



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 05:29 am BST

PDB ID : 4CX0
Title : Structure of bovine endothelial nitric oxide synthase Y477A mutant heme domain in complex with 6-((((3S, 5R)-5-(((6-AMINO-4-METHYLPYRIDIN-2-YL)METHOXY)METHYL)PYRROLIDIN-3-YL)OXY)METHYL)-4-METHYLPYRIDIN-2-AMINE
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-04-03
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

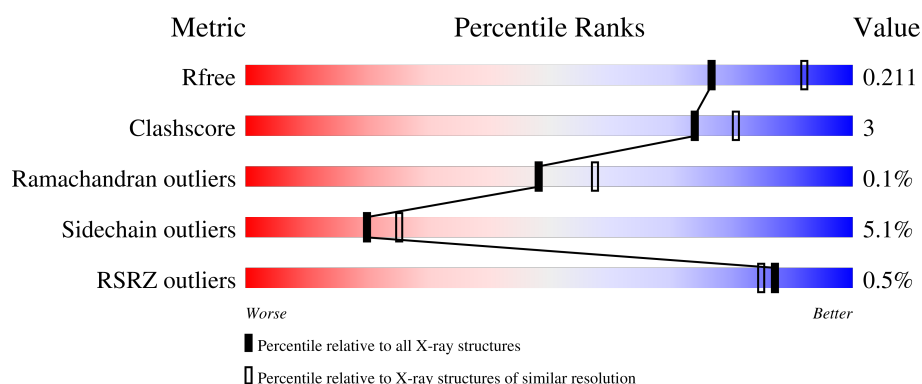
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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 $\leq 5\%$. 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	443	<div> <div style="width: 81%;"></div> <div style="width: 9%;"></div> <div style="width: 9%;"></div> <div style="width: 9%;"></div> </div> <div>81% 9% • 9%</div>
1	B	443	<div> <div style="width: 84%;"></div> <div style="width: 7%;"></div> <div style="width: 9%;"></div> </div> <div>84% 7% 9%</div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7054 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.

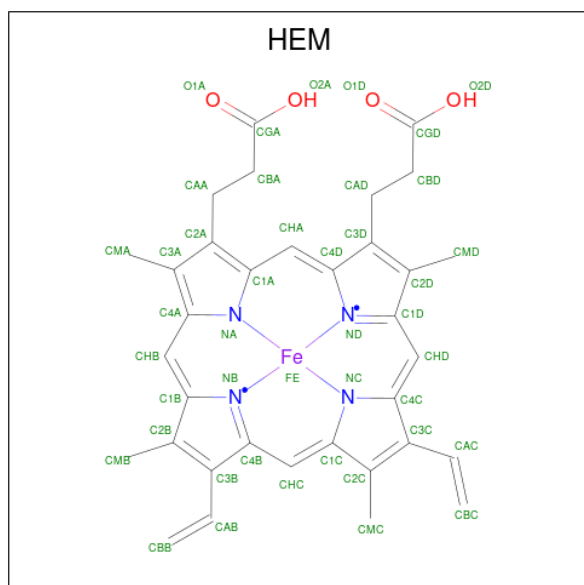
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	1	0
			3221	1	2046	568	590	16			
1	B	403	Total	As	C	N	O	S	0	0	0
			3205	1	2036	566	586	16			

There are 4 discrepancies between the modelled and reference sequences:

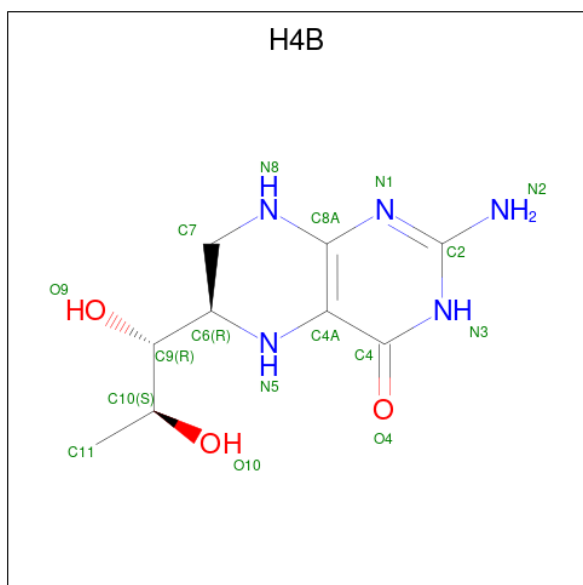
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
A	477	ALA	TYR	engineered mutation	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	477	ALA	TYR	engineered mutation	UNP P29473

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



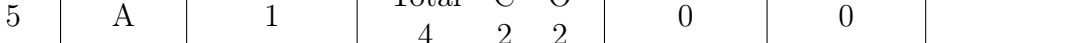
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 4 is 6-((((3S, 5R)-5-((((6-amino-4-methylpyridin-2-yl)methoxy)methyl)pyrrolidin-3-yl)oxy)methyl)-4-methylpyridin-2-amine (three-letter code: Q16) (formula: $C_{19}H_{27}N_5O_2$).



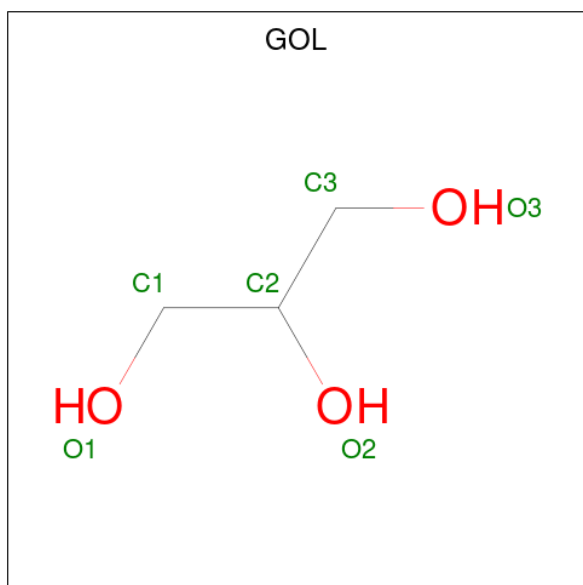
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	232	Total	O	0	0
			232	232		
8	B	195	Total	O	0	0
			195	195		

- Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL

	L126	R130	S143	Q146	L152	Q153	E154	V155	E156	A157	E158	V159	H166	L167	R168	P238	G239	R240	G241	W246	L293	L294	P298	H319	P320	L328	R331	N340	C370	L378	R390	D398	V402	K416	W449	L458	E465				
ARG																																									
ALA																																									
PRO																																									
ALA																																									
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LEU																																									
THR																																									

- Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL

D202	D202	ARG
C214	ALA	ALA
K218	PRO	PRO
F233	ALA	ALA
P234	THR	THR
Q235	PRO	PRO
R236	HIS	HIS
R240	ALA	ALA
G241	PRO	PRO
D242	ASP	ASP
W281	HIS	HIS
R287	SER	SER
L304	PRO	PRO
P308	THR	THR
L311	LEU	LEU
E323	THR	THR
L330	ARG	ARG
L378	PRO	PRO
L378	GLU	GLU
T389	GLY	GLY
L414	PRO	PRO
I419	PRO	PRO
E465	PRO	PRO
W482	GLY	GLY
	GLN	GLN
	LEU	LEU
	LYS	LYS
	R109	R109
	L105	L105
	L102	L102
	C101	C101
	R99	R99
	K69	K69

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.71Å 106.46Å 156.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.68 – 2.20 38.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.68-2.20) 99.4 (38.68-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.155 , 0.203 0.164 , 0.211	Depositor DCC
R_{free} test set	2466 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7054	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, ACT, Q16, ZN, CAS, H4B, 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	0.64	0/3303	0.77	2/4497 (0.0%)
1	B	0.63	0/3283	0.76	2/4469 (0.0%)
All	All	0.64	0/6586	0.76	4/8966 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	240	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	240	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	100	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3221	0	3127	23	0
1	B	3205	0	3113	14	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	17	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	0	0
4	A	26	0	27	0	0
4	B	26	0	27	0	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	232	0	0	1	0
8	B	195	0	0	3	0
All	All	7054	0	6412	39	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (39) 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)
2:B:500:HEM:HMC2	2:B:500:HEM:HBC2	1.63	0.79
1:A:126:LEU:HD23	1:A:130:ARG:NH2	2.10	0.66
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.78	0.65
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.83	0.61
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.00	0.61
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.84	0.60
1:B:287:ARG:HD3	8:B:2122:HOH:O	2.03	0.59
1:A:126:LEU:HD21	1:A:156:GLU:HB3	1.85	0.59
1:A:70:PHE:HB3	1:A:84:ASP:O	2.05	0.57
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.86	0.57
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.43	0.57
1:B:240:ARG:HD2	1:B:241:GLY:O	2.05	0.56
1:A:240:ARG:HD2	1:A:241:GLY:O	2.06	0.55
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.88	0.55
1:A:449:TRP:HA	3:A:600:H4B:N1	2.23	0.54
1:A:152:LEU:O	1:A:156:GLU:HG2	2.07	0.53
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.39	0.53
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.39	0.52
1:A:69:LYS:HA	1:A:69:LYS:HE2	1.91	0.52
1:B:378:LEU:HB2	8:B:2152:HOH:O	2.10	0.51
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.52	0.49
1:B:366:THR:O	1:B:370:CYS:HB2	2.12	0.49
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:CYS:SG	8:B:2081:HOH:O	2.59	0.48
1:A:126:LEU:HD13	1:A:159:VAL:HG11	1.96	0.48
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.41	0.47
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.97	0.46
1:A:378:LEU:HB2	8:A:2173:HOH:O	2.16	0.46
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.51	0.46
1:A:158:GLU:OE2	1:A:166:HIS:HD2	1.99	0.46
1:B:134:ASN:OD1	1:B:148:HIS:NE2	2.50	0.45
1:A:340:ASN:H	1:A:340:ASN:HD22	1.66	0.44
1:A:126:LEU:HD12	1:A:159:VAL:HG21	2.00	0.44
1:B:281:TRP:HB2	1:B:304:LEU:HD21	2.01	0.42
1:B:202:ASP:CG	1:B:202:ASP:O	2.58	0.42
1:A:105:LEU:HD23	1:A:105:LEU:N	2.35	0.41
1:A:154:GLU:OE1	1:A:168:ARG:NH2	2.54	0.40
1:A:126:LEU:HD11	1:A:156:GLU:HA	2.04	0.40
1:A:398:ASP:O	1:A:402:VAL:HG23	2.22	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	401/443 (90%)	390 (97%)	10 (2%)	1 (0%)	44	52
1	B	398/443 (90%)	384 (96%)	14 (4%)	0	100	100
All	All	799/886 (90%)	774 (97%)	24 (3%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA

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	343/374 (92%)	323 (94%)	20 (6%)	17	20
1	B	341/374 (91%)	326 (96%)	15 (4%)	24	31
All	All	684/748 (91%)	649 (95%)	35 (5%)	20	25

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	72	ARG
1	A	99	ARG
1	A	100	ARG
1	A	102	LEU
1	A	109	ARG
1	A	123	GLU
1	A	125	LEU
1	A	143	SER
1	A	146	GLN
1	A	156	GLU
1	A	238	PRO
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	390	ARG
1	A	416	LYS
1	A	458	LEU
1	B	99	ARG
1	B	100	ARG
1	B	102	LEU
1	B	109	ARG
1	B	124	GLN
1	B	131	ASP
1	B	202	ASP

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Mol	Chain	Res	Type
1	B	218	LYS
1	B	240	ARG
1	B	323	GLU
1	B	330	LEU
1	B	340	ASN
1	B	389	THR
1	B	414	LEU
1	B	419	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CAS	A	384	1	5,8,9	0.91	0	1,9,11	0.31	0
1	CAS	B	384	1	5,8,9	1.19	0	1,9,11	0.15	0

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
1	CAS	A	384	1	-	0/0/7/9	-
1	CAS	B	384	1	-	0/0/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z > 2$
5	ACT	B	861	-	3,3,3	0.97	0	3,3,3	0.52	0
4	Q16	B	800	-	26,28,28	0.66	0	33,38,38	1.83	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	Q16	A	800	-	26,28,28	0.78	0	33,38,38	1.39	4 (12%)
5	ACT	A	861	-	3,3,3	0.84	0	3,3,3	0.86	0
5	ACT	A	860	-	3,3,3	0.79	0	3,3,3	0.66	0
5	ACT	B	860	-	3,3,3	0.79	0	3,3,3	1.02	0
2	HEM	B	500	1	41,50,50	1.37	4 (9%)	45,82,82	2.19	14 (31%)
2	HEM	A	500	1	41,50,50	1.39	6 (14%)	45,82,82	2.00	16 (35%)
3	H4B	B	600	-	16,18,18	0.75	0	11,26,26	2.59	6 (54%)
6	GOL	B	880	-	5,5,5	0.32	0	5,5,5	0.59	0
6	GOL	A	880	-	5,5,5	0.37	0	5,5,5	0.76	0
3	H4B	A	600	-	16,18,18	0.95	0	11,26,26	3.06	7 (63%)

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
4	Q16	B	800	-	-	2/11/20/20	0/3/3/3
4	Q16	A	800	-	-	1/11/20/20	0/3/3/3
2	HEM	B	500	1	-	1/12/54/54	-
2	HEM	A	500	1	-	0/12/54/54	-
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
6	GOL	B	880	-	-	1/4/4/4	-
6	GOL	A	880	-	-	0/4/4/4	-
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C1B-NB	-4.84	1.32	1.40
2	A	500	HEM	C1B-NB	-3.39	1.34	1.40
2	A	500	HEM	C3B-C4B	2.86	1.50	1.44
2	A	500	HEM	C4B-NB	-2.45	1.33	1.38
2	A	500	HEM	C1D-ND	-2.40	1.33	1.38
2	B	500	HEM	C4D-ND	-2.27	1.36	1.40
2	A	500	HEM	FE-NB	2.16	2.07	1.96
2	B	500	HEM	CHB-C1B	2.08	1.40	1.35
2	A	500	HEM	C3C-C2C	2.06	1.43	1.40
2	B	500	HEM	C3B-C4B	2.04	1.48	1.44

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CBA-CAA-C2A	-6.60	101.36	112.62
3	A	600	H4B	C8A-C4A-C4	5.29	119.27	114.57
3	A	600	H4B	C4-C4A-N5	5.28	123.55	119.12
3	B	600	H4B	C4-C4A-N5	5.21	123.49	119.12
2	B	500	HEM	C1B-NB-C4B	5.14	110.39	105.07
4	B	800	Q16	C02-N01-C06	4.91	121.82	118.10
4	B	800	Q16	C3'-C4'-C5'	4.47	107.66	103.65
2	A	500	HEM	CBA-CAA-C2A	-4.32	105.24	112.62
4	B	800	Q16	C10-C2'-N1'	-4.23	104.12	111.58
2	B	500	HEM	CHD-C1D-ND	4.12	128.90	124.43
3	A	600	H4B	C2-N3-C4	3.96	122.22	115.93
2	B	500	HEM	CHC-C4B-NB	3.94	128.71	124.43
2	A	500	HEM	C1B-NB-C4B	3.74	108.93	105.07
2	A	500	HEM	CHB-C1B-NB	3.73	128.99	124.38
2	B	500	HEM	CHD-C1D-C2D	-3.72	119.17	124.98
2	A	500	HEM	CHA-C4D-C3D	-3.66	118.47	125.33
4	A	800	Q16	C24-C25-C26	-3.45	118.06	120.32
2	A	500	HEM	CAD-C3D-C4D	3.44	130.67	124.66
2	B	500	HEM	CHB-C1B-NB	3.38	128.56	124.38
3	A	600	H4B	N1-C2-N3	-3.24	120.34	125.42
4	A	800	Q16	C3'-C4'-C5'	3.24	106.55	103.65
3	B	600	H4B	C8A-C4A-C4	3.23	117.44	114.57
2	A	500	HEM	CHA-C4D-ND	3.14	128.26	124.38
2	B	500	HEM	CHA-C4D-C3D	-3.06	119.58	125.33
3	B	600	H4B	N2-C2-N3	2.99	121.91	117.25
2	B	500	HEM	CHA-C4D-ND	2.96	128.04	124.38
3	B	600	H4B	N1-C2-N3	-2.96	120.78	125.42
4	A	800	Q16	C10-C2'-N1'	-2.94	106.39	111.58
4	B	800	Q16	C24-C25-C26	-2.94	118.40	120.32
2	B	500	HEM	C4B-C3B-C2B	-2.92	104.80	107.11
3	B	600	H4B	C2-N3-C4	2.82	120.40	115.93
2	A	500	HEM	CHC-C4B-NB	2.77	127.44	124.43
2	B	500	HEM	C3B-C2B-C1B	2.58	108.40	106.49
2	A	500	HEM	C3D-C4D-ND	2.56	113.01	110.17
3	B	600	H4B	C2-N1-C8A	2.52	120.20	114.54
3	A	600	H4B	N2-C2-N3	2.51	121.16	117.25
3	A	600	H4B	C2-N1-C8A	2.50	120.14	114.54
2	A	500	HEM	CHD-C1D-C2D	-2.48	121.10	124.98
4	B	800	Q16	O09-C10-C2'	-2.47	102.01	109.28
2	A	500	HEM	CMA-C3A-C4A	-2.46	124.68	128.46
4	B	800	Q16	C05-C06-N01	-2.42	120.33	122.90
2	A	500	HEM	CHB-C1B-C2B	-2.38	120.14	126.72
4	A	800	Q16	C3'-C2'-C10	-2.34	109.14	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	O2D-CGD-O1D	-2.33	117.49	123.30
3	A	600	H4B	C4A-C4-N3	-2.32	117.41	124.01
2	A	500	HEM	CMC-C2C-C3C	2.28	128.94	124.68
2	A	500	HEM	O2A-CGA-O1A	-2.18	117.86	123.30
2	B	500	HEM	O2A-CGA-CBA	2.10	120.77	114.03
2	B	500	HEM	CAD-C3D-C4D	2.09	128.32	124.66
4	B	800	Q16	C08-C06-C05	2.07	123.96	121.08
2	B	500	HEM	O2D-CGD-CBD	2.07	120.68	114.03
2	A	500	HEM	CHD-C1D-ND	2.04	126.65	124.43
4	B	800	Q16	C04-C05-C06	-2.04	118.98	120.32
2	B	500	HEM	O2D-CGD-O1D	-2.01	118.30	123.30
2	A	500	HEM	CMB-C2B-C1B	2.00	128.09	125.04

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	800	Q16	C5'-C4'-O11-C12
2	B	500	HEM	C4B-C3B-CAB-CBB
4	B	800	Q16	O09-C10-C2'-N1'
4	A	800	Q16	C06-C08-O09-C10
6	B	880	GOL	O1-C1-C2-C3

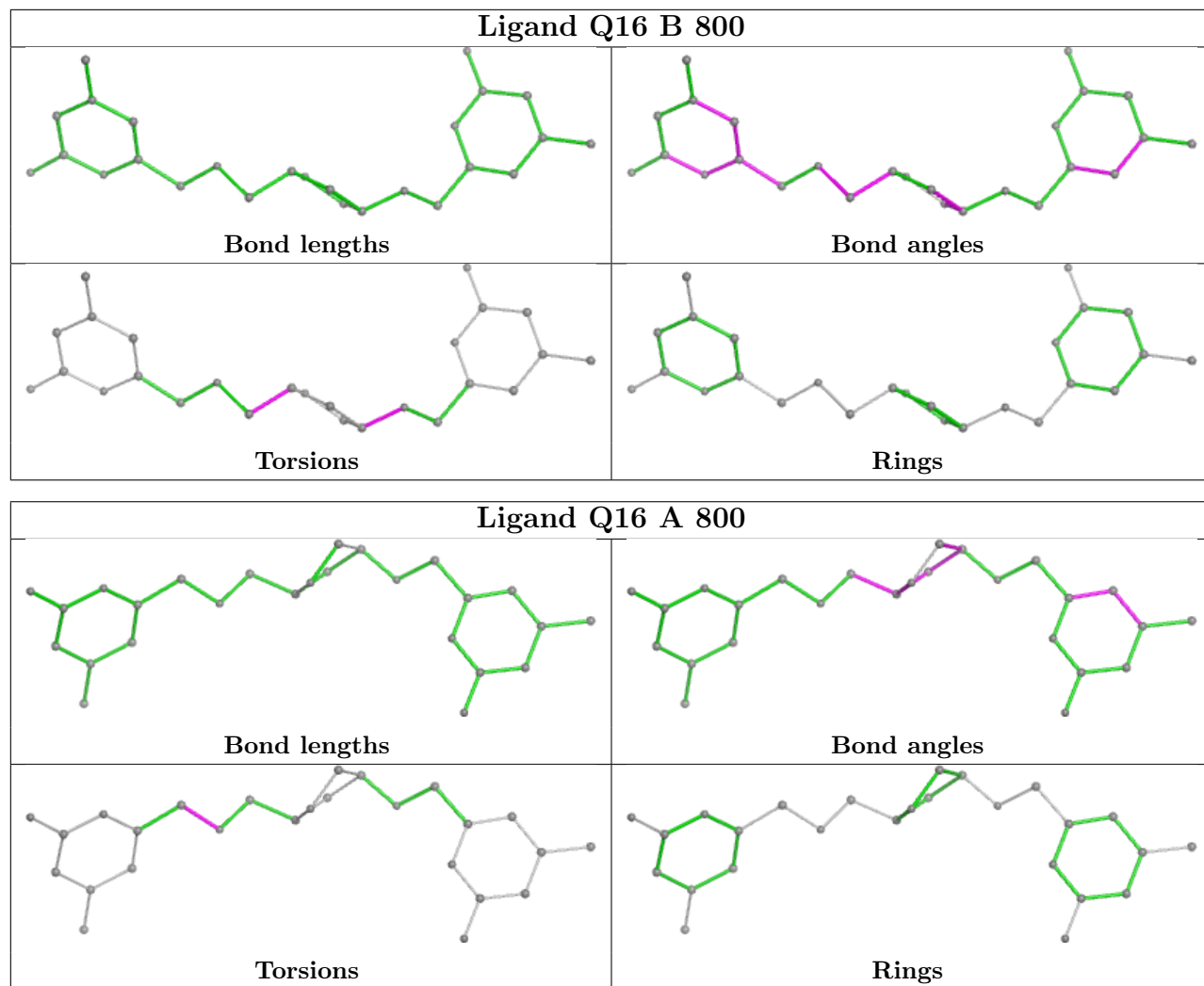
There are no ring outliers.

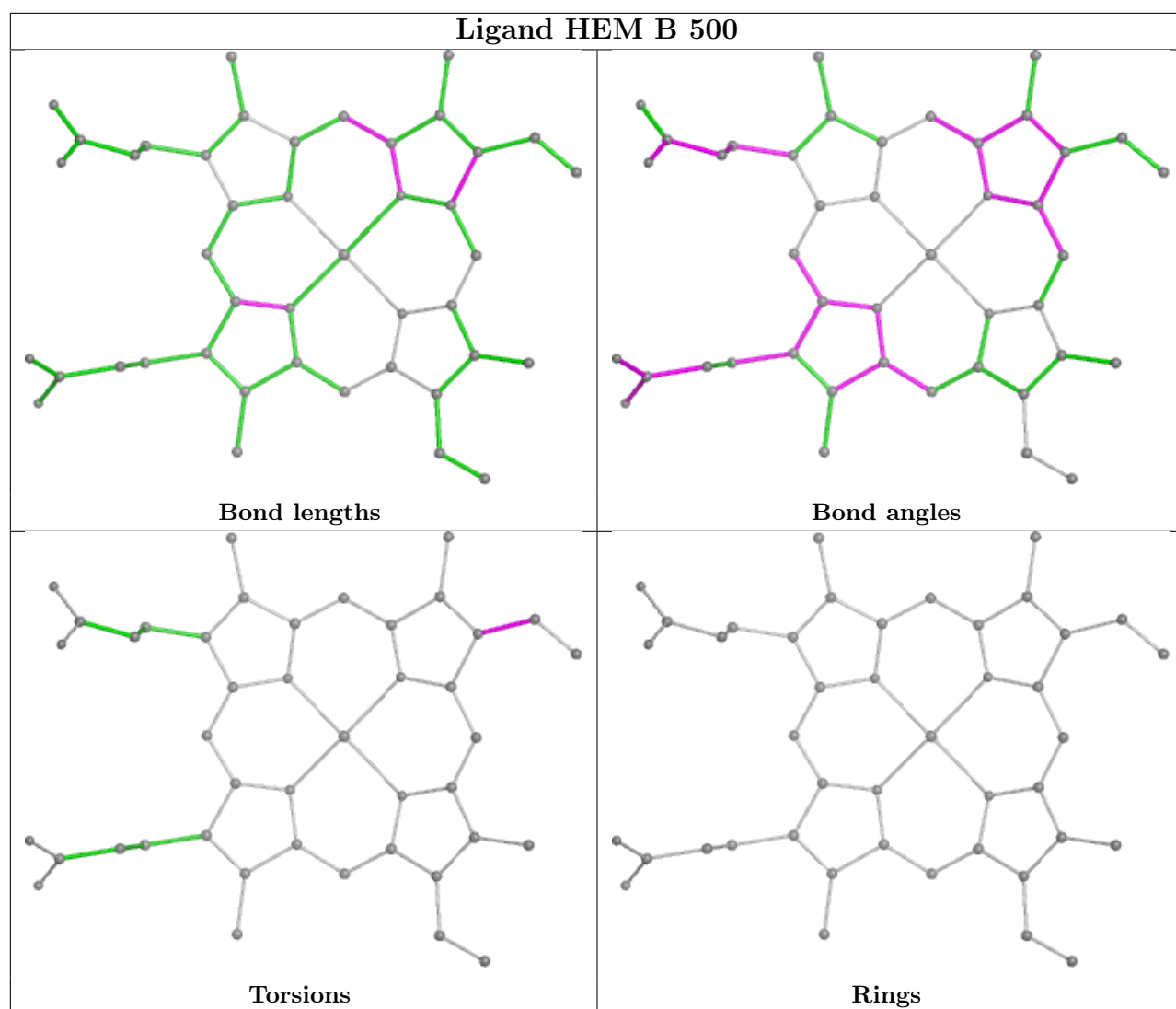
3 monomers are involved in 5 short contacts:

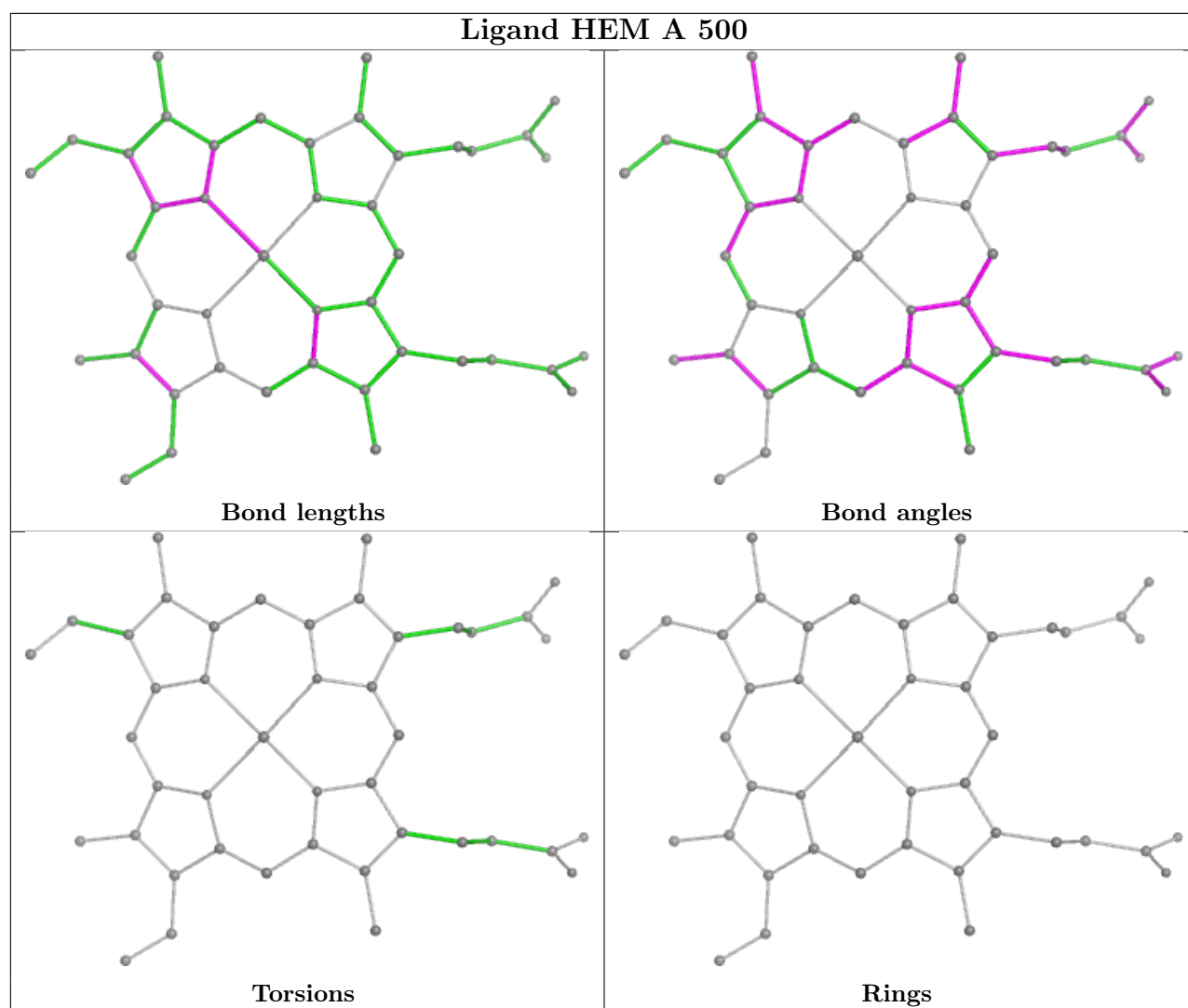
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	HEM	3	0
2	A	500	HEM	1	0
3	A	600	H4B	1	0

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 than 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.







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	404/443 (91%)	-0.57	2 (0%) 87 85	20, 34, 60, 94	1 (0%)
1	B	402/443 (90%)	-0.49	2 (0%) 87 85	23, 36, 64, 98	0
All	All	806/886 (90%)	-0.53	4 (0%) 87 85	20, 35, 62, 98	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ARG	3.1
1	B	69	LYS	3.0
1	B	109	ARG	2.9
1	A	121	PRO	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CAS	A	384	9/10	0.98	0.07	33,34,52,53	0
1	CAS	B	384	9/10	0.98	0.08	43,44,51,52	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

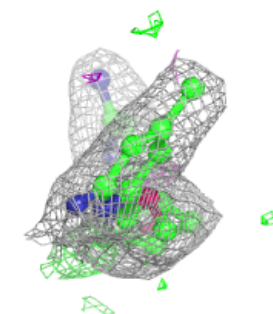
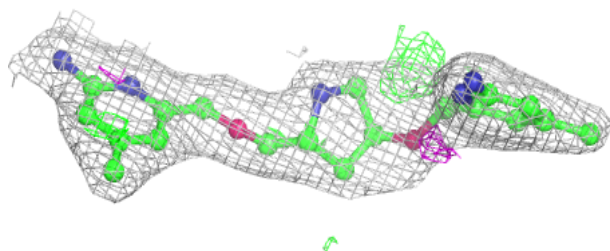
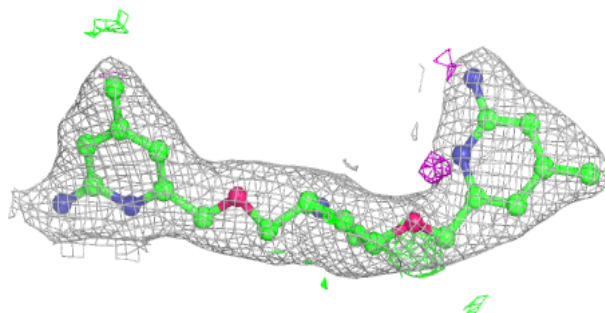
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	880	6/6	0.87	0.14	53,57,60,66	0
6	GOL	B	880	6/6	0.87	0.14	51,55,57,64	0
5	ACT	A	860	4/4	0.93	0.11	35,42,47,47	0
5	ACT	B	860	4/4	0.94	0.12	44,45,46,48	0
4	Q16	B	800	26/26	0.94	0.08	26,36,43,45	0
4	Q16	A	800	26/26	0.94	0.08	22,33,43,44	0
3	H4B	B	600	17/17	0.96	0.06	27,30,32,34	0
5	ACT	B	861	4/4	0.97	0.09	27,28,29,30	0
5	ACT	A	861	4/4	0.97	0.06	28,32,33,33	0
3	H4B	A	600	17/17	0.97	0.05	26,29,31,31	0
2	HEM	A	500	43/43	0.98	0.07	24,27,29,31	0
2	HEM	B	500	43/43	0.98	0.06	25,28,32,36	0
7	ZN	A	900	1/1	1.00	0.02	28,28,28,28	0

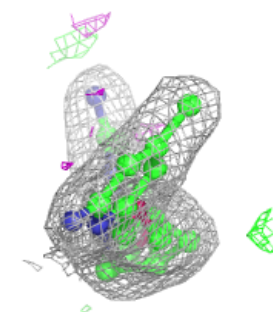
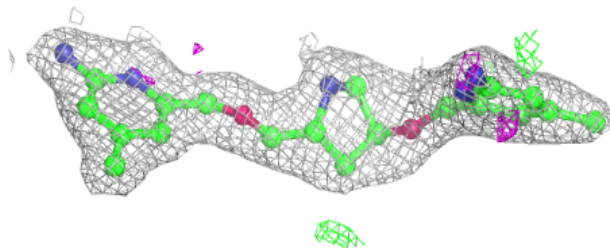
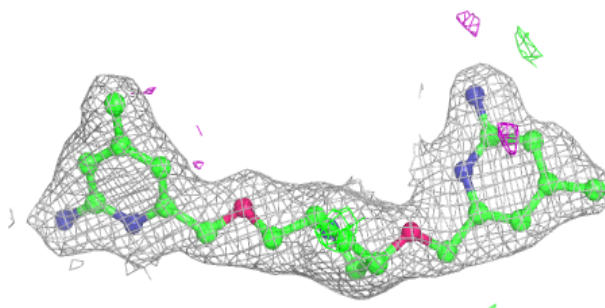
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Q16 B 800:

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

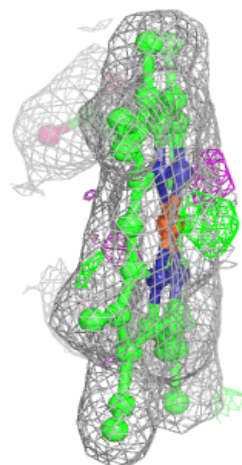
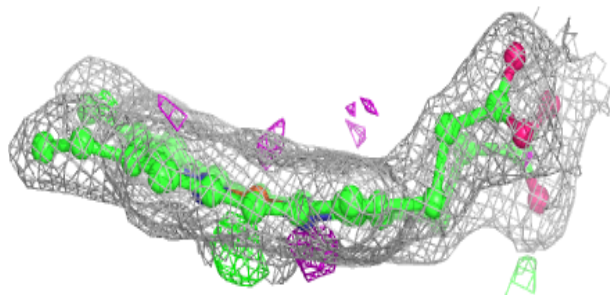
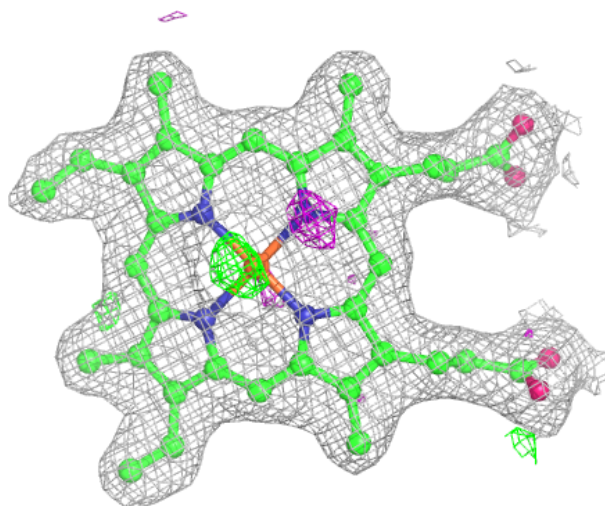
**Electron density around Q16 A 800:**

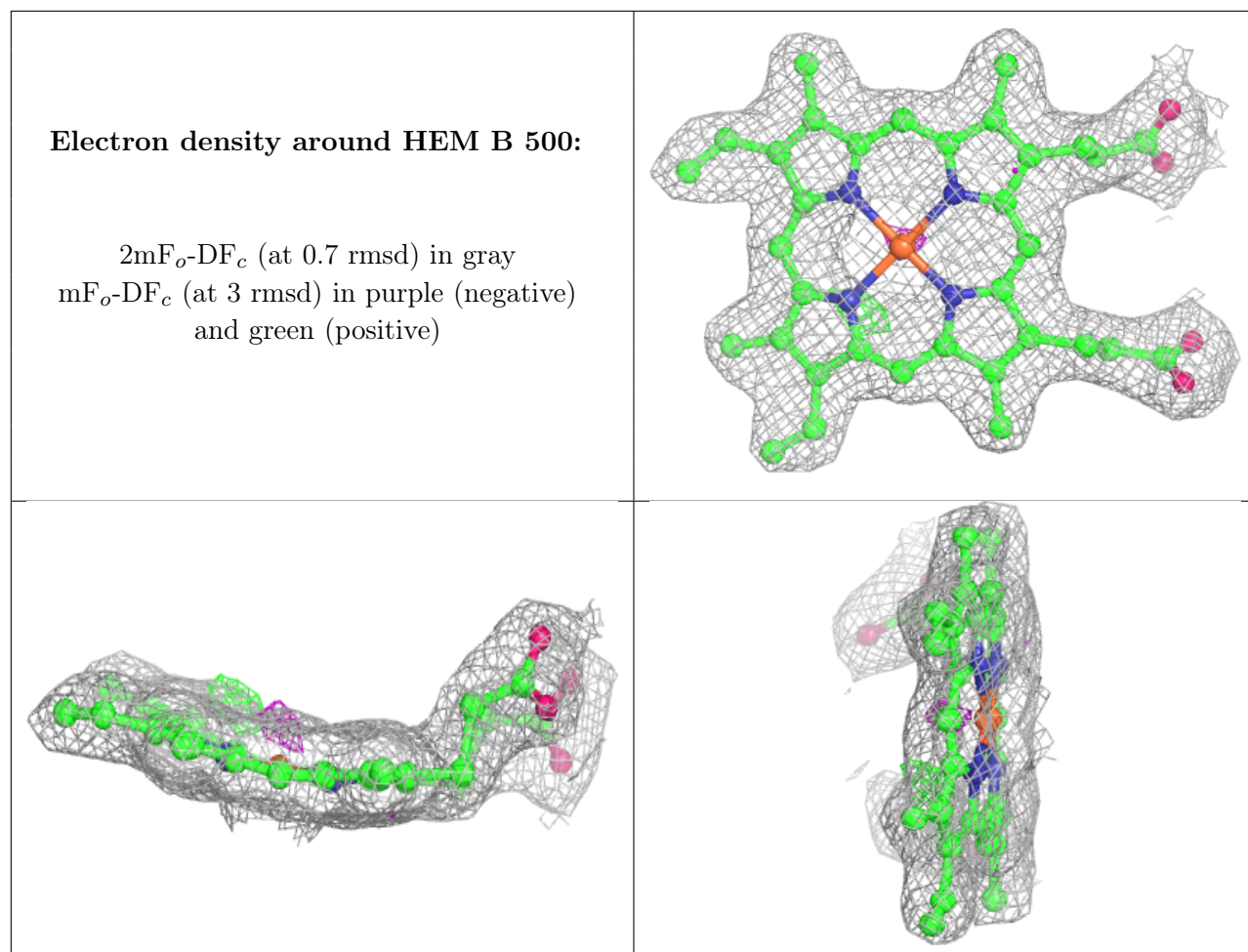
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 500:

$2mF_o-DF_c$ (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.