Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 09:25 PM EST

PDB ID	:	4R21
Title	:	Zebra fish cytochrome P450 17A2 with Progesterone
Authors	:	Pallan, P.S.; Egli, M.
Deposited on	:	2014-08-08
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
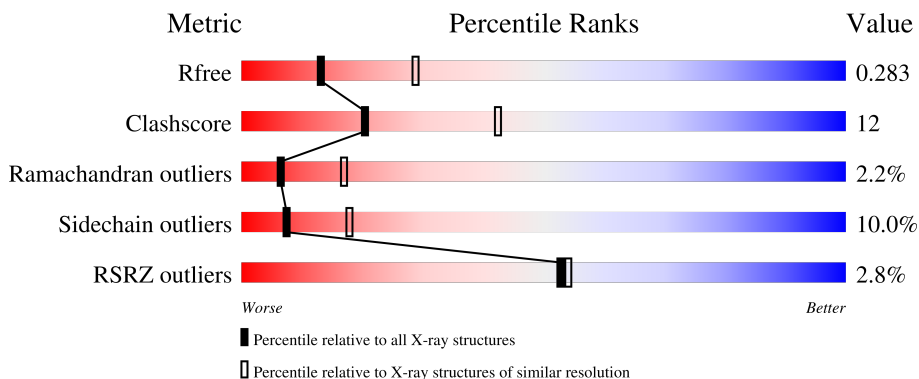
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	486	2% / 60% / 22% / · · / 13%
1	B	486	2% / 62% / 21% / · · / 13%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6752 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 family 17 polypeptide 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total 3301	C 2099	N 581	O 606	S 15	5	0	0
1	B	423	Total 3304	C 2096	N 582	O 611	S 15	9	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP A7U483
A	17	ALA	-	expression tag	UNP A7U483
A	18	LYS	-	expression tag	UNP A7U483
A	19	LYS	-	expression tag	UNP A7U483
A	20	THR	-	expression tag	UNP A7U483
A	21	SER	-	expression tag	UNP A7U483
A	22	SER	-	expression tag	UNP A7U483
A	23	LYS	-	expression tag	UNP A7U483
A	24	GLY	-	expression tag	UNP A7U483
A	25	LYS	-	expression tag	UNP A7U483
A	496	HIS	-	expression tag	UNP A7U483
A	497	HIS	-	expression tag	UNP A7U483
A	498	HIS	-	expression tag	UNP A7U483
A	499	HIS	-	expression tag	UNP A7U483
A	500	HIS	-	expression tag	UNP A7U483
A	501	HIS	-	expression tag	UNP A7U483
B	16	MET	-	expression tag	UNP A7U483
B	17	ALA	-	expression tag	UNP A7U483
B	18	LYS	-	expression tag	UNP A7U483
B	19	LYS	-	expression tag	UNP A7U483
B	20	THR	-	expression tag	UNP A7U483
B	21	SER	-	expression tag	UNP A7U483
B	22	SER	-	expression tag	UNP A7U483
B	23	LYS	-	expression tag	UNP A7U483
B	24	GLY	-	expression tag	UNP A7U483

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	LYS	-	expression tag	UNP A7U483
B	496	HIS	-	expression tag	UNP A7U483
B	497	HIS	-	expression tag	UNP A7U483
B	498	HIS	-	expression tag	UNP A7U483
B	499	HIS	-	expression tag	UNP A7U483
B	500	HIS	-	expression tag	UNP A7U483
B	501	HIS	-	expression tag	UNP A7U483

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
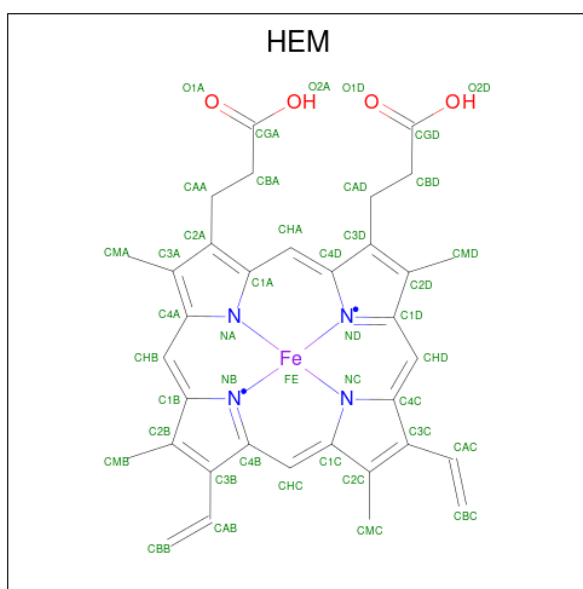
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			42	34	1	4	3		
2	B	1	Total	C	Fe	N	O	0	0
			42	34	1	4	3		

- Molecule 3 is PROGESTERONE (three-letter code: STR) (formula: $C_{21}H_{30}O_2$).

STR
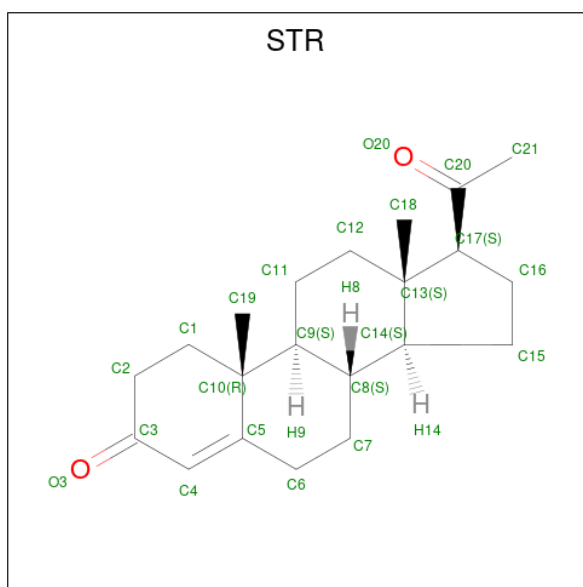
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 23	C 21	O 2	0	0
3	B	1	Total 23	C 21	O 2	0	0

• Molecule 4 is water.

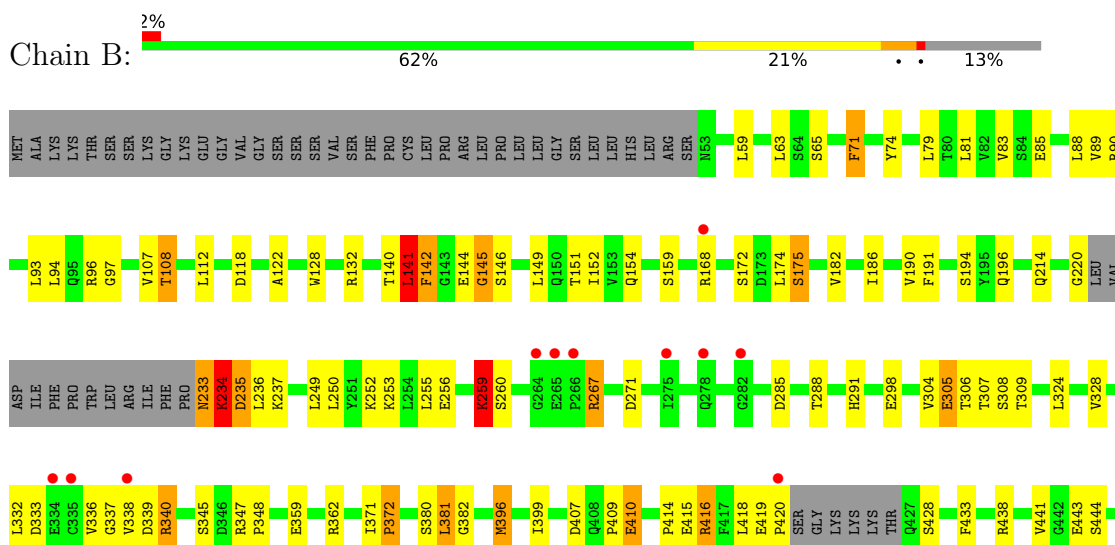| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	10	Total 10	O 10	0	0

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: Cytochrome P450 family 17 polypeptide 2

• Molecule 1: Cytochrome P450 family 17 polypeptide 2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.94Å 78.63Å 95.41Å 90.00° 92.03° 90.00°	Depositor
Resolution (Å)	17.08 – 2.70 48.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (17.08-2.70) 98.8 (48.99-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.205 , 0.283 0.209 , 0.283	Depositor DCC
R_{free} test set	1159 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6752	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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, STR

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	0.57	0/3373	0.79	2/4581 (0.0%)
1	B	0.55	1/3377 (0.0%)	0.78	2/4588 (0.0%)
All	All	0.56	1/6750 (0.0%)	0.78	4/9169 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	ASN	C-N	-5.68	1.21	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	233	ASN	O-C-N	-6.88	111.69	122.70
1	B	420	PRO	N-CA-CB	5.38	109.75	103.30
1	A	191	PHE	CB-CA-C	-5.18	100.05	110.40
1	A	416	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	GLY	Peptide
1	A	266	PRO	Peptide
1	A	456	ARG	Sidechain
1	B	142	PHE	Peptide
1	B	145	GLY	Peptide
1	B	234	LYS	Peptide
1	B	235	ASP	Peptide
1	B	267	ARG	Sidechain
1	B	418	LEU	Peptide

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	3301	0	3321	90	0
1	B	3304	0	3308	70	0
2	A	42	0	30	5	0
2	B	42	0	30	3	0
3	A	23	0	30	3	0
3	B	23	0	30	2	0
4	A	7	0	0	0	0
4	B	10	0	0	0	0
All	All	6752	0	6749	166	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 12.

All (166) 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:234:LYS:HA	1:A:235:ASP:HB3	1.17	1.16
1:A:453:PHE:O	1:A:457:PRO:HD3	1.56	1.03
1:A:338:VAL:HG21	1:A:494:ARG:NH1	1.87	0.89
1:A:234:LYS:CA	1:A:235:ASP:HB3	2.02	0.87
1:A:234:LYS:HA	1:A:235:ASP:CB	2.03	0.87
1:B:453:PHE:O	1:B:457:PRO:CD	2.23	0.85
1:A:453:PHE:O	1:A:457:PRO:CD	2.25	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:VAL:CG2	1:A:494:ARG:NH1	2.42	0.82
1:A:266:PRO:HB2	1:A:267:ARG:HA	1.63	0.79
1:B:339:ASP:O	1:B:340:ARG:HB3	1.83	0.77
1:B:453:PHE:O	1:B:457:PRO:HD2	1.82	0.77
1:A:450:LEU:O	1:A:454:VAL:HG23	1.86	0.74
1:B:362:ARG:NH2	1:B:409:PRO:O	2.24	0.71
1:A:189:LEU:CD2	1:A:445:LEU:HD11	2.22	0.69
1:A:379:THR:OG1	1:A:380:SER:N	2.25	0.68
1:B:141:LEU:O	1:B:145:GLY:HA3	1.95	0.67
1:A:338:VAL:CG2	1:A:494:ARG:HH12	2.08	0.66
1:A:265:GLU:HB3	1:A:266:PRO:HA	1.78	0.66
1:A:362:ARG:NH2	1:A:409:PRO:O	2.30	0.65
1:B:453:PHE:O	1:B:457:PRO:HD3	1.97	0.65
1:A:266:PRO:HB2	1:A:267:ARG:CA	2.27	0.64
1:A:106:MET:SD	1:A:221:LEU:O	2.56	0.64
1:A:407:ASP:O	1:A:416:ARG:NH2	2.31	0.64
1:A:174:LEU:O	1:A:175:SER:CB	2.48	0.62
1:A:122:ALA:O	1:A:438:ARG:NH2	2.32	0.62
1:B:144:GLU:HA	1:B:144:GLU:OE1	1.99	0.62
1:B:450:LEU:O	1:B:454:VAL:HG23	1.98	0.62
1:B:233:ASN:O	1:B:234:LYS:C	2.36	0.61
2:B:600:HEM:HBB2	2:B:600:HEM:HHC	1.83	0.61
1:B:304:VAL:O	1:B:305:GLU:CB	2.46	0.60
1:B:122:ALA:O	1:B:438:ARG:NH2	2.25	0.60
2:A:600:HEM:HBB2	2:A:600:HEM:HHC	1.83	0.59
1:A:338:VAL:HG21	1:A:494:ARG:CZ	2.33	0.59
1:A:208:TYR:CE1	1:A:246:ARG:HG3	2.38	0.59
1:A:359:GLU:CD	1:A:362:ARG:NH1	2.56	0.58
1:A:154:GLN:O	1:A:456:ARG:NH1	2.36	0.58
1:B:128:TRP:CH2	1:B:132:ARG:HD2	2.39	0.58
1:B:174:LEU:O	1:B:175:SER:CB	2.52	0.58
1:B:396:MET:HE2	1:B:399:ILE:HD11	1.84	0.58
1:B:259:LYS:HG3	1:B:260:SER:H	1.69	0.57
1:A:275:ILE:O	1:A:278:GLN:HB2	2.03	0.57
1:A:371:ILE:HD11	3:A:601:STR:H181	1.87	0.57
1:A:142:PHE:CD2	1:A:148:LYS:HD3	2.40	0.57
1:A:191:PHE:HB3	1:A:253:LYS:HG2	1.87	0.56
1:A:174:LEU:O	1:A:175:SER:HB2	2.05	0.56
1:A:454:VAL:O	1:A:457:PRO:HD2	2.06	0.56
1:B:359:GLU:OE1	1:B:416:ARG:HD2	2.05	0.56
1:A:167:CYS:O	1:A:170:GLN:HG2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:600:HEM:HBC2	2:A:600:HEM:HHD	1.88	0.55
1:B:407:ASP:O	1:B:416:ARG:NH2	2.39	0.55
1:A:64:SER:HA	1:A:68:GLY:O	2.07	0.54
1:A:251:TYR:CZ	1:B:252:LYS:HD2	2.42	0.54
1:A:359:GLU:OE1	1:A:362:ARG:NH1	2.41	0.54
1:B:63:LEU:HD13	1:B:71:PHE:CZ	2.42	0.54
1:A:254:LEU:CD1	1:A:274:LEU:HD21	2.38	0.54
1:B:307:THR:HG21	1:B:449:GLU:OE1	2.08	0.54
1:A:359:GLU:CD	1:A:362:ARG:HH12	2.11	0.53
1:B:108:THR:HG21	1:B:220:GLY:HA3	1.89	0.53
1:A:132:ARG:CZ	1:A:441:VAL:HG12	2.38	0.53
1:B:140:THR:C	1:B:142:PHE:H	2.11	0.53
1:B:85:GLU:O	1:B:89:VAL:HG13	2.08	0.53
1:B:492:THR:OG1	1:B:493:PRO:HD3	2.08	0.53
1:A:118:ASP:OD2	1:A:298:GLU:OE2	2.27	0.52
1:A:324:LEU:HD21	1:A:414:PRO:HG2	1.91	0.52
2:B:600:HEM:HHD	2:B:600:HEM:HBC2	1.91	0.52
1:B:233:ASN:O	1:B:234:LYS:O	2.27	0.52
1:A:254:LEU:HD11	1:A:274:LEU:HD21	1.91	0.52
1:B:90:ARG:NH1	1:B:428:SER:O	2.43	0.52
1:B:252:LYS:HE3	1:B:256:GLU:OE2	2.10	0.52
1:A:81:LEU:HD22	1:A:390:THR:HG21	1.91	0.51
1:A:191:PHE:HB3	1:A:253:LYS:CG	2.40	0.51
1:B:260:SER:CB	1:B:267:ARG:HH21	2.23	0.51
1:A:66:GLN:HG3	1:A:67:TYR:CE2	2.46	0.51
1:A:265:GLU:CB	1:A:266:PRO:HA	2.41	0.51
1:B:347:ARG:HB2	1:B:348:PRO:HD3	1.93	0.50
1:A:263:PRO:HG3	1:A:278:GLN:HE22	1.76	0.50
1:B:260:SER:O	1:B:267:ARG:NH2	2.43	0.50
1:A:257:HIS:HD2	1:A:271:ASP:OD1	1.95	0.50
1:A:164:LEU:O	1:A:167:CYS:SG	2.62	0.50
1:B:260:SER:HB3	1:B:267:ARG:HH21	1.76	0.50
1:A:147:ASN:OD1	1:A:147:ASN:N	2.44	0.49
1:A:453:PHE:O	1:A:457:PRO:CG	2.59	0.49
1:B:83:VAL:CG1	1:B:88:LEU:HB3	2.42	0.49
1:B:174:LEU:O	1:B:175:SER:OG	2.26	0.49
1:A:148:LYS:O	1:A:152:ILE:HG13	2.12	0.49
1:B:93:LEU:O	1:B:97:GLY:HA3	2.13	0.49
1:B:144:GLU:C	1:B:146:SER:HA	2.34	0.48
1:B:333:ASP:O	1:B:336:VAL:O	2.31	0.48
1:A:406:TRP:HB2	1:A:409:PRO:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:HB2	1:A:348:PRO:HD3	1.96	0.48
1:B:288:THR:HG22	1:B:291:HIS:ND1	2.27	0.48
1:A:153:VAL:HB	1:A:452:LEU:HD23	1.96	0.48
1:B:371:ILE:O	1:B:372:PRO:C	2.52	0.47
1:A:149:LEU:HD23	1:A:448:ILE:HG21	1.96	0.47
1:A:203:GLN:O	1:A:207:GLN:HG2	2.14	0.47
1:B:81:LEU:HD23	1:B:381:LEU:HD13	1.97	0.47
1:B:186:ILE:O	1:B:190:VAL:HG23	2.15	0.47
2:B:600:HEM:C2A	3:B:601:STR:H212	2.50	0.47
1:A:189:LEU:HD21	1:A:445:LEU:HD11	1.97	0.47
1:A:441:VAL:HG22	2:A:600:HEM:CMD	2.45	0.46
1:B:337:GLY:C	1:B:339:ASP:H	2.19	0.46
1:B:172:SER:O	1:B:488:THR:HA	2.15	0.46
1:B:233:ASN:O	1:B:233:ASN:OD1	2.34	0.46
1:B:249:LEU:C	1:B:249:LEU:HD23	2.36	0.46
1:A:454:VAL:C	1:A:457:PRO:HD2	2.36	0.46
1:B:149:LEU:HD23	1:B:448:ILE:HG21	1.97	0.46
1:A:112:LEU:HD13	1:A:239:LEU:HD21	1.97	0.46
3:A:601:STR:H213	3:A:601:STR:H183	1.98	0.45
1:A:96:ARG:NH1	1:A:380:SER:OG	2.50	0.45
1:A:223:ASP:OD1	1:A:223:ASP:C	2.54	0.45
3:A:601:STR:H213	3:A:601:STR:C18	2.46	0.45
1:A:381:LEU:HB2	1:A:386:VAL:HG21	1.98	0.45
1:B:396:MET:CE	1:B:399:ILE:HD11	2.46	0.45
1:B:433:PHE:CD2	1:B:443:GLU:HG3	2.51	0.45
1:A:264:GLY:O	1:A:265:GLU:HG2	2.17	0.45
1:A:441:VAL:CG2	2:A:600:HEM:HMD2	2.47	0.45
1:A:66:GLN:HG3	1:A:67:TYR:CD2	2.52	0.45
1:B:83:VAL:HG13	1:B:88:LEU:HB3	1.99	0.44
1:B:154:GLN:O	1:B:456:ARG:NH2	2.50	0.44
1:A:413:ASN:OD1	1:A:415:GLU:HB2	2.17	0.44
1:A:149:LEU:CD2	1:A:448:ILE:HG21	2.48	0.44
1:A:138:SER:O	1:A:142:PHE:HD1	2.00	0.44
1:A:336:VAL:HG12	1:A:337:GLY:N	2.33	0.43
1:A:373:HIS:HE1	2:A:600:HEM:O1A	2.02	0.43
1:A:283:GLY:O	1:A:284:ALA:C	2.56	0.43
1:A:139:PHE:CE1	1:A:269:LEU:HD11	2.53	0.43
1:A:450:LEU:O	1:A:454:VAL:CG2	2.64	0.43
1:B:140:THR:O	1:B:142:PHE:N	2.41	0.43
1:B:305:GLU:O	1:B:309:THR:CB	2.67	0.43
1:B:466:PRO:O	1:B:467:SER:C	2.55	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:PHE:CD1	1:A:191:PHE:N	2.86	0.43
1:A:320:HIS:CG	1:A:474:LEU:HD11	2.54	0.43
1:B:74:TYR:CE2	1:B:79:LEU:HD13	2.54	0.42
1:B:259:LYS:HG3	1:B:260:SER:N	2.34	0.42
1:A:191:PHE:CG	1:A:253:LYS:HG2	2.54	0.42
1:B:410:GLU:H	1:B:410:GLU:CD	2.23	0.42
1:A:355:ALA:HB1	1:A:414:PRO:O	2.20	0.42
1:A:381:LEU:HD23	1:A:382:GLY:H	1.85	0.42
1:B:359:GLU:OE1	1:B:416:ARG:CD	2.67	0.42
1:A:288:THR:HG1	1:A:290:ASP:H	1.65	0.42
1:A:396:MET:CE	1:A:399:ILE:HD11	2.50	0.42
1:B:140:THR:C	1:B:142:PHE:N	2.73	0.42
1:B:371:ILE:HD11	3:B:601:STR:H181	2.01	0.42
1:A:307:THR:HG21	1:A:449:GLU:OE1	2.20	0.41
1:B:151:THR:O	1:B:152:ILE:C	2.58	0.41
1:B:304:VAL:O	1:B:305:GLU:HB2	2.19	0.41
1:B:340:ARG:O	1:B:459:GLN:NE2	2.39	0.41
1:A:359:GLU:OE2	1:A:362:ARG:NH1	2.48	0.41
1:B:144:GLU:HG3	1:B:145:GLY:H	1.85	0.41
1:B:324:LEU:O	1:B:328:VAL:HG23	2.20	0.41
1:B:324:LEU:HD21	1:B:414:PRO:HG2	2.02	0.41
1:A:113:THR:O	1:A:114:GLN:C	2.59	0.41
1:A:434:GLY:O	1:A:435:ALA:HB2	2.21	0.41
1:A:189:LEU:HD21	1:A:445:LEU:CD1	2.50	0.41
1:A:303:GLY:O	1:A:307:THR:OG1	2.30	0.41
1:A:352:LEU:O	1:A:353:LEU:C	2.59	0.41
1:B:142:PHE:CD1	1:B:149:LEU:HB2	2.56	0.40
1:B:174:LEU:HD11	1:B:489:VAL:HG11	2.03	0.40
1:B:456:ARG:HB2	1:B:457:PRO:HD3	2.02	0.40
1:A:158:ASP:OD1	1:A:456:ARG:CZ	2.69	0.40
1:A:255:LEU:HD12	1:A:255:LEU:HA	1.92	0.40
1:A:344:LEU:HD23	1:A:452:LEU:HD13	2.03	0.40
1:B:381:LEU:HD23	1:B:382:GLY:N	2.37	0.40
1:B:118:ASP:OD2	1:B:298:GLU:OE2	2.40	0.40
1:A:313:TRP:CZ3	1:A:484:PRO:HB3	2.56	0.40
1:B:396:MET:HE2	1:B:396:MET:HA	2.04	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	414/486 (85%)	383 (92%)	25 (6%)	6 (1%)	11	28
1	B	417/486 (86%)	387 (93%)	18 (4%)	12 (3%)	4	10
All	All	831/972 (86%)	770 (93%)	43 (5%)	18 (2%)	6	17

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	PRO
1	B	492	THR
1	A	175	SER
1	A	281	SER
1	B	175	SER
1	B	259	LYS
1	B	305	GLU
1	B	467	SER
1	A	284	ALA
1	B	234	LYS
1	B	338	VAL
1	B	372	PRO
1	B	141	LEU
1	A	493	PRO
1	B	340	ARG
1	B	419	GLU
1	B	466	PRO
1	A	222	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	369/427 (86%)	335 (91%)	34 (9%)	9	21
1	B	369/427 (86%)	329 (89%)	40 (11%)	6	15
All	All	738/854 (86%)	664 (90%)	74 (10%)	7	18

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	81	LEU
1	A	89	VAL
1	A	94	LEU
1	A	96	ARG
1	A	112	LEU
1	A	137	SER
1	A	174	LEU
1	A	182	VAL
1	A	188	ARG
1	A	191	PHE
1	A	214	GLN
1	A	236	LEU
1	A	238	ARG
1	A	253	LYS
1	A	254	LEU
1	A	255	LEU
1	A	267	ARG
1	A	268	ASP
1	A	271	ASP
1	A	278	GLN
1	A	288	THR
1	A	380	SER
1	A	385	SER
1	A	396	MET
1	A	416	ARG
1	A	419	GLU
1	A	452	LEU
1	A	453	PHE
1	A	460	ARG
1	A	462	SER
1	A	477	ARG
1	A	489	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	492	THR
1	B	59	LEU
1	B	65	SER
1	B	71	PHE
1	B	94	LEU
1	B	96	ARG
1	B	107	VAL
1	B	108	THR
1	B	112	LEU
1	B	141	LEU
1	B	159	SER
1	B	168	ARG
1	B	182	VAL
1	B	191	PHE
1	B	194	SER
1	B	196	GLN
1	B	214	GLN
1	B	235	ASP
1	B	236	LEU
1	B	237	LYS
1	B	250	LEU
1	B	253	LYS
1	B	255	LEU
1	B	259	LYS
1	B	271	ASP
1	B	285	ASP
1	B	306	THR
1	B	308	SER
1	B	332	LEU
1	B	345	SER
1	B	380	SER
1	B	381	LEU
1	B	396	MET
1	B	410	GLU
1	B	415	GLU
1	B	416	ARG
1	B	441	VAL
1	B	444	SER
1	B	452	LEU
1	B	460	ARG
1	B	475	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	291	HIS
1	A	373	HIS
1	B	114	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 ⓘ

4 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	STR	B	601	-	26,26,26	2.29	7 (26%)	42,42,42	1.67	13 (30%)
2	HEM	B	600	1	40,49,50	1.45	5 (12%)	42,80,82	2.01	13 (30%)
2	HEM	A	600	1	40,49,50	1.49	8 (20%)	42,80,82	2.27	15 (35%)
3	STR	A	601	-	26,26,26	2.55	8 (30%)	42,42,42	1.60	8 (19%)

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	STR	B	601	-	-	2/4/62/62	0/4/4/4
2	HEM	B	600	1	-	6/10/53/54	-
2	HEM	A	600	1	-	4/10/53/54	-
3	STR	A	601	-	-	2/4/62/62	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	STR	C2-C3	-5.61	1.37	1.49
3	A	601	STR	C6-C5	-5.39	1.41	1.50
3	A	601	STR	C10-C5	-5.24	1.42	1.52
3	A	601	STR	C17-C20	4.95	1.58	1.51
3	B	601	STR	C10-C5	-4.84	1.43	1.52
2	A	600	HEM	C1B-NB	-4.77	1.32	1.40
2	B	600	HEM	C1B-NB	-4.74	1.32	1.40
3	B	601	STR	C6-C5	-4.72	1.42	1.50
3	B	601	STR	C4-C5	4.64	1.41	1.34
3	B	601	STR	C2-C3	-4.59	1.39	1.49
3	A	601	STR	C4-C5	4.06	1.40	1.34
3	B	601	STR	C13-C17	-3.56	1.50	1.56
2	A	600	HEM	C4D-ND	-3.42	1.34	1.40
3	A	601	STR	C4-C3	-3.06	1.39	1.45
3	A	601	STR	C11-C9	3.01	1.58	1.53
2	B	600	HEM	C4D-ND	-2.98	1.35	1.40
3	B	601	STR	C4-C3	-2.79	1.39	1.45
3	A	601	STR	C21-C20	2.71	1.56	1.49
2	B	600	HEM	FE-NB	2.49	2.09	1.96
2	B	600	HEM	C4B-NB	-2.42	1.33	1.38
2	A	600	HEM	FE-NB	2.41	2.08	1.96
2	A	600	HEM	C1D-ND	-2.27	1.34	1.38
2	A	600	HEM	O2A-CGA	-2.18	1.23	1.30
2	A	600	HEM	C3D-C2D	-2.18	1.32	1.36
2	A	600	HEM	C4B-NB	-2.16	1.34	1.38
3	B	601	STR	C11-C9	2.12	1.57	1.53
2	A	600	HEM	FE-ND	-2.12	1.86	1.96
2	B	600	HEM	FE-ND	-2.02	1.86	1.96

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	CHD-C1D-ND	6.08	131.03	124.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	HEM	CHD-C1D-ND	4.82	129.67	124.43
2	A	600	HEM	C1B-NB-C4B	4.42	109.64	105.07
2	B	600	HEM	CHA-C4D-ND	4.40	129.82	124.38
3	B	601	STR	C13-C17-C20	-4.00	109.34	114.98
2	A	600	HEM	CHA-C4D-ND	3.98	129.30	124.38
2	B	600	HEM	C1B-NB-C4B	3.88	109.08	105.07
2	A	600	HEM	CHC-C4B-NB	3.86	128.62	124.43
3	A	601	STR	C14-C8-C9	-3.84	103.95	109.09
2	B	600	HEM	CMB-C2B-C1B	3.66	130.62	125.04
2	A	600	HEM	CHD-C1D-C2D	-3.66	119.27	124.98
2	A	600	HEM	CAA-CBA-CGA	-3.60	103.68	113.76
3	B	601	STR	C12-C11-C9	-3.51	107.03	113.11
3	A	601	STR	C2-C3-C4	3.45	122.06	116.74
2	B	600	HEM	CHC-C4B-NB	3.28	127.99	124.43
2	B	600	HEM	CHD-C1D-C2D	-3.22	119.96	124.98
2	A	600	HEM	CAD-C3D-C4D	3.20	130.26	124.66
3	A	601	STR	C13-C14-C8	-3.19	109.65	114.38
3	A	601	STR	C1-C10-C9	-3.04	104.47	108.73
2	A	600	HEM	CMA-C3A-C4A	-3.00	123.86	128.46
2	A	600	HEM	CHB-C1B-NB	2.97	128.06	124.38
2	A	600	HEM	CHA-C4D-C3D	-2.94	119.81	125.33
2	B	600	HEM	CHA-C4D-C3D	-2.92	119.85	125.33
3	B	601	STR	C2-C3-C4	2.79	121.03	116.74
3	B	601	STR	C13-C14-C8	-2.78	110.26	114.38
3	A	601	STR	C12-C11-C9	-2.77	108.31	113.11
2	A	600	HEM	CBA-CAA-C2A	2.67	117.17	112.62
2	A	600	HEM	CMB-C2B-C1B	2.60	128.99	125.04
3	A	601	STR	C21-C20-C17	2.59	121.33	117.56
2	A	600	HEM	CMD-C2D-C1D	2.48	128.81	125.04
2	A	600	HEM	CAB-C3B-C2B	-2.45	120.53	128.60
3	B	601	STR	C7-C8-C14	-2.44	107.91	112.08
2	B	600	HEM	CMA-C3A-C4A	-2.42	124.74	128.46
2	B	600	HEM	CAB-C3B-C2B	-2.32	120.97	128.60
3	B	601	STR	C9-C10-C5	-2.30	106.04	109.65
3	A	601	STR	C17-C13-C14	2.30	102.18	99.72
3	B	601	STR	C15-C14-C8	-2.23	115.41	119.08
2	B	600	HEM	CMB-C2B-C3B	-2.22	122.88	128.30
3	A	601	STR	C16-C17-C13	-2.18	102.27	104.21
2	B	600	HEM	CHB-C1B-NB	2.18	127.07	124.38
2	B	600	HEM	C4B-CHC-C1C	2.18	125.43	122.56
2	A	600	HEM	CMA-C3A-C2A	2.15	129.00	124.94
3	B	601	STR	C16-C17-C13	-2.09	102.34	104.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	STR	C2-C1-C10	2.06	117.32	113.45
3	B	601	STR	C14-C8-C9	-2.04	106.36	109.09
3	B	601	STR	C11-C12-C13	-2.03	109.29	112.78
3	B	601	STR	C18-C13-C14	2.03	115.49	111.71
2	B	600	HEM	O2A-CGA-CBA	2.03	120.54	114.03
3	B	601	STR	C6-C5-C4	-2.01	117.50	120.87

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	HEM	C3A-C2A-CAA-CBA
2	B	600	HEM	C3D-CAD-CBD-CGD
2	A	600	HEM	C4B-C3B-CAB-CBB
2	B	600	HEM	C4B-C3B-CAB-CBB
3	A	601	STR	C16-C17-C20-O20
3	A	601	STR	C16-C17-C20-C21
3	B	601	STR	C16-C17-C20-C21
2	A	600	HEM	C3A-C2A-CAA-CBA
2	B	600	HEM	C1A-C2A-CAA-CBA
3	B	601	STR	C16-C17-C20-O20
2	B	600	HEM	CAA-CBA-CGA-O1A
2	A	600	HEM	CAA-CBA-CGA-O1A
2	A	600	HEM	CAA-CBA-CGA-O2A
2	B	600	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.
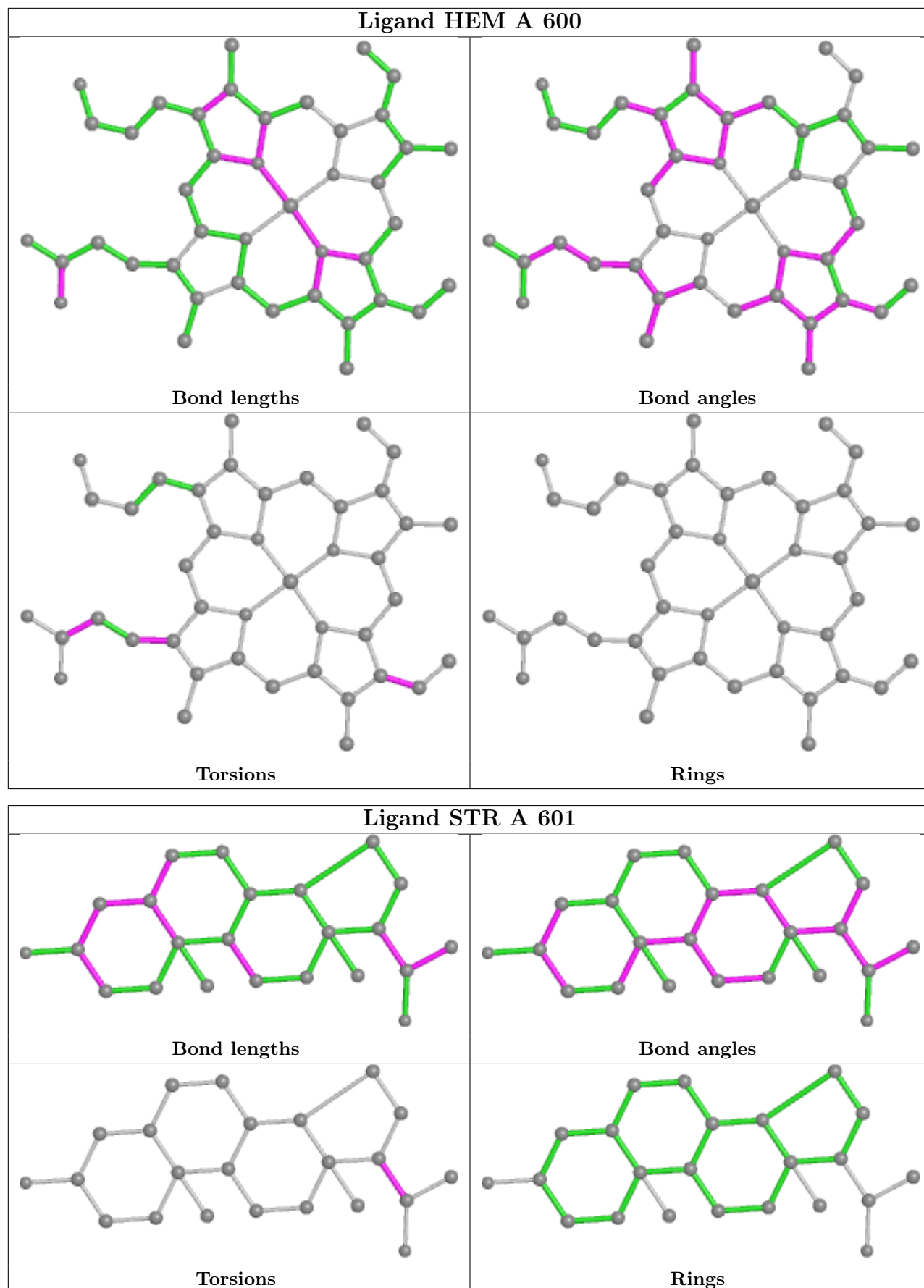
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	STR	2	0
2	B	600	HEM	3	0
2	A	600	HEM	5	0
3	A	601	STR	3	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 STR B 601

Bond lengths   Bond angles

Torsions   Rings

Ligand HEM B 600

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand STR A 601

Bond lengths

Bond angles

Torsions

Rings
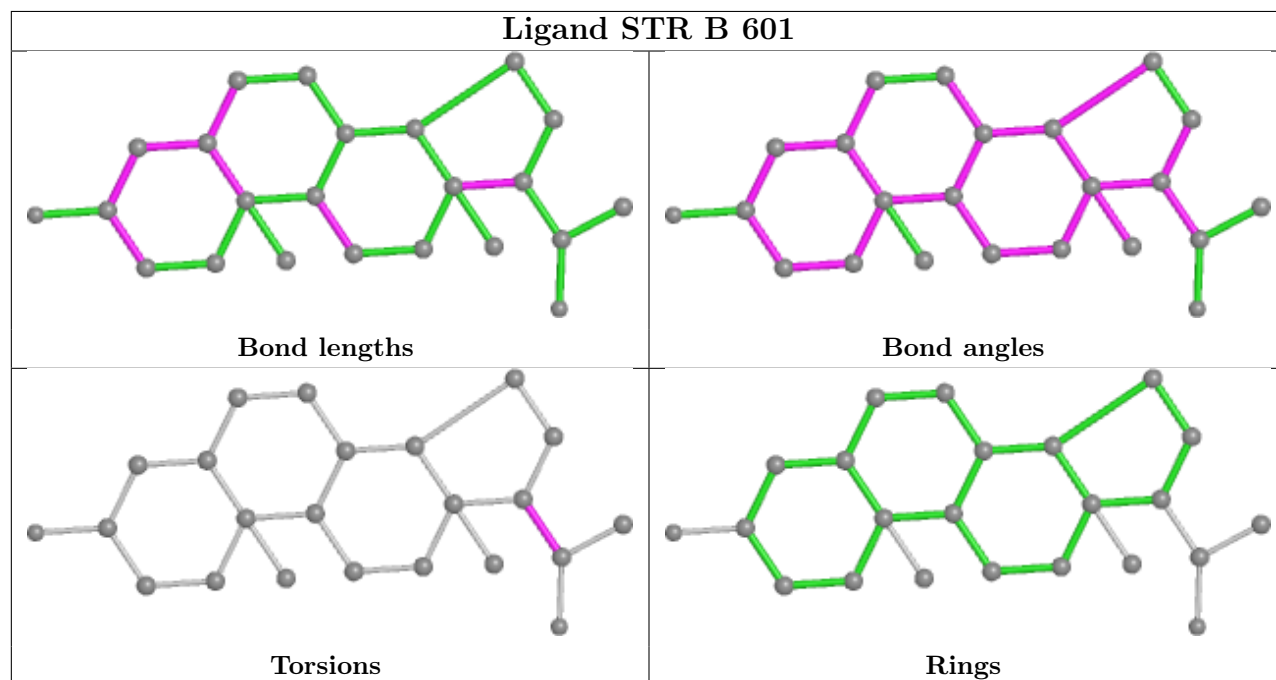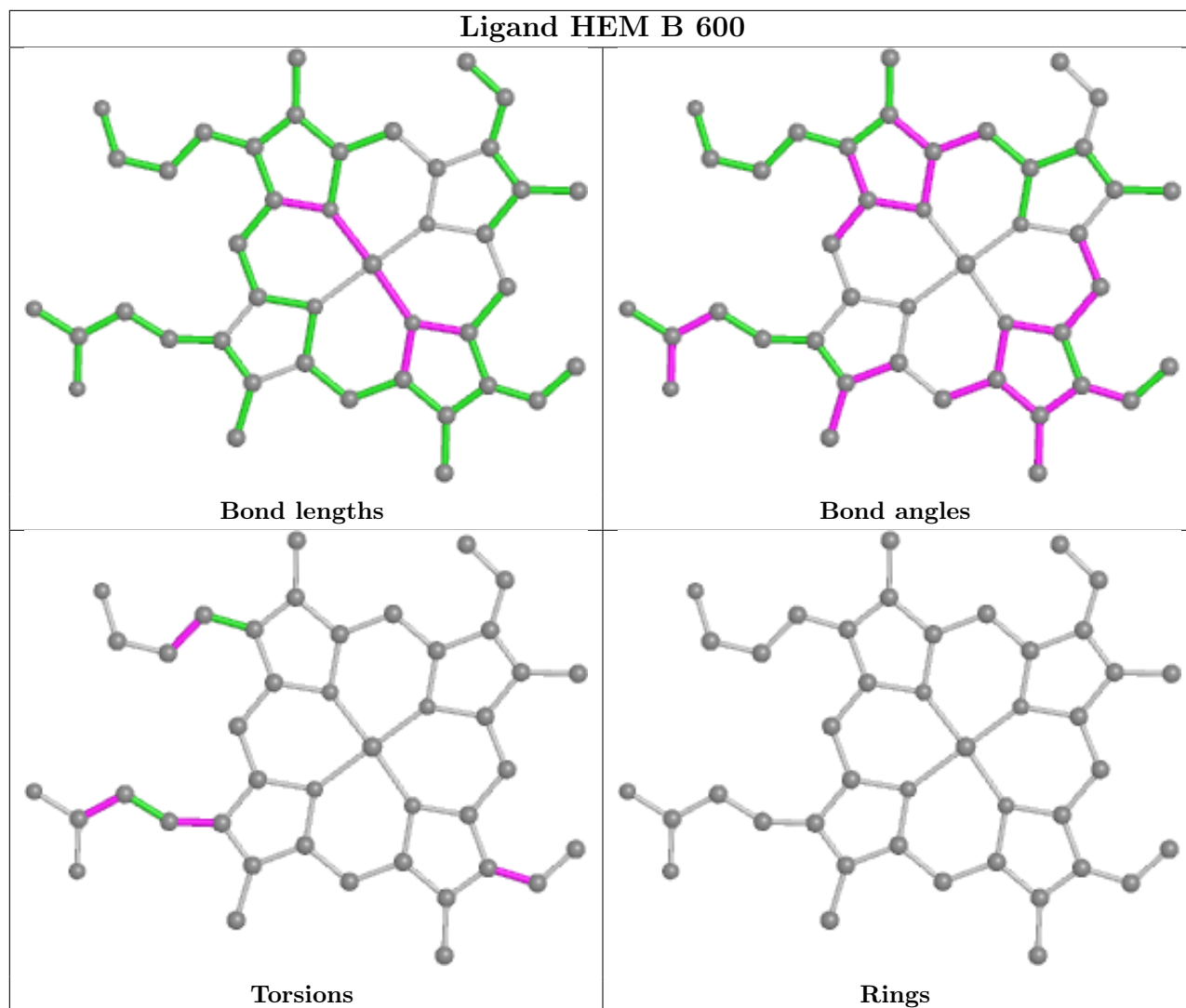
5.7 Other polymers ⓘ

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	422/486 (86%)	-0.08	12 (2%)	53	54	30, 52, 86, 125	1 (0%)
1	B	423/486 (87%)	0.05	12 (2%)	53	54	35, 62, 108, 130	2 (0%)
All	All	845/972 (86%)	-0.02	24 (2%)	53	54	30, 57, 102, 130	3 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	GLU	4.5
1	A	167	CYS	3.4
1	B	265	GLU	3.4
1	B	338	VAL	3.4
1	A	53	ASN	3.3
1	B	335	CYS	3.3
1	A	264	GLY	3.3
1	B	275	ILE	3.1
1	A	146	SER	2.8
1	B	334	GLU	2.7
1	A	169	GLY	2.6
1	B	168	ARG	2.6
1	B	266	PRO	2.5
1	A	419	GLU	2.5
1	A	236	LEU	2.5
1	B	278	GLN	2.4
1	A	168	ARG	2.4
1	A	266	PRO	2.3
1	B	282	GLY	2.2
1	B	264	GLY	2.2
1	A	338	VAL	2.2
1	A	262	THR	2.1
1	B	420	PRO	2.0
1	B	468	GLU	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.

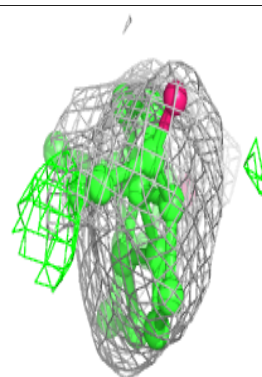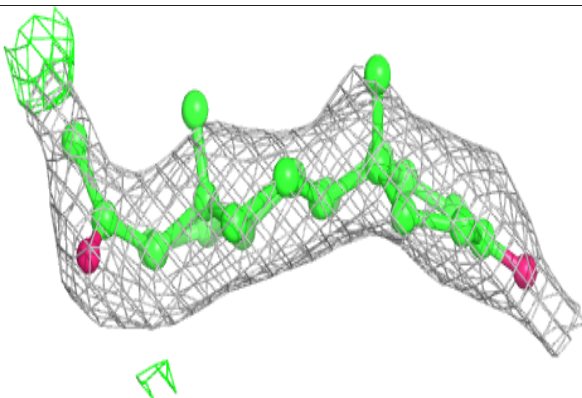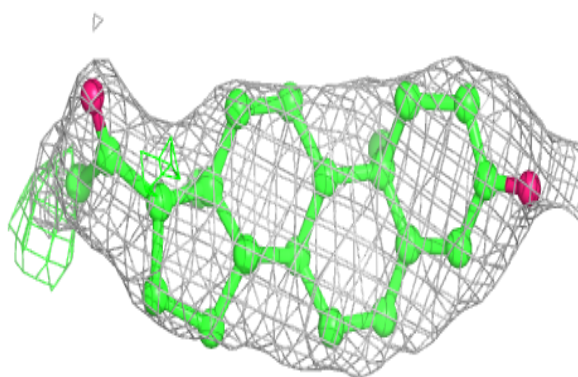| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	STR	B	601	23/23	0.91	0.21	36,39,41,45	0
3	STR	A	601	23/23	0.93	0.19	42,44,50,51	0
2	HEM	B	600	42/43	0.96	0.17	24,26,30,31	0
2	HEM	A	600	42/43	0.97	0.13	18,24,27,32	0

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.
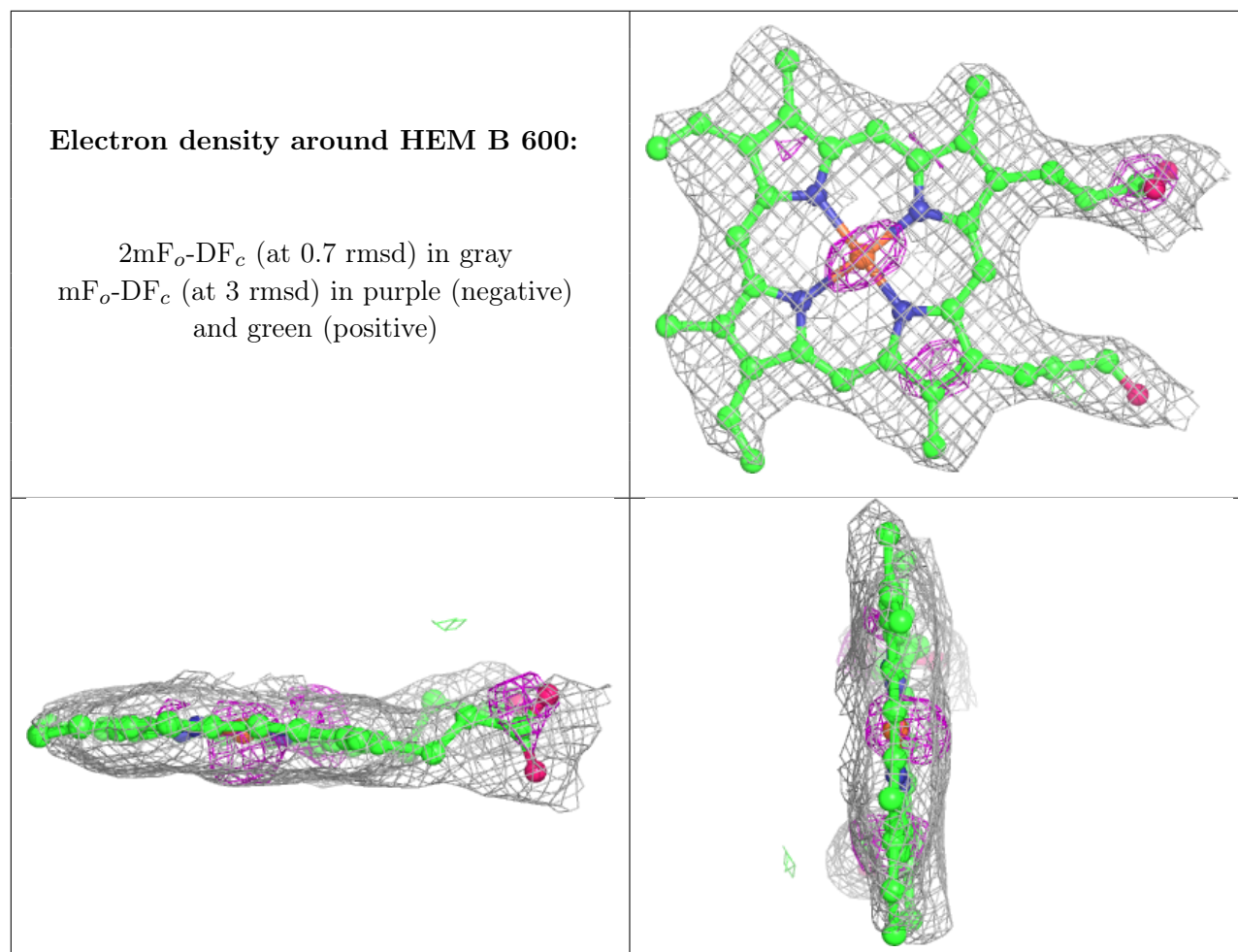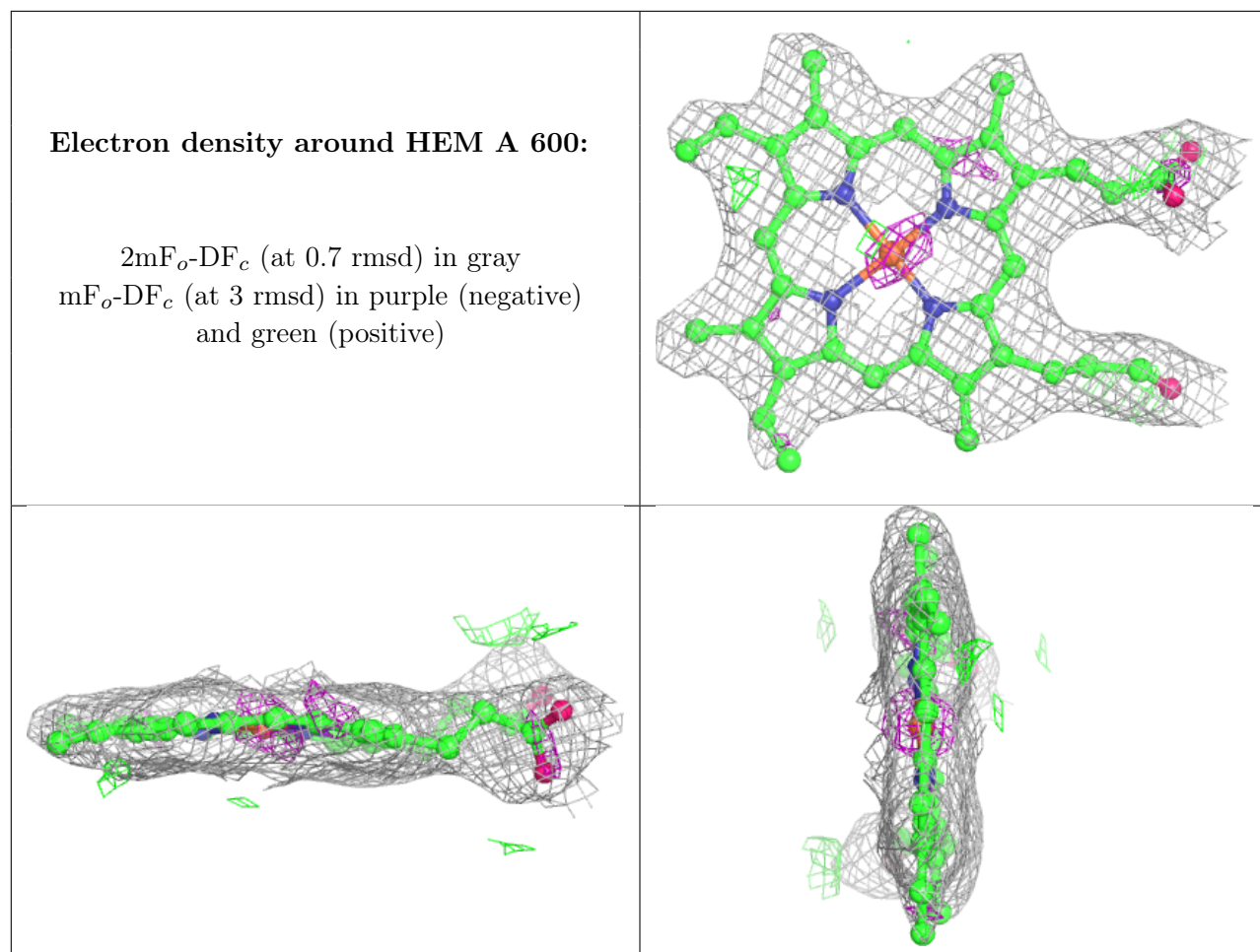
Electron density around STR B 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
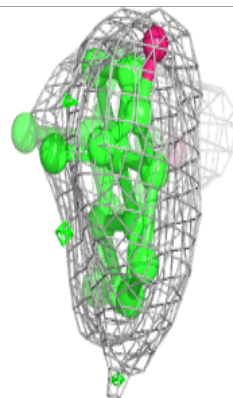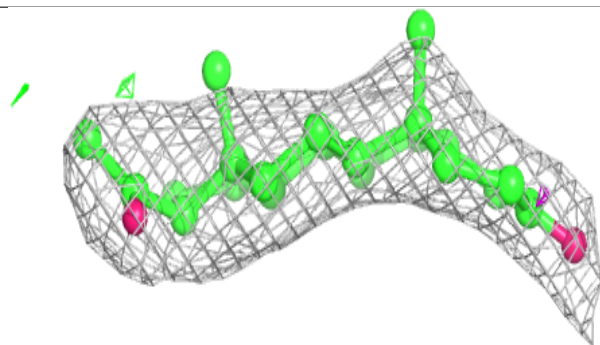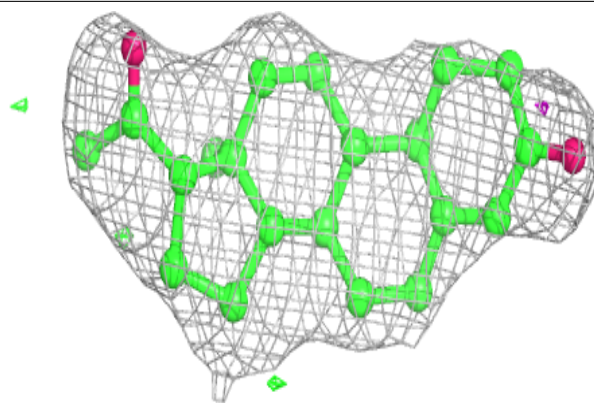
Electron density around STR A 601:

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

Electron density around HEM B 600:

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 600:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.