WORLDWIDE wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 11:51 PM JST

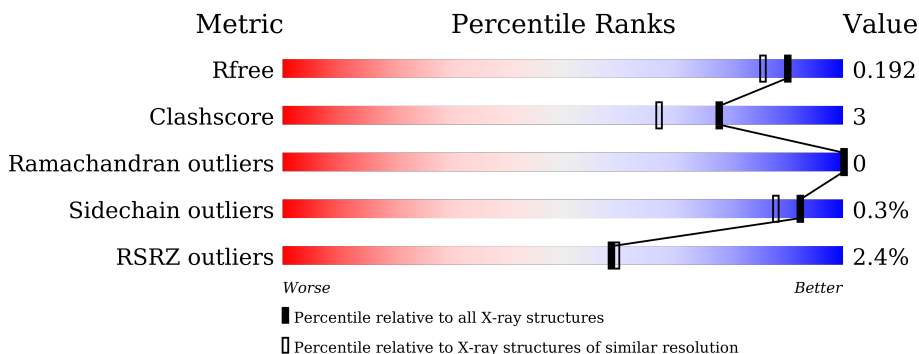|		
PDB ID	:	7YDD
Title	:	Crystal structure of the P450 BM3 heme domain mutant F87A/T268P/V78I in complex with N-imidazolyl-pentanoyl-L-phenylalanine,propylbenzene and hydroxylamine
Authors	:	Dong, S.; Chen, J.; Jiang, Y.; Cong, Z.; Feng, Y.
Deposited on	:	2022-07-04
Resolution	:	1.66 Å(reported)

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 1.66 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		0.192
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.3%
RSRZ outliers		2.4%

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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	3% ... 94% ...
1	B	466	2% ... 91% ... 6% ·

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	3H0	A	503	-	-	-	X
4	3H0	B	501	-	-	X	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8463 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 P450 BM3 heme domain mutant F87A/T268P/V78I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total 3656	C 2337	N 621	O 681	S 17	0	1	0
1	B	453	Total 3643	C 2328	N 621	O 677	S 17	0	0	0

There are 26 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	78	ILE	VAL	engineered mutation	UNP P14779
A	87	ALA	PHE	engineered mutation	UNP P14779
A	268	PRO	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	78	ILE	VAL	engineered mutation	UNP P14779
B	87	ALA	PHE	engineered mutation	UNP P14779
B	268	PRO	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
B	461	HIS	-	expression tag	UNP P14779
B	462	HIS	-	expression tag	UNP P14779

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

- Molecule 2 is HYDROXYAMINE (three-letter code: HOA) (formula: H_3NO) (labeled as "Ligand of Interest" by depositor).

HOA

$_NH_2N$ ——— OH_O
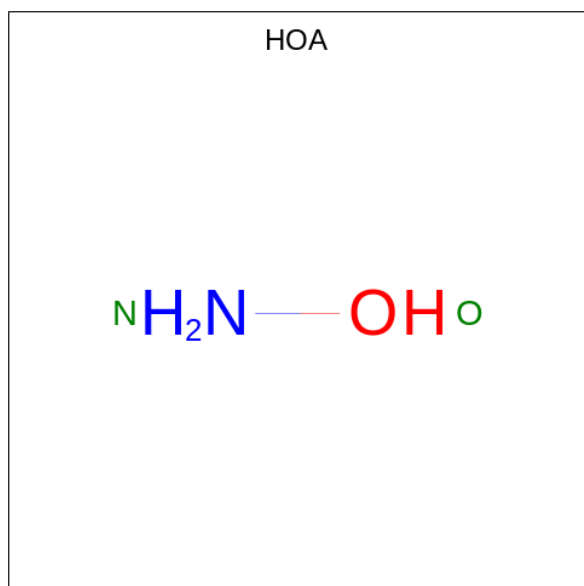
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 2	N 1	O 1	0	0
2	B	1	Total 2	N 1	O 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).
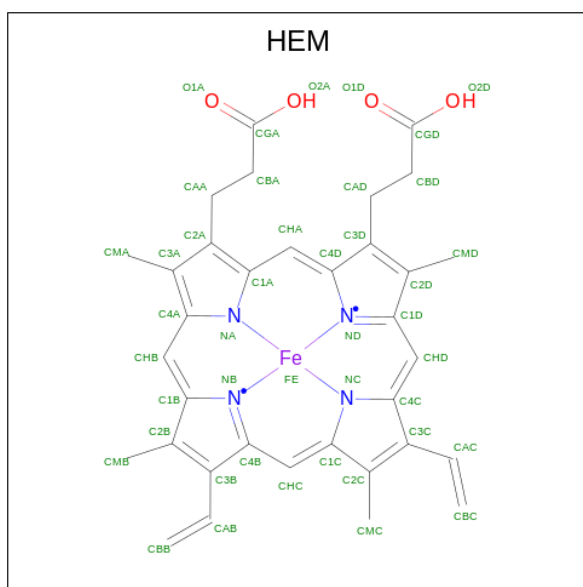
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is propylbenzene (three-letter code: 3H0) (formula: C_9H_{12}) (labeled as "Ligand of Interest" by depositor).
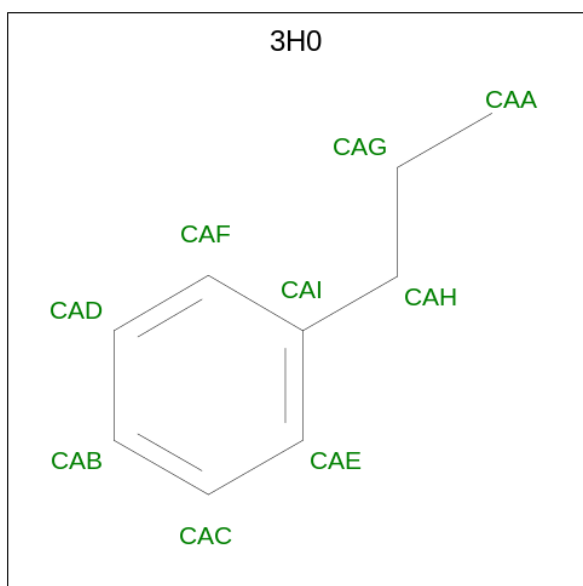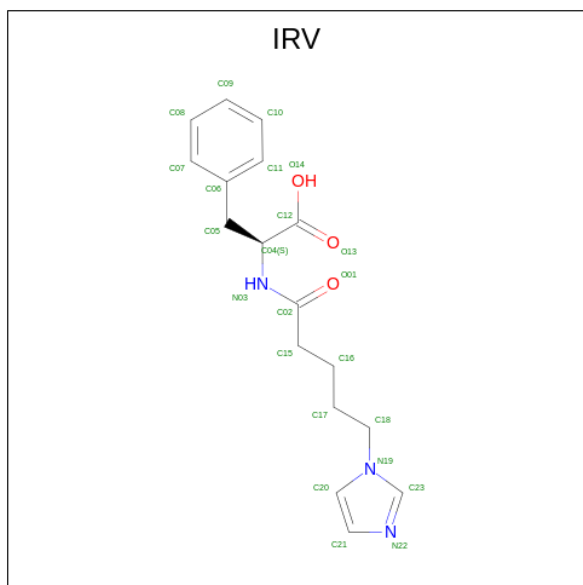

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total C 9 9		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 N O 46 34 6 6				0	1
5	B	1	Total C N O 46 34 6 6				0	1

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	507	Total O 507 507		0	0
6	B	457	Total O 457 457		0	0

Full wwPDB X-ray Structure Validation Report

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: P450 BM3 heme domain mutant F87A/T268P/V78I
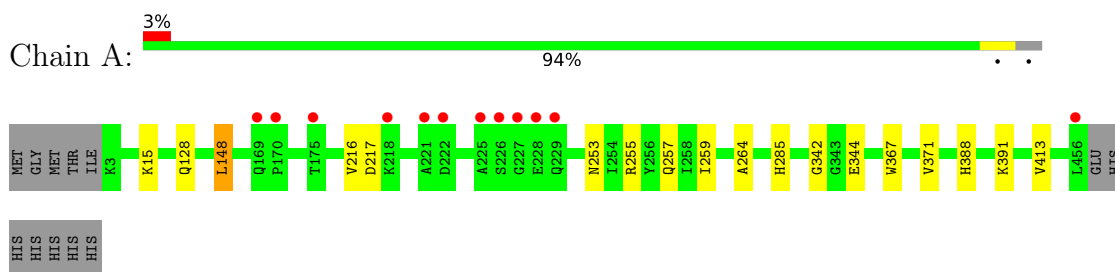
• Molecule 1: P450 BM3 heme domain mutant F87A/T268P/V78I
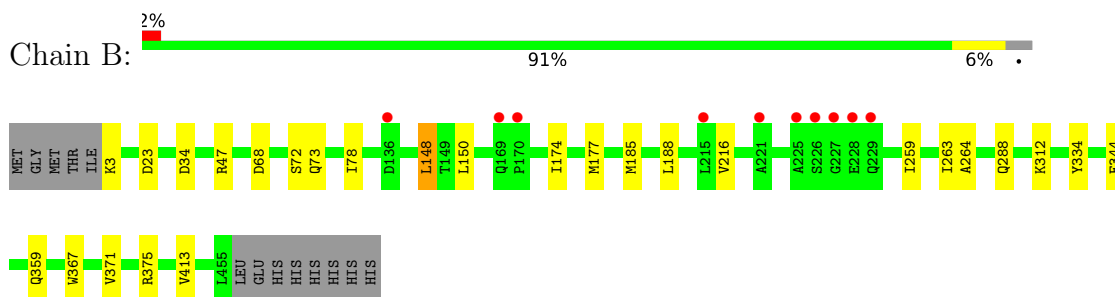
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.44Å 148.26Å 63.90Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	37.51 – 1.66 57.97 – 1.66	Depositor EDS
% Data completeness (in resolution range)	88.0 (37.51-1.66) 89.7 (57.97-1.66)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.66Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.156 , 0.193 0.157 , 0.192	Depositor DCC
R_{free} test set	1904 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.3	EDS
L-test for twinning [2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8463	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HOA, HEM, IRV, 3H0

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	0.74	0/3744	0.82	0/5063
1	B	0.75	0/3728	0.82	0/5041
All	All	0.75	0/7472	0.82	0/10104

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 (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	3656	0	3629	11	0
1	B	3643	0	3616	22	0
2	A	2	0	0	1	0
2	B	2	0	0	1	0
3	A	43	0	30	1	0
3	B	43	0	30	0	0
4	A	9	0	12	5	0
4	B	9	0	12	9	0
5	A	46	0	0	3	0
5	B	46	0	0	6	0
6	A	507	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	457	0	0	3	0
All	All	8463	0	7329	43	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 3.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASP:OD1	1:A:255:ARG:NH2	2.14	0.80
1:B:23:ASP:OD2	6:B:601:HOH:O	2.09	0.69
4:A:503:3H0:H3	5:A:504[B]:IRV:N22	2.11	0.65
4:B:501:3H0:H7	5:B:504[B]:IRV:N22	2.10	0.65
1:B:185:MET:O	1:B:188:LEU:HD12	2.02	0.60
2:A:501:HOA:N	4:A:503:3H0:H5	2.21	0.56
1:B:288:GLN:NE2	6:B:605:HOH:O	2.41	0.54
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.90	0.53
4:A:503:3H0:H7	5:A:504[B]:IRV:N22	2.24	0.53
1:B:73:GLN:HB3	1:B:188:LEU:CD2	2.39	0.52
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.91	0.52
1:A:342:GLY:O	1:A:344:GLU:HG3	2.13	0.49
4:B:501:3H0:H5	2:B:502:HOA:N	2.28	0.49
1:B:264:ALA:HB2	4:B:501:3H0:H8	1.95	0.49
1:B:78:ILE:HG21	4:B:501:3H0:H10	1.95	0.48
1:B:150:LEU:HD22	1:B:174:ILE:HG13	1.96	0.48
1:B:177:MET:CE	1:B:263:ILE:HG12	2.44	0.48
1:A:285:HIS:HD2	6:A:845:HOH:O	1.96	0.47
4:B:501:3H0:H3	5:B:504[B]:IRV:C23	2.44	0.47
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.97	0.47
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.97	0.47
4:B:501:3H0:H3	5:B:504[B]:IRV:N22	2.30	0.47
4:A:503:3H0:H7	5:A:504[B]:IRV:C21	2.44	0.46
6:A:743:HOH:O	1:B:312:LYS:HD3	2.17	0.45
1:B:367:TRP:HB2	1:B:371:VAL:HG12	1.99	0.44
1:B:73:GLN:HG2	1:B:188:LEU:HD23	1.98	0.44
1:B:78:ILE:CG2	4:B:501:3H0:H10	2.48	0.44
1:A:216:VAL:HG21	1:A:259:ILE:HG13	2.00	0.44
4:B:501:3H0:H7	5:B:504[B]:IRV:C21	2.49	0.43
1:B:375:ARG:HD3	6:B:636:HOH:O	2.18	0.43
1:A:15:LYS:HE3	6:A:841:HOH:O	2.19	0.42
1:B:78:ILE:HG21	4:B:501:3H0:CAB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502:HEM:CMC	3:A:502:HEM:HBC2	2.49	0.42
1:B:68:ASP:HB3	1:B:334:TYR:CZ	2.54	0.42
1:B:216:VAL:HG21	1:B:259:ILE:HG13	2.02	0.42
1:A:128:GLN:NE2	6:A:607:HOH:O	2.37	0.41
1:B:72:SER:HB2	5:B:504[A]:IRV:C12	2.50	0.41
1:B:47:ARG:NH1	5:B:504[A]:IRV:O13	2.44	0.41
1:B:150:LEU:HD13	1:B:174:ILE:HD11	2.03	0.41
1:A:264:ALA:HB2	4:A:503:3H0:H8	2.02	0.41
1:B:34:ASP:OD1	1:B:359:GLN:NE2	2.52	0.41
1:B:3:LYS:HB2	1:B:344:GLU:HB3	2.03	0.40
1:A:253:ASN:O	1:A:257:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/466 (97%)	439 (97%)	14 (3%)	0	100	100
1	B	451/466 (97%)	441 (98%)	10 (2%)	0	100	100
All	All	904/932 (97%)	880 (97%)	24 (3%)	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	396/408 (97%)	395 (100%)	1 (0%)	92	88
1	B	394/408 (97%)	393 (100%)	1 (0%)	92	88
All	All	790/816 (97%)	788 (100%)	2 (0%)	92	88

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

Mol	Chain	Res	Type
1	A	148	LEU
1	B	148	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	404	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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
4	3H0	B	501	-	9,9,9	0.27	0	10,10,10	1.04	1 (10%)
3	HEM	B	503	2,1	41,50,50	1.54	5 (12%)	45,82,82	1.52	8 (17%)
5	IRV	A	504[B]	-	23,24,24	1.53	2 (8%)	28,30,30	1.20	3 (10%)
5	IRV	B	504[A]	-	23,24,24	1.69	3 (13%)	28,30,30	1.23	4 (14%)
3	HEM	A	502	2,1	41,50,50	1.54	6 (14%)	45,82,82	1.60	10 (22%)
5	IRV	A	504[A]	-	23,24,24	1.73	3 (13%)	28,30,30	1.15	4 (14%)
2	HOA	A	501	3	0,1,1	-	-	-		
4	3H0	A	503	-	9,9,9	0.30	0	10,10,10	0.88	0
2	HOA	B	502	3	0,1,1	-	-	-		
5	IRV	B	504[B]	-	23,24,24	1.64	4 (17%)	28,30,30	1.20	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	503	2,1	-	2/12/54/54	-
5	IRV	A	504[B]	-	-	0/19/19/19	0/2/2/2
5	IRV	B	504[A]	-	-	6/19/19/19	0/2/2/2
3	HEM	A	502	2,1	-	2/12/54/54	-
5	IRV	A	504[A]	-	-	6/19/19/19	0/2/2/2
4	3H0	A	503	-	-	1/3/3/3	0/1/1/1
5	IRV	B	504[B]	-	-	0/19/19/19	0/2/2/2
4	3H0	B	501	-	-	1/3/3/3	0/1/1/1

All (23) bond length outliers are listed below:

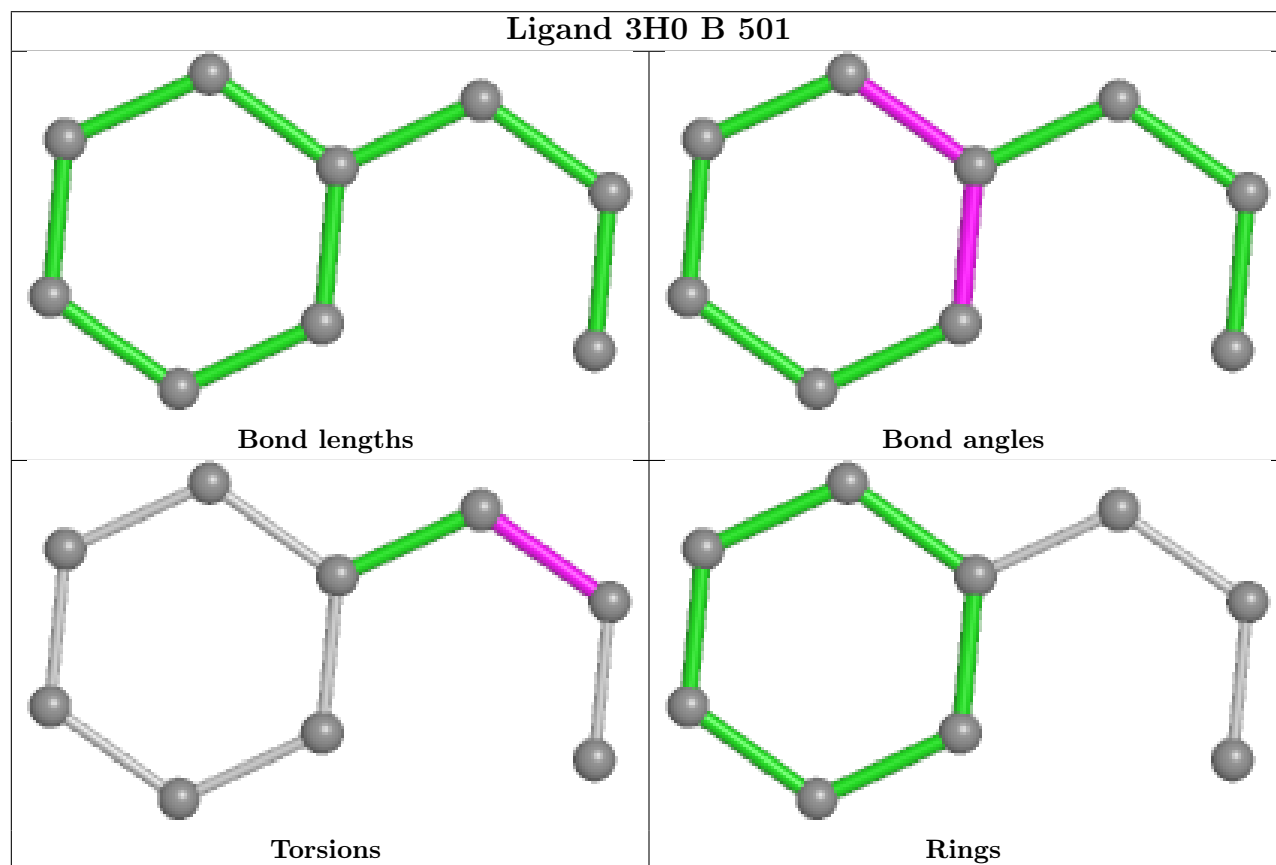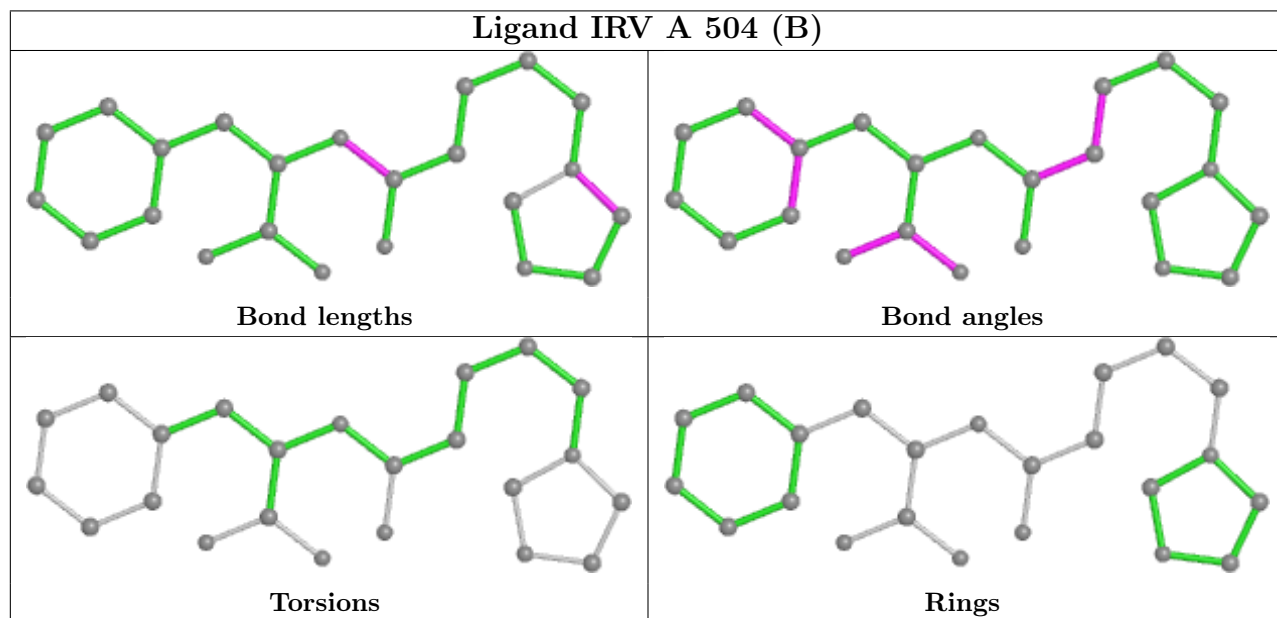| Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	504[A]	IRV	C02-N03	6.47	1.47	1.34
5	A	504[A]	IRV	C02-N03	6.32	1.47	1.34
5	B	504[B]	IRV	C02-N03	5.82	1.46	1.34
5	A	504[B]	IRV	C02-N03	5.74	1.46	1.34
3	B	503	HEM	C3C-C2C	-5.58	1.32	1.40
3	A	502	HEM	C3C-C2C	-4.16	1.34	1.40
5	A	504[A]	IRV	C20-N19	-3.67	1.30	1.37
3	A	502	HEM	C3C-CAC	3.45	1.54	1.47
3	B	503	HEM	C3C-CAC	3.42	1.54	1.47
3	A	502	HEM	CAB-C3B	3.28	1.56	1.47
3	B	503	HEM	CAB-C3B	2.79	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	504[A]	IRV	C20-N19	-2.78	1.32	1.37
5	B	504[B]	IRV	C20-N19	-2.68	1.32	1.37
5	A	504[B]	IRV	C20-N19	-2.64	1.32	1.37
5	B	504[A]	IRV	O01-C02	-2.60	1.18	1.23
3	B	503	HEM	CMD-C2D	2.55	1.56	1.50
3	A	502	HEM	CAA-C2A	2.38	1.55	1.52
5	B	504[B]	IRV	O13-C12	2.19	1.28	1.22
3	A	502	HEM	CMA-C3A	2.17	1.56	1.51
5	A	504[A]	IRV	O01-C02	-2.16	1.18	1.23
5	B	504[B]	IRV	O01-C02	-2.05	1.19	1.23
3	B	503	HEM	CMC-C2C	2.04	1.56	1.51
3	A	502	HEM	CHB-C1B	2.01	1.40	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	HEM	CHD-C1D-ND	3.65	128.40	124.43
3	A	502	HEM	CMA-C3A-C4A	-3.59	122.94	128.46
3	A	502	HEM	CBA-CAA-C2A	-3.29	107.00	112.62
3	B	503	HEM	C1B-NB-C4B	3.29	108.47	105.07
5	B	504[B]	IRV	C16-C15-C02	-3.11	104.53	113.26
5	B	504[A]	IRV	C15-C02-N03	2.92	120.89	115.83
3	B	503	HEM	CHB-C1B-NB	2.81	127.85	124.38
3	A	502	HEM	C4B-C3B-C2B	2.76	109.31	107.11
5	A	504[A]	IRV	C04-N03-C02	2.75	128.72	121.65
3	B	503	HEM	C4D-ND-C1D	2.74	107.91	105.07
5	B	504[A]	IRV	C05-C04-C12	-2.73	103.86	110.42
3	A	502	HEM	CMC-C2C-C3C	2.70	129.72	124.68
5	A	504[B]	IRV	C16-C15-C02	-2.62	105.90	113.26
3	A	502	HEM	CBD-CAD-C3D	-2.58	105.47	112.63
5	A	504[A]	IRV	O01-C02-C15	-2.54	117.37	122.02
3	B	503	HEM	CBA-CAA-C2A	-2.41	108.51	112.62
5	B	504[B]	IRV	C11-C06-C07	2.41	121.95	118.17
5	A	504[B]	IRV	C11-C06-C07	2.40	121.94	118.17
3	B	503	HEM	CHC-C4B-NB	2.38	127.02	124.43
3	A	502	HEM	CHB-C1B-NB	2.32	127.25	124.38
3	A	502	HEM	C4D-ND-C1D	2.31	107.46	105.07
3	A	502	HEM	CMA-C3A-C2A	2.27	129.23	124.94
3	B	503	HEM	CBD-CAD-C3D	-2.27	106.32	112.63
5	B	504[A]	IRV	O01-C02-C15	-2.27	117.87	122.02
3	B	503	HEM	O2A-CGA-CBA	2.23	121.20	114.03
5	A	504[A]	IRV	C12-C04-N03	-2.21	105.30	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	504[A]	IRV	C15-C02-N03	2.12	119.51	115.83
3	A	502	HEM	O2D-CGD-CBD	2.08	120.72	114.03
4	B	501	3H0	CAF-CAI-CAE	2.06	121.41	118.17
3	B	503	HEM	O1A-CGA-CBA	-2.03	116.56	123.08
5	A	504[B]	IRV	O14-C12-O13	-2.03	119.48	124.09
5	B	504[A]	IRV	C04-N03-C02	2.00	126.80	121.65

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	3H0	CAA-CAG-CAH-CAI
5	A	504[A]	IRV	C17-C18-N19-C20
5	B	504[A]	IRV	C17-C18-N19-C20
5	A	504[A]	IRV	C16-C17-C18-N19
5	B	504[A]	IRV	C02-C15-C16-C17
4	B	501	3H0	CAA-CAG-CAH-CAI
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[A]	IRV	N03-C02-C15-C16
5	B	504[A]	IRV	O01-C02-C15-C16
5	B	504[A]	IRV	C17-C18-N19-C23
5	A	504[A]	IRV	C02-C15-C16-C17
5	B	504[A]	IRV	C16-C17-C18-N19
3	A	502	HEM	CAD-CBD-CGD-O2D
3	B	503	HEM	CAD-CBD-CGD-O2D
3	B	503	HEM	CAD-CBD-CGD-O1D
3	A	502	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	3H0	9	0
5	A	504[B]	IRV	3	0
5	B	504[A]	IRV	2	0
3	A	502	HEM	1	0
2	A	501	HOA	1	0
4	A	503	3H0	5	0
2	B	502	HOA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504[B]	IRV	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 3H0 B 501

Ligand HEM B 503

Bond lengths

Bond angles

Torsions

Rings

Ligand IRV A 504 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand IRV B 504 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand IRV A 504 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand HOA A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 3H0 A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HOA B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand IRV B 504 (B)

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(Å²)	Q<0.9
1	A	454/466 (97%)	-0.30	12 (2%) 56	56	18, 25, 49, 106	0
1	B	453/466 (97%)	-0.30	10 (2%) 62	63	18, 26, 54, 98	0
All	All	907/932 (97%)	-0.30	22 (2%) 59	59	18, 26, 52, 106	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	GLU	6.9
1	A	227	GLY	5.6
1	B	226	SER	5.1
1	A	226	SER	5.0
1	B	225	ALA	4.5
1	B	169	GLN	4.1
1	A	169	GLN	3.8
1	B	227	GLY	3.7
1	B	228	GLU	3.6
1	A	225	ALA	3.3
1	B	229	GLN	2.9
1	A	170	PRO	2.8
1	A	229	GLN	2.6
1	A	222	ASP	2.5
1	A	218	LYS	2.5
1	A	456	LEU	2.5
1	B	221	ALA	2.4
1	B	215	LEU	2.4
1	B	170	PRO	2.3
1	A	221	ALA	2.2
1	A	175	THR	2.2
1	B	136	ASP	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
4	3H0	A	503	9/9	0.59	0.49	79,94,97,100	0
4	3H0	B	501	9/9	0.66	0.52	101,108,110,110	0
5	IRV	B	504[A]	23/23	0.88	0.17	12,19,29,32	23
5	IRV	B	504[B]	23/23	0.88	0.17	13,20,29,31	23
5	IRV	A	504[A]	23/23	0.90	0.17	11,21,28,33	23
5	IRV	A	504[B]	23/23	0.90	0.17	10,19,26,29	23
2	HOA	B	502	2/2	0.97	0.07	19,19,19,26	0
2	HOA	A	501	2/2	0.98	0.10	21,21,21,27	0
3	HEM	A	502	43/43	0.98	0.07	15,18,22,30	0
3	HEM	B	503	43/43	0.99	0.08	14,17,23,29	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 3H0 A 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
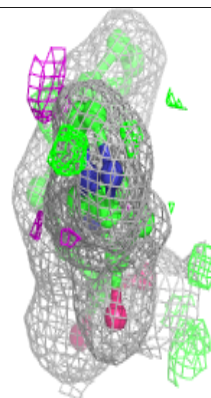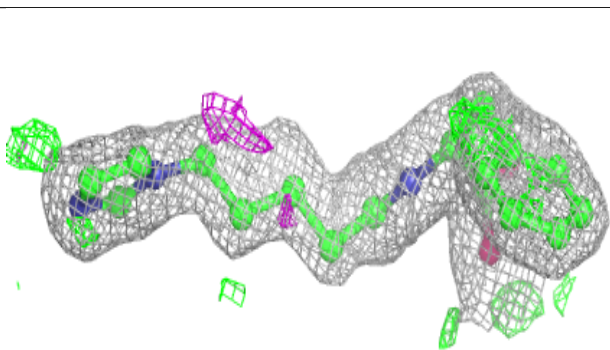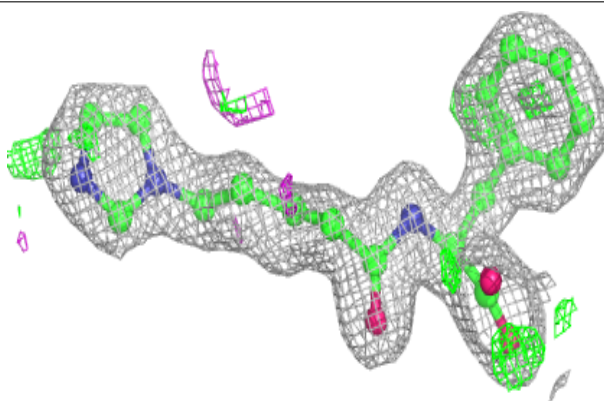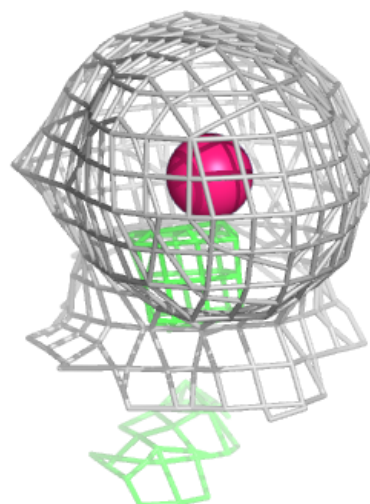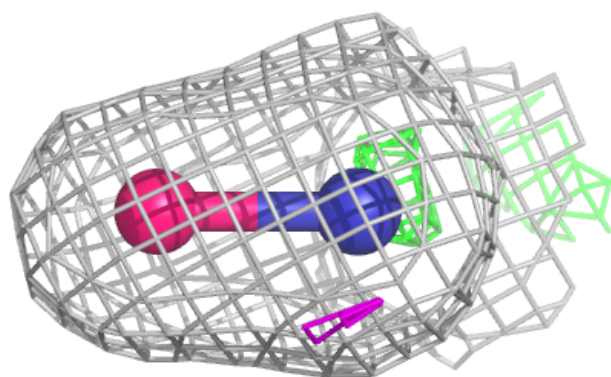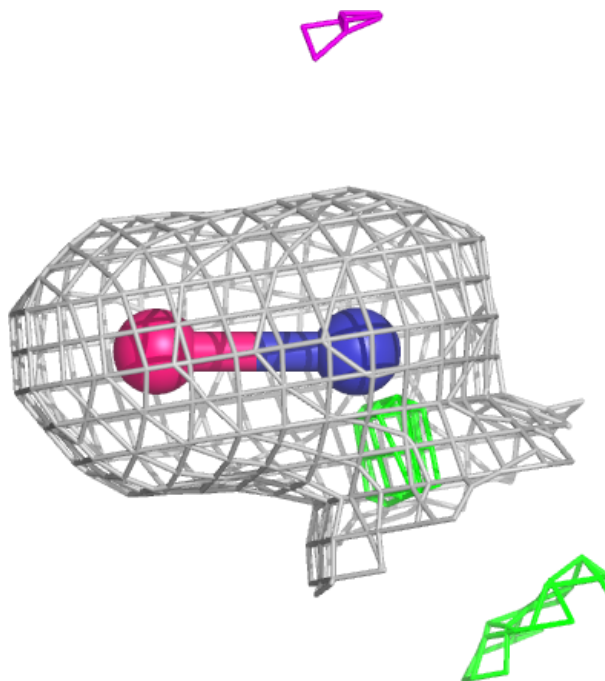$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
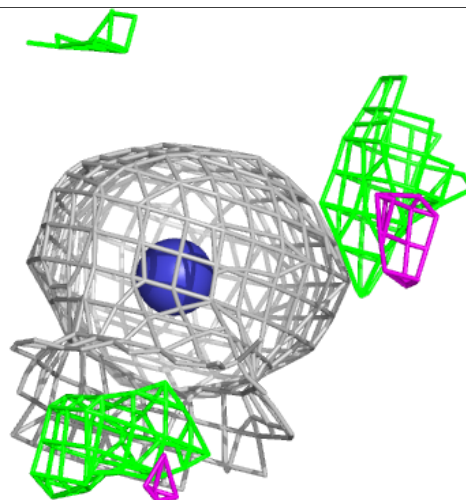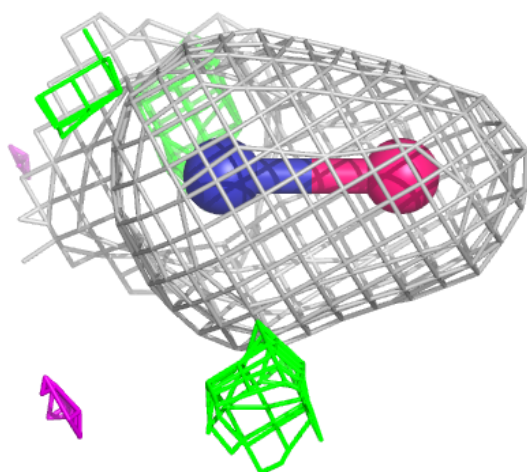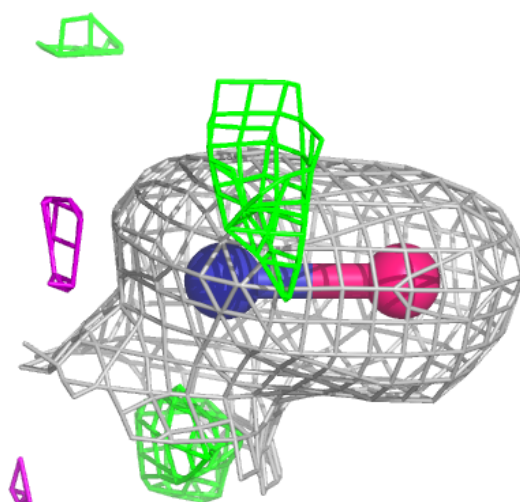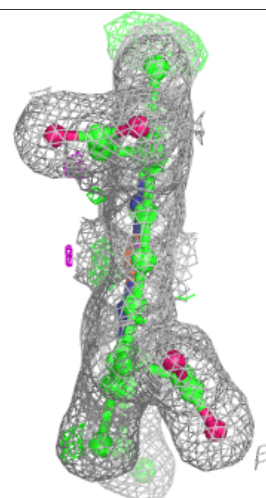and green (positive)
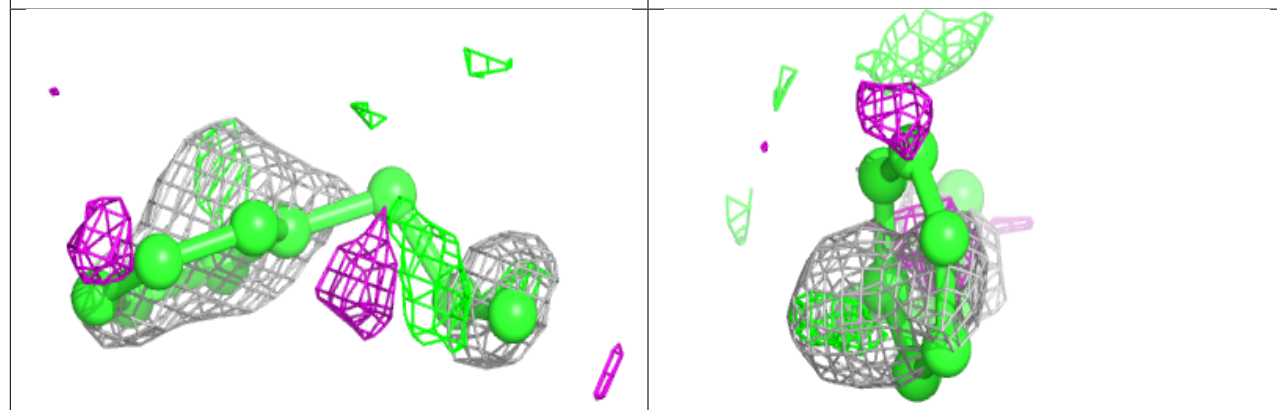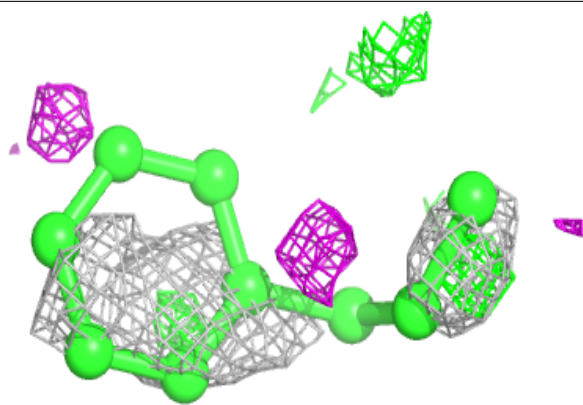
Electron density around 3H0 B 501:

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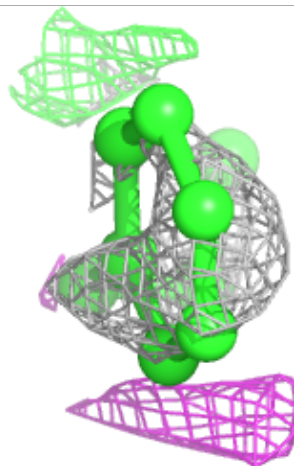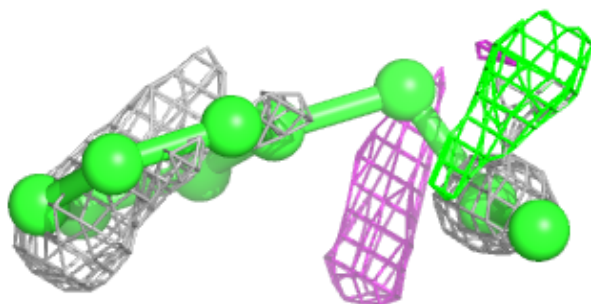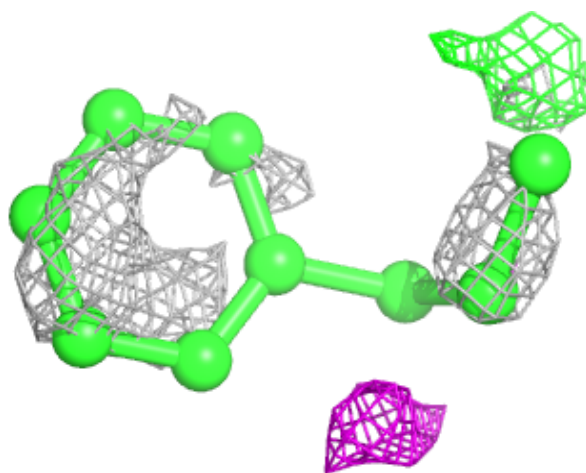
Electron density around IRV B 504 (A):

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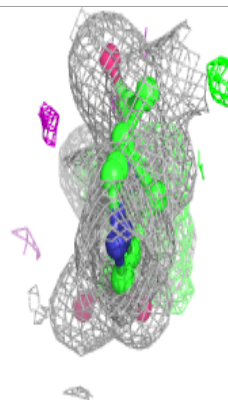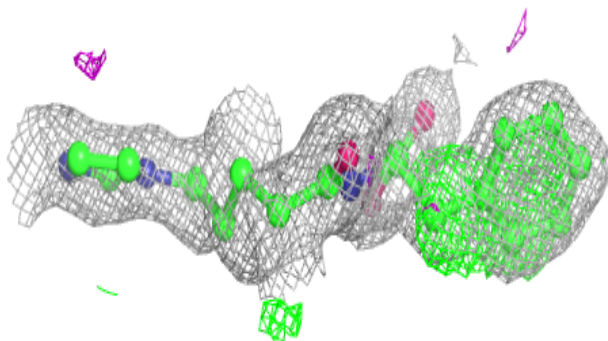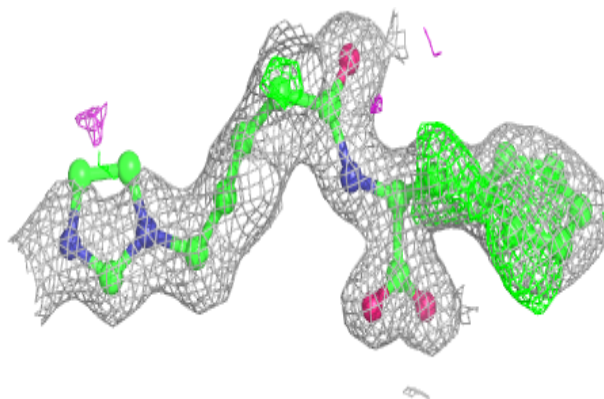
Electron density around IRV B 504 (B):

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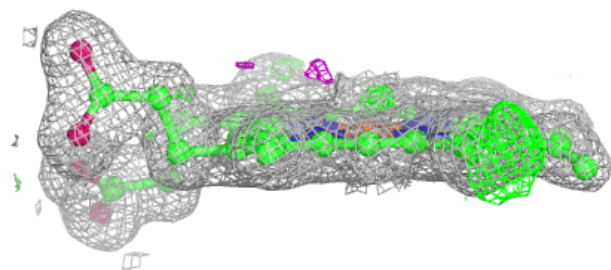and green (positive)
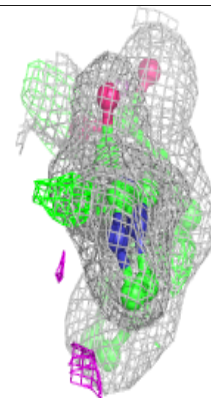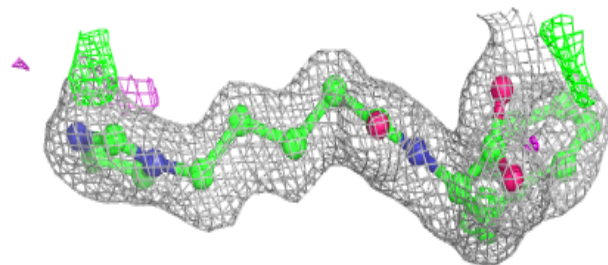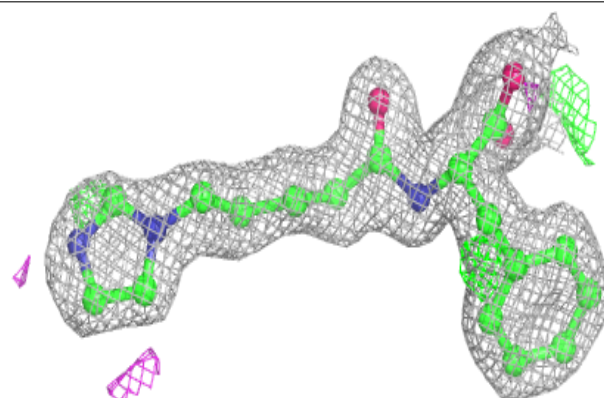
Electron density around IRV A 504 (A):

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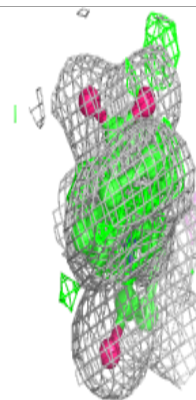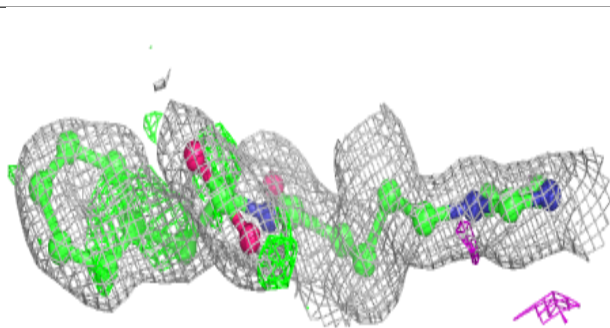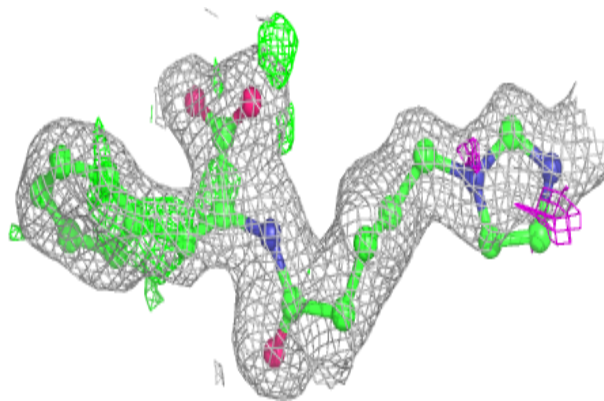
Electron density around IRV A 504 (B):

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

Electron density around HOA B 502:

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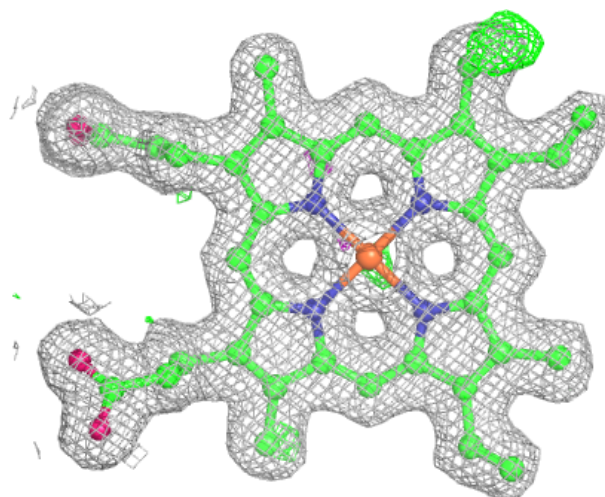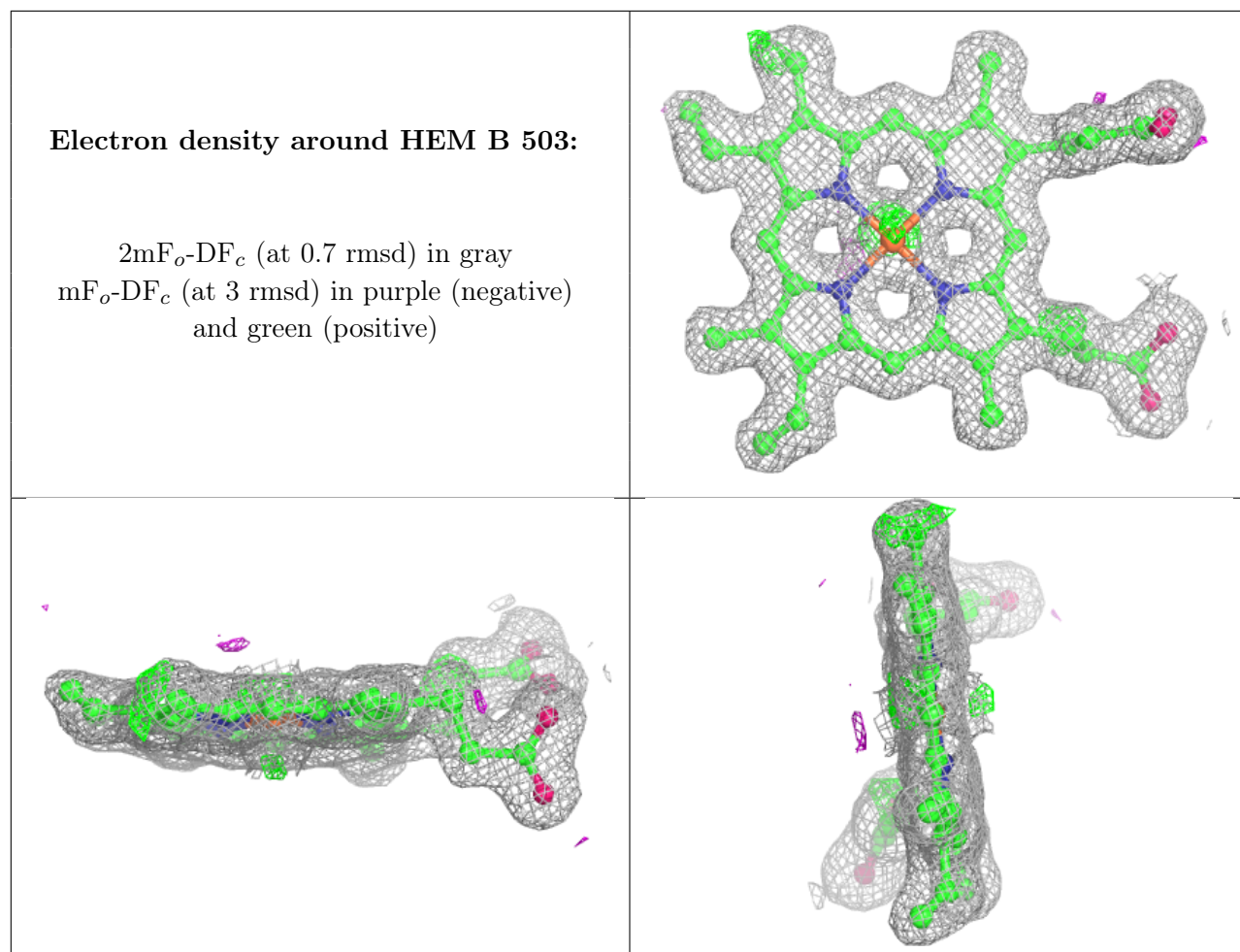and green (positive)

Electron density around HOA 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 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 B 503:

$2mF_o$-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.