Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 10:05 PM EDT

PDB ID	:	4K9U
Title	:	Complex of human CYP3A4 with a desoxyritonavir analog
Authors	:	Sevrioukova, I.F.; Poulos, T.L.
Deposited on	:	2013-04-21
Resolution	:	2.85 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	:	2.35.1
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 2.85 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		0.278
Clashscore		24
Ramachandran outliers		2.9%
Sidechain outliers		10.9%
RSRZ outliers		4.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
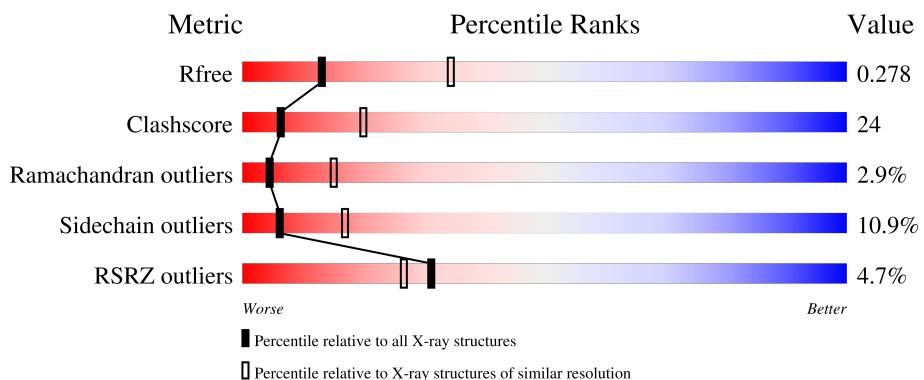
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	487	4% 53% 32% 6% · 8%
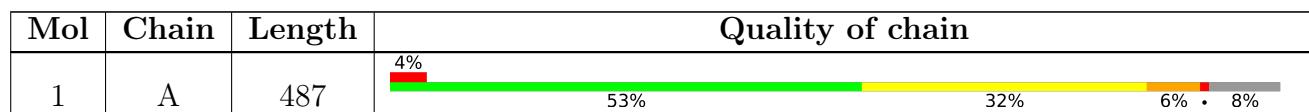
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	5AW	A	602	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	5AW	A	603	-	-	X	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3730 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 Cytochrome P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3613	2349	592	648	24	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P08684
A	?	-	ILE	deletion	UNP P08684
A	?	-	PRO	deletion	UNP P08684
A	?	-	ASP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	MET	deletion	UNP P08684
A	?	-	GLU	deletion	UNP P08684
A	?	-	THR	deletion	UNP P08684
A	?	-	TRP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	VAL	deletion	UNP P08684
A	?	-	SER	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	VAL	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	504	HIS	-	expression tag	UNP P08684
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684
A	507	HIS	-	expression tag	UNP P08684

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

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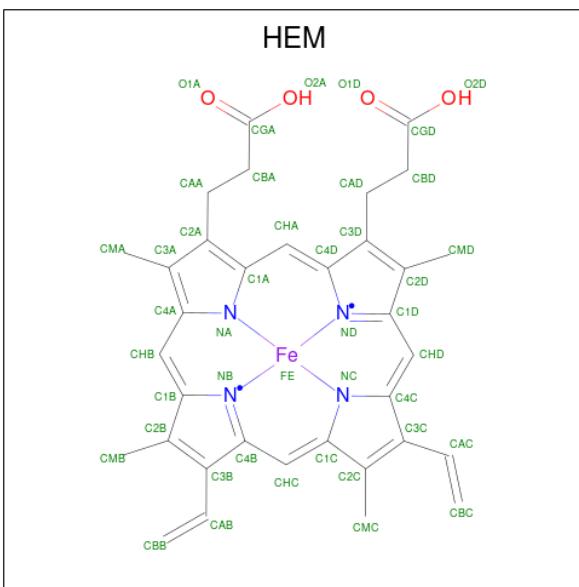
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is N 2 -(methyl{[2-(propan-2-yl)-1,3-thiazol-4-yl]methyl}carbamoyl)-N-[(2S,5S)-5-{[(1,3-thiazol-5-ylmethoxy)carbonyl]amino}hexan-2-yl]-D-valinamide (three-letter code: 5AW) (formula: $C_{25}H_{40}N_6O_4S_2$).
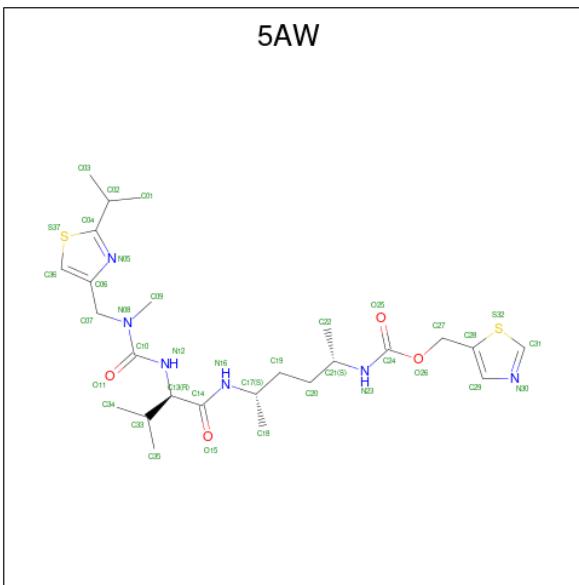
5AW

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			37	25	6	4	2		
3	A	1	Total	C	N	O	S	0	0
			37	25	6	4	2		

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: Cytochrome P450 3A4
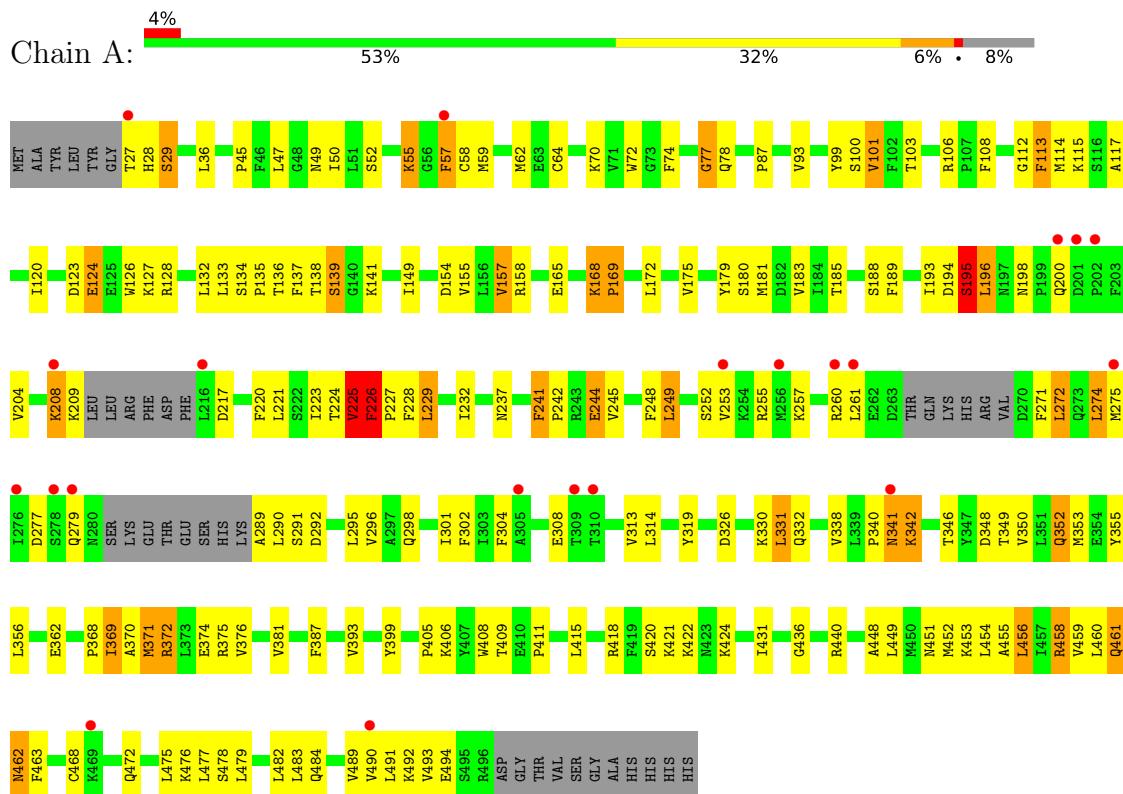
4　Data and refinement statistics　ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	77.53Å　　99.88Å　　130.16Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	32.25　–　2.85 32.25　–　2.85	Depositor EDS
% Data completeness (in resolution range)	97.8 (32.25-2.85) 97.9 (32.25-2.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.213　,　0.279 0.223　,　0.278	Depositor DCC
R_{free} test set	572 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	86.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 75.1	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3730	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: 5AW, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	0.53	0/3699	0.67	0/5003

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	3613	0	3691	169	0
2	A	43	0	30	5	0
3	A	74	0	80	33	0
All	All	3730	0	3801	182	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 24.

All (182) 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:58:CYS:SG	1:A:371:MET:CG	2.40	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:CYS:SG	1:A:371:MET:HG3	2.01	0.98
1:A:371:MET:SD	1:A:483:LEU:HD13	2.05	0.97
1:A:149:ILE:HG12	1:A:183:VAL:HG13	1.47	0.94
1:A:58:CYS:SG	1:A:371:MET:HG2	2.10	0.90
3:A:602:5AW:H32	3:A:602:5AW:H22	1.54	0.89
1:A:484:GLN:HE22	3:A:603:5AW:H22	1.38	0.87
1:A:340:PRO:O	1:A:341:ASN:HB2	1.76	0.86
1:A:369:ILE:CG2	1:A:482:LEU:HD22	2.05	0.85
1:A:221:LEU:O	1:A:225:VAL:HG22	1.77	0.84
1:A:369:ILE:CG2	1:A:482:LEU:CD2	2.59	0.80
1:A:225:VAL:HB	1:A:226:PHE:CD1	2.20	0.76
1:A:220:PHE:HE2	3:A:602:5AW:H21	1.51	0.75
1:A:117:ALA:HB1	1:A:301:ILE:HG13	1.67	0.74
1:A:181:MET:HG2	1:A:204:VAL:HG23	1.70	0.74
1:A:209:LYS:HA	3:A:602:5AW:H33	1.69	0.74
1:A:279:GLN:HG2	1:A:290:LEU:O	1.87	0.74
1:A:304:PHE:CE1	3:A:603:5AW:H17	2.22	0.73
1:A:55:LYS:O	1:A:479:LEU:HD22	1.89	0.72
1:A:375:ARG:NH2	2:A:601:HEM:O1A	2.20	0.72
1:A:369:ILE:HG23	1:A:482:LEU:HD22	1.70	0.72
1:A:462:ASN:O	1:A:463:PHE:CG	2.42	0.72
1:A:188:SER:O	1:A:271:PHE:HB3	1.88	0.71
1:A:369:ILE:HG22	1:A:482:LEU:CD2	2.20	0.71
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.70	0.71
1:A:149:ILE:HG12	1:A:183:VAL:CG1	2.19	0.71
3:A:602:5AW:C14	3:A:603:5AW:H14	2.22	0.70
1:A:436:GLY:HA3	2:A:601:HEM:HBA1	1.73	0.70
3:A:602:5AW:H12	3:A:603:5AW:H13	1.74	0.70
1:A:217:ASP:H	3:A:603:5AW:H34	1.55	0.69
1:A:313:VAL:HG23	1:A:369:ILE:CD1	2.22	0.69
1:A:375:ARG:HH22	2:A:601:HEM:CGA	2.05	0.69
1:A:368:PRO:O	1:A:370:ALA:N	2.26	0.68
1:A:409:THR:O	1:A:418:ARG:NH2	2.27	0.68
1:A:249:LEU:HA	1:A:252:SER:HB2	1.76	0.67
1:A:313:VAL:HG23	1:A:369:ILE:HD11	1.76	0.67
1:A:331:LEU:HD13	1:A:460:LEU:CD1	2.25	0.67
1:A:226:PHE:HB3	1:A:228:PHE:CE2	2.30	0.66
1:A:225:VAL:O	1:A:227:PRO:HD3	1.96	0.66
1:A:87:PRO:HG3	1:A:431:ILE:HD11	1.78	0.65
1:A:27:THR:O	1:A:29:SER:N	2.30	0.65
1:A:126:TRP:CZ2	1:A:440:ARG:HG2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:HA	3:A:602:5AW:C36	2.27	0.64
1:A:226:PHE:CD1	1:A:226:PHE:N	2.62	0.63
1:A:220:PHE:CE2	3:A:602:5AW:C35	2.82	0.62
1:A:27:THR:C	1:A:29:SER:H	2.01	0.62
1:A:220:PHE:HE2	3:A:602:5AW:C35	2.13	0.62
1:A:27:THR:C	1:A:29:SER:N	2.53	0.61
1:A:57:PHE:H	1:A:57:PHE:HD2	1.47	0.61
1:A:137:PHE:HZ	1:A:302:PHE:CE2	2.18	0.60
1:A:245:VAL:O	1:A:248:PHE:HB3	2.03	0.59
1:A:220:PHE:CE2	3:A:602:5AW:H21	2.37	0.59
1:A:252:SER:O	1:A:255:ARG:HB2	2.02	0.59
1:A:226:PHE:N	1:A:226:PHE:HD1	2.01	0.58
3:A:602:5AW:H30	3:A:603:5AW:C35	2.33	0.58
1:A:138:THR:O	1:A:139:SER:C	2.40	0.58
1:A:275:MET:HB3	1:A:290:LEU:CD2	2.33	0.57
1:A:179:TYR:CE1	1:A:455:ALA:HB2	2.40	0.57
1:A:458:ARG:HA	1:A:461:GLN:HG2	1.88	0.56
1:A:449:LEU:O	1:A:453:LYS:HG3	2.06	0.56
3:A:602:5AW:H12	3:A:603:5AW:C19	2.35	0.56
1:A:225:VAL:HB	1:A:226:PHE:HD1	1.67	0.56
1:A:482:LEU:HD12	3:A:603:5AW:C14	2.36	0.55
1:A:134:SER:N	1:A:135:PRO:CD	2.70	0.55
1:A:58:CYS:SG	1:A:399:TYR:CG	2.95	0.54
1:A:292:ASP:O	1:A:296:VAL:HG23	2.06	0.54
1:A:168:LYS:O	1:A:169:PRO:C	2.46	0.54
1:A:369:ILE:HG22	1:A:369:ILE:O	2.07	0.54
1:A:460:LEU:C	1:A:462:ASN:H	2.12	0.53
1:A:99:TYR:CE2	1:A:127:LYS:HD3	2.44	0.53
1:A:249:LEU:HD12	1:A:253:VAL:HG23	1.91	0.53
1:A:112:GLY:O	1:A:115:LYS:HG2	2.09	0.52
1:A:304:PHE:CD1	3:A:603:5AW:H17	2.44	0.52
3:A:603:5AW:N05	3:A:603:5AW:H28	2.25	0.52
1:A:124:GLU:OE2	1:A:127:LYS:NZ	2.43	0.52
1:A:220:PHE:HA	1:A:223:ILE:HG12	1.92	0.52
3:A:603:5AW:H25	3:A:603:5AW:H18	1.75	0.52
1:A:194:ASP:C	1:A:196:LEU:H	2.13	0.52
1:A:217:ASP:CB	3:A:603:5AW:S37	2.98	0.51
1:A:57:PHE:CD2	1:A:57:PHE:N	2.75	0.51
1:A:257:LYS:O	1:A:261:LEU:HG	2.11	0.51
1:A:472:GLN:NE2	1:A:476:LYS:H	2.09	0.51
1:A:181:MET:HG2	1:A:204:VAL:CG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HB	1:A:196:LEU:HD23	1.92	0.51
1:A:208:LYS:O	3:A:602:5AW:H29	2.10	0.51
1:A:338:VAL:O	1:A:340:PRO:HD3	2.11	0.51
2:A:601:HEM:NC	3:A:602:5AW:C31	2.74	0.51
1:A:369:ILE:CG2	1:A:369:ILE:O	2.58	0.51
1:A:415:LEU:HB2	1:A:418:ARG:HD2	1.93	0.51
1:A:477:LEU:HD13	1:A:483:LEU:HD11	1.93	0.51
1:A:209:LYS:HB3	3:A:602:5AW:S37	2.51	0.50
1:A:332:GLN:NE2	1:A:463:PHE:O	2.44	0.50
1:A:482:LEU:HD12	3:A:603:5AW:H19	1.94	0.50
1:A:313:VAL:HG23	1:A:369:ILE:HD12	1.93	0.50
1:A:27:THR:N	1:A:78:GLN:NE2	2.60	0.50
1:A:461:GLN:O	1:A:462:ASN:HB3	2.11	0.50
1:A:154:ASP:O	1:A:157:VAL:HG22	2.11	0.50
1:A:330:LYS:HE3	1:A:355:TYR:CE2	2.47	0.50
1:A:136:THR:O	1:A:141:LYS:HG3	2.12	0.50
1:A:168:LYS:O	1:A:169:PRO:O	2.30	0.50
1:A:408:TRP:HB2	1:A:411:PRO:HB3	1.94	0.50
1:A:114:MET:HG3	1:A:241:PHE:CZ	2.47	0.49
1:A:242:PRO:C	1:A:244:GLU:H	2.16	0.49
1:A:137:PHE:CZ	1:A:302:PHE:HE2	2.31	0.49
1:A:459:VAL:O	1:A:463:PHE:HB2	2.12	0.49
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.94	0.49
1:A:198:ASN:HB3	1:A:200:GLN:O	2.13	0.49
1:A:346:THR:O	1:A:350:VAL:HG23	2.13	0.49
1:A:179:TYR:CZ	1:A:455:ALA:HB2	2.48	0.48
1:A:185:THR:HG21	1:A:193:ILE:CD1	2.44	0.48
1:A:108:PHE:HE2	1:A:120:ILE:HG12	1.78	0.48
1:A:64:CYS:HB3	1:A:72:TRP:CE2	2.48	0.47
1:A:223:ILE:HG13	1:A:224:THR:N	2.29	0.47
1:A:64:CYS:HB3	1:A:72:TRP:NE1	2.30	0.47
1:A:172:LEU:HD12	1:A:489:VAL:CG1	2.45	0.47
1:A:113:PHE:C	1:A:113:PHE:CD2	2.88	0.47
1:A:482:LEU:HD12	3:A:603:5AW:O15	2.15	0.47
1:A:137:PHE:HZ	1:A:302:PHE:HE2	1.61	0.46
3:A:602:5AW:H30	3:A:603:5AW:H20	1.97	0.46
1:A:217:ASP:OD1	1:A:220:PHE:HD2	1.98	0.46
1:A:189:PHE:HA	1:A:272:LEU:HB2	1.98	0.46
1:A:463:PHE:HA	1:A:494:GLU:O	2.15	0.46
1:A:137:PHE:CZ	1:A:302:PHE:CE2	3.02	0.46
1:A:195:SER:O	1:A:198:ASN:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ARG:HE	1:A:461:GLN:HE21	1.63	0.46
1:A:458:ARG:NE	1:A:461:GLN:NE2	2.62	0.46
1:A:217:ASP:HB3	3:A:603:5AW:S37	2.56	0.46
1:A:225:VAL:HB	1:A:226:PHE:CE1	2.51	0.46
1:A:275:MET:HE3	1:A:295:LEU:HG	1.97	0.46
3:A:602:5AW:H11	3:A:603:5AW:H5	1.80	0.46
1:A:275:MET:HB3	1:A:290:LEU:HD23	1.97	0.46
1:A:185:THR:HG21	1:A:193:ILE:HD13	1.97	0.46
1:A:106:ARG:HH21	1:A:374:GLU:CD	2.18	0.45
1:A:217:ASP:HB3	3:A:603:5AW:H37	1.98	0.45
1:A:172:LEU:HD12	1:A:489:VAL:HG12	1.98	0.45
1:A:463:PHE:CD1	1:A:493:VAL:HG12	2.52	0.45
1:A:169:PRO:HG3	1:A:468:CYS:SG	2.56	0.45
1:A:371:MET:C	1:A:372:ARG:CG	2.85	0.45
1:A:362:GLU:OE2	1:A:418:ARG:HD3	2.16	0.45
1:A:47:LEU:HD23	1:A:225:VAL:HG11	1.99	0.45
1:A:376:VAL:HG22	1:A:393:VAL:HG22	2.00	0.44
1:A:319:TYR:CZ	1:A:475:LEU:HB2	2.52	0.44
1:A:132:LEU:HD21	1:A:290:LEU:HB2	2.00	0.44
1:A:157:VAL:CG2	1:A:158:ARG:N	2.80	0.44
1:A:189:PHE:O	1:A:260:ARG:NH2	2.51	0.44
1:A:349:THR:O	1:A:353:MET:HG3	2.18	0.44
1:A:58:CYS:SG	1:A:371:MET:SD	3.16	0.44
1:A:274:LEU:O	1:A:277:ASP:HB2	2.18	0.44
1:A:52:SER:O	1:A:55:LYS:HG3	2.18	0.44
1:A:448:ALA:O	1:A:452:MET:HG3	2.19	0.43
1:A:463:PHE:HD1	1:A:494:GLU:O	2.02	0.43
1:A:331:LEU:HD21	1:A:356:LEU:HD13	1.99	0.43
1:A:462:ASN:O	1:A:463:PHE:CD2	2.71	0.43
1:A:352:GLN:HE21	1:A:352:GLN:HB3	1.65	0.43
1:A:194:ASP:O	1:A:196:LEU:N	2.51	0.43
1:A:128:ARG:HH21	1:A:289:ALA:C	2.22	0.42
1:A:314:LEU:HD22	1:A:456:LEU:HD13	1.99	0.42
1:A:420:SER:O	1:A:424:LYS:HB2	2.20	0.42
1:A:308:GLU:HG2	3:A:603:5AW:H26	2.00	0.42
1:A:126:TRP:CH2	1:A:440:ARG:HG2	2.54	0.42
1:A:128:ARG:NH2	1:A:290:LEU:HA	2.35	0.42
1:A:172:LEU:HD11	1:A:491:LEU:CD1	2.46	0.42
1:A:331:LEU:HD13	1:A:460:LEU:HD13	2.00	0.42
1:A:47:LEU:O	1:A:77:GLY:HA2	2.19	0.42
1:A:179:TYR:O	1:A:183:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CZ	3:A:602:5AW:H20	2.54	0.42
3:A:602:5AW:O11	3:A:603:5AW:H15	2.20	0.41
1:A:217:ASP:HB2	3:A:603:5AW:S37	2.61	0.41
1:A:100:SER:OG	1:A:101:VAL:HG12	2.19	0.41
1:A:381:VAL:O	1:A:387:PHE:HA	2.20	0.41
1:A:461:GLN:O	1:A:461:GLN:HG3	2.19	0.41
1:A:58:CYS:SG	1:A:399:TYR:CD1	3.14	0.41
1:A:183:VAL:HG11	1:A:451:ASN:ND2	2.36	0.41
1:A:103:THR:HG21	1:A:123:ASP:HA	2.03	0.41
1:A:117:ALA:HB1	1:A:301:ILE:CG1	2.45	0.41
1:A:133:LEU:HD11	1:A:298:GLN:HG3	2.02	0.41
1:A:229:LEU:O	1:A:232:ILE:HB	2.20	0.41
3:A:602:5AW:H30	3:A:603:5AW:C33	2.51	0.40
1:A:45:PRO:O	1:A:47:LEU:N	2.50	0.40
1:A:49:ASN:OD1	1:A:74:PHE:HB2	2.21	0.40
1:A:196:LEU:C	1:A:198:ASN:N	2.74	0.40
1:A:342:LYS:HE2	1:A:342:LYS:HB3	1.98	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	442/487 (91%)	383 (87%)	46 (10%)	13 (3%)	4	15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	ASN
1	A	28	HIS
1	A	169	PRO
1	A	369	ILE

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Mol	Chain	Res	Type
1	A	139	SER
1	A	195	SER
1	A	225	VAL
1	A	226	PHE
1	A	341	ASN
1	A	77	GLY
1	A	406	LYS
1	A	461	GLN
1	A	405	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/443 (93%)	366 (89%)	45 (11%)	6	17

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	36	LEU
1	A	50	ILE
1	A	55	LYS
1	A	57	PHE
1	A	59	MET
1	A	62	MET
1	A	70	LYS
1	A	93	VAL
1	A	101	VAL
1	A	113	PHE
1	A	124	GLU
1	A	157	VAL
1	A	165	GLU
1	A	168	LYS
1	A	175	VAL
1	A	180	SER

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Mol	Chain	Res	Type
1	A	195	SER
1	A	196	LEU
1	A	208	LYS
1	A	225	VAL
1	A	226	PHE
1	A	229	LEU
1	A	237	ASN
1	A	241	PHE
1	A	244	GLU
1	A	249	LEU
1	A	272	LEU
1	A	274	LEU
1	A	291	SER
1	A	326	ASP
1	A	331	LEU
1	A	342	LYS
1	A	348	ASP
1	A	352	GLN
1	A	371	MET
1	A	372	ARG
1	A	421	LYS
1	A	422	LYS
1	A	454	LEU
1	A	456	LEU
1	A	458	ARG
1	A	478	SER
1	A	490	VAL
1	A	492	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	78	GLN
1	A	237	ASN
1	A	279	GLN
1	A	352	GLN
1	A	426	ASN
1	A	451	ASN
1	A	461	GLN
1	A	472	GLN
1	A	484	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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	HEM	A	601	3,1	41,50,50	2.45	16 (39%)	45,82,82	3.23	20 (44%)
3	5AW	A	602	2	33,38,38	1.46	3 (9%)	35,51,51	2.25	14 (40%)
3	5AW	A	603	-	33,38,38	1.23	1 (3%)	35,51,51	2.26	10 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	601	3,1	-	0/12/54/54	-
3	5AW	A	602	2	-	20/38/42/42	0/2/2/2
3	5AW	A	603	-	-	21/38/42/42	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	5AW	O26-C24	6.41	1.47	1.35
3	A	603	5AW	O26-C24	6.12	1.47	1.35
2	A	601	HEM	C3C-C2C	5.48	1.48	1.40
2	A	601	HEM	C4A-NA	5.06	1.46	1.36
2	A	601	HEM	C1A-NA	4.97	1.46	1.36
2	A	601	HEM	C3B-C2B	4.74	1.46	1.37
2	A	601	HEM	C3D-C2D	4.08	1.45	1.36
2	A	601	HEM	CHA-C4D	3.84	1.44	1.35
2	A	601	HEM	CHB-C1B	3.59	1.44	1.35
2	A	601	HEM	C4D-ND	-3.08	1.35	1.40
2	A	601	HEM	C2C-C1C	3.05	1.49	1.42
2	A	601	HEM	C2A-C3A	3.05	1.46	1.37
2	A	601	HEM	FE-NB	2.94	2.11	1.96
2	A	601	HEM	FE-ND	2.91	2.11	1.96
2	A	601	HEM	C1D-C2D	2.84	1.50	1.44
2	A	601	HEM	C4D-C3D	2.81	1.49	1.45
2	A	601	HEM	C1B-NB	-2.27	1.36	1.40
3	A	602	5AW	C28-S32	-2.19	1.69	1.73
3	A	602	5AW	C27-C28	2.07	1.52	1.50
2	A	601	HEM	C4B-NB	-2.05	1.34	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C3B-C2B-C1B	-9.21	99.65	106.49
2	A	601	HEM	C2B-C1B-NB	7.66	118.92	109.84
2	A	601	HEM	C3D-C4D-ND	7.21	118.19	110.17
3	A	603	5AW	C29-N30-C31	7.17	116.97	105.78
2	A	601	HEM	C2D-C1D-ND	6.64	117.83	109.88
3	A	602	5AW	C29-N30-C31	5.34	114.11	105.78
3	A	603	5AW	C07-C06-C36	-5.04	122.03	129.62
2	A	601	HEM	C4D-ND-C1D	-4.81	100.10	105.07
3	A	602	5AW	O26-C24-N23	4.80	120.27	110.50
2	A	601	HEM	C1D-C2D-C3D	-4.70	102.02	106.96
3	A	602	5AW	C02-C04-N05	4.67	133.98	125.08
3	A	603	5AW	C02-C04-N05	4.56	133.76	125.08
2	A	601	HEM	C4A-C3A-C2A	-4.30	104.00	107.00
3	A	603	5AW	O26-C24-N23	4.19	119.02	110.50
2	A	601	HEM	C1B-NB-C4B	-4.01	100.94	105.07
2	A	601	HEM	CMD-C2D-C1D	3.72	130.71	125.04
3	A	602	5AW	C07-C06-C36	-3.70	124.06	129.62
2	A	601	HEM	CHD-C1D-C2D	-3.56	119.41	124.98
2	A	601	HEM	C4D-C3D-C2D	-3.55	101.72	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	5AW	O26-C24-O25	-3.55	117.44	124.25
2	A	601	HEM	CAD-C3D-C4D	3.46	130.70	124.66
2	A	601	HEM	CHB-C1B-C2B	-3.40	117.32	126.72
2	A	601	HEM	C4B-C3B-C2B	-3.24	104.54	107.11
2	A	601	HEM	CAA-CBA-CGA	-3.19	104.80	113.76
3	A	603	5AW	C19-C17-N16	3.12	116.01	110.49
2	A	601	HEM	CBD-CAD-C3D	-3.11	103.98	112.63
3	A	602	5AW	C27-O26-C24	3.11	122.87	115.93
3	A	602	5AW	C17-N16-C14	3.04	130.92	123.46
3	A	602	5AW	C14-C13-N12	2.98	118.47	110.36
3	A	602	5AW	C21-N23-C24	2.97	127.20	122.44
2	A	601	HEM	CHA-C4D-C3D	-2.80	120.07	125.33
3	A	603	5AW	O26-C24-O25	-2.78	118.92	124.25
2	A	601	HEM	CMC-C2C-C3C	2.54	129.44	124.68
3	A	602	5AW	O15-C14-C13	-2.38	115.82	120.74
2	A	601	HEM	CHA-C4D-ND	-2.37	121.45	124.38
3	A	603	5AW	C17-N16-C14	2.32	129.14	123.46
3	A	602	5AW	C20-C21-N23	2.29	114.54	110.49
3	A	603	5AW	C27-O26-C24	2.28	121.02	115.93
3	A	602	5AW	O26-C27-C28	2.18	115.21	109.76
3	A	602	5AW	C19-C17-N16	2.17	114.33	110.49
3	A	603	5AW	C13-C14-N16	2.10	121.02	116.48
3	A	602	5AW	C13-C14-N16	2.07	120.95	116.48
2	A	601	HEM	CHC-C4B-NB	-2.06	122.20	124.43
3	A	603	5AW	C21-N23-C24	2.05	125.72	122.44

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	5AW	O25-C24-N23-C21
3	A	602	5AW	O26-C24-N23-C21
3	A	602	5AW	C22-C21-N23-C24
3	A	602	5AW	C19-C20-C21-N23
3	A	602	5AW	C19-C20-C21-C22
3	A	602	5AW	C17-C19-C20-C21
3	A	602	5AW	C18-C17-C19-C20
3	A	602	5AW	C18-C17-N16-C14
3	A	602	5AW	O11-C10-N12-C13
3	A	602	5AW	N08-C10-N12-C13
3	A	602	5AW	N12-C10-N08-C09
3	A	602	5AW	N12-C10-N08-C07

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Mol	Chain	Res	Type	Atoms
3	A	602	5AW	O11-C10-N08-C09
3	A	602	5AW	O11-C10-N08-C07
3	A	603	5AW	O26-C24-N23-C21
3	A	603	5AW	C22-C21-N23-C24
3	A	603	5AW	C19-C20-C21-N23
3	A	603	5AW	C19-C20-C21-C22
3	A	603	5AW	C33-C13-C14-N16
3	A	603	5AW	C33-C13-C14-O15
3	A	603	5AW	N12-C10-N08-C09
3	A	603	5AW	N12-C10-N08-C07
3	A	603	5AW	O11-C10-N08-C09
3	A	603	5AW	O11-C10-N08-C07
3	A	603	5AW	C06-C07-N08-C10
3	A	603	5AW	C06-C07-N08-C09
3	A	603	5AW	O15-C14-N16-C17
3	A	603	5AW	C13-C14-N16-C17
3	A	603	5AW	O25-C24-N23-C21
3	A	602	5AW	C14-C13-C33-C34
3	A	602	5AW	C14-C13-C33-C35
3	A	602	5AW	N12-C13-C33-C34
3	A	602	5AW	N12-C13-C33-C35
3	A	603	5AW	C18-C17-N16-C14
3	A	602	5AW	N05-C06-C07-N08
3	A	603	5AW	N12-C13-C14-O15
3	A	603	5AW	C28-C27-O26-C24
3	A	603	5AW	C20-C21-N23-C24
3	A	603	5AW	N12-C13-C14-N16
3	A	603	5AW	C36-C06-C07-N08
3	A	602	5AW	C33-C13-N12-C10

There are no ring outliers.

3 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	5	0
3	A	602	5AW	19	0
3	A	603	5AW	22	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 HEM A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand 5AW A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand 5AW A 603

Bond lengths

Bond angles

Torsions

Rings
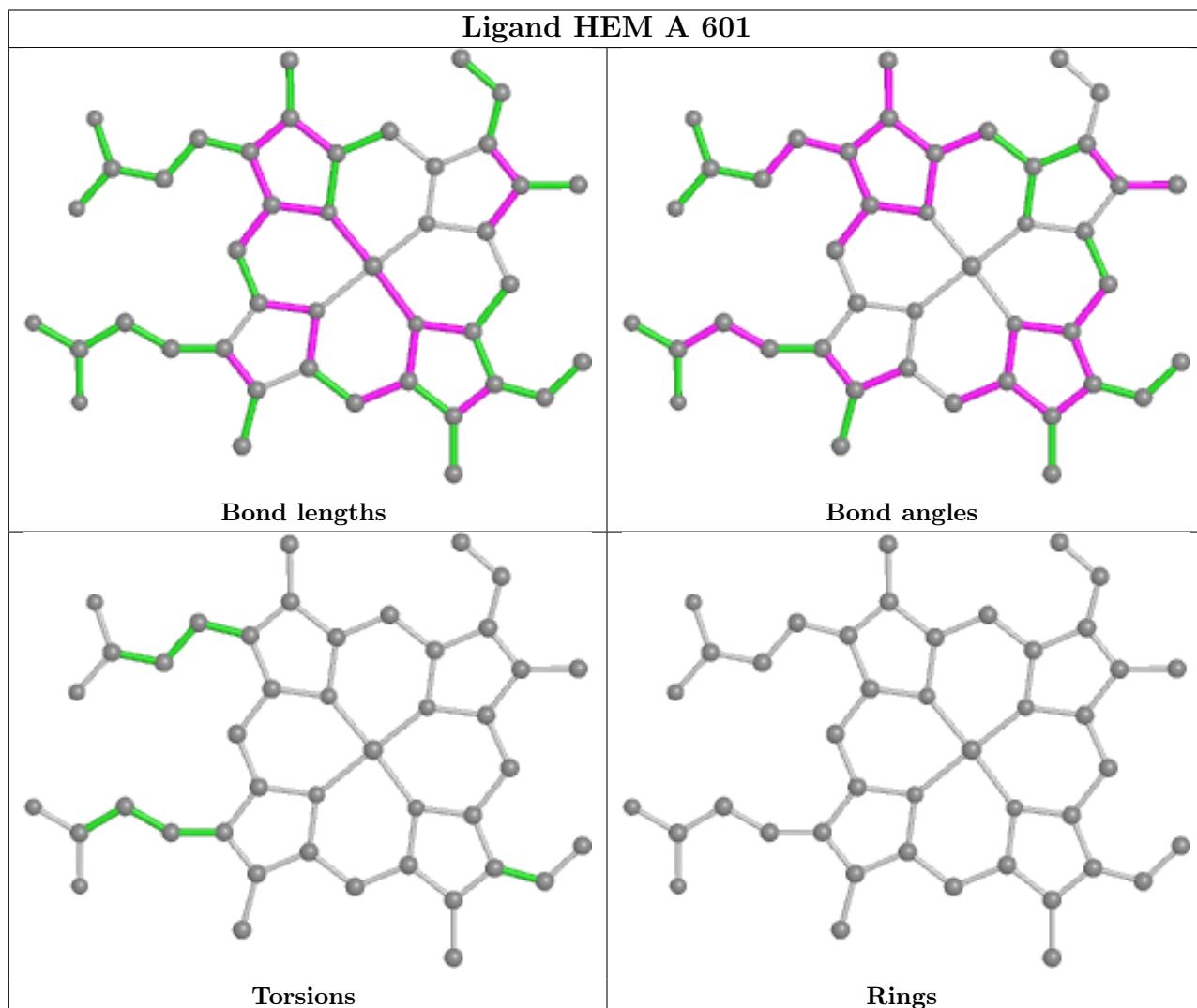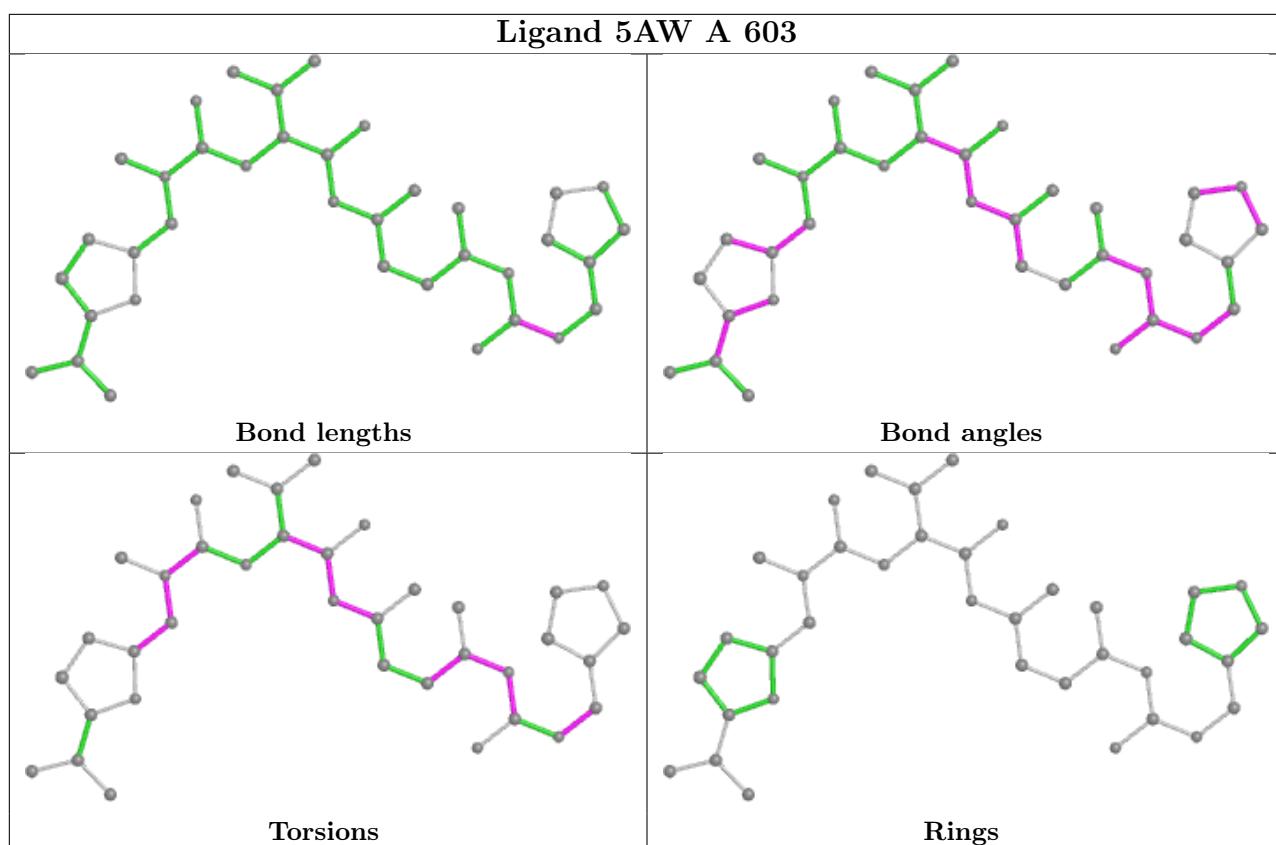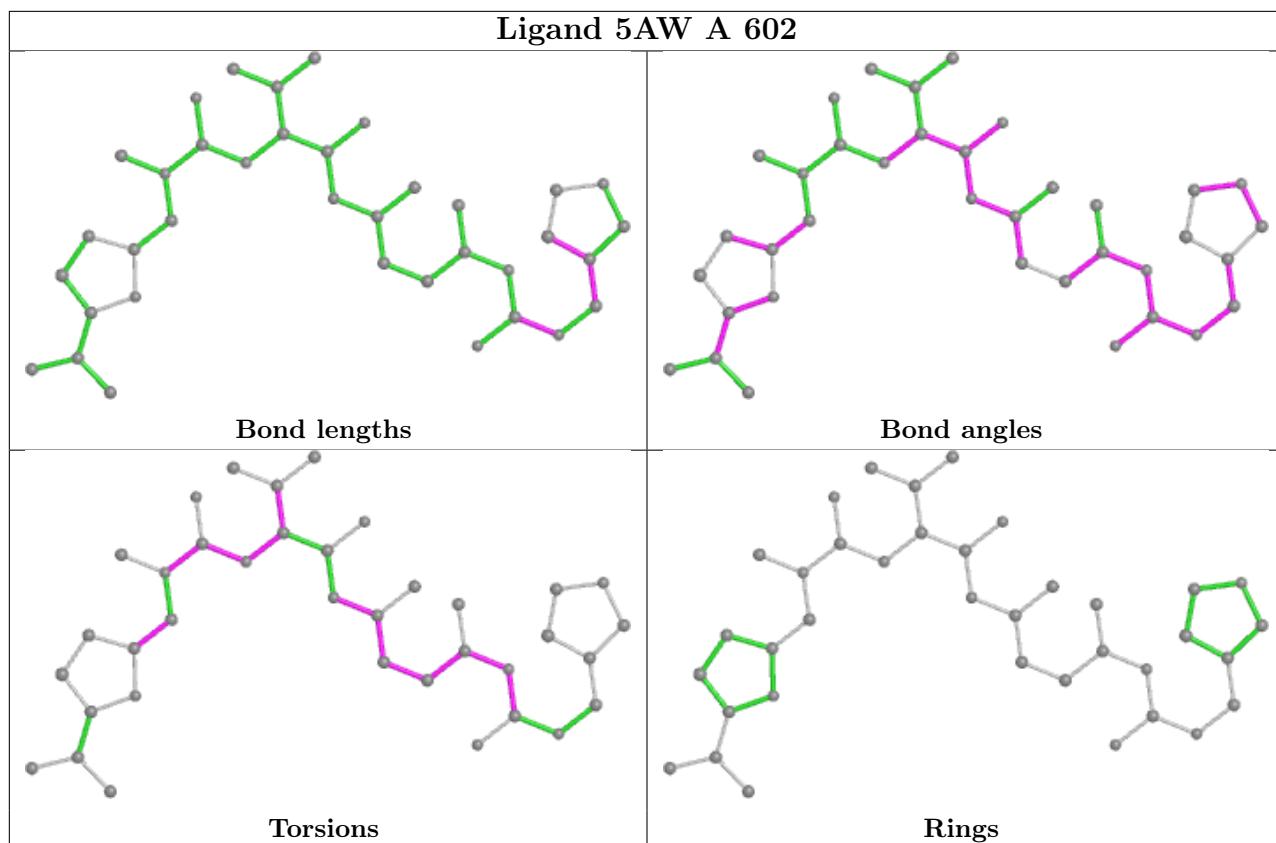
5.7 Other polymers ⓘ

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	450/487 (92%)	0.17	21 (4%)	31	27	53, 91, 162, 204	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	PRO	4.8
1	A	201	ASP	4.7
1	A	278	SER	4.5
1	A	256	MET	4.0
1	A	261	LEU	3.8
1	A	260	ARG	3.6
1	A	279	GLN	3.6
1	A	216	LEU	3.3
1	A	309	THR	3.2
1	A	27	THR	2.8
1	A	276	ILE	2.8
1	A	469	LYS	2.7
1	A	208	LYS	2.7
1	A	200	GLN	2.6
1	A	253	VAL	2.4
1	A	310	THR	2.4
1	A	275	MET	2.3
1	A	305	ALA	2.2
1	A	490	VAL	2.1
1	A	57	PHE	2.1
1	A	341	ASN	2.1

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(Å²)	Q<0.9
3	5AW	A	603	37/37	0.41	0.72	124,194,278,282	0
3	5AW	A	602	37/37	0.74	0.53	64,176,196,199	0
2	HEM	A	601	43/43	0.97	0.27	51,59,69,74	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 5AW A 603:

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

Electron density around 5AW A 602:

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

Electron density around HEM A 601:

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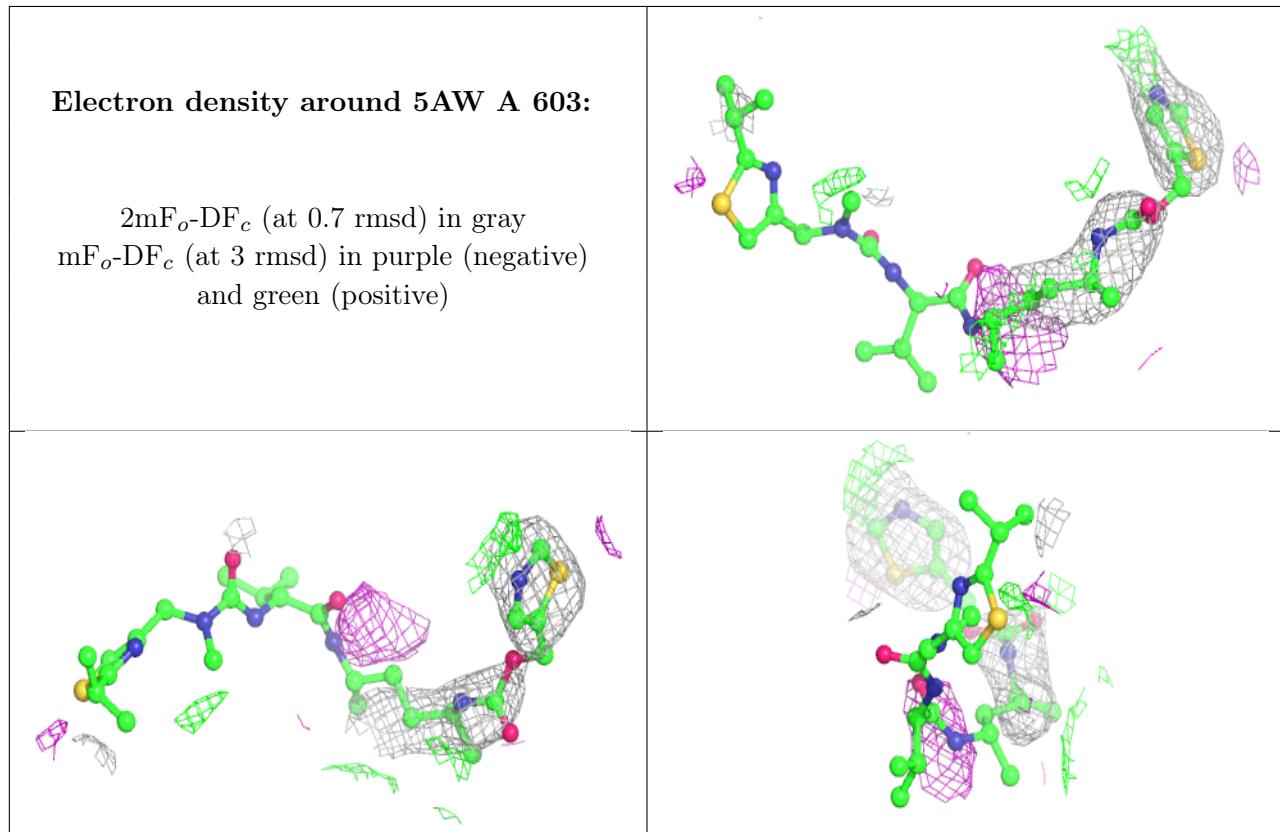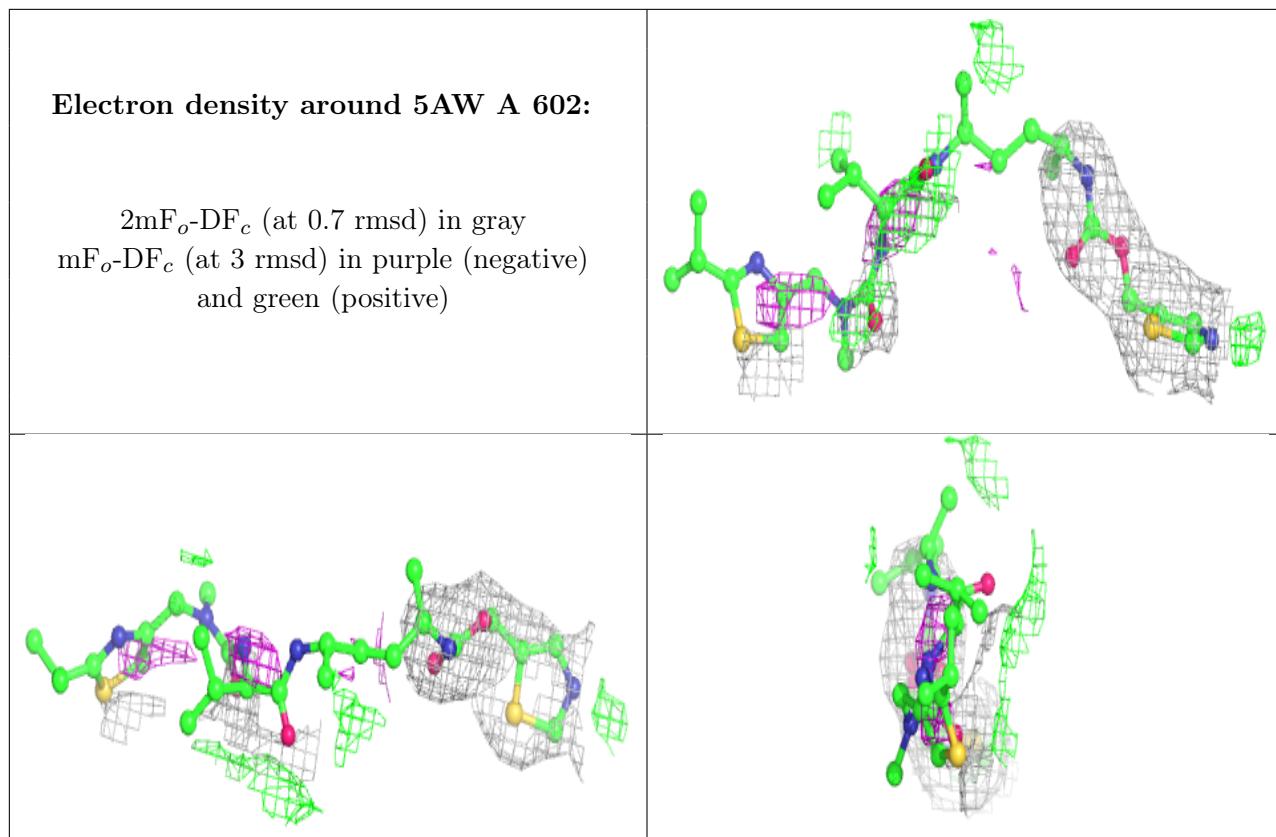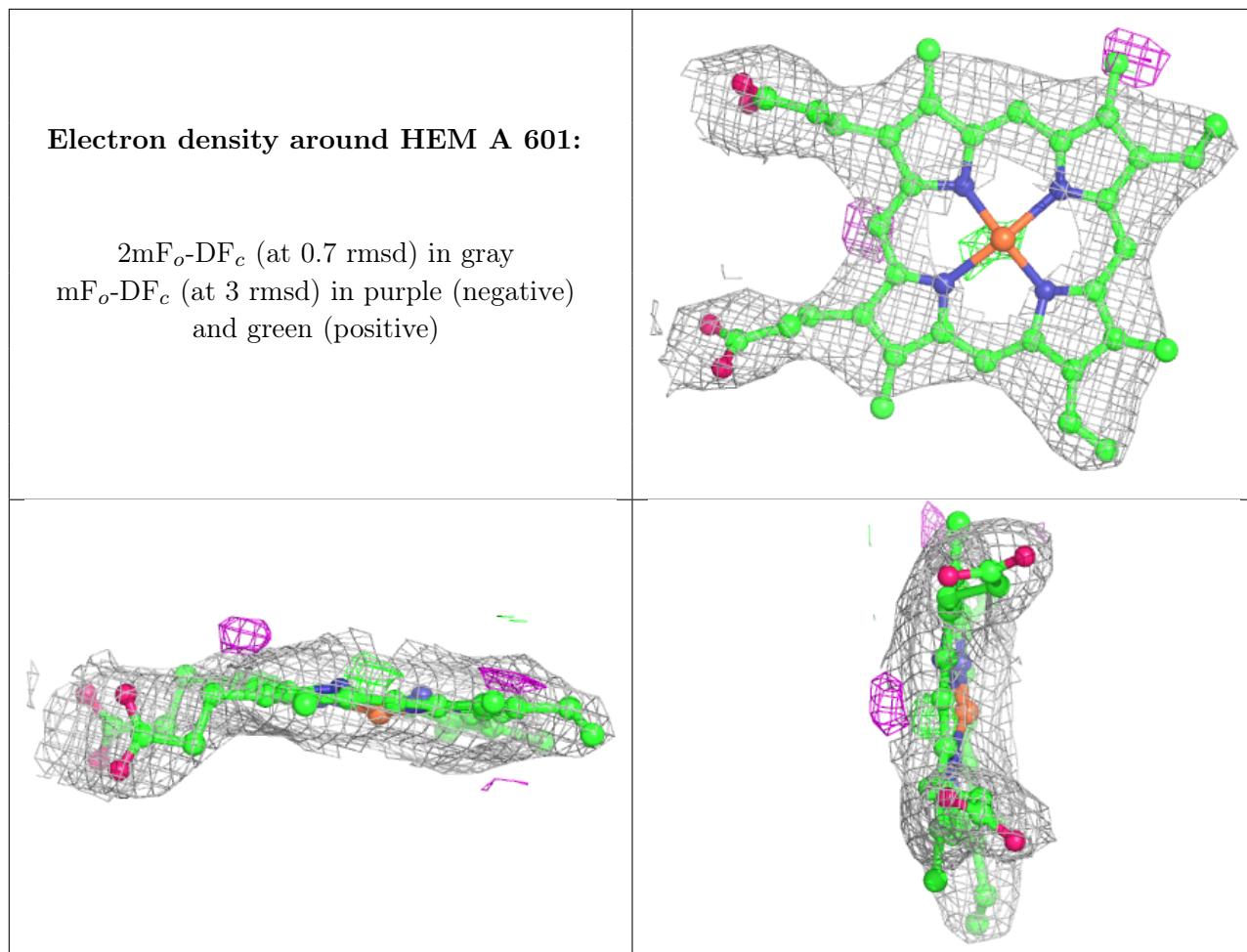
6.5 Other polymers (i)

There are no such residues in this entry.