W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 23, 2023 – 12:34 AM JST

PDB ID	:	7YFT
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 (i) 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 (i)) were used in the production of this report:

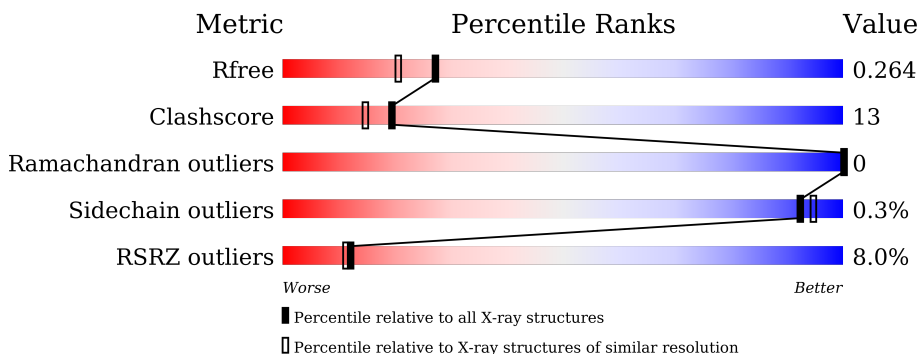|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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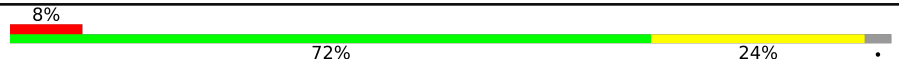*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Rfree		0.264
Clashscore		13
Ramachandran outliers		0
Sidechain outliers		0.3%
RSRZ outliers		8.0%

Worse   *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	8% 72% 24% ·
1	B	466	8% 71% 26% ·

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	X
5	IRV	A	504[A]	-	-	-	X
5	IRV	A	504[B]	-	-	-	X
5	IRV	B	504[A]	-	-	-	X
5	IRV	B	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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).


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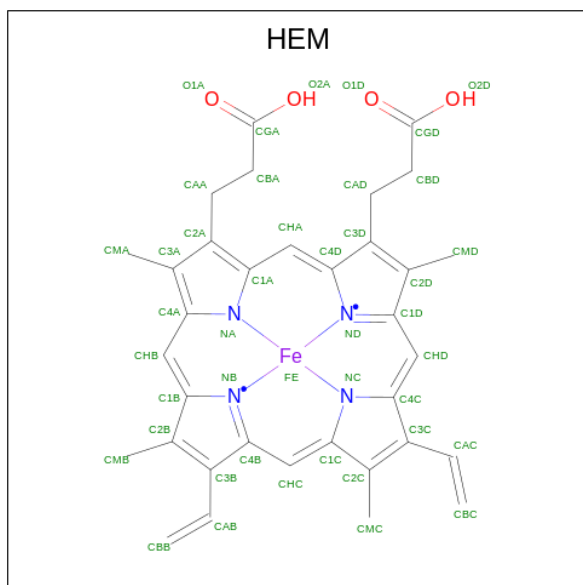
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total C Fe N O 43 34 1 4 4				0	0
2	B	1	Total C Fe N O 43 34 1 4 4				0	0

- Molecule 3 is HYDROXYAMINE (three-letter code: HOA) (formula: H_3NO) (labeled as "Ligand of Interest" by depositor).
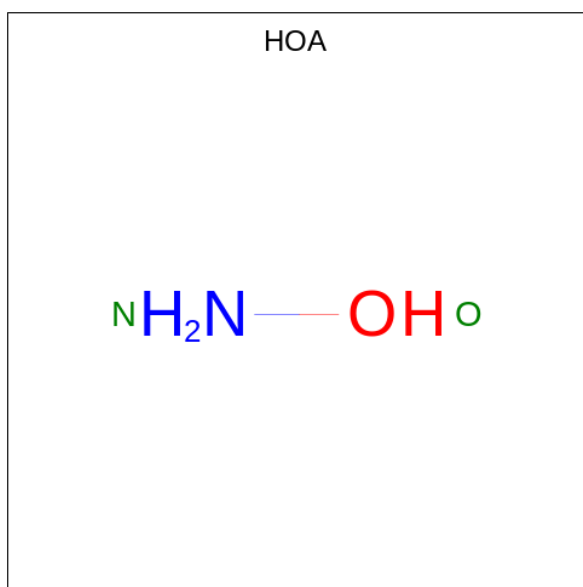
HOA

$_NH_2N$ —— OH_O

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 (three-letter code: 16N) (formula: C_9H_{10}) (labeled as "Ligand of Interest" by depositor).
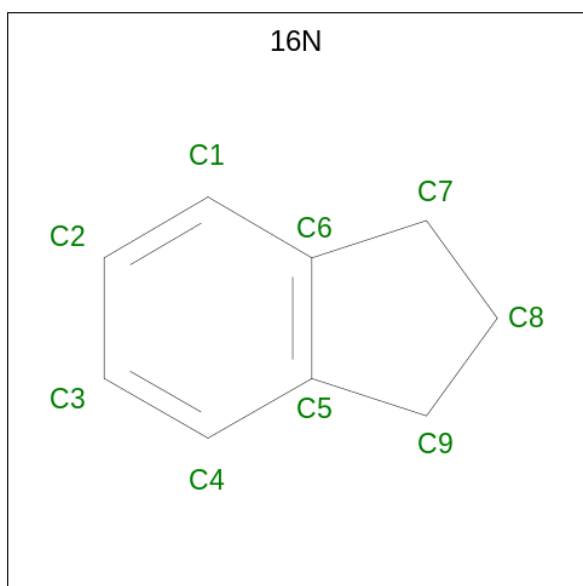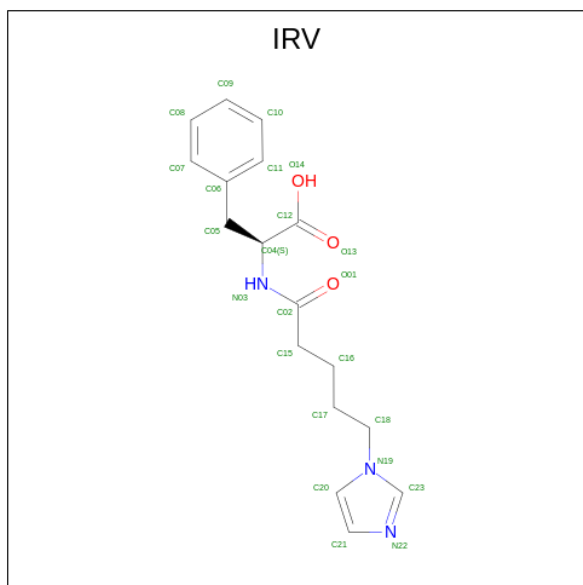
16N

C1
C7
C2   C6
C8
C3   C5
C9
C4

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 19　9　10			0	0

- Molecule 5 is (2 {S})-2-(5-imidazol-1-ylpentanoylamino)-3-phenyl-propanoic acid (three-letter code: IRV) (formula: $C_{17}H_{21}N_3O_3$) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is water.

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

# 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
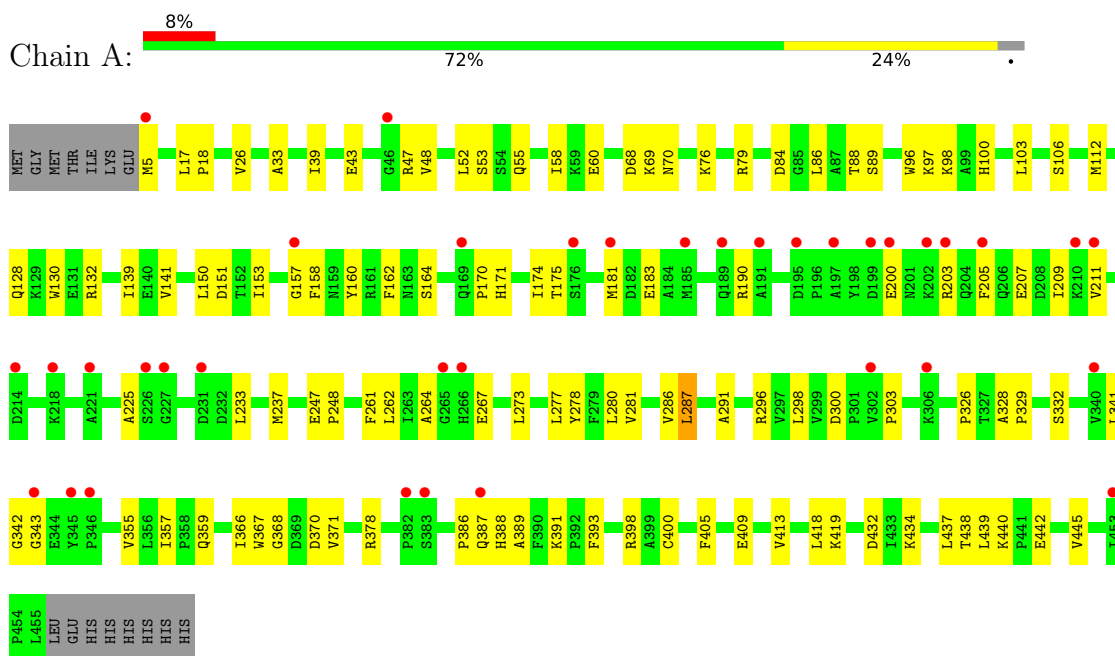
- Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase
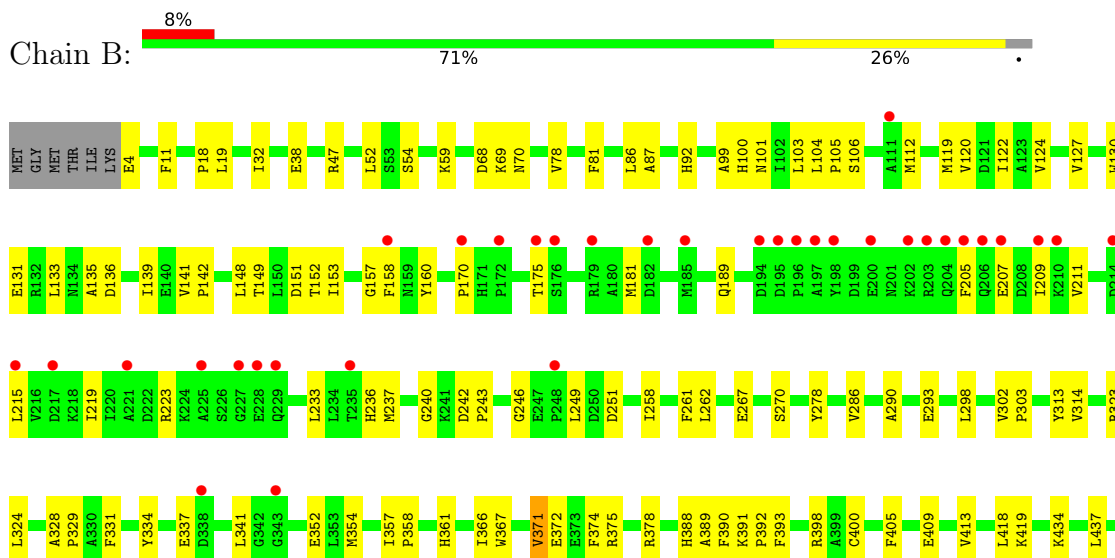
K440 P441 E442 G443 F444 K449 S450 K451 K452 I453 P454 L455 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	4.92 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.241 , 0.266 0.244 , 0.264	Depositor DCC
R_{free} test set	1824 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 41.8	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
HEM, IRV, HOA, 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	0.60	0/3704	0.61	0/5011
1	B	0.56	0/3717	0.60	0/5028
All	All	0.58	0/7421	0.60	0/10039

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3620	3562	3575	81	0
1	B	3633	3576	3585	96	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	8	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	357	0	0	16	1
All	All	8120	7244	7240	188	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 (188) 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: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: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: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:A:151:ASP:OD1	1:A:164:SER:OG	2.18	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:5:MET:HE3	1:A:39:ILE:HG12	1.97	0.47
1:A:86:LEU:HD21	1:A:100:HIS:N	2.30	0.47
1:B:181:MET:HE3	1:B:437:LEU:HD12	1.97	0.47
1:B:393:PHE:HB3	1:B:400:CYS:HB3	1.96	0.47
1:A:432:ASP:O	1:A:442:GLU:N	2.44	0.47
1:B:354:MET:HE1	6:B:625:HOH:O	2.15	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
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:354:MET:CE	6:B:625:HOH:O	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:76:LYS:NZ	6:A:619:HOH:O	2.34	0.43
1:B:158:PHE:CZ	1:B:262:LEU:HD11	2.53	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:160:TYR:HH	1:A:171:HIS:HE2	1.68	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: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:181:MET:HE1	4:B:503:16N:H10	2.03	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:181:MET:HE2	1:A:437:LEU:HD12	2.02	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
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: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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	92	95
1	B	394/409 (96%)	393 (100%)	1 (0%)	92	95
All	All	786/818 (96%)	784 (100%)	2 (0%)	92	95

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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
5	IRV	A	504[A]	-	23,24,24	1.52	2 (8%)	28,30,30	0.86	2 (7%)
5	IRV	B	504[A]	-	23,24,24	1.48	2 (8%)	28,30,30	1.07	2 (7%)
2	HEM	A	501	1,3	41,50,50	1.53	7 (17%)	45,82,82	1.92	10 (22%)
4	16N	A	503	-	10,10,10	2.28	3 (30%)	13,13,13	2.40	6 (46%)
3	HOA	B	501	2	0,1,1	-	-	-		
5	IRV	A	504[B]	-	23,24,24	1.51	3 (13%)	28,30,30	0.89	3 (10%)
2	HEM	B	502	1,3	41,50,50	1.49	7 (17%)	45,82,82	1.94	13 (28%)
3	HOA	A	502	2	0,1,1	-	-	-		
5	IRV	B	504[B]	-	23,24,24	1.52	3 (13%)	28,30,30	1.17	4 (14%)
4	16N	B	503	-	10,10,10	1.89	2 (20%)	13,13,13	1.14	0

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
5	IRV	A	504[A]	-	-	8/19/19/19	0/2/2/2
5	IRV	B	504[A]	-	-	6/19/19/19	0/2/2/2
2	HEM	A	501	1,3	-	0/12/54/54	-
4	16N	A	503	-	-		0/2/2/2
5	IRV	A	504[B]	-	-	8/19/19/19	0/2/2/2
2	HEM	B	502	1,3	-	0/12/54/54	-
5	IRV	B	504[B]	-	-	5/19/19/19	0/2/2/2
4	16N	B	503	-	-		0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504[A]	IRV	C02-N03	5.74	1.46	1.34
5	B	504[B]	IRV	C02-N03	5.64	1.46	1.34
5	A	504[B]	IRV	C02-N03	5.52	1.45	1.34
5	B	504[A]	IRV	C02-N03	5.40	1.45	1.34
4	A	503	16N	C2-C1	-4.46	1.29	1.38
2	A	501	HEM	C4D-ND	-4.26	1.33	1.40
4	A	503	16N	C1-C6	-4.08	1.32	1.39
2	B	502	HEM	C1B-NB	-3.99	1.33	1.40
2	A	501	HEM	C1B-NB	-3.98	1.33	1.40
4	B	503	16N	C9-C5	3.95	1.57	1.51
2	B	502	HEM	C4D-ND	-3.83	1.33	1.40
4	B	503	16N	C7-C6	3.67	1.56	1.51
4	A	503	16N	C8-C7	-3.10	1.44	1.53
2	B	502	HEM	FE-NB	2.93	2.11	1.96
2	A	501	HEM	C1D-ND	-2.79	1.33	1.38
2	A	501	HEM	FE-NB	2.75	2.10	1.96
5	A	504[B]	IRV	C20-N19	-2.63	1.32	1.37
2	A	501	HEM	C4B-NB	-2.55	1.33	1.38
5	B	504[B]	IRV	C20-N19	-2.47	1.33	1.37
5	B	504[A]	IRV	C20-N19	-2.42	1.33	1.37
5	A	504[A]	IRV	C20-N19	-2.41	1.33	1.37
2	B	502	HEM	C4B-NB	-2.37	1.33	1.38
2	B	502	HEM	O2D-CGD	-2.36	1.22	1.30
2	B	502	HEM	C1D-ND	-2.34	1.34	1.38
2	B	502	HEM	O2A-CGA	-2.23	1.23	1.30
5	B	504[B]	IRV	O01-C02	-2.18	1.18	1.23
2	A	501	HEM	O2D-CGD	-2.18	1.23	1.30
5	A	504[B]	IRV	O01-C02	-2.12	1.19	1.23
2	A	501	HEM	O2A-CGA	-2.10	1.23	1.30

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	HEM	CBA-CAA-C2A	-5.00	104.09	112.62
2	A	501	HEM	CHC-C4B-NB	4.85	129.70	124.43
2	A	501	HEM	CBA-CAA-C2A	-4.66	104.66	112.62
2	B	502	HEM	CHC-C4B-NB	4.51	129.33	124.43
2	A	501	HEM	C1B-NB-C4B	4.28	109.49	105.07
4	A	503	16N	C8-C7-C6	-4.16	97.92	103.78
2	A	501	HEM	CHD-C1D-ND	4.05	128.83	124.43
2	B	502	HEM	CHA-C4D-ND	3.97	129.29	124.38
2	B	502	HEM	CHD-C1D-ND	3.92	128.69	124.43
2	B	502	HEM	C1B-NB-C4B	3.91	109.12	105.07
2	A	501	HEM	CHA-C4D-ND	3.90	129.20	124.38
4	A	503	16N	C9-C8-C7	3.60	114.38	107.08
4	A	503	16N	C3-C2-C1	3.51	125.53	120.19
2	A	501	HEM	CHB-C1B-NB	3.43	128.62	124.38
4	A	503	16N	C7-C6-C5	2.90	114.78	110.16
2	B	502	HEM	CHB-C1B-NB	2.87	127.93	124.38
2	A	501	HEM	CBD-CAD-C3D	-2.83	104.77	112.63
2	B	502	HEM	CAD-CBD-CGD	-2.81	107.56	113.60
4	A	503	16N	C2-C3-C4	-2.79	115.94	120.19
2	B	502	HEM	CBD-CAD-C3D	-2.74	105.01	112.63
5	B	504[A]	IRV	O14-C12-C04	2.69	122.33	113.40
5	B	504[A]	IRV	O14-C12-O13	-2.57	118.26	124.09
2	B	502	HEM	CMD-C2D-C1D	2.51	128.85	125.04
2	A	501	HEM	CHD-C1D-C2D	-2.50	121.07	124.98
2	A	501	HEM	CHA-C4D-C3D	-2.48	120.67	125.33
2	B	502	HEM	C4D-ND-C1D	2.41	107.57	105.07
5	B	504[B]	IRV	C17-C18-N19	2.40	118.29	111.64
2	B	502	HEM	CHD-C1D-C2D	-2.33	121.34	124.98
2	B	502	HEM	CHA-C4D-C3D	-2.28	121.04	125.33
5	B	504[B]	IRV	O14-C12-C04	2.27	120.94	113.40
5	B	504[B]	IRV	C15-C02-N03	2.27	119.76	115.83
5	B	504[B]	IRV	O14-C12-O13	-2.25	118.97	124.09
5	A	504[B]	IRV	O14-C12-C04	2.25	120.88	113.40
4	A	503	16N	C8-C9-C5	-2.25	100.62	103.78
2	A	501	HEM	C4D-ND-C1D	2.22	107.36	105.07
5	A	504[A]	IRV	C16-C15-C02	-2.17	107.17	113.26
5	A	504[A]	IRV	O14-C12-C04	2.14	120.51	113.40
5	A	504[B]	IRV	C15-C02-N03	2.12	119.51	115.83
5	A	504[B]	IRV	O14-C12-O13	-2.09	119.35	124.09
2	B	502	HEM	C4B-C3B-C2B	-2.05	105.49	107.11

There are no chirality outliers.

All (27) torsion outliers are listed below:

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

There are no ring outliers.

8 monomers are involved in 23 short contacts:

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

Bond lengths — Bond angles — Torsions — Rings

Ligand IRV B 504 (A)

Bond lengths — Bond angles — Torsions — Rings

Ligand HEM A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 16N A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HOA B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand IRV A 504 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HOA A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand IRV B 504 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 16N B 503

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.62	36 (7%)	12	11	12, 24, 51, 65	0
1	B	452/466 (96%)	0.62	36 (7%)	12	11	13, 23, 48, 59	0
All	All	903/932 (96%)	0.62	72 (7%)	12	11	12, 24, 49, 65	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	GLY	5.5
1	A	197	ALA	5.1
1	B	225	ALA	5.0
1	B	221	ALA	4.9
1	A	200	GLU	4.8
1	A	227	GLY	4.8
1	A	231	ASP	4.6
1	B	214	ASP	4.2
1	A	211	VAL	4.0
1	B	210	LYS	3.7
1	B	228	GLU	3.6
1	A	5	MET	3.5
1	A	218	LYS	3.4
1	A	203	ARG	3.3
1	B	203	ARG	3.3
1	A	205	PHE	3.3
1	B	200	GLU	3.2
1	A	345	TYR	3.2
1	A	346	PRO	3.1
1	B	197	ALA	3.1
1	B	229	GLN	3.1
1	B	196	PRO	3.1
1	B	185	MET	3.0
1	B	205	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	387	GLN	2.9
1	A	202	LYS	2.9
1	B	198	TYR	2.9
1	B	206	GLN	2.8
1	B	170	PRO	2.8
1	A	199	ASP	2.8
1	B	209	ILE	2.7
1	A	176	SER	2.7
1	B	182	ASP	2.7
1	B	194	ASP	2.7
1	B	207	GLU	2.7
1	A	46	GLY	2.7
1	A	195	ASP	2.6
1	A	340	VAL	2.6
1	B	202	LYS	2.5
1	B	195	ASP	2.5
1	A	453	ILE	2.5
1	A	214	ASP	2.5
1	A	382	PRO	2.5
1	B	158	PHE	2.4
1	A	226	SER	2.4
1	B	215	LEU	2.4
1	B	343	GLY	2.4
1	B	111	ALA	2.4
1	B	176	SER	2.4
1	A	210	LYS	2.4
1	A	343	GLY	2.4
1	A	266	HIS	2.3
1	A	265	GLY	2.3
1	B	248	PRO	2.3
1	A	189	GLN	2.3
1	A	169	GLN	2.3
1	B	204	GLN	2.3
1	B	175	THR	2.2
1	A	185	MET	2.2
1	A	157	GLY	2.2
1	B	217	ASP	2.2
1	A	181	MET	2.2
1	B	179	ARG	2.2
1	A	302	VAL	2.1
1	A	191	ALA	2.1
1	A	306	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	453	ILE	2.1
1	A	383	SER	2.1
1	B	172	PRO	2.1
1	B	338	ASP	2.1
1	A	221	ALA	2.0
1	B	235	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	IRV	A	504[A]	23/23	0.40	0.70	89,90,108,108	43
5	IRV	A	504[B]	23/23	0.40	0.70	87,91,108,108	43
4	16N	B	503	9/9	0.49	0.53	79,80,97,97	0
5	IRV	B	504[A]	23/23	0.58	0.65	68,78,89,91	43
5	IRV	B	504[B]	23/23	0.58	0.65	68,76,91,92	43
4	16N	A	503	9/9	0.69	0.35	82,82,98,98	0
3	HOA	A	502	2/2	0.91	0.37	33,34,40,41	0
2	HEM	A	501	43/43	0.94	0.18	9,16,29,41	0
3	HOA	B	501	2/2	0.95	0.25	27,29,33,35	0
2	HEM	B	502	43/43	0.96	0.17	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.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Electron density around IRV A 504 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
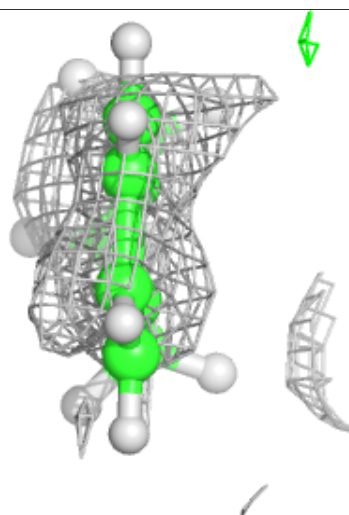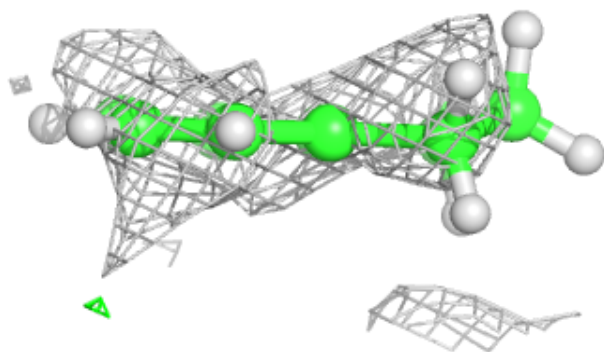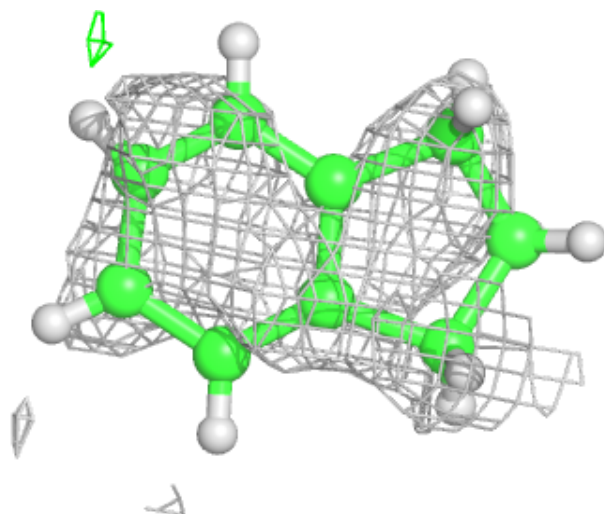$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
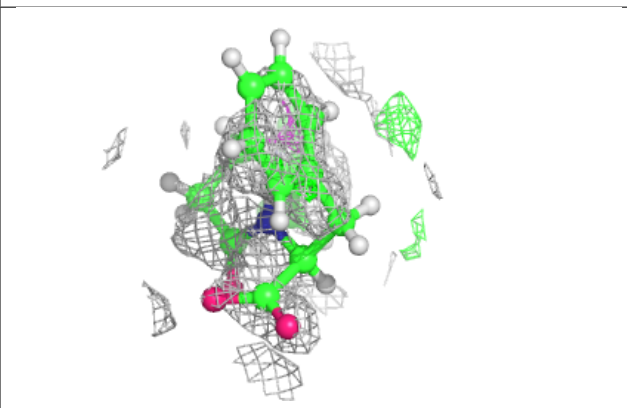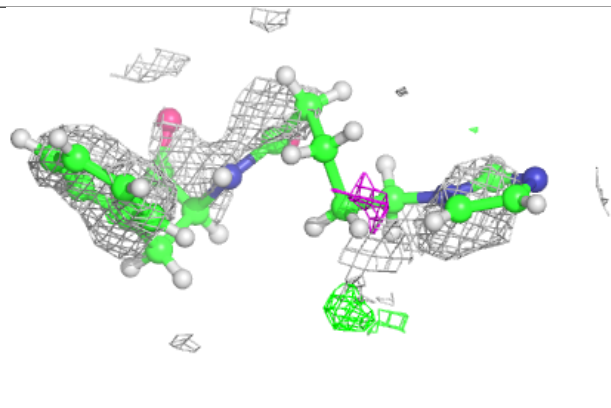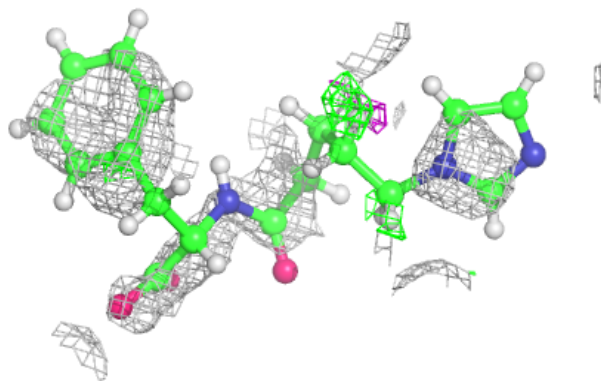
Electron density around IRV A 504 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
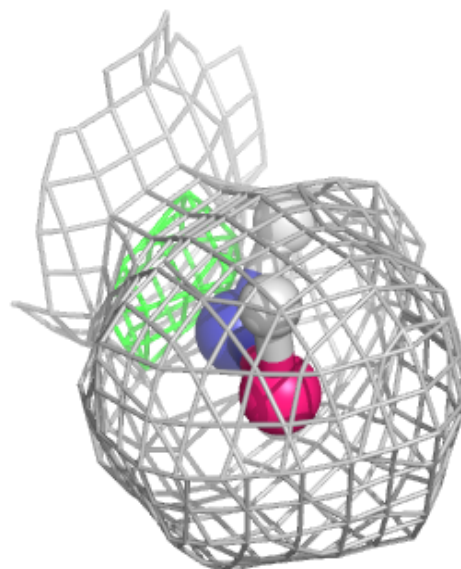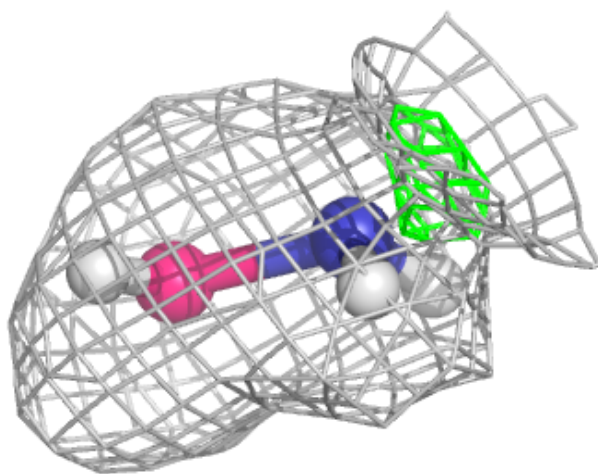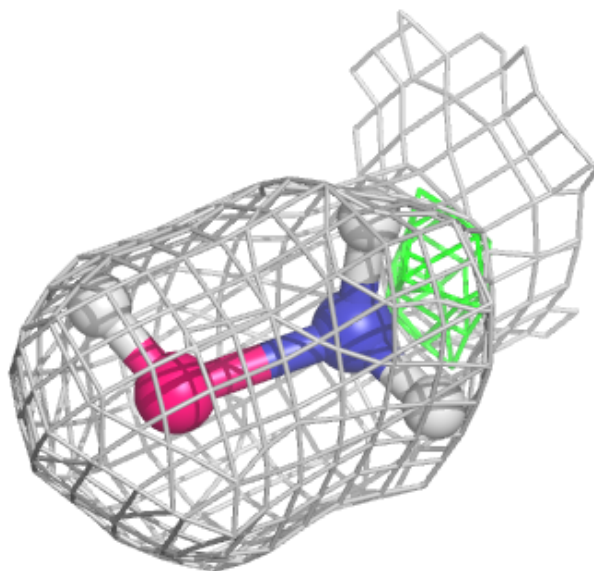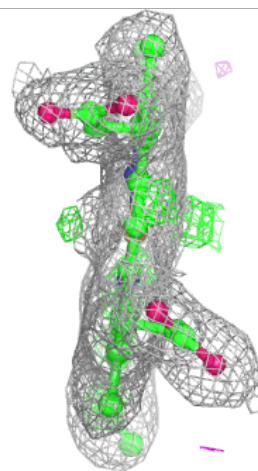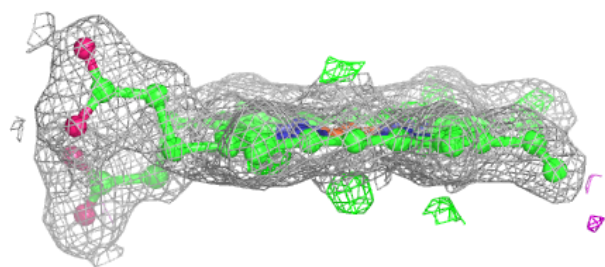and green (positive)
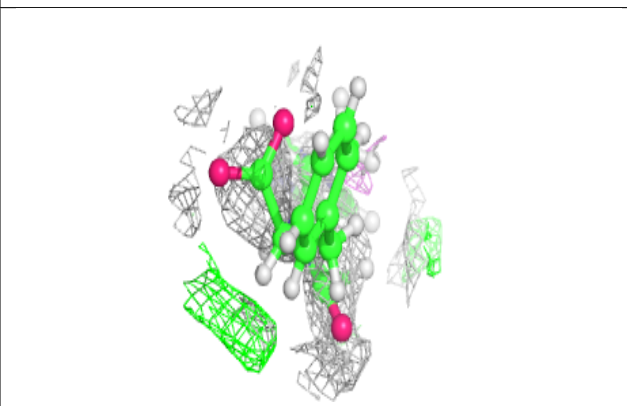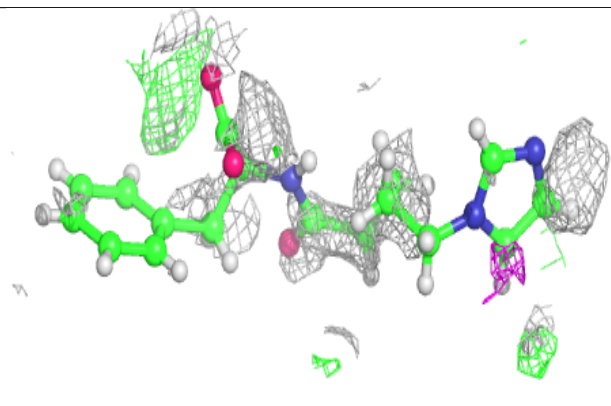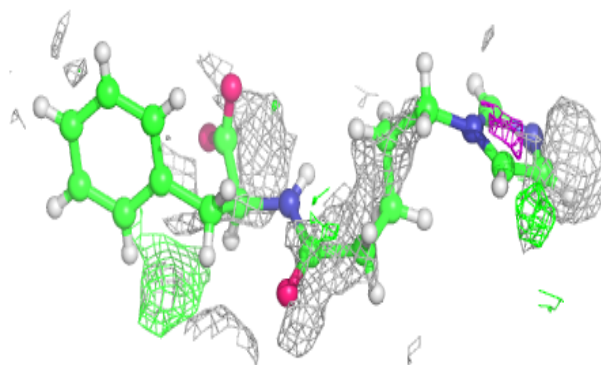
Electron density around 16N B 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
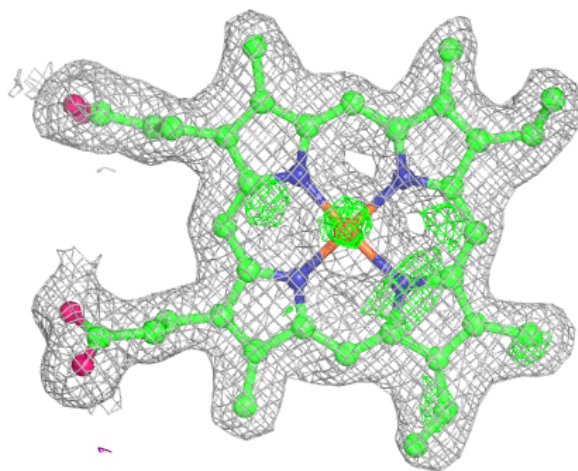and green (positive)
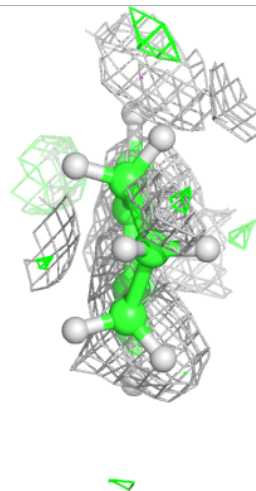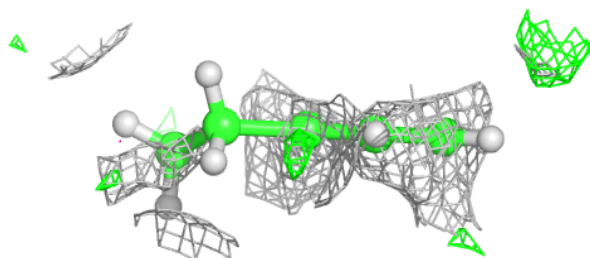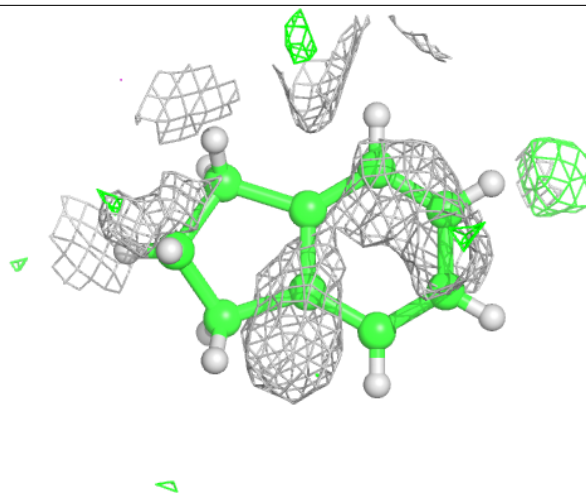
Electron density around IRV B 504 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
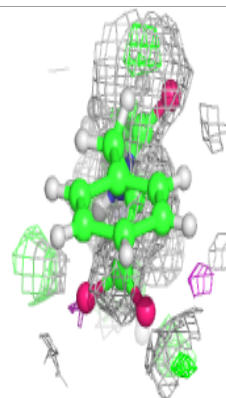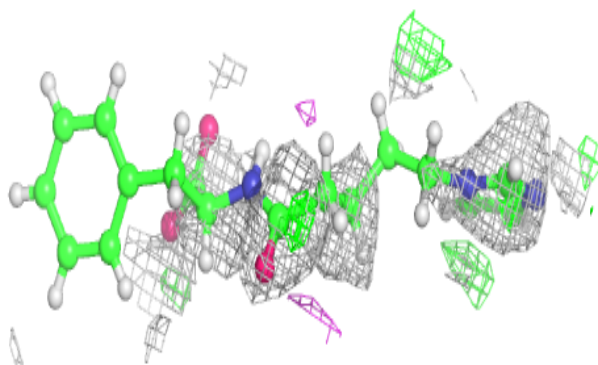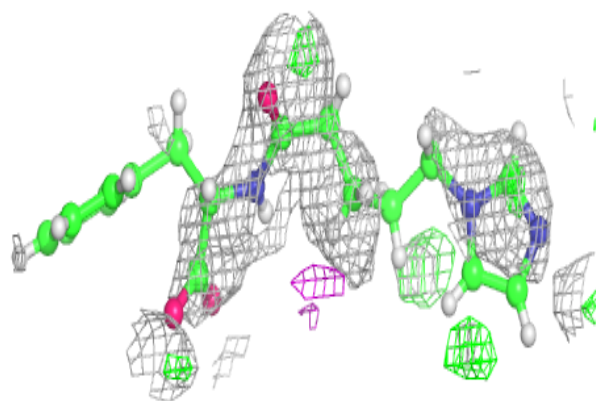
Electron density around IRV B 504 (B):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
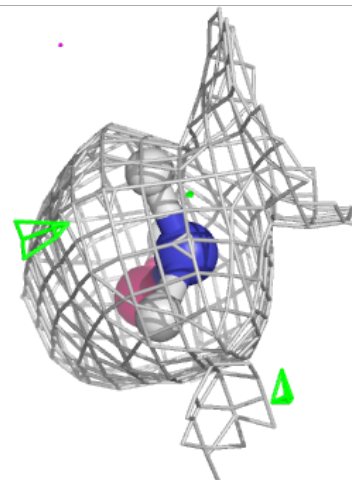mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
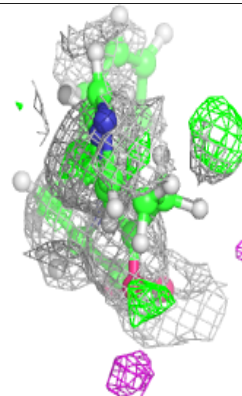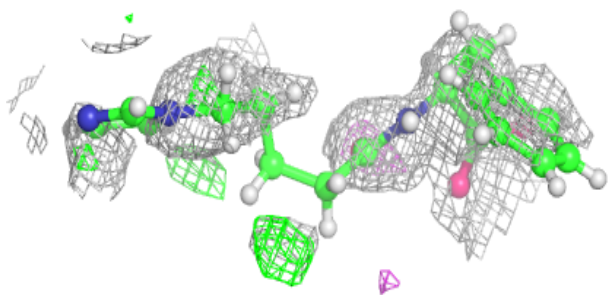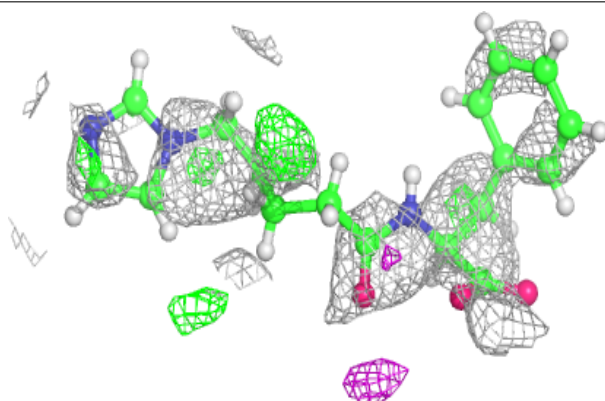
Electron density around 16N A 503:

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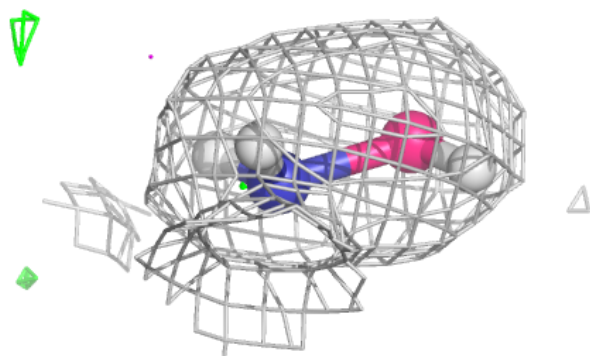and green (positive)

Electron density around HOA A 502:

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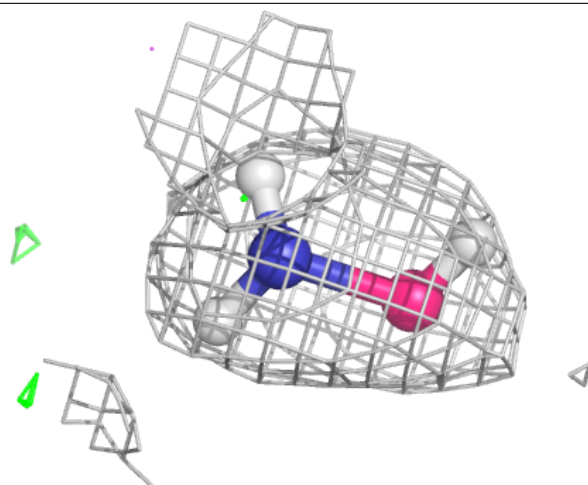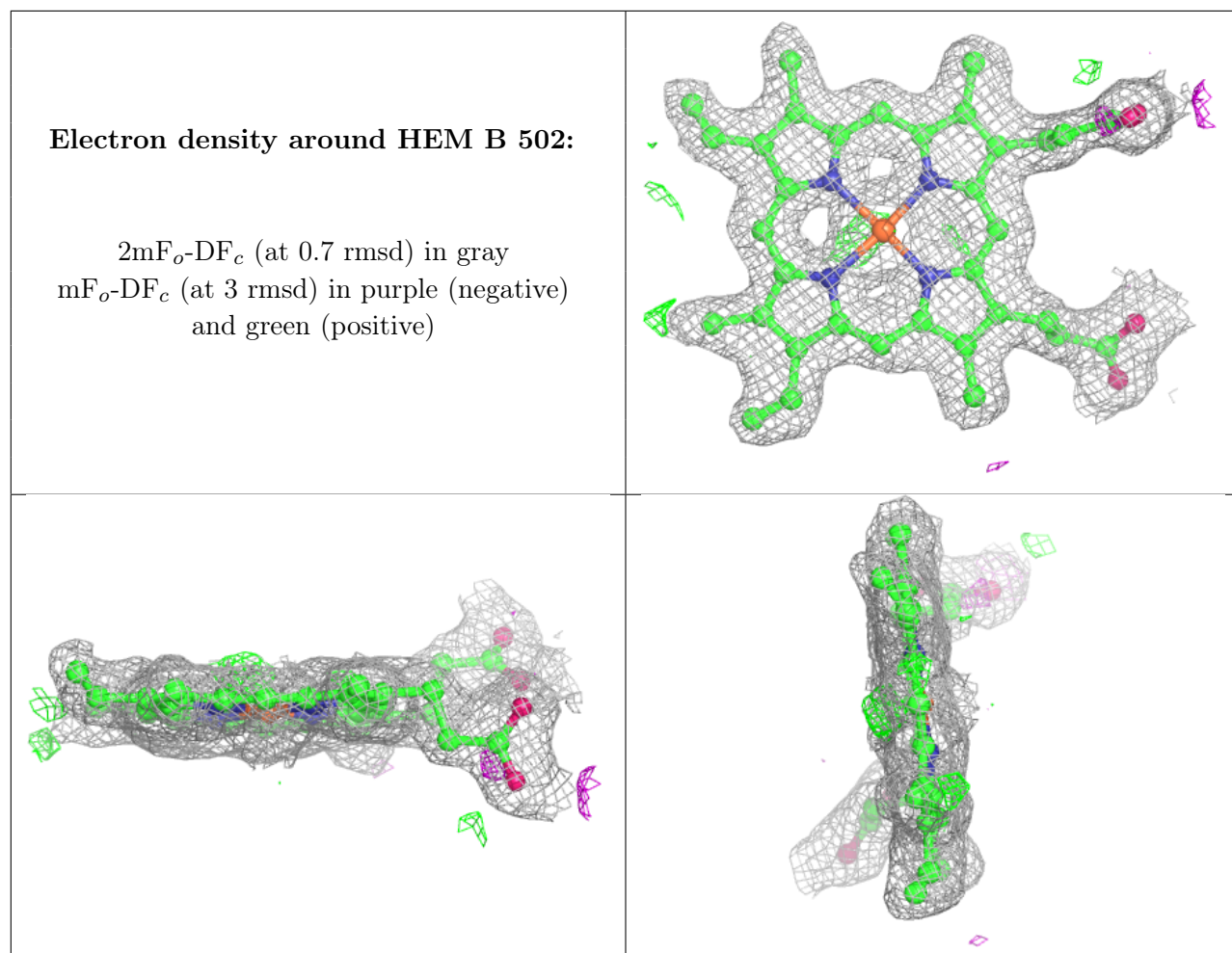and green (positive)

Electron density around 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 HOA B 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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 ⓘ

There are no such residues in this entry.