



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:48 AM UTC

PDB ID : 7YFT / pdb_00007yft
Title : Crystal structure of the P450 BM3 heme domain mutant F87A/T268V/A82 C/L181M in complex with N-imidazolyl-pentanoyl-L-phenylalanine, indane and hydroxylamine
Authors : Dong, S.; Chen, J.; Jiang, Y.; Cong, Z.; Feng, Y.
Deposited on : 2022-07-09
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

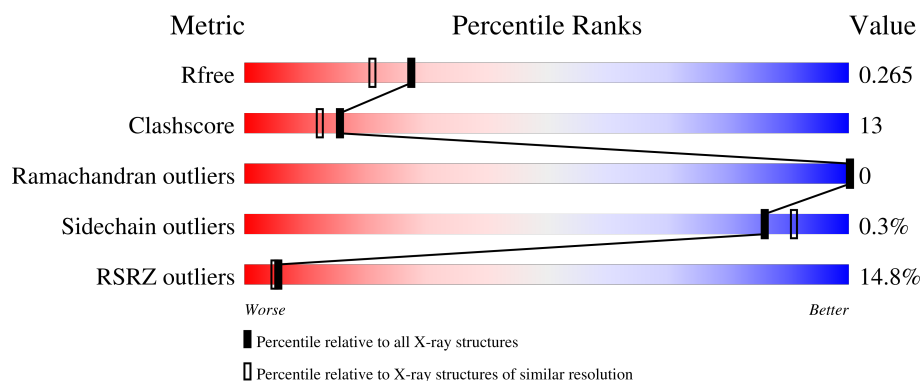
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	466	16% 71% 25% .
1	B	466	13% 69% 28% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	16N	A	503	-	-	X	-
4	16N	B	503	-	-	X	-
5	IRV	A	504[A]	-	-	-	X
5	IRV	A	504[B]	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15364 atoms, of which 7244 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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	451	Total	C	H	N	O	S	0	0	0
			7182	2310	3562	616	675	19			
1	B	452	Total	C	H	N	O	S	0	0	0
			7209	2317	3576	617	680	19			

There are 28 discrepancies between the modelled and reference sequences:

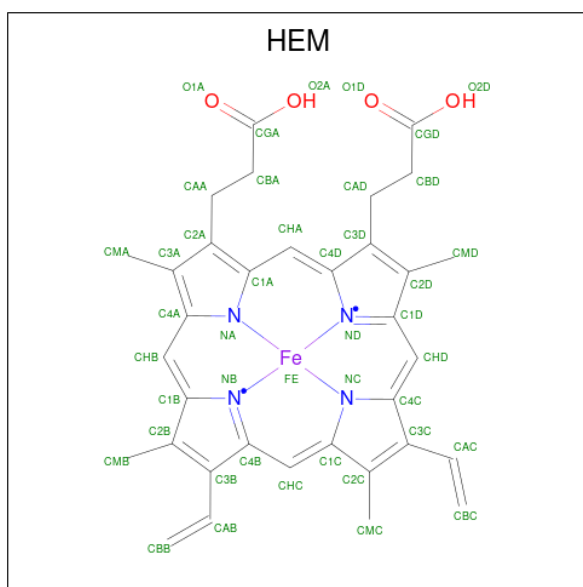
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P14779
A	-1	GLY	-	expression tag	UNP P14779
A	82	CYS	ALA	engineered mutation	UNP P14779
A	87	ALA	PHE	engineered mutation	UNP P14779
A	181	MET	LEU	engineered mutation	UNP P14779
A	268	VAL	THR	engineered mutation	UNP P14779
A	456	LEU	-	expression tag	UNP P14779
A	457	GLU	-	expression tag	UNP P14779
A	458	HIS	-	expression tag	UNP P14779
A	459	HIS	-	expression tag	UNP P14779
A	460	HIS	-	expression tag	UNP P14779
A	461	HIS	-	expression tag	UNP P14779
A	462	HIS	-	expression tag	UNP P14779
A	463	HIS	-	expression tag	UNP P14779
B	-2	MET	-	initiating methionine	UNP P14779
B	-1	GLY	-	expression tag	UNP P14779
B	82	CYS	ALA	engineered mutation	UNP P14779
B	87	ALA	PHE	engineered mutation	UNP P14779
B	181	MET	LEU	engineered mutation	UNP P14779
B	268	VAL	THR	engineered mutation	UNP P14779
B	456	LEU	-	expression tag	UNP P14779
B	457	GLU	-	expression tag	UNP P14779
B	458	HIS	-	expression tag	UNP P14779
B	459	HIS	-	expression tag	UNP P14779
B	460	HIS	-	expression tag	UNP P14779

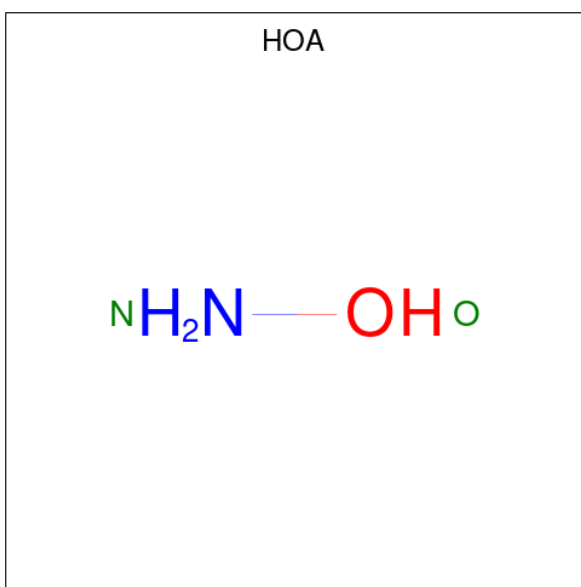
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Chain	Residue	Modelled	Actual	Comment	Reference
B	461	HIS	-	expression tag	UNP P14779
B	462	HIS	-	expression tag	UNP P14779
B	463	HIS	-	expression tag	UNP P14779

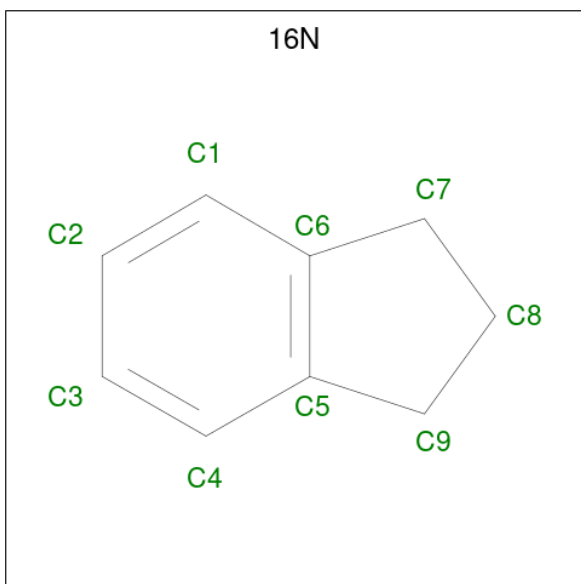
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	H	N	O	0	0
			5	3	1	1		
3	B	1	Total	H	N	O	0	0
			5	3	1	1		

- Molecule 4 is 2,3-dihydro-1H-indene (CCD ID: 16N) (formula: C₉H₁₀) (labeled as "Ligand of Interest" by depositor).



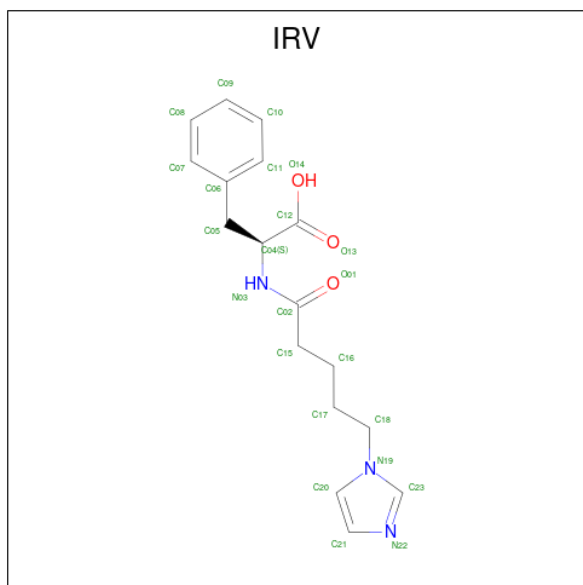
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	H	0	0
			19	9	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	H	0	0
			19	9	10		

- Molecule 5 is (2 {S})-2-(5-imidazol-1-ylpentanoylamino)-3-phenyl-propanoic acid (CCD ID: IRV) (formula: C₁₇H₂₁N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	1
			86	34	40	6	6		
5	B	1	Total	C	H	N	O	0	1
			86	34	40	6	6		

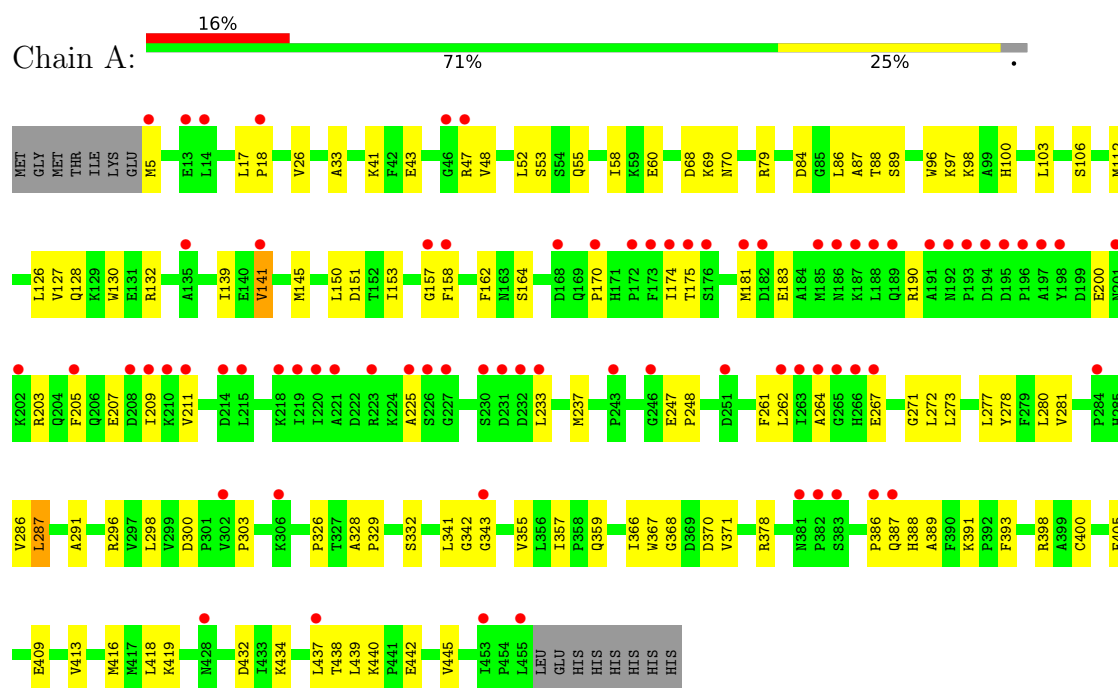
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	310	Total	O	0	0
			310	310		
6	B	357	Total	O	0	0
			357	357		

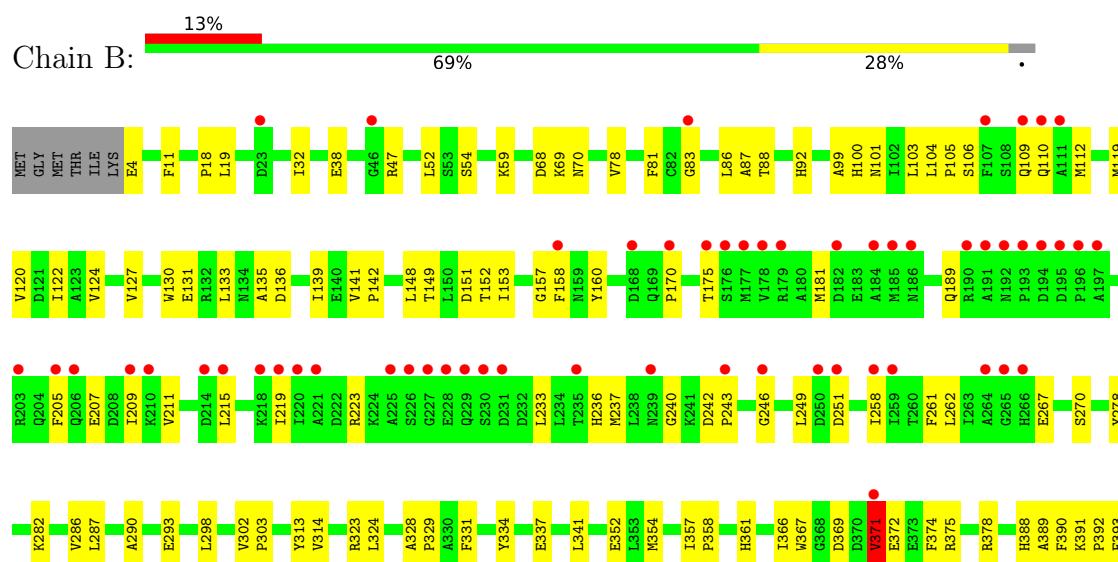
3 Residue-property plots

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: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.93Å 143.73Å 62.44Å 90.00° 100.01° 90.00°	Depositor
Resolution (Å)	38.48 – 2.00 38.48 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.2 (38.48-2.00) 85.7 (38.48-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.241 , 0.266 0.245 , 0.265	Depositor DCC
R_{free} test set	1824 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15364	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7516e-03.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, HOA, IRV, 16N

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	0.68	3/3704 (0.1%)	0.62	0/5011
1	B	0.61	2/3717 (0.1%)	0.62	2/5028 (0.0%)
All	All	0.65	5/7421 (0.1%)	0.62	2/10039 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	VAL	C-O	-7.05	1.15	1.24
1	A	272	LEU	C-O	-5.75	1.17	1.24
1	B	413	VAL	C-O	-5.74	1.17	1.24
1	B	371	VAL	C-O	-5.64	1.17	1.24
1	A	271	GLY	C-O	-5.38	1.17	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	GLN	N-CA-CB	5.79	118.41	110.01
1	B	109	GLN	N-CA-C	-5.64	105.28	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3620	3562	3575	82	0
1	B	3633	3576	3585	102	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
3	A	2	3	0	0	0
3	B	2	3	0	0	0
4	A	9	10	10	4	0
4	B	9	10	10	8	0
5	A	46	40	0	5	0
5	B	46	40	0	9	0
6	A	310	0	0	7	1
6	B	357	0	0	17	1
All	All	8120	7244	7240	195	1

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 13.

All (195) 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:52:LEU:HD21	1:B:341:LEU:HD21	1.69	0.74
4:A:503:16N:C4	5:A:504[A]:IRV:C21	2.66	0.73
4:B:503:16N:H1	5:B:504[B]:IRV:C23	2.23	0.67
1:B:367:TRP:HB2	1:B:371:VAL:HG23	1.78	0.66
2:B:502:HEM:HBC2	2:B:502:HEM:HMC2	1.78	0.65
1:A:128:GLN:O	1:A:132:ARG:HG3	1.96	0.65
1:A:205:PHE:CE2	1:A:209:ILE:HD11	2.31	0.64
1:A:183:GLU:OE1	1:A:190:ARG:NH2	2.29	0.64
1:A:280:LEU:HB3	1:A:287:LEU:HD23	1.81	0.63
1:A:150:LEU:HD21	1:A:174:ILE:HD11	1.80	0.62
1:B:148:LEU:HD13	1:B:413:VAL:HG21	1.81	0.62
1:B:127:VAL:HG21	1:B:416:MET:HE2	1.81	0.62
1:B:366:ILE:HG21	1:B:389:ALA:HB1	1.81	0.62
1:B:87:ALA:CB	4:B:503:16N:H5	2.30	0.61
1:B:354:MET:HE1	6:B:625:HOH:O	2.00	0.61
1:A:181:MET:CE	1:A:437:LEU:HD12	2.31	0.61
1:A:203:ARG:NH1	1:A:207:GLU:OE1	2.33	0.60
1:A:52:LEU:HD21	1:A:341:LEU:HD21	1.84	0.59
1:A:400:CYS:HB2	2:A:501:HEM:NA	2.16	0.59
2:B:502:HEM:HBC2	2:B:502:HEM:CMC	2.31	0.59
1:B:103:LEU:HD13	1:B:261:PHE:HZ	1.68	0.59
1:A:126:LEU:HD21	1:A:145:MET:HE1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.86	0.58
4:B:503:16N:H1	5:B:504[B]:IRV:C20	2.33	0.58
4:B:503:16N:H1	5:B:504[B]:IRV:N19	2.19	0.57
1:B:127:VAL:O	1:B:131:GLU:HG2	2.04	0.57
1:B:205:PHE:CE2	1:B:209:ILE:HD11	2.41	0.56
1:A:47:ARG:NH2	6:A:630:HOH:O	2.39	0.56
1:A:170:PRO:HG2	1:A:175:THR:HG22	1.87	0.56
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.88	0.56
1:A:183:GLU:OE2	1:A:190:ARG:NH1	2.37	0.55
1:B:434:LYS:HD3	1:B:440:LYS:HE2	1.87	0.55
1:A:343:GLY:N	6:A:623:HOH:O	2.35	0.54
1:B:47:ARG:NH2	5:B:504[A]:IRV:O14	2.32	0.54
1:A:434:LYS:HB2	1:A:442:GLU:HB2	1.88	0.54
1:A:200:GLU:N	1:A:200:GLU:OE1	2.40	0.54
1:A:264:ALA:HB1	2:A:501:HEM:C4C	2.42	0.54
1:B:92:HIS:O	6:B:601:HOH:O	2.17	0.54
1:B:100:HIS:NE2	1:B:104:LEU:HD11	2.23	0.54
1:B:331:PHE:HD1	1:B:357:ILE:HD11	1.72	0.54
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.89	0.53
1:B:70:ASN:OD1	6:B:602:HOH:O	2.18	0.53
1:B:4:GLU:N	6:B:658:HOH:O	2.42	0.53
1:A:273:LEU:HD11	1:A:413:VAL:HG11	1.91	0.53
1:A:298:LEU:HD22	1:A:303:PRO:HB3	1.90	0.53
1:B:236:HIS:O	1:B:240:GLY:N	2.41	0.53
1:B:133:LEU:HD12	6:B:768:HOH:O	2.09	0.52
1:B:328:ALA:CB	5:B:504[B]:IRV:C23	2.88	0.52
1:B:124:VAL:HG13	1:B:455:LEU:HD13	1.89	0.52
1:B:153:ILE:O	1:B:157:GLY:N	2.42	0.52
1:A:60:GLU:OE1	1:A:342:GLY:N	2.42	0.51
1:A:158:PHE:CZ	1:A:262:LEU:HD11	2.45	0.51
1:B:78:VAL:HG11	4:B:503:16N:H9	1.91	0.51
1:A:103:LEU:HD13	1:A:261:PHE:HZ	1.75	0.51
1:B:149:THR:HA	1:B:409:GLU:OE2	2.11	0.51
4:A:503:16N:H9	5:A:504[A]:IRV:N22	2.25	0.51
1:B:267:GLU:HA	1:B:270:SER:OG	2.10	0.51
1:B:328:ALA:O	1:B:357:ILE:HD12	2.11	0.51
1:A:98:LYS:CE	1:A:248:PRO:O	2.59	0.50
1:A:103:LEU:HD21	1:A:237:MET:HG2	1.94	0.50
1:A:326:PRO:HG3	1:A:357:ILE:HG22	1.92	0.50
1:A:68:ASP:OD1	1:A:69:LYS:N	2.45	0.50
1:A:328:ALA:O	1:A:357:ILE:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:O	1:A:211:VAL:HG23	2.10	0.50
1:B:158:PHE:CD1	1:B:258:ILE:HD12	2.47	0.50
1:B:158:PHE:CD2	1:B:219:ILE:HG21	2.47	0.50
1:B:70:ASN:ND2	6:B:602:HOH:O	2.43	0.50
1:B:251:ASP:N	6:B:666:HOH:O	2.44	0.50
1:B:223:ARG:HB2	6:B:630:HOH:O	2.11	0.50
1:B:68:ASP:OD1	1:B:69:LYS:N	2.45	0.49
1:B:170:PRO:HG2	1:B:175:THR:HG22	1.94	0.49
1:A:98:LYS:NZ	1:A:248:PRO:O	2.45	0.49
1:B:293:GLU:OE1	1:B:314:VAL:HG23	2.12	0.49
1:A:112:MET:SD	1:A:405:PHE:HA	2.52	0.49
1:B:181:MET:CE	1:B:437:LEU:HD12	2.41	0.49
1:B:120:VAL:HG11	1:B:302:VAL:CG1	2.42	0.49
1:B:328:ALA:HB1	5:B:504[B]:IRV:C21	2.42	0.49
1:A:103:LEU:HD21	1:A:237:MET:CG	2.43	0.49
1:B:83:GLY:O	1:B:88:THR:OG1	2.25	0.49
1:B:181:MET:HE1	1:B:437:LEU:HD12	1.95	0.48
1:A:106:SER:HB3	1:A:233:LEU:HD23	1.94	0.48
1:B:120:VAL:HG11	1:B:302:VAL:HG11	1.95	0.48
1:A:158:PHE:CE1	1:A:262:LEU:HD21	2.48	0.48
1:A:296:ARG:HD3	1:B:59:LYS:HE3	1.95	0.48
1:B:160:TYR:CD1	1:B:219:ILE:HD11	2.48	0.48
1:B:158:PHE:CE1	1:B:262:LEU:HD21	2.49	0.47
4:A:503:16N:C4	5:A:504[A]:IRV:N22	2.77	0.47
1:A:69:LYS:NZ	1:A:87:ALA:O	2.46	0.47
1:B:47:ARG:NH2	1:B:352:GLU:OE2	2.43	0.47
1:B:112:MET:SD	1:B:405:PHE:HA	2.55	0.47
1:A:86:LEU:HD21	1:A:100:HIS:N	2.30	0.47
1:B:393:PHE:HB3	1:B:400:CYS:HB3	1.96	0.47
1:A:127:VAL:HG21	1:A:416:MET:HE2	1.97	0.47
1:A:432:ASP:O	1:A:442:GLU:N	2.44	0.47
1:A:296:ARG:NH2	6:A:613:HOH:O	2.32	0.46
1:A:267:GLU:OE1	6:A:601:HOH:O	2.20	0.46
4:B:503:16N:H1	5:B:504[A]:IRV:C21	2.45	0.46
1:B:103:LEU:HD21	1:B:237:MET:CG	2.46	0.46
4:A:503:16N:H9	5:A:504[A]:IRV:C23	2.45	0.46
1:A:98:LYS:HE3	1:A:247:GLU:HB2	1.97	0.46
1:B:104:LEU:N	1:B:105:PRO:CD	2.78	0.46
1:A:141:VAL:HG21	1:A:277:LEU:HD23	1.97	0.46
1:B:141:VAL:HB	1:B:142:PRO:HD3	1.97	0.46
1:A:139:ILE:O	1:A:445:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:503:16N:H1	5:B:504[B]:IRV:C21	2.45	0.46
1:A:434:LYS:HD3	1:A:440:LYS:HE2	1.97	0.46
1:B:286:VAL:HG11	1:B:374:PHE:HE2	1.81	0.46
1:B:449:LYS:HE2	6:B:841:HOH:O	2.16	0.45
1:A:273:LEU:CD1	1:A:413:VAL:HG11	2.45	0.45
1:B:181:MET:HE1	4:B:503:16N:H10	1.98	0.45
1:B:130:TRP:CZ2	1:B:139:ILE:HG21	2.52	0.45
1:B:242:ASP:O	1:B:246:GLY:N	2.45	0.45
1:B:298:LEU:HD22	1:B:303:PRO:HB3	1.98	0.45
1:A:55:GLN:NE2	1:A:387:GLN:O	2.46	0.45
1:A:96:TRP:CZ2	1:A:398:ARG:HD2	2.52	0.45
1:A:153:ILE:O	1:A:157:GLY:N	2.45	0.45
1:A:368:GLY:O	1:A:371:VAL:HG13	2.16	0.45
1:B:251:ASP:HB2	6:B:666:HOH:O	2.17	0.45
1:B:331:PHE:CD1	1:B:357:ILE:HD11	2.52	0.44
1:B:375:ARG:O	1:B:378:ARG:HG3	2.17	0.44
1:B:101:ASN:HB3	1:B:243:PRO:HD2	2.00	0.44
1:B:290:ALA:HB1	1:B:418:LEU:HD13	1.99	0.44
1:B:130:TRP:CD2	1:B:139:ILE:HD13	2.53	0.44
1:A:47:ARG:NH2	5:A:504[B]:IRV:O14	2.36	0.44
1:A:151:ASP:OD1	1:A:164:SER:OG	2.18	0.44
1:A:225:ALA:HB2	6:A:636:HOH:O	2.18	0.44
1:B:86:LEU:O	1:B:398:ARG:NH2	2.51	0.44
1:B:211:VAL:O	1:B:215:LEU:HD13	2.18	0.44
1:B:106:SER:HB3	1:B:233:LEU:HD23	1.99	0.43
1:B:286:VAL:HG13	1:B:313:TYR:OH	2.17	0.43
1:B:323:ARG:HH22	1:B:324:LEU:HD21	1.83	0.43
1:A:5:MET:HE2	1:A:41:LYS:N	2.33	0.43
1:B:323:ARG:HG2	1:B:361:HIS:HB3	2.00	0.43
1:B:390:PHE:CZ	1:B:392:PRO:HG3	2.53	0.43
1:B:158:PHE:CZ	1:B:262:LEU:HD11	2.53	0.43
1:A:5:MET:HE2	1:A:41:LYS:HB2	2.01	0.43
1:A:287:LEU:HD13	1:A:287:LEU:O	2.18	0.43
1:B:11:PHE:HB2	1:B:18:PRO:HG2	1.99	0.43
1:B:19:LEU:HD13	1:B:32:ILE:HD11	2.01	0.43
1:B:328:ALA:HB1	5:B:504[B]:IRV:C23	2.49	0.43
1:A:33:ALA:CB	1:A:359:GLN:HG2	2.49	0.43
1:A:366:ILE:HG23	1:A:386:PRO:HG2	2.00	0.43
1:A:79:ARG:NH1	1:A:88:THR:O	2.47	0.43
1:A:17:LEU:HB3	1:A:18:PRO:HD3	1.99	0.43
1:B:70:ASN:CG	6:B:602:HOH:O	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:PHE:CZ	1:B:262:LEU:HD21	2.53	0.43
1:A:53:SER:HB3	1:A:359:GLN:CG	2.49	0.42
1:B:323:ARG:NH2	1:B:324:LEU:HD21	2.34	0.42
1:B:290:ALA:CB	1:B:418:LEU:HD13	2.48	0.42
1:A:43:GLU:HG2	1:A:48:VAL:HG22	2.02	0.42
1:A:370:ASP:O	1:A:378:ARG:NH2	2.53	0.42
1:B:434:LYS:CD	1:B:440:LYS:HE2	2.49	0.42
2:B:502:HEM:HMC2	2:B:502:HEM:CBC	2.48	0.42
1:B:282:LYS:NZ	1:B:425:ASP:OD2	2.44	0.42
1:B:329:PRO:O	1:B:358:PRO:HD3	2.20	0.42
1:B:290:ALA:HB1	1:B:418:LEU:CD1	2.50	0.42
1:B:331:PHE:CA	6:B:625:HOH:O	2.67	0.42
1:A:280:LEU:CD2	1:A:286:VAL:HG12	2.50	0.42
1:B:375:ARG:HB3	1:B:375:ARG:CZ	2.50	0.42
1:B:103:LEU:HD21	1:B:237:MET:HG2	2.01	0.42
1:B:419:LYS:O	1:B:451:LYS:HD2	2.20	0.42
1:A:33:ALA:HB1	1:A:359:GLN:HG2	2.00	0.41
1:A:97:LYS:HG3	6:A:687:HOH:O	2.20	0.41
1:A:150:LEU:HD13	1:A:162:PHE:CD2	2.55	0.41
1:B:189:GLN:OE1	6:B:603:HOH:O	2.21	0.41
1:A:291:ALA:HA	1:A:418:LEU:HB3	2.03	0.41
1:B:38:GLU:HB2	1:B:54:SER:OG	2.20	0.41
1:A:393:PHE:HB3	1:A:400:CYS:HB3	2.01	0.41
1:B:119:MET:HG2	1:B:152:THR:HG23	2.01	0.41
1:A:300:ASP:O	1:A:419:LYS:NZ	2.54	0.41
1:A:84:ASP:O	1:A:89:SER:OG	2.38	0.41
1:A:130:TRP:CD2	1:A:139:ILE:HD13	2.56	0.41
1:B:81:PHE:HB3	1:B:209:ILE:HG12	2.02	0.41
1:B:207:GLU:O	1:B:211:VAL:HG23	2.21	0.41
1:B:430:GLU:CD	6:B:617:HOH:O	2.64	0.41
1:A:400:CYS:HB2	2:A:501:HEM:C1A	2.56	0.41
1:B:86:LEU:HD11	1:B:103:LEU:HD12	2.02	0.41
1:B:434:LYS:HB2	1:B:442:GLU:HB2	2.03	0.41
1:A:70:ASN:HB3	1:A:332:SER:OG	2.21	0.40
1:A:278:TYR:O	1:A:281:VAL:HG22	2.21	0.40
1:A:367:TRP:HB2	1:A:371:VAL:HG12	2.02	0.40
1:B:287:LEU:C	1:B:287:LEU:HD23	2.46	0.40
1:B:334:TYR:HB3	6:B:774:HOH:O	2.21	0.40
1:B:372:GLU:HB3	6:B:733:HOH:O	2.21	0.40
1:A:58:ILE:HD13	1:A:355:VAL:HG13	2.03	0.40
1:B:122:ILE:HD12	1:B:151:ASP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ALA:O	1:B:136:ASP:HB2	2.22	0.40
1:B:278:TYR:HA	1:B:444:PHE:CZ	2.56	0.40
1:A:26:VAL:HG21	1:A:329:PRO:CG	2.50	0.40
1:A:391:LYS:HA	6:A:761:HOH:O	2.21	0.40
1:A:409:GLU:O	1:A:413:VAL:HG12	2.22	0.40
1:B:99:ALA:HA	1:B:249:LEU:HD21	2.02	0.40
1:B:369:ASP:C	1:B:371:VAL:H	2.29	0.40
1:A:438:THR:OG1	1:A:439:LEU:N	2.55	0.40
1:B:337:GLU:HB3	6:B:686:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:737:HOH:O	6:B:860:HOH:O[1_454]	2.13	0.07

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	449/466 (96%)	431 (96%)	18 (4%)	0	100	100
1	B	450/466 (97%)	432 (96%)	18 (4%)	0	100	100
All	All	899/932 (96%)	863 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	392/409 (96%)	391 (100%)	1 (0%)	86	91
1	B	394/409 (96%)	393 (100%)	1 (0%)	86	91
All	All	786/818 (96%)	784 (100%)	2 (0%)	86	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	LEU
1	B	371	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	204	GLN
1	A	288	GLN
1	A	359	GLN
1	A	403	GLN
1	B	110	GLN
1	B	204	GLN
1	B	229	GLN
1	B	239	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

10 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	A	501	3,1	50,50,50	1.78	12 (24%)	67,82,82	1.66	13 (19%)
5	IRV	A	504[A]	-	24,24,24	1.48	1 (4%)	30,30,30	0.96	2 (6%)
5	IRV	A	504[B]	-	24,24,24	1.46	2 (8%)	30,30,30	0.99	3 (10%)
3	HOA	A	502	2	0,1,1	-	-	-	-	-
5	IRV	B	504[A]	-	24,24,24	1.44	1 (4%)	30,30,30	1.14	2 (6%)
4	16N	A	503	-	10,10,10	2.56	4 (40%)	13,13,13	2.68	7 (53%)
2	HEM	B	502	3,1	50,50,50	1.76	13 (26%)	67,82,82	1.64	14 (20%)
4	16N	B	503	-	10,10,10	1.88	2 (20%)	13,13,13	1.24	0
5	IRV	B	504[B]	-	24,24,24	1.49	2 (8%)	30,30,30	1.28	6 (20%)
3	HOA	B	501	2	0,1,1	-	-	-	-	-

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	A	501	3,1	-	0/14/54/54	-
5	IRV	A	504[A]	-	-	9/19/19/19	0/2/2/2
5	IRV	A	504[B]	-	-	8/19/19/19	0/2/2/2
5	IRV	B	504[A]	-	-	6/19/19/19	0/2/2/2
4	16N	A	503	-	-	-	0/2/2/2
2	HEM	B	502	3,1	-	0/14/54/54	-
5	IRV	B	504[B]	-	-	5/19/19/19	0/2/2/2
4	16N	B	503	-	-	-	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504[A]	IRV	C02-N03	5.78	1.46	1.34
5	B	504[B]	IRV	C02-N03	5.68	1.46	1.34
5	A	504[B]	IRV	C02-N03	5.56	1.45	1.34
4	A	503	16N	C2-C1	-5.48	1.29	1.38
5	B	504[A]	IRV	C02-N03	5.44	1.45	1.34
2	B	502	HEM	FE-NB	5.34	2.11	1.94
2	A	501	HEM	FE-NB	5.06	2.10	1.94
2	B	502	HEM	FE-NC	4.50	2.10	1.95
2	A	501	HEM	FE-NC	4.31	2.09	1.95
4	A	503	16N	C1-C6	-4.27	1.32	1.39
2	A	501	HEM	C4D-ND	-4.20	1.33	1.40
2	B	502	HEM	C1B-NB	-3.94	1.33	1.40
2	A	501	HEM	C1B-NB	-3.93	1.33	1.40
4	B	503	16N	C9-C5	3.85	1.57	1.51
2	B	502	HEM	C4D-ND	-3.78	1.33	1.40
4	B	503	16N	C7-C6	3.57	1.56	1.51
4	A	503	16N	C8-C7	-3.30	1.44	1.53
2	A	501	HEM	C1D-ND	-2.96	1.33	1.38
2	A	501	HEM	C4B-NB	-2.70	1.33	1.38
2	A	501	HEM	FE-ND	-2.52	1.87	1.94
2	B	502	HEM	C4B-NB	-2.51	1.33	1.38
2	B	502	HEM	C1D-ND	-2.48	1.34	1.38
2	B	502	HEM	FE-ND	-2.46	1.87	1.94
2	B	502	HEM	O2D-CGD	-2.42	1.22	1.30
2	A	501	HEM	C1A-C2A	-2.32	1.40	1.44
2	B	502	HEM	O2A-CGA	-2.29	1.23	1.30
2	A	501	HEM	C1C-NC	-2.27	1.35	1.39
2	A	501	HEM	O2D-CGD	-2.24	1.23	1.30
5	B	504[B]	IRV	O01-C02	-2.23	1.18	1.23
2	B	502	HEM	C1A-C2A	-2.22	1.40	1.44
2	B	502	HEM	C1C-NC	-2.19	1.35	1.39
5	A	504[B]	IRV	O01-C02	-2.17	1.19	1.23
2	A	501	HEM	O2A-CGA	-2.16	1.23	1.30
2	A	501	HEM	C1C-C2C	-2.11	1.41	1.45
2	B	502	HEM	C1C-C2C	-2.09	1.41	1.45
4	A	503	16N	C4-C5	-2.07	1.36	1.39
2	B	502	HEM	C4C-NC	-2.01	1.35	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CHC-C4B-NB	4.90	129.70	124.42
2	B	502	HEM	CHC-C4B-NB	4.56	129.33	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	16N	C8-C7-C6	-4.48	97.92	103.79
4	A	503	16N	C3-C2-C1	4.29	125.53	120.24
2	A	501	HEM	CHD-C1D-ND	4.10	128.83	124.42
2	B	502	HEM	CHA-C4D-ND	3.98	129.29	124.37
2	B	502	HEM	CHD-C1D-ND	3.97	128.69	124.42
2	A	501	HEM	CHA-C4D-ND	3.91	129.20	124.37
4	A	503	16N	C9-C8-C7	3.75	114.38	107.08
2	A	501	HEM	C1B-NB-C4B	3.62	109.49	105.21
4	A	503	16N	C2-C3-C4	-3.48	115.94	120.24
2	A	501	HEM	CHB-C1B-NB	3.44	128.62	124.37
2	B	502	HEM	C1B-NB-C4B	3.30	109.12	105.21
4	A	503	16N	C7-C6-C5	3.23	114.78	110.19
2	B	502	HEM	CBA-CAA-C2A	-3.05	104.09	112.53
2	B	502	HEM	CHB-C1B-NB	2.88	127.93	124.37
2	A	501	HEM	CBA-CAA-C2A	-2.85	104.66	112.53
2	A	501	HEM	CBD-CAD-C3D	-2.81	104.77	112.53
2	B	502	HEM	CBD-CAD-C3D	-2.72	105.01	112.53
5	B	504[A]	IRV	O14-C12-C04	2.61	122.33	113.51
5	B	504[A]	IRV	O14-C12-O13	-2.57	118.26	124.08
2	A	501	HEM	C3B-C4B-NB	-2.55	107.64	109.47
2	A	501	HEM	CHD-C1D-C2D	-2.51	121.07	125.03
2	A	501	HEM	CHA-C4D-C3D	-2.47	120.67	125.23
2	B	502	HEM	CMD-C2D-C1D	2.44	128.85	125.03
2	B	502	HEM	C1A-CHA-C4D	-2.43	120.53	126.25
4	A	503	16N	C8-C9-C5	-2.43	100.62	103.79
2	B	502	HEM	CHA-C1A-NA	2.41	128.23	123.86
2	B	502	HEM	CHD-C1D-C2D	-2.34	121.34	125.03
5	B	504[B]	IRV	C20-N19-C23	2.32	109.60	106.71
2	B	502	HEM	CAD-CBD-CGD	-2.30	107.56	113.67
2	B	502	HEM	CHA-C4D-C3D	-2.27	121.04	125.23
5	B	504[B]	IRV	O14-C12-O13	-2.25	118.97	124.08
4	A	503	16N	C9-C5-C6	-2.24	107.01	110.19
5	B	504[B]	IRV	C21-N22-C23	2.23	109.75	105.47
5	B	504[B]	IRV	C15-C02-N03	2.21	119.76	115.86
2	B	502	HEM	CHD-C4C-NC	2.20	126.85	124.45
5	B	504[B]	IRV	O14-C12-C04	2.20	120.94	113.51
2	A	501	HEM	C1A-CHA-C4D	-2.19	121.11	126.25
5	A	504[B]	IRV	O14-C12-C04	2.18	120.88	113.51
5	A	504[A]	IRV	C16-C15-C02	-2.17	107.17	113.19
5	B	504[B]	IRV	C20-C21-N22	-2.11	105.91	109.92
2	A	501	HEM	CHA-C1A-NA	2.09	127.65	123.86
5	A	504[B]	IRV	O14-C12-O13	-2.09	119.35	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504[A]	IRV	O14-C12-C04	2.07	120.51	113.51
5	A	504[B]	IRV	C15-C02-N03	2.07	119.51	115.86
2	A	501	HEM	CHD-C4C-NC	2.06	126.69	124.45

There are no chirality outliers.

All (28) torsion outliers are listed below:

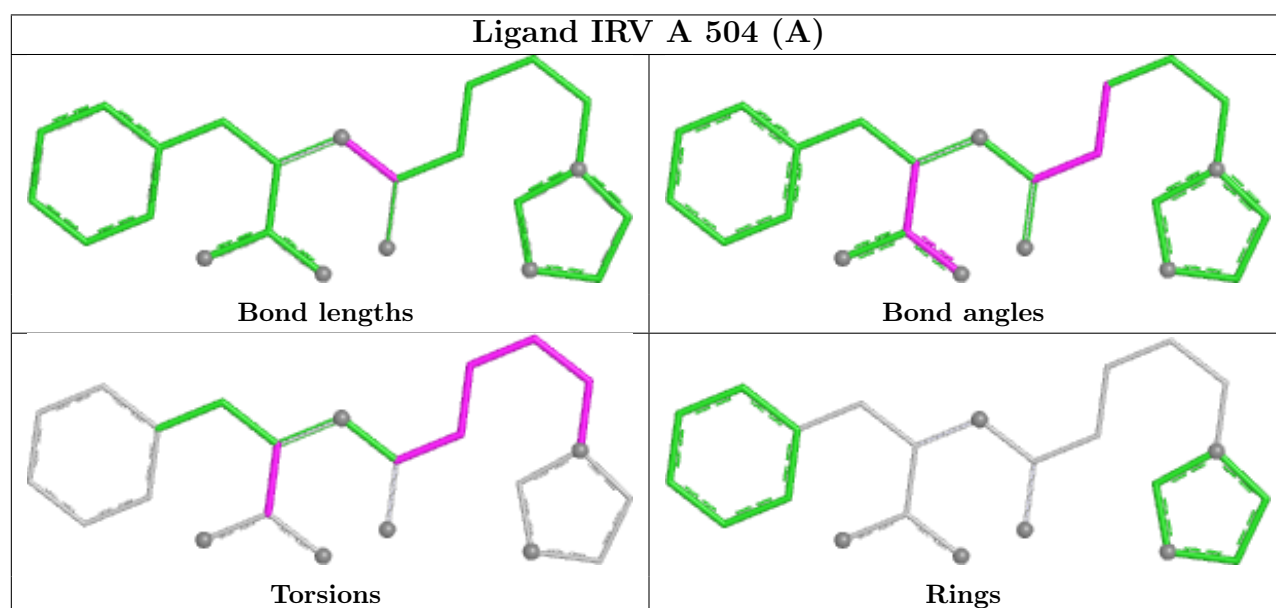
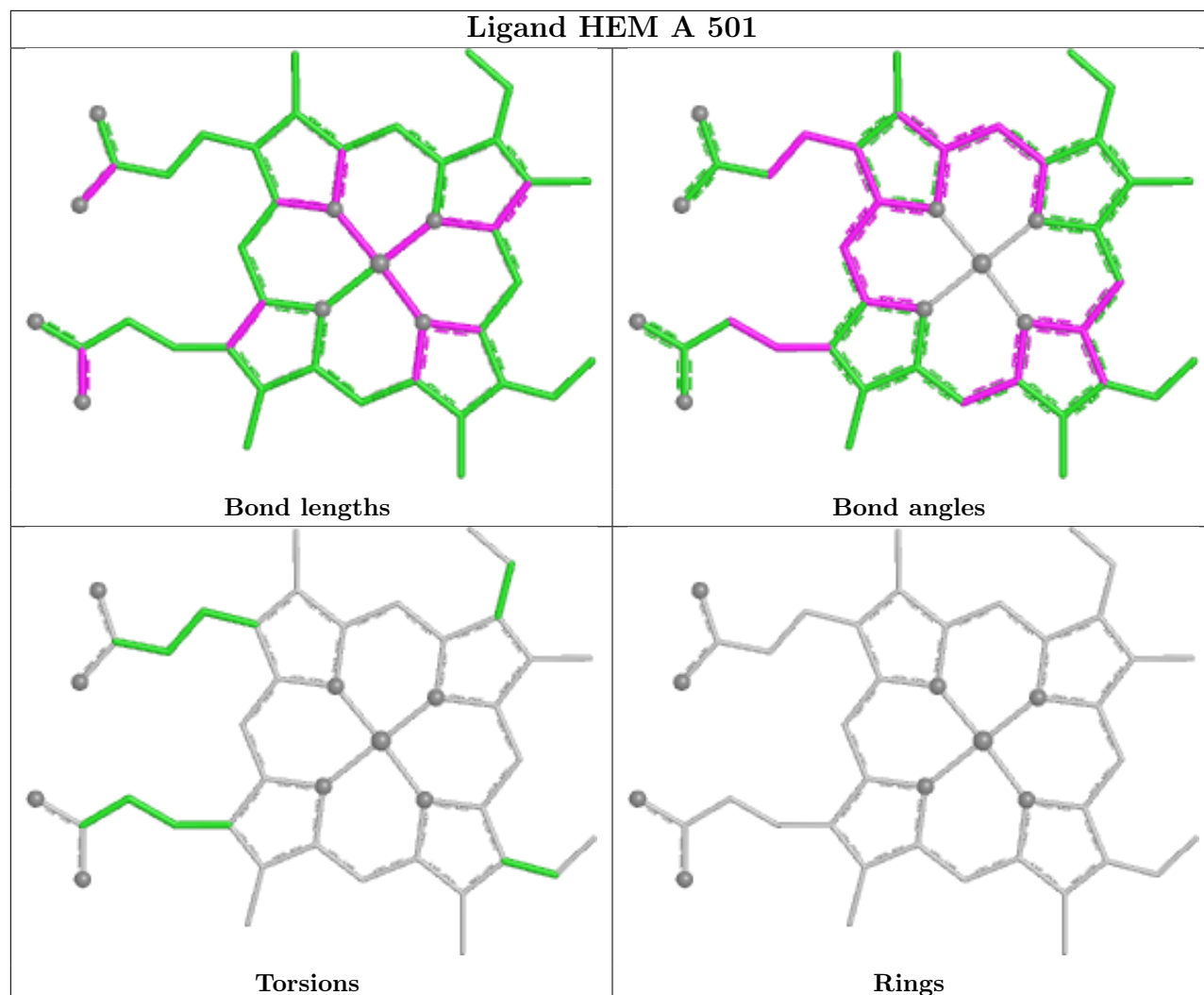
Mol	Chain	Res	Type	Atoms
5	B	504[A]	IRV	C16-C17-C18-N19
5	A	504[B]	IRV	C05-C04-N03-C02
5	A	504[B]	IRV	N03-C02-C15-C16
5	A	504[B]	IRV	O01-C02-C15-C16
5	B	504[B]	IRV	C17-C18-N19-C20
5	B	504[B]	IRV	C17-C18-N19-C23
5	B	504[B]	IRV	C15-C16-C17-C18
5	A	504[A]	IRV	C17-C18-N19-C20
5	A	504[B]	IRV	C12-C04-C05-C06
5	A	504[A]	IRV	N03-C02-C15-C16
5	B	504[A]	IRV	C17-C18-N19-C20
5	A	504[B]	IRV	N03-C04-C12-O14
5	A	504[A]	IRV	C17-C18-N19-C23
5	B	504[A]	IRV	C17-C18-N19-C23
5	A	504[A]	IRV	O01-C02-C15-C16
5	A	504[B]	IRV	N03-C04-C12-O13
5	A	504[B]	IRV	N03-C04-C05-C06
5	A	504[A]	IRV	C16-C17-C18-N19
5	B	504[A]	IRV	C02-C15-C16-C17
5	A	504[B]	IRV	C15-C16-C17-C18
5	B	504[B]	IRV	C05-C04-C12-O14
5	B	504[A]	IRV	O01-C02-C15-C16
5	B	504[A]	IRV	N03-C02-C15-C16
5	B	504[B]	IRV	C05-C04-C12-O13
5	A	504[A]	IRV	C02-C15-C16-C17
5	A	504[A]	IRV	C05-C04-C12-O14
5	A	504[A]	IRV	C15-C16-C17-C18
5	A	504[A]	IRV	C05-C04-C12-O13

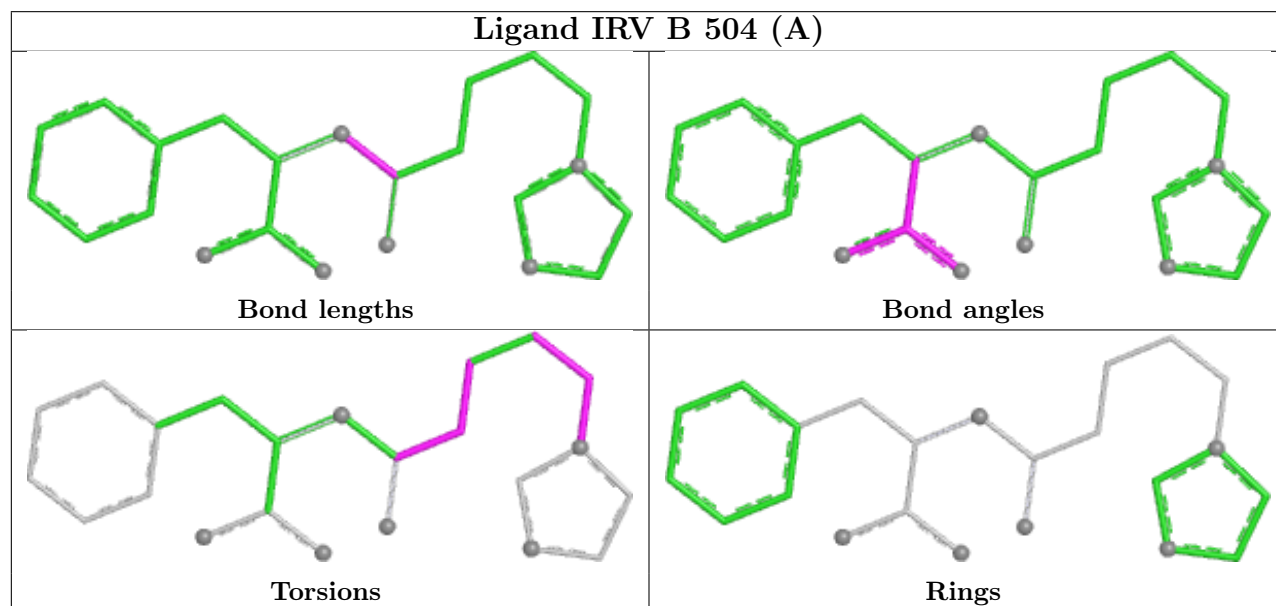
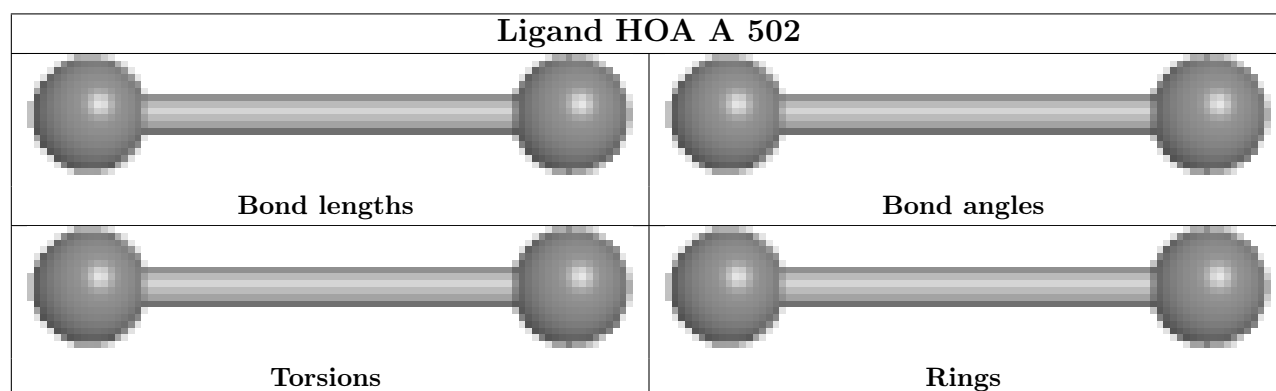
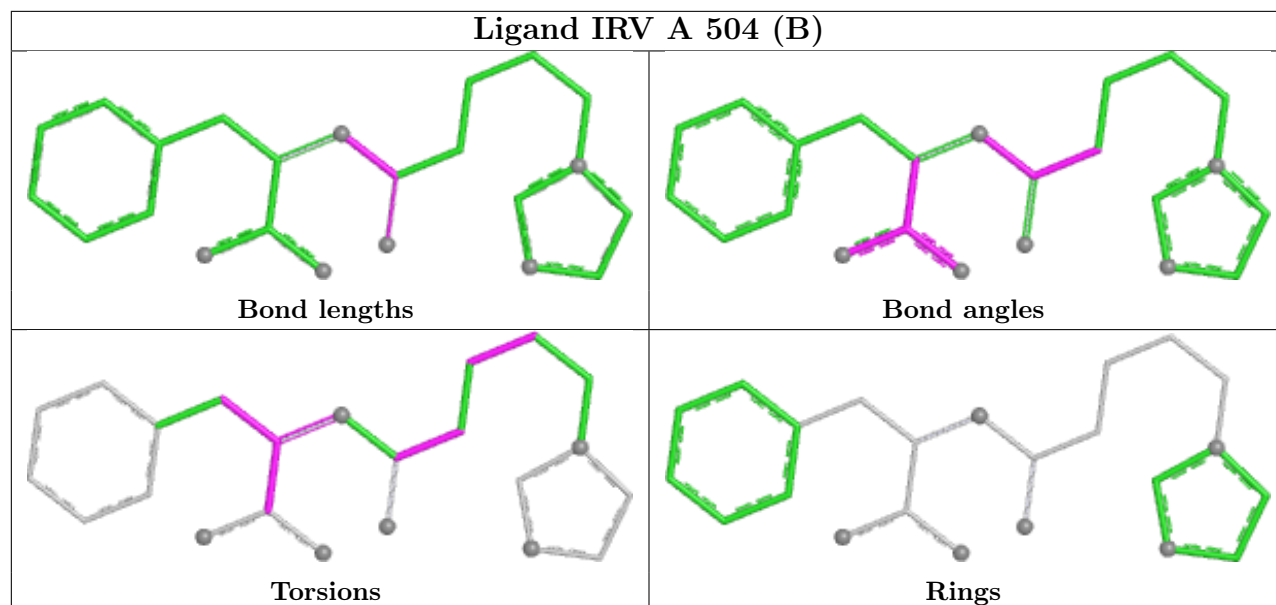
There are no ring outliers.

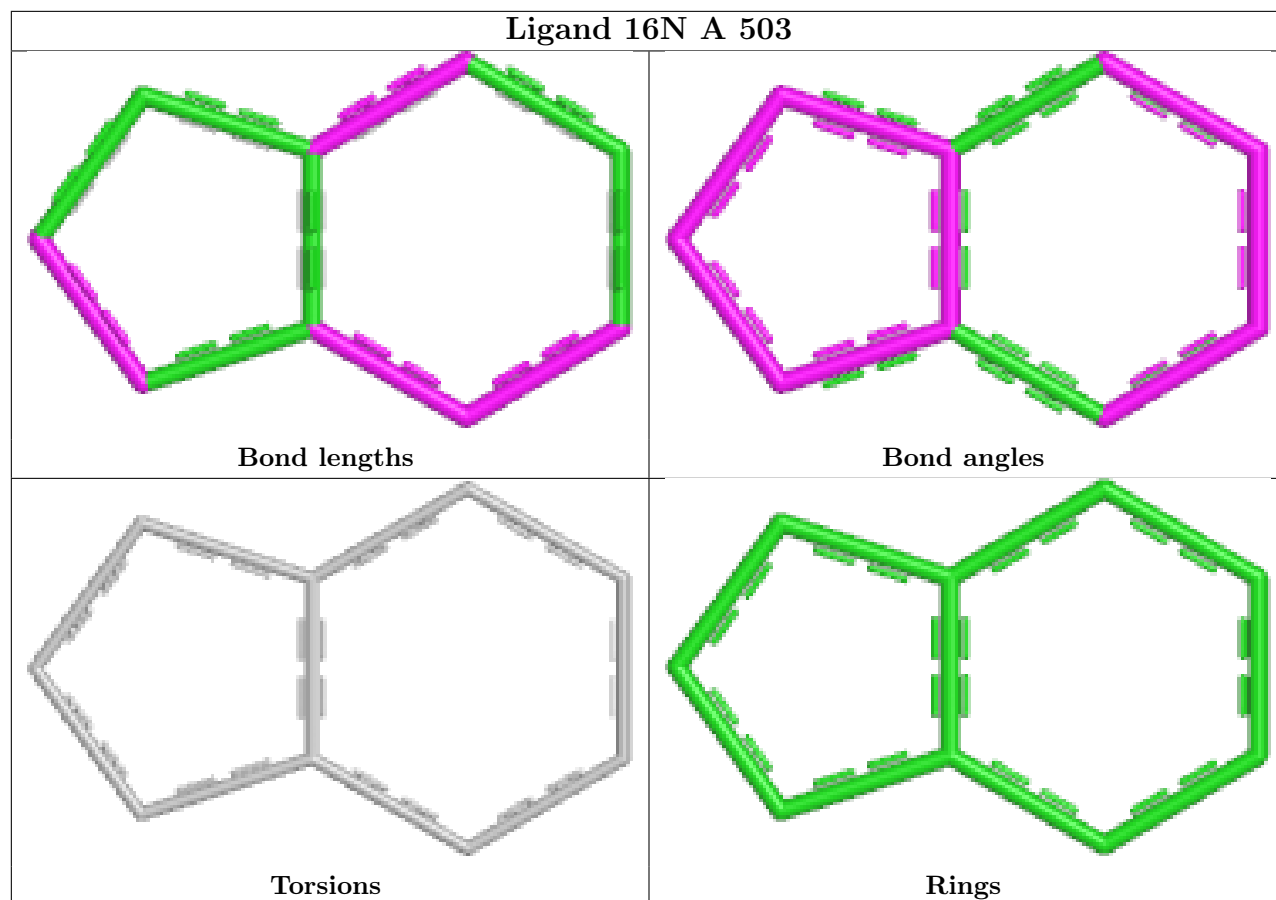
8 monomers are involved in 23 short contacts:

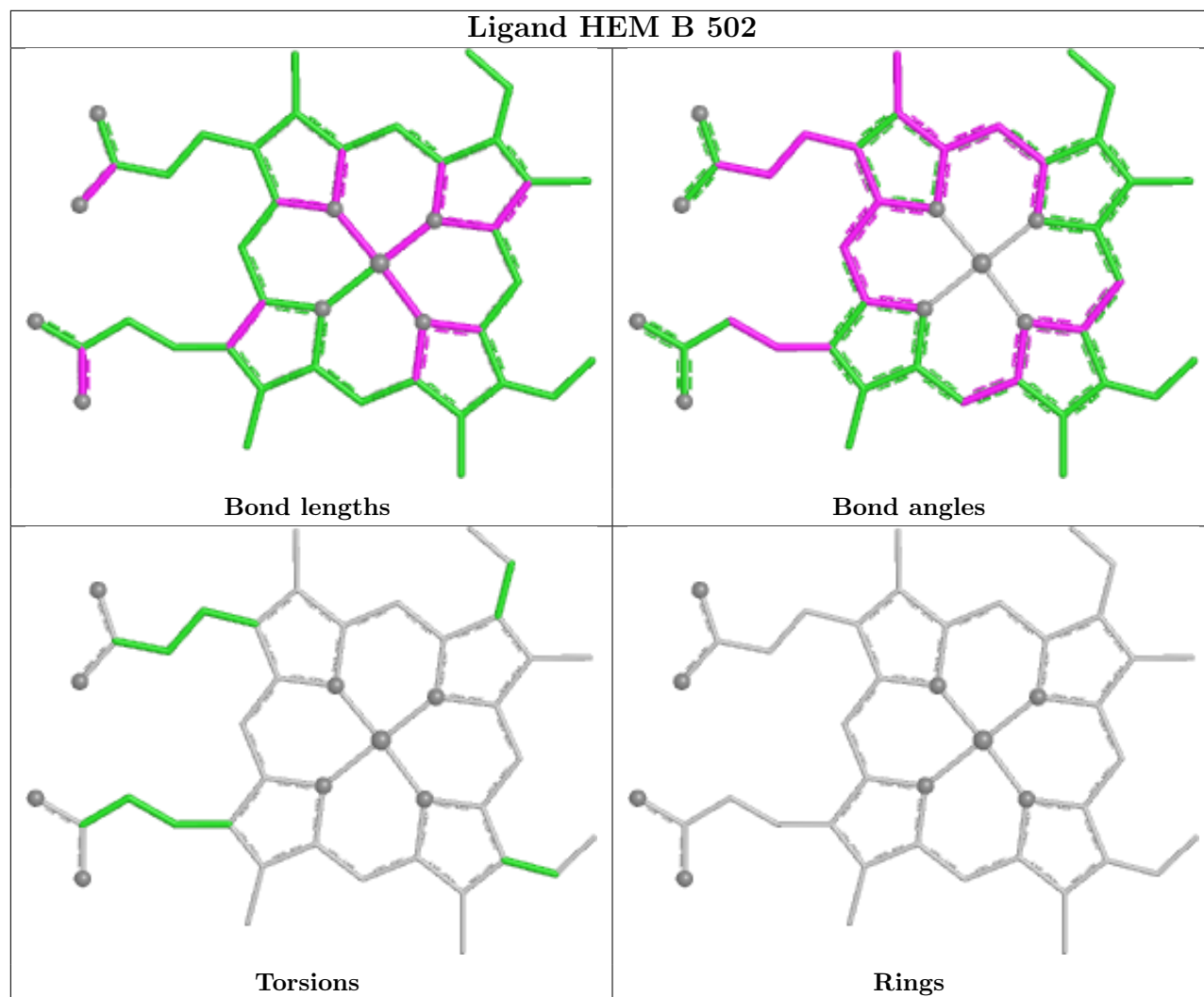
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	3	0
5	A	504[A]	IRV	4	0
5	A	504[B]	IRV	1	0
5	B	504[A]	IRV	2	0
4	A	503	16N	4	0
2	B	502	HEM	3	0
4	B	503	16N	8	0
5	B	504[B]	IRV	7	0

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.

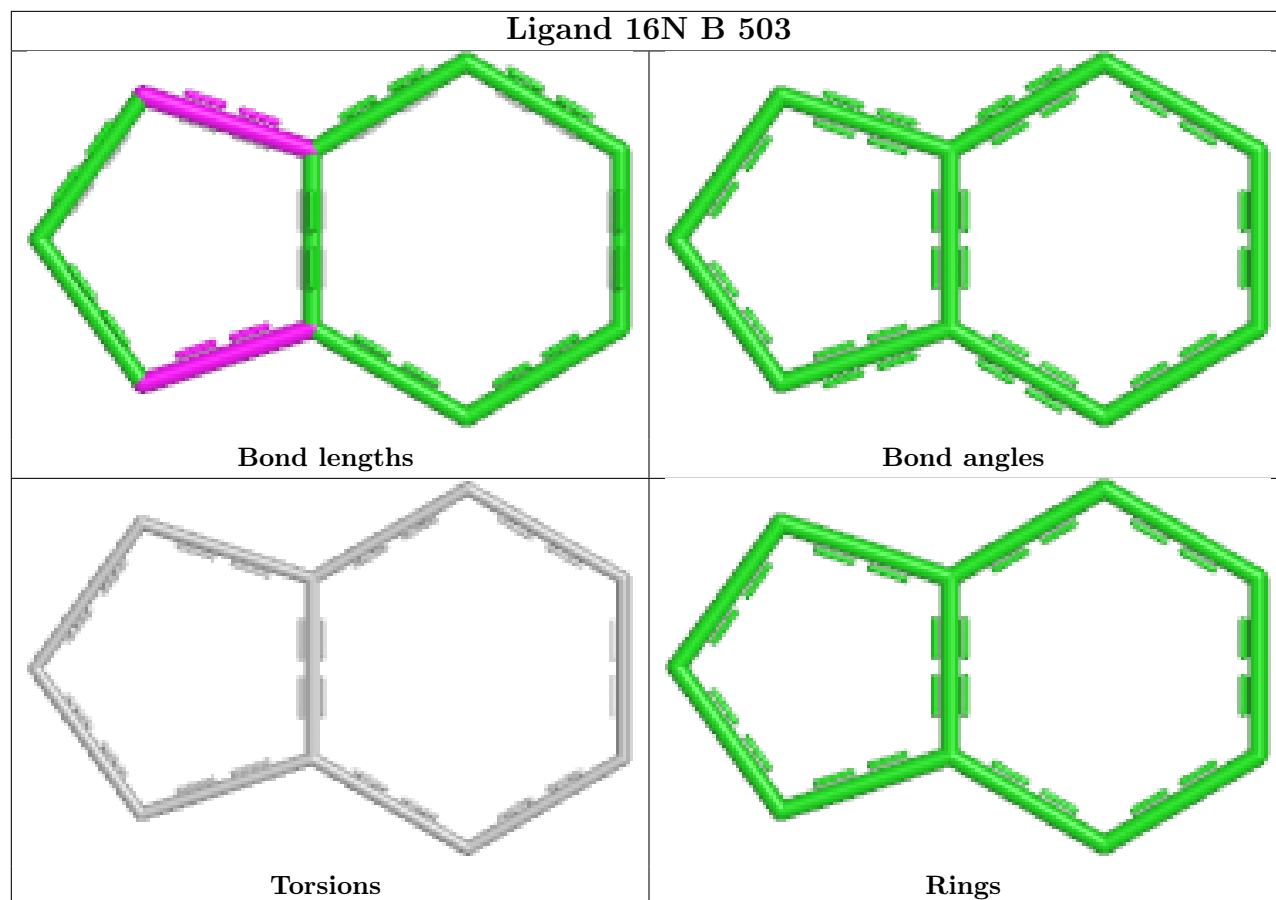




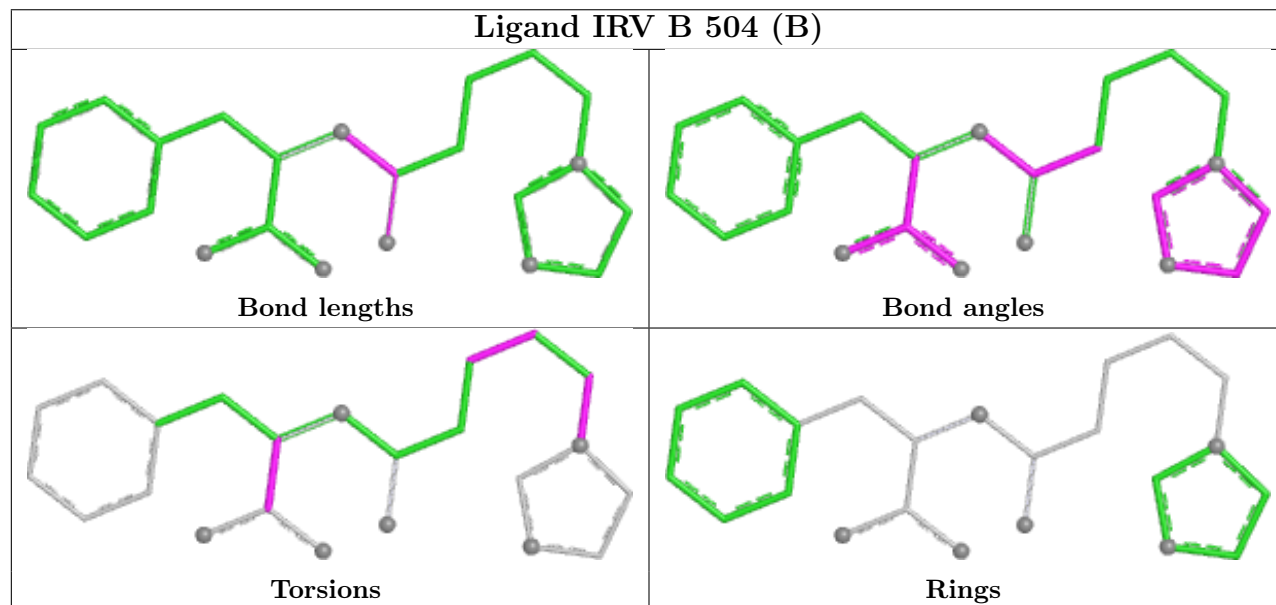




Ligand 16N B 503



Ligand IRV B 504 (B)



Ligand HOA B 501			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	451/466 (96%)	1.06	75 (16%) 4 4	13, 27, 55, 68	0
1	B	452/466 (96%)	0.93	59 (13%) 7 6	15, 26, 52, 65	0
All	All	903/932 (96%)	0.99	134 (14%) 5 5	13, 27, 53, 68	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	ALA	6.0
1	A	218	LYS	5.1
1	B	230	SER	5.0
1	A	266	HIS	4.4
1	B	191	ALA	4.2
1	A	227	GLY	4.1
1	A	202	LYS	4.1
1	A	211	VAL	4.1
1	A	189	GLN	4.1
1	A	176	SER	4.0
1	A	215	LEU	3.9
1	B	158	PHE	3.8
1	A	181	MET	3.8
1	B	182	ASP	3.7
1	B	195	ASP	3.7
1	A	192	ASN	3.7
1	A	382	PRO	3.7
1	B	185	MET	3.7
1	B	221	ALA	3.7
1	B	225	ALA	3.7
1	A	196	PRO	3.6
1	A	197	ALA	3.6
1	A	135	ALA	3.6
1	A	210	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	230	SER	3.6
1	A	5	MET	3.5
1	A	265	GLY	3.5
1	B	177	MET	3.5
1	B	229	GLN	3.5
1	B	219	ILE	3.4
1	B	194	ASP	3.4
1	A	185	MET	3.4
1	A	182	ASP	3.4
1	B	186	ASN	3.3
1	A	193	PRO	3.3
1	B	178	VAL	3.3
1	B	215	LEU	3.3
1	A	263	ILE	3.2
1	A	231	ASP	3.2
1	A	226	SER	3.2
1	B	210	LYS	3.2
1	A	267	GLU	3.1
1	A	387	GLN	3.1
1	A	157	GLY	3.1
1	A	158	PHE	3.1
1	B	175	THR	3.1
1	A	383	SER	3.1
1	B	228	GLU	3.1
1	B	197	ALA	3.1
1	A	186	ASN	3.0
1	A	194	ASP	3.0
1	A	232	ASP	3.0
1	B	111	ALA	3.0
1	A	174	ILE	2.9
1	B	259	ILE	2.9
1	B	437	LEU	2.9
1	B	110	GLN	2.9
1	A	187	LYS	2.8
1	B	250	ASP	2.8
1	A	343	GLY	2.8
1	B	196	PRO	2.8
1	A	223	ARG	2.8
1	B	266	HIS	2.8
1	B	227	GLY	2.7
1	A	46	GLY	2.7
1	A	219	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	225	ALA	2.7
1	B	371	VAL	2.7
1	B	170	PRO	2.6
1	A	198	TYR	2.6
1	A	453	ILE	2.6
1	B	193	PRO	2.6
1	A	208	ASP	2.6
1	B	214	ASP	2.6
1	A	195	ASP	2.6
1	B	455	LEU	2.6
1	A	209	ILE	2.5
1	A	306	LYS	2.5
1	A	381	ASN	2.5
1	A	188	LEU	2.5
1	B	226	SER	2.5
1	B	107	PHE	2.5
1	A	220	ILE	2.5
1	A	175	THR	2.4
1	A	205	PHE	2.4
1	A	437	LEU	2.4
1	B	251	ASP	2.3
1	B	220	ILE	2.3
1	A	233	LEU	2.3
1	A	214	ASP	2.3
1	A	13	GLU	2.3
1	B	206	GLN	2.3
1	A	455	LEU	2.3
1	B	205	PHE	2.3
1	A	172	PRO	2.3
1	B	235	THR	2.3
1	B	192	ASN	2.3
1	B	203	ARG	2.3
1	B	168	ASP	2.3
1	A	141	VAL	2.2
1	A	201	ASN	2.2
1	B	190	ARG	2.2
1	B	218	LYS	2.2
1	B	231	ASP	2.2
1	A	168	ASP	2.2
1	B	265	GLY	2.2
1	B	23	ASP	2.2
1	B	176	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	239	ASN	2.2
1	B	109	GLN	2.1
1	A	221	ALA	2.1
1	A	264	ALA	2.1
1	B	264	ALA	2.1
1	A	170	PRO	2.1
1	A	386	PRO	2.1
1	B	179	ARG	2.1
1	A	262	LEU	2.1
1	A	18	PRO	2.1
1	B	243	PRO	2.1
1	A	246	GLY	2.1
1	B	83	GLY	2.1
1	A	284	PRO	2.1
1	B	209	ILE	2.1
1	B	184	ALA	2.1
1	B	46	GLY	2.0
1	B	246	GLY	2.0
1	B	258	ILE	2.0
1	A	173	PHE	2.0
1	A	302	VAL	2.0
1	A	428	ASN	2.0
1	A	14	LEU	2.0
1	A	251	ASP	2.0
1	A	47	ARG	2.0
1	A	243	PRO	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](#)

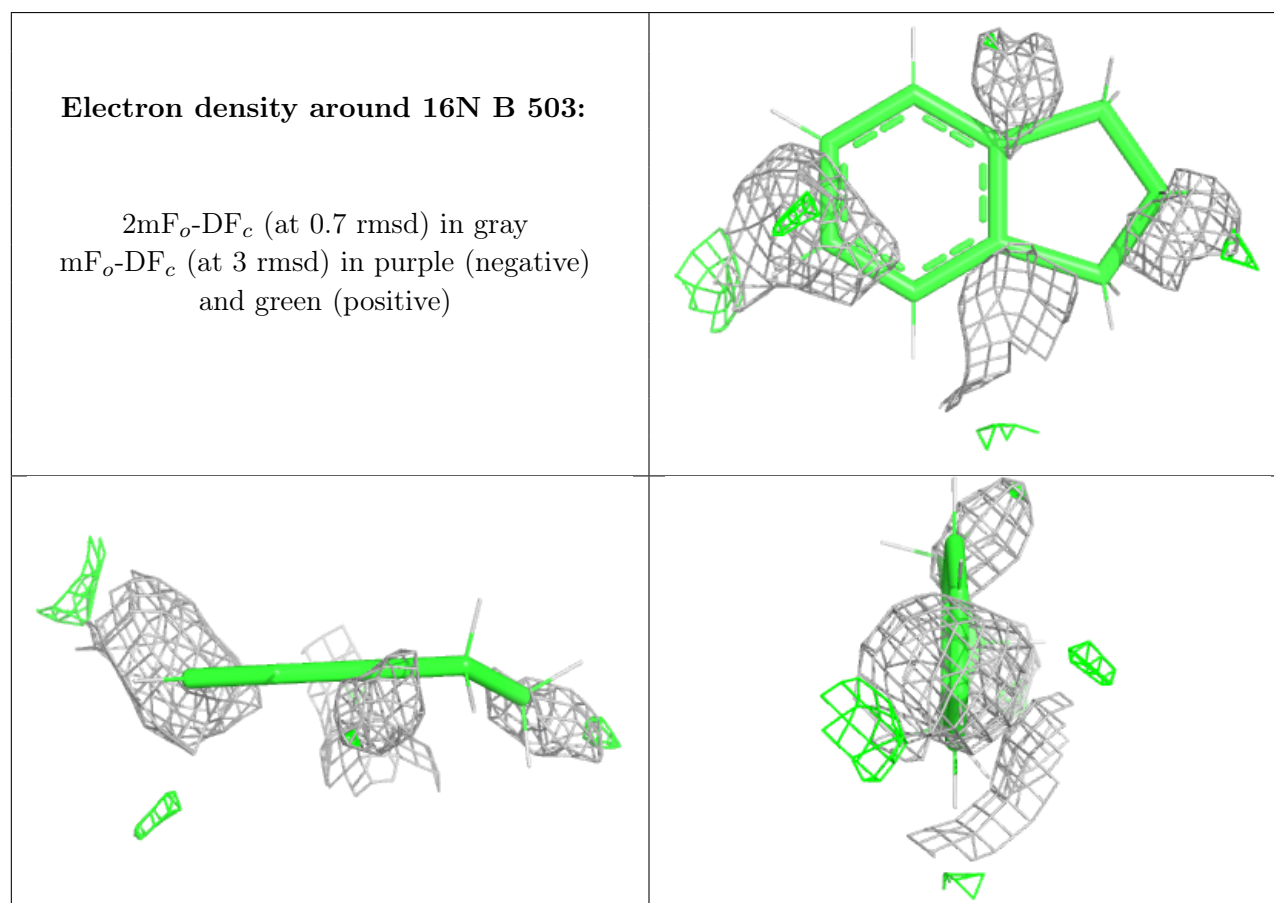
There are no oligosaccharides in this entry.

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.

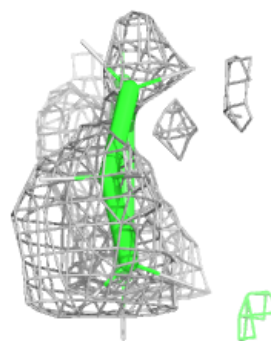
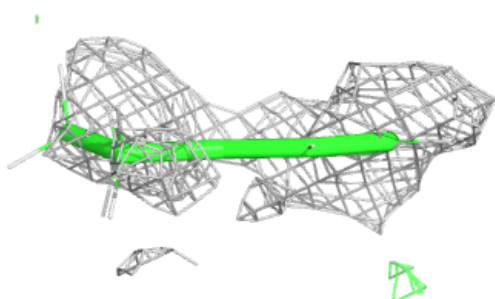
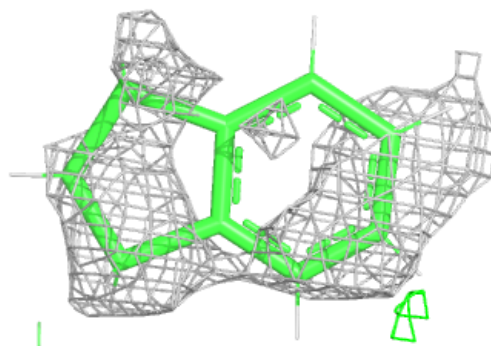
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	16N	B	503	9/9	0.67	0.40	79,80,97,97	0
4	16N	A	503	9/9	0.74	0.23	82,82,98,98	0
5	IRV	A	504[A]	23/23	0.76	0.42	89,90,108,108	43
5	IRV	A	504[B]	23/23	0.76	0.42	87,91,108,108	43
5	IRV	B	504[A]	23/23	0.76	0.33	68,78,89,91	43
5	IRV	B	504[B]	23/23	0.76	0.33	68,76,91,92	43
3	HOA	A	502	2/2	0.79	0.17	33,34,40,41	0
3	HOA	B	501	2/2	0.87	0.12	27,29,33,35	0
2	HEM	A	501	43/43	0.94	0.12	9,16,29,41	0
2	HEM	B	502	43/43	0.95	0.09	8,13,15,18	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.

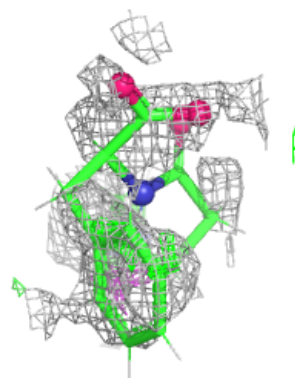
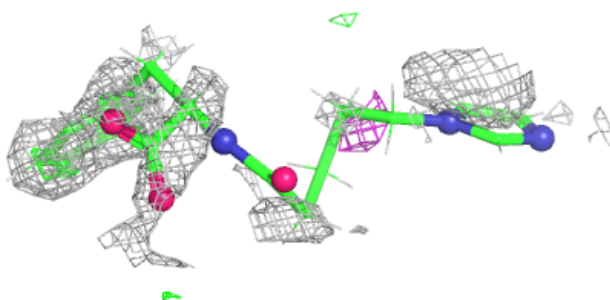
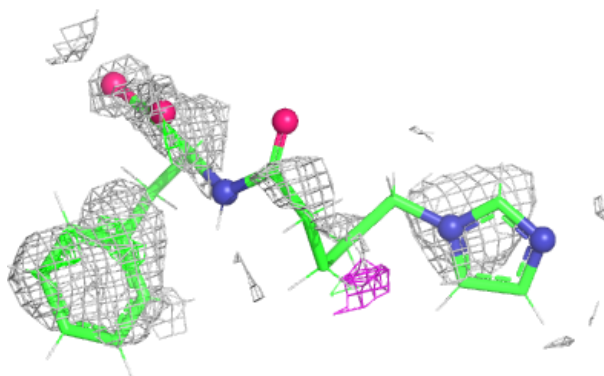


Electron density around 16N A 503:

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

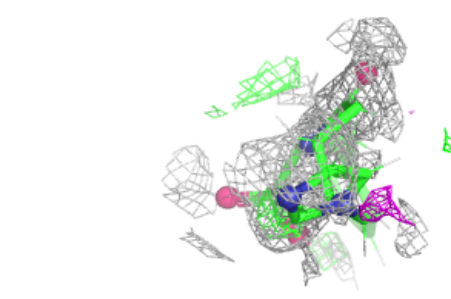
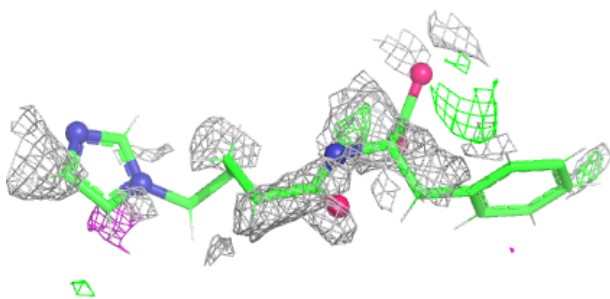
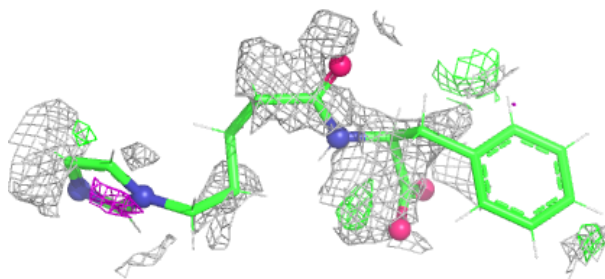
**Electron density around IRV A 504 (A):**

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

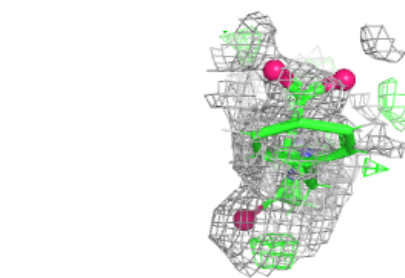
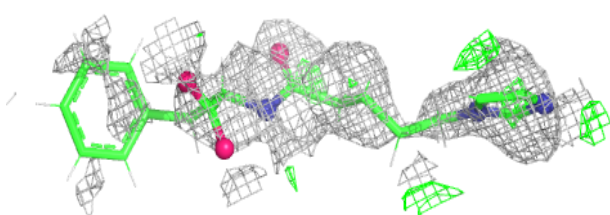
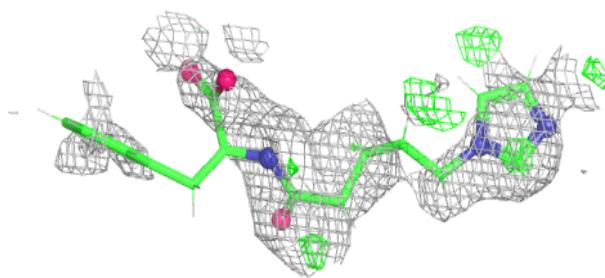


Electron density around IRV A 504 (B):

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

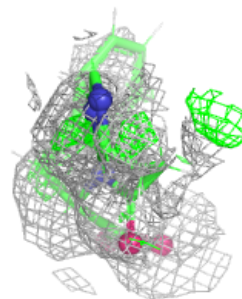
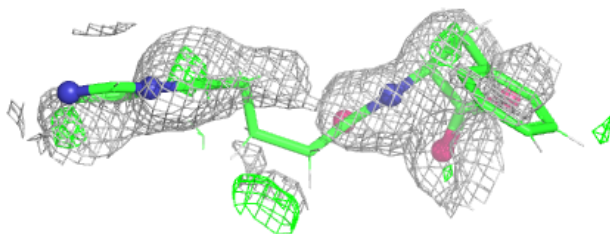
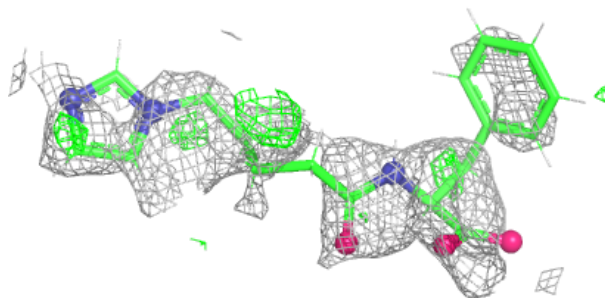
**Electron density around IRV B 504 (A):**

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

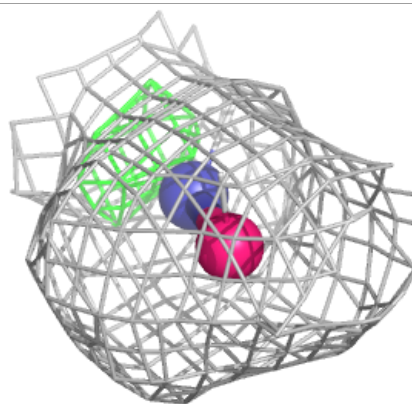
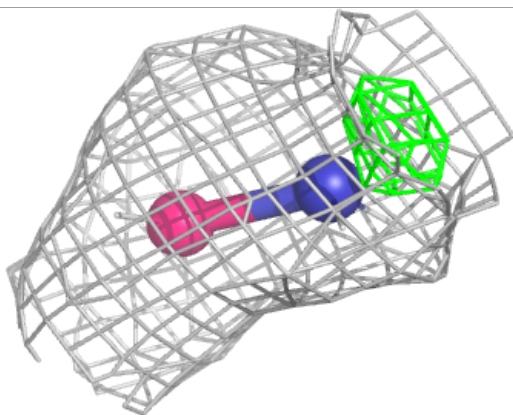
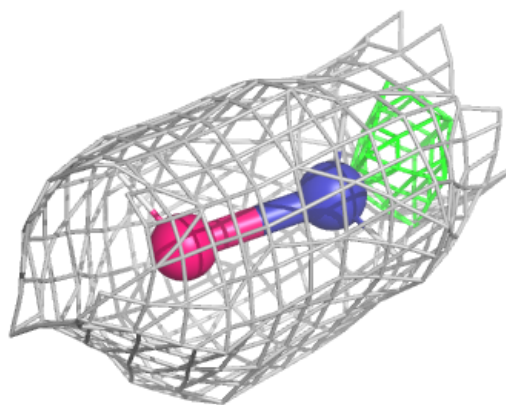


Electron density around IRV B 504 (B):

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

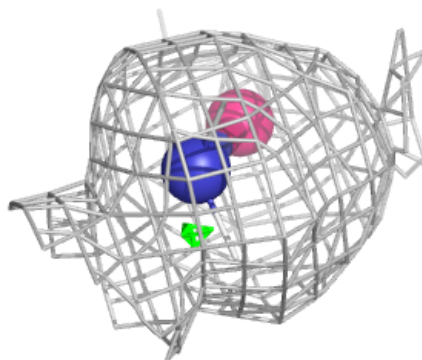
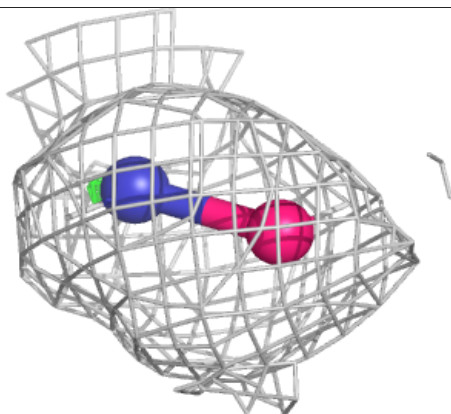
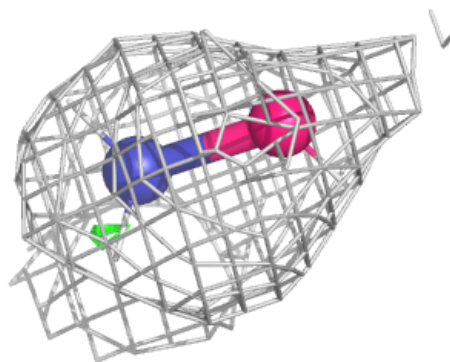
**Electron density around HOA A 502:**

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



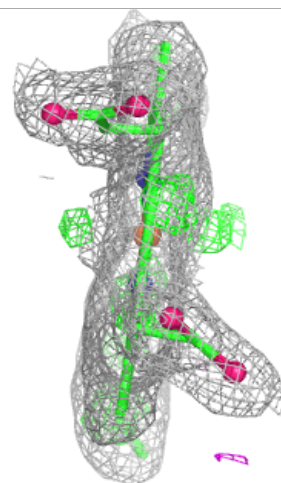
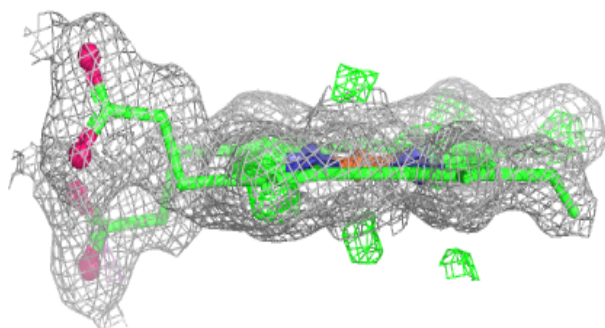
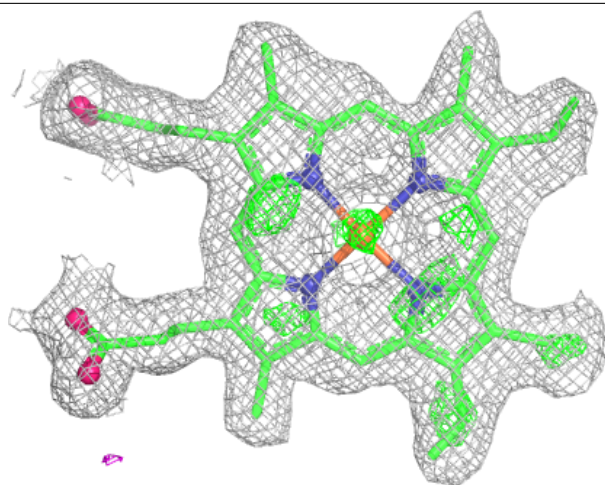
Electron density around HOA B 501:

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



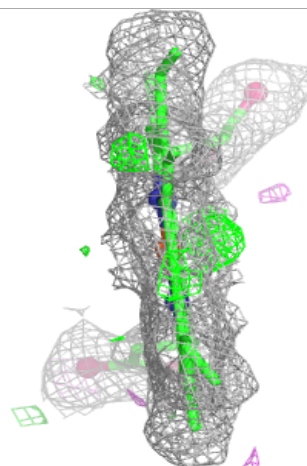
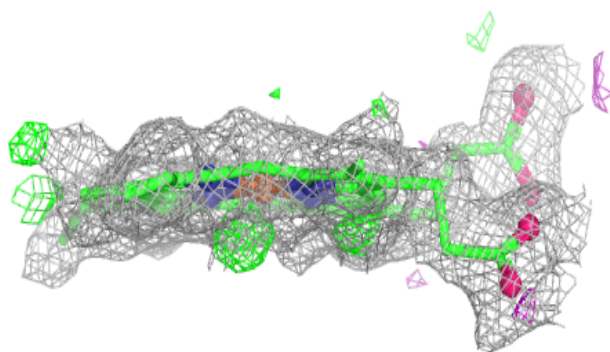
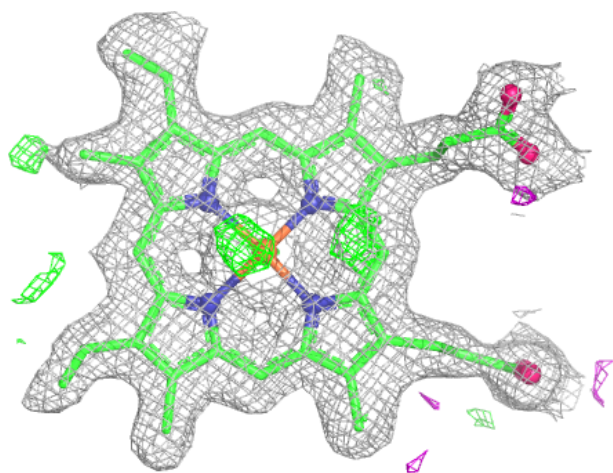
Electron density around HEM A 501:

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



Electron density around HEM B 502:

$2mF_o-DF_c$ (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.