



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 05:04 PM EDT

PDB ID : 3G5N
Title : Triple ligand occupancy crystal structure of cytochrome P450 2B4 in complex with the inhibitor 1-biphenyl-4-methyl-1H-imidazole
Authors : Gay, S.C.; Sun, L.; Maekawa, K.; Halpert, J.R.; Stout, C.D.
Deposited on : 2009-02-05
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

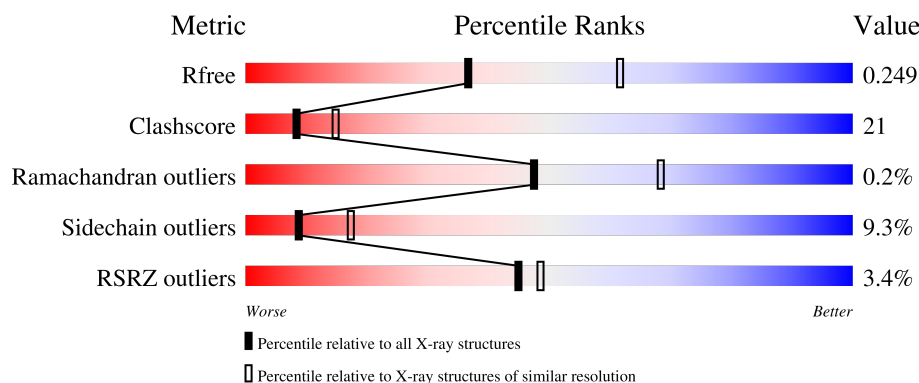
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	476	 4% 67% 24% 5% 5%
1	B	476	 2% 65% 25% 5% 5%
1	C	476	 5% 61% 29% 5% 5%
1	D	476	 3% 64% 27% 5% 5%

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	PB2	A	503	-	-	X	-
3	PB2	B	502	-	-	X	-
3	PB2	B	503	-	-	X	-
3	PB2	C	502	-	-	X	-
3	PB2	C	503	-	-	X	X
3	PB2	D	502	-	-	X	-
3	PB2	D	503	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14746 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3573	2310	607	646	10			
1	B	451	Total	C	N	O	S	0	1	0
			3511	2269	596	637	9			
1	C	452	Total	C	N	O	S	0	1	0
			3504	2265	599	631	9			
1	D	451	Total	C	N	O	S	0	0	0
			3526	2277	600	639	10			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	engineered mutation	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	SER	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	GLY	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	ARG	deletion	UNP P00178
A	22	LYS	GLY	engineered mutation	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LYS	HIS	engineered mutation	UNP P00178
A	24	THR	PRO	engineered mutation	UNP P00178
A	25	SER	LYS	engineered mutation	UNP P00178
A	26	SER	ALA	engineered mutation	UNP P00178
A	27	LYS	HIS	engineered mutation	UNP P00178
A	29	LYS	ARG	engineered mutation	UNP P00178
A	221	SER	PRO	SEE REMARK 999	UNP P00178
A	226	TYR	HIS	engineered mutation	UNP P00178
A	492	HIS	-	expression tag	UNP P00178
A	493	HIS	-	expression tag	UNP P00178
A	494	HIS	-	expression tag	UNP P00178
A	495	HIS	-	expression tag	UNP P00178
B	21	ALA	GLU	engineered mutation	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	SER	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	ALA	deletion	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	ALA	deletion	UNP P00178
B	?	-	GLY	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	ARG	deletion	UNP P00178
B	22	LYS	GLY	engineered mutation	UNP P00178
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B	25	SER	LYS	engineered mutation	UNP P00178
B	26	SER	ALA	engineered mutation	UNP P00178
B	27	LYS	HIS	engineered mutation	UNP P00178
B	29	LYS	ARG	engineered mutation	UNP P00178
B	221	SER	PRO	SEE REMARK 999	UNP P00178
B	226	TYR	HIS	engineered mutation	UNP P00178
B	492	HIS	-	expression tag	UNP P00178

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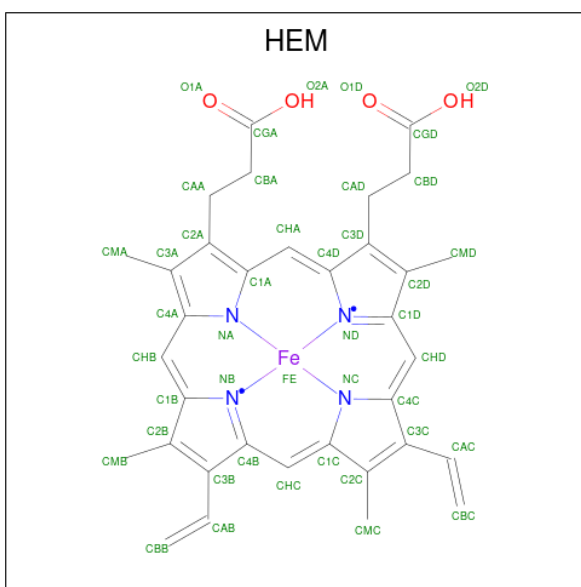
Chain	Residue	Modelled	Actual	Comment	Reference
B	493	HIS	-	expression tag	UNP P00178
B	494	HIS	-	expression tag	UNP P00178
B	495	HIS	-	expression tag	UNP P00178
C	21	ALA	GLU	engineered mutation	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	SER	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	ALA	deletion	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	ALA	deletion	UNP P00178
C	?	-	GLY	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	ARG	deletion	UNP P00178
C	22	LYS	GLY	engineered mutation	UNP P00178
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C	24	THR	PRO	engineered mutation	UNP P00178
C	25	SER	LYS	engineered mutation	UNP P00178
C	26	SER	ALA	engineered mutation	UNP P00178
C	27	LYS	HIS	engineered mutation	UNP P00178
C	29	LYS	ARG	engineered mutation	UNP P00178
C	221	SER	PRO	SEE REMARK 999	UNP P00178
C	226	TYR	HIS	engineered mutation	UNP P00178
C	492	HIS	-	expression tag	UNP P00178
C	493	HIS	-	expression tag	UNP P00178
C	494	HIS	-	expression tag	UNP P00178
C	495	HIS	-	expression tag	UNP P00178
D	21	ALA	GLU	engineered mutation	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	SER	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178

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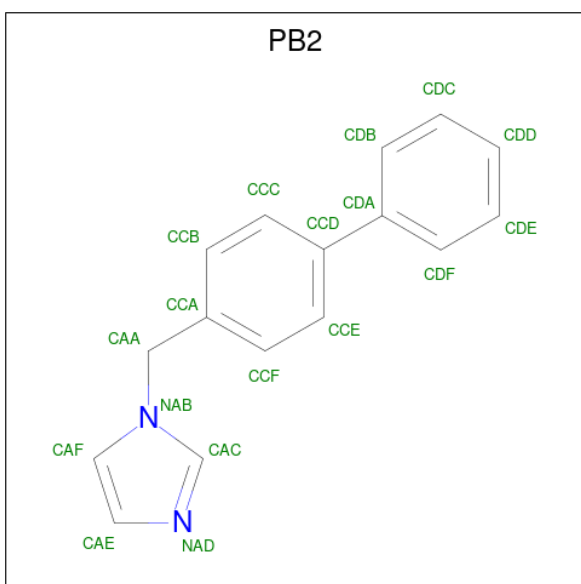
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	ALA	deletion	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	ALA	deletion	UNP P00178
D	?	-	GLY	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	ARG	deletion	UNP P00178
D	22	LYS	GLY	engineered mutation	UNP P00178
D	23	LYS	HIS	engineered mutation	UNP P00178
D	24	THR	PRO	engineered mutation	UNP P00178
D	25	SER	LYS	engineered mutation	UNP P00178
D	26	SER	ALA	engineered mutation	UNP P00178
D	27	LYS	HIS	engineered mutation	UNP P00178
D	29	LYS	ARG	engineered mutation	UNP P00178
D	221	SER	PRO	SEE REMARK 999	UNP P00178
D	226	TYR	HIS	engineered mutation	UNP P00178
D	492	HIS	-	expression tag	UNP P00178
D	493	HIS	-	expression tag	UNP P00178
D	494	HIS	-	expression tag	UNP P00178
D	495	HIS	-	expression tag	UNP P00178

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



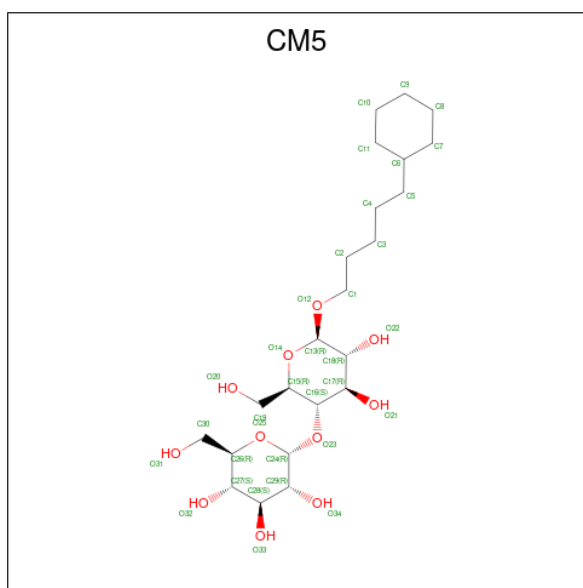
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 1-(biphenyl-4-ylmethyl)-1H-imidazole (three-letter code: PB2) (formula: $\text{C}_{16}\text{H}_{14}\text{N}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 18 16 2	0	0
3	A	1	Total C 12 12	0	0
3	B	1	Total C N 18 16 2	0	0
3	B	1	Total C N 18 16 2	0	0
3	B	1	Total C N 18 16 2	0	0
3	B	1	Total C 12 12	0	0
3	C	1	Total C N 18 16 2	0	0
3	C	1	Total C N 18 16 2	0	0
3	C	1	Total C 12 12	0	0
3	D	1	Total C N 18 16 2	0	0
3	D	1	Total C N 18 16 2	0	0
3	D	1	Total C 12 12	0	0

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (three-letter code: CM5) (formula: C₂₃H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	17	5		
4	B	1	Total	C	O	0	0
			22	17	5		
4	C	1	Total	C	O	0	0
			22	17	5		
4	D	1	Total	C	O	0	0
			22	17	5		

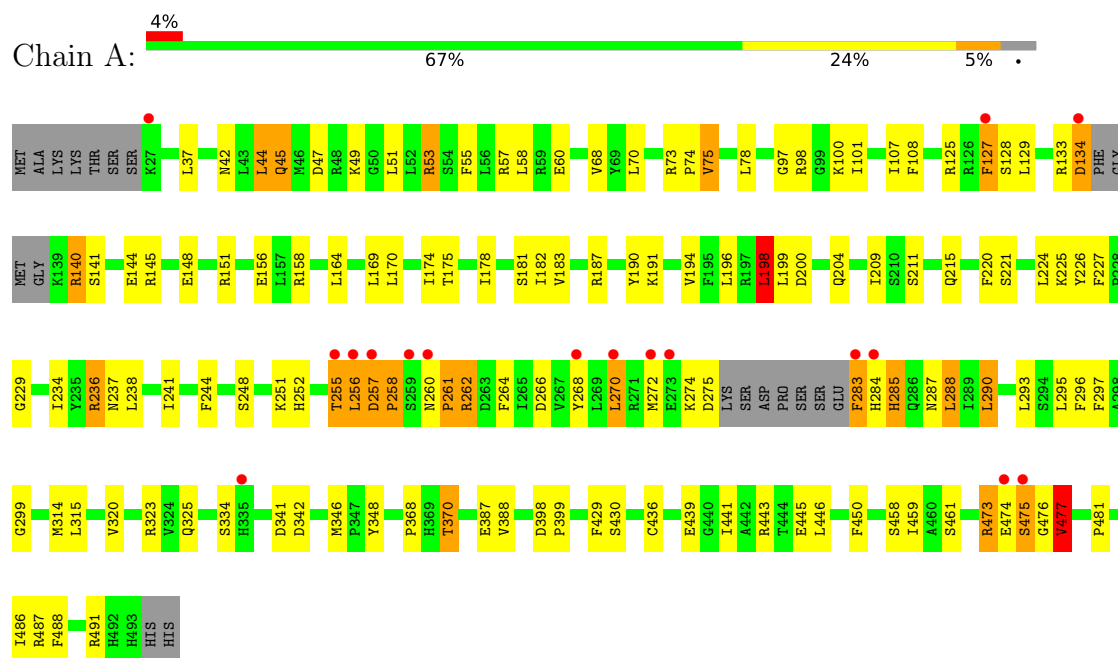
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	40	Total	O	0	0
			40	40		
5	C	30	Total	O	0	0
			30	30		
5	D	54	Total	O	0	0
			54	54		

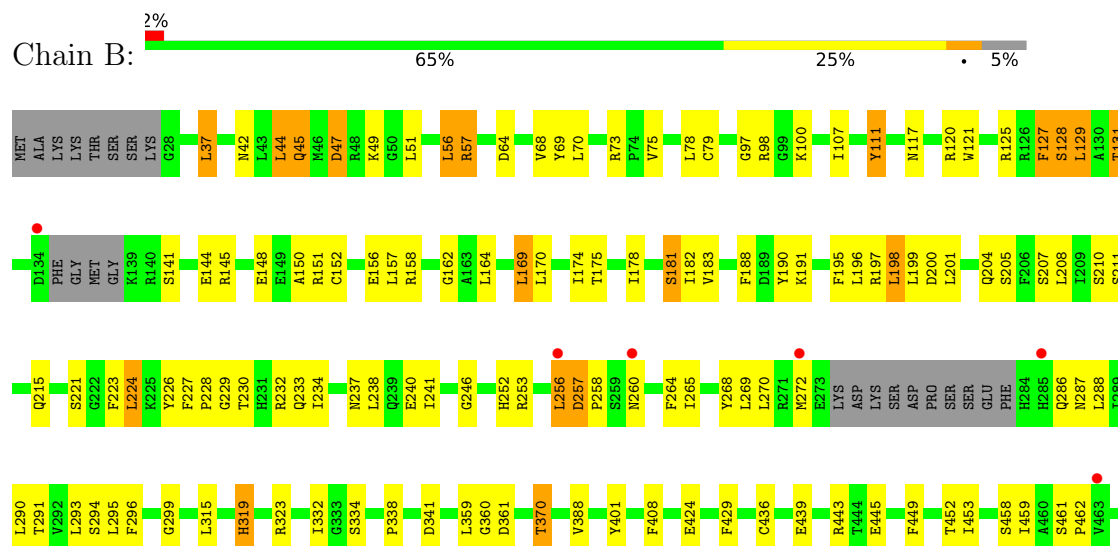
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome P450 2B4

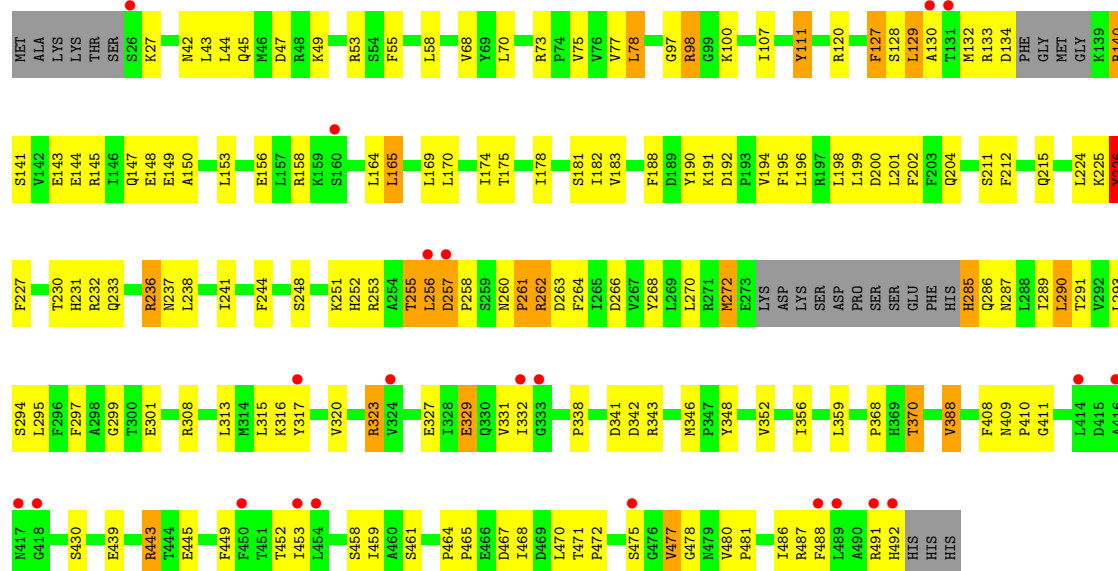


• Molecule 1: Cytochrome P450 2B4

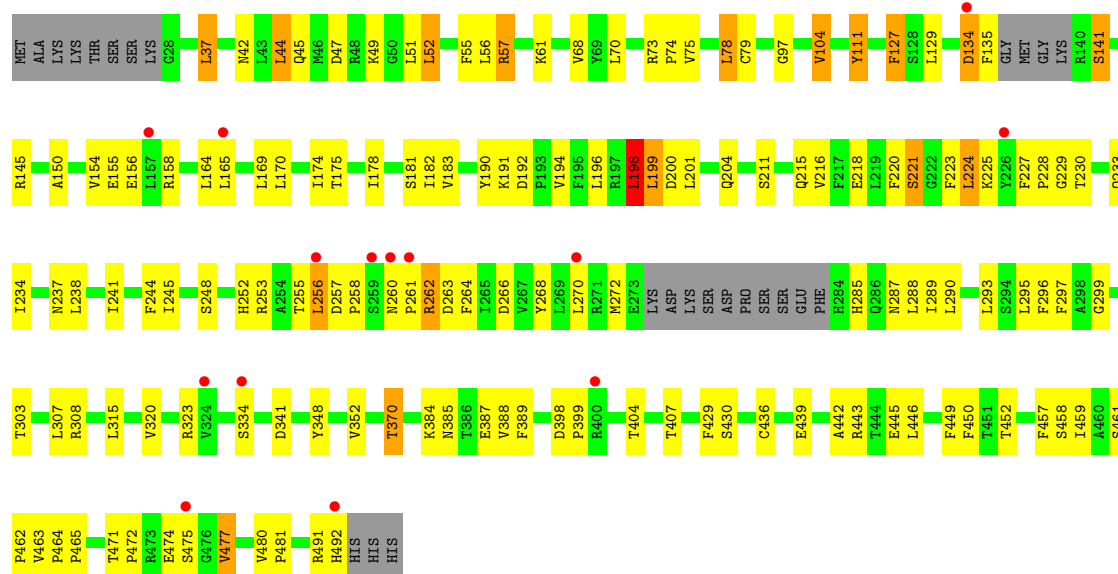




• Molecule 1: Cytochrome P450 2B4



• Molecule 1: Cytochrome P450 2B4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.70Å 152.53Å 181.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.48 – 2.50 45.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (45.48-2.50) 97.0 (45.48-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.218 , 0.247 0.222 , 0.249	Depositor DCC
R_{free} test set	4089 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14746	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, CM5, PB2

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	0.95	2/3661 (0.1%)	0.92	3/4974 (0.1%)
1	B	0.90	1/3598 (0.0%)	0.86	2/4893 (0.0%)
1	C	0.90	2/3592 (0.1%)	0.91	4/4888 (0.1%)
1	D	0.90	2/3613 (0.1%)	0.88	3/4912 (0.1%)
All	All	0.91	7/14464 (0.0%)	0.89	12/19667 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	VAL	CB-CG1	-5.96	1.40	1.52
1	D	79	CYS	CB-SG	-5.94	1.72	1.81
1	A	388	VAL	CB-CG1	-5.76	1.40	1.52
1	B	388	VAL	CB-CG1	-5.56	1.41	1.52
1	C	388	VAL	CB-CG1	-5.25	1.41	1.52
1	C	226	TYR	CB-CG	5.20	1.59	1.51
1	D	104	VAL	CB-CG1	-5.17	1.42	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	TYR	N-CA-C	-5.81	95.32	111.00
1	D	198	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	98	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	D	111	TYR	N-CA-C	-5.68	95.67	111.00
1	C	443	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	198	LEU	CA-CB-CG	5.49	127.92	115.30
1	D	111	TYR	C-N-CA	-5.43	110.89	122.30
1	A	285	HIS	N-CA-C	5.37	125.51	111.00
1	B	111	TYR	N-CA-C	-5.19	96.98	111.00
1	B	111	TYR	C-N-CA	-5.10	111.58	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	PRO	N-CA-C	-5.05	98.98	112.10
1	C	120	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3573	0	3494	146	0
1	B	3511	0	3429	139	0
1	C	3504	0	3407	183	0
1	D	3526	0	3440	139	0
2	A	43	0	30	9	0
2	B	43	0	30	11	0
2	C	43	0	30	5	0
2	D	43	0	30	12	0
3	A	30	0	23	11	0
3	B	66	0	51	22	0
3	C	48	0	37	19	0
3	D	48	0	37	18	0
4	A	22	0	30	1	0
4	B	22	0	30	4	0
4	C	22	0	30	7	0
4	D	22	0	30	1	0
5	A	56	0	0	3	0
5	B	40	0	0	6	0
5	C	30	0	0	0	0
5	D	54	0	0	3	0
All	All	14746	0	14158	600	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 21.

All (600) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:SER:OG	1:C:144:GLU:HG3	1.33	1.26
1:B:56:LEU:HD12	1:B:56:LEU:O	1.35	1.21
1:C:164:LEU:HD23	1:C:487:ARG:CG	1.72	1.19
1:A:141:SER:OG	1:A:144:GLU:HG3	1.42	1.19
1:C:327:GLU:O	1:C:331:VAL:HG23	1.43	1.18
1:C:164:LEU:CD2	1:C:487:ARG:HG3	1.75	1.16
1:B:198:LEU:HD23	1:B:241:ILE:HD12	1.29	1.13
1:C:231:HIS:CE1	1:C:233[B]:GLN:HG2	1.86	1.09
1:C:165:LEU:HD12	1:C:165:LEU:O	1.51	1.08
1:C:256:LEU:O	1:C:256:LEU:HD13	1.52	1.08
1:D:474:GLU:OE1	1:D:474:GLU:HA	1.47	1.06
1:C:164:LEU:CD2	1:C:487:ARG:CG	2.32	1.03
1:C:164:LEU:HD23	1:C:487:ARG:HG2	1.39	1.03
1:C:164:LEU:HD21	1:C:487:ARG:NE	1.75	1.01
2:D:500:HEM:HBC2	2:D:500:HEM:HHD	1.39	1.01
3:C:503:PB2:HDD	1:D:224:LEU:O	1.59	1.01
1:C:231:HIS:CE1	1:C:233[B]:GLN:CG	2.44	1.00
1:B:73:ARG:HB2	3:B:503:PB2:HCB	1.42	1.00
1:A:314:MET:CE	1:A:450:PHE:CZ	2.47	0.98
1:A:44:LEU:HD23	1:B:287:ASN:HD22	1.28	0.97
1:C:165:LEU:HD12	1:C:165:LEU:C	1.82	0.96
1:A:258:PRO:HA	1:A:260:ASN:H	1.29	0.95
1:C:129:LEU:CD1	1:C:129:LEU:N	2.30	0.95
1:A:314:MET:HE1	1:A:450:PHE:CZ	2.04	0.92
3:A:503:PB2:HDF	5:B:525:HOH:O	1.66	0.92
1:A:283:PHE:O	1:A:287:ASN:HB2	1.68	0.92
1:D:266:ASP:O	1:D:270:LEU:HD13	1.70	0.91
1:C:129:LEU:N	1:C:129:LEU:HD13	1.86	0.90
1:B:164:LEU:HD23	1:B:487:ARG:HG3	1.54	0.89
1:A:97:GLY:HA3	1:A:370:THR:HG22	1.52	0.89
1:B:97:GLY:HA3	1:B:370:THR:HG22	1.54	0.89
1:A:145:ARG:HD3	1:A:181:SER:OG	1.74	0.88
1:C:231:HIS:HE1	1:C:233[B]:GLN:CG	1.87	0.87
1:C:129:LEU:HD13	1:C:129:LEU:H	1.37	0.87
1:C:47:ASP:HB3	1:C:49:LYS:H	1.41	0.85
1:D:134:ASP:HB3	1:D:135:PHE:CB	2.06	0.85
1:C:477:VAL:O	1:C:477:VAL:HG13	1.77	0.85
1:B:197:ARG:HG2	1:B:237:ASN:OD1	1.76	0.85
1:C:301:GLU:HG3	5:D:507:HOH:O	1.75	0.84
1:A:314:MET:CE	1:A:450:PHE:HZ	1.90	0.84
1:B:319:HIS:H	1:B:319:HIS:CD2	1.94	0.84
1:B:47:ASP:CG	1:B:57:ARG:NH1	2.31	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LEU:H	1:D:256:LEU:HD12	1.40	0.84
1:C:231:HIS:ND1	1:C:233[B]:GLN:HG2	1.93	0.83
2:A:500:HEM:HBB2	2:A:500:HEM:HMB2	1.59	0.83
1:B:258:PRO:HA	1:B:260:ASN:H	1.43	0.83
1:C:165:LEU:C	1:C:165:LEU:CD1	2.47	0.82
1:B:200:ASP:O	1:B:204:GLN:HB3	1.79	0.82
1:B:230:THR:CG2	3:B:502:PB2:CCE	2.58	0.82
1:D:56:LEU:HD12	1:D:56:LEU:O	1.80	0.82
1:B:117:ASN:HB3	4:B:504:CM5:H32A	1.59	0.81
1:A:44:LEU:HD23	1:B:287:ASN:ND2	1.93	0.81
1:A:200:ASP:O	1:A:204:GLN:HB3	1.81	0.81
1:A:133:ARG:HA	1:A:141:SER:HB2	1.63	0.81
1:D:97:GLY:HA3	1:D:370:THR:HG22	1.61	0.81
1:A:226:TYR:CD2	1:B:226:TYR:HB3	2.16	0.80
1:A:283:PHE:CD2	1:A:285:HIS:CB	2.64	0.80
1:B:56:LEU:HD12	1:B:56:LEU:C	1.97	0.80
1:B:127:PHE:O	1:B:131:THR:CG2	2.30	0.80
1:B:269:LEU:O	1:B:272:MET:CB	2.30	0.80
1:C:251:LYS:O	1:C:255:THR:HG23	1.82	0.80
1:B:258:PRO:HA	1:B:260:ASN:N	1.96	0.79
1:C:257:ASP:OD1	1:C:258:PRO:CD	2.30	0.79
1:C:129:LEU:O	1:C:132:MET:CB	2.30	0.79
1:A:258:PRO:CG	1:A:258:PRO:O	2.30	0.79
1:B:73:ARG:HG3	3:B:503:PB2:CCA	2.12	0.79
1:D:477:VAL:CG1	1:D:477:VAL:O	2.30	0.79
1:B:230:THR:CG2	3:B:502:PB2:HCE	2.12	0.78
1:A:387:GLU:OE1	3:A:503:PB2:CCE	2.31	0.78
1:B:491:ARG:O	1:B:492:HIS:CB	2.29	0.78
1:C:141:SER:O	1:C:145:ARG:HG3	1.84	0.78
1:A:258:PRO:O	1:A:258:PRO:HG2	1.82	0.77
1:A:258:PRO:CA	1:A:260:ASN:H	1.96	0.77
1:C:97:GLY:HA3	1:C:370:THR:HG22	1.67	0.77
1:C:327:GLU:O	1:C:331:VAL:CG2	2.30	0.77
1:A:227:PHE:CE1	1:B:70:LEU:HB3	2.21	0.76
1:C:200:ASP:O	1:C:204:GLN:HB3	1.85	0.76
3:C:503:PB2:CDD	1:D:224:LEU:O	2.33	0.76
1:D:42:ASN:HD22	1:D:45:GLN:NE2	1.84	0.76
1:A:283:PHE:N	1:A:283:PHE:CD1	2.52	0.76
1:C:133:ARG:O	1:C:134:ASP:CB	2.34	0.76
1:A:474:GLU:O	1:A:475:SER:HB3	1.84	0.76
1:C:231:HIS:CE1	1:C:233[B]:GLN:HG3	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:N	1:A:288:LEU:CD2	2.47	0.75
2:A:500:HEM:HBB2	2:A:500:HEM:CMB	2.16	0.75
1:B:164:LEU:HD23	1:B:487:ARG:CG	2.17	0.75
1:B:288:LEU:HD13	4:B:504:CM5:H92	1.67	0.75
1:A:258:PRO:HA	1:A:260:ASN:N	2.01	0.74
1:C:475:SER:HA	1:C:478:GLY:O	1.87	0.74
1:D:200:ASP:O	1:D:204:GLN:HB3	1.88	0.74
1:C:449:PHE:O	1:C:453:ILE:HG13	1.87	0.73
1:A:474:GLU:O	1:A:475:SER:CB	2.36	0.73
1:B:73:ARG:CB	3:B:503:PB2:HCB	2.16	0.73
3:C:502:PB2:CDE	3:C:503:PB2:HDC	2.19	0.73
1:B:47:ASP:HB3	1:B:49:LYS:H	1.54	0.73
1:A:288:LEU:N	1:A:288:LEU:HD23	2.04	0.72
1:C:257:ASP:OD1	1:C:258:PRO:HD3	1.88	0.72
1:A:47:ASP:HB3	1:A:49:LYS:H	1.54	0.72
1:C:262:ARG:HG3	1:C:266:ASP:OD1	1.90	0.72
1:C:164:LEU:HD21	1:C:487:ARG:HE	1.53	0.72
1:A:44:LEU:CD2	1:B:287:ASN:HD22	2.01	0.72
1:A:53:ARG:HH11	1:A:53:ARG:HB3	1.55	0.72
1:B:170:LEU:O	1:B:174:ILE:HG23	1.89	0.72
1:B:246:GLY:HA2	1:B:286:GLN:OE1	1.91	0.71
1:B:230:THR:HG23	3:B:502:PB2:HCF	1.71	0.71
1:A:164:LEU:HD23	1:A:487:ARG:HG3	1.73	0.70
1:C:227:PHE:CE1	1:D:70:LEU:HB3	2.26	0.70
1:D:477:VAL:O	1:D:477:VAL:HG13	1.90	0.70
1:C:251:LYS:O	1:C:255:THR:CG2	2.39	0.70
1:A:283:PHE:HD2	1:A:285:HIS:CB	2.04	0.69
1:B:258:PRO:CA	1:B:260:ASN:H	2.05	0.69
1:C:226:TYR:CD2	1:C:226:TYR:C	2.66	0.69
1:C:70:LEU:HB3	1:D:227:PHE:CE1	2.27	0.69
1:C:332:ILE:HG22	1:C:332:ILE:O	1.92	0.69
1:C:253:ARG:O	1:C:256:LEU:CD1	2.41	0.69
1:B:47:ASP:CG	1:B:57:ARG:HH12	1.96	0.69
1:C:257:ASP:OD1	1:C:258:PRO:HD2	1.90	0.69
1:C:164:LEU:CD2	1:C:487:ARG:NE	2.54	0.69
1:A:387:GLU:OE1	3:A:503:PB2:HCE	1.92	0.69
1:D:253:ARG:O	1:D:256:LEU:HD12	1.93	0.69
1:A:225:LYS:HG2	1:B:477:VAL:HG11	1.75	0.68
1:D:150:ALA:O	1:D:154:VAL:HG23	1.93	0.68
1:B:152:CYS:HB3	5:B:498:HOH:O	1.94	0.68
1:A:70:LEU:HD12	3:A:503:PB2:HDC	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ARG:O	1:C:256:LEU:HD12	1.93	0.68
1:D:134:ASP:CB	1:D:135:PHE:CB	2.71	0.68
1:A:258:PRO:O	1:A:258:PRO:CD	2.41	0.68
1:A:446:LEU:O	1:A:450:PHE:HB2	1.94	0.68
1:C:332:ILE:O	1:C:332:ILE:CG2	2.40	0.68
1:A:476:GLY:O	1:A:477:VAL:HG12	1.93	0.68
1:B:230:THR:CG2	3:B:502:PB2:CCF	2.72	0.67
1:A:73:ARG:HG3	3:A:503:PB2:CCF	2.24	0.67
2:C:500:HEM:HBB2	2:C:500:HEM:HMB2	1.75	0.67
1:D:256:LEU:HD12	1:D:256:LEU:N	2.10	0.67
1:C:475:SER:CA	1:C:478:GLY:O	2.42	0.67
1:B:237:ASN:O	1:B:241:ILE:HG12	1.95	0.67
1:D:73:ARG:HG3	3:D:503:PB2:HCB	1.77	0.67
3:C:502:PB2:CCC	1:D:230:THR:CG2	2.73	0.66
1:D:73:ARG:CB	3:D:503:PB2:HCB	2.25	0.66
1:B:127:PHE:O	1:B:131:THR:HG23	1.93	0.66
1:C:164:LEU:HD21	1:C:487:ARG:CG	2.23	0.66
1:C:141:SER:HG	1:C:144:GLU:HG3	1.56	0.66
1:C:477:VAL:O	1:C:477:VAL:CG1	2.42	0.66
1:D:446:LEU:O	1:D:450:PHE:HB2	1.95	0.66
1:B:230:THR:HG23	3:B:502:PB2:CCF	2.26	0.66
3:A:503:PB2:CDF	5:B:525:HOH:O	2.32	0.66
1:C:128:SER:OG	1:C:129:LEU:HD13	1.96	0.66
1:B:127:PHE:O	1:B:131:THR:HG22	1.95	0.66
1:C:315:LEU:HD23	1:C:459:ILE:HD12	1.78	0.66
1:B:230:THR:HG22	3:B:502:PB2:CCE	2.25	0.66
1:D:73:ARG:HG3	3:D:503:PB2:CCB	2.24	0.66
1:C:140:ARG:NH2	1:C:148:GLU:OE2	2.29	0.65
1:A:476:GLY:O	1:A:477:VAL:CB	2.44	0.65
3:C:503:PB2:HDE	1:D:224:LEU:N	2.12	0.65
2:B:500:HEM:HBB2	2:B:500:HEM:HMB2	1.77	0.65
1:C:258:PRO:HA	1:C:260:ASN:H	1.61	0.65
1:D:47:ASP:OD2	1:D:57:ARG:NH2	2.30	0.65
1:A:140:ARG:NH2	1:A:148:GLU:OE2	2.30	0.65
3:C:502:PB2:CCC	1:D:230:THR:HG23	2.26	0.65
1:B:150:ALA:HB1	1:B:452:THR:HG21	1.79	0.65
1:B:439:GLU:O	1:B:443:ARG:HG3	1.96	0.65
1:A:204:GLN:HE21	1:A:236:ARG:HH12	1.45	0.65
1:C:129:LEU:N	1:C:129:LEU:HD12	2.12	0.65
1:C:320:VAL:HG13	1:C:348:TYR:OH	1.97	0.65
3:C:502:PB2:HCC	1:D:230:THR:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LEU:H	1:D:256:LEU:CD1	2.10	0.64
1:C:129:LEU:O	1:C:132:MET:N	2.31	0.64
1:C:256:LEU:O	1:C:256:LEU:CD1	2.39	0.64
1:D:145:ARG:HD3	1:D:181:SER:OG	1.98	0.64
1:D:255:THR:OG1	1:D:262:ARG:NH2	2.31	0.64
1:B:208:LEU:HD22	1:B:226:TYR:HD1	1.63	0.64
1:C:70:LEU:HD22	3:C:502:PB2:CAC	2.28	0.64
1:C:143:GLU:O	1:C:147:GLN:HG3	1.98	0.64
3:C:503:PB2:HDE	1:D:224:LEU:H	1.61	0.64
1:C:204:GLN:HE21	1:C:236:ARG:HH12	1.46	0.63
1:A:42:ASN:HD22	1:A:45:GLN:NE2	1.96	0.63
1:A:475:SER:HB3	1:B:232:ARG:NH1	2.14	0.63
1:B:121:TRP:HZ2	2:B:500:HEM:O1D	1.81	0.63
1:C:129:LEU:O	1:C:132:MET:CA	2.45	0.63
1:C:178:ILE:O	1:C:182:ILE:HG13	1.99	0.63
1:D:154:VAL:HG13	1:D:457:PHE:HE2	1.62	0.63
1:C:491:ARG:O	1:C:492:HIS:CB	2.45	0.63
1:A:125:ARG:O	1:A:129:LEU:HD13	1.99	0.63
1:B:56:LEU:O	1:B:56:LEU:CD1	2.30	0.63
1:B:145:ARG:HD3	1:B:181:SER:OG	1.99	0.63
1:C:129:LEU:O	1:C:133:ARG:N	2.31	0.63
1:D:258:PRO:HA	1:D:260:ASN:H	1.64	0.63
1:D:387:GLU:OE1	3:D:503:PB2:CCC	2.47	0.63
1:C:255:THR:OG1	1:C:262:ARG:NH1	2.32	0.63
1:A:164:LEU:HD23	1:A:487:ARG:CG	2.28	0.62
1:C:127:PHE:C	1:C:127:PHE:CD1	2.72	0.62
1:D:268:TYR:CD1	1:D:289:ILE:HD11	2.34	0.62
1:C:198:LEU:CD2	1:C:202:PHE:HD1	2.10	0.62
1:C:128:SER:OG	1:C:129:LEU:CD1	2.47	0.62
1:B:125:ARG:O	1:B:129:LEU:HD22	2.00	0.62
1:A:141:SER:OG	1:A:144:GLU:CG	2.35	0.62
1:A:266:ASP:O	1:A:270:LEU:HD22	1.99	0.62
1:B:198:LEU:HD23	1:B:241:ILE:CD1	2.20	0.62
1:C:226:TYR:C	1:C:226:TYR:HD2	2.02	0.62
1:C:308:ARG:NH2	1:C:481:PRO:O	2.32	0.62
1:A:255:THR:OG1	1:A:262:ARG:NH2	2.30	0.62
2:D:500:HEM:ND	3:D:501:PB2:HAE	2.14	0.61
3:C:502:PB2:CCB	1:D:230:THR:HG23	2.30	0.61
1:C:439:GLU:O	1:C:443:ARG:HG3	1.99	0.61
3:C:502:PB2:HDE	3:C:503:PB2:HDD	1.82	0.61
1:C:164:LEU:HD21	1:C:487:ARG:HG3	1.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:O	1:D:174:ILE:HG23	2.00	0.61
1:B:257:ASP:OD1	1:B:258:PRO:HD2	2.01	0.61
1:B:164:LEU:HD21	1:B:462:PRO:HD3	1.82	0.60
1:A:133:ARG:HA	1:A:141:SER:CB	2.30	0.60
1:A:486:ILE:HD13	1:A:488:PHE:CZ	2.36	0.60
1:C:164:LEU:HD23	1:C:487:ARG:HG3	1.45	0.60
1:D:253:ARG:O	1:D:256:LEU:CD1	2.49	0.60
3:D:502:PB2:CDE	3:D:503:PB2:HDD	2.32	0.60
1:C:170:LEU:O	1:C:174:ILE:HG23	2.01	0.60
1:B:256:LEU:HD13	1:B:256:LEU:O	2.02	0.59
1:C:342:ASP:O	1:C:346:MET:HG3	2.01	0.59
1:C:164:LEU:HD21	1:C:487:ARG:CD	2.33	0.59
2:B:500:HEM:ND	3:B:501:PB2:HAE	2.16	0.59
1:D:481:PRO:HA	5:D:543:HOH:O	2.02	0.59
2:D:500:HEM:HBD1	2:D:500:HEM:HHA	1.84	0.59
1:C:42:ASN:HD22	1:C:45:GLN:NE2	2.00	0.59
1:D:127:PHE:CD1	1:D:127:PHE:C	2.74	0.59
1:A:314:MET:SD	1:A:450:PHE:CZ	2.94	0.59
1:A:314:MET:HE2	1:A:450:PHE:HZ	1.66	0.59
1:B:162:GLY:HA2	1:B:488:PHE:O	2.03	0.59
2:B:500:HEM:HBB2	2:B:500:HEM:CMB	2.33	0.59
2:B:500:HEM:HBC2	2:B:500:HEM:HHH	1.83	0.59
3:C:502:PB2:HCC	1:D:230:THR:HG23	1.85	0.59
1:D:270:LEU:N	1:D:270:LEU:HD12	2.17	0.59
1:B:449:PHE:O	1:B:453:ILE:HG13	2.02	0.59
1:B:42:ASN:HD22	1:B:45:GLN:NE2	2.00	0.58
1:D:268:TYR:CE1	1:D:289:ILE:HD11	2.38	0.58
1:A:314:MET:SD	1:A:450:PHE:CE1	2.96	0.58
1:B:141:SER:OG	1:B:144:GLU:HG3	2.02	0.58
1:A:283:PHE:N	1:A:283:PHE:HD1	2.01	0.58
1:A:175:THR:HG22	1:A:445:GLU:OE1	2.04	0.58
1:C:237:ASN:O	1:C:241:ILE:HG12	2.03	0.58
1:A:284:HIS:O	1:A:288:LEU:HD23	2.04	0.58
1:B:201:LEU:HD22	1:B:241:ILE:HG13	1.86	0.58
1:D:320:VAL:HG13	1:D:348:TYR:OH	2.03	0.58
1:A:439:GLU:O	1:A:443:ARG:HG3	2.03	0.57
1:C:145:ARG:HD3	1:C:181:SER:OG	2.04	0.57
1:C:230:THR:CG2	3:D:502:PB2:CCE	2.81	0.57
1:D:296:PHE:CD1	2:D:500:HEM:HBC1	2.39	0.57
1:C:198:LEU:CD2	1:C:202:PHE:CD1	2.87	0.57
1:A:191:LYS:HA	1:A:196:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:504:CM5:H11	4:C:504:CM5:H191	1.85	0.57
1:C:368:PRO:HB2	1:D:223:PHE:CD2	2.40	0.57
1:A:441:ILE:HG13	5:A:522:HOH:O	2.05	0.57
1:A:476:GLY:O	1:A:477:VAL:CG1	2.53	0.57
1:B:198:LEU:CD2	1:B:241:ILE:HD12	2.21	0.57
1:C:464:PRO:HD2	1:C:467:ASP:HB2	1.87	0.57
1:B:47:ASP:OD1	1:B:57:ARG:NH1	2.38	0.57
1:D:73:ARG:HB3	3:D:503:PB2:HCB	1.87	0.57
1:A:476:GLY:O	1:A:477:VAL:HB	2.03	0.56
1:B:56:LEU:C	1:B:56:LEU:CD1	2.69	0.56
1:B:315:LEU:HD23	1:B:459:ILE:HD12	1.86	0.56
1:A:315:LEU:HD23	1:A:459:ILE:HD12	1.87	0.56
1:D:308:ARG:NH2	1:D:481:PRO:O	2.38	0.56
1:A:475:SER:CB	1:B:232:ARG:NH1	2.69	0.56
2:C:500:HEM:HBB2	2:C:500:HEM:CMB	2.36	0.56
1:C:293:LEU:HG	1:C:297:PHE:HE2	1.70	0.56
1:D:141:SER:O	1:D:145:ARG:HG3	2.05	0.56
1:B:121:TRP:CZ2	2:B:500:HEM:O1D	2.59	0.56
1:C:198:LEU:HD21	1:C:202:PHE:CD1	2.41	0.56
1:A:53:ARG:HB3	1:A:53:ARG:NH1	2.19	0.56
1:A:299:GLY:HA3	2:A:500:HEM:C1C	2.41	0.56
1:A:70:LEU:HD12	3:A:503:PB2:CDC	2.36	0.55
1:A:215:GLN:HB3	1:B:228:PRO:HB3	1.88	0.55
1:C:331:VAL:HG21	1:C:346:MET:HG2	1.87	0.55
1:C:198:LEU:HD23	1:C:202:PHE:HD1	1.71	0.55
1:A:98:ARG:NH2	4:A:504:CM5:O20	2.40	0.55
1:D:73:ARG:CG	3:D:503:PB2:HCB	2.36	0.55
1:C:253:ARG:C	1:C:256:LEU:HD12	2.27	0.55
1:A:148:GLU:HG3	1:A:151:ARG:NH2	2.22	0.55
1:A:287:ASN:HB2	1:B:37:LEU:HD21	1.88	0.55
1:C:198:LEU:HD23	1:C:198:LEU:C	2.27	0.55
1:D:293:LEU:HG	1:D:297:PHE:HE2	1.71	0.55
1:B:73:ARG:CG	3:B:503:PB2:CCA	2.84	0.55
1:C:55:PHE:HE2	1:C:77:VAL:HG21	1.72	0.55
1:C:231:HIS:ND1	1:C:233[A]:GLN:HB2	2.21	0.55
1:D:262:ARG:NH1	1:D:266:ASP:OD1	2.39	0.54
1:A:477:VAL:HG13	1:A:477:VAL:O	2.07	0.54
3:C:502:PB2:HDE	3:C:503:PB2:CDD	2.36	0.54
1:A:148:GLU:HG3	1:A:151:ARG:HH22	1.73	0.54
2:B:500:HEM:C1D	3:B:501:PB2:HAE	2.42	0.54
1:B:230:THR:HG22	3:B:502:PB2:CCF	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:HD23	1:C:198:LEU:O	2.07	0.54
1:A:283:PHE:O	1:B:37:LEU:HD21	2.06	0.54
1:A:314:MET:HE2	1:A:450:PHE:CZ	2.40	0.54
1:B:211:SER:O	1:B:215:GLN:HG3	2.08	0.54
1:B:141:SER:O	1:B:145:ARG:HG3	2.08	0.54
1:B:191:LYS:HA	1:B:196:LEU:HD21	1.90	0.54
1:D:439:GLU:O	1:D:443:ARG:HG3	2.08	0.54
1:B:299:GLY:HA3	2:B:500:HEM:C1C	2.43	0.53
1:B:183:VAL:HA	1:B:264:PHE:HB3	1.89	0.53
3:B:496:PB2:CDC	3:B:503:PB2:HDD	2.39	0.53
1:B:97:GLY:CA	1:B:370:THR:HG22	2.34	0.53
1:B:111:TYR:OH	1:C:107:ILE:HD13	2.09	0.53
1:C:294:SER:HB3	1:D:216:VAL:HG11	1.90	0.53
1:C:149:GLU:OE1	1:C:190:TYR:OH	2.23	0.53
1:C:480:VAL:HG12	1:C:480:VAL:O	2.08	0.53
1:A:194:VAL:HG11	1:A:244:PHE:CD2	2.44	0.53
1:D:183:VAL:HA	1:D:264:PHE:HB3	1.90	0.53
1:A:170:LEU:O	1:A:174:ILE:HG23	2.08	0.53
1:A:51:LEU:O	1:A:55:PHE:HD1	1.91	0.53
1:A:134:ASP:H	1:A:141:SER:CB	2.22	0.52
1:B:51:LEU:HD13	3:B:496:PB2:CCB	2.39	0.52
1:B:230:THR:HG23	3:B:502:PB2:CCE	2.39	0.52
1:A:178:ILE:O	1:A:182:ILE:HG13	2.09	0.52
1:B:253:ARG:O	1:B:256:LEU:HD12	2.08	0.52
1:C:262:ARG:CG	1:C:266:ASP:OD1	2.56	0.52
1:C:43:LEU:CD1	1:D:229:GLY:HA3	2.40	0.52
1:D:134:ASP:CA	1:D:135:PHE:CB	2.87	0.52
2:D:500:HEM:HBC2	2:D:500:HEM:CHD	2.17	0.52
1:D:178:ILE:O	1:D:182:ILE:HG13	2.09	0.52
2:A:500:HEM:HMB2	2:A:500:HEM:CBB	2.35	0.52
1:C:191:LYS:HA	1:C:196:LEU:HD21	1.92	0.52
1:D:256:LEU:N	1:D:256:LEU:CD1	2.70	0.52
1:C:268:TYR:O	1:C:272:MET:HB2	2.10	0.52
1:B:319:HIS:H	1:B:319:HIS:HD2	1.53	0.51
1:C:98:ARG:HD2	4:C:504:CM5:H18	1.91	0.51
1:D:293:LEU:HG	1:D:297:PHE:CE2	2.45	0.51
1:C:268:TYR:CD1	1:C:289:ILE:HD11	2.45	0.51
1:D:164:LEU:HD21	1:D:462:PRO:HD3	1.91	0.51
1:D:201:LEU:HD22	1:D:241:ILE:HG13	1.93	0.51
1:D:474:GLU:OE1	1:D:474:GLU:CA	2.30	0.51
1:D:237:ASN:O	1:D:241:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:HIS:CE1	1:C:233[A]:GLN:HB2	2.45	0.51
1:A:73:ARG:HG3	3:A:503:PB2:CCA	2.41	0.51
1:C:150:ALA:HB1	1:C:452:THR:HG21	1.92	0.51
1:B:265:ILE:O	1:B:268:TYR:HB3	2.10	0.51
3:C:502:PB2:HCB	1:D:230:THR:HG23	1.93	0.51
1:B:47:ASP:HB3	1:B:49:LYS:N	2.22	0.51
1:C:430:SER:CB	2:C:500:HEM:HBA1	2.41	0.51
1:D:73:ARG:HG3	3:D:503:PB2:CCA	2.41	0.51
1:A:198:LEU:C	1:A:198:LEU:HD12	2.32	0.50
1:B:47:ASP:CB	1:B:57:ARG:HH12	2.24	0.50
1:C:317:TYR:HB3	1:C:320:VAL:HG23	1.93	0.50
1:A:293:LEU:HG	1:A:297:PHE:HE2	1.76	0.50
1:B:230:THR:HG21	3:B:502:PB2:HCE	1.93	0.50
1:B:70:LEU:HD22	3:B:496:PB2:CAE	2.41	0.50
1:C:475:SER:O	1:C:478:GLY:O	2.30	0.50
1:A:274:LYS:O	1:A:275:ASP:O	2.30	0.50
1:D:165:LEU:HD12	1:D:165:LEU:O	2.11	0.50
1:D:491:ARG:O	1:D:492:HIS:O	2.30	0.50
1:C:293:LEU:HG	1:C:297:PHE:CE2	2.46	0.50
3:C:502:PB2:CDE	3:C:503:PB2:CDC	2.90	0.50
1:D:477:VAL:O	1:D:477:VAL:HG12	2.10	0.50
1:A:194:VAL:HG11	1:A:244:PHE:CE2	2.47	0.50
1:C:174:ILE:HD12	1:C:449:PHE:CD1	2.47	0.50
1:A:262:ARG:HG3	1:A:266:ASP:OD1	2.11	0.50
1:D:288:LEU:HD13	4:D:504:CM5:H92	1.92	0.50
1:D:303:THR:HA	2:D:500:HEM:CBB	2.42	0.50
1:A:299:GLY:HA3	2:A:500:HEM:C2C	2.46	0.50
1:B:319:HIS:CD2	1:B:319:HIS:N	2.69	0.50
3:B:496:PB2:HDC	3:B:503:PB2:HDD	1.94	0.50
1:C:255:THR:OG1	1:C:256:LEU:N	2.45	0.50
1:D:348:TYR:O	1:D:352:VAL:HG23	2.12	0.50
1:A:134:ASP:H	1:A:141:SER:HB3	1.77	0.50
1:C:78:LEU:HD22	1:C:388:VAL:CG1	2.42	0.50
1:C:256:LEU:O	1:C:257:ASP:OD2	2.30	0.50
1:D:198:LEU:HD12	1:D:198:LEU:C	2.32	0.50
1:C:477:VAL:HG11	1:D:225:LYS:HG2	1.93	0.49
1:C:226:TYR:HD2	1:C:226:TYR:O	1.94	0.49
1:A:133:ARG:O	1:A:134:ASP:O	2.30	0.49
2:A:500:HEM:HBD1	2:A:500:HEM:HHA	1.95	0.49
1:D:78:LEU:HD22	1:D:388:VAL:CG1	2.42	0.49
1:B:488:PHE:N	1:B:488:PHE:CD2	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:LEU:N	1:D:270:LEU:CD1	2.75	0.49
1:C:194:VAL:HG11	1:C:244:PHE:CD2	2.48	0.49
2:D:500:HEM:HHD	2:D:500:HEM:CBC	2.25	0.49
1:C:194:VAL:HG11	1:C:244:PHE:CE2	2.48	0.49
1:D:47:ASP:HB3	1:D:49:LYS:H	1.77	0.49
1:A:107:ILE:HD13	1:D:111:TYR:OH	2.13	0.49
1:C:252:HIS:NE2	1:C:263:ASP:OD2	2.34	0.49
1:A:237:ASN:O	1:A:241:ILE:HG12	2.13	0.49
1:C:258:PRO:HA	1:C:260:ASN:N	2.27	0.49
1:C:248:SER:O	1:C:252:HIS:ND1	2.45	0.49
1:C:268:TYR:CE1	1:C:289:ILE:HD11	2.47	0.49
1:A:145:ARG:NH1	1:A:181:SER:OG	2.36	0.48
1:A:314:MET:HE1	1:A:450:PHE:CE1	2.44	0.48
1:B:175:THR:HG22	1:B:445:GLU:OE1	2.13	0.48
1:B:291:THR:O	1:B:294:SER:HB2	2.14	0.48
1:A:288:LEU:HD23	1:A:288:LEU:H	1.78	0.48
1:B:70:LEU:HD22	3:B:496:PB2:CAF	2.43	0.48
1:D:204:GLN:HG3	1:D:233:GLN:HE22	1.78	0.48
1:A:70:LEU:HB3	1:B:227:PHE:CZ	2.49	0.48
1:A:209:ILE:HD12	1:B:474:GLU:OE1	2.12	0.48
1:A:473:ARG:NH2	1:A:481:PRO:O	2.46	0.48
4:C:504:CM5:H11	4:C:504:CM5:C19	2.44	0.48
1:D:200:ASP:O	1:D:204:GLN:CB	2.61	0.48
1:C:127:PHE:CD1	1:C:127:PHE:O	2.66	0.48
1:C:348:TYR:O	1:C:352:VAL:HG23	2.14	0.48
1:D:47:ASP:C	1:D:49:LYS:N	2.66	0.48
1:D:252:HIS:NE2	1:D:263:ASP:OD2	2.34	0.48
1:D:47:ASP:C	1:D:49:LYS:H	2.17	0.48
1:A:251:LYS:HB2	1:A:251:LYS:HE3	1.52	0.48
1:B:229:GLY:HA2	1:B:234:ILE:HD13	1.96	0.47
1:C:290:LEU:HD12	1:D:44:LEU:HD21	1.95	0.47
1:C:316:LYS:HB2	1:C:468:ILE:HB	1.95	0.47
1:D:303:THR:HA	2:D:500:HEM:HBB1	1.96	0.47
1:D:471:THR:HA	1:D:472:PRO:HD3	1.78	0.47
2:D:500:HEM:C1D	3:D:501:PB2:HAE	2.48	0.47
1:A:257:ASP:O	1:A:258:PRO:C	2.48	0.47
1:C:256:LEU:C	1:C:256:LEU:HD22	2.34	0.47
1:D:429:PHE:CD2	1:D:439:GLU:HG3	2.49	0.47
1:A:293:LEU:HG	1:A:297:PHE:CE2	2.49	0.47
1:A:211:SER:O	1:A:215:GLN:HG3	2.14	0.47
1:D:248:SER:O	1:D:252:HIS:ND1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:LEU:HD23	1:D:450:PHE:CE2	2.50	0.47
1:B:183:VAL:HG11	1:B:293:LEU:HD21	1.97	0.47
1:C:164:LEU:CD2	1:C:487:ARG:CD	2.91	0.47
1:C:230:THR:HG23	3:D:502:PB2:CCF	2.45	0.47
1:C:260:ASN:N	1:C:261:PRO:CD	2.77	0.47
1:C:299:GLY:HA3	2:C:500:HEM:C1C	2.50	0.47
4:C:504:CM5:H20	4:C:504:CM5:C13	2.28	0.47
1:A:226:TYR:HB3	1:B:226:TYR:CD2	2.49	0.47
1:A:227:PHE:CZ	1:B:70:LEU:HB3	2.48	0.47
1:B:252:HIS:O	1:B:256:LEU:HB3	2.15	0.47
1:A:187:ARG:NH1	5:A:508:HOH:O	2.47	0.47
1:A:368:PRO:HB2	1:B:223:PHE:CD2	2.49	0.47
1:D:404:THR:HB	1:D:407:THR:HB	1.97	0.47
1:A:57:ARG:NH1	1:A:60:GLU:OE1	2.48	0.46
1:C:329:GLU:CA	1:C:329:GLU:OE2	2.61	0.46
1:D:429:PHE:HB3	1:D:436:CYS:HB3	1.96	0.46
1:A:314:MET:SD	1:A:450:PHE:HZ	2.35	0.46
1:C:329:GLU:OE2	1:C:329:GLU:HA	2.16	0.46
1:B:73:ARG:CB	3:B:503:PB2:CCB	2.91	0.46
1:B:178:ILE:O	1:B:182:ILE:HG13	2.15	0.46
3:C:502:PB2:HDE	3:C:503:PB2:CDC	2.45	0.46
1:C:183:VAL:HA	1:C:264:PHE:HB3	1.97	0.46
1:C:475:SER:C	1:C:478:GLY:O	2.54	0.46
1:A:342:ASP:O	1:A:346:MET:HG3	2.15	0.46
1:D:51:LEU:O	1:D:55:PHE:HD1	1.99	0.46
1:D:57:ARG:HE	1:D:57:ARG:HB3	1.47	0.46
1:D:211:SER:O	1:D:215:GLN:HG3	2.15	0.46
1:B:227:PHE:CD1	1:B:228:PRO:HD2	2.51	0.46
1:C:252:HIS:O	1:C:256:LEU:HB3	2.16	0.46
1:D:174:ILE:HD12	1:D:449:PHE:CD1	2.51	0.46
1:A:70:LEU:CD1	3:A:503:PB2:HDC	2.43	0.46
1:B:477:VAL:O	1:B:477:VAL:HG13	2.15	0.46
1:D:229:GLY:HA2	1:D:234:ILE:CD1	2.45	0.46
1:D:285:HIS:C	1:D:287:ASN:N	2.68	0.46
1:A:70:LEU:HB3	1:B:227:PHE:CE1	2.52	0.45
1:B:188:PHE:CG	1:B:195:PHE:HB2	2.51	0.45
1:B:107:ILE:HD13	1:C:111:TYR:OH	2.16	0.45
1:D:442:ALA:HB2	2:D:500:HEM:HMC2	1.98	0.45
1:B:148:GLU:HG3	1:B:151:ARG:HH22	1.81	0.45
1:D:253:ARG:HH11	1:D:253:ARG:HG3	1.80	0.45
1:C:408:PHE:CE1	1:C:410:PRO:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:HEM:HMB2	2:B:500:HEM:CBB	2.46	0.45
1:C:192:ASP:O	1:C:196:LEU:HD23	2.16	0.45
1:D:194:VAL:HG11	1:D:244:PHE:CD2	2.51	0.45
1:B:156:GLU:HG3	1:B:190:TYR:CD2	2.51	0.45
1:C:253:ARG:O	1:C:256:LEU:HD11	2.15	0.45
1:C:285:HIS:C	1:C:287:ASN:N	2.70	0.45
1:D:429:PHE:O	1:D:430:SER:HB3	2.16	0.45
1:A:183:VAL:HA	1:A:264:PHE:HB3	1.97	0.45
1:B:257:ASP:OD1	1:B:258:PRO:CD	2.63	0.45
1:B:183:VAL:HG21	1:B:293:LEU:CD2	2.47	0.45
1:C:156:GLU:HG3	1:C:190:TYR:CD2	2.52	0.45
4:C:504:CM5:O12	4:C:504:CM5:O20	2.30	0.45
1:D:389:PHE:CZ	3:D:503:PB2:HDE	2.51	0.45
1:A:73:ARG:HD3	1:B:100:LYS:O	2.17	0.45
1:A:156:GLU:HG3	1:A:190:TYR:CD2	2.52	0.45
1:B:258:PRO:C	1:B:260:ASN:H	2.19	0.44
1:A:255:THR:CB	1:A:262:ARG:NH2	2.79	0.44
1:A:429:PHE:O	1:A:430:SER:HB3	2.17	0.44
1:B:476:GLY:CA	5:B:527:HOH:O	2.64	0.44
1:B:229:GLY:HA2	1:B:234:ILE:CD1	2.48	0.44
1:C:215:GLN:HB3	1:D:228:PRO:HB3	2.00	0.44
1:D:156:GLU:HG3	1:D:190:TYR:CE2	2.53	0.44
1:A:475:SER:O	1:A:475:SER:OG	2.30	0.44
1:C:73:ARG:HG3	3:C:503:PB2:CCA	2.47	0.44
1:D:191:LYS:HA	1:D:196:LEU:HD21	1.99	0.44
1:A:296:PHE:CD1	2:A:500:HEM:CBC	3.01	0.44
1:A:296:PHE:CD1	2:A:500:HEM:HBC1	2.53	0.44
1:B:401:TYR:CE2	1:B:424:GLU:HB2	2.53	0.44
1:C:257:ASP:CB	1:C:258:PRO:CD	2.95	0.44
1:D:296:PHE:CD1	2:D:500:HEM:CBC	3.01	0.44
1:B:270:LEU:C	1:B:272:MET:N	2.70	0.44
1:C:98:ARG:NH1	1:D:220:PHE:CE2	2.86	0.44
1:C:227:PHE:CZ	1:D:70:LEU:HB3	2.53	0.44
1:A:288:LEU:N	1:A:288:LEU:HD22	2.25	0.43
1:A:272:MET:O	1:A:275:ASP:CB	2.66	0.43
1:C:188:PHE:CG	1:C:195:PHE:HB2	2.53	0.43
1:C:244:PHE:CD1	1:C:244:PHE:C	2.92	0.43
1:D:218:GLU:O	1:D:221:SER:HB2	2.17	0.43
1:C:464:PRO:O	1:C:465:PRO:C	2.57	0.43
1:C:98:ARG:HD2	4:C:504:CM5:C18	2.49	0.43
1:C:287:ASN:HB2	1:D:37:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ASN:N	1:D:261:PRO:HD3	2.32	0.43
1:D:389:PHE:HZ	3:D:503:PB2:HDE	1.81	0.43
1:B:429:PHE:HB3	1:B:436:CYS:HB3	2.00	0.43
1:C:294:SER:CB	1:D:216:VAL:HG11	2.47	0.43
1:C:486:ILE:HG12	1:C:487:ARG:N	2.34	0.43
1:B:332:ILE:HD13	1:B:338:PRO:HB3	2.00	0.43
1:C:130:ALA:O	1:C:134:ASP:C	2.57	0.43
4:B:504:CM5:H41	4:B:504:CM5:H71	1.24	0.43
1:D:192:ASP:O	1:D:196:LEU:HD23	2.19	0.43
1:B:64:ASP:HB3	1:B:79:CYS:O	2.19	0.43
1:C:232:ARG:HH21	1:C:232:ARG:HB3	1.84	0.43
1:A:100:LYS:O	1:B:73:ARG:HD3	2.19	0.43
1:A:229:GLY:HA2	1:A:234:ILE:CD1	2.48	0.43
1:B:164:LEU:HG	1:B:487:ARG:CZ	2.49	0.43
1:C:27:LYS:H	1:C:27:LYS:HG2	1.46	0.42
1:C:323:ARG:HE	1:C:323:ARG:HB3	1.26	0.42
4:C:504:CM5:C19	4:C:504:CM5:C1	2.97	0.42
1:B:120:ARG:HD2	4:B:504:CM5:H82	2.00	0.42
1:C:153:LEU:CD1	1:C:170:LEU:HD21	2.49	0.42
1:C:313:LEU:HD23	1:C:470:LEU:HD11	2.00	0.42
1:D:464:PRO:O	1:D:465:PRO:C	2.56	0.42
1:A:73:ARG:HG3	3:A:503:PB2:HCF	1.98	0.42
1:D:150:ALA:HB1	1:D:452:THR:HG21	2.01	0.42
1:D:165:LEU:HD12	1:D:165:LEU:C	2.39	0.42
1:A:133:ARG:C	1:A:134:ASP:O	2.57	0.42
3:A:503:PB2:CDE	5:B:525:HOH:O	2.64	0.42
1:C:230:THR:CG2	3:D:502:PB2:CCF	2.98	0.42
1:C:260:ASN:N	1:C:261:PRO:HD3	2.35	0.42
1:D:480:VAL:HA	1:D:481:PRO:HD3	1.81	0.42
1:A:288:LEU:HD22	1:A:288:LEU:HA	1.54	0.42
1:C:149:GLU:OE1	1:C:190:TYR:CE1	2.73	0.42
1:C:200:ASP:O	1:C:204:GLN:CB	2.61	0.42
1:C:359:LEU:HD11	1:C:408:PHE:HA	1.99	0.42
1:A:314:MET:SD	1:A:450:PHE:HE1	2.41	0.42
1:C:211:SER:O	1:C:215:GLN:HG3	2.20	0.42
2:C:500:HEM:C1B	3:C:501:PB2:HAC	2.54	0.42
1:A:398:ASP:HA	1:A:399:PRO:HD3	1.94	0.42
1:B:169:LEU:HD12	1:B:169:LEU:O	2.19	0.42
1:C:471:THR:HA	1:C:472:PRO:HD3	1.74	0.42
1:D:175:THR:HG22	1:D:445:GLU:OE1	2.19	0.42
1:A:476:GLY:CA	5:A:539:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:THR:HA	1:B:472:PRO:HD3	1.79	0.42
1:C:175:THR:HG22	1:C:445:GLU:OE1	2.19	0.42
1:D:194:VAL:HG11	1:D:244:PHE:CE2	2.55	0.42
1:A:220:PHE:CE2	1:B:98:ARG:NH2	2.88	0.42
1:A:226:TYR:CE2	1:B:226:TYR:HB3	2.54	0.42
1:C:486:ILE:HD13	1:C:488:PHE:CZ	2.55	0.42
1:A:58:LEU:HA	1:A:58:LEU:HD23	1.75	0.42
1:A:101:ILE:HD13	1:B:224:LEU:HD13	2.02	0.41
1:D:52:LEU:HD12	1:D:52:LEU:HA	1.84	0.41
1:D:155:GLU:OE1	5:D:512:HOH:O	2.22	0.41
1:A:256:LEU:H	1:A:256:LEU:HG	1.59	0.41
1:B:128:SER:OG	1:B:129:LEU:HD13	2.20	0.41
1:B:296:PHE:CD1	2:B:500:HEM:HBC1	2.54	0.41
1:C:70:LEU:HB3	1:D:227:PHE:CZ	2.55	0.41
1:C:70:LEU:HD22	3:C:502:PB2:NAD	2.35	0.41
1:D:244:PHE:CD1	1:D:244:PHE:C	2.94	0.41
1:A:108:PHE:HB3	1:B:69:TYR:OH	2.20	0.41
1:C:313:LEU:HD12	1:C:356:ILE:HG12	2.02	0.41
1:D:70:LEU:HD22	3:D:502:PB2:CAF	2.50	0.41
1:A:248:SER:O	1:A:252:HIS:ND1	2.43	0.41
1:A:287:ASN:HD22	1:A:287:ASN:HA	1.59	0.41
1:C:212:PHE:CD2	1:D:234:ILE:HG23	2.55	0.41
1:A:436:CYS:HA	2:A:500:HEM:CHA	2.50	0.41
1:D:398:ASP:HA	1:D:399:PRO:HD3	1.89	0.41
1:A:283:PHE:CE2	1:A:285:HIS:CB	3.03	0.41
1:B:230:THR:CG2	3:B:502:PB2:HCF	2.40	0.41
1:B:360:GLY:O	1:B:361:ASP:C	2.59	0.41
1:D:70:LEU:HD22	3:D:502:PB2:CAE	2.51	0.41
1:A:209:ILE:HG23	1:B:205:SER:HB3	2.03	0.41
1:A:320:VAL:HG13	1:A:348:TYR:OH	2.21	0.41
1:B:246:GLY:CA	1:B:286:GLN:OE1	2.66	0.41
1:C:262:ARG:CD	1:C:266:ASP:OD1	2.68	0.41
1:C:409:ASN:C	1:C:411:GLY:H	2.23	0.41
1:C:409:ASN:C	1:C:411:GLY:N	2.73	0.41
1:D:262:ARG:HG2	1:D:266:ASP:OD1	2.20	0.41
1:A:128:SER:OG	1:A:129:LEU:HD12	2.20	0.41
1:A:323:ARG:HE	1:A:323:ARG:HB3	1.39	0.41
1:C:230:THR:HG22	3:D:502:PB2:CCE	2.51	0.41
1:D:73:ARG:HA	1:D:74:PRO:HD3	1.94	0.41
2:B:500:HEM:HBC2	2:B:500:HEM:CHD	2.50	0.41
1:C:201:LEU:HD22	1:C:241:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:THR:O	1:C:294:SER:HB2	2.21	0.41
1:C:338:PRO:HD2	1:C:452:THR:OG1	2.21	0.41
1:D:315:LEU:HD23	1:D:459:ILE:HD12	2.02	0.41
1:D:323:ARG:HE	1:D:323:ARG:HB3	1.32	0.41
1:A:141:SER:O	1:A:145:ARG:HG3	2.21	0.41
1:A:260:ASN:N	1:A:261:PRO:HD3	2.36	0.41
1:D:199:LEU:HD12	1:D:199:LEU:HA	1.92	0.41
1:D:463:VAL:HA	1:D:464:PRO:HD3	1.76	0.41
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.95	0.40
1:A:127:PHE:CZ	1:A:264:PHE:HD2	2.39	0.40
1:A:290:LEU:HD12	1:B:44:LEU:HD21	2.03	0.40
1:B:152:CYS:CB	5:B:498:HOH:O	2.62	0.40
1:B:359:LEU:HD11	1:B:408:PHE:HA	2.02	0.40
1:C:58:LEU:HD23	1:C:58:LEU:HA	1.86	0.40
1:C:100:LYS:O	1:D:73:ARG:HD3	2.21	0.40
1:D:241:ILE:O	1:D:245:ILE:HG13	2.22	0.40
1:D:299:GLY:HA3	2:D:500:HEM:C1C	2.56	0.40
1:C:257:ASP:CB	1:C:258:PRO:HD2	2.52	0.40
1:A:156:GLU:HG3	1:A:190:TYR:CE2	2.56	0.40
1:A:325:GLN:HG2	1:A:491:ARG:NH1	2.37	0.40
1:C:225:LYS:HG2	1:D:477:VAL:HG11	2.02	0.40
1:D:384:LYS:O	1:D:385:ASN:HB2	2.22	0.40
1:B:253:ARG:HH11	1:B:253:ARG:HG3	1.86	0.40
1:B:323:ARG:HE	1:B:323:ARG:HB3	1.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	450/476 (94%)	427 (95%)	21 (5%)	2 (0%)	34 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	446/476 (94%)	417 (94%)	29 (6%)	0	100	100
1	C	447/476 (94%)	418 (94%)	27 (6%)	2 (0%)	34	54
1	D	445/476 (94%)	417 (94%)	28 (6%)	0	100	100
All	All	1788/1904 (94%)	1679 (94%)	105 (6%)	4 (0%)	47	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	VAL
1	C	286	GLN
1	C	261	PRO
1	A	261	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	A	381/421 (90%)	344 (90%)	37 (10%)	8	16
1	B	372/421 (88%)	336 (90%)	36 (10%)	8	16
1	C	368/421 (87%)	335 (91%)	33 (9%)	9	19
1	D	376/421 (89%)	343 (91%)	33 (9%)	10	19
All	All	1497/1684 (89%)	1358 (91%)	139 (9%)	9	17

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	44	LEU
1	A	45	GLN
1	A	53	ARG
1	A	68	VAL
1	A	74	PRO
1	A	75	VAL

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Mol	Chain	Res	Type
1	A	78	LEU
1	A	127	PHE
1	A	134	ASP
1	A	140	ARG
1	A	158	ARG
1	A	169	LEU
1	A	198	LEU
1	A	199	LEU
1	A	221	SER
1	A	224	LEU
1	A	236	ARG
1	A	238	LEU
1	A	255	THR
1	A	256	LEU
1	A	257	ASP
1	A	262	ARG
1	A	268	TYR
1	A	270	LEU
1	A	283	PHE
1	A	288	LEU
1	A	290	LEU
1	A	295	LEU
1	A	334	SER
1	A	341	ASP
1	A	370	THR
1	A	458	SER
1	A	461	SER
1	A	473	ARG
1	A	475	SER
1	A	477	VAL
1	B	37	LEU
1	B	44	LEU
1	B	45	GLN
1	B	47	ASP
1	B	56	LEU
1	B	57	ARG
1	B	68	VAL
1	B	75	VAL
1	B	78	LEU
1	B	127	PHE
1	B	128	SER
1	B	129	LEU

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Mol	Chain	Res	Type
1	B	131	THR
1	B	158	ARG
1	B	169	LEU
1	B	181	SER
1	B	198	LEU
1	B	199	LEU
1	B	207	SER
1	B	210	SER
1	B	221	SER
1	B	224	LEU
1	B	233	GLN
1	B	238	LEU
1	B	240	GLU
1	B	256	LEU
1	B	257	ASP
1	B	290	LEU
1	B	295	LEU
1	B	319	HIS
1	B	334	SER
1	B	341	ASP
1	B	370	THR
1	B	458	SER
1	B	461	SER
1	B	477	VAL
1	C	44	LEU
1	C	53	ARG
1	C	68	VAL
1	C	75	VAL
1	C	78	LEU
1	C	127	PHE
1	C	129	LEU
1	C	140	ARG
1	C	158	ARG
1	C	165	LEU
1	C	169	LEU
1	C	199	LEU
1	C	224	LEU
1	C	226	TYR
1	C	236	ARG
1	C	238	LEU
1	C	255	THR
1	C	256	LEU

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Mol	Chain	Res	Type
1	C	257	ASP
1	C	262	ARG
1	C	270	LEU
1	C	272	MET
1	C	285	HIS
1	C	290	LEU
1	C	295	LEU
1	C	323	ARG
1	C	329	GLU
1	C	341	ASP
1	C	343	ARG
1	C	370	THR
1	C	458	SER
1	C	461	SER
1	C	477	VAL
1	D	37	LEU
1	D	44	LEU
1	D	52	LEU
1	D	57	ARG
1	D	61	LYS
1	D	68	VAL
1	D	75	VAL
1	D	78	LEU
1	D	104	VAL
1	D	127	PHE
1	D	129	LEU
1	D	134	ASP
1	D	141	SER
1	D	158	ARG
1	D	169	LEU
1	D	198	LEU
1	D	199	LEU
1	D	221	SER
1	D	224	LEU
1	D	238	LEU
1	D	256	LEU
1	D	257	ASP
1	D	262	ARG
1	D	272	MET
1	D	290	LEU
1	D	295	LEU
1	D	334	SER

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Mol	Chain	Res	Type
1	D	341	ASP
1	D	370	THR
1	D	458	SER
1	D	461	SER
1	D	475	SER
1	D	477	VAL

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

Mol	Chain	Res	Type
1	A	45	GLN
1	A	204	GLN
1	A	233	GLN
1	A	385	ASN
1	B	45	GLN
1	B	233	GLN
1	B	287	ASN
1	B	319	HIS
1	B	456	ASN
1	C	45	GLN
1	C	204	GLN
1	C	287	ASN
1	D	45	GLN
1	D	233	GLN
1	D	287	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

20 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
3	PB2	A	503	-	13,13,20	1.88	3 (23%)	16,16,26	0.92	0
3	PB2	C	503	-	13,13,20	1.97	4 (30%)	16,16,26	1.21	1 (6%)
2	HEM	C	500	1,3	27,50,50	2.57	8 (29%)	17,82,82	1.24	3 (17%)
3	PB2	C	502	-	19,20,20	2.02	4 (21%)	24,26,26	0.93	0
4	CM5	A	504	-	23,23,36	0.49	0	28,29,49	2.06	9 (32%)
4	CM5	B	504	-	23,23,36	0.54	0	28,29,49	2.09	9 (32%)
3	PB2	B	502	-	19,20,20	1.99	5 (26%)	24,26,26	0.86	0
3	PB2	C	501	2	19,20,20	2.10	8 (42%)	24,26,26	1.47	2 (8%)
3	PB2	B	503	-	13,13,20	1.93	3 (23%)	16,16,26	0.96	0
2	HEM	B	500	1,3	27,50,50	2.58	9 (33%)	17,82,82	1.52	4 (23%)
2	HEM	D	500	1,3	27,50,50	2.64	7 (25%)	17,82,82	1.54	5 (29%)
3	PB2	B	496	-	19,20,20	2.01	6 (31%)	24,26,26	1.30	4 (16%)
3	PB2	D	502	-	19,20,20	2.00	4 (21%)	24,26,26	0.69	0
3	PB2	D	503	-	13,13,20	2.01	4 (30%)	16,16,26	0.98	0
3	PB2	A	501	2	19,20,20	2.13	6 (31%)	24,26,26	0.80	0
3	PB2	B	501	2	19,20,20	2.36	7 (36%)	24,26,26	0.99	1 (4%)
2	HEM	A	500	1,3	27,50,50	2.57	9 (33%)	17,82,82	1.50	1 (5%)
4	CM5	C	504	-	23,23,36	0.48	0	28,29,49	1.66	4 (14%)
3	PB2	D	501	2	19,20,20	2.16	7 (36%)	24,26,26	1.45	4 (16%)
4	CM5	D	504	-	23,23,36	0.52	0	28,29,49	2.36	9 (32%)

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
3	PB2	A	503	-	-	0/4/4/8	0/2/2/3
3	PB2	C	503	-	-	0/4/4/8	0/2/2/3
2	HEM	C	500	1,3	-	0/6/54/54	-
3	PB2	C	502	-	-	1/8/8/8	0/3/3/3
4	CM5	A	504	-	-	8/11/35/65	0/2/2/3
4	CM5	B	504	-	-	8/11/35/65	0/2/2/3
3	PB2	B	502	-	-	0/8/8/8	0/3/3/3
3	PB2	C	501	2	-	0/8/8/8	0/3/3/3
3	PB2	B	503	-	-	0/4/4/8	0/2/2/3
2	HEM	B	500	1,3	-	0/6/54/54	-
2	HEM	D	500	1,3	-	2/6/54/54	-
3	PB2	B	496	-	-	2/8/8/8	0/3/3/3
3	PB2	D	502	-	-	0/8/8/8	0/3/3/3
3	PB2	D	503	-	-	0/4/4/8	0/2/2/3
3	PB2	A	501	2	-	2/8/8/8	0/3/3/3
3	PB2	B	501	2	-	0/8/8/8	0/3/3/3
2	HEM	A	500	1,3	-	2/6/54/54	-
4	CM5	C	504	-	-	7/11/35/65	1/2/2/3
3	PB2	D	501	2	-	2/8/8/8	0/3/3/3
4	CM5	D	504	-	-	5/11/35/65	0/2/2/3

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3C-C2C	-8.61	1.28	1.40
2	C	500	HEM	C3C-C2C	-8.35	1.28	1.40
2	D	500	HEM	C3C-C2C	-7.87	1.29	1.40
2	B	500	HEM	C3C-C2C	-7.69	1.29	1.40
2	D	500	HEM	C3B-C2B	-7.66	1.29	1.40
2	B	500	HEM	C3B-C2B	-7.41	1.30	1.40
2	A	500	HEM	C3B-C2B	-6.92	1.30	1.40
2	C	500	HEM	C3B-C2B	-6.68	1.31	1.40
3	B	501	PB2	CDB-CDA	5.39	1.50	1.39
3	A	501	PB2	CDB-CDA	5.20	1.50	1.39
3	B	501	PB2	CCC-CCD	4.95	1.49	1.39
3	D	501	PB2	CDB-CDA	4.85	1.49	1.39
3	D	502	PB2	CCC-CCD	4.76	1.49	1.39
3	C	501	PB2	CCC-CCD	4.61	1.49	1.39
3	B	496	PB2	CCC-CCD	4.56	1.49	1.39
3	D	502	PB2	CDB-CDA	4.46	1.48	1.39
3	C	502	PB2	CAF-NAB	-4.37	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	C3D-C2D	4.35	1.50	1.37
3	B	502	PB2	CAF-NAB	-4.26	1.29	1.37
2	B	500	HEM	C3D-C2D	4.25	1.50	1.37
3	B	496	PB2	CDB-CDA	4.17	1.48	1.39
3	D	501	PB2	CCC-CCD	4.07	1.48	1.39
2	C	500	HEM	C3D-C2D	4.03	1.49	1.37
3	A	501	PB2	CCC-CCD	4.01	1.47	1.39
3	B	501	PB2	CAF-NAB	-3.90	1.30	1.37
3	C	502	PB2	CDB-CDA	3.84	1.47	1.39
3	D	503	PB2	CDB-CDA	3.83	1.47	1.39
3	A	503	PB2	CCC-CCD	3.81	1.47	1.39
3	C	501	PB2	CDB-CDA	3.80	1.47	1.39
3	B	503	PB2	CDB-CDA	3.79	1.47	1.39
3	B	502	PB2	CDB-CDA	3.73	1.47	1.39
3	C	503	PB2	CDB-CDA	3.71	1.47	1.39
3	D	503	PB2	CCC-CCD	3.62	1.47	1.39
3	B	502	PB2	CCC-CCD	3.58	1.47	1.39
2	A	500	HEM	C3D-C2D	3.56	1.48	1.37
3	C	502	PB2	CCC-CCD	3.51	1.46	1.39
3	C	503	PB2	CCC-CCD	3.45	1.46	1.39
3	A	503	PB2	CDB-CDA	3.36	1.46	1.39
3	B	503	PB2	CCC-CCD	3.18	1.46	1.39
2	D	500	HEM	C3B-CAB	3.17	1.54	1.47
2	B	500	HEM	C3C-CAC	2.97	1.53	1.47
3	D	501	PB2	CDE-CDD	2.93	1.45	1.38
3	C	501	PB2	CCF-CCA	2.92	1.45	1.38
2	C	500	HEM	C3B-CAB	2.92	1.53	1.47
3	A	501	PB2	CAF-NAB	-2.85	1.32	1.37
3	B	501	PB2	CCF-CCE	2.80	1.43	1.38
3	D	501	PB2	CCB-CCA	2.70	1.44	1.38
3	B	501	PB2	CCF-CCA	2.68	1.44	1.38
2	B	500	HEM	C3B-CAB	2.65	1.53	1.47
2	D	500	HEM	C2A-C3A	-2.64	1.29	1.37
2	C	500	HEM	C3C-CAC	2.63	1.53	1.47
3	D	501	PB2	CCF-CCA	2.62	1.44	1.38
2	C	500	HEM	C4B-CHC	-2.62	1.33	1.41
2	D	500	HEM	C4A-CHB	-2.60	1.33	1.41
3	D	501	PB2	CCF-CCE	2.60	1.43	1.38
3	B	502	PB2	CAA-NAB	-2.59	1.43	1.49
3	C	502	PB2	CAA-NAB	-2.57	1.43	1.49
3	B	496	PB2	CAF-NAB	-2.57	1.32	1.37
2	A	500	HEM	C2A-C3A	-2.56	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PB2	CCF-CCA	2.55	1.44	1.38
3	B	496	PB2	CCF-CCA	2.55	1.44	1.38
3	B	503	PB2	CDF-CDA	-2.52	1.33	1.39
3	C	501	PB2	CCF-CCE	2.49	1.43	1.38
3	D	501	PB2	CAF-NAB	-2.46	1.33	1.37
2	B	500	HEM	C4B-CHC	-2.43	1.34	1.41
3	C	501	PB2	CAF-NAB	-2.41	1.33	1.37
2	A	500	HEM	C1A-CHA	-2.37	1.34	1.41
2	A	500	HEM	C3B-CAB	2.34	1.52	1.47
3	D	503	PB2	CDF-CDA	-2.32	1.34	1.39
3	D	502	PB2	CCF-CCA	2.31	1.43	1.38
2	A	500	HEM	C3C-CAC	2.31	1.52	1.47
2	C	500	HEM	C2A-C3A	-2.31	1.30	1.37
2	B	500	HEM	C2A-C3A	-2.27	1.30	1.37
2	A	500	HEM	C4A-CHB	-2.25	1.34	1.41
2	A	500	HEM	C4B-CHC	-2.25	1.34	1.41
3	B	501	PB2	CDE-CDD	2.24	1.44	1.38
2	B	500	HEM	C1A-CHA	-2.23	1.34	1.41
3	A	503	PB2	CCE-CCD	-2.21	1.34	1.39
2	B	500	HEM	C4A-CHB	-2.20	1.34	1.41
3	B	501	PB2	CCB-CCA	2.18	1.43	1.38
3	C	501	PB2	CAA-NAB	-2.17	1.44	1.49
3	C	503	PB2	CDE-CDD	2.15	1.43	1.38
3	B	496	PB2	CAA-NAB	-2.15	1.44	1.49
2	D	500	HEM	C3C-CAC	2.13	1.52	1.47
3	B	496	PB2	CDE-CDD	2.12	1.43	1.38
2	C	500	HEM	C4A-CHB	-2.10	1.35	1.41
3	A	501	PB2	CAA-CCA	2.08	1.56	1.51
3	D	502	PB2	CDE-CDD	2.06	1.43	1.38
3	D	503	PB2	CCA-CCF	2.05	1.43	1.38
3	A	501	PB2	CDE-CDD	2.03	1.43	1.38
3	C	501	PB2	CCB-CCA	2.03	1.43	1.38
3	B	502	PB2	CCE-CCD	-2.03	1.35	1.39
3	C	503	PB2	CCE-CCD	-2.02	1.35	1.39
3	C	501	PB2	CCD-CDA	2.02	1.54	1.49

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	504	CM5	C13-O14-C15	-7.07	105.30	113.13
4	B	504	CM5	C13-O14-C15	-4.86	107.75	113.13
4	A	504	CM5	C13-O14-C15	-4.54	108.11	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	CM5	C1-O12-C13	-4.53	106.33	113.84
4	A	504	CM5	O14-C15-C19	4.51	114.06	106.83
4	D	504	CM5	C1-O12-C13	-4.28	106.75	113.84
3	C	501	PB2	CCC-CCD-CDA	-4.27	113.96	121.36
4	C	504	CM5	C17-C16-C15	-4.12	104.13	111.22
4	D	504	CM5	O14-C15-C16	-4.03	103.60	110.04
2	A	500	HEM	CAD-CBD-CGD	-3.99	105.98	112.67
4	B	504	CM5	C16-C17-C18	-3.93	104.97	110.69
4	B	504	CM5	O14-C15-C19	3.71	112.78	106.83
4	A	504	CM5	C17-C16-C15	-3.70	104.85	111.22
4	D	504	CM5	O14-C15-C19	3.54	112.51	106.83
4	D	504	CM5	C17-C16-C15	-3.51	105.18	111.22
4	C	504	CM5	O14-C15-C19	3.48	112.42	106.83
3	D	501	PB2	CCE-CCF-CCA	-3.46	116.26	121.03
4	C	504	CM5	C13-O14-C15	3.46	116.96	113.13
4	D	504	CM5	O22-C18-C17	-3.09	104.08	109.99
4	D	504	CM5	C11-C6-C7	-3.05	101.87	109.33
4	C	504	CM5	C1-O12-C13	-3.01	108.84	113.84
2	B	500	HEM	CMA-C3A-C4A	-3.01	123.84	128.46
4	B	504	CM5	C17-C16-C15	-2.96	106.13	111.22
4	B	504	CM5	C5-C6-C7	-2.92	105.14	112.11
3	B	501	PB2	CDC-CDB-CDA	-2.85	116.98	120.56
4	B	504	CM5	C1-O12-C13	-2.75	109.28	113.84
3	B	496	PB2	CCC-CCD-CDA	-2.74	116.61	121.36
3	D	501	PB2	CCC-CCD-CDA	-2.70	116.67	121.36
2	D	500	HEM	CAA-CBA-CGA	-2.66	108.21	112.67
2	C	500	HEM	C3B-C4B-NB	2.45	112.38	109.21
4	B	504	CM5	O12-C13-C18	2.45	112.12	108.30
2	D	500	HEM	C4C-C3C-C2C	2.44	108.60	106.90
2	C	500	HEM	CMA-C3A-C4A	-2.43	124.72	128.46
2	D	500	HEM	CAD-CBD-CGD	-2.43	108.59	112.67
4	D	504	CM5	O14-C13-C18	2.43	115.49	110.35
3	B	496	PB2	CDF-CDA-CCD	-2.39	117.21	121.36
2	B	500	HEM	CAD-CBD-CGD	-2.38	108.67	112.67
2	D	500	HEM	C1D-C2D-C3D	-2.38	105.34	107.00
4	D	504	CM5	C10-C11-C6	-2.38	107.65	112.15
3	C	501	PB2	CCE-CCD-CDA	2.37	125.46	121.36
3	C	503	PB2	CDF-CDA-CDB	2.34	122.26	117.59
2	C	500	HEM	CBD-CAD-C3D	-2.30	108.23	112.48
4	B	504	CM5	C10-C9-C8	-2.28	104.15	111.18
2	B	500	HEM	C1D-C2D-C3D	-2.23	105.45	107.00
4	A	504	CM5	C5-C6-C7	-2.22	106.80	112.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	496	PB2	CCF-CCE-CCD	-2.21	117.95	121.13
3	D	501	PB2	CCB-CCC-CCD	-2.19	117.97	121.13
4	A	504	CM5	C3-C4-C5	-2.19	105.89	113.62
4	A	504	CM5	O14-C15-C16	-2.19	106.55	110.04
2	B	500	HEM	C3B-C4B-NB	2.19	112.03	109.21
4	A	504	CM5	C10-C11-C6	-2.14	108.10	112.15
3	D	501	PB2	CDD-CDE-CDF	-2.14	116.93	120.19
4	B	504	CM5	C9-C8-C7	-2.13	107.06	111.42
2	D	500	HEM	CMA-C3A-C4A	-2.12	125.21	128.46
3	B	496	PB2	CCC-CCB-CCA	-2.11	118.12	121.03
4	A	504	CM5	C4-C5-C6	-2.00	104.67	115.89

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500	HEM	C2D-C3D-CAD-CBD
2	D	500	HEM	C4D-C3D-CAD-CBD
4	A	504	CM5	C18-C13-O12-C1
4	A	504	CM5	O14-C13-O12-C1
4	A	504	CM5	O14-C15-C19-O20
4	A	504	CM5	C16-C15-C19-O20
4	B	504	CM5	C2-C1-O12-C13
4	B	504	CM5	O14-C15-C19-O20
4	B	504	CM5	C16-C15-C19-O20
4	C	504	CM5	C2-C1-O12-C13
4	C	504	CM5	C18-C13-O12-C1
4	C	504	CM5	O14-C15-C19-O20
4	C	504	CM5	C16-C15-C19-O20
4	D	504	CM5	O14-C13-O12-C1
4	D	504	CM5	O14-C15-C19-O20
4	D	504	CM5	C16-C15-C19-O20
4	A	504	CM5	C2-C3-C4-C5
4	B	504	CM5	C4-C5-C6-C7
4	C	504	CM5	O12-C1-C2-C3
4	C	504	CM5	C2-C3-C4-C5
4	A	504	CM5	C2-C1-O12-C13
4	B	504	CM5	C4-C5-C6-C11
4	B	504	CM5	C3-C4-C5-C6
4	C	504	CM5	O14-C13-O12-C1
4	B	504	CM5	C2-C3-C4-C5
3	D	501	PB2	CCE-CCD-CDA-CDF

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Mol	Chain	Res	Type	Atoms
4	A	504	CM5	C4-C5-C6-C7
4	B	504	CM5	C1-C2-C3-C4
2	A	500	HEM	C2D-C3D-CAD-CBD
2	A	500	HEM	C4D-C3D-CAD-CBD
3	D	501	PB2	CCE-CCD-CDA-CDB
3	A	501	PB2	CCC-CCD-CDA-CDB
4	A	504	CM5	C4-C5-C6-C11
3	A	501	PB2	CCC-CCD-CDA-CDF
4	D	504	CM5	C3-C4-C5-C6
3	B	496	PB2	NAB-CAA-CCA-CCB
3	B	496	PB2	NAB-CAA-CCA-CCF
3	C	502	PB2	CCA-CAA-NAB-CAF
4	D	504	CM5	C2-C3-C4-C5

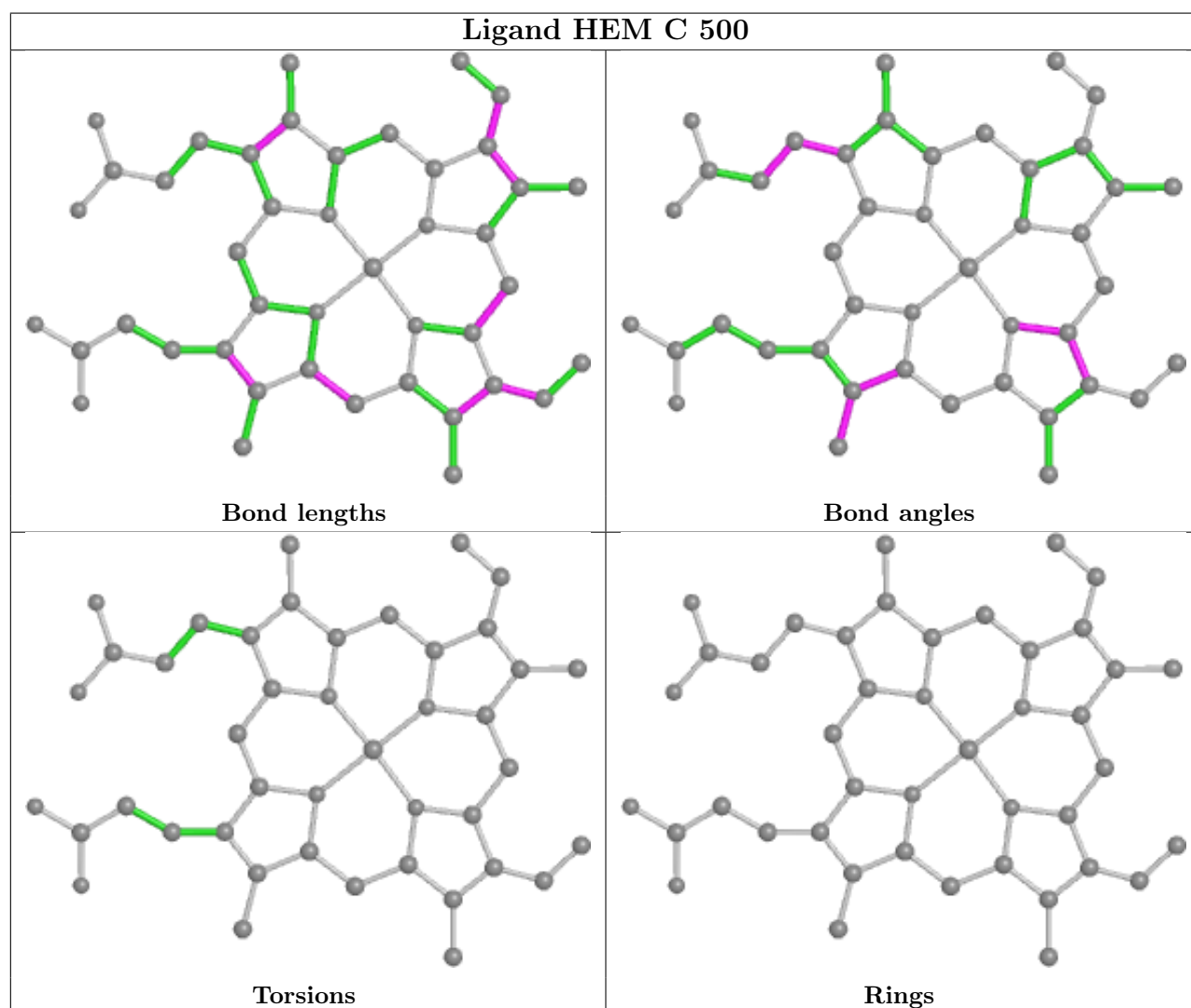
All (1) ring outliers are listed below:

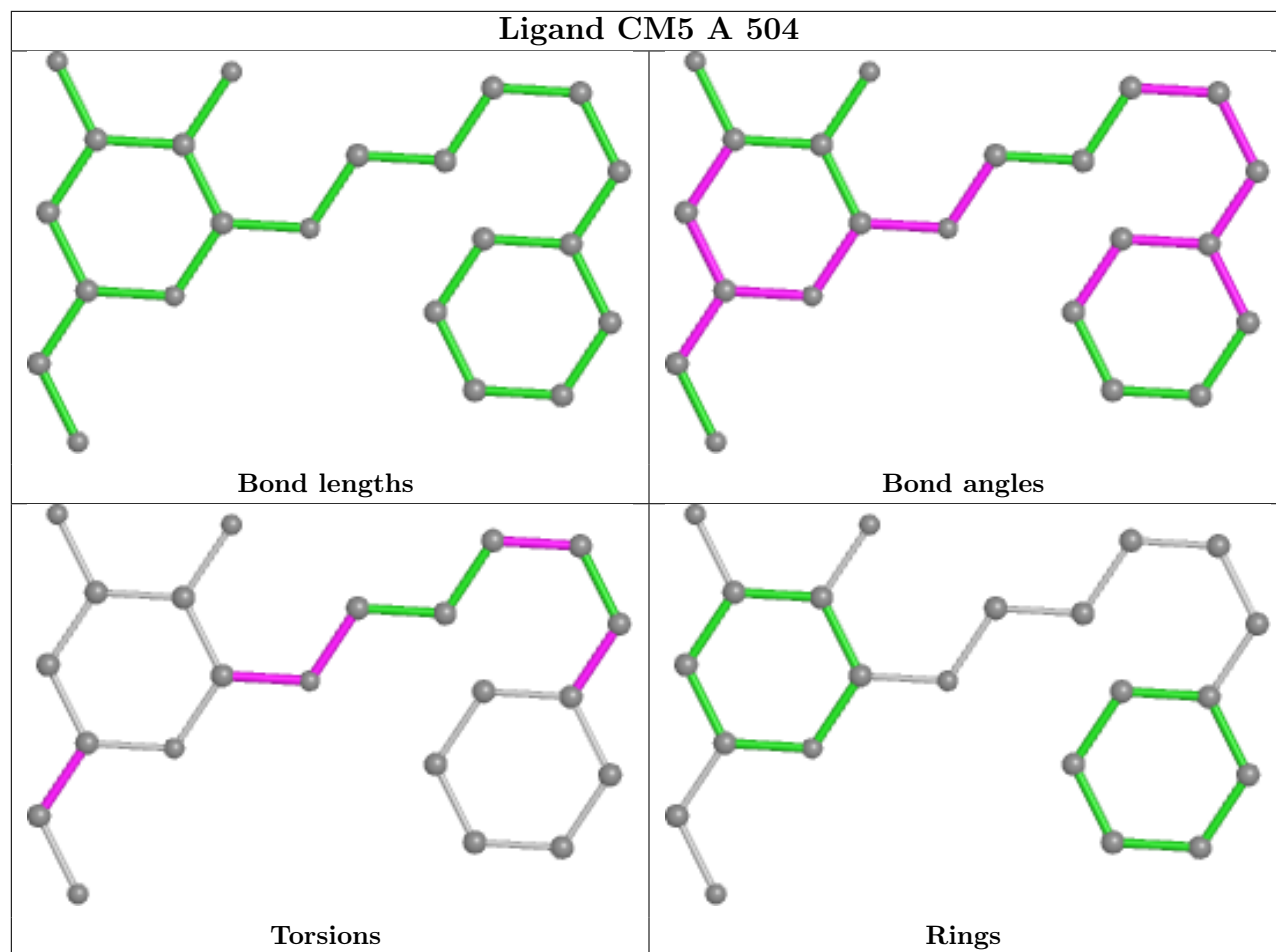
Mol	Chain	Res	Type	Atoms
4	C	504	CM5	C13-C15-C16-C17-C18-O14

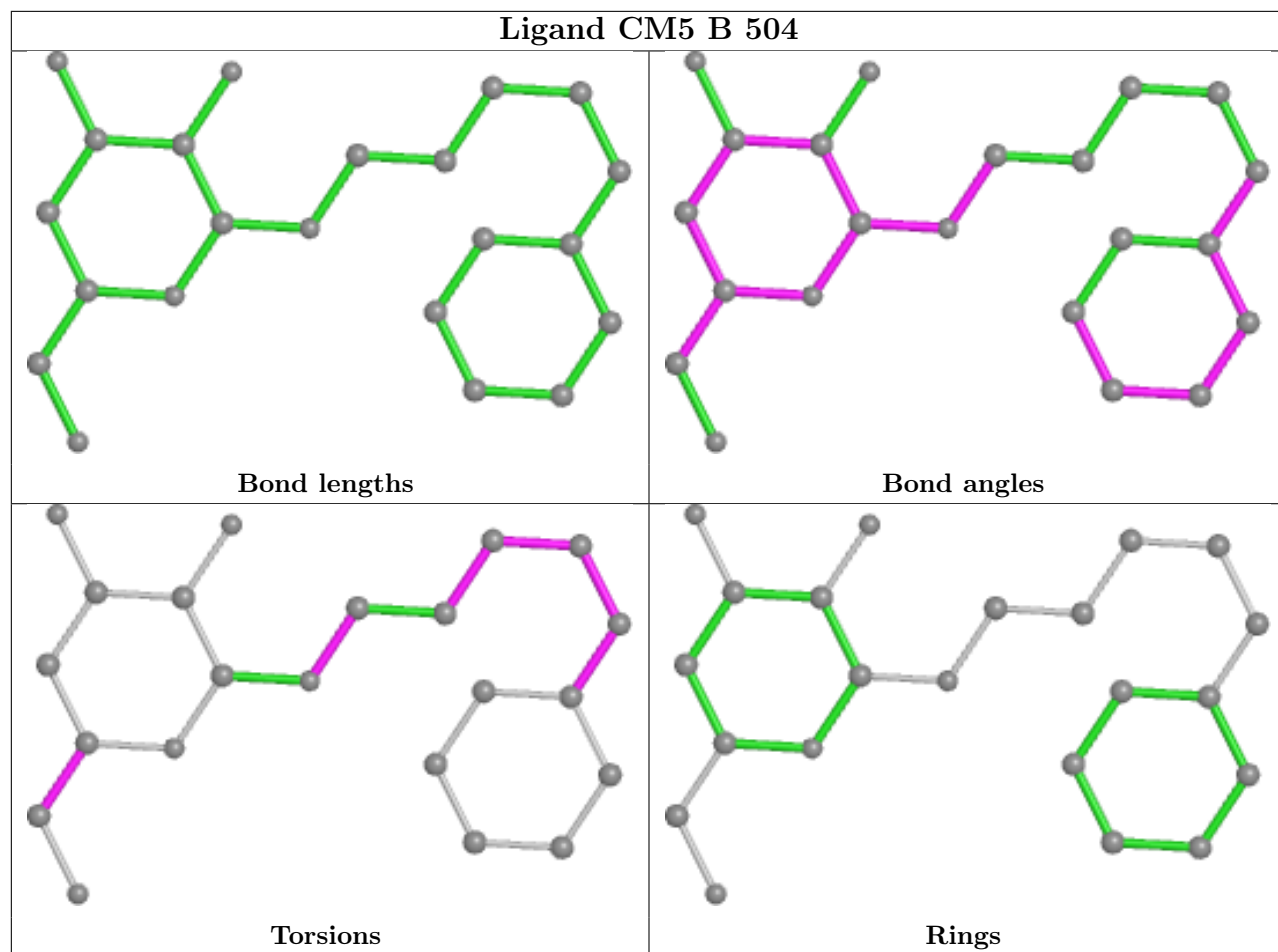
19 monomers are involved in 115 short contacts:

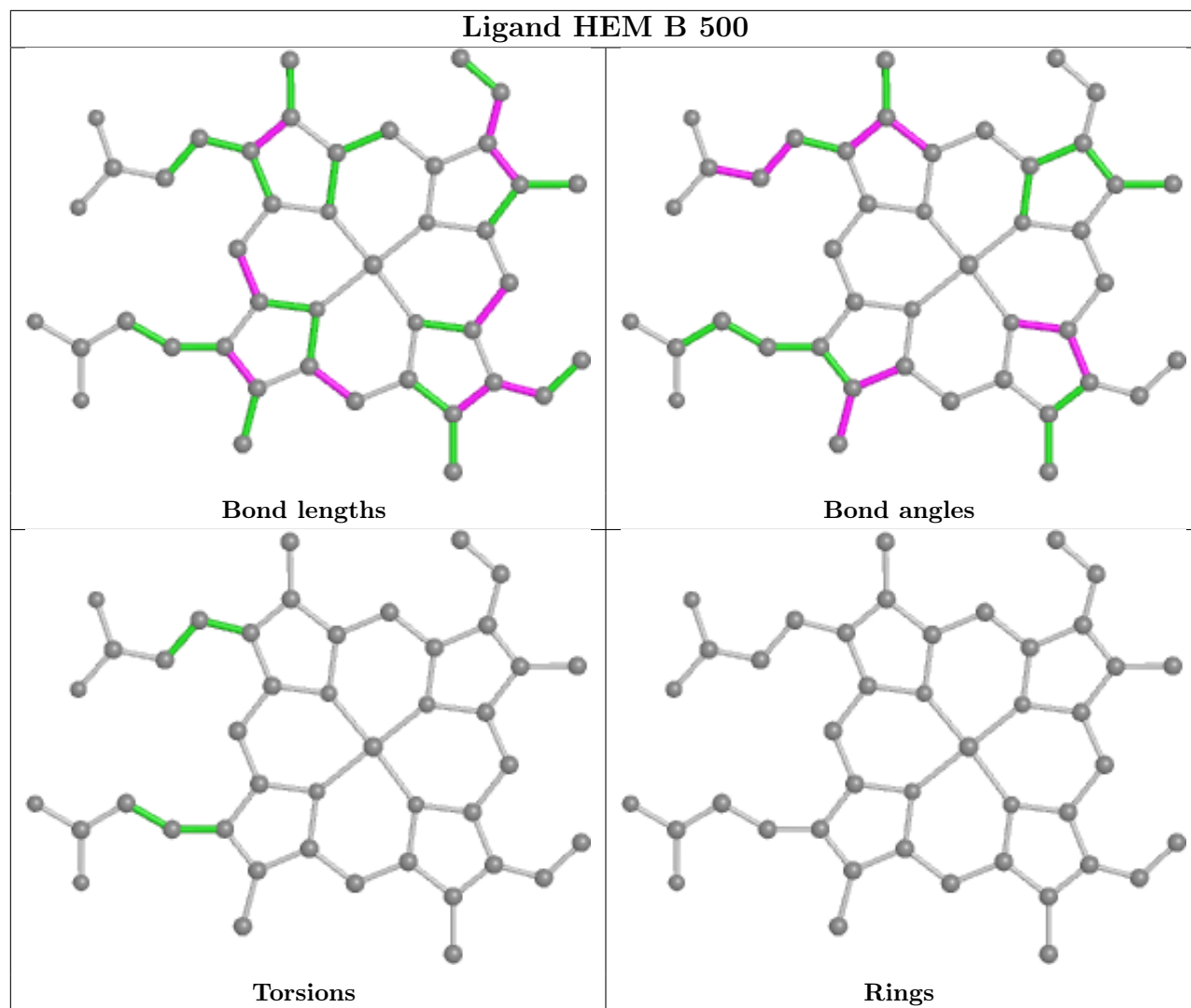
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	PB2	11	0
3	C	503	PB2	10	0
2	C	500	HEM	5	0
3	C	502	PB2	13	0
4	A	504	CM5	1	0
4	B	504	CM5	4	0
3	B	502	PB2	10	0
3	C	501	PB2	1	0
3	B	503	PB2	7	0
2	B	500	HEM	11	0
2	D	500	HEM	12	0
3	B	496	PB2	5	0
3	D	502	PB2	7	0
3	D	503	PB2	10	0
3	B	501	PB2	2	0
2	A	500	HEM	9	0
4	C	504	CM5	7	0
3	D	501	PB2	2	0
4	D	504	CM5	1	0

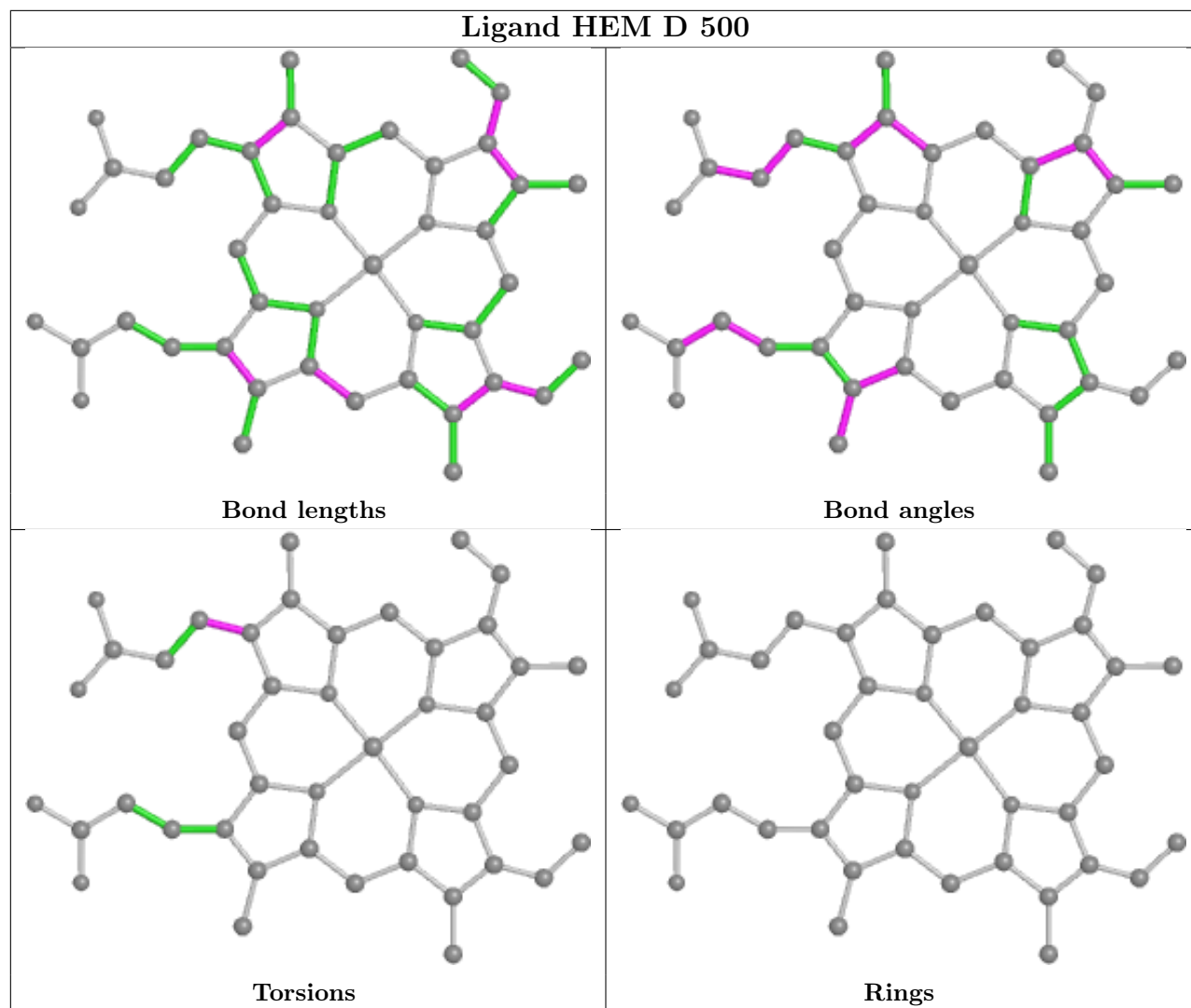
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

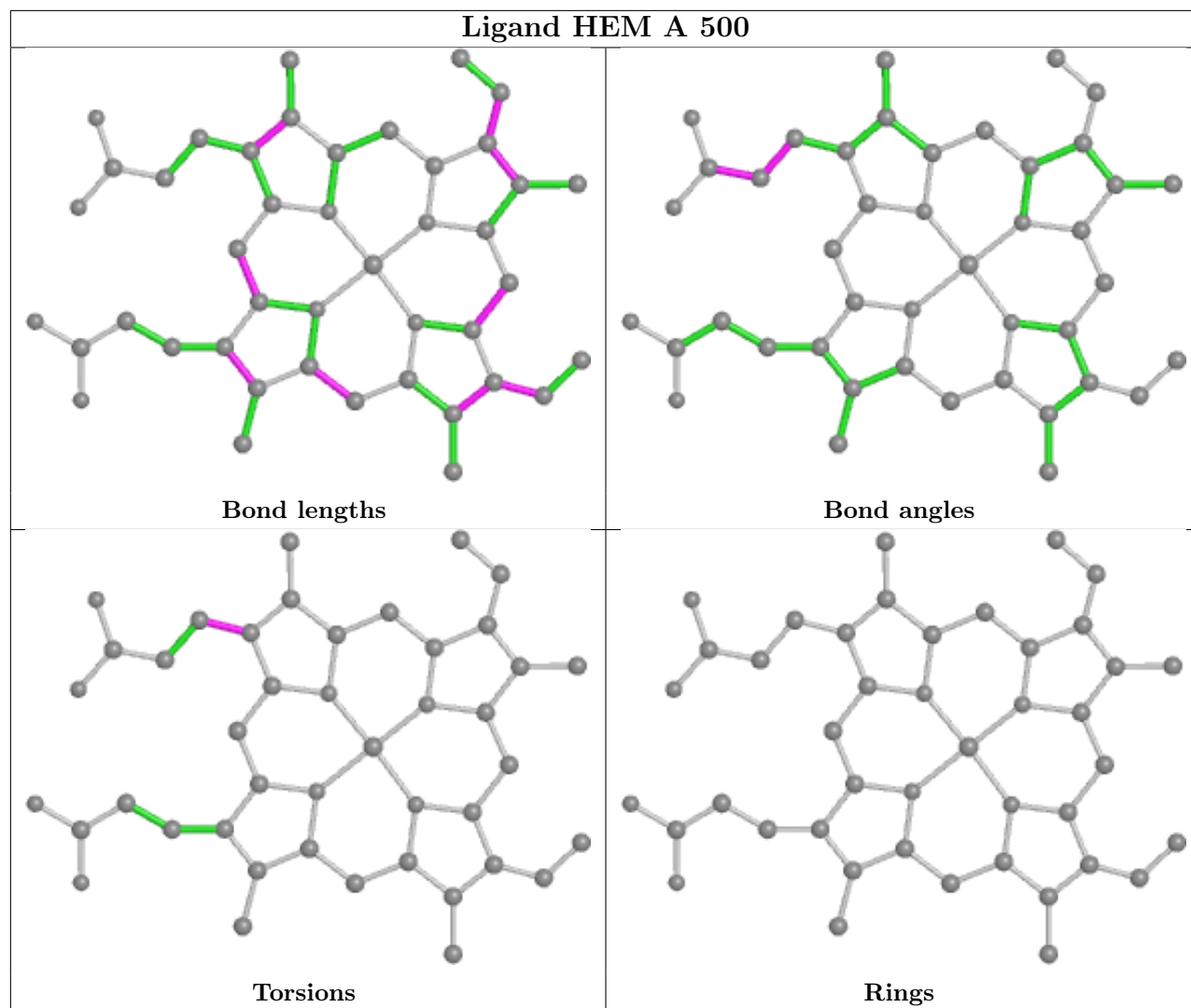


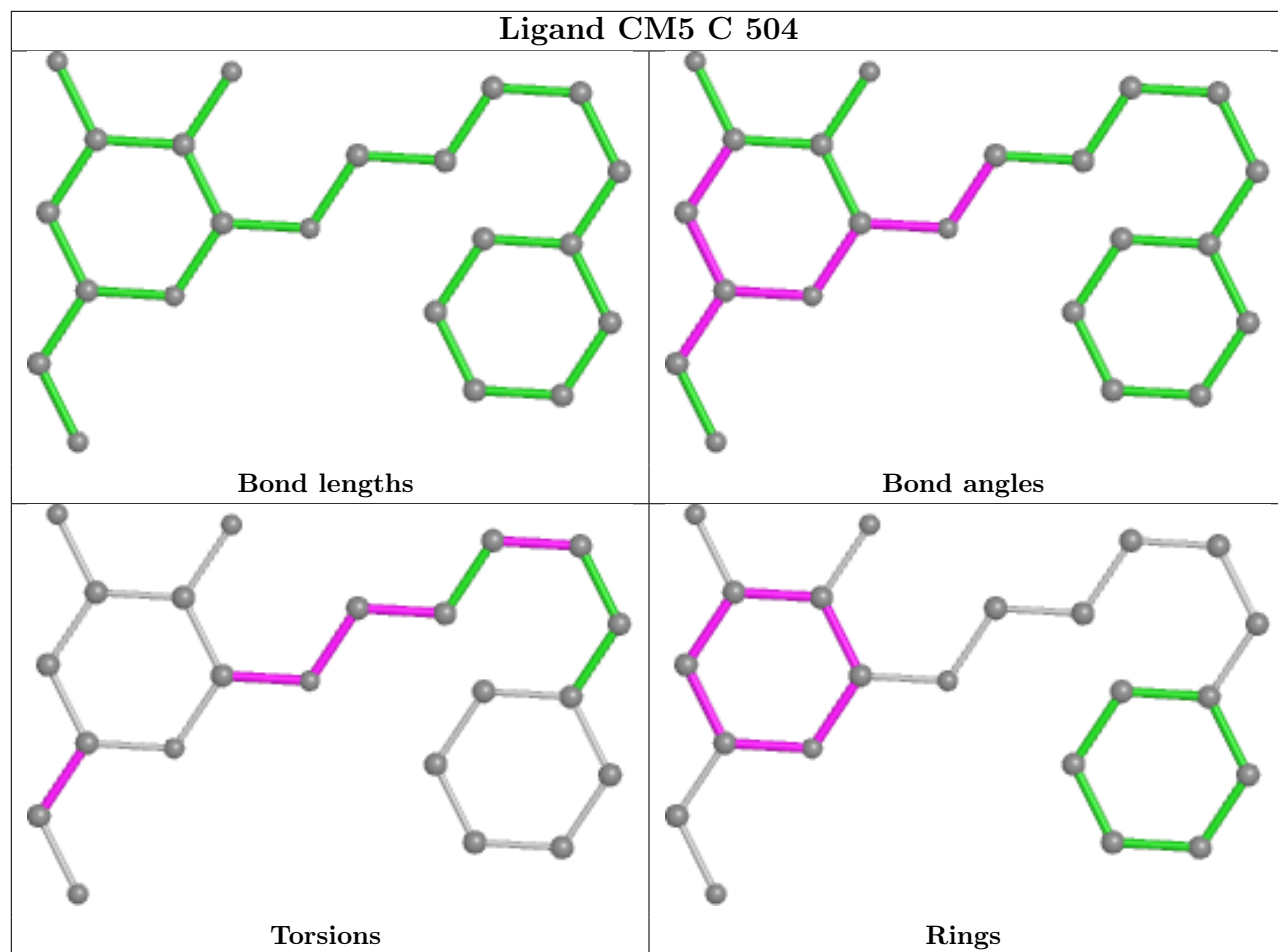


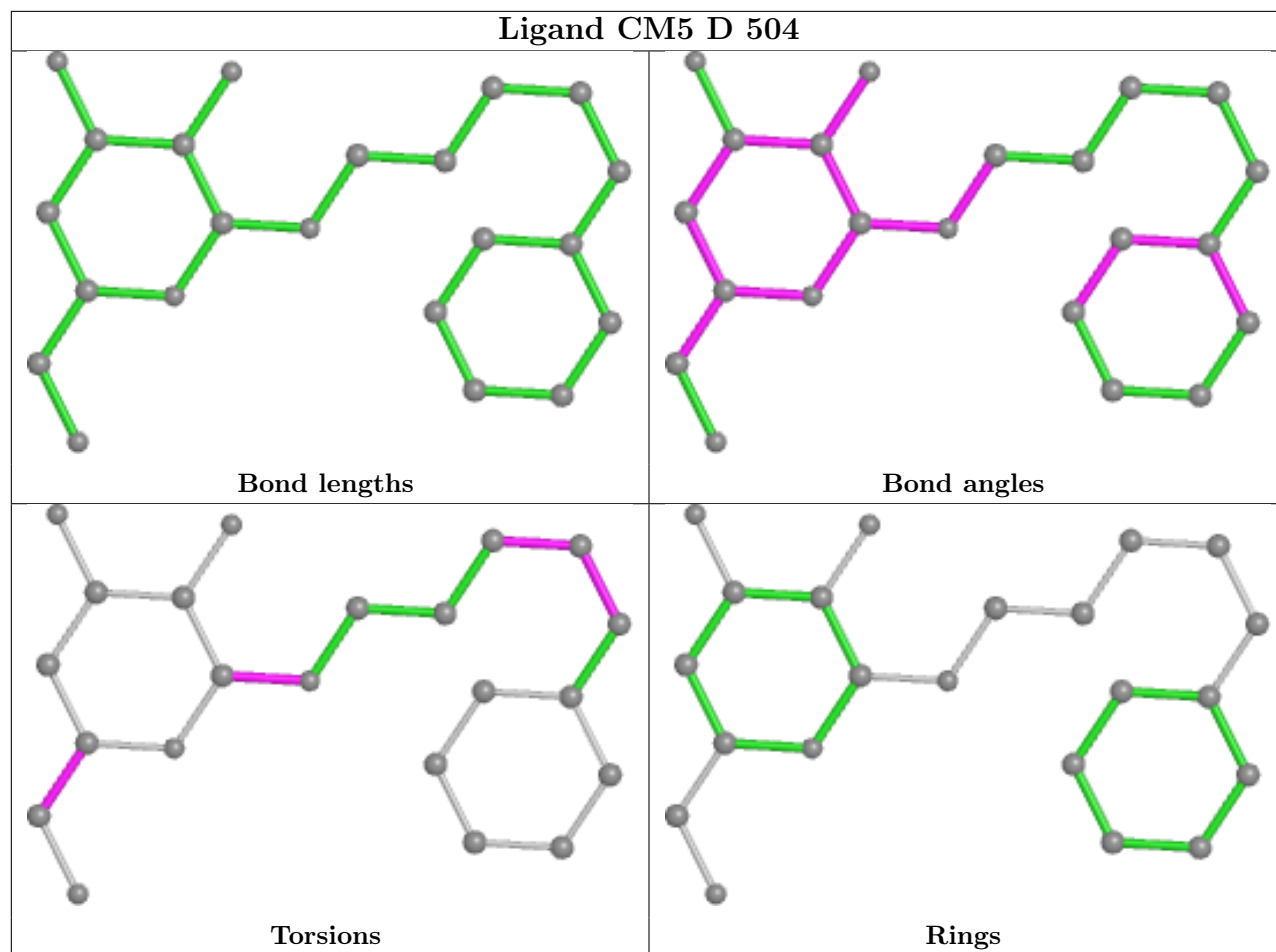












5.7 Other polymers [i](#)

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	456/476 (95%)	0.06	17 (3%) 41 45	34, 59, 97, 128	0
1	B	451/476 (94%)	-0.00	8 (1%) 68 71	27, 61, 98, 125	0
1	C	452/476 (94%)	0.14	22 (4%) 29 31	31, 62, 100, 123	0
1	D	451/476 (94%)	0.04	14 (3%) 49 52	27, 60, 96, 121	0
All	All	1810/1904 (95%)	0.06	61 (3%) 45 48	27, 61, 98, 128	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	SER	6.7
1	C	416	ALA	6.2
1	A	283	PHE	5.9
1	C	130	ALA	4.9
1	C	26	SER	4.8
1	A	256	LEU	4.7
1	A	127	PHE	4.6
1	A	273	GLU	3.8
1	D	260	ASN	3.6
1	D	259	SER	3.4
1	A	474	GLU	3.4
1	A	260	ASN	3.3
1	B	272	MET	3.3
1	A	268	TYR	3.3
1	B	256	LEU	3.2
1	C	324	VAL	3.2
1	C	418	GLY	3.2
1	C	454	LEU	3.2
1	A	335	HIS	3.1
1	D	270	LEU	3.0
1	C	332	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	468	ILE	2.9
1	D	226	TYR	2.8
1	C	488	PHE	2.8
1	C	317	TYR	2.8
1	B	285	HIS	2.8
1	D	492	HIS	2.8
1	A	257	ASP	2.8
1	A	255	THR	2.8
1	B	134	ASP	2.7
1	A	270	LEU	2.7
1	C	492	HIS	2.6
1	D	261	PRO	2.6
1	B	488	PHE	2.6
1	D	256	LEU	2.6
1	C	417	ASN	2.6
1	D	475	SER	2.5
1	D	324	VAL	2.5
1	C	131	THR	2.5
1	C	453	ILE	2.5
1	C	257	ASP	2.5
1	D	165	LEU	2.4
1	B	463	VAL	2.4
1	A	134	ASP	2.4
1	C	160	SER	2.4
1	B	260	ASN	2.4
1	C	414	LEU	2.4
1	C	450	PHE	2.3
1	A	259	SER	2.3
1	D	134	ASP	2.3
1	C	489	LEU	2.3
1	D	400	ARG	2.2
1	D	157	LEU	2.2
1	C	333	GLY	2.2
1	A	284	HIS	2.1
1	A	27	LYS	2.1
1	C	475	SER	2.1
1	C	491	ARG	2.1
1	C	256	LEU	2.0
1	D	334	SER	2.0
1	A	272	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

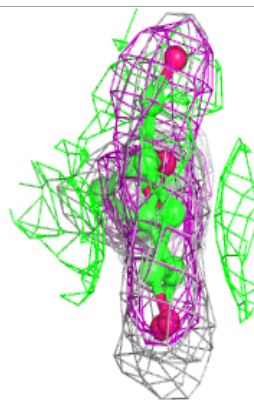
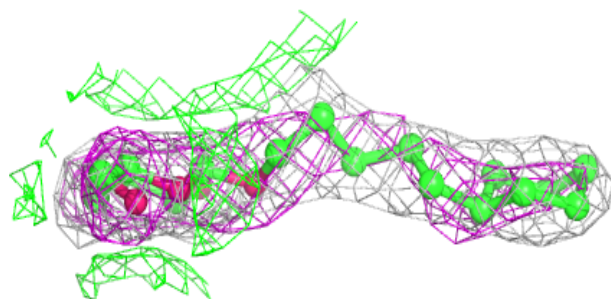
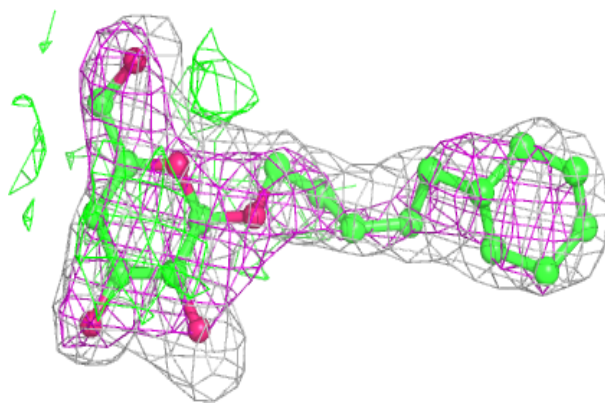
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PB2	C	503	12/18	0.78	0.40	57,66,72,72	12
3	PB2	D	503	12/18	0.82	0.44	62,69,83,85	12
4	CM5	B	504	22/34	0.86	0.34	20,20,20,20	0
4	CM5	C	504	22/34	0.86	0.45	20,20,20,20	0
3	PB2	A	503	12/18	0.87	0.36	53,63,77,78	12
4	CM5	A	504	22/34	0.88	0.28	20,20,20,20	0
3	PB2	B	503	12/18	0.90	0.24	61,73,81,85	12
3	PB2	C	502	18/18	0.91	0.29	54,78,87,89	0
4	CM5	D	504	22/34	0.91	0.37	20,20,20,20	0
3	PB2	D	502	18/18	0.93	0.17	43,65,73,74	0
3	PB2	B	502	18/18	0.94	0.18	53,68,82,87	0
3	PB2	B	496	18/18	0.95	0.21	53,60,74,76	0
3	PB2	C	501	18/18	0.97	0.15	30,46,52,52	0
2	HEM	C	500	43/43	0.98	0.14	32,51,61,66	0
2	HEM	D	500	43/43	0.98	0.17	36,51,59,63	0
3	PB2	B	501	18/18	0.98	0.16	30,40,46,51	0
3	PB2	D	501	18/18	0.98	0.19	27,39,50,51	0
2	HEM	A	500	43/43	0.98	0.13	31,42,51,63	0
3	PB2	A	501	18/18	0.99	0.15	32,35,47,49	0
2	HEM	B	500	43/43	0.99	0.13	31,43,58,63	0

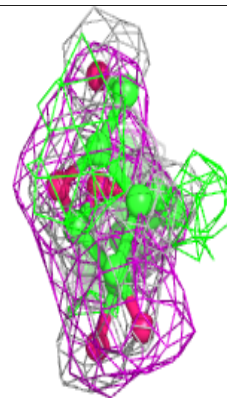
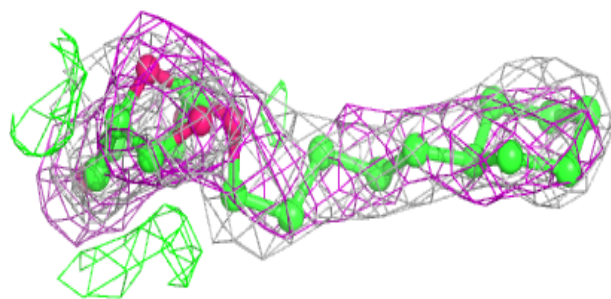
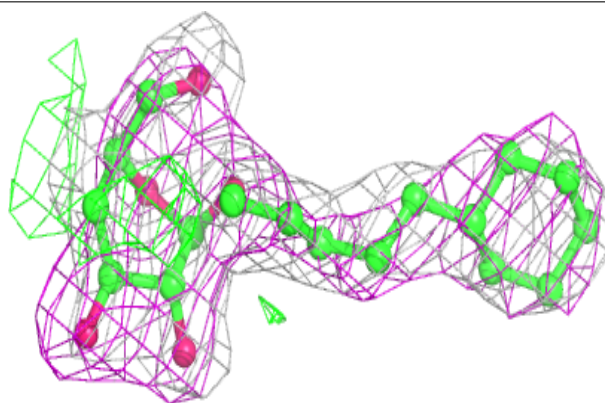
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CM5 B 504:

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

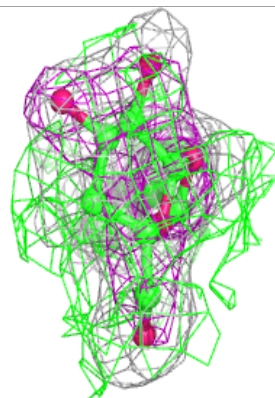
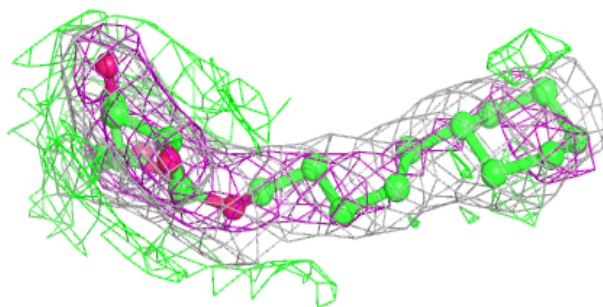
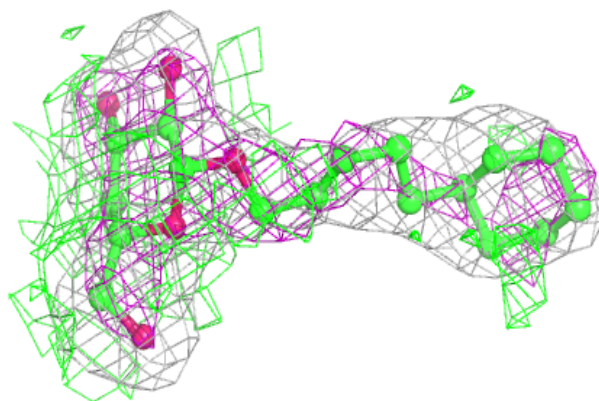
**Electron density around CM5 C 504:**

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

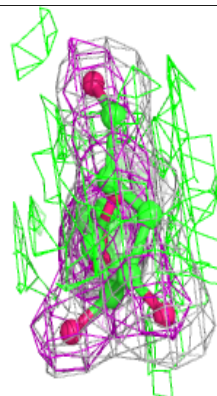
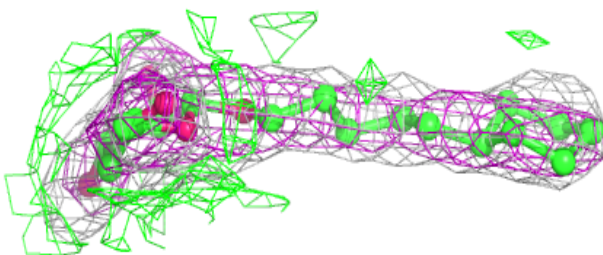
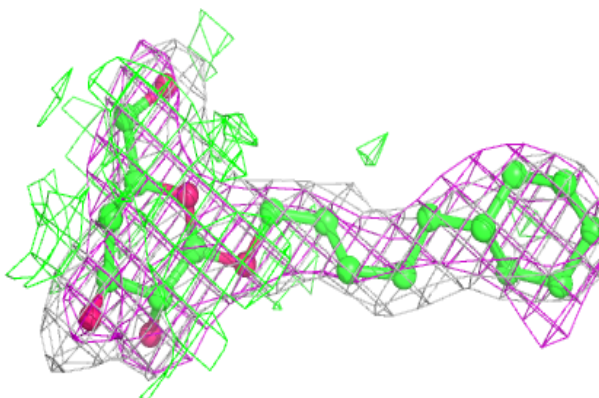


Electron density around CM5 A 504:

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

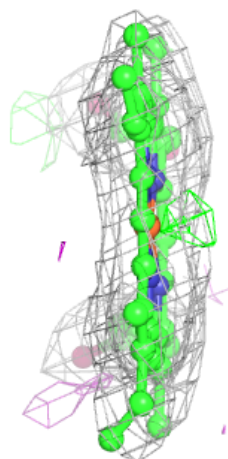
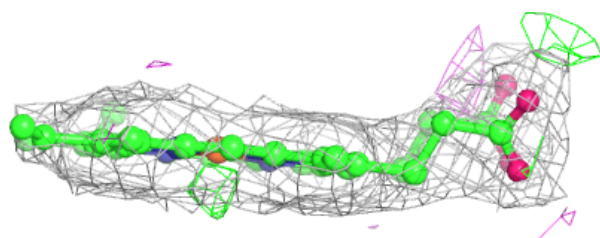
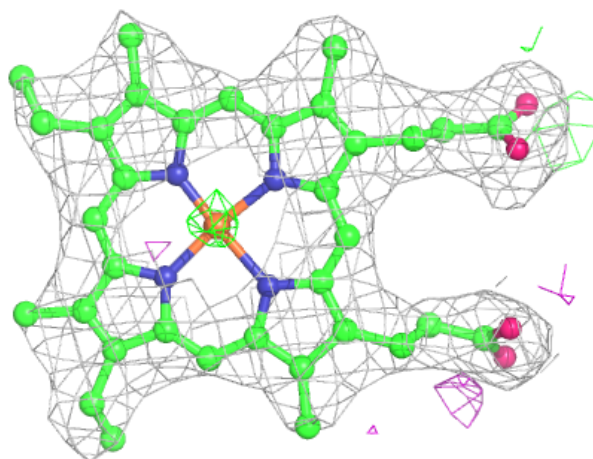
**Electron density around CM5 D 504:**

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



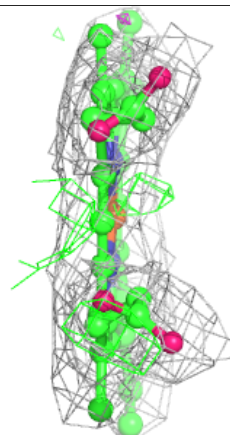
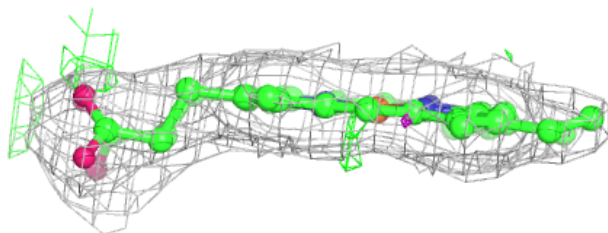
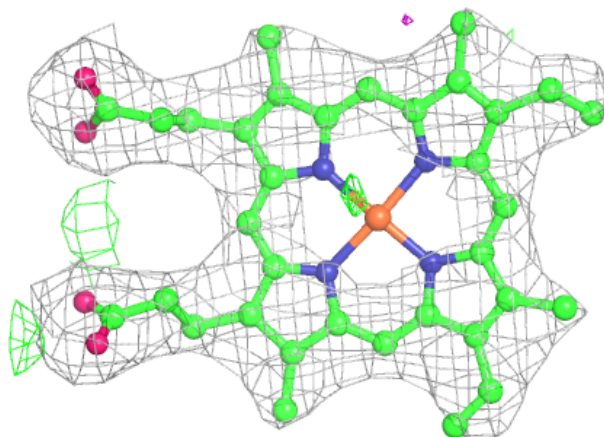
Electron density around HEM C 500:

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



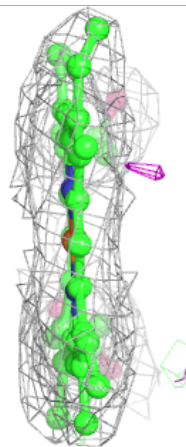
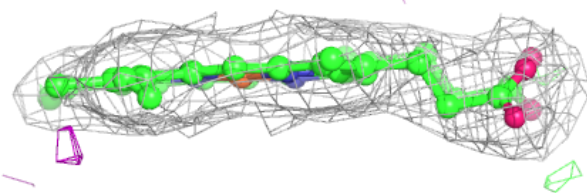
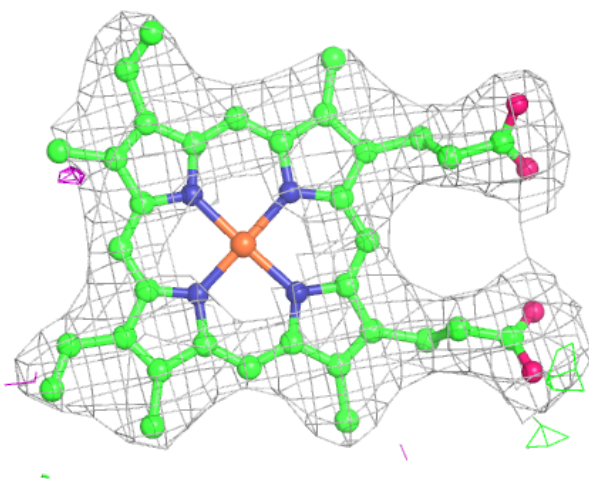
Electron density around HEM D 500:

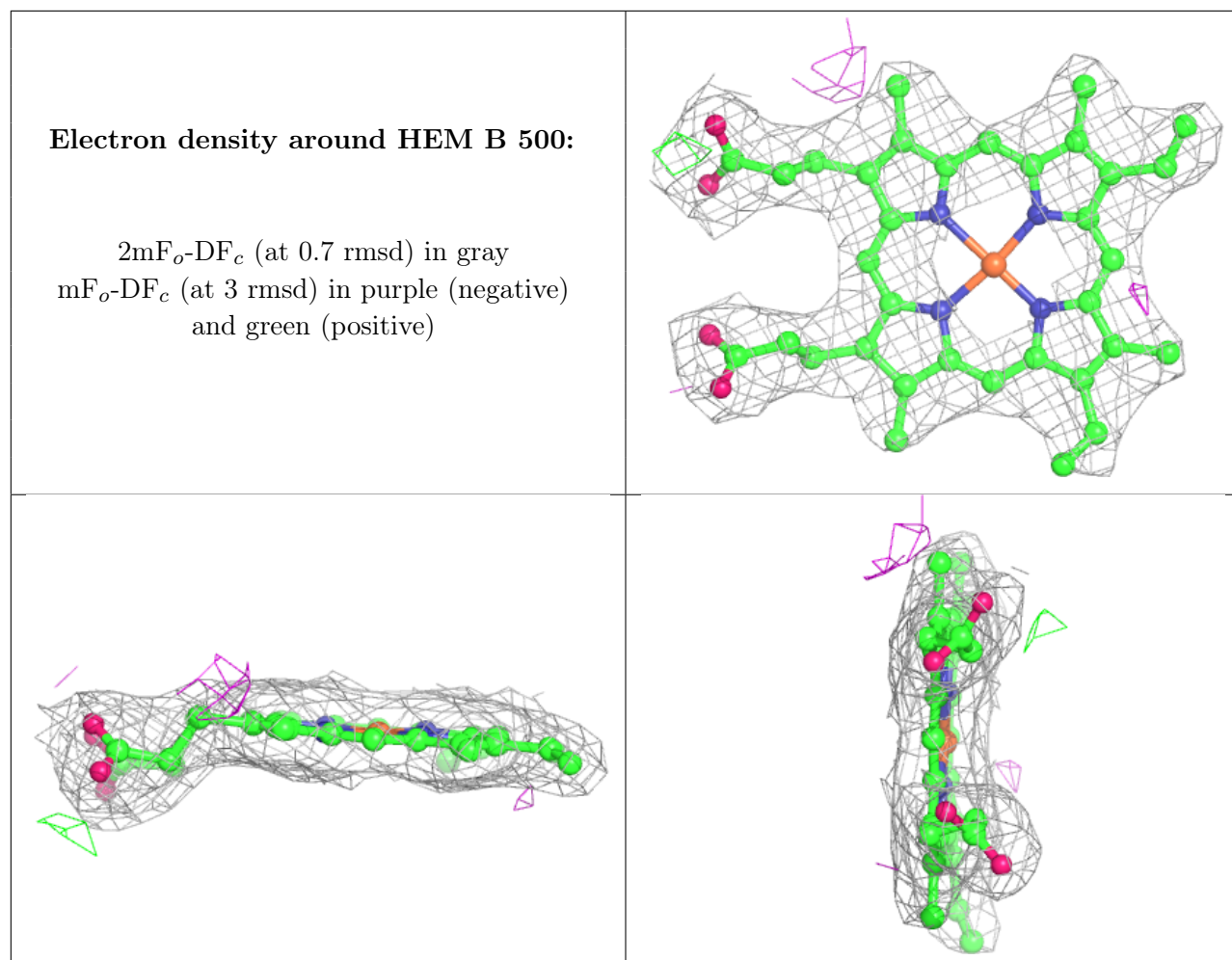
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 500:

$2mF_o-DF_c$ (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.