287:ASP:OD1	1:D:287:ASP:N	2.44	0.50
1:G:42:VAL:HG11	1:G:105:GLN:HG3	1.94	0.50
1:A:292:TRP:HZ3	2:A:354:HEM:HBC2	1.77	0.49
1:B:218:ARG:HA	1:B:279:ASN:O	2.13	0.49
1:F:218:ARG:HA	1:F:279:ASN:O	2.12	0.49
1:D:218:ARG:HG3	1:D:278:TYR:CD2	2.48	0.49
1:A:29:MET:HE1	3:A:355:BXO:H4	1.94	0.49
1:D:31:VAL:HG13	1:D:166:ILE:HG12	1.93	0.49
1:H:72:LEU:HB3	1:H:73:PRO:HD2	1.95	0.49
1:A:302:ILE:HD12	2:A:354:HEM:HBB2	1.94	0.49
1:D:218:ARG:HA	1:D:279:ASN:O	2.13	0.49
1:D:246:MET:HE2	1:D:246:MET:HA	1.94	0.49
1:A:29:MET:CE	3:A:355:BXO:H4	2.44	0.48
1:F:174:SER:O	1:F:178:ARG:HG3	2.13	0.48
1:H:218:ARG:HA	1:H:279:ASN:O	2.13	0.48
1:E:287:ASP:O	1:E:291:ARG:HG2	2.13	0.48
1:F:29:MET:HE3	1:F:145:LEU:HG	1.95	0.48
1:C:220:GLY:HA3	1:C:319:TYR:CE1	2.49	0.47
1:H:145:LEU:HD23	3:H:355:BXO:H4A	1.95	0.47
1:C:117:TRP:O	1:C:123:ARG:NH1	2.47	0.47
1:D:320:HIS:CD2	1:D:320:HIS:C	2.92	0.47
1:F:1:MET:HE1	1:F:25:PRO:CG	2.44	0.47
1:A:29:MET:HE3	1:A:145:LEU:HG	1.95	0.47
1:E:215:ALA:HA	1:E:323:SER:O	2.15	0.47
1:C:215:ALA:HA	1:C:323:SER:O	2.14	0.47
1:E:302:ILE:HD12	2:E:354:HEM:HBB2	1.96	0.47
1:H:222:ASP:HB3	1:H:317:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:HIS:CE1	1:H:92:ASN:HB2	2.49	0.47
1:B:287:ASP:OD1	1:B:287:ASP:N	2.44	0.47
1:D:218:ARG:HB3	1:D:321:GLU:HG2	1.96	0.47
1:A:220:GLY:HA3	1:A:319:TYR:CE1	2.50	0.46
1:D:62:ALA:O	1:D:66:ILE:HG13	2.16	0.46
1:B:222:ASP:HB3	1:B:317:ARG:HB2	1.96	0.46
1:G:152:LEU:HD21	1:G:162:ILE:HD13	1.98	0.46
1:A:215:ALA:HA	1:A:323:SER:O	2.16	0.46
1:D:222:ASP:HB3	1:D:317:ARG:HB2	1.97	0.46
1:G:215:ALA:HA	1:G:323:SER:O	2.15	0.46
1:E:218:ARG:HA	1:E:279:ASN:O	2.16	0.46
1:F:152:LEU:HD21	1:F:162:ILE:HD13	1.98	0.46
1:C:211:HIS:CE1	1:C:214:ILE:HG13	2.52	0.45
1:F:216:LEU:HB3	1:F:325:PHE:HZ	1.80	0.45
1:A:236:ASP:OD1	1:D:-3[B]:ARG:HD3	2.17	0.45
1:D:84:HIS:CE1	1:D:92:ASN:HB2	2.51	0.45
1:G:53:GLU:CD	1:G:56:ARG:HH21	2.25	0.45
1:F:193:LEU:O	1:F:348:VAL:HG12	2.17	0.45
1:F:218:ARG:HB3	1:F:321:GLU:HG2	1.99	0.44
1:A:287:ASP:O	1:A:291:ARG:HG2	2.16	0.44
1:D:143:GLU:OE2	1:D:175:MET:HG3	2.18	0.44
1:G:220:GLY:HA3	1:G:319:TYR:CE1	2.53	0.44
1:H:249:LEU:HD21	1:H:292:TRP:CE2	2.52	0.44
1:D:11:CYS:HB2	1:D:12:PRO:HD2	1.99	0.44
1:E:308:ARG:NE	1:E:309:VAL:HG22	2.31	0.44
1:G:150:GLU:N	1:G:150:GLU:OE1	2.49	0.44
1:G:218:ARG:HA	1:G:279:ASN:O	2.18	0.44
1:G:47:GLY:HA3	1:G:131:PHE:CZ	2.53	0.44
1:A:145:LEU:HD22	1:A:178:ARG:NH2	2.33	0.44
1:B:216:LEU:HB3	1:B:325:PHE:HZ	1.83	0.44
1:D:39:GLN:HG2	4:D:514:HOH:O	2.17	0.44
1:A:186:TRP:HH2	1:B:17:ARG:O	1.99	0.43
1:H:306:PHE:C	1:H:306:PHE:CD1	2.96	0.43
1:B:218:ARG:HB3	1:B:321:GLU:HG2	2.00	0.43
1:H:173:GLY:HA2	4:H:374:HOH:O	2.18	0.43
1:E:18:ARG:HD2	1:F:18:ARG:HD2	2.00	0.43
1:G:29:MET:HE3	1:G:145:LEU:HG	2.01	0.43
1:A:194:ARG:HG2	1:A:348:VAL:CG2	2.49	0.43
1:C:17:ARG:O	1:D:186:TRP:HH2	2.01	0.43
1:F:81:LEU:N	1:F:81:LEU:HD23	2.33	0.43
1:G:196:ILE:HD13	1:G:209:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LEU:HA	1:C:237:GLU:HG3	2.01	0.43
1:G:145:LEU:HD22	1:G:178:ARG:NH2	2.34	0.43
1:G:56:ARG:HB3	1:G:57:PRO:HD3	2.00	0.43
1:A:132:ARG:HG2	1:A:333:GLU:HB2	2.01	0.42
1:B:84:HIS:CE1	1:B:92:ASN:HB2	2.54	0.42
1:B:246:MET:HA	1:B:246:MET:HE2	2.00	0.42
1:D:1:MET:HE1	1:D:25:PRO:HG2	2.00	0.42
1:F:62:ALA:O	1:F:66:ILE:HG13	2.19	0.42
1:A:331:LEU:C	1:A:331:LEU:HD23	2.44	0.42
1:C:218:ARG:HA	1:C:279:ASN:O	2.19	0.42
1:C:241:THR:HG21	1:C:301:ARG:HB3	2.01	0.42
1:E:56:ARG:HB3	1:E:57:PRO:HD3	2.00	0.42
1:H:222:ASP:OD1	1:H:222:ASP:C	2.62	0.42
1:B:173:GLY:HA2	4:B:367:HOH:O	2.20	0.42
1:D:152:LEU:HD21	1:D:162:ILE:HD13	2.01	0.42
1:C:29:MET:HE3	1:C:145:LEU:HG	2.02	0.42
1:A:218:ARG:HA	1:A:279:ASN:O	2.19	0.42
1:F:222:ASP:OD1	1:F:222:ASP:C	2.62	0.42
1:D:11:CYS:HB2	1:D:12:PRO:CD	2.49	0.41
1:D:24:THR:HA	1:D:25:PRO:HD3	1.95	0.41
1:A:56:ARG:HB3	1:A:57:PRO:HD3	2.02	0.41
1:C:18:ARG:HD2	1:D:18:ARG:HD2	2.01	0.41
1:C:42:VAL:HG11	1:C:105:GLN:HG3	2.02	0.41
1:H:143:GLU:OE2	1:H:175:MET:HG3	2.20	0.41
1:C:302:ILE:HD12	2:C:354:HEM:HBB2	2.02	0.41
1:E:152:LEU:HD21	1:E:162:ILE:HD13	2.02	0.41
1:C:76:PRO:HD3	1:C:99:TRP:CZ2	2.55	0.41
1:D:216:LEU:HB3	1:D:325:PHE:HZ	1.86	0.41
1:H:62:ALA:O	1:H:66:ILE:HG13	2.20	0.41
1:A:209:ARG:NE	4:A:588:HOH:O	2.52	0.41
1:D:218:ARG:HB3	1:D:321:GLU:CG	2.50	0.41
2:D:354:HEM:C4A	3:D:355:BXO:H1	2.56	0.41
1:E:47:GLY:HA3	1:E:131:PHE:CZ	2.56	0.41
1:F:258:CYS:SG	1:F:261:ASN:HB2	2.61	0.41
1:A:254:PRO:HD3	1:A:345:ARG:NH2	2.36	0.41
1:H:152:LEU:HD21	1:H:162:ILE:HD13	2.02	0.41
2:B:354:HEM:C4A	3:B:355:BXO:H1	2.56	0.41
1:F:320:HIS:C	1:F:320:HIS:CD2	2.98	0.41
1:H:241:THR:HG21	1:H:301:ARG:HD3	2.03	0.41
1:A:123:ARG:HA	1:A:123:ARG:HD3	1.92	0.41
1:B:8:HIS:CE1	1:B:9:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:CYS:SG	1:B:261:ASN:HB2	2.61	0.41
1:H:56:ARG:HB3	1:H:57:PRO:HD3	2.03	0.41
1:H:197:ALA:HB3	1:H:207:VAL:HB	2.03	0.41
1:D:12:PRO:HD3	4:D:598:HOH:O	2.20	0.41
1:B:152:LEU:HD21	1:B:162:ILE:HD13	2.02	0.40
2:H:354:HEM:C4A	3:H:355:BXO:H1	2.56	0.40
1:A:196:ILE:HD13	1:A:209:ARG:HB2	2.02	0.40
1:D:64:ARG:HG2	1:D:269:ILE:HD11	2.04	0.40
1:G:284:ALA:HB3	1:G:288:GLN:HE22	1.87	0.40
1:H:279:ASN:OD1	2:H:354:HEM:HAC	2.22	0.40
2:F:354:HEM:C4A	3:F:355:BXO:H1	2.56	0.40
1:G:241:THR:OG1	1:G:302:ILE:HG23	2.22	0.40
1:H:8:HIS:CE1	1:H:9:LEU:HG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	348/373 (93%)	346 (99%)	2 (1%)	0	100	100
1	B	357/373 (96%)	354 (99%)	3 (1%)	0	100	100
1	C	351/373 (94%)	346 (99%)	5 (1%)	0	100	100
1	D	359/373 (96%)	357 (99%)	2 (1%)	0	100	100
1	E	350/373 (94%)	346 (99%)	4 (1%)	0	100	100
1	F	357/373 (96%)	354 (99%)	3 (1%)	0	100	100
1	G	351/373 (94%)	347 (99%)	4 (1%)	0	100	100
1	H	357/373 (96%)	357 (100%)	0	0	100	100
All	All	2830/2984 (95%)	2807 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/312 (94%)	286 (98%)	7 (2%)	43	70
1	B	300/312 (96%)	288 (96%)	12 (4%)	28	54
1	C	295/312 (95%)	285 (97%)	10 (3%)	32	60
1	D	301/312 (96%)	286 (95%)	15 (5%)	22	44
1	E	294/312 (94%)	288 (98%)	6 (2%)	48	75
1	F	300/312 (96%)	285 (95%)	15 (5%)	22	44
1	G	295/312 (95%)	286 (97%)	9 (3%)	35	62
1	H	300/312 (96%)	286 (95%)	14 (5%)	23	47
All	All	2378/2496 (95%)	2290 (96%)	88 (4%)	30	57

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	109	SER
1	A	123	ARG
1	A	150	GLU
1	A	304	THR
1	A	325	PHE
1	A	349	THR
1	B	46	LEU
1	B	81	LEU
1	B	101	ASP
1	B	134	ILE
1	B	241	THR
1	B	287	ASP
1	B	301	ARG
1	B	308	ARG
1	B	313	LEU

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Mol	Chain	Res	Type
1	B	315	LYS
1	B	320	HIS
1	B	325	PHE
1	C	53	GLU
1	C	81	LEU
1	C	150	GLU
1	C	237	GLU
1	C	309	VAL
1	C	325	PHE
1	C	343	MET
1	C	348	VAL
1	C	350	ILE
1	C	352	GLU
1	D	-3[A]	ARG
1	D	-3[B]	ARG
1	D	24	THR
1	D	38	LEU
1	D	46	LEU
1	D	81	LEU
1	D	101	ASP
1	D	109	SER
1	D	121	GLU
1	D	150	GLU
1	D	287	ASP
1	D	313	LEU
1	D	314	SER
1	D	320	HIS
1	D	325	PHE
1	E	81	LEU
1	E	121	GLU
1	E	193	LEU
1	E	309	VAL
1	E	325	PHE
1	E	350	ILE
1	F	-3	ARG
1	F	24	THR
1	F	46	LEU
1	F	81	LEU
1	F	101	ASP
1	F	109	SER
1	F	150	GLU
1	F	241	THR

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Mol	Chain	Res	Type
1	F	287	ASP
1	F	313	LEU
1	F	314	SER
1	F	315	LYS
1	F	320	HIS
1	F	325	PHE
1	F	349	THR
1	G	38	LEU
1	G	81	LEU
1	G	123	ARG
1	G	166	ILE
1	G	287	ASP
1	G	305	THR
1	G	325	PHE
1	G	343	MET
1	G	348	VAL
1	H	24	THR
1	H	46	LEU
1	H	81	LEU
1	H	101	ASP
1	H	109	SER
1	H	121	GLU
1	H	188	GLN
1	H	194	ARG
1	H	241	THR
1	H	287	ASP
1	H	313	LEU
1	H	314	SER
1	H	320	HIS
1	H	325	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	279	ASN
1	B	39	GLN
1	B	106	HIS
1	B	243	GLN
1	C	61	GLN
1	D	105	GLN
1	E	8	HIS

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Mol	Chain	Res	Type
1	E	61	GLN
1	E	105	GLN
1	E	188	GLN
1	E	288	GLN
1	F	106	HIS
1	G	61	GLN
1	G	105	GLN
1	G	149	GLN
1	G	188	GLN
1	G	288	GLN
1	H	105	GLN
1	H	106	HIS

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	B	354	3,1	50,50,50	1.81	10 (20%)	67,82,82	1.33	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	354	3,1	50,50,50	1.65	8 (16%)	67,82,82	1.39	8 (11%)
2	HEM	F	354	3,1	50,50,50	1.82	12 (24%)	67,82,82	1.37	6 (8%)
2	HEM	H	354	3,1	50,50,50	1.75	8 (16%)	67,82,82	1.30	6 (8%)
3	BXO	F	355	2	5,5,5	1.74	1 (20%)	4,4,4	3.41	3 (75%)
3	BXO	G	355	2	5,5,5	2.05	2 (40%)	4,4,4	3.72	2 (50%)
3	BXO	C	355	2	5,5,5	2.23	2 (40%)	4,4,4	4.23	2 (50%)
3	BXO	E	355	2	5,5,5	2.18	2 (40%)	4,4,4	3.80	2 (50%)
2	HEM	G	354	3,1	50,50,50	1.68	9 (18%)	67,82,82	1.34	7 (10%)
3	BXO	D	355	2	5,5,5	1.89	2 (40%)	4,4,4	3.58	3 (75%)
2	HEM	D	354	3,1	50,50,50	1.77	9 (18%)	67,82,82	1.34	6 (8%)
3	BXO	A	355	2	5,5,5	1.32	1 (20%)	4,4,4	5.37	1 (25%)
2	HEM	C	354	3,1	50,50,50	1.67	9 (18%)	67,82,82	1.35	8 (11%)
3	BXO	B	355	2	5,5,5	1.73	1 (20%)	4,4,4	3.68	3 (75%)
2	HEM	E	354	3,1	50,50,50	1.69	9 (18%)	67,82,82	1.38	7 (10%)
3	BXO	H	355	2	5,5,5	1.62	1 (20%)	4,4,4	3.54	3 (75%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	354	3,1	-	6/14/54/54	-
2	HEM	A	354	3,1	-	8/14/54/54	-
2	HEM	F	354	3,1	-	6/14/54/54	-
2	HEM	H	354	3,1	-	6/14/54/54	-
3	BXO	F	355	2	-	2/2/3/3	-
3	BXO	G	355	2	-	0/2/3/3	-
3	BXO	C	355	2	-	0/2/3/3	-
3	BXO	E	355	2	-	0/2/3/3	-
2	HEM	G	354	3,1	-	8/14/54/54	-
3	BXO	D	355	2	-	2/2/3/3	-
2	HEM	D	354	3,1	-	6/14/54/54	-
3	BXO	A	355	2	-	0/2/3/3	-
2	HEM	C	354	3,1	-	8/14/54/54	-
3	BXO	B	355	2	-	2/2/3/3	-
2	HEM	E	354	3,1	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BXO	H	355	2	-	2/2/3/3	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	354	HEM	C3D-C2D	7.52	1.53	1.36
2	C	354	HEM	C3D-C2D	7.50	1.52	1.36
2	G	354	HEM	C3D-C2D	7.42	1.52	1.36
2	A	354	HEM	C3D-C2D	7.35	1.52	1.36
2	B	354	HEM	C3D-C2D	7.29	1.52	1.36
2	F	354	HEM	C3D-C2D	7.29	1.52	1.36
2	H	354	HEM	C3D-C2D	7.16	1.52	1.36
2	D	354	HEM	C3D-C2D	7.07	1.52	1.36
3	C	355	BXO	C2-C1	4.36	1.53	1.49
3	E	355	BXO	C2-C1	4.26	1.53	1.49
2	H	354	HEM	FE-NB	4.22	2.07	1.94
3	G	355	BXO	C2-C1	3.82	1.52	1.49
2	F	354	HEM	FE-NB	3.79	2.06	1.94
3	D	355	BXO	C2-C1	3.66	1.52	1.49
2	B	354	HEM	FE-ND	3.51	2.05	1.94
2	D	354	HEM	FE-NB	3.49	2.05	1.94
2	B	354	HEM	FE-NC	3.46	2.06	1.95
2	G	354	HEM	FE-NB	3.38	2.05	1.94
2	E	354	HEM	FE-NB	3.36	2.05	1.94
2	D	354	HEM	FE-ND	3.36	2.05	1.94
3	F	355	BXO	C2-C1	3.35	1.52	1.49
2	H	354	HEM	FE-NC	3.31	2.06	1.95
3	B	355	BXO	C2-C1	3.27	1.52	1.49
2	F	354	HEM	FE-ND	3.25	2.04	1.94
2	B	354	HEM	FE-NB	3.22	2.04	1.94
2	F	354	HEM	CAC-C3C	3.21	1.55	1.47
2	D	354	HEM	FE-NA	3.19	2.05	1.95
3	H	355	BXO	C2-C1	3.19	1.52	1.49
2	A	354	HEM	FE-ND	3.18	2.04	1.94
2	B	354	HEM	CAB-C3B	3.16	1.55	1.47
2	H	354	HEM	CAC-C3C	3.11	1.55	1.47
2	C	354	HEM	FE-NA	3.11	2.05	1.95
2	D	354	HEM	CAB-C3B	2.99	1.55	1.47
2	B	354	HEM	CAC-C3C	2.97	1.55	1.47
2	D	354	HEM	CAC-C3C	2.95	1.55	1.47
2	E	354	HEM	CAB-C3B	2.95	1.55	1.47
2	C	354	HEM	FE-ND	2.91	2.03	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	354	HEM	CMC-C2C	2.91	1.56	1.50
2	A	354	HEM	CAB-C3B	2.90	1.55	1.47
2	H	354	HEM	CAB-C3B	2.90	1.55	1.47
2	F	354	HEM	CAB-C3B	2.86	1.55	1.47
2	G	354	HEM	CAB-C3B	2.85	1.55	1.47
3	A	355	BXO	C2-C1	2.82	1.51	1.49
2	C	354	HEM	CAB-C3B	2.80	1.54	1.47
2	F	354	HEM	FE-NC	2.75	2.04	1.95
2	C	354	HEM	FE-NB	2.66	2.03	1.94
2	H	354	HEM	CMB-C2B	2.63	1.56	1.50
2	C	354	HEM	CAC-C3C	2.58	1.54	1.47
2	F	354	HEM	CMB-C2B	2.56	1.56	1.50
2	B	354	HEM	CMB-C2B	2.55	1.56	1.50
2	A	354	HEM	CAC-C3C	2.55	1.54	1.47
2	E	354	HEM	CAC-C3C	2.53	1.54	1.47
2	F	354	HEM	CMA-C3A	2.52	1.55	1.50
2	F	354	HEM	CMC-C2C	2.52	1.55	1.50
2	E	354	HEM	FE-NA	2.52	2.03	1.95
2	D	354	HEM	CMC-C2C	2.51	1.55	1.50
3	G	355	BXO	C1-N1	2.50	1.28	1.26
2	A	354	HEM	FE-NB	2.47	2.02	1.94
2	D	354	HEM	CMB-C2B	2.47	1.55	1.50
2	A	354	HEM	FE-NA	2.47	2.03	1.95
2	E	354	HEM	CMA-C3A	2.47	1.55	1.50
2	H	354	HEM	FE-ND	2.42	2.02	1.94
2	H	354	HEM	CMC-C2C	2.41	1.55	1.50
2	D	354	HEM	CMA-C3A	2.39	1.55	1.50
3	C	355	BXO	C1-N1	2.39	1.28	1.26
2	G	354	HEM	CAC-C3C	2.38	1.53	1.47
2	A	354	HEM	CMB-C2B	2.38	1.55	1.50
2	G	354	HEM	CMB-C2B	2.33	1.55	1.50
3	E	355	BXO	C1-N1	2.32	1.28	1.26
2	E	354	HEM	FE-ND	2.31	2.02	1.94
2	G	354	HEM	CMC-C2C	2.31	1.55	1.50
2	B	354	HEM	CMA-C3A	2.30	1.55	1.50
2	G	354	HEM	FE-NA	2.29	2.02	1.95
2	G	354	HEM	FE-ND	2.29	2.02	1.94
2	C	354	HEM	CMA-C3A	2.27	1.55	1.50
2	F	354	HEM	CMD-C2D	2.25	1.55	1.50
2	E	354	HEM	CMB-C2B	2.20	1.55	1.50
2	C	354	HEM	CMB-C2B	2.20	1.55	1.50
2	G	354	HEM	CMA-C3A	2.19	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	354	HEM	FE-NA	2.19	2.02	1.95
2	A	354	HEM	CMA-C3A	2.15	1.55	1.50
2	B	354	HEM	CAD-C3D	2.07	1.56	1.51
2	E	354	HEM	CMC-C2C	2.05	1.55	1.50
2	C	354	HEM	CMC-C2C	2.04	1.54	1.50
3	D	355	BXO	C1-N1	2.04	1.28	1.26
2	F	354	HEM	CAD-C3D	2.02	1.56	1.51

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	355	BXO	O1-N1-C1	10.51	121.55	111.70
3	C	355	BXO	O1-N1-C1	8.02	119.22	111.70
3	E	355	BXO	O1-N1-C1	7.00	118.26	111.70
3	G	355	BXO	O1-N1-C1	6.84	118.12	111.70
3	B	355	BXO	O1-N1-C1	6.44	117.74	111.70
3	D	355	BXO	O1-N1-C1	6.16	117.48	111.70
3	H	355	BXO	O1-N1-C1	6.07	117.39	111.70
3	F	355	BXO	O1-N1-C1	5.70	117.05	111.70
2	F	354	HEM	C4D-ND-C1D	5.65	111.89	105.21
2	D	354	HEM	C4D-ND-C1D	5.34	111.54	105.21
2	B	354	HEM	C4D-ND-C1D	5.31	111.50	105.21
2	G	354	HEM	C4D-ND-C1D	5.22	111.39	105.21
2	E	354	HEM	C4D-ND-C1D	5.19	111.36	105.21
2	H	354	HEM	C4D-ND-C1D	5.15	111.30	105.21
2	A	354	HEM	C4D-ND-C1D	5.12	111.28	105.21
2	C	354	HEM	C4D-ND-C1D	5.12	111.27	105.21
2	C	354	HEM	CBA-CAA-C2A	-3.52	102.81	112.53
2	A	354	HEM	CBA-CAA-C2A	-3.49	102.88	112.53
2	E	354	HEM	CBA-CAA-C2A	-3.45	102.99	112.53
2	F	354	HEM	CAD-C3D-C4D	3.44	130.69	124.70
2	G	354	HEM	CBA-CAA-C2A	-3.42	103.07	112.53
2	D	354	HEM	CAD-C3D-C4D	3.39	130.60	124.70
2	H	354	HEM	CAD-C3D-C4D	3.30	130.44	124.70
2	B	354	HEM	CAD-C3D-C4D	3.27	130.40	124.70
3	D	355	BXO	C2-C1-N1	2.99	126.43	121.40
3	F	355	BXO	C2-C1-N1	2.96	126.38	121.40
3	H	355	BXO	C2-C1-N1	2.87	126.23	121.40
3	B	355	BXO	C2-C1-N1	2.86	126.22	121.40
2	D	354	HEM	CAA-CBA-CGA	-2.63	106.69	113.67
3	E	355	BXO	C2-C1-N1	2.60	125.78	121.40
2	F	354	HEM	CAA-CBA-CGA	-2.49	107.05	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	354	HEM	C2A-C1A-NA	-2.46	107.42	110.15
3	G	355	BXO	C2-C1-N1	2.46	125.54	121.40
2	A	354	HEM	C2A-C1A-NA	-2.36	107.53	110.15
2	H	354	HEM	CAA-CBA-CGA	-2.36	107.42	113.67
3	C	355	BXO	C2-C1-N1	2.35	125.36	121.40
2	B	354	HEM	CAA-CBA-CGA	-2.35	107.44	113.67
2	A	354	HEM	C1B-NB-C4B	2.32	107.96	105.21
2	C	354	HEM	CAD-C3D-C4D	2.32	128.75	124.70
2	A	354	HEM	CAD-CBD-CGD	-2.32	107.51	113.67
2	E	354	HEM	CAD-C3D-C4D	2.32	128.74	124.70
2	F	354	HEM	CMD-C2D-C1D	2.30	128.63	125.03
2	F	354	HEM	C4D-C3D-C2D	-2.29	103.55	106.89
2	G	354	HEM	CAD-CBD-CGD	-2.27	107.65	113.67
2	C	354	HEM	C2A-C1A-NA	-2.26	107.65	110.15
3	F	355	BXO	C3-C2-C1	-2.26	107.72	114.14
2	D	354	HEM	C4D-C3D-C2D	-2.25	103.62	106.89
2	A	354	HEM	CAD-C3D-C4D	2.23	128.59	124.70
2	G	354	HEM	C1B-NB-C4B	2.23	107.85	105.21
2	B	354	HEM	C2A-C1A-NA	-2.22	107.69	110.15
3	H	355	BXO	C3-C2-C1	-2.22	107.84	114.14
2	D	354	HEM	CMD-C2D-C1D	2.21	128.49	125.03
2	E	354	HEM	CMD-C2D-C1D	2.21	128.49	125.03
2	C	354	HEM	CAD-CBD-CGD	-2.21	107.81	113.67
2	B	354	HEM	C4D-C3D-C2D	-2.19	103.71	106.89
2	G	354	HEM	C2A-C1A-NA	-2.18	107.73	110.15
2	G	354	HEM	CMD-C2D-C1D	2.17	128.43	125.03
2	D	354	HEM	C2A-C1A-NA	-2.17	107.74	110.15
2	B	354	HEM	CMD-C2D-C1D	2.15	128.40	125.03
2	H	354	HEM	C4D-C3D-C2D	-2.15	103.76	106.89
2	H	354	HEM	CHC-C4B-NB	2.13	126.71	124.42
2	E	354	HEM	C1B-NB-C4B	2.13	107.72	105.21
2	C	354	HEM	CMD-C2D-C1D	2.12	128.35	125.03
2	E	354	HEM	CAD-CBD-CGD	-2.12	108.05	113.67
3	B	355	BXO	C3-C2-C1	-2.11	108.14	114.14
2	A	354	HEM	C2B-C1B-NB	-2.11	107.42	109.84
2	A	354	HEM	CMD-C2D-C1D	2.11	128.33	125.03
2	H	354	HEM	C2A-C1A-NA	-2.10	107.82	110.15
2	G	354	HEM	CAD-C3D-C4D	2.08	128.31	124.70
2	C	354	HEM	C1B-NB-C4B	2.04	107.63	105.21
2	F	354	HEM	C1B-NB-C4B	2.04	107.62	105.21
2	C	354	HEM	CBC-CAC-C3C	-2.02	117.43	127.53
3	D	355	BXO	C3-C2-C1	-2.02	108.41	114.14

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	354	HEM	C2B-C3B-CAB-CBB
2	A	354	HEM	C4B-C3B-CAB-CBB
2	B	354	HEM	C2B-C3B-CAB-CBB
2	C	354	HEM	C2B-C3B-CAB-CBB
2	C	354	HEM	C4B-C3B-CAB-CBB
2	D	354	HEM	C2B-C3B-CAB-CBB
2	E	354	HEM	C2B-C3B-CAB-CBB
2	E	354	HEM	C4B-C3B-CAB-CBB
2	F	354	HEM	C2B-C3B-CAB-CBB
2	G	354	HEM	C2B-C3B-CAB-CBB
2	G	354	HEM	C4B-C3B-CAB-CBB
2	H	354	HEM	C2B-C3B-CAB-CBB
3	B	355	BXO	C1-C2-C3-C4
3	D	355	BXO	C1-C2-C3-C4
3	F	355	BXO	C1-C2-C3-C4
3	H	355	BXO	C1-C2-C3-C4
2	A	354	HEM	C2C-C3C-CAC-CBC
2	C	354	HEM	C2C-C3C-CAC-CBC
2	E	354	HEM	C2C-C3C-CAC-CBC
2	G	354	HEM	C2C-C3C-CAC-CBC
2	B	354	HEM	C4B-C3B-CAB-CBB
2	D	354	HEM	C4B-C3B-CAB-CBB
2	F	354	HEM	C4B-C3B-CAB-CBB
2	H	354	HEM	C4B-C3B-CAB-CBB
2	F	354	HEM	CAD-CBD-CGD-O2D
2	A	354	HEM	C4C-C3C-CAC-CBC
2	C	354	HEM	C4C-C3C-CAC-CBC
2	E	354	HEM	C4C-C3C-CAC-CBC
2	G	354	HEM	C4C-C3C-CAC-CBC
2	B	354	HEM	CAD-CBD-CGD-O2D
2	H	354	HEM	CAD-CBD-CGD-O2D
2	B	354	HEM	CAD-CBD-CGD-O1D
2	D	354	HEM	CAD-CBD-CGD-O2D
2	F	354	HEM	CAD-CBD-CGD-O1D
2	H	354	HEM	CAD-CBD-CGD-O1D
2	D	354	HEM	CAD-CBD-CGD-O1D
2	A	354	HEM	CAA-CBA-CGA-O2A
2	D	354	HEM	CAA-CBA-CGA-O1A
2	F	354	HEM	CAA-CBA-CGA-O1A
2	G	354	HEM	CAA-CBA-CGA-O2A

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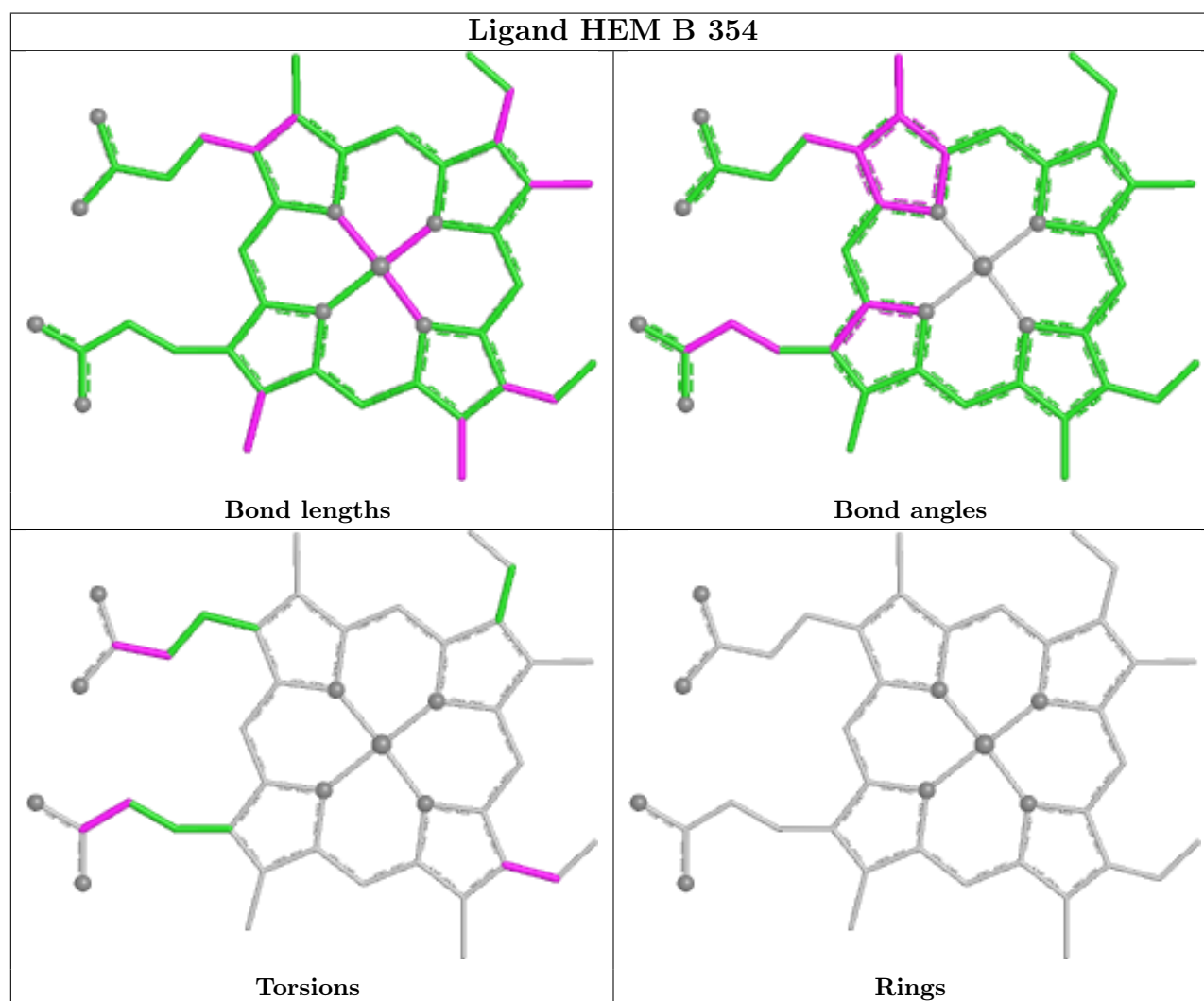
Mol	Chain	Res	Type	Atoms
2	H	354	HEM	CAA-CBA-CGA-O1A
2	C	354	HEM	CAA-CBA-CGA-O2A
2	E	354	HEM	CAA-CBA-CGA-O2A
2	B	354	HEM	CAA-CBA-CGA-O1A
2	D	354	HEM	CAA-CBA-CGA-O2A
2	F	354	HEM	CAA-CBA-CGA-O2A
2	B	354	HEM	CAA-CBA-CGA-O2A
2	H	354	HEM	CAA-CBA-CGA-O2A
2	C	354	HEM	CAD-CBD-CGD-O2D
2	A	354	HEM	CAD-CBD-CGD-O2D
2	A	354	HEM	CAA-CBA-CGA-O1A
2	C	354	HEM	CAA-CBA-CGA-O1A
2	E	354	HEM	CAD-CBD-CGD-O2D
2	G	354	HEM	CAA-CBA-CGA-O1A
2	G	354	HEM	CAD-CBD-CGD-O2D
2	E	354	HEM	CAA-CBA-CGA-O1A
2	C	354	HEM	CAD-CBD-CGD-O1D
2	A	354	HEM	CAD-CBD-CGD-O1D
2	E	354	HEM	CAD-CBD-CGD-O1D
2	G	354	HEM	CAD-CBD-CGD-O1D
3	B	355	BXO	N1-C1-C2-C3
3	D	355	BXO	N1-C1-C2-C3
3	F	355	BXO	N1-C1-C2-C3
3	H	355	BXO	N1-C1-C2-C3

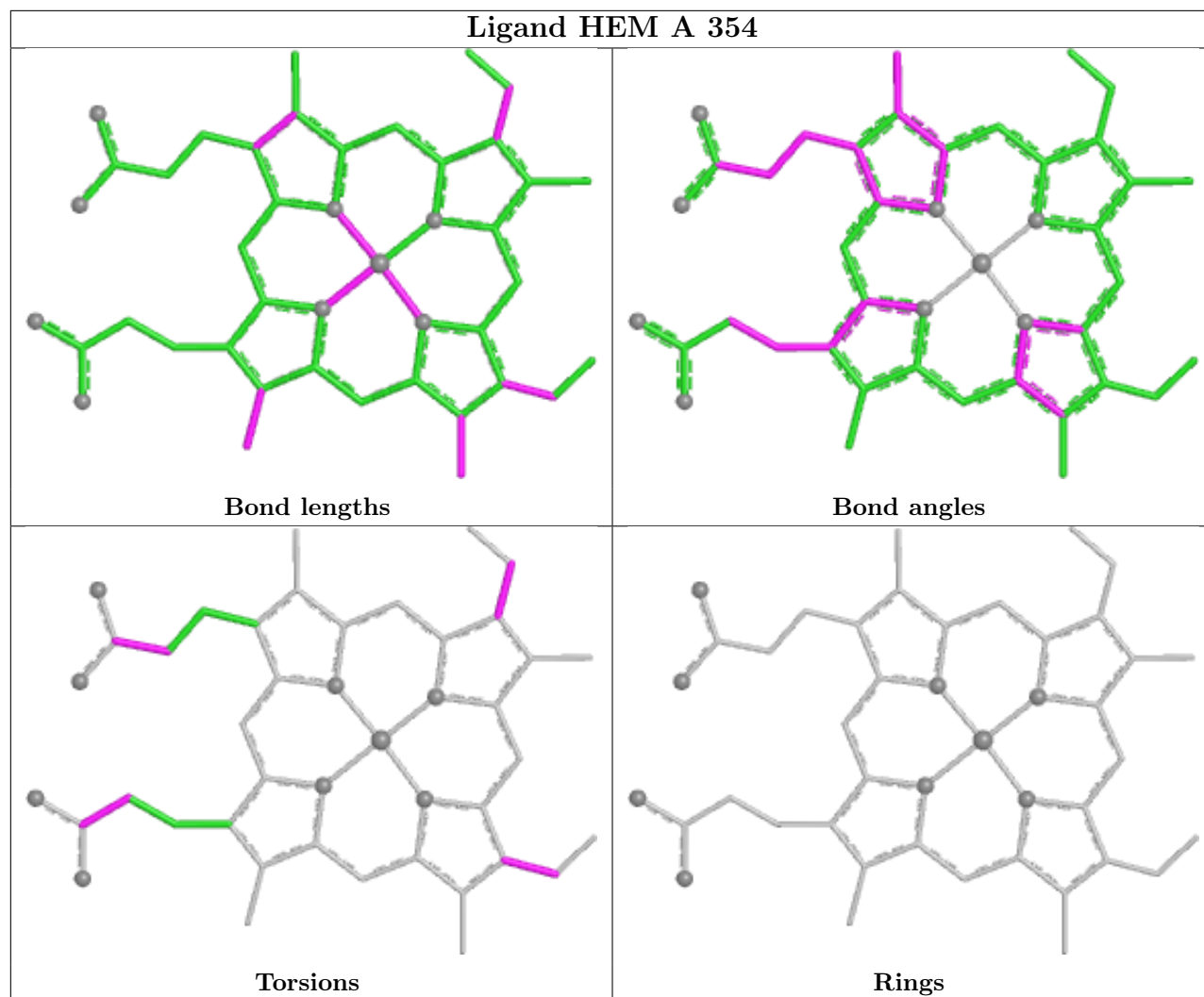
There are no ring outliers.

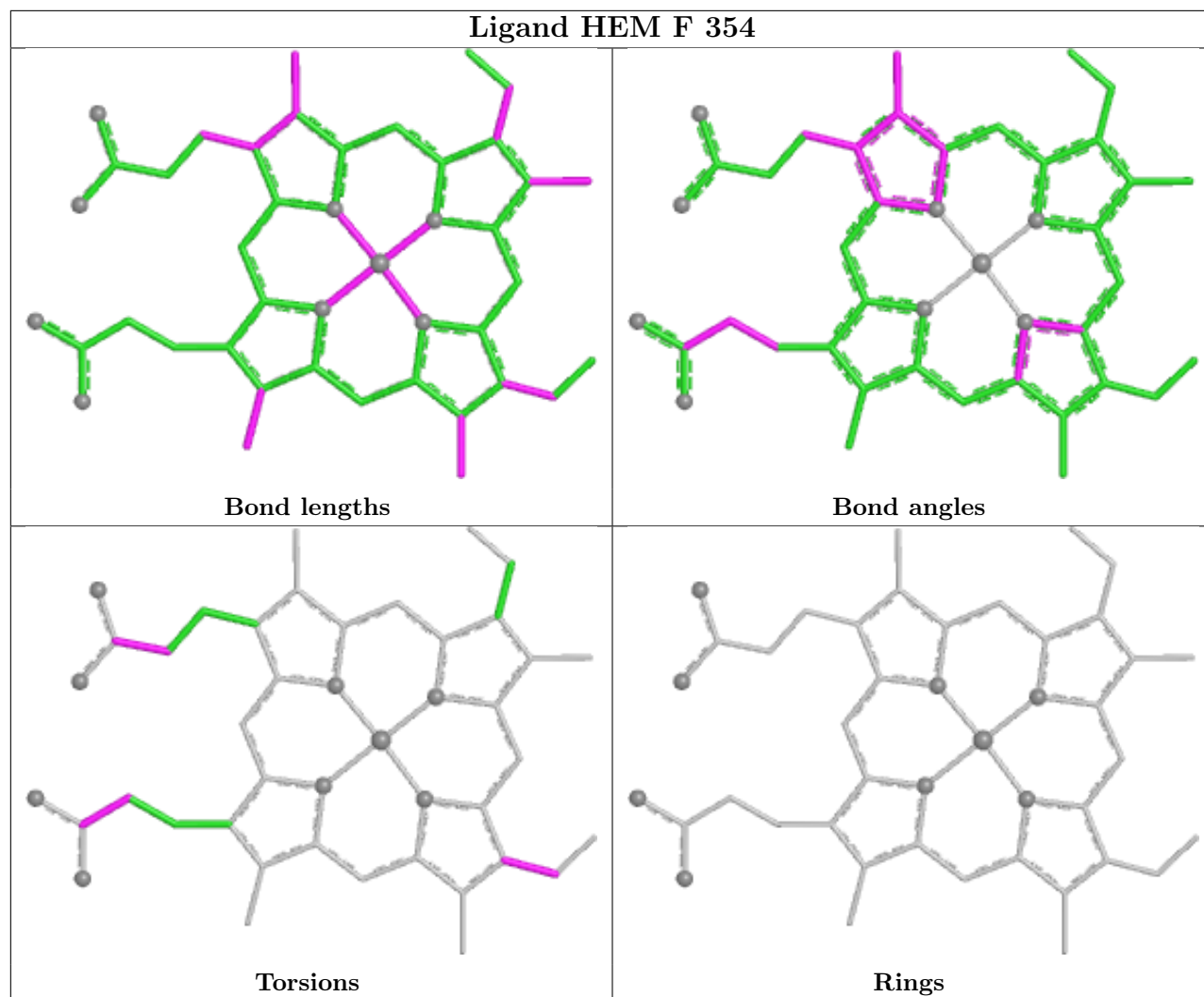
13 monomers are involved in 28 short contacts:

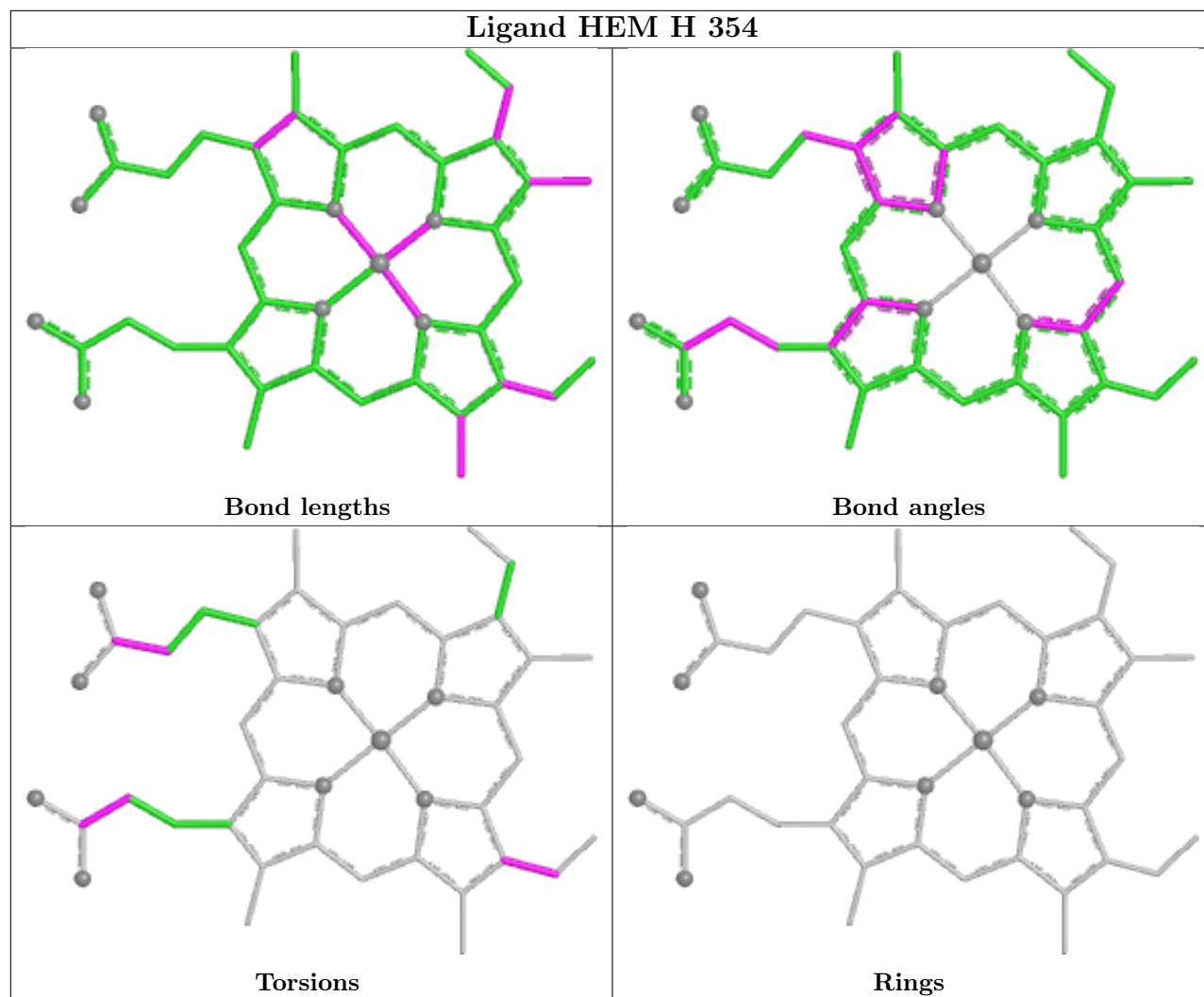
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	354	HEM	2	0
2	A	354	HEM	4	0
2	F	354	HEM	2	0
2	H	354	HEM	3	0
3	F	355	BXO	1	0
2	G	354	HEM	4	0
3	D	355	BXO	1	0
2	D	354	HEM	1	0
3	A	355	BXO	2	0
2	C	354	HEM	4	0
3	B	355	BXO	1	0
2	E	354	HEM	4	0
3	H	355	BXO	3	0

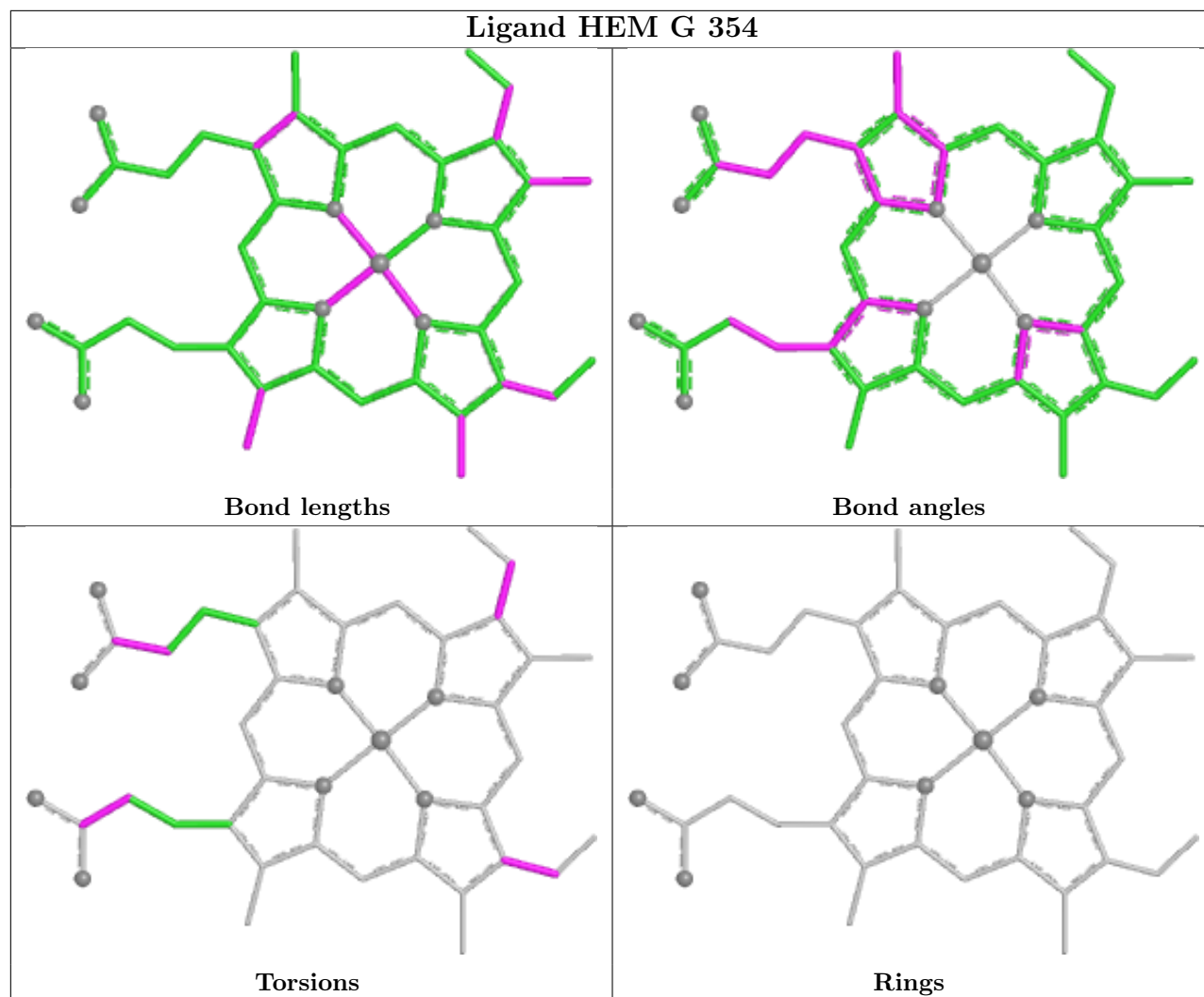
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

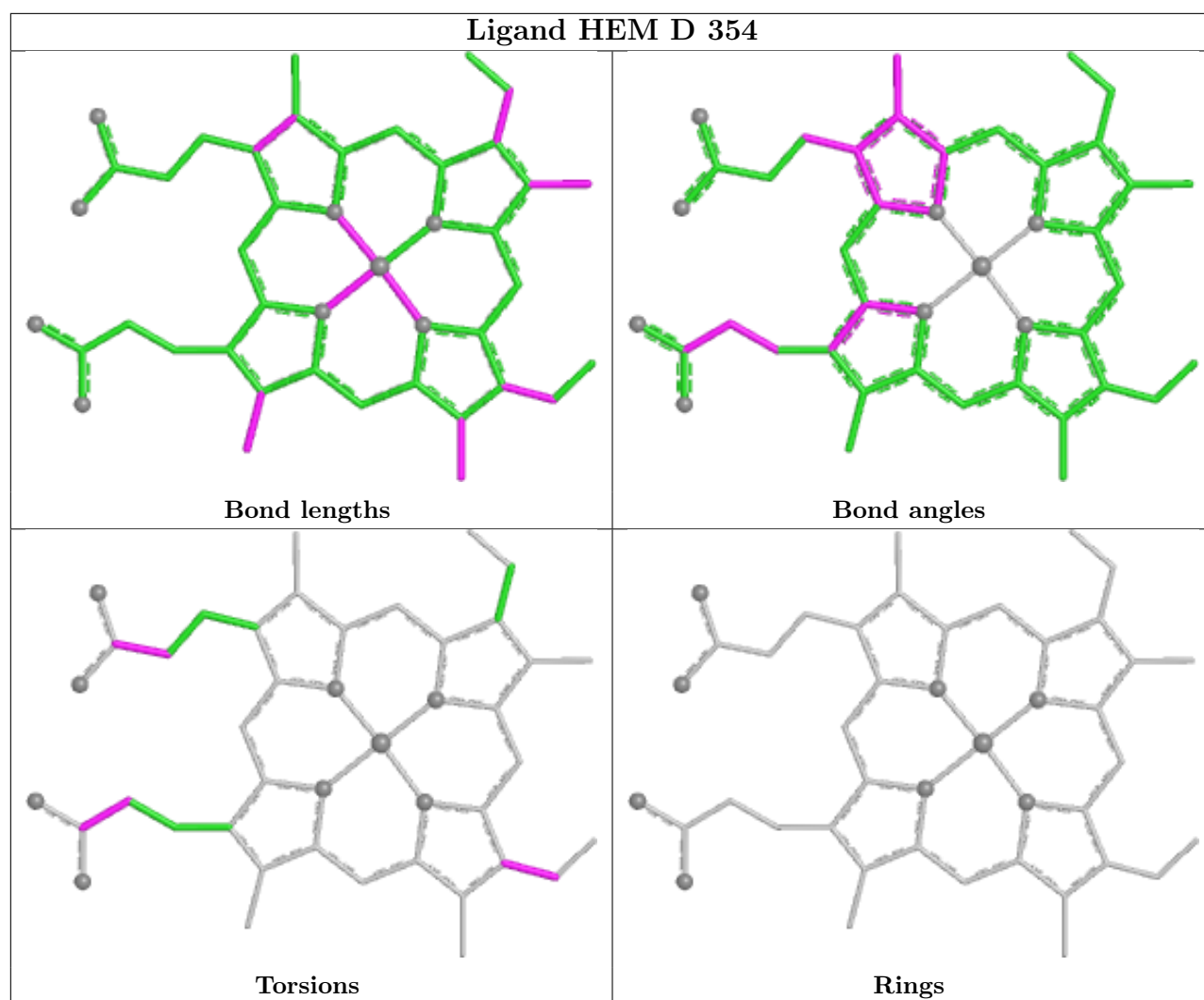


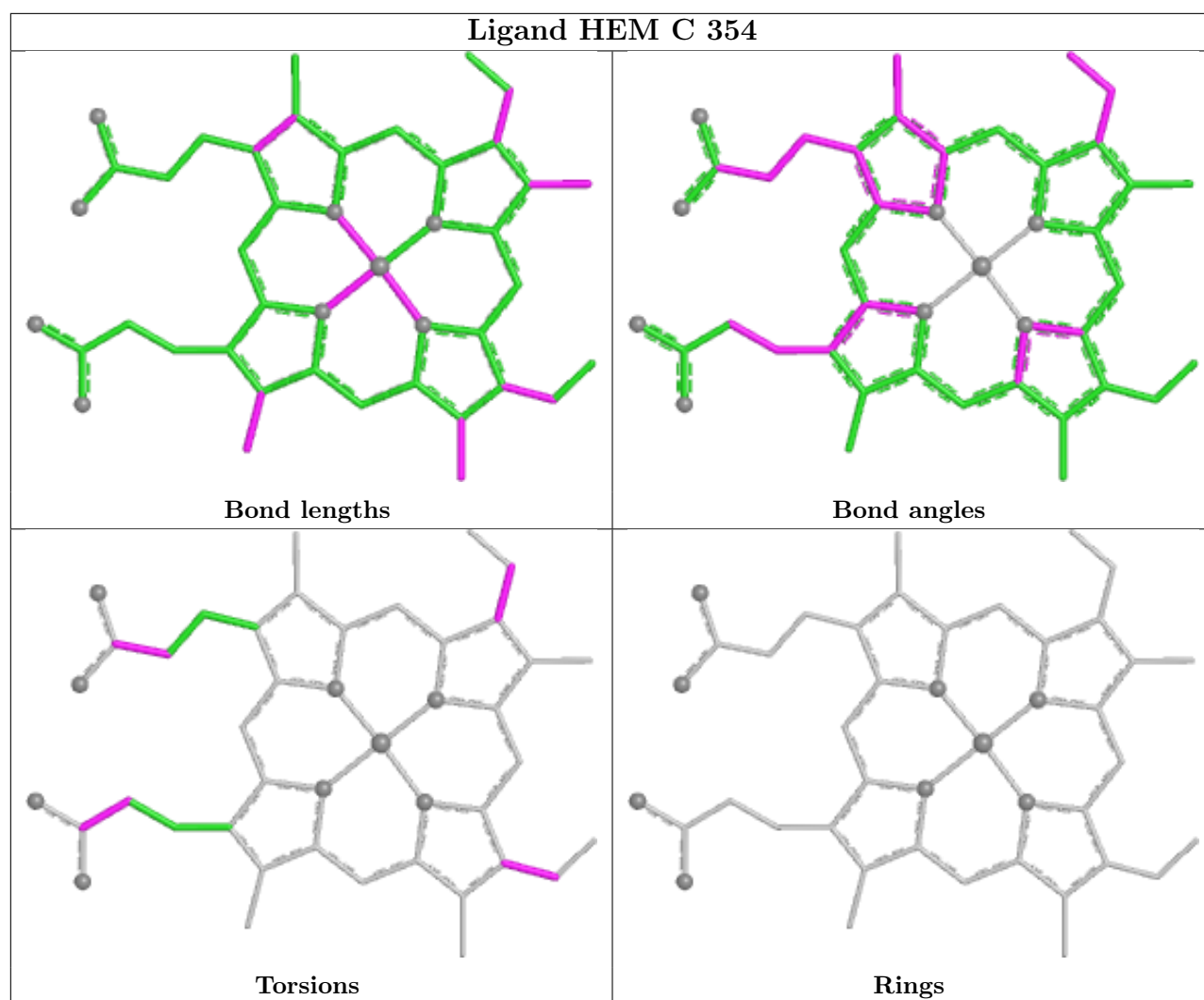


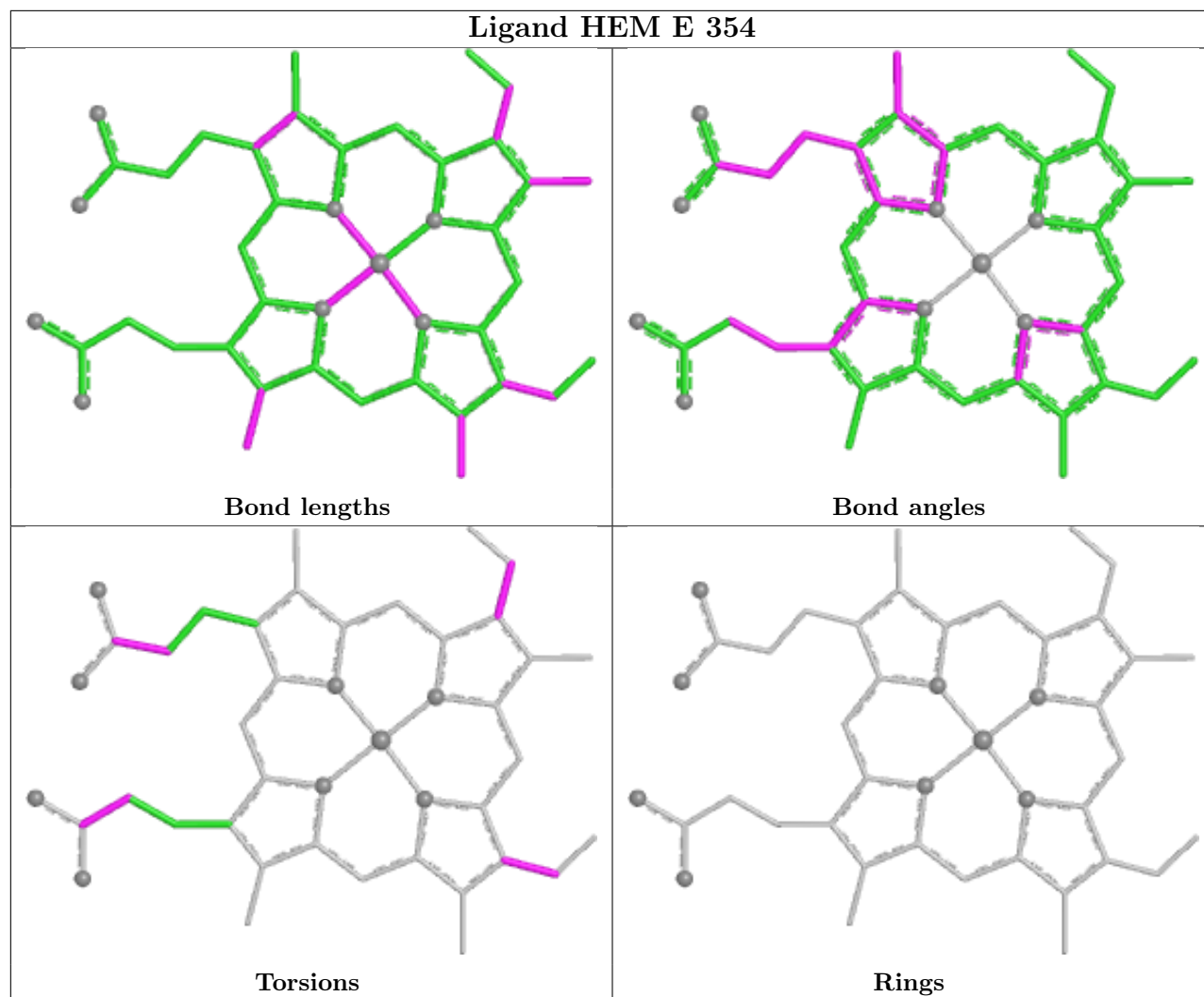












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	350/373 (93%)	0.23	6 (1%) 69 65	13, 25, 39, 55	0
1	B	359/373 (96%)	0.59	29 (8%) 18 15	15, 31, 57, 67	0
1	C	352/373 (94%)	0.22	10 (2%) 55 50	14, 25, 40, 55	1 (0%)
1	D	360/373 (96%)	0.61	23 (6%) 25 22	15, 31, 57, 68	1 (0%)
1	E	351/373 (94%)	0.24	10 (2%) 55 50	14, 25, 40, 55	1 (0%)
1	F	359/373 (96%)	0.57	30 (8%) 17 15	15, 31, 57, 68	0
1	G	353/373 (94%)	0.24	7 (1%) 65 61	13, 25, 41, 55	0
1	H	359/373 (96%)	0.52	21 (5%) 29 25	15, 31, 57, 68	0
All	All	2843/2984 (95%)	0.41	136 (4%) 35 31	13, 26, 55, 68	3 (0%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	351	ALA	6.3
1	C	351	ALA	5.3
1	G	353	HIS	4.9
1	B	63	MET	4.3
1	H	75	GLY	4.1
1	B	201	ALA	4.0
1	D	112	THR	3.9
1	F	118	TRP	3.7
1	B	126	ASP	3.7
1	H	350	ILE	3.7
1	B	112	THR	3.6
1	F	126	ASP	3.5
1	H	118	TRP	3.4
1	B	350	ILE	3.4
1	G	126	ASP	3.3
1	B	194	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	103	SER	3.2
1	D	350	ILE	3.2
1	B	115	ALA	3.2
1	D	106	HIS	3.2
1	E	350	ILE	3.1
1	H	129	GLY	3.1
1	D	196	ILE	3.1
1	E	126	ASP	3.0
1	B	192	GLU	3.0
1	F	127	GLY	3.0
1	F	349	THR	3.0
1	G	352	GLU	3.0
1	A	123	ARG	3.0
1	D	75	GLY	3.0
1	D	63	MET	3.0
1	F	121	GLU	2.9
1	D	113	PRO	2.9
1	E	351	ALA	2.9
1	C	192	GLU	2.9
1	H	120	SER	2.9
1	E	51	ARG	2.9
1	D	118	TRP	2.9
1	F	347	ALA	2.8
1	F	128	LEU	2.8
1	B	196	ILE	2.8
1	F	114	ILE	2.7
1	D	351	ALA	2.7
1	F	192	GLU	2.7
1	F	115	ALA	2.7
1	B	118	TRP	2.7
1	B	202	VAL	2.7
1	F	201	ALA	2.7
1	F	106	HIS	2.7
1	E	124	LEU	2.6
1	B	58	ALA	2.6
1	B	128	LEU	2.6
1	F	120	SER	2.6
1	H	194	ARG	2.5
1	B	62	ALA	2.5
1	D	115	ALA	2.5
1	D	124	LEU	2.5
1	C	150	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	124	LEU	2.5
1	D	201	ALA	2.5
1	F	103	SER	2.5
1	F	62	ALA	2.5
1	D	104	SER	2.5
1	B	121	GLU	2.4
1	C	126	ASP	2.4
1	C	12	PRO	2.4
1	B	106	HIS	2.4
1	F	58	ALA	2.4
1	H	112	THR	2.4
1	H	109	SER	2.4
1	F	350	ILE	2.4
1	B	124	LEU	2.4
1	B	116	SER	2.3
1	F	202	VAL	2.3
1	C	350	ILE	2.3
1	D	335	ILE	2.3
1	E	192	GLU	2.3
1	B	113	PRO	2.3
1	A	124	LEU	2.3
1	E	150	GLU	2.3
1	F	119	GLU	2.3
1	B	132	ARG	2.3
1	C	123	ARG	2.3
1	F	129	GLY	2.3
1	D	150	GLU	2.3
1	A	12	PRO	2.3
1	D	62	ALA	2.2
1	D	-8	SER	2.2
1	F	125	SER	2.2
1	H	128	LEU	2.2
1	A	126	ASP	2.2
1	D	194	ARG	2.2
1	G	123	ARG	2.2
1	E	4	ALA	2.2
1	F	122	ASP	2.2
1	D	192	GLU	2.2
1	D	70	PHE	2.2
1	H	57	PRO	2.2
1	C	124	LEU	2.2
1	D	203	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	203	GLY	2.2
1	F	74	ASP	2.2
1	F	51	ARG	2.2
1	B	195	VAL	2.1
1	B	347	ALA	2.1
1	H	61	GLN	2.1
1	H	62	ALA	2.1
1	H	63	MET	2.1
1	B	114	ILE	2.1
1	H	106	HIS	2.1
1	A	349	THR	2.1
1	B	199	ASP	2.1
1	B	55	GLN	2.1
1	F	110	THR	2.1
1	C	301	ARG	2.1
1	F	197	ALA	2.1
1	H	115	ALA	2.1
1	B	90	TYR	2.1
1	F	151	ASP	2.1
1	A	125	SER	2.1
1	B	125	SER	2.1
1	E	201	ALA	2.0
1	C	253	GLY	2.0
1	H	117	TRP	2.0
1	F	116	SER	2.0
1	H	103	SER	2.0
1	F	55	GLN	2.0
1	H	70	PHE	2.0
1	H	195	VAL	2.0
1	D	328	ALA	2.0
1	H	58	ALA	2.0
1	H	201	ALA	2.0
1	E	53	GLU	2.0
1	G	121	GLU	2.0
1	G	192	GLU	2.0
1	D	36	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

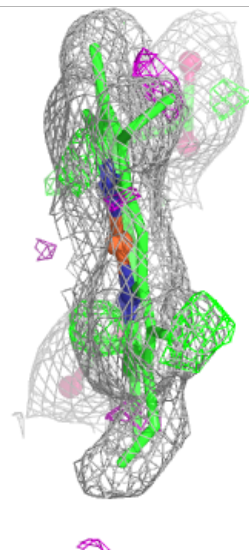
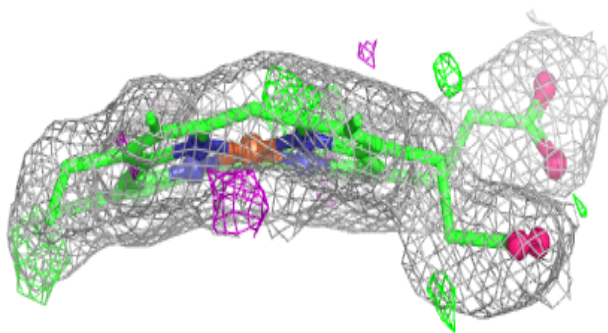
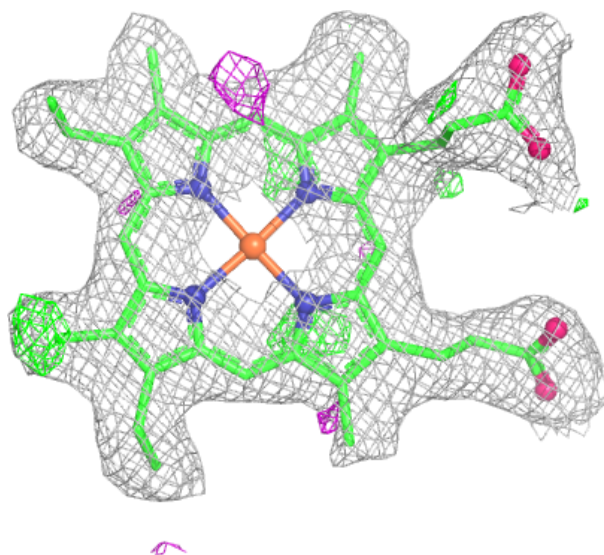
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BXO	B	355	6/6	0.93	0.11	25,26,27,28	0
3	BXO	D	355	6/6	0.94	0.10	25,26,27,28	0
3	BXO	F	355	6/6	0.94	0.09	25,26,27,28	0
2	HEM	F	354	43/43	0.95	0.09	12,13,17,17	0
3	BXO	E	355	6/6	0.95	0.10	18,20,21,21	0
2	HEM	D	354	43/43	0.95	0.09	12,13,17,17	0
3	BXO	G	355	6/6	0.95	0.11	18,20,21,21	0
3	BXO	H	355	6/6	0.95	0.09	25,26,27,28	0
3	BXO	C	355	6/6	0.96	0.07	18,20,21,21	0
2	HEM	H	354	43/43	0.96	0.08	12,13,17,17	0
2	HEM	B	354	43/43	0.96	0.08	12,13,17,17	0
2	HEM	G	354	43/43	0.97	0.07	13,15,18,18	0
2	HEM	A	354	43/43	0.97	0.08	13,15,18,18	0
3	BXO	A	355	6/6	0.97	0.09	18,20,21,21	0
2	HEM	E	354	43/43	0.97	0.08	13,15,18,18	0
2	HEM	C	354	43/43	0.97	0.08	13,15,18,18	0

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

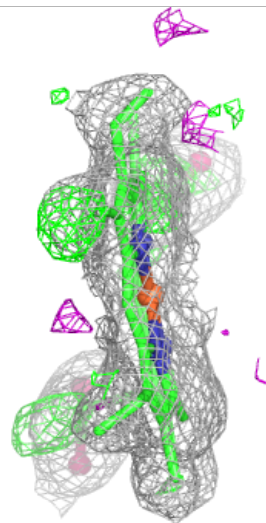
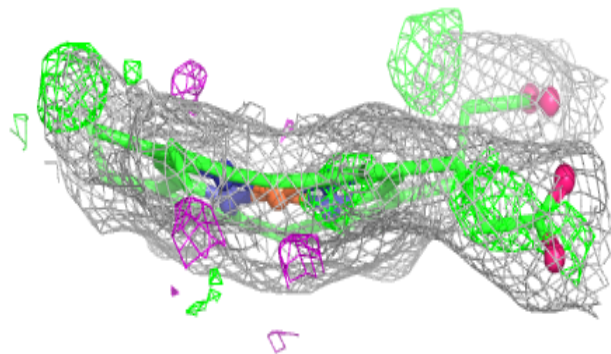
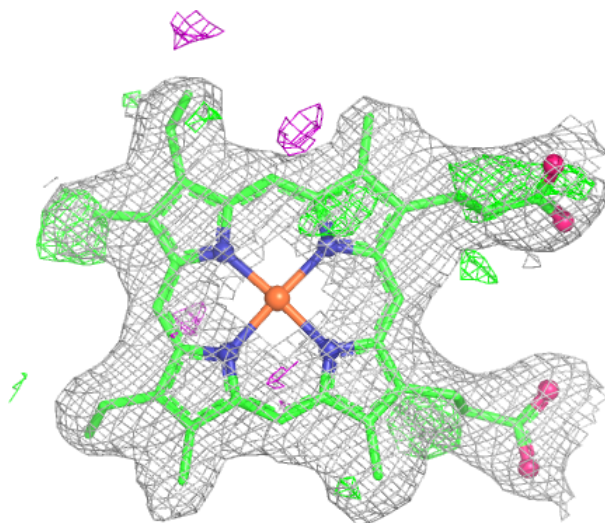
Electron density around HEM F 354:

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



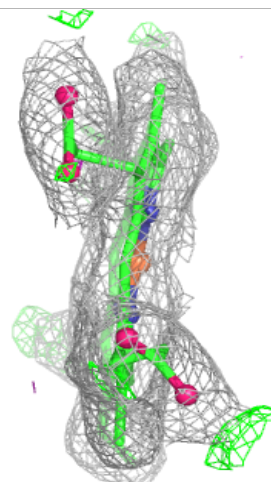
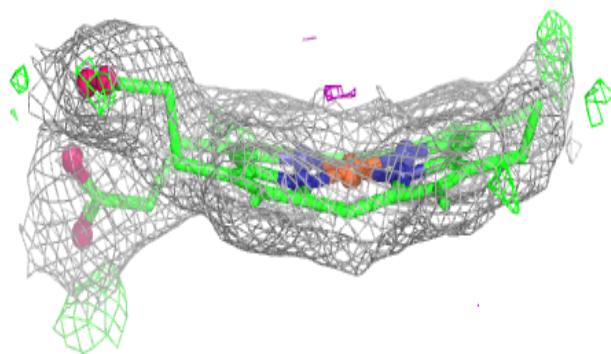
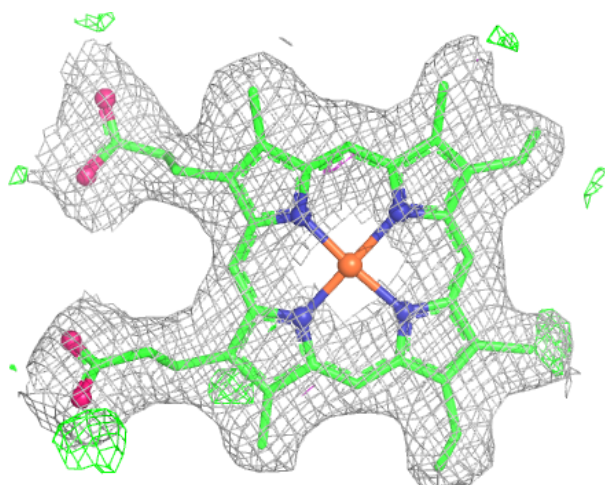
Electron density around HEM D 354:

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



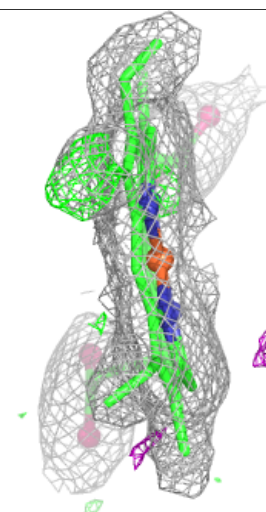
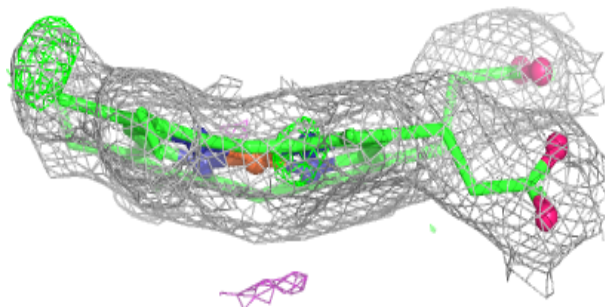
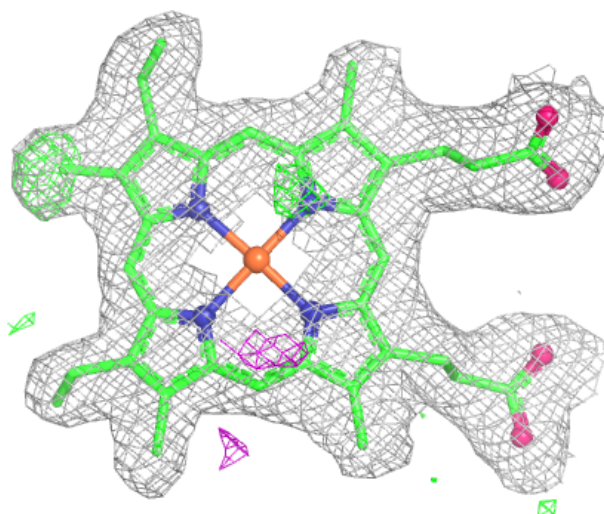
Electron density around HEM H 354:

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



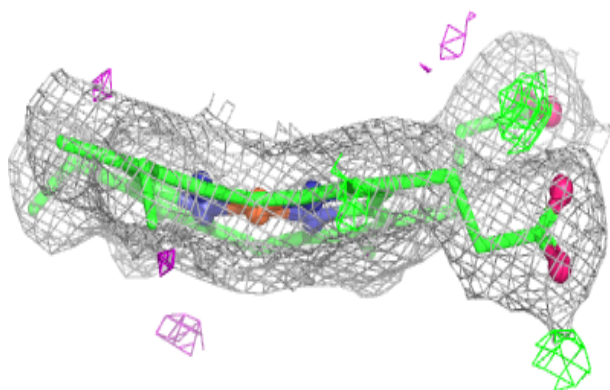
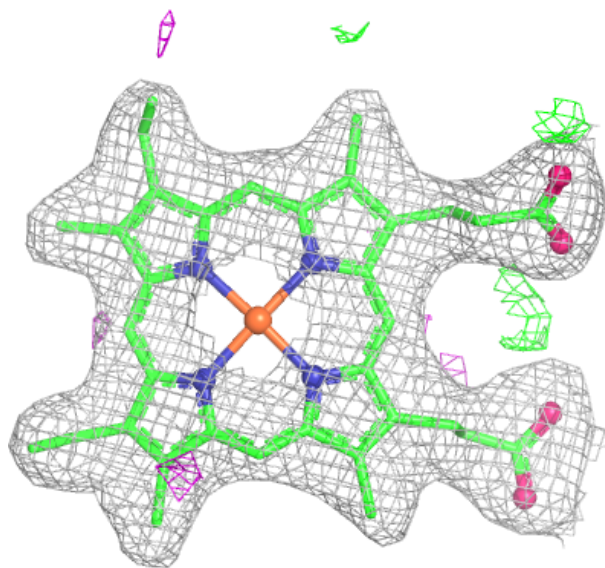
Electron density around HEM B 354:

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



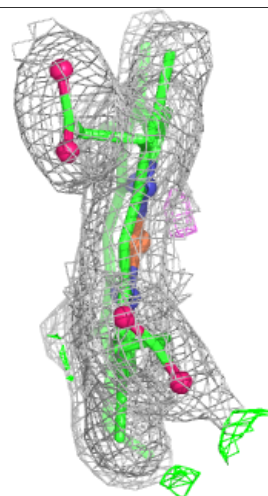
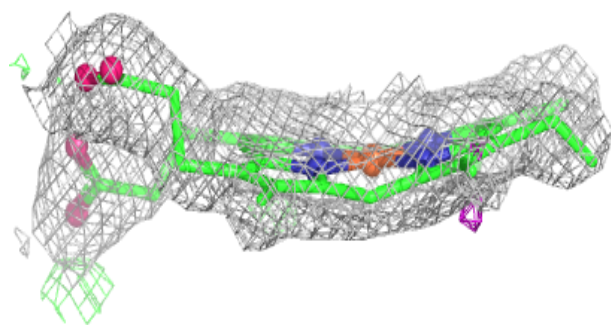
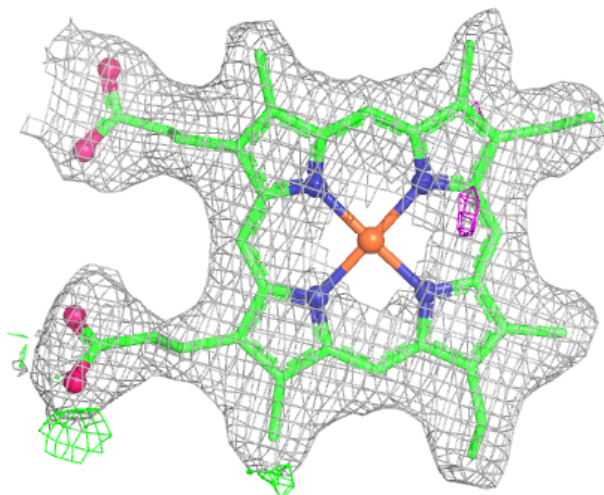
Electron density around HEM G 354:

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



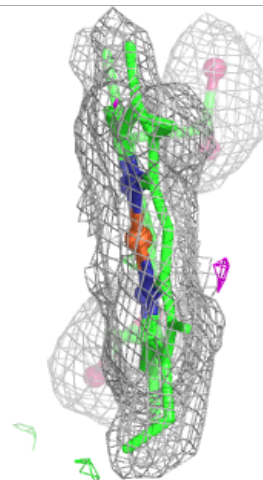
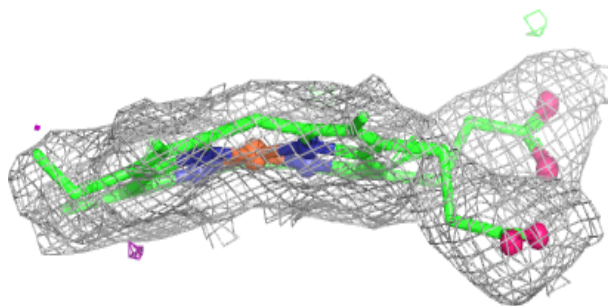
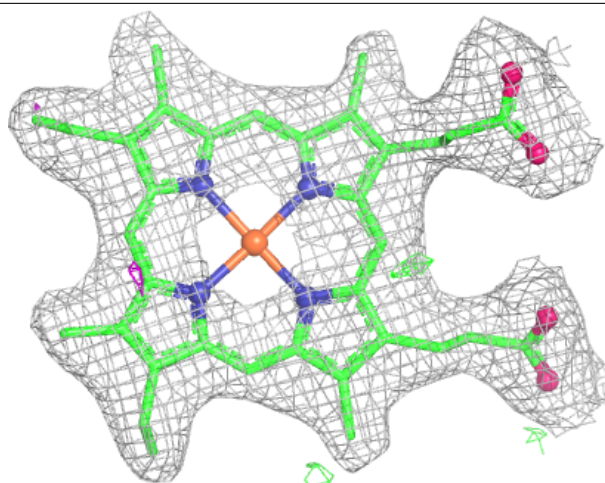
Electron density around HEM A 354:

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



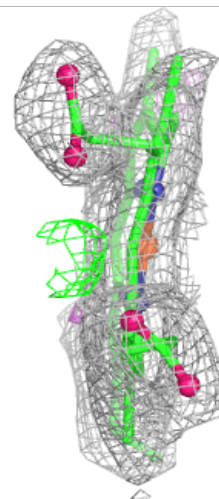
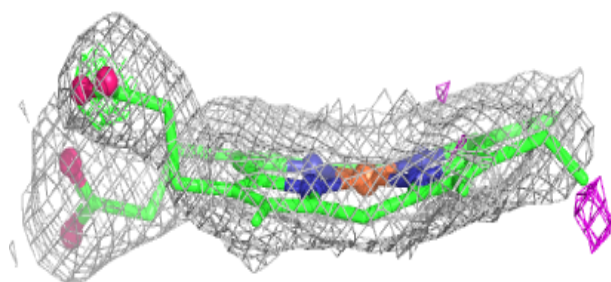
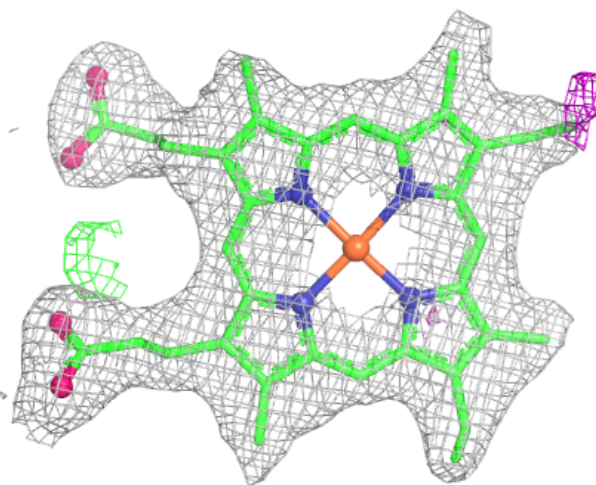
Electron density around HEM E 354:

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



Electron density around HEM C 354:

$2mF_o-DF_c$ (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.