



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:19 AM UTC

PDB ID : 3TIK / pdb_00003tik
Title : Sterol 14-alpha demethylase (CYP51) from Trypanosoma brucei in complex with the tipifarnib derivative 6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-4-(2,6-difluorophenyl)-1-methylquinolin-2(1H)-one
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Deposited on : 2011-08-20
Resolution : 2.05 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](#) ①) were used in the production of this report:

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

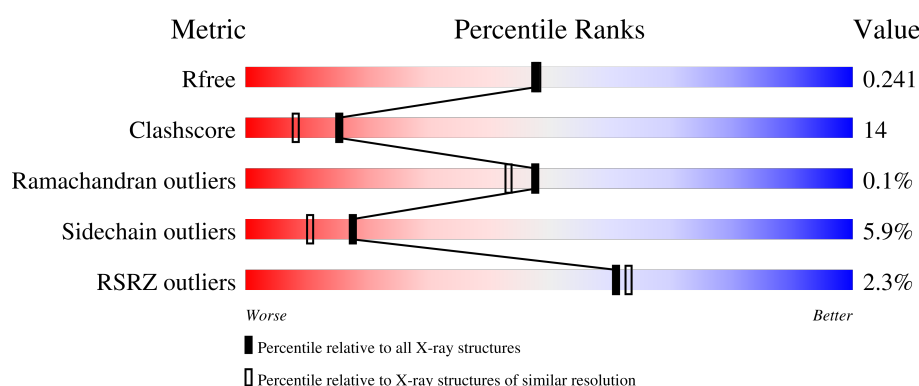
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	454	2% 76% 22% ..
1	B	454	3% 76% 20% ..
1	C	454	2% 78% 19% ..
1	D	454	2% 79% 17% ..

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	JKF	C	490	-	-	X	-
3	JKF	D	490	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14911 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.

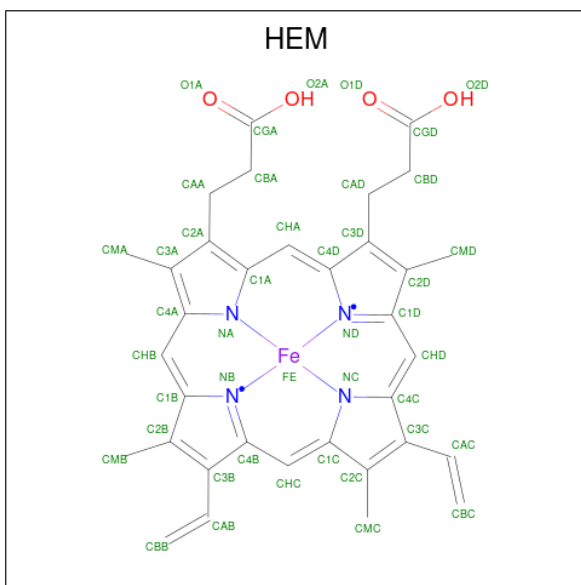
- Molecule 1 is a protein called sterol 14-alpha demethylase (CYP51).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3575	2283	625	640	27			
1	B	450	Total	C	N	O	S	0	0	0
			3575	2283	625	640	27			
1	C	450	Total	C	N	O	S	0	0	0
			3575	2283	625	640	27			
1	D	450	Total	C	N	O	S	0	0	0
			3575	2283	625	640	27			

There are 16 discrepancies between the modelled and reference sequences:

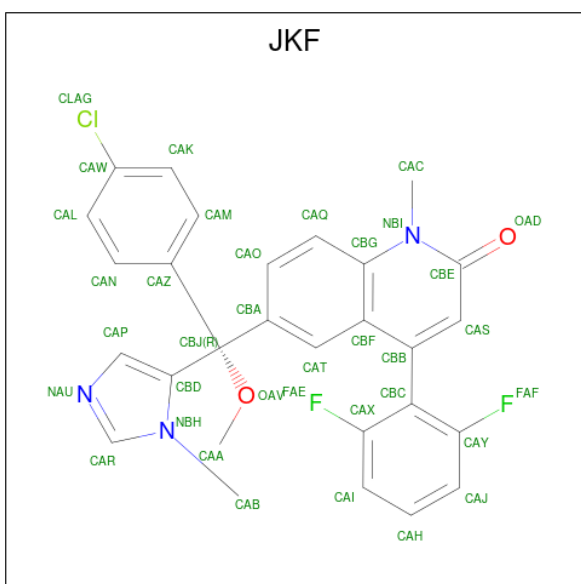
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	LYS	-	expression tag	UNP Q385E8
A	29	GLY	-	expression tag	UNP Q385E8
A	30	LYS	-	expression tag	UNP Q385E8
A	31	LEU	-	expression tag	UNP Q385E8
B	28	LYS	-	expression tag	UNP Q385E8
B	29	GLY	-	expression tag	UNP Q385E8
B	30	LYS	-	expression tag	UNP Q385E8
B	31	LEU	-	expression tag	UNP Q385E8
C	28	LYS	-	expression tag	UNP Q385E8
C	29	GLY	-	expression tag	UNP Q385E8
C	30	LYS	-	expression tag	UNP Q385E8
C	31	LEU	-	expression tag	UNP Q385E8
D	28	LYS	-	expression tag	UNP Q385E8
D	29	GLY	-	expression tag	UNP Q385E8
D	30	LYS	-	expression tag	UNP Q385E8
D	31	LEU	-	expression tag	UNP Q385E8

- 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

- Molecule 3 is 6-[(R)-(4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl]-4-(2,6-difluorophenyl)-1-methylquinolin-2(1H)-one (CCD ID: JKF) (formula: $C_{28}H_{22}ClF_2N_3O_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			36	28	1	2	3	2		
3	B	1	Total	C	Cl	F	N	O	0	0
			36	28	1	2	3	2		
3	C	1	Total	C	Cl	F	N	O	0	0
			36	28	1	2	3	2		
3	D	1	Total	C	Cl	F	N	O	0	0
			36	28	1	2	3	2		

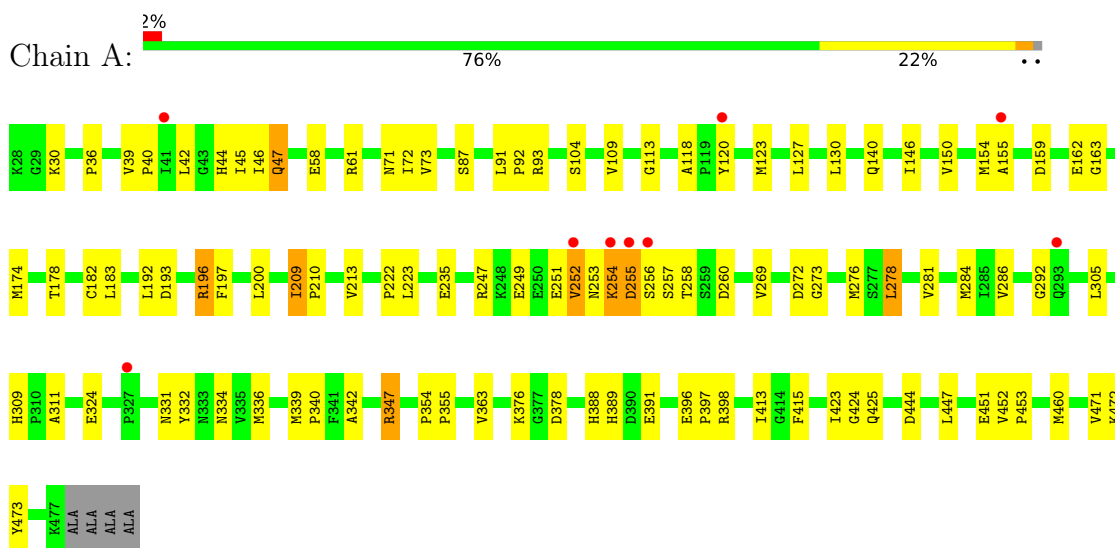
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	76	Total	O	0	0
			76	76		
4	C	59	Total	O	0	0
			59	59		
4	D	113	Total	O	0	0
			113	113		

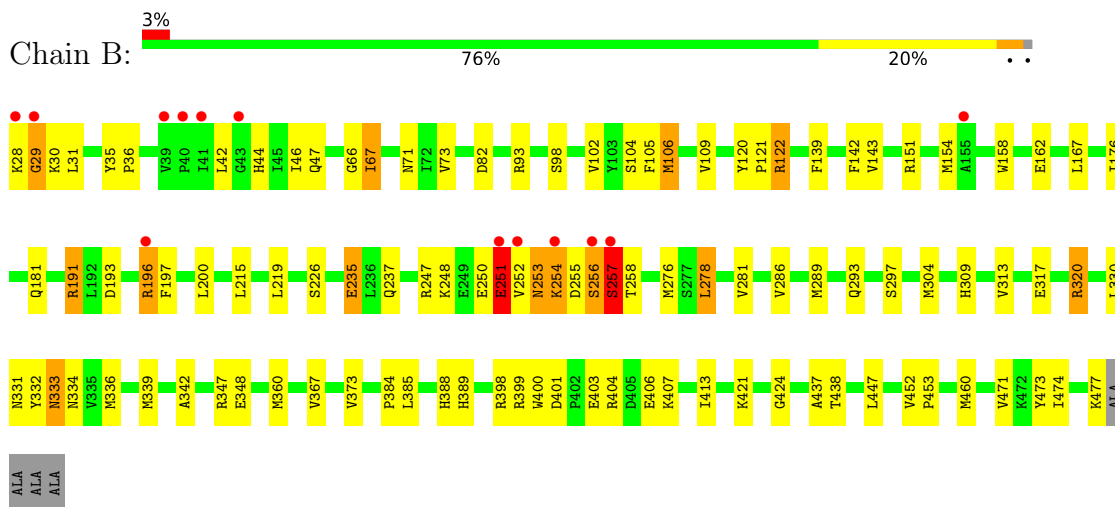
3 Residue-property plots [i](#)

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.

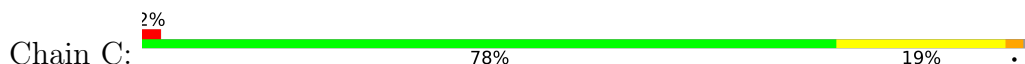
- Molecule 1: sterol 14-alpha demethylase (CYP51)

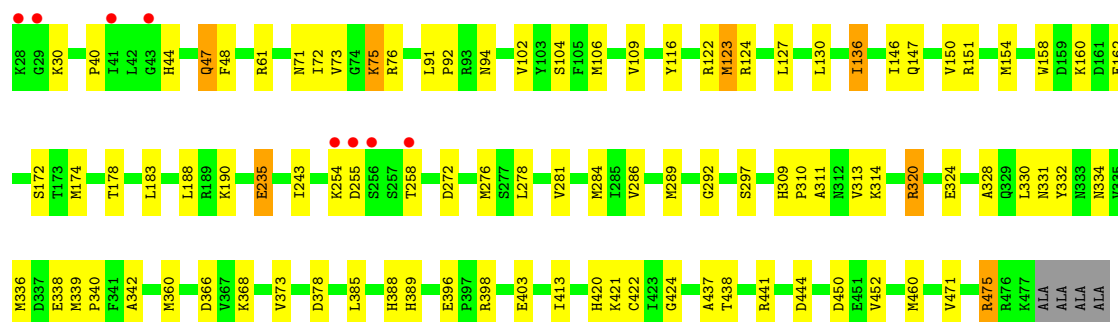


- Molecule 1: sterol 14-alpha demethylase (CYP51)

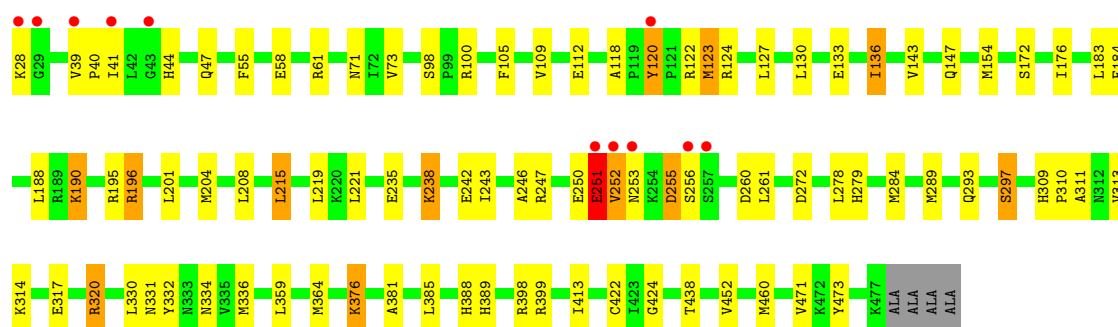
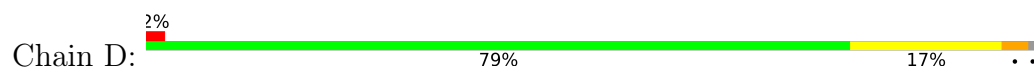


- Molecule 1: sterol 14-alpha demethylase (CYP51)





● Molecule 1: sterol 14-alpha demethylase (CYP51)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.72Å 79.72Å 117.52Å 74.47° 81.58° 68.05°	Depositor
Resolution (Å)	30.00 – 2.05 30.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.05) 99.7 (30.00-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.243 0.185 , 0.241	Depositor DCC
R_{free} test set	6082 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14911	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: JKF, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/3657	0.84	4/4944 (0.1%)
1	B	0.57	0/3657	0.84	8/4944 (0.2%)
1	C	0.52	0/3657	0.78	0/4944
1	D	0.64	2/3657 (0.1%)	0.86	1/4944 (0.0%)
All	All	0.57	2/14628 (0.0%)	0.83	13/19776 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	120	TYR	C-O	-5.71	1.19	1.24
1	D	143	VAL	CA-CB	5.53	1.57	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	251	GLU	N-CA-C	9.81	121.98	111.28
1	B	251	GLU	N-CA-C	9.50	121.72	111.36
1	A	209	ILE	CA-C-N	6.70	126.96	119.32
1	A	209	ILE	C-N-CA	6.70	126.96	119.32
1	A	39	VAL	CA-C-N	6.30	127.71	119.84
1	A	39	VAL	C-N-CA	6.30	127.71	119.84
1	B	143	VAL	CA-C-N	-6.08	113.42	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	VAL	C-N-CA	-6.08	113.42	119.56
1	B	250	GLU	CA-C-N	5.99	128.80	120.29
1	B	250	GLU	C-N-CA	5.99	128.80	120.29
1	B	29	GLY	N-CA-C	-5.65	106.20	114.90
1	B	257	SER	N-CA-C	-5.42	106.26	112.92
1	B	367	VAL	N-CA-C	5.07	116.01	108.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	251	GLU	Peptide

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	3575	0	3620	81	0
1	B	3575	0	3620	108	0
1	C	3575	0	3620	89	0
1	D	3575	0	3620	89	0
2	A	43	0	30	6	0
2	B	43	0	30	5	0
2	C	43	0	30	10	0
2	D	43	0	30	5	0
3	A	36	0	22	7	0
3	B	36	0	22	7	0
3	C	36	0	22	15	0
3	D	36	0	22	10	0
4	A	47	0	0	1	0
4	B	76	0	0	0	0
4	C	59	0	0	1	0
4	D	113	0	0	0	0
All	All	14911	0	14688	396	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 14.

All (396) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:HH11	1:B:191:ARG:CG	1.61	1.14
1:A:196:ARG:CB	1:A:196:ARG:HH11	1.59	1.12
1:D:320:ARG:HH21	1:D:320:ARG:HG2	1.08	1.10
1:B:28:LYS:HD2	1:B:30:LYS:HB3	1.34	1.08
1:A:196:ARG:HB3	1:A:196:ARG:NH1	1.67	1.08
1:B:320:ARG:HG2	1:B:320:ARG:HH21	1.08	1.07
1:A:196:ARG:HH11	1:A:196:ARG:HB3	1.04	1.07
1:D:250:GLU:HB2	1:D:256:SER:HB2	1.12	1.06
1:D:250:GLU:CB	1:D:256:SER:HB2	1.86	1.05
1:B:191:ARG:HG2	1:B:191:ARG:NH1	1.50	1.04
1:B:254:LYS:HE2	1:B:254:LYS:HA	1.39	0.99
1:C:320:ARG:HG2	1:C:320:ARG:HH21	1.24	0.98
1:D:123:MET:HE3	1:D:127:LEU:HD12	1.46	0.98
1:C:75:LYS:HB2	1:C:75:LYS:NZ	1.80	0.96
1:C:75:LYS:HB2	1:C:75:LYS:HZ2	1.33	0.93
1:B:73:VAL:HG12	1:B:73:VAL:O	1.68	0.93
1:D:251:GLU:HA	1:D:256:SER:HB3	1.51	0.93
1:C:276:MET:HE2	1:C:281:VAL:HG22	1.49	0.92
1:D:250:GLU:HB2	1:D:256:SER:CB	1.98	0.92
1:C:44:HIS:HD2	1:C:71:ASN:H	1.07	0.92
1:D:320:ARG:HH21	1:D:320:ARG:CG	1.84	0.91
1:A:47:GLN:H	1:A:47:GLN:HE21	1.15	0.90
1:D:44:HIS:HD2	1:D:71:ASN:H	1.13	0.90
1:B:320:ARG:HH21	1:B:320:ARG:CG	1.85	0.90
1:C:389:HIS:HE1	1:C:398:ARG:HH11	1.20	0.89
1:B:122:ARG:HG2	1:B:122:ARG:HH11	1.36	0.89
1:D:388:HIS:HE1	1:D:413:ILE:H	1.19	0.89
1:D:196:ARG:HB3	1:D:196:ARG:HH11	1.37	0.89
1:C:475:ARG:CG	1:C:475:ARG:HH11	1.86	0.88
1:B:388:HIS:HE1	1:B:413:ILE:H	1.17	0.87
1:A:196:ARG:HH11	1:A:196:ARG:CG	1.88	0.87
1:C:388:HIS:HE1	1:C:413:ILE:H	1.20	0.86
1:B:193:ASP:OD1	1:B:196:ARG:HG3	1.75	0.85
1:D:136:ILE:HG22	1:D:336:MET:HE2	1.58	0.85
1:B:251:GLU:HA	1:B:256:SER:HB2	1.59	0.85
1:C:123:MET:HE3	1:C:127:LEU:HD12	1.59	0.85
1:B:122:ARG:HH11	1:B:122:ARG:CG	1.89	0.84
1:B:320:ARG:HG2	1:B:320:ARG:NH2	1.90	0.84
1:B:109:VAL:HG13	1:B:286:VAL:HG11	1.59	0.83
1:A:388:HIS:HE1	1:A:413:ILE:H	1.23	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:HIS:CE1	1:C:398:ARG:HH11	1.98	0.82
1:D:309:HIS:HD2	1:D:311:ALA:H	1.25	0.81
1:B:191:ARG:HH11	1:B:191:ARG:HG2	0.69	0.81
1:D:320:ARG:HG2	1:D:320:ARG:NH2	1.90	0.81
1:B:122:ARG:HG2	1:B:122:ARG:NH1	1.94	0.81
1:B:253:ASN:HB2	1:B:255:ASP:H	1.45	0.81
1:C:460:MET:CE	3:C:490:JKF:CAJ	2.59	0.81
1:C:320:ARG:HH21	1:C:320:ARG:CG	1.94	0.80
1:C:47:GLN:H	1:C:47:GLN:HE21	1.30	0.80
1:A:309:HIS:CD2	1:A:311:ALA:H	2.00	0.80
1:B:28:LYS:HB3	1:B:30:LYS:H	1.47	0.79
1:B:102:VAL:HG11	1:B:360:MET:HB2	1.65	0.79
1:A:260:ASP:HA	4:A:517:HOH:O	1.81	0.79
1:B:200:LEU:HD21	1:B:235:GLU:HG2	1.64	0.78
1:B:247:ARG:O	1:B:251:GLU:HB2	1.82	0.78
1:D:389:HIS:HE1	1:D:398:ARG:HH11	1.27	0.78
1:D:247:ARG:O	1:D:251:GLU:HB2	1.83	0.78
1:A:44:HIS:HD2	1:A:71:ASN:H	1.31	0.77
1:C:332:TYR:CE1	1:C:336:MET:HG3	2.20	0.77
1:C:320:ARG:O	1:C:324:GLU:HG3	1.85	0.77
1:C:460:MET:CE	3:C:490:JKF:CAY	2.64	0.76
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.49	0.76
1:B:28:LYS:HD2	1:B:30:LYS:CB	2.14	0.76
1:C:460:MET:HE1	3:C:490:JKF:HAJ	1.66	0.76
1:C:276:MET:HE2	1:C:281:VAL:CG2	2.16	0.75
1:B:44:HIS:HD2	1:B:71:ASN:H	1.32	0.75
1:B:251:GLU:CD	1:B:251:GLU:O	2.30	0.75
1:C:475:ARG:HH11	1:C:475:ARG:HG2	1.52	0.74
1:B:196:ARG:NH1	1:B:196:ARG:HB3	2.03	0.74
1:B:42:LEU:HD13	1:B:46:ILE:HD11	1.70	0.74
1:D:331:ASN:H	1:D:334:ASN:HD22	1.36	0.74
3:B:490:JKF:CAM	3:B:490:JKF:HAAB	2.18	0.73
3:B:490:JKF:CAO	3:B:490:JKF:HAN	2.17	0.73
1:A:253:ASN:C	1:A:254:LYS:HG2	2.12	0.73
1:C:44:HIS:CD2	1:C:71:ASN:H	1.99	0.73
1:D:399:ARG:HG3	1:D:399:ARG:HH11	1.52	0.73
1:D:44:HIS:CD2	1:D:71:ASN:H	2.02	0.72
1:C:460:MET:HE2	3:C:490:JKF:CAJ	2.18	0.72
2:B:482:HEM:HMC2	2:B:482:HEM:HBC2	1.71	0.72
1:C:460:MET:HE1	3:C:490:JKF:CAJ	2.18	0.72
1:B:401:ASP:O	1:B:404:ARG:HG2	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:MET:HE2	3:C:490:JKF:CAY	2.19	0.71
1:A:309:HIS:HD2	1:A:311:ALA:H	1.35	0.71
1:D:251:GLU:CA	1:D:256:SER:HB3	2.21	0.70
1:A:47:GLN:H	1:A:47:GLN:NE2	1.89	0.70
1:A:251:GLU:O	1:A:254:LYS:HD3	1.92	0.70
1:D:123:MET:HE3	1:D:127:LEU:CD1	2.21	0.70
1:C:183:LEU:HD12	1:C:289:MET:HE1	1.74	0.69
1:B:251:GLU:CD	1:B:251:GLU:C	2.61	0.69
1:B:333:ASN:HD22	1:B:333:ASN:H	1.41	0.69
1:A:30:LYS:HG2	1:B:181:GLN:HE22	1.57	0.69
1:D:196:ARG:HH11	1:D:196:ARG:CB	2.05	0.69
1:A:155:ALA:O	1:A:159:ASP:HB3	1.94	0.68
1:B:197:PHE:CZ	1:B:289:MET:HG3	2.28	0.68
1:B:389:HIS:HE1	1:B:398:ARG:HH11	1.42	0.68
1:A:200:LEU:HD21	1:A:235:GLU:OE1	1.93	0.68
1:D:389:HIS:CE1	1:D:398:ARG:HH11	2.10	0.68
1:C:75:LYS:NZ	1:C:75:LYS:CB	2.54	0.68
1:D:188:LEU:HD13	1:D:243:ILE:HG13	1.76	0.68
1:B:196:ARG:CB	1:B:196:ARG:HH11	2.07	0.67
1:D:320:ARG:CG	1:D:320:ARG:NH2	2.49	0.67
3:A:490:JKF:HAN	3:A:490:JKF:CAO	2.22	0.67
1:C:309:HIS:CD2	1:C:311:ALA:H	2.13	0.67
1:B:73:VAL:O	1:B:73:VAL:CG1	2.41	0.66
1:A:210:PRO:O	1:A:213:VAL:HG23	1.96	0.66
1:A:388:HIS:CE1	1:A:413:ILE:H	2.10	0.66
1:D:388:HIS:CE1	1:D:413:ILE:H	2.10	0.66
1:D:309:HIS:CD2	1:D:311:ALA:H	2.11	0.66
1:B:196:ARG:HB3	1:B:196:ARG:HH11	1.60	0.66
1:A:58:GLU:OE1	1:A:61:ARG:NH1	2.29	0.66
1:C:320:ARG:HG2	1:C:320:ARG:NH2	2.04	0.65
1:B:388:HIS:CE1	1:B:413:ILE:H	2.06	0.65
2:D:482:HEM:HBC2	2:D:482:HEM:HMC2	1.79	0.65
1:C:424:GLY:HA3	2:C:482:HEM:C3C	2.32	0.65
1:D:136:ILE:CG2	1:D:336:MET:HE2	2.27	0.65
1:B:248:LYS:HA	1:B:251:GLU:HB2	1.78	0.65
1:C:331:ASN:H	1:C:334:ASN:HD22	1.46	0.64
1:A:127:LEU:HD23	1:A:284:MET:HE1	1.77	0.64
1:D:196:ARG:HB3	1:D:196:ARG:NH1	2.11	0.64
1:B:331:ASN:H	1:B:334:ASN:HD22	1.46	0.64
1:C:276:MET:CE	1:C:281:VAL:HG22	2.26	0.64
1:D:247:ARG:O	1:D:251:GLU:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:HG2	1:A:93:ARG:NH1	2.10	0.64
1:B:139:PHE:HA	1:B:142:PHE:HB2	1.80	0.64
1:B:385:LEU:O	1:B:389:HIS:HD2	1.80	0.64
1:C:136:ILE:HD12	1:C:136:ILE:C	2.23	0.64
1:D:399:ARG:HG3	1:D:399:ARG:NH1	2.12	0.63
1:B:36:PRO:O	1:B:44:HIS:HE1	1.81	0.63
1:A:309:HIS:HD2	1:A:311:ALA:N	1.97	0.62
1:C:320:ARG:CG	1:C:320:ARG:NH2	2.57	0.62
1:D:253:ASN:HB3	1:D:255:ASP:OD1	1.99	0.62
2:B:482:HEM:HMB2	2:B:482:HEM:HBB2	1.81	0.62
2:C:482:HEM:CMB	2:C:482:HEM:HBB2	2.30	0.62
1:B:197:PHE:CE2	1:B:289:MET:HG3	2.35	0.61
1:A:196:ARG:NH1	1:A:196:ARG:CG	2.56	0.61
2:C:482:HEM:HBB2	2:C:482:HEM:HMB2	1.81	0.61
1:C:388:HIS:CE1	1:C:413:ILE:H	2.10	0.61
1:C:75:LYS:HB2	1:C:75:LYS:HZ3	1.66	0.60
1:D:58:GLU:HA	1:D:61:ARG:NH1	2.16	0.60
1:B:254:LYS:HA	1:B:254:LYS:CE	2.11	0.60
3:C:490:JKF:HAAB	3:C:490:JKF:CAM	2.30	0.60
1:D:332:TYR:CE1	1:D:336:MET:HG3	2.37	0.59
1:A:113:GLY:O	1:A:118:ALA:HB2	2.03	0.59
1:B:389:HIS:CE1	1:B:398:ARG:HH11	2.20	0.59
1:C:75:LYS:HZ2	1:C:75:LYS:CB	2.10	0.59
1:D:252:VAL:O	1:D:252:VAL:HG13	2.01	0.59
3:A:490:JKF:HAT	3:A:490:JKF:CAA	2.31	0.59
1:B:253:ASN:OD1	1:B:253:ASN:N	2.28	0.59
2:D:482:HEM:HBC2	2:D:482:HEM:CMC	2.33	0.59
1:B:320:ARG:CG	1:B:320:ARG:NH2	2.50	0.59
1:D:253:ASN:C	1:D:255:ASP:H	2.10	0.59
1:B:154:MET:HE1	1:B:438:THR:HG22	1.85	0.58
1:C:475:ARG:HH11	1:C:475:ARG:HG3	1.66	0.58
1:A:255:ASP:OD2	1:A:255:ASP:N	2.36	0.58
1:C:460:MET:CE	3:C:490:JKF:FAF	2.42	0.58
1:C:460:MET:CE	3:C:490:JKF:HAJ	2.32	0.58
3:A:490:JKF:CAO	3:A:490:JKF:CAN	2.81	0.58
1:B:105:PHE:HA	1:B:219:LEU:HD21	1.85	0.58
1:B:406:GLU:O	1:C:136:ILE:HD11	2.04	0.58
1:A:45:ILE:HG23	1:A:46:ILE:HD12	1.85	0.57
1:B:30:LYS:HG2	1:B:31:LEU:H	1.68	0.57
1:C:76:ARG:NH2	1:C:378:ASP:OD2	2.37	0.57
1:C:190:LYS:NZ	1:C:190:LYS:HB3	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:490:JKF:CAO	3:B:490:JKF:CAN	2.81	0.57
1:C:309:HIS:HD2	1:C:311:ALA:H	1.51	0.57
3:A:490:JKF:HAT	3:A:490:JKF:HAAA	1.85	0.57
1:A:42:LEU:HD13	1:A:46:ILE:CD1	2.34	0.57
1:C:328:ALA:HA	1:C:441:ARG:HH21	1.70	0.57
1:D:246:ALA:O	1:D:250:GLU:HG3	2.03	0.57
1:A:309:HIS:CD2	1:A:311:ALA:HB3	2.40	0.57
1:B:333:ASN:H	1:B:333:ASN:ND2	2.02	0.57
1:D:331:ASN:H	1:D:334:ASN:ND2	2.03	0.57
1:C:310:PRO:O	1:C:313:VAL:HG13	2.05	0.56
1:D:251:GLU:N	1:D:256:SER:HB3	2.21	0.56
1:D:460:MET:CE	3:D:490:JKF:CAY	2.84	0.56
3:D:490:JKF:CAO	3:D:490:JKF:HAN	2.35	0.56
1:A:305:LEU:HD13	1:A:453:PRO:HG2	1.87	0.56
2:A:482:HEM:CMB	2:A:482:HEM:HBB2	2.36	0.56
2:B:482:HEM:HBB2	2:B:482:HEM:CMB	2.35	0.56
3:C:490:JKF:HAN	3:C:490:JKF:CAO	2.35	0.56
2:A:482:HEM:HBB2	2:A:482:HEM:HMB2	1.86	0.56
1:A:460:MET:HE2	3:A:490:JKF:HAS	1.88	0.56
1:B:30:LYS:CG	1:B:31:LEU:H	2.19	0.56
1:B:109:VAL:CG1	1:B:286:VAL:HG11	2.33	0.56
1:D:127:LEU:HD23	1:D:284:MET:HE1	1.87	0.55
1:A:127:LEU:CD2	1:A:284:MET:HE1	2.36	0.55
1:D:253:ASN:HB3	1:D:255:ASP:CG	2.31	0.55
1:C:116:TYR:OH	2:C:482:HEM:O2D	2.23	0.55
1:C:437:ALA:O	1:C:441:ARG:HB2	2.07	0.55
1:D:154:MET:HE1	1:D:438:THR:HG22	1.89	0.55
1:A:109:VAL:CG1	1:A:286:VAL:HG11	2.37	0.55
1:C:94:ASN:OD1	1:C:420:HIS:NE2	2.39	0.55
2:C:482:HEM:HBC2	2:C:482:HEM:CMC	2.37	0.55
1:C:47:GLN:HE21	1:C:47:GLN:N	2.01	0.54
1:B:331:ASN:H	1:B:334:ASN:ND2	2.05	0.54
1:C:314:LYS:HB2	4:C:522:HOH:O	2.06	0.54
1:A:278:LEU:O	1:A:278:LEU:HD22	2.07	0.54
1:D:253:ASN:O	1:D:255:ASP:OD2	2.25	0.54
1:A:252:VAL:HG13	1:A:252:VAL:O	2.06	0.54
3:B:490:JKF:CAM	3:B:490:JKF:CAA	2.85	0.54
1:D:130:LEU:HD22	1:D:284:MET:HE3	1.90	0.54
1:D:105:PHE:HA	1:D:219:LEU:HD21	1.89	0.54
1:A:109:VAL:HG13	1:A:286:VAL:HG11	1.90	0.53
1:C:475:ARG:CG	1:C:475:ARG:NH1	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLY:HA2	1:B:373:VAL:HG23	1.90	0.53
1:D:208:LEU:CD1	3:D:490:JKF:HAJ	2.38	0.53
1:B:251:GLU:HA	1:B:256:SER:CB	2.36	0.53
1:D:252:VAL:O	1:D:252:VAL:CG1	2.57	0.53
3:A:490:JKF:HAAA	3:A:490:JKF:CAT	2.38	0.53
1:B:200:LEU:CD2	1:B:235:GLU:HG2	2.37	0.53
1:A:272:ASP:C	1:A:272:ASP:OD1	2.52	0.52
1:C:30:LYS:O	1:C:373:VAL:HG12	2.09	0.52
1:D:98:SER:OG	1:D:120:TYR:OH	2.21	0.52
1:B:46:ILE:HD12	1:B:46:ILE:H	1.74	0.52
1:D:385:LEU:O	1:D:389:HIS:HD2	1.92	0.52
1:A:252:VAL:O	1:A:252:VAL:CG1	2.58	0.52
1:B:399:ARG:HG3	1:B:399:ARG:HH11	1.74	0.52
1:C:475:ARG:HG3	1:C:475:ARG:NH1	2.25	0.51
1:D:123:MET:HE2	1:D:124:ARG:HA	1.92	0.51
1:A:276:MET:HE2	1:A:281:VAL:HA	1.92	0.51
1:D:172:SER:HA	1:D:297:SER:HB2	1.93	0.51
1:B:460:MET:CE	3:B:490:JKF:CAY	2.88	0.50
2:A:482:HEM:HBC2	2:A:482:HEM:CMC	2.41	0.50
1:B:399:ARG:HG3	1:B:399:ARG:NH1	2.26	0.50
1:B:66:GLY:C	1:B:67:ILE:HD13	2.37	0.50
1:B:237:GLN:CG	1:B:278:LEU:HD13	2.41	0.50
1:B:257:SER:O	1:B:258:THR:C	2.50	0.50
1:C:422:CYS:HB2	2:C:482:HEM:NA	2.26	0.50
1:D:123:MET:HE2	1:D:124:ARG:N	2.27	0.50
1:B:424:GLY:HA3	2:B:482:HEM:C3C	2.47	0.50
1:A:45:ILE:HD13	1:D:221:LEU:HD22	1.94	0.50
1:A:36:PRO:O	1:A:44:HIS:HE1	1.95	0.49
1:B:309:HIS:HD2	1:B:452:VAL:HG23	1.77	0.49
3:C:490:JKF:CAO	3:C:490:JKF:CAN	2.90	0.49
1:D:460:MET:HE1	3:D:490:JKF:CAJ	2.42	0.49
1:A:120:TYR:O	1:A:123:MET:HE2	2.12	0.49
1:B:67:ILE:HD13	1:B:67:ILE:N	2.26	0.49
1:C:320:ARG:NH1	1:C:444:ASP:OD2	2.44	0.49
1:D:133:GLU:HG3	1:D:261:LEU:HD12	1.94	0.49
1:A:389:HIS:HE1	1:A:398:ARG:HH11	1.60	0.49
1:C:292:GLY:HA3	2:C:482:HEM:HMC3	1.94	0.49
1:C:123:MET:HE2	1:C:124:ARG:N	2.28	0.49
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.74	0.49
1:B:347:ARG:HH11	1:B:347:ARG:HB3	1.78	0.49
1:A:247:ARG:NH2	1:A:258:THR:HG21	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:VAL:CG1	1:C:286:VAL:HG11	2.43	0.49
1:A:256:SER:OG	1:A:257:SER:N	2.46	0.49
1:C:276:MET:CE	1:C:281:VAL:HA	2.43	0.49
1:C:460:MET:HE1	3:C:490:JKF:CAY	2.41	0.49
1:D:183:LEU:O	1:D:260:ASP:HB2	2.13	0.49
1:A:42:LEU:HD13	1:A:46:ILE:HD13	1.95	0.49
1:D:255:ASP:OD2	1:D:255:ASP:N	2.45	0.49
1:B:35:TYR:HD2	1:B:44:HIS:CE1	2.31	0.48
1:C:154:MET:HE1	1:C:438:THR:HG22	1.95	0.48
1:D:460:MET:HE1	3:D:490:JKF:CAY	2.43	0.48
1:B:251:GLU:O	1:B:251:GLU:OE2	2.30	0.48
1:B:473:TYR:C	1:B:474:ILE:HG13	2.38	0.48
1:A:162:GLU:HA	1:A:473:TYR:O	2.13	0.48
3:D:490:JKF:CAM	3:D:490:JKF:HAAB	2.43	0.48
1:C:47:GLN:H	1:C:47:GLN:NE2	2.04	0.48
3:A:490:JKF:CAA	3:A:490:JKF:CAT	2.90	0.48
1:C:44:HIS:HD2	1:C:71:ASN:N	1.92	0.48
3:C:490:JKF:CAM	3:C:490:JKF:CAP	2.88	0.48
1:B:347:ARG:HB3	1:B:347:ARG:NH1	2.29	0.48
1:C:172:SER:HB2	1:C:297:SER:OG	2.13	0.48
1:D:147:GLN:HE22	1:D:330:LEU:HG	1.78	0.48
1:A:42:LEU:HD13	1:A:46:ILE:HD11	1.96	0.48
1:C:123:MET:HE2	1:C:124:ARG:CA	2.44	0.48
1:B:255:ASP:O	1:B:257:SER:N	2.44	0.47
1:D:183:LEU:HD12	1:D:289:MET:HE1	1.96	0.47
1:A:222:PRO:O	1:A:223:LEU:HD23	2.14	0.47
1:B:407:LYS:HA	1:C:136:ILE:HD11	1.96	0.47
1:A:347:ARG:HH11	1:A:347:ARG:HB3	1.80	0.47
1:A:424:GLY:HA3	2:A:482:HEM:C3C	2.48	0.47
1:A:209:ILE:HA	1:A:210:PRO:HD2	1.60	0.47
1:B:98:SER:HG	1:B:120:TYR:HH	1.60	0.47
1:D:208:LEU:HD13	3:D:490:JKF:HAJ	1.95	0.47
1:B:154:MET:HG2	1:B:158:TRP:CE3	2.50	0.47
1:D:188:LEU:CD1	1:D:243:ILE:HG13	2.42	0.47
1:C:174:MET:O	1:C:178:THR:HG23	2.14	0.47
1:D:460:MET:HE2	3:D:490:JKF:CAY	2.44	0.47
1:B:196:ARG:NH1	1:B:196:ARG:CB	2.72	0.47
1:C:154:MET:HG2	1:C:158:TRP:CE3	2.48	0.47
1:B:151:ARG:HA	1:B:154:MET:HE2	1.97	0.47
1:C:338:GLU:C	1:C:340:PRO:HD3	2.40	0.47
1:A:309:HIS:CD2	1:A:311:ALA:CB	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLU:C	1:D:256:SER:HB3	2.39	0.47
2:A:482:HEM:HBC2	2:A:482:HEM:HMC1	1.97	0.46
1:B:237:GLN:HG3	1:B:278:LEU:HD13	1.96	0.46
1:C:123:MET:HE2	1:C:124:ARG:HA	1.97	0.46
1:C:339:MET:N	1:C:340:PRO:HD3	2.31	0.46
1:A:276:MET:CE	1:A:281:VAL:HA	2.46	0.46
1:C:146:ILE:O	1:C:150:VAL:HG23	2.15	0.46
1:C:314:LYS:HE3	1:C:314:LYS:HB3	1.63	0.46
1:B:251:GLU:OE1	1:B:252:VAL:HA	2.16	0.46
1:B:332:TYR:CE1	1:B:336:MET:HG3	2.51	0.46
1:B:46:ILE:HD12	1:B:46:ILE:N	2.31	0.46
1:B:313:VAL:O	1:B:317:GLU:HB2	2.15	0.46
1:D:253:ASN:CB	1:D:255:ASP:CG	2.89	0.45
1:A:150:VAL:O	1:A:154:MET:HG3	2.16	0.45
3:D:490:JKF:CAO	3:D:490:JKF:CAN	2.93	0.45
1:B:36:PRO:O	1:B:44:HIS:CE1	2.66	0.45
1:B:109:VAL:HG13	1:B:286:VAL:CG1	2.40	0.45
1:B:167:LEU:HD21	1:B:304:MET:HB2	1.99	0.45
1:D:100:ARG:NH2	1:D:118:ALA:O	2.50	0.45
1:D:332:TYR:CD2	1:D:332:TYR:C	2.94	0.45
1:A:130:LEU:HD23	1:A:423:ILE:HD11	1.98	0.45
1:B:385:LEU:O	1:B:389:HIS:CD2	2.66	0.45
1:C:276:MET:CE	1:C:281:VAL:CG2	2.92	0.45
3:C:490:JKF:CAX	3:C:490:JKF:HAT	2.45	0.45
1:A:331:ASN:H	1:A:334:ASN:HD22	1.64	0.45
1:B:406:GLU:O	1:C:136:ILE:CD1	2.65	0.45
2:C:482:HEM:HMB2	2:C:482:HEM:CBB	2.46	0.45
3:C:490:JKF:CAM	3:C:490:JKF:HAP	2.47	0.45
1:B:330:LEU:HD11	1:B:437:ALA:HB3	1.98	0.45
1:A:363:VAL:HG12	1:A:376:LYS:HA	1.99	0.45
1:B:460:MET:HE1	3:B:490:JKF:CAY	2.47	0.45
1:C:424:GLY:HA3	2:C:482:HEM:C2C	2.52	0.45
1:D:123:MET:HE2	1:D:124:ARG:CA	2.46	0.45
1:B:333:ASN:ND2	1:B:333:ASN:N	2.65	0.44
1:B:348:GLU:HG3	1:B:400:TRP:CD1	2.53	0.44
1:B:452:VAL:HG13	1:B:453:PRO:HD2	2.00	0.44
1:C:147:GLN:NE2	1:C:151:ARG:HH12	2.14	0.44
1:D:364:MET:O	1:D:376:LYS:HE2	2.16	0.44
1:B:253:ASN:CG	1:B:255:ASP:HB3	2.42	0.44
1:C:106:MET:HE2	1:C:106:MET:HB3	1.75	0.44
1:A:87:SER:HB2	1:A:91:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LYS:HD3	1:B:31:LEU:N	2.33	0.44
1:D:310:PRO:O	1:D:313:VAL:HG13	2.17	0.44
1:A:183:LEU:O	1:A:260:ASP:HB2	2.18	0.43
1:A:415:PHE:CD2	1:A:425:GLN:HB2	2.53	0.43
2:D:482:HEM:HBB2	2:D:482:HEM:CMB	2.47	0.43
1:B:460:MET:HE2	3:B:490:JKF:CAY	2.48	0.43
1:D:112:GLU:O	1:D:279:HIS:HE1	2.01	0.43
1:C:48:PHE:C	1:C:48:PHE:CD2	2.96	0.43
1:C:130:LEU:HB2	1:C:284:MET:HE3	1.98	0.43
1:D:253:ASN:C	1:D:255:ASP:N	2.74	0.43
1:A:249:GLU:O	1:A:253:ASN:ND2	2.51	0.43
1:D:184:PHE:CZ	1:D:289:MET:HE3	2.54	0.43
1:D:272:ASP:OD1	1:D:272:ASP:C	2.61	0.43
1:A:196:ARG:NH1	1:A:196:ARG:HG2	2.29	0.43
1:B:106:MET:HB3	1:B:106:MET:HE2	1.76	0.43
1:A:174:MET:O	1:A:178:THR:HG23	2.19	0.43
1:A:396:GLU:N	1:A:397:PRO:CD	2.81	0.43
1:A:192:LEU:HD11	1:A:197:PHE:HA	2.01	0.43
1:C:109:VAL:HG13	1:C:286:VAL:HG11	2.01	0.43
1:C:235:GLU:O	1:C:235:GLU:HG3	2.18	0.43
1:C:385:LEU:O	1:C:389:HIS:HD2	2.01	0.43
1:A:163:GLY:O	1:A:472:LYS:HG3	2.19	0.43
1:A:332:TYR:CE1	1:A:336:MET:HG3	2.53	0.43
1:C:102:VAL:HG13	1:C:360:MET:HE3	2.01	0.43
1:D:424:GLY:HA3	2:D:482:HEM:C3C	2.54	0.43
1:A:451:GLU:OE2	1:A:451:GLU:HA	2.19	0.42
1:B:339:MET:HE2	1:B:342:ALA:CB	2.49	0.42
1:C:91:LEU:N	1:C:92:PRO:CD	2.82	0.42
1:D:176:ILE:HB	1:D:293:GLN:OE1	2.18	0.42
1:D:460:MET:CE	3:D:490:JKF:CAJ	2.96	0.42
1:A:91:LEU:N	1:A:92:PRO:CD	2.82	0.42
1:C:72:ILE:O	1:C:73:VAL:HG22	2.19	0.42
1:B:398:ARG:HA	1:B:398:ARG:HD2	1.84	0.42
1:B:30:LYS:CG	1:B:31:LEU:N	2.82	0.42
1:D:44:HIS:HB3	1:D:55:PHE:CZ	2.54	0.42
1:B:120:TYR:N	1:B:121:PRO:CD	2.83	0.42
1:D:250:GLU:HB3	1:D:256:SER:HB2	1.92	0.42
1:B:109:VAL:CG1	1:B:286:VAL:CG1	2.98	0.42
2:C:482:HEM:CMC	2:C:482:HEM:CBC	2.97	0.42
1:A:292:GLY:HA3	2:A:482:HEM:HMC3	2.02	0.42
1:D:422:CYS:HA	2:D:482:HEM:C4D	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:VAL:HA	1:D:40:PRO:HD3	1.75	0.41
1:D:190:LYS:HE2	1:D:190:LYS:HB3	1.68	0.41
1:A:45:ILE:HB	1:A:72:ILE:HG23	2.01	0.41
1:D:58:GLU:HA	1:D:61:ARG:HH12	1.83	0.41
1:B:424:GLY:HA3	2:B:482:HEM:C2C	2.55	0.41
1:D:473:TYR:CD1	1:D:473:TYR:C	2.98	0.41
1:A:389:HIS:CE1	1:A:398:ARG:HH11	2.38	0.41
1:C:272:ASP:OD1	1:C:272:ASP:C	2.63	0.41
1:B:28:LYS:CD	1:B:30:LYS:HB3	2.26	0.41
1:B:253:ASN:HB2	1:B:255:ASP:HB3	2.03	0.41
1:B:276:MET:HE2	1:B:281:VAL:HA	2.02	0.41
1:A:309:HIS:HD2	1:A:311:ALA:CB	2.33	0.41
1:B:67:ILE:HD11	1:B:82:ASP:HB3	2.03	0.41
1:D:201:LEU:HA	1:D:204:MET:HE3	2.03	0.41
1:D:359:LEU:O	1:D:381:ALA:HA	2.21	0.41
1:A:354:PRO:HA	1:A:355:PRO:HD3	1.96	0.41
1:D:238:LYS:HD3	1:D:242:GLU:OE2	2.21	0.41
1:A:339:MET:N	1:A:340:PRO:CD	2.84	0.41
1:D:73:VAL:HG11	1:D:215:LEU:HD21	2.03	0.41
1:A:146:ILE:HG13	1:A:182:CYS:SG	2.62	0.40
1:A:339:MET:HE2	1:A:342:ALA:CB	2.52	0.40
1:D:136:ILE:CG2	1:D:336:MET:CE	2.98	0.40
1:B:176:ILE:HB	1:B:293:GLN:OE1	2.21	0.40
1:C:147:GLN:NE2	1:C:330:LEU:HG	2.36	0.40
1:A:309:HIS:HD2	1:A:311:ALA:HB3	1.82	0.40
1:A:269:VAL:HG13	1:A:273:GLY:O	2.21	0.40
1:C:188:LEU:HD13	1:C:243:ILE:HG13	2.04	0.40
1:C:339:MET:HE2	1:C:342:ALA:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/454 (99%)	432 (96%)	15 (3%)	1 (0%)	43	37
1	B	448/454 (99%)	434 (97%)	14 (3%)	0	100	100
1	C	448/454 (99%)	429 (96%)	18 (4%)	1 (0%)	43	37
1	D	448/454 (99%)	436 (97%)	12 (3%)	0	100	100
All	All	1792/1816 (99%)	1731 (97%)	59 (3%)	2 (0%)	48	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	PRO
1	A	40	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	392/392 (100%)	374 (95%)	18 (5%)	24	18
1	B	392/392 (100%)	366 (93%)	26 (7%)	15	9
1	C	392/392 (100%)	368 (94%)	24 (6%)	17	10
1	D	392/392 (100%)	368 (94%)	24 (6%)	17	10
All	All	1568/1568 (100%)	1476 (94%)	92 (6%)	18	10

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	73	VAL
1	A	104	SER
1	A	140	GLN
1	A	193	ASP
1	A	196	ARG
1	A	252	VAL
1	A	254	LYS
1	A	255	ASP

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Mol	Chain	Res	Type
1	A	278	LEU
1	A	324	GLU
1	A	347	ARG
1	A	378	ASP
1	A	391	GLU
1	A	444	ASP
1	A	447	LEU
1	A	452	VAL
1	A	471	VAL
1	B	47	GLN
1	B	67	ILE
1	B	93	ARG
1	B	104	SER
1	B	106	MET
1	B	122	ARG
1	B	162	GLU
1	B	191	ARG
1	B	196	ARG
1	B	215	LEU
1	B	226	SER
1	B	235	GLU
1	B	253	ASN
1	B	254	LYS
1	B	256	SER
1	B	257	SER
1	B	278	LEU
1	B	297	SER
1	B	320	ARG
1	B	333	ASN
1	B	384	PRO
1	B	403	GLU
1	B	421	LYS
1	B	447	LEU
1	B	471	VAL
1	B	477	LYS
1	C	47	GLN
1	C	61	ARG
1	C	75	LYS
1	C	104	SER
1	C	122	ARG
1	C	123	MET
1	C	136	ILE

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Mol	Chain	Res	Type
1	C	160	LYS
1	C	162	GLU
1	C	235	GLU
1	C	254	LYS
1	C	255	ASP
1	C	258	THR
1	C	278	LEU
1	C	320	ARG
1	C	366	ASP
1	C	368	LYS
1	C	396	GLU
1	C	403	GLU
1	C	421	LYS
1	C	450	ASP
1	C	452	VAL
1	C	471	VAL
1	C	475	ARG
1	D	28	LYS
1	D	41	ILE
1	D	47	GLN
1	D	109	VAL
1	D	122	ARG
1	D	123	MET
1	D	136	ILE
1	D	190	LYS
1	D	195	ARG
1	D	196	ARG
1	D	215	LEU
1	D	235	GLU
1	D	238	LYS
1	D	251	GLU
1	D	252	VAL
1	D	255	ASP
1	D	278	LEU
1	D	297	SER
1	D	314	LYS
1	D	317	GLU
1	D	320	ARG
1	D	376	LYS
1	D	452	VAL
1	D	471	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	47	GLN
1	A	253	ASN
1	A	279	HIS
1	A	309	HIS
1	A	388	HIS
1	A	389	HIS
1	A	431	GLN
1	B	44	HIS
1	B	181	GLN
1	B	279	HIS
1	B	306	HIS
1	B	329	GLN
1	B	333	ASN
1	B	334	ASN
1	B	388	HIS
1	B	389	HIS
1	B	446	GLN
1	C	44	HIS
1	C	47	GLN
1	C	140	GLN
1	C	279	HIS
1	C	309	HIS
1	C	333	ASN
1	C	334	ASN
1	C	388	HIS
1	C	389	HIS
1	C	446	GLN
1	D	44	HIS
1	D	279	HIS
1	D	309	HIS
1	D	334	ASN
1	D	388	HIS
1	D	389	HIS

5.3.3 RNA ⓘ

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](#)

8 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	482	3,1	50,50,50	1.76	10 (20%)	67,82,82	1.33	7 (10%)
3	JKF	D	490	2	38,40,40	2.33	9 (23%)	50,60,60	1.99	5 (10%)
2	HEM	D	482	3,1	50,50,50	1.75	10 (20%)	67,82,82	1.27	4 (5%)
3	JKF	A	490	2	38,40,40	2.58	7 (18%)	50,60,60	2.00	10 (20%)
2	HEM	B	482	3,1	50,50,50	1.72	9 (18%)	67,82,82	1.34	9 (13%)
3	JKF	C	490	2	38,40,40	2.44	7 (18%)	50,60,60	1.96	8 (16%)
2	HEM	A	482	3,1	50,50,50	1.70	10 (20%)	67,82,82	1.16	4 (5%)
3	JKF	B	490	2	38,40,40	2.65	8 (21%)	50,60,60	1.94	7 (14%)

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	482	3,1	-	0/14/54/54	-
3	JKF	D	490	2	-	5/24/25/25	0/5/5/5
2	HEM	D	482	3,1	-	0/14/54/54	-
3	JKF	A	490	2	-	5/24/25/25	0/5/5/5
2	HEM	B	482	3,1	-	0/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	JKF	C	490	2	-	10/24/25/25	0/5/5/5
2	HEM	A	482	3,1	-	2/14/54/54	-
3	JKF	B	490	2	-	7/24/25/25	0/5/5/5

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	490	JKF	CBJ-CBA	-9.41	1.38	1.53
3	C	490	JKF	CBJ-CBA	-8.92	1.38	1.53
3	A	490	JKF	CBJ-CAZ	-8.20	1.39	1.53
3	B	490	JKF	CBJ-CBA	-7.51	1.41	1.53
3	B	490	JKF	CBJ-CAZ	-7.49	1.41	1.53
2	C	482	HEM	C3D-C2D	7.44	1.52	1.36
2	D	482	HEM	C3D-C2D	7.32	1.52	1.36
3	D	490	JKF	CBJ-CBA	-7.29	1.41	1.53
2	B	482	HEM	C3D-C2D	7.28	1.52	1.36
3	D	490	JKF	CBJ-CAZ	-7.14	1.41	1.53
2	A	482	HEM	C3D-C2D	7.13	1.52	1.36
3	C	490	JKF	CBJ-CAZ	-7.08	1.41	1.53
3	C	490	JKF	CBC-CBB	-6.11	1.39	1.50
3	B	490	JKF	FAF-CAY	-5.88	1.19	1.35
3	A	490	JKF	CBC-CBB	-5.74	1.39	1.50
3	B	490	JKF	FAE-CAX	-5.71	1.20	1.35
3	B	490	JKF	CBC-CBB	-5.66	1.40	1.50
3	D	490	JKF	CBC-CBB	-4.78	1.41	1.50
3	D	490	JKF	CAS-CBB	4.03	1.40	1.35
2	C	482	HEM	FE-ND	3.88	2.06	1.94
3	A	490	JKF	FAF-CAY	-3.88	1.25	1.35
2	B	482	HEM	FE-ND	3.55	2.05	1.94
3	B	490	JKF	CBF-CBB	-3.54	1.40	1.47
3	D	490	JKF	FAF-CAY	-3.49	1.26	1.35
2	A	482	HEM	FE-ND	3.44	2.05	1.94
3	B	490	JKF	CAS-CBB	3.36	1.39	1.35
3	C	490	JKF	CAS-CBB	3.33	1.39	1.35
3	D	490	JKF	CBF-CBB	-3.33	1.40	1.47
2	B	482	HEM	CAC-C3C	3.30	1.56	1.47
2	D	482	HEM	FE-ND	3.29	2.05	1.94
3	A	490	JKF	CBF-CBB	-3.27	1.40	1.47
2	D	482	HEM	CAB-C3B	3.14	1.55	1.47
2	B	482	HEM	FE-NA	3.06	2.05	1.95
2	C	482	HEM	FE-NA	3.01	2.05	1.95
2	A	482	HEM	CMC-C2C	3.00	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	490	JKF	CBF-CBB	-2.97	1.41	1.47
2	A	482	HEM	CAC-C3C	2.93	1.55	1.47
2	B	482	HEM	CAB-C3B	2.90	1.55	1.47
3	B	490	JKF	CBG-NBI	-2.86	1.35	1.40
2	D	482	HEM	CAC-C3C	2.84	1.55	1.47
2	C	482	HEM	FE-NB	2.84	2.03	1.94
3	C	490	JKF	CAW-CLAG	2.79	1.80	1.74
3	A	490	JKF	CAS-CBB	2.78	1.38	1.35
2	C	482	HEM	CAB-C3B	2.77	1.54	1.47
3	D	490	JKF	CBG-NBI	-2.72	1.35	1.40
3	A	490	JKF	CBG-NBI	-2.69	1.35	1.40
2	D	482	HEM	CMC-C2C	2.66	1.56	1.50
2	A	482	HEM	CAB-C3B	2.58	1.54	1.47
2	D	482	HEM	CMB-C2B	2.51	1.55	1.50
2	C	482	HEM	CAC-C3C	2.45	1.53	1.47
2	D	482	HEM	FE-NA	2.43	2.03	1.95
2	C	482	HEM	CMC-C2C	2.40	1.55	1.50
2	B	482	HEM	CMB-C2B	2.37	1.55	1.50
2	A	482	HEM	CMB-C2B	2.37	1.55	1.50
2	A	482	HEM	FE-NC	2.35	2.02	1.95
2	B	482	HEM	CMD-C2D	2.33	1.55	1.50
2	D	482	HEM	C2A-C3A	-2.31	1.32	1.38
3	D	490	JKF	CAB-NBH	2.27	1.51	1.46
2	B	482	HEM	FE-NB	2.26	2.01	1.94
3	C	490	JKF	CBG-NBI	-2.26	1.36	1.40
2	D	482	HEM	FE-NB	2.26	2.01	1.94
2	C	482	HEM	CMB-C2B	2.23	1.55	1.50
2	B	482	HEM	CMC-C2C	2.23	1.55	1.50
2	A	482	HEM	CMD-C2D	2.23	1.55	1.50
2	D	482	HEM	FE-NC	2.21	2.02	1.95
2	A	482	HEM	FE-NB	2.17	2.01	1.94
2	A	482	HEM	CMA-C3A	2.16	1.55	1.50
3	D	490	JKF	CBJ-CBD	2.12	1.55	1.51
2	C	482	HEM	C3C-C2C	-2.12	1.32	1.37
2	C	482	HEM	CMD-C2D	2.05	1.55	1.50

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	490	JKF	NBH-CAR-NAU	-8.99	107.59	112.94
3	B	490	JKF	NBH-CAR-NAU	-8.60	107.82	112.94
3	C	490	JKF	NBH-CAR-NAU	-8.59	107.83	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	490	JKF	NBH-CAR-NAU	-8.34	107.98	112.94
3	A	490	JKF	CAS-CBE-NBI	6.38	121.67	115.44
3	B	490	JKF	CAS-CBE-NBI	6.19	121.49	115.44
3	D	490	JKF	CAS-CBE-NBI	5.99	121.29	115.44
3	C	490	JKF	CAS-CBE-NBI	5.38	120.69	115.44
2	C	482	HEM	C4D-ND-C1D	5.05	111.19	105.21
2	B	482	HEM	C4D-ND-C1D	4.32	110.33	105.21
2	D	482	HEM	C4D-ND-C1D	4.14	110.11	105.21
2	A	482	HEM	C4D-ND-C1D	4.02	109.97	105.21
3	B	490	JKF	CBB-CAS-CBE	-3.03	119.19	122.87
2	D	482	HEM	CHD-C4C-NC	3.00	127.72	124.45
3	A	490	JKF	CBB-CAS-CBE	-2.98	119.24	122.87
3	C	490	JKF	CAP-NAU-CAR	2.96	109.12	105.24
3	A	490	JKF	CAP-NAU-CAR	2.92	109.06	105.24
2	C	482	HEM	CHD-C1D-ND	2.78	127.41	124.42
2	A	482	HEM	CHC-C4B-NB	2.73	127.37	124.42
3	D	490	JKF	CBG-NBI-CBE	-2.73	120.34	122.93
3	A	490	JKF	CAX-CBC-CBB	-2.72	118.72	122.28
3	B	490	JKF	CAX-CBC-CBB	-2.72	118.72	122.28
3	D	490	JKF	CAP-NAU-CAR	2.68	108.75	105.24
3	D	490	JKF	CBB-CAS-CBE	-2.68	119.61	122.87
2	B	482	HEM	CBD-CAD-C3D	-2.63	105.26	112.53
3	A	490	JKF	OAD-CBE-CAS	-2.62	119.15	125.61
2	B	482	HEM	CHD-C4C-NC	2.60	127.29	124.45
3	A	490	JKF	CBG-NBI-CBE	-2.58	120.48	122.93
2	B	482	HEM	O1D-CGD-CBD	-2.57	114.95	123.09
3	B	490	JKF	CAP-NAU-CAR	2.56	108.59	105.24
3	C	490	JKF	CAN-CAL-CAW	2.54	121.80	119.24
2	C	482	HEM	CBD-CAD-C3D	-2.53	105.54	112.53
3	C	490	JKF	OAD-CBE-CAS	-2.53	119.37	125.61
2	B	482	HEM	CHD-C1D-ND	2.53	127.14	124.42
3	B	490	JKF	OAD-CBE-CAS	-2.50	119.44	125.61
3	B	490	JKF	CBG-NBI-CBE	-2.47	120.59	122.93
2	B	482	HEM	O2A-CGA-CBA	2.40	121.58	114.00
3	C	490	JKF	CBB-CAS-CBE	-2.36	119.99	122.87
3	C	490	JKF	CAY-CBC-CAX	2.34	118.95	114.93
3	A	490	JKF	CAY-CBC-CAX	2.30	118.90	114.93
2	B	482	HEM	C1B-NB-C4B	2.28	107.91	105.21
2	C	482	HEM	C4C-C3C-C2C	2.27	108.78	106.81
2	D	482	HEM	CHC-C4B-NB	2.24	126.83	124.42
3	A	490	JKF	CBJ-CBD-CAP	-2.16	125.09	131.31
3	A	490	JKF	CAQ-CAO-CBA	-2.15	118.20	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	482	HEM	C4C-C3C-C2C	2.14	108.67	106.81
2	C	482	HEM	CHC-C4B-NB	2.12	126.71	124.42
3	C	490	JKF	CBG-NBI-CBE	-2.11	120.92	122.93
2	A	482	HEM	CMD-C2D-C1D	2.08	128.28	125.03
2	B	482	HEM	O2D-CGD-CBD	2.06	120.50	114.00
2	B	482	HEM	CAA-CBA-CGA	-2.05	108.22	113.67
2	C	482	HEM	C4A-C3A-C2A	2.04	109.16	106.82
2	C	482	HEM	CBC-CAC-C3C	-2.03	117.37	127.53
2	D	482	HEM	O2D-CGD-CBD	2.01	120.35	114.00

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	490	JKF	CAZ-CBJ-OAV-CAA
3	C	490	JKF	CBA-CBJ-OAV-CAA
3	C	490	JKF	CBF-CBB-CBC-CAY
3	C	490	JKF	CBF-CBB-CBC-CAX
3	B	490	JKF	CAN-CAZ-CBJ-OAV
3	D	490	JKF	CAN-CAZ-CBJ-OAV
3	A	490	JKF	CAN-CAZ-CBJ-OAV
3	B	490	JKF	CAZ-CBJ-OAV-CAA
3	A	490	JKF	CAP-CBD-CBJ-CBA
3	C	490	JKF	CAP-CBD-CBJ-CBA
3	D	490	JKF	CAP-CBD-CBJ-CBA
3	B	490	JKF	CAM-CAZ-CBJ-OAV
3	D	490	JKF	CAM-CAZ-CBJ-OAV
3	A	490	JKF	CAM-CAZ-CBJ-OAV
3	C	490	JKF	CAN-CAZ-CBJ-OAV
3	A	490	JKF	CAM-CAZ-CBJ-CBA
3	A	490	JKF	CAN-CAZ-CBJ-CBA
3	B	490	JKF	CAM-CAZ-CBJ-CBA
3	B	490	JKF	CAN-CAZ-CBJ-CBA
3	C	490	JKF	CAM-CAZ-CBJ-CBA
3	C	490	JKF	CAN-CAZ-CBJ-CBA
3	D	490	JKF	CAM-CAZ-CBJ-CBA
3	D	490	JKF	CAN-CAZ-CBJ-CBA
2	A	482	HEM	CAD-CBD-CGD-O2D
3	B	490	JKF	CBA-CBJ-OAV-CAA
2	A	482	HEM	CAD-CBD-CGD-O1D
3	C	490	JKF	CAS-CBB-CBC-CAY
3	C	490	JKF	CAP-CBD-CBJ-OAV

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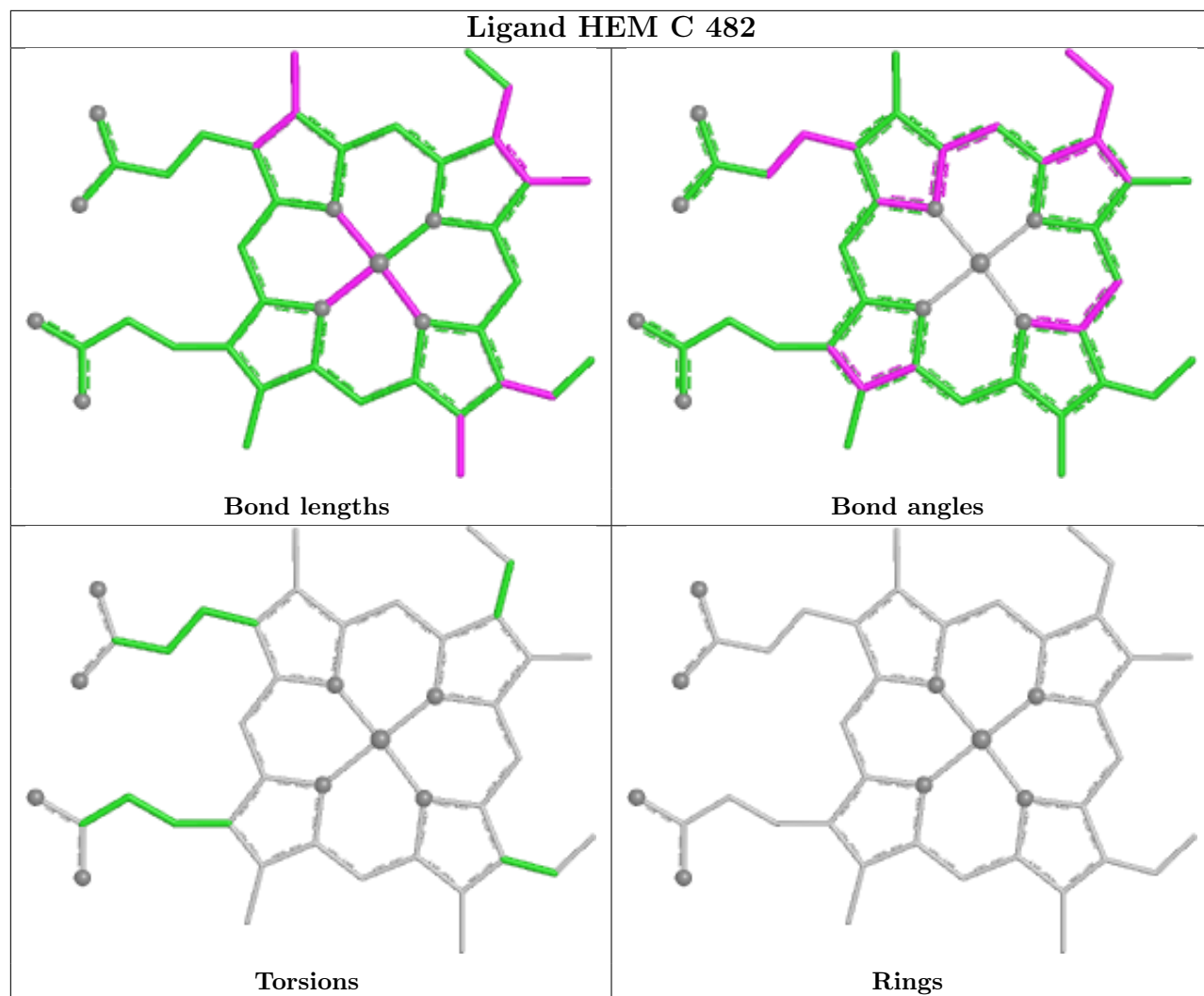
Mol	Chain	Res	Type	Atoms
3	B	490	JKF	CAP-CBD-CBJ-CBA

There are no ring outliers.

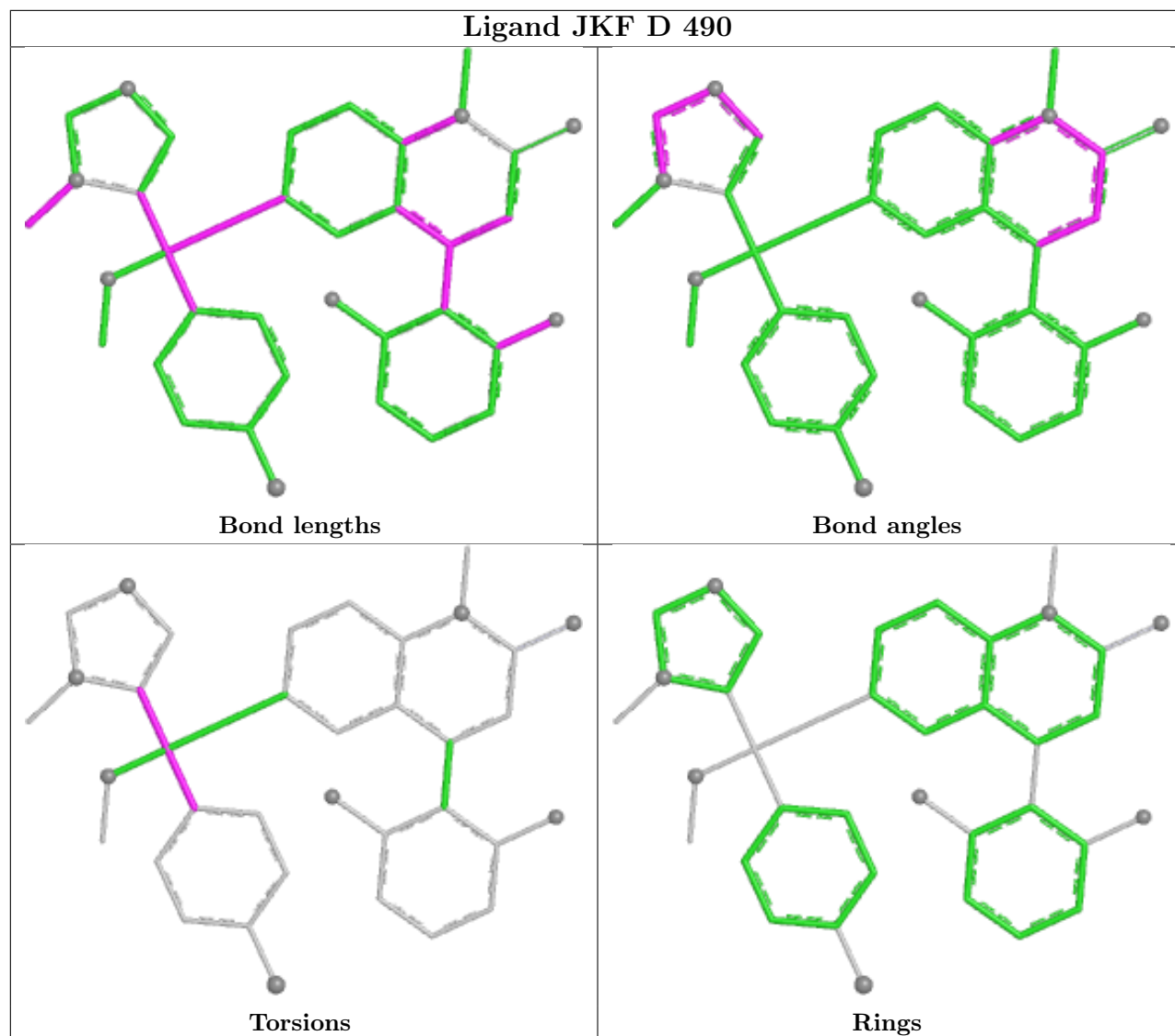
8 monomers are involved in 65 short contacts:

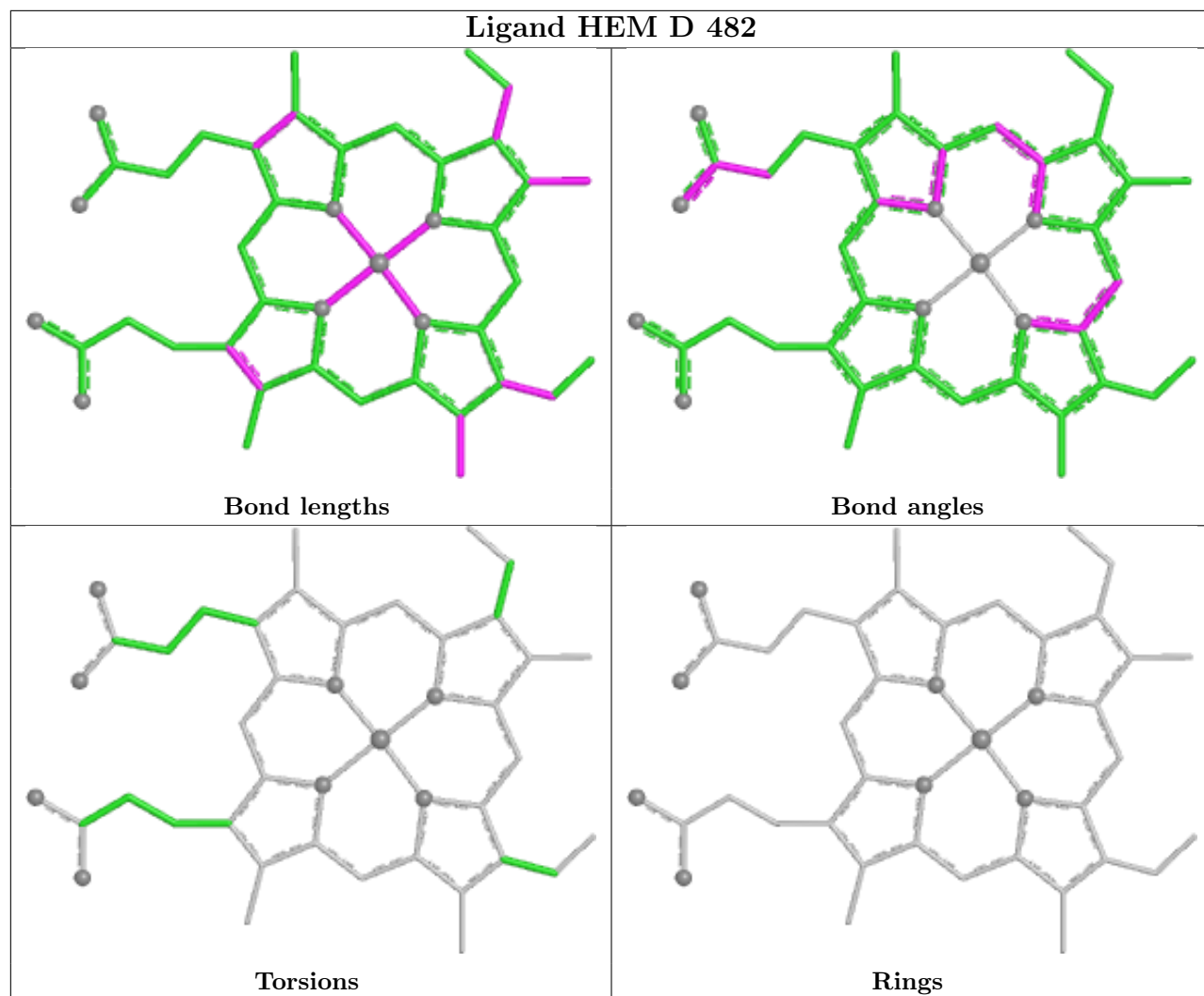
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	482	HEM	10	0
3	D	490	JKF	10	0
2	D	482	HEM	5	0
3	A	490	JKF	7	0
2	B	482	HEM	5	0
3	C	490	JKF	15	0
2	A	482	HEM	6	0
3	B	490	JKF	7	0

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

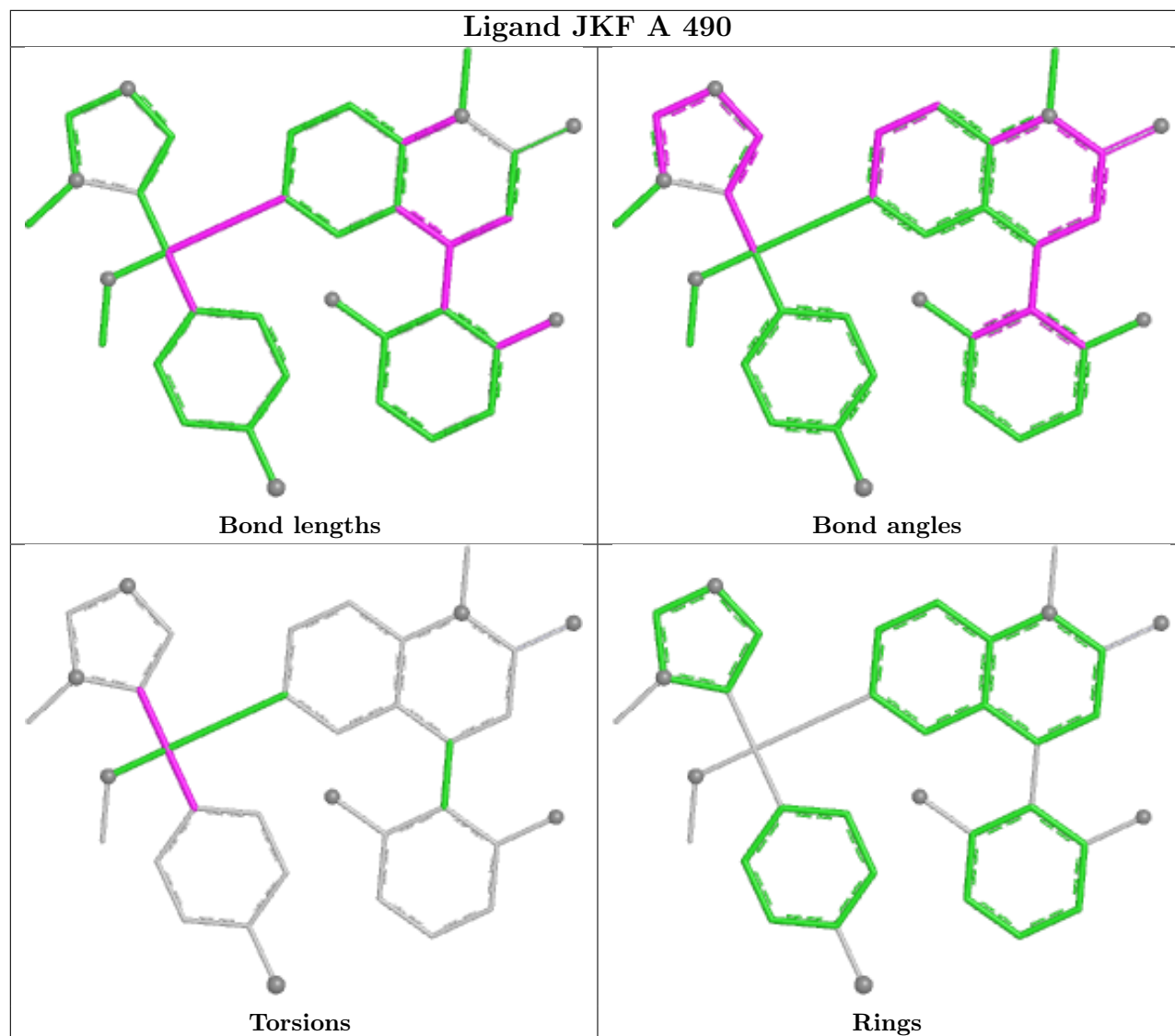


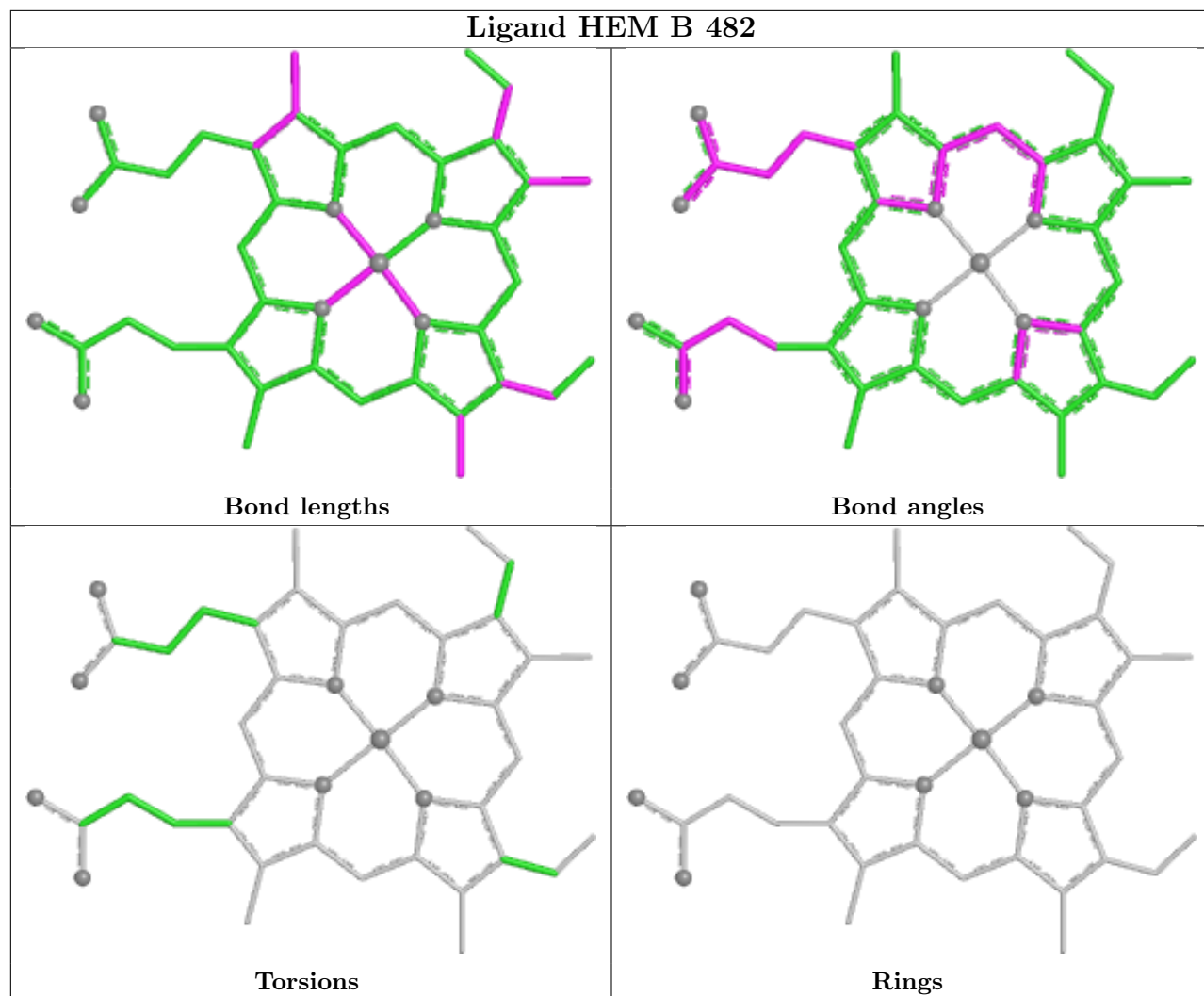
Ligand JKF D 490



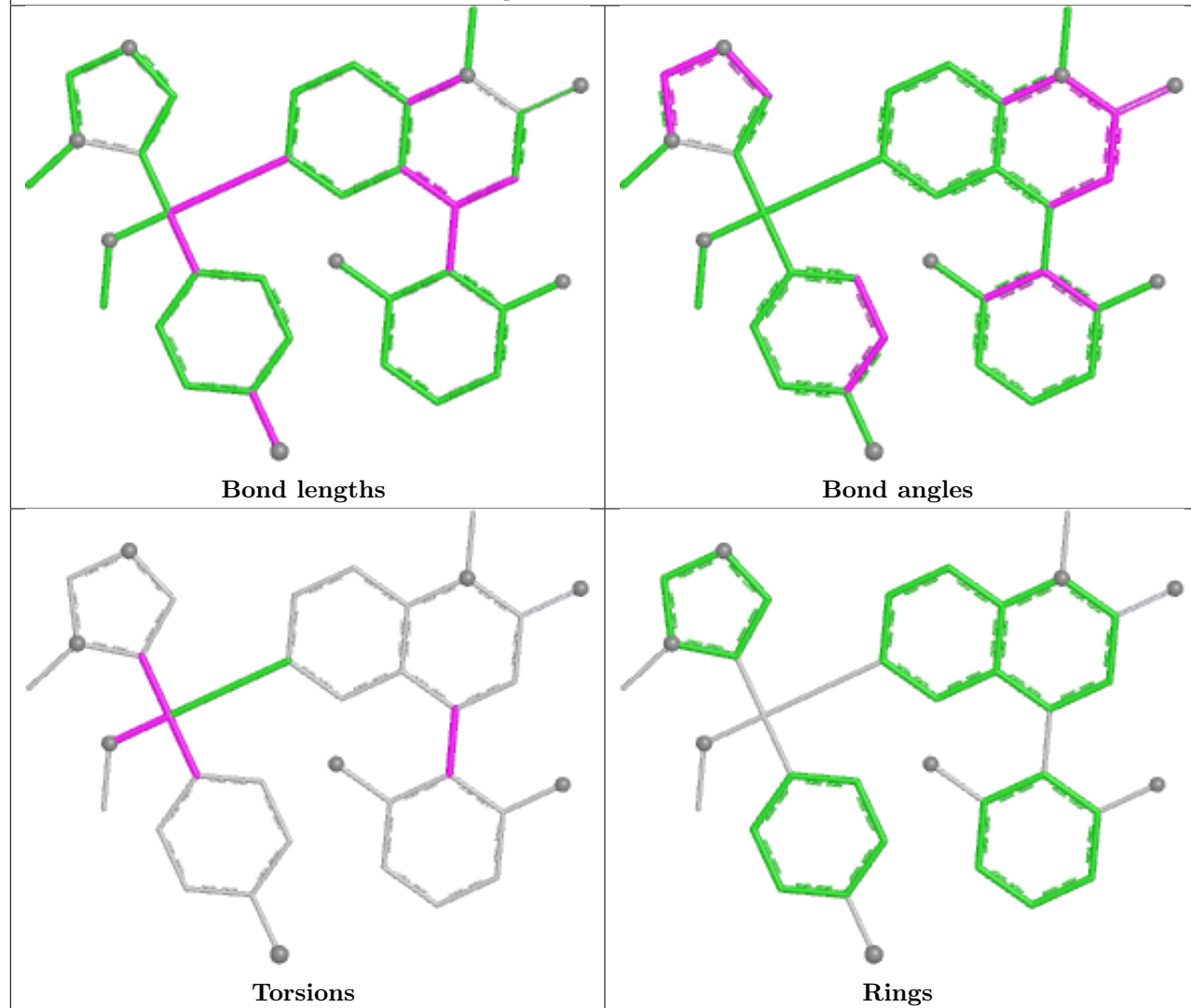


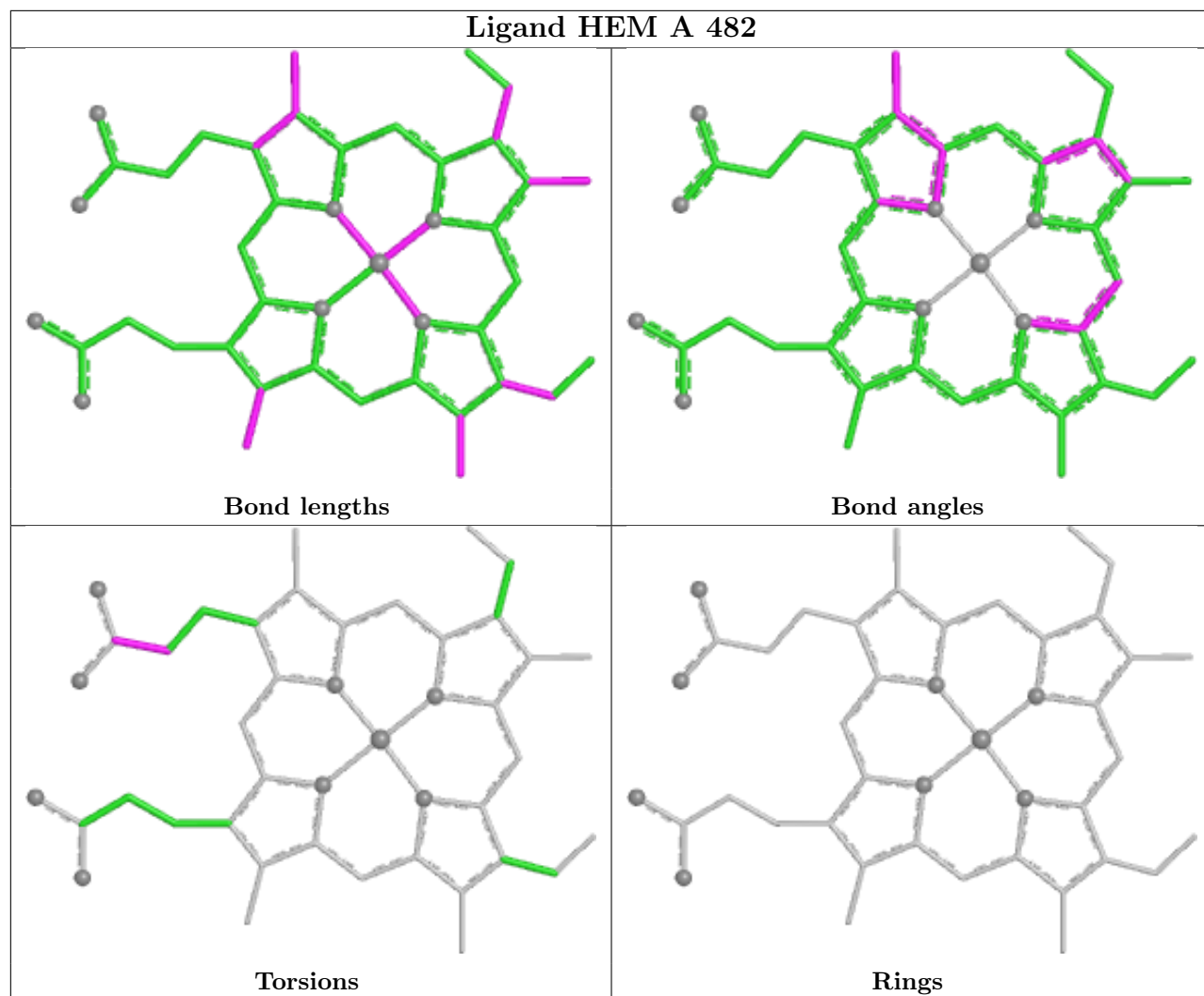
Ligand JKF A 490

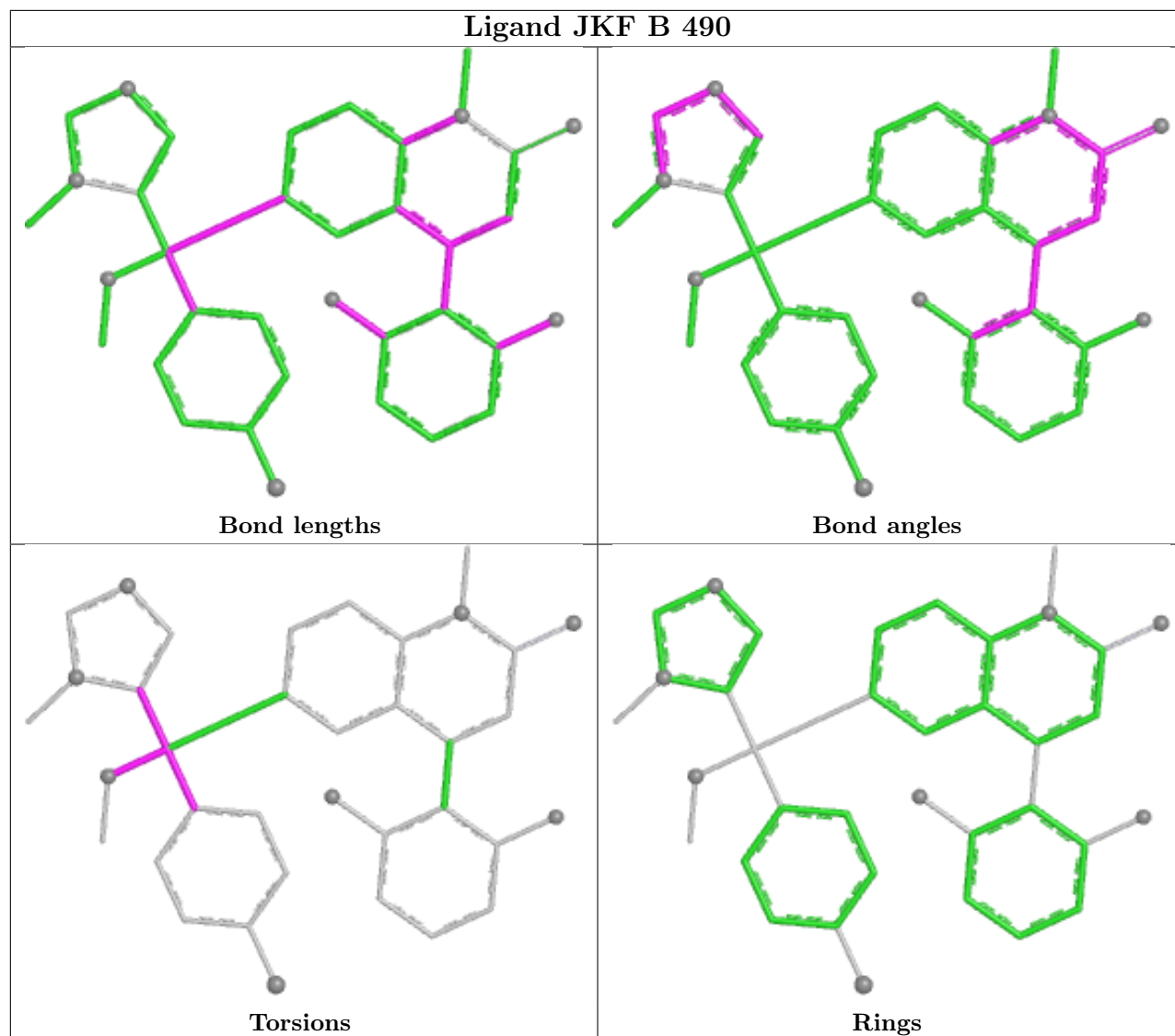




Ligand JKF C 490







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	450/454 (99%)	0.16	9 (2%) 65 67	33, 53, 75, 88	0
1	B	450/454 (99%)	0.06	13 (2%) 53 55	27, 47, 70, 95	0
1	C	450/454 (99%)	0.05	8 (1%) 67 69	33, 52, 73, 93	0
1	D	450/454 (99%)	-0.23	11 (2%) 59 61	25, 41, 62, 85	0
All	All	1800/1816 (99%)	0.01	41 (2%) 61 63	25, 48, 72, 95	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	252	VAL	5.4
1	C	29	GLY	5.0
1	C	256	SER	4.5
1	D	256	SER	4.3
1	B	254	LYS	4.2
1	D	29	GLY	4.1
1	B	256	SER	3.7
1	D	28	LYS	3.6
1	B	252	VAL	3.5
1	C	41	ILE	3.3
1	A	155	ALA	3.3
1	C	255	ASP	3.3
1	A	254	LYS	3.2
1	D	41	ILE	3.1
1	A	256	SER	3.0
1	B	251	GLU	2.9
1	C	254	LYS	2.9
1	B	28	LYS	2.8
1	A	293	GLN	2.8
1	B	41	ILE	2.7
1	B	29	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	155	ALA	2.6
1	A	41	ILE	2.6
1	D	251	GLU	2.6
1	D	257	SER	2.6
1	A	120	TYR	2.5
1	D	253	ASN	2.5
1	B	196	ARG	2.4
1	B	40	PRO	2.4
1	D	43	GLY	2.3
1	A	255	ASP	2.3
1	C	258	THR	2.3
1	B	39	VAL	2.3
1	A	327	PRO	2.3
1	C	28	LYS	2.3
1	C	43	GLY	2.2
1	A	252	VAL	2.1
1	D	39	VAL	2.1
1	B	43	GLY	2.1
1	B	257	SER	2.0
1	D	120	TYR	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	JKF	C	490	36/36	0.92	0.09	38,49,58,64	0
3	JKF	A	490	36/36	0.95	0.07	33,41,60,66	0
3	JKF	D	490	36/36	0.95	0.07	21,39,56,66	0

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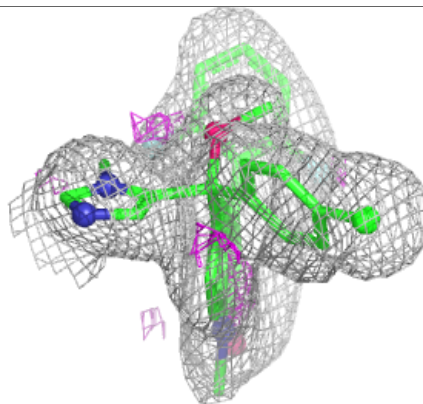
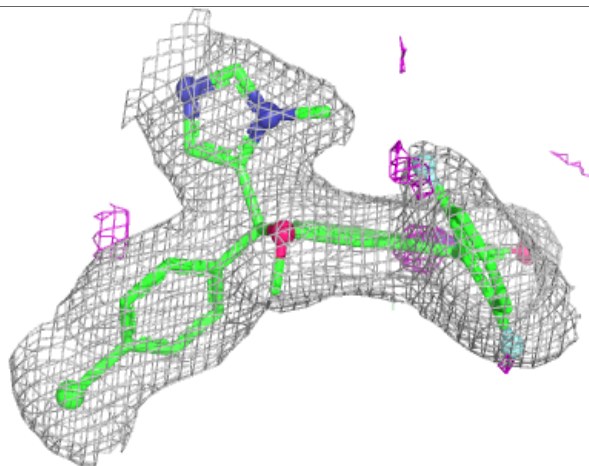
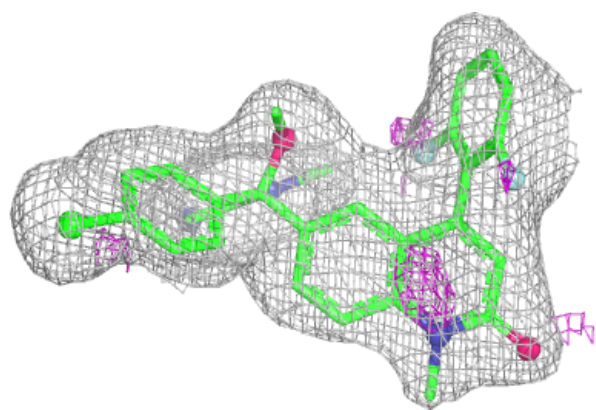
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JKF	B	490	36/36	0.96	0.07	31,42,57,65	0
2	HEM	A	482	43/43	0.98	0.06	29,32,39,45	0
2	HEM	C	482	43/43	0.98	0.07	35,40,48,55	0
2	HEM	B	482	43/43	0.99	0.05	23,31,37,41	0
2	HEM	D	482	43/43	0.99	0.05	23,27,38,43	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.

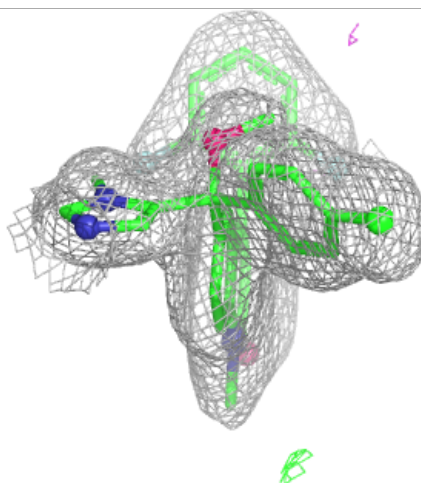
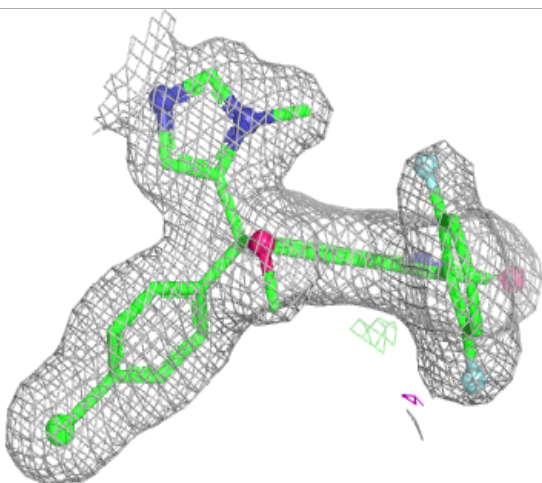
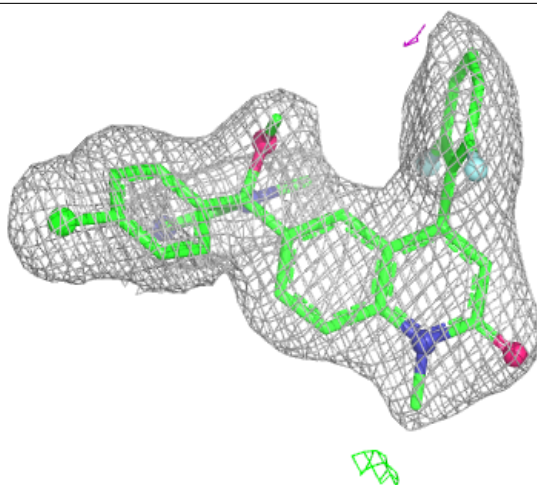
Electron density around JKF C 490:

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



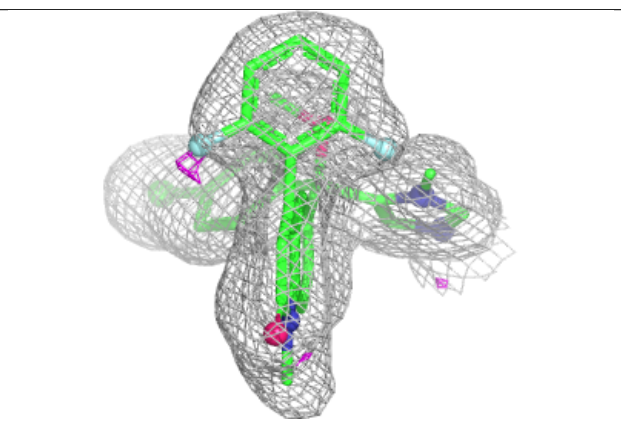
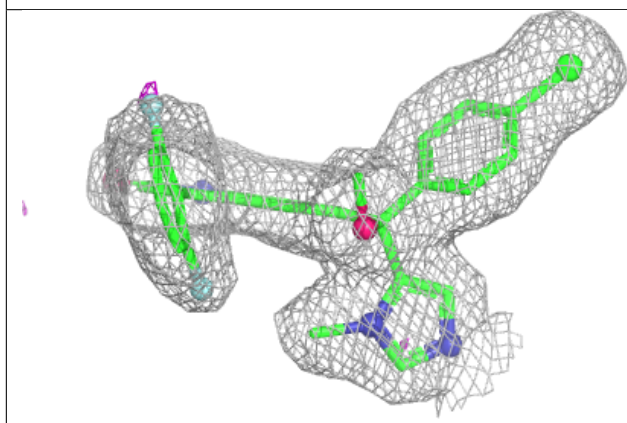
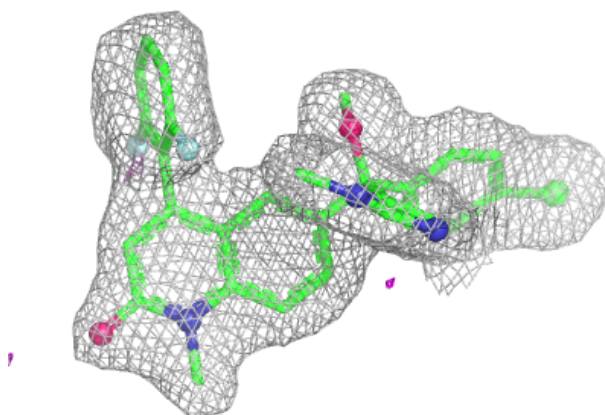
Electron density around JKF A 490:

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



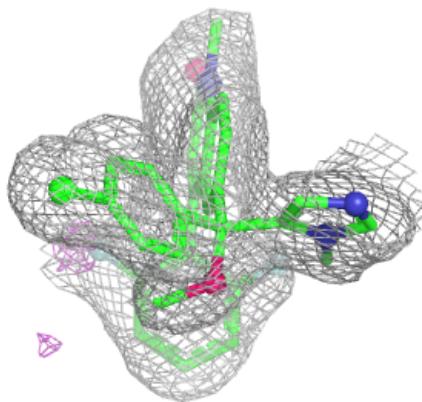
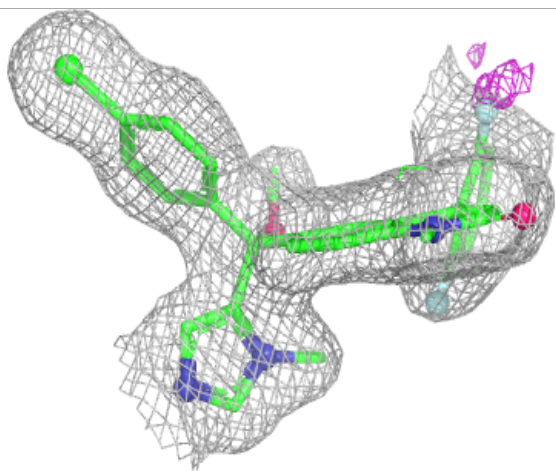
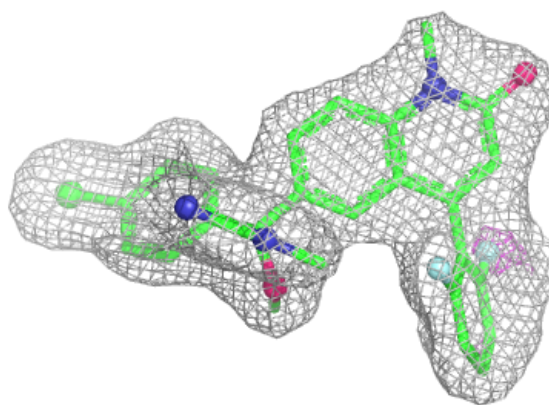
Electron density around JKF D 490:

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



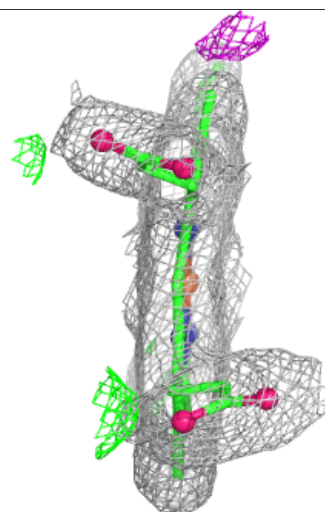
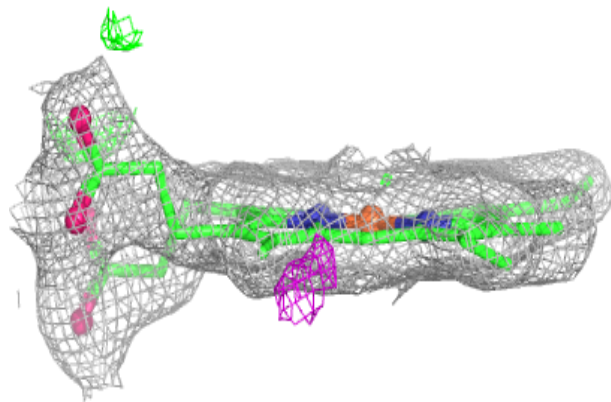
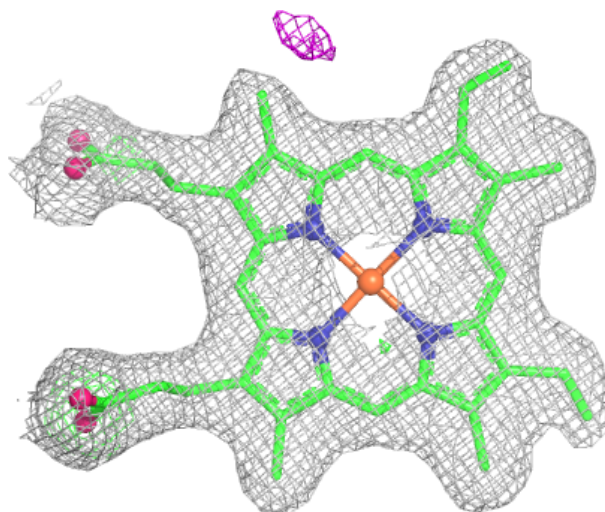
Electron density around JKF B 490:

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



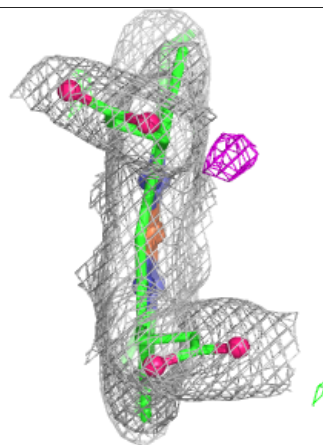
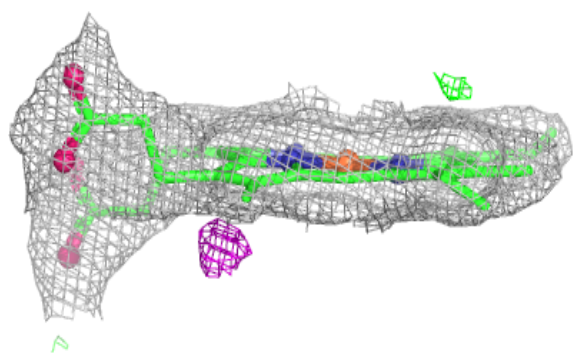
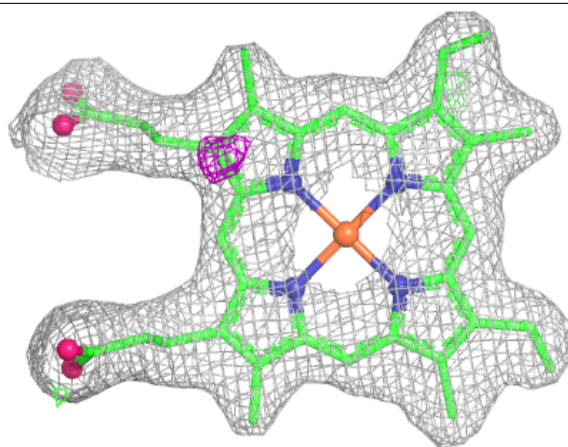
Electron density around HEM A 482:

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



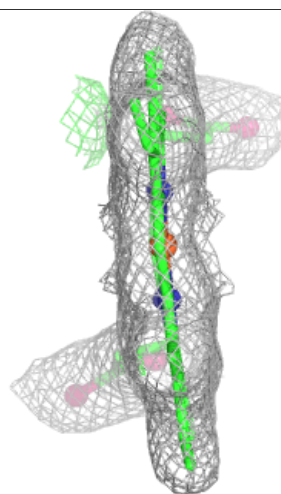
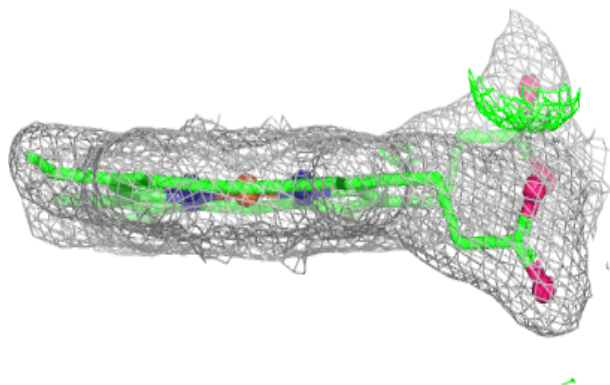
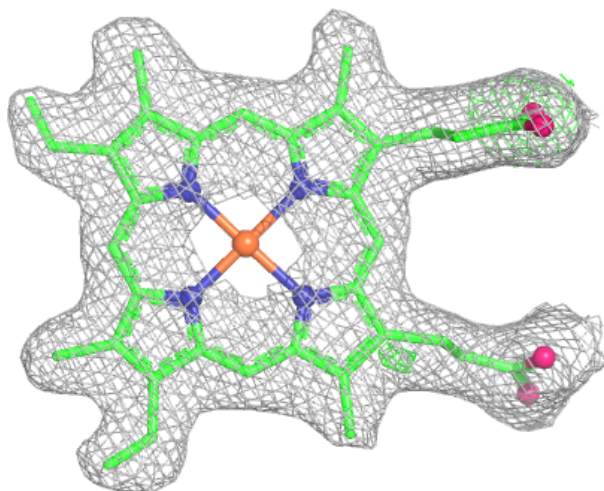
Electron density around HEM C 482:

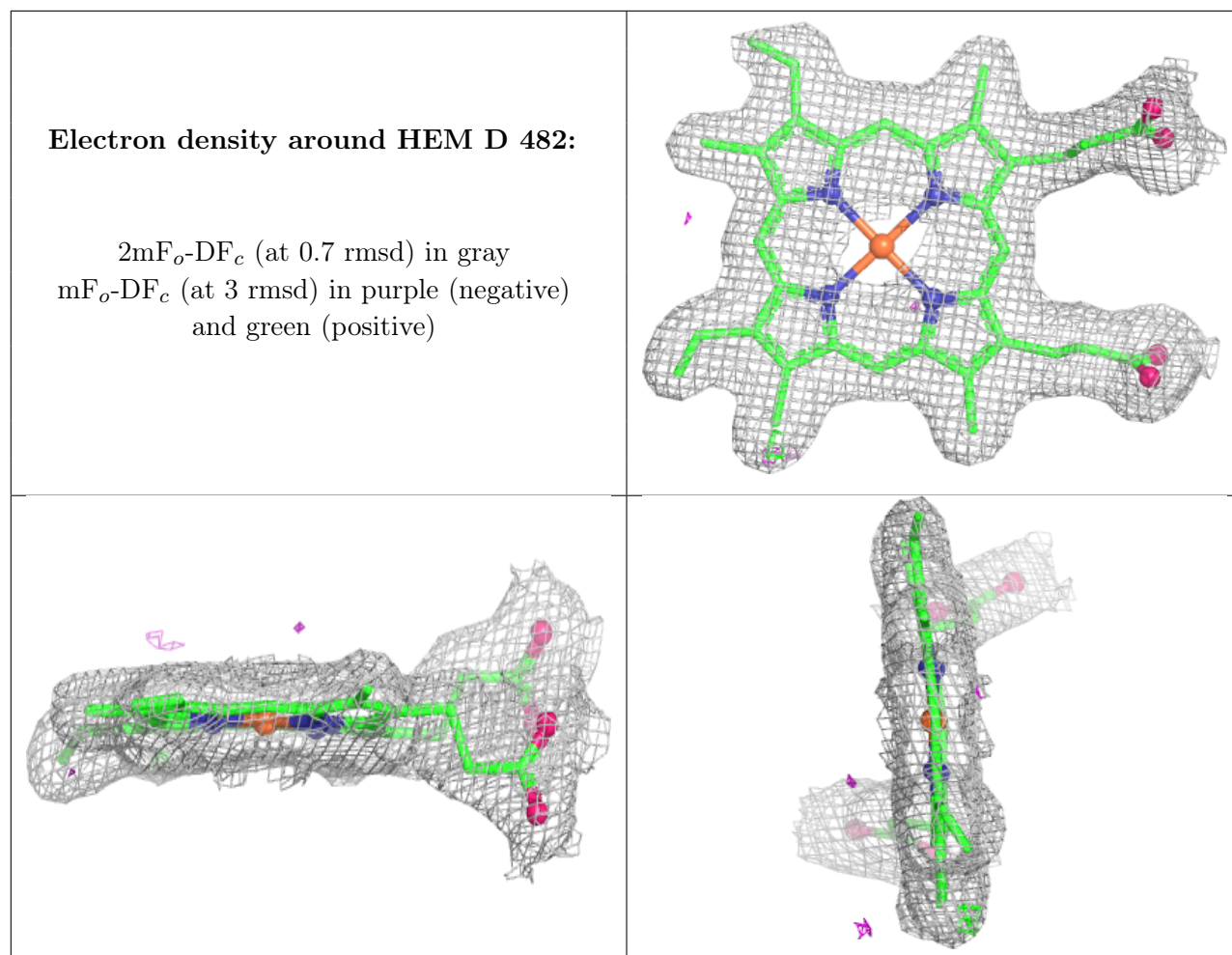
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 482:

$2mF_o-DF_c$ (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.