



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:55 PM BST

PDB ID : 4EJG
Title : Human Cytochrome P450 2A13 in complex with Nicotine
Authors : DeVore, N.M.; Scott, E.E.
Deposited on : 2012-04-06
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

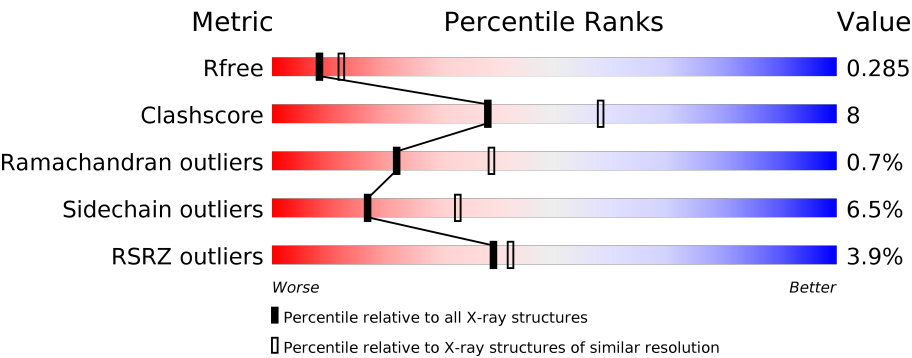
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	476	<div><div></div><div>80%17%..</div></div>
1	B	476	<div><div></div><div>81%16%.</div></div>
1	C	476	<div><div></div><div>75%22%..</div></div>
1	D	476	<div><div></div><div>75%20%..</div></div>
1	E	476	<div><div>2%</div><div></div><div>79%17%..</div></div>
1	F	476	<div><div>8%</div><div></div><div>72%24%..</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	476	
1	H	476	

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	H	502	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30618 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 2A13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	1	0
			3772	2426	652	676	18			
1	B	464	Total	C	N	O	S	0	5	0
			3812	2448	663	683	18			
1	C	464	Total	C	N	O	S	0	4	0
			3798	2441	659	680	18			
1	D	465	Total	C	N	O	S	0	3	0
			3797	2441	658	680	18			
1	E	465	Total	C	N	O	S	0	3	0
			3798	2443	659	678	18			
1	F	465	Total	C	N	O	S	0	0	0
			3772	2427	652	675	18			
1	G	463	Total	C	N	O	S	0	0	0
			3735	2403	643	671	18			
1	H	458	Total	C	N	O	S	0	0	0
			3687	2365	638	666	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	EXPRESSION TAG	UNP Q16696
A	24	ALA	-	EXPRESSION TAG	UNP Q16696
A	25	LYS	-	EXPRESSION TAG	UNP Q16696
A	26	LYS	-	EXPRESSION TAG	UNP Q16696
A	27	THR	-	EXPRESSION TAG	UNP Q16696
A	28	SER	-	EXPRESSION TAG	UNP Q16696
A	29	SER	-	EXPRESSION TAG	UNP Q16696
A	30	LYS	-	EXPRESSION TAG	UNP Q16696
A	495	HIS	-	EXPRESSION TAG	UNP Q16696
A	496	HIS	-	EXPRESSION TAG	UNP Q16696
A	497	HIS	-	EXPRESSION TAG	UNP Q16696
A	498	HIS	-	EXPRESSION TAG	UNP Q16696
B	23	MET	-	EXPRESSION TAG	UNP Q16696

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	ALA	-	EXPRESSION TAG	UNP Q16696
B	25	LYS	-	EXPRESSION TAG	UNP Q16696
B	26	LYS	-	EXPRESSION TAG	UNP Q16696
B	27	THR	-	EXPRESSION TAG	UNP Q16696
B	28	SER	-	EXPRESSION TAG	UNP Q16696
B	29	SER	-	EXPRESSION TAG	UNP Q16696
B	30	LYS	-	EXPRESSION TAG	UNP Q16696
B	495	HIS	-	EXPRESSION TAG	UNP Q16696
B	496	HIS	-	EXPRESSION TAG	UNP Q16696
B	497	HIS	-	EXPRESSION TAG	UNP Q16696
B	498	HIS	-	EXPRESSION TAG	UNP Q16696
C	23	MET	-	EXPRESSION TAG	UNP Q16696
C	24	ALA	-	EXPRESSION TAG	UNP Q16696
C	25	LYS	-	EXPRESSION TAG	UNP Q16696
C	26	LYS	-	EXPRESSION TAG	UNP Q16696
C	27	THR	-	EXPRESSION TAG	UNP Q16696
C	28	SER	-	EXPRESSION TAG	UNP Q16696
C	29	SER	-	EXPRESSION TAG	UNP Q16696
C	30	LYS	-	EXPRESSION TAG	UNP Q16696
C	495	HIS	-	EXPRESSION TAG	UNP Q16696
C	496	HIS	-	EXPRESSION TAG	UNP Q16696
C	497	HIS	-	EXPRESSION TAG	UNP Q16696
C	498	HIS	-	EXPRESSION TAG	UNP Q16696
D	23	MET	-	EXPRESSION TAG	UNP Q16696
D	24	ALA	-	EXPRESSION TAG	UNP Q16696
D	25	LYS	-	EXPRESSION TAG	UNP Q16696
D	26	LYS	-	EXPRESSION TAG	UNP Q16696
D	27	THR	-	EXPRESSION TAG	UNP Q16696
D	28	SER	-	EXPRESSION TAG	UNP Q16696
D	29	SER	-	EXPRESSION TAG	UNP Q16696
D	30	LYS	-	EXPRESSION TAG	UNP Q16696
D	495	HIS	-	EXPRESSION TAG	UNP Q16696
D	496	HIS	-	EXPRESSION TAG	UNP Q16696
D	497	HIS	-	EXPRESSION TAG	UNP Q16696
D	498	HIS	-	EXPRESSION TAG	UNP Q16696
E	23	MET	-	EXPRESSION TAG	UNP Q16696
E	24	ALA	-	EXPRESSION TAG	UNP Q16696
E	25	LYS	-	EXPRESSION TAG	UNP Q16696
E	26	LYS	-	EXPRESSION TAG	UNP Q16696
E	27	THR	-	EXPRESSION TAG	UNP Q16696
E	28	SER	-	EXPRESSION TAG	UNP Q16696
E	29	SER	-	EXPRESSION TAG	UNP Q16696

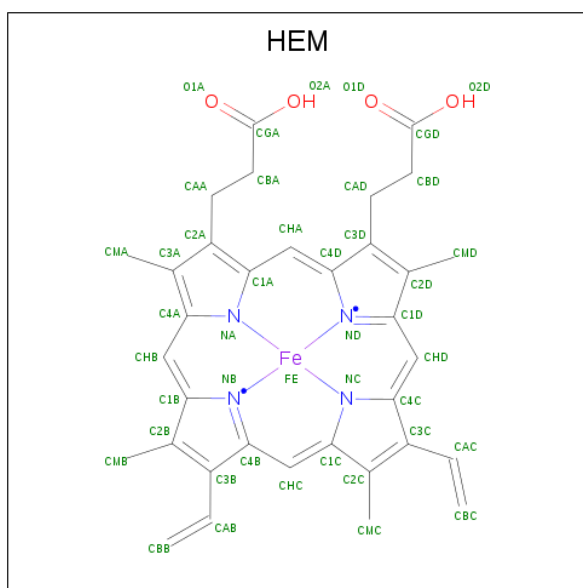
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	30	LYS	-	EXPRESSION TAG	UNP Q16696
E	495	HIS	-	EXPRESSION TAG	UNP Q16696
E	496	HIS	-	EXPRESSION TAG	UNP Q16696
E	497	HIS	-	EXPRESSION TAG	UNP Q16696
E	498	HIS	-	EXPRESSION TAG	UNP Q16696
F	23	MET	-	EXPRESSION TAG	UNP Q16696
F	24	ALA	-	EXPRESSION TAG	UNP Q16696
F	25	LYS	-	EXPRESSION TAG	UNP Q16696
F	26	LYS	-	EXPRESSION TAG	UNP Q16696
F	27	THR	-	EXPRESSION TAG	UNP Q16696
F	28	SER	-	EXPRESSION TAG	UNP Q16696
F	29	SER	-	EXPRESSION TAG	UNP Q16696
F	30	LYS	-	EXPRESSION TAG	UNP Q16696
F	495	HIS	-	EXPRESSION TAG	UNP Q16696
F	496	HIS	-	EXPRESSION TAG	UNP Q16696
F	497	HIS	-	EXPRESSION TAG	UNP Q16696
F	498	HIS	-	EXPRESSION TAG	UNP Q16696
G	23	MET	-	EXPRESSION TAG	UNP Q16696
G	24	ALA	-	EXPRESSION TAG	UNP Q16696
G	25	LYS	-	EXPRESSION TAG	UNP Q16696
G	26	LYS	-	EXPRESSION TAG	UNP Q16696
G	27	THR	-	EXPRESSION TAG	UNP Q16696
G	28	SER	-	EXPRESSION TAG	UNP Q16696
G	29	SER	-	EXPRESSION TAG	UNP Q16696
G	30	LYS	-	EXPRESSION TAG	UNP Q16696
G	495	HIS	-	EXPRESSION TAG	UNP Q16696
G	496	HIS	-	EXPRESSION TAG	UNP Q16696
G	497	HIS	-	EXPRESSION TAG	UNP Q16696
G	498	HIS	-	EXPRESSION TAG	UNP Q16696
H	23	MET	-	EXPRESSION TAG	UNP Q16696
H	24	ALA	-	EXPRESSION TAG	UNP Q16696
H	25	LYS	-	EXPRESSION TAG	UNP Q16696
H	26	LYS	-	EXPRESSION TAG	UNP Q16696
H	27	THR	-	EXPRESSION TAG	UNP Q16696
H	28	SER	-	EXPRESSION TAG	UNP Q16696
H	29	SER	-	EXPRESSION TAG	UNP Q16696
H	30	LYS	-	EXPRESSION TAG	UNP Q16696
H	495	HIS	-	EXPRESSION TAG	UNP Q16696
H	496	HIS	-	EXPRESSION TAG	UNP Q16696
H	497	HIS	-	EXPRESSION TAG	UNP Q16696
H	498	HIS	-	EXPRESSION TAG	UNP Q16696

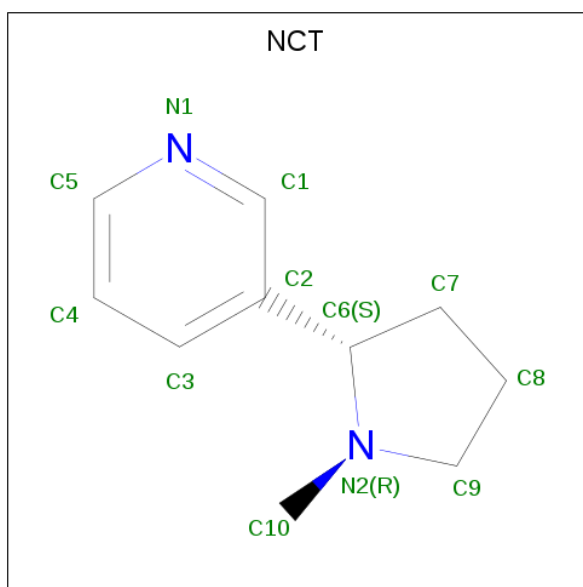
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: $C_{34}H_{32}FeN_4O_4$).



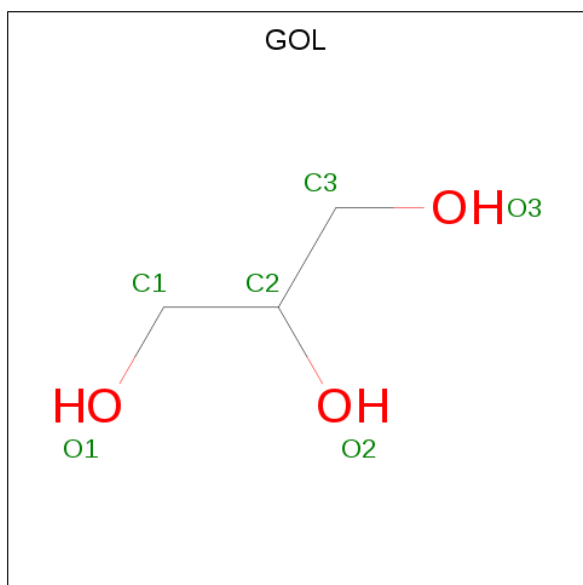
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 3 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (three-letter code: NCT) (formula: $C_{10}H_{14}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			12	10	2		
3	B	1	Total	C	N	0	0
			12	10	2		
3	C	1	Total	C	N	0	0
			12	10	2		
3	D	1	Total	C	N	0	0
			12	10	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		

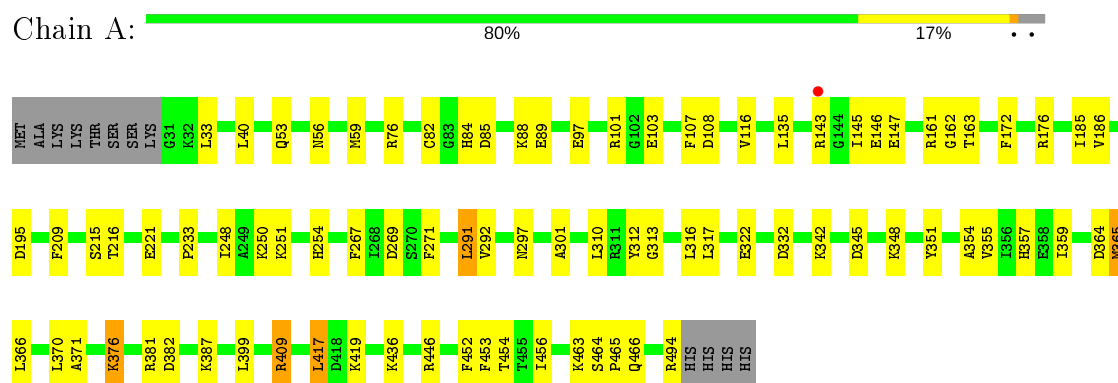
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	5	Total	O	0	0
			5	5		
5	C	6	Total	O	0	0
			6	6		
5	D	14	Total	O	0	0
			14	14		
5	E	2	Total	O	0	0
			2	2		
5	F	2	Total	O	0	0
			2	2		
5	G	9	Total	O	0	0
			9	9		
5	H	2	Total	O	0	0
			2	2		

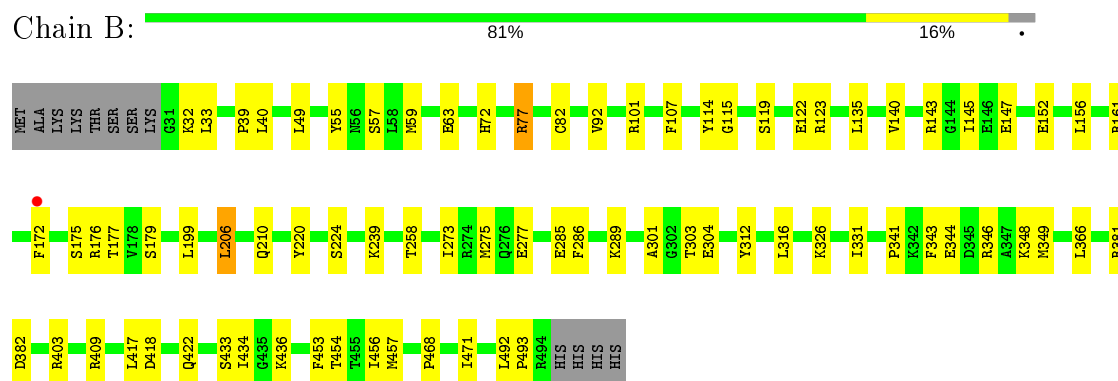
3 Residue-property plots

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.

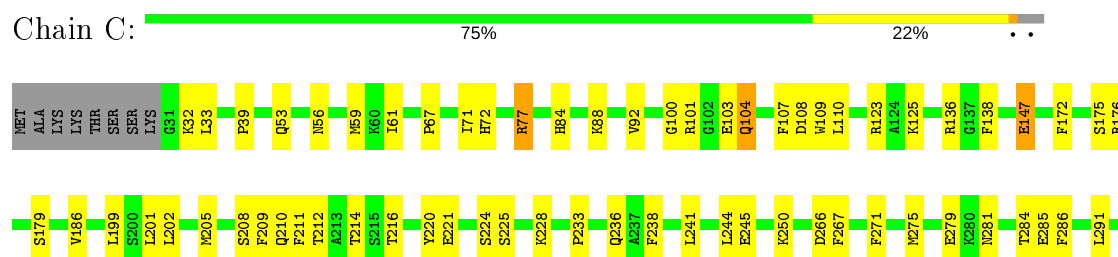
• Molecule 1: Cytochrome P450 2A13

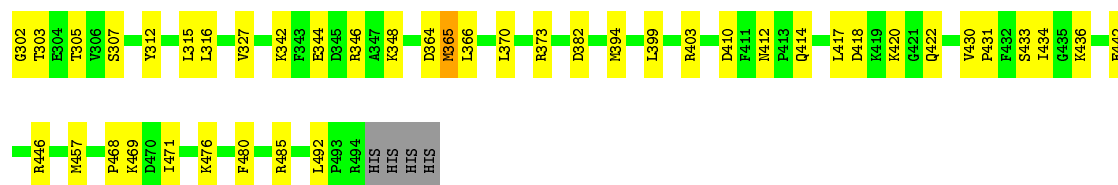


• Molecule 1: Cytochrome P450 2A13



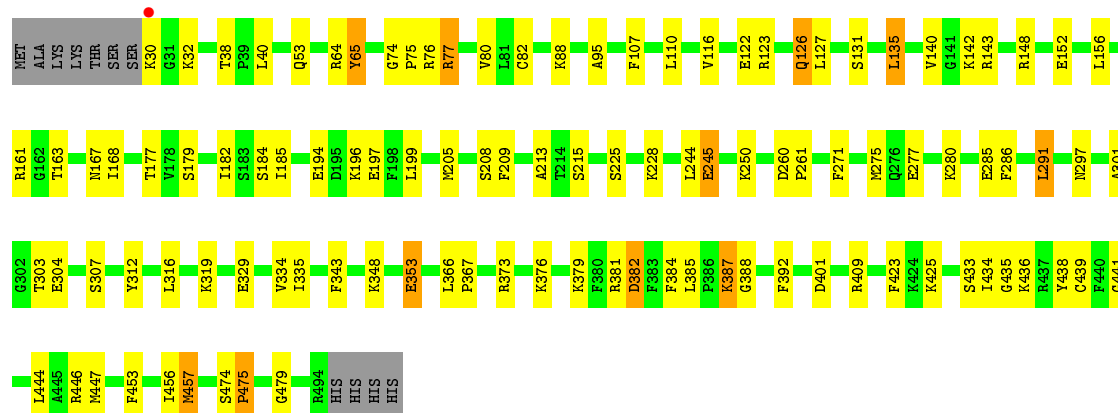
• Molecule 1: Cytochrome P450 2A13





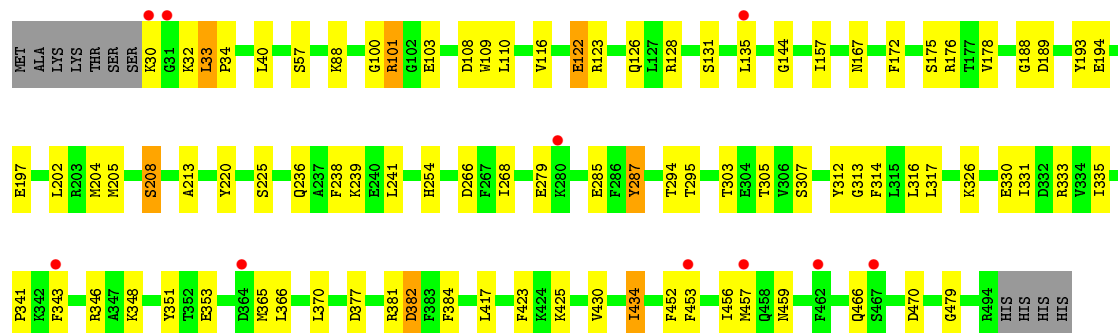
• Molecule 1: Cytochrome P450 2A13

Chain D: 75% 20% • •



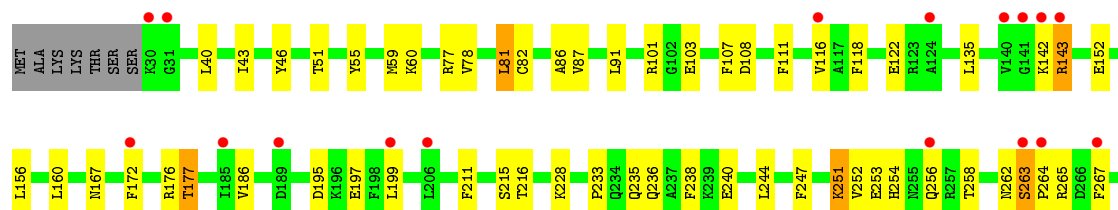
• Molecule 1: Cytochrome P450 2A13

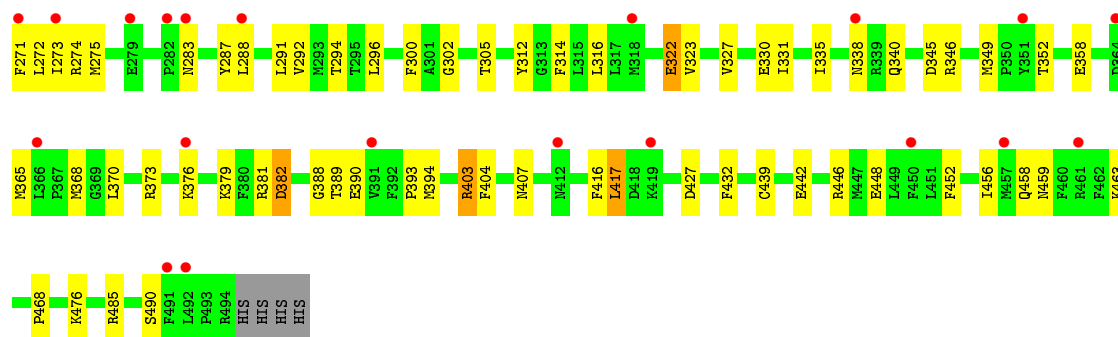
Chain E: 79% 17% • •



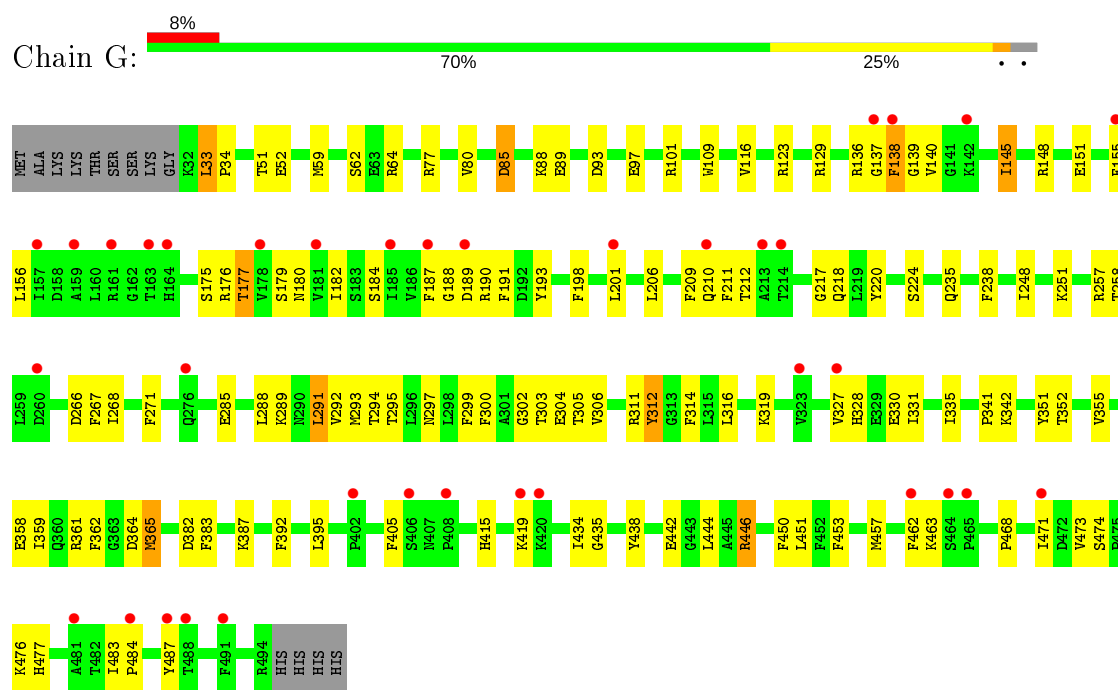
• Molecule 1: Cytochrome P450 2A13

Chain F: 72% 24% • •

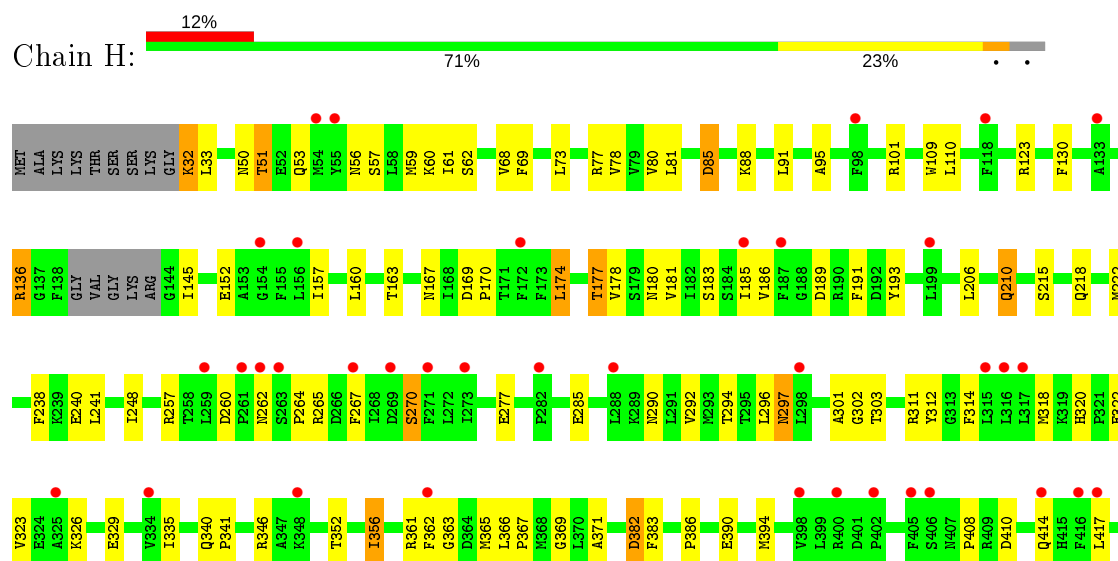


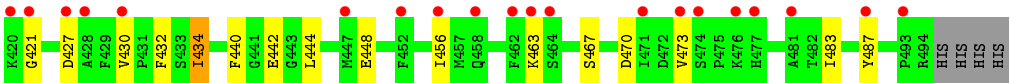


• Molecule 1: Cytochrome P450 2A13



• Molecule 1: Cytochrome P450 2A13





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.66Å 120.32Å 153.73Å 100.62° 101.82° 93.73°	Depositor
Resolution (Å)	102.58 – 2.50 102.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (102.58-2.50) 96.7 (102.59-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.52Å)	Xtriage
Refinement program	REFMAC 6.1.13	Depositor
R, R_{free}	0.224 , 0.285 0.222 , 0.285	Depositor DCC
R_{free} test set	8224 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30618	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NCT, 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	0.98	1/3869 (0.0%)	0.88	2/5210 (0.0%)
1	B	0.97	0/3909	0.88	0/5262
1	C	0.95	1/3898 (0.0%)	0.85	1/5248 (0.0%)
1	D	0.96	4/3897 (0.1%)	0.87	6/5246 (0.1%)
1	E	0.84	3/3898 (0.1%)	0.79	0/5246
1	F	0.78	1/3869 (0.0%)	0.77	0/5209
1	G	0.73	0/3832	0.76	0/5166
1	H	0.70	0/3780	0.72	0/5094
All	All	0.87	10/30952 (0.0%)	0.82	9/41681 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	65	TYR	CD2-CE2	-5.98	1.30	1.39
1	F	46	TYR	CD1-CE1	-5.93	1.30	1.39
1	E	100	GLY	C-N	-5.86	1.20	1.34
1	D	475	PRO	N-CD	5.67	1.55	1.47
1	E	101	ARG	C-N	-5.61	1.23	1.33
1	E	122	GLU	CG-CD	5.53	1.60	1.51
1	A	322	GLU	CG-CD	5.13	1.59	1.51
1	C	211	PHE	CE2-CZ	5.13	1.47	1.37
1	D	439	CYS	CB-SG	5.10	1.91	1.82
1	D	65	TYR	CD1-CE1	-5.07	1.31	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	316	LEU	CA-CB-CG	5.70	128.41	115.30
1	D	401	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	195	ASP	CB-CG-OD1	5.35	123.12	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	387	LYS	CD-CE-NZ	-5.32	99.47	111.70
1	C	315	LEU	CB-CG-CD2	-5.24	102.10	111.00
1	D	382	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	269	ASP	CB-CG-OD1	5.16	122.95	118.30
1	D	161	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	76	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3772	0	3735	53	0
1	B	3812	0	3771	45	0
1	C	3798	0	3762	57	0
1	D	3797	0	3764	56	0
1	E	3798	0	3772	44	0
1	F	3772	0	3741	71	0
1	G	3735	0	3670	77	0
1	H	3687	0	3614	54	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
2	G	43	0	30	0	0
2	H	43	0	30	2	0
3	A	12	0	14	3	0
3	B	12	0	14	3	0
3	C	12	0	14	3	0
3	D	12	0	14	3	0
4	H	6	0	8	1	0
5	A	9	0	0	0	0
5	B	5	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	6	0	0	0	0
5	D	14	0	0	1	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	9	0	0	1	0
5	H	2	0	0	0	0
All	All	30618	0	30133	459	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 (459) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LYS:HD2	1:C:33:LEU:H	1.19	1.07
1:D:77:ARG:HH11	1:D:77:ARG:HG2	1.23	1.03
1:B:32:LYS:HD2	1:B:33:LEU:H	1.25	0.96
1:C:32:LYS:HD2	1:C:33:LEU:N	1.81	0.95
1:H:352:THR:O	1:H:356:ILE:HD13	1.72	0.90
1:B:77:ARG:HH11	1:B:77:ARG:HG2	1.37	0.89
1:G:476:LYS:HG3	1:G:477:HIS:H	1.39	0.87
1:F:403:ARG:HH11	1:F:403:ARG:HG3	1.40	0.85
1:G:190:ARG:HH22	1:G:193:TYR:HE1	1.23	0.84
1:F:186:VAL:HA	1:F:267:PHE:HB3	1.58	0.84
1:A:53[B]:GLN:HG3	1:A:56:ASN:HB2	1.62	0.82
1:F:172:PHE:O	1:F:176:ARG:HG3	1.80	0.81
1:A:376:LYS:HA	1:A:387:LYS:HG3	1.62	0.81
1:H:215:SER:HB3	4:H:502:GOL:H2	1.61	0.81
1:A:216:THR:HG21	1:A:233:PRO:HG2	1.61	0.80
1:G:305:THR:HG22	1:G:365:MET:HG3	1.63	0.79
1:A:59:MET:HE1	1:A:82:CYS:SG	2.23	0.78
1:A:271:PHE:HB3	1:A:291:LEU:HD22	1.66	0.77
1:F:305:THR:HA	1:F:365:MET:CE	2.14	0.77
1:F:253:GLU:HA	1:F:256:GLN:OE1	1.85	0.77
1:A:59:MET:CE	1:A:82:CYS:SG	2.73	0.77
1:G:190:ARG:NH2	1:G:193:TYR:HE1	1.83	0.76
1:D:381:ARG:O	1:D:382:ASP:HB2	1.86	0.76
1:E:303:THR:O	1:E:307:SER:HB2	1.87	0.75
1:E:33:LEU:HD12	1:E:34:PRO:HD2	1.67	0.75
1:G:442:GLU:OE2	1:G:446:ARG:NH1	2.20	0.74
1:B:32:LYS:HD2	1:B:33:LEU:N	2.02	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.70	0.74
1:C:77:ARG:HG2	1:C:77:ARG:HH11	1.52	0.73
1:F:442:GLU:O	1:F:446:ARG:HG3	1.89	0.73
1:G:311:ARG:HH11	1:G:484:PRO:HD2	1.54	0.72
1:G:140:VAL:HG21	1:G:444:LEU:HB2	1.70	0.72
1:H:170:PRO:O	1:H:174:LEU:HB2	1.88	0.72
1:G:457:MET:HE2	1:G:462:PHE:HE2	1.53	0.72
1:F:305:THR:HA	1:F:365:MET:HE3	1.72	0.71
1:C:92:VAL:HG23	1:C:434:ILE:HD12	1.70	0.71
1:B:273:ILE:O	1:B:277:GLU:HG3	1.91	0.71
1:E:101:ARG:NH1	1:E:370:LEU:HB3	2.05	0.70
1:F:216:THR:HG21	1:F:233:PRO:HG2	1.73	0.70
1:C:364:ASP:OD1	1:C:399:LEU:HD12	1.92	0.69
1:H:51:THR:HG23	1:H:218:GLN:HG3	1.73	0.69
1:F:186:VAL:HA	1:F:267:PHE:CB	2.23	0.68
1:C:53[B]:GLN:HG3	1:C:56:ASN:HB2	1.75	0.68
1:C:303:THR:O	1:C:307:SER:HB2	1.94	0.67
1:B:172:PHE:O	1:B:176[B]:ARG:HG3	1.94	0.67
1:A:101:ARG:NH1	1:A:370:LEU:HB3	2.09	0.67
1:H:365:MET:O	1:H:367:PRO:HD3	1.94	0.67
1:C:216:THR:HG21	1:C:233:PRO:HG2	1.77	0.66
1:H:366:LEU:HB3	1:H:369:GLY:HA2	1.77	0.66
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.01	0.66
1:B:179:SER:HB2	1:B:303:THR:HG23	1.76	0.66
1:G:209:PHE:HE2	1:G:300:PHE:HD1	1.41	0.65
1:G:156:LEU:HB2	1:G:177:THR:HG21	1.79	0.65
1:E:101:ARG:HH12	1:E:370:LEU:HB3	1.60	0.65
1:H:123:ARG:HA	1:H:285:GLU:HG2	1.80	0.64
1:E:331:ILE:HG23	1:E:335:ILE:HD12	1.78	0.64
1:G:88:LYS:HE2	5:G:603:HOH:O	1.96	0.64
1:B:92:VAL:HG23	1:B:434:ILE:HD12	1.80	0.64
1:F:368:MET:HG2	1:F:394:MET:CE	2.28	0.64
1:G:209:PHE:CE2	1:G:300:PHE:HD1	2.15	0.63
1:F:40:LEU:HD22	1:F:43:ILE:HD11	1.79	0.63
1:H:180:ASN:OD1	1:H:191:PHE:HB2	1.98	0.63
1:H:248:ILE:HG22	1:H:292:VAL:HG13	1.80	0.63
1:H:59:MET:C	1:H:61:ILE:H	2.01	0.62
1:B:206:LEU:O	1:B:210[B]:GLN:HG3	1.99	0.62
1:G:182:ILE:HD11	1:G:302:GLY:C	2.19	0.62
1:H:356:ILE:CD1	1:H:356:ILE:N	2.62	0.62
1:F:403:ARG:CG	1:F:403:ARG:HH11	2.09	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:351:TYR:O	1:G:355:VAL:HG23	2.00	0.61
1:C:107:PHE:CE1	3:C:501:NCT:HC4	2.35	0.61
1:D:152:GLU:HG3	1:D:177:THR:HG23	1.81	0.61
1:G:116:VAL:CG1	1:G:294:THR:HG23	2.31	0.61
1:G:311:ARG:NH1	1:G:484:PRO:HD2	2.15	0.61
1:D:280:LYS:HE3	5:D:612:HOH:O	2.00	0.61
1:G:327:VAL:HG21	1:G:355:VAL:HG21	1.83	0.61
1:A:143:ARG:O	1:A:147:GLU:HG2	2.00	0.61
1:H:240:GLU:HA	1:H:240:GLU:OE1	2.01	0.61
1:D:271:PHE:CD1	1:D:291:LEU:HB2	2.36	0.61
1:D:209:PHE:CD2	1:D:304:GLU:HG3	2.36	0.61
1:D:64:ARG:HG2	1:D:65:TYR:CE2	2.36	0.60
1:A:381:ARG:O	1:A:382:ASP:HB2	2.01	0.60
1:B:101:ARG:NH1	2:B:500:HEM:O2A	2.31	0.60
1:D:376:LYS:HA	1:D:387:LYS:HG3	1.84	0.60
1:B:39:PRO:HG3	1:B:72:HIS:CE1	2.37	0.60
1:H:180:ASN:HA	1:H:183:SER:HB2	1.83	0.60
1:D:142:LYS:HG2	1:D:143:ARG:N	2.17	0.59
1:F:403:ARG:O	1:F:403:ARG:HG3	2.01	0.59
1:G:64:ARG:HG3	1:G:64:ARG:O	2.02	0.59
1:B:206:LEU:HD12	1:B:304:GLU:OE2	2.02	0.59
1:G:355:VAL:O	1:G:359:ILE:HG12	2.02	0.59
1:A:351:TYR:O	1:A:355:VAL:HG23	2.02	0.59
1:A:59:MET:HE3	1:A:82:CYS:SG	2.41	0.59
1:G:176:ARG:O	1:G:180:ASN:ND2	2.33	0.59
3:C:501:NCT:H102	3:C:501:NCT:HC3	1.84	0.59
1:G:175:SER:O	1:G:179:SER:HB2	2.02	0.59
1:B:143:ARG:O	1:B:147:GLU:HG2	2.03	0.59
5:B:605:HOH:O	1:C:403:ARG:HD2	2.01	0.59
1:F:432:PHE:HB3	1:F:439:CYS:HB3	1.84	0.59
1:G:235:GLN:OE1	1:G:238:PHE:HD2	1.85	0.59
1:A:452:PHE:O	1:A:456:ILE:HD12	2.03	0.58
1:B:122:GLU:HA	1:B:122:GLU:OE1	2.01	0.58
1:E:172:PHE:O	1:E:176:ARG:HG3	2.04	0.58
1:C:302:GLY:HA2	2:C:500:HEM:HMC2	1.86	0.58
1:A:107:PHE:CZ	3:A:501:NCT:HC4	2.38	0.58
1:G:116:VAL:HG12	1:G:294:THR:HG23	1.85	0.58
1:B:107:PHE:CE1	3:B:501:NCT:HC4	2.38	0.58
1:A:271:PHE:HB3	1:A:291:LEU:CD2	2.33	0.58
1:E:220:TYR:HH	1:E:238:PHE:HZ	1.52	0.58
1:C:172:PHE:O	1:C:176:ARG:HG3	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:GLU:HG3	1:F:177:THR:HG22	1.86	0.57
1:G:312:TYR:O	1:G:316:LEU:HD12	2.05	0.57
1:A:271:PHE:CG	1:A:291:LEU:HD22	2.39	0.57
1:G:34:PRO:HD3	1:G:383:PHE:HB3	1.87	0.57
1:D:179:SER:HB2	1:D:303:THR:HG23	1.86	0.57
1:C:100:GLY:HA3	1:C:373:ARG:O	2.05	0.56
1:E:335:ILE:HD13	1:E:341:PRO:HB3	1.87	0.56
1:A:271:PHE:CB	1:A:291:LEU:HD22	2.34	0.56
1:E:123:ARG:HA	1:E:285:GLU:HG3	1.86	0.56
1:C:209:PHE:HZ	1:C:365:MET:HE3	1.70	0.56
1:H:109:TRP:CH2	1:H:238:PHE:HB3	2.41	0.56
1:H:444:LEU:O	1:H:448:GLU:HG3	2.06	0.56
1:A:313:GLY:O	1:A:317:LEU:HG	2.05	0.56
1:G:335:ILE:HD13	1:G:341:PRO:HB3	1.88	0.56
1:D:301:ALA:HB2	3:D:501:NCT:HC6	1.88	0.55
1:E:313:GLY:O	1:E:317:LEU:HG	2.06	0.55
1:B:453:PHE:O	1:B:457:MET:HG3	2.07	0.55
1:B:49:LEU:HD23	1:B:57:SER:HB3	1.88	0.55
1:C:209:PHE:HZ	1:C:365:MET:CE	2.19	0.55
1:F:302:GLY:HA2	2:F:500:HEM:HMC2	1.88	0.55
1:G:473:VAL:HG23	1:G:474:SER:H	1.71	0.55
1:G:139:GLY:HA2	1:G:145:ILE:HB	1.88	0.55
1:G:211:PHE:CZ	1:G:217:GLY:HA2	2.41	0.55
1:C:305:THR:HG22	1:C:365:MET:HE2	1.87	0.55
1:D:213:ALA:HA	1:D:479:GLY:HA3	1.88	0.55
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.89	0.55
1:A:209:PHE:CZ	1:A:365:MET:HE3	2.42	0.54
1:A:464:SER:HB2	1:A:465:PRO:HD2	1.89	0.54
1:A:355:VAL:O	1:A:359:ILE:HG13	2.08	0.54
1:C:175:SER:O	1:C:179:SER:HB2	2.08	0.54
1:E:381:ARG:O	1:E:382:ASP:OD2	2.25	0.54
1:H:311:ARG:HH12	1:H:483:ILE:HG23	1.72	0.54
1:C:103:GLU:HB2	1:C:108:ASP:OD2	2.08	0.54
1:D:182:ILE:HA	1:D:185:ILE:HD12	1.89	0.54
1:D:95:ALA:HB1	1:D:436:LYS:HG2	1.89	0.53
1:E:430:VAL:HG11	1:E:434:ILE:HD13	1.90	0.53
1:F:458:GLN:HG3	1:F:459:ASN:N	2.23	0.53
1:A:89:GLU:OE1	1:A:381:ARG:NE	2.38	0.53
1:D:435:GLY:O	1:D:438:TYR:HD1	1.91	0.53
1:E:305:THR:HA	1:E:365:MET:CE	2.39	0.53
1:F:358:GLU:OE1	1:F:358:GLU:HA	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:THR:O	1:G:297:ASN:HB2	2.09	0.53
1:B:32:LYS:CD	1:B:33:LEU:H	2.12	0.53
1:F:448:GLU:O	1:F:452:PHE:HD2	1.91	0.53
1:A:354:ALA:HB2	1:A:417:LEU:HD13	1.91	0.52
1:F:296:LEU:O	1:F:300:PHE:HB2	2.09	0.52
1:F:302:GLY:HA2	2:F:500:HEM:CMC	2.39	0.52
1:H:110:LEU:HD22	1:H:241:LEU:HB3	1.91	0.52
1:G:148:ARG:HD3	1:G:184:SER:OG	2.10	0.52
1:A:357:HIS:NE2	1:A:446:ARG:NH2	2.57	0.52
1:C:430:VAL:N	1:C:431:PRO:CD	2.73	0.52
1:E:33:LEU:HD12	1:E:34:PRO:CD	2.36	0.52
1:C:39:PRO:HG3	1:C:72:HIS:CE1	2.45	0.52
1:E:326:LYS:HB2	1:E:351:TYR:CE1	2.44	0.52
1:A:409:ARG:HH11	1:A:409:ARG:HB3	1.75	0.52
1:B:172:PHE:O	1:B:176[A]:ARG:HB2	2.10	0.52
1:C:109:TRP:CH2	1:C:238:PHE:HB3	2.45	0.52
1:C:342:LYS:HG3	1:C:344:GLU:HG2	1.92	0.52
1:F:416:PHE:O	1:F:417:LEU:HD13	2.09	0.52
1:A:172:PHE:O	1:A:176:ARG:HG3	2.10	0.52
1:H:101:ARG:HD3	1:H:371:ALA:O	2.10	0.52
1:A:145:ILE:HD11	1:A:185:ILE:HD11	1.91	0.51
1:A:381:ARG:O	1:A:382:ASP:CB	2.58	0.51
1:C:136:ARG:NH1	1:D:277:GLU:OE2	2.41	0.51
1:A:271:PHE:CD1	1:A:291:LEU:HD22	2.46	0.51
1:F:247:PHE:CZ	1:F:251:LYS:HG2	2.45	0.51
1:G:51:THR:HG23	1:G:218:GLN:HB2	1.92	0.51
1:E:452:PHE:O	1:E:456:ILE:HG13	2.10	0.51
1:H:206:LEU:O	1:H:210:GLN:HB2	2.10	0.51
1:C:271:PHE:CE1	1:C:291:LEU:HB2	2.45	0.51
1:C:250:LYS:HB2	1:C:250:LYS:NZ	2.25	0.51
1:G:123:ARG:HA	1:G:285:GLU:HG3	1.93	0.51
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.76	0.51
1:E:109:TRP:CH2	1:E:238:PHE:HB3	2.46	0.51
1:F:211:PHE:HE1	1:F:233:PRO:HB2	1.76	0.51
1:E:305:THR:HA	1:E:365:MET:HE2	1.93	0.51
1:F:107:PHE:O	1:F:111:PHE:HD2	1.94	0.51
1:E:188:GLY:N	1:E:266:ASP:HB3	2.26	0.51
1:C:61:ILE:HD13	1:C:71:ILE:HD13	1.92	0.50
1:D:122:GLU:O	1:D:126:GLN:HB2	2.11	0.50
1:E:305:THR:HB	2:E:500:HEM:CAB	2.42	0.50
1:F:40:LEU:CD2	1:F:43:ILE:HD11	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:VAL:HG22	1:H:390:GLU:HB2	1.92	0.50
1:E:205:MET:HE1	1:E:303:THR:HG21	1.93	0.50
1:G:405:PHE:HD1	1:G:415:HIS:HB3	1.77	0.50
1:H:302:GLY:HA2	2:H:501:HEM:CMC	2.41	0.50
1:D:140:VAL:HG13	1:D:444:LEU:HD13	1.92	0.50
1:D:453:PHE:O	1:D:457:MET:HG3	2.12	0.50
1:H:356:ILE:HD12	1:H:356:ILE:N	2.27	0.50
1:B:156:LEU:CD2	1:B:456:ILE:HD11	2.42	0.50
1:G:138:PHE:CD2	1:G:138:PHE:N	2.79	0.50
1:F:271:PHE:CD1	1:F:291:LEU:HB2	2.47	0.50
1:E:202:LEU:HA	1:E:205:MET:HE2	1.94	0.49
1:F:118:PHE:HE1	1:F:370:LEU:HD11	1.77	0.49
1:G:442:GLU:CD	1:G:446:ARG:HH11	2.15	0.49
1:C:476:LYS:HB2	1:C:485:ARG:HA	1.94	0.49
1:G:89:GLU:O	1:G:93:ASP:HB2	2.12	0.49
1:B:114:TYR:CD1	1:B:289:LYS:HE3	2.47	0.49
1:H:88:LYS:HG2	1:H:434:ILE:HD13	1.93	0.49
1:H:152:GLU:HG3	1:H:177:THR:HG22	1.95	0.49
1:H:414:GLN:OE1	1:H:417:LEU:HD12	2.13	0.49
1:E:131:SER:O	1:E:135:LEU:HB2	2.11	0.49
1:F:55:TYR:CE1	1:F:59:MET:HG3	2.48	0.49
1:A:76:ARG:NH1	1:A:221:GLU:O	2.45	0.49
1:C:412:ASN:HD21	1:C:414:GLN:HB2	1.78	0.49
1:D:441:GLY:HA2	2:D:500:HEM:HBC2	1.95	0.49
1:G:188:GLY:H	1:G:266:ASP:HB3	1.77	0.49
1:G:140:VAL:CG2	1:G:444:LEU:HB2	2.40	0.49
1:H:440:PHE:O	1:H:440:PHE:HD1	1.96	0.49
1:F:305:THR:HA	1:F:365:MET:HE2	1.95	0.48
1:B:115:GLY:O	1:B:119:SER:HB3	2.13	0.48
1:A:146:GLU:OE2	1:A:342:LYS:HB2	2.14	0.48
1:B:63:GLU:O	1:C:67:PRO:HG3	2.13	0.48
1:A:186:VAL:HA	1:A:267:PHE:HB3	1.95	0.48
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.95	0.48
1:C:77:ARG:HH11	1:C:77:ARG:CG	2.21	0.48
1:H:440:PHE:CD1	1:H:440:PHE:O	2.67	0.48
1:C:84:HIS:NE2	1:C:88:LYS:HD3	2.28	0.48
1:D:225:SER:HA	1:D:228:LYS:HE2	1.96	0.48
1:F:327:VAL:O	1:F:331:ILE:HG13	2.13	0.48
1:F:381:ARG:O	1:F:382:ASP:HB2	2.14	0.48
1:B:275:MET:HG2	1:B:286:PHE:O	2.14	0.48
1:C:186:VAL:HA	1:C:267:PHE:HB3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:PHE:CZ	3:D:501:NCT:HC4	2.48	0.47
1:G:187:PHE:HZ	1:G:248:ILE:HD13	1.79	0.47
1:G:271:PHE:CD1	1:G:291:LEU:HB2	2.48	0.47
1:G:316:LEU:HD21	1:G:362:PHE:CD2	2.49	0.47
1:H:73:LEU:HB3	1:H:222:MET:HG2	1.95	0.47
1:A:85:ASP:O	1:A:89:GLU:HB2	2.15	0.47
1:C:275:MET:HG2	1:C:286:PHE:O	2.15	0.47
1:G:189:ASP:OD1	1:G:190:ARG:N	2.45	0.47
1:A:107:PHE:CE2	3:A:501:NCT:HC4	2.50	0.47
1:B:156:LEU:HD21	1:B:456:ILE:HD11	1.95	0.47
1:G:33:LEU:HD21	1:G:77:ARG:HD2	1.96	0.47
1:H:59:MET:C	1:H:61:ILE:N	2.65	0.47
1:A:84:HIS:CE1	1:A:88:LYS:HD3	2.50	0.47
1:F:314:PHE:HZ	1:F:456:ILE:HD13	1.78	0.47
1:A:310:LEU:HD23	1:A:453:PHE:CE1	2.49	0.47
1:E:343:PHE:CE1	1:E:346:ARG:HD3	2.49	0.47
1:E:377:ASP:HB3	1:E:384:PHE:CE1	2.49	0.47
1:A:53[B]:GLN:HG3	1:A:56:ASN:CB	2.40	0.47
1:F:235:GLN:OE1	1:F:238:PHE:HD2	1.97	0.47
1:G:182:ILE:HD11	1:G:302:GLY:O	2.15	0.47
1:H:186:VAL:HA	1:H:267:PHE:HB2	1.96	0.47
1:D:334:VAL:HG12	1:D:335:ILE:HG13	1.97	0.47
1:G:193:TYR:HD1	1:G:193:TYR:N	2.13	0.47
1:G:288:LEU:O	1:G:292:VAL:HG23	2.14	0.47
1:F:271:PHE:HB3	1:F:291:LEU:HD13	1.97	0.47
1:D:131:SER:O	1:D:135:LEU:HB2	2.15	0.46
1:F:211:PHE:CE1	1:F:233:PRO:HB2	2.50	0.46
1:G:268:ILE:HG23	1:G:291:LEU:HD11	1.96	0.46
1:H:88:LYS:HE3	1:H:434:ILE:HG21	1.96	0.46
1:F:152:GLU:HG3	1:F:177:THR:CG2	2.45	0.46
1:G:193:TYR:CD1	1:G:193:TYR:N	2.83	0.46
1:B:301:ALA:HB2	3:B:501:NCT:HC6	1.98	0.46
1:H:262:ASN:O	1:H:264:PRO:HD3	2.15	0.46
1:B:72:HIS:NE2	1:B:77:ARG:HD3	2.31	0.46
1:D:343:PHE:CE1	1:D:447:MET:HA	2.51	0.46
1:G:358:GLU:OE2	1:G:361:ARG:NH2	2.44	0.46
1:D:110:LEU:HD11	1:D:245:GLU:HB2	1.98	0.46
1:E:204:MET:O	1:E:208:SER:HB2	2.16	0.46
1:G:450:PHE:HD2	1:G:451:LEU:HD23	1.79	0.46
1:E:285:GLU:HA	1:E:287:TYR:CE2	2.51	0.46
1:F:51:THR:OG1	1:F:215:SER:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:SER:HB2	1:D:475:PRO:HD2	1.98	0.46
1:F:448:GLU:O	1:F:452:PHE:CD2	2.68	0.46
1:A:248:ILE:HG22	1:A:292:VAL:HG13	1.97	0.46
1:G:191:PHE:CD1	1:G:198:PHE:HB2	2.51	0.45
1:B:140:VAL:HA	1:B:145:ILE:HG21	1.98	0.45
1:H:301:ALA:O	2:H:501:HEM:C1C	2.70	0.45
1:D:156:LEU:CD2	1:D:456:ILE:HD11	2.46	0.45
1:H:77:ARG:NH2	1:H:386:PRO:HG2	2.30	0.45
1:C:104:GLN:NE2	1:C:221:GLU:OE2	2.49	0.45
1:D:319:LYS:O	1:D:319:LYS:HG3	2.16	0.45
2:E:500:HEM:HMB2	2:E:500:HEM:HBB2	1.99	0.45
1:G:266:ASP:HB2	1:G:267:PHE:H	1.62	0.45
1:G:327:VAL:CG2	1:G:355:VAL:HG21	2.47	0.45
1:H:265:ARG:HB3	1:H:265:ARG:CZ	2.46	0.45
1:D:275:MET:HG2	1:D:286:PHE:O	2.16	0.45
1:F:156:LEU:O	1:F:160:LEU:N	2.49	0.45
1:H:260:ASP:OD1	1:H:262:ASN:HB2	2.16	0.45
1:C:201:LEU:HD22	1:C:244:LEU:HD23	1.99	0.45
1:D:123:ARG:O	1:D:127:LEU:HG	2.17	0.45
1:D:384:PHE:C	1:D:385:LEU:HD12	2.37	0.45
1:F:373:ARG:NH1	1:F:388:GLY:O	2.48	0.45
1:G:182:ILE:HD13	1:G:299:PHE:HA	1.99	0.45
1:H:432:PHE:CG	1:H:442:GLU:HG3	2.52	0.45
1:A:301:ALA:HB2	3:A:501:NCT:HC6	1.98	0.45
1:C:220:TYR:O	1:C:224:SER:HB3	2.17	0.45
1:C:110:LEU:HD22	1:C:241:LEU:HB3	1.99	0.45
1:C:365:MET:HG3	1:C:366:LEU:HD13	1.99	0.45
1:F:82:CYS:O	1:F:86:ALA:HB3	2.17	0.45
1:G:450:PHE:CD2	1:G:451:LEU:HD23	2.52	0.45
1:A:161:ARG:C	1:A:163:THR:H	2.20	0.44
1:A:209:PHE:HZ	1:A:365:MET:HE3	1.81	0.44
1:H:290:ASN:O	1:H:294:THR:OG1	2.30	0.44
1:G:193:TYR:HD1	1:G:193:TYR:H	1.64	0.44
1:A:342:LYS:O	1:A:345:ASP:HB2	2.17	0.44
1:F:403:ARG:O	1:F:403:ARG:CG	2.65	0.44
1:G:206:LEU:O	1:G:210:GLN:HB2	2.18	0.44
1:G:80:VAL:HG22	1:G:392:PHE:HB2	1.99	0.44
1:A:101:ARG:HD3	1:A:371:ALA:O	2.18	0.44
1:B:418:ASP:OD2	1:B:422:GLN:HB2	2.17	0.44
1:C:101:ARG:NH1	2:C:500:HEM:O2A	2.45	0.44
1:E:314:PHE:HE1	1:E:453:PHE:CE1	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:PHE:CE2	1:E:425:LYS:HG2	2.52	0.44
1:F:240:GLU:O	1:F:244:LEU:HG	2.18	0.44
1:F:258:THR:O	1:F:265:ARG:NH2	2.50	0.44
1:G:220:TYR:CE1	1:G:224:SER:HB3	2.52	0.44
1:G:330:GLU:OE2	1:G:352:THR:N	2.51	0.44
1:H:178:VAL:CG1	1:H:303:THR:HA	2.48	0.44
1:C:101:ARG:O	1:C:373:ARG:HG2	2.17	0.44
1:F:403:ARG:CG	1:F:403:ARG:NH1	2.73	0.44
1:A:332:ASP:OD2	1:A:494:ARG:NH2	2.46	0.44
1:H:340:GLN:HA	1:H:341:PRO:HD3	1.78	0.44
1:D:205:MET:HG3	1:D:244:LEU:HD11	2.00	0.44
1:D:107:PHE:CE2	3:D:501:NCT:HC4	2.53	0.44
1:D:156:LEU:HD23	1:D:456:ILE:HD11	2.00	0.44
1:H:181:VAL:O	1:H:185:ILE:HG13	2.18	0.44
1:C:327:VAL:HG11	1:C:457:MET:CE	2.48	0.44
1:F:288:LEU:O	1:F:292:VAL:HG23	2.18	0.44
1:F:78:VAL:HG22	1:F:390:GLU:HB2	2.00	0.44
1:A:103:GLU:HB2	1:A:108:ASP:OD2	2.18	0.43
1:D:148:ARG:HD3	1:D:184:SER:OG	2.17	0.43
1:E:157:ILE:HD12	1:E:459:ASN:HB2	2.00	0.43
1:G:476:LYS:HG3	1:G:477:HIS:N	2.18	0.43
1:A:419:LYS:HD2	1:A:419:LYS:HA	1.88	0.43
1:B:381:ARG:O	1:B:382:ASP:CB	2.66	0.43
1:G:235:GLN:OE1	1:G:238:PHE:CD2	2.68	0.43
3:C:501:NCT:C3	3:C:501:NCT:C10	2.96	0.43
1:F:368:MET:HG2	1:F:394:MET:HE3	2.00	0.43
1:H:136:ARG:HA	1:H:136:ARG:HE	1.83	0.43
1:A:366:LEU:HD12	2:A:500:HEM:HMA2	2.01	0.43
1:A:101:ARG:NH1	1:A:370:LEU:HD23	2.34	0.43
1:C:138:PHE:CZ	1:C:266:ASP:HA	2.54	0.43
1:C:418:ASP:OD2	1:C:422[A]:GLN:HB2	2.19	0.43
1:B:77:ARG:NH1	1:B:77:ARG:HG2	2.15	0.43
1:C:250:LYS:HB2	1:C:250:LYS:HZ2	1.83	0.43
1:C:281:ASN:HB3	1:C:284:THR:HB	2.00	0.43
1:D:205:MET:CG	1:D:244:LEU:HD11	2.48	0.43
1:E:116:VAL:CG1	1:E:294:THR:HG23	2.49	0.43
1:F:77:ARG:NH1	1:F:389:THR:OG1	2.52	0.43
1:G:85:ASP:O	1:G:89:GLU:HB2	2.19	0.43
1:H:130:PHE:HZ	1:H:270:SER:HB3	1.84	0.43
1:A:101:ARG:HH12	1:A:370:LEU:HB3	1.79	0.43
1:D:453:PHE:O	1:D:457:MET:CG	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:PHE:HE2	1:E:425:LYS:HG2	1.83	0.43
1:H:32:LYS:O	1:H:383:PHE:HA	2.19	0.43
1:D:80:VAL:HG22	1:D:392:PHE:HB2	2.00	0.42
1:A:116:VAL:HG12	1:A:297:ASN:HD22	1.85	0.42
1:G:435:GLY:O	1:G:438:TYR:HD2	2.02	0.42
1:G:59:MET:HA	1:G:62:SER:HB3	2.00	0.42
1:B:331:ILE:HG12	1:B:349:MET:HE1	2.01	0.42
1:B:343:PHE:O	1:B:346:ARG:HB2	2.18	0.42
1:D:260:ASP:HA	1:D:261:PRO:HD3	1.84	0.42
1:G:209:PHE:CE1	1:G:304:GLU:HG2	2.54	0.42
1:E:103:GLU:HB2	1:E:108:ASP:OD2	2.19	0.42
1:G:109:TRP:CH2	1:G:238:PHE:HB3	2.53	0.42
1:H:297:ASN:HD22	1:H:297:ASN:HA	1.63	0.42
1:D:423:PHE:HE1	1:D:425:LYS:HG3	1.85	0.42
1:E:353:GLU:OE1	1:E:353:GLU:HA	2.19	0.42
1:F:143:ARG:C	1:F:143:ARG:HD2	2.40	0.42
1:A:251:LYS:O	1:A:254:HIS:HB3	2.19	0.42
1:A:101:ARG:NH2	2:A:500:HEM:O2D	2.53	0.42
1:B:107:PHE:CZ	3:B:501:NCT:HC4	2.55	0.42
1:C:250:LYS:NZ	1:C:250:LYS:CB	2.82	0.42
1:D:197:GLU:OE2	1:D:250:LYS:NZ	2.53	0.42
1:H:320:HIS:HB3	1:H:323:VAL:HG22	2.01	0.42
1:F:103:GLU:HB2	1:F:108:ASP:OD2	2.19	0.42
1:F:195:ASP:OD2	1:F:197:GLU:HB3	2.19	0.42
1:F:272:LEU:HA	1:F:275:MET:HB3	2.01	0.42
1:G:314:PHE:HB2	1:G:487:TYR:OH	2.19	0.42
1:B:220:TYR:CZ	1:B:224:SER:HB2	2.54	0.42
1:D:53[B]:GLN:OE1	1:D:53[B]:GLN:C	2.57	0.42
1:E:205:MET:CE	1:E:303:THR:HG21	2.49	0.42
1:E:330:GLU:HG3	1:E:333[A]:ARG:NH2	2.34	0.42
1:F:463:LYS:HB3	1:F:490:SER:HB2	2.02	0.42
1:F:81:LEU:HB2	1:F:87:VAL:HG22	2.02	0.42
1:C:210[B]:GLN:O	1:C:214:THR:HG23	2.19	0.42
1:G:248:ILE:HD12	1:G:295:THR:HG22	2.02	0.42
1:H:314:PHE:HB2	1:H:487:TYR:OH	2.20	0.42
1:H:53:GLN:OE1	1:H:56:ASN:ND2	2.53	0.42
1:C:442:GLU:OE2	1:C:446:ARG:NH1	2.53	0.42
1:D:366:LEU:HA	1:D:367:PRO:HD3	1.88	0.42
1:F:322:GLU:H	1:F:322:GLU:CD	2.23	0.42
1:A:464:SER:C	1:A:466:GLN:H	2.24	0.41
1:F:271:PHE:CG	1:F:291:LEU:HD13	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:ILE:HG23	1:F:335:ILE:HD12	2.02	0.41
1:G:328:HIS:HA	1:G:331:ILE:HD12	2.02	0.41
1:H:157:ILE:HD11	1:H:456:ILE:HA	2.02	0.41
1:A:364:ASP:OD1	1:A:399:LEU:HD12	2.20	0.41
1:B:152:GLU:HG3	1:B:177:THR:HG23	2.03	0.41
1:D:353:GLU:HG2	1:D:423:PHE:CD2	2.56	0.41
1:B:32:LYS:CD	1:B:33:LEU:N	2.78	0.41
1:B:468:PRO:HA	1:B:471:ILE:HD12	2.01	0.41
1:F:271:PHE:CB	1:F:291:LEU:HD13	2.51	0.41
1:G:190:ARG:NH2	1:G:193:TYR:CE1	2.67	0.41
1:G:457:MET:HE2	1:G:462:PHE:CE2	2.44	0.41
1:C:202:LEU:HD23	1:C:205:MET:HE3	2.01	0.41
1:D:433:SER:HB3	2:D:500:HEM:HBA1	2.03	0.41
1:E:116:VAL:HG12	1:E:294:THR:HG23	2.02	0.41
1:F:116:VAL:HG12	1:F:294:THR:HG23	2.02	0.41
1:F:271:PHE:CE1	1:F:291:LEU:HB2	2.56	0.41
1:F:323:VAL:O	1:F:327:VAL:HG23	2.20	0.41
1:B:436:LYS:HD3	1:B:436:LYS:HA	1.84	0.41
1:C:59:MET:CE	1:C:394:MET:HE2	2.51	0.41
1:D:163:THR:HG21	1:D:168:ILE:HD13	2.02	0.41
1:E:101:ARG:NH1	1:E:370:LEU:CB	2.81	0.41
1:F:314:PHE:CZ	1:F:456:ILE:HD13	2.54	0.41
1:H:382:ASP:OD2	1:H:382:ASP:N	2.51	0.41
1:C:147:GLU:OE2	1:D:143:ARG:NH1	2.52	0.41
1:E:110:LEU:HD13	1:E:241:LEU:HB3	2.01	0.41
1:E:101:ARG:NH1	1:E:370:LEU:CG	2.84	0.41
1:F:263:SER:HA	1:F:264:PRO:HD3	1.76	0.41
1:H:81:LEU:O	1:H:394:MET:HG2	2.21	0.41
1:B:344:GLU:C	1:B:346:ARG:H	2.23	0.41
1:D:381:ARG:O	1:D:382:ASP:CB	2.56	0.41
1:G:289:LYS:O	1:G:293:MET:HG2	2.21	0.41
1:B:341:PRO:HB3	1:B:454:THR:HG21	2.03	0.41
1:C:225:SER:HA	1:C:228:LYS:HE3	2.02	0.41
1:D:116:VAL:HG12	1:D:297:ASN:HD22	1.86	0.41
1:D:303:THR:O	1:D:307:SER:HB3	2.21	0.41
1:D:373:ARG:NH1	1:D:388:GLY:O	2.54	0.41
1:D:74:GLY:HA3	1:D:75:PRO:HD2	1.89	0.41
1:F:476:LYS:HB2	1:F:485:ARG:HA	2.02	0.41
1:G:138:PHE:HD2	1:G:138:PHE:N	2.18	0.41
1:H:109:TRP:CZ2	1:H:238:PHE:HB3	2.56	0.41
1:F:452:PHE:O	1:F:456:ILE:HD12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:500:HEM:HBD2	2:F:500:HEM:HHA	2.01	0.41
1:B:492:LEU:HA	1:B:493:PRO:HD3	1.95	0.40
1:E:213:ALA:HA	1:E:479:GLY:HA3	2.02	0.40
1:G:395:LEU:HA	1:G:395:LEU:HD23	1.91	0.40
1:H:69:PHE:CE1	1:H:80:VAL:HB	2.56	0.40
1:C:199:LEU:HD12	1:C:199:LEU:HA	1.92	0.40
1:C:468:PRO:HA	1:C:471:ILE:HD12	2.03	0.40
1:E:178:VAL:HG12	1:E:303:THR:HA	2.04	0.40
1:F:330:GLU:OE1	1:F:349:MET:HB3	2.21	0.40
1:H:68:VAL:HA	1:H:80:VAL:O	2.21	0.40
1:B:175:SER:O	1:B:179:SER:CB	2.69	0.40
1:D:64:ARG:HG2	1:D:65:TYR:CD2	2.56	0.40
1:B:55:TYR:CE1	1:B:59:MET:HG3	2.56	0.40
1:C:370:LEU:HD12	1:C:370:LEU:HA	1.86	0.40
1:E:122:GLU:O	1:E:126:GLN:HB2	2.22	0.40
1:F:116:VAL:CG1	1:F:294:THR:HG23	2.51	0.40
1:C:212:THR:HB	1:C:480:PHE:HB3	2.04	0.40
2:D:500:HEM:HBB2	2:D:500:HEM:HMB1	2.02	0.40
1:E:268:ILE:HD11	1:E:295:THR:HG21	2.04	0.40
1:F:142:LYS:H	1:F:142:LYS:HG2	1.69	0.40
1:F:458:GLN:CG	1:F:459:ASN:N	2.85	0.40
1:G:473:VAL:HG23	1:G:474:SER:N	2.36	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%)	441 (95%)	21 (4%)	1 (0%)	47 68
1	B	467/476 (98%)	433 (93%)	33 (7%)	1 (0%)	47 68
1	C	466/476 (98%)	438 (94%)	26 (6%)	2 (0%)	34 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	466/476 (98%)	445 (96%)	21 (4%)	0	100	100
1	E	466/476 (98%)	448 (96%)	16 (3%)	2 (0%)	34	54
1	F	463/476 (97%)	413 (89%)	44 (10%)	6 (1%)	12	21
1	G	461/476 (97%)	404 (88%)	52 (11%)	5 (1%)	14	26
1	H	454/476 (95%)	396 (87%)	49 (11%)	9 (2%)	7	12
All	All	3706/3808 (97%)	3418 (92%)	262 (7%)	26 (1%)	22	39

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	262	ASN
1	F	338	ASN
1	H	95	ALA
1	H	408	PRO
1	F	345	ASP
1	G	364	ASP
1	H	277	GLU
1	H	421	GLY
1	F	382	ASP
1	H	60	LYS
1	B	433	SER
1	C	433	SER
1	G	387	LYS
1	G	468	PRO
1	H	362	PHE
1	C	365	MET
1	E	193	TYR
1	H	85	ASP
1	H	193	TYR
1	F	393	PRO
1	F	468	PRO
1	G	137	GLY
1	G	471	ILE
1	A	162	GLY
1	E	144	GLY
1	H	363	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	409/419 (98%)	392 (96%)	17 (4%)	30	54
1	B	413/419 (99%)	397 (96%)	16 (4%)	32	57
1	C	412/419 (98%)	393 (95%)	19 (5%)	27	50
1	D	412/419 (98%)	386 (94%)	26 (6%)	18	34
1	E	412/419 (98%)	382 (93%)	30 (7%)	14	27
1	F	409/419 (98%)	376 (92%)	33 (8%)	11	23
1	G	402/419 (96%)	371 (92%)	31 (8%)	13	25
1	H	396/419 (94%)	356 (90%)	40 (10%)	7	14
All	All	3265/3352 (97%)	3053 (94%)	212 (6%)	17	33

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	40	LEU
1	A	97	GLU
1	A	135	LEU
1	A	215	SER
1	A	250	LYS
1	A	291	LEU
1	A	312	TYR
1	A	316	LEU
1	A	348	LYS
1	A	365	MET
1	A	376	LYS
1	A	409	ARG
1	A	417	LEU
1	A	436	LYS
1	A	454	THR
1	A	463	LYS
1	B	40	LEU
1	B	77	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	82	CYS
1	B	135	LEU
1	B	199	LEU
1	B	206	LEU
1	B	239	LYS
1	B	258	THR
1	B	312	TYR
1	B	316	LEU
1	B	326	LYS
1	B	348	LYS
1	B	366	LEU
1	B	403	ARG
1	B	409	ARG
1	B	417	LEU
1	C	77	ARG
1	C	104	GLN
1	C	125	LYS
1	C	147	GLU
1	C	208	SER
1	C	236	GLN
1	C	245	GLU
1	C	279	GLU
1	C	312	TYR
1	C	316	LEU
1	C	346	ARG
1	C	348	LYS
1	C	382	ASP
1	C	410	ASP
1	C	417	LEU
1	C	420	LYS
1	C	436	LYS
1	C	469	LYS
1	C	492	LEU
1	D	30	LYS
1	D	32	LYS
1	D	38	THR
1	D	40	LEU
1	D	77	ARG
1	D	82	CYS
1	D	88	LYS
1	D	126	GLN
1	D	135	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	167	ASN
1	D	194	GLU
1	D	196	LYS
1	D	199	LEU
1	D	208	SER
1	D	215	SER
1	D	245	GLU
1	D	291	LEU
1	D	312	TYR
1	D	329	GLU
1	D	348	LYS
1	D	353	GLU
1	D	379	LYS
1	D	409	ARG
1	D	434	ILE
1	D	446	ARG
1	D	457	MET
1	E	30	LYS
1	E	32	LYS
1	E	33	LEU
1	E	40	LEU
1	E	57	SER
1	E	88	LYS
1	E	128	ARG
1	E	167	ASN
1	E	175	SER
1	E	189	ASP
1	E	194	GLU
1	E	197	GLU
1	E	208	SER
1	E	225	SER
1	E	236	GLN
1	E	239[A]	LYS
1	E	239[B]	LYS
1	E	254	HIS
1	E	279	GLU
1	E	287	TYR
1	E	312	TYR
1	E	316	LEU
1	E	348	LYS
1	E	366	LEU
1	E	382	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	417	LEU
1	E	434	ILE
1	E	457	MET
1	E	466	GLN
1	E	470	ASP
1	F	60	LYS
1	F	81	LEU
1	F	91	LEU
1	F	101	ARG
1	F	122	GLU
1	F	135	LEU
1	F	143	ARG
1	F	167	ASN
1	F	177	THR
1	F	199	LEU
1	F	228	LYS
1	F	236	GLN
1	F	251	LYS
1	F	252	VAL
1	F	254	HIS
1	F	263	SER
1	F	273	ILE
1	F	274	ARG
1	F	283	ASN
1	F	287	TYR
1	F	312	TYR
1	F	316	LEU
1	F	322	GLU
1	F	340	GLN
1	F	346	ARG
1	F	352	THR
1	F	376	LYS
1	F	379	LYS
1	F	403	ARG
1	F	404	PHE
1	F	407	ASN
1	F	417	LEU
1	F	427	ASP
1	G	33	LEU
1	G	52	GLU
1	G	85	ASP
1	G	97	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	101	ARG
1	G	129	ARG
1	G	136	ARG
1	G	138	PHE
1	G	145	ILE
1	G	151	GLU
1	G	155	PHE
1	G	177	THR
1	G	201	LEU
1	G	212	THR
1	G	251	LYS
1	G	257	ARG
1	G	258	THR
1	G	291	LEU
1	G	303	THR
1	G	306	VAL
1	G	312	TYR
1	G	319	LYS
1	G	342	LYS
1	G	365	MET
1	G	382	ASP
1	G	419	LYS
1	G	434	ILE
1	G	446	ARG
1	G	453	PHE
1	G	463	LYS
1	G	483	ILE
1	H	32	LYS
1	H	33	LEU
1	H	50	ASN
1	H	51	THR
1	H	57	SER
1	H	62	SER
1	H	85	ASP
1	H	91	LEU
1	H	136	ARG
1	H	145	ILE
1	H	160	LEU
1	H	163	THR
1	H	167	ASN
1	H	169	ASP
1	H	174	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	177	THR
1	H	189	ASP
1	H	210	GLN
1	H	257	ARG
1	H	270	SER
1	H	296	LEU
1	H	297	ASN
1	H	312	TYR
1	H	318	MET
1	H	322	GLU
1	H	326	LYS
1	H	329	GLU
1	H	335	ILE
1	H	346	ARG
1	H	356	ILE
1	H	361	ARG
1	H	382	ASP
1	H	410	ASP
1	H	427	ASP
1	H	430	VAL
1	H	434	ILE
1	H	463	LYS
1	H	467	SER
1	H	470	ASP
1	H	473	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	B	297	ASN
1	C	297	ASN
1	D	297	ASN
1	E	255	ASN
1	E	297	ASN
1	F	375	ASN
1	F	414	GLN
1	F	477	HIS
1	G	340	GLN
1	G	486	ASN
1	H	120	ASN
1	H	477	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 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	NCT	B	501	-	13,13,13	1.20	1 (7%)	17,17,17	2.30	6 (35%)
3	NCT	A	501	-	13,13,13	0.82	0	17,17,17	2.18	7 (41%)
4	GOL	H	502	-	5,5,5	0.97	0	5,5,5	2.05	3 (60%)
2	HEM	A	500	1	27,50,50	2.30	8 (29%)	17,82,82	1.44	5 (29%)
2	HEM	H	501	1	27,50,50	2.18	9 (33%)	17,82,82	1.70	4 (23%)
2	HEM	F	500	1	27,50,50	2.28	7 (25%)	17,82,82	1.35	3 (17%)
2	HEM	D	500	1	27,50,50	2.17	9 (33%)	17,82,82	1.54	4 (23%)
2	HEM	G	500	1	27,50,50	2.33	7 (25%)	17,82,82	1.79	4 (23%)
2	HEM	B	500	1	27,50,50	2.19	8 (29%)	17,82,82	1.57	5 (29%)
2	HEM	E	500	1	27,50,50	2.24	7 (25%)	17,82,82	2.02	7 (41%)
2	HEM	C	500	1	27,50,50	2.33	8 (29%)	17,82,82	1.85	5 (29%)
3	NCT	D	501	-	13,13,13	0.76	1 (7%)	17,17,17	1.88	6 (35%)
3	NCT	C	501	-	13,13,13	1.15	1 (7%)	17,17,17	2.35	6 (35%)

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	NCT	B	501	-	-	0/4/14/14	0/2/2/2
3	NCT	A	501	-	-	0/4/14/14	0/2/2/2
4	GOL	H	502	-	-	4/4/4/4	-
2	HEM	A	500	1	-	0/6/54/54	-
2	HEM	H	501	1	-	1/6/54/54	-
2	HEM	F	500	1	-	3/6/54/54	-
2	HEM	D	500	1	-	0/6/54/54	-
2	HEM	G	500	1	-	0/6/54/54	-
2	HEM	B	500	1	-	0/6/54/54	-
2	HEM	E	500	1	-	0/6/54/54	-
2	HEM	C	500	1	-	0/6/54/54	-
3	NCT	D	501	-	-	0/4/14/14	0/2/2/2
3	NCT	C	501	-	-	0/4/14/14	0/2/2/2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	HEM	C3D-C2D	5.94	1.55	1.37
2	F	500	HEM	C3D-C2D	5.68	1.54	1.37
2	C	500	HEM	C3C-C2C	-5.61	1.32	1.40
2	C	500	HEM	C3D-C2D	5.45	1.53	1.37
2	G	500	HEM	C3C-C2C	-5.40	1.32	1.40
2	E	500	HEM	C3D-C2D	5.31	1.53	1.37
2	A	500	HEM	C3C-C2C	-5.20	1.33	1.40
2	H	501	HEM	C3D-C2D	5.10	1.52	1.37
2	A	500	HEM	C3D-C2D	4.78	1.51	1.37
2	E	500	HEM	C3C-C2C	-4.71	1.33	1.40
2	B	500	HEM	C3C-C2C	-4.65	1.33	1.40
2	B	500	HEM	C3D-C2D	4.62	1.51	1.37
2	D	500	HEM	C3C-C2C	-4.58	1.34	1.40
2	F	500	HEM	C3C-CAC	4.44	1.56	1.47
2	H	501	HEM	C3C-CAC	4.42	1.56	1.47
2	E	500	HEM	C3B-C2B	-4.31	1.34	1.40
2	D	500	HEM	C3D-C2D	4.30	1.50	1.37
2	G	500	HEM	C3B-CAB	4.30	1.56	1.47
2	E	500	HEM	C3B-CAB	4.25	1.56	1.47
2	H	501	HEM	C3B-C2B	-4.23	1.34	1.40
2	E	500	HEM	C3C-CAC	4.19	1.56	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	C3B-CAB	4.18	1.56	1.47
2	F	500	HEM	C3C-C2C	-4.12	1.34	1.40
2	A	500	HEM	C3B-CAB	4.11	1.56	1.47
2	D	500	HEM	C3C-CAC	4.06	1.56	1.47
2	C	500	HEM	C3B-CAB	4.04	1.56	1.47
2	B	500	HEM	C3B-CAB	4.03	1.56	1.47
2	G	500	HEM	C3B-C2B	-4.00	1.34	1.40
2	C	500	HEM	C3B-C2B	-3.98	1.34	1.40
2	D	500	HEM	C3B-C2B	-3.95	1.34	1.40
2	A	500	HEM	C3C-CAC	3.91	1.55	1.47
2	A	500	HEM	CAA-C2A	3.87	1.57	1.52
2	F	500	HEM	C3B-CAB	3.82	1.55	1.47
2	B	500	HEM	C3C-CAC	3.81	1.55	1.47
2	H	501	HEM	C3B-CAB	3.79	1.55	1.47
2	F	500	HEM	C3B-C2B	-3.69	1.35	1.40
2	B	500	HEM	C3B-C2B	-3.67	1.35	1.40
2	C	500	HEM	C3C-CAC	3.66	1.55	1.47
2	B	500	HEM	CAA-C2A	3.47	1.57	1.52
2	H	501	HEM	C3C-C2C	-3.34	1.35	1.40
3	C	501	NCT	C2-C6	-3.32	1.46	1.51
2	A	500	HEM	C3B-C2B	-2.95	1.36	1.40
2	A	500	HEM	CMA-C3A	2.91	1.57	1.51
2	B	500	HEM	CMB-C2B	2.83	1.58	1.51
2	G	500	HEM	C3C-CAC	2.83	1.53	1.47
3	B	501	NCT	C1-C2	2.82	1.43	1.39
2	C	500	HEM	CAA-C2A	2.73	1.56	1.52
2	D	500	HEM	CMB-C2B	2.64	1.57	1.51
2	F	500	HEM	CAA-C2A	2.50	1.55	1.52
2	E	500	HEM	CMA-C3A	2.47	1.56	1.51
2	G	500	HEM	CAD-C3D	2.46	1.56	1.52
2	C	500	HEM	CAD-C3D	2.38	1.56	1.52
2	A	500	HEM	CMB-C2B	2.31	1.57	1.51
2	F	500	HEM	CAD-C3D	2.31	1.56	1.52
2	H	501	HEM	CMB-C2B	2.29	1.57	1.51
2	D	500	HEM	C1D-ND	2.24	1.40	1.36
2	C	500	HEM	CMC-C2C	2.23	1.56	1.51
2	H	501	HEM	CAA-C2A	2.16	1.55	1.52
2	E	500	HEM	CMB-C2B	2.15	1.56	1.51
3	D	501	NCT	C2-C6	-2.12	1.48	1.51
2	D	500	HEM	CMC-C2C	2.11	1.56	1.51
2	G	500	HEM	CMD-C2D	2.10	1.56	1.51
2	B	500	HEM	CMC-C2C	2.04	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	HEM	C1D-CHD	-2.03	1.35	1.41
2	D	500	HEM	C2A-C3A	-2.02	1.31	1.37
2	H	501	HEM	C1C-C2C	2.02	1.47	1.42

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	NCT	C10-N2-C6	5.82	130.53	112.83
3	B	501	NCT	C10-N2-C6	5.68	130.09	112.83
3	A	501	NCT	C10-N2-C6	5.11	128.37	112.83
2	G	500	HEM	CAA-CBA-CGA	-4.68	104.83	112.67
3	D	501	NCT	C10-N2-C6	4.43	126.29	112.83
2	E	500	HEM	CAA-CBA-CGA	-4.02	105.92	112.67
2	C	500	HEM	C4A-C3A-C2A	3.96	109.75	107.00
3	C	501	NCT	C3-C2-C1	3.87	120.99	116.88
3	B	501	NCT	C2-C6-N2	3.82	122.18	112.37
2	H	501	HEM	CAA-CBA-CGA	-3.71	106.45	112.67
3	A	501	NCT	C4-C3-C2	-3.55	116.26	120.65
2	D	500	HEM	CAA-CBA-CGA	-3.36	107.03	112.67
2	E	500	HEM	CBD-CAD-C3D	-3.27	106.46	112.48
2	G	500	HEM	C1D-C2D-C3D	-3.22	104.75	107.00
3	C	501	NCT	C4-C3-C2	-3.19	116.70	120.65
2	E	500	HEM	C1D-C2D-C3D	-3.19	104.77	107.00
3	A	501	NCT	C10-N2-C9	3.17	122.63	112.70
2	C	500	HEM	CBD-CAD-C3D	-3.10	106.77	112.48
3	C	501	NCT	C10-N2-C9	3.03	122.19	112.70
2	B	500	HEM	C4A-C3A-C2A	3.02	109.09	107.00
4	H	502	GOL	O2-C2-C3	-2.98	96.02	109.12
3	D	501	NCT	C9-N2-C6	2.96	113.33	104.37
2	C	500	HEM	C4C-C3C-C2C	2.83	108.87	106.90
2	E	500	HEM	C4C-C3C-C2C	2.82	108.86	106.90
2	C	500	HEM	CMA-C3A-C4A	-2.81	124.15	128.46
2	A	500	HEM	CAD-CBD-CGD	-2.78	108.02	112.67
2	H	501	HEM	CMA-C3A-C4A	-2.74	124.25	128.46
3	B	501	NCT	C4-C3-C2	-2.72	117.29	120.65
2	F	500	HEM	C4A-C3A-C2A	2.60	108.80	107.00
2	B	500	HEM	CMB-C2B-C3B	2.57	129.48	124.68
2	F	500	HEM	CMA-C3A-C4A	-2.52	124.60	128.46
2	H	501	HEM	CBD-CAD-C3D	-2.51	107.86	112.48
2	E	500	HEM	C3C-C4C-NC	-2.49	106.25	110.94
3	B	501	NCT	C10-N2-C9	2.46	120.42	112.70
3	D	501	NCT	C10-N2-C9	2.45	120.36	112.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	HEM	C1D-C2D-C3D	-2.44	105.30	107.00
2	D	500	HEM	CBA-CAA-C2A	-2.37	108.11	112.49
2	G	500	HEM	C4C-C3C-C2C	2.36	108.55	106.90
2	E	500	HEM	CBA-CAA-C2A	-2.36	108.14	112.49
2	F	500	HEM	CAA-CBA-CGA	-2.33	108.77	112.67
2	E	500	HEM	CMB-C2B-C3B	2.30	128.98	124.68
3	B	501	NCT	C8-C9-N2	-2.29	97.42	103.85
4	H	502	GOL	C3-C2-C1	-2.28	102.83	111.70
2	D	500	HEM	C4C-C3C-C2C	2.28	108.49	106.90
4	H	502	GOL	O3-C3-C2	-2.27	99.32	110.20
3	D	501	NCT	C4-C3-C2	-2.26	117.85	120.65
3	A	501	NCT	C3-C4-C5	2.25	122.24	118.91
2	A	500	HEM	C1D-C2D-C3D	-2.24	105.44	107.00
3	A	501	NCT	C8-C9-N2	-2.22	97.62	103.85
3	A	501	NCT	C2-C6-N2	2.15	117.89	112.37
2	B	500	HEM	CMD-C2D-C1D	2.15	131.76	128.46
2	A	500	HEM	CBD-CAD-C3D	-2.14	108.53	112.48
2	B	500	HEM	CBD-CAD-C3D	-2.14	108.53	112.48
2	A	500	HEM	CMB-C2B-C3B	2.13	128.67	124.68
3	B	501	NCT	C1-C2-C6	-2.12	116.92	121.40
2	D	500	HEM	C3C-C4C-NC	-2.12	106.94	110.94
3	D	501	NCT	C3-C2-C1	2.10	119.12	116.88
3	C	501	NCT	C1-C2-C6	-2.10	116.97	121.40
2	A	500	HEM	CMD-C2D-C1D	2.08	131.66	128.46
2	C	500	HEM	C1D-C2D-C3D	-2.07	105.55	107.00
3	A	501	NCT	C3-C2-C1	2.07	119.09	116.88
3	D	501	NCT	C5-N1-C1	2.07	120.43	116.85
2	G	500	HEM	C3C-C4C-NC	-2.03	107.11	110.94
2	B	500	HEM	CMD-C2D-C3D	-2.02	121.13	124.94
3	C	501	NCT	C8-C9-N2	-2.00	98.23	103.85

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	502	GOL	O1-C1-C2-C3
4	H	502	GOL	C1-C2-C3-O3
2	H	501	HEM	C3D-CAD-CBD-CGD
2	F	500	HEM	C2D-C3D-CAD-CBD
2	F	500	HEM	C4D-C3D-CAD-CBD
2	F	500	HEM	C3D-CAD-CBD-CGD
4	H	502	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

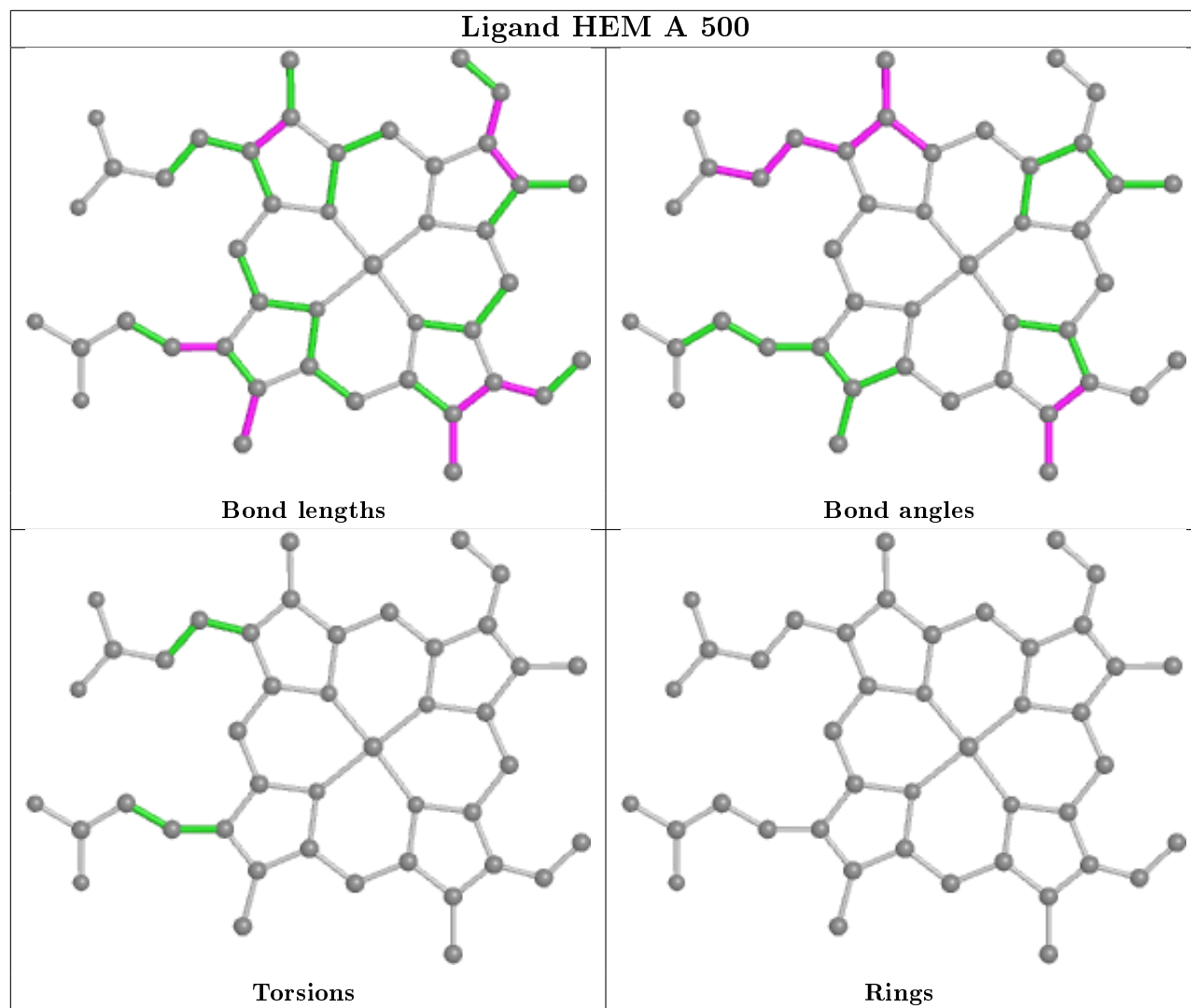
Mol	Chain	Res	Type	Atoms
4	H	502	GOL	O2-C2-C3-O3

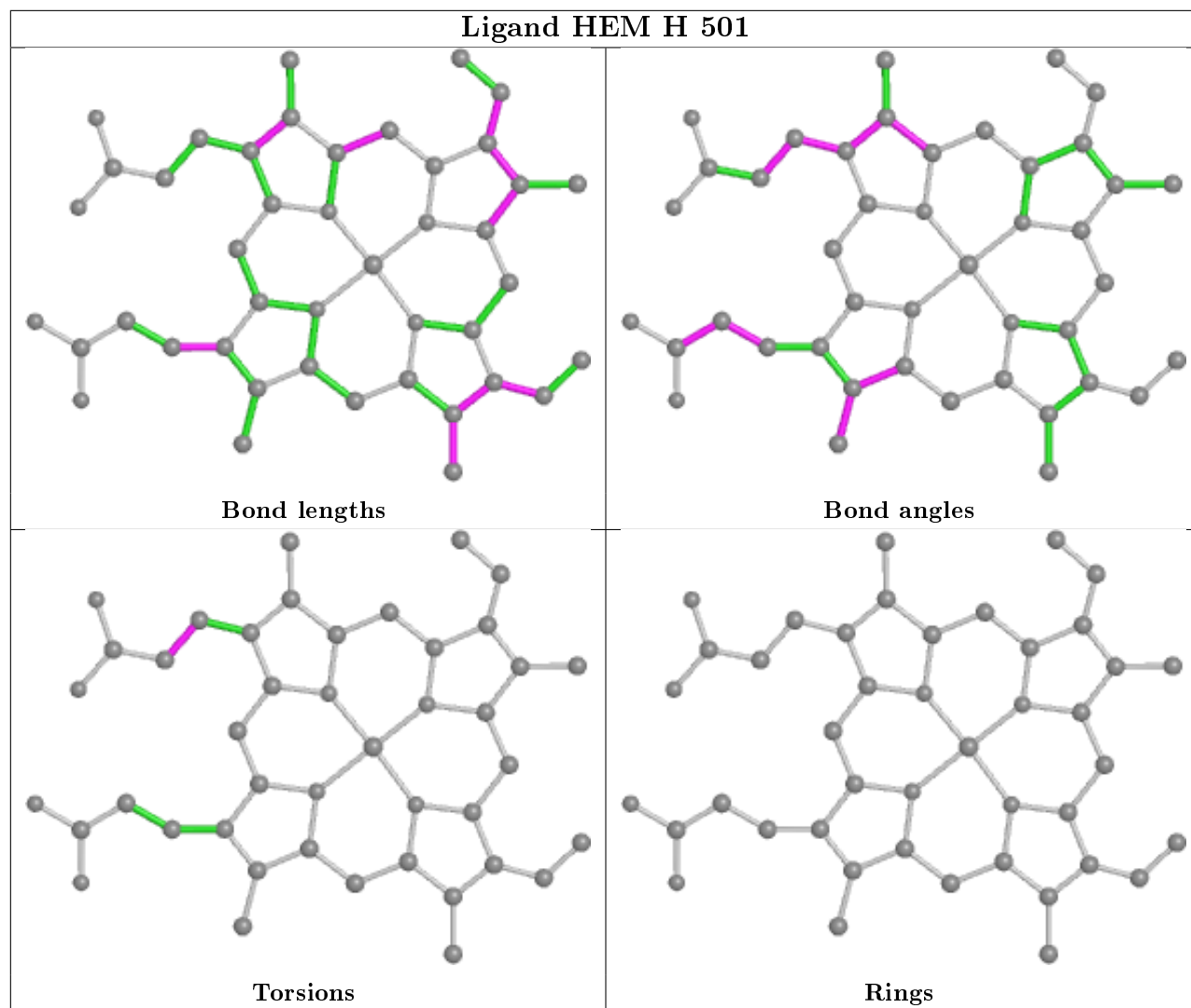
There are no ring outliers.

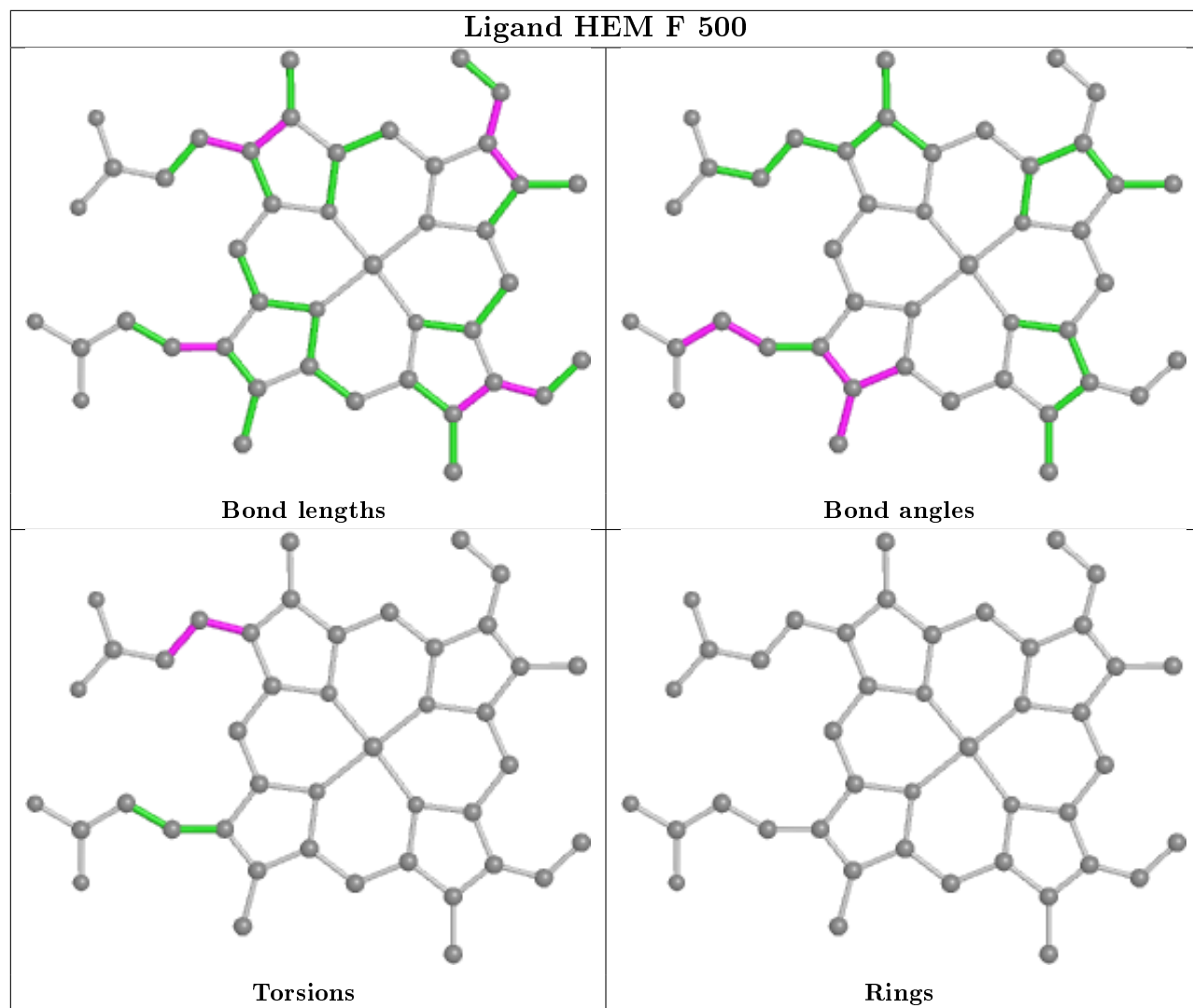
12 monomers are involved in 28 short contacts:

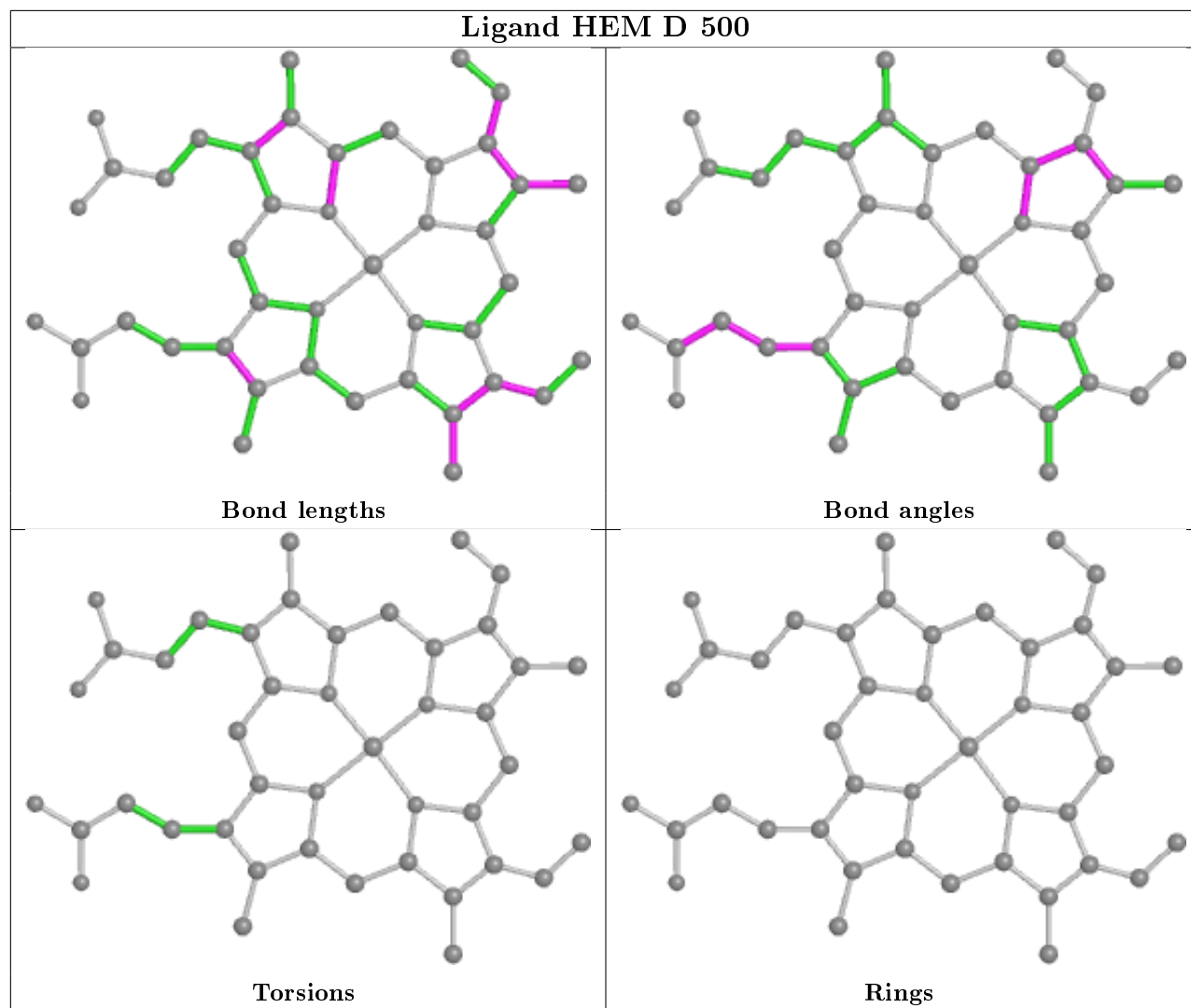
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	NCT	3	0
3	A	501	NCT	3	0
4	H	502	GOL	1	0
2	A	500	HEM	2	0
2	H	501	HEM	2	0
2	F	500	HEM	3	0
2	D	500	HEM	3	0
2	B	500	HEM	1	0
2	E	500	HEM	2	0
2	C	500	HEM	2	0
3	D	501	NCT	3	0
3	C	501	NCT	3	0

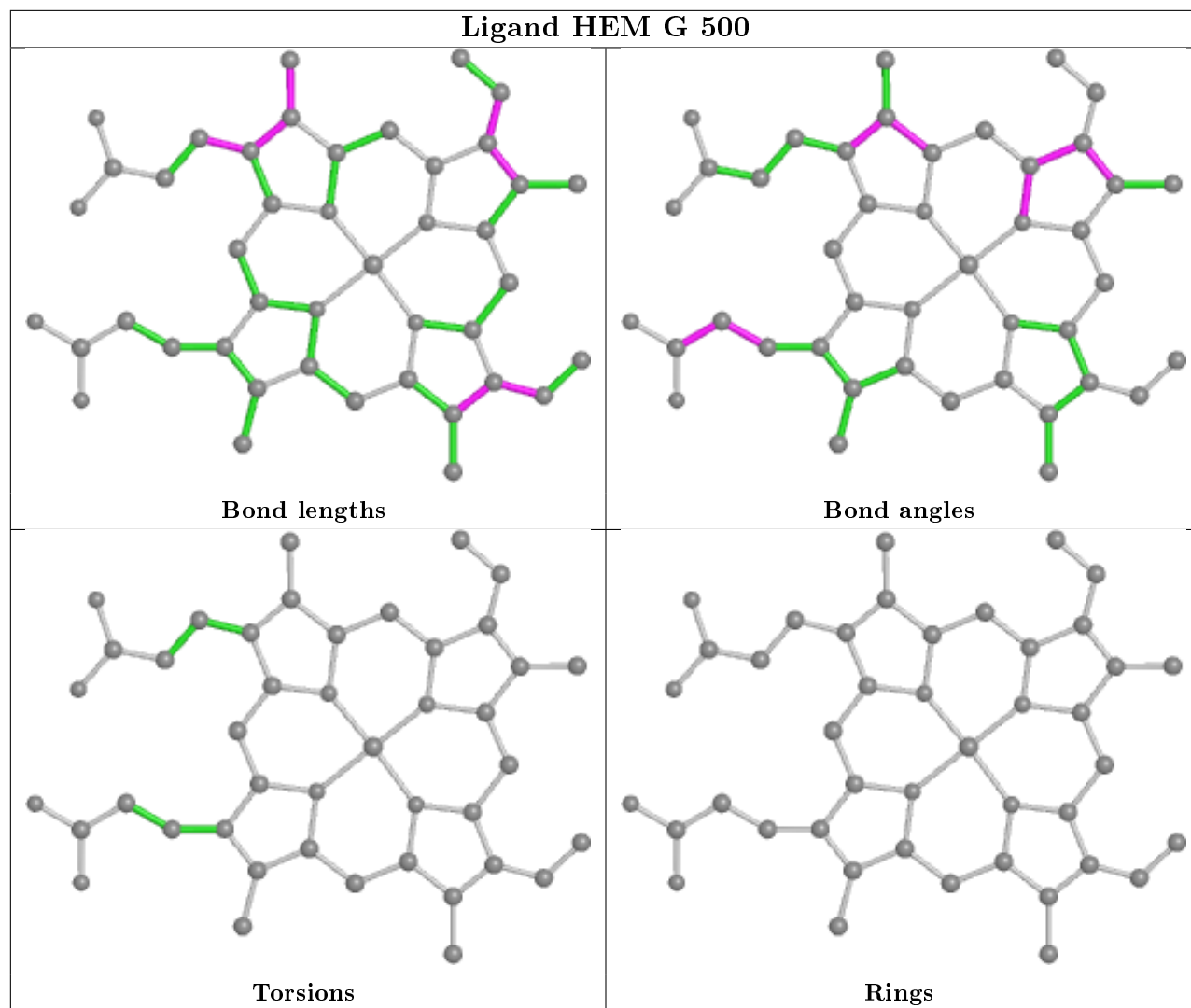
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

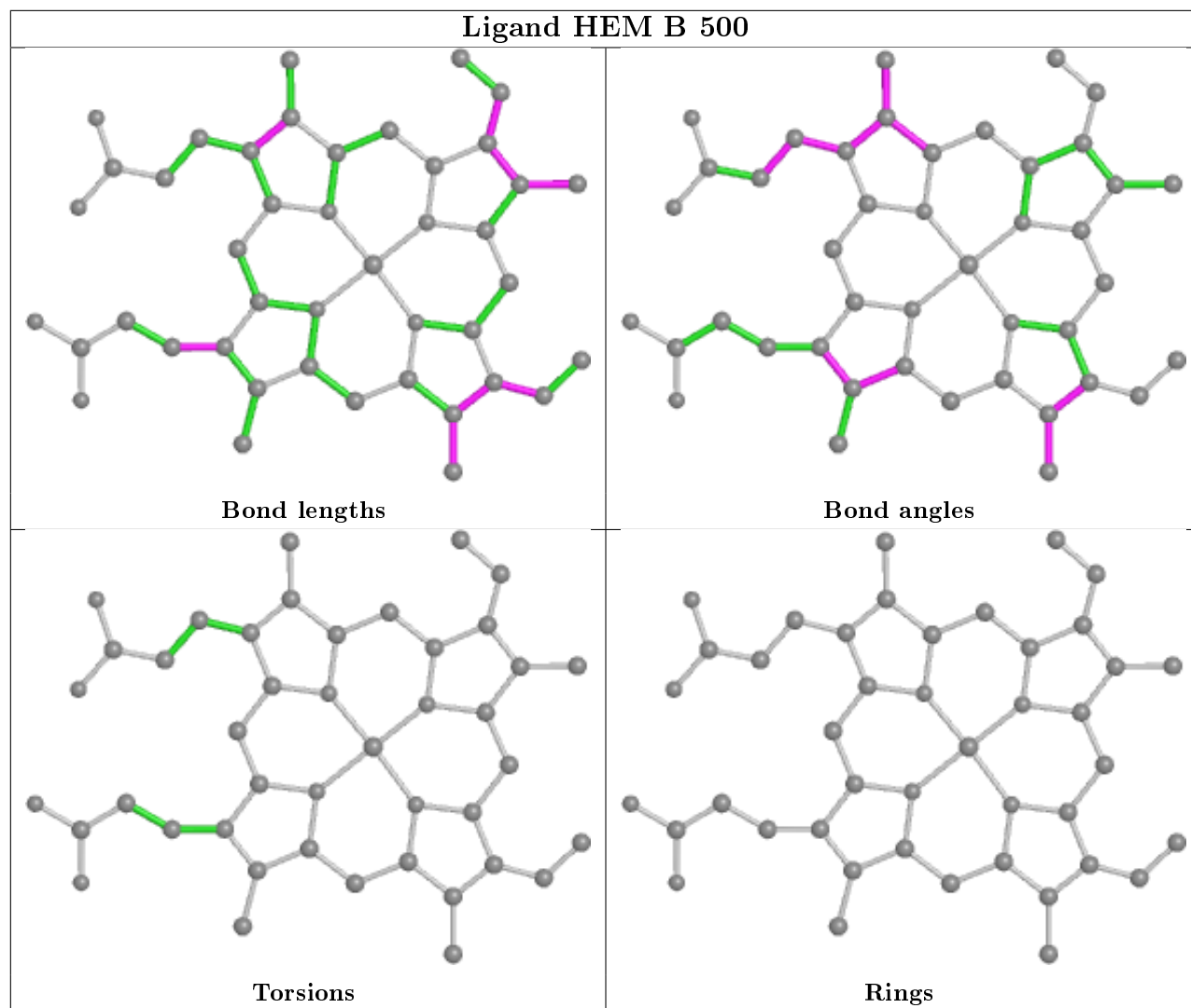


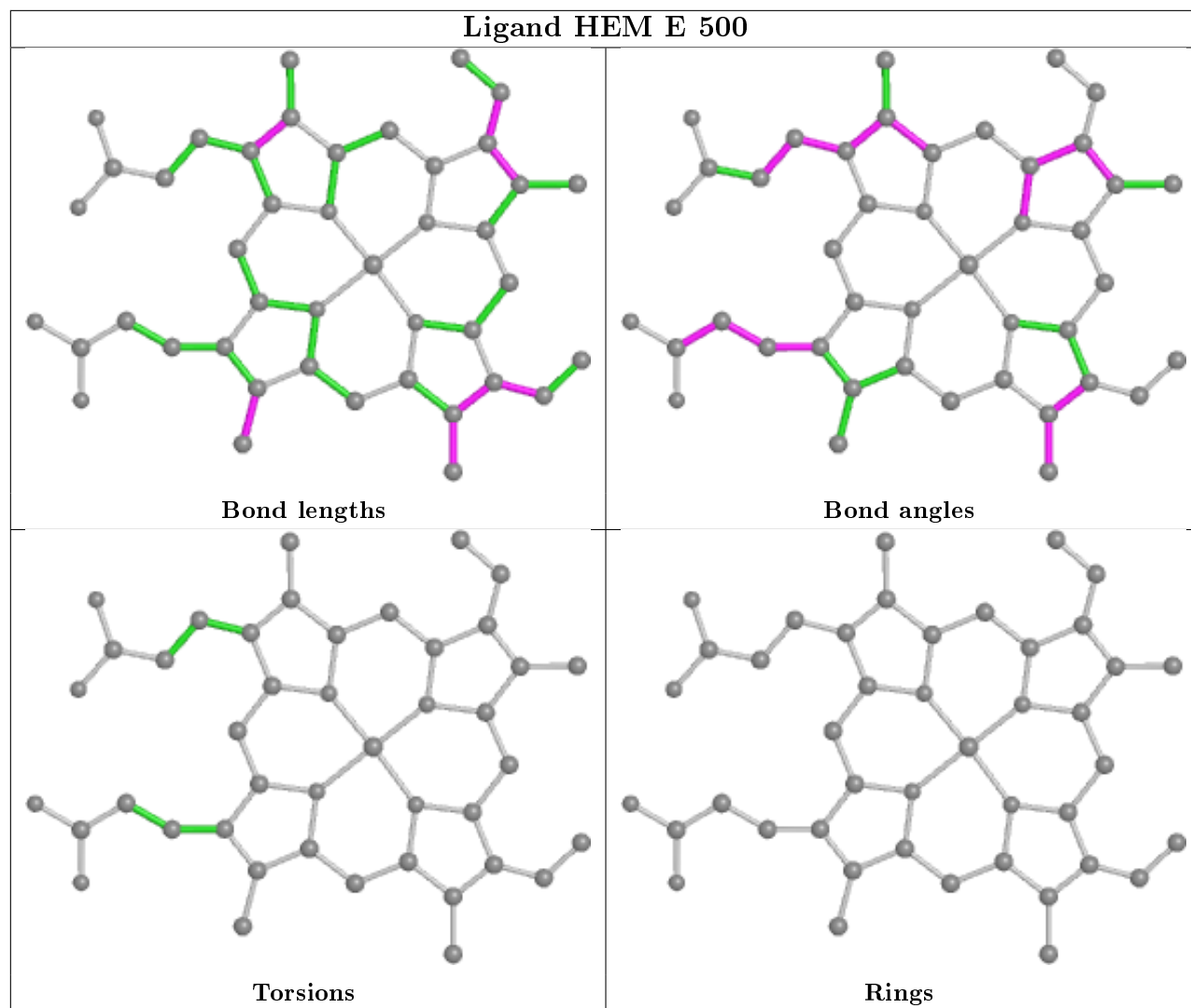


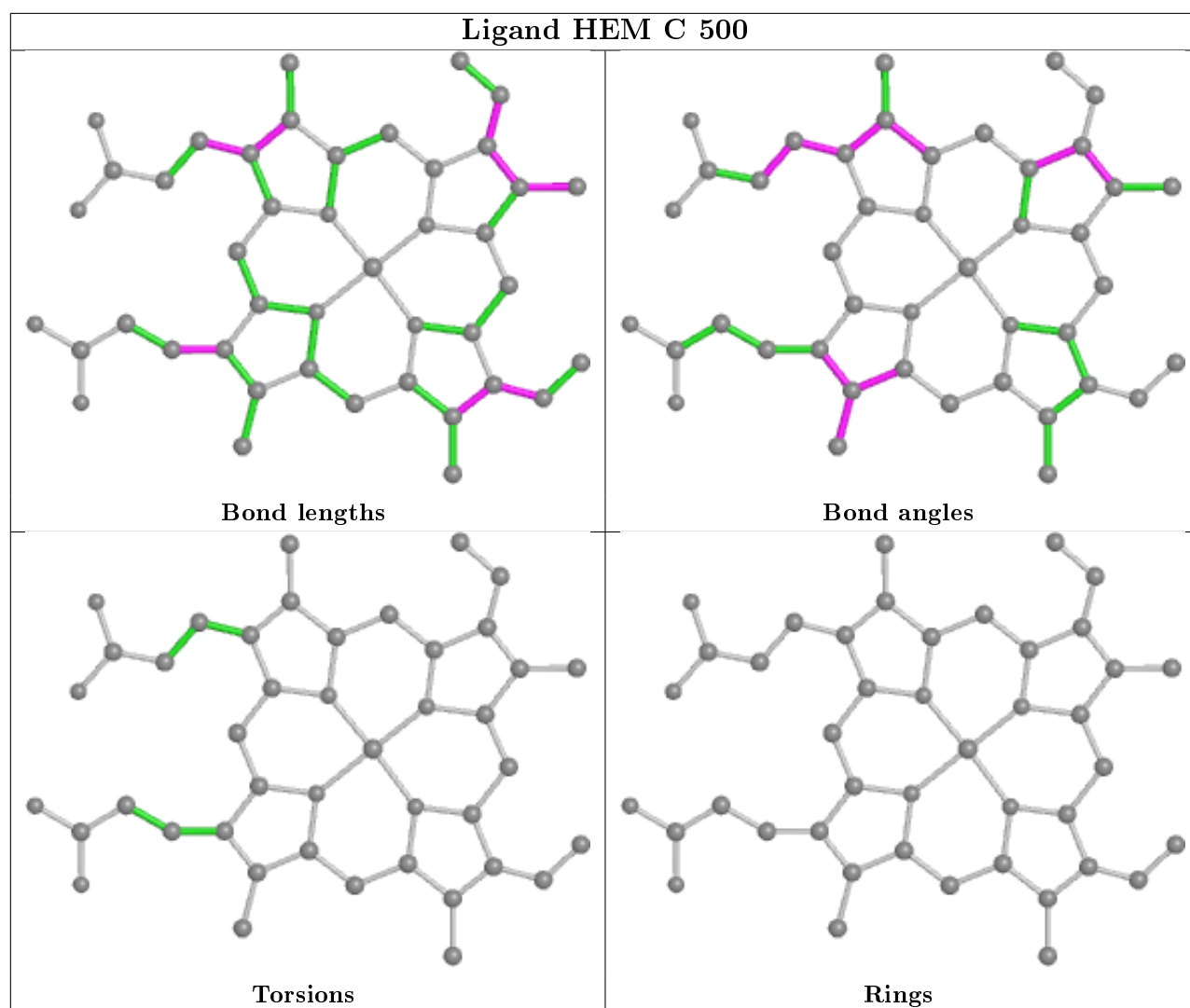












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	464/476 (97%)	0.15	1 (0%) 95 95	17, 33, 53, 58	0
1	B	464/476 (97%)	0.11	1 (0%) 95 95	18, 33, 52, 61	0
1	C	464/476 (97%)	0.09	0 100 100	17, 33, 49, 58	0
1	D	465/476 (97%)	0.16	1 (0%) 95 95	19, 34, 52, 59	0
1	E	465/476 (97%)	0.20	10 (2%) 62 65	22, 48, 66, 74	0
1	F	465/476 (97%)	0.60	37 (7%) 12 12	23, 61, 83, 90	0
1	G	463/476 (97%)	0.63	36 (7%) 13 13	29, 65, 85, 95	0
1	H	458/476 (96%)	0.83	57 (12%) 4 3	23, 75, 94, 99	0
All	All	3708/3808 (97%)	0.34	143 (3%) 39 42	17, 45, 85, 99	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	141	GLY	7.7
1	H	133	ALA	6.0
1	H	282	PRO	5.4
1	G	157	ILE	5.4
1	G	491	PHE	5.0
1	H	462	PHE	4.9
1	F	140	VAL	4.8
1	G	420	LYS	4.7
1	H	267	PHE	4.7
1	G	137	GLY	4.6
1	H	430	VAL	4.1
1	H	400	ARG	4.0
1	G	471	ILE	3.9
1	F	492	LEU	3.8
1	H	417	LEU	3.7
1	E	462	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	30	LYS	3.7
1	H	273	ILE	3.7
1	H	334	VAL	3.6
1	H	316	LEU	3.6
1	H	487	TYR	3.6
1	H	458	GLN	3.6
1	H	263	SER	3.5
1	H	477	HIS	3.5
1	F	31	GLY	3.5
1	G	210	GLN	3.4
1	G	419	LYS	3.4
1	G	187	PHE	3.3
1	H	420	LYS	3.3
1	H	406	SER	3.3
1	H	473	VAL	3.3
1	H	463	LYS	3.2
1	G	155	PHE	3.2
1	G	213	ALA	3.2
1	F	282	PRO	3.1
1	F	189	ASP	3.1
1	H	456	ILE	3.1
1	F	264	PRO	3.1
1	F	271	PHE	3.1
1	G	408	PRO	3.0
1	D	30	LYS	3.0
1	F	263	SER	3.0
1	H	362	PHE	3.0
1	F	491	PHE	3.0
1	H	476	LYS	3.0
1	F	116	VAL	3.0
1	H	416	PHE	3.0
1	F	124	ALA	2.9
1	F	143	ARG	2.9
1	G	276	GLN	2.9
1	G	323	VAL	2.9
1	H	259	LEU	2.9
1	H	262	ASN	2.9
1	E	135	LEU	2.9
1	H	156	LEU	2.9
1	H	288	LEU	2.9
1	H	271	PHE	2.9
1	F	351	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	427	ASP	2.8
1	H	421	GLY	2.8
1	H	54	MET	2.8
1	G	487	TYR	2.8
1	H	428	ALA	2.8
1	H	317	LEU	2.8
1	G	464	SER	2.8
1	F	273	ILE	2.7
1	H	325	ALA	2.7
1	G	488	THR	2.7
1	A	143	ARG	2.7
1	G	462	PHE	2.7
1	H	315	LEU	2.7
1	H	481	ALA	2.6
1	F	288	LEU	2.6
1	H	405	PHE	2.6
1	H	474	SER	2.6
1	H	269	ASP	2.6
1	H	414	GLN	2.5
1	G	481	ALA	2.5
1	H	261	PRO	2.5
1	G	164	HIS	2.5
1	H	98	PHE	2.5
1	G	406	SER	2.5
1	F	412	ASN	2.5
1	F	172	PHE	2.5
1	F	279	GLU	2.5
1	F	185	ILE	2.4
1	F	142	LYS	2.4
1	H	154	GLY	2.4
1	H	452	PHE	2.4
1	F	376	LYS	2.4
1	G	189	ASP	2.4
1	F	256	GLN	2.4
1	F	338	ASN	2.4
1	H	464	SER	2.4
1	E	457	MET	2.4
1	F	283	ASN	2.3
1	H	493	PRO	2.3
1	G	159	ALA	2.3
1	H	55	TYR	2.3
1	F	206	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	260	ASP	2.3
1	H	447	MET	2.3
1	H	471	ILE	2.3
1	F	267	PHE	2.3
1	H	185	ILE	2.3
1	G	181	VAL	2.3
1	E	364	ASP	2.3
1	G	138	PHE	2.3
1	G	402	PRO	2.2
1	G	163	THR	2.2
1	H	187	PHE	2.2
1	F	199	LEU	2.2
1	G	185	ILE	2.2
1	B	172	PHE	2.2
1	G	484	PRO	2.2
1	F	318	MET	2.2
1	F	419	LYS	2.2
1	E	31	GLY	2.2
1	G	214	THR	2.2
1	H	298	LEU	2.2
1	H	398	VAL	2.1
1	G	201	LEU	2.1
1	E	280	LYS	2.1
1	G	465	PRO	2.1
1	E	453	PHE	2.1
1	G	161	ARG	2.1
1	H	172	PHE	2.1
1	E	343	PHE	2.1
1	F	461	ARG	2.1
1	F	30	LYS	2.1
1	H	348	LYS	2.1
1	G	327	VAL	2.1
1	H	402	PRO	2.1
1	F	391	VAL	2.0
1	G	178	VAL	2.0
1	F	450	PHE	2.0
1	H	118	PHE	2.0
1	F	364	ASP	2.0
1	G	142	LYS	2.0
1	E	467	SER	2.0
1	F	366	LEU	2.0
1	H	199	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	457	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

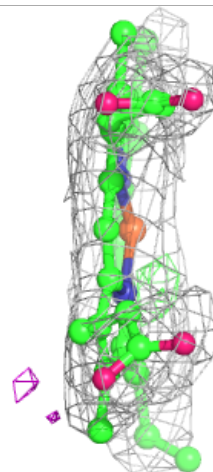
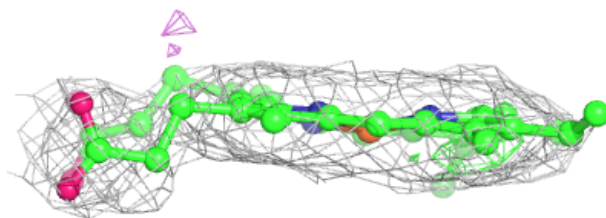
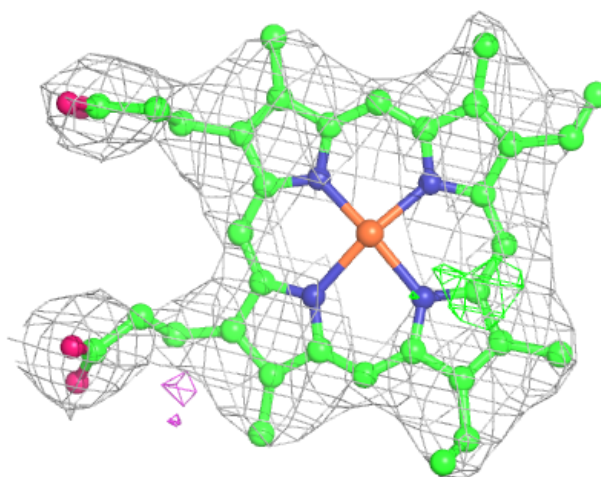
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NCT	D	501	12/12	0.88	0.35	80,81,82,82	0
4	GOL	H	502	6/6	0.89	0.27	28,32,35,37	0
3	NCT	A	501	12/12	0.91	0.23	50,52,53,54	0
3	NCT	C	501	12/12	0.91	0.31	61,62,67,68	0
3	NCT	B	501	12/12	0.92	0.23	40,43,44,47	0
2	HEM	H	501	43/43	0.93	0.22	58,61,67,68	0
2	HEM	G	500	43/43	0.97	0.16	32,38,43,49	0
2	HEM	E	500	43/43	0.97	0.16	26,33,35,35	0
2	HEM	F	500	43/43	0.97	0.18	44,48,50,51	0
2	HEM	D	500	43/43	0.97	0.19	16,26,28,28	0
2	HEM	C	500	43/43	0.98	0.17	15,23,27,29	0
2	HEM	B	500	43/43	0.98	0.16	13,23,25,28	0
2	HEM	A	500	43/43	0.98	0.19	16,23,27,31	0

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

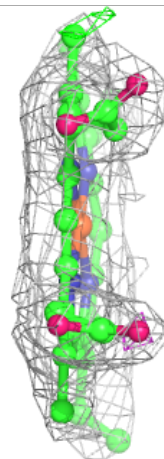
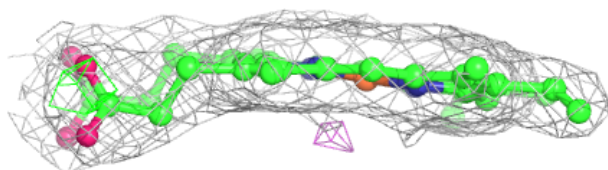
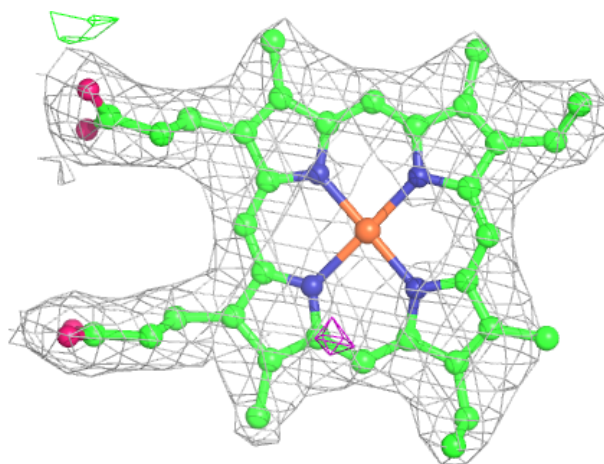
Electron density around HEM H 501:

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



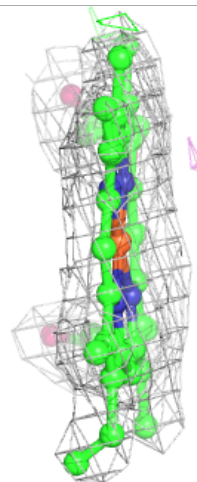
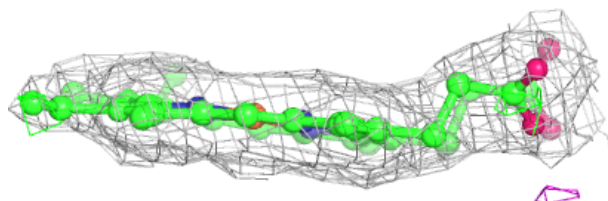
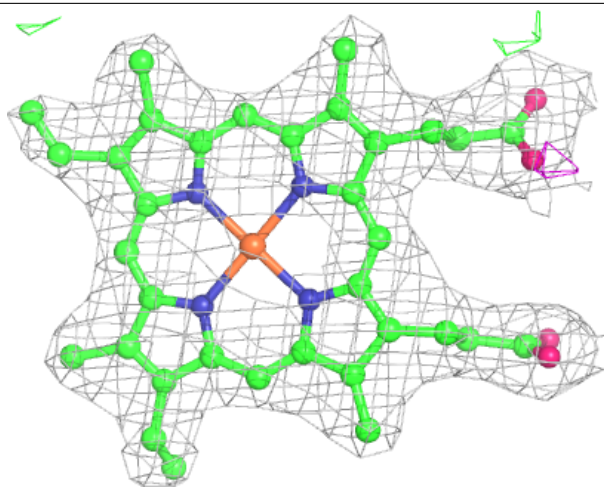
Electron density around HEM G 500:

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



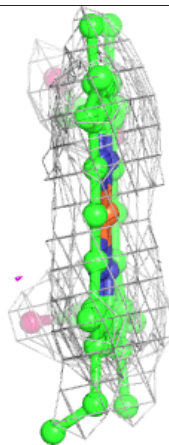
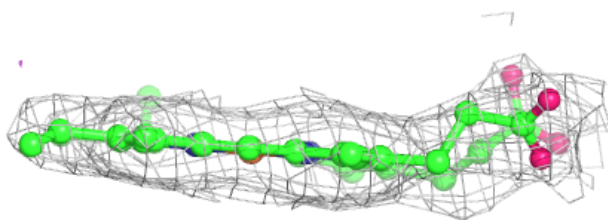
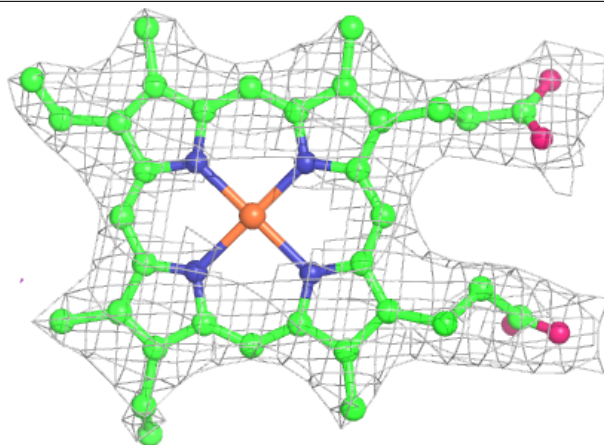
Electron density around HEM E 500:

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



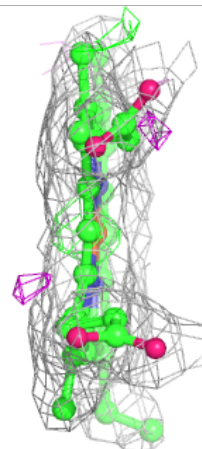
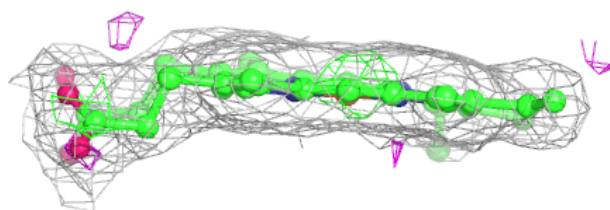
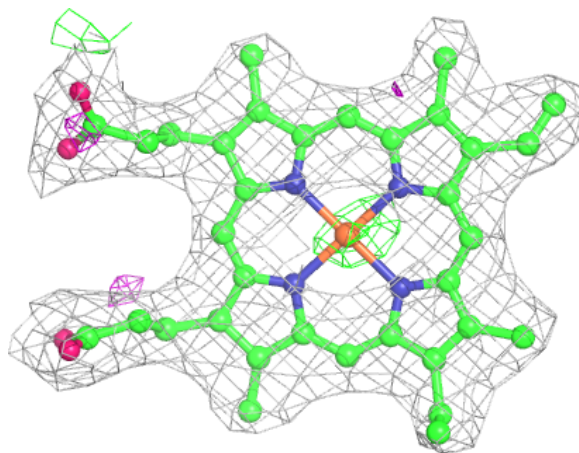
Electron density around HEM F 500:

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



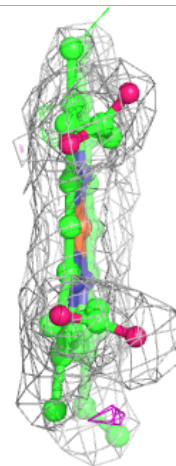
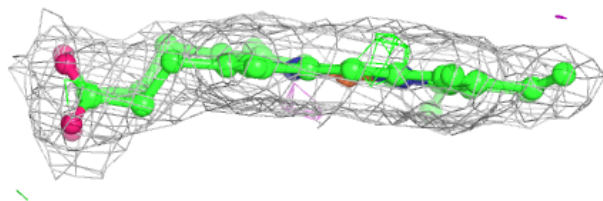
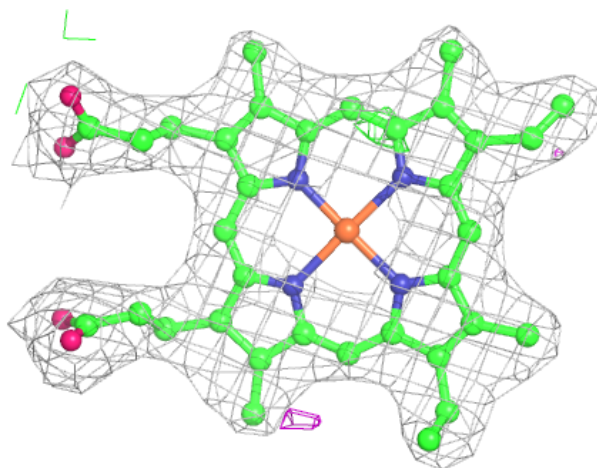
Electron density around HEM D 500:

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



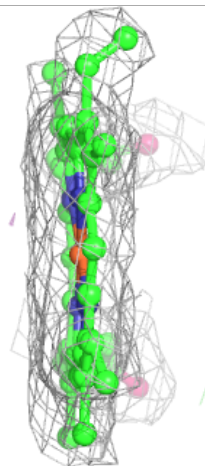
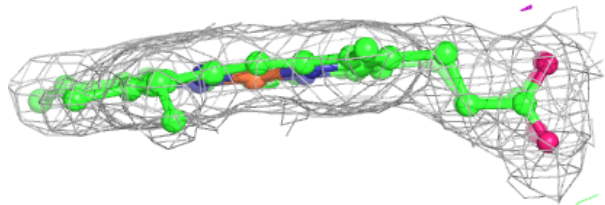
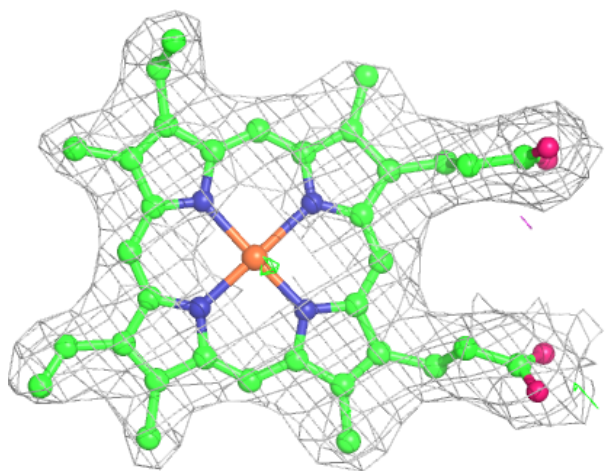
Electron density around HEM C 500:

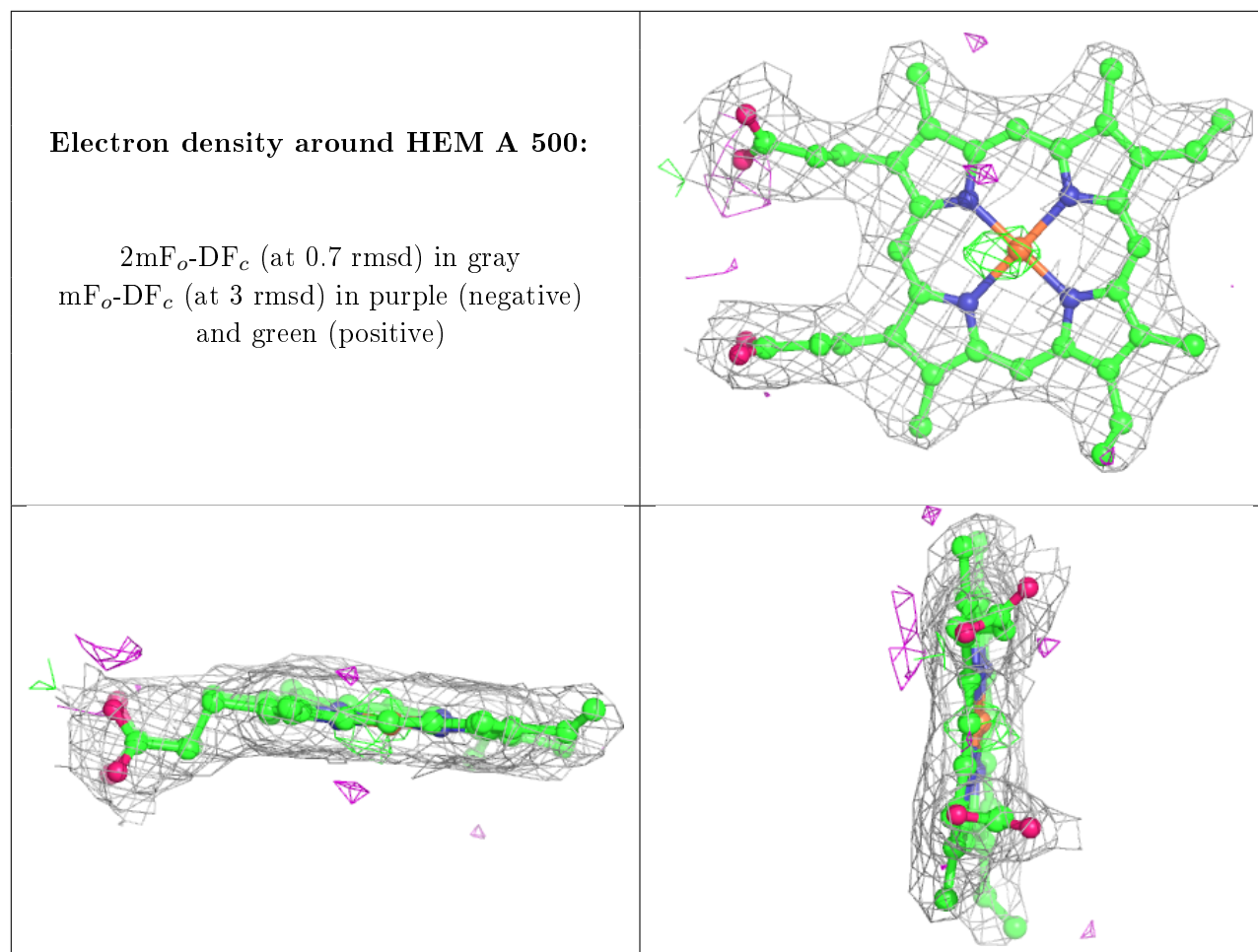
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 500:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.