Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 07:42 PM EDT

PDB ID	:	7RTQ
Title	:	Sterol 14alpha demethylase (CYP51) from Naegleria fowleri in complex with an inhibitor R)-N-(1-(3,4'-difluorobiphenyl-4-yl)-2-(1H-imidazol-1-yl)ethyl)-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide
Authors	:	Lepesheva, G.I.; Hargrove, T.Y.; Wawrzak, Z.
Deposited on	:	2021-08-13
Resolution	:	2.11 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:

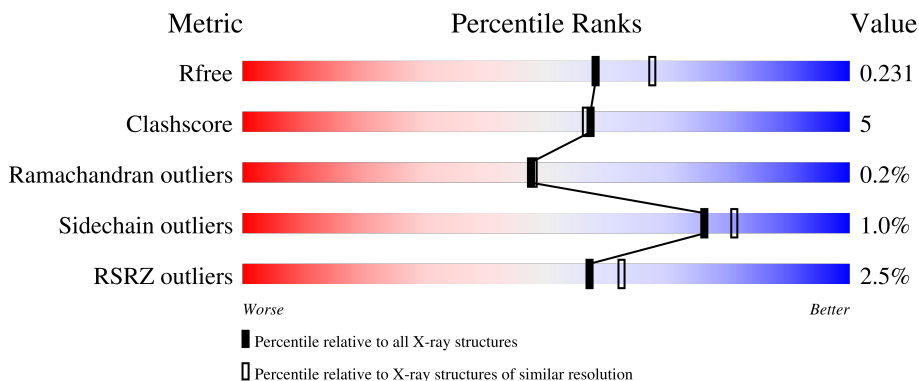|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.11 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		0.231
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		1.0%
RSRZ outliers		2.5%

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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	2% / 89% 7% •
1	B	466	2% / 88% 8% •
1	C	466	3% / 89% 7% •
1	D	466	3% / 89% 7% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15917 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 Protein CYP51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total 3617	C 2319	N 614	O 662	S 22	0	0	0
1	B	449	Total 3617	C 2319	N 614	O 662	S 22	0	0	0
1	C	449	Total 3617	C 2319	N 614	O 662	S 22	0	0	0
1	D	449	Total 3617	C 2319	N 614	O 662	S 22	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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

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

- Molecule 3 is N-[(1R)-2-(1H-imidazol-1-yl)-1-(3,4',5-trifluoro[1,1'-biphenyl]-4-yl)ethyl]-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide (three-letter code: 7PW) (formula: $C_{32}H_{22}F_3N_5O_2$) (labeled as "Ligand of Interest" by depositor).

7PW
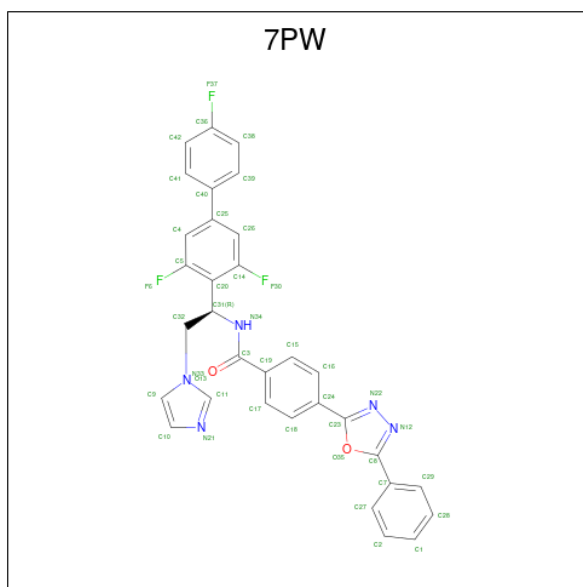
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	1
			84	64	6	10	4		
3	B	1	Total	C	F	N	O	0	1
			84	64	6	10	4		
3	C	1	Total	C	F	N	O	0	1
			84	64	6	10	4		
3	D	1	Total	C	F	N	O	0	1
			84	64	6	10	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	214	Total	O	0	0
			214	214		
4	B	249	Total	O	0	0
			249	249		

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| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	245	Total O 245 245	0	0
4	D	233	Total O 233 233	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.
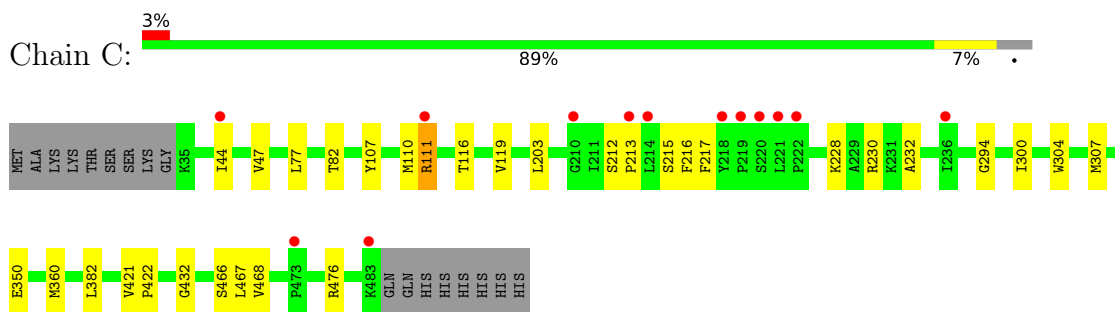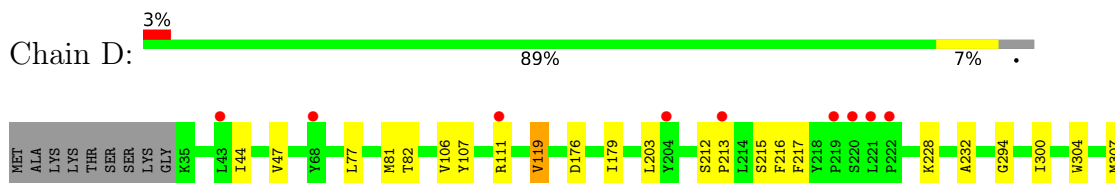
- Molecule 1: Protein CYP51
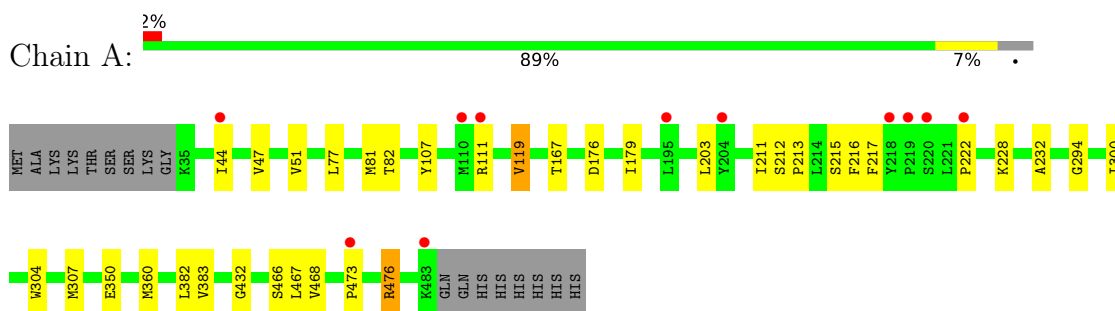
Chain A:

- Molecule 1: Protein CYP51

Chain B:

- Molecule 1: Protein CYP51

Chain C:

- Molecule 1: Protein CYP51

Chain D:
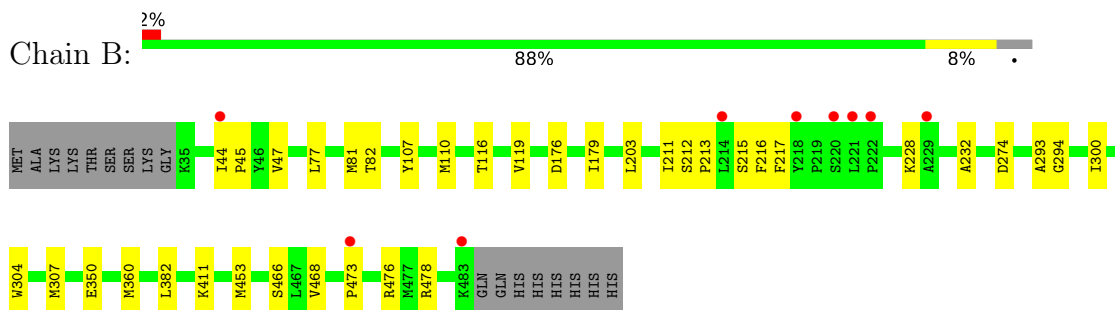
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.06Å 75.22Å 105.95Å 89.49° 74.63° 63.98°	Depositor
Resolution (Å)	64.63 – 2.11 64.54 – 2.11	Depositor EDS
% Data completeness (in resolution range)	96.8 (64.63-2.11) 96.8 (64.54-2.11)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.237 0.218 , 0.231	Depositor DCC
R_{free} test set	5529 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15917	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 15.14% 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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 7PW

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	0.67	0/3695	0.77	0/4981
1	B	0.68	0/3695	0.77	0/4981
1	C	0.69	0/3695	0.76	0/4981
1	D	0.68	0/3695	0.77	0/4981
All	All	0.68	0/14780	0.77	0/19924

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	3617	0	3680	35	0
1	B	3617	0	3680	39	0
1	C	3617	0	3680	36	0
1	D	3617	0	3680	37	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
3	A	84	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	84	0	0	17	0
3	C	84	0	0	17	0
3	D	84	0	0	14	0
4	A	214	0	0	2	0
4	B	249	0	0	5	0
4	C	245	0	0	4	0
4	D	233	0	0	3	0
All	All	15917	0	14840	147	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 5.

All (147) 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:D:107:TYR:CE1	3:D:502[A]:7PW:N22	2.40	0.90
1:C:213:PRO:O	3:C:502[A]:7PW:C1	2.19	0.89
1:B:217:PHE:CE1	3:B:502[A]:7PW:C2	2.60	0.84
1:D:360:MET:SD	1:D:383:VAL:HG11	2.19	0.82
1:B:217:PHE:HE1	3:B:502[A]:7PW:C2	1.93	0.81
1:C:111:ARG:NH1	3:C:502[B]:7PW:C1	2.45	0.79
1:D:294:GLY:HA2	2:D:501:HEM:HMC2	1.66	0.77
1:D:213:PRO:O	3:D:502[A]:7PW:C28	2.33	0.77
1:A:217:PHE:CE1	3:A:502[A]:7PW:C2	2.70	0.75
1:A:213:PRO:O	3:A:502[A]:7PW:C28	2.35	0.74
1:B:294:GLY:HA2	2:B:501:HEM:HMC2	1.69	0.74
1:D:107:TYR:HE1	3:D:502[A]:7PW:N22	1.85	0.74
1:B:360:MET:CE	3:B:502[A]:7PW:C28	2.66	0.73
1:B:213:PRO:O	3:B:502[A]:7PW:C28	2.37	0.73
1:A:467:LEU:HD11	3:A:502[A]:7PW:C18	2.20	0.72
1:C:360:MET:HE3	3:C:502[A]:7PW:C28	2.20	0.71
1:B:360:MET:HE3	3:B:502[A]:7PW:C28	2.20	0.71
1:B:360:MET:HE1	3:B:502[A]:7PW:C1	2.20	0.71
1:B:107:TYR:HE1	3:B:502[A]:7PW:N22	1.89	0.70
1:A:51:VAL:HG22	4:A:634:HOH:O	1.92	0.69
1:D:217:PHE:CE1	3:D:502[A]:7PW:C2	2.76	0.69
1:C:360:MET:CE	3:C:502[A]:7PW:C28	2.71	0.68
1:B:213:PRO:O	3:B:502[A]:7PW:C1	2.42	0.68
1:C:213:PRO:O	3:C:502[A]:7PW:C28	2.43	0.66
1:C:467:LEU:HD11	3:C:502[A]:7PW:C24	2.28	0.64
1:A:360:MET:HE1	3:A:502[A]:7PW:C1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:SER:OG	3:D:502[B]:7PW:C2	2.47	0.63
1:D:217:PHE:HE1	3:D:502[A]:7PW:C1	2.12	0.62
1:B:360:MET:HE1	3:B:502[A]:7PW:C28	2.30	0.61
1:A:217:PHE:HE1	3:A:502[A]:7PW:C2	2.13	0.61
1:A:217:PHE:HE1	3:A:502[A]:7PW:C1	2.13	0.60
1:C:213:PRO:HB2	3:C:502[A]:7PW:C28	2.32	0.60
1:A:467:LEU:HD11	3:A:502[A]:7PW:C24	2.32	0.60
1:A:294:GLY:HA2	2:A:501:HEM:HMC2	1.84	0.60
1:C:213:PRO:O	3:C:502[A]:7PW:C2	2.50	0.60
1:A:360:MET:CE	3:A:502[A]:7PW:C1	2.80	0.59
1:A:304:TRP:HA	1:A:307:MET:HE3	1.85	0.59
1:A:213:PRO:O	3:A:502[A]:7PW:C1	2.51	0.59
1:A:213:PRO:HD3	1:A:466:SER:O	2.03	0.59
1:B:81:MET:HE1	1:B:216:PHE:HE2	1.68	0.58
1:B:213:PRO:HD3	1:B:466:SER:O	2.03	0.58
1:C:111:ARG:HE	1:C:111:ARG:H	1.52	0.58
1:C:217:PHE:CE1	3:C:502[A]:7PW:C2	2.86	0.58
1:D:81:MET:HE1	1:D:216:PHE:HE2	1.69	0.57
1:D:213:PRO:HD3	1:D:466:SER:O	2.03	0.57
1:B:107:TYR:CE1	3:B:502[A]:7PW:N22	2.70	0.57
1:B:213:PRO:HB2	3:B:502[A]:7PW:C28	2.35	0.57
1:C:213:PRO:HD3	1:C:466:SER:O	2.04	0.57
1:B:304:TRP:HA	1:B:307:MET:HE3	1.87	0.57
1:A:44:ILE:HG22	1:A:47:VAL:HG22	1.87	0.56
1:C:44:ILE:HG22	1:C:47:VAL:HG22	1.88	0.56
1:C:304:TRP:HA	1:C:307:MET:HE3	1.87	0.56
1:D:44:ILE:HG22	1:D:47:VAL:HG22	1.88	0.55
1:D:216:PHE:CD2	3:D:502[A]:7PW:C27	2.90	0.55
1:D:304:TRP:HA	1:D:307:MET:HE3	1.88	0.54
1:C:230:ARG:HG2	4:C:768:HOH:O	2.07	0.54
1:D:360:MET:SD	1:D:383:VAL:CG1	2.94	0.54
1:A:222:PRO:HA	4:A:700:HOH:O	2.07	0.53
1:C:47:VAL:HA	1:C:77:LEU:HD23	1.90	0.53
1:D:47:VAL:HA	1:D:77:LEU:HD23	1.90	0.53
1:B:47:VAL:HA	1:B:77:LEU:HD23	1.89	0.53
1:B:411:LYS:NZ	4:B:605:HOH:O	2.29	0.53
1:B:293:ALA:HA	4:B:603:HOH:O	2.09	0.53
1:D:106:VAL:HG12	1:D:107:TYR:CE1	2.44	0.53
1:A:47:VAL:HA	1:A:77:LEU:HD23	1.90	0.52
1:C:360:MET:HE1	3:C:502[A]:7PW:C28	2.38	0.52
1:B:215:SER:OG	3:B:502[B]:7PW:C2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:PHE:CB	3:C:502[A]:7PW:C27	2.87	0.51
1:B:110:MET:HB2	4:B:817:HOH:O	2.09	0.51
1:A:81:MET:HE1	1:A:216:PHE:HE2	1.74	0.51
1:C:432:GLY:HA3	2:C:501:HEM:C3C	2.44	0.51
1:D:107:TYR:CZ	3:D:502[A]:7PW:N22	2.78	0.51
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.93	0.51
1:D:119:VAL:HG22	3:D:502[B]:7PW:C38	2.41	0.51
1:D:360:MET:CE	3:D:502[A]:7PW:C1	2.89	0.51
1:C:116:THR:HG21	4:C:830:HOH:O	2.11	0.51
1:C:110:MET:SD	3:C:502[B]:7PW:O35	2.69	0.50
1:D:217:PHE:CE1	3:D:502[A]:7PW:C1	2.94	0.50
1:B:116:THR:HG23	4:B:772:HOH:O	2.12	0.49
1:A:215:SER:OG	3:A:502[B]:7PW:C2	2.61	0.49
1:A:360:MET:SD	1:A:383:VAL:HG11	2.52	0.49
1:B:211:ILE:HD12	3:B:502[B]:7PW:C29	2.43	0.49
1:D:106:VAL:HG12	1:D:107:TYR:CD1	2.48	0.49
1:A:107:TYR:HE1	3:A:502[A]:7PW:N22	2.11	0.48
1:B:360:MET:CE	3:B:502[A]:7PW:C1	2.91	0.48
1:A:211:ILE:HD12	3:A:502[B]:7PW:C29	2.43	0.48
1:D:106:VAL:HG11	1:D:362:MET:HE3	1.94	0.48
1:C:116:THR:CG2	4:C:830:HOH:O	2.60	0.48
1:B:217:PHE:HE1	3:B:502[A]:7PW:C1	2.25	0.47
1:B:44:ILE:HB	1:B:47:VAL:HG22	1.96	0.47
1:C:111:ARG:H	1:C:111:ARG:NE	2.12	0.47
1:B:81:MET:CE	1:B:216:PHE:HE2	2.27	0.47
1:C:116:THR:HG22	4:C:766:HOH:O	2.13	0.47
1:D:119:VAL:HG13	3:D:502[B]:7PW:C39	2.45	0.47
1:C:467:LEU:HD21	3:C:502[B]:7PW:C17	2.45	0.47
1:C:107:TYR:HE1	3:C:502[A]:7PW:N22	2.12	0.47
1:C:213:PRO:CB	3:C:502[A]:7PW:C28	2.93	0.47
1:A:44:ILE:CG2	1:A:47:VAL:HG22	2.45	0.47
1:C:350:GLU:OE1	1:C:350:GLU:HA	2.16	0.46
1:C:44:ILE:CG2	1:C:47:VAL:HG22	2.45	0.46
1:A:350:GLU:HA	1:A:350:GLU:OE1	2.16	0.46
1:A:467:LEU:CD1	3:A:502[A]:7PW:C18	2.92	0.45
1:D:350:GLU:HA	1:D:350:GLU:OE1	2.17	0.45
1:B:300:ILE:HD12	1:B:468:VAL:HG12	1.98	0.45
1:D:44:ILE:CG2	1:D:47:VAL:HG22	2.46	0.45
1:A:432:GLY:HA3	2:A:501:HEM:C3C	2.52	0.45
1:B:350:GLU:HA	1:B:350:GLU:OE1	2.17	0.45
1:D:467:LEU:HD21	3:D:502[B]:7PW:C17	2.47	0.45

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:MET:CE	1:D:216:PHE:HE2	2.28	0.45
1:B:274:ASP:OD2	4:B:601:HOH:O	2.21	0.44
1:A:300:ILE:HD12	1:A:468:VAL:HG12	2.00	0.44
1:D:217:PHE:CZ	3:D:502[A]:7PW:C2	3.01	0.44
1:B:44:ILE:HD11	1:C:44:ILE:HG12	2.00	0.43
1:D:334:ASP:OD2	4:D:601:HOH:O	2.21	0.43
1:B:44:ILE:HB	1:B:47:VAL:CG2	2.47	0.43
1:A:82:THR:O	1:A:382:LEU:HA	2.19	0.43
1:A:360:MET:HE2	3:A:502[A]:7PW:C28	2.48	0.43
1:B:82:THR:O	1:B:382:LEU:HA	2.18	0.43
1:D:106:VAL:CG1	1:D:362:MET:HE3	2.49	0.43
1:D:421:VAL:N	1:D:422:PRO:CD	2.82	0.43
1:C:421:VAL:N	1:C:422:PRO:CD	2.82	0.43
1:D:82:THR:O	1:D:382:LEU:HA	2.19	0.43
1:C:203:LEU:HD22	1:C:232:ALA:CB	2.49	0.43
1:D:300:ILE:HD12	1:D:468:VAL:HG12	2.00	0.43
1:B:203:LEU:HD22	1:B:232:ALA:CB	2.49	0.43
1:C:294:GLY:HA2	2:C:501:HEM:HMC2	2.01	0.43
1:A:107:TYR:CE1	3:A:502[A]:7PW:N22	2.87	0.42
1:C:300:ILE:HD12	1:C:468:VAL:HG12	2.00	0.42
1:D:203:LEU:HD22	1:D:232:ALA:CB	2.49	0.42
1:B:44:ILE:HG23	1:B:45:PRO:HD2	2.01	0.42
1:C:82:THR:O	1:C:382:LEU:HA	2.19	0.42
1:B:213:PRO:CB	3:B:502[A]:7PW:C28	2.98	0.42
1:B:211:ILE:CD1	3:B:502[B]:7PW:C28	2.97	0.42
1:C:111:ARG:NH1	3:C:502[B]:7PW:C2	2.82	0.42
1:C:215:SER:OG	3:C:502[B]:7PW:C2	2.68	0.42
1:A:203:LEU:HD22	1:A:232:ALA:CB	2.49	0.42
1:B:453:MET:HA	1:B:478:ARG:O	2.21	0.41
1:D:410:ARG:O	4:D:602:HOH:O	2.21	0.41
1:A:119:VAL:HG22	3:A:502[A]:7PW:C38	2.51	0.41
1:A:119:VAL:HG13	3:A:502[A]:7PW:C39	2.51	0.41
1:A:167:THR:OG1	1:A:476:ARG:NH1	2.54	0.41
1:B:107:TYR:O	1:B:110:MET:HB3	2.21	0.41
1:A:176:ASP:O	1:A:179:ILE:HG22	2.22	0.40
1:B:176:ASP:O	1:B:179:ILE:HG22	2.21	0.40
1:D:410:ARG:HB3	4:D:602:HOH:O	2.21	0.40
1:D:176:ASP:O	1:D:179:ILE:HG22	2.21	0.40
1:A:216:PHE:CB	3:A:502[A]:7PW:C27	2.99	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	447/466 (96%)	435 (97%)	11 (2%)	1 (0%)	47	48
1	B	447/466 (96%)	434 (97%)	12 (3%)	1 (0%)	47	48
1	C	447/466 (96%)	436 (98%)	10 (2%)	1 (0%)	47	48
1	D	447/466 (96%)	435 (97%)	11 (2%)	1 (0%)	47	48
All	All	1788/1864 (96%)	1740 (97%)	44 (2%)	4 (0%)	47	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	VAL
1	B	119	VAL
1	C	119	VAL
1	D	119	VAL

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	403/418 (96%)	398 (99%)	5 (1%)	71	77
1	B	403/418 (96%)	399 (99%)	4 (1%)	76	81
1	C	403/418 (96%)	399 (99%)	4 (1%)	76	81
1	D	403/418 (96%)	400 (99%)	3 (1%)	84	88
All	All	1612/1672 (96%)	1596 (99%)	16 (1%)	76	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	212	SER
1	A	228	LYS
1	A	473	PRO
1	A	476	ARG
1	B	212	SER
1	B	228	LYS
1	B	473	PRO
1	B	476	ARG
1	C	111	ARG
1	C	212	SER
1	C	228	LYS
1	C	476	ARG
1	D	111	ARG
1	D	212	SER
1	D	228	LYS

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 ⓘ

12 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	$\#\|Z\| > 2$
3	7PW	D	502[A]	2	38,47,47	1.57	6 (15%)	57,66,66	1.99	15 (26%)
2	HEM	C	501	1,3	41,50,50	1.36	6 (14%)	45,82,82	1.73	12 (26%)
2	HEM	B	501	1,3	41,50,50	1.39	6 (14%)	45,82,82	1.77	11 (24%)
3	7PW	B	502[B]	2	38,47,47	1.35	6 (15%)	57,66,66	1.37	10 (17%)
3	7PW	C	502[A]	2	38,47,47	2.33	7 (18%)	57,66,66	1.89	15 (26%)
3	7PW	A	502[B]	2	38,47,47	1.53	5 (13%)	57,66,66	1.48	10 (17%)
2	HEM	D	501	1,3	41,50,50	1.40	6 (14%)	45,82,82	1.81	12 (26%)
2	HEM	A	501	1,3	41,50,50	1.41	6 (14%)	45,82,82	1.81	12 (26%)
3	7PW	D	502[B]	2	38,47,47	1.30	4 (10%)	57,66,66	1.52	12 (21%)
3	7PW	B	502[A]	2	38,47,47	1.53	5 (13%)	57,66,66	1.83	16 (28%)
3	7PW	A	502[A]	2	38,47,47	1.75	7 (18%)	57,66,66	1.95	20 (35%)
3	7PW	C	502[B]	2	38,47,47	2.05	5 (13%)	57,66,66	1.47	10 (17%)

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	7PW	D	502[A]	2	-	3/24/28/28	0/6/6/6
2	HEM	C	501	1,3	-	2/12/54/54	-
2	HEM	B	501	1,3	-	2/12/54/54	-
3	7PW	B	502[B]	2	-	2/24/28/28	0/6/6/6
3	7PW	C	502[A]	2	-	4/24/28/28	0/6/6/6
3	7PW	A	502[B]	2	-	4/24/28/28	0/6/6/6
2	HEM	D	501	1,3	-	0/12/54/54	-
2	HEM	A	501	1,3	-	0/12/54/54	-
3	7PW	D	502[B]	2	-	1/24/28/28	0/6/6/6
3	7PW	B	502[A]	2	-	3/24/28/28	0/6/6/6
3	7PW	A	502[A]	2	-	4/24/28/28	0/6/6/6
3	7PW	C	502[B]	2	-	3/24/28/28	0/6/6/6

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502[A]	7PW	F30-C14	-10.40	1.08	1.35
3	C	502[B]	7PW	F30-C14	-9.69	1.10	1.35
3	C	502[A]	7PW	C19-C3	-6.24	1.37	1.50
3	A	502[A]	7PW	C19-C3	-6.18	1.37	1.50
3	D	502[A]	7PW	C19-C3	-6.17	1.37	1.50
3	B	502[A]	7PW	C19-C3	-5.84	1.38	1.50
3	A	502[B]	7PW	F6-C5	-4.63	1.23	1.35
3	B	502[B]	7PW	C19-C3	-4.54	1.40	1.50
3	A	502[B]	7PW	C19-C3	-4.20	1.41	1.50
2	D	501	HEM	C1B-NB	-4.14	1.33	1.40
3	A	502[A]	7PW	F6-C5	-4.11	1.25	1.35
2	A	501	HEM	C1B-NB	-4.11	1.33	1.40
3	C	502[B]	7PW	C19-C3	-4.02	1.41	1.50
3	D	502[B]	7PW	C19-C3	-4.00	1.41	1.50
2	B	501	HEM	C1B-NB	-3.89	1.33	1.40
3	C	502[A]	7PW	C25-C40	-3.83	1.39	1.49
2	C	501	HEM	C1B-NB	-3.82	1.33	1.40
3	B	502[A]	7PW	C25-C40	-3.82	1.39	1.49
3	A	502[B]	7PW	C25-C40	-3.81	1.39	1.49
3	D	502[A]	7PW	C25-C40	-3.81	1.39	1.49
3	C	502[B]	7PW	C25-C40	-3.74	1.39	1.49
3	A	502[A]	7PW	C25-C40	-3.73	1.39	1.49
2	A	501	HEM	C4D-ND	-3.60	1.34	1.40
3	D	502[B]	7PW	C25-C40	-3.56	1.40	1.49
2	D	501	HEM	C4D-ND	-3.50	1.34	1.40
2	C	501	HEM	C4D-ND	-3.45	1.34	1.40
3	B	502[B]	7PW	C25-C40	-3.44	1.40	1.49
3	A	502[A]	7PW	F37-C36	3.37	1.44	1.36
2	B	501	HEM	C4D-ND	-3.24	1.34	1.40
3	C	502[A]	7PW	N12-N22	-3.16	1.31	1.37
3	D	502[B]	7PW	F30-C14	-3.04	1.27	1.35
3	B	502[A]	7PW	N12-N22	-3.02	1.31	1.37
2	C	501	HEM	FE-NB	3.02	2.11	1.96
3	C	502[A]	7PW	C32-N33	-3.00	1.45	1.48
2	B	501	HEM	FE-NB	2.98	2.11	1.96
3	B	502[A]	7PW	C32-N33	-2.95	1.45	1.48
2	D	501	HEM	FE-NB	2.94	2.11	1.96
3	A	502[A]	7PW	N12-N22	-2.93	1.31	1.37
2	A	501	HEM	FE-NB	2.93	2.11	1.96
3	C	502[B]	7PW	C9-N33	-2.85	1.32	1.37
3	C	502[A]	7PW	C9-N33	-2.80	1.32	1.37
3	D	502[A]	7PW	N12-N22	-2.80	1.32	1.37
3	D	502[A]	7PW	C32-N33	-2.66	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502[B]	7PW	C20-C5	2.66	1.41	1.38
3	A	502[A]	7PW	C9-N33	-2.65	1.32	1.37
3	A	502[A]	7PW	C32-N33	-2.61	1.45	1.48
3	D	502[A]	7PW	F30-C14	-2.58	1.29	1.35
3	D	502[A]	7PW	C9-N33	-2.57	1.32	1.37
3	A	502[B]	7PW	C9-N33	-2.53	1.33	1.37
3	B	502[A]	7PW	C9-N33	-2.52	1.33	1.37
2	A	501	HEM	C4B-NB	-2.43	1.33	1.38
3	A	502[B]	7PW	F37-C36	2.41	1.42	1.36
3	B	502[B]	7PW	C31-N34	2.35	1.49	1.46
2	B	501	HEM	C4B-NB	-2.34	1.34	1.38
3	C	502[A]	7PW	C20-C5	2.32	1.41	1.38
2	D	501	HEM	C4B-NB	-2.31	1.34	1.38
3	B	502[B]	7PW	C20-C5	2.31	1.41	1.38
3	D	502[B]	7PW	C9-N33	-2.28	1.33	1.37
3	B	502[B]	7PW	C9-N33	-2.26	1.33	1.37
2	D	501	HEM	C1D-ND	-2.21	1.34	1.38
3	B	502[B]	7PW	N12-N22	-2.18	1.33	1.37
2	B	501	HEM	C1D-ND	-2.17	1.34	1.38
2	A	501	HEM	CHB-C1B	2.14	1.40	1.35
2	A	501	HEM	C1D-ND	-2.12	1.34	1.38
2	B	501	HEM	CHB-C1B	2.10	1.40	1.35
2	C	501	HEM	C4B-NB	-2.07	1.34	1.38
2	C	501	HEM	CHB-C1B	2.07	1.40	1.35
2	D	501	HEM	CHB-C1B	2.02	1.40	1.35
2	C	501	HEM	C1D-ND	-2.00	1.34	1.38

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502[A]	7PW	C32-C31-N34	-5.82	100.29	110.45
3	C	502[A]	7PW	C32-C31-N34	-5.53	100.80	110.45
3	A	502[A]	7PW	C32-C31-N34	-5.53	100.81	110.45
3	D	502[A]	7PW	C5-C20-C14	5.31	119.26	114.16
3	B	502[A]	7PW	C32-C31-N34	-5.02	101.68	110.45
2	D	501	HEM	CHC-C4B-NB	4.87	129.73	124.43
2	C	501	HEM	CHC-C4B-NB	4.85	129.70	124.43
3	A	502[A]	7PW	C31-N34-C3	-4.77	116.19	122.34
3	C	502[A]	7PW	C31-N34-C3	-4.74	116.23	122.34
2	A	501	HEM	CHC-C4B-NB	4.69	129.53	124.43
3	B	502[A]	7PW	C5-C20-C14	4.69	118.67	114.16
2	B	501	HEM	CHC-C4B-NB	4.57	129.40	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502[A]	7PW	C5-C20-C14	4.46	118.45	114.16
3	D	502[B]	7PW	C5-C20-C14	4.03	118.03	114.16
2	D	501	HEM	CHD-C1D-ND	3.93	128.71	124.43
3	C	502[A]	7PW	F6-C5-C20	3.91	121.96	118.13
3	A	502[A]	7PW	C5-C20-C14	3.88	117.89	114.16
3	C	502[B]	7PW	C5-C20-C14	3.82	117.84	114.16
2	B	501	HEM	CHD-C1D-ND	3.76	128.52	124.43
2	C	501	HEM	CHD-C1D-ND	3.73	128.49	124.43
3	A	502[B]	7PW	C31-N34-C3	-3.73	117.53	122.34
3	C	502[B]	7PW	F6-C5-C20	3.70	121.75	118.13
3	D	502[A]	7PW	C31-N34-C3	-3.64	117.65	122.34
2	A	501	HEM	C1B-NB-C4B	3.63	108.82	105.07
3	C	502[A]	7PW	C4-C5-C20	-3.58	120.13	124.63
2	D	501	HEM	C1B-NB-C4B	3.56	108.75	105.07
3	B	502[A]	7PW	C26-C14-C20	-3.56	120.15	124.63
3	D	502[B]	7PW	C31-N34-C3	-3.52	117.80	122.34
3	B	502[A]	7PW	C31-N34-C3	-3.50	117.83	122.34
2	A	501	HEM	CHD-C1D-ND	3.48	128.21	124.43
3	A	502[A]	7PW	C16-C15-C19	-3.41	116.81	120.78
3	D	502[A]	7PW	C16-C24-C18	3.36	124.29	117.59
3	A	502[A]	7PW	C15-C19-C17	3.34	123.35	118.59
3	B	502[B]	7PW	C5-C20-C14	3.34	117.37	114.16
2	C	501	HEM	C1B-NB-C4B	3.33	108.52	105.07
2	B	501	HEM	C1B-NB-C4B	3.33	108.51	105.07
3	A	502[B]	7PW	C5-C20-C14	3.32	117.35	114.16
2	A	501	HEM	CMC-C2C-C3C	3.32	130.88	124.68
3	D	502[A]	7PW	O13-C3-C19	-3.31	115.03	120.94
3	C	502[B]	7PW	C31-C32-N33	-3.29	107.99	112.25
3	B	502[B]	7PW	C31-N34-C3	-3.26	118.14	122.34
3	D	502[A]	7PW	C4-C5-C20	-3.24	120.55	124.63
3	D	502[A]	7PW	C16-C15-C19	-3.24	117.01	120.78
3	B	502[B]	7PW	C26-C14-C20	-3.24	120.56	124.63
3	C	502[A]	7PW	C15-C19-C17	3.23	123.19	118.59
3	A	502[A]	7PW	C16-C24-C18	3.18	123.93	117.59
3	C	502[B]	7PW	C4-C5-C20	-3.16	120.65	124.63
3	D	502[A]	7PW	C17-C18-C24	-3.16	116.59	121.13
2	D	501	HEM	CMC-C2C-C3C	3.14	130.55	124.68
3	C	502[B]	7PW	C26-C14-C20	-3.13	120.69	124.63
3	A	502[A]	7PW	C17-C18-C24	-3.13	116.63	121.13
3	D	502[A]	7PW	C15-C19-C17	3.12	123.03	118.59
3	B	502[A]	7PW	C4-C5-C20	-3.12	120.71	124.63
3	D	502[A]	7PW	C26-C14-C20	-3.11	120.72	124.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502[B]	7PW	C31-N34-C3	-3.11	118.34	122.34
2	B	501	HEM	CHA-C4D-ND	3.10	128.21	124.38
3	B	502[A]	7PW	F6-C5-C20	3.09	121.15	118.13
2	B	501	HEM	C4B-C3B-C2B	-3.06	104.69	107.11
3	C	502[B]	7PW	F30-C14-C20	3.05	121.11	118.13
3	A	502[A]	7PW	C4-C25-C40	3.03	125.87	120.86
2	C	501	HEM	C4B-C3B-C2B	-3.02	104.72	107.11
2	C	501	HEM	CHA-C4D-ND	3.01	128.09	124.38
2	D	501	HEM	C4B-C3B-C2B	-2.99	104.74	107.11
3	A	502[B]	7PW	C25-C4-C5	2.99	122.13	119.59
3	C	502[A]	7PW	C16-C15-C19	-2.99	117.31	120.78
3	A	502[A]	7PW	C4-C5-C20	-2.94	120.93	124.63
2	A	501	HEM	CHA-C4D-ND	2.94	128.01	124.38
3	A	502[B]	7PW	C19-C3-N34	2.93	122.69	117.06
2	A	501	HEM	C4B-C3B-C2B	-2.90	104.81	107.11
3	D	502[B]	7PW	C4-C5-C20	-2.88	121.01	124.63
3	D	502[A]	7PW	C28-C29-C7	-2.87	116.96	120.56
3	A	502[B]	7PW	C4-C5-C20	-2.84	121.06	124.63
3	B	502[A]	7PW	C16-C15-C19	-2.84	117.48	120.78
2	D	501	HEM	CHA-C4D-ND	2.81	127.86	124.38
3	B	502[B]	7PW	F6-C5-C20	2.79	120.86	118.13
3	D	502[B]	7PW	C32-C31-N34	-2.77	105.62	110.45
3	C	502[A]	7PW	C16-C24-C18	2.77	123.11	117.59
2	B	501	HEM	CHA-C4D-C3D	-2.76	120.15	125.33
3	A	502[A]	7PW	C26-C14-C20	-2.75	121.17	124.63
3	C	502[B]	7PW	C25-C4-C5	2.74	121.92	119.59
2	D	501	HEM	CHD-C1D-C2D	-2.74	120.70	124.98
3	A	502[B]	7PW	C26-C14-C20	-2.73	121.20	124.63
2	A	501	HEM	CHA-C4D-C3D	-2.73	120.21	125.33
3	A	502[B]	7PW	C25-C26-C14	2.71	121.90	119.59
3	B	502[B]	7PW	C25-C26-C14	2.69	121.88	119.59
3	B	502[A]	7PW	C16-C24-C18	2.68	122.93	117.59
3	B	502[A]	7PW	F30-C14-C20	2.67	120.75	118.13
3	D	502[B]	7PW	C42-C36-C38	-2.65	119.30	122.83
3	A	502[B]	7PW	C4-C25-C40	2.65	125.25	120.86
3	C	502[A]	7PW	C26-C14-C20	-2.64	121.30	124.63
3	D	502[B]	7PW	C26-C14-C20	-2.63	121.32	124.63
2	C	501	HEM	CHA-C4D-C3D	-2.63	120.39	125.33
3	D	502[A]	7PW	C17-C19-C3	-2.63	112.09	120.62
3	B	502[A]	7PW	C17-C19-C3	-2.63	112.10	120.62
3	B	502[B]	7PW	F30-C14-C20	2.61	120.68	118.13
3	B	502[A]	7PW	C15-C19-C17	2.58	122.26	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CHD-C1D-C2D	-2.54	121.02	124.98
3	A	502[A]	7PW	C27-C7-C8	-2.53	116.58	120.44
3	D	502[B]	7PW	O13-C3-N34	-2.52	117.82	122.45
2	A	501	HEM	CHD-C1D-C2D	-2.52	121.05	124.98
3	A	502[A]	7PW	C26-C25-C40	-2.52	116.70	120.86
2	D	501	HEM	CHA-C4D-C3D	-2.51	120.61	125.33
3	B	502[A]	7PW	C29-C7-C27	2.51	122.59	117.59
3	B	502[A]	7PW	C17-C18-C24	-2.51	117.53	121.13
3	B	502[B]	7PW	C19-C3-N34	2.50	121.86	117.06
3	D	502[A]	7PW	C29-C7-C27	2.50	122.56	117.59
3	C	502[A]	7PW	C17-C19-C3	-2.49	112.57	120.62
3	D	502[B]	7PW	C32-N33-C9	2.47	131.00	125.92
2	B	501	HEM	CHD-C1D-C2D	-2.45	121.15	124.98
3	D	502[B]	7PW	C25-C4-C5	2.41	121.64	119.59
3	A	502[A]	7PW	C42-C36-C38	-2.39	119.65	122.83
2	B	501	HEM	CHB-C1B-NB	2.38	127.32	124.38
3	B	502[A]	7PW	C28-C29-C7	-2.38	117.57	120.56
2	B	501	HEM	CMC-C2C-C3C	2.37	129.11	124.68
2	A	501	HEM	O2A-CGA-CBA	2.36	121.61	114.03
2	A	501	HEM	CHB-C1B-NB	2.35	127.29	124.38
3	B	502[B]	7PW	C4-C5-C20	-2.35	121.67	124.63
2	D	501	HEM	O2A-CGA-CBA	2.33	121.51	114.03
2	C	501	HEM	CMC-C2C-C3C	2.32	129.02	124.68
3	B	502[A]	7PW	C27-C7-C8	-2.28	116.96	120.44
3	D	502[B]	7PW	C4-C25-C40	2.27	124.62	120.86
3	C	502[A]	7PW	O13-C3-C19	-2.26	116.90	120.94
3	B	502[A]	7PW	O13-C3-C19	-2.26	116.91	120.94
2	D	501	HEM	CHB-C1B-NB	2.24	127.14	124.38
3	A	502[A]	7PW	C25-C26-C14	2.23	121.49	119.59
3	C	502[B]	7PW	C25-C26-C14	2.23	121.49	119.59
3	C	502[A]	7PW	C27-C7-C8	-2.22	117.06	120.44
3	C	502[A]	7PW	C17-C18-C24	-2.20	117.97	121.13
3	B	502[B]	7PW	O13-C3-N34	-2.19	118.41	122.45
2	C	501	HEM	CHC-C4B-C3B	-2.18	121.23	124.57
3	B	502[B]	7PW	C41-C42-C36	2.16	120.60	118.36
2	B	501	HEM	O2A-CGA-CBA	2.16	120.97	114.03
3	D	502[A]	7PW	C18-C24-C23	-2.16	117.14	120.44
2	B	501	HEM	C4A-C3A-C2A	2.16	108.50	107.00
2	D	501	HEM	CHC-C4B-C3B	-2.15	121.28	124.57
3	D	502[A]	7PW	C42-C36-C38	-2.15	119.97	122.83
3	A	502[A]	7PW	C17-C19-C3	-2.14	113.67	120.62
3	D	502[B]	7PW	C32-N33-C11	-2.12	121.58	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502[B]	7PW	C32-N33-C9	2.12	130.29	125.92
3	A	502[A]	7PW	C25-C4-C5	2.12	121.39	119.59
2	D	501	HEM	O2D-CGD-O1D	-2.12	118.03	123.30
3	C	502[A]	7PW	C18-C24-C23	-2.11	117.22	120.44
3	A	502[A]	7PW	C29-C7-C27	2.10	121.78	117.59
3	C	502[A]	7PW	C29-C7-C27	2.09	121.77	117.59
2	A	501	HEM	O2D-CGD-CBD	2.09	120.76	114.03
3	A	502[A]	7PW	C16-C24-C23	-2.09	117.26	120.44
2	A	501	HEM	C4A-C3A-C2A	2.07	108.44	107.00
2	C	501	HEM	O2D-CGD-O1D	-2.07	118.14	123.30
2	C	501	HEM	CHB-C1B-NB	2.05	126.92	124.38
3	A	502[A]	7PW	C39-C38-C36	2.03	120.47	118.36
2	C	501	HEM	O2A-CGA-CBA	2.03	120.55	114.03
3	A	502[B]	7PW	C32-N33-C9	2.03	130.09	125.92
3	D	502[B]	7PW	C19-C3-N34	2.02	120.94	117.06
3	A	502[B]	7PW	C18-C17-C19	2.02	123.13	120.78
3	A	502[A]	7PW	O13-C3-C19	-2.02	117.33	120.94

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502[A]	7PW	C20-C31-N34-C3
3	C	502[B]	7PW	C14-C20-C31-N34
3	C	502[B]	7PW	C5-C20-C31-N34
3	A	502[A]	7PW	C20-C31-N34-C3
3	C	502[A]	7PW	C20-C31-N34-C3
3	D	502[A]	7PW	C20-C31-N34-C3
3	A	502[B]	7PW	C14-C20-C31-N34
3	A	502[B]	7PW	C5-C20-C31-C32
3	A	502[B]	7PW	C5-C20-C31-N34
3	B	502[A]	7PW	C5-C20-C31-C32
3	B	502[B]	7PW	C5-C20-C31-C32
3	B	502[B]	7PW	C5-C20-C31-N34
3	C	502[A]	7PW	C5-C20-C31-N34
3	D	502[A]	7PW	C5-C20-C31-C32
3	D	502[B]	7PW	C5-C20-C31-C32
3	C	502[A]	7PW	C15-C19-C3-N34
3	D	502[A]	7PW	C15-C19-C3-N34
3	A	502[B]	7PW	C32-C31-N34-C3
3	A	502[A]	7PW	C15-C19-C3-N34
3	B	502[A]	7PW	C15-C19-C3-N34

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Mol	Chain	Res	Type	Atoms
3	A	502[A]	7PW	C17-C19-C3-N34
3	A	502[A]	7PW	C5-C20-C31-C32
3	C	502[A]	7PW	C5-C20-C31-C32
3	C	502[B]	7PW	C5-C20-C31-C32
2	B	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

12 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502[A]	7PW	10	0
2	C	501	HEM	2	0
2	B	501	HEM	1	0
3	B	502[B]	7PW	3	0
3	C	502[A]	7PW	12	0
3	A	502[B]	7PW	2	0
2	D	501	HEM	1	0
2	A	501	HEM	3	0
3	D	502[B]	7PW	4	0
3	B	502[A]	7PW	14	0
3	A	502[A]	7PW	16	0
3	C	502[B]	7PW	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 7PW D 502 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 7PW B 502 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 7PW C 502 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand 7PW A 502 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 7PW D 502 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 7PW B 502 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand 7PW A 502 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand 7PW C 502 (B)

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	449/466 (96%)	0.04	11 (2%)	59	64	12, 27, 56, 100	0
1	B	449/466 (96%)	-0.04	9 (2%)	65	69	11, 25, 52, 100	0
1	C	449/466 (96%)	0.07	13 (2%)	51	57	12, 27, 56, 99	0
1	D	449/466 (96%)	0.03	12 (2%)	54	60	12, 26, 56, 98	0
All	All	1796/1864 (96%)	0.02	45 (2%)	57	62	11, 26, 56, 100	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	220	SER	5.8
1	A	220	SER	5.6
1	D	222	PRO	5.2
1	A	222	PRO	5.1
1	B	220	SER	5.1
1	C	220	SER	4.5
1	C	222	PRO	4.4
1	A	111	ARG	4.2
1	C	210	GLY	4.2
1	C	44	ILE	4.1
1	A	218	TYR	4.1
1	D	219	PRO	3.8
1	C	218	TYR	3.7
1	B	483	LYS	3.7
1	C	213	PRO	3.6
1	A	44	ILE	3.5
1	A	483	LYS	3.5
1	C	111	ARG	3.4
1	A	473	PRO	3.4
1	A	219	PRO	3.4
1	B	222	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	44	ILE	3.0
1	D	473	PRO	2.9
1	C	219	PRO	2.9
1	D	213	PRO	2.8
1	C	221	LEU	2.6
1	A	204	TYR	2.6
1	B	221	LEU	2.6
1	C	214	LEU	2.6
1	C	483	LYS	2.5
1	C	473	PRO	2.4
1	D	111	ARG	2.4
1	D	204	TYR	2.4
1	B	214	LEU	2.3
1	D	472	SER	2.3
1	B	218	TYR	2.3
1	A	110	MET	2.3
1	B	229	ALA	2.2
1	D	483	LYS	2.1
1	A	195	LEU	2.1
1	D	221	LEU	2.1
1	C	236	ILE	2.0
1	D	68	TYR	2.0
1	B	473	PRO	2.0
1	D	43	LEU	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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	7PW	A	502[A]	42/42	0.90	0.18	17,22,45,46	42
3	7PW	A	502[B]	42/42	0.90	0.18	15,20,37,37	42
3	7PW	B	502[A]	42/42	0.91	0.17	15,19,43,47	42
3	7PW	B	502[B]	42/42	0.91	0.17	13,17,37,38	42
3	7PW	D	502[A]	42/42	0.91	0.19	17,24,54,56	42
3	7PW	D	502[B]	42/42	0.91	0.19	15,21,40,42	42
3	7PW	C	502[A]	42/42	0.93	0.17	16,22,44,47	42
3	7PW	C	502[B]	42/42	0.93	0.17	14,20,36,40	42
2	HEM	C	501	43/43	0.95	0.13	10,12,16,18	0
2	HEM	D	501	43/43	0.97	0.12	8,10,15,18	0
2	HEM	B	501	43/43	0.97	0.12	8,10,14,17	0
2	HEM	A	501	43/43	0.97	0.12	8,10,16,17	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 7PW A 502 (A):

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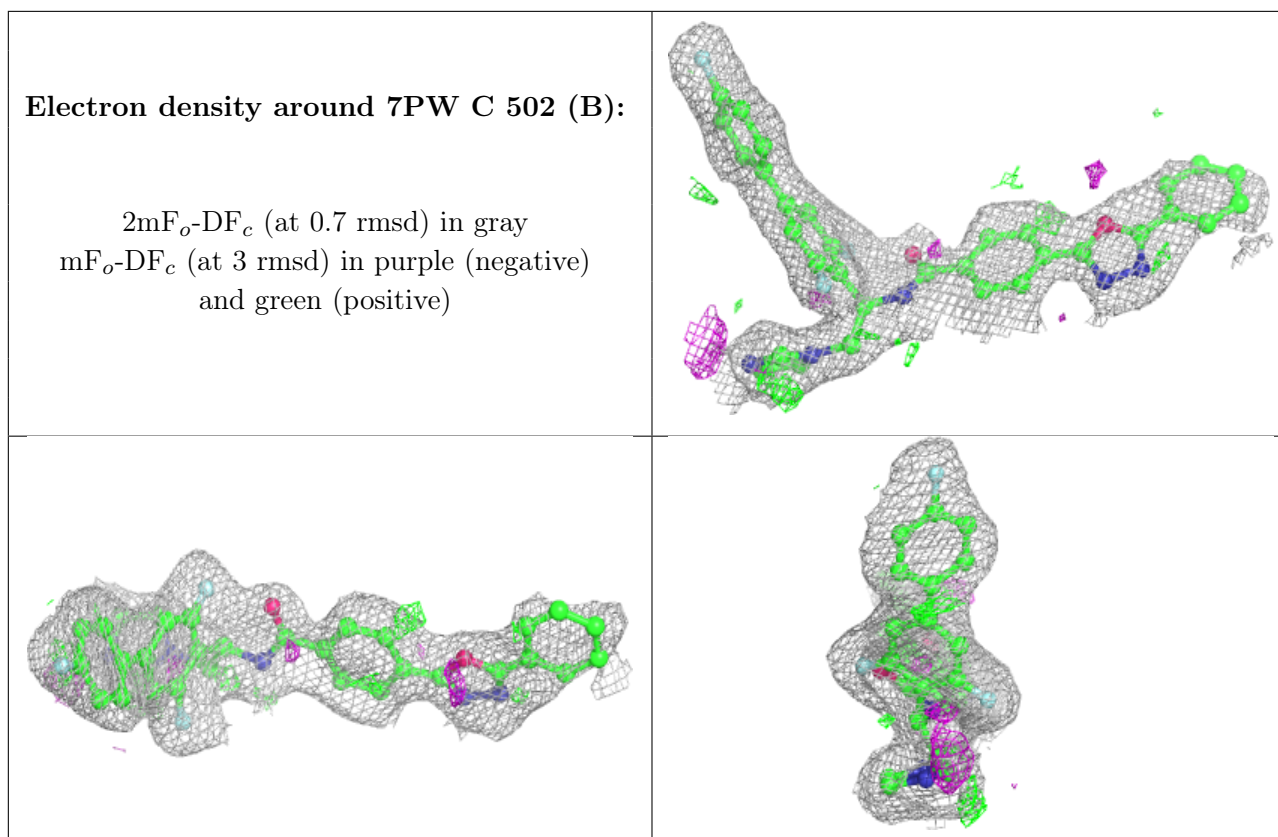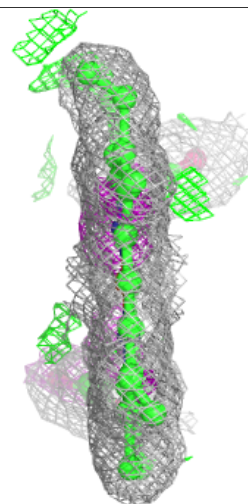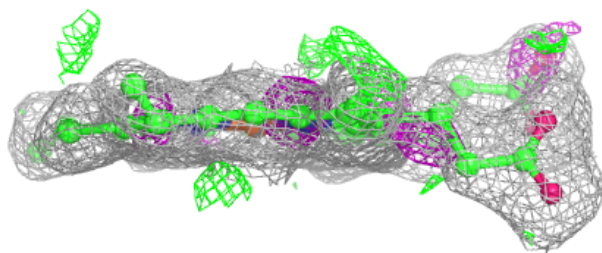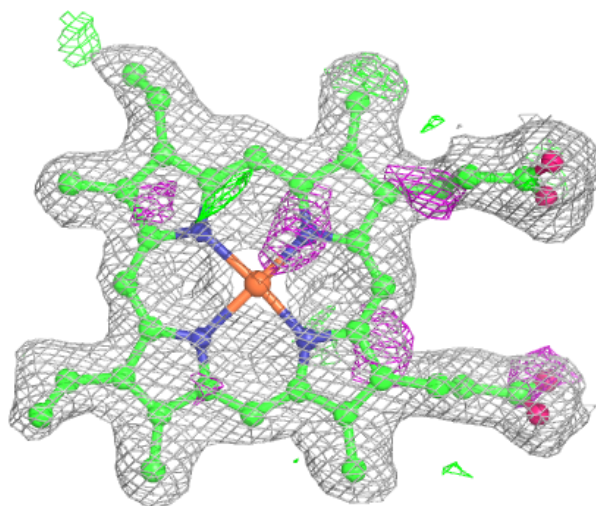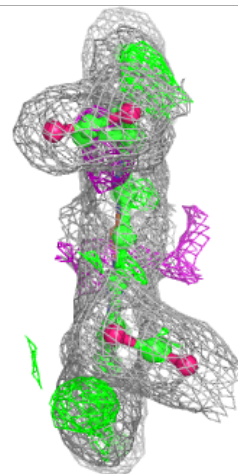mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

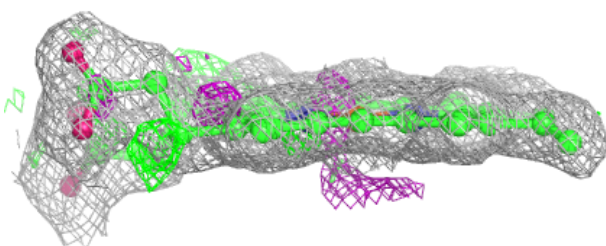**Electron density around 7PW A 502 (B):**

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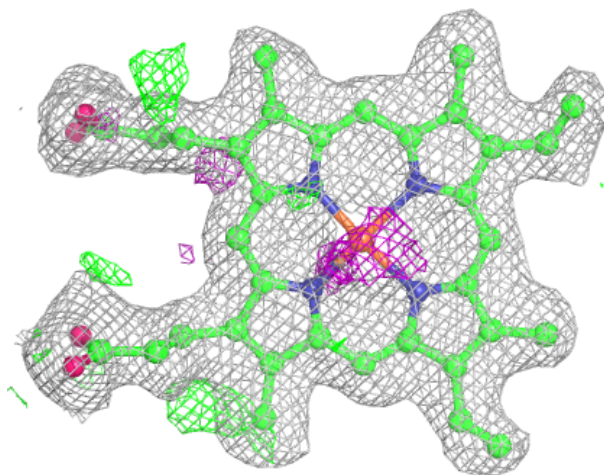and green (positive)

Electron density around 7PW B 502 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
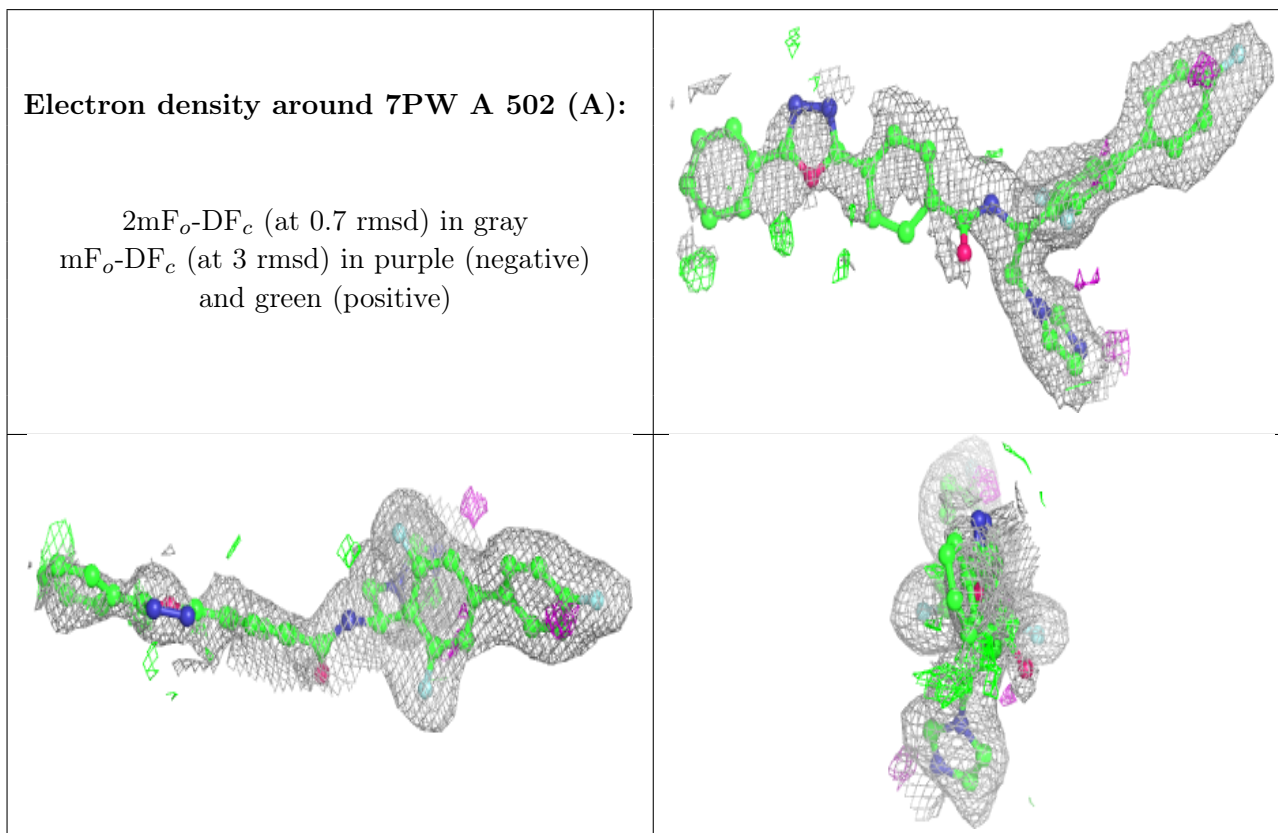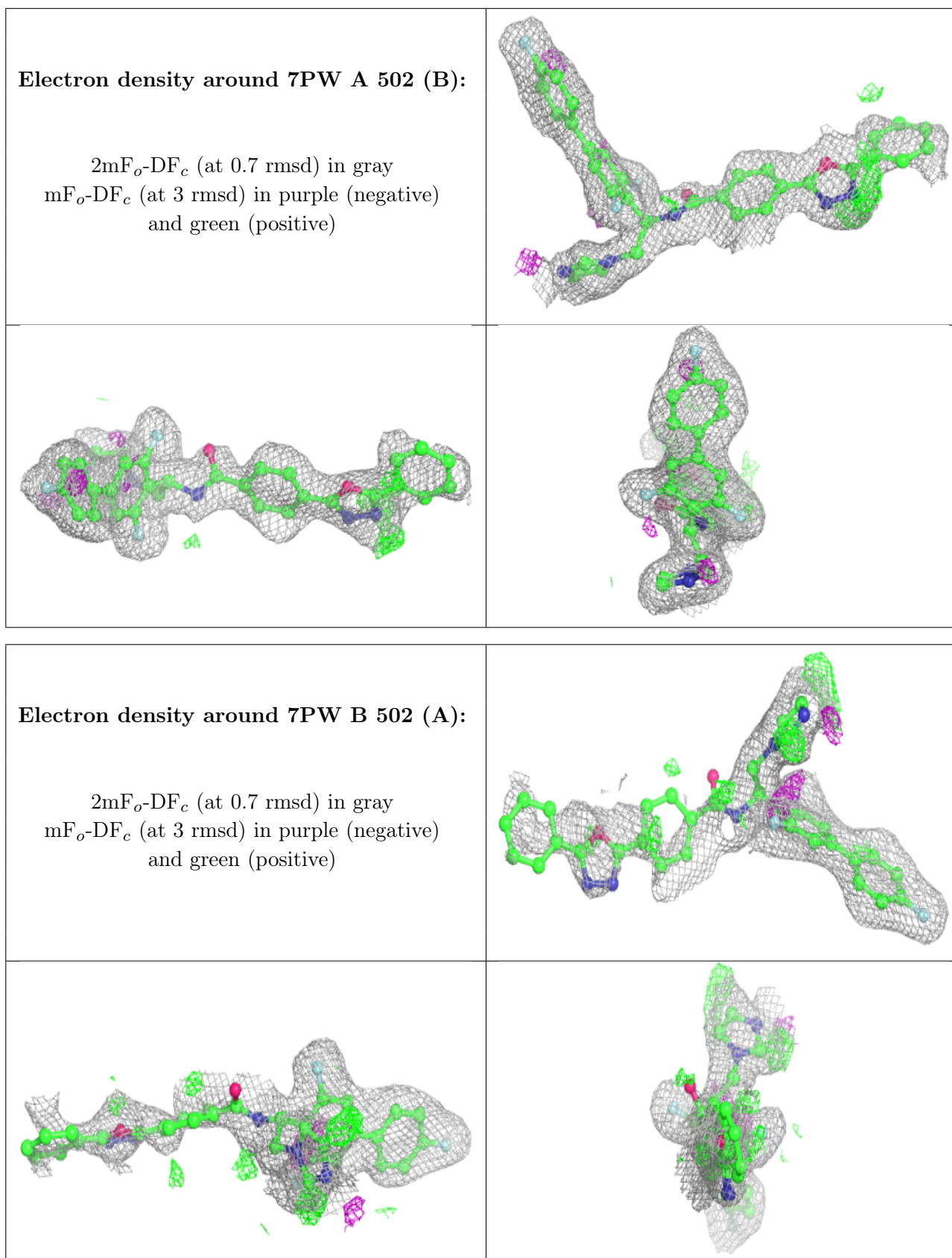
Electron density around 7PW B 502 (B):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
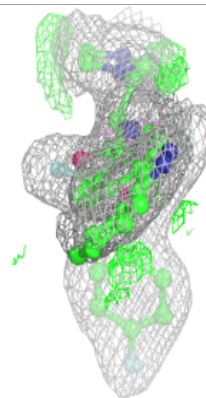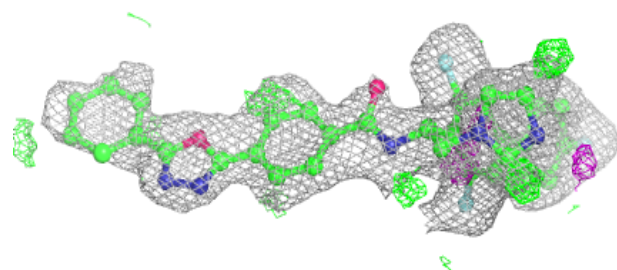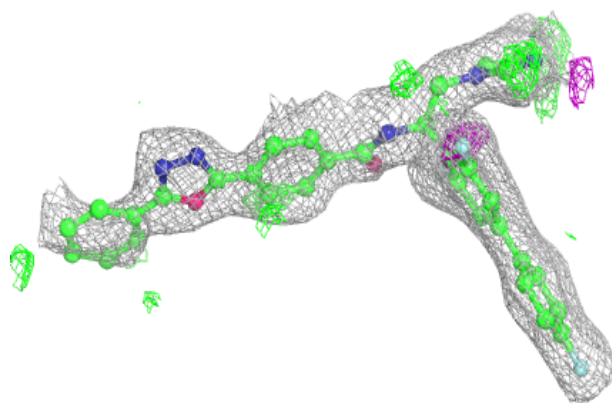
Electron density around 7PW D 502 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
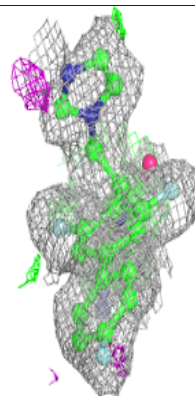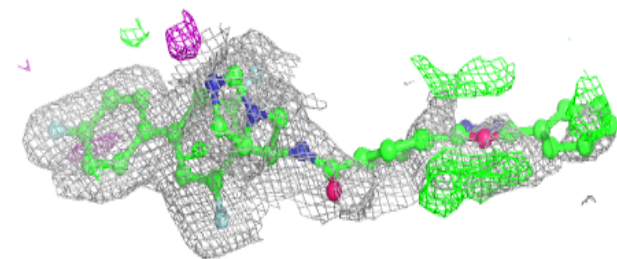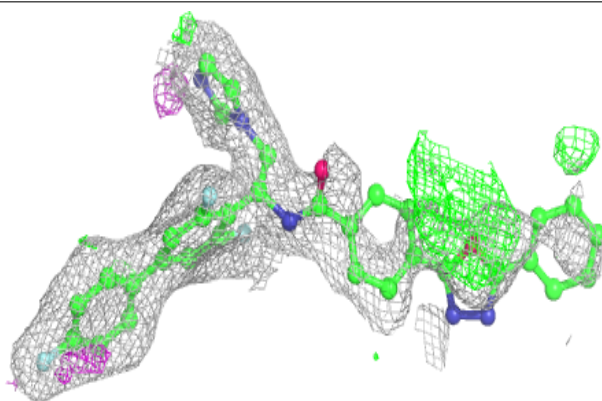
Electron density around 7PW D 502 (B):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
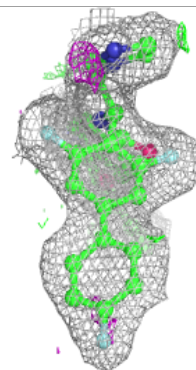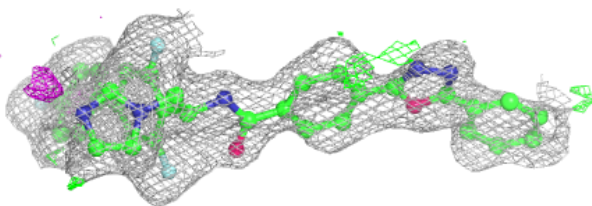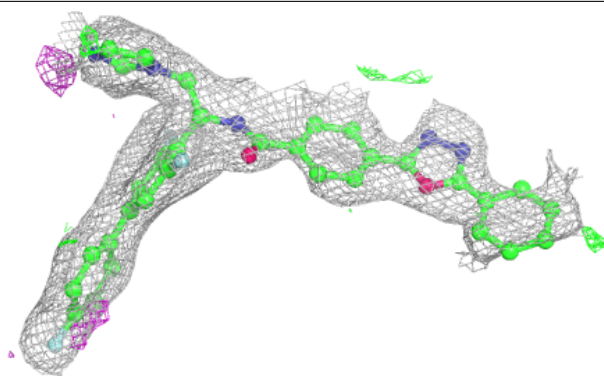
Electron density around 7PW C 502 (A):

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 7PW C 502 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
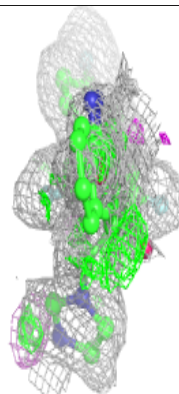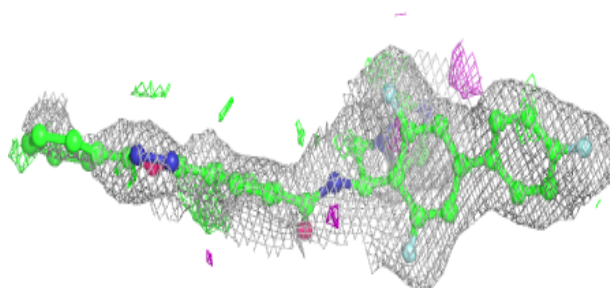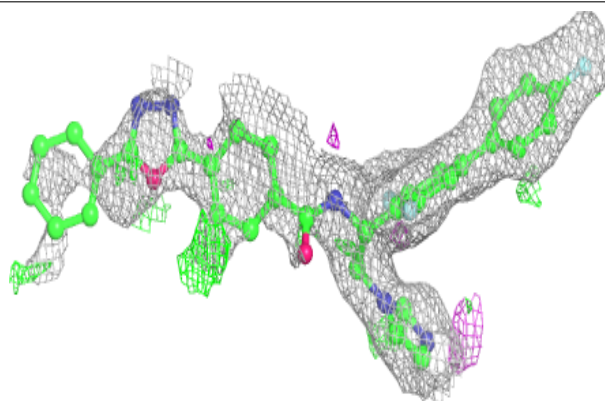
Electron density around HEM C 501:

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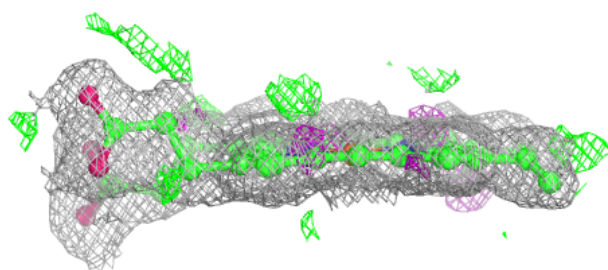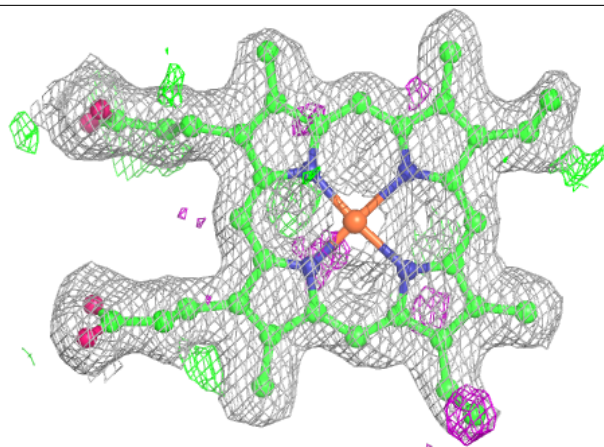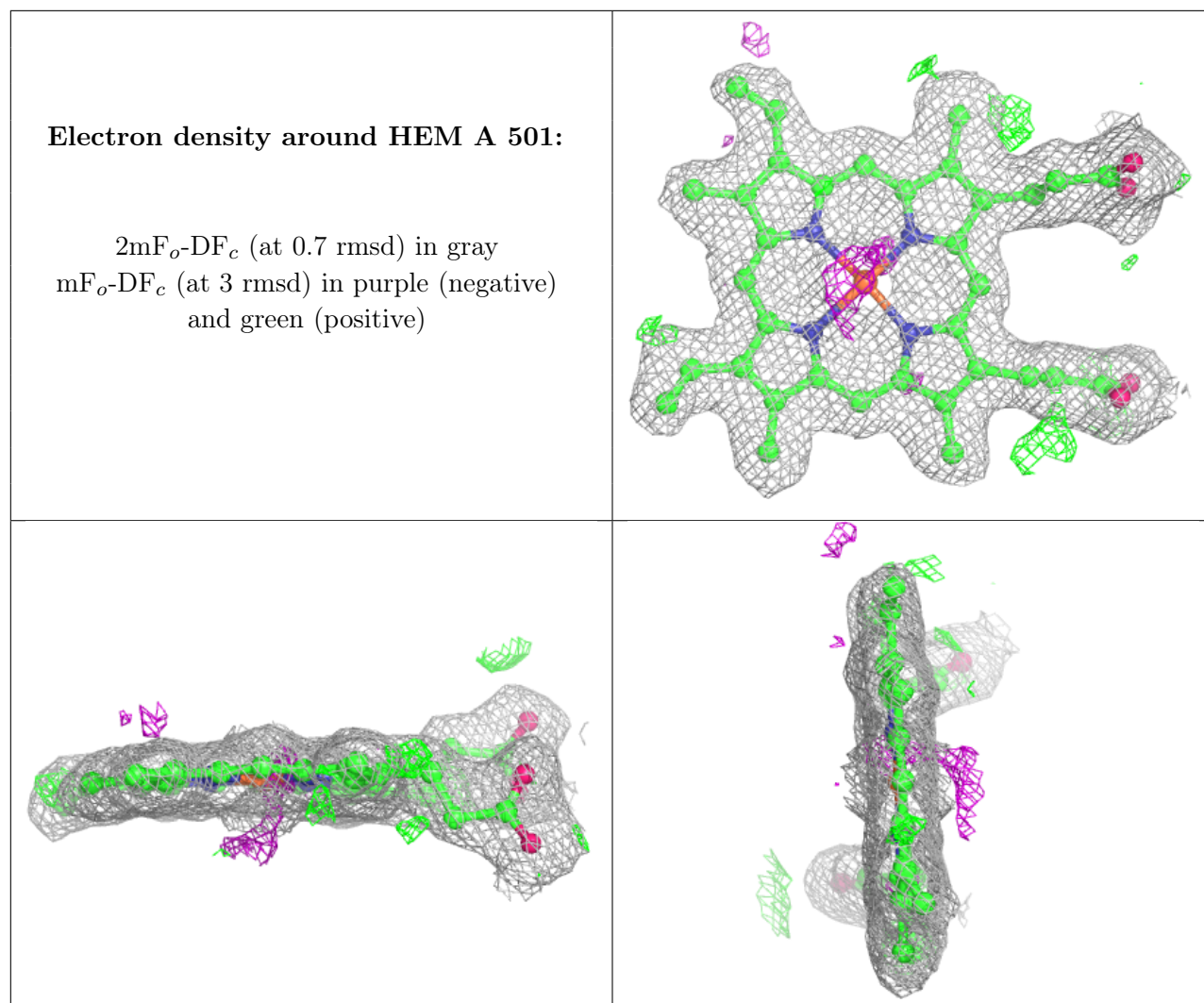and green (positive)

Electron density around HEM D 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 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)
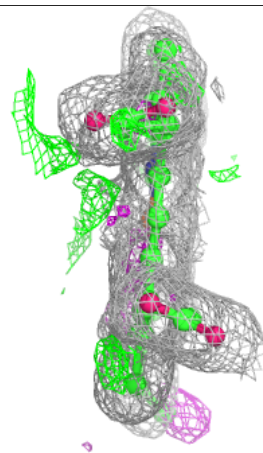
6.5 Other polymers (i)

There are no such residues in this entry.