



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:20 PM UTC

PDB ID : 3TBG / pdb_00003tbg
Title : Human cytochrome P450 2D6 with two thioridazines bound in active site
Authors : Wang, A.; Stout, C.D.; Johnson, E.F.
Deposited on : 2011-08-05
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

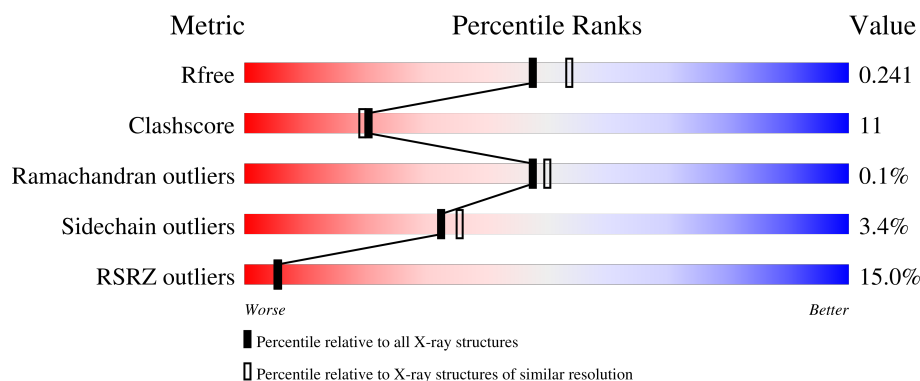
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	479	12% 75% 20% • •
1	B	479	17% 73% 21% • 5%
1	C	479	14% 73% 22% • •
1	D	479	14% 71% 22% • 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
4	GOL	B	750	-	-	X	-
4	GOL	D	750	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15538 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 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3690	2367	654	655	14			
1	B	456	Total	C	N	O	S	0	0	0
			3614	2317	640	643	14			
1	C	467	Total	C	N	O	S	0	0	0
			3690	2367	654	655	14			
1	D	456	Total	C	N	O	S	0	0	0
			3614	2317	640	643	14			

There are 60 discrepancies between the modelled and reference sequences:

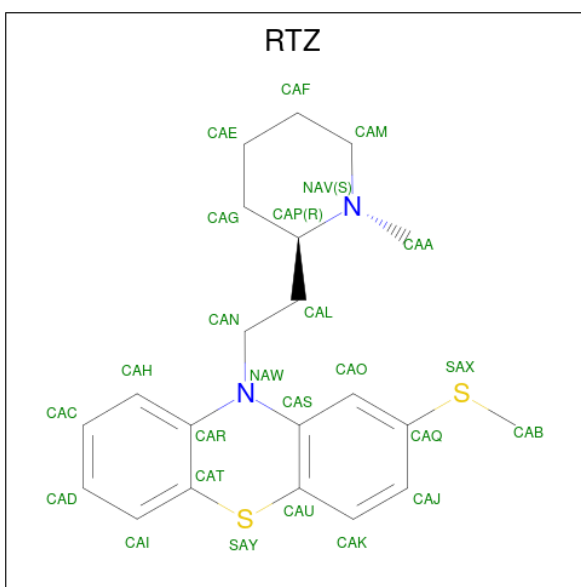
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP P10635
A	24	ALA	-	expression tag	UNP P10635
A	25	LYS	-	expression tag	UNP P10635
A	26	LYS	-	expression tag	UNP P10635
A	27	THR	-	expression tag	UNP P10635
A	28	SER	-	expression tag	UNP P10635
A	29	SER	-	expression tag	UNP P10635
A	30	LYS	-	expression tag	UNP P10635
A	31	GLY	-	expression tag	UNP P10635
A	32	LYS	-	expression tag	UNP P10635
A	33	LEU	-	expression tag	UNP P10635
A	498	HIS	-	expression tag	UNP P10635
A	499	HIS	-	expression tag	UNP P10635
A	500	HIS	-	expression tag	UNP P10635
A	501	HIS	-	expression tag	UNP P10635
B	23	MET	-	expression tag	UNP P10635
B	24	ALA	-	expression tag	UNP P10635
B	25	LYS	-	expression tag	UNP P10635
B	26	LYS	-	expression tag	UNP P10635
B	27	THR	-	expression tag	UNP P10635
B	28	SER	-	expression tag	UNP P10635

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP P10635
B	30	LYS	-	expression tag	UNP P10635
B	31	GLY	-	expression tag	UNP P10635
B	32	LYS	-	expression tag	UNP P10635
B	33	LEU	-	expression tag	UNP P10635
B	498	HIS	-	expression tag	UNP P10635
B	499	HIS	-	expression tag	UNP P10635
B	500	HIS	-	expression tag	UNP P10635
B	501	HIS	-	expression tag	UNP P10635
C	23	MET	-	expression tag	UNP P10635
C	24	ALA	-	expression tag	UNP P10635
C	25	LYS	-	expression tag	UNP P10635
C	26	LYS	-	expression tag	UNP P10635
C	27	THR	-	expression tag	UNP P10635
C	28	SER	-	expression tag	UNP P10635
C	29	SER	-	expression tag	UNP P10635
C	30	LYS	-	expression tag	UNP P10635
C	31	GLY	-	expression tag	UNP P10635
C	32	LYS	-	expression tag	UNP P10635
C	33	LEU	-	expression tag	UNP P10635
C	498	HIS	-	expression tag	UNP P10635
C	499	HIS	-	expression tag	UNP P10635
C	500	HIS	-	expression tag	UNP P10635
C	501	HIS	-	expression tag	UNP P10635
D	23	MET	-	expression tag	UNP P10635
D	24	ALA	-	expression tag	UNP P10635
D	25	LYS	-	expression tag	UNP P10635
D	26	LYS	-	expression tag	UNP P10635
D	27	THR	-	expression tag	UNP P10635
D	28	SER	-	expression tag	UNP P10635
D	29	SER	-	expression tag	UNP P10635
D	30	LYS	-	expression tag	UNP P10635
D	31	GLY	-	expression tag	UNP P10635
D	32	LYS	-	expression tag	UNP P10635
D	33	LEU	-	expression tag	UNP P10635
D	498	HIS	-	expression tag	UNP P10635
D	499	HIS	-	expression tag	UNP P10635
D	500	HIS	-	expression tag	UNP P10635
D	501	HIS	-	expression tag	UNP P10635

- Molecule 2 is 10-{2-[(2R)-1-methylpiperidin-2-yl]ethyl}-2-(methylsulfanyl)-10H-phenothiazine (CCD ID: RTZ) (formula: C₂₁H₂₆N₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			25	21	2	2		
2	A	1	Total	C	N	S	0	0
			25	21	2	2		
2	B	1	Total	C	N	S	0	0
			25	21	2	2		
2	B	1	Total	C	N	S	0	0
			25	21	2	2		
2	C	1	Total	C	N	S	0	0
			25	21	2	2		
2	C	1	Total	C	N	S	0	0
			25	21	2	2		
2	D	1	Total	C	N	S	0	0
			25	21	2	2		
2	D	1	Total	C	N	S	0	0
			25	21	2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

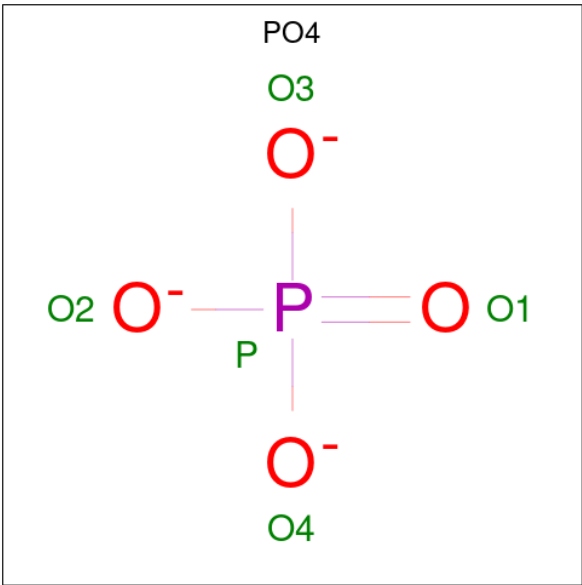
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		
3	B	1	Total	Zn	0	0
			1	1		
3	C	2	Total	Zn	0	0
			2	2		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



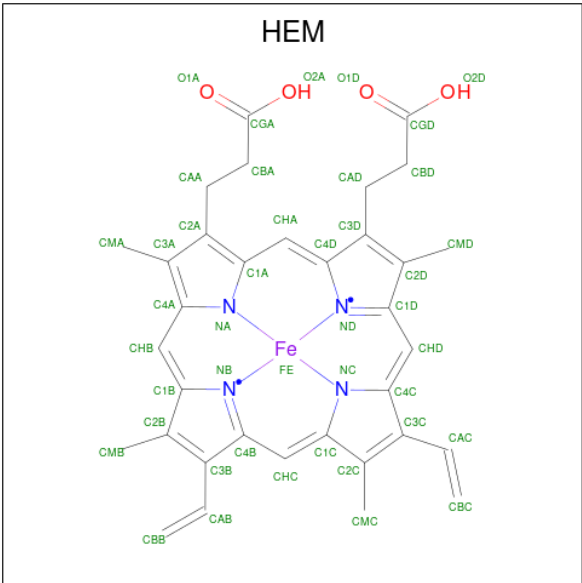
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	O	P		0	0
			5	4	1			

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

Continued on next page...

Continued from previous page...

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

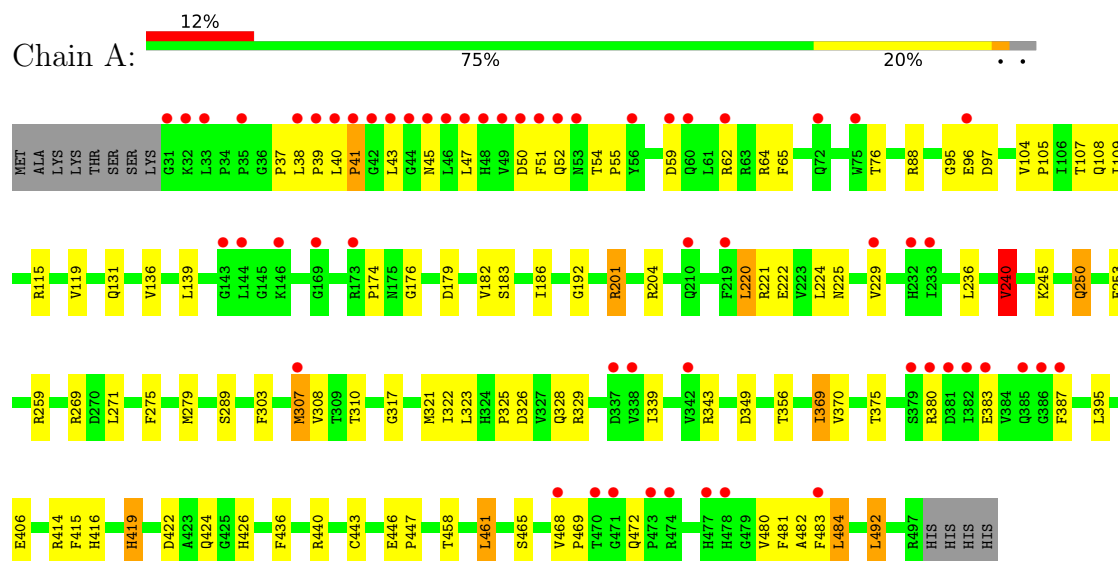
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	146	Total	O	0	0
			146	146		
7	B	109	Total	O	0	0
			109	109		
7	C	134	Total	O	0	0
			134	134		
7	D	115	Total	O	0	0
			115	115		

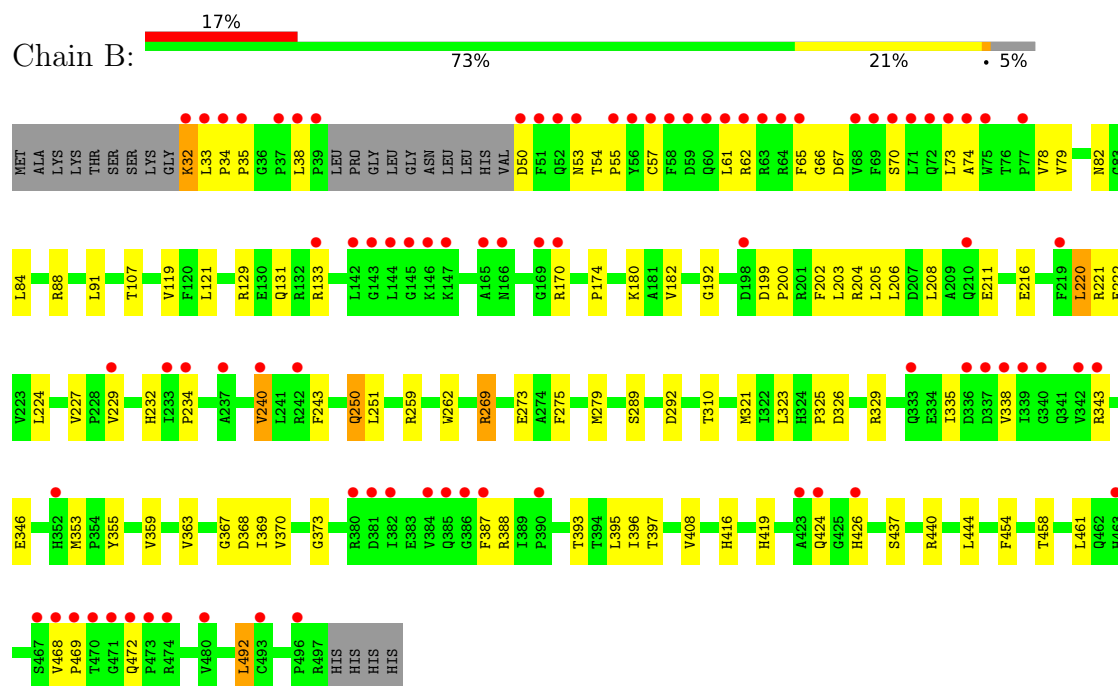
3 Residue-property plots

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.

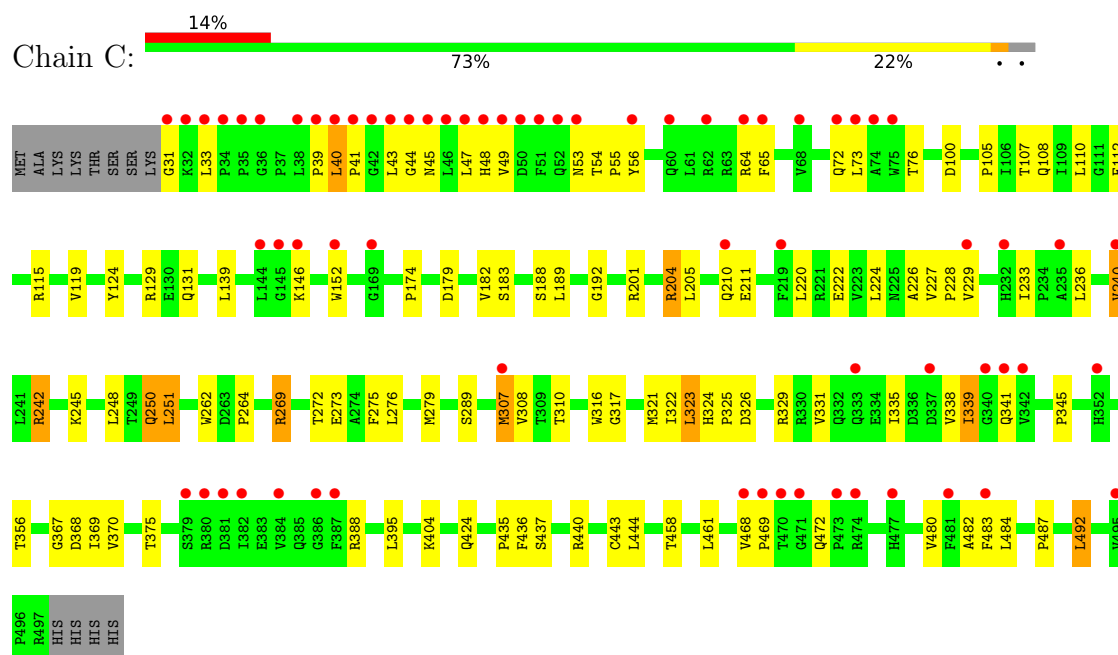
• Molecule 1: Cytochrome P450 2D6



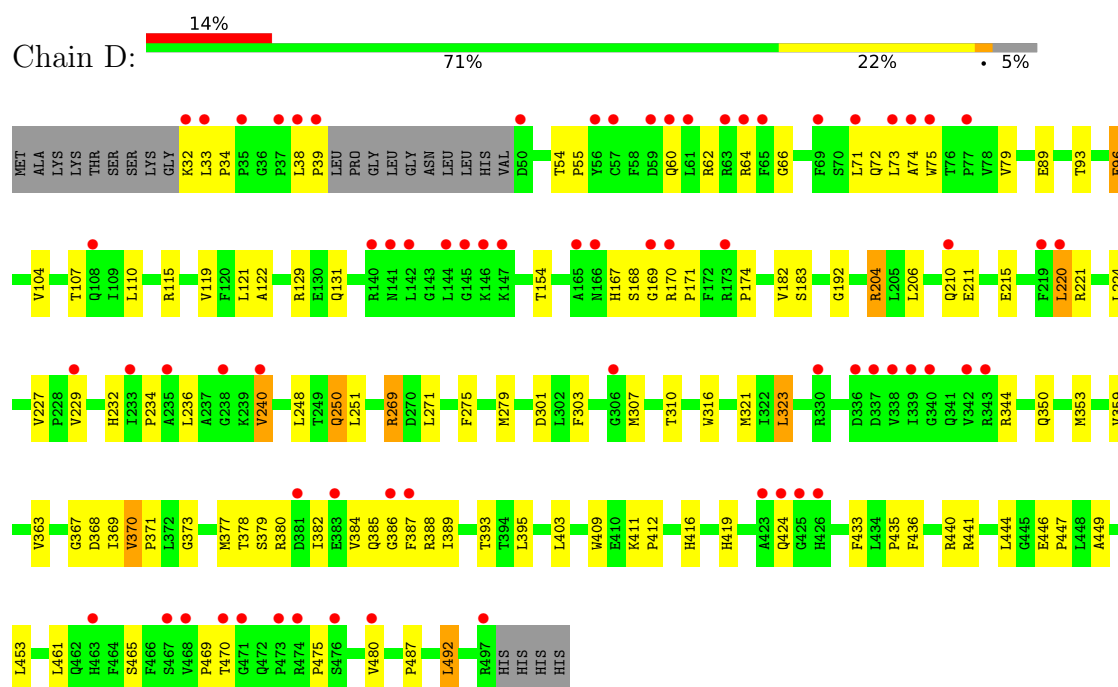
• Molecule 1: Cytochrome P450 2D6



● Molecule 1: Cytochrome P450 2D6



● Molecule 1: Cytochrome P450 2D6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.19Å 191.96Å 249.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.90 – 2.10 36.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (36.90-2.10) 99.4 (36.90-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.05Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.222 , 0.247 0.215 , 0.241	Depositor DCC
R_{free} test set	8054 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.514	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15538	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8395e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4, ZN, GOL, RTZ, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/3790	0.89	9/5155 (0.2%)
1	B	0.39	0/3711	0.86	4/5045 (0.1%)
1	C	0.41	0/3790	0.89	6/5155 (0.1%)
1	D	0.39	0/3711	0.87	5/5045 (0.1%)
All	All	0.41	0/15002	0.88	24/20400 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	339	ILE	N-CA-C	6.30	117.00	111.90
1	D	353	MET	CA-C-N	5.78	125.47	119.05
1	D	353	MET	C-N-CA	5.78	125.47	119.05
1	A	465	SER	N-CA-C	-5.53	99.50	108.52
1	A	415	PHE	N-CA-C	-5.52	100.11	108.67
1	A	484	LEU	N-CA-C	-5.50	100.75	109.76
1	A	369	ILE	N-CA-C	5.47	117.92	111.09
1	A	419	HIS	N-CA-C	-5.44	105.90	112.54
1	B	408	VAL	N-CA-C	5.36	115.62	110.74
1	B	289	SER	N-CA-C	-5.33	106.45	113.17
1	A	289	SER	N-CA-C	-5.30	106.49	113.17
1	D	370	VAL	CA-C-N	5.30	126.46	119.84
1	D	370	VAL	C-N-CA	5.30	126.46	119.84
1	C	338	VAL	N-CA-C	5.20	116.67	111.00
1	C	324	HIS	CA-C-N	5.17	125.21	119.32
1	C	324	HIS	C-N-CA	5.17	125.21	119.32
1	B	74	ALA	CB-CA-C	-5.15	110.23	117.23
1	A	240	VAL	CB-CA-C	-5.09	105.37	112.04
1	C	76	THR	N-CA-C	5.08	117.57	109.64
1	A	76	THR	N-CA-C	5.06	116.96	109.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	VAL	N-CA-C	5.06	116.16	111.81
1	C	289	SER	N-CA-C	-5.02	106.84	113.17
1	A	95	GLY	N-CA-C	5.02	118.96	112.83
1	D	74	ALA	CB-CA-C	-5.01	110.41	117.23

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	3690	0	3679	79	0
1	B	3614	0	3596	84	0
1	C	3690	0	3679	86	0
1	D	3614	0	3596	87	0
2	A	50	0	52	2	0
2	B	50	0	52	1	0
2	C	50	0	52	3	0
2	D	50	0	52	1	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	24	0	32	4	0
4	B	6	0	8	4	0
4	C	6	0	8	0	0
4	D	6	0	8	6	0
5	A	5	0	0	0	0
6	A	43	0	30	0	0
6	B	43	0	30	1	0
6	C	43	0	30	1	0
6	D	43	0	30	0	0
7	A	146	0	0	3	0
7	B	109	0	0	2	0
7	C	134	0	0	5	0
7	D	115	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15538	0	14934	335	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 11.

All (335) 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:B:32:LYS:HE3	1:B:32:LYS:HA	1.47	0.96
1:A:38:LEU:HD12	1:A:39:PRO:HD2	1.56	0.86
1:A:406:GLU:O	1:D:411:LYS:HE3	1.76	0.85
1:D:220:LEU:HD22	1:D:240:VAL:HG13	1.63	0.81
2:A:1:RTZ:HAI	7:A:628:HOH:O	1.79	0.81
1:A:179:ASP:HB3	1:A:307:MET:HE1	1.65	0.78
1:B:170:ARG:HB2	1:B:170:ARG:HH11	1.49	0.78
1:B:224:LEU:HD12	1:B:240:VAL:HG11	1.66	0.78
1:A:204:ARG:HH11	1:A:204:ARG:HG2	1.49	0.77
1:D:224:LEU:HD12	1:D:240:VAL:HG11	1.66	0.77
1:C:179:ASP:HB3	1:C:307:MET:HE1	1.67	0.77
1:D:71:LEU:HD11	1:D:73:LEU:HG	1.67	0.76
1:C:40:LEU:HG	1:C:41:PRO:HD2	1.70	0.71
1:D:221:ARG:NH2	4:D:750:GOL:O1	2.22	0.71
1:D:38:LEU:HB2	1:D:39:PRO:HD3	1.73	0.70
1:B:424:GLN:O	1:D:424:GLN:HG3	1.92	0.69
1:D:183:SER:OG	1:D:206:LEU:HD21	1.91	0.69
1:C:339:ILE:HD13	1:C:345:PRO:HB3	1.73	0.69
1:A:43:LEU:HD22	1:A:47:LEU:HD11	1.75	0.69
1:A:105:PRO:O	1:A:108:GLN:HG3	1.93	0.69
1:B:35:PRO:HB2	1:B:65:PHE:HD2	1.56	0.69
1:A:339:ILE:HG23	1:A:343:ARG:NH1	2.08	0.68
1:B:204:ARG:NH1	1:B:208:LEU:HD11	2.08	0.68
1:A:369:ILE:HG13	1:A:370:VAL:HG23	1.76	0.68
1:A:224:LEU:HD12	1:A:240:VAL:HG11	1.76	0.68
1:B:34:PRO:HG2	1:B:70:SER:OG	1.94	0.68
1:D:378:THR:HG23	1:D:395:LEU:HD11	1.76	0.67
1:A:307:MET:HG3	1:A:308:VAL:N	2.10	0.67
1:B:204:ARG:NH1	1:B:250:GLN:HG2	2.10	0.66
1:A:139:LEU:HD13	7:A:590:HOH:O	1.96	0.65
1:B:129:ARG:NH1	7:B:601:HOH:O	2.30	0.65
1:C:192:GLY:O	1:C:269:ARG:NH2	2.29	0.65
1:B:170:ARG:HB2	1:B:170:ARG:NH1	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PRO:HG2	1:B:65:PHE:HB3	1.79	0.65
1:D:224:LEU:HD12	1:D:240:VAL:CG1	2.26	0.64
1:C:369:ILE:HG13	1:C:370:VAL:HG23	1.79	0.63
1:C:250:GLN:HE21	1:C:250:GLN:HA	1.62	0.63
1:C:204:ARG:HH11	1:C:204:ARG:HG2	1.63	0.63
1:C:469:PRO:HB2	1:C:472:GLN:NE2	2.14	0.62
1:A:192:GLY:O	1:A:269:ARG:NH2	2.32	0.62
1:D:204:ARG:HG2	1:D:204:ARG:HH11	1.65	0.62
1:B:133:ARG:HG2	1:B:133:ARG:HH11	1.63	0.62
1:C:222:GLU:OE1	2:C:2:RTZ:HAAA	1.99	0.62
1:A:275:PHE:HE2	1:A:279:MET:HE2	1.65	0.62
1:C:129:ARG:NH1	7:C:4:HOH:O	2.32	0.61
1:D:104:VAL:HG11	4:D:750:GOL:H11	1.83	0.60
1:C:250:GLN:HE21	1:C:250:GLN:CA	2.14	0.60
1:B:227:VAL:HG12	1:B:229:VAL:HG12	1.82	0.60
1:B:202:PHE:O	1:B:206:LEU:HD13	2.02	0.60
1:D:174:PRO:HD3	1:D:492:LEU:HD22	1.84	0.60
1:C:307:MET:HG3	1:C:308:VAL:N	2.16	0.59
1:D:227:VAL:HG12	1:D:229:VAL:HG12	1.83	0.59
1:C:224:LEU:HD12	1:C:240:VAL:HG11	1.84	0.58
1:D:54:THR:HB	1:D:55:PRO:HD3	1.83	0.58
1:D:369:ILE:HG13	1:D:370:VAL:HG23	1.84	0.58
1:C:39:PRO:HA	1:C:45:ASN:ND2	2.17	0.58
1:A:224:LEU:HD12	1:A:240:VAL:CG1	2.32	0.58
1:D:359:VAL:O	1:D:363:VAL:HG23	2.04	0.57
1:A:204:ARG:HG2	1:A:204:ARG:NH1	2.18	0.57
1:D:38:LEU:HB2	1:D:39:PRO:CD	2.35	0.57
1:C:139:LEU:HD13	7:C:623:HOH:O	2.05	0.56
1:C:233:ILE:N	1:C:233:ILE:HD12	2.19	0.56
1:D:170:ARG:HB2	1:D:170:ARG:NH1	2.20	0.56
1:C:224:LEU:HD12	1:C:240:VAL:CG1	2.35	0.56
1:B:182:VAL:HG11	1:B:310:THR:HB	1.87	0.56
1:B:204:ARG:HH11	1:B:250:GLN:HG2	1.70	0.56
1:A:422:ASP:HB3	1:C:424:GLN:HG3	1.87	0.56
1:B:174:PRO:HD3	1:B:492:LEU:HD22	1.86	0.56
1:D:236:LEU:O	1:D:240:VAL:HG22	2.06	0.56
1:D:71:LEU:C	1:D:71:LEU:HD12	2.31	0.56
1:A:136:VAL:HG13	4:A:753:GOL:H12	1.88	0.56
1:A:220:LEU:HD13	1:A:240:VAL:HG13	1.87	0.56
1:C:182:VAL:HG11	1:C:310:THR:HB	1.88	0.56
1:D:33:LEU:HD11	1:D:388:ARG:NH1	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:VAL:HG12	1:D:373:GLY:HA2	1.88	0.56
1:A:109:ILE:CG2	1:A:245:LYS:HD2	2.36	0.55
1:B:355:TYR:O	1:B:359:VAL:HG23	2.07	0.55
1:D:232:HIS:O	1:D:234:PRO:HD3	2.07	0.55
1:B:54:THR:HB	1:B:55:PRO:HD3	1.88	0.55
1:B:84:LEU:HD11	1:B:88:ARG:HD2	1.88	0.55
1:B:369:ILE:HG13	1:B:370:VAL:HG23	1.88	0.54
1:D:250:GLN:HE21	1:D:250:GLN:HA	1.72	0.54
1:B:192:GLY:O	1:B:269:ARG:NH2	2.41	0.54
1:C:227:VAL:HG12	1:C:229:VAL:HG12	1.88	0.54
1:C:275:PHE:CE2	1:C:279:MET:HE2	2.42	0.54
1:B:91:LEU:HD11	1:B:397:THR:HG21	1.88	0.54
1:A:469:PRO:HB2	1:A:472:GLN:NE2	2.22	0.54
1:B:38:LEU:HD22	1:B:38:LEU:N	2.23	0.54
1:C:40:LEU:CD2	1:C:47:LEU:HD12	2.38	0.54
1:A:96:GLU:HG2	1:A:440:ARG:NH1	2.22	0.54
1:A:482:ALA:O	1:A:483:PHE:HB3	2.07	0.54
1:B:221:ARG:HG3	1:B:222:GLU:N	2.23	0.54
1:A:174:PRO:HD3	1:A:492:LEU:HD22	1.90	0.54
1:B:121:LEU:CD1	4:B:750:GOL:H11	2.38	0.54
1:A:43:LEU:N	1:A:43:LEU:HD12	2.24	0.53
1:A:40:LEU:HG	1:A:41:PRO:HD2	1.89	0.53
1:A:97:ASP:OD2	1:A:380:ARG:HD2	2.09	0.53
1:B:32:LYS:HE3	1:B:32:LYS:CA	2.31	0.53
1:C:119:VAL:HG22	1:C:131:GLN:HB3	1.90	0.53
1:C:275:PHE:HE2	1:C:279:MET:HE2	1.72	0.53
1:D:384:VAL:HG12	1:D:385:GLN:HG3	1.90	0.53
1:A:236:LEU:O	1:A:240:VAL:HG22	2.08	0.53
1:A:50:ASP:OD1	1:A:52:GLN:HG2	2.07	0.53
1:B:262:TRP:CD1	1:B:273:GLU:HG2	2.44	0.53
1:D:60:GLN:O	1:D:64:ARG:HG3	2.08	0.53
1:D:275:PHE:CE2	1:D:279:MET:HE2	2.44	0.53
1:A:322:ILE:HD12	1:A:468:VAL:HG12	1.91	0.53
1:B:454:PHE:O	1:B:458:THR:HG23	2.09	0.53
1:D:168:SER:C	1:D:170:ARG:H	2.17	0.53
1:B:199:ASP:O	1:B:203:LEU:HG	2.09	0.52
1:A:104:VAL:HG11	4:A:750:GOL:H11	1.92	0.52
1:A:326:ASP:N	1:A:326:ASP:OD2	2.42	0.52
1:C:31:GLY:HA2	1:C:388:ARG:HD3	1.92	0.52
1:D:379:SER:O	1:D:380:ARG:HG3	2.10	0.52
1:C:440:ARG:HH21	1:C:440:ARG:HG3	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HB2	1:C:44:GLY:O	2.09	0.52
1:D:170:ARG:HB2	1:D:170:ARG:HH11	1.73	0.52
1:B:204:ARG:HH11	1:B:250:GLN:CG	2.22	0.52
1:B:62:ARG:HD2	1:B:82:ASN:HB3	1.91	0.52
1:D:440:ARG:HG3	7:D:609:HOH:O	2.10	0.52
1:B:62:ARG:HH11	1:B:82:ASN:HB2	1.75	0.51
1:B:359:VAL:O	1:B:363:VAL:HG23	2.10	0.51
1:D:119:VAL:CG2	1:D:131:GLN:HB3	2.40	0.51
1:A:37:PRO:HG2	1:A:45:ASN:HD22	1.76	0.51
1:C:110:LEU:HD22	1:C:248:LEU:HD12	1.91	0.51
1:C:49:VAL:HG21	1:C:73:LEU:HD21	1.93	0.51
1:D:182:VAL:HG11	1:D:310:THR:HB	1.92	0.51
1:A:339:ILE:HG23	1:A:343:ARG:HH12	1.75	0.51
1:B:440:ARG:HG3	7:B:548:HOH:O	2.10	0.51
1:C:325:PRO:O	1:C:329:ARG:HG3	2.12	0.50
1:A:422:ASP:CB	1:C:424:GLN:HG3	2.41	0.50
1:B:224:LEU:HD12	1:B:240:VAL:CG1	2.39	0.50
1:B:444:LEU:C	1:B:444:LEU:HD12	2.37	0.50
1:A:275:PHE:CE2	1:A:279:MET:HE2	2.45	0.50
1:C:469:PRO:O	1:C:472:GLN:HB2	2.12	0.50
1:A:221:ARG:HG3	1:A:222:GLU:N	2.27	0.50
1:B:170:ARG:HH11	1:B:170:ARG:CB	2.24	0.50
1:C:119:VAL:CG2	1:C:131:GLN:HB3	2.42	0.49
1:A:186:ILE:HD13	1:A:303:PHE:HA	1.94	0.49
1:D:367:GLY:O	1:D:368:ASP:C	2.56	0.49
1:A:105:PRO:HD2	1:A:225:ASN:OD1	2.12	0.49
1:C:40:LEU:CG	1:C:41:PRO:HD2	2.42	0.49
1:D:129:ARG:NH2	7:D:512:HOH:O	2.45	0.49
1:D:221:ARG:HH22	4:D:750:GOL:C1	2.25	0.49
1:A:328:GLN:HG3	1:A:461:LEU:CD1	2.42	0.49
1:C:45:ASN:HA	1:C:48:HIS:ND1	2.27	0.49
1:B:121:LEU:HD11	4:B:750:GOL:H11	1.95	0.49
1:A:271:LEU:C	1:A:271:LEU:HD23	2.38	0.49
1:A:325:PRO:O	1:A:329:ARG:HG3	2.12	0.49
1:A:416:HIS:HB3	1:A:419:HIS:CE1	2.48	0.49
1:D:275:PHE:HE2	1:D:279:MET:HE2	1.76	0.49
1:C:226:ALA:C	1:C:228:PRO:HD3	2.37	0.49
1:A:59:ASP:HA	1:A:62:ARG:NH1	2.27	0.49
1:D:89:GLU:O	1:D:93:THR:HB	2.12	0.48
1:A:250:GLN:HE21	1:A:250:GLN:CA	2.25	0.48
1:A:424:GLN:HG2	1:A:426:HIS:CE1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:THR:HB	1:C:55:PRO:HD3	1.94	0.48
1:B:424:GLN:CD	1:B:424:GLN:H	2.22	0.48
1:C:236:LEU:O	1:C:240:VAL:HG22	2.13	0.48
1:A:64:ARG:HD2	1:A:65:PHE:CE1	2.48	0.48
1:C:210:GLN:NE2	1:C:211:GLU:HG2	2.28	0.48
1:A:356:THR:HG21	1:A:458:THR:HG22	1.96	0.48
1:D:121:LEU:CD1	4:D:750:GOL:H12	2.44	0.48
1:A:40:LEU:HD23	1:A:41:PRO:N	2.29	0.48
1:B:88:ARG:HB3	1:B:88:ARG:NH1	2.29	0.48
1:A:119:VAL:CG2	1:A:131:GLN:HB3	2.43	0.48
1:D:444:LEU:C	1:D:444:LEU:HD12	2.39	0.48
1:A:183:SER:OG	1:A:307:MET:HE2	2.14	0.48
1:A:229:VAL:HG13	7:A:604:HOH:O	2.13	0.48
1:A:414:ARG:HD3	7:D:595:HOH:O	2.13	0.48
1:B:275:PHE:CE2	1:B:279:MET:HE2	2.48	0.47
1:C:356:THR:HG21	1:C:458:THR:HG22	1.94	0.47
1:C:482:ALA:O	1:C:483:PHE:CB	2.62	0.47
1:D:122:ALA:O	1:D:441:ARG:NH2	2.37	0.47
1:B:275:PHE:HE2	1:B:279:MET:HE2	1.79	0.47
1:A:107:THR:HG22	4:A:750:GOL:H32	1.96	0.47
1:C:210:GLN:HB3	7:C:603:HOH:O	2.15	0.47
1:D:321:MET:HE2	1:D:321:MET:HA	1.96	0.47
1:B:335:ILE:HG12	1:B:353:MET:HE1	1.96	0.47
1:B:78:VAL:HG11	1:B:396:ILE:HD12	1.96	0.47
1:A:37:PRO:HG2	1:A:45:ASN:ND2	2.29	0.47
1:B:321:MET:HE2	1:B:321:MET:HA	1.97	0.47
1:A:326:ASP:HA	1:A:329:ARG:NH2	2.30	0.47
1:D:210:GLN:HG3	1:D:211:GLU:N	2.29	0.47
1:B:326:ASP:OD2	1:B:326:ASP:N	2.47	0.47
1:C:40:LEU:HD22	1:C:47:LEU:HD12	1.97	0.47
1:B:326:ASP:HA	1:B:329:ARG:NH1	2.30	0.46
1:D:110:LEU:HD22	1:D:248:LEU:HD12	1.97	0.46
1:D:220:LEU:HD22	1:D:240:VAL:CG1	2.39	0.46
1:A:40:LEU:HD22	1:A:43:LEU:HD13	1.96	0.46
1:A:383:GLU:HA	1:A:387:PHE:O	2.15	0.46
1:B:119:VAL:HG22	1:B:131:GLN:HB3	1.97	0.46
1:D:119:VAL:HG22	1:D:131:GLN:HB3	1.96	0.46
1:A:88:ARG:NH1	1:A:88:ARG:HB3	2.31	0.46
1:B:416:HIS:HB3	1:B:419:HIS:CE1	2.51	0.46
1:D:71:LEU:CD1	1:D:73:LEU:HG	2.39	0.46
1:A:307:MET:CG	1:A:308:VAL:N	2.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ARG:HH21	1:B:346:GLU:CD	2.23	0.46
1:C:174:PRO:HD3	1:C:492:LEU:HD22	1.98	0.46
1:C:262:TRP:CD1	1:C:273:GLU:HG2	2.50	0.46
1:D:435:PRO:HG2	1:D:436:PHE:CD1	2.50	0.46
1:C:204:ARG:HG2	1:C:204:ARG:NH1	2.28	0.46
1:C:436:PHE:HB3	1:C:443:CYS:HB3	1.97	0.46
1:D:107:THR:HG22	4:D:750:GOL:H32	1.96	0.46
1:D:192:GLY:O	1:D:269:ARG:NH2	2.48	0.46
1:B:211:GLU:HB3	1:B:243:PHE:CD2	2.51	0.46
1:B:35:PRO:HD3	1:B:387:PHE:CE1	2.51	0.46
1:C:205:LEU:HD11	1:C:251:LEU:HD13	1.98	0.46
1:B:367:GLY:O	1:B:368:ASP:C	2.57	0.46
1:B:469:PRO:HB2	1:B:472:GLN:CD	2.41	0.45
1:C:245:LYS:HE2	1:C:245:LYS:HB3	1.84	0.45
1:B:33:LEU:HD23	1:B:388:ARG:O	2.16	0.45
1:C:183:SER:OG	1:C:307:MET:HE2	2.17	0.45
1:B:220:LEU:HD22	1:B:240:VAL:HG13	1.99	0.45
1:C:316:TRP:CD1	1:C:487:PRO:HD3	2.51	0.45
1:C:375:THR:HG23	2:C:2:RTZ:CAJ	2.47	0.45
1:D:370:VAL:HG12	1:D:373:GLY:CA	2.47	0.45
1:D:121:LEU:HD11	4:D:750:GOL:H12	1.98	0.45
1:A:375:THR:HG23	2:A:2:RTZ:CAJ	2.47	0.45
1:D:368:ASP:OD1	1:D:403:LEU:HD12	2.16	0.45
1:A:303:PHE:O	1:A:307:MET:HB3	2.18	0.44
1:D:62:ARG:HA	1:D:66:GLY:O	2.17	0.44
1:C:33:LEU:HD23	1:C:388:ARG:O	2.18	0.44
1:D:168:SER:O	1:D:170:ARG:N	2.51	0.44
1:A:54:THR:HB	1:A:55:PRO:HD3	2.00	0.44
1:D:96:GLU:CD	1:D:96:GLU:H	2.26	0.44
1:D:433:PHE:CZ	1:D:435:PRO:HG3	2.52	0.44
1:C:100:ASP:HA	1:C:124:TYR:HB2	2.00	0.44
1:C:321:MET:HE2	1:C:321:MET:HA	2.00	0.44
1:D:71:LEU:HD12	1:D:72:GLN:N	2.33	0.44
1:D:382:ILE:HG13	1:D:389:ILE:HB	1.99	0.44
1:D:416:HIS:HB3	1:D:419:HIS:CE1	2.53	0.44
1:C:251:LEU:HD12	1:C:251:LEU:HA	1.87	0.44
1:A:436:PHE:HB3	1:A:443:CYS:HB3	1.98	0.44
1:C:404:LYS:NZ	7:C:586:HOH:O	2.49	0.43
1:B:180:LYS:HE2	1:B:203:LEU:CD2	2.48	0.43
1:C:492:LEU:HD23	1:C:492:LEU:O	2.18	0.43
1:D:75:TRP:CD1	1:D:75:TRP:N	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:MET:HA	1:D:393:THR:O	2.18	0.43
1:A:201:ARG:HD2	1:A:253:GLU:OE2	2.18	0.43
1:B:220:LEU:HD13	1:B:240:VAL:HG13	2.01	0.43
1:D:204:ARG:HG2	1:D:204:ARG:NH1	2.32	0.43
1:B:62:ARG:HA	1:B:66:GLY:O	2.18	0.43
1:B:205:LEU:HD11	1:B:251:LEU:HD13	2.01	0.43
1:C:119:VAL:HG22	1:C:131:GLN:CB	2.47	0.43
1:C:250:GLN:HA	1:C:250:GLN:NE2	2.32	0.43
1:C:331:VAL:O	1:C:335:ILE:HG13	2.18	0.43
1:D:79:VAL:HG21	1:D:389:ILE:HD12	2.01	0.43
1:D:446:GLU:HB3	1:D:447:PRO:HD3	2.00	0.43
1:A:119:VAL:HG22	1:A:131:GLN:HB3	2.00	0.43
1:C:53:ASN:HB3	1:C:56:TYR:HD2	1.84	0.43
1:D:154:THR:HG22	1:D:344:ARG:HD3	2.01	0.43
1:A:51:PHE:HA	1:A:54:THR:OG1	2.19	0.43
1:A:317:GLY:O	1:A:321:MET:HG2	2.19	0.43
1:B:78:VAL:HG11	1:B:396:ILE:CD1	2.49	0.43
1:B:437:SER:HB3	6:B:800:HEM:HBA1	2.00	0.43
1:A:97:ASP:CG	1:A:380:ARG:HD2	2.43	0.43
1:B:232:HIS:O	1:B:234:PRO:HD3	2.18	0.43
1:B:269:ARG:HG2	1:B:273:GLU:OE1	2.19	0.43
1:D:271:LEU:C	1:D:271:LEU:HD23	2.44	0.43
1:D:350:GLN:NE2	7:D:603:HOH:O	2.52	0.43
1:A:469:PRO:O	1:A:472:GLN:HB2	2.19	0.42
1:D:369:ILE:C	1:D:371:PRO:HD3	2.43	0.42
1:D:33:LEU:HD12	1:D:33:LEU:N	2.34	0.42
1:D:167:HIS:O	1:D:170:ARG:HB3	2.20	0.42
1:A:176:GLY:HA2	4:A:751:GOL:H11	2.00	0.42
1:C:40:LEU:HD13	1:C:48:HIS:HE1	1.85	0.42
1:B:424:GLN:HB2	1:B:426:HIS:ND1	2.34	0.42
1:C:152:TRP:CD2	1:C:188:SER:HB3	2.55	0.42
1:D:303:PHE:O	1:D:307:MET:HB2	2.19	0.42
1:D:449:ALA:O	1:D:453:LEU:HG	2.19	0.42
1:A:37:PRO:O	1:A:45:ASN:ND2	2.51	0.42
1:A:182:VAL:HG11	1:A:310:THR:HB	2.02	0.42
1:C:323:LEU:HD12	1:C:323:LEU:HA	1.85	0.42
1:B:62:ARG:NH1	1:B:67:ASP:OD2	2.52	0.42
1:B:107:THR:HG22	4:B:750:GOL:H32	2.01	0.42
1:C:226:ALA:O	1:C:228:PRO:HD3	2.19	0.42
1:B:57:CYS:O	1:B:61:LEU:HG	2.20	0.42
1:C:179:ASP:CB	1:C:307:MET:HE1	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TRP:O	1:C:264:PRO:HD3	2.20	0.42
1:C:326:ASP:OD2	1:C:326:ASP:N	2.52	0.42
1:D:32:LYS:HD2	1:D:386:GLY:O	2.20	0.42
1:D:301:ASP:OD2	2:D:1:RTZ:NAV	2.53	0.42
1:B:54:THR:N	1:B:55:PRO:CD	2.82	0.42
1:B:119:VAL:CG2	1:B:131:GLN:HB3	2.50	0.42
1:B:259:ARG:HH22	1:B:292:ASP:CG	2.27	0.42
1:C:64:ARG:HD2	1:C:65:PHE:CE1	2.55	0.42
1:C:435:PRO:HG2	1:C:436:PHE:CD1	2.55	0.42
1:C:105:PRO:O	1:C:108:GLN:HG3	2.20	0.41
1:C:444:LEU:HD12	1:C:444:LEU:C	2.45	0.41
1:A:446:GLU:HB3	1:A:447:PRO:HD3	2.02	0.41
1:B:133:ARG:HG2	1:B:133:ARG:NH1	2.33	0.41
1:B:204:ARG:NH1	1:B:250:GLN:CG	2.81	0.41
1:D:215:GLU:O	1:D:221:ARG:NH1	2.52	0.41
1:A:40:LEU:CG	1:A:41:PRO:HD2	2.50	0.41
1:C:272:THR:O	1:C:276:LEU:HG	2.20	0.41
1:C:322:ILE:HD12	1:C:468:VAL:HG12	2.02	0.41
1:D:409:TRP:O	1:D:412:PRO:HD3	2.21	0.41
1:A:481:PHE:CZ	1:A:483:PHE:HA	2.55	0.41
2:B:1:RTZ:HAG	2:B:1:RTZ:HABA	2.02	0.41
1:C:482:ALA:O	1:C:483:PHE:HB3	2.21	0.41
1:B:370:VAL:HG12	1:B:373:GLY:HA2	2.01	0.41
1:C:43:LEU:CD1	1:C:47:LEU:HD11	2.51	0.41
1:C:107:THR:HB	1:C:112:PHE:CG	2.56	0.41
1:B:62:ARG:HH11	1:B:62:ARG:HG3	1.85	0.41
1:B:325:PRO:O	1:B:329:ARG:HG3	2.20	0.41
1:A:343:ARG:NH2	1:A:349:ASP:OD2	2.54	0.41
1:B:50:ASP:OD2	1:B:53:ASN:ND2	2.49	0.41
1:B:216:GLU:OE2	4:B:750:GOL:H12	2.20	0.41
1:D:307:MET:C	1:D:307:MET:SD	3.04	0.41
1:D:316:TRP:CD1	1:D:487:PRO:HD3	2.55	0.41
1:D:469:PRO:O	1:D:470:THR:C	2.64	0.41
1:C:242:ARG:HB2	1:C:242:ARG:HH11	1.86	0.41
1:C:317:GLY:O	1:C:321:MET:HG2	2.21	0.41
1:C:367:GLY:O	1:C:368:ASP:C	2.64	0.41
1:D:171:PRO:HA	1:D:492:LEU:O	2.21	0.41
1:B:79:VAL:HG23	1:B:393:THR:HG21	2.03	0.40
1:C:307:MET:CG	1:C:308:VAL:N	2.82	0.40
1:C:437:SER:HB3	6:C:800:HEM:HBA1	2.02	0.40
1:D:34:PRO:HG3	1:D:387:PHE:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:VAL:O	1:D:480:VAL:HG13	2.22	0.40
1:A:307:MET:HG3	1:A:308:VAL:H	1.84	0.40
1:B:73:LEU:HD12	1:B:78:VAL:HG21	2.02	0.40
1:B:199:ASP:HA	1:B:200:PRO:HD3	1.96	0.40
1:D:323:LEU:CD1	1:D:475:PRO:HG2	2.51	0.40
1:A:492:LEU:HD23	1:A:492:LEU:O	2.22	0.40
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.84	0.40
1:C:341:GLN:O	1:C:341:GLN:HG2	2.21	0.40
1:C:468:VAL:O	1:C:468:VAL:HG23	2.21	0.40
1:D:71:LEU:HD11	1:D:73:LEU:CG	2.42	0.40
1:A:40:LEU:HD22	1:A:43:LEU:H	1.87	0.40
1:B:62:ARG:NH1	1:B:82:ASN:HB2	2.36	0.40
1:C:440:ARG:HG3	1:C:440:ARG:NH2	2.37	0.40
2:C:2:RTZ:HAA	7:C:613:HOH:O	2.21	0.40
1:D:461:LEU:HD23	1:D:461:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/479 (97%)	452 (97%)	13 (3%)	0	100	100
1	B	452/479 (94%)	437 (97%)	15 (3%)	0	100	100
1	C	465/479 (97%)	449 (97%)	16 (3%)	0	100	100
1	D	452/479 (94%)	435 (96%)	16 (4%)	1 (0%)	43	44
All	All	1834/1916 (96%)	1773 (97%)	60 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	169	GLY

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	398/409 (97%)	384 (96%)	14 (4%)	32	35
1	B	390/409 (95%)	381 (98%)	9 (2%)	44	51
1	C	398/409 (97%)	378 (95%)	20 (5%)	22	22
1	D	390/409 (95%)	379 (97%)	11 (3%)	38	43
All	All	1576/1636 (96%)	1522 (97%)	54 (3%)	32	35

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	A	115	ARG
1	A	201	ARG
1	A	220	LEU
1	A	240	VAL
1	A	250	GLN
1	A	259	ARG
1	A	307	MET
1	A	323	LEU
1	A	395	LEU
1	A	461	LEU
1	A	480	VAL
1	A	484	LEU
1	A	492	LEU
1	B	32	LYS
1	B	220	LEU
1	B	240	VAL
1	B	250	GLN
1	B	269	ARG
1	B	323	LEU
1	B	395	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	468	VAL
1	B	492	LEU
1	C	40	LEU
1	C	72	GLN
1	C	115	ARG
1	C	146	LYS
1	C	189	LEU
1	C	201	ARG
1	C	204	ARG
1	C	220	LEU
1	C	240	VAL
1	C	242	ARG
1	C	250	GLN
1	C	251	LEU
1	C	269	ARG
1	C	307	MET
1	C	323	LEU
1	C	395	LEU
1	C	461	LEU
1	C	480	VAL
1	C	484	LEU
1	C	492	LEU
1	D	96	GLU
1	D	115	ARG
1	D	204	ARG
1	D	220	LEU
1	D	240	VAL
1	D	250	GLN
1	D	251	LEU
1	D	269	ARG
1	D	323	LEU
1	D	465	SER
1	D	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	463	HIS
1	A	472	GLN
1	B	60	GLN
1	B	108	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	167	HIS
1	B	232	HIS
1	B	333	GLN
1	B	352	HIS
1	B	426	HIS
1	B	472	GLN
1	B	478	HIS
1	C	53	ASN
1	C	210	GLN
1	C	232	HIS
1	C	250	GLN
1	C	333	GLN
1	C	352	HIS
1	C	472	GLN
1	D	167	HIS
1	D	333	GLN
1	D	462	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 7 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RTZ	A	1	-	28,28,28	2.04	12 (42%)	36,39,39	1.24	4 (11%)
2	RTZ	A	2	-	28,28,28	2.13	12 (42%)	36,39,39	1.42	4 (11%)
5	PO4	A	790	-	4,4,4	1.70	0	6,6,6	0.47	0
4	GOL	B	750	-	5,5,5	0.25	0	5,5,5	0.32	0
2	RTZ	D	1	-	28,28,28	2.06	11 (39%)	36,39,39	1.21	4 (11%)
6	HEM	B	800	1,7	50,50,50	2.40	23 (46%)	67,82,82	1.33	9 (13%)
4	GOL	A	750	-	5,5,5	0.31	0	5,5,5	0.30	0
2	RTZ	B	1	-	28,28,28	2.03	13 (46%)	36,39,39	1.20	4 (11%)
2	RTZ	C	1	-	28,28,28	1.93	11 (39%)	36,39,39	1.21	4 (11%)
4	GOL	A	753	-	5,5,5	0.39	0	5,5,5	0.28	0
6	HEM	D	800	1	50,50,50	2.40	23 (46%)	67,82,82	1.31	12 (17%)
4	GOL	D	750	-	5,5,5	0.34	0	5,5,5	0.41	0
4	GOL	C	750	-	5,5,5	0.35	0	5,5,5	0.36	0
2	RTZ	B	2	-	28,28,28	2.02	12 (42%)	36,39,39	1.03	2 (5%)
6	HEM	C	800	1,7	50,50,50	2.37	21 (42%)	67,82,82	1.29	11 (16%)
2	RTZ	D	2	-	28,28,28	2.00	11 (39%)	36,39,39	1.02	2 (5%)
4	GOL	A	752	-	5,5,5	0.33	0	5,5,5	0.26	0
2	RTZ	C	2	-	28,28,28	2.15	13 (46%)	36,39,39	1.49	4 (11%)
6	HEM	A	800	1,7	50,50,50	2.46	23 (46%)	67,82,82	1.36	10 (14%)
4	GOL	A	751	-	5,5,5	0.32	0	5,5,5	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RTZ	A	1	-	-	6/7/30/30	0/4/4/4
2	RTZ	A	2	-	-	7/7/30/30	0/4/4/4
4	GOL	B	750	-	-	0/4/4/4	-
2	RTZ	D	1	-	-	6/7/30/30	0/4/4/4
6	HEM	B	800	1,7	-	4/14/54/54	-
4	GOL	A	750	-	-	2/4/4/4	-
2	RTZ	B	1	-	-	6/7/30/30	0/4/4/4
2	RTZ	C	1	-	-	6/7/30/30	0/4/4/4
4	GOL	A	753	-	-	4/4/4/4	-
6	HEM	D	800	1	-	4/14/54/54	-
4	GOL	D	750	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	750	-	-	1/4/4/4	-
2	RTZ	B	2	-	-	2/7/30/30	0/4/4/4
6	HEM	C	800	1,7	-	2/14/54/54	-
2	RTZ	D	2	-	-	2/7/30/30	0/4/4/4
4	GOL	A	752	-	-	4/4/4/4	-
2	RTZ	C	2	-	-	7/7/30/30	0/4/4/4
6	HEM	A	800	1,7	-	4/14/54/54	-
4	GOL	A	751	-	-	4/4/4/4	-

All (185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	800	HEM	FE-ND	4.95	2.10	1.94
6	A	800	HEM	C1D-ND	-4.85	1.29	1.38
6	C	800	HEM	FE-ND	4.72	2.09	1.94
6	A	800	HEM	FE-ND	4.66	2.09	1.94
6	D	800	HEM	FE-ND	4.45	2.08	1.94
6	B	800	HEM	CMA-C3A	4.39	1.59	1.50
6	C	800	HEM	C1D-ND	-4.28	1.30	1.38
6	A	800	HEM	FE-NB	4.28	2.08	1.94
6	D	800	HEM	C1D-ND	-4.25	1.30	1.38
6	B	800	HEM	C1D-ND	-4.20	1.30	1.38
6	D	800	HEM	C4A-NA	-4.15	1.31	1.39
6	B	800	HEM	C1B-NB	-4.14	1.33	1.40
6	D	800	HEM	C1B-NB	-4.10	1.33	1.40
6	A	800	HEM	C1B-NB	-4.08	1.33	1.40
6	C	800	HEM	FE-NB	4.06	2.07	1.94
6	C	800	HEM	C1B-NB	-4.05	1.33	1.40
6	D	800	HEM	CMA-C3A	3.97	1.58	1.50
6	A	800	HEM	C1C-NC	-3.96	1.32	1.39
6	B	800	HEM	C1C-NC	-3.90	1.32	1.39
6	C	800	HEM	CMA-C3A	3.90	1.58	1.50
6	A	800	HEM	CMA-C3A	3.89	1.58	1.50
6	D	800	HEM	C4D-ND	-3.89	1.33	1.40
6	B	800	HEM	FE-NB	3.89	2.06	1.94
2	A	2	RTZ	CAT-SAY	3.87	1.82	1.76
6	B	800	HEM	C4A-NA	-3.87	1.32	1.39
6	D	800	HEM	FE-NB	3.87	2.06	1.94
6	A	800	HEM	C4A-NA	-3.85	1.32	1.39
6	D	800	HEM	CBB-CAB	3.79	1.48	1.30
2	C	2	RTZ	CAR-CAT	3.79	1.44	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	800	HEM	C4D-ND	-3.77	1.33	1.40
6	C	800	HEM	CBB-CAB	3.75	1.48	1.30
6	C	800	HEM	C4A-NA	-3.74	1.32	1.39
2	C	2	RTZ	CAT-SAY	3.74	1.82	1.76
6	C	800	HEM	C1C-NC	-3.73	1.32	1.39
6	D	800	HEM	FE-NA	3.70	2.07	1.95
6	B	800	HEM	FE-NA	3.70	2.07	1.95
6	A	800	HEM	CBB-CAB	3.67	1.48	1.30
6	B	800	HEM	CBB-CAB	3.66	1.48	1.30
2	B	2	RTZ	CAR-CAT	3.65	1.44	1.40
6	D	800	HEM	C1C-NC	-3.63	1.32	1.39
2	A	2	RTZ	CAR-CAT	3.62	1.44	1.40
2	D	2	RTZ	CAR-CAT	3.62	1.44	1.40
6	C	800	HEM	CMC-C2C	3.62	1.58	1.50
6	D	800	HEM	CAC-C3C	-3.62	1.37	1.47
2	D	1	RTZ	CAT-SAY	3.60	1.82	1.76
6	A	800	HEM	C4D-ND	-3.57	1.34	1.40
6	A	800	HEM	C1C-C2C	-3.56	1.38	1.45
6	A	800	HEM	C4B-NB	-3.54	1.31	1.38
2	A	1	RTZ	CAS-CAU	3.53	1.44	1.40
2	D	2	RTZ	CAT-SAY	3.53	1.82	1.76
2	A	1	RTZ	CAR-CAT	3.52	1.44	1.40
2	D	1	RTZ	CAS-CAU	3.50	1.44	1.40
6	A	800	HEM	CAC-C3C	-3.49	1.38	1.47
2	D	1	RTZ	CAR-CAT	3.48	1.44	1.40
6	C	800	HEM	FE-NA	3.48	2.06	1.95
6	A	800	HEM	FE-NA	3.48	2.06	1.95
2	B	1	RTZ	CAS-CAU	3.47	1.44	1.40
2	A	1	RTZ	CAT-SAY	3.41	1.82	1.76
2	C	2	RTZ	CAS-CAU	3.41	1.44	1.40
6	B	800	HEM	C4B-NB	-3.40	1.32	1.38
2	B	1	RTZ	CAR-CAT	3.39	1.44	1.40
6	C	800	HEM	CAC-C3C	-3.37	1.38	1.47
2	A	2	RTZ	CAS-CAU	3.37	1.44	1.40
2	B	1	RTZ	CAT-SAY	3.36	1.82	1.76
6	D	800	HEM	FE-NC	3.34	2.06	1.95
6	C	800	HEM	C4D-ND	-3.33	1.34	1.40
6	B	800	HEM	CAC-C3C	-3.33	1.38	1.47
6	A	800	HEM	CMC-C2C	3.32	1.57	1.50
6	C	800	HEM	C1C-C2C	-3.31	1.38	1.45
2	C	1	RTZ	CAS-CAU	3.27	1.44	1.40
6	D	800	HEM	C4B-NB	-3.27	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	800	HEM	CMC-C2C	3.25	1.57	1.50
2	D	2	RTZ	CAS-CAU	3.18	1.44	1.40
2	C	1	RTZ	CAR-CAT	3.17	1.44	1.40
6	A	800	HEM	C4D-C3D	-3.17	1.39	1.45
2	B	2	RTZ	CAM-NAV	3.16	1.53	1.47
2	C	1	RTZ	CAT-SAY	3.16	1.81	1.76
2	B	2	RTZ	CAT-SAY	3.16	1.81	1.76
6	C	800	HEM	C4B-NB	-3.10	1.32	1.38
6	A	800	HEM	FE-NC	3.07	2.05	1.95
2	B	2	RTZ	CAS-CAU	3.05	1.43	1.40
6	C	800	HEM	FE-NC	3.04	2.05	1.95
2	D	2	RTZ	CAM-NAV	3.03	1.52	1.47
6	B	800	HEM	C3B-C2B	3.01	1.43	1.37
6	B	800	HEM	FE-NC	3.00	2.05	1.95
2	D	1	RTZ	CAH-CAR	2.99	1.44	1.39
2	C	1	RTZ	CAM-NAV	2.97	1.52	1.47
2	A	1	RTZ	CAM-NAV	2.94	1.52	1.47
6	D	800	HEM	C3B-C2B	2.94	1.43	1.37
6	B	800	HEM	CMC-C2C	2.93	1.56	1.50
2	A	2	RTZ	CAS-NAW	2.88	1.45	1.40
6	B	800	HEM	C1C-C2C	-2.88	1.39	1.45
2	C	2	RTZ	CAS-NAW	2.88	1.45	1.40
2	C	2	RTZ	CAC-CAH	2.87	1.43	1.38
2	D	1	RTZ	CAM-NAV	2.87	1.52	1.47
6	D	800	HEM	C1C-C2C	-2.85	1.39	1.45
2	A	2	RTZ	CAC-CAH	2.80	1.43	1.38
2	C	1	RTZ	CAH-CAR	2.79	1.44	1.39
6	A	800	HEM	CMD-C2D	2.79	1.56	1.50
2	B	2	RTZ	CAR-NAW	2.79	1.45	1.40
2	A	2	RTZ	CAM-NAV	2.78	1.52	1.47
2	A	1	RTZ	CAH-CAR	2.76	1.43	1.39
2	C	2	RTZ	CAM-NAV	2.76	1.52	1.47
2	B	1	RTZ	CAR-NAW	2.76	1.45	1.40
2	D	1	RTZ	CAS-NAW	2.76	1.45	1.40
2	B	1	RTZ	CAS-NAW	2.74	1.45	1.40
2	B	1	RTZ	CAM-NAV	2.73	1.52	1.47
2	B	2	RTZ	CAH-CAR	2.72	1.43	1.39
6	C	800	HEM	O2A-CGA	-2.71	1.21	1.30
2	D	1	RTZ	CAC-CAH	2.71	1.43	1.38
6	B	800	HEM	C4D-C3D	-2.71	1.40	1.45
6	A	800	HEM	C3B-C2B	2.69	1.42	1.37
2	D	2	RTZ	CAH-CAR	2.69	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	RTZ	CAS-NAW	2.68	1.44	1.40
2	B	2	RTZ	CAS-NAW	2.66	1.44	1.40
6	C	800	HEM	C4D-C3D	-2.65	1.40	1.45
2	B	1	RTZ	CAH-CAR	2.65	1.43	1.39
2	A	1	RTZ	CAC-CAH	2.65	1.43	1.38
2	D	2	RTZ	CAS-NAW	2.64	1.44	1.40
2	D	1	RTZ	CAR-NAW	2.64	1.44	1.40
2	B	1	RTZ	CAO-CAS	2.64	1.43	1.39
2	B	2	RTZ	CAC-CAH	2.63	1.43	1.38
6	C	800	HEM	C3B-C2B	2.62	1.42	1.37
2	B	1	RTZ	CAC-CAH	2.62	1.43	1.38
6	A	800	HEM	O2A-CGA	-2.61	1.22	1.30
6	D	800	HEM	C4D-C3D	-2.59	1.40	1.45
2	A	2	RTZ	CAO-CAS	2.56	1.43	1.39
2	A	2	RTZ	CAD-CAI	2.56	1.43	1.38
2	C	1	RTZ	CAR-NAW	2.54	1.44	1.40
2	C	1	RTZ	CAC-CAH	2.51	1.43	1.38
2	C	2	RTZ	CAO-CAS	2.50	1.43	1.39
6	B	800	HEM	O2A-CGA	-2.50	1.22	1.30
2	C	2	RTZ	CAD-CAI	2.49	1.43	1.38
2	D	2	RTZ	CAR-NAW	2.49	1.44	1.40
2	D	2	RTZ	CAC-CAH	2.46	1.43	1.38
6	D	800	HEM	O2A-CGA	-2.45	1.22	1.30
6	C	800	HEM	CBC-CAC	2.45	1.42	1.30
6	C	800	HEM	CMD-C2D	2.44	1.55	1.50
2	A	1	RTZ	CAR-NAW	2.42	1.44	1.40
2	B	2	RTZ	CAO-CAS	2.41	1.43	1.39
2	B	2	RTZ	CAO-CAQ	2.40	1.43	1.39
2	C	2	RTZ	CAO-CAQ	2.40	1.43	1.39
2	C	2	RTZ	CAU-SAY	2.40	1.80	1.76
6	D	800	HEM	CBC-CAC	2.39	1.41	1.30
2	A	2	RTZ	CAO-CAQ	2.38	1.43	1.39
2	A	1	RTZ	CAD-CAI	2.37	1.43	1.38
2	A	2	RTZ	CAH-CAR	2.36	1.43	1.39
6	A	800	HEM	CBC-CAC	2.33	1.41	1.30
2	C	1	RTZ	CAU-SAY	2.31	1.80	1.76
2	D	2	RTZ	CAO-CAS	2.30	1.43	1.39
6	B	800	HEM	CBC-CAC	2.30	1.41	1.30
2	C	1	RTZ	CAS-NAW	2.29	1.44	1.40
2	C	2	RTZ	CAH-CAR	2.29	1.43	1.39
2	A	2	RTZ	CAU-SAY	2.27	1.80	1.76
2	D	1	RTZ	CAO-CAS	2.26	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	RTZ	CAD-CAI	2.25	1.42	1.38
6	A	800	HEM	C3C-C4C	-2.23	1.42	1.46
2	D	1	RTZ	CAD-CAI	2.23	1.42	1.38
2	B	2	RTZ	CAD-CAI	2.23	1.42	1.38
6	A	800	HEM	C4C-NC	-2.21	1.35	1.39
6	B	800	HEM	C1D-C2D	-2.21	1.40	1.44
2	D	2	RTZ	CAO-CAQ	2.20	1.43	1.39
6	D	800	HEM	C1D-C2D	-2.19	1.40	1.44
2	B	1	RTZ	CAO-CAQ	2.19	1.43	1.39
2	A	1	RTZ	CAU-SAY	2.18	1.80	1.76
6	D	800	HEM	CMD-C2D	2.16	1.55	1.50
2	B	1	RTZ	CAD-CAI	2.14	1.42	1.38
6	B	800	HEM	CMD-C2D	2.13	1.55	1.50
2	D	1	RTZ	CAU-SAY	2.11	1.79	1.76
2	C	1	RTZ	CAE-CAG	2.10	1.58	1.53
2	B	1	RTZ	CAE-CAG	2.09	1.58	1.53
6	B	800	HEM	C3C-C2C	2.07	1.41	1.37
2	A	1	RTZ	CAE-CAG	2.07	1.58	1.53
2	C	1	RTZ	CAO-CAS	2.06	1.43	1.39
2	C	2	RTZ	CAJ-CAQ	2.06	1.43	1.39
6	C	800	HEM	C4C-NC	-2.05	1.35	1.39
2	B	1	RTZ	CAU-SAY	2.04	1.79	1.76
6	D	800	HEM	C4C-NC	-2.03	1.35	1.39
6	D	800	HEM	C3C-C4C	-2.03	1.42	1.46
2	A	1	RTZ	CAO-CAS	2.02	1.42	1.39
2	A	2	RTZ	CAE-CAG	2.02	1.58	1.53
2	B	2	RTZ	CAE-CAG	2.01	1.58	1.53
2	C	2	RTZ	CAQ-SAX	2.01	1.81	1.76
6	A	800	HEM	C3C-C2C	2.01	1.41	1.37
6	B	800	HEM	C3C-C4C	-2.01	1.42	1.46

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	RTZ	CAA-NAV-CAM	-4.65	102.94	110.61
2	A	2	RTZ	CAA-NAV-CAM	-4.50	103.20	110.61
2	A	2	RTZ	CAN-NAW-CAS	4.40	125.16	119.03
2	C	2	RTZ	CAN-NAW-CAS	4.37	125.12	119.03
2	A	1	RTZ	CAA-NAV-CAM	-4.33	103.47	110.61
2	C	1	RTZ	CAA-NAV-CAM	-4.33	103.48	110.61
2	B	1	RTZ	CAA-NAV-CAM	-4.28	103.55	110.61
2	D	1	RTZ	CAA-NAV-CAM	-4.22	103.65	110.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	800	HEM	C3B-C4B-NB	3.32	111.85	109.47
6	B	800	HEM	CHD-C4C-NC	-3.29	120.87	124.45
6	A	800	HEM	CHD-C4C-NC	-3.25	120.91	124.45
2	D	1	RTZ	CAL-CAP-CAG	-3.11	107.94	112.65
2	B	1	RTZ	CAL-CAP-CAG	-3.08	107.98	112.65
2	A	1	RTZ	CAL-CAP-CAG	-3.05	108.03	112.65
2	A	2	RTZ	CAL-CAN-NAW	2.98	122.64	111.30
6	C	800	HEM	C3B-C4B-NB	2.96	111.59	109.47
2	C	2	RTZ	CAL-CAN-NAW	2.93	122.45	111.30
6	A	800	HEM	C4B-C3B-C2B	-2.93	104.59	107.28
6	B	800	HEM	C4B-C3B-C2B	-2.93	104.59	107.28
6	D	800	HEM	CHD-C4C-NC	-2.91	121.28	124.45
6	D	800	HEM	C4B-C3B-C2B	-2.88	104.63	107.28
2	C	1	RTZ	CAL-CAP-CAG	-2.88	108.28	112.65
2	B	2	RTZ	CAA-NAV-CAM	-2.83	105.94	110.61
2	A	1	RTZ	CAL-CAN-NAW	2.77	121.82	111.30
2	D	2	RTZ	CAA-NAV-CAM	-2.72	106.13	110.61
2	C	1	RTZ	CAL-CAN-NAW	2.71	121.61	111.30
6	D	800	HEM	C3B-C4B-NB	2.68	111.39	109.47
6	B	800	HEM	C3B-C4B-NB	2.66	111.38	109.47
6	C	800	HEM	CHD-C4C-NC	-2.63	121.59	124.45
6	B	800	HEM	C1C-CHC-C4B	2.62	131.59	126.02
6	A	800	HEM	C3B-C2B-C1B	-2.61	104.45	106.41
6	D	800	HEM	C4D-ND-C1D	2.59	108.27	105.21
6	A	800	HEM	C1C-CHC-C4B	2.59	131.52	126.02
6	C	800	HEM	C4B-C3B-C2B	-2.58	104.91	107.28
6	A	800	HEM	C4D-ND-C1D	2.57	108.25	105.21
6	B	800	HEM	C4D-ND-C1D	2.57	108.25	105.21
6	B	800	HEM	C3B-C2B-C1B	-2.54	104.50	106.41
6	A	800	HEM	C4C-C3C-C2C	-2.54	104.61	106.81
6	D	800	HEM	C1C-CHC-C4B	2.53	131.40	126.02
2	A	1	RTZ	CAN-NAW-CAS	2.50	122.51	119.03
6	B	800	HEM	CHC-C1C-NC	-2.49	121.74	124.45
6	B	800	HEM	C4C-C3C-C2C	-2.47	104.67	106.81
6	C	800	HEM	C3B-C2B-C1B	-2.47	104.56	106.41
6	D	800	HEM	C1B-NB-C4B	2.46	108.12	105.21
2	D	1	RTZ	CAL-CAN-NAW	2.46	120.65	111.30
6	C	800	HEM	C4C-C3C-C2C	-2.44	104.69	106.81
6	D	800	HEM	C4C-C3C-C2C	-2.44	104.69	106.81
2	B	1	RTZ	CAL-CAN-NAW	2.43	120.55	111.30
6	B	800	HEM	C1B-NB-C4B	2.43	108.08	105.21
6	C	800	HEM	C1C-CHC-C4B	2.42	131.16	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	800	HEM	C3B-C2B-C1B	-2.41	104.60	106.41
2	D	2	RTZ	CAA-NAV-CAP	2.41	115.25	111.87
2	C	2	RTZ	CAS-NAW-CAR	-2.34	114.75	120.18
6	C	800	HEM	C1B-NB-C4B	2.32	107.96	105.21
6	C	800	HEM	C4A-CHB-C1B	2.30	131.66	126.25
6	C	800	HEM	C4D-ND-C1D	2.30	107.93	105.21
2	B	2	RTZ	CAA-NAV-CAP	2.29	115.09	111.87
6	A	800	HEM	C4A-CHB-C1B	2.29	131.63	126.25
2	C	1	RTZ	CAN-NAW-CAS	2.28	122.20	119.03
6	A	800	HEM	C1B-NB-C4B	2.16	107.76	105.21
2	B	1	RTZ	CAN-NAW-CAS	2.13	122.00	119.03
6	C	800	HEM	C4C-CHD-C1D	2.11	130.51	126.02
2	D	1	RTZ	CAN-NAW-CAS	2.10	121.95	119.03
6	D	800	HEM	C4A-CHB-C1B	2.08	131.14	126.25
6	D	800	HEM	CHC-C1C-NC	-2.07	122.20	124.45
2	A	2	RTZ	CAS-NAW-CAR	-2.05	115.42	120.18
6	A	800	HEM	CHB-C1B-NB	-2.04	121.84	124.37
6	D	800	HEM	CHB-C1B-NB	-2.04	121.84	124.37
6	C	800	HEM	CHB-C1B-NB	-2.01	121.88	124.37
6	D	800	HEM	O2A-CGA-CBA	2.00	120.33	114.00

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	RTZ	CAN-CAL-CAP-CAG
2	A	1	RTZ	CAN-CAL-CAP-NAV
2	A	2	RTZ	CAP-CAL-CAN-NAW
2	A	2	RTZ	CAN-CAL-CAP-CAG
2	A	2	RTZ	CAL-CAN-NAW-CAR
2	A	2	RTZ	CAL-CAN-NAW-CAS
2	B	1	RTZ	CAN-CAL-CAP-CAG
2	B	1	RTZ	CAN-CAL-CAP-NAV
2	B	2	RTZ	CAP-CAL-CAN-NAW
2	C	1	RTZ	CAN-CAL-CAP-CAG
2	C	1	RTZ	CAN-CAL-CAP-NAV
2	C	2	RTZ	CAP-CAL-CAN-NAW
2	C	2	RTZ	CAL-CAN-NAW-CAR
2	C	2	RTZ	CAL-CAN-NAW-CAS
2	D	1	RTZ	CAN-CAL-CAP-CAG
2	D	1	RTZ	CAN-CAL-CAP-NAV
2	D	2	RTZ	CAP-CAL-CAN-NAW

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	750	GOL	O1-C1-C2-C3
4	A	751	GOL	O1-C1-C2-O2
4	A	751	GOL	O1-C1-C2-C3
4	A	753	GOL	O1-C1-C2-C3
4	A	753	GOL	C1-C2-C3-O3
4	D	750	GOL	O1-C1-C2-C3
2	B	1	RTZ	CAO-CAQ-SAX-CAB
2	B	1	RTZ	CAJ-CAQ-SAX-CAB
2	A	1	RTZ	CAJ-CAQ-SAX-CAB
4	A	751	GOL	C1-C2-C3-O3
4	A	752	GOL	O1-C1-C2-C3
4	A	752	GOL	C1-C2-C3-O3
2	A	1	RTZ	CAO-CAQ-SAX-CAB
2	C	1	RTZ	CAO-CAQ-SAX-CAB
4	A	751	GOL	O2-C2-C3-O3
4	A	752	GOL	O1-C1-C2-O2
4	A	752	GOL	O2-C2-C3-O3
4	A	753	GOL	O1-C1-C2-O2
4	A	753	GOL	O2-C2-C3-O3
4	D	750	GOL	O1-C1-C2-O2
2	C	1	RTZ	CAJ-CAQ-SAX-CAB
2	D	1	RTZ	CAO-CAQ-SAX-CAB
6	D	800	HEM	C2C-C3C-CAC-CBC
4	A	750	GOL	O1-C1-C2-O2
2	D	1	RTZ	CAJ-CAQ-SAX-CAB
2	A	2	RTZ	CAN-CAL-CAP-NAV
2	A	2	RTZ	CAJ-CAQ-SAX-CAB
4	C	750	GOL	O1-C1-C2-O2
2	A	2	RTZ	CAO-CAQ-SAX-CAB
6	A	800	HEM	C2C-C3C-CAC-CBC
6	B	800	HEM	C2C-C3C-CAC-CBC
6	D	800	HEM	C4C-C3C-CAC-CBC
2	A	1	RTZ	CAL-CAN-NAW-CAS
2	D	1	RTZ	CAL-CAN-NAW-CAS
2	A	1	RTZ	CAP-CAL-CAN-NAW
2	B	1	RTZ	CAP-CAL-CAN-NAW
2	C	1	RTZ	CAP-CAL-CAN-NAW
2	D	1	RTZ	CAP-CAL-CAN-NAW
2	C	2	RTZ	CAJ-CAQ-SAX-CAB
2	C	2	RTZ	CAO-CAQ-SAX-CAB
2	C	2	RTZ	CAN-CAL-CAP-NAV
2	B	2	RTZ	CAL-CAN-NAW-CAS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	800	HEM	C4C-C3C-CAC-CBC
2	D	2	RTZ	CAL-CAN-NAW-CAS
6	C	800	HEM	CAA-CBA-CGA-O2A
6	A	800	HEM	CAA-CBA-CGA-O2A
2	C	1	RTZ	CAL-CAN-NAW-CAS
6	B	800	HEM	CAA-CBA-CGA-O2A
6	C	800	HEM	CAA-CBA-CGA-O1A
2	C	2	RTZ	CAN-CAL-CAP-CAG
6	A	800	HEM	CAA-CBA-CGA-O1A
6	D	800	HEM	CAA-CBA-CGA-O2A
6	A	800	HEM	C4C-C3C-CAC-CBC
6	D	800	HEM	CAA-CBA-CGA-O1A
6	B	800	HEM	CAA-CBA-CGA-O1A
2	B	1	RTZ	CAL-CAN-NAW-CAS

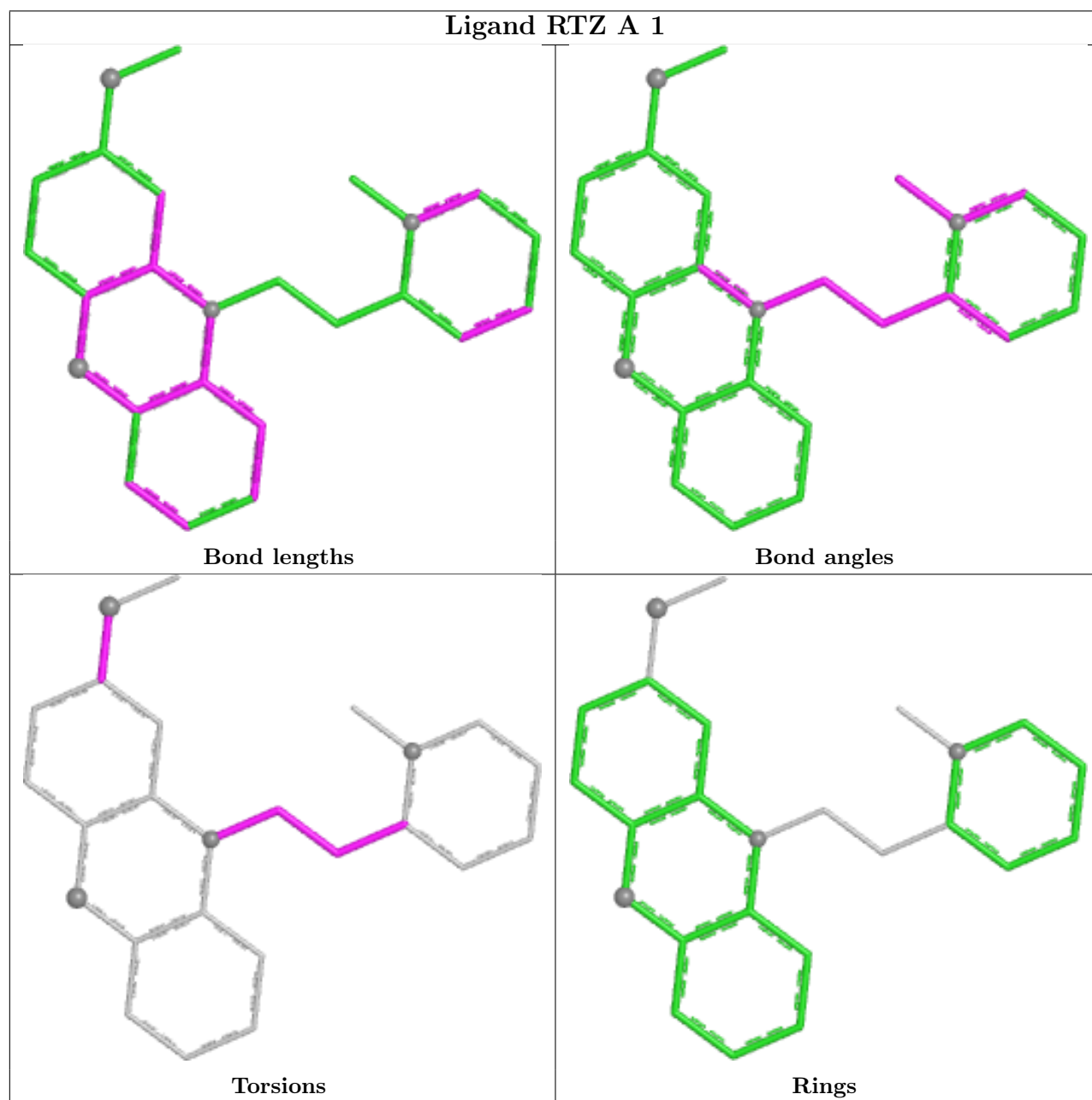
There are no ring outliers.

12 monomers are involved in 23 short contacts:

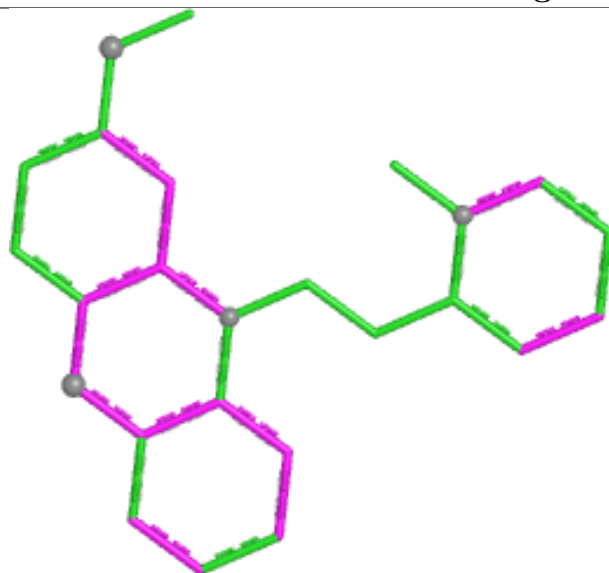
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	RTZ	1	0
2	A	2	RTZ	1	0
4	B	750	GOL	4	0
2	D	1	RTZ	1	0
6	B	800	HEM	1	0
4	A	750	GOL	2	0
2	B	1	RTZ	1	0
4	A	753	GOL	1	0
4	D	750	GOL	6	0
6	C	800	HEM	1	0
2	C	2	RTZ	3	0
4	A	751	GOL	1	0

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.

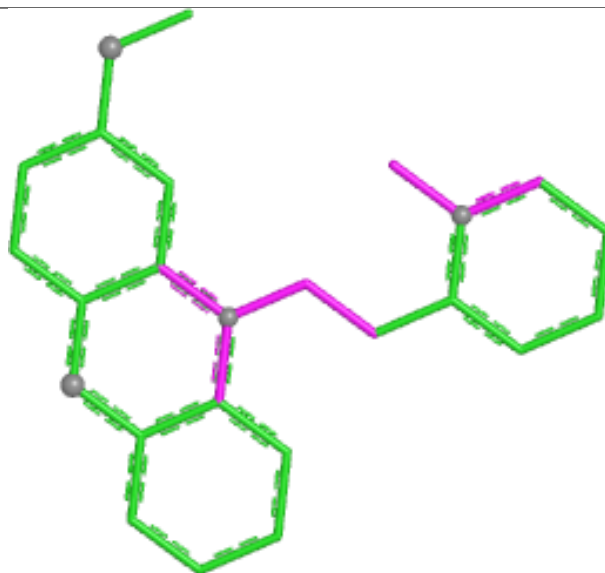
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



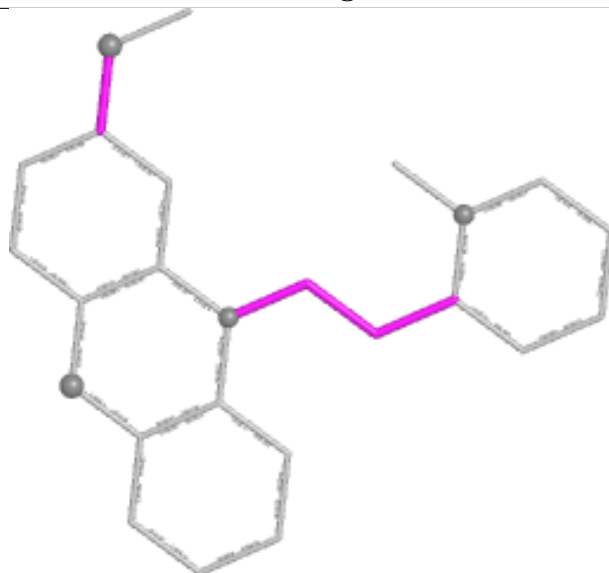
Ligand RTZ A 2



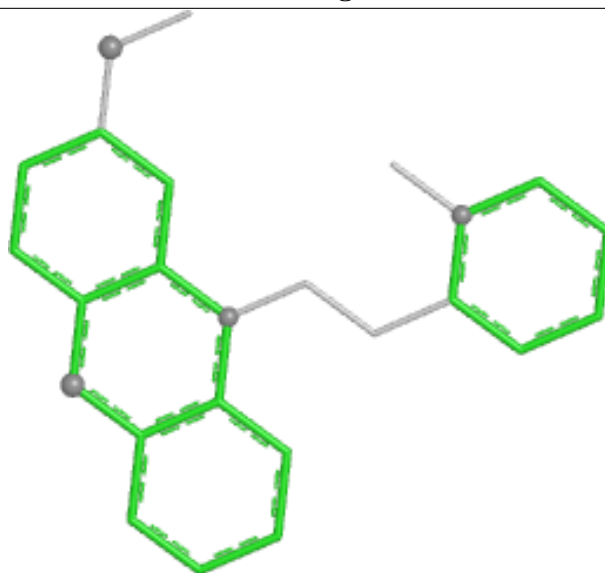
Bond lengths



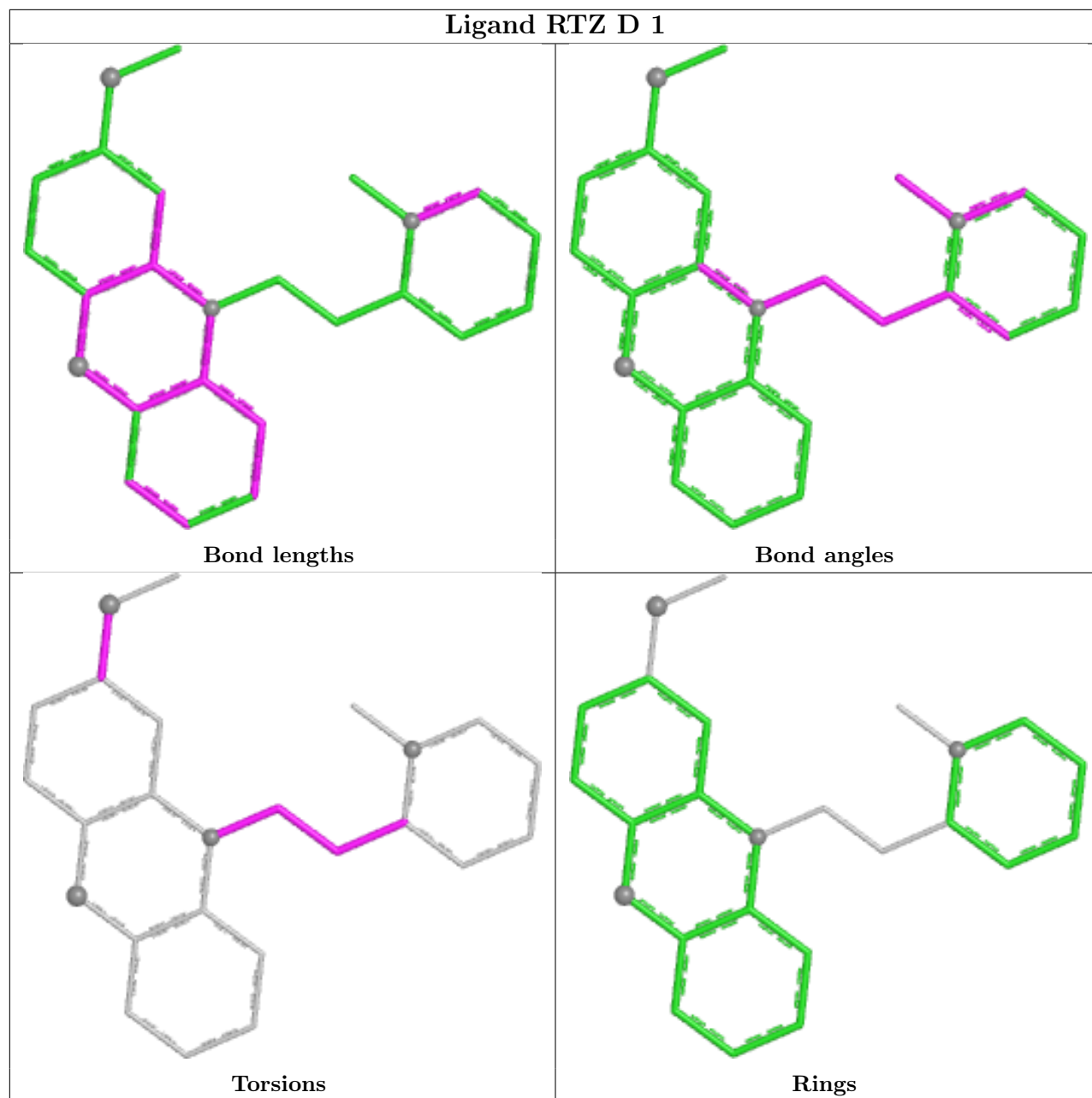
Bond angles

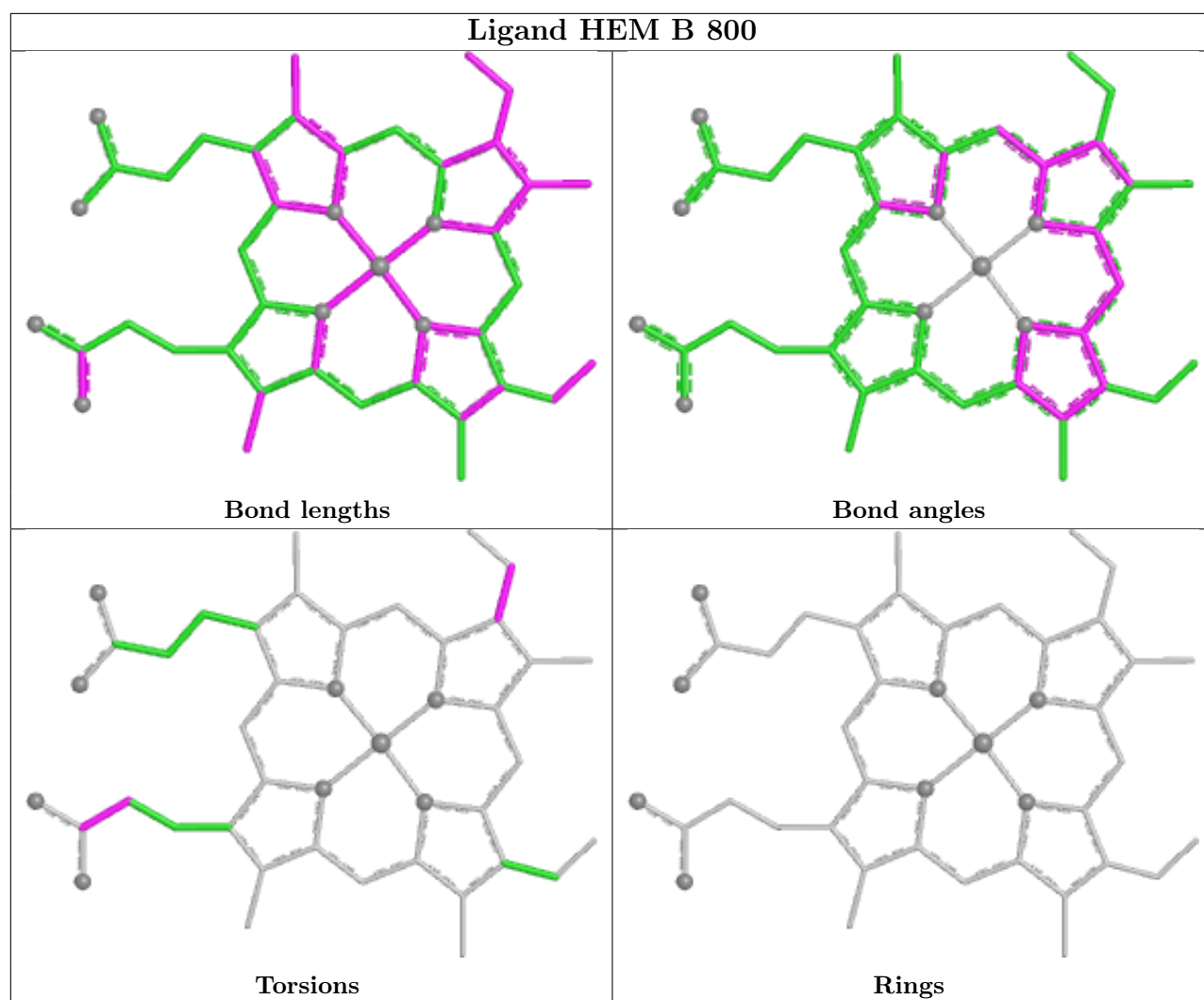


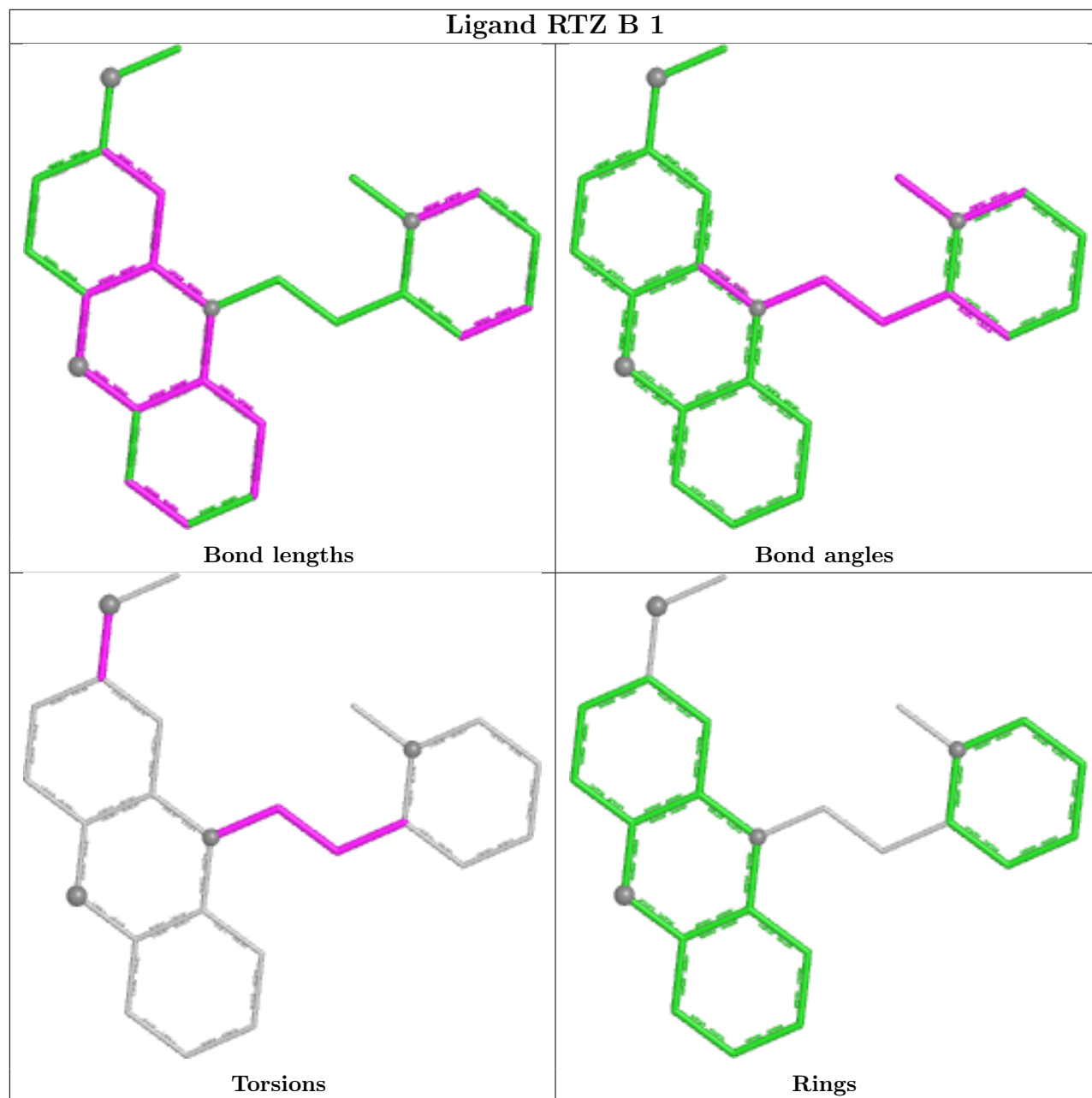
Torsions

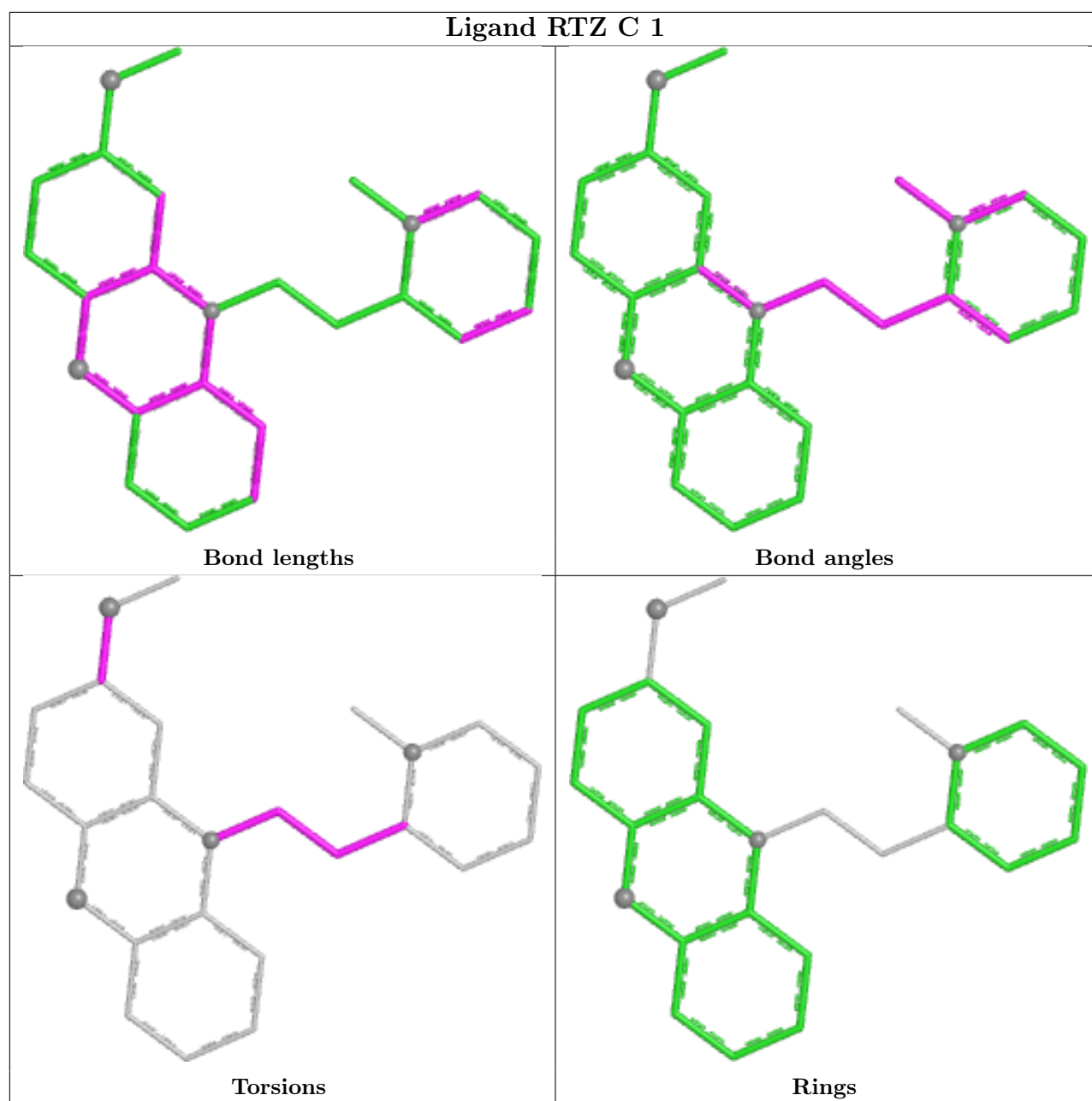


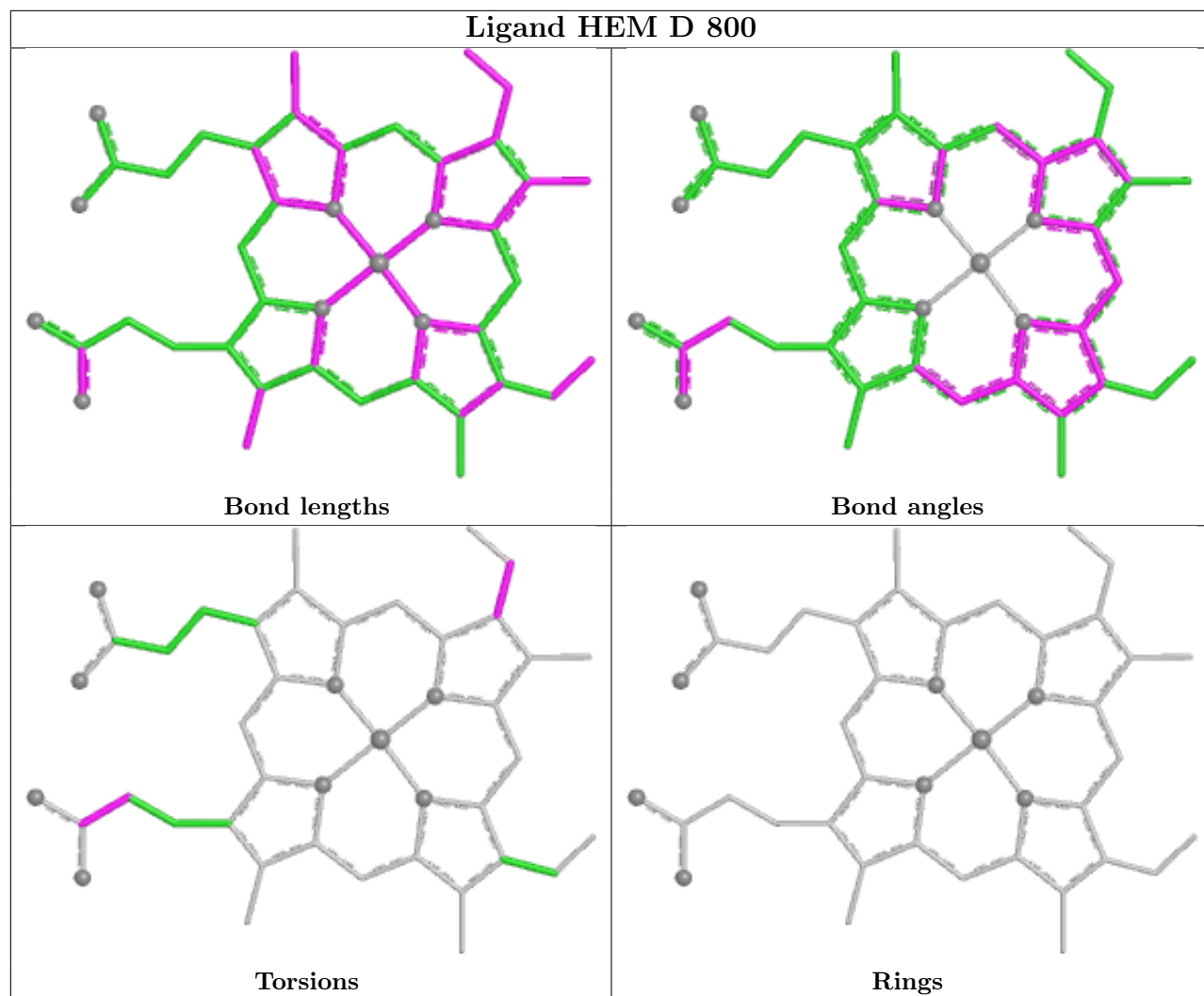
Rings

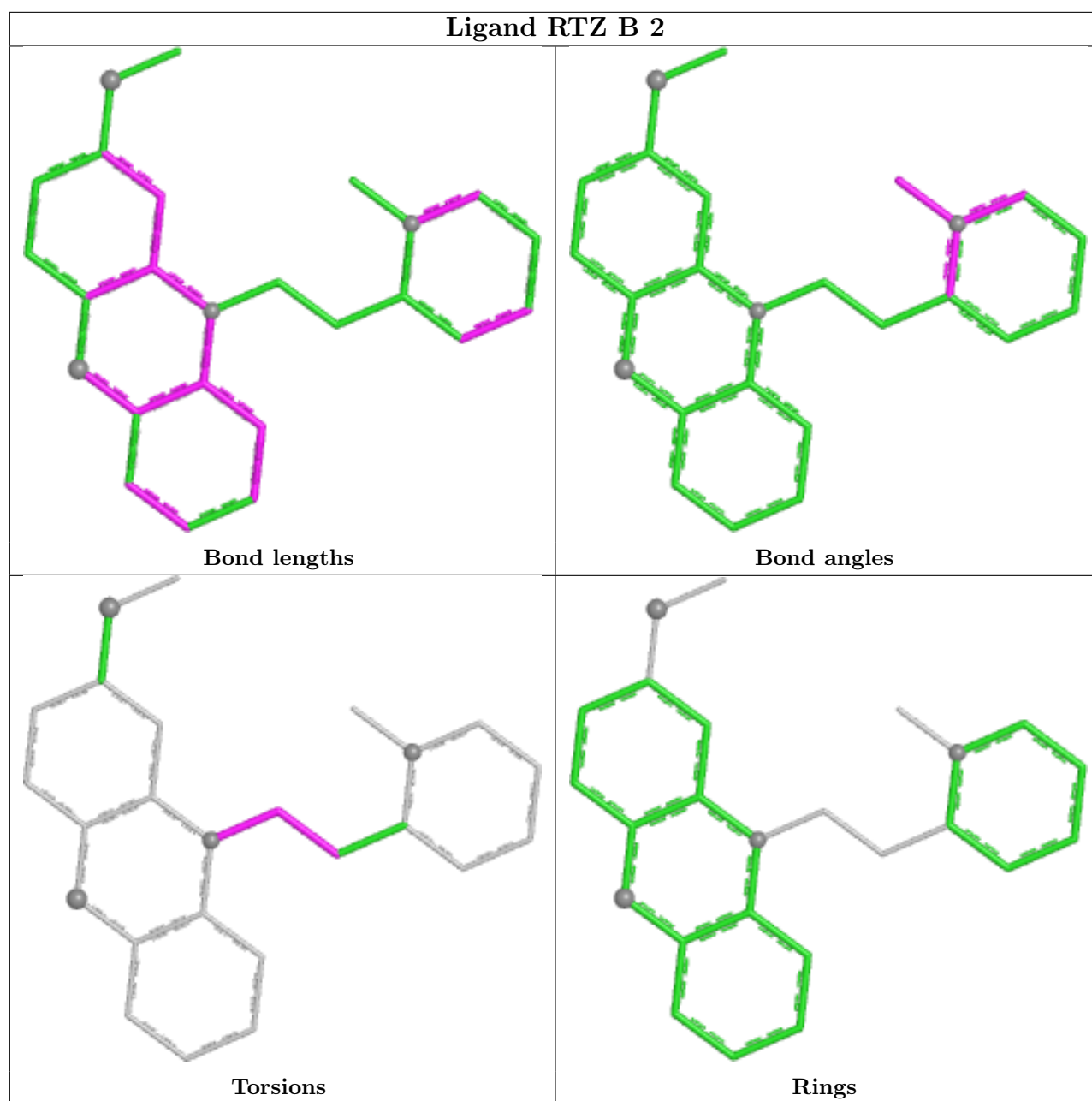


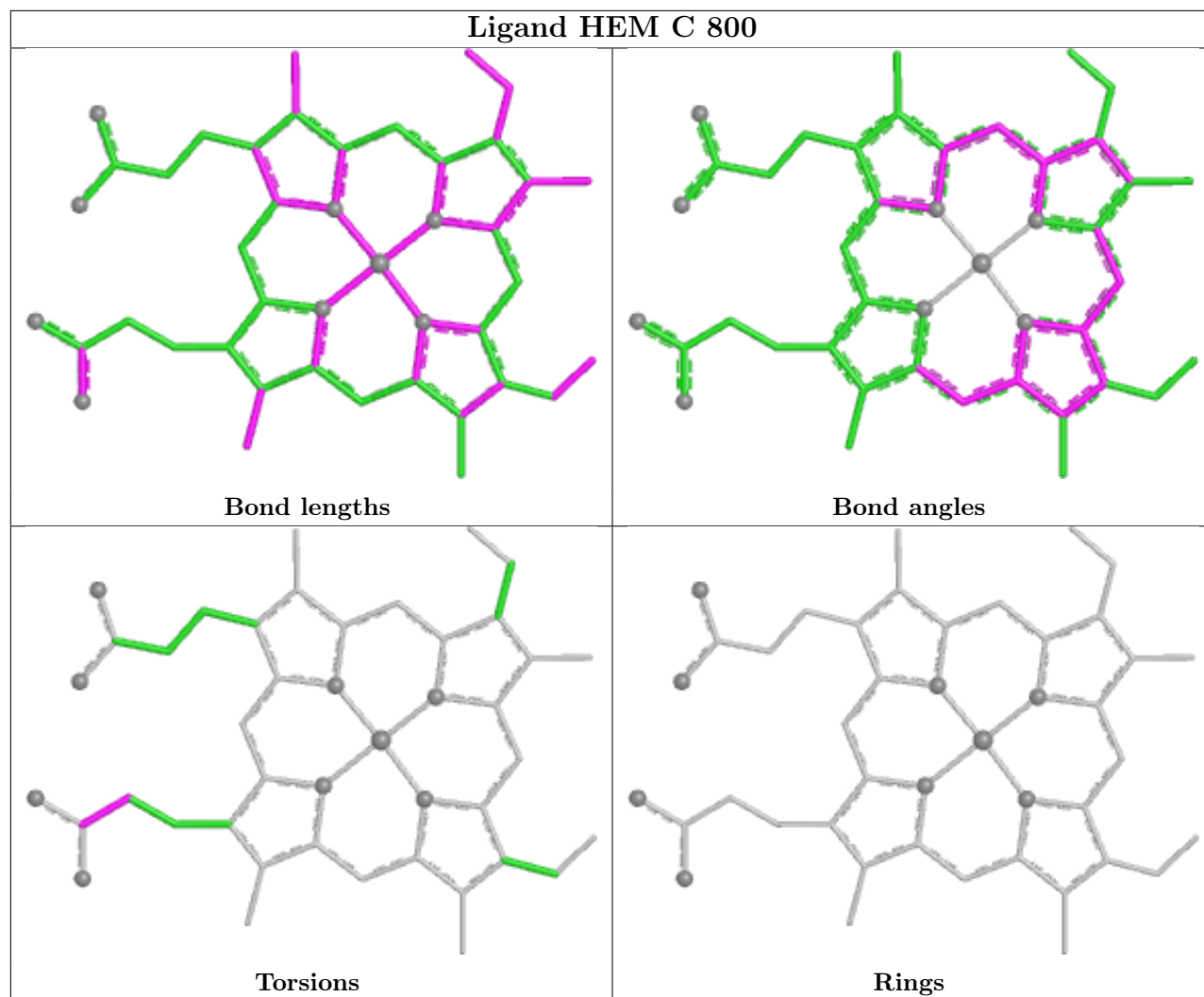


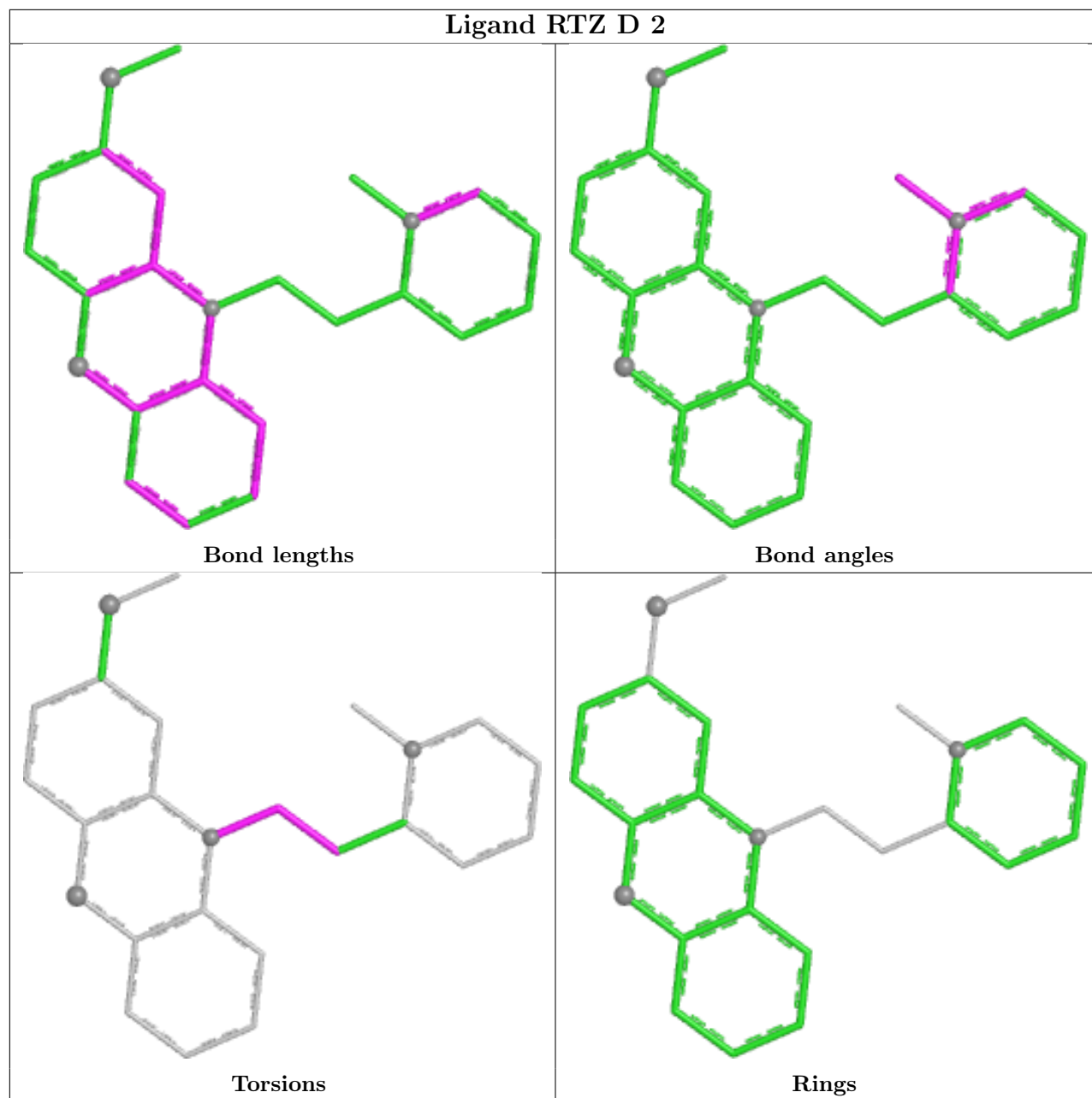




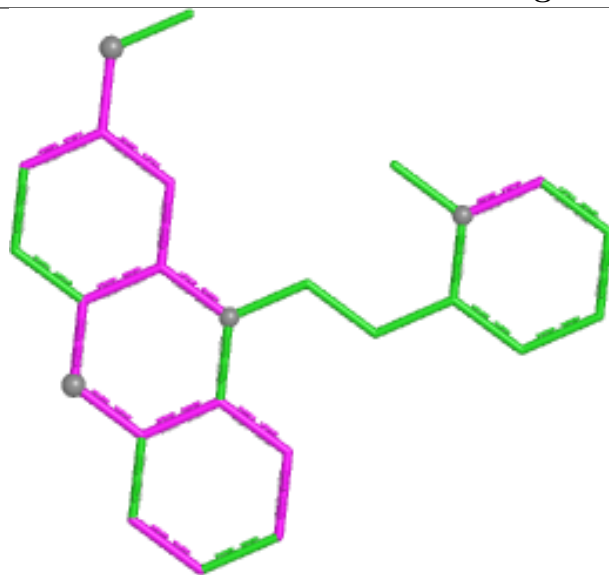




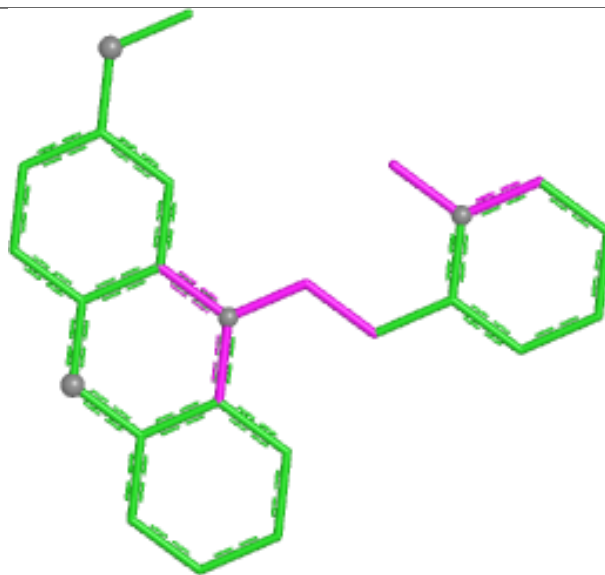




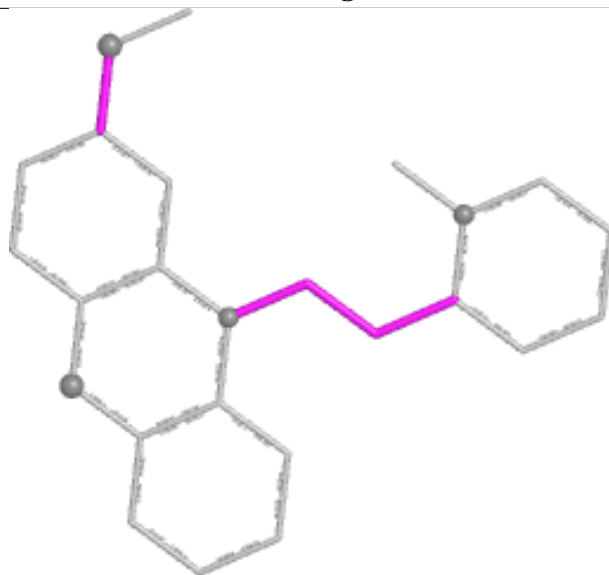
Ligand RTZ C 2



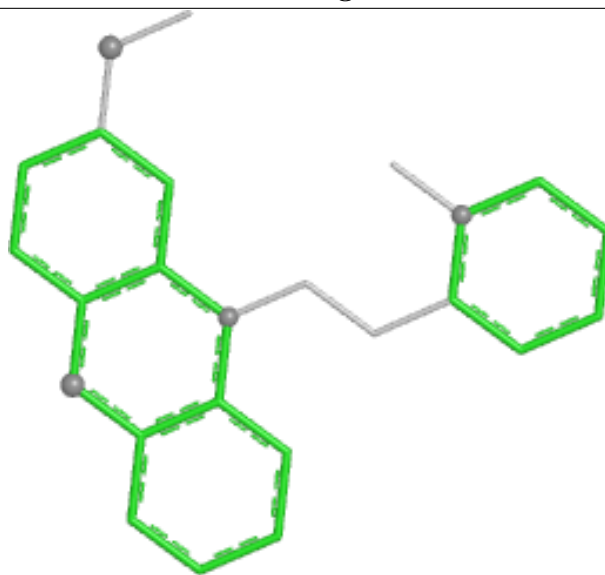
Bond lengths



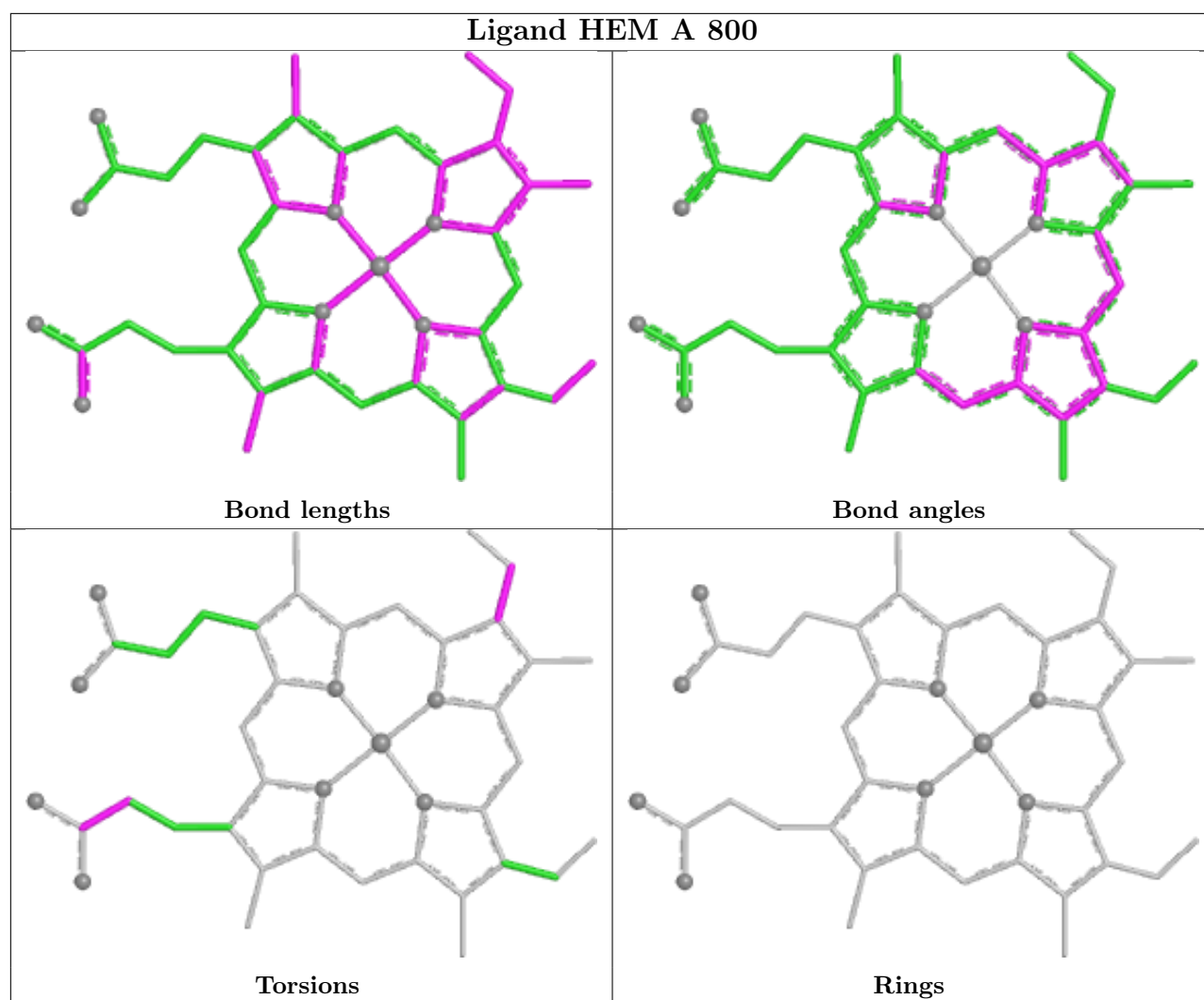
Bond angles



Torsions



Rings



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	467/479 (97%)	0.61	57 (12%) 8 8	15, 29, 53, 80	0
1	B	456/479 (95%)	0.87	83 (18%) 3 3	17, 34, 62, 82	0
1	C	467/479 (97%)	0.68	67 (14%) 6 6	15, 30, 57, 94	0
1	D	456/479 (95%)	0.85	69 (15%) 5 5	18, 34, 57, 82	0
All	All	1846/1916 (96%)	0.75	276 (14%) 5 5	15, 32, 58, 94	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	39	PRO	8.1
1	D	38	LEU	7.2
1	C	47	LEU	6.8
1	C	38	LEU	6.7
1	C	43	LEU	6.5
1	A	40	LEU	6.4
1	D	63	ARG	6.2
1	B	38	LEU	6.1
1	C	48	HIS	6.1
1	A	48	HIS	5.8
1	C	40	LEU	5.7
1	C	46	LEU	5.5
1	B	75	TRP	5.5
1	C	41	PRO	5.2
1	D	169	GLY	5.1
1	B	63	ARG	5.1
1	A	38	LEU	4.9
1	A	75	TRP	4.9
1	D	142	LEU	4.8
1	C	219	PHE	4.8
1	D	65	PHE	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	49	VAL	4.8
1	B	39	PRO	4.7
1	C	483	PHE	4.7
1	D	219	PHE	4.6
1	B	144	LEU	4.6
1	A	41	PRO	4.6
1	C	75	TRP	4.5
1	A	219	PHE	4.4
1	D	144	LEU	4.4
1	D	75	TRP	4.4
1	B	424	GLN	4.4
1	C	52	GLN	4.3
1	D	166	ASN	4.3
1	D	424	GLN	4.3
1	D	60	GLN	4.2
1	C	56	TYR	4.2
1	A	46	LEU	4.2
1	A	47	LEU	4.2
1	A	483	PHE	4.1
1	B	145	GLY	4.1
1	B	480	VAL	4.1
1	C	39	PRO	4.1
1	A	471	GLY	4.1
1	B	51	PHE	3.9
1	A	337	ASP	3.9
1	A	51	PHE	3.9
1	B	73	LEU	3.9
1	B	337	ASP	3.9
1	C	169	GLY	3.8
1	D	145	GLY	3.8
1	B	33	LEU	3.8
1	B	53	ASN	3.7
1	A	56	TYR	3.7
1	B	56	TYR	3.7
1	D	64	ARG	3.7
1	A	49	VAL	3.6
1	B	74	ALA	3.6
1	A	39	PRO	3.6
1	C	51	PHE	3.6
1	A	144	LEU	3.6
1	C	42	GLY	3.6
1	B	64	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	44	GLY	3.6
1	D	32	LYS	3.5
1	A	52	GLN	3.5
1	B	77	PRO	3.5
1	A	44	GLY	3.5
1	D	146	LYS	3.5
1	B	387	PHE	3.5
1	B	471	GLY	3.4
1	B	146	LYS	3.4
1	B	32	LYS	3.4
1	B	470	THR	3.4
1	C	33	LEU	3.4
1	B	463	HIS	3.3
1	A	32	LYS	3.3
1	C	45	ASN	3.3
1	A	307	MET	3.3
1	D	37	PRO	3.3
1	B	229	VAL	3.3
1	A	43	LEU	3.3
1	D	463	HIS	3.2
1	B	61	LEU	3.2
1	C	50	ASP	3.2
1	B	386	GLY	3.2
1	C	35	PRO	3.2
1	C	468	VAL	3.2
1	B	59	ASP	3.2
1	B	240	VAL	3.1
1	D	423	ALA	3.1
1	B	339	ILE	3.1
1	C	381	ASP	3.1
1	C	307	MET	3.1
1	C	341	GLN	3.1
1	D	57	CYS	3.1
1	B	133	ARG	3.1
1	B	343	ARG	3.1
1	C	53	ASN	3.1
1	B	71	LEU	3.1
1	C	144	LEU	3.1
1	D	471	GLY	3.0
1	B	68	VAL	3.0
1	B	493	CYS	3.0
1	A	96	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	58	PHE	3.0
1	D	340	GLY	2.9
1	C	340	GLY	2.9
1	A	59	ASP	2.9
1	A	477	HIS	2.9
1	C	380	ARG	2.9
1	B	237	ALA	2.9
1	C	34	PRO	2.9
1	B	219	PHE	2.9
1	A	45	ASN	2.9
1	C	146	LYS	2.9
1	C	473	PRO	2.8
1	B	50	ASP	2.8
1	C	235	ALA	2.8
1	B	55	PRO	2.8
1	D	339	ILE	2.8
1	A	380	ARG	2.8
1	B	333	GLN	2.8
1	D	426	HIS	2.8
1	A	50	ASP	2.8
1	B	210	GLN	2.7
1	B	423	ALA	2.7
1	C	32	LYS	2.7
1	D	73	LEU	2.7
1	D	220	LEU	2.7
1	D	233	ILE	2.7
1	C	379	SER	2.7
1	B	381	ASP	2.7
1	C	481	PHE	2.7
1	A	33	LEU	2.7
1	B	62	ARG	2.7
1	C	470	THR	2.7
1	B	37	PRO	2.7
1	A	232	HIS	2.7
1	A	382	ILE	2.7
1	B	467	SER	2.7
1	D	238	GLY	2.7
1	D	74	ALA	2.7
1	A	473	PRO	2.7
1	D	240	VAL	2.7
1	D	468	VAL	2.7
1	B	57	CYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	42	GLY	2.7
1	C	386	GLY	2.7
1	C	72	GLN	2.6
1	A	53	ASN	2.6
1	C	31	GLY	2.6
1	C	387	PHE	2.6
1	A	379	SER	2.6
1	D	50	ASP	2.6
1	D	61	LEU	2.6
1	B	70	SER	2.6
1	D	387	PHE	2.6
1	A	72	GLN	2.6
1	A	381	ASP	2.6
1	D	467	SER	2.6
1	A	60	GLN	2.5
1	B	60	GLN	2.5
1	C	60	GLN	2.5
1	B	342	VAL	2.5
1	D	229	VAL	2.5
1	A	31	GLY	2.5
1	C	337	ASP	2.5
1	B	165	ALA	2.5
1	D	383	GLU	2.5
1	C	152	TRP	2.5
1	A	143	GLY	2.5
1	A	342	VAL	2.5
1	A	383	GLU	2.5
1	B	169	GLY	2.5
1	B	170	ARG	2.5
1	B	338	VAL	2.5
1	B	382	ILE	2.5
1	C	229	VAL	2.5
1	D	170	ARG	2.5
1	D	470	THR	2.5
1	D	497	ARG	2.5
1	D	337	ASP	2.4
1	B	384	VAL	2.4
1	D	59	ASP	2.4
1	D	342	VAL	2.4
1	B	35	PRO	2.4
1	B	473	PRO	2.4
1	B	380	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	147	LYS	2.4
1	D	235	ALA	2.4
1	B	72	GLN	2.4
1	B	336	ASP	2.4
1	C	145	GLY	2.4
1	D	425	GLY	2.4
1	B	474	ARG	2.4
1	C	495	VAL	2.4
1	C	477	HIS	2.4
1	A	62	ARG	2.3
1	B	65	PHE	2.3
1	C	62	ARG	2.3
1	D	338	VAL	2.3
1	A	470	THR	2.3
1	D	56	TYR	2.3
1	D	165	ALA	2.3
1	C	73	LEU	2.3
1	D	71	LEU	2.3
1	D	140	ARG	2.3
1	D	306	GLY	2.3
1	D	330	ARG	2.3
1	D	386	GLY	2.3
1	A	233	ILE	2.3
1	D	480	VAL	2.3
1	B	242	ARG	2.3
1	B	198	ASP	2.3
1	D	381	ASP	2.3
1	A	386	GLY	2.3
1	B	143	GLY	2.3
1	B	472	GLN	2.2
1	B	69	PHE	2.2
1	B	166	ASN	2.2
1	D	173	ARG	2.2
1	A	478	HIS	2.2
1	C	210	GLN	2.2
1	C	333	GLN	2.2
1	B	147	LYS	2.2
1	C	240	VAL	2.2
1	C	471	GLY	2.2
1	D	33	LEU	2.2
1	D	474	ARG	2.2
1	A	146	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	141	ASN	2.2
1	C	36	GLY	2.2
1	C	232	HIS	2.2
1	D	108	GLN	2.2
1	A	173	ARG	2.2
1	B	34	PRO	2.1
1	D	35	PRO	2.1
1	C	65	PHE	2.1
1	C	68	VAL	2.1
1	A	169	GLY	2.1
1	B	234	PRO	2.1
1	B	390	PRO	2.1
1	B	496	PRO	2.1
1	A	210	GLN	2.1
1	A	387	PHE	2.1
1	B	233	ILE	2.1
1	B	385	GLN	2.1
1	B	142	LEU	2.1
1	D	476	SER	2.1
1	C	469	PRO	2.1
1	B	352	HIS	2.1
1	C	352	HIS	2.1
1	A	468	VAL	2.1
1	A	385	GLN	2.1
1	D	210	GLN	2.1
1	A	35	PRO	2.1
1	A	474	ARG	2.1
1	B	468	VAL	2.1
1	D	69	PHE	2.1
1	B	52	GLN	2.0
1	D	336	ASP	2.0
1	C	474	ARG	2.0
1	B	426	HIS	2.0
1	B	469	PRO	2.0
1	D	77	PRO	2.0
1	D	473	PRO	2.0
1	B	340	GLY	2.0
1	C	382	ILE	2.0
1	A	229	VAL	2.0
1	A	338	VAL	2.0
1	C	342	VAL	2.0
1	C	384	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	74	ALA	2.0
1	C	64	ARG	2.0
1	D	343	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	A	790	5/5	0.61	0.29	109,109,110,110	0
4	GOL	A	752	6/6	0.79	0.18	55,58,59,60	0
4	GOL	A	751	6/6	0.81	0.17	70,71,71,72	0
2	RTZ	C	2	25/25	0.82	0.18	51,62,64,64	0
3	ZN	A	602	1/1	0.85	0.17	90,90,90,90	0
4	GOL	A	753	6/6	0.86	0.18	31,42,46,47	0
2	RTZ	A	2	25/25	0.86	0.16	46,57,63,63	0
2	RTZ	B	2	25/25	0.87	0.15	53,54,55,57	0
3	ZN	C	602	1/1	0.87	0.12	79,79,79,79	0
2	RTZ	D	2	25/25	0.87	0.14	48,50,52,55	0
4	GOL	D	750	6/6	0.92	0.16	46,47,48,49	0
4	GOL	C	750	6/6	0.92	0.12	33,36,37,38	0
2	RTZ	B	1	25/25	0.93	0.10	28,34,37,41	0
2	RTZ	D	1	25/25	0.93	0.11	29,35,38,39	0
4	GOL	B	750	6/6	0.93	0.15	42,51,52,55	0
4	GOL	A	750	6/6	0.94	0.13	34,41,42,45	0
2	RTZ	A	1	25/25	0.95	0.09	26,29,33,36	0
2	RTZ	C	1	25/25	0.96	0.07	25,29,32,35	0
3	ZN	A	601	1/1	0.98	0.04	27,27,27,27	0
6	HEM	A	800	43/43	0.98	0.06	9,14,17,19	0

Continued on next page...

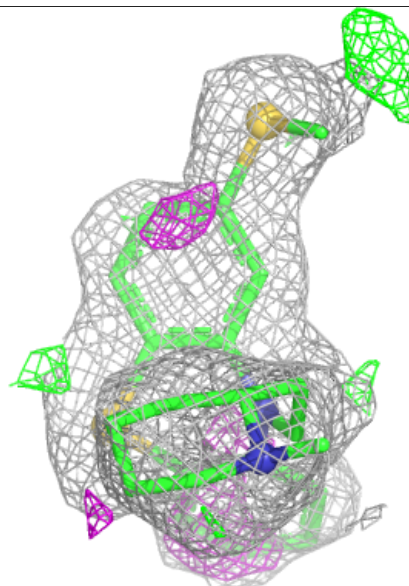
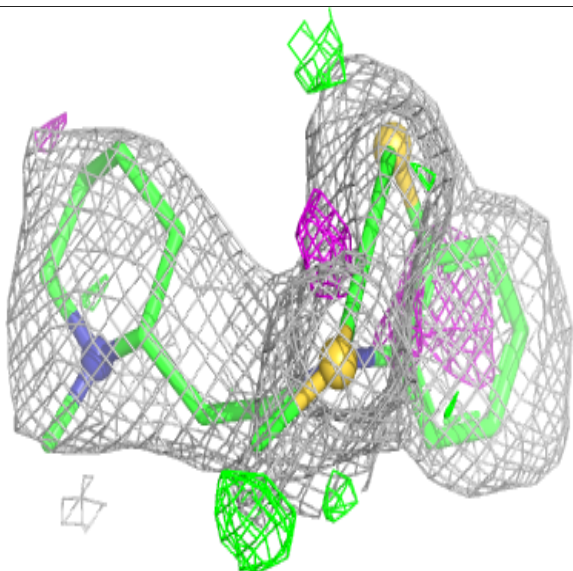
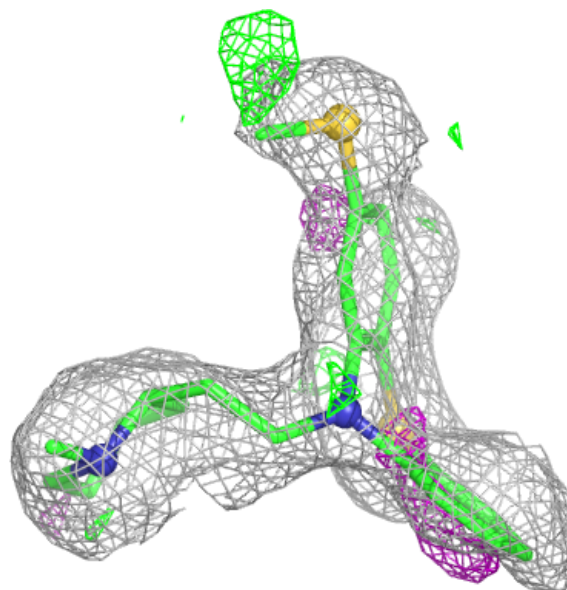
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	HEM	B	800	43/43	0.98	0.06	10,17,20,22	0
6	HEM	C	800	43/43	0.98	0.05	9,14,18,21	0
6	HEM	D	800	43/43	0.98	0.06	16,22,23,24	0
3	ZN	B	600	1/1	1.00	0.01	23,23,23,23	0
3	ZN	C	600	1/1	1.00	0.02	24,24,24,24	0
3	ZN	A	600	1/1	1.00	0.01	21,21,21,21	0
3	ZN	D	600	1/1	1.00	0.01	26,26,26,26	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.

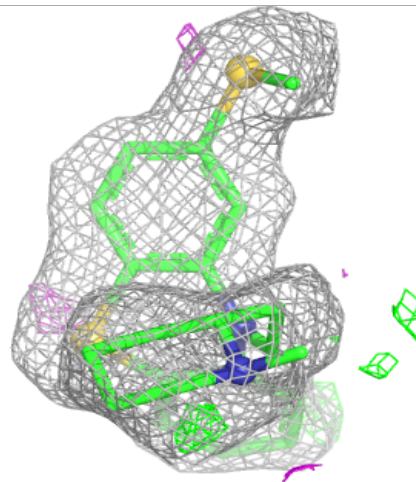
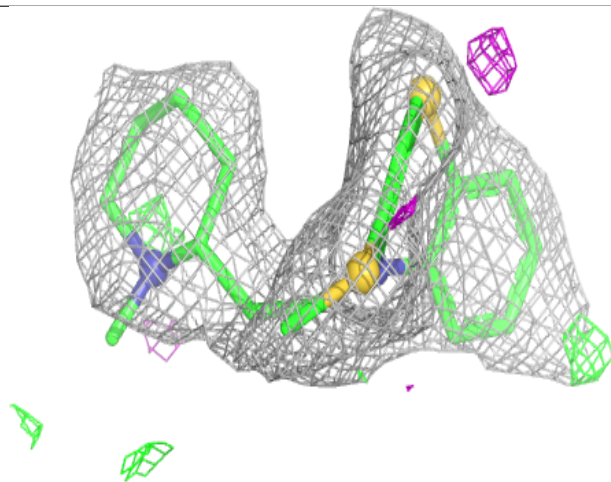
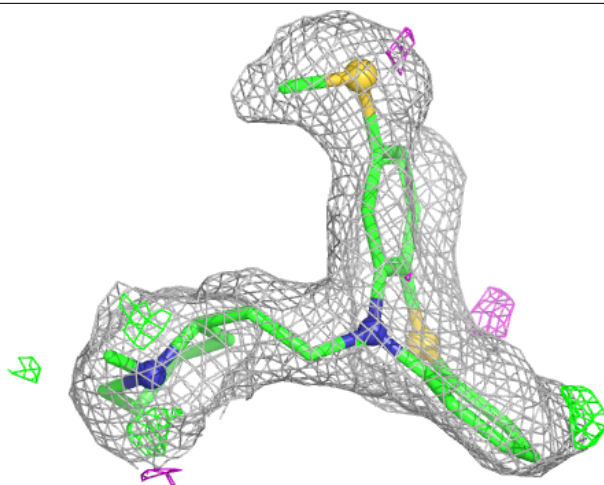
Electron density around RTZ C 2:

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



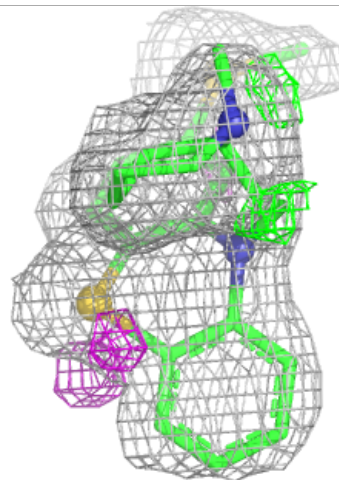
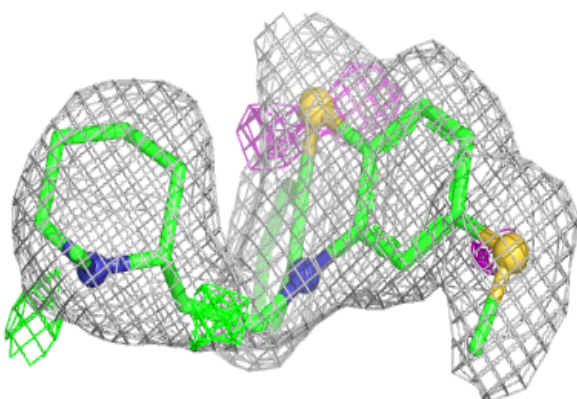
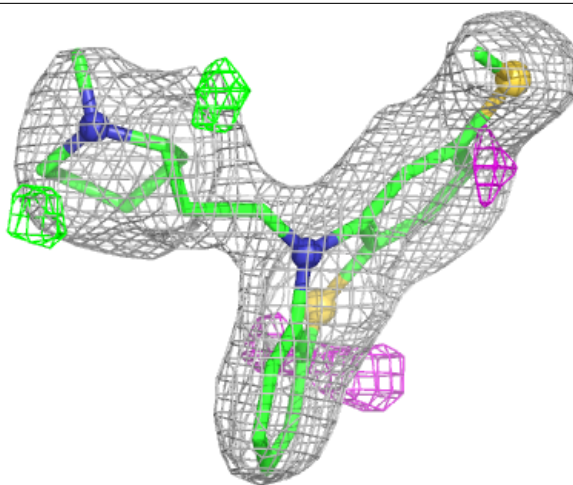
Electron density around RTZ A 2:

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



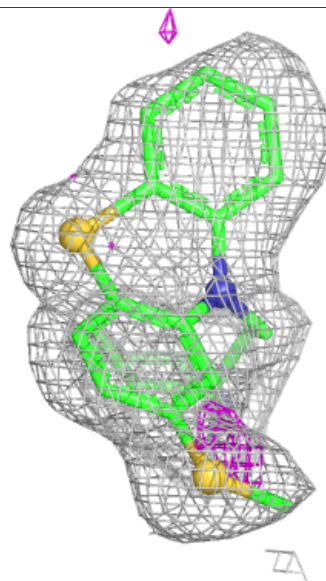
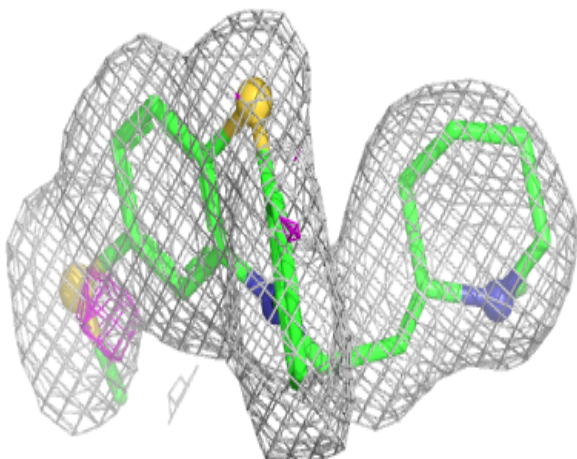
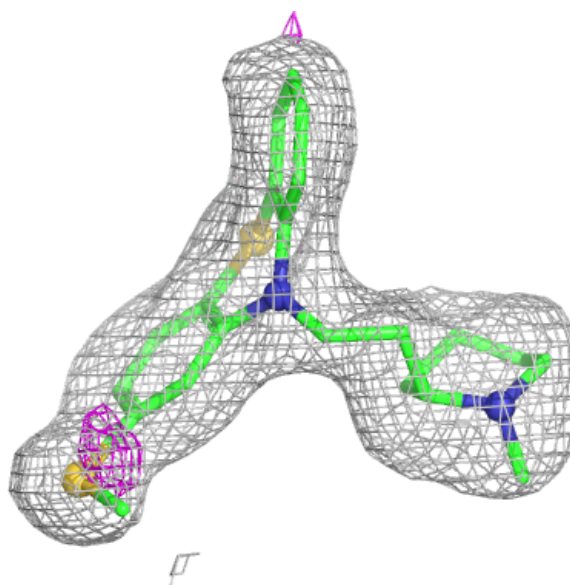
Electron density around RTZ B 2:

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



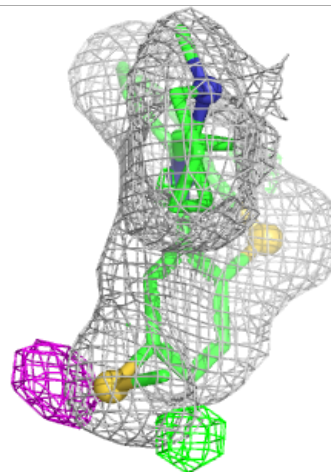
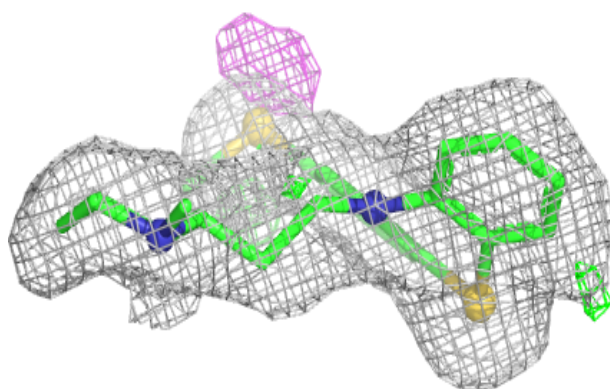
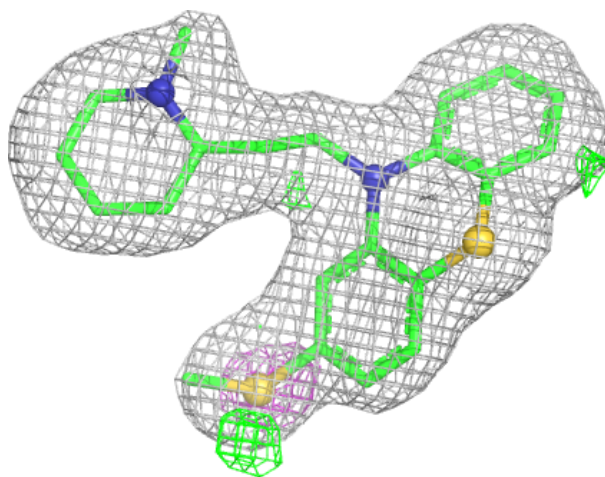
Electron density around RTZ D 2:

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



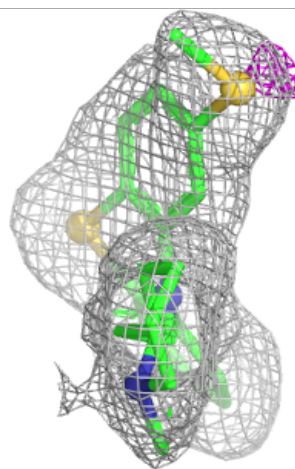
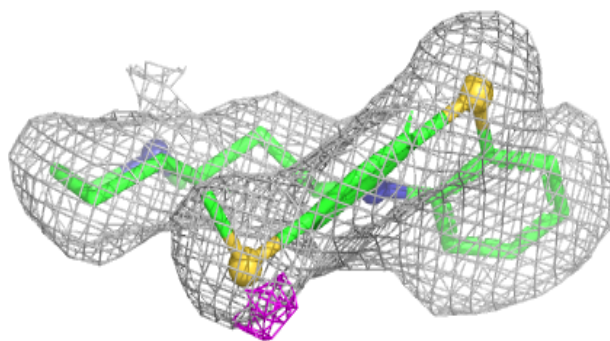
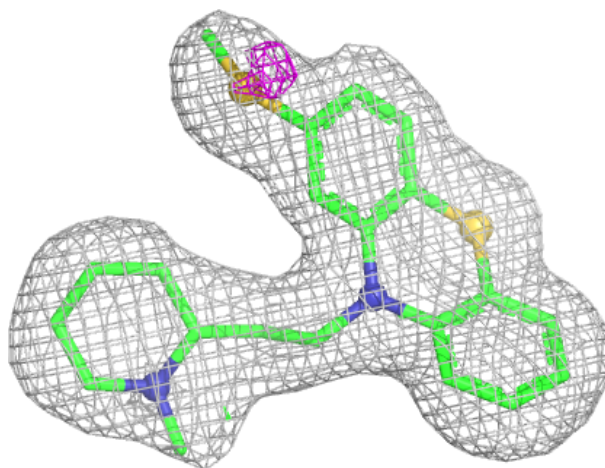
Electron density around RTZ B 1:

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



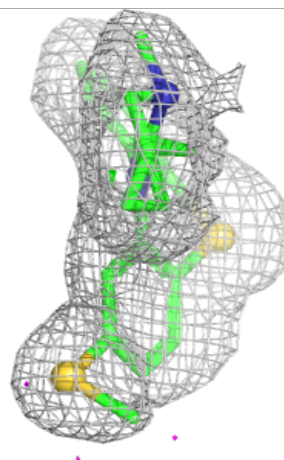
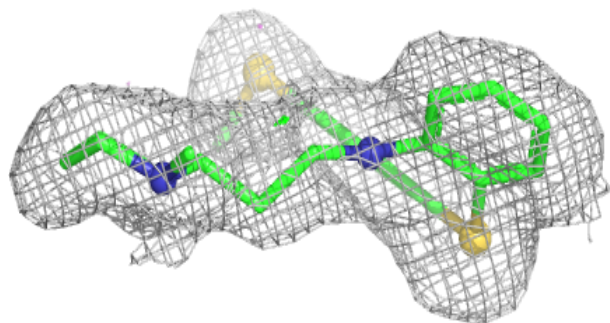
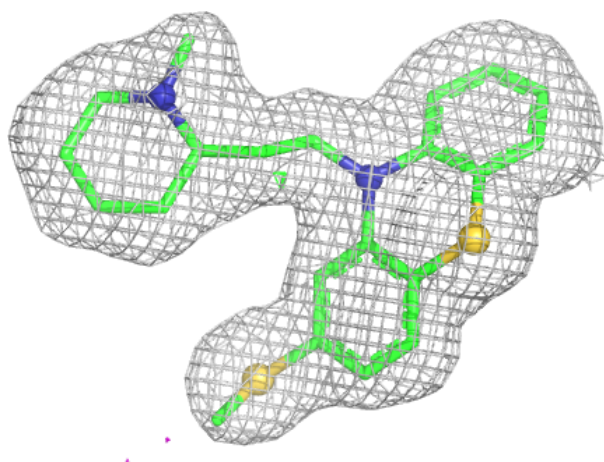
Electron density around RTZ D 1:

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



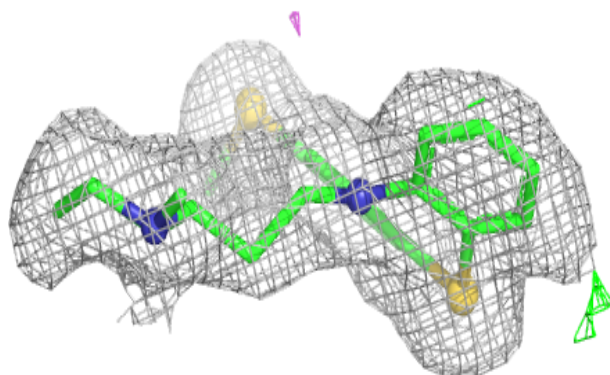
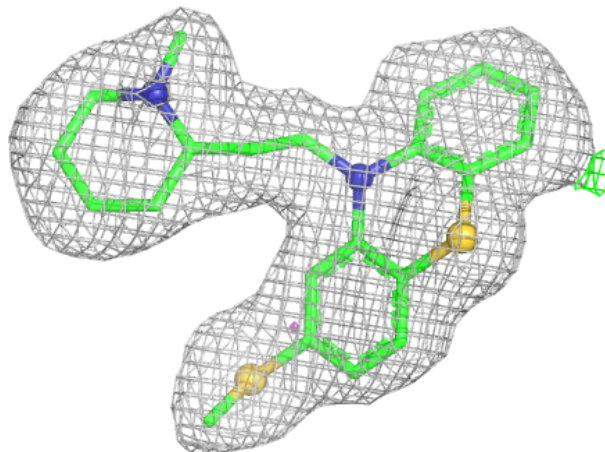
Electron density around RTZ A 1:

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



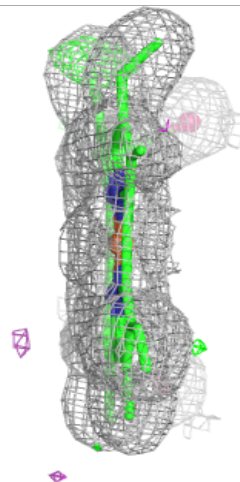
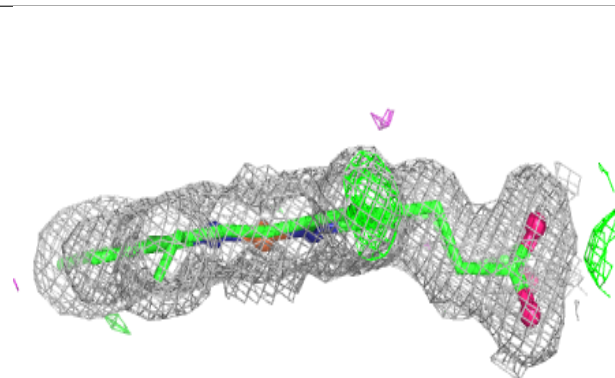
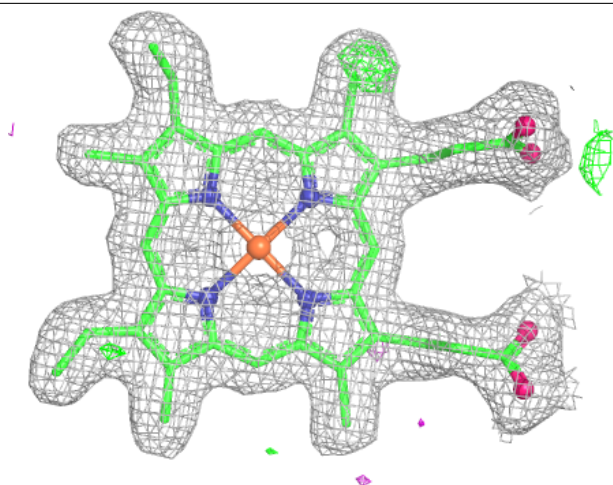
Electron density around RTZ C 1:

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



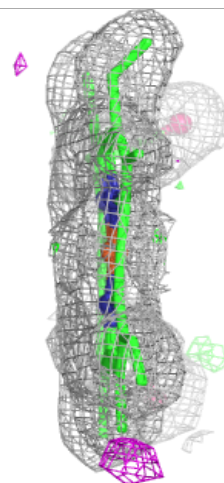
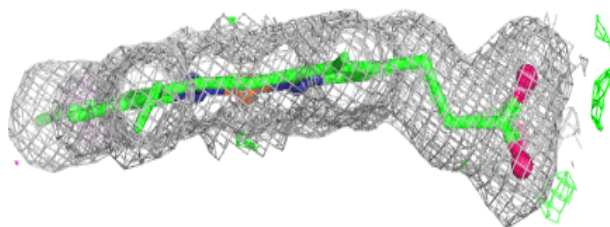
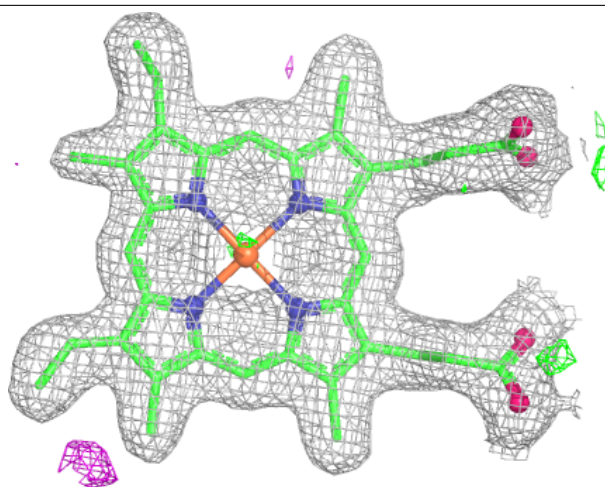
Electron density around HEM A 800:

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



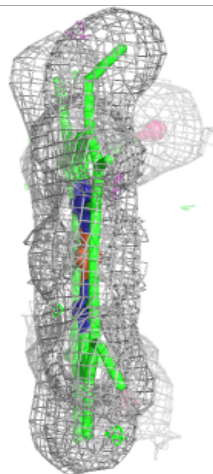
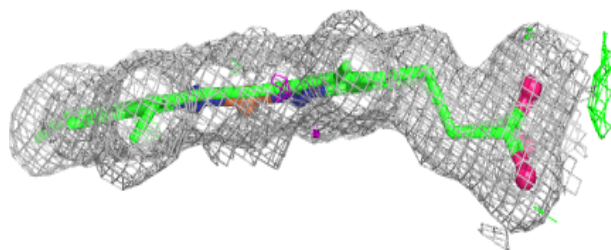
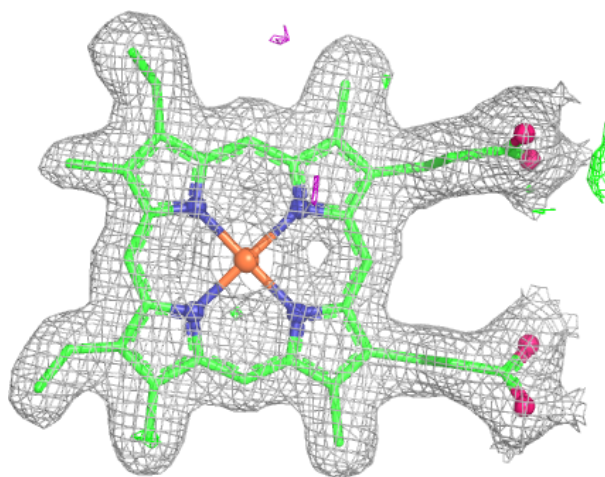
Electron density around HEM B 800:

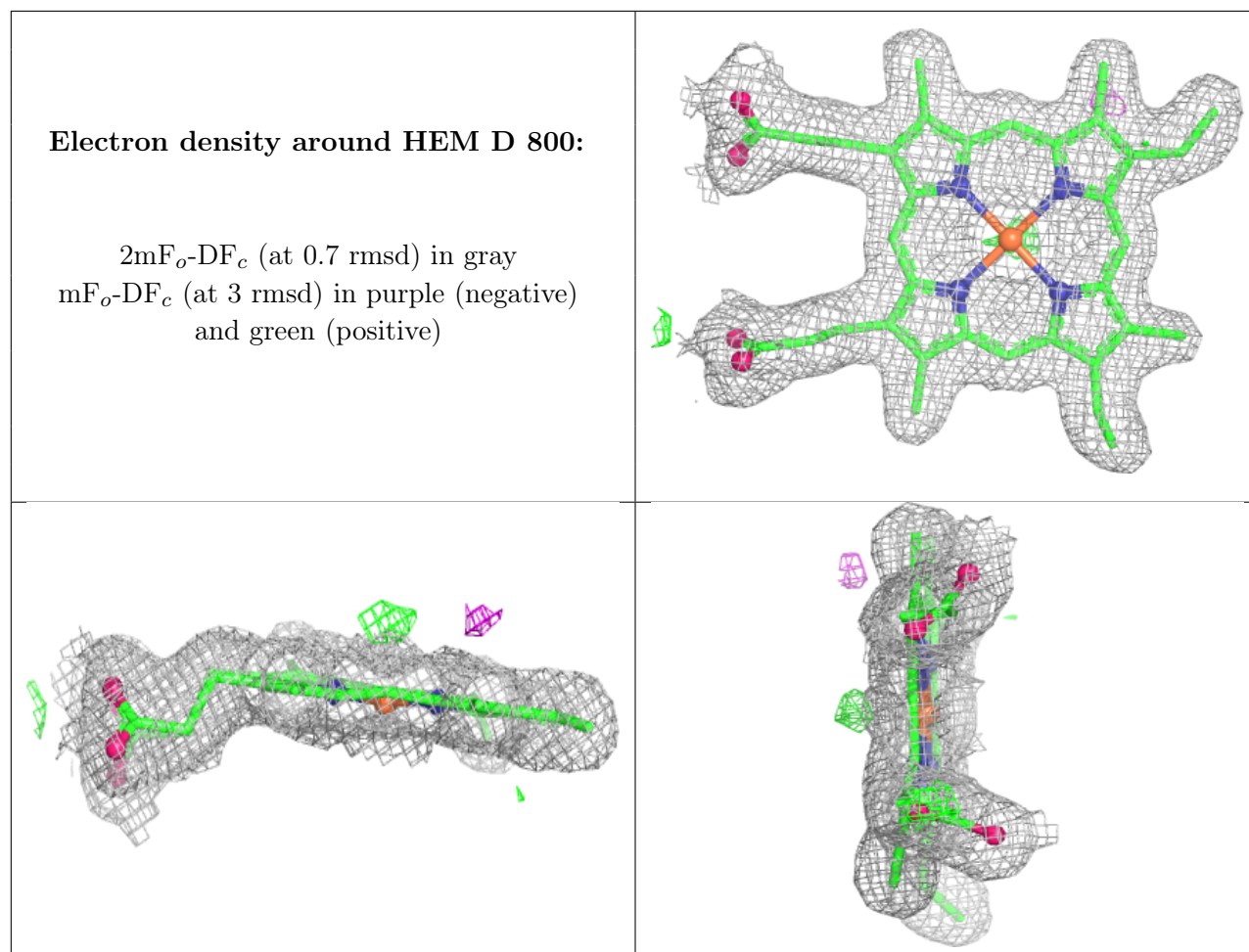
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 800:

$2mF_o-DF_c$ (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.