



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:43 PM UTC

PDB ID : 6FMO / pdb_00006fmo
Title : Crystal structure of the substrate (obtusifoliol)-bound and ligand-free I105F mutant of sterol 14- α demethylase (CYP51) from *Trypanosoma cruzi*
Authors : Hargrove, T.Y.; Wawrzak, Z.; Lepesheva, G.I.
Deposited on : 2018-02-01
Resolution : 3.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

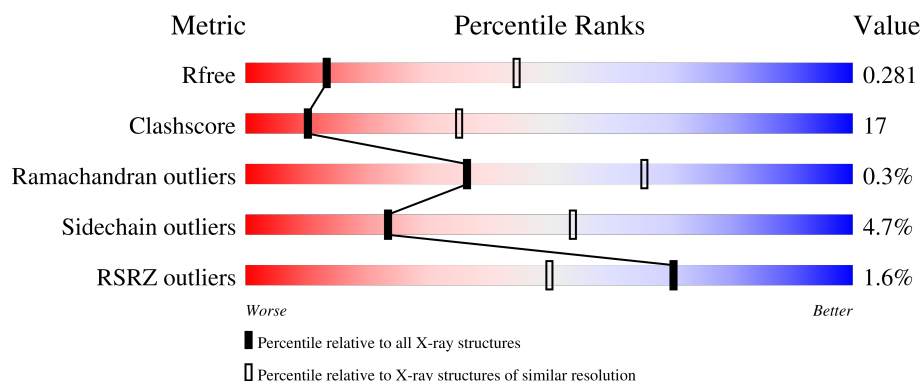
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	485	% 71% 19% • 8%
1	B	485	2% 69% 20% • 8%
1	C	485	3% 71% 19% • 8%
1	D	485	% 68% 22% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14445 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 Sterol 14alpha-demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3585	2292	627	638	28			
1	B	448	Total	C	N	O	S	0	0	0
			3518	2234	622	636	26			
1	C	448	Total	C	N	O	S	0	0	0
			3487	2210	616	637	24			
1	D	448	Total	C	N	O	S	0	0	0
			3585	2292	627	638	28			

There are 28 discrepancies between the modelled and reference sequences:

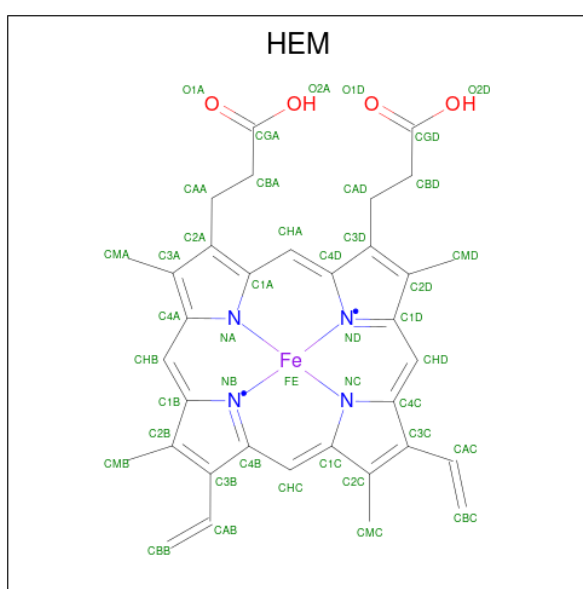
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	LEU	ASP	conflict	UNP M1FYE4
A	105	PHE	ILE	engineered mutation	UNP M1FYE4
A	355	PRO	SER	conflict	UNP M1FYE4
A	482	HIS	-	expression tag	UNP M1FYE4
A	483	HIS	-	expression tag	UNP M1FYE4
A	484	HIS	-	expression tag	UNP M1FYE4
A	485	HIS	-	expression tag	UNP M1FYE4
B	31	LEU	ASP	conflict	UNP M1FYE4
B	105	PHE	ILE	engineered mutation	UNP M1FYE4
B	355	PRO	SER	conflict	UNP M1FYE4
B	482	HIS	-	expression tag	UNP M1FYE4
B	483	HIS	-	expression tag	UNP M1FYE4
B	484	HIS	-	expression tag	UNP M1FYE4
B	485	HIS	-	expression tag	UNP M1FYE4
C	31	LEU	ASP	conflict	UNP M1FYE4
C	105	PHE	ILE	engineered mutation	UNP M1FYE4
C	355	PRO	SER	conflict	UNP M1FYE4
C	482	HIS	-	expression tag	UNP M1FYE4
C	483	HIS	-	expression tag	UNP M1FYE4
C	484	HIS	-	expression tag	UNP M1FYE4
C	485	HIS	-	expression tag	UNP M1FYE4

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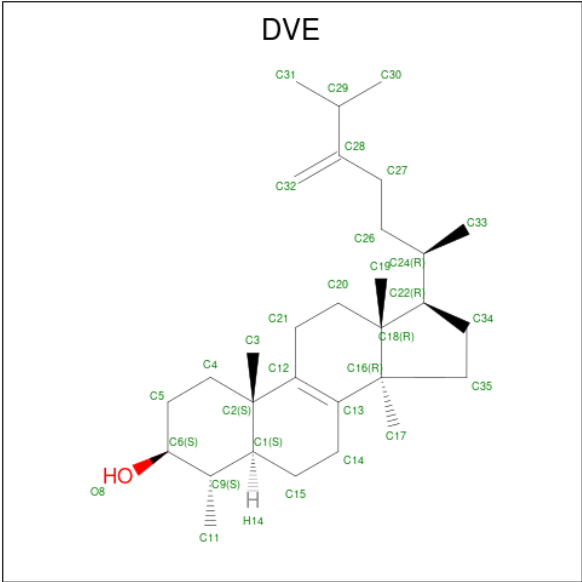
Chain	Residue	Modelled	Actual	Comment	Reference
D	31	LEU	ASP	conflict	UNP M1FYE4
D	105	PHE	ILE	engineered mutation	UNP M1FYE4
D	355	PRO	SER	conflict	UNP M1FYE4
D	482	HIS	-	expression tag	UNP M1FYE4
D	483	HIS	-	expression tag	UNP M1FYE4
D	484	HIS	-	expression tag	UNP M1FYE4
D	485	HIS	-	expression tag	UNP M1FYE4

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 3 is Obtusifoliol (CCD ID: DVE) (formula: $\text{C}_{30}\text{H}_{50}\text{O}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			31	30	1		
3	B	1	Total	C	O	0	0
			31	30	1		
3	C	1	Total	C	O	0	0
			31	30	1		

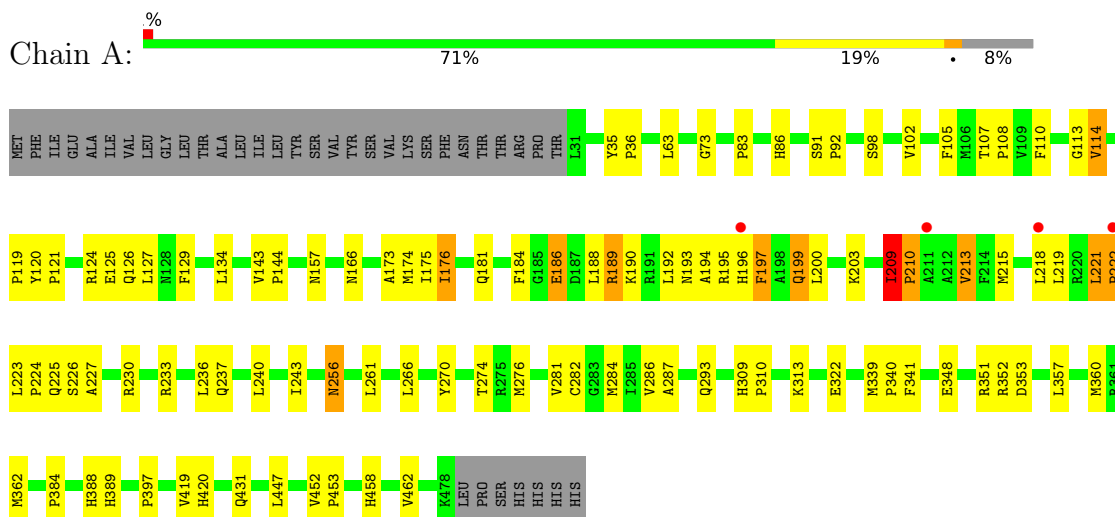
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	5	Total	O	0	0
			5	5		

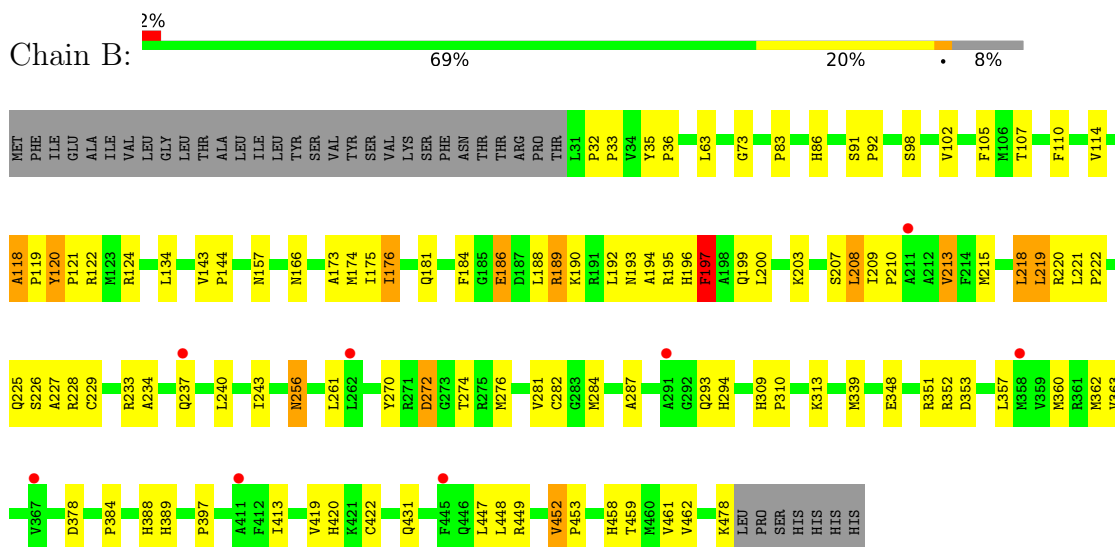
3 Residue-property plots

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: Sterol 14alpha-demethylase

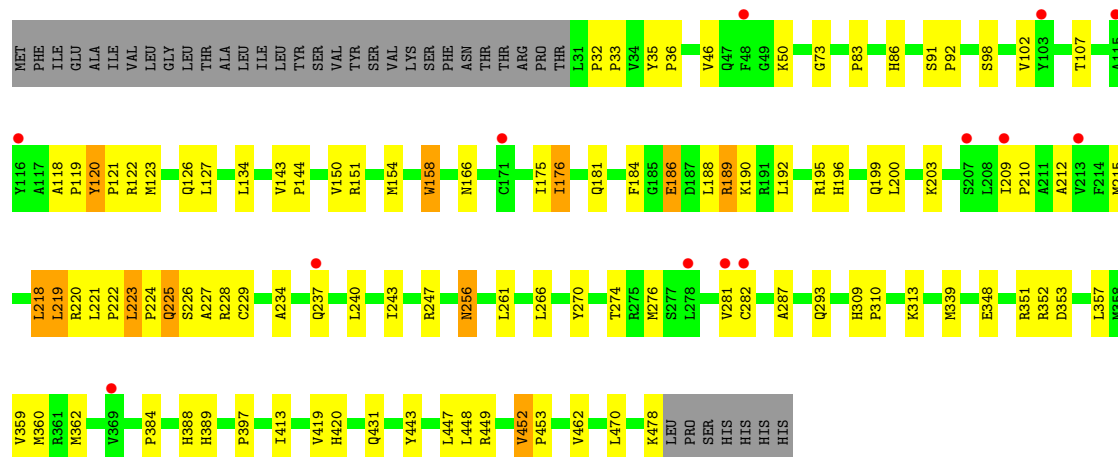


• Molecule 1: Sterol 14alpha-demethylase

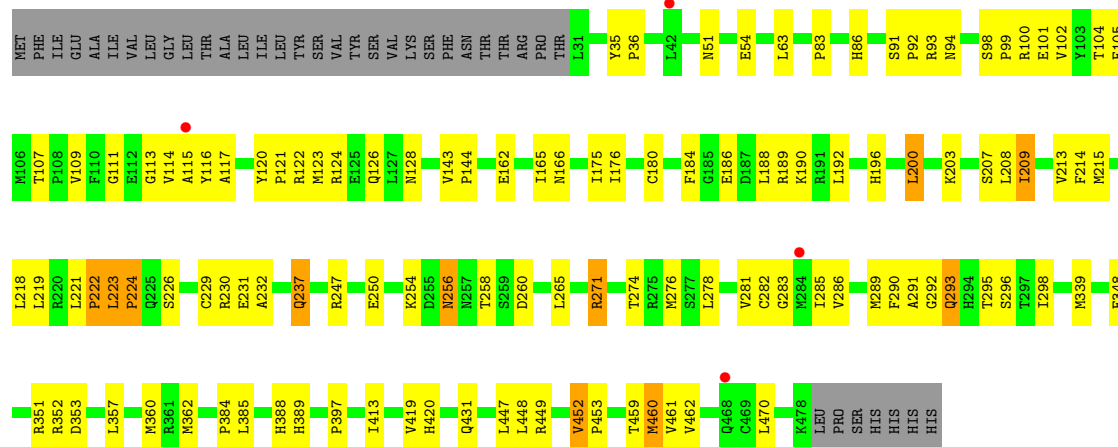


• Molecule 1: Sterol 14alpha-demethylase





• Molecule 1: Sterol 14alpha-demethylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	154.31Å 154.31Å 178.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	133.64 – 3.18 133.64 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.2 (133.64-3.18) 99.2 (133.64-3.18)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.260 , 0.293 0.271 , 0.281	Depositor DCC
R_{free} test set	2027 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	137.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 143.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14445	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

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

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, DVE

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	0.28	0/3671	0.75	9/4963 (0.2%)
1	B	0.31	0/3603	0.79	7/4875 (0.1%)
1	C	0.29	0/3569	0.74	2/4835 (0.0%)
1	D	0.29	0/3671	0.77	4/4963 (0.1%)
All	All	0.29	0/14514	0.76	22/19636 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	339	MET	CA-C-N	10.40	130.19	118.85
1	D	339	MET	C-N-CA	10.40	130.19	118.85
1	B	339	MET	CA-C-N	10.02	129.77	118.85
1	B	339	MET	C-N-CA	10.02	129.77	118.85
1	C	339	MET	CA-C-N	9.80	129.53	118.85
1	C	339	MET	C-N-CA	9.80	129.53	118.85
1	B	120	TYR	CA-C-N	-8.06	109.77	119.84
1	B	120	TYR	C-N-CA	-8.06	109.77	119.84
1	A	199	GLN	N-CA-C	7.73	119.49	111.14
1	A	339	MET	CA-C-N	6.92	128.48	119.84
1	A	339	MET	C-N-CA	6.92	128.48	119.84
1	B	118	ALA	CA-C-N	6.15	127.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ALA	C-N-CA	6.15	127.53	119.84
1	A	209	ILE	CA-C-N	6.02	127.36	119.84
1	A	209	ILE	C-N-CA	6.02	127.36	119.84
1	A	221	LEU	CA-C-N	5.93	127.25	119.84
1	A	221	LEU	C-N-CA	5.93	127.25	119.84
1	D	223	LEU	CA-C-N	5.88	127.19	119.84
1	D	223	LEU	C-N-CA	5.88	127.19	119.84
1	A	125	GLU	N-CA-C	5.87	117.36	111.07
1	A	127	LEU	N-CA-CB	5.14	117.52	110.07
1	B	197	PHE	N-CA-C	-5.13	105.69	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	PHE	Sidechain

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	3585	0	3608	105	0
1	B	3518	0	3435	128	0
1	C	3487	0	3385	114	0
1	D	3585	0	3608	126	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
2	C	43	0	30	10	0
2	D	43	0	30	4	0
3	A	31	0	0	0	0
3	B	31	0	0	1	0
3	C	31	0	0	2	0
4	D	5	0	0	0	0
All	All	14445	0	14156	488	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 (488) 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:A:221:LEU:CG	1:A:222:PRO:HD3	1.06	1.51
1:A:221:LEU:CD1	1:A:222:PRO:HD3	1.47	1.42
1:A:221:LEU:CG	1:A:222:PRO:CD	2.02	1.36
1:A:221:LEU:HG	1:A:222:PRO:CD	1.53	1.35
1:A:221:LEU:CD1	1:A:222:PRO:CD	2.08	1.31
1:B:193:ASN:CG	1:B:194:ALA:H	1.45	1.14
1:A:223:LEU:HD11	1:A:227:ALA:H	1.00	1.13
1:A:221:LEU:HD12	1:A:222:PRO:CD	1.74	1.12
1:A:221:LEU:CD1	1:A:222:PRO:CG	2.29	1.11
1:B:118:ALA:HB1	1:B:119:PRO:HD2	1.33	1.10
1:A:221:LEU:HD11	1:A:222:PRO:HG3	1.23	1.08
1:B:222:PRO:HG3	1:C:46:VAL:HA	1.29	1.08
1:C:219:LEU:HA	1:C:223:LEU:HD13	1.34	1.07
1:A:223:LEU:HD11	1:A:227:ALA:N	1.70	1.04
1:C:225:GLN:OE1	1:C:227:ALA:HB2	1.57	1.03
1:D:460:MET:SD	1:D:460:MET:N	2.31	1.03
1:A:221:LEU:CD1	1:A:222:PRO:HG3	1.87	1.02
1:B:119:PRO:HG2	1:B:121:PRO:HD2	1.43	1.01
1:B:195:ARG:O	1:B:199:GLN:N	1.94	1.00
1:B:193:ASN:CG	1:B:194:ALA:N	2.17	1.00
1:A:210:PRO:HB3	1:A:458:HIS:O	1.64	0.97
1:C:151:ARG:HA	1:C:154:MET:SD	2.08	0.94
1:A:105:PHE:CD2	1:A:213:VAL:HG12	2.02	0.94
1:A:193:ASN:CG	1:A:194:ALA:H	1.74	0.93
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.49	0.92
1:B:225:GLN:HE21	1:B:227:ALA:CB	1.82	0.92
1:C:219:LEU:CA	1:C:223:LEU:HD13	1.99	0.91
1:A:221:LEU:HD12	1:A:222:PRO:CG	1.95	0.91
1:C:154:MET:HG2	1:C:158:TRP:CZ3	2.06	0.91
1:C:154:MET:HG2	1:C:158:TRP:CH2	2.06	0.90
1:A:108:PRO:O	1:A:230:ARG:HD3	1.72	0.89
1:A:195:ARG:O	1:A:199:GLN:CB	2.21	0.89
1:A:108:PRO:O	1:A:230:ARG:CD	2.20	0.89
1:A:195:ARG:O	1:A:199:GLN:HB3	1.73	0.89
1:C:118:ALA:HB3	1:C:122:ARG:HB2	1.55	0.88
1:D:419:VAL:HG23	1:D:420:HIS:CD2	2.10	0.87
1:A:221:LEU:HG	1:A:222:PRO:HD3	0.89	0.87
1:C:218:LEU:C	1:C:223:LEU:CD1	2.48	0.86
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.56	0.86
1:B:105:PHE:CD2	1:B:213:VAL:HG12	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:HD23	1:A:196:HIS:ND1	1.91	0.84
1:A:221:LEU:CB	1:A:222:PRO:HD3	2.00	0.84
1:C:118:ALA:CB	1:C:122:ARG:HB2	2.07	0.84
1:A:192:LEU:HB3	1:A:196:HIS:HB2	1.59	0.84
1:D:419:VAL:HG23	1:D:420:HIS:HD2	1.42	0.84
1:B:118:ALA:CB	1:B:122:ARG:HB2	2.07	0.84
1:B:119:PRO:CG	1:B:121:PRO:HD2	2.09	0.83
1:D:207:SER:HB3	1:D:229:CYS:SG	2.18	0.83
1:A:221:LEU:HG	1:A:222:PRO:HD2	1.57	0.83
1:A:105:PHE:CE2	1:A:213:VAL:HG12	2.14	0.82
1:B:208:LEU:HD21	1:B:461:VAL:HB	1.62	0.82
1:A:195:ARG:O	1:A:199:GLN:N	2.11	0.81
1:B:225:GLN:HE21	1:B:227:ALA:HB2	1.45	0.81
1:D:203:LYS:O	1:D:229:CYS:SG	2.39	0.80
1:D:298:ILE:CD1	1:D:461:VAL:HG12	2.11	0.80
1:C:218:LEU:O	1:C:223:LEU:HD12	1.82	0.80
1:D:223:LEU:N	1:D:224:PRO:HD2	1.96	0.80
1:D:176:ILE:HD13	1:D:293:GLN:HE21	1.46	0.80
1:A:193:ASN:CG	1:A:194:ALA:N	2.39	0.80
1:D:298:ILE:CD1	1:D:461:VAL:CG1	2.59	0.79
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.64	0.79
1:C:209:ILE:HB	1:C:210:PRO:HD2	1.64	0.79
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.65	0.79
1:A:210:PRO:CB	1:A:458:HIS:O	2.31	0.79
1:B:221:LEU:HG	1:C:50:LYS:NZ	1.98	0.79
1:A:221:LEU:HD11	1:A:222:PRO:CG	1.99	0.78
1:D:292:GLY:O	1:D:296:SER:HB2	1.82	0.78
1:D:124:ARG:HH22	1:D:420:HIS:CE1	2.01	0.78
1:A:157:ASN:HD21	1:A:197:PHE:HZ	1.32	0.78
1:D:207:SER:HB2	1:D:226:SER:HA	1.64	0.77
1:B:192:LEU:HB3	1:B:196:HIS:HB2	1.64	0.77
1:A:226:SER:O	1:A:230:ARG:HG2	1.84	0.77
1:B:118:ALA:HB1	1:B:122:ARG:HB2	1.67	0.77
1:C:150:VAL:O	1:C:154:MET:HG3	1.85	0.77
1:C:225:GLN:OE1	1:C:227:ALA:CB	2.33	0.77
1:D:102:VAL:O	1:D:213:VAL:CG1	2.33	0.76
1:D:192:LEU:HD12	1:D:192:LEU:O	1.85	0.76
1:B:363:VAL:HG23	1:B:378:ASP:O	1.86	0.76
1:D:109:VAL:HG11	1:D:290:PHE:CE2	2.20	0.75
1:B:118:ALA:HB1	1:B:119:PRO:CD	2.16	0.75
1:A:221:LEU:HD12	1:A:222:PRO:N	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ASN:OD1	1:B:194:ALA:N	2.19	0.74
1:C:218:LEU:C	1:C:223:LEU:HD13	2.12	0.74
2:C:501:HEM:CBD	2:C:501:HEM:HHA	2.17	0.74
1:A:192:LEU:HB3	1:A:196:HIS:CB	2.18	0.73
1:C:218:LEU:C	1:C:223:LEU:HD12	2.13	0.73
1:D:292:GLY:O	1:D:296:SER:CB	2.37	0.73
1:D:298:ILE:HD11	1:D:461:VAL:HG12	1.69	0.73
1:B:208:LEU:HD23	1:B:459:THR:HB	1.69	0.73
1:C:219:LEU:N	1:C:223:LEU:HD13	2.03	0.72
1:A:192:LEU:HB3	1:A:196:HIS:CG	2.24	0.72
1:D:124:ARG:NH2	1:D:420:HIS:CE1	2.57	0.72
1:B:192:LEU:HB3	1:B:196:HIS:CG	2.24	0.71
1:D:460:MET:SD	1:D:461:VAL:N	2.63	0.71
1:B:105:PHE:CE2	1:B:213:VAL:HG12	2.25	0.71
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.70	0.70
1:D:448:LEU:HD12	1:D:448:LEU:O	1.90	0.70
1:D:176:ILE:CD1	1:D:293:GLN:HE21	2.04	0.70
1:B:192:LEU:HB3	1:B:196:HIS:CB	2.21	0.70
1:D:100:ARG:HG3	1:D:116:TYR:O	1.92	0.70
1:C:176:ILE:HG21	1:C:196:HIS:HA	1.72	0.70
1:D:221:LEU:HD23	1:D:230:ARG:HH22	1.56	0.69
1:D:291:ALA:O	1:D:295:THR:OG1	2.10	0.69
1:A:223:LEU:C	1:A:223:LEU:HD12	2.16	0.69
1:D:203:LYS:HD2	1:D:232:ALA:HB2	1.74	0.69
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.74	0.69
1:C:154:MET:CG	1:C:158:TRP:CZ3	2.75	0.68
1:B:208:LEU:CD2	1:B:459:THR:HB	2.23	0.68
1:A:196:HIS:HA	1:A:200:LEU:H	1.56	0.68
1:C:158:TRP:CE3	1:C:443:TYR:CE2	2.82	0.68
1:B:196:HIS:HA	1:B:200:LEU:H	1.58	0.68
1:B:221:LEU:HG	1:C:50:LYS:HZ1	1.58	0.68
1:B:157:ASN:HD21	1:B:197:PHE:HZ	1.41	0.67
1:C:122:ARG:O	1:C:126:GLN:CG	2.43	0.66
1:A:176:ILE:HD12	1:A:293:GLN:HG3	1.76	0.66
1:D:209:ILE:N	1:D:209:ILE:HD12	2.10	0.66
1:A:108:PRO:O	1:A:230:ARG:HD2	1.96	0.66
1:C:247:ARG:NH2	1:D:186:GLU:OE2	2.28	0.66
1:D:113:GLY:H	1:D:117:ALA:CB	2.09	0.66
1:A:224:PRO:HB2	1:A:225:GLN:OE1	1.96	0.66
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.25	0.66
1:D:207:SER:CB	1:D:226:SER:HA	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PHE:CG	1:B:213:VAL:HG12	2.30	0.65
1:C:195:ARG:HA	1:C:199:GLN:HB2	1.78	0.65
1:B:272:ASP:OD1	1:B:272:ASP:N	2.25	0.65
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.79	0.65
1:C:176:ILE:HD12	1:C:293:GLN:HG3	1.78	0.65
1:D:51:ASN:ND2	1:D:54:GLU:HG3	2.12	0.65
1:B:176:ILE:HD12	1:B:293:GLN:HG3	1.78	0.64
1:B:363:VAL:HG21	1:B:378:ASP:HB2	1.78	0.64
3:B:502:DVE:C21	3:B:502:DVE:C17	2.72	0.64
1:A:322:GLU:CD	1:A:340:PRO:HD2	2.22	0.64
1:C:218:LEU:O	1:C:223:LEU:CD1	2.44	0.64
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.27	0.64
1:C:154:MET:HB3	1:C:158:TRP:CZ3	2.33	0.63
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.28	0.63
1:D:105:PHE:HA	1:D:219:LEU:HD11	1.81	0.63
1:D:109:VAL:CG1	1:D:290:PHE:CE2	2.81	0.63
1:D:102:VAL:O	1:D:213:VAL:HG11	1.99	0.62
1:A:195:ARG:O	1:A:199:GLN:CA	2.47	0.62
1:B:225:GLN:HE21	1:B:227:ALA:HB3	1.63	0.62
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.80	0.62
1:B:351:ARG:HA	1:B:388:HIS:HD2	1.65	0.62
1:A:105:PHE:CG	1:A:213:VAL:HG12	2.35	0.62
1:C:154:MET:CB	1:C:158:TRP:CZ3	2.83	0.62
1:D:113:GLY:H	1:D:117:ALA:HB3	1.65	0.62
1:A:357:LEU:HD21	1:A:462:VAL:HG21	1.82	0.62
1:B:195:ARG:O	1:B:199:GLN:CB	2.48	0.62
1:D:111:GLY:C	1:D:114:VAL:HG23	2.25	0.61
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.29	0.61
1:C:123:MET:O	1:C:127:LEU:HB2	2.01	0.61
1:C:287:ALA:HB1	3:C:502:DVE:C32	2.30	0.61
1:D:448:LEU:HD21	1:D:470:LEU:HB3	1.83	0.61
1:A:221:LEU:HD12	1:A:222:PRO:CB	2.29	0.61
1:B:194:ALA:HA	1:B:197:PHE:HB3	1.83	0.61
1:D:122:ARG:O	1:D:126:GLN:HG3	2.00	0.60
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.31	0.60
1:C:120:TYR:CB	1:C:121:PRO:HD3	2.31	0.60
1:C:228:ARG:HD2	1:C:228:ARG:N	2.16	0.60
1:D:351:ARG:HA	1:D:388:HIS:HD2	1.65	0.60
1:B:215:MET:HB3	1:B:218:LEU:CD2	2.31	0.60
1:B:228:ARG:HD2	1:B:228:ARG:N	2.17	0.60
1:B:221:LEU:HB3	1:B:222:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ILE:HD11	1:D:461:VAL:CG1	2.29	0.60
1:D:292:GLY:O	1:D:296:SER:OG	2.20	0.60
1:D:207:SER:HB2	1:D:226:SER:CB	2.32	0.60
2:C:501:HEM:HHA	2:C:501:HEM:HBD1	1.83	0.59
1:D:109:VAL:CG1	1:D:290:PHE:HE2	2.15	0.59
1:C:234:ALA:HA	1:C:282:CYS:SG	2.43	0.59
1:B:221:LEU:HD21	1:C:50:LYS:HE2	1.84	0.59
1:B:222:PRO:HG3	1:C:46:VAL:CA	2.19	0.59
1:A:223:LEU:CD1	1:A:227:ALA:H	1.93	0.59
1:D:51:ASN:HD21	1:D:54:GLU:HG3	1.68	0.59
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.33	0.59
1:B:357:LEU:HD21	1:B:462:VAL:HG21	1.84	0.59
1:D:222:PRO:CG	1:D:226:SER:HB3	2.32	0.59
1:D:384:PRO:O	1:D:388:HIS:ND1	2.35	0.59
1:D:207:SER:HB2	1:D:226:SER:CA	2.32	0.58
1:D:114:VAL:O	1:D:126:GLN:NE2	2.37	0.58
1:D:207:SER:HB3	1:D:229:CYS:CB	2.34	0.58
1:A:193:ASN:OD1	1:A:194:ALA:N	2.35	0.58
1:C:384:PRO:O	1:C:388:HIS:ND1	2.36	0.58
1:A:105:PHE:CE2	1:A:213:VAL:CG1	2.84	0.58
1:A:192:LEU:CD2	1:A:196:HIS:ND1	2.63	0.58
1:C:351:ARG:HA	1:C:388:HIS:HD2	1.68	0.58
1:B:270:TYR:HB3	1:B:272:ASP:OD1	2.04	0.58
1:B:384:PRO:O	1:B:388:HIS:ND1	2.37	0.58
1:C:357:LEU:HD21	1:C:462:VAL:HG21	1.86	0.57
1:D:120:TYR:HB2	1:D:121:PRO:HD3	1.85	0.57
1:D:221:LEU:CD2	1:D:230:ARG:HH22	2.16	0.57
1:B:363:VAL:HG23	1:B:378:ASP:C	2.29	0.57
2:D:501:HEM:HBB2	2:D:501:HEM:CMB	2.34	0.57
1:C:158:TRP:CZ3	1:C:443:TYR:CE2	2.93	0.57
2:C:501:HEM:HHA	2:C:501:HEM:HBD2	1.87	0.57
1:B:199:GLN:HE21	1:B:203:LYS:HE2	1.70	0.56
1:A:419:VAL:HG23	1:A:420:HIS:CD2	2.41	0.56
1:B:118:ALA:HB1	1:B:122:ARG:HD2	1.87	0.56
1:D:176:ILE:HD13	1:D:293:GLN:NE2	2.18	0.56
1:D:286:VAL:CG1	1:D:290:PHE:CE2	2.88	0.56
1:C:215:MET:HB3	1:C:218:LEU:CD2	2.36	0.56
1:A:113:GLY:O	1:A:126:GLN:NE2	2.38	0.56
1:C:219:LEU:HA	1:C:223:LEU:CD1	2.23	0.56
1:D:223:LEU:N	1:D:224:PRO:CD	2.68	0.56
1:A:105:PHE:CZ	1:A:213:VAL:CG1	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PRO:CB	1:B:121:PRO:HD2	2.35	0.55
1:D:256:ASN:HD22	1:D:256:ASN:C	2.13	0.55
1:B:208:LEU:HD11	1:B:294:HIS:CD2	2.42	0.55
1:B:419:VAL:HG23	1:B:420:HIS:CD2	2.42	0.55
2:C:501:HEM:HBB2	2:C:501:HEM:CMB	2.35	0.55
1:A:192:LEU:HD23	1:A:196:HIS:CG	2.42	0.55
1:D:184:PHE:CE2	1:D:289:MET:HE3	2.42	0.55
1:B:234:ALA:HA	1:B:282:CYS:SG	2.46	0.54
1:B:105:PHE:CZ	1:B:213:VAL:CG1	2.90	0.54
1:C:175:ILE:HG21	1:C:293:GLN:HA	1.89	0.54
1:B:102:VAL:HG11	1:B:360:MET:HB2	1.90	0.54
1:D:448:LEU:HG	1:D:470:LEU:O	2.08	0.54
1:A:256:ASN:HD22	1:A:256:ASN:C	2.12	0.54
1:A:322:GLU:OE1	1:A:340:PRO:HD2	2.08	0.54
1:B:105:PHE:CE2	1:B:213:VAL:CG1	2.90	0.54
1:D:94:ASN:HB3	1:D:120:TYR:CE1	2.42	0.54
1:B:175:ILE:CG2	1:B:293:GLN:HA	2.38	0.54
1:B:208:LEU:CD1	1:B:294:HIS:NE2	2.71	0.54
1:D:357:LEU:HD21	1:D:462:VAL:HG21	1.88	0.54
1:B:197:PHE:CD1	1:B:197:PHE:C	2.85	0.54
1:C:73:GLY:HA3	1:C:215:MET:SD	2.48	0.54
1:D:120:TYR:HA	1:D:123:MET:HG2	1.90	0.54
1:A:120:TYR:HB3	1:A:121:PRO:HD3	1.90	0.54
1:B:175:ILE:HG21	1:B:293:GLN:HA	1.89	0.54
1:C:175:ILE:CG2	1:C:293:GLN:HA	2.38	0.53
1:D:180:CYS:HA	1:D:289:MET:HE1	1.90	0.53
1:B:118:ALA:CB	1:B:122:ARG:HD2	2.38	0.53
1:A:143:VAL:HB	1:A:144:PRO:HD3	1.91	0.53
1:A:175:ILE:HG21	1:A:293:GLN:HA	1.90	0.53
1:C:123:MET:O	1:C:127:LEU:CB	2.56	0.53
1:A:384:PRO:O	1:A:388:HIS:CD2	2.61	0.53
1:C:83:PRO:HA	1:C:86:HIS:CE1	2.43	0.53
1:C:102:VAL:HG11	1:C:360:MET:HB2	1.90	0.53
1:C:123:MET:O	1:C:127:LEU:CG	2.56	0.53
1:C:359:VAL:HG13	2:C:501:HEM:CGA	2.39	0.53
1:B:389:HIS:HD2	1:B:397:PRO:HB2	1.73	0.53
1:C:419:VAL:HG23	1:C:420:HIS:CD2	2.44	0.53
1:B:193:ASN:ND2	1:B:194:ALA:H	2.03	0.53
1:B:225:GLN:NE2	1:B:227:ALA:CB	2.64	0.53
1:D:237:GLN:HB2	1:D:282:CYS:SG	2.49	0.53
1:C:118:ALA:CB	1:C:122:ARG:CB	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:HH21	1:A:286:VAL:HG11	1.74	0.52
1:B:193:ASN:O	1:B:197:PHE:CB	2.57	0.52
1:C:91:SER:HB2	1:C:92:PRO:HD3	1.92	0.52
1:C:143:VAL:HB	1:C:144:PRO:HD3	1.91	0.52
1:D:99:PRO:HG3	1:D:420:HIS:CE1	2.44	0.52
1:D:143:VAL:HB	1:D:144:PRO:HD3	1.90	0.52
1:A:175:ILE:CG2	1:A:293:GLN:HA	2.38	0.52
1:B:143:VAL:HB	1:B:144:PRO:HD3	1.90	0.52
1:D:51:ASN:HD22	1:D:54:GLU:HB2	1.74	0.52
1:A:240:LEU:HA	1:A:243:ILE:HG22	1.91	0.52
1:B:83:PRO:HA	1:B:86:HIS:CE1	2.44	0.52
1:D:258:THR:HG22	1:D:260:ASP:CG	2.34	0.52
1:D:192:LEU:O	1:D:192:LEU:CD1	2.57	0.52
1:C:118:ALA:HB2	1:C:122:ARG:HG3	1.91	0.52
1:D:175:ILE:HG21	1:D:293:GLN:HA	1.92	0.52
1:B:193:ASN:O	1:B:197:PHE:HB2	2.10	0.52
1:D:83:PRO:HA	1:D:86:HIS:CE1	2.45	0.52
1:A:83:PRO:HA	1:A:86:HIS:CE1	2.45	0.52
1:A:192:LEU:CB	1:A:196:HIS:CG	2.92	0.52
1:B:118:ALA:CB	1:B:119:PRO:HD2	2.17	0.52
1:A:73:GLY:HA3	1:A:215:MET:SD	2.50	0.51
1:A:102:VAL:HG11	1:A:360:MET:HB2	1.91	0.51
1:A:226:SER:O	1:A:230:ARG:CG	2.57	0.51
1:D:91:SER:HB2	1:D:92:PRO:HD3	1.93	0.51
1:B:73:GLY:HA3	1:B:215:MET:SD	2.51	0.51
1:B:118:ALA:HB3	1:B:122:ARG:HB2	1.91	0.51
1:B:240:LEU:HA	1:B:243:ILE:HG22	1.93	0.51
1:D:111:GLY:C	1:D:114:VAL:CG2	2.84	0.51
1:D:109:VAL:CG2	1:D:208:LEU:HD21	2.40	0.51
1:B:208:LEU:HD11	1:B:294:HIS:NE2	2.25	0.51
1:C:256:ASN:HD22	1:C:256:ASN:C	2.13	0.51
1:D:213:VAL:HG23	1:D:214:PHE:N	2.26	0.51
1:B:195:ARG:O	1:B:199:GLN:CA	2.59	0.51
1:D:222:PRO:CB	1:D:226:SER:HB3	2.41	0.50
2:A:501:HEM:HBD2	2:A:501:HEM:HHA	1.94	0.50
1:B:119:PRO:HB2	1:B:121:PRO:HD2	1.94	0.50
1:D:196:HIS:CE1	1:D:200:LEU:HD11	2.46	0.50
1:C:158:TRP:HE3	1:C:443:TYR:CZ	2.30	0.50
1:D:459:THR:HB	1:D:460:MET:SD	2.51	0.50
1:D:298:ILE:HD12	1:D:461:VAL:CG1	2.42	0.50
1:A:91:SER:HB2	1:A:92:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:MET:HG2	1:D:218:LEU:HD11	1.93	0.50
1:B:210:PRO:CB	1:B:458:HIS:O	2.60	0.50
1:B:192:LEU:HG	1:B:196:HIS:CE1	2.47	0.50
1:D:184:PHE:CZ	1:D:289:MET:HE3	2.47	0.50
1:C:209:ILE:HB	1:C:210:PRO:CD	2.39	0.50
1:C:240:LEU:HA	1:C:243:ILE:HG22	1.93	0.50
1:C:154:MET:HB3	1:C:158:TRP:CE3	2.46	0.49
1:A:35:TYR:CG	1:A:36:PRO:HD2	2.46	0.49
1:B:35:TYR:CG	1:B:36:PRO:HD2	2.46	0.49
1:B:98:SER:O	1:B:362:MET:N	2.37	0.49
1:C:192:LEU:HG	1:C:195:ARG:CB	2.42	0.49
1:D:35:TYR:CG	1:D:36:PRO:HD2	2.47	0.49
1:D:256:ASN:O	1:D:256:ASN:ND2	2.26	0.49
1:D:271:ARG:O	1:D:271:ARG:HD3	2.12	0.49
1:B:192:LEU:CB	1:B:196:HIS:CG	2.94	0.49
1:D:102:VAL:HG11	1:D:360:MET:HB2	1.95	0.49
1:A:126:GLN:HA	1:A:129:PHE:CD2	2.47	0.49
1:B:210:PRO:HB3	1:B:458:HIS:O	2.13	0.49
1:A:237:GLN:NE2	1:A:282:CYS:O	2.46	0.49
1:B:188:LEU:O	1:B:192:LEU:HD13	2.13	0.49
1:C:35:TYR:CG	1:C:36:PRO:HD2	2.47	0.49
1:C:176:ILE:HG21	1:C:196:HIS:CA	2.42	0.48
1:D:113:GLY:N	1:D:117:ALA:HB3	2.27	0.48
1:B:91:SER:HB2	1:B:92:PRO:HD3	1.94	0.48
1:C:256:ASN:O	1:C:256:ASN:ND2	2.25	0.48
1:A:219:LEU:C	1:A:219:LEU:HD12	2.37	0.48
1:A:351:ARG:HA	1:A:388:HIS:HD1	1.77	0.48
1:C:123:MET:O	1:C:127:LEU:HD12	2.13	0.48
1:B:237:GLN:NE2	1:B:282:CYS:O	2.46	0.48
1:D:111:GLY:CA	1:D:114:VAL:HG21	2.44	0.48
1:B:221:LEU:CD2	1:C:50:LYS:HE2	2.44	0.48
1:C:237:GLN:NE2	1:C:282:CYS:O	2.46	0.48
1:A:194:ALA:HA	1:A:197:PHE:HB3	1.97	0.47
1:A:196:HIS:CE1	1:A:200:LEU:HD13	2.49	0.47
1:A:340:PRO:HG2	1:A:341:PHE:H	1.79	0.47
1:A:256:ASN:O	1:A:256:ASN:ND2	2.25	0.47
1:C:154:MET:CE	1:C:158:TRP:HZ3	2.27	0.47
1:D:184:PHE:CE1	1:D:285:ILE:HG23	2.49	0.47
1:D:51:ASN:ND2	1:D:54:GLU:CG	2.77	0.47
1:D:215:MET:HG3	1:D:218:LEU:HG	1.96	0.47
1:C:120:TYR:H	1:C:121:PRO:CD	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:GLU:HA	1:D:104:THR:HG23	1.96	0.47
1:D:115:ALA:O	1:D:116:TYR:HB2	2.14	0.47
1:B:194:ALA:CA	1:B:197:PHE:HB3	2.44	0.47
1:B:256:ASN:HD22	1:B:256:ASN:C	2.13	0.47
1:C:181:GLN:HE21	1:C:181:GLN:HA	1.80	0.47
1:D:109:VAL:HG12	1:D:290:PHE:HE2	1.80	0.47
1:B:120:TYR:N	1:B:121:PRO:CD	2.77	0.46
1:C:226:SER:HB2	1:C:229:CYS:HB2	1.97	0.46
1:A:223:LEU:HD12	1:A:223:LEU:O	2.15	0.46
1:C:218:LEU:HB3	1:C:223:LEU:CD1	2.45	0.46
1:C:270:TYR:HD2	1:C:274:THR:HG23	1.80	0.46
1:C:120:TYR:CB	1:C:121:PRO:CD	2.94	0.46
1:D:98:SER:O	1:D:362:MET:N	2.37	0.46
1:D:351:ARG:HA	1:D:388:HIS:CD2	2.49	0.46
1:A:98:SER:O	1:A:362:MET:N	2.37	0.46
1:D:207:SER:HB2	1:D:226:SER:OG	2.15	0.46
1:B:351:ARG:HA	1:B:388:HIS:CD2	2.49	0.46
1:C:50:LYS:HD3	1:C:50:LYS:HA	1.78	0.46
1:C:158:TRP:HE3	1:C:443:TYR:CE2	2.31	0.46
1:A:120:TYR:CE2	1:A:124:ARG:HG3	2.50	0.46
1:D:175:ILE:CG2	1:D:293:GLN:HA	2.46	0.46
1:D:298:ILE:CD1	1:D:461:VAL:HG11	2.44	0.46
1:C:150:VAL:HG12	1:C:154:MET:SD	2.56	0.46
1:C:218:LEU:HB3	1:C:223:LEU:HD11	1.98	0.46
1:B:32:PRO:HA	1:B:33:PRO:HD3	1.85	0.46
1:C:118:ALA:HB2	1:C:122:ARG:CG	2.46	0.46
1:A:181:GLN:HA	1:A:181:GLN:HE21	1.81	0.45
1:B:196:HIS:CE1	1:B:200:LEU:HD13	2.50	0.45
1:B:215:MET:HE3	1:B:218:LEU:HD21	1.98	0.45
1:B:270:TYR:HD2	1:B:274:THR:HG23	1.81	0.45
1:D:109:VAL:HG23	1:D:208:LEU:HD21	1.98	0.45
1:D:219:LEU:O	1:D:219:LEU:HD23	2.17	0.45
1:B:221:LEU:HG	1:C:50:LYS:HZ3	1.80	0.45
1:B:225:GLN:NE2	1:B:227:ALA:HB2	2.24	0.45
1:C:220:ARG:O	1:C:221:LEU:C	2.59	0.45
1:B:184:PHE:CZ	1:B:261:LEU:HD23	2.51	0.45
1:C:210:PRO:C	1:C:212:ALA:H	2.25	0.45
1:A:184:PHE:CZ	1:A:261:LEU:HD23	2.51	0.45
1:D:250:GLU:N	1:D:250:GLU:OE1	2.50	0.45
1:A:218:LEU:O	1:A:222:PRO:HD2	2.17	0.45
1:B:220:ARG:O	1:B:221:LEU:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:TYR:H	1:C:121:PRO:HD2	1.81	0.45
1:D:389:HIS:ND1	1:D:397:PRO:HB2	2.32	0.45
1:C:221:LEU:HB3	1:C:222:PRO:HD3	1.98	0.45
1:A:102:VAL:HG11	1:A:360:MET:CB	2.47	0.45
1:A:270:TYR:HD2	1:A:274:THR:HG23	1.81	0.45
1:A:389:HIS:ND1	1:A:397:PRO:HB2	2.32	0.45
1:B:194:ALA:C	1:B:197:PHE:HB3	2.41	0.45
1:B:256:ASN:O	1:B:256:ASN:ND2	2.25	0.45
1:A:192:LEU:HG	1:A:196:HIS:CE1	2.52	0.45
1:D:113:GLY:H	1:D:117:ALA:HB1	1.82	0.45
1:B:181:GLN:HA	1:B:181:GLN:HE21	1.80	0.45
1:B:188:LEU:O	1:B:189:ARG:C	2.60	0.45
1:C:223:LEU:HD23	1:C:224:PRO:HD2	1.99	0.45
1:A:196:HIS:ND1	1:A:200:LEU:HB2	2.32	0.44
1:A:309:HIS:CD2	1:A:310:PRO:HD2	2.52	0.44
1:B:276:MET:HB3	1:B:281:VAL:HG13	1.99	0.44
1:C:158:TRP:CE3	1:C:443:TYR:CZ	3.03	0.44
1:C:276:MET:HB3	1:C:281:VAL:HG13	1.99	0.44
1:D:51:ASN:ND2	1:D:54:GLU:HB2	2.33	0.44
1:C:122:ARG:O	1:C:126:GLN:CB	2.66	0.44
1:C:309:HIS:CD2	1:C:310:PRO:HD2	2.53	0.44
1:D:222:PRO:HB2	1:D:226:SER:HB3	2.00	0.44
1:B:215:MET:HB3	1:B:218:LEU:HD23	1.98	0.44
1:C:195:ARG:CB	1:C:200:LEU:HB2	2.47	0.44
1:C:184:PHE:CZ	1:C:261:LEU:HD23	2.53	0.44
1:A:209:ILE:HA	1:A:210:PRO:HD3	1.64	0.44
1:B:102:VAL:HG11	1:B:360:MET:CB	2.47	0.44
1:C:388:HIS:CE1	1:C:413:ILE:H	2.36	0.44
1:C:389:HIS:ND1	1:C:397:PRO:HB2	2.32	0.44
1:C:188:LEU:O	1:C:189:ARG:C	2.61	0.44
1:B:192:LEU:HD23	1:B:196:HIS:ND1	2.33	0.43
1:C:192:LEU:HB3	1:C:196:HIS:NE2	2.33	0.43
1:B:389:HIS:CD2	1:B:397:PRO:HB2	2.52	0.43
1:D:254:LYS:HE2	1:D:254:LYS:HA	1.99	0.43
1:A:114:VAL:HG12	1:A:284:MET:HG2	2.00	0.43
1:B:199:GLN:HE21	1:B:203:LYS:CE	2.31	0.43
1:C:32:PRO:HA	1:C:33:PRO:HD3	1.85	0.43
1:C:118:ALA:CB	1:C:122:ARG:CG	2.97	0.43
1:D:109:VAL:HG11	1:D:290:PHE:CZ	2.52	0.43
1:D:388:HIS:CE1	1:D:413:ILE:H	2.36	0.43
1:B:225:GLN:CD	1:B:225:GLN:C	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:HIS:CD2	1:B:310:PRO:HD2	2.53	0.43
1:B:422:CYS:HA	2:B:501:HEM:C4D	2.53	0.43
1:D:213:VAL:CG2	1:D:214:PHE:N	2.81	0.43
1:D:265:LEU:HD13	1:D:281:VAL:HG13	2.00	0.43
1:B:225:GLN:NE2	1:B:227:ALA:HB3	2.29	0.43
1:B:226:SER:HB2	1:B:229:CYS:HB2	2.00	0.43
1:C:448:LEU:HD12	1:C:470:LEU:HB3	2.00	0.43
1:C:195:ARG:CA	1:C:200:LEU:H	2.32	0.43
1:A:188:LEU:O	1:A:189:ARG:C	2.60	0.43
1:C:452:VAL:HG13	1:C:453:PRO:HD2	2.01	0.43
1:D:120:TYR:HA	1:D:123:MET:CG	2.48	0.43
1:B:157:ASN:ND2	1:B:197:PHE:HZ	2.12	0.43
1:B:188:LEU:C	1:B:190:LYS:N	2.77	0.43
1:C:102:VAL:HG11	1:C:360:MET:CB	2.48	0.43
1:C:98:SER:O	1:C:362:MET:N	2.37	0.42
1:C:287:ALA:CB	3:C:502:DVE:C32	2.97	0.42
1:C:352:ARG:NH1	1:C:353:ASP:OD2	2.52	0.42
1:D:94:ASN:HB3	1:D:120:TYR:CD1	2.53	0.42
1:D:352:ARG:NH1	1:D:353:ASP:OD2	2.52	0.42
1:A:223:LEU:CD1	1:A:227:ALA:N	2.60	0.42
1:B:388:HIS:CE1	1:B:413:ILE:H	2.36	0.42
1:C:223:LEU:HG	1:C:224:PRO:HD2	2.02	0.42
1:B:209:ILE:HD12	1:B:219:LEU:HD23	2.01	0.42
1:B:448:LEU:O	1:B:449:ARG:HG3	2.20	0.42
1:C:199:GLN:O	1:C:203:LYS:N	2.31	0.42
1:D:357:LEU:HD22	1:D:385:LEU:HD22	2.01	0.42
1:A:197:PHE:CD1	1:A:197:PHE:C	2.97	0.42
1:B:348:GLU:OE1	1:B:348:GLU:HA	2.20	0.42
1:B:352:ARG:NH1	1:B:353:ASP:OD2	2.53	0.42
1:C:122:ARG:O	1:C:126:GLN:HG2	2.19	0.42
1:A:196:HIS:HE2	1:A:236:LEU:CD2	2.32	0.42
1:B:120:TYR:O	1:B:124:ARG:HB2	2.19	0.42
1:C:448:LEU:O	1:C:449:ARG:HG3	2.19	0.42
1:B:105:PHE:CZ	1:B:213:VAL:HG11	2.54	0.42
1:C:186:GLU:HA	1:C:186:GLU:OE2	2.20	0.42
1:A:199:GLN:HE21	1:A:203:LYS:CE	2.33	0.42
1:A:352:ARG:NH1	1:A:353:ASP:OD2	2.53	0.42
1:C:348:GLU:HA	1:C:348:GLU:OE1	2.20	0.42
1:D:105:PHE:HA	1:D:219:LEU:CD1	2.48	0.42
1:D:276:MET:HE2	1:D:276:MET:HB3	1.95	0.42
1:A:348:GLU:HA	1:A:348:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HG13	1:A:453:PRO:HD2	2.02	0.41
1:B:173:ALA:O	1:B:174:MET:C	2.64	0.41
2:C:501:HEM:HMC2	2:C:501:HEM:CBC	2.45	0.41
1:D:114:VAL:O	1:D:126:GLN:CD	2.64	0.41
1:D:348:GLU:OE1	1:D:348:GLU:HA	2.20	0.41
1:C:122:ARG:O	1:C:126:GLN:HG3	2.17	0.41
1:D:114:VAL:HG11	1:D:283:GLY:HA3	2.02	0.41
1:D:188:LEU:O	1:D:189:ARG:C	2.63	0.41
1:A:276:MET:HB3	1:A:281:VAL:HG13	2.02	0.41
1:A:119:PRO:O	1:A:120:TYR:C	2.62	0.41
1:A:188:LEU:C	1:A:190:LYS:N	2.76	0.41
1:A:199:GLN:HE21	1:A:203:LYS:HE2	1.85	0.41
1:C:126:GLN:NE2	1:C:270:TYR:OH	2.53	0.41
1:B:195:ARG:O	1:B:199:GLN:HB2	2.20	0.41
1:A:186:GLU:OE2	1:A:186:GLU:HA	2.20	0.41
1:B:363:VAL:HG21	1:B:378:ASP:CB	2.48	0.41
1:D:209:ILE:N	1:D:209:ILE:CD1	2.79	0.41
1:D:215:MET:HG2	1:D:218:LEU:CD1	2.51	0.41
1:D:448:LEU:O	1:D:449:ARG:HG3	2.21	0.41
1:B:114:VAL:HG12	1:B:284:MET:HG2	2.02	0.41
1:B:449:ARG:HD2	1:D:162:GLU:OE1	2.20	0.41
1:B:452:VAL:HG13	1:B:453:PRO:HD2	2.03	0.41
1:C:188:LEU:C	1:C:190:LYS:N	2.77	0.41
2:C:501:HEM:CBD	2:C:501:HEM:CHA	2.89	0.41
1:D:124:ARG:NH2	1:D:420:HIS:NE2	2.65	0.41
1:A:110:PHE:CD1	1:A:287:ALA:HB2	2.56	0.41
1:C:351:ARG:HA	1:C:388:HIS:CD2	2.51	0.41
1:D:286:VAL:HG12	1:D:290:PHE:CE2	2.55	0.41
1:B:186:GLU:HA	1:B:186:GLU:OE2	2.20	0.40
1:D:452:VAL:HG13	1:D:453:PRO:HD2	2.03	0.40
1:B:207:SER:OG	1:B:233:ARG:NH2	2.54	0.40
1:D:188:LEU:C	1:D:190:LYS:N	2.77	0.40
1:B:110:PHE:CD1	1:B:287:ALA:HB2	2.56	0.40
2:B:501:HEM:HHA	2:B:501:HEM:HBD2	2.03	0.40
1:D:247:ARG:NH2	1:D:260:ASP:OD2	2.47	0.40
1:A:173:ALA:O	1:A:174:MET:C	2.64	0.40
1:B:105:PHE:CE1	1:B:213:VAL:CG1	3.05	0.40
1:B:196:HIS:ND1	1:B:200:LEU:HD22	2.37	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	446/485 (92%)	421 (94%)	23 (5%)	2 (0%)	30	60
1	B	446/485 (92%)	417 (94%)	29 (6%)	0	100	100
1	C	446/485 (92%)	417 (94%)	27 (6%)	2 (0%)	30	60
1	D	446/485 (92%)	419 (94%)	25 (6%)	2 (0%)	30	60
All	All	1784/1940 (92%)	1674 (94%)	104 (6%)	6 (0%)	36	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	224	PRO
1	C	120	TYR
1	A	222	PRO
1	D	222	PRO
1	C	119	PRO
1	A	210	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	391/425 (92%)	376 (96%)	15 (4%)	29	59
1	B	370/425 (87%)	351 (95%)	19 (5%)	21	51
1	C	364/425 (86%)	346 (95%)	18 (5%)	22	52
1	D	391/425 (92%)	372 (95%)	19 (5%)	22	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1516/1700 (89%)	1445 (95%)	71 (5%)	23 54

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	107	THR
1	A	114	VAL
1	A	134	LEU
1	A	166	ASN
1	A	176	ILE
1	A	186	GLU
1	A	189	ARG
1	A	209	ILE
1	A	213	VAL
1	A	256	ASN
1	A	266	LEU
1	A	313	LYS
1	A	431	GLN
1	A	447	LEU
1	B	63	LEU
1	B	107	THR
1	B	134	LEU
1	B	166	ASN
1	B	176	ILE
1	B	186	GLU
1	B	189	ARG
1	B	197	PHE
1	B	208	LEU
1	B	213	VAL
1	B	218	LEU
1	B	219	LEU
1	B	256	ASN
1	B	272	ASP
1	B	313	LYS
1	B	431	GLN
1	B	447	LEU
1	B	452	VAL
1	B	478	LYS
1	C	107	THR
1	C	134	LEU
1	C	158	TRP

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Mol	Chain	Res	Type
1	C	166	ASN
1	C	176	ILE
1	C	186	GLU
1	C	189	ARG
1	C	218	LEU
1	C	219	LEU
1	C	223	LEU
1	C	225	GLN
1	C	256	ASN
1	C	266	LEU
1	C	313	LYS
1	C	431	GLN
1	C	447	LEU
1	C	452	VAL
1	C	478	LYS
1	D	63	LEU
1	D	93	ARG
1	D	107	THR
1	D	128	ASN
1	D	165	ILE
1	D	166	ASN
1	D	200	LEU
1	D	209	ILE
1	D	231	GLU
1	D	237	GLN
1	D	256	ASN
1	D	271	ARG
1	D	274	THR
1	D	278	LEU
1	D	293	GLN
1	D	431	GLN
1	D	447	LEU
1	D	452	VAL
1	D	460	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	237	GLN
1	A	257	ASN
1	A	306	HIS

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Mol	Chain	Res	Type
1	A	309	HIS
1	A	396	ASN
1	B	157	ASN
1	B	181	GLN
1	B	225	GLN
1	B	306	HIS
1	B	388	HIS
1	B	396	ASN
1	C	140	GLN
1	C	181	GLN
1	C	193	ASN
1	C	199	GLN
1	C	237	GLN
1	C	257	ASN
1	C	294	HIS
1	C	306	HIS
1	C	334	ASN
1	C	388	HIS
1	C	396	ASN
1	C	425	GLN
1	D	51	ASN
1	D	257	ASN
1	D	306	HIS
1	D	388	HIS
1	D	396	ASN
1	D	431	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

7 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
2	HEM	C	501	1	50,50,50	1.57	8 (16%)	67,82,82	1.73	13 (19%)
2	HEM	B	501	1	50,50,50	1.56	8 (16%)	67,82,82	1.93	14 (20%)
3	DVE	C	502	-	34,34,34	3.22	8 (23%)	53,55,55	1.64	12 (22%)
3	DVE	B	502	-	34,34,34	3.22	8 (23%)	53,55,55	1.85	14 (26%)
3	DVE	A	502	-	34,34,34	3.22	8 (23%)	53,55,55	1.65	12 (22%)
2	HEM	D	501	1	50,50,50	1.57	8 (16%)	67,82,82	1.65	11 (16%)
2	HEM	A	501	1	50,50,50	1.54	8 (16%)	67,82,82	1.88	15 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	501	1	-	6/14/54/54	-
2	HEM	B	501	1	-	2/14/54/54	-
3	DVE	C	502	-	-	1/13/81/81	0/4/4/4
3	DVE	B	502	-	-	2/13/81/81	0/4/4/4
3	DVE	A	502	-	-	1/13/81/81	0/4/4/4
2	HEM	D	501	1	-	2/14/54/54	-
2	HEM	A	501	1	-	2/14/54/54	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	DVE	C32-C28	10.19	1.53	1.32
3	A	502	DVE	C32-C28	10.19	1.53	1.32
3	C	502	DVE	C32-C28	10.19	1.53	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	DVE	C2-C12	-9.52	1.39	1.53
3	C	502	DVE	C2-C12	-9.48	1.40	1.53
3	A	502	DVE	C2-C12	-9.45	1.40	1.53
3	B	502	DVE	C21-C12	-6.66	1.40	1.51
3	A	502	DVE	C14-C13	-6.64	1.40	1.51
3	C	502	DVE	C14-C13	-6.61	1.40	1.51
3	A	502	DVE	C21-C12	-6.60	1.40	1.51
3	B	502	DVE	C14-C13	-6.60	1.40	1.51
3	C	502	DVE	C21-C12	-6.59	1.40	1.51
3	B	502	DVE	C16-C13	-6.27	1.39	1.52
3	A	502	DVE	C16-C13	-6.18	1.39	1.52
3	C	502	DVE	C16-C13	-6.18	1.39	1.52
2	C	501	HEM	FE-NB	5.05	2.10	1.94
2	B	501	HEM	FE-NB	5.02	2.10	1.94
2	D	501	HEM	FE-NB	4.92	2.10	1.94
2	A	501	HEM	FE-NB	4.74	2.09	1.94
2	C	501	HEM	FE-NC	4.51	2.10	1.95
2	B	501	HEM	FE-NC	4.43	2.09	1.95
2	A	501	HEM	FE-NC	4.41	2.09	1.95
2	D	501	HEM	FE-NC	4.40	2.09	1.95
2	A	501	HEM	C1B-NB	-3.71	1.33	1.40
2	D	501	HEM	C1B-NB	-3.68	1.33	1.40
2	B	501	HEM	C1B-NB	-3.56	1.34	1.40
2	C	501	HEM	C1B-NB	-3.49	1.34	1.40
2	D	501	HEM	C4D-ND	-3.23	1.34	1.40
2	C	501	HEM	C4D-ND	-2.98	1.35	1.40
2	B	501	HEM	C4D-ND	-2.86	1.35	1.40
2	A	501	HEM	C4D-ND	-2.82	1.35	1.40
3	A	502	DVE	C12-C13	2.82	1.40	1.34
3	C	502	DVE	C12-C13	2.82	1.40	1.34
3	B	502	DVE	C12-C13	2.67	1.39	1.34
2	D	501	HEM	FE-ND	-2.57	1.87	1.94
2	C	501	HEM	FE-ND	-2.52	1.87	1.94
3	C	502	DVE	C18-C16	-2.50	1.51	1.56
2	A	501	HEM	C4B-NB	-2.48	1.34	1.38
3	A	502	DVE	C18-C16	-2.46	1.51	1.56
2	B	501	HEM	FE-ND	-2.43	1.87	1.94
2	D	501	HEM	C4B-NB	-2.39	1.34	1.38
2	B	501	HEM	C4B-NB	-2.36	1.34	1.38
2	A	501	HEM	FE-ND	-2.31	1.87	1.94
2	C	501	HEM	C4B-NB	-2.31	1.34	1.38
3	A	502	DVE	C2-C1	-2.29	1.52	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	DVE	C2-C1	-2.28	1.52	1.56
3	B	502	DVE	C2-C1	-2.26	1.52	1.56
2	C	501	HEM	C1C-C2C	-2.25	1.40	1.45
3	B	502	DVE	C18-C16	-2.24	1.52	1.56
2	C	501	HEM	C1D-ND	-2.22	1.34	1.38
2	D	501	HEM	C1C-C2C	-2.20	1.41	1.45
2	B	501	HEM	C1D-ND	-2.18	1.34	1.38
2	A	501	HEM	C1C-C2C	-2.17	1.41	1.45
2	D	501	HEM	C1D-ND	-2.17	1.34	1.38
2	B	501	HEM	C1C-C2C	-2.15	1.41	1.45
2	A	501	HEM	C1D-ND	-2.12	1.34	1.38

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CHD-C1D-ND	6.18	131.07	124.42
2	A	501	HEM	CHD-C1D-ND	5.57	130.42	124.42
2	B	501	HEM	CAD-C3D-C4D	5.50	134.28	124.70
2	C	501	HEM	CHD-C1D-ND	5.43	130.27	124.42
3	A	502	DVE	C18-C22-C24	-5.43	112.89	119.28
3	C	502	DVE	C18-C22-C24	-5.40	112.92	119.28
3	B	502	DVE	C18-C22-C24	-5.27	113.08	119.28
2	C	501	HEM	CHC-C4B-NB	5.11	129.92	124.42
2	D	501	HEM	CHC-C4B-NB	4.94	129.74	124.42
2	A	501	HEM	CHC-C4B-NB	4.93	129.73	124.42
2	A	501	HEM	C1B-NB-C4B	4.89	111.00	105.21
2	B	501	HEM	CHC-C4B-NB	4.85	129.64	124.42
2	D	501	HEM	CHD-C1D-ND	4.84	129.63	124.42
2	B	501	HEM	CAD-C3D-C2D	-4.50	119.45	127.87
2	B	501	HEM	CHD-C1D-C2D	-4.45	118.00	125.03
2	A	501	HEM	CHD-C1D-C2D	-4.21	118.38	125.03
2	D	501	HEM	C1B-NB-C4B	4.20	110.18	105.21
2	A	501	HEM	CAD-C3D-C4D	4.17	131.97	124.70
2	B	501	HEM	C1B-NB-C4B	3.89	109.82	105.21
2	C	501	HEM	CHD-C1D-C2D	-3.86	118.93	125.03
2	D	501	HEM	CHA-C4D-ND	3.86	129.14	124.37
3	A	502	DVE	C5-C4-C2	-3.80	104.70	112.78
2	C	501	HEM	CAD-C3D-C4D	3.79	131.31	124.70
3	C	502	DVE	C5-C4-C2	-3.79	104.71	112.78
3	B	502	DVE	C21-C12-C2	3.77	121.61	116.05
2	A	501	HEM	C3B-C4B-NB	-3.60	106.88	109.47
2	D	501	HEM	CHD-C1D-C2D	-3.46	119.56	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	DVE	C15-C1-C2	-3.45	107.22	111.53
2	C	501	HEM	C1B-NB-C4B	3.37	109.20	105.21
2	C	501	HEM	CHA-C4D-ND	3.28	128.43	124.37
3	B	502	DVE	C16-C13-C12	-3.22	112.87	120.76
3	B	502	DVE	C14-C13-C16	3.14	120.72	116.56
3	B	502	DVE	C4-C2-C1	3.13	112.87	108.26
2	A	501	HEM	CAD-C3D-C2D	-3.08	122.09	127.87
2	D	501	HEM	CHA-C4D-C3D	-3.08	119.54	125.23
3	A	502	DVE	C15-C1-C2	-3.03	107.76	111.53
3	C	502	DVE	C15-C1-C2	-3.00	107.79	111.53
2	A	501	HEM	CHA-C4D-ND	3.00	128.07	124.37
2	D	501	HEM	C3B-C4B-NB	-2.99	107.32	109.47
3	A	502	DVE	C27-C26-C24	-2.88	109.08	114.46
3	C	502	DVE	C27-C26-C24	-2.87	109.10	114.46
3	A	502	DVE	C4-C2-C1	-2.86	104.05	108.26
3	C	502	DVE	C4-C2-C1	-2.85	104.06	108.26
2	A	501	HEM	CHA-C4D-C3D	-2.74	120.17	125.23
2	C	501	HEM	CHB-C1B-NB	2.73	127.74	124.37
3	B	502	DVE	C20-C18-C16	2.70	111.83	108.51
2	C	501	HEM	CHA-C4D-C3D	-2.69	120.27	125.23
3	A	502	DVE	C11-C9-C6	-2.68	108.21	111.35
2	B	501	HEM	CHA-C4D-ND	2.68	127.69	124.37
3	B	502	DVE	C27-C26-C24	-2.67	109.46	114.46
3	B	502	DVE	C21-C20-C18	-2.67	107.62	112.44
3	C	502	DVE	C11-C9-C6	-2.67	108.23	111.35
3	B	502	DVE	C18-C16-C13	-2.65	107.58	110.88
2	C	501	HEM	CAA-CBA-CGA	-2.64	106.67	113.67
2	D	501	HEM	CHB-C1B-NB	2.62	127.61	124.37
2	B	501	HEM	C3B-C4B-NB	-2.54	107.64	109.47
2	B	501	HEM	CHB-C1B-NB	2.54	127.51	124.37
2	A	501	HEM	CHB-C1B-NB	2.51	127.47	124.37
2	B	501	HEM	CAD-CBD-CGD	-2.49	107.06	113.67
2	A	501	HEM	C4C-CHD-C1D	-2.46	120.79	126.02
2	B	501	HEM	C4C-CHD-C1D	-2.45	120.80	126.02
2	D	501	HEM	C4C-CHD-C1D	-2.41	120.91	126.02
2	C	501	HEM	C1A-CHA-C4D	-2.40	120.60	126.25
3	C	502	DVE	C14-C15-C1	-2.36	107.12	111.70
2	D	501	HEM	C1A-CHA-C4D	-2.36	120.70	126.25
2	C	501	HEM	CAD-C3D-C2D	-2.35	123.46	127.87
3	B	502	DVE	C21-C12-C13	-2.35	116.45	121.99
2	A	501	HEM	C1A-CHA-C4D	-2.34	120.74	126.25
3	A	502	DVE	C14-C15-C1	-2.34	107.17	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	DVE	C35-C16-C13	-2.22	115.03	118.03
2	B	501	HEM	C1A-CHA-C4D	-2.22	121.04	126.25
3	A	502	DVE	C35-C16-C13	-2.20	115.06	118.03
3	A	502	DVE	C16-C13-C12	-2.20	115.37	120.76
3	C	502	DVE	C16-C13-C12	-2.19	115.39	120.76
3	C	502	DVE	C29-C28-C32	-2.15	117.25	123.59
3	B	502	DVE	C33-C24-C22	-2.15	109.66	112.88
3	A	502	DVE	C29-C28-C32	-2.15	117.27	123.59
2	A	501	HEM	CAA-CBA-CGA	-2.14	107.98	113.67
2	B	501	HEM	O2D-CGD-CBD	2.11	120.67	114.00
2	B	501	HEM	CHA-C4D-C3D	-2.08	121.39	125.23
2	C	501	HEM	C4C-CHD-C1D	-2.07	121.62	126.02
3	B	502	DVE	C1-C2-C12	-2.06	106.38	109.29
2	A	501	HEM	O2A-CGA-CBA	2.06	120.50	114.00
2	A	501	HEM	O2D-CGD-CBD	2.05	120.48	114.00
3	A	502	DVE	C15-C14-C13	-2.03	108.38	113.19
2	C	501	HEM	C3B-C4B-NB	-2.02	108.02	109.47
2	D	501	HEM	O2D-CGD-CBD	2.02	120.38	114.00
3	C	502	DVE	C15-C14-C13	-2.02	108.41	113.19
3	C	502	DVE	C18-C16-C13	-2.02	108.37	110.88
3	B	502	DVE	C15-C14-C13	-2.01	108.43	113.19
3	A	502	DVE	C18-C16-C13	-2.01	108.38	110.88

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2D-C3D-CAD-CBD
2	B	501	HEM	C2D-C3D-CAD-CBD
2	B	501	HEM	C4D-C3D-CAD-CBD
2	C	501	HEM	C2D-C3D-CAD-CBD
2	C	501	HEM	C4D-C3D-CAD-CBD
3	B	502	DVE	C27-C28-C29-C30
2	A	501	HEM	C4D-C3D-CAD-CBD
3	B	502	DVE	C18-C22-C24-C33
2	C	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O1D
3	A	502	DVE	C24-C26-C27-C28
3	C	502	DVE	C24-C26-C27-C28
2	C	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAA-CBA-CGA-O2A

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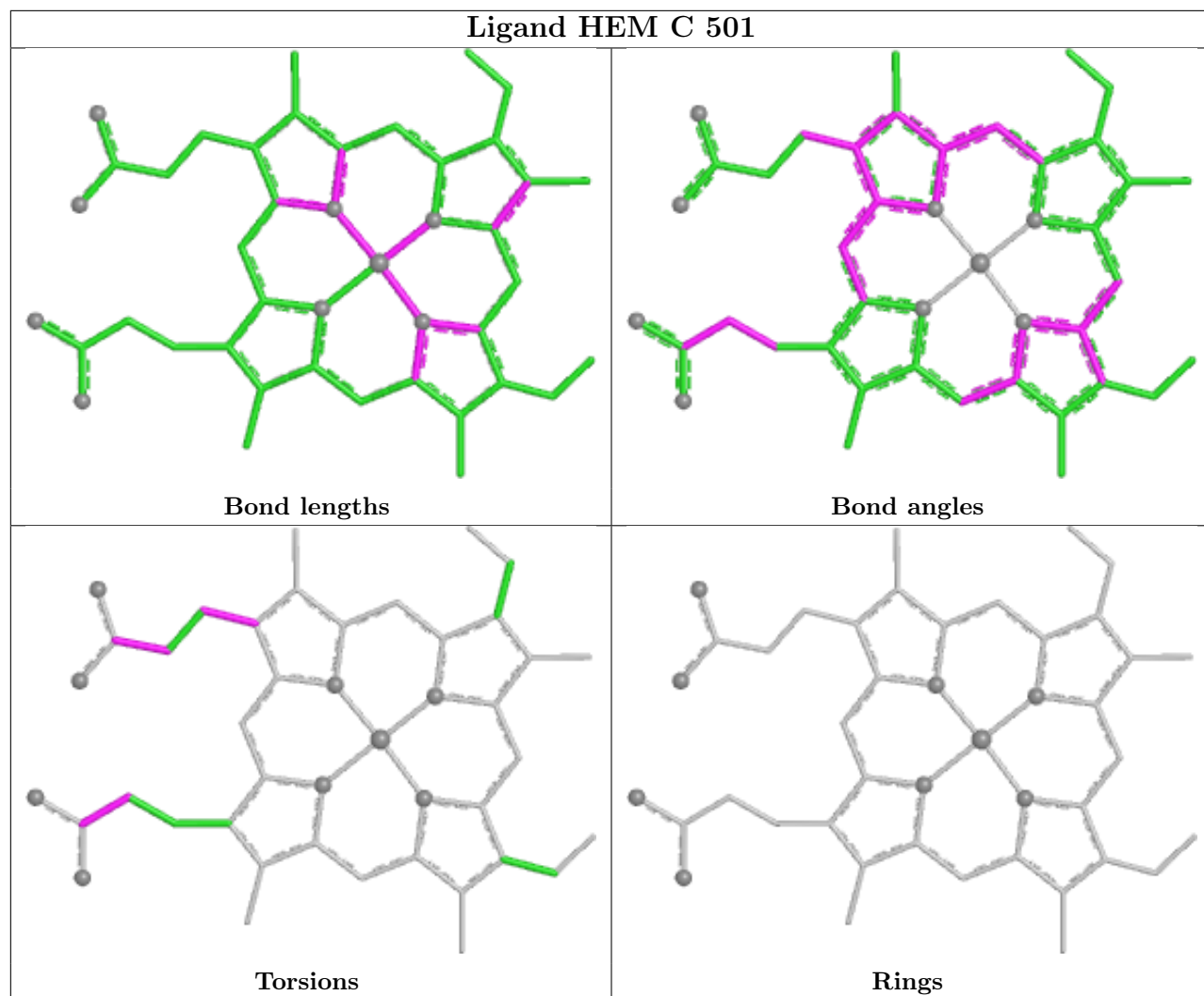
Mol	Chain	Res	Type	Atoms
2	C	501	HEM	CAA-CBA-CGA-O1A

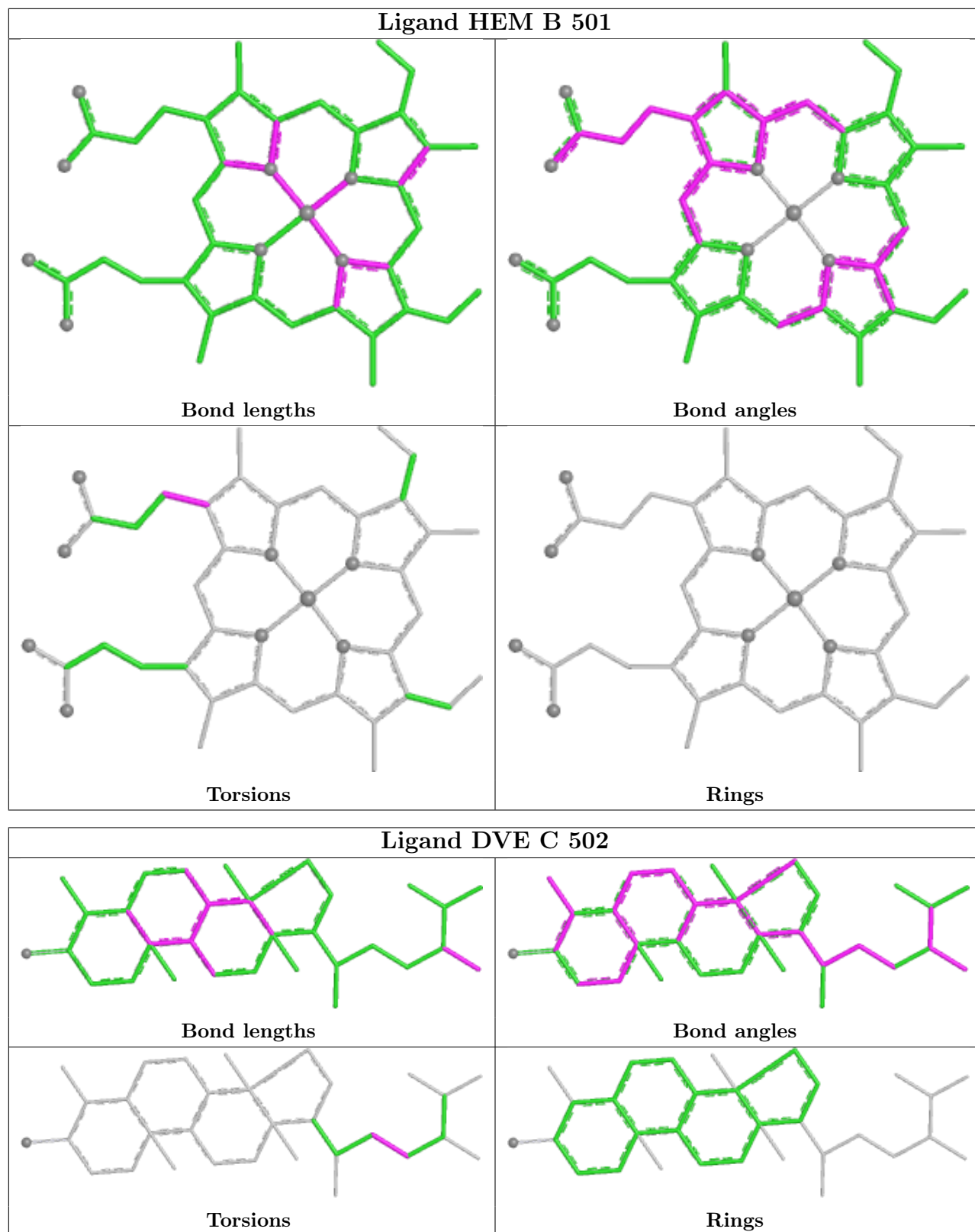
There are no ring outliers.

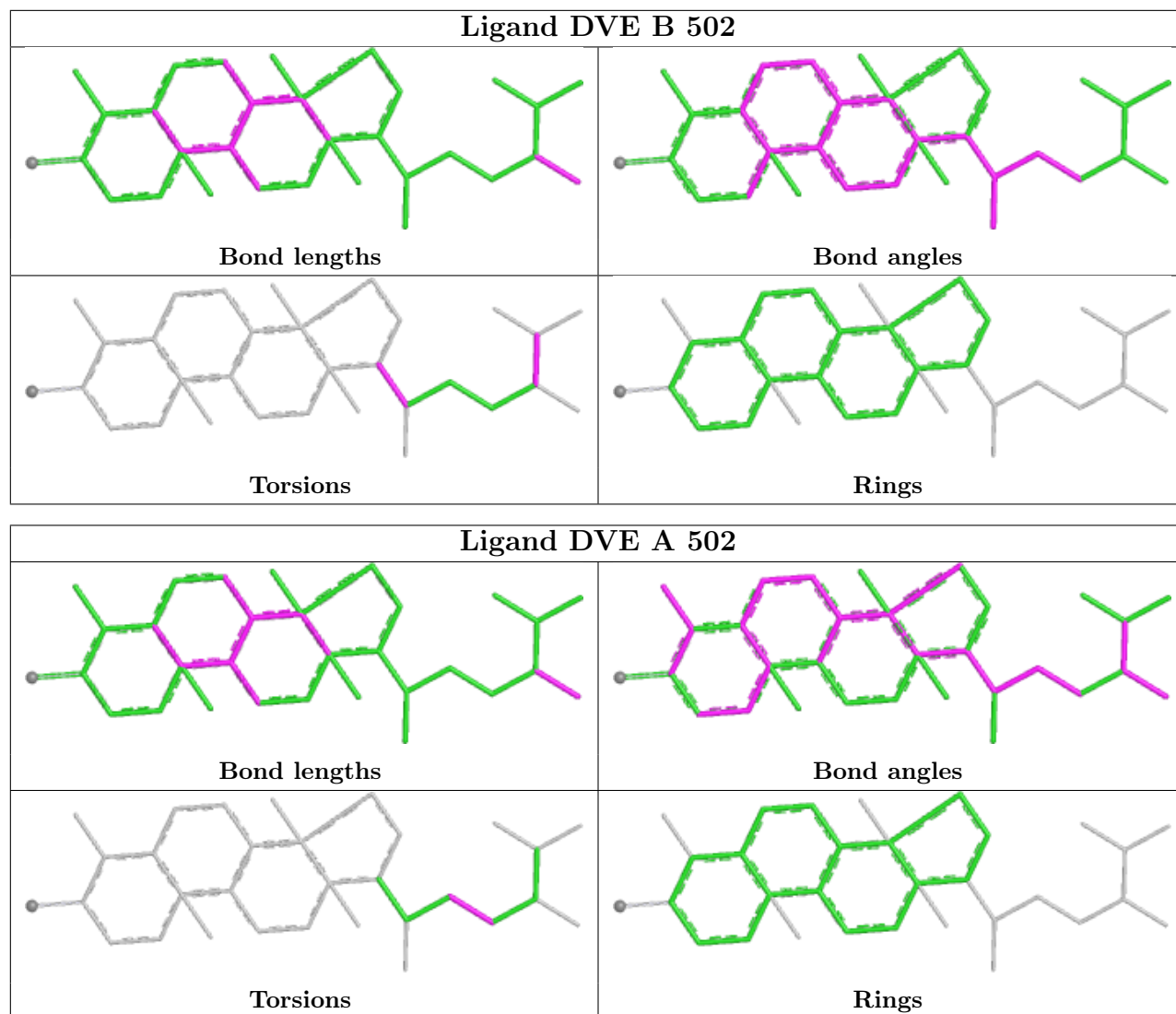
6 monomers are involved in 28 short contacts:

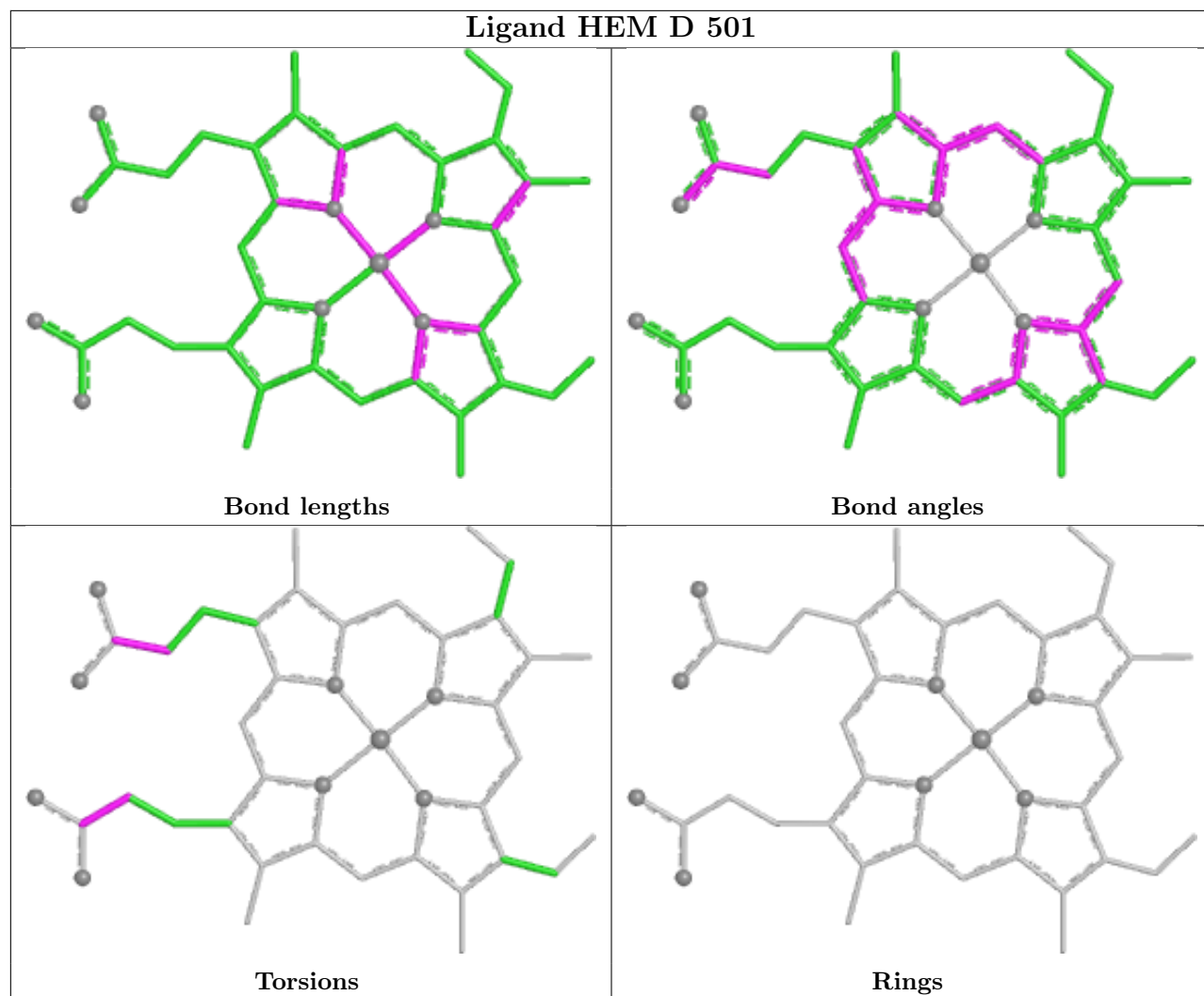
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	10	0
2	B	501	HEM	6	0
3	C	502	DVE	2	0
3	B	502	DVE	1	0
2	D	501	HEM	4	0
2	A	501	HEM	5	0

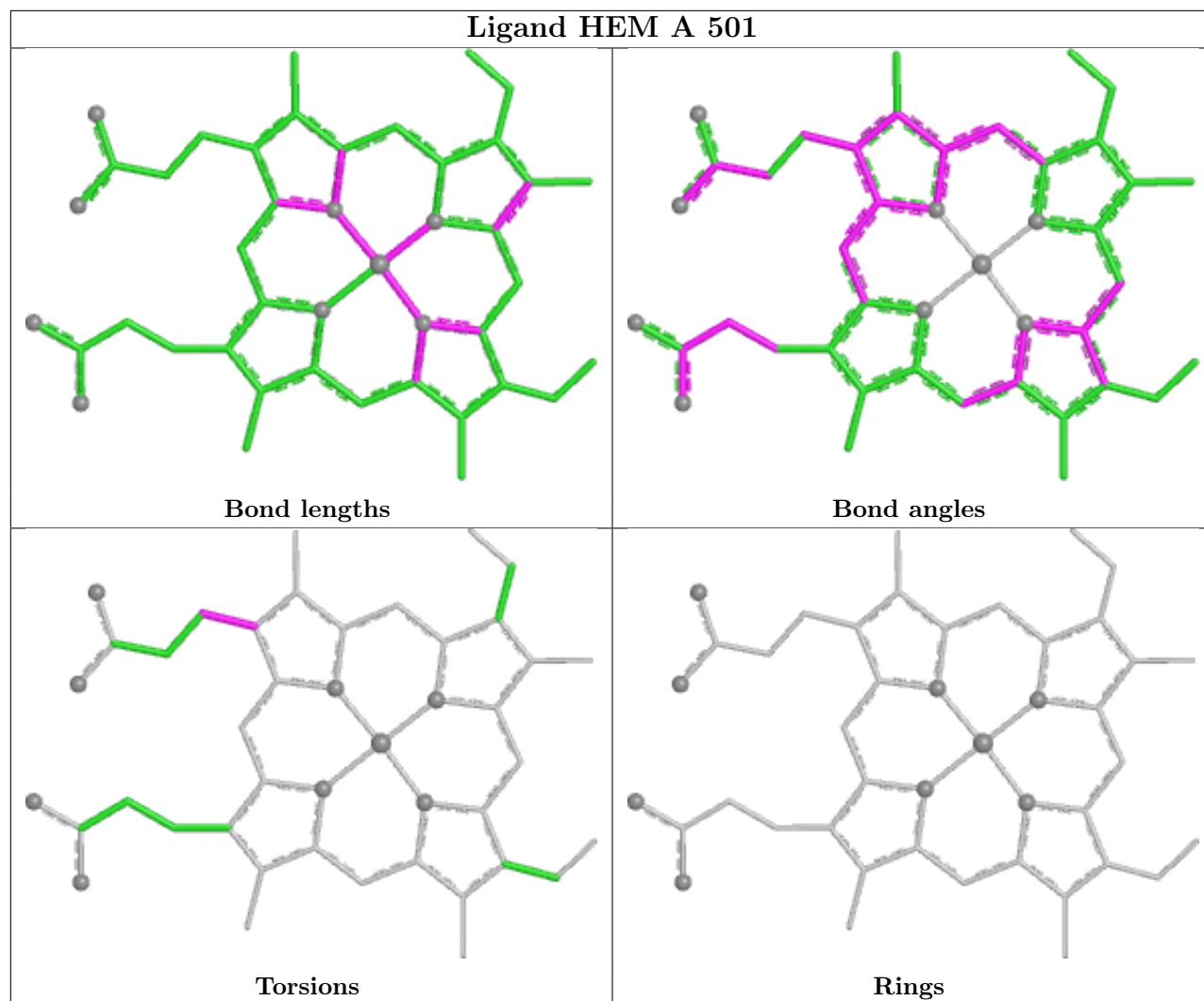
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	448/485 (92%)	-0.19	4 (0%) 81 64	88, 130, 199, 324	0
1	B	448/485 (92%)	-0.05	8 (1%) 67 47	95, 156, 234, 303	0
1	C	448/485 (92%)	0.01	13 (2%) 53 34	86, 167, 245, 325	0
1	D	448/485 (92%)	-0.14	4 (0%) 81 64	98, 166, 218, 337	0
All	All	1792/1940 (92%)	-0.09	29 (1%) 70 50	86, 154, 232, 337	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	282	CYS	4.5
1	C	281	VAL	4.1
1	C	369	VAL	3.5
1	B	411	ALA	3.3
1	A	211	ALA	2.8
1	A	218	LEU	2.8
1	C	237	GLN	2.7
1	B	211	ALA	2.7
1	B	262	LEU	2.7
1	B	358	MET	2.6
1	A	196	HIS	2.5
1	C	115	ALA	2.5
1	C	207	SER	2.5
1	C	171	CYS	2.4
1	B	291	ALA	2.4
1	C	278	LEU	2.4
1	D	115	ALA	2.4
1	B	237	GLN	2.4
1	C	103	TYR	2.3
1	C	48	PHE	2.3
1	B	367	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	222	PRO	2.2
1	C	116	TYR	2.2
1	D	284	MET	2.1
1	D	468	GLN	2.1
1	B	445	PHE	2.1
1	C	209	ILE	2.0
1	D	42	LEU	2.0
1	C	213	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

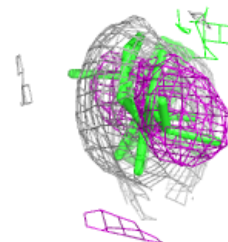
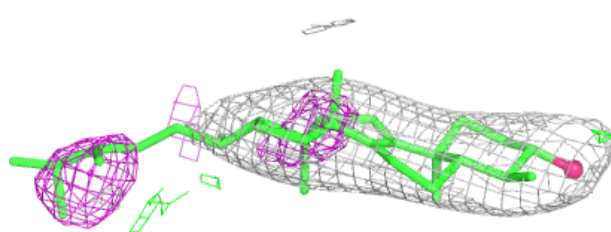
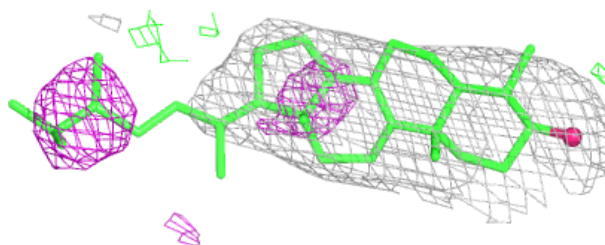
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DVE	C	502	31/31	0.89	0.15	79,100,110,122	0
3	DVE	B	502	31/31	0.96	0.13	104,123,137,151	0
3	DVE	A	502	31/31	0.97	0.10	79,100,110,122	0
2	HEM	C	501	43/43	0.97	0.09	83,114,163,176	0
2	HEM	D	501	43/43	0.97	0.08	86,108,136,165	0
2	HEM	B	501	43/43	0.98	0.07	73,91,123,137	0
2	HEM	A	501	43/43	0.98	0.07	70,86,119,124	0

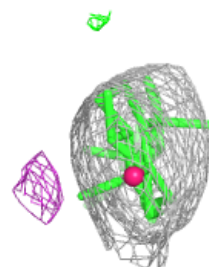
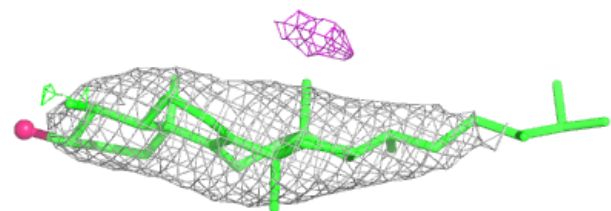
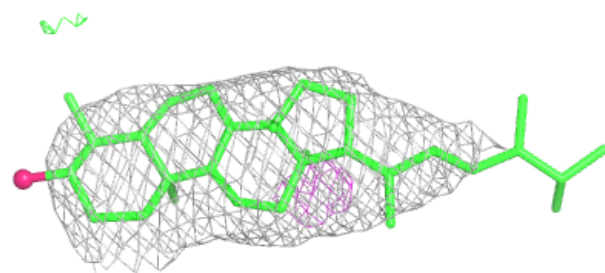
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DVE C 502:

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

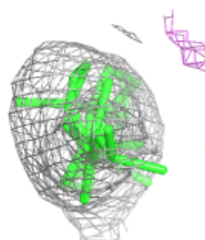
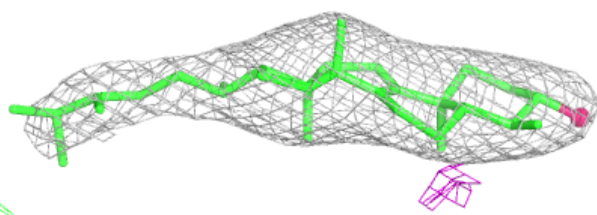
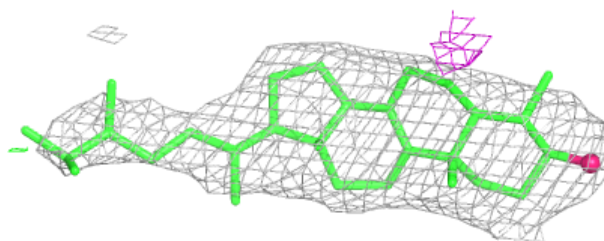
**Electron density around DVE B 502:**

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

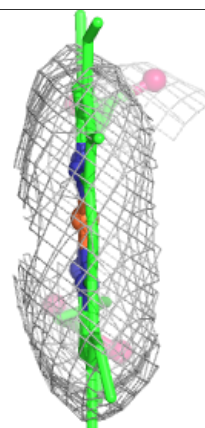
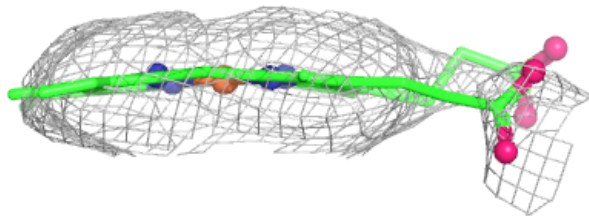
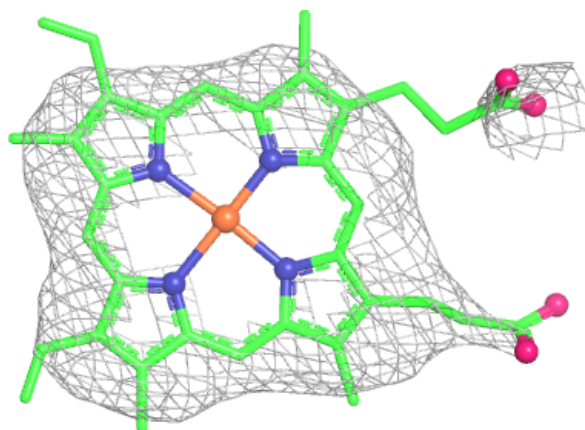


Electron density around DVE A 502:

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

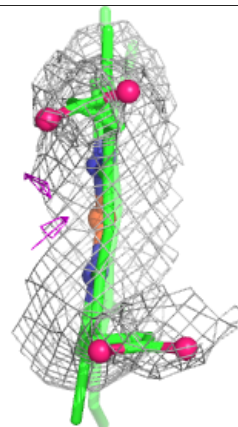
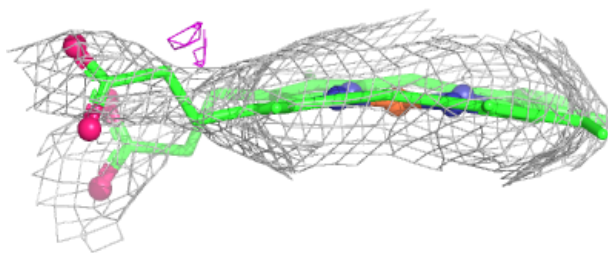
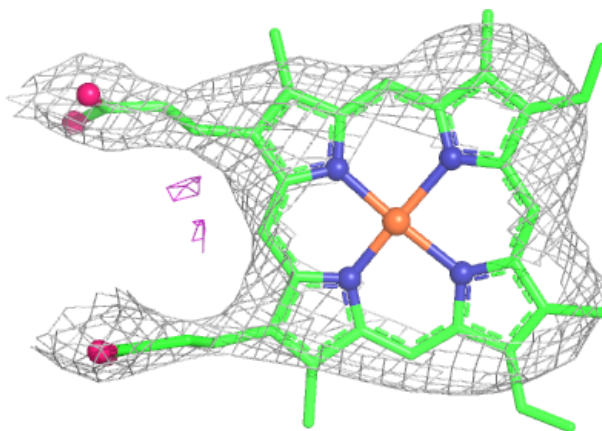
**Electron density around HEM C 501:**

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



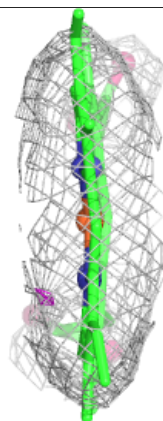
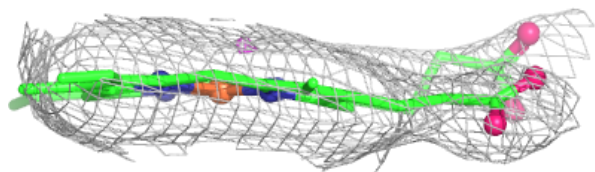
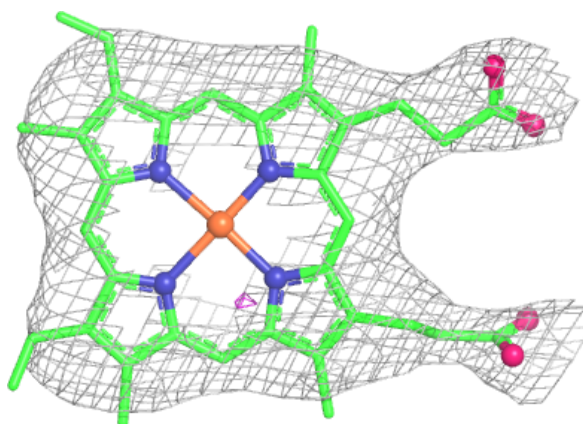
Electron density around HEM D 501:

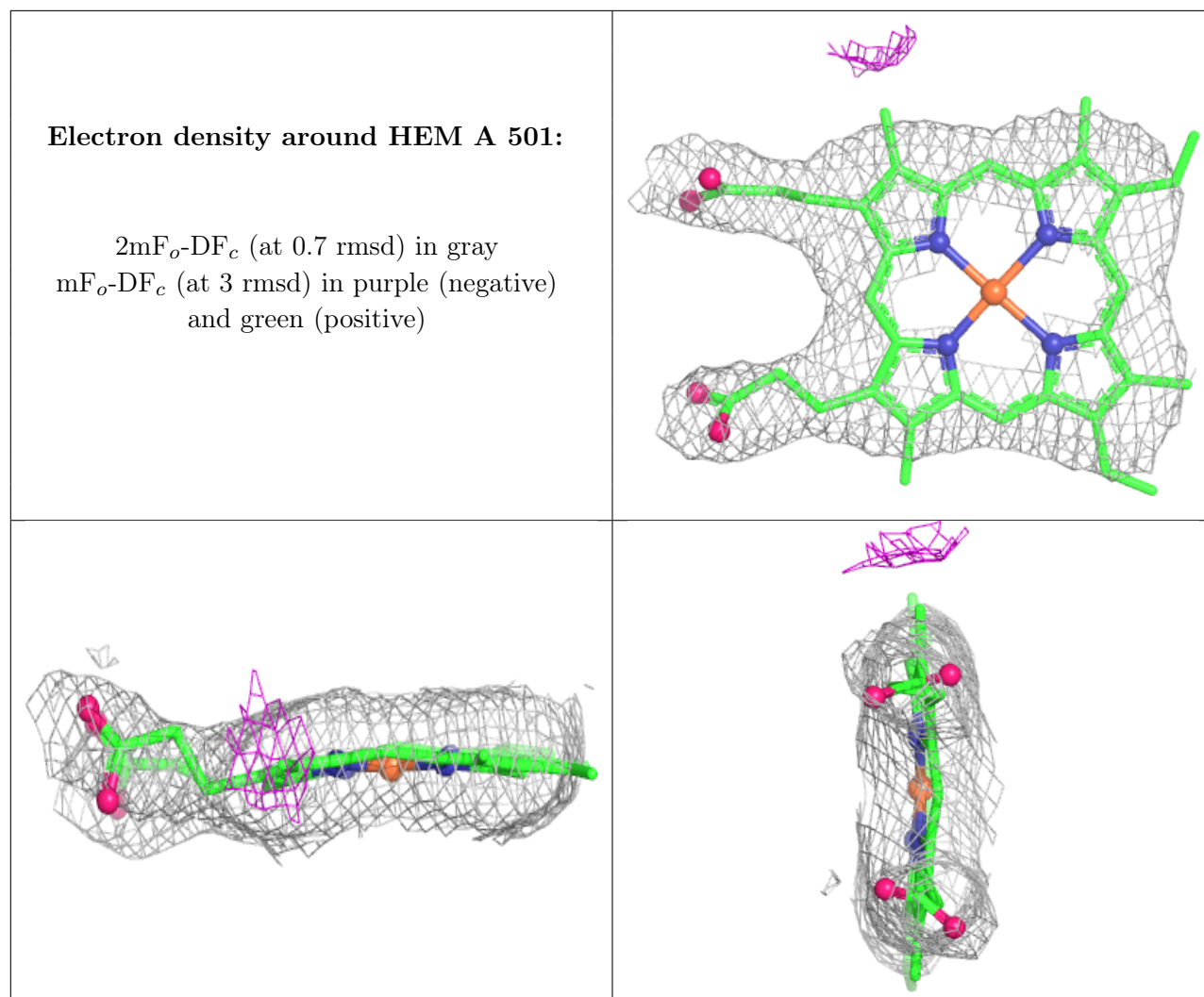
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.