



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:29 AM UTC

PDB ID : 2P85 / pdb_00002p85
Title : Structure of Human Lung Cytochrome P450 2A13 with indole bound in two alternate conformations
Authors : Scott, E.E.; Stout, C.D.
Deposited on : 2007-03-21
Resolution : 2.35 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:

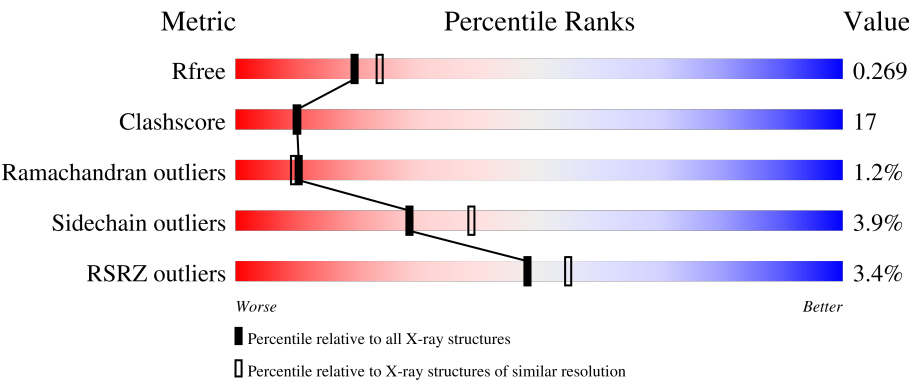
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	476	73%21% . .
1	B	476	4% 67%28% . .
1	C	476	7% 56%35%6% .
1	D	476	% 67%28% . .
1	E	476	2% 67%28% . .

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Mol	Chain	Length	Quality of chain
1	F	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
3	IND	B	508[B]	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23541 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	0	0
			3763	2421	650	674	18			
1	B	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	C	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	D	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	E	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	F	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	VAL	engineered mutation	UNP Q16696
A	24	ALA	TRP	engineered mutation	UNP Q16696
A	25	LYS	ARG	engineered mutation	UNP Q16696
A	26	LYS	GLN	engineered mutation	UNP Q16696
A	27	THR	ARG	engineered mutation	UNP Q16696
A	28	SER	LYS	engineered mutation	UNP Q16696
A	30	LYS	ARG	engineered mutation	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	VAL	engineered mutation	UNP Q16696
B	24	ALA	TRP	engineered mutation	UNP Q16696
B	25	LYS	ARG	engineered mutation	UNP Q16696
B	26	LYS	GLN	engineered mutation	UNP Q16696
B	27	THR	ARG	engineered mutation	UNP Q16696
B	28	SER	LYS	engineered mutation	UNP Q16696

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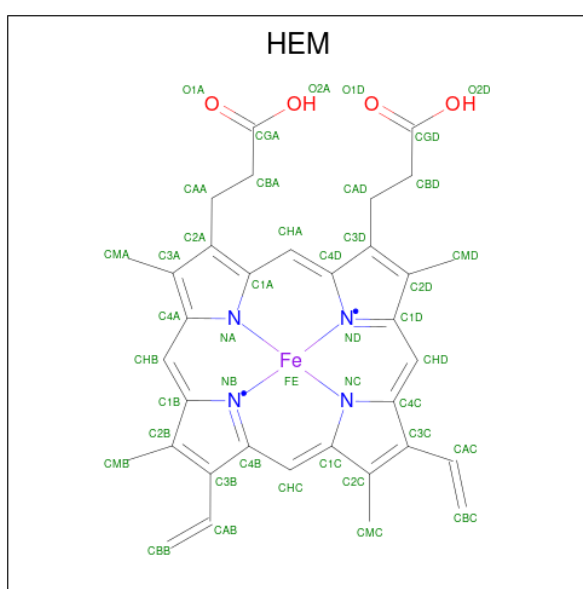
Chain	Residue	Modelled	Actual	Comment	Reference
B	30	LYS	ARG	engineered mutation	UNP Q16696
B	495	HIS	-	expression tag	UNP Q16696
B	496	HIS	-	expression tag	UNP Q16696
B	497	HIS	-	expression tag	UNP Q16696
B	498	HIS	-	expression tag	UNP Q16696
C	23	MET	VAL	engineered mutation	UNP Q16696
C	24	ALA	TRP	engineered mutation	UNP Q16696
C	25	LYS	ARG	engineered mutation	UNP Q16696
C	26	LYS	GLN	engineered mutation	UNP Q16696
C	27	THR	ARG	engineered mutation	UNP Q16696
C	28	SER	LYS	engineered mutation	UNP Q16696
C	30	LYS	ARG	engineered mutation	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	VAL	engineered mutation	UNP Q16696
D	24	ALA	TRP	engineered mutation	UNP Q16696
D	25	LYS	ARG	engineered mutation	UNP Q16696
D	26	LYS	GLN	engineered mutation	UNP Q16696
D	27	THR	ARG	engineered mutation	UNP Q16696
D	28	SER	LYS	engineered mutation	UNP Q16696
D	30	LYS	ARG	engineered mutation	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	VAL	engineered mutation	UNP Q16696
E	24	ALA	TRP	engineered mutation	UNP Q16696
E	25	LYS	ARG	engineered mutation	UNP Q16696
E	26	LYS	GLN	engineered mutation	UNP Q16696
E	27	THR	ARG	engineered mutation	UNP Q16696
E	28	SER	LYS	engineered mutation	UNP Q16696
E	30	LYS	ARG	engineered mutation	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	VAL	engineered mutation	UNP Q16696
F	24	ALA	TRP	engineered mutation	UNP Q16696
F	25	LYS	ARG	engineered mutation	UNP Q16696
F	26	LYS	GLN	engineered mutation	UNP Q16696

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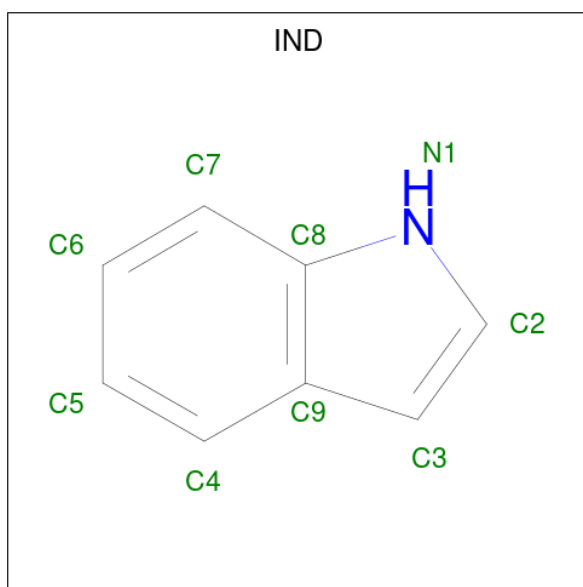
Chain	Residue	Modelled	Actual	Comment	Reference
F	27	THR	ARG	engineered mutation	UNP Q16696
F	28	SER	LYS	engineered mutation	UNP Q16696
F	30	LYS	ARG	engineered mutation	UNP Q16696
F	495	HIS	-	expression tag	UNP Q16696
F	496	HIS	-	expression tag	UNP Q16696
F	497	HIS	-	expression tag	UNP Q16696
F	498	HIS	-	expression tag	UNP Q16696

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



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

- Molecule 3 is INDOLE (CCD ID: IND) (formula: C_8H_7N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	1
			9	8	1		
3	A	1	Total	C	N	0	1
			9	8	1		
3	B	1	Total	C	N	0	1
			9	8	1		
3	B	1	Total	C	N	0	1
			9	8	1		
3	C	1	Total	C	N	0	1
			9	8	1		
3	C	1	Total	C	N	0	1
			9	8	1		
3	D	1	Total	C	N	0	1
			9	8	1		
3	D	1	Total	C	N	0	1
			9	8	1		
3	E	1	Total	C	N	0	1
			9	8	1		
3	E	1	Total	C	N	0	1
			9	8	1		
3	F	1	Total	C	N	0	1
			9	8	1		
3	F	1	Total	C	N	0	1
			9	8	1		

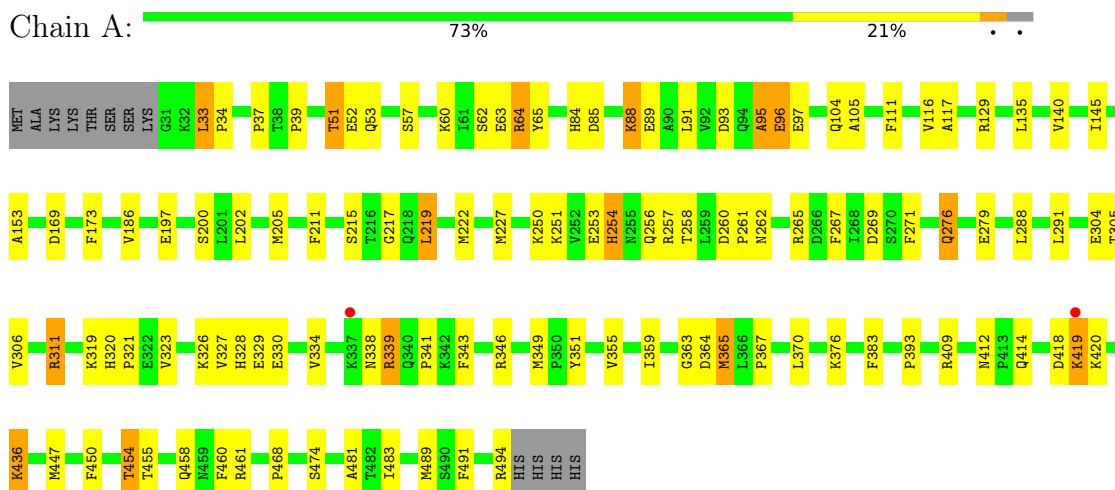
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total 161	O 161	0	1
4	B	75	Total 75	O 75	0	1
4	C	89	Total 89	O 89	0	1
4	D	96	Total 96	O 96	0	1
4	E	99	Total 99	O 99	0	1
4	F	77	Total 77	O 77	0	1

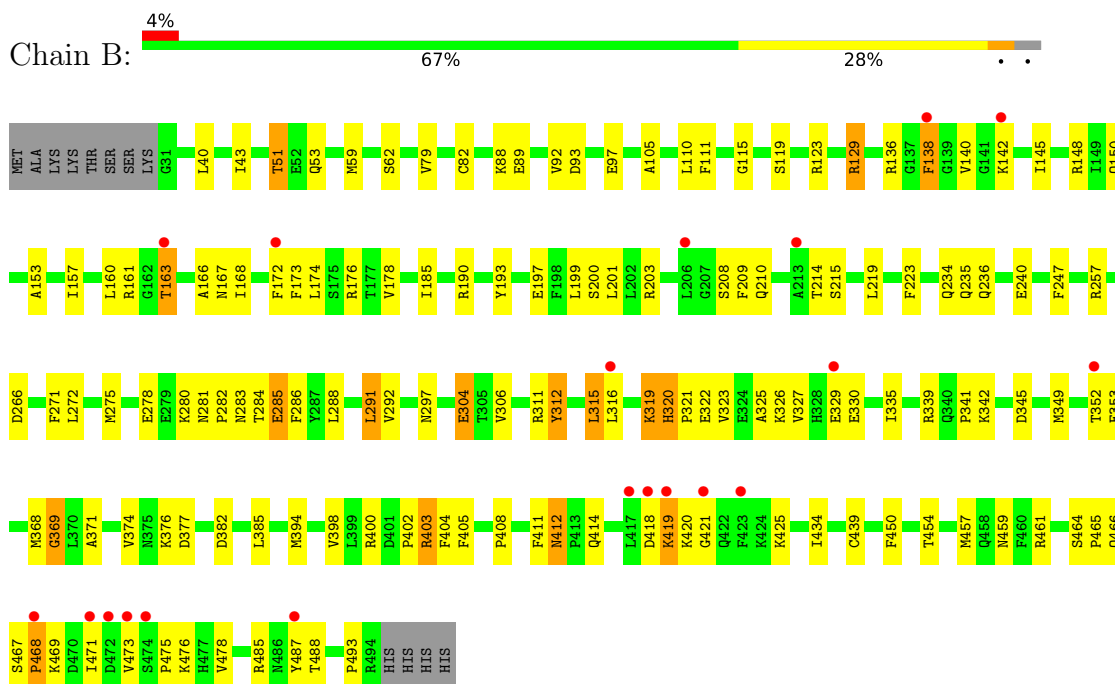
3 Residue-property plots

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.

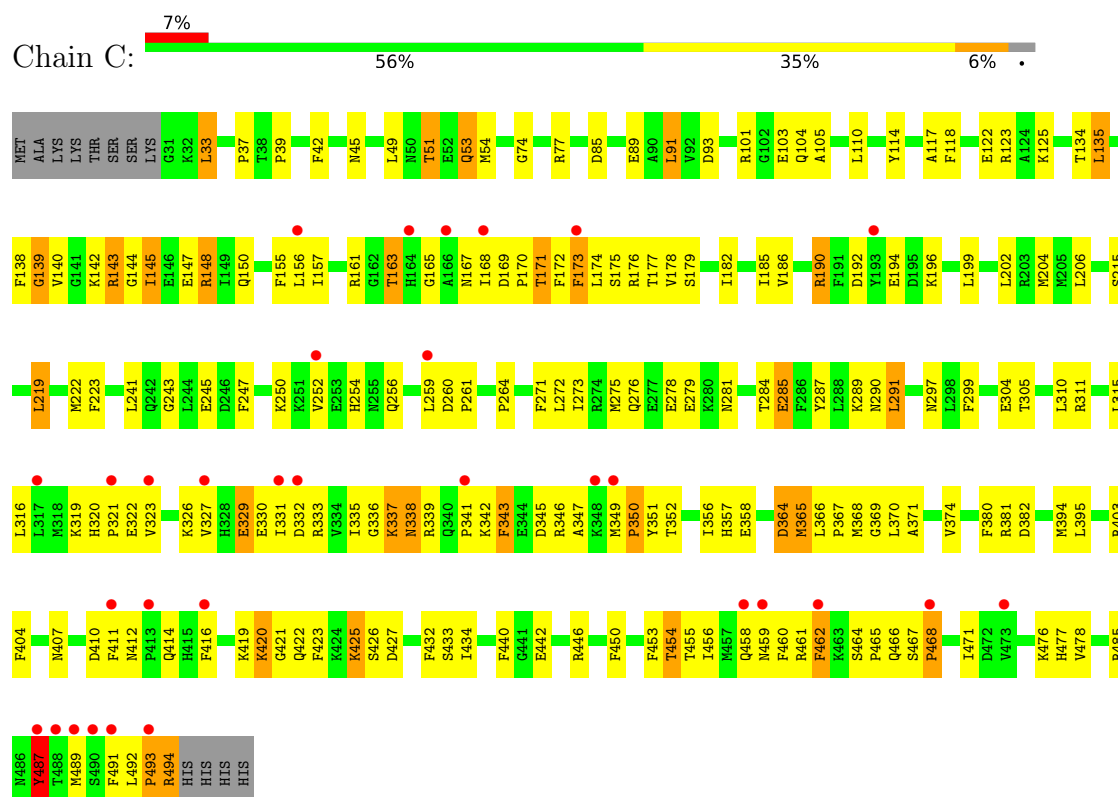
• Molecule 1: Cytochrome P450 2A13



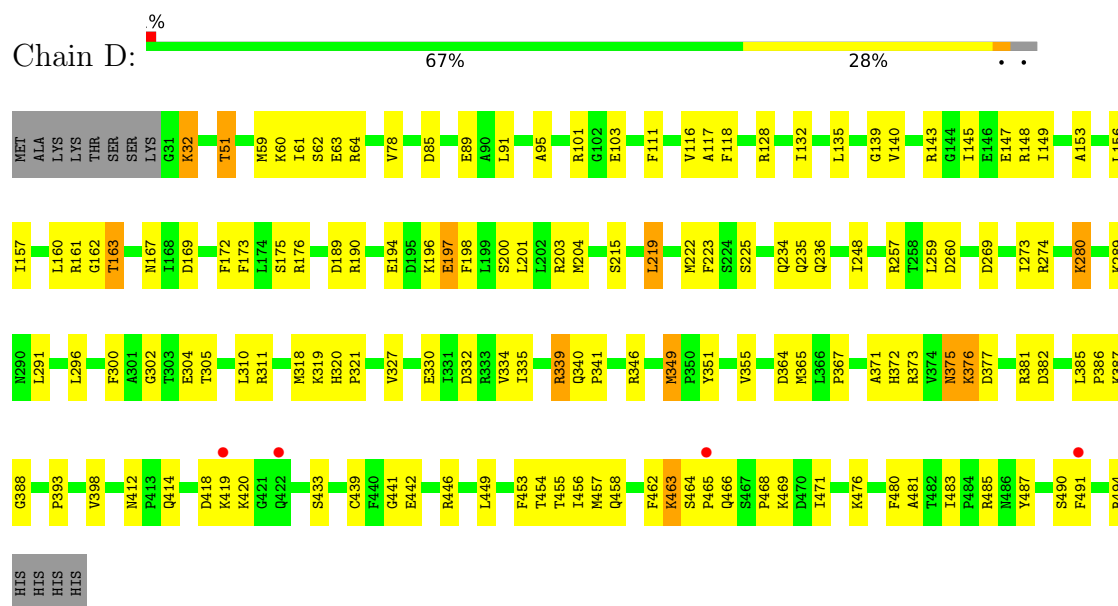
• Molecule 1: Cytochrome P450 2A13



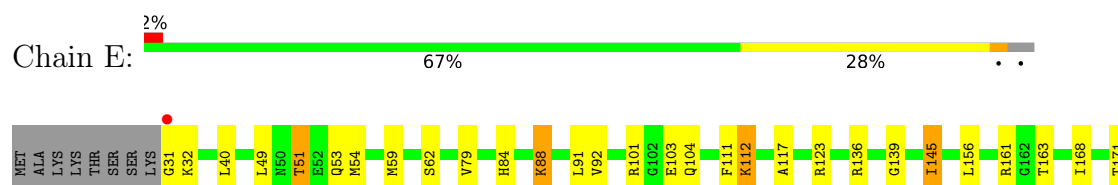
- Molecule 1: Cytochrome P450 2A13

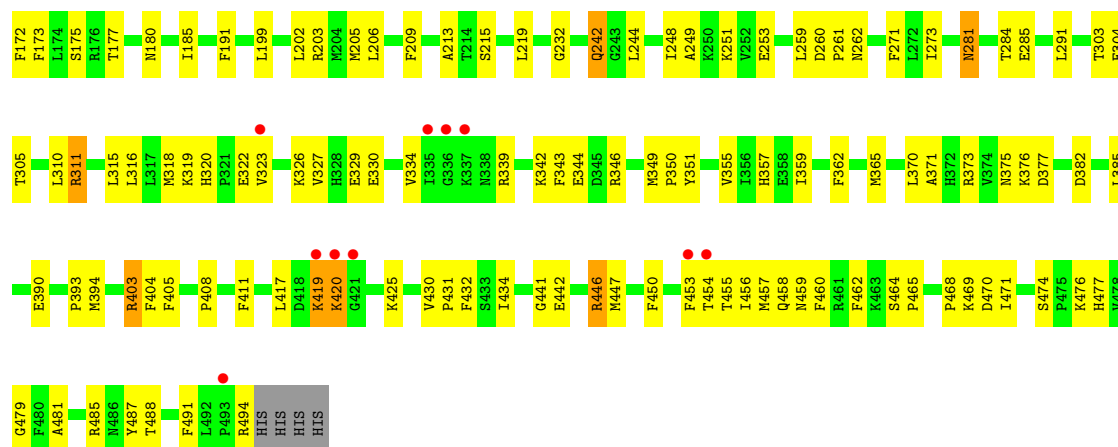


- Molecule 1: Cytochrome P450 2A13

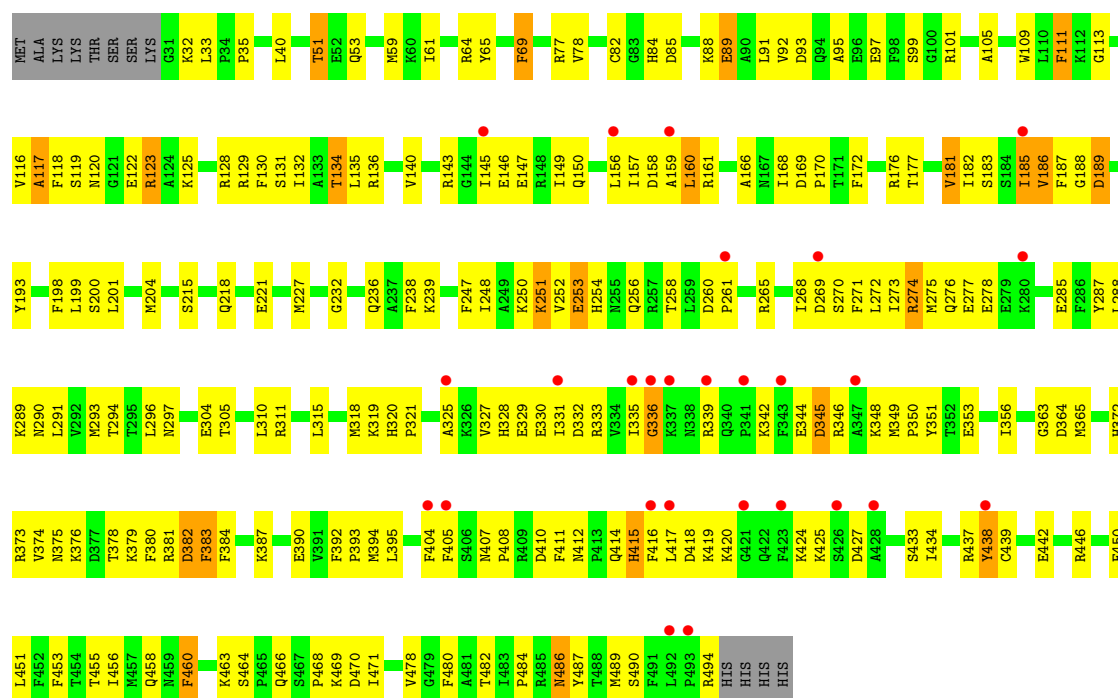


- Molecule 1: Cytochrome P450 2A13





● Molecule 1: Cytochrome P450 2A13



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.32Å 110.28Å 142.00Å 90.00° 110.28° 90.00°	Depositor
Resolution (Å)	29.34 – 2.35 29.34 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.34-2.35) 97.1 (29.34-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.277 0.211 , 0.269	Depositor DCC
R_{free} test set	19677 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23541	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.60	0/3860	1.05	27/5198 (0.5%)
1	B	0.53	0/3860	1.04	19/5198 (0.4%)
1	C	0.50	0/3860	1.01	27/5198 (0.5%)
1	D	0.53	0/3860	1.05	29/5198 (0.6%)
1	E	0.51	0/3860	0.98	15/5198 (0.3%)
1	F	0.48	0/3860	0.97	18/5198 (0.3%)
All	All	0.53	0/23160	1.02	135/31188 (0.4%)

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ALA	N-CA-C	9.74	121.98	111.36
1	C	143	ARG	N-CA-C	-8.50	104.93	114.62
1	D	320	HIS	CA-C-N	8.46	128.44	119.05
1	D	320	HIS	C-N-CA	8.46	128.44	119.05
1	E	304	GLU	N-CA-C	8.21	120.23	111.28
1	B	223	PHE	N-CA-C	8.03	121.16	110.88
1	C	370	LEU	N-CA-C	-7.98	96.55	109.96
1	C	117	ALA	N-CA-C	7.94	121.03	111.82
1	A	288	LEU	N-CA-C	7.81	120.48	111.11
1	F	304	GLU	N-CA-C	7.35	119.93	111.11
1	D	304	GLU	N-CA-C	7.26	120.06	111.71
1	A	105	ALA	N-CA-C	7.19	119.74	111.11
1	E	117	ALA	N-CA-C	7.11	118.82	111.14
1	A	169	ASP	N-CA-C	-7.11	99.36	109.24
1	A	173	PHE	N-CA-C	-7.07	103.65	111.36
1	C	338	ASN	N-CA-C	7.04	118.74	111.14
1	A	116	VAL	N-CA-C	6.92	117.70	110.72
1	F	345	ASP	N-CA-C	-6.89	103.97	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	LYS	N-CA-C	-6.89	104.61	112.87
1	A	304	GLU	N-CA-C	6.85	119.59	111.71
1	A	104	GLN	N-CA-C	-6.76	96.17	107.32
1	C	458	GLN	N-CA-C	-6.70	103.90	111.14
1	D	78	VAL	N-CA-C	6.68	118.41	108.46
1	B	173	PHE	N-CA-C	-6.67	104.09	111.36
1	B	461	ARG	N-CA-C	-6.63	99.41	109.95
1	E	104	GLN	N-CA-C	-6.57	96.49	107.32
1	A	219	LEU	N-CA-C	-6.54	104.19	111.71
1	A	117	ALA	N-CA-C	6.46	119.29	111.40
1	F	232	GLY	CA-C-N	6.40	126.32	119.28
1	F	232	GLY	C-N-CA	6.40	126.32	119.28
1	D	349	MET	CA-C-N	6.38	126.14	119.05
1	D	349	MET	C-N-CA	6.38	126.14	119.05
1	C	199	LEU	N-CA-C	-6.32	104.49	111.82
1	F	89	GLU	N-CA-C	6.28	117.79	111.07
1	F	169	ASP	CA-C-N	6.27	126.39	119.87
1	F	169	ASP	C-N-CA	6.27	126.39	119.87
1	A	365	MET	N-CA-C	6.23	118.59	111.11
1	D	169	ASP	CA-C-N	6.21	125.89	119.56
1	D	169	ASP	C-N-CA	6.21	125.89	119.56
1	D	116	VAL	N-CA-C	6.19	116.35	110.53
1	A	461	ARG	N-CA-C	-6.16	98.95	109.24
1	D	103	GLU	N-CA-C	6.16	119.97	110.42
1	D	173	PHE	N-CA-C	-6.15	103.90	112.45
1	E	370	LEU	N-CA-C	-6.14	99.19	109.07
1	D	371	ALA	N-CA-C	6.12	118.87	110.24
1	D	197	GLU	N-CA-C	-6.09	104.20	111.69
1	D	334	VAL	N-CA-C	6.05	116.69	110.82
1	E	474	SER	N-CA-C	-6.03	102.47	110.07
1	D	85	ASP	N-CA-C	6.03	117.53	111.07
1	D	259	LEU	N-CA-C	6.01	118.91	109.96
1	C	304	GLU	N-CA-C	6.01	117.50	111.07
1	C	74	GLY	N-CA-C	-6.01	100.09	112.34
1	D	480	PHE	N-CA-C	-6.00	104.74	111.28
1	C	487	TYR	N-CA-C	5.99	116.00	108.45
1	B	285	GLU	N-CA-C	-5.99	105.74	113.16
1	B	219	LEU	N-CA-C	-5.96	104.87	111.36
1	C	285	GLU	N-CA-C	-5.89	105.67	112.92
1	A	85	ASP	N-CA-C	5.89	117.37	111.07
1	D	219	LEU	N-CA-C	-5.86	104.90	111.28
1	D	260	ASP	CA-C-N	5.83	125.97	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	260	ASP	C-N-CA	5.83	125.97	119.32
1	A	227	MET	N-CA-C	5.83	118.41	111.71
1	A	370	LEU	N-CA-C	-5.82	99.70	109.07
1	B	168	ILE	N-CA-C	5.80	116.53	108.23
1	A	460	PHE	N-CA-C	5.78	118.66	109.81
1	A	436	LYS	N-CA-C	5.77	119.58	112.54
1	B	320	HIS	CA-C-N	5.76	127.04	119.84
1	B	320	HIS	C-N-CA	5.76	127.04	119.84
1	A	458	GLN	N-CA-C	-5.74	105.17	111.82
1	C	33	LEU	CA-C-N	5.73	123.84	119.66
1	C	33	LEU	C-N-CA	5.73	123.84	119.66
1	D	483	ILE	N-CA-C	5.68	114.08	107.89
1	C	139	GLY	N-CA-C	5.66	121.50	114.37
1	F	456	ILE	N-CA-C	5.64	115.83	110.53
1	F	69	PHE	N-CA-C	5.60	117.31	108.96
1	B	304	GLU	N-CA-C	5.60	117.38	111.28
1	A	91	LEU	N-CA-C	5.58	117.36	111.28
1	E	232	GLY	CA-C-N	5.58	126.81	119.84
1	E	232	GLY	C-N-CA	5.58	126.81	119.84
1	C	173	PHE	N-CA-C	-5.55	104.05	112.04
1	A	474	SER	N-CA-C	-5.54	102.43	110.08
1	A	95	ALA	N-CA-C	5.54	117.00	111.07
1	C	105	ALA	N-CA-C	5.52	118.01	111.33
1	A	153	ALA	N-CA-C	-5.50	105.28	111.28
1	B	105	ALA	N-CA-C	5.50	117.71	111.11
1	B	398	VAL	N-CA-C	-5.50	105.75	111.58
1	A	393	PRO	N-CA-C	-5.49	101.16	112.47
1	E	173	PHE	N-CA-C	-5.49	104.94	111.69
1	B	138	PHE	N-CA-C	-5.47	105.22	112.94
1	A	483	ILE	N-CA-C	5.47	113.85	107.89
1	E	219	LEU	N-CA-C	-5.46	105.33	111.28
1	F	185	ILE	N-CA-C	5.45	115.65	110.53
1	D	111	PHE	N-CA-C	5.42	117.26	111.36
1	B	148	ARG	N-CA-C	-5.39	105.44	112.23
1	C	104	GLN	N-CA-C	-5.39	96.22	107.37
1	E	111	PHE	N-CA-C	5.39	118.07	111.82
1	F	460	PHE	N-CA-C	5.38	117.37	109.24
1	E	479	GLY	N-CA-C	-5.37	100.46	113.18
1	D	223	PHE	N-CA-C	5.37	117.75	110.88
1	B	412	ASN	CA-C-N	5.34	126.51	119.84
1	B	412	ASN	C-N-CA	5.34	126.51	119.84
1	C	320	HIS	CA-C-N	5.34	126.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	320	HIS	C-N-CA	5.34	126.51	119.84
1	A	111	PHE	N-CA-C	5.33	118.00	111.82
1	E	441	GLY	N-CA-C	-5.32	106.54	115.80
1	E	281	ASN	CA-C-N	5.30	125.39	119.87
1	E	281	ASN	C-N-CA	5.30	125.39	119.87
1	A	334	VAL	N-CA-C	5.30	116.37	111.81
1	F	480	PHE	N-CA-C	-5.30	105.62	111.71
1	F	415	HIS	N-CA-C	-5.28	106.54	112.87
1	C	223	PHE	N-CA-C	5.27	118.84	111.56
1	A	320	HIS	CA-C-N	5.24	125.55	119.47
1	A	320	HIS	C-N-CA	5.24	125.55	119.47
1	D	441	GLY	N-CA-C	-5.23	106.94	115.46
1	F	111	PHE	N-CA-C	5.23	116.98	111.28
1	C	260	ASP	CA-C-N	5.22	126.37	119.84
1	C	260	ASP	C-N-CA	5.22	126.37	119.84
1	C	462	PHE	N-CA-C	5.20	117.21	108.73
1	C	163	THR	N-CA-C	-5.19	106.90	114.12
1	F	117	ALA	N-CA-C	5.17	116.99	111.36
1	B	403	ARG	N-CA-C	-5.16	106.25	113.37
1	C	371	ALA	N-CA-C	5.12	117.86	110.28
1	F	227	MET	N-CA-C	5.12	118.62	112.38
1	B	475	PRO	N-CA-C	5.08	119.17	111.19
1	C	103	GLU	N-CA-C	5.05	118.25	110.42
1	C	169	ASP	CA-C-N	5.05	124.49	119.24
1	C	169	ASP	C-N-CA	5.05	124.49	119.24
1	D	248	ILE	CB-CA-C	-5.04	105.52	111.97
1	F	260	ASP	CA-C-N	5.04	126.13	119.84
1	F	260	ASP	C-N-CA	5.04	126.13	119.84
1	D	91	LEU	N-CA-C	5.03	117.65	111.82
1	D	462	PHE	N-CA-C	5.01	117.41	109.24
1	D	398	VAL	N-CA-C	-5.01	106.79	111.45
1	B	371	ALA	N-CA-C	5.01	117.50	110.23
1	E	393	PRO	N-CA-C	-5.00	102.17	112.47

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	3763	0	3728	70	0
1	B	3763	0	3728	115	0
1	C	3763	0	3728	175	0
1	D	3763	0	3728	119	0
1	E	3763	0	3728	112	0
1	F	3763	0	3728	189	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
2	E	43	0	30	0	0
2	F	43	0	30	5	0
3	A	18	0	14	1	0
3	B	18	0	14	5	0
3	C	18	0	14	2	0
3	D	18	0	14	0	0
3	E	18	0	14	2	0
3	F	18	0	14	2	0
4	A	161	0	0	5	0
4	B	75	0	0	1	0
4	C	89	0	0	4	0
4	D	96	0	0	2	0
4	E	99	0	0	3	0
4	F	77	0	0	2	0
All	All	23541	0	22632	785	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 17.

All (785) 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:204:MET:HE1	1:C:243:GLY:HA3	1.19	1.16
1:D:280:LYS:H	1:D:280:LYS:HE3	1.07	1.15
1:A:419:LYS:H	1:A:419:LYS:HD2	1.10	1.12
1:D:419:LYS:H	1:D:419:LYS:HD2	1.01	1.12
1:D:51:THR:HG23	1:D:215:SER:HB2	1.40	1.03
1:F:143:ARG:HH12	1:F:147:GLU:HB3	1.22	1.02
1:A:57:SER:HA	1:A:60:LYS:HE3	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:LYS:H	1:D:32:LYS:CE	1.76	0.98
1:B:419:LYS:H	1:B:419:LYS:HD2	1.30	0.97
1:D:32:LYS:H	1:D:32:LYS:HE2	1.33	0.93
1:F:274:ARG:HH21	1:F:274:ARG:HB3	1.35	0.92
1:C:157:ILE:HG23	1:C:460:PHE:HE1	1.34	0.92
1:D:419:LYS:HD2	1:D:419:LYS:N	1.86	0.90
1:C:247:PHE:HD1	1:C:250:LYS:HE2	1.37	0.90
1:C:204:MET:CE	1:C:243:GLY:HA3	2.04	0.87
1:F:156:LEU:HD12	1:F:177:THR:OG1	1.73	0.87
1:A:420:LYS:H	1:A:420:LYS:HD2	1.40	0.87
1:D:280:LYS:HE3	1:D:280:LYS:N	1.91	0.85
1:F:143:ARG:NH1	1:F:147:GLU:HB3	1.91	0.85
1:E:242:GLN:HG2	4:E:1128:HOH:O	1.75	0.85
1:A:265:ARG:HD3	1:A:269:ASP:OD1	1.74	0.85
1:D:32:LYS:HE3	1:D:382:ASP:O	1.75	0.85
1:C:175:SER:HB2	1:C:202:LEU:HD11	1.59	0.84
1:C:247:PHE:CD1	1:C:250:LYS:HE2	2.13	0.84
1:C:144:GLY:O	1:C:147:GLU:HG2	1.78	0.83
1:E:450:PHE:O	1:E:454:THR:HG22	1.78	0.83
1:D:376:LYS:NZ	1:D:376:LYS:HB3	1.96	0.81
1:F:130:PHE:O	1:F:134:THR:HG22	1.80	0.81
1:D:468:PRO:HB2	1:D:469:LYS:HE3	1.62	0.81
1:F:420:LYS:N	1:F:420:LYS:HD2	1.96	0.80
1:B:330:GLU:OE1	1:B:352:THR:HG22	1.82	0.80
1:B:53:GLN:NE2	1:B:478:VAL:HB	1.97	0.79
1:C:461:ARG:HE	1:C:494:ARG:HB2	1.47	0.79
1:B:419:LYS:HD2	1:B:419:LYS:N	1.98	0.79
1:C:450:PHE:O	1:C:454:THR:HB	1.82	0.78
1:C:247:PHE:O	1:C:250:LYS:HG2	1.83	0.78
1:E:31:GLY:O	1:E:32:LYS:HD2	1.84	0.78
1:C:335:ILE:HD13	1:C:341:PRO:HG3	1.64	0.77
1:B:53:GLN:HE21	1:B:478:VAL:HB	1.49	0.77
1:C:442:GLU:O	1:C:446:ARG:HG3	1.83	0.77
1:F:33:LEU:HD11	1:F:77:ARG:NH2	1.99	0.77
1:A:254:HIS:O	1:A:257:ARG:HG2	1.84	0.77
1:D:419:LYS:H	1:D:419:LYS:CD	1.86	0.77
1:A:419:LYS:HD2	1:A:419:LYS:N	1.94	0.77
1:F:201:LEU:HA	1:F:204:MET:HE3	1.66	0.77
1:F:442:GLU:O	1:F:446:ARG:HG3	1.85	0.77
1:E:156:LEU:HD21	1:E:456:ILE:HD11	1.67	0.76
1:E:205:MET:HE1	1:E:303:THR:HG21	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HA	1:D:222:MET:HE3	1.68	0.76
1:C:168:ILE:HD12	1:C:173:PHE:CE2	2.21	0.75
1:B:172:PHE:O	1:B:176:ARG:HG3	1.87	0.75
1:C:315:LEU:HB2	1:C:487:TYR:HE2	1.50	0.75
1:D:201:LEU:HD23	1:D:204:MET:CE	2.15	0.75
1:B:197:GLU:O	1:B:200:SER:HB3	1.87	0.75
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.53	0.74
1:F:130:PHE:CE2	1:F:274:ARG:HG3	2.22	0.73
1:C:315:LEU:HD13	1:C:487:TYR:CD2	2.23	0.73
1:F:274:ARG:HA	1:F:277:GLU:HG2	1.71	0.73
1:C:461:ARG:HH22	1:C:492:LEU:CD1	2.01	0.73
1:C:297:ASN:HD22	3:C:503[A]:IND:HN1	1.35	0.72
1:F:32:LYS:H	1:F:384:PHE:HB3	1.53	0.72
1:E:405:PHE:O	1:E:408:PRO:HD3	1.89	0.72
1:D:60:LYS:O	1:D:63:GLU:HG2	1.90	0.71
1:C:412:ASN:OD1	1:C:414:GLN:HB2	1.90	0.71
1:C:460:PHE:HA	1:C:492:LEU:O	1.90	0.71
1:A:51:THR:HG23	1:A:215:SER:OG	1.90	0.71
1:B:209:PHE:CD2	1:B:304:GLU:HG2	2.26	0.71
1:E:92:VAL:HG23	1:E:434:ILE:HD12	1.72	0.70
1:C:172:PHE:HA	1:C:175:SER:OG	1.91	0.70
1:D:201:LEU:HD23	1:D:204:MET:HE3	1.73	0.69
1:A:305:THR:HB	1:A:365:MET:HE1	1.75	0.69
1:E:323:VAL:O	1:E:327:VAL:HG23	1.91	0.69
1:D:376:LYS:HB3	1:D:376:LYS:HZ3	1.56	0.68
1:B:53:GLN:HE22	1:B:478:VAL:HG11	1.57	0.68
1:F:236:GLN:OE1	1:F:239:LYS:HE3	1.93	0.68
1:C:310:LEU:HD23	1:C:453:PHE:CE1	2.29	0.68
1:C:476:LYS:HE2	1:C:477:HIS:NE2	2.08	0.68
1:B:88:LYS:HG2	1:B:92:VAL:HG21	1.74	0.68
1:D:89:GLU:CD	1:D:381:ARG:HH11	2.02	0.68
1:C:157:ILE:HG23	1:C:460:PHE:CE1	2.24	0.67
1:B:209:PHE:CE1	3:B:508[B]:IND:H2	2.30	0.67
1:C:271:PHE:O	1:C:275:MET:HG3	1.95	0.67
1:F:254:HIS:O	1:F:258:THR:HG22	1.94	0.67
1:D:219:LEU:HD12	1:D:222:MET:HE3	1.77	0.66
1:B:129:ARG:HG3	1:B:129:ARG:NH1	2.09	0.66
1:F:310:LEU:HD23	1:F:453:PHE:CE1	2.30	0.66
1:C:51:THR:HG21	1:C:219:LEU:CD1	2.26	0.66
1:F:132:ILE:O	1:F:136:ARG:HG2	1.96	0.66
1:C:156:LEU:HD13	1:C:177:THR:OG1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:MET:HE2	1:C:491:PHE:CE1	2.31	0.66
1:E:355:VAL:O	1:E:359:ILE:HG13	1.95	0.66
1:F:88:LYS:HZ2	1:F:92:VAL:HG21	1.59	0.65
1:C:461:ARG:HH22	1:C:492:LEU:HD12	1.60	0.65
1:D:201:LEU:HA	1:D:204:MET:HE3	1.78	0.65
1:F:188:GLY:O	1:F:189:ASP:HB2	1.95	0.65
1:F:64:ARG:HD3	1:F:65:TYR:CE1	2.31	0.65
1:C:352:THR:O	1:C:356:ILE:HG13	1.97	0.65
1:D:176:ARG:HG3	1:D:198:PHE:CE2	2.31	0.65
1:E:357:HIS:CE1	1:E:446:ARG:HH22	2.15	0.65
1:F:486:ASN:HD22	1:F:486:ASN:N	1.94	0.65
1:A:419:LYS:H	1:A:419:LYS:CD	1.96	0.65
1:D:311:ARG:HH21	1:D:311:ARG:HG3	1.62	0.65
1:D:32:LYS:HE2	1:D:32:LYS:N	2.09	0.65
1:C:315:LEU:HD13	1:C:487:TYR:HD2	1.62	0.64
1:B:402:PRO:C	1:B:404:PHE:H	2.05	0.64
1:D:466:GLN:HE21	1:D:471:ILE:HG12	1.62	0.64
1:E:123:ARG:HA	1:E:285:GLU:HG3	1.80	0.64
1:B:51:THR:HG22	1:B:215:SER:HB2	1.80	0.64
1:F:328:HIS:O	1:F:331:ILE:HB	1.96	0.64
1:D:364:ASP:OD2	1:D:367:PRO:HB3	1.98	0.64
1:E:419:LYS:HD3	1:E:419:LYS:N	2.11	0.64
1:C:148:ARG:HE	1:C:148:ARG:CA	2.11	0.64
1:D:161:ARG:HG2	1:D:161:ARG:HH11	1.62	0.64
1:E:49:LEU:HD13	1:E:54:MET:HE1	1.80	0.64
1:E:202:LEU:HD23	1:E:205:MET:CE	2.28	0.64
1:E:51:THR:HG23	1:E:215:SER:OG	1.98	0.64
1:C:461:ARG:HE	1:C:494:ARG:CB	2.11	0.63
1:A:420:LYS:HD2	1:A:420:LYS:N	2.12	0.63
1:B:419:LYS:H	1:B:419:LYS:CD	2.08	0.63
1:C:460:PHE:HD2	1:C:491:PHE:HB3	1.63	0.63
1:D:51:THR:CG2	1:D:215:SER:HB2	2.24	0.63
1:F:64:ARG:HH11	1:F:64:ARG:HG2	1.62	0.63
1:C:423:PHE:HE1	1:C:425:LYS:HG2	1.63	0.63
1:C:460:PHE:CD2	1:C:491:PHE:HB3	2.34	0.63
1:B:51:THR:CG2	1:B:215:SER:HB2	2.29	0.63
1:B:342:LYS:HG3	1:B:345:ASP:OD1	1.99	0.63
1:B:400:ARG:HG3	1:B:400:ARG:HH11	1.64	0.62
1:F:248:ILE:O	1:F:252:VAL:HG23	1.98	0.62
1:F:330:GLU:OE2	1:F:350:PRO:HD2	1.99	0.62
1:F:88:LYS:HZ1	1:F:92:VAL:HG11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:LYS:HD2	1:B:377:ASP:O	2.00	0.62
1:D:269:ASP:O	1:D:273:ILE:HG13	2.00	0.62
1:D:373:ARG:NH1	1:D:388:GLY:O	2.33	0.62
1:F:59:MET:HE1	1:F:82:CYS:SG	2.39	0.62
1:E:419:LYS:H	1:E:419:LYS:HZ2	1.46	0.62
1:F:458:GLN:O	1:F:494:ARG:HD3	1.98	0.62
1:C:156:LEU:HD22	1:C:177:THR:HG21	1.82	0.62
1:B:201:LEU:HD11	1:B:247:PHE:CZ	2.35	0.61
1:C:167:ASN:ND2	1:C:465:PRO:HB3	2.15	0.61
1:F:330:GLU:CD	1:F:350:PRO:HD2	2.26	0.61
1:C:305:THR:HG22	1:C:365:MET:HE1	1.82	0.61
1:B:208:SER:N	1:B:240:GLU:OE2	2.33	0.61
1:D:442:GLU:O	1:D:446:ARG:HG3	2.00	0.61
1:B:138:PHE:CZ	1:B:185:ILE:HA	2.35	0.61
1:F:157:ILE:HD11	1:F:455:THR:HG22	1.82	0.61
1:C:489:MET:HE2	1:C:491:PHE:CZ	2.36	0.61
1:F:327:VAL:O	1:F:331:ILE:HG13	2.01	0.61
1:D:319:LYS:O	1:D:321:PRO:HD3	2.00	0.61
1:A:51:THR:CG2	1:A:215:SER:OG	2.49	0.61
1:A:420:LYS:H	1:A:420:LYS:CD	2.12	0.61
1:D:51:THR:HG23	1:D:215:SER:CB	2.25	0.61
1:B:174:LEU:HD12	1:B:311:ARG:HG2	1.83	0.60
1:C:196:LYS:HE3	1:C:196:LYS:HA	1.83	0.60
1:F:265:ARG:HD3	1:F:269:ASP:OD1	2.01	0.60
1:B:53:GLN:HE22	1:B:478:VAL:CG1	2.14	0.60
1:F:51:THR:HG23	1:F:215:SER:HB2	1.82	0.60
1:F:136:ARG:HG3	1:F:136:ARG:HH11	1.65	0.60
1:F:270:SER:O	1:F:273:ILE:HB	2.01	0.60
1:B:450:PHE:O	1:B:454:THR:HG22	2.02	0.60
1:C:342:LYS:HD3	4:C:1031:HOH:O	2.01	0.60
1:B:53:GLN:NE2	1:B:478:VAL:CB	2.64	0.59
1:C:342:LYS:HG3	1:C:345:ASP:OD1	2.02	0.59
1:D:310:LEU:HD23	1:D:453:PHE:CE1	2.37	0.59
1:D:291:LEU:C	1:D:291:LEU:HD23	2.28	0.59
1:E:346:ARG:HB3	1:E:450:PHE:CE1	2.38	0.59
1:F:130:PHE:O	1:F:134:THR:CG2	2.51	0.59
1:F:130:PHE:CE1	1:F:134:THR:HG21	2.38	0.59
1:B:210:GLN:O	1:B:214:THR:HG23	2.02	0.59
1:B:89:GLU:HA	1:B:93:ASP:OD2	2.03	0.59
1:D:296:LEU:HD12	1:D:296:LEU:O	2.03	0.59
1:D:327:VAL:HG11	1:D:457:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:373:ARG:HH21	1:F:373:ARG:HB2	1.67	0.59
1:C:487:TYR:C	1:C:487:TYR:HD1	2.10	0.58
1:E:101:ARG:O	1:E:373:ARG:HD2	2.03	0.58
1:F:176:ARG:HD3	1:F:193:TYR:HA	1.85	0.58
1:C:425:LYS:HD3	1:C:426:SER:H	1.68	0.58
1:C:487:TYR:C	1:C:487:TYR:CD1	2.81	0.58
1:D:51:THR:O	1:D:215:SER:HA	2.03	0.58
1:D:332:ASP:OD2	1:D:494:ARG:NH2	2.37	0.58
1:D:341:PRO:HG2	1:D:454:THR:HG22	1.85	0.58
1:C:323:VAL:O	1:C:327:VAL:HG23	2.03	0.58
1:F:329:GLU:C	1:F:331:ILE:H	2.11	0.58
1:B:374:VAL:HG23	1:B:374:VAL:O	2.03	0.58
1:F:147:GLU:HA	1:F:150:GLN:OE1	2.04	0.58
1:D:219:LEU:HD12	1:D:222:MET:CE	2.34	0.57
1:F:433:SER:HB3	2:F:500:HEM:HBA1	1.86	0.57
1:D:161:ARG:C	1:D:163:THR:H	2.12	0.57
1:E:51:THR:CG2	1:E:215:SER:OG	2.52	0.57
1:F:250:LYS:O	1:F:253:GLU:HG3	2.03	0.57
1:C:85:ASP:O	1:C:89:GLU:HG3	2.03	0.57
1:A:219:LEU:HA	1:A:222:MET:HE2	1.87	0.57
1:C:155:PHE:HD2	1:C:190:ARG:NH2	2.01	0.57
1:C:172:PHE:O	1:C:176:ARG:HG3	2.05	0.57
1:F:382:ASP:OD2	1:F:382:ASP:N	2.36	0.57
1:A:311:ARG:HG3	4:A:648:HOH:O	2.04	0.57
1:C:462:PHE:CD2	1:C:489:MET:HE1	2.39	0.57
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.69	0.57
1:B:51:THR:HG23	1:B:215:SER:O	2.04	0.57
1:C:51:THR:HG21	1:C:219:LEU:HD12	1.87	0.57
1:E:59:MET:O	1:E:62:SER:HB3	2.04	0.57
1:E:156:LEU:CD2	1:E:456:ILE:HD11	2.33	0.57
1:F:91:LEU:O	1:F:95:ALA:HA	2.05	0.57
1:A:341:PRO:HG2	1:A:454:THR:HG23	1.86	0.57
1:B:319:LYS:NZ	1:B:471:ILE:O	2.37	0.57
1:C:89:GLU:O	1:C:93:ASP:HB2	2.05	0.57
1:C:174:LEU:HD22	1:C:310:LEU:HD13	1.87	0.57
1:E:172:PHE:HA	1:E:175:SER:OG	2.04	0.57
1:F:161:ARG:HG2	1:F:161:ARG:HH11	1.69	0.57
1:C:134:THR:O	1:C:138:PHE:HD1	1.88	0.57
1:A:219:LEU:HD12	1:A:222:MET:CE	2.35	0.56
1:F:418:ASP:CA	1:F:424:LYS:HD2	2.34	0.56
1:C:259:LEU:O	1:C:261:PRO:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:PHE:HB3	1:E:291:LEU:HD13	1.87	0.56
1:F:135:LEU:O	1:F:140:VAL:HB	2.05	0.56
1:F:405:PHE:O	1:F:408:PRO:HD3	2.05	0.56
1:A:409:ARG:HH21	1:A:409:ARG:HG3	1.69	0.56
1:D:32:LYS:CE	1:D:32:LYS:N	2.59	0.56
1:D:148:ARG:HH21	1:D:148:ARG:HG3	1.70	0.56
1:D:341:PRO:HB3	1:D:454:THR:HG21	1.86	0.56
1:E:92:VAL:CG2	1:E:434:ILE:HD12	2.35	0.56
1:E:112:LYS:HE3	4:E:758:HOH:O	2.03	0.56
1:F:418:ASP:C	1:F:420:LYS:H	2.12	0.56
1:B:418:ASP:C	1:B:420:LYS:H	2.12	0.56
1:F:251:LYS:HB3	1:F:251:LYS:NZ	2.19	0.56
1:B:400:ARG:HG3	1:B:400:ARG:NH1	2.20	0.56
1:C:333:ARG:HG2	1:C:333:ARG:HH21	1.69	0.56
1:F:88:LYS:NZ	1:F:92:VAL:HG21	2.21	0.56
1:A:338:ASN:CG	1:A:339:ARG:H	2.14	0.56
1:F:156:LEU:C	1:F:156:LEU:HD23	2.31	0.56
1:E:31:GLY:C	1:E:32:LYS:HD2	2.31	0.56
1:D:375:ASN:HB3	4:D:613:HOH:O	2.05	0.56
1:F:105:ALA:HB3	1:F:221:GLU:OE2	2.05	0.56
1:F:130:PHE:HE2	1:F:274:ARG:HG3	1.67	0.56
1:B:167:ASN:OD1	1:B:488:THR:HB	2.06	0.56
1:E:261:PRO:HA	1:E:273:ILE:CD1	2.36	0.56
1:C:358:GLU:OE1	1:C:358:GLU:HA	2.05	0.55
1:C:419:LYS:C	1:C:421:GLY:H	2.13	0.55
1:A:253:GLU:HA	1:A:256:GLN:OE1	2.07	0.55
1:E:209:PHE:HE1	3:E:511[B]:IND:H3	1.72	0.55
1:E:403:ARG:HG3	1:E:404:PHE:CD2	2.41	0.55
1:F:335:ILE:HG23	1:F:339:ARG:NH2	2.22	0.55
1:B:319:LYS:HE3	1:B:468:PRO:O	2.06	0.55
1:C:168:ILE:HD12	1:C:173:PHE:HE2	1.69	0.55
1:C:461:ARG:HH22	1:C:492:LEU:HD13	1.71	0.55
1:F:149:ILE:HG21	1:F:451:LEU:HD12	1.88	0.55
1:F:172:PHE:O	1:F:176:ARG:HB2	2.06	0.55
1:C:219:LEU:HA	1:C:222:MET:HE3	1.87	0.55
1:E:419:LYS:O	1:E:420:LYS:HB2	2.06	0.55
1:F:325:ALA:O	1:F:328:HIS:HB2	2.06	0.55
1:F:128:ARG:O	1:F:132:ILE:HG13	2.06	0.55
1:B:59:MET:HE3	1:B:394:MET:HE3	1.89	0.55
1:B:418:ASP:C	1:B:420:LYS:N	2.63	0.55
1:D:327:VAL:HG11	1:D:457:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PHE:CG	1:B:291:LEU:HD23	2.42	0.55
1:C:37:PRO:HG2	1:C:45:ASN:ND2	2.22	0.55
1:E:343:PHE:CE1	1:E:447:MET:HA	2.42	0.55
1:E:365:MET:O	1:E:481:ALA:HA	2.07	0.55
1:F:372:HIS:HD2	1:F:393:PRO:HG2	1.72	0.55
1:A:62:SER:C	1:A:64:ARG:H	2.14	0.54
1:A:89:GLU:O	1:A:93:ASP:HB2	2.07	0.54
1:B:412:ASN:OD1	1:B:414:GLN:HB2	2.07	0.54
1:F:318:MET:SD	1:F:464:SER:HB2	2.47	0.54
1:D:148:ARG:HG3	1:D:148:ARG:NH2	2.21	0.54
1:B:288:LEU:HD13	1:B:292:VAL:HG23	1.90	0.54
1:A:328:HIS:HB3	1:A:494:ARG:NH2	2.22	0.54
1:B:349:MET:HB3	1:B:352:THR:CG2	2.37	0.54
1:C:49:LEU:HD13	1:C:54:MET:HE1	1.89	0.54
1:F:156:LEU:HD12	1:F:177:THR:CB	2.36	0.54
1:F:329:GLU:C	1:F:331:ILE:N	2.65	0.54
1:B:153:ALA:O	1:B:157:ILE:HG12	2.08	0.54
1:E:79:VAL:HG21	1:E:385:LEU:HD22	1.89	0.54
1:E:419:LYS:HB2	1:E:419:LYS:NZ	2.23	0.54
1:F:375:ASN:O	1:F:376:LYS:HG3	2.07	0.54
1:B:349:MET:HB3	1:B:352:THR:HG22	1.90	0.54
1:C:315:LEU:HB2	1:C:487:TYR:CE2	2.38	0.54
1:D:219:LEU:HA	1:D:222:MET:CE	2.37	0.54
1:D:469:LYS:CA	1:D:469:LYS:HE2	2.38	0.54
1:D:469:LYS:HE2	1:D:469:LYS:N	2.23	0.54
1:C:135:LEU:O	1:C:140:VAL:HG23	2.08	0.53
1:D:135:LEU:HD22	1:D:140:VAL:HG21	1.90	0.53
1:D:466:GLN:NE2	1:D:471:ILE:HG12	2.23	0.53
1:B:405:PHE:O	1:B:408:PRO:HD3	2.08	0.53
1:C:461:ARG:N	1:C:492:LEU:O	2.37	0.53
1:C:461:ARG:NH2	1:C:492:LEU:HD12	2.22	0.53
1:F:156:LEU:HD23	1:F:156:LEU:O	2.08	0.53
1:F:331:ILE:HA	1:F:349:MET:HE3	1.90	0.53
1:B:325:ALA:O	1:B:329:GLU:HG3	2.08	0.53
1:F:123:ARG:HA	1:F:285:GLU:HG3	1.91	0.53
1:F:344:GLU:C	1:F:346:ARG:N	2.64	0.53
1:A:95:ALA:HB1	1:A:436:LYS:HG3	1.91	0.53
1:B:234:GLN:HG2	1:B:235:GLN:N	2.23	0.53
1:A:186:VAL:HA	1:A:267:PHE:HB3	1.91	0.53
1:B:467:SER:C	1:B:469:LYS:H	2.17	0.53
1:D:160:LEU:HD22	1:D:491:PHE:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:THR:HG22	1:F:365:MET:HE1	1.91	0.53
1:F:414:GLN:NE2	1:F:417:LEU:HB2	2.23	0.53
1:D:420:LYS:HD3	1:D:420:LYS:N	2.24	0.52
1:E:322:GLU:O	1:E:326:LYS:HG3	2.10	0.52
1:F:97:GLU:O	1:F:374:VAL:HA	2.09	0.52
1:E:271:PHE:CB	1:E:291:LEU:HD13	2.40	0.52
1:E:419:LYS:HB2	1:E:419:LYS:HZ3	1.74	0.52
1:F:418:ASP:HA	1:F:424:LYS:HD2	1.90	0.52
1:D:418:ASP:OD2	1:D:418:ASP:C	2.52	0.52
1:F:378:THR:HG22	1:F:379:LYS:N	2.24	0.52
1:D:89:GLU:OE2	1:D:381:ARG:NH1	2.42	0.52
1:E:457:MET:HG2	1:E:462:PHE:CZ	2.45	0.52
1:C:350:PRO:HG2	1:C:351:TYR:H	1.75	0.52
1:D:420:LYS:HD3	1:D:420:LYS:H	1.74	0.52
1:A:271:PHE:CG	1:A:291:LEU:HD13	2.44	0.52
1:B:476:LYS:HB2	1:B:485:ARG:HA	1.92	0.52
1:C:53:GLN:NE2	1:C:478:VAL:HB	2.25	0.52
1:F:95:ALA:O	1:F:99:SER:HB3	2.10	0.52
1:F:335:ILE:HG22	1:F:335:ILE:O	2.10	0.52
1:B:376:LYS:O	1:B:377:ASP:C	2.52	0.52
1:E:319:LYS:HB2	1:E:471:ILE:HG21	1.90	0.52
1:E:454:THR:HG23	1:E:455:THR:H	1.75	0.52
1:F:342:LYS:HE2	1:F:344:GLU:CG	2.40	0.52
1:C:148:ARG:HE	1:C:148:ARG:HA	1.73	0.52
1:D:161:ARG:HG2	1:D:161:ARG:NH1	2.24	0.52
1:F:335:ILE:HD11	1:F:345:ASP:CB	2.40	0.52
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.91	0.51
1:E:344:GLU:HA	1:E:344:GLU:OE1	2.10	0.51
1:A:276:GLN:O	1:A:279:GLU:HG3	2.11	0.51
1:C:461:ARG:NH2	1:C:492:LEU:CD1	2.72	0.51
1:E:458:GLN:C	1:E:459:ASN:HD22	2.18	0.51
1:B:288:LEU:HD13	1:B:288:LEU:C	2.34	0.51
1:E:205:MET:CE	1:E:303:THR:HG21	2.39	0.51
1:F:442:GLU:HG2	1:F:446:ARG:HD2	1.91	0.51
1:E:84:HIS:O	1:E:88:LYS:HB2	2.10	0.51
1:E:249:ALA:O	1:E:253:GLU:HG3	2.11	0.51
1:B:178:VAL:HG11	1:B:306:VAL:HB	1.93	0.51
1:C:466:GLN:HG2	1:C:467:SER:N	2.26	0.51
1:B:53:GLN:NE2	1:B:478:VAL:CG1	2.73	0.51
1:D:128:ARG:O	1:D:132:ILE:HG13	2.11	0.51
2:A:500:HEM:C4D	3:A:507[B]:IND:H5	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:GLN:O	1:C:279:GLU:HG3	2.11	0.51
1:C:462:PHE:CE2	1:C:489:MET:HE1	2.45	0.51
1:B:138:PHE:CD2	1:B:138:PHE:O	2.64	0.51
1:E:88:LYS:HD3	1:E:92:VAL:HB	1.93	0.51
1:B:320:HIS:O	1:B:323:VAL:HB	2.11	0.51
1:B:439:CYS:HB2	2:B:500:HEM:NA	2.25	0.51
1:F:486:ASN:N	1:F:486:ASN:ND2	2.58	0.51
1:A:197:GLU:O	1:A:200:SER:HB3	2.11	0.51
1:B:271:PHE:CD2	1:B:291:LEU:HB2	2.46	0.51
1:B:322:GLU:O	1:B:326:LYS:HG3	2.11	0.51
1:C:91:LEU:HB3	1:C:434:ILE:HG13	1.93	0.51
1:D:32:LYS:HE2	1:D:32:LYS:O	2.11	0.51
1:A:64:ARG:HG3	1:A:65:TYR:CD2	2.46	0.50
1:B:136:ARG:C	1:B:138:PHE:H	2.19	0.50
1:D:341:PRO:CG	1:D:454:THR:HG22	2.41	0.50
1:F:182:ILE:O	1:F:186:VAL:HG13	2.11	0.50
1:B:199:LEU:HD21	1:B:203:ARG:NH1	2.26	0.50
1:F:158:ASP:HA	1:F:161:ARG:HD2	1.93	0.50
1:F:363:GLY:O	1:F:364:ASP:C	2.55	0.50
1:B:209:PHE:CD1	3:B:508[B]:IND:H2	2.46	0.50
1:C:333:ARG:HG2	1:C:333:ARG:O	2.11	0.50
1:E:323:VAL:HG13	1:E:351:TYR:OH	2.12	0.50
1:D:335:ILE:HG23	1:D:339:ARG:NH1	2.26	0.50
1:C:170:PRO:CG	1:C:487:TYR:HE1	2.25	0.50
1:D:463:LYS:HB3	1:D:490:SER:OG	2.11	0.50
1:B:402:PRO:C	1:B:404:PHE:N	2.69	0.50
1:D:351:TYR:O	1:D:355:VAL:HG23	2.12	0.50
1:E:476:LYS:HB2	1:E:485:ARG:HA	1.93	0.50
1:F:84:HIS:C	1:F:84:HIS:ND1	2.69	0.50
1:A:202:LEU:HD23	1:A:205:MET:HE3	1.94	0.50
1:F:247:PHE:O	1:F:251:LYS:HG2	2.12	0.50
1:A:323:VAL:O	1:A:327:VAL:HG23	2.11	0.49
1:B:275:MET:HG2	1:B:286:PHE:O	2.12	0.49
1:C:440:PHE:HD1	1:C:440:PHE:O	1.95	0.49
1:E:199:LEU:HD21	1:E:203:ARG:HH11	1.76	0.49
1:E:316:LEU:HD13	1:E:411:PHE:CD2	2.47	0.49
1:E:319:LYS:HD2	1:E:468:PRO:O	2.12	0.49
1:F:274:ARG:HB3	1:F:274:ARG:NH2	2.14	0.49
1:F:438:TYR:C	1:F:438:TYR:CD2	2.90	0.49
1:D:197:GLU:O	1:D:200:SER:HB3	2.13	0.49
1:D:439:CYS:HB2	2:D:500:HEM:NA	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:LYS:HB2	4:E:773:HOH:O	2.12	0.49
1:F:335:ILE:O	1:F:336:GLY:C	2.55	0.49
1:C:252:VAL:O	1:C:256:GLN:HG3	2.11	0.49
1:C:341:PRO:HG2	1:C:454:THR:HG23	1.94	0.49
1:D:382:ASP:OD2	1:D:382:ASP:N	2.39	0.49
1:F:418:ASP:N	1:F:424:LYS:HD2	2.26	0.49
1:A:84:HIS:O	1:A:88:LYS:HB2	2.12	0.49
1:D:143:ARG:CZ	1:D:147:GLU:HG2	2.43	0.49
1:F:289:LYS:HE2	4:F:1225:HOH:O	2.13	0.49
1:F:380:PHE:O	1:F:381:ARG:C	2.55	0.49
1:A:412:ASN:OD1	1:A:414:GLN:HB2	2.12	0.49
1:E:339:ARG:NH1	1:E:342:LYS:NZ	2.61	0.49
1:B:161:ARG:C	1:B:163:THR:H	2.20	0.49
1:C:170:PRO:O	1:C:171:THR:C	2.56	0.49
1:D:143:ARG:NH1	1:D:147:GLU:HG2	2.27	0.49
1:F:146:GLU:OE2	1:F:342:LYS:HB2	2.12	0.49
1:D:365:MET:O	1:D:481:ALA:HA	2.13	0.49
1:F:101:ARG:N	1:F:120:ASN:OD1	2.37	0.49
1:F:332:ASP:O	1:F:336:GLY:HA2	2.12	0.49
1:F:372:HIS:HE1	1:F:437:ARG:HB2	1.76	0.49
1:B:257:ARG:NH2	1:C:403:ARG:HB3	2.28	0.49
1:B:271:PHE:CE2	1:B:291:LEU:HB2	2.48	0.49
1:B:319:LYS:HG2	1:B:471:ILE:HD12	1.95	0.49
1:F:268:ILE:O	1:F:272:LEU:HB2	2.13	0.49
1:C:336:GLY:O	1:C:338:ASN:N	2.45	0.48
1:D:469:LYS:HE2	1:D:469:LYS:HA	1.94	0.48
1:E:339:ARG:HH22	1:E:342:LYS:HG2	1.78	0.48
1:F:128:ARG:HG2	1:F:132:ILE:HD11	1.95	0.48
1:F:464:SER:C	1:F:466:GLN:H	2.21	0.48
1:C:432:PHE:CD2	1:C:442:GLU:HG3	2.48	0.48
1:F:331:ILE:HG22	1:F:332:ASP:N	2.28	0.48
1:F:419:LYS:C	1:F:420:LYS:HD2	2.37	0.48
1:A:57:SER:HA	1:A:60:LYS:CE	2.29	0.48
1:E:163:THR:HG21	1:E:168:ILE:HD13	1.93	0.48
1:F:251:LYS:HB3	1:F:251:LYS:HZ2	1.77	0.48
1:B:319:LYS:HE3	1:B:469:LYS:HA	1.96	0.48
1:E:271:PHE:CG	1:E:291:LEU:HD13	2.48	0.48
1:F:89:GLU:O	1:F:93:ASP:HB2	2.13	0.48
1:F:201:LEU:CA	1:F:204:MET:HE3	2.42	0.48
1:A:33:LEU:N	1:A:33:LEU:HD22	2.28	0.48
1:A:260:ASP:HB3	4:A:1238:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:SER:C	1:B:466:GLN:H	2.20	0.48
1:D:449:LEU:O	1:D:453:PHE:HD1	1.96	0.48
1:A:37:PRO:HD3	1:A:65:TYR:CE2	2.48	0.48
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.95	0.48
1:C:461:ARG:HG2	1:C:461:ARG:HH11	1.79	0.48
1:D:145:ILE:O	1:D:149:ILE:HG13	2.14	0.48
1:E:244:LEU:O	1:E:248:ILE:HG12	2.14	0.48
1:E:465:PRO:HG3	1:E:488:THR:OG1	2.14	0.48
1:F:116:VAL:CG1	1:F:294:THR:HG23	2.44	0.48
1:F:158:ASP:O	1:F:161:ARG:HB2	2.14	0.48
1:A:343:PHE:O	1:A:346:ARG:HG2	2.13	0.48
1:B:201:LEU:HD21	1:B:247:PHE:CG	2.48	0.48
1:D:234:GLN:HG2	1:D:235:GLN:N	2.29	0.48
1:E:454:THR:HG23	1:E:455:THR:N	2.29	0.48
1:F:330:GLU:HA	1:F:333:ARG:HH21	1.79	0.48
1:C:271:PHE:CD2	1:C:291:LEU:HG	2.49	0.48
1:D:280:LYS:H	1:D:280:LYS:CE	1.99	0.48
1:F:183:SER:O	1:F:187:PHE:HB2	2.13	0.48
1:B:403:ARG:HH21	1:B:403:ARG:HG3	1.79	0.48
1:C:327:VAL:O	1:C:331:ILE:HG13	2.14	0.48
1:E:320:HIS:HB3	1:E:323:VAL:HG23	1.94	0.48
1:D:32:LYS:H	1:D:32:LYS:CD	2.26	0.47
1:D:161:ARG:C	1:D:163:THR:N	2.71	0.47
1:D:302:GLY:CA	2:D:500:HEM:HBC2	2.43	0.47
1:B:316:LEU:HD12	1:B:411:PHE:CG	2.49	0.47
1:C:322:GLU:O	1:C:326:LYS:HG3	2.15	0.47
1:E:199:LEU:O	1:E:203:ARG:HB2	2.14	0.47
1:F:160:LEU:HB2	1:F:460:PHE:CE1	2.49	0.47
1:A:135:LEU:HB3	1:A:140:VAL:HG21	1.97	0.47
1:A:305:THR:CB	1:A:365:MET:HE1	2.43	0.47
1:C:51:THR:O	1:C:215:SER:HA	2.13	0.47
1:E:316:LEU:HD13	1:E:411:PHE:CE2	2.48	0.47
1:E:419:LYS:HD3	1:E:419:LYS:H	1.76	0.47
1:F:88:LYS:NZ	1:F:92:VAL:HG11	2.29	0.47
1:C:174:LEU:O	1:C:178:VAL:HG23	2.15	0.47
1:E:305:THR:CG2	1:E:365:MET:HE1	2.44	0.47
1:F:161:ARG:HG2	1:F:161:ARG:NH1	2.29	0.47
1:F:478:VAL:HG22	1:F:482:THR:HG23	1.97	0.47
1:B:190:ARG:NH2	1:B:193:TYR:CE1	2.82	0.47
1:E:156:LEU:HD22	1:E:177:THR:HG21	1.96	0.47
1:A:257:ARG:HG3	1:A:258:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:PHE:HD1	1:C:155:PHE:H	1.62	0.47
1:C:272:LEU:O	1:C:275:MET:HB2	2.14	0.47
1:C:433:SER:CB	2:C:500:HEM:HBA1	2.45	0.47
1:E:311:ARG:HH21	1:E:311:ARG:HG3	1.80	0.47
1:C:91:LEU:HA	1:C:91:LEU:HD12	1.72	0.47
1:C:364:ASP:OD2	1:C:367:PRO:HB3	2.15	0.47
1:E:316:LEU:HD21	1:E:362:PHE:CE2	2.49	0.47
1:F:274:ARG:HH21	1:F:274:ARG:CB	2.18	0.47
1:F:393:PRO:O	1:F:395:LEU:N	2.46	0.47
1:F:417:LEU:N	1:F:424:LYS:HG2	2.30	0.47
1:F:420:LYS:N	1:F:420:LYS:CD	2.70	0.47
1:B:272:LEU:O	1:B:275:MET:HB2	2.15	0.47
1:F:288:LEU:O	1:F:291:LEU:HB3	2.15	0.47
1:F:287:TYR:CE1	1:F:290:ASN:ND2	2.83	0.47
1:F:356:ILE:CD1	1:F:450:PHE:HA	2.45	0.47
1:B:51:THR:O	1:B:215:SER:HA	2.15	0.47
1:B:376:LYS:HD2	1:B:376:LYS:C	2.40	0.47
1:C:155:PHE:CD1	1:C:155:PHE:N	2.83	0.47
1:F:469:LYS:HE3	1:F:470:ASP:OD1	2.15	0.47
1:A:355:VAL:O	1:A:359:ILE:HG13	2.14	0.46
1:C:206:LEU:HD12	4:C:1165:HOH:O	2.13	0.46
1:C:333:ARG:HG2	1:C:333:ARG:NH2	2.29	0.46
1:E:171:THR:OG1	1:E:311:ARG:HD3	2.15	0.46
1:E:460:PHE:CD2	1:E:491:PHE:HB3	2.50	0.46
1:F:136:ARG:HG3	1:F:136:ARG:NH1	2.30	0.46
1:F:176:ARG:HG3	1:F:198:PHE:CE2	2.50	0.46
1:D:330:GLU:OE2	1:D:349:MET:HB3	2.15	0.46
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.97	0.46
1:E:329:GLU:OE2	1:E:330:GLU:N	2.47	0.46
1:C:165:GLY:HA2	1:C:491:PHE:O	2.16	0.46
1:C:464:SER:C	1:C:466:GLN:H	2.23	0.46
1:D:172:PHE:HA	1:D:175:SER:OG	2.14	0.46
1:E:139:GLY:O	1:E:145:ILE:HB	2.15	0.46
1:D:346:ARG:HG2	1:D:346:ARG:HH21	1.80	0.46
1:A:34:PRO:HA	1:A:383:PHE:CE2	2.51	0.46
1:E:261:PRO:HA	1:E:273:ILE:HD11	1.97	0.46
1:E:326:LYS:HB2	1:E:351:TYR:CE2	2.49	0.46
1:E:469:LYS:HG3	1:E:470:ASP:N	2.30	0.46
1:F:88:LYS:HD3	1:F:92:VAL:HB	1.96	0.46
1:B:161:ARG:C	1:B:163:THR:N	2.74	0.46
1:C:278:GLU:O	1:C:281:ASN:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:HD21	1:C:456:ILE:HD11	1.98	0.46
1:C:170:PRO:HG3	1:C:487:TYR:HE1	1.81	0.46
1:D:189:ASP:OD2	1:D:190:ARG:N	2.49	0.46
1:C:332:ASP:OD1	1:C:337:LYS:HE3	2.15	0.46
1:F:258:THR:HG23	1:F:265:ARG:HH22	1.80	0.46
1:C:281:ASN:O	1:C:284:THR:HG22	2.16	0.46
1:B:278:GLU:C	1:B:280:LYS:H	2.24	0.46
1:B:138:PHE:CE2	1:B:185:ILE:HA	2.51	0.45
1:B:320:HIS:N	1:B:321:PRO:HD3	2.31	0.45
1:B:327:VAL:HG11	1:B:457:MET:HE1	1.98	0.45
1:E:432:PHE:CD2	1:E:442:GLU:HG3	2.50	0.45
1:B:281:ASN:ND2	1:B:284:THR:N	2.64	0.45
1:C:468:PRO:HA	1:C:471:ILE:CD1	2.46	0.45
1:E:209:PHE:CE1	3:E:511[B]:IND:H3	2.51	0.45
1:E:343:PHE:O	1:E:346:ARG:HG2	2.16	0.45
1:B:138:PHE:HE1	1:B:266:ASP:HA	1.80	0.45
1:D:153:ALA:O	1:D:157:ILE:HG12	2.16	0.45
1:F:418:ASP:C	1:F:420:LYS:N	2.72	0.45
2:F:500:HEM:NA	3:F:512[B]:IND:H5	2.32	0.45
1:B:327:VAL:HG11	1:B:457:MET:CE	2.45	0.45
1:C:135:LEU:HG	1:C:140:VAL:HG21	1.96	0.45
1:C:161:ARG:C	1:C:163:THR:H	2.24	0.45
1:C:339:ARG:O	1:C:339:ARG:HG3	2.16	0.45
1:F:405:PHE:HD1	1:F:415:HIS:HB3	1.82	0.45
1:B:368:MET:C	1:B:369:GLY:O	2.59	0.45
1:C:337:LYS:H	1:C:337:LYS:HD2	1.82	0.45
1:D:32:LYS:N	1:D:32:LYS:CD	2.79	0.45
1:D:257:ARG:NE	1:D:257:ARG:HA	2.32	0.45
1:E:305:THR:HG22	1:E:365:MET:CE	2.47	0.45
1:F:271:PHE:CD2	1:F:291:LEU:HD13	2.51	0.45
1:F:412:ASN:OD1	1:F:414:GLN:HB2	2.16	0.45
1:F:433:SER:CB	2:F:500:HEM:HBA1	2.46	0.45
1:A:330:GLU:OE2	1:A:349:MET:HB3	2.17	0.45
1:B:97:GLU:O	1:B:374:VAL:HA	2.17	0.45
1:C:174:LEU:HD12	1:C:311:ARG:HG2	1.99	0.45
1:E:419:LYS:O	1:E:420:LYS:CB	2.65	0.45
1:E:459:ASN:HD22	1:E:459:ASN:N	2.12	0.45
1:F:176:ARG:CG	1:F:198:PHE:HE2	2.30	0.45
1:C:155:PHE:HD1	1:C:155:PHE:N	2.14	0.45
1:E:305:THR:HG22	1:E:365:MET:HE1	1.98	0.45
1:F:318:MET:HE1	1:F:489:MET:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:469:LYS:HG3	1:F:470:ASP:OD1	2.17	0.45
1:B:79:VAL:HG21	1:B:385:LEU:HD22	1.99	0.45
1:F:156:LEU:O	1:F:159:ALA:HB3	2.17	0.45
1:F:271:PHE:HB3	1:F:291:LEU:HD13	1.99	0.45
1:C:182:ILE:O	1:C:186:VAL:HG22	2.17	0.45
1:C:369:GLY:HA2	1:C:395:LEU:HD12	1.98	0.45
1:E:103:GLU:HG2	1:E:390:GLU:CD	2.42	0.45
1:F:315:LEU:HB2	1:F:487:TYR:CE2	2.52	0.45
1:F:342:LYS:N	1:F:345:ASP:OD2	2.44	0.45
1:F:373:ARG:HH22	1:F:390:GLU:HG2	1.80	0.45
1:B:92:VAL:CG2	1:B:434:ILE:HD12	2.46	0.45
1:B:315:LEU:O	1:B:316:LEU:C	2.60	0.45
1:F:61:ILE:HG22	1:F:61:ILE:O	2.17	0.45
1:F:166:ALA:O	1:F:168:ILE:HG23	2.17	0.45
1:F:276:GLN:C	1:F:278:GLU:H	2.25	0.45
1:C:264:PRO:HB3	1:C:273:ILE:HD12	1.99	0.44
1:D:318:MET:SD	1:D:464:SER:HB2	2.56	0.44
1:D:376:LYS:HB3	1:D:376:LYS:HZ2	1.81	0.44
1:F:92:VAL:HG23	1:F:434:ILE:HD12	1.98	0.44
1:A:219:LEU:HD12	1:A:222:MET:HE3	1.98	0.44
1:B:319:LYS:C	1:B:321:PRO:HD3	2.41	0.44
1:B:335:ILE:HG23	1:B:339:ARG:NH1	2.33	0.44
1:C:316:LEU:HD13	1:C:411:PHE:CE1	2.52	0.44
1:D:339:ARG:HG2	1:D:339:ARG:HH11	1.82	0.44
1:E:339:ARG:HH12	1:E:342:LYS:NZ	2.16	0.44
1:F:78:VAL:HG11	1:F:392:PHE:CD2	2.52	0.44
1:F:258:THR:CG2	1:F:265:ARG:HH22	2.29	0.44
1:B:40:LEU:HD12	1:B:43:ILE:HD11	1.99	0.44
1:C:271:PHE:HD2	1:C:275:MET:HG3	1.82	0.44
1:C:420:LYS:O	1:C:422:GLN:HG2	2.17	0.44
1:E:180:ASN:OD1	1:E:191:PHE:HB2	2.17	0.44
1:E:351:TYR:O	1:E:355:VAL:HG23	2.17	0.44
1:F:101:ARG:HG2	1:F:118:PHE:HA	1.99	0.44
1:B:412:ASN:OD1	1:B:414:GLN:CB	2.66	0.44
1:C:139:GLY:C	1:C:145:ILE:HB	2.43	0.44
1:C:271:PHE:CG	1:C:291:LEU:HG	2.51	0.44
1:E:403:ARG:HG3	1:E:404:PHE:CE2	2.52	0.44
1:F:176:ARG:HG2	1:F:198:PHE:HE2	1.82	0.44
1:F:463:LYS:HB3	1:F:490:SER:HB2	1.98	0.44
1:C:101:ARG:HG2	1:C:118:PHE:HA	1.99	0.44
1:D:156:LEU:CD2	1:D:456:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:GLN:OE1	1:D:236:GLN:HA	2.18	0.44
1:D:300:PHE:C	1:D:300:PHE:CD2	2.96	0.44
1:F:51:THR:O	1:F:215:SER:HA	2.18	0.44
1:F:145:ILE:HD11	1:F:181:VAL:HG13	1.98	0.44
1:F:458:GLN:HA	1:F:494:ARG:HH11	1.82	0.44
1:D:61:ILE:HG13	4:D:734:HOH:O	2.18	0.44
1:A:363:GLY:O	1:A:364:ASP:C	2.60	0.44
1:F:170:PRO:HG3	1:F:487:TYR:CE1	2.52	0.44
1:B:115:GLY:O	1:B:119:SER:HB3	2.17	0.44
1:B:459:ASN:O	1:B:493:PRO:HA	2.18	0.44
1:C:343:PHE:O	1:C:346:ARG:HG2	2.18	0.44
1:F:168:ILE:HA	4:F:1119:HOH:O	2.18	0.44
1:F:404:PHE:CD1	1:F:404:PHE:N	2.86	0.44
1:A:271:PHE:CE2	1:A:291:LEU:HB2	2.53	0.43
1:D:167:ASN:HD21	1:D:465:PRO:HD3	1.82	0.43
1:E:259:LEU:HD12	1:E:260:ASP:N	2.33	0.43
1:E:315:LEU:HD13	1:E:487:TYR:CD2	2.53	0.43
1:E:318:MET:SD	1:E:464:SER:HB2	2.58	0.43
1:A:62:SER:O	1:A:64:ARG:N	2.51	0.43
1:A:326:LYS:HB2	1:A:351:TYR:CE2	2.54	0.43
1:F:84:HIS:ND1	1:F:85:ASP:N	2.67	0.43
1:F:469:LYS:HG3	1:F:470:ASP:N	2.31	0.43
1:A:62:SER:C	1:A:64:ARG:N	2.77	0.43
1:B:349:MET:HE2	1:B:352:THR:HG21	1.99	0.43
2:B:500:HEM:CHA	3:B:508[B]:IND:H5	2.47	0.43
1:D:300:PHE:C	1:D:300:PHE:HD2	2.26	0.43
1:C:150:GLN:NE2	1:C:341:PRO:O	2.48	0.43
1:C:171:THR:HA	1:C:311:ARG:HD3	2.00	0.43
1:C:374:VAL:O	1:C:374:VAL:HG23	2.19	0.43
1:C:466:GLN:CG	1:C:467:SER:N	2.80	0.43
1:E:339:ARG:HH12	1:E:342:LYS:HZ3	1.65	0.43
1:F:199:LEU:O	1:F:200:SER:C	2.61	0.43
1:F:342:LYS:HE2	1:F:344:GLU:HG3	1.98	0.43
1:F:468:PRO:HA	1:F:471:ILE:HD12	2.00	0.43
1:A:97:GLU:HG3	1:A:376:LYS:HE2	2.00	0.43
1:A:343:PHE:CE1	1:A:447:MET:HA	2.53	0.43
1:C:148:ARG:HA	1:C:148:ARG:NE	2.33	0.43
1:C:155:PHE:CD2	1:C:190:ARG:NH2	2.84	0.43
1:C:476:LYS:HB2	1:C:485:ARG:HA	2.01	0.43
1:F:318:MET:HE2	1:F:489:MET:HE3	2.00	0.43
1:C:190:ARG:HG3	1:C:190:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:LEU:HD23	1:C:272:LEU:HA	1.80	0.43
1:C:493:PRO:HG2	1:C:494:ARG:H	1.84	0.43
1:E:145:ILE:HD11	1:E:185:ILE:HD11	2.01	0.43
1:B:312:TYR:O	1:B:316:LEU:HD23	2.19	0.43
1:E:199:LEU:CD2	1:E:203:ARG:HH11	2.31	0.43
1:E:376:LYS:O	1:E:377:ASP:C	2.62	0.43
1:F:275:MET:HE3	1:F:287:TYR:HA	2.00	0.43
1:A:96:GLU:HG2	1:A:436:LYS:HE3	2.01	0.43
1:C:365:MET:O	1:C:366:LEU:HD23	2.19	0.43
1:A:260:ASP:C	1:A:262:ASN:H	2.27	0.43
1:A:319:LYS:C	1:A:321:PRO:HD3	2.43	0.43
1:D:59:MET:O	1:D:62:SER:HB3	2.18	0.43
1:D:139:GLY:O	1:D:145:ILE:HB	2.18	0.43
1:D:487:TYR:CD1	1:D:487:TYR:C	2.96	0.43
1:E:199:LEU:C	1:E:199:LEU:HD23	2.44	0.43
1:F:35:PRO:O	1:F:69:PHE:HB2	2.18	0.43
1:B:382:ASP:OD2	1:B:382:ASP:N	2.48	0.43
1:C:51:THR:HG23	1:C:215:SER:OG	2.19	0.43
1:D:172:PHE:O	1:D:176:ARG:HB2	2.19	0.43
1:D:305:THR:HG22	1:D:365:MET:CE	2.49	0.43
1:E:487:TYR:CD1	1:E:487:TYR:C	2.97	0.43
1:F:319:LYS:C	1:F:321:PRO:HD3	2.44	0.43
1:C:175:SER:HB2	1:C:202:LEU:CD1	2.40	0.42
1:C:414:GLN:C	1:C:416:PHE:H	2.26	0.42
1:D:32:LYS:H	1:D:32:LYS:NZ	2.14	0.42
1:A:145:ILE:HD12	1:A:145:ILE:HA	1.85	0.42
1:B:140:VAL:C	1:B:142:LYS:H	2.27	0.42
1:C:419:LYS:O	1:C:421:GLY:N	2.52	0.42
1:C:440:PHE:O	1:C:440:PHE:CD1	2.72	0.42
1:D:157:ILE:HD11	1:D:455:THR:HG22	2.01	0.42
1:C:110:LEU:HD22	1:C:241:LEU:HB3	2.00	0.42
1:D:161:ARG:O	1:D:163:THR:N	2.53	0.42
1:F:116:VAL:HG13	1:F:117:ALA:N	2.35	0.42
1:F:344:GLU:C	1:F:346:ARG:H	2.27	0.42
1:F:350:PRO:HG2	1:F:351:TYR:H	1.84	0.42
1:B:62:SER:OG	1:B:82:CYS:SG	2.75	0.42
1:B:150:GLN:NE2	1:B:341:PRO:O	2.43	0.42
1:B:368:MET:O	1:B:369:GLY:O	2.37	0.42
1:B:469:LYS:C	1:B:471:ILE:H	2.27	0.42
1:C:357:HIS:CE1	1:C:446:ARG:NH2	2.87	0.42
1:E:382:ASP:OD2	1:E:382:ASP:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:HEM:C1A	3:B:508[B]:IND:H5	2.54	0.42
1:C:33:LEU:HD11	1:C:77:ARG:CZ	2.50	0.42
1:C:122:GLU:O	1:C:125:LYS:HB3	2.18	0.42
1:C:173:PHE:CD1	1:C:176:ARG:NH2	2.88	0.42
1:C:192:ASP:OD1	1:C:194:GLU:HG2	2.19	0.42
1:C:264:PRO:HB3	1:C:273:ILE:CD1	2.48	0.42
1:C:403:ARG:HG3	4:C:912:HOH:O	2.18	0.42
1:C:433:SER:HB2	2:C:500:HEM:HBA1	2.01	0.42
1:D:311:ARG:HG3	1:D:311:ARG:NH2	2.32	0.42
1:E:319:LYS:HD3	1:E:471:ILE:HG22	2.01	0.42
1:E:351:TYR:HD1	1:E:417:LEU:HD11	1.84	0.42
1:F:88:LYS:HD3	1:F:88:LYS:O	2.20	0.42
3:B:508[B]:IND:H7	4:B:1242[B]:HOH:O	2.19	0.42
1:C:168:ILE:HD11	1:C:491:PHE:CE1	2.55	0.42
1:C:254:HIS:CD2	1:C:254:HIS:C	2.96	0.42
1:C:278:GLU:O	1:C:279:GLU:C	2.62	0.42
1:C:380:PHE:O	1:C:381:ARG:C	2.59	0.42
1:C:468:PRO:HA	1:C:471:ILE:HD12	2.01	0.42
1:D:376:LYS:O	1:D:377:ASP:C	2.61	0.42
1:C:414:GLN:C	1:C:416:PHE:N	2.76	0.42
1:C:467:SER:O	1:C:471:ILE:HG13	2.20	0.42
1:D:101:ARG:HG2	1:D:118:PHE:HA	2.02	0.42
1:D:203:ARG:HG2	1:D:203:ARG:HH11	1.83	0.42
1:E:351:TYR:CD1	1:E:417:LEU:HD11	2.54	0.42
1:A:339:ARG:HG2	1:A:339:ARG:HH21	1.85	0.42
1:C:175:SER:OG	1:C:202:LEU:HD21	2.19	0.42
1:C:321:PRO:C	1:C:323:VAL:N	2.78	0.42
1:C:454:THR:CG2	1:C:455:THR:N	2.83	0.42
2:C:500:HEM:C1A	3:C:509[B]:IND:H5	2.55	0.42
1:D:302:GLY:HA3	2:D:500:HEM:HBC2	2.01	0.42
1:F:353:GLU:OE1	1:F:353:GLU:HA	2.20	0.42
1:B:89:GLU:O	1:B:93:ASP:HB2	2.19	0.42
1:C:145:ILE:HD11	1:C:185:ILE:HD11	2.01	0.42
1:C:287:TYR:CZ	1:C:290:ASN:ND2	2.88	0.42
1:D:372:HIS:CD2	1:D:393:PRO:HG2	2.55	0.42
1:D:433:SER:CB	2:D:500:HEM:HBA1	2.49	0.42
1:F:311:ARG:NH1	1:F:484:PRO:HG2	2.34	0.42
1:A:88:LYS:HE3	4:A:949:HOH:O	2.20	0.42
1:A:211:PHE:CZ	1:A:217:GLY:HA2	2.55	0.42
1:A:365:MET:O	1:A:481:ALA:HA	2.20	0.42
1:C:175:SER:CB	1:C:202:LEU:HD21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:SER:OG	1:C:299:PHE:HE1	2.03	0.42
1:E:281:ASN:HD22	1:E:284:THR:HB	1.84	0.42
1:F:111:PHE:HD2	1:F:293:MET:HB3	1.84	0.42
1:C:368:MET:N	4:C:731:HOH:O	2.44	0.41
1:E:310:LEU:HD23	1:E:453:PHE:CE1	2.55	0.41
1:E:403:ARG:HD2	1:E:403:ARG:O	2.20	0.41
1:F:109:TRP:CH2	1:F:238:PHE:HB3	2.55	0.41
1:F:145:ILE:HD13	1:F:185:ILE:HD11	2.02	0.41
1:A:346:ARG:HB3	1:A:450:PHE:CE2	2.55	0.41
1:C:114:TYR:CD2	1:C:289:LYS:HD2	2.55	0.41
1:C:114:TYR:CE2	1:C:289:LYS:HD2	2.55	0.41
1:C:382:ASP:OD2	1:C:382:ASP:N	2.45	0.41
1:E:101:ARG:HD3	1:E:371:ALA:O	2.20	0.41
1:E:403:ARG:O	1:E:403:ARG:CG	2.68	0.41
1:F:464:SER:OG	1:F:466:GLN:HG2	2.19	0.41
4:A:989:HOH:O	1:D:64:ARG:HD2	2.20	0.41
1:B:201:LEU:HD11	1:B:247:PHE:CE2	2.55	0.41
1:F:407:ASN:HB3	1:F:410:ASP:HB2	2.00	0.41
1:B:281:ASN:OD1	1:B:282:PRO:HD2	2.20	0.41
1:B:352:THR:HG23	1:B:353:GLU:N	2.35	0.41
1:C:461:ARG:NE	1:C:494:ARG:HB2	2.24	0.41
1:E:456:ILE:O	1:E:460:PHE:HD1	2.04	0.41
1:A:489:MET:HE2	1:A:491:PHE:CZ	2.55	0.41
1:C:329:GLU:HG3	1:C:330:GLU:N	2.36	0.41
1:C:404:PHE:CD1	1:C:404:PHE:N	2.89	0.41
1:D:203:ARG:HG2	1:D:203:ARG:NH1	2.35	0.41
1:E:161:ARG:HH11	1:E:161:ARG:HG2	1.86	0.41
1:E:213:ALA:O	1:E:477:HIS:HB3	2.21	0.41
1:F:348:LYS:HD3	1:F:348:LYS:N	2.36	0.41
1:C:331:ILE:HA	1:C:349:MET:CE	2.51	0.41
1:C:407:ASN:HB3	1:C:410:ASP:OD2	2.20	0.41
1:F:305:THR:CG2	1:F:365:MET:HE1	2.50	0.41
1:C:331:ILE:HA	1:C:349:MET:HE3	2.03	0.41
1:D:386:PRO:O	1:D:387:LYS:C	2.64	0.41
1:E:349:MET:N	1:E:350:PRO:CD	2.84	0.41
1:F:111:PHE:CD2	1:F:293:MET:HB3	2.56	0.41
1:F:160:LEU:N	1:F:160:LEU:CD1	2.83	0.41
1:A:341:PRO:CG	1:A:454:THR:HG23	2.51	0.41
1:F:416:PHE:C	1:F:424:LYS:HG2	2.45	0.41
1:A:305:THR:OG1	1:A:306:VAL:N	2.54	0.41
1:B:145:ILE:HD12	1:B:145:ILE:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:O	1:B:163:THR:HG22	2.21	0.41
1:B:335:ILE:HG23	1:B:339:ARG:CZ	2.51	0.41
1:C:346:ARG:HG3	1:C:347:ALA:N	2.35	0.41
1:D:145:ILE:HD12	1:D:145:ILE:HA	1.90	0.41
1:D:289:LYS:HE3	1:D:289:LYS:HB2	1.84	0.41
1:D:300:PHE:HD2	1:D:300:PHE:O	2.03	0.41
1:D:319:LYS:C	1:D:321:PRO:HD3	2.45	0.41
1:E:430:VAL:N	1:E:431:PRO:CD	2.84	0.41
1:F:113:GLY:O	1:F:119:SER:HB3	2.20	0.41
1:F:256:GLN:HB2	1:F:272:LEU:HD21	2.03	0.41
1:A:351:TYR:O	1:A:355:VAL:HG23	2.21	0.41
1:A:418:ASP:OD2	1:A:418:ASP:C	2.64	0.41
1:B:43:ILE:HD13	1:F:40:LEU:HD11	2.03	0.41
1:F:122:GLU:O	1:F:125:LYS:N	2.54	0.41
1:F:201:LEU:HD23	1:F:204:MET:CE	2.51	0.41
1:F:439:CYS:HB2	2:F:500:HEM:NA	2.35	0.41
1:A:254:HIS:ND1	1:A:254:HIS:C	2.79	0.40
1:B:315:LEU:HD13	1:B:487:TYR:CE2	2.56	0.40
1:F:218:GLN:NE2	1:F:218:GLN:HA	2.35	0.40
1:F:332:ASP:O	1:F:336:GLY:CA	2.70	0.40
1:A:454:THR:CG2	1:A:455:THR:N	2.83	0.40
1:B:111:PHE:CE2	1:B:297:ASN:ND2	2.90	0.40
1:F:375:ASN:O	1:F:387:LYS:HG3	2.22	0.40
1:A:265:ARG:HD2	4:A:1238:HOH:O	2.21	0.40
1:B:342:LYS:HG3	1:B:345:ASP:CG	2.45	0.40
1:C:245:GLU:O	1:C:245:GLU:HG2	2.21	0.40
1:C:319:LYS:HA	1:C:471:ILE:HD12	2.04	0.40
1:D:176:ARG:HG3	1:D:198:PHE:HE2	1.84	0.40
1:E:459:ASN:N	1:E:459:ASN:ND2	2.68	0.40
2:F:500:HEM:C1A	3:F:512[B]:IND:H5	2.56	0.40
1:A:364:ASP:O	1:A:367:PRO:HD3	2.22	0.40
1:D:412:ASN:OD1	1:D:414:GLN:HG2	2.22	0.40
1:D:463:LYS:C	1:D:463:LYS:HD3	2.46	0.40
1:E:156:LEU:HD13	1:E:177:THR:OG1	2.20	0.40
1:F:320:HIS:CD2	1:F:411:PHE:CD2	3.10	0.40
1:F:438:TYR:CD2	1:F:438:TYR:O	2.74	0.40
1:E:330:GLU:O	1:E:334:VAL:HG23	2.22	0.40
1:F:296:LEU:O	1:F:297:ASN:C	2.65	0.40
1:F:332:ASP:HA	1:F:336:GLY:HA2	2.03	0.40
1:F:373:ARG:HB2	1:F:373:ARG:NH2	2.32	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	462/476 (97%)	434 (94%)	26 (6%)	2 (0%)	30	34
1	B	462/476 (97%)	416 (90%)	40 (9%)	6 (1%)	9	8
1	C	462/476 (97%)	403 (87%)	47 (10%)	12 (3%)	4	2
1	D	462/476 (97%)	441 (96%)	19 (4%)	2 (0%)	30	34
1	E	462/476 (97%)	424 (92%)	36 (8%)	2 (0%)	30	34
1	F	462/476 (97%)	407 (88%)	47 (10%)	8 (2%)	7	6
All	All	2772/2856 (97%)	2525 (91%)	215 (8%)	32 (1%)	10	9

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	C	142	LYS
1	C	171	THR
1	C	337	LYS
1	E	420	LYS
1	B	369	GLY
1	C	394	MET
1	C	459	ASN
1	C	493	PRO
1	F	189	ASP
1	F	425	LYS
1	B	425	LYS
1	C	364	ASP
1	F	123	ARG
1	F	383	PHE
1	A	261	PRO
1	C	420	LYS
1	E	394	MET
1	F	394	MET
1	B	166	ALA

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Mol	Chain	Res	Type
1	B	468	PRO
1	C	42	PHE
1	C	190	ARG
1	F	261	PRO
1	B	421	GLY
1	D	95	ALA
1	C	350	PRO
1	C	468	PRO
1	F	181	VAL
1	F	336	GLY
1	D	162	GLY
1	B	465	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	408/419 (97%)	390 (96%)	18 (4%)	25	33
1	B	408/419 (97%)	397 (97%)	11 (3%)	39	52
1	C	408/419 (97%)	390 (96%)	18 (4%)	25	33
1	D	408/419 (97%)	393 (96%)	15 (4%)	30	40
1	E	408/419 (97%)	390 (96%)	18 (4%)	25	33
1	F	408/419 (97%)	393 (96%)	15 (4%)	30	40
All	All	2448/2514 (97%)	2353 (96%)	95 (4%)	28	39

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	39	PRO
1	A	51	THR
1	A	52	GLU
1	A	53	GLN
1	A	64	ARG

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Mol	Chain	Res	Type
1	A	88	LYS
1	A	96	GLU
1	A	250	LYS
1	A	251	LYS
1	A	254	HIS
1	A	276	GLN
1	A	311	ARG
1	A	329	GLU
1	A	339	ARG
1	A	419	LYS
1	A	454	THR
1	A	468	PRO
1	B	51	THR
1	B	110	LEU
1	B	129	ARG
1	B	163	THR
1	B	236	GLN
1	B	283	ASN
1	B	291	LEU
1	B	312	TYR
1	B	315	LEU
1	B	319	LYS
1	B	473	VAL
1	C	39	PRO
1	C	51	THR
1	C	53	GLN
1	C	91	LEU
1	C	135	LEU
1	C	143	ARG
1	C	145	ILE
1	C	148	ARG
1	C	219	LEU
1	C	291	LEU
1	C	329	GLU
1	C	343	PHE
1	C	365	MET
1	C	425	LYS
1	C	427	ASP
1	C	454	THR
1	C	487	TYR
1	C	494	ARG
1	D	32	LYS

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Mol	Chain	Res	Type
1	D	51	THR
1	D	163	THR
1	D	194	GLU
1	D	196	LYS
1	D	225	SER
1	D	274	ARG
1	D	280	LYS
1	D	339	ARG
1	D	340	GLN
1	D	375	ASN
1	D	376	LYS
1	D	385	LEU
1	D	458	GLN
1	D	463	LYS
1	E	40	LEU
1	E	51	THR
1	E	53	GLN
1	E	88	LYS
1	E	91	LEU
1	E	112	LYS
1	E	136	ARG
1	E	145	ILE
1	E	206	LEU
1	E	242	GLN
1	E	251	LYS
1	E	262	ASN
1	E	311	ARG
1	E	375	ASN
1	E	403	ARG
1	E	419	LYS
1	E	446	ARG
1	E	494	ARG
1	F	51	THR
1	F	53	GLN
1	F	129	ARG
1	F	131	SER
1	F	134	THR
1	F	160	LEU
1	F	186	VAL
1	F	251	LYS
1	F	253	GLU
1	F	274	ARG

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Mol	Chain	Res	Type
1	F	382	ASP
1	F	383	PHE
1	F	427	ASP
1	F	438	TYR
1	F	486	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	72	HIS
1	A	210	GLN
1	A	283	ASN
1	A	414	GLN
1	A	466	GLN
1	B	72	HIS
1	B	104	GLN
1	B	210	GLN
1	B	255	ASN
1	B	276	GLN
1	B	297	ASN
1	B	328	HIS
1	B	338	ASN
1	B	466	GLN
1	C	229	HIS
1	C	254	HIS
1	C	297	ASN
1	C	328	HIS
1	C	486	ASN
1	D	56	ASN
1	D	167	ASN
1	D	262	ASN
1	D	276	GLN
1	D	283	ASN
1	D	297	ASN
1	D	414	GLN
1	D	458	GLN
1	D	466	GLN
1	E	167	ASN
1	E	236	GLN
1	E	242	GLN
1	E	276	GLN

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Mol	Chain	Res	Type
1	E	297	ASN
1	E	328	HIS
1	E	340	GLN
1	E	459	ASN
1	E	486	ASN
1	F	218	GLN
1	F	256	GLN
1	F	276	GLN
1	F	320	HIS
1	F	340	GLN
1	F	372	HIS
1	F	407	ASN
1	F	486	ASN

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](#)

18 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	IND	C	509[B]	-	10,10,10	1.06	1 (10%)	13,13,13	1.22	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	500	1	50,50,50	2.35	23 (46%)	67,82,82	1.36	12 (17%)
2	HEM	C	500	1	50,50,50	2.37	23 (46%)	67,82,82	1.43	12 (17%)
3	IND	A	501[A]	-	10,10,10	1.31	1 (10%)	13,13,13	1.20	1 (7%)
3	IND	B	502[A]	-	10,10,10	1.18	0	13,13,13	1.15	1 (7%)
2	HEM	E	500	1	50,50,50	2.47	24 (48%)	67,82,82	1.33	12 (17%)
3	IND	B	508[B]	-	10,10,10	1.10	1 (10%)	13,13,13	1.13	1 (7%)
3	IND	D	504[A]	-	10,10,10	1.15	1 (10%)	13,13,13	1.16	1 (7%)
3	IND	E	511[B]	-	10,10,10	1.13	1 (10%)	13,13,13	1.24	1 (7%)
3	IND	D	510[B]	-	10,10,10	1.02	0	13,13,13	1.23	1 (7%)
3	IND	F	512[B]	-	10,10,10	1.02	0	13,13,13	1.22	1 (7%)
3	IND	C	503[A]	-	10,10,10	1.31	1 (10%)	13,13,13	1.20	1 (7%)
3	IND	A	507[B]	-	10,10,10	1.03	0	13,13,13	1.23	1 (7%)
2	HEM	F	500	1	50,50,50	2.31	21 (42%)	67,82,82	1.39	13 (19%)
2	HEM	B	500	1	50,50,50	2.35	24 (48%)	67,82,82	1.38	9 (13%)
3	IND	E	505[A]	-	10,10,10	1.20	0	13,13,13	1.15	1 (7%)
2	HEM	D	500	1	50,50,50	2.46	23 (46%)	67,82,82	1.33	11 (16%)
3	IND	F	506[A]	-	10,10,10	1.27	1 (10%)	13,13,13	1.16	1 (7%)

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	IND	C	509[B]	-	-	-	0/2/2/2
2	HEM	A	500	1	-	4/14/54/54	-
2	HEM	C	500	1	-	4/14/54/54	-
3	IND	A	501[A]	-	-	-	0/2/2/2
3	IND	B	502[A]	-	-	-	0/2/2/2
2	HEM	E	500	1	-	4/14/54/54	-
3	IND	B	508[B]	-	-	-	0/2/2/2
3	IND	D	504[A]	-	-	-	0/2/2/2
3	IND	E	511[B]	-	-	-	0/2/2/2
3	IND	D	510[B]	-	-	-	0/2/2/2
3	IND	F	512[B]	-	-	-	0/2/2/2
3	IND	C	503[A]	-	-	-	0/2/2/2
3	IND	A	507[B]	-	-	-	0/2/2/2
2	HEM	F	500	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	500	1	-	4/14/54/54	-
3	IND	E	505[A]	-	-	-	0/2/2/2
2	HEM	D	500	1	-	4/14/54/54	-
3	IND	F	506[A]	-	-	-	0/2/2/2

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	HEM	C4A-NA	-4.90	1.30	1.39
2	C	500	HEM	C1C-NC	-4.80	1.30	1.39
2	A	500	HEM	C1C-NC	-4.72	1.30	1.39
2	D	500	HEM	C1D-ND	-4.56	1.29	1.38
2	D	500	HEM	C1C-NC	-4.41	1.31	1.39
2	E	500	HEM	C1B-NB	-4.33	1.32	1.40
2	C	500	HEM	C1D-ND	-4.32	1.30	1.38
2	B	500	HEM	C4D-ND	-4.24	1.32	1.40
2	A	500	HEM	FE-NC	4.17	2.08	1.95
2	F	500	HEM	C4A-NA	-4.16	1.31	1.39
2	D	500	HEM	C4D-ND	-4.15	1.33	1.40
2	D	500	HEM	C4A-NA	-4.12	1.31	1.39
2	E	500	HEM	FE-NC	4.09	2.08	1.95
2	A	500	HEM	FE-NB	4.08	2.07	1.94
2	F	500	HEM	CBB-CAB	4.05	1.49	1.30
2	E	500	HEM	C1D-ND	-4.04	1.30	1.38
2	C	500	HEM	C4A-NA	-4.03	1.32	1.39
2	A	500	HEM	C1D-ND	-4.02	1.30	1.38
2	C	500	HEM	CBB-CAB	4.01	1.49	1.30
2	B	500	HEM	C1B-NB	-3.98	1.33	1.40
2	F	500	HEM	FE-NA	3.97	2.08	1.95
2	E	500	HEM	C4D-ND	-3.95	1.33	1.40
2	E	500	HEM	CBB-CAB	3.95	1.49	1.30
2	F	500	HEM	FE-NB	3.92	2.07	1.94
2	A	500	HEM	C4A-NA	-3.91	1.32	1.39
2	F	500	HEM	FE-NC	3.91	2.08	1.95
2	B	500	HEM	CAC-C3C	-3.88	1.37	1.47
2	B	500	HEM	C1D-ND	-3.87	1.31	1.38
2	E	500	HEM	CMA-C3A	3.86	1.58	1.50
2	D	500	HEM	FE-NC	3.86	2.07	1.95
2	D	500	HEM	C1B-NB	-3.85	1.33	1.40
2	B	500	HEM	FE-NB	3.84	2.06	1.94
2	E	500	HEM	C1C-NC	-3.84	1.32	1.39
2	F	500	HEM	CMA-C3A	3.79	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	FE-NA	3.78	2.07	1.95
2	E	500	HEM	FE-NB	3.78	2.06	1.94
2	D	500	HEM	C1C-C2C	-3.78	1.37	1.45
2	B	500	HEM	C4A-NA	-3.77	1.32	1.39
2	D	500	HEM	C4B-NB	-3.74	1.31	1.38
2	C	500	HEM	C1B-NB	-3.73	1.33	1.40
2	B	500	HEM	C4B-NB	-3.71	1.31	1.38
2	F	500	HEM	CAC-C3C	-3.71	1.37	1.47
2	E	500	HEM	FE-ND	3.70	2.06	1.94
2	D	500	HEM	FE-ND	3.67	2.06	1.94
2	F	500	HEM	C1B-NB	-3.67	1.33	1.40
2	B	500	HEM	CBB-CAB	3.65	1.47	1.30
2	D	500	HEM	CBB-CAB	3.64	1.47	1.30
2	F	500	HEM	C1D-ND	-3.63	1.31	1.38
2	D	500	HEM	CAC-C3C	-3.63	1.37	1.47
2	D	500	HEM	FE-NB	3.62	2.06	1.94
2	B	500	HEM	C1C-NC	-3.61	1.32	1.39
2	C	500	HEM	CAC-C3C	-3.59	1.37	1.47
2	D	500	HEM	CMA-C3A	3.56	1.58	1.50
2	A	500	HEM	FE-ND	3.55	2.05	1.94
2	C	500	HEM	FE-NA	3.54	2.06	1.95
2	E	500	HEM	CAC-C3C	-3.53	1.38	1.47
2	D	500	HEM	CMC-C2C	3.51	1.58	1.50
2	B	500	HEM	CMA-C3A	3.51	1.58	1.50
2	E	500	HEM	CMC-C2C	3.51	1.58	1.50
2	E	500	HEM	FE-NA	3.49	2.06	1.95
2	B	500	HEM	CMC-C2C	3.49	1.57	1.50
2	B	500	HEM	FE-NC	3.48	2.06	1.95
2	C	500	HEM	FE-NB	3.48	2.05	1.94
2	A	500	HEM	CAC-C3C	-3.47	1.38	1.47
2	F	500	HEM	C1C-C2C	-3.47	1.38	1.45
2	A	500	HEM	C1B-NB	-3.45	1.34	1.40
2	F	500	HEM	C1C-NC	-3.45	1.33	1.39
2	C	500	HEM	FE-NC	3.45	2.06	1.95
2	F	500	HEM	FE-ND	3.43	2.05	1.94
2	C	500	HEM	C1C-C2C	-3.43	1.38	1.45
2	A	500	HEM	CBB-CAB	3.42	1.46	1.30
2	E	500	HEM	C1C-C2C	-3.37	1.38	1.45
2	C	500	HEM	C4B-NB	-3.37	1.32	1.38
2	C	500	HEM	CMA-C3A	3.33	1.57	1.50
2	A	500	HEM	C4B-NB	-3.29	1.32	1.38
2	B	500	HEM	FE-ND	3.19	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	HEM	C3B-C2B	3.17	1.43	1.37
2	B	500	HEM	C1C-C2C	-3.16	1.39	1.45
2	A	500	HEM	C4D-ND	-3.11	1.34	1.40
2	D	500	HEM	C4D-C3D	-3.09	1.39	1.45
2	C	500	HEM	C4D-ND	-3.07	1.34	1.40
2	C	500	HEM	CBD-CGD	3.07	1.57	1.50
2	F	500	HEM	C4D-ND	-3.05	1.35	1.40
2	C	500	HEM	C4C-NC	-2.96	1.34	1.39
2	F	500	HEM	C4B-NB	-2.89	1.33	1.38
2	B	500	HEM	C4C-NC	-2.88	1.34	1.39
2	A	500	HEM	C4D-C3D	-2.88	1.40	1.45
2	D	500	HEM	C3B-C2B	2.86	1.43	1.37
2	D	500	HEM	FE-NA	2.83	2.04	1.95
2	F	500	HEM	CMC-C2C	2.82	1.56	1.50
2	A	500	HEM	C1C-C2C	-2.80	1.39	1.45
2	A	500	HEM	C3B-C2B	2.80	1.42	1.37
2	A	500	HEM	CMC-C2C	2.76	1.56	1.50
2	A	500	HEM	CMD-C2D	2.76	1.56	1.50
2	C	500	HEM	FE-ND	2.73	2.03	1.94
2	E	500	HEM	C4B-NB	-2.69	1.33	1.38
2	F	500	HEM	C3B-C2B	2.66	1.42	1.37
2	E	500	HEM	C4C-NC	-2.66	1.34	1.39
2	D	500	HEM	C4C-NC	-2.65	1.34	1.39
2	C	500	HEM	C3B-C2B	2.62	1.42	1.37
2	E	500	HEM	CBC-CAC	2.61	1.42	1.30
2	F	500	HEM	C4C-NC	-2.61	1.34	1.39
2	A	500	HEM	CMA-C3A	2.61	1.56	1.50
2	C	500	HEM	CMC-C2C	2.54	1.56	1.50
2	F	500	HEM	CBC-CAC	2.53	1.42	1.30
2	E	500	HEM	C1A-C2A	-2.53	1.39	1.44
2	C	500	HEM	CBC-CAC	2.52	1.42	1.30
2	A	500	HEM	CBC-CAC	2.51	1.42	1.30
2	D	500	HEM	C3C-C4C	-2.47	1.41	1.46
2	C	500	HEM	C3C-C4C	-2.47	1.41	1.46
2	C	500	HEM	CAD-C3D	2.46	1.57	1.51
2	E	500	HEM	O2A-CGA	-2.45	1.22	1.30
2	A	500	HEM	CAD-C3D	2.40	1.57	1.51
2	B	500	HEM	C3B-C2B	2.38	1.42	1.37
2	D	500	HEM	O2A-CGA	-2.38	1.22	1.30
2	B	500	HEM	CBC-CAC	2.37	1.41	1.30
2	B	500	HEM	CMD-C2D	2.37	1.55	1.50
2	F	500	HEM	O2A-CGA	-2.36	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	O2A-CGA	-2.36	1.23	1.30
2	D	500	HEM	CBC-CAC	2.35	1.41	1.30
2	F	500	HEM	CMD-C2D	2.28	1.55	1.50
2	E	500	HEM	C3C-C4C	-2.26	1.42	1.46
2	B	500	HEM	FE-NA	2.24	2.02	1.95
2	D	500	HEM	O2D-CGD	-2.22	1.23	1.30
2	C	500	HEM	O2A-CGA	-2.19	1.23	1.30
2	B	500	HEM	CBD-CGD	2.18	1.55	1.50
3	F	506[A]	IND	C7-C8	2.15	1.43	1.39
2	A	500	HEM	CBD-CGD	2.14	1.55	1.50
2	B	500	HEM	C3C-C4C	-2.13	1.42	1.46
3	E	511[B]	IND	C9-C8	2.11	1.44	1.41
3	B	508[B]	IND	C9-C8	2.10	1.44	1.41
3	A	501[A]	IND	C7-C8	2.08	1.43	1.39
2	E	500	HEM	C3C-C2C	2.08	1.41	1.37
2	A	500	HEM	O2A-CGA	-2.07	1.24	1.30
2	C	500	HEM	C4D-C3D	-2.06	1.41	1.45
2	D	500	HEM	C1A-C2A	-2.05	1.40	1.44
3	C	509[B]	IND	C9-C8	2.05	1.44	1.41
2	B	500	HEM	CAD-C3D	2.04	1.56	1.51
3	C	503[A]	IND	C6-C5	2.03	1.42	1.38
2	F	500	HEM	CBD-CGD	2.03	1.55	1.50
2	A	500	HEM	C1A-C2A	-2.02	1.40	1.44
3	D	504[A]	IND	C7-C8	2.01	1.43	1.39
2	E	500	HEM	O2D-CGD	-2.01	1.24	1.30
2	B	500	HEM	O2D-CGD	-2.00	1.24	1.30
2	E	500	HEM	C4D-C3D	-2.00	1.41	1.45

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	CHD-C4C-NC	-3.63	120.50	124.45
2	F	500	HEM	CHD-C4C-NC	-3.27	120.89	124.45
2	C	500	HEM	C4C-C3C-C2C	-3.26	103.99	106.81
2	B	500	HEM	CHD-C4C-NC	-3.23	120.93	124.45
2	D	500	HEM	CHD-C4C-NC	-3.14	121.03	124.45
2	E	500	HEM	CHD-C4C-NC	-3.14	121.03	124.45
2	C	500	HEM	C1C-CHC-C4B	3.13	132.68	126.02
3	A	501[A]	IND	C7-C8-C9	-3.09	119.33	122.13
3	C	503[A]	IND	C7-C8-C9	-3.09	119.33	122.13
3	A	507[B]	IND	C7-C8-C9	-3.09	119.34	122.13
2	D	500	HEM	C3B-C4B-NB	3.07	111.67	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	HEM	C3B-C2B-C1B	-3.03	104.14	106.41
3	D	504[A]	IND	C7-C8-C9	-3.02	119.39	122.13
3	B	502[A]	IND	C7-C8-C9	-3.02	119.40	122.13
2	A	500	HEM	CHD-C4C-NC	-3.00	121.18	124.45
3	E	511[B]	IND	C7-C8-C9	-3.00	119.41	122.13
3	E	505[A]	IND	C7-C8-C9	-3.00	119.42	122.13
3	F	506[A]	IND	C7-C8-C9	-2.99	119.42	122.13
3	F	512[B]	IND	C7-C8-C9	-2.98	119.44	122.13
2	B	500	HEM	C3B-C4B-NB	2.96	111.59	109.47
3	C	509[B]	IND	C7-C8-C9	-2.95	119.46	122.13
2	D	500	HEM	C1C-CHC-C4B	2.95	132.28	126.02
3	D	510[B]	IND	C7-C8-C9	-2.94	119.46	122.13
2	E	500	HEM	C4B-C3B-C2B	-2.93	104.58	107.28
2	A	500	HEM	C3B-C2B-C1B	-2.92	104.22	106.41
2	F	500	HEM	C4B-C3B-C2B	-2.92	104.60	107.28
2	B	500	HEM	C3B-C2B-C1B	-2.92	104.22	106.41
2	F	500	HEM	C1C-CHC-C4B	2.85	132.07	126.02
2	C	500	HEM	C3B-C2B-C1B	-2.83	104.28	106.41
2	F	500	HEM	C3B-C4B-NB	2.81	111.49	109.47
2	A	500	HEM	C4C-C3C-C2C	-2.81	104.38	106.81
2	B	500	HEM	CHC-C1C-NC	-2.70	121.51	124.45
2	E	500	HEM	C1B-NB-C4B	2.69	108.39	105.21
3	B	508[B]	IND	C7-C8-C9	-2.67	119.71	122.13
2	B	500	HEM	C4B-C3B-C2B	-2.67	104.83	107.28
2	A	500	HEM	C1C-CHC-C4B	2.66	131.67	126.02
2	A	500	HEM	O2A-CGA-CBA	2.64	122.33	114.00
2	E	500	HEM	C1C-CHC-C4B	2.57	131.48	126.02
2	B	500	HEM	O2A-CGA-CBA	2.56	122.09	114.00
2	E	500	HEM	CHB-C1B-NB	-2.54	121.22	124.37
2	C	500	HEM	O2A-CGA-CBA	2.53	121.98	114.00
2	E	500	HEM	C3B-C4B-NB	2.52	111.28	109.47
2	F	500	HEM	O2A-CGA-CBA	2.51	121.94	114.00
2	A	500	HEM	C3B-C4B-NB	2.48	111.25	109.47
2	D	500	HEM	C4C-C3C-C2C	-2.45	104.69	106.81
2	F	500	HEM	C4A-CHB-C1B	2.45	132.00	126.25
2	D	500	HEM	C4B-C3B-C2B	-2.44	105.04	107.28
2	D	500	HEM	C1B-NB-C4B	2.43	108.09	105.21
2	F	500	HEM	C3B-C2B-C1B	-2.43	104.59	106.41
2	E	500	HEM	C4C-C3C-C2C	-2.41	104.72	106.81
2	B	500	HEM	C1C-CHC-C4B	2.41	131.15	126.02
2	C	500	HEM	C3B-C4B-NB	2.41	111.20	109.47
2	A	500	HEM	CHB-C1B-NB	-2.39	121.41	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	C1B-NB-C4B	2.37	108.01	105.21
2	E	500	HEM	O2A-CGA-CBA	2.35	121.43	114.00
2	C	500	HEM	CHD-C4C-C3C	2.32	129.12	125.21
2	C	500	HEM	C4B-C3B-C2B	-2.32	105.15	107.28
2	C	500	HEM	CHC-C1C-NC	-2.32	121.93	124.45
2	C	500	HEM	C1B-NB-C4B	2.29	107.92	105.21
2	A	500	HEM	CHC-C1C-NC	-2.29	121.96	124.45
2	E	500	HEM	C3B-C2B-C1B	-2.27	104.71	106.41
2	A	500	HEM	C4B-C3B-C2B	-2.25	105.21	107.28
2	C	500	HEM	C4D-C3D-C2D	-2.24	103.62	106.89
2	F	500	HEM	CHC-C1C-NC	-2.24	122.01	124.45
2	D	500	HEM	O2A-CGA-CBA	2.24	121.07	114.00
2	F	500	HEM	CHD-C4C-C3C	2.23	128.96	125.21
2	A	500	HEM	C4D-ND-C1D	2.21	107.82	105.21
2	F	500	HEM	CHB-C1B-NB	-2.20	121.65	124.37
2	C	500	HEM	CHB-C1B-NB	-2.17	121.68	124.37
2	D	500	HEM	CHB-C1B-NB	-2.15	121.71	124.37
2	F	500	HEM	C4C-C3C-C2C	-2.13	104.97	106.81
2	D	500	HEM	C4D-ND-C1D	2.11	107.70	105.21
2	D	500	HEM	C4A-CHB-C1B	2.10	131.19	126.25
2	A	500	HEM	C4C-CHD-C1D	2.07	130.42	126.02
2	B	500	HEM	CHB-C1B-NB	-2.06	121.82	124.37
2	E	500	HEM	C4A-CHB-C1B	2.04	131.05	126.25
2	E	500	HEM	C4C-CHD-C1D	2.04	130.36	126.02
2	F	500	HEM	C4D-ND-C1D	2.02	107.60	105.21
2	B	500	HEM	C4A-CHB-C1B	2.02	131.00	126.25
2	E	500	HEM	C4D-ND-C1D	2.02	107.60	105.21
2	F	500	HEM	C4C-CHD-C1D	2.01	130.30	126.02

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2C-C3C-CAC-CBC
2	A	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	C2C-C3C-CAC-CBC
2	C	500	HEM	C2C-C3C-CAC-CBC
2	C	500	HEM	C4C-C3C-CAC-CBC
2	E	500	HEM	C2C-C3C-CAC-CBC
2	E	500	HEM	C4C-C3C-CAC-CBC
2	F	500	HEM	C2C-C3C-CAC-CBC
2	F	500	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	D	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC
2	D	500	HEM	C4C-C3C-CAC-CBC
2	E	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O2A
2	F	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAA-CBA-CGA-O2A
2	D	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAA-CBA-CGA-O1A
2	F	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAA-CBA-CGA-O2A
2	E	500	HEM	CAA-CBA-CGA-O2A

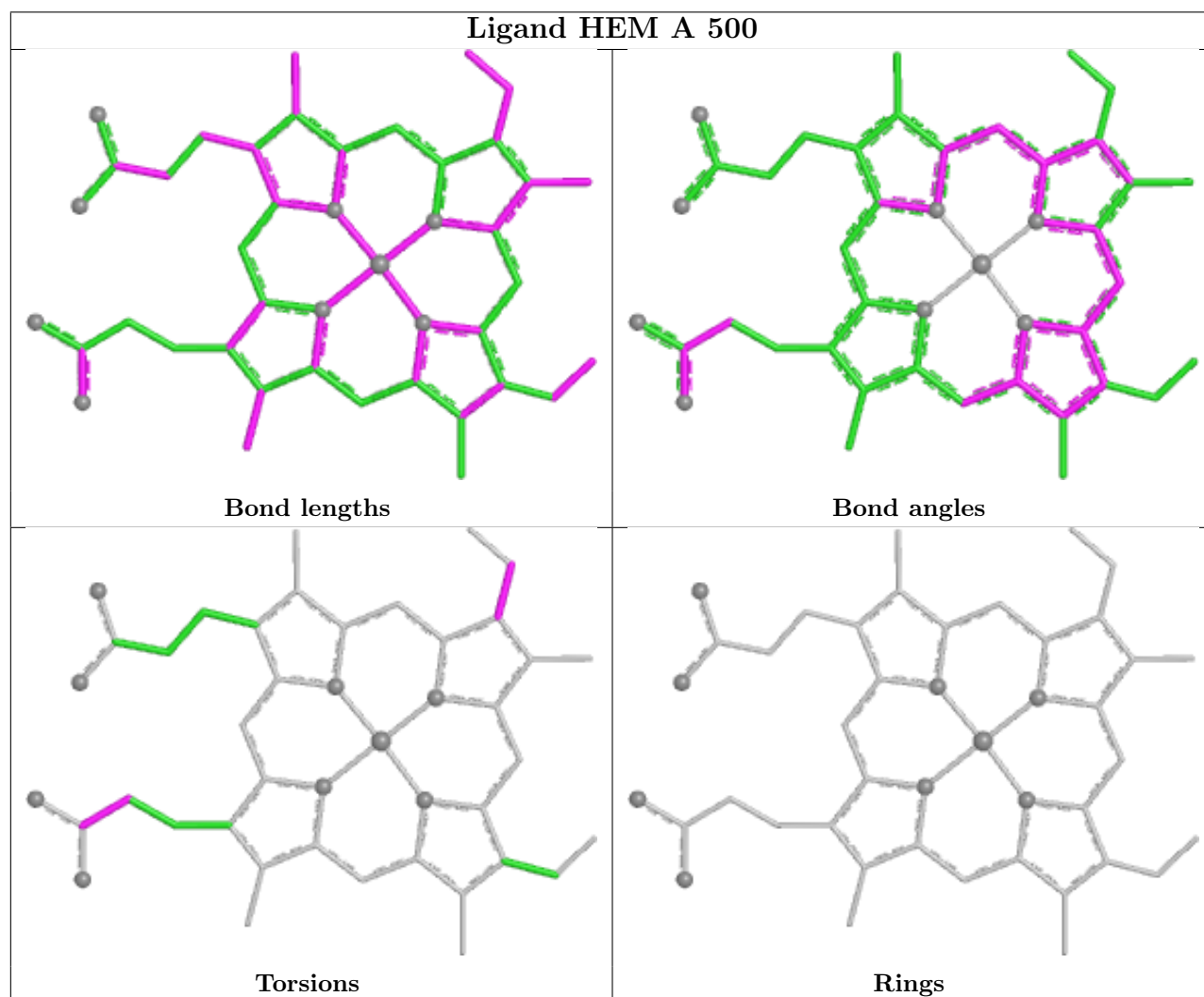
There are no ring outliers.

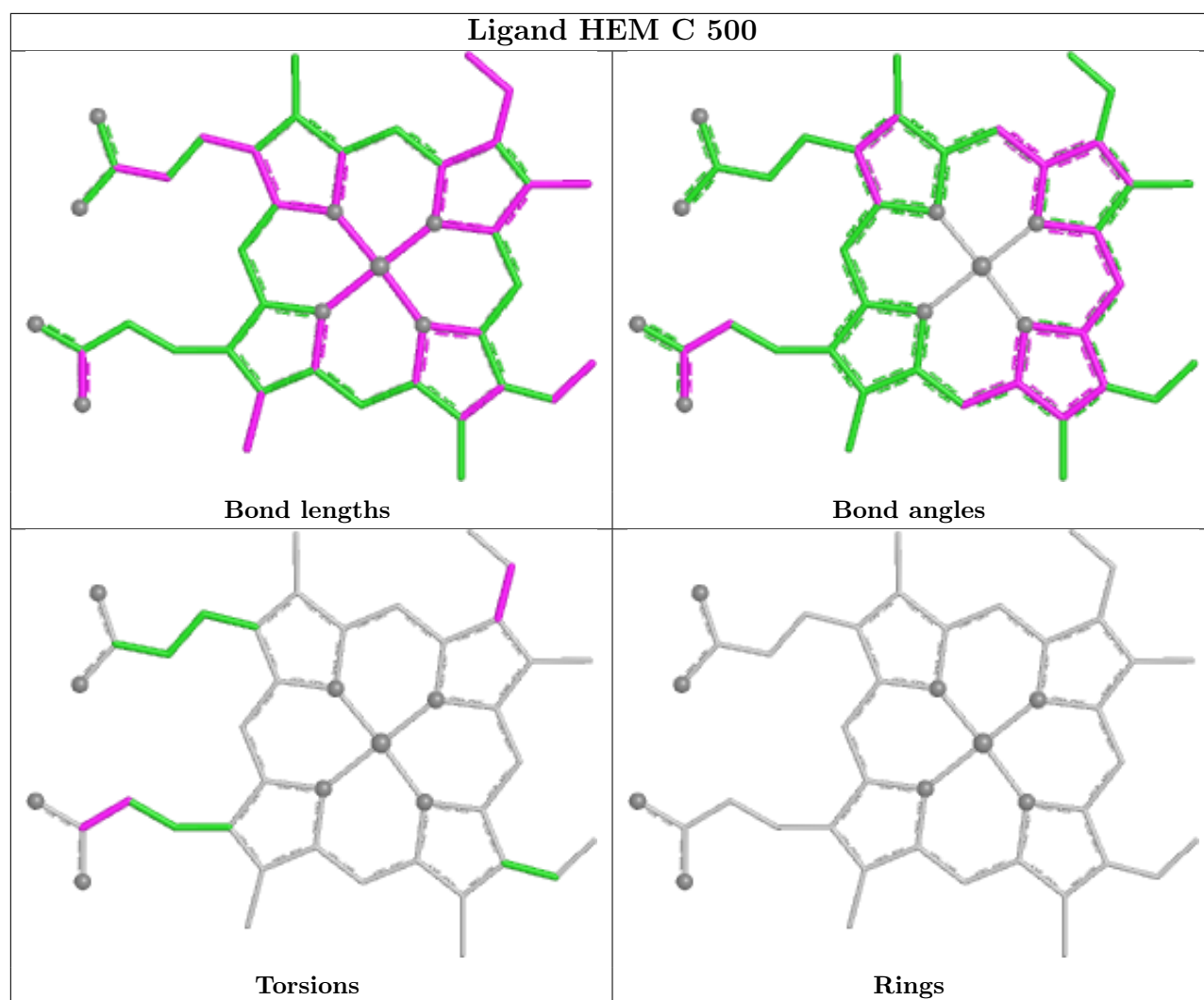
11 monomers are involved in 22 short contacts:

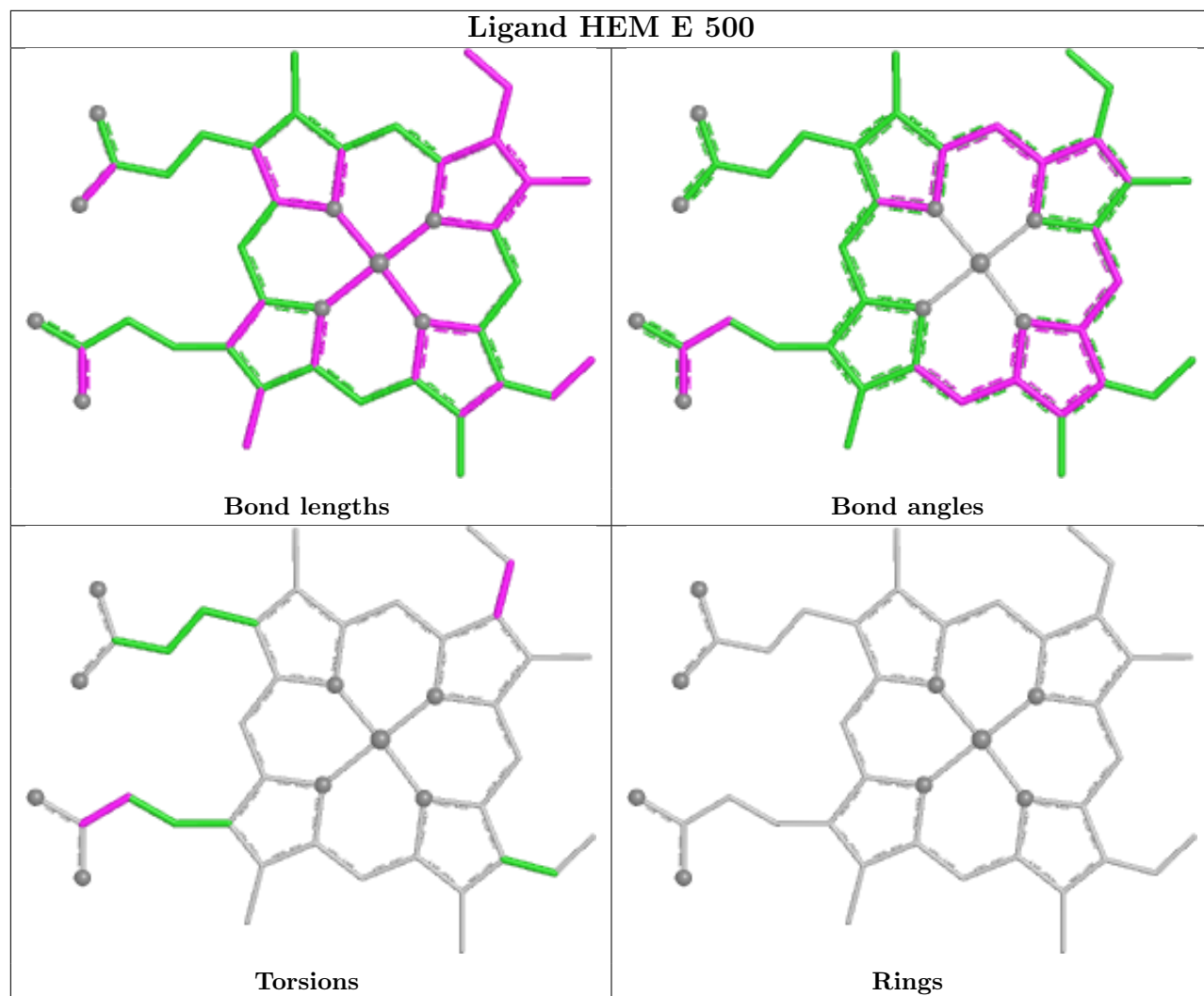
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	509[B]	IND	1	0
2	A	500	HEM	1	0
2	C	500	HEM	3	0
3	B	508[B]	IND	5	0
3	E	511[B]	IND	2	0
3	F	512[B]	IND	2	0
3	C	503[A]	IND	1	0
3	A	507[B]	IND	1	0
2	F	500	HEM	5	0
2	B	500	HEM	3	0
2	D	500	HEM	4	0

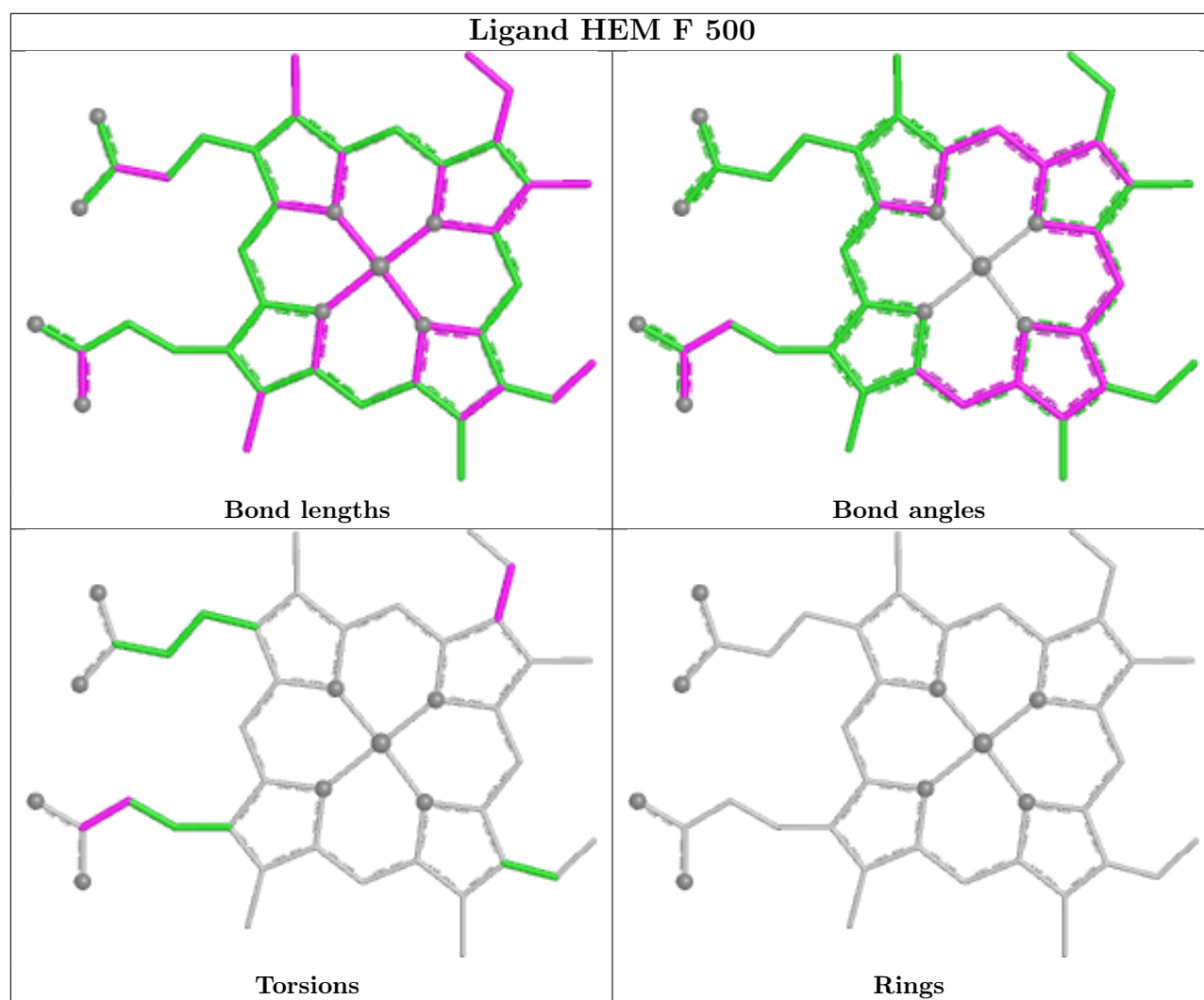
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

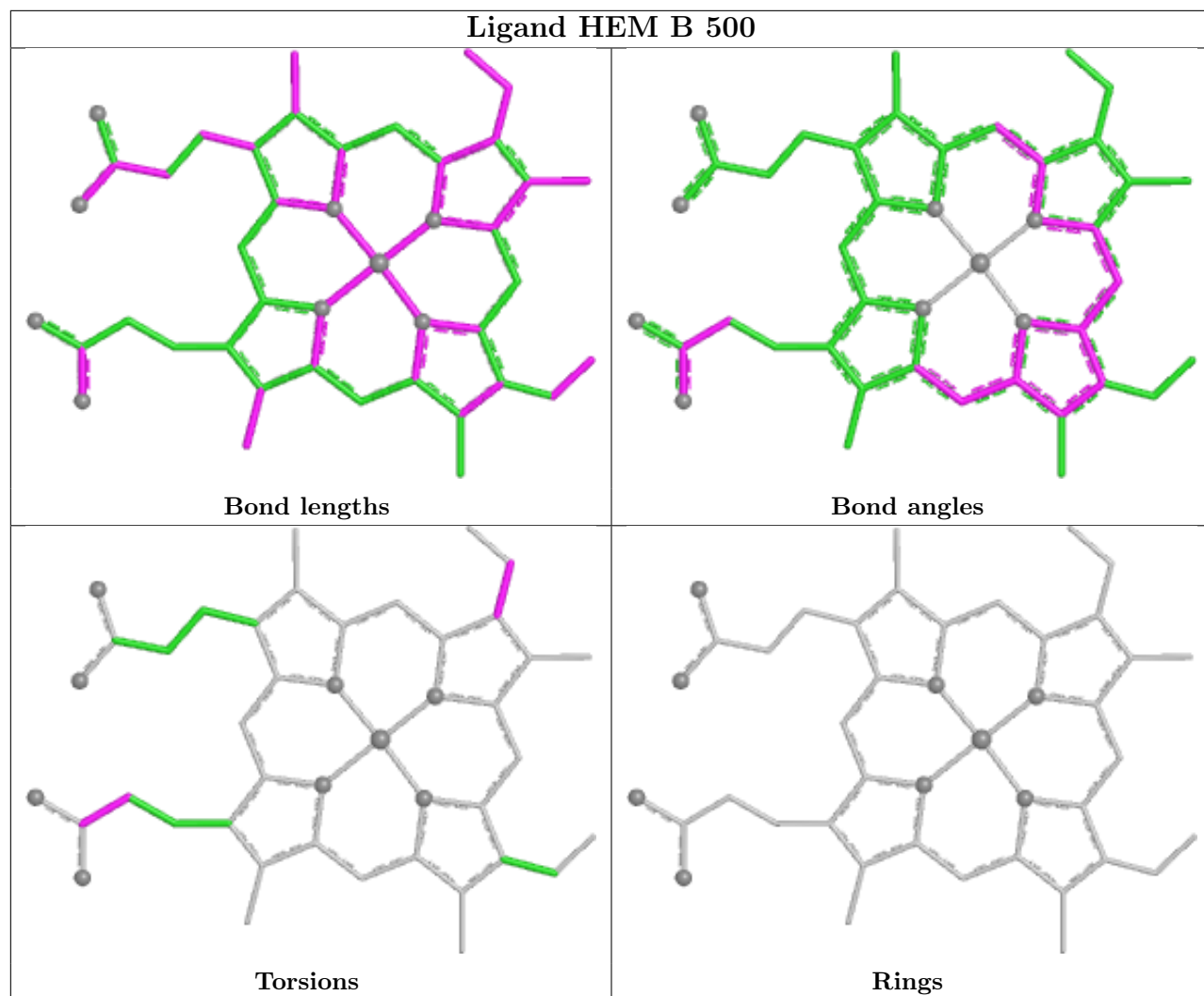
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

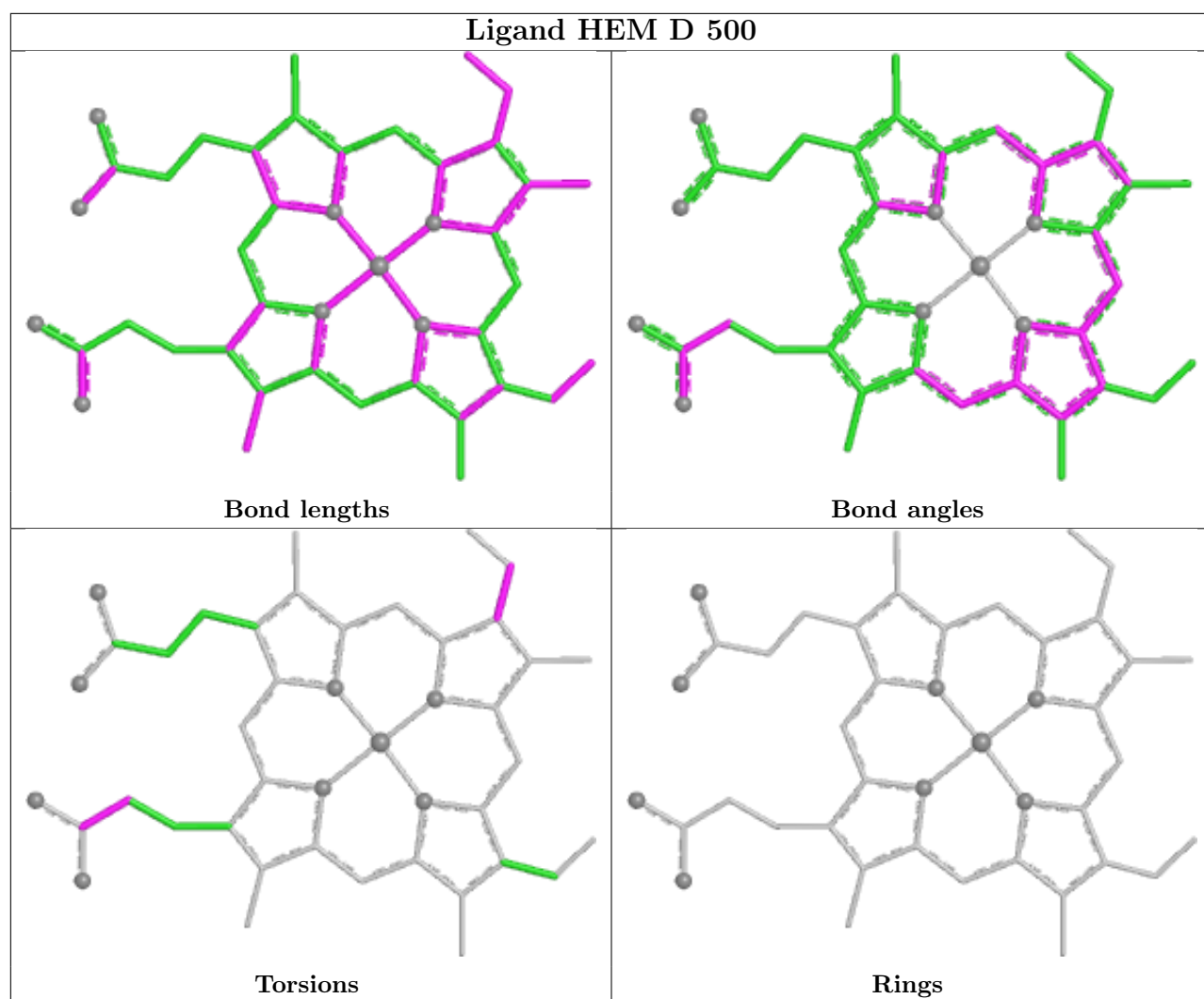












5.7 Other polymers [i](#)

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%)	-0.22	2 (0%) 88 91	15, 31, 56, 76	0
1	B	464/476 (97%)	0.31	20 (4%) 40 45	16, 43, 73, 86	0
1	C	464/476 (97%)	0.55	31 (6%) 24 27	19, 49, 79, 90	0
1	D	464/476 (97%)	0.02	4 (0%) 81 84	20, 39, 67, 79	0
1	E	464/476 (97%)	0.23	11 (2%) 59 66	22, 41, 72, 84	0
1	F	464/476 (97%)	0.73	27 (5%) 29 33	19, 52, 79, 91	0
All	All	2784/2856 (97%)	0.27	95 (3%) 48 55	15, 42, 75, 91	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	PHE	3.8
1	C	491	PHE	3.6
1	F	421	GLY	3.4
1	F	331	ILE	3.3
1	F	428	ALA	3.1
1	B	417	LEU	3.1
1	F	343	PHE	3.1
1	C	341	PRO	3.0
1	B	419	LYS	2.9
1	F	417	LEU	2.9
1	C	473	VAL	2.9
1	B	316	LEU	2.8
1	F	423	PHE	2.8
1	F	492	LEU	2.8
1	F	156	LEU	2.8
1	C	173	PHE	2.8
1	E	323	VAL	2.8
1	F	335	ILE	2.7
1	C	168	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	426	SER	2.7
1	C	468	PRO	2.6
1	E	419	LYS	2.6
1	F	337	LYS	2.6
1	C	156	LEU	2.6
1	C	416	PHE	2.6
1	B	487	TYR	2.6
1	C	166	ALA	2.5
1	F	325	ALA	2.5
1	C	459	ASN	2.5
1	B	468	PRO	2.5
1	F	493	PRO	2.5
1	B	472	ASP	2.5
1	F	261	PRO	2.5
1	B	352	THR	2.5
1	B	474	SER	2.5
1	C	490	SER	2.5
1	B	423	PHE	2.4
1	C	493	PRO	2.4
1	E	493	PRO	2.4
1	C	323	VAL	2.4
1	F	405	PHE	2.4
1	C	332	ASP	2.4
1	B	471	ILE	2.4
1	E	335	ILE	2.4
1	B	473	VAL	2.3
1	C	321	PRO	2.3
1	C	349	MET	2.3
1	C	462	PHE	2.3
1	E	337	LYS	2.3
1	D	465	PRO	2.3
1	C	487	TYR	2.3
1	B	213	ALA	2.3
1	A	419	LYS	2.3
1	B	142	LYS	2.3
1	E	420	LYS	2.3
1	C	413	PRO	2.2
1	F	347	ALA	2.2
1	B	163	THR	2.2
1	B	329	GLU	2.2
1	E	454	THR	2.2
1	C	348	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	172	PHE	2.2
1	E	31	GLY	2.2
1	D	419	LYS	2.2
1	B	206	LEU	2.2
1	F	339	ARG	2.2
1	F	280	LYS	2.2
1	B	421	GLY	2.2
1	E	421	GLY	2.2
1	B	418	ASP	2.1
1	A	337	LYS	2.1
1	F	341	PRO	2.1
1	C	164	HIS	2.1
1	E	336	GLY	2.1
1	C	488	THR	2.1
1	F	145	ILE	2.1
1	C	411	PHE	2.1
1	D	491	PHE	2.1
1	F	416	PHE	2.1
1	F	159	ALA	2.1
1	C	331	ILE	2.1
1	F	269	ASP	2.1
1	E	453	PHE	2.1
1	C	259	LEU	2.1
1	C	458	GLN	2.1
1	F	185	ILE	2.1
1	C	327	VAL	2.1
1	F	404	PHE	2.1
1	C	489	MET	2.0
1	C	193	TYR	2.0
1	F	438	TYR	2.0
1	C	252	VAL	2.0
1	F	336	GLY	2.0
1	D	422	GLN	2.0
1	C	317	LEU	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

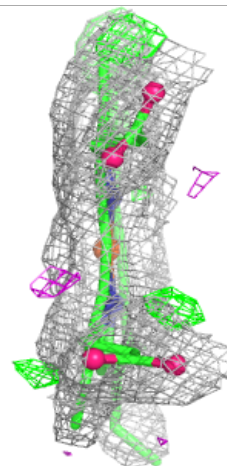
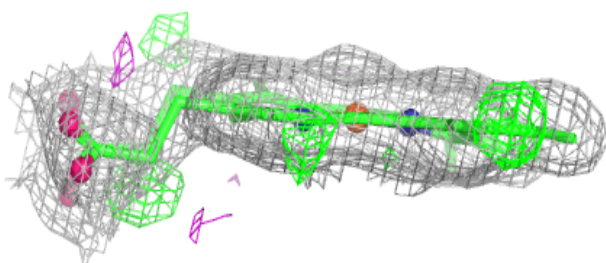
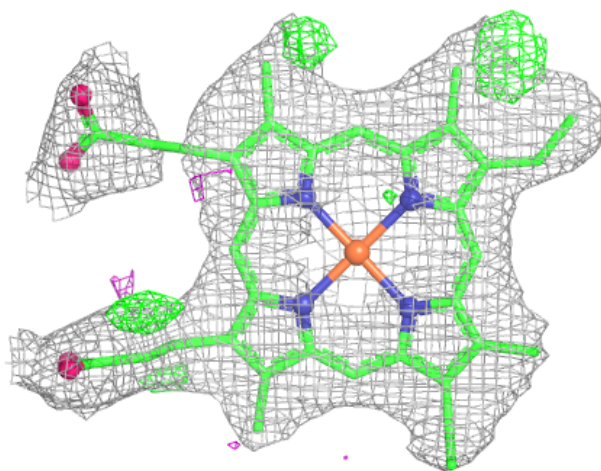
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IND	A	507[B]	9/9	0.72	0.22	31,31,31,31	9
3	IND	C	509[B]	9/9	0.74	0.22	31,31,31,31	9
3	IND	E	511[B]	9/9	0.76	0.20	31,31,31,31	9
3	IND	D	510[B]	9/9	0.77	0.20	31,31,31,31	9
3	IND	E	505[A]	9/9	0.84	0.14	31,31,31,31	9
3	IND	F	506[A]	9/9	0.86	0.15	31,31,31,31	9
3	IND	D	504[A]	9/9	0.87	0.15	31,31,31,31	9
3	IND	B	502[A]	9/9	0.89	0.13	31,31,31,31	9
3	IND	F	512[B]	9/9	0.90	0.12	31,31,31,31	9
3	IND	C	503[A]	9/9	0.91	0.10	31,31,31,31	9
3	IND	A	501[A]	9/9	0.93	0.11	31,31,31,31	9
3	IND	B	508[B]	9/9	0.94	0.09	31,31,31,31	9
2	HEM	F	500	43/43	0.95	0.10	23,41,54,61	0
2	HEM	D	500	43/43	0.97	0.07	18,27,33,35	0
2	HEM	C	500	43/43	0.97	0.07	12,30,41,45	0
2	HEM	E	500	43/43	0.98	0.07	26,34,39,41	0
2	HEM	B	500	43/43	0.98	0.06	9,22,34,41	0
2	HEM	A	500	43/43	0.99	0.05	14,20,28,38	0

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

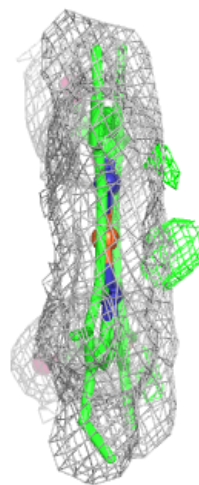
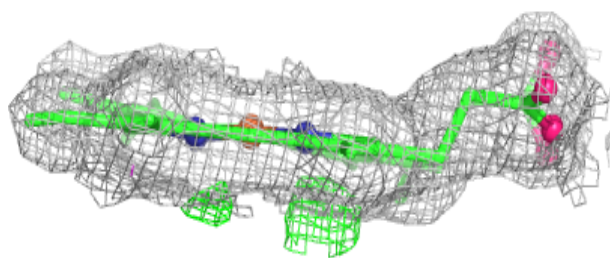
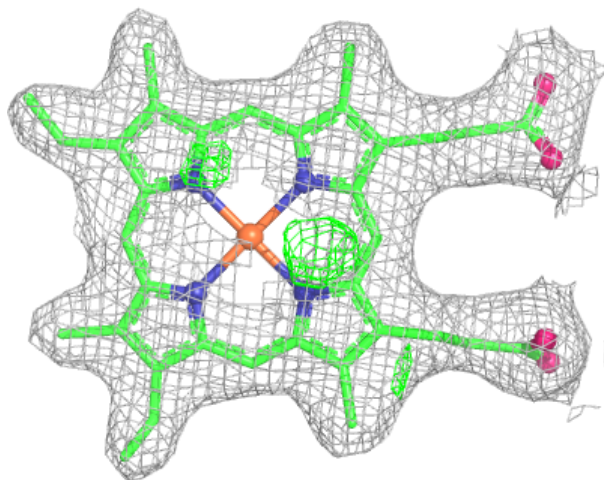
Electron density around HEM F 500:

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



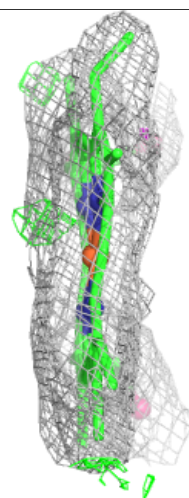
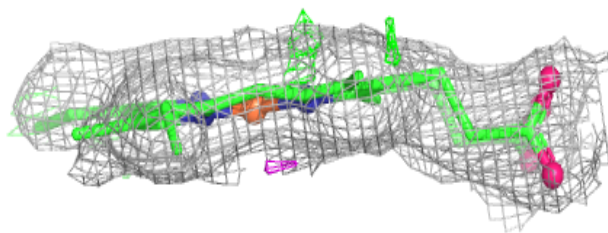
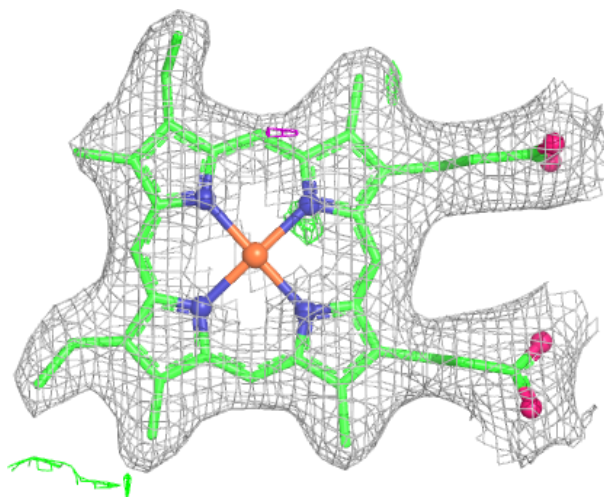
Electron density around HEM D 500:

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



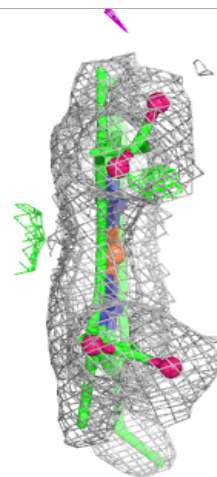
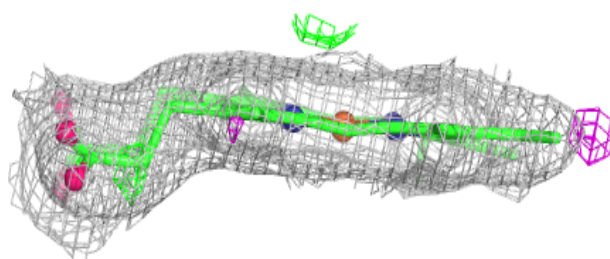
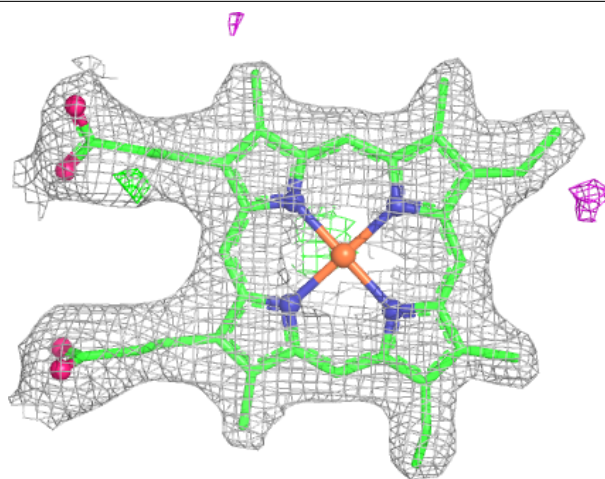
Electron density around HEM C 500:

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



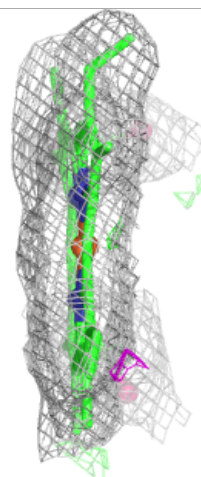
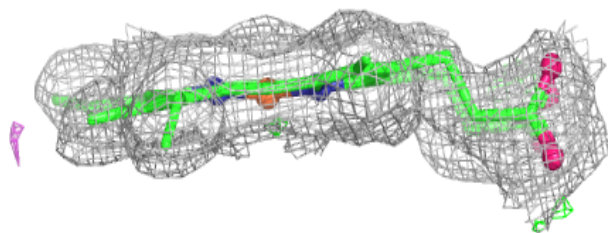
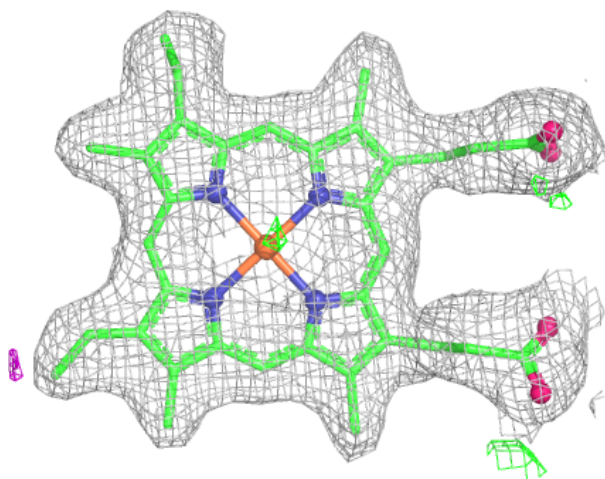
Electron density around HEM E 500:

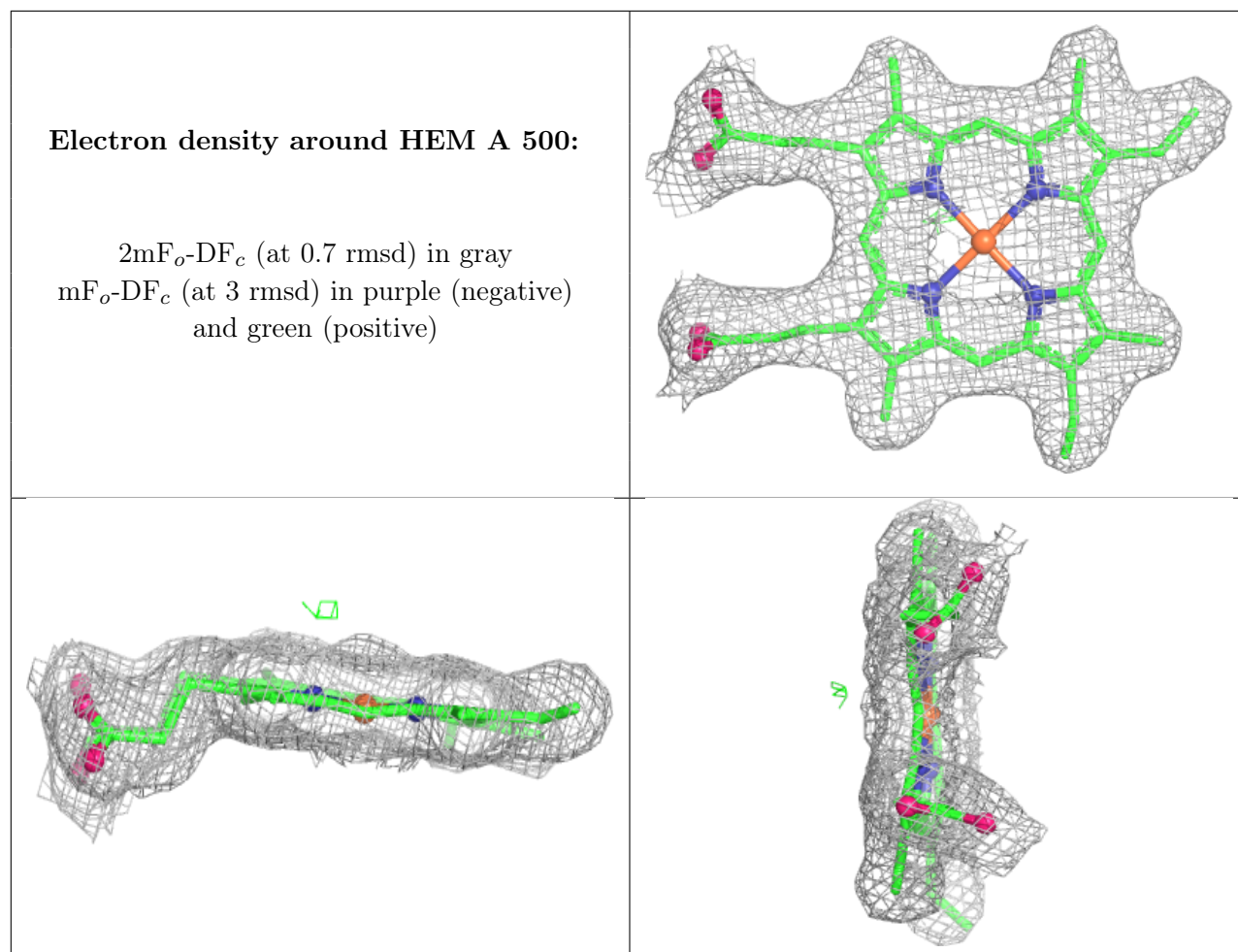
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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.