



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:47 pm BST

PDB ID : 4RQL  
Title : Crystal structure of a human cytochrome P450 2B6 (Y226H/K262R) in complex with a monoterpene - sabinene  
Authors : Shah, M.B.  
Deposited on : 2014-11-03  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

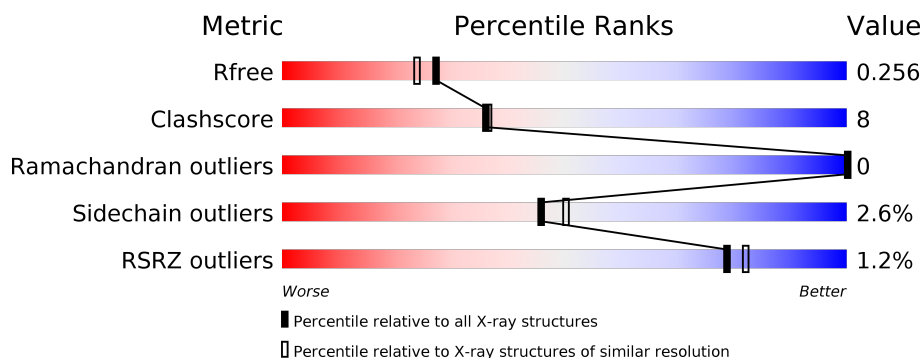
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	476	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; right: 0;">83%13%..</div> </div> </div>
1	B	476	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; right: 0;">84%13%..</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8202 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 2B6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3746	2426	643	661	16			
1	B	465	Total	C	N	O	S	0	0	0
			3753	2430	646	661	16			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	ENGINEERED MUTATION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	SER	DELETION	UNP P20813
A	?	-	VAL	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	PHE	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	ALA	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	THR	DELETION	UNP P20813
A	?	-	GLY	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	VAL	DELETION	UNP P20813
A	?	-	GLN	DELETION	UNP P20813
A	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
A	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
A	26	SER	THR	ENGINEERED MUTATION	UNP P20813

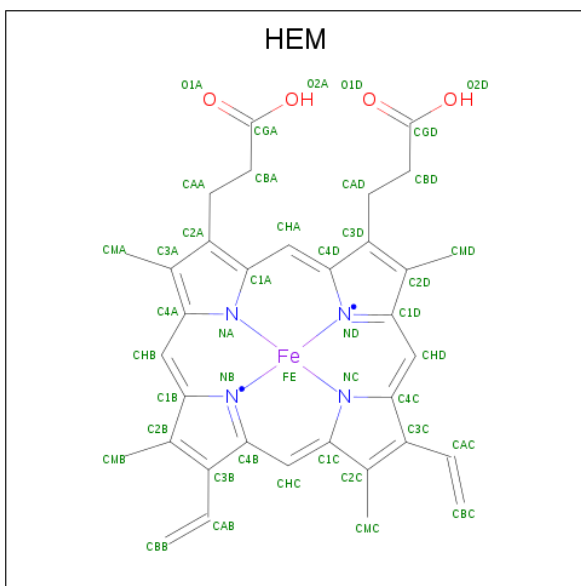
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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	29	LYS	ASP	ENGINEERED MUTATION	UNP P20813
A	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
A	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
A	492	HIS	-	EXPRESSION TAG	UNP P20813
A	493	HIS	-	EXPRESSION TAG	UNP P20813
A	494	HIS	-	EXPRESSION TAG	UNP P20813
A	495	HIS	-	EXPRESSION TAG	UNP P20813
B	21	ALA	GLU	ENGINEERED MUTATION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	SER	DELETION	UNP P20813
B	?	-	VAL	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	PHE	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	ALA	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	THR	DELETION	UNP P20813
B	?	-	GLY	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	VAL	DELETION	UNP P20813
B	?	-	GLN	DELETION	UNP P20813
B	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
B	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
B	26	SER	THR	ENGINEERED MUTATION	UNP P20813
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	29	LYS	ASP	ENGINEERED MUTATION	UNP P20813
B	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
B	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
B	492	HIS	-	EXPRESSION TAG	UNP P20813
B	493	HIS	-	EXPRESSION TAG	UNP P20813
B	494	HIS	-	EXPRESSION TAG	UNP P20813
B	495	HIS	-	EXPRESSION TAG	UNP P20813

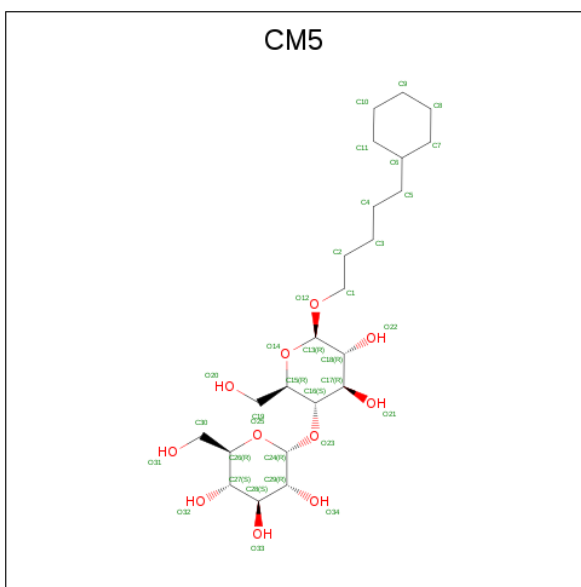
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



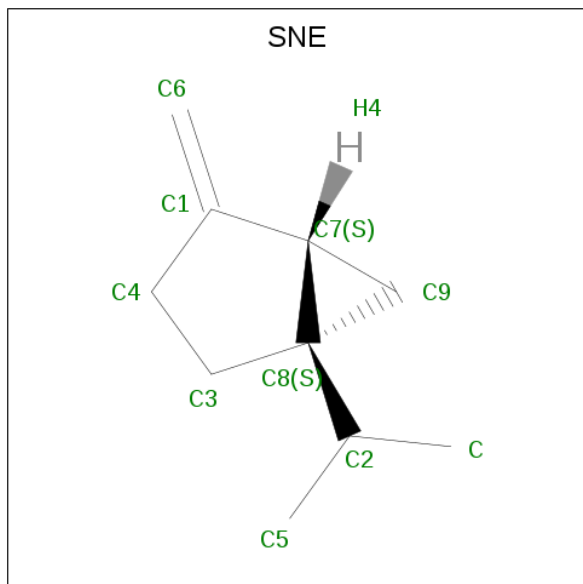
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (three-letter code: CM5) (formula:  $C_{23}H_{42}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			34	23	11		
3	A	1	Total	C	O	0	0
			34	23	11		
3	A	1	Total	C	O	0	0
			13	12	1		
3	B	1	Total	C	O	0	0
			34	23	11		
3	B	1	Total	C	O	0	0
			13	12	1		
3	B	1	Total	C	O	0	0
			13	12	1		

- Molecule 4 is Sabinene (three-letter code: SNE) (formula: C<sub>10</sub>H<sub>16</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			10	10		
4	B	1	Total	C	0	0
			10	10		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

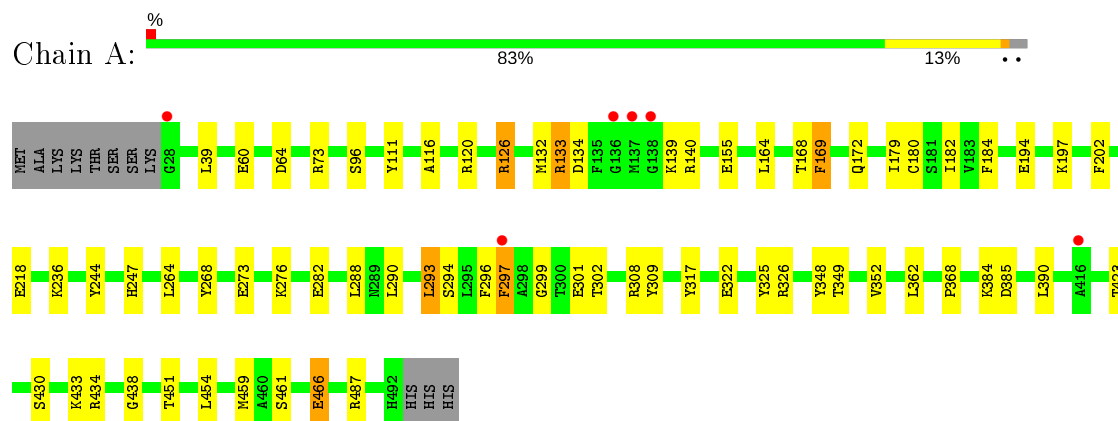
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	225	Total	O	0	0
			225	225		
6	B	223	Total	O	0	0
			223	223		

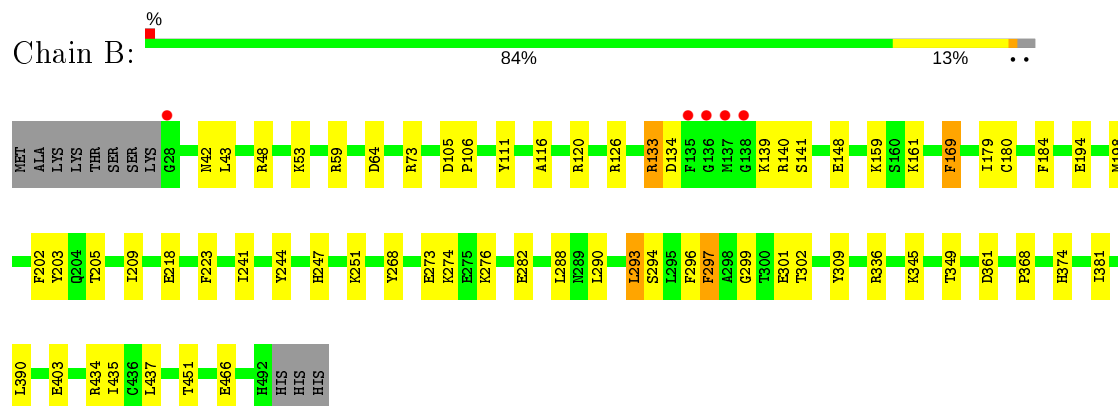
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Cytochrome P450 2B6



#### • Molecule 1: Cytochrome P450 2B6





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.33Å 78.33Å 202.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.86 – 2.10 24.86 – 2.11	Depositor EDS
% Data completeness (in resolution range)	96.0 (24.86-2.10) 95.9 (24.86-2.11)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.211 , 0.258 0.211 , 0.256	Depositor DCC
$R_{free}$ test set	3895 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 28.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.469 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CM5, SNE, EDO

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	1.15	6/3848 (0.2%)	0.90	2/5206 (0.0%)
1	B	1.12	4/3855 (0.1%)	0.91	4/5214 (0.1%)
All	All	1.13	10/7703 (0.1%)	0.90	6/10420 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	TYR	CD2-CE2	-5.91	1.30	1.39
1	A	294	SER	CB-OG	-5.80	1.34	1.42
1	B	294	SER	CB-OG	-5.79	1.34	1.42
1	A	466	GLU	CG-CD	5.72	1.60	1.51
1	A	155	GLU	CG-CD	5.57	1.60	1.51
1	B	203	TYR	CG-CD1	5.27	1.46	1.39
1	B	301	GLU	CD-OE1	-5.26	1.19	1.25
1	B	403	GLU	CG-CD	5.20	1.59	1.51
1	A	317	TYR	CD2-CE2	5.09	1.47	1.39
1	A	322	GLU	CB-CG	5.00	1.61	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	336	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	326	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	59	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	361	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	64	ASP	CB-CG-OD1	5.13	122.91	118.30

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	3746	0	3723	61	0
1	B	3753	0	3739	51	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
3	A	81	0	97	8	0
3	B	60	0	81	10	0
4	A	10	0	16	1	0
4	B	10	0	16	1	0
5	A	4	0	6	1	0
5	B	4	0	6	1	0
6	A	225	0	0	11	0
6	B	223	0	0	7	0
All	All	8202	0	7744	124	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 8.

All (124) 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)
3:A:502:CM5:C13	3:A:502:CM5:O12	1.63	1.43
3:B:503:CM5:C13	3:B:503:CM5:O12	1.63	1.43
3:A:503:CM5:C13	3:A:503:CM5:O12	1.63	1.43
1:B:435:ILE:HG23	6:B:715:HOH:O	1.54	1.07
1:A:126:ARG:NH1	1:A:126:ARG:HG2	1.60	0.99
1:A:126:ARG:HH11	1:A:126:ARG:CG	1.75	0.98
1:A:126:ARG:HH11	1:A:126:ARG:HG2	0.82	0.97
1:B:184:PHE:CE2	1:B:296:PHE:CE2	2.54	0.96
3:A:502:CM5:C1	3:A:502:CM5:C13	2.45	0.94
3:A:503:CM5:C13	3:A:503:CM5:C1	2.49	0.90
3:B:503:CM5:C1	3:B:503:CM5:C13	2.49	0.90
1:B:184:PHE:CE2	1:B:296:PHE:CZ	2.61	0.88
1:A:184:PHE:CE2	1:A:296:PHE:CE2	2.66	0.84
1:A:169:PHE:CE1	6:A:736:HOH:O	2.33	0.81
1:B:184:PHE:HE2	1:B:296:PHE:CZ	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PHE:CE2	1:A:296:PHE:CZ	2.69	0.80
1:A:273:GLU:OE2	1:A:276:LYS:HE2	1.87	0.74
1:A:116:ALA:O	1:A:434:ARG:NH2	2.20	0.73
1:A:169:PHE:CD2	6:A:647:HOH:O	2.41	0.72
1:A:184:PHE:HE2	1:A:296:PHE:CZ	2.07	0.72
1:B:247:HIS:CD2	1:B:251:LYS:HZ1	2.07	0.72
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.72	0.71
1:A:244:TYR:CD2	3:A:503:CM5:H72	2.27	0.70
1:B:184:PHE:HE2	1:B:296:PHE:CE2	2.04	0.67
1:A:169:PHE:CD1	6:A:736:HOH:O	2.48	0.66
1:B:169:PHE:CD2	6:B:639:HOH:O	2.50	0.65
1:B:247:HIS:CD2	1:B:251:LYS:NZ	2.65	0.65
1:B:111:TYR:HB2	1:B:290:LEU:HD12	1.82	0.62
1:A:133:ARG:NH2	6:A:779:HOH:O	2.28	0.62
1:A:111:TYR:HB2	1:A:290:LEU:HD12	1.79	0.62
1:A:169:PHE:HZ	6:A:735:HOH:O	1.84	0.61
1:A:133:ARG:HG3	1:A:134:ASP:OD1	2.01	0.60
1:B:184:PHE:CE2	1:B:296:PHE:HE2	2.16	0.60
1:A:60:GLU:HG2	6:A:618:HOH:O	2.00	0.60
1:B:349:THR:HG21	1:B:451:THR:HG22	1.83	0.60
1:B:244:TYR:CD2	3:B:503:CM5:H72	2.37	0.59
1:B:268:TYR:CE2	1:B:288:LEU:HB2	2.39	0.57
3:A:502:CM5:O34	3:A:502:CM5:H191	2.04	0.57
1:A:96:SER:CB	1:A:433:LYS:HD2	2.35	0.57
6:A:730:HOH:O	1:B:169:PHE:HE2	1.88	0.56
1:B:194:GLU:OE2	3:B:503:CM5:O22	2.23	0.56
1:B:244:TYR:HA	3:B:503:CM5:H192	1.88	0.56
1:B:202:PHE:CD1	1:B:297:PHE:CD1	2.93	0.55
1:A:197:LYS:HD3	6:A:739:HOH:O	2.05	0.55
1:A:132:MET:HE3	1:A:264:LEU:CD1	2.37	0.55
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.88	0.55
1:A:368:PRO:CG	5:A:506:EDO:H12	2.37	0.55
1:A:120:ARG:HA	1:A:282:GLU:HG3	1.89	0.54
1:B:434:ARG:O	2:B:501:HEM:HBA2	2.07	0.54
1:A:132:MET:HE3	1:A:264:LEU:HD13	1.90	0.54
1:B:141:SER:HB2	6:B:793:HOH:O	2.06	0.54
1:A:126:ARG:NH1	1:A:126:ARG:CG	2.44	0.53
1:A:236:LYS:HE3	6:A:660:HOH:O	2.08	0.53
1:A:132:MET:CE	1:A:182:ILE:HG21	2.38	0.52
1:A:169:PHE:HE1	6:A:736:HOH:O	1.82	0.52
1:A:390:LEU:HD22	1:A:390:LEU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:TYR:CE2	1:A:288:LEU:HB2	2.45	0.52
1:A:247:HIS:HB2	6:A:745:HOH:O	2.09	0.52
1:A:302:THR:CG2	4:A:505:SNE:H1	2.39	0.52
1:A:202:PHE:CD1	1:A:297:PHE:CD1	2.98	0.52
1:A:434:ARG:O	2:A:501:HEM:HBA2	2.11	0.51
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.39	0.51
1:A:132:MET:HE2	1:A:132:MET:HA	1.92	0.51
1:A:202:PHE:HD1	1:A:297:PHE:CD1	2.29	0.50
1:B:273:GLU:OE2	1:B:276:LYS:HE2	2.12	0.50
1:B:202:PHE:CE1	1:B:241:ILE:HD13	2.46	0.50
1:A:194:GLU:OE2	3:A:503:CM5:O22	2.29	0.50
1:B:126:ARG:NH1	6:B:752:HOH:O	2.44	0.50
1:B:198:MET:HG3	3:B:503:CM5:H52	1.93	0.49
1:B:223:PHE:HB2	3:B:505:CM5:H21A	1.94	0.49
1:A:349:THR:HG21	1:A:451:THR:HG22	1.95	0.49
1:A:184:PHE:CE2	1:A:296:PHE:HE2	2.28	0.49
1:A:184:PHE:HE2	1:A:296:PHE:CE2	2.21	0.49
1:A:466:GLU:H	1:A:466:GLU:CD	2.16	0.49
1:A:179:ILE:HG13	1:A:299:GLY:HA3	1.95	0.49
1:A:132:MET:HE2	1:A:182:ILE:HG21	1.96	0.48
1:B:73:ARG:NH2	1:B:218:GLU:HG3	2.28	0.48
1:A:454:LEU:HD21	1:A:459:MET:CE	2.44	0.48
1:B:105:ASP:N	1:B:106:PRO:CD	2.77	0.48
1:B:116:ALA:O	1:B:434:ARG:NH2	2.25	0.48
1:B:302:THR:CG2	4:B:502:SNE:H1	2.43	0.48
1:B:368:PRO:HG3	5:B:506:EDO:H21	1.95	0.47
1:B:133:ARG:NH1	6:B:630:HOH:O	2.42	0.47
1:A:430:SER:HB2	2:A:501:HEM:HBA1	1.97	0.46
1:A:164:LEU:HD23	1:A:487:ARG:HG3	1.97	0.46
3:A:502:CM5:H191	3:A:502:CM5:H28	1.97	0.46
1:A:438:GLY:HA3	2:A:501:HEM:C3C	2.50	0.46
1:B:120:ARG:HA	1:B:282:GLU:HG3	1.97	0.46
1:B:159:LYS:HE3	6:B:635:HOH:O	2.15	0.46
1:A:168:THR:HG23	1:A:308:ARG:HD2	1.98	0.46
1:B:345:LYS:HE2	1:B:345:LYS:HB2	1.70	0.45
1:A:293:LEU:HD12	1:A:293:LEU:O	2.16	0.45
1:B:140:ARG:HD2	1:B:148:GLU:OE2	2.16	0.45
1:B:293:LEU:HD12	1:B:293:LEU:O	2.16	0.45
1:A:172:GLN:NE2	1:A:301:GLU:OE2	2.49	0.45
1:B:179:ILE:HG13	1:B:299:GLY:HA3	1.99	0.45
1:B:194:GLU:CD	3:B:503:CM5:H22	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:THR:HG21	1:B:451:THR:CG2	2.48	0.44
1:B:179:ILE:HG23	1:B:179:ILE:HD12	1.67	0.44
1:A:430:SER:CB	2:A:501:HEM:HBA1	2.48	0.44
1:B:202:PHE:HD1	1:B:297:PHE:CD1	2.35	0.44
1:B:180:CYS:HG	1:B:296:PHE:HE1	1.59	0.44
1:B:274:LYS:HE2	1:B:274:LYS:HB2	1.84	0.44
1:A:180:CYS:HG	1:A:296:PHE:HE1	1.61	0.43
1:A:140:ARG:HB2	1:A:140:ARG:HE	1.37	0.43
1:B:194:GLU:CD	3:B:503:CM5:O22	2.57	0.43
1:B:437:LEU:C	1:B:437:LEU:HD12	2.39	0.43
1:B:42:ASN:O	1:B:43:LEU:C	2.57	0.42
1:A:302:THR:HG22	1:A:362:LEU:HD21	2.01	0.42
1:A:179:ILE:HD12	1:A:179:ILE:HG23	1.55	0.42
1:B:205:THR:HG22	1:B:209:ILE:CD1	2.50	0.42
1:A:454:LEU:HD21	1:A:459:MET:HE3	2.00	0.41
1:B:133:ARG:HG3	1:B:134:ASP:OD1	2.20	0.41
1:A:348:TYR:O	1:A:352:VAL:HG23	2.21	0.41
1:A:384:LYS:O	1:A:385:ASP:HB2	2.21	0.41
1:A:180:CYS:SG	1:A:296:PHE:HE1	2.44	0.41
1:B:179:ILE:HA	1:B:179:ILE:HD13	1.74	0.41
1:B:466:GLU:CD	1:B:466:GLU:H	2.24	0.41
3:B:503:CM5:H12	3:B:503:CM5:C13	2.47	0.41
1:A:180:CYS:SG	1:A:296:PHE:CE1	3.12	0.41
1:B:169:PHE:CD1	6:B:640:HOH:O	2.73	0.40
1:A:73:ARG:NH2	1:A:218:GLU:HG3	2.36	0.40
1:B:161:LYS:HD3	1:B:161:LYS:HA	1.93	0.40
1:A:454:LEU:HA	1:A:454:LEU:HD23	1.80	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	463/476 (97%)	452 (98%)	11 (2%)	0	100	100
1	B	463/476 (97%)	453 (98%)	10 (2%)	0	100	100
All	All	926/952 (97%)	905 (98%)	21 (2%)	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	403/418 (96%)	393 (98%)	10 (2%)	47	52
1	B	405/418 (97%)	394 (97%)	11 (3%)	44	48
All	All	808/836 (97%)	787 (97%)	21 (3%)	46	50

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	126	ARG
1	A	133	ARG
1	A	139	LYS
1	A	169	PHE
1	A	293	LEU
1	A	297	PHE
1	A	309	TYR
1	A	423	THR
1	A	461	SER
1	B	48	ARG
1	B	53	LYS
1	B	133	ARG
1	B	139	LYS
1	B	169	PHE
1	B	293	LEU
1	B	297	PHE
1	B	309	TYR

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Mol	Chain	Res	Type
1	B	374	HIS
1	B	381	ILE
1	B	390	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	HIS
1	B	247	HIS
1	B	374	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	CM5	A	504	-	13,13,36	1.02	0	14,14,49	0.65	0
5	EDO	B	506	-	3,3,3	0.50	0	2,2,2	0.94	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SNE	B	502	-	10,11,11	0.72	0	9,18,18	3.24	4 (44%)
3	CM5	A	503	-	36,36,36	3.41	15 (41%)	49,49,49	4.71	21 (42%)
3	CM5	B	503	-	36,36,36	3.28	14 (38%)	49,49,49	4.74	23 (46%)
3	CM5	B	504	-	13,13,36	1.11	0	14,14,49	1.08	2 (14%)
3	CM5	A	502	-	36,36,36	3.69	16 (44%)	49,49,49	4.74	21 (42%)
4	SNE	A	505	-	10,11,11	0.73	0	9,18,18	3.25	4 (44%)
2	HEM	A	501	1	27,50,50	1.94	6 (22%)	17,82,82	2.31	6 (35%)
5	EDO	A	506	-	3,3,3	0.51	0	2,2,2	0.59	0
3	CM5	B	505	-	13,13,36	1.07	1 (7%)	14,14,49	1.01	2 (14%)
2	HEM	B	501	1	27,50,50	2.03	8 (29%)	17,82,82	2.50	8 (47%)

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	CM5	A	504	-	-	4/7/15/65	0/1/1/3
5	EDO	B	506	-	-	1/1/1/1	-
4	SNE	B	502	-	-	3/6/24/24	0/2/2/2
3	CM5	A	503	-	-	4/17/65/65	0/3/3/3
3	CM5	B	503	-	-	4/17/65/65	0/3/3/3
3	CM5	B	504	-	-	2/7/15/65	0/1/1/3
3	CM5	A	502	-	-	6/17/65/65	0/3/3/3
4	SNE	A	505	-	-	3/6/24/24	0/2/2/2
2	HEM	A	501	1	-	0/6/54/54	-
5	EDO	A	506	-	-	1/1/1/1	-
3	CM5	B	505	-	-	4/7/15/65	0/1/1/3
2	HEM	B	501	1	-	0/6/54/54	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	CM5	O12-C13	13.84	1.63	1.40
3	A	503	CM5	O12-C13	13.82	1.63	1.40
3	A	502	CM5	O12-C13	13.79	1.63	1.40
3	A	502	CM5	O12-C1	-8.74	1.18	1.43
3	A	502	CM5	O22-C18	-5.69	1.29	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	CM5	O25-C24	5.67	1.56	1.41
3	A	503	CM5	O25-C24	5.66	1.56	1.41
3	A	503	CM5	O22-C18	-5.66	1.29	1.43
3	A	502	CM5	O25-C24	5.66	1.56	1.41
2	A	501	HEM	C3B-C2B	-5.08	1.33	1.40
3	A	502	CM5	C30-C26	-4.95	1.35	1.51
3	A	503	CM5	C30-C26	-4.94	1.35	1.51
3	B	503	CM5	C30-C26	-4.93	1.35	1.51
2	B	501	HEM	C3B-C2B	-4.62	1.34	1.40
2	B	501	HEM	C3D-C2D	4.41	1.50	1.37
3	A	503	CM5	O14-C13	-4.38	1.30	1.41
3	B	503	CM5	O14-C13	-4.38	1.30	1.41
3	A	502	CM5	O14-C13	-4.36	1.30	1.41
2	A	501	HEM	C3D-C2D	4.32	1.50	1.37
3	A	503	CM5	C16-C15	4.17	1.64	1.52
3	A	502	CM5	C16-C15	4.17	1.64	1.52
3	B	503	CM5	C16-C15	4.15	1.63	1.52
2	B	501	HEM	C3C-C2C	-4.08	1.34	1.40
3	B	503	CM5	C17-C16	3.82	1.62	1.52
3	A	503	CM5	C17-C16	3.79	1.62	1.52
3	A	502	CM5	O25-C26	3.76	1.53	1.44
3	A	503	CM5	O25-C26	3.76	1.53	1.44
3	A	502	CM5	C17-C16	3.75	1.62	1.52
3	B	503	CM5	O25-C26	3.74	1.53	1.44
3	A	502	CM5	O21-C17	3.30	1.50	1.43
3	A	503	CM5	O21-C17	3.27	1.50	1.43
3	B	503	CM5	O21-C17	3.25	1.50	1.43
2	A	501	HEM	C3C-CAC	3.24	1.54	1.47
3	B	503	CM5	O34-C29	3.21	1.50	1.43
3	A	502	CM5	O34-C29	3.20	1.50	1.43
3	A	503	CM5	O34-C29	3.19	1.50	1.43
2	A	501	HEM	C3C-C2C	-3.12	1.36	1.40
3	B	503	CM5	C29-C28	3.08	1.60	1.52
3	A	503	CM5	C29-C28	3.07	1.60	1.52
3	A	503	CM5	O23-C24	3.05	1.50	1.41
3	A	502	CM5	C29-C28	3.03	1.60	1.52
3	B	503	CM5	O23-C24	3.03	1.50	1.41
3	A	502	CM5	O23-C24	3.03	1.50	1.41
3	A	502	CM5	C27-C26	2.90	1.59	1.53
3	B	503	CM5	C27-C26	2.88	1.59	1.53
3	A	503	CM5	C27-C26	2.87	1.59	1.53
2	B	501	HEM	C3C-CAC	2.81	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-CAB	2.79	1.53	1.47
2	B	501	HEM	CMA-C3A	2.75	1.57	1.51
2	B	501	HEM	C3B-CAB	2.58	1.53	1.47
2	A	501	HEM	CMA-C3A	2.53	1.56	1.51
3	A	502	CM5	C28-C27	2.35	1.58	1.52
3	A	503	CM5	O23-C16	-2.35	1.37	1.43
3	B	503	CM5	C28-C27	2.33	1.58	1.52
3	A	502	CM5	O23-C16	-2.33	1.37	1.43
3	A	503	CM5	C28-C27	2.33	1.58	1.52
3	B	503	CM5	O23-C16	-2.32	1.37	1.43
2	B	501	HEM	CMC-C2C	2.10	1.56	1.51
2	B	501	HEM	C4B-CHC	-2.01	1.35	1.41
3	B	505	CM5	O12-C1	2.00	1.52	1.40

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	CM5	O33-C28-C27	-15.75	73.93	110.35
3	B	503	CM5	O33-C28-C27	-15.74	73.96	110.35
3	A	503	CM5	O33-C28-C27	-15.73	73.98	110.35
3	B	503	CM5	O23-C24-C29	-14.52	70.47	108.10
3	A	503	CM5	O23-C24-C29	-14.52	70.48	108.10
3	A	502	CM5	O23-C24-C29	-14.51	70.49	108.10
3	A	502	CM5	O14-C13-C18	11.56	134.82	110.35
3	A	503	CM5	O14-C13-C18	11.56	134.82	110.35
3	B	503	CM5	O14-C13-C18	11.54	134.78	110.35
3	A	503	CM5	O34-C29-C24	9.11	132.18	110.05
3	B	503	CM5	O34-C29-C24	9.10	132.15	110.05
3	A	502	CM5	O34-C29-C24	9.10	132.15	110.05
3	A	502	CM5	C24-O25-C26	8.72	130.81	113.69
3	B	503	CM5	C24-O25-C26	8.72	130.81	113.69
3	A	503	CM5	C24-O25-C26	8.71	130.78	113.69
3	A	502	CM5	C24-C29-C28	8.59	127.88	110.00
3	B	503	CM5	C24-C29-C28	8.59	127.88	110.00
3	A	503	CM5	C24-C29-C28	8.58	127.86	110.00
3	A	502	CM5	O21-C17-C18	-7.07	94.01	110.35
3	A	503	CM5	O21-C17-C18	-7.07	94.01	110.35
3	B	503	CM5	O21-C17-C18	-7.05	94.04	110.35
4	A	505	SNE	C4-C1-C7	6.14	115.07	108.31
4	B	502	SNE	C4-C1-C7	6.14	115.06	108.31
3	B	503	CM5	O34-C29-C28	-5.87	96.78	110.35
3	A	503	CM5	O34-C29-C28	-5.86	96.79	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	CM5	O34-C29-C28	-5.85	96.81	110.35
4	A	505	SNE	C9-C7-C1	-5.59	110.03	117.62
4	B	502	SNE	C9-C7-C1	-5.56	110.07	117.62
2	B	501	HEM	CAA-CBA-CGA	-5.04	104.21	112.67
3	B	503	CM5	O32-C27-C28	-4.77	99.32	110.35
3	A	503	CM5	O32-C27-C28	-4.75	99.36	110.35
3	A	502	CM5	O32-C27-C28	-4.74	99.38	110.35
2	A	501	HEM	CAA-CBA-CGA	-4.56	105.02	112.67
2	B	501	HEM	CBD-CAD-C3D	-4.15	104.83	112.48
3	B	503	CM5	O23-C16-C15	3.99	120.38	109.45
3	B	503	CM5	C19-C15-C16	-3.99	101.72	113.33
3	A	503	CM5	O23-C16-C15	3.99	120.37	109.45
3	A	502	CM5	O23-C16-C15	3.98	120.36	109.45
3	A	503	CM5	C19-C15-C16	-3.98	101.75	113.33
3	A	502	CM5	C19-C15-C16	-3.97	101.77	113.33
3	A	503	CM5	O23-C16-C17	3.96	117.82	107.28
3	A	502	CM5	O23-C16-C17	3.96	117.81	107.28
3	B	503	CM5	O23-C16-C17	3.95	117.79	107.28
3	B	503	CM5	C1-O12-C13	-3.79	107.55	113.84
3	A	503	CM5	C1-O12-C13	-3.78	107.57	113.84
2	B	501	HEM	CAD-CBD-CGD	-3.77	106.35	112.67
3	A	503	CM5	O32-C27-C26	3.73	118.56	109.30
3	B	503	CM5	O32-C27-C26	3.72	118.53	109.30
3	A	502	CM5	O32-C27-C26	3.71	118.50	109.30
4	B	502	SNE	C7-C1-C6	-3.70	122.46	126.16
4	A	505	SNE	C7-C1-C6	-3.67	122.49	126.16
2	B	501	HEM	C1D-C2D-C3D	-3.59	104.50	107.00
3	A	502	CM5	C1-O12-C13	3.58	119.78	113.84
2	A	501	HEM	CBD-CAD-C3D	-3.58	105.88	112.48
3	B	503	CM5	C28-C27-C26	3.51	116.51	110.24
3	A	503	CM5	C28-C27-C26	3.51	116.50	110.24
3	A	502	CM5	C28-C27-C26	3.50	116.48	110.24
3	B	503	CM5	O25-C26-C30	3.36	114.79	106.44
3	A	502	CM5	O25-C26-C30	3.36	114.78	106.44
3	A	503	CM5	O25-C26-C30	3.36	114.78	106.44
2	A	501	HEM	CAD-CBD-CGD	-3.33	107.08	112.67
2	A	501	HEM	C1D-C2D-C3D	-3.32	104.69	107.00
3	A	502	CM5	C24-O23-C16	3.15	125.75	117.96
3	A	503	CM5	C24-O23-C16	3.13	125.70	117.96
3	B	503	CM5	C24-O23-C16	3.12	125.67	117.96
3	B	503	CM5	O14-C15-C16	3.10	116.29	109.75
3	A	503	CM5	O14-C15-C16	3.10	116.29	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	CM5	O14-C15-C16	3.09	116.27	109.75
2	A	501	HEM	CMA-C3A-C4A	-3.00	123.85	128.46
2	A	501	HEM	C4A-C3A-C2A	3.00	109.08	107.00
4	A	505	SNE	C4-C1-C6	-2.96	122.45	125.51
4	B	502	SNE	C4-C1-C6	-2.93	122.48	125.51
2	B	501	HEM	CMA-C3A-C4A	-2.92	123.97	128.46
3	B	503	CM5	O22-C18-C17	-2.88	103.69	110.35
3	B	503	CM5	O25-C26-C27	2.79	114.76	109.69
3	A	503	CM5	O25-C26-C27	2.79	114.76	109.69
3	A	502	CM5	O25-C26-C27	2.78	114.74	109.69
3	B	503	CM5	O21-C17-C16	-2.52	103.27	109.94
3	A	503	CM5	O21-C17-C16	-2.51	103.29	109.94
3	A	502	CM5	O21-C17-C16	-2.49	103.34	109.94
3	B	503	CM5	O22-C18-C13	-2.49	104.00	110.05
2	B	501	HEM	CMD-C2D-C3D	2.49	129.63	124.94
3	A	502	CM5	C29-C28-C27	2.38	114.98	110.82
3	A	503	CM5	C29-C28-C27	2.38	114.97	110.82
3	B	503	CM5	C29-C28-C27	2.35	114.93	110.82
3	B	504	CM5	C10-C11-C6	2.25	116.40	112.15
2	B	501	HEM	C4A-C3A-C2A	2.20	108.53	107.00
3	B	505	CM5	C11-C6-C7	-2.14	104.09	109.33
3	B	504	CM5	O12-C1-C2	2.10	119.16	109.94
3	B	505	CM5	O12-C1-C2	2.05	118.97	109.94
2	B	501	HEM	CMC-C2C-C3C	2.02	128.46	124.68

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	502	SNE	C-C2-C8-C9
4	B	502	SNE	C5-C2-C8-C9
4	A	505	SNE	C-C2-C8-C9
4	A	505	SNE	C5-C2-C8-C9
3	A	502	CM5	C18-C13-O12-C1
3	A	502	CM5	O25-C24-O23-C16
3	A	502	CM5	C3-C4-C5-C6
3	B	504	CM5	O12-C1-C2-C3
3	A	502	CM5	C2-C3-C4-C5
3	A	502	CM5	O14-C13-O12-C1
3	A	504	CM5	C1-C2-C3-C4
3	B	505	CM5	C1-C2-C3-C4
3	B	505	CM5	C2-C3-C4-C5

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
5	B	506	EDO	O1-C1-C2-O2
5	A	506	EDO	O1-C1-C2-O2
3	A	504	CM5	C4-C5-C6-C7
3	A	503	CM5	C17-C16-O23-C24
3	A	502	CM5	C17-C16-O23-C24
3	B	505	CM5	C2-C1-O12-C13
3	B	504	CM5	C1-C2-C3-C4
3	A	504	CM5	C4-C5-C6-C11
3	B	505	CM5	C4-C5-C6-C11
3	A	503	CM5	O14-C13-O12-C1
3	B	503	CM5	O14-C13-O12-C1
3	A	503	CM5	C1-C2-C3-C4
3	B	503	CM5	C1-C2-C3-C4
3	B	503	CM5	C17-C16-O23-C24
3	A	504	CM5	O12-C1-C2-C3
4	B	502	SNE	C-C2-C8-C7
4	A	505	SNE	C-C2-C8-C7
3	A	503	CM5	O12-C1-C2-C3
3	B	503	CM5	O12-C1-C2-C3

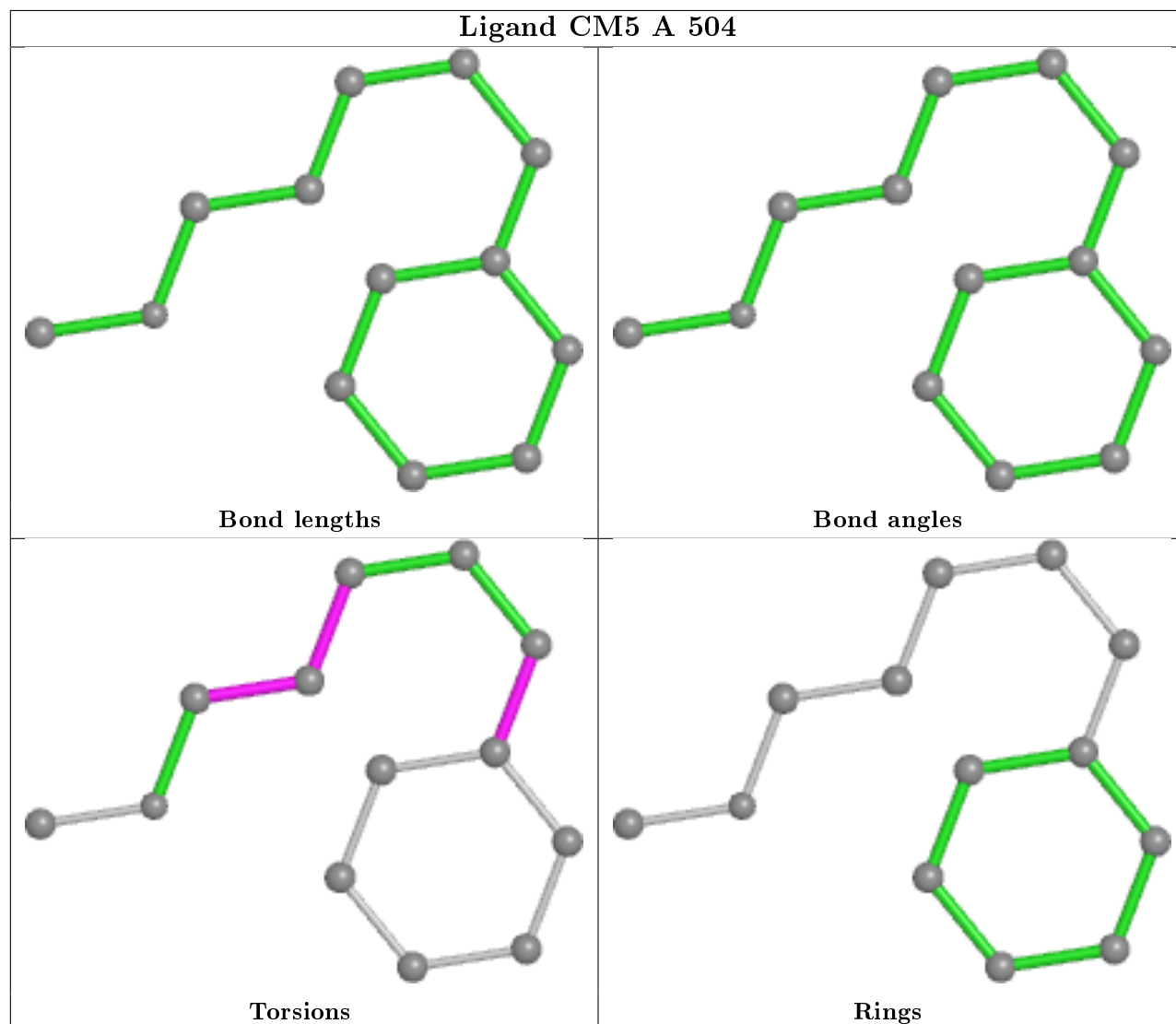
There are no ring outliers.

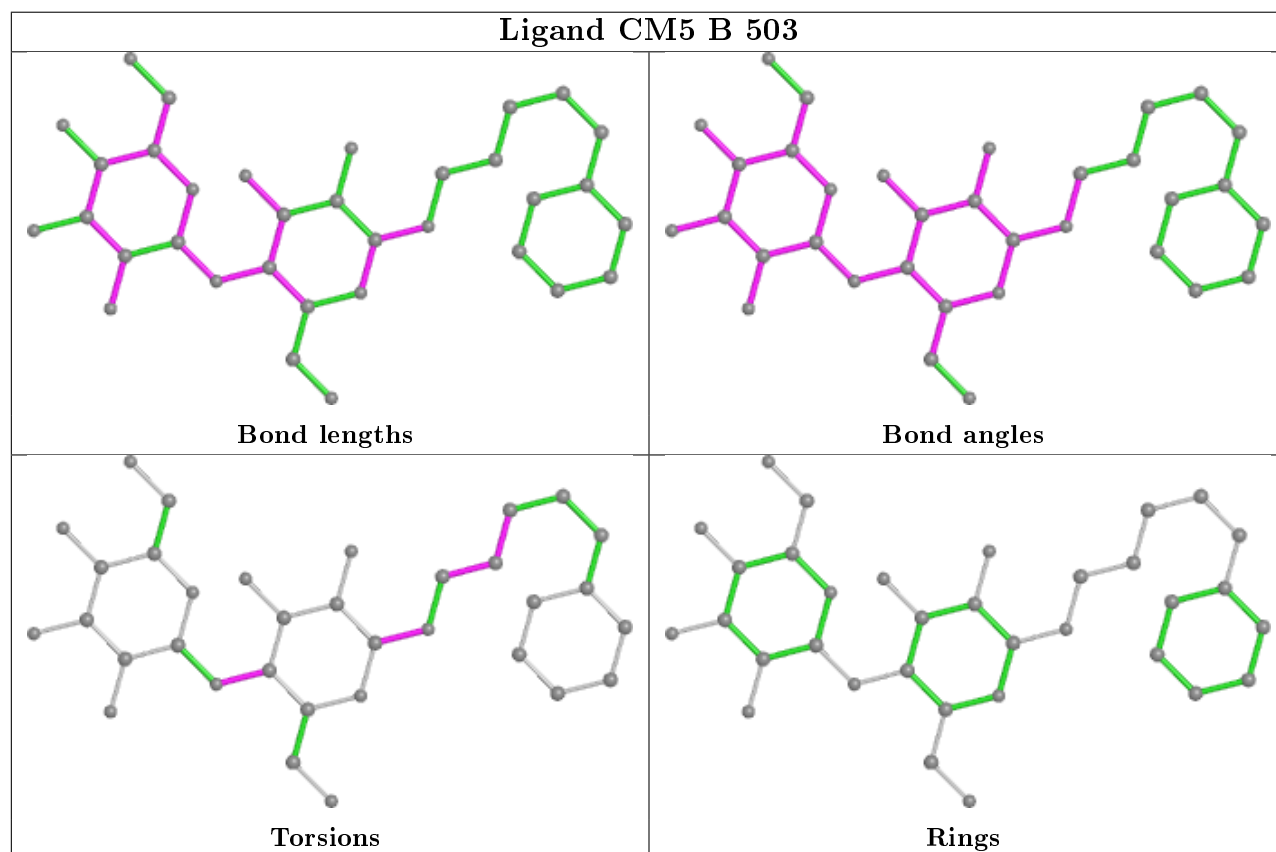
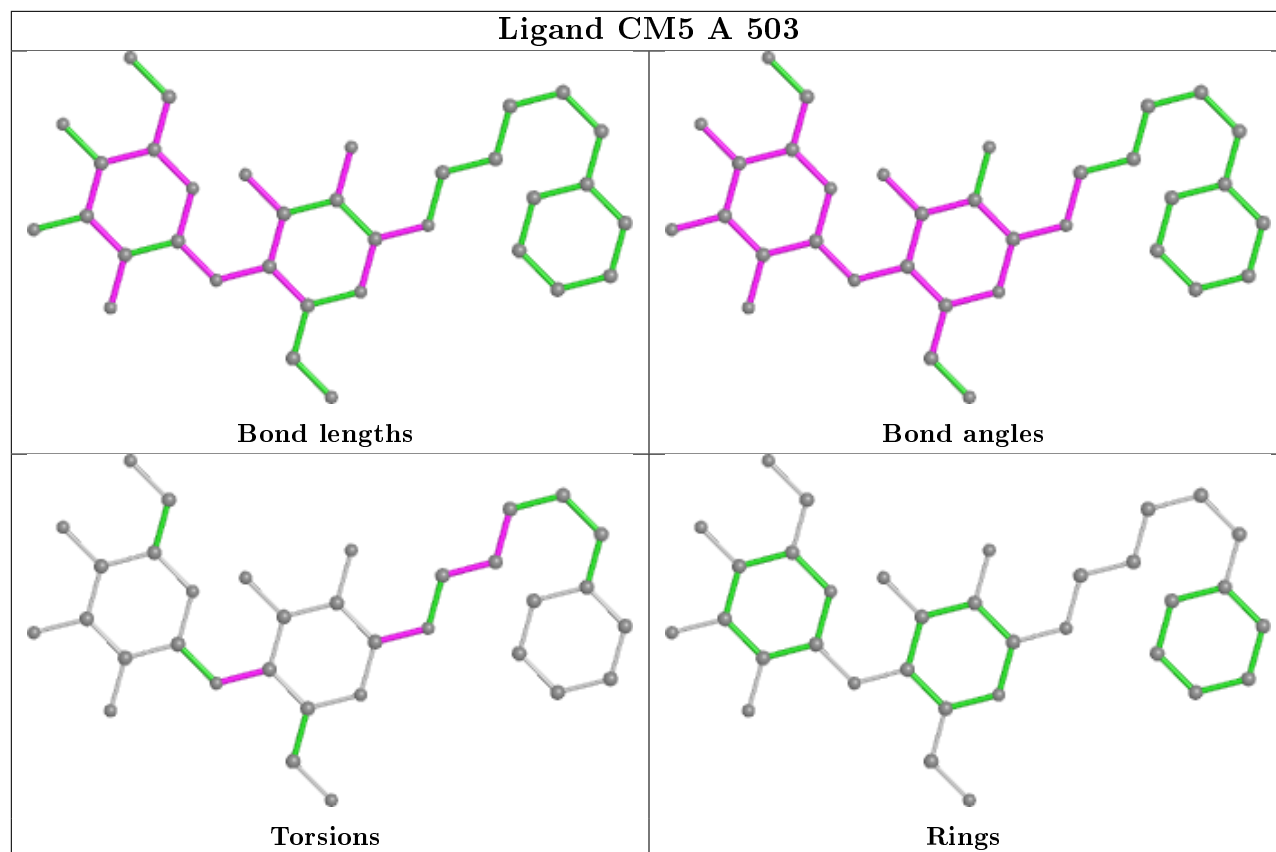
10 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	506	EDO	1	0
4	B	502	SNE	1	0
3	A	503	CM5	4	0
3	B	503	CM5	9	0
3	A	502	CM5	4	0
4	A	505	SNE	1	0
2	A	501	HEM	5	0
5	A	506	EDO	1	0
3	B	505	CM5	1	0
2	B	501	HEM	3	0

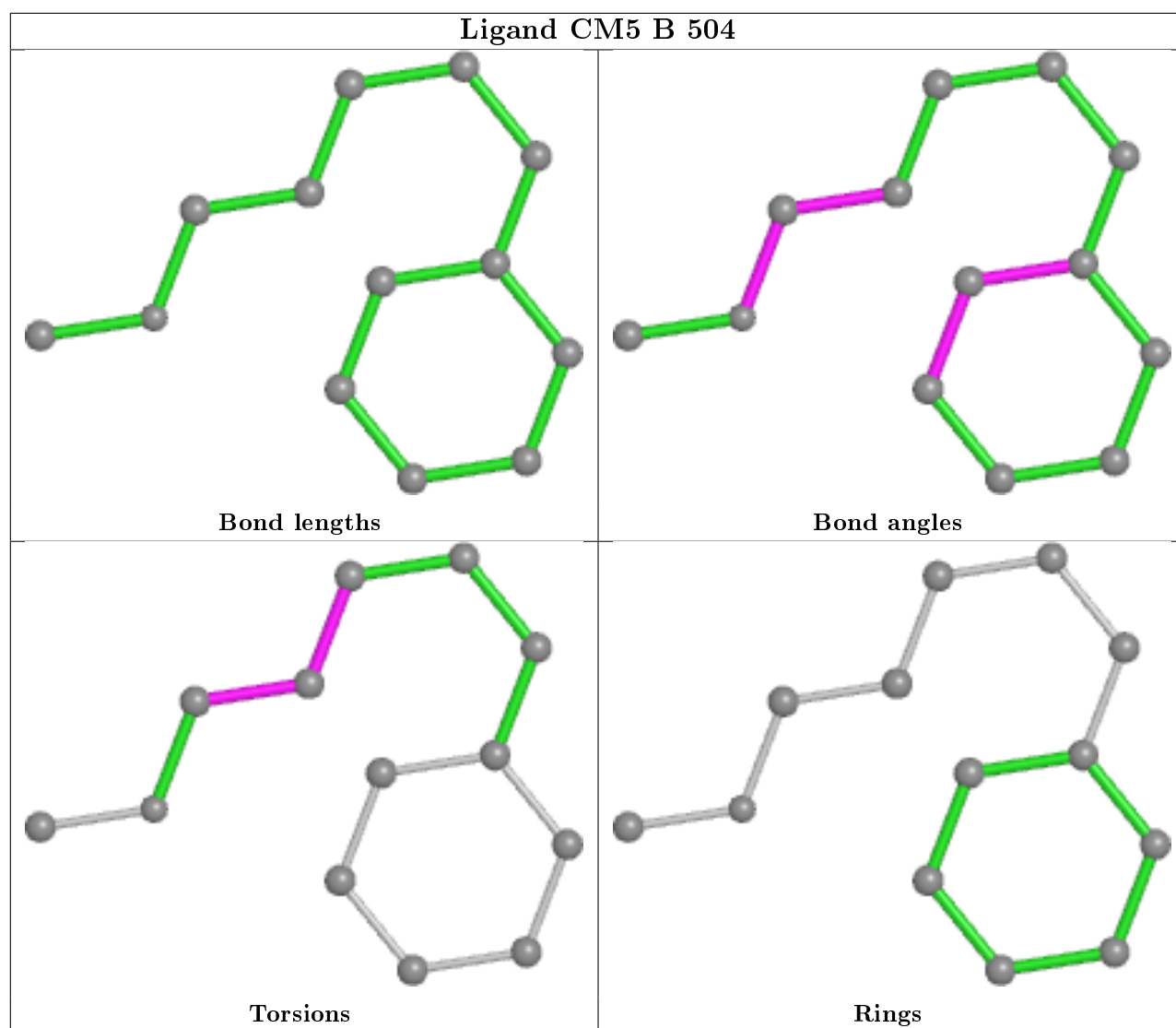
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

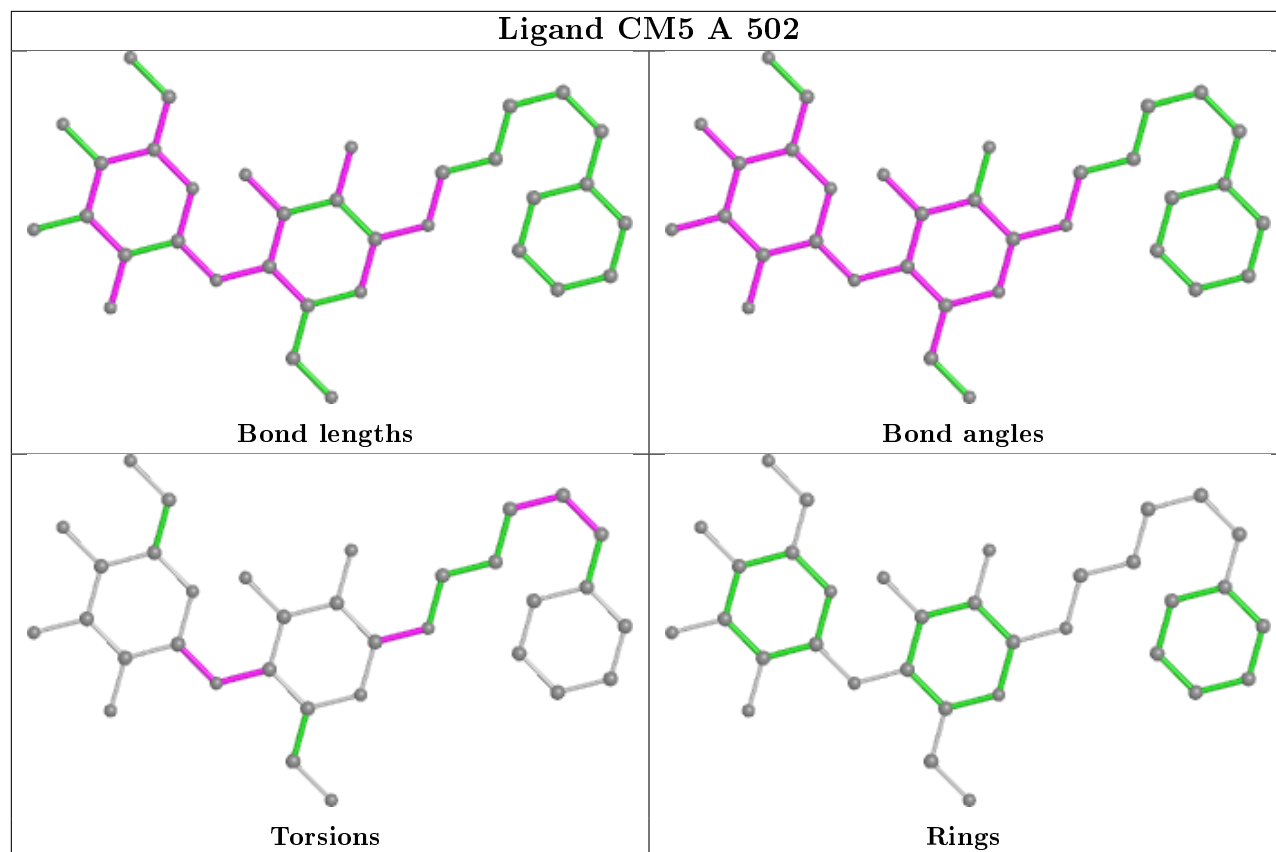
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

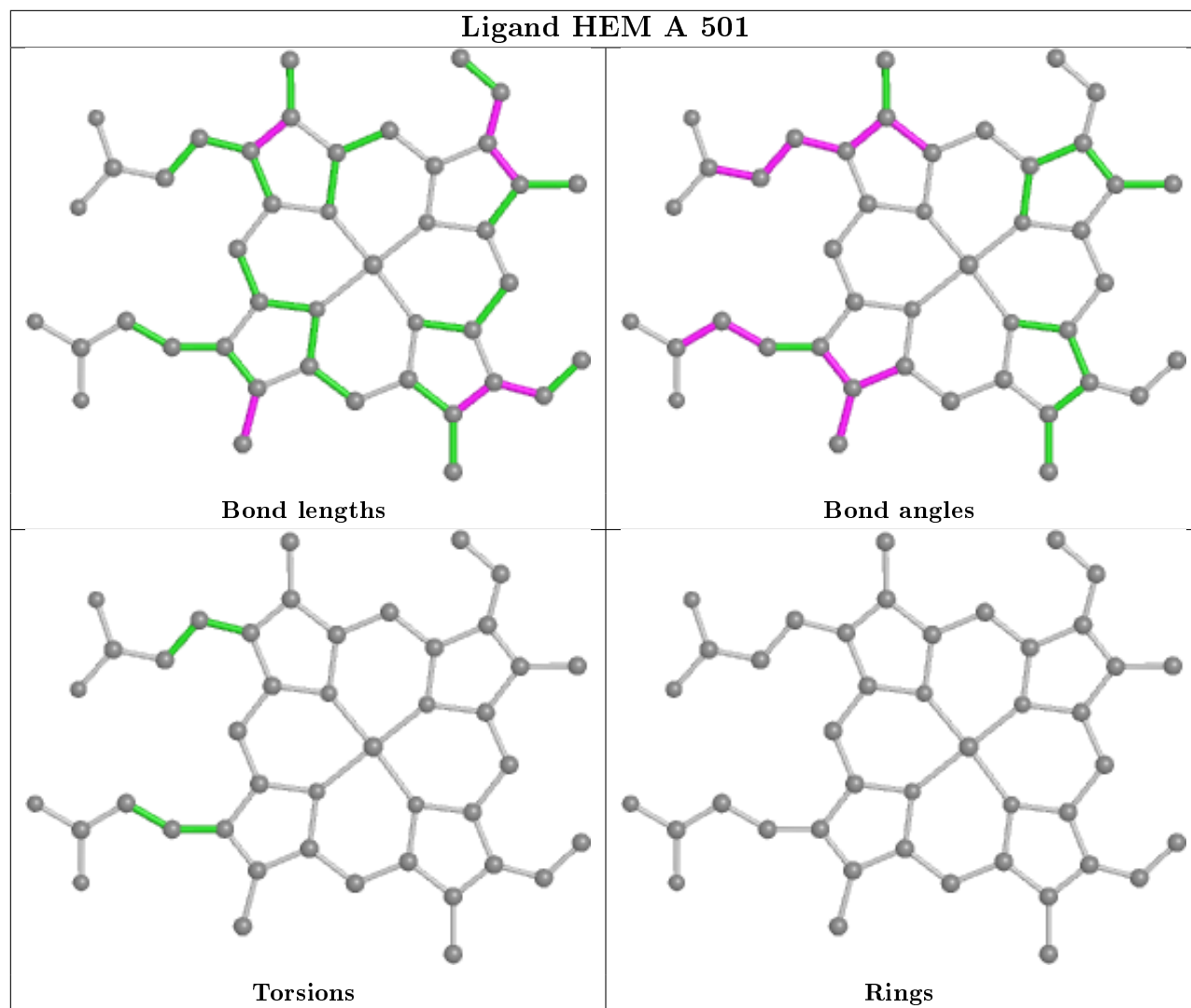


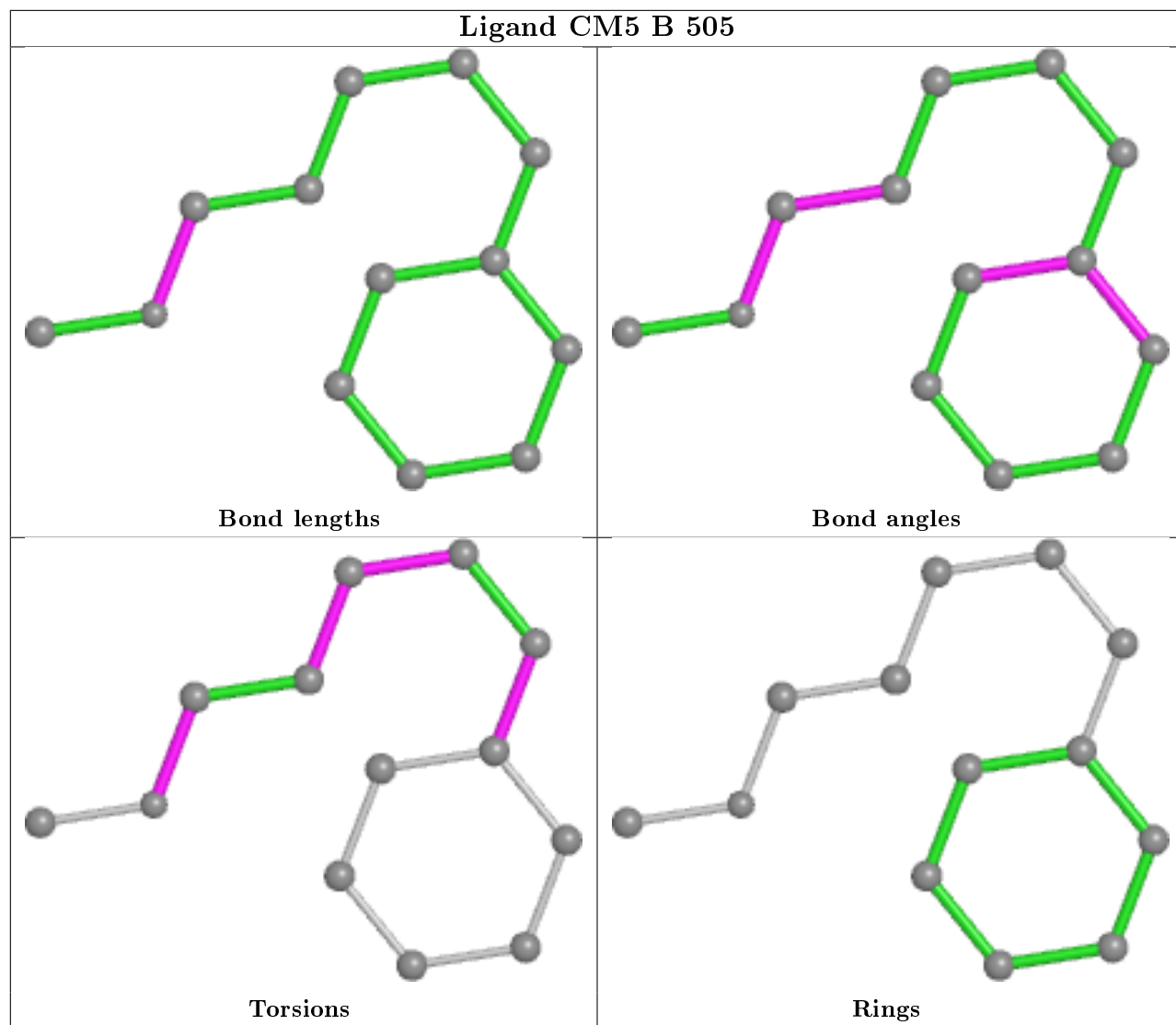


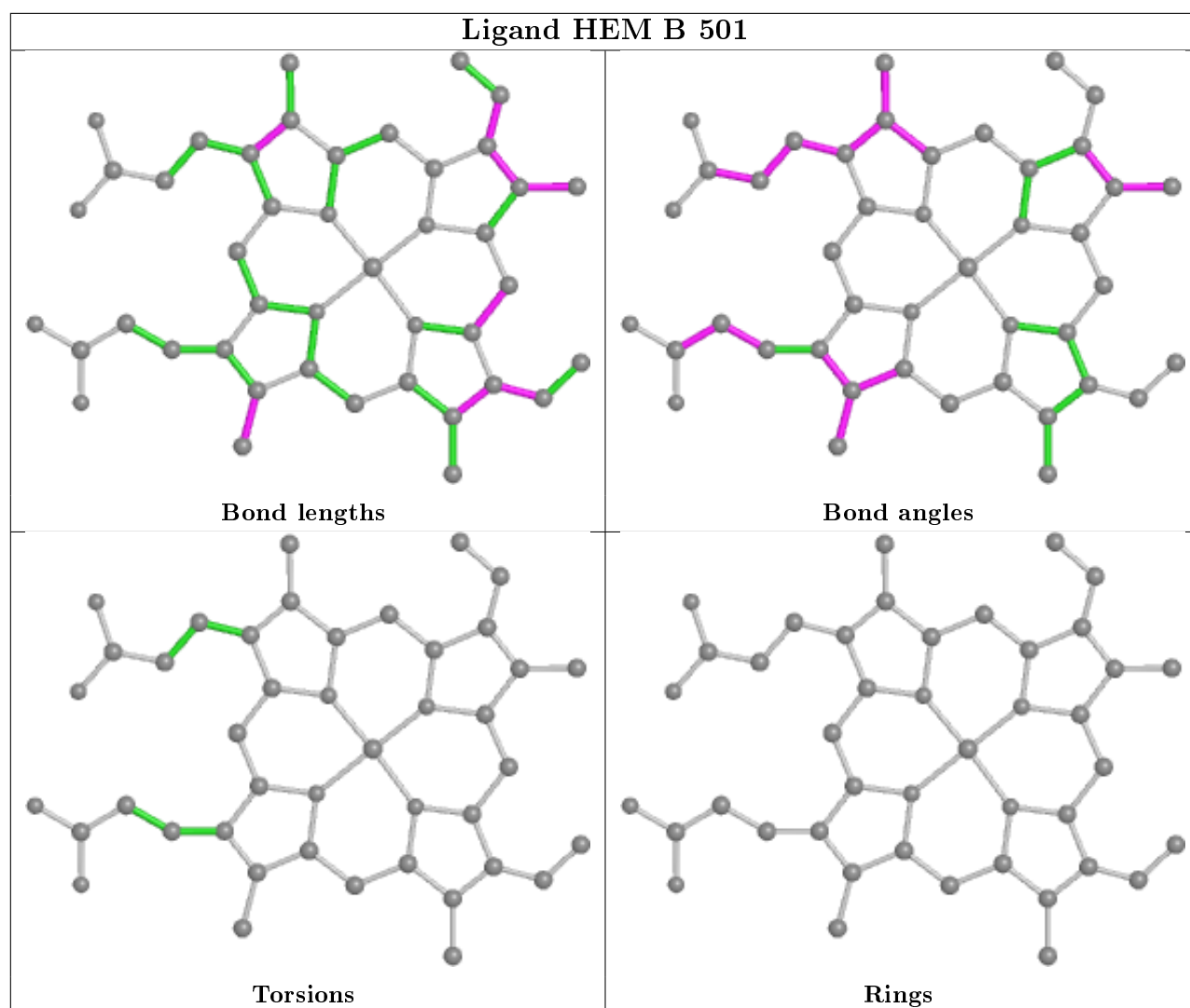












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	465/476 (97%)	-0.23	6 (1%) 77 80	14, 23, 41, 66	8 (1%)
1	B	465/476 (97%)	-0.23	5 (1%) 80 84	14, 23, 42, 65	8 (1%)
All	All	930/952 (97%)	-0.23	11 (1%) 79 82	14, 23, 41, 66	16 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	GLY	4.2
1	B	138	GLY	3.6
1	A	137	MET	3.4
1	B	137	MET	2.9
1	B	136	GLY	2.8
1	A	138	GLY	2.7
1	A	28	GLY	2.4
1	A	297	PHE	2.3
1	B	135	PHE	2.2
1	B	28	GLY	2.0
1	A	416	ALA	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 carbohydrates in this entry.

## 6.4 Ligands

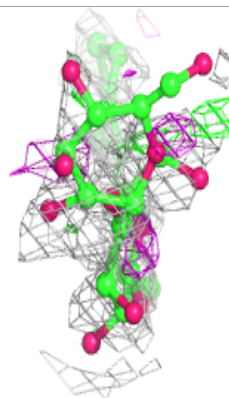
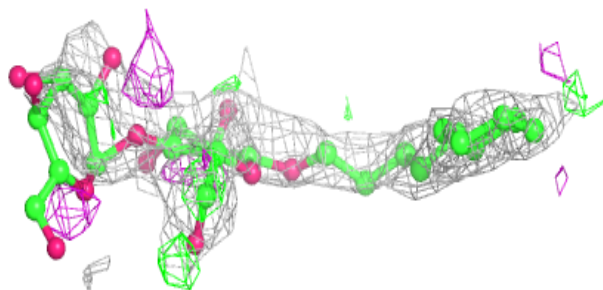
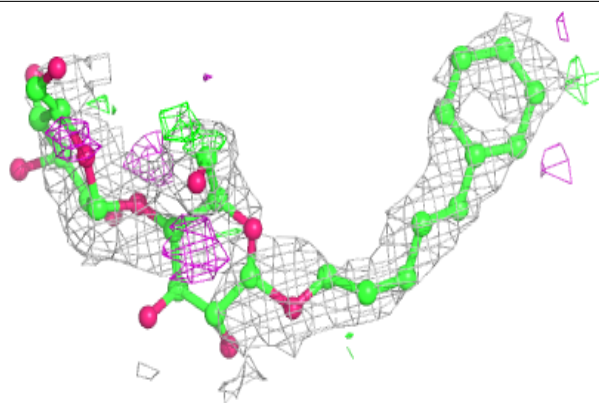
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CM5	B	503	34/34	0.55	0.38	52,90,100,101	0
3	CM5	A	503	34/34	0.59	0.36	47,83,94,94	0
3	CM5	A	502	34/34	0.70	0.31	59,97,109,109	0
3	CM5	B	504	13/34	0.70	0.34	57,63,76,77	0
3	CM5	A	504	13/34	0.74	0.32	55,62,83,84	0
4	SNE	A	505	10/10	0.76	0.33	53,55,55,56	0
4	SNE	B	502	10/10	0.78	0.32	53,55,55,56	0
3	CM5	B	505	13/34	0.79	0.23	53,54,62,64	0
5	EDO	A	506	4/4	0.93	0.22	45,46,46,51	0
5	EDO	B	506	4/4	0.93	0.24	42,45,47,50	0
2	HEM	A	501	43/43	0.98	0.11	9,15,20,29	0
2	HEM	B	501	43/43	0.98	0.10	9,15,18,28	0

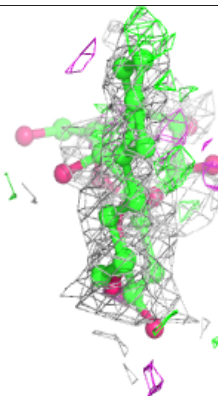
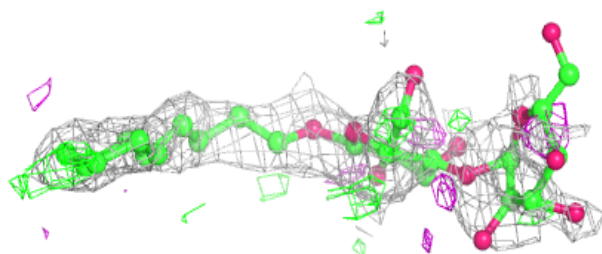
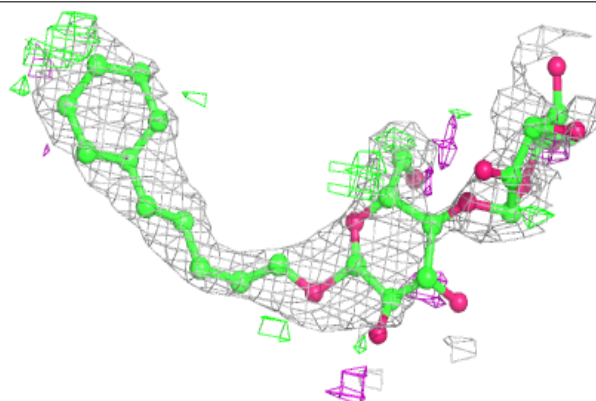
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CM5 B 503:**

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

**Electron density around CM5 A 503:**

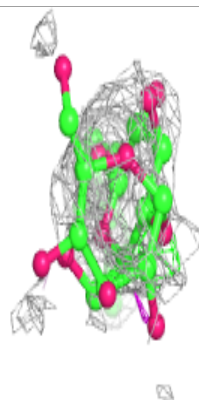
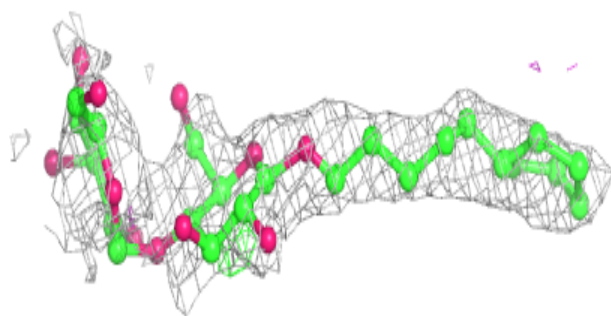
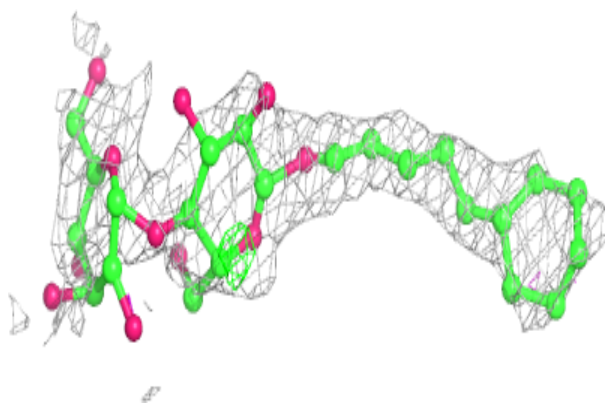
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



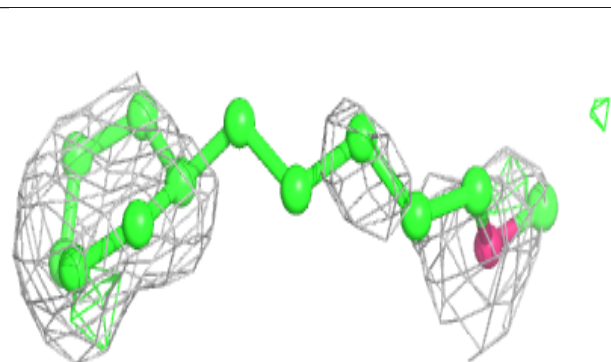
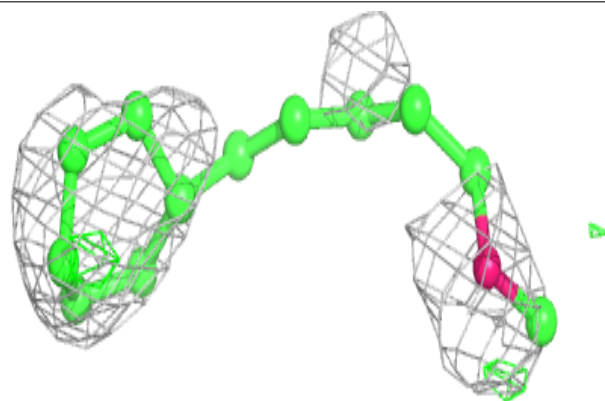


**Electron density around CM5 A 502:**

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

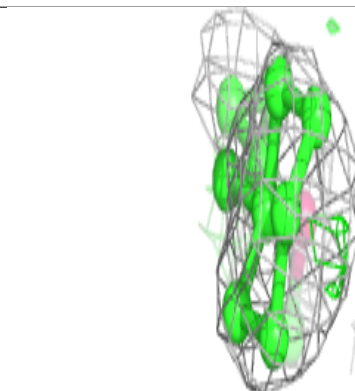
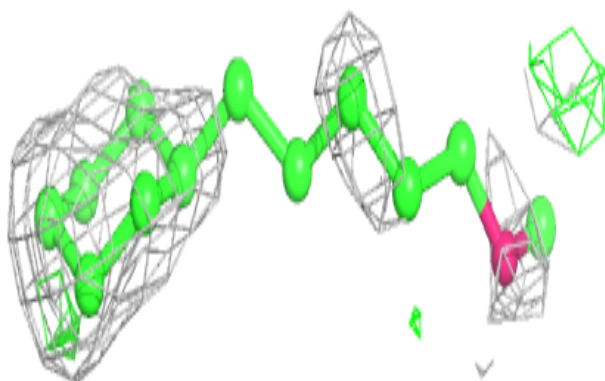
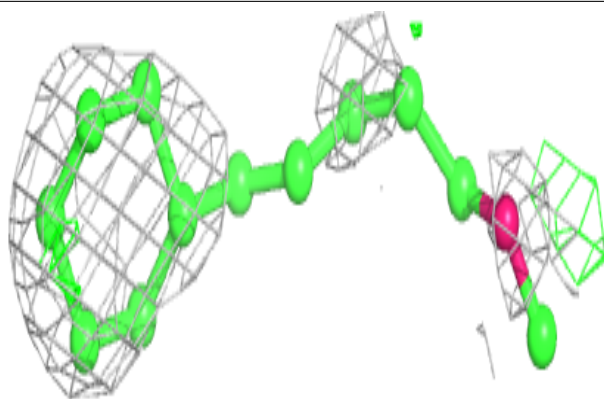
**Electron density around CM5 B 504:**

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

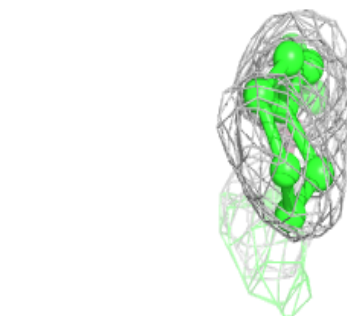
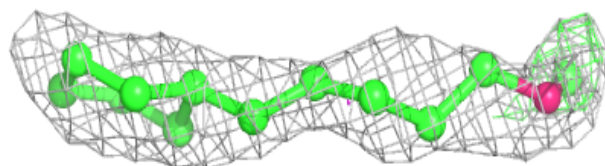
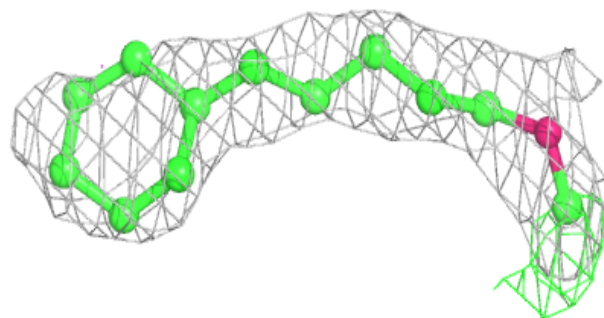


**Electron density around CM5 A 504:**

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

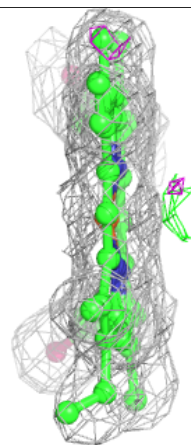
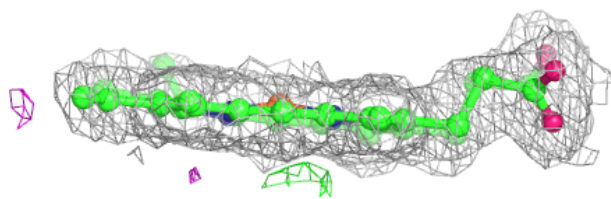
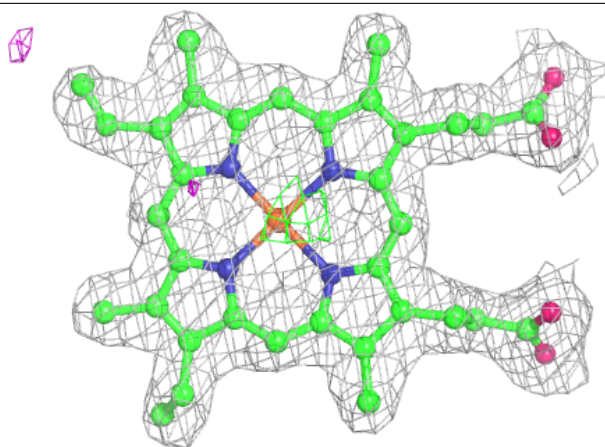
**Electron density around CM5 B 505:**

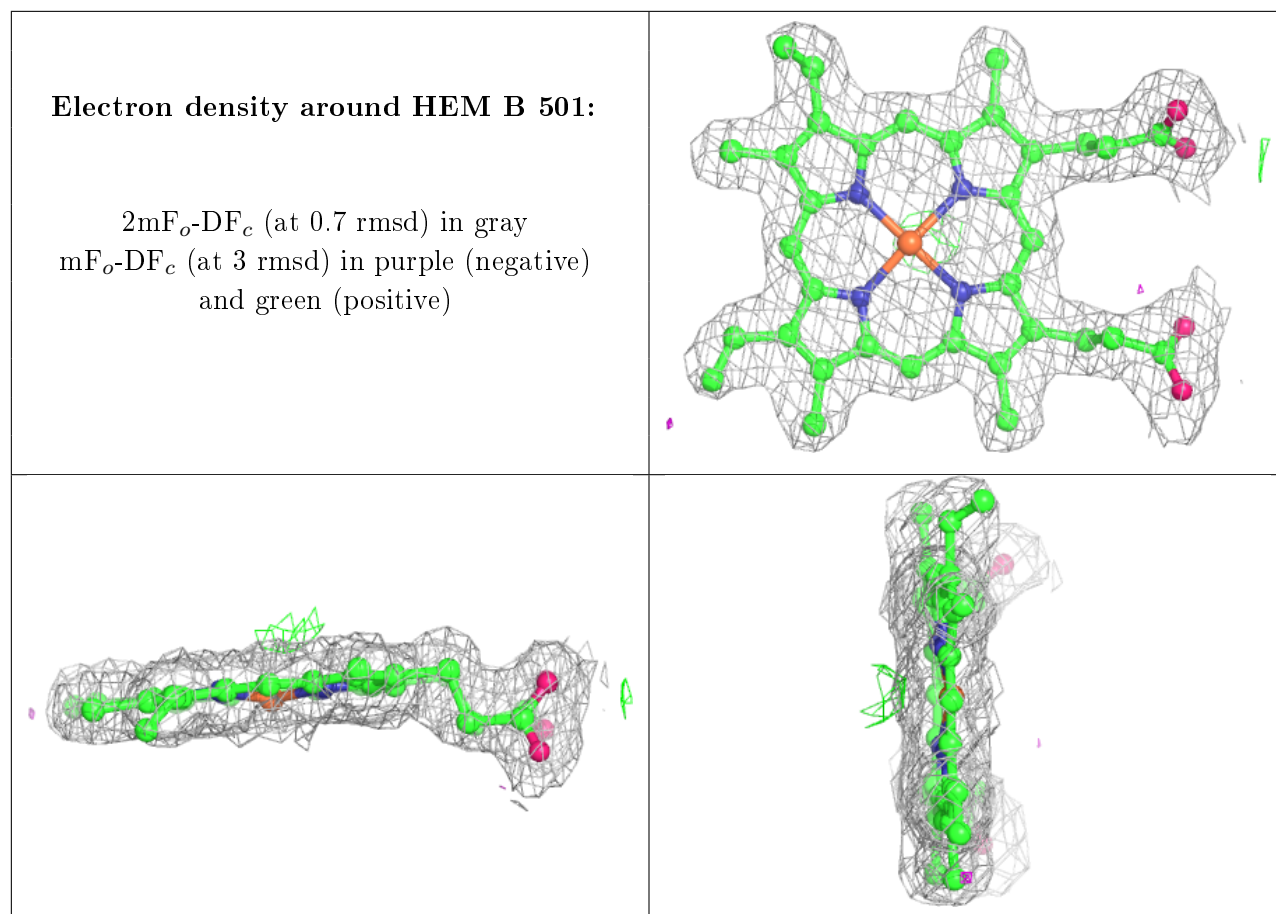
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 501:**

$2mF_o - DF_c$  (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.