Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 02:23 AM EDT

PDB ID	:	1Q2O
Title	:	Bovine endothelial nitric oxide synthase N368D mutant heme domain dimer with L-N(omega)-nitroarginine-2,4-L-diaminobutyramide bound
Authors	:	Flinspach, M.L.; Li, H.; Jamal, J.; Yang, W.; Huang, H.; Hah, J.M.; Gomez-Vidal, J.A.; Litzinger, E.A.; Silverman, R.B.; Poulos, T.L.
Deposited on	:	2003-07-25
Resolution	:	1.74 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 following versions of software and data (see references (i)) were used in the production of this report:

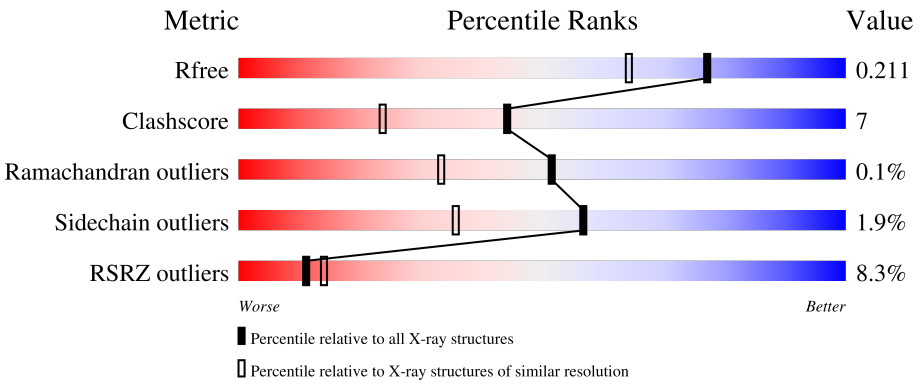
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	416	11% 87% 9% • •
1	B	416	6% 86% 11% • •

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
2	CAC	B	851	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7278 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.

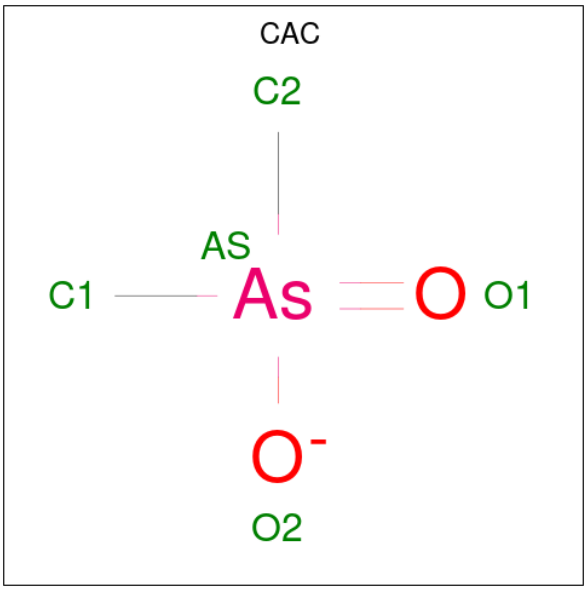
- Molecule 1 is a protein called Nitric-oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	3216	2046	564	590	16	0	0	0
1	B	405	3223	2050	567	590	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

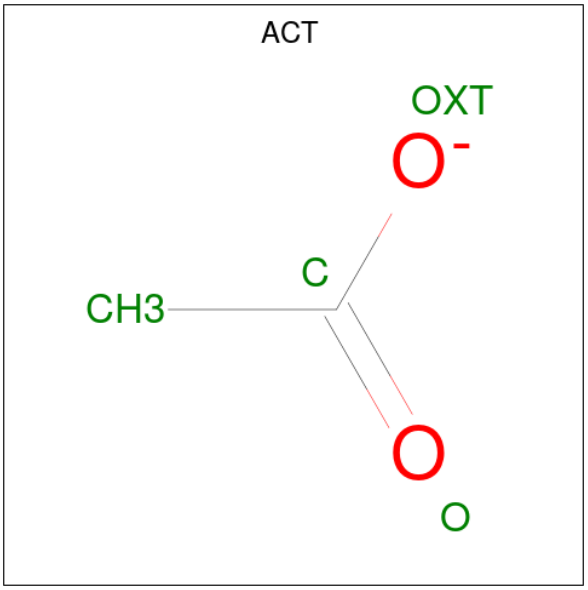
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	conflict	UNP P29473
A	368	ASP	ASN	engineered mutation	UNP P29473
B	100	ARG	CYS	conflict	UNP P29473
B	368	ASP	ASN	engineered mutation	UNP P29473

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	As	C		
2	A	1	3	1	2	0	0
			Total	As	C		
2	B	1	3	1	2	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

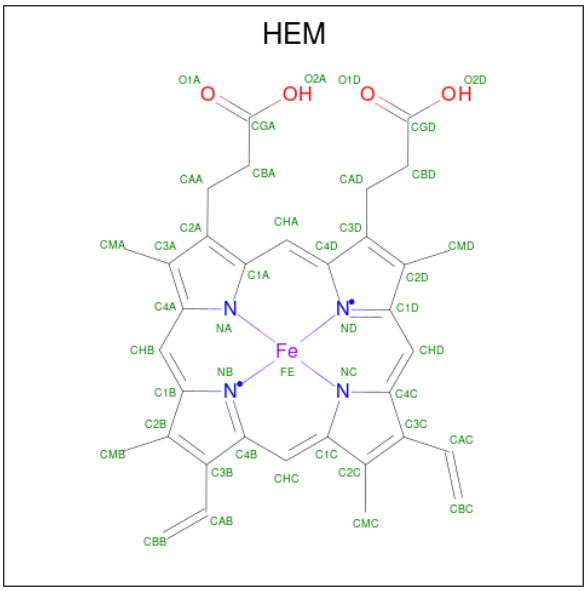


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

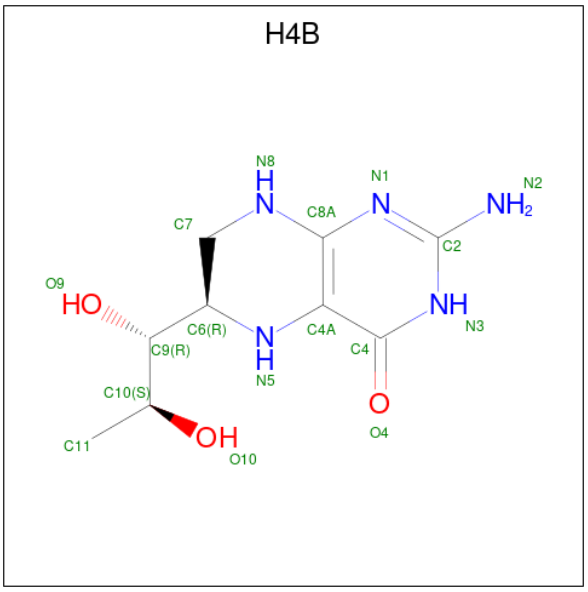
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	17	9	5	3	0	0

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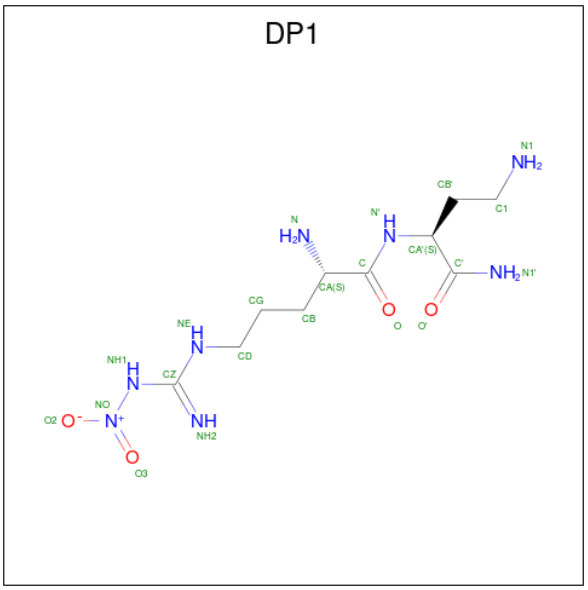
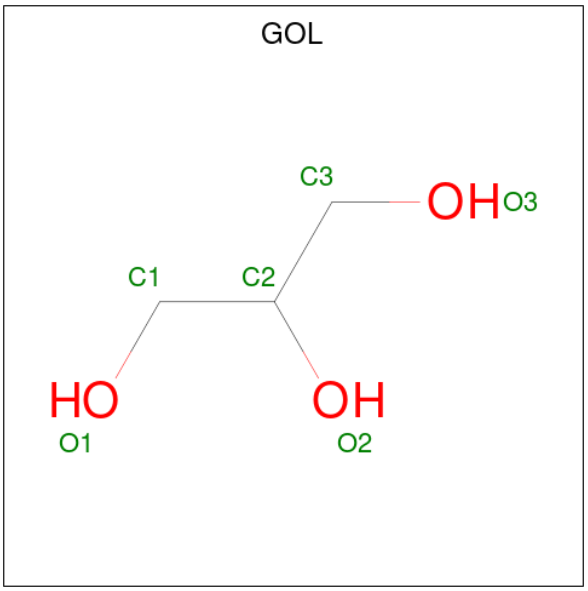
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	17	9	5	3	0	0

- Molecule 7 is L-N(OMEGA)-NITROARGININE-2,4-L-DIAMINOBUTYRIC AMIDE (three-letter code: DP1) (formula: $C_{10}H_{22}N_8O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	44	20	16	8	0	1
			Total	C	N	O		
7	B	1	44	20	16	8	0	1

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0
			Total	C	O		
8	B	1	6	3	3	0	0

- Molecule 9 is water.

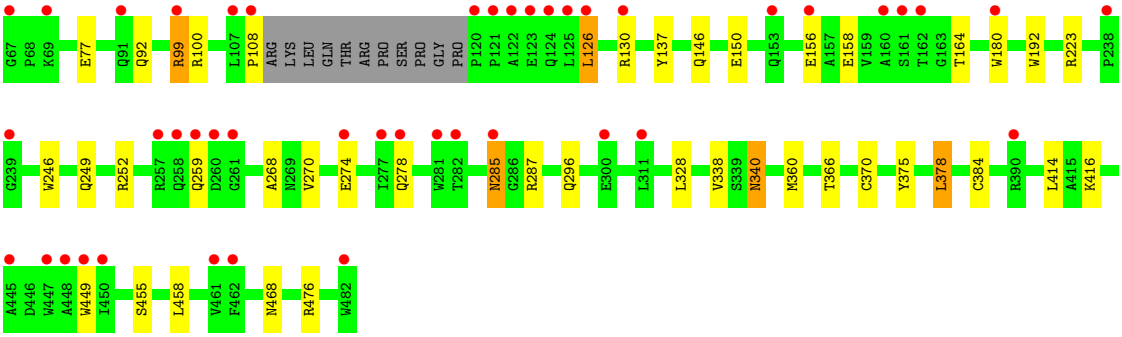
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	320	320	320	0	5
			Total	O		
9	B	284	284	284	0	4

3 Residue-property plots (i)

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.

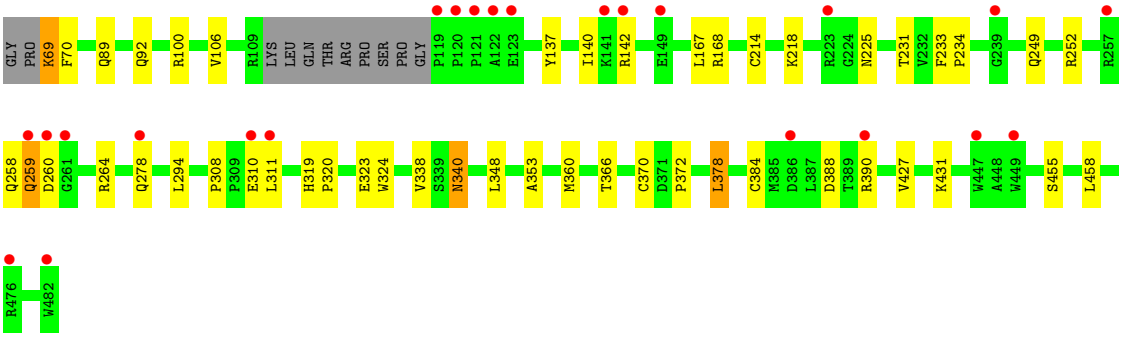
• Molecule 1: Nitric-oxide synthase, endothelial

Chain A:



• Molecule 1: Nitric-oxide synthase, endothelial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.91Å 106.99Å 156.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.44 – 1.74 48.44 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.44-1.74) 97.7 (48.44-1.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.74Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193 , 0.220 0.185 , 0.211	Depositor DCC
R_{free} test set	4908 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.6	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	0.95	EDS
Total number of atoms	7278	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, DP1, HEM, GOL, H4B, ZN, ACT

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	0.36	0/3307	0.63	1/4506 (0.0%)
1	B	0.35	0/3314	0.63	1/4515 (0.0%)
All	All	0.35	0/6621	0.63	2/9021 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	360	MET	N-CA-C	-6.03	94.71	111.00
1	A	360	MET	N-CA-C	-5.56	95.98	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	TYR	Sidechain
1	B	137	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3216	0	3120	40	0
1	B	3223	0	3130	44	0
2	A	3	0	0	1	0
2	B	3	0	0	2	0
3	A	4	0	3	1	0
3	B	4	0	3	0	0
4	A	1	0	0	0	0
5	A	43	0	30	1	0
5	B	43	0	30	0	0
6	A	17	0	15	1	0
6	B	17	0	15	0	0
7	A	44	0	42	1	0
7	B	44	0	42	2	0
8	A	6	0	8	0	0
8	B	6	0	8	1	0
9	A	320	0	0	9	0
9	B	284	0	0	8	0
All	All	7278	0	6446	87	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 7.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PRO:HB2	1:B:311:LEU:HD13	1.41	1.03
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.30	0.95
1:B:259:GLN:HG2	1:B:260:ASP:H	1.31	0.94
1:B:384:CYS:SG	2:B:851:CAC:AS	2.93	0.87
1:A:384:CYS:SG	2:A:850:CAC:AS	2.95	0.84
1:A:126:LEU:HD12	1:A:130:ARG:HE	1.46	0.79
1:B:259:GLN:HG2	1:B:260:ASP:N	2.01	0.76
1:B:310:GLU:HG2	1:B:311:LEU:HD12	1.73	0.70
1:B:323:GLU:H	1:B:323:GLU:CD	1.98	0.66
1:B:388:ASP:OD1	1:B:390:ARG:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.76	0.66
1:A:99:ARG:HB2	1:A:99:ARG:NH1	2.08	0.65
1:A:259:GLN:CD	1:A:259:GLN:H	2.01	0.64
1:B:378:LEU:HB2	9:B:941:HOH:O	1.98	0.64
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.82	0.61
1:A:268:ALA:HB3	9:A:1125:HOH:O	2.00	0.60
1:A:126:LEU:O	1:A:130:ARG:HG3	2.05	0.57
1:B:140:ILE:HD12	1:B:142:ARG:HD2	1.85	0.57
1:A:146:GLN:HG2	1:A:150:GLU:OE2	2.06	0.56
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.88	0.55
1:A:378:LEU:HB2	9:A:919:HOH:O	2.05	0.55
1:A:252:ARG:NH2	9:A:1125:HOH:O	2.39	0.54
1:A:99:ARG:HH11	1:A:99:ARG:CB	2.10	0.54
1:B:340:ASN:HD22	1:B:340:ASN:H	1.55	0.54
1:B:89:GLN:HE21	1:B:89:GLN:HA	1.73	0.54
1:B:427:VAL:HG12	1:B:431:LYS:NZ	2.23	0.53
1:B:106:VAL:HG21	8:B:881:GOL:H12	1.91	0.52
1:B:366:THR:O	1:B:370:CYS:HB2	2.09	0.52
1:A:414:LEU:O	1:A:414:LEU:HD23	2.09	0.52
1:B:249:GLN:HB2	1:B:252:ARG:HD3	1.90	0.52
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.44	0.52
1:B:89:GLN:HA	1:B:89:GLN:NE2	2.25	0.52
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.75	0.51
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.93	0.51
1:B:278:GLN:HB2	9:B:1015:HOH:O	2.10	0.51
1:A:338:VAL:HG23	9:A:1115:HOH:O	2.10	0.51
1:B:259:GLN:CG	1:B:260:ASP:H	2.14	0.50
1:B:324:TRP:HB2	2:B:851:CAC:C1	2.40	0.50
1:A:108:PRO:HD2	9:A:1060:HOH:O	2.12	0.50
1:A:108:PRO:HG3	9:A:1008:HOH:O	2.12	0.50
1:A:270:VAL:O	1:A:274:GLU:HG3	2.12	0.49
1:A:246:TRP:HE1	1:A:296:GLN:NE2	2.10	0.49
1:B:427:VAL:HG12	1:B:431:LYS:HZ2	1.76	0.49
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.52	0.49
1:A:274:GLU:O	1:A:278:GLN:HG3	2.13	0.48
1:B:214:CYS:O	1:B:218:LYS:HG3	2.14	0.48
1:A:92:GLN:HE22	1:A:476:ARG:HH22	1.62	0.47
1:B:249:GLN:NE2	1:B:252:ARG:HH21	2.13	0.47
1:A:340:ASN:H	1:A:340:ASN:HD22	1.63	0.47
1:B:69:LYS:HE2	1:B:70:PHE:CD1	2.50	0.47
1:B:89:GLN:HE21	1:B:89:GLN:CA	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:NH2	9:A:1113:HOH:O	2.48	0.46
7:B:791[A]:DP1:HB'2	9:B:1053[A]:HOH:O	2.15	0.46
1:B:92:GLN:NE2	9:B:1164:HOH:O	2.48	0.46
1:B:252:ARG:NH2	9:B:1097:HOH:O	2.49	0.46
1:A:366:THR:O	1:A:370:CYS:HB2	2.16	0.46
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.96	0.46
7:B:791[B]:DP1:HB'1	9:B:1107[B]:HOH:O	2.16	0.45
1:A:449:TRP:HA	6:A:760:H4B:N1	2.31	0.45
1:A:285:ASN:H	1:A:285:ASN:HD22	1.64	0.44
1:A:287:ARG:HG2	1:A:375:TYR:HE2	1.82	0.44
1:A:126:LEU:HD11	1:A:156:GLU:CG	2.47	0.44
1:A:252:ARG:NH1	9:A:1126[B]:HOH:O	2.51	0.44
1:B:252:ARG:NH2	9:B:1096:HOH:O	2.50	0.43
1:A:158:GLU:HG2	1:A:164:THR:O	2.19	0.43
3:A:860:ACT:H2	5:A:700:HEM:HMB3	2.01	0.43
1:A:249:GLN:HB2	1:A:252:ARG:CG	2.48	0.43
1:B:310:GLU:HG2	1:B:311:LEU:CD1	2.46	0.43
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.49	0.42
1:B:340:ASN:HD22	1:B:340:ASN:N	2.14	0.42
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.59	0.42
1:A:249:GLN:HB2	1:A:252:ARG:HG2	2.01	0.42
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.54	0.42
1:B:249:GLN:NE2	1:B:252:ARG:NH2	2.68	0.42
1:A:285:ASN:HD22	1:A:285:ASN:N	2.18	0.41
7:A:790[A]:DP1:HB'2	9:A:1016:HOH:O	2.20	0.41
1:B:338:VAL:HG23	9:B:1087:HOH:O	2.20	0.41
1:B:258:GLN:NE2	1:B:264:ARG:HB2	2.36	0.41
1:B:323:GLU:CD	1:B:323:GLU:N	2.71	0.41
1:A:259:GLN:CD	1:A:259:GLN:N	2.70	0.40
1:A:340:ASN:HD22	1:A:340:ASN:N	2.18	0.40
1:A:416:LYS:HB3	1:A:416:LYS:HE2	1.88	0.40
1:B:168:ARG:HD3	1:B:168:ARG:HA	1.79	0.40
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.93	0.40
1:B:340:ASN:H	1:B:340:ASN:ND2	2.19	0.40
1:B:140:ILE:O	1:B:142:ARG:HG3	2.21	0.40
1:B:231:THR:O	1:B:353:ALA:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	401/416 (96%)	393 (98%)	8 (2%)	0	100	100
1	B	401/416 (96%)	391 (98%)	9 (2%)	1 (0%)	47	29
All	All	802/832 (96%)	784 (98%)	17 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLN

5.3.2 Protein sidechains (i)

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	344/354 (97%)	336 (98%)	8 (2%)	50	27
1	B	345/354 (98%)	340 (99%)	5 (1%)	67	50
All	All	689/708 (97%)	676 (98%)	13 (2%)	57	36

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	100	ARG
1	A	126	LEU
1	A	285	ASN
1	A	328	LEU

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Mol	Chain	Res	Type
1	A	340	ASN
1	A	378	LEU
1	A	468	ASN
1	B	69	LYS
1	B	100	ARG
1	B	225	ASN
1	B	340	ASN
1	B	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	191	GLN
1	A	207	GLN
1	A	278	GLN
1	A	279	HIS
1	A	285	ASN
1	A	296	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	89	GLN
1	B	92	GLN
1	B	146	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	249	GLN
1	B	258	GLN
1	B	278	GLN
1	B	279	HIS
1	B	405	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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	$\#\|Z\| > 2$
7	DP1	B	791[B]	-	17,21,21	0.91	1 (5%)	20,26,26	1.06	1 (5%)
3	ACT	A	860	-	1,3,3	3.02	1 (100%)	0,3,3	-	-
2	CAC	B	851	-	0,2,4	-	-	0,1,6	-	-
7	DP1	A	790[B]	-	17,21,21	0.95	1 (5%)	20,26,26	1.06	0
6	H4B	A	760	-	16,18,18	2.07	4 (25%)	11,26,26	4.29	9 (81%)
6	H4B	B	761	-	16,18,18	1.92	3 (18%)	11,26,26	4.34	9 (81%)
8	GOL	B	881	-	5,5,5	0.28	0	5,5,5	0.23	0
2	CAC	A	850	-	0,2,4	-	-	0,1,6	-	-
5	HEM	B	700	1	27,50,50	1.53	4 (14%)	17,82,82	1.57	4 (23%)
8	GOL	A	880	-	5,5,5	0.31	0	5,5,5	0.32	0
3	ACT	B	861	-	1,3,3	3.19	1 (100%)	0,3,3	-	-
7	DP1	A	790[A]	-	17,21,21	0.90	1 (5%)	20,26,26	0.99	1 (5%)
7	DP1	B	791[A]	-	17,21,21	1.00	1 (5%)	20,26,26	0.98	1 (5%)
5	HEM	A	700	1	27,50,50	1.58	6 (22%)	17,82,82	1.40	2 (11%)

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
7	DP1	B	791[B]	-	-	5/23/26/26	-
8	GOL	B	881	-	-	2/4/4/4	-
7	DP1	A	790[B]	-	-	7/23/26/26	-
6	H4B	A	760	-	-	0/8/17/17	0/2/2/2
6	H4B	B	761	-	-	0/8/17/17	0/2/2/2
5	HEM	B	700	1	-	0/6/54/54	-
8	GOL	A	880	-	-	2/4/4/4	-
7	DP1	A	790[A]	-	-	9/23/26/26	-
7	DP1	B	791[A]	-	-	6/23/26/26	-
5	HEM	A	700	1	-	0/6/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	760	H4B	C4-N3	4.90	1.41	1.33
6	B	761	H4B	C4-N3	4.81	1.41	1.33
6	A	760	H4B	C4A-N5	4.36	1.46	1.38
6	B	761	H4B	C4A-N5	4.00	1.46	1.38
5	A	700	HEM	C3B-CAB	-3.38	1.41	1.47
5	B	700	HEM	C3B-C2B	-3.27	1.35	1.40
6	B	761	H4B	C6-N5	3.27	1.52	1.45
3	B	861	ACT	CH3-C	3.19	1.52	1.48
6	A	760	H4B	C6-N5	3.17	1.52	1.45
5	B	700	HEM	C3B-CAB	-3.13	1.41	1.47
3	A	860	ACT	CH3-C	3.02	1.52	1.48
5	A	700	HEM	C3C-C2C	-2.98	1.36	1.40
5	B	700	HEM	C1D-ND	2.85	1.42	1.36
5	B	700	HEM	C3C-CAC	-2.75	1.42	1.47
5	A	700	HEM	C3B-C2B	-2.70	1.36	1.40
7	A	790[B]	DP1	CZ-NH1	-2.67	1.28	1.35
7	B	791[B]	DP1	CZ-NH1	-2.67	1.28	1.35
5	A	700	HEM	C3C-CAC	-2.60	1.42	1.47
5	A	700	HEM	C4A-NA	2.60	1.41	1.36
7	A	790[A]	DP1	CZ-NH1	-2.49	1.28	1.35
7	B	791[A]	DP1	CZ-NH1	-2.49	1.28	1.35
5	A	700	HEM	C4B-NB	2.13	1.40	1.36
6	A	760	H4B	C7-N8	2.04	1.48	1.44

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	761	H4B	C4-C4A-C8A	9.24	122.77	114.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	760	H4B	C4-C4A-C8A	8.94	122.51	114.57
6	A	760	H4B	C4-N3-C2	5.86	125.24	115.93
6	B	761	H4B	C4-N3-C2	5.82	125.18	115.93
6	A	760	H4B	N3-C2-N1	-4.75	117.97	125.42
6	B	761	H4B	N3-C2-N1	-4.73	118.00	125.42
6	A	760	H4B	C4A-C4-N3	-3.68	113.56	124.01
6	B	761	H4B	C4A-C4-N3	-3.64	113.65	124.01
6	A	760	H4B	C2-N1-C8A	3.51	122.40	114.54
6	B	761	H4B	N2-C2-N1	3.50	122.69	117.25
6	A	760	H4B	N2-C2-N1	3.42	122.58	117.25
6	B	761	H4B	C4-C4A-N5	-3.34	116.32	119.12
6	B	761	H4B	C2-N1-C8A	3.34	122.02	114.54
6	B	761	H4B	C4A-N5-C6	-3.09	112.75	121.16
5	B	700	HEM	CBA-CAA-C2A	-3.09	106.79	112.49
5	B	700	HEM	CBD-CAD-C3D	-3.08	106.81	112.48
6	A	760	H4B	C4-C4A-N5	-3.06	116.56	119.12
5	A	700	HEM	C4A-C3A-C2A	-2.97	104.93	107.00
6	A	760	H4B	C4A-N5-C6	-2.91	113.24	121.16
6	A	760	H4B	O9-C9-C6	2.89	115.88	108.98
6	B	761	H4B	O9-C9-C6	2.63	115.27	108.98
5	A	700	HEM	CBA-CAA-C2A	-2.28	108.29	112.49
7	B	791[A]	DP1	CB'-CA'-N'	-2.18	106.46	110.88
7	A	790[A]	DP1	CB'-CA'-N'	-2.16	106.50	110.88
5	B	700	HEM	CMC-C2C-C3C	2.09	128.59	124.68
7	B	791[B]	DP1	CB'-CA'-N'	-2.05	106.73	110.88
5	B	700	HEM	CMD-C2D-C1D	-2.01	125.38	128.46

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	790[A]	DP1	N'-CA'-CB'-C1
7	A	790[B]	DP1	CZ-NH1-NO-O3
7	A	790[B]	DP1	O'-C'-CA'-CB'
7	A	790[B]	DP1	N1'-C'-CA'-CB'
7	B	791[A]	DP1	N-CA-CB-CG
8	A	880	GOL	O1-C1-C2-C3
7	A	790[B]	DP1	NE-CD-CG-CB
8	B	881	GOL	O1-C1-C2-C3
7	B	791[A]	DP1	C-CA-CB-CG
7	A	790[A]	DP1	O'-C'-CA'-N'
7	A	790[A]	DP1	N1'-C'-CA'-N'

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Mol	Chain	Res	Type	Atoms
7	B	791[A]	DP1	O'-C'-CA'-N'
7	B	791[A]	DP1	N1'-C'-CA'-N'
7	B	791[B]	DP1	N1'-C'-CA'-N'
8	B	881	GOL	O1-C1-C2-O2
7	A	790[A]	DP1	N1'-C'-CA'-CB'
7	B	791[A]	DP1	N1'-C'-CA'-CB'
7	A	790[B]	DP1	O-C-CA-N
8	A	880	GOL	O1-C1-C2-O2
7	A	790[B]	DP1	N'-C-CA-N
7	A	790[A]	DP1	C'-CA'-CB'-C1
7	B	791[B]	DP1	NE-CD-CG-CB
7	A	790[A]	DP1	C-CA-CB-CG
7	B	791[B]	DP1	O'-C'-CA'-N'
7	A	790[A]	DP1	O'-C'-CA'-CB'
7	B	791[A]	DP1	O'-C'-CA'-CB'
7	A	790[A]	DP1	N-CA-CB-CG
7	B	791[B]	DP1	O'-C'-CA'-CB'
7	A	790[B]	DP1	C-CA-CB-CG
7	B	791[B]	DP1	C-CA-CB-CG
7	A	790[A]	DP1	CA-CB-CG-CD

There are no ring outliers.

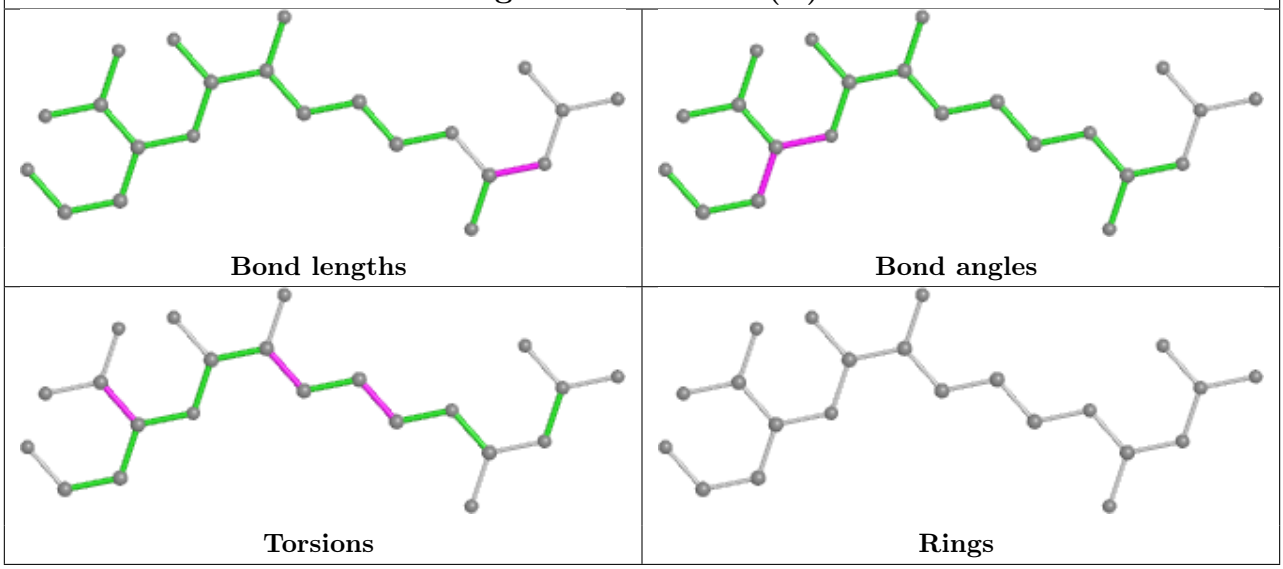
9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	791[B]	DP1	1	0
3	A	860	ACT	1	0
2	B	851	CAC	2	0
6	A	760	H4B	1	0
8	B	881	GOL	1	0
2	A	850	CAC	1	0
7	A	790[A]	DP1	1	0
7	B	791[A]	DP1	1	0
5	A	700	HEM	1	0

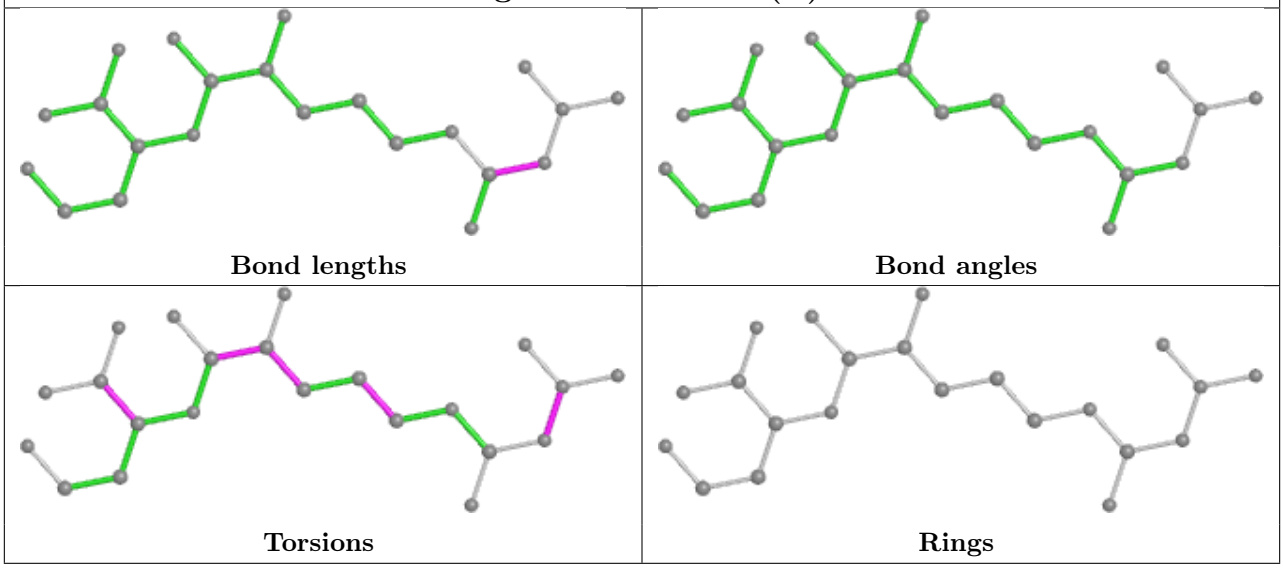
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

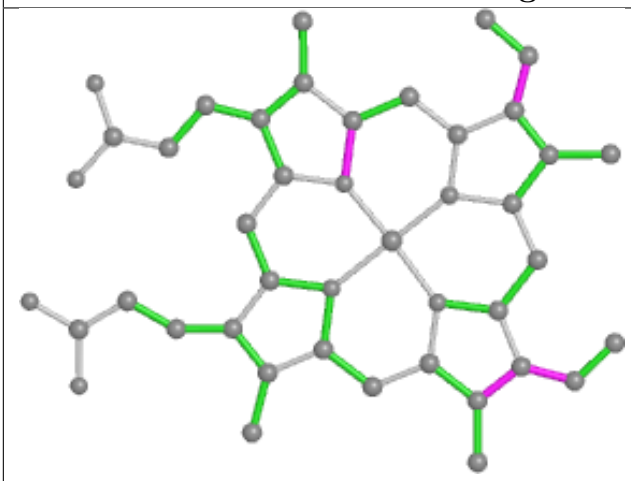
Ligand DP1 B 791 (B)



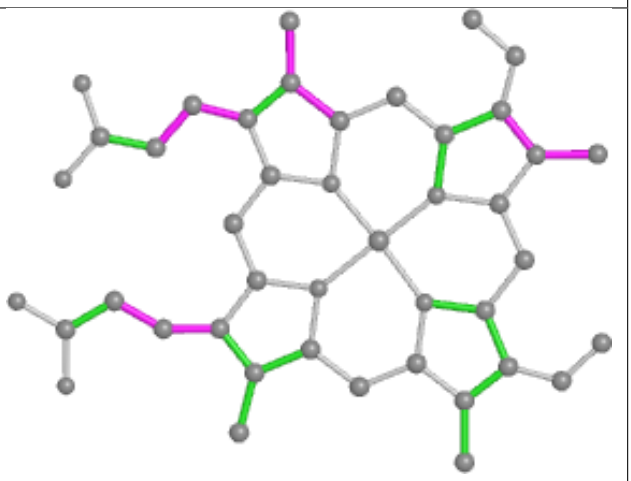
Ligand DP1 A 790 (B)



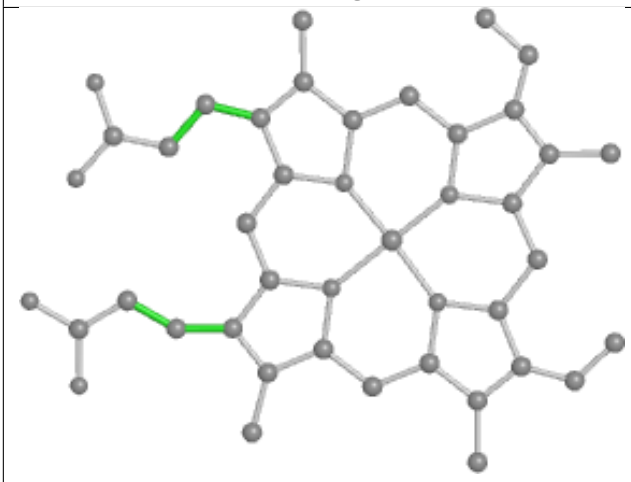
Ligand HEM B 700



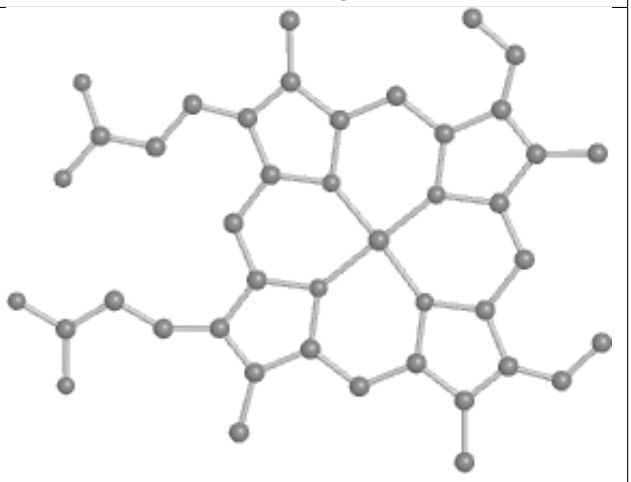
Bond lengths



Bond angles

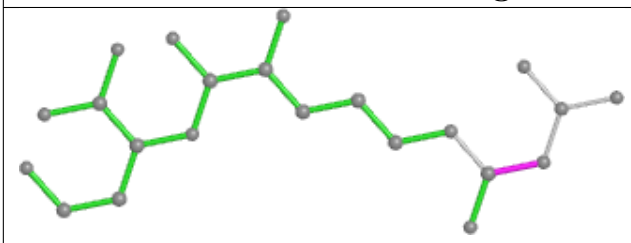


Torsions

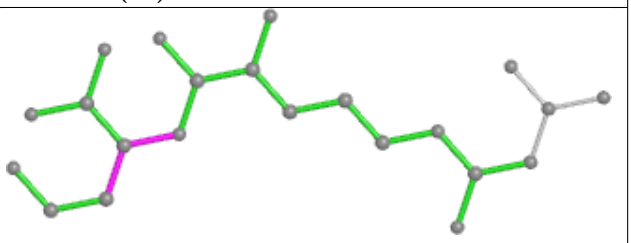


Rings

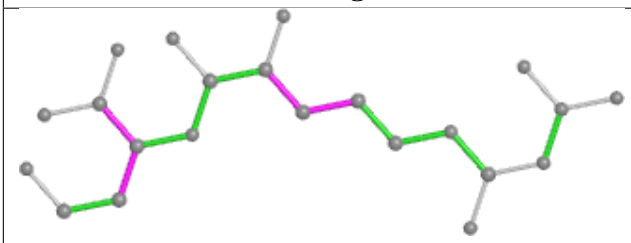
Ligand DP1 A 790 (A)



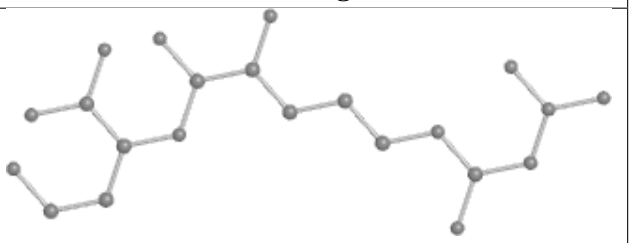
Bond lengths



Bond angles

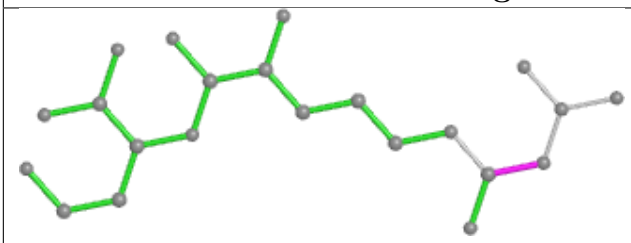


Torsions

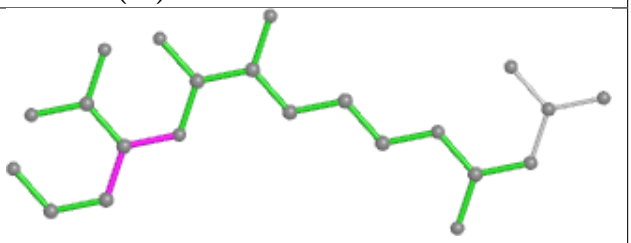


Rings

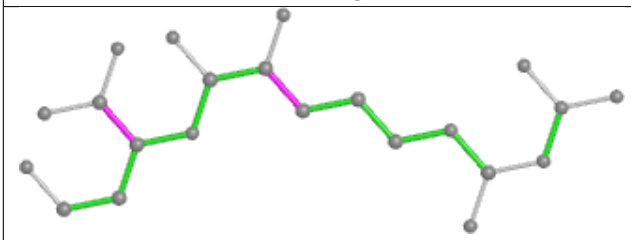
Ligand DP1 B 791 (A)



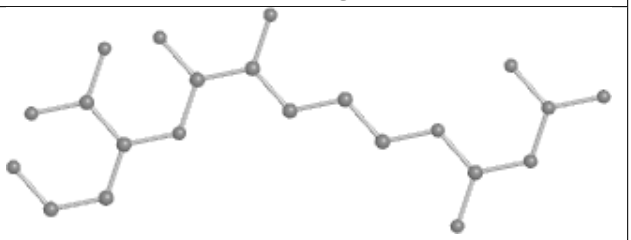
Bond lengths



Bond angles

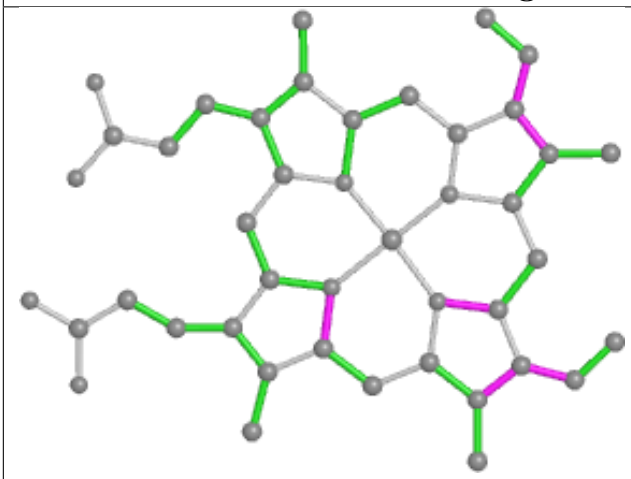


Torsions

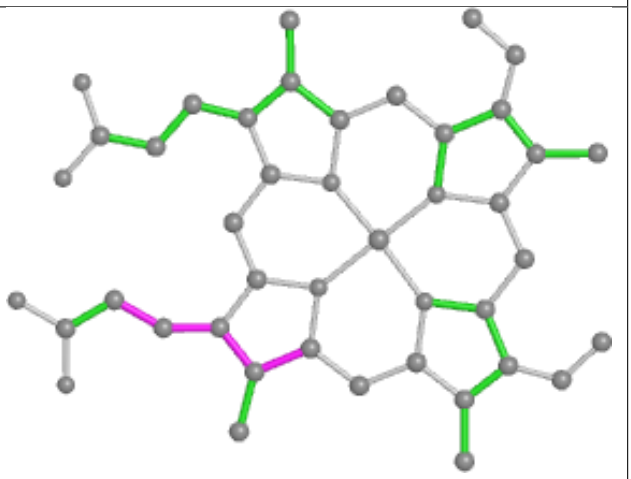


Rings

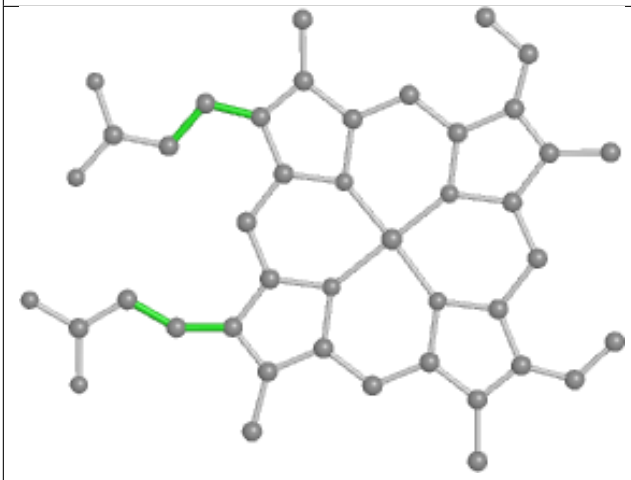
Ligand HEM A 700



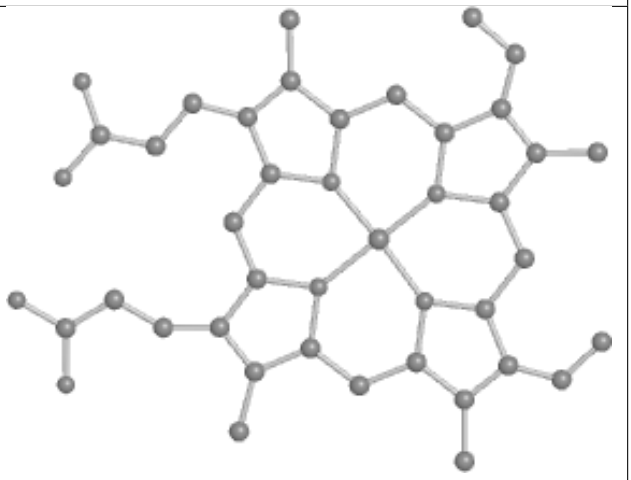
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	405/416 (97%)	0.65	44 (10%)	5	7	13, 22, 39, 58	0
1	B	405/416 (97%)	0.42	23 (5%)	23	28	14, 23, 39, 56	0
All	All	810/832 (97%)	0.54	67 (8%)	11	14	13, 23, 39, 58	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	PRO	8.0
1	A	121	PRO	7.9
1	A	259	GLN	7.1
1	A	120	PRO	6.8
1	B	260	ASP	6.4
1	B	120	PRO	5.7
1	A	122	ALA	5.4
1	B	121	PRO	5.1
1	B	259	GLN	5.0
1	A	123	GLU	4.9
1	A	239	GLY	4.9
1	B	390	ARG	4.5
1	A	238	PRO	4.2
1	A	108	PRO	4.0
1	A	107	LEU	4.0
1	B	261	GLY	4.0
1	B	257	ARG	3.9
1	A	260	ASP	3.9
1	A	261	GLY	3.9
1	A	153	GLN	3.9
1	A	124	GLN	3.9
1	A	67	GLY	3.8
1	A	126	LEU	3.6
1	A	311	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	278	GLN	3.3
1	A	91	GLN	3.2
1	A	257	ARG	3.2
1	A	285	ASN	3.2
1	B	142	ARG	3.1
1	A	160	ALA	3.1
1	B	386	ASP	3.0
1	B	223	ARG	3.0
1	A	161	SER	2.9
1	A	482	TRP	2.9
1	B	311	LEU	2.9
1	A	69	LYS	2.8
1	A	450	ILE	2.7
1	A	130	ARG	2.7
1	A	156	GLU	2.7
1	A	282	THR	2.7
1	A	162	THR	2.7
1	B	447	TRP	2.6
1	A	461	VAL	2.6
1	A	449	TRP	2.5
1	B	122	ALA	2.5
1	A	448	ALA	2.5
1	A	99	ARG	2.5
1	B	123	GLU	2.4
1	A	258	GLN	2.4
1	B	476	ARG	2.3
1	B	141	LYS	2.3
1	A	445	ALA	2.3
1	A	274	GLU	2.3
1	B	239	GLY	2.3
1	B	310	GLU	2.3
1	B	278	GLN	2.2
1	B	149	GLU	2.2
1	A	390	ARG	2.2
1	A	447	TRP	2.2
1	A	462	PHE	2.2
1	A	281	TRP	2.2
1	B	449	TRP	2.2
1	A	277	ILE	2.1
1	A	180	TRP	2.1
1	B	482	TRP	2.1
1	A	125	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	300	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

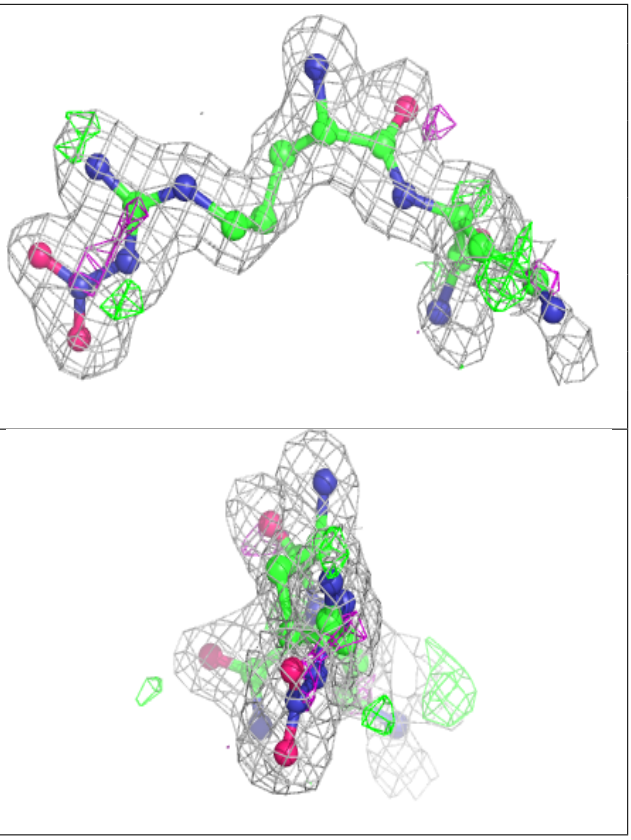
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CAC	A	850	3/5	0.69	0.39	92,92,93,93	0
2	CAC	B	851	3/5	0.73	0.40	97,97,98,98	0
8	GOL	A	880	6/6	0.78	0.16	38,42,43,44	0
8	GOL	B	881	6/6	0.82	0.14	32,34,37,39	0
7	DP1	B	791[A]	22/22	0.91	0.18	15,19,23,28	22
7	DP1	B	791[B]	22/22	0.91	0.18	45,46,47,47	22
7	DP1	A	790[A]	22/22	0.91	0.17	19,25,28,32	22
7	DP1	A	790[B]	22/22	0.91	0.17	25,28,31,32	22
3	ACT	B	861	4/4	0.92	0.14	36,38,39,39	0
3	ACT	A	860	4/4	0.96	0.17	39,40,41,42	0
6	H4B	A	760	17/17	0.97	0.16	14,15,19,20	0
6	H4B	B	761	17/17	0.97	0.15	12,14,18,19	0
5	HEM	A	700	43/43	0.98	0.15	13,16,21,26	0
5	HEM	B	700	43/43	0.98	0.12	14,16,20,26	0
4	ZN	A	900	1/1	1.00	0.07	20,20,20,20	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.

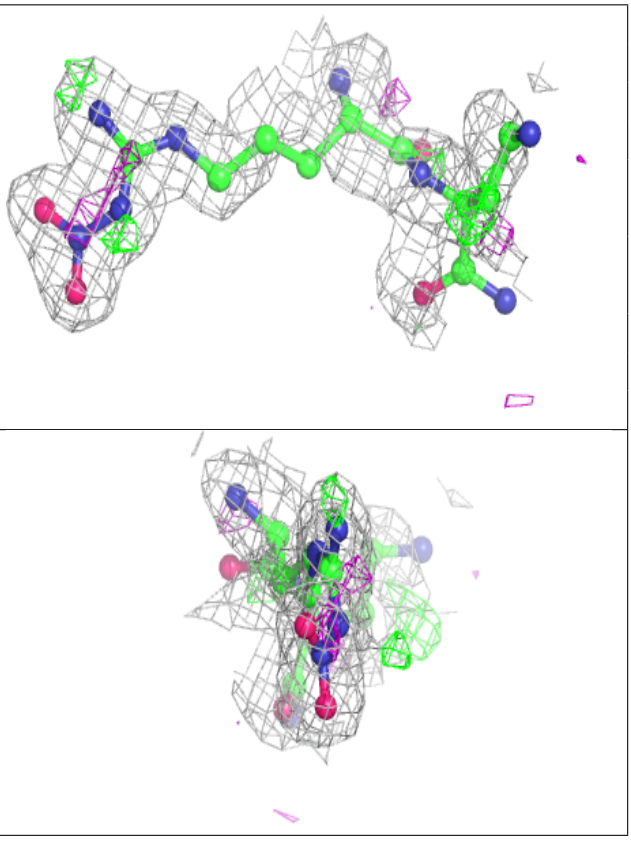
Electron density around DP1 B 791 (A):

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



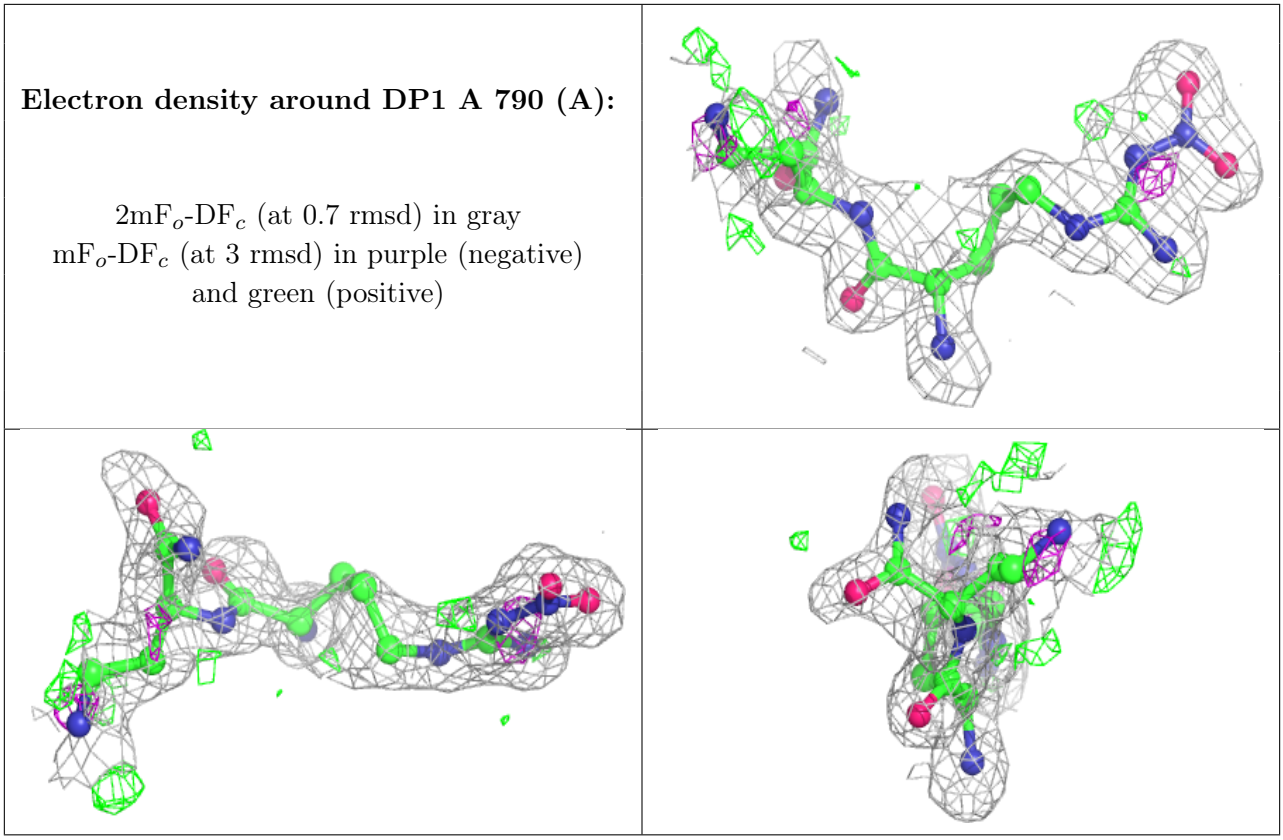
Electron density around DP1 B 791 (B):

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



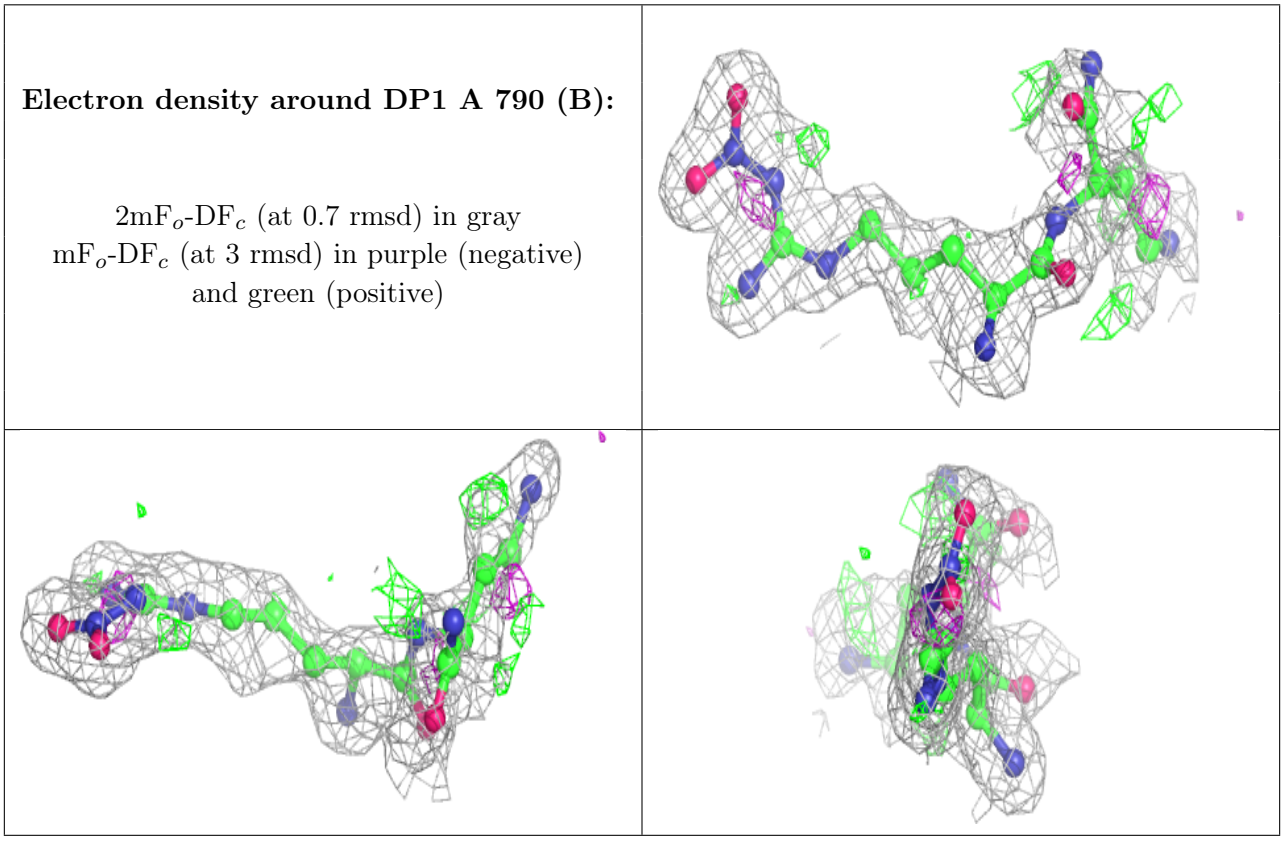
Electron density around DP1 A 790 (A):

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



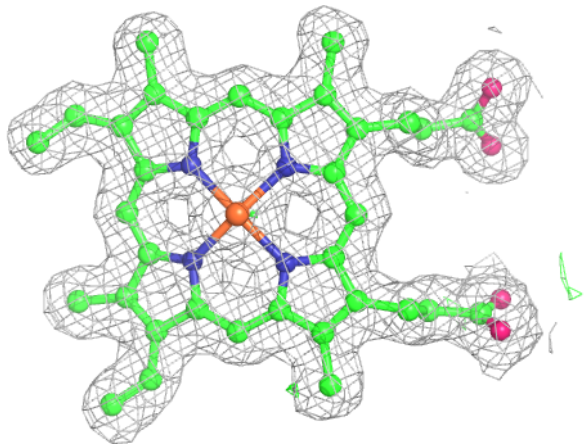
Electron density around DP1 A 790 (B):

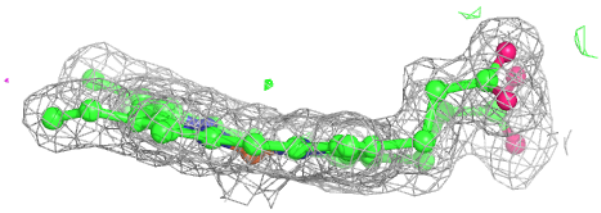
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

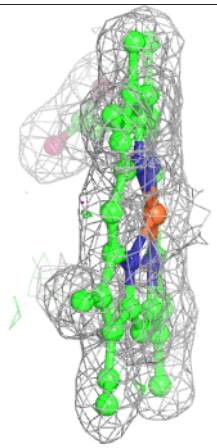


Electron density around HEM A 700:

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

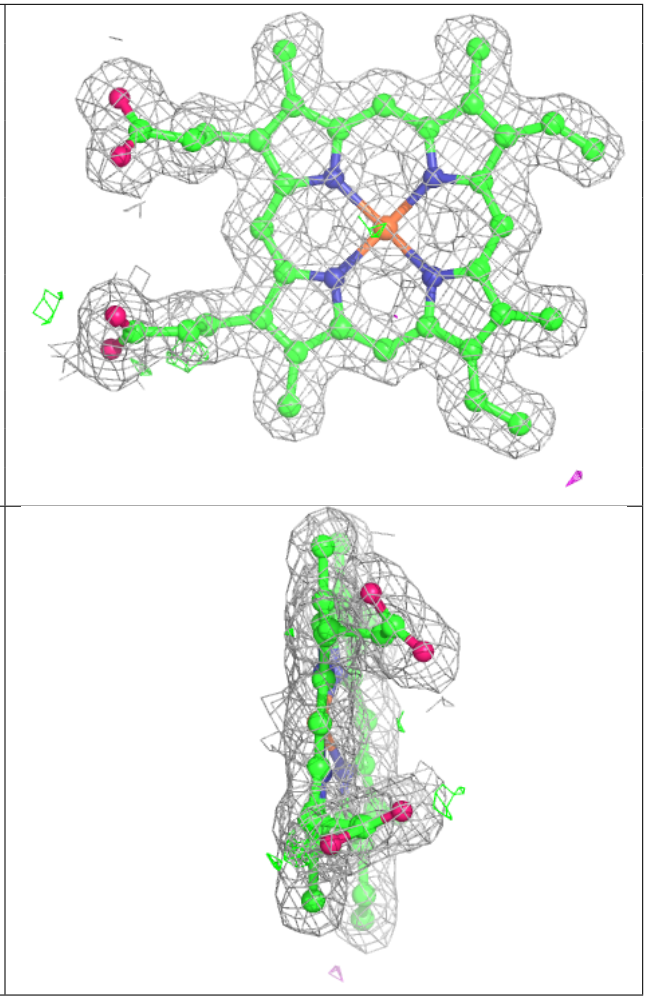






Electron density around HEM B 700:

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.