



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:23 PM UTC

PDB ID : 3N6C / pdb_00003n6c
Title : Structure of endothelial nitric oxide synthase H373S single mutant heme domain complexed with 4-(2-(6-(2-(6-amino-4-methylpyridin-2-yl)ethyl)pyridin-2-yl)ethyl)-6-methylpyridin-2-amine
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Deposited on : 2010-05-25
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

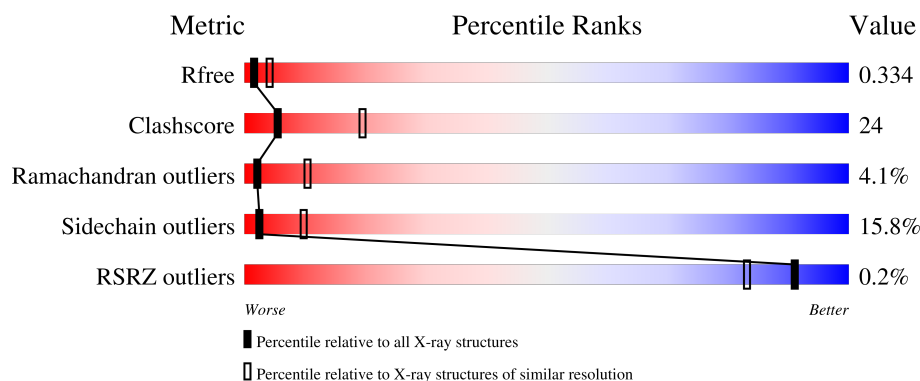
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	444	
1	B	444	

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
8	ZN	B	900	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6621 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.

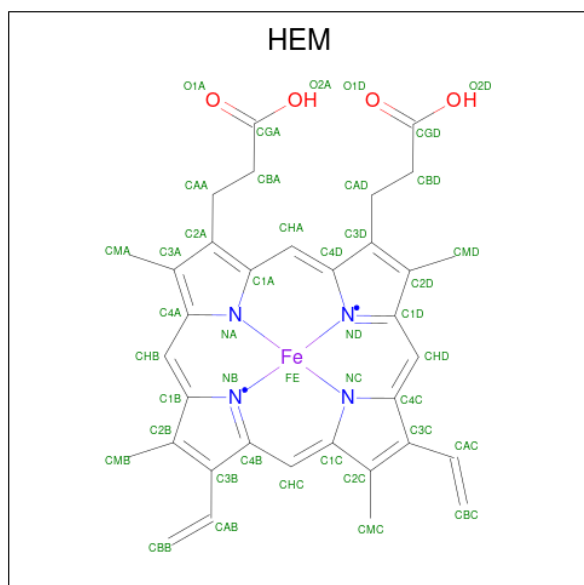
- Molecule 1 is a protein called Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3205	2038	562	589	16			
1	B	401	Total	C	N	O	S	0	0	0
			3187	2026	559	586	16			

There are 4 discrepancies between the modelled and reference sequences:

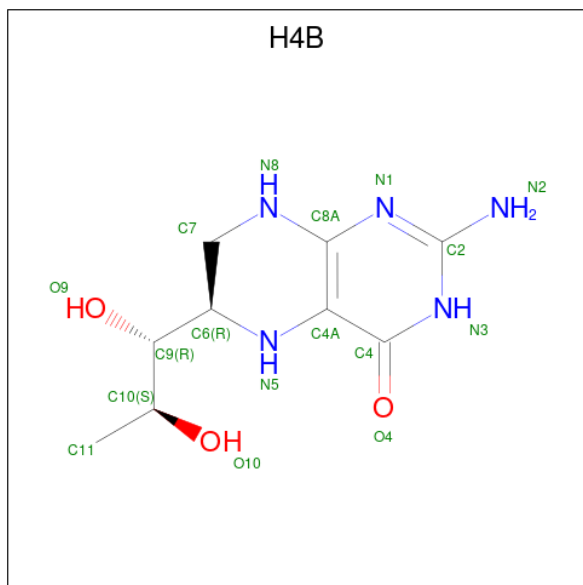
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29476
A	373	SER	HIS	engineered mutation	UNP P29476
B	100	ARG	CYS	SEE REMARK 999	UNP P29476
B	373	SER	HIS	engineered mutation	UNP P29476

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



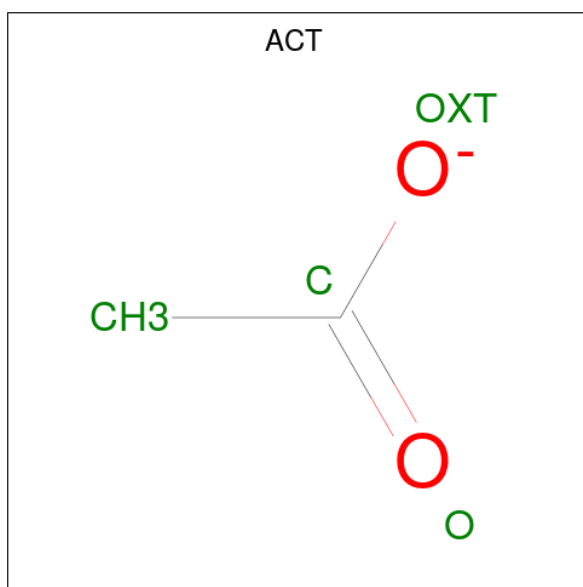
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



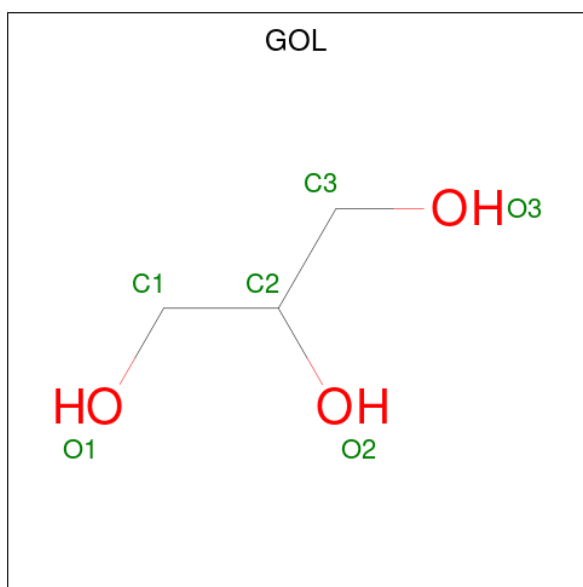
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



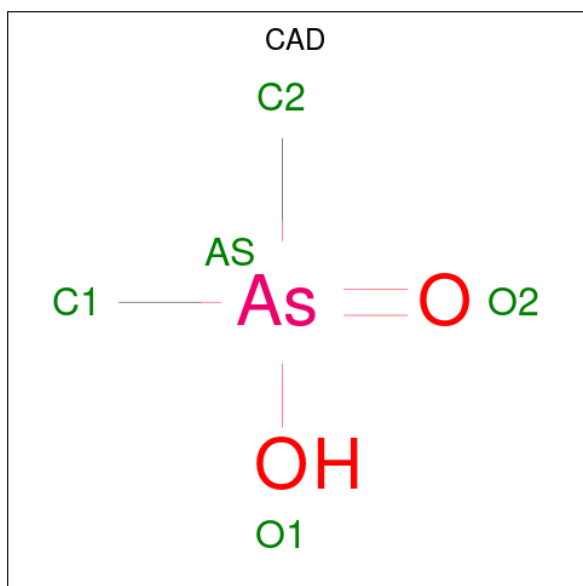
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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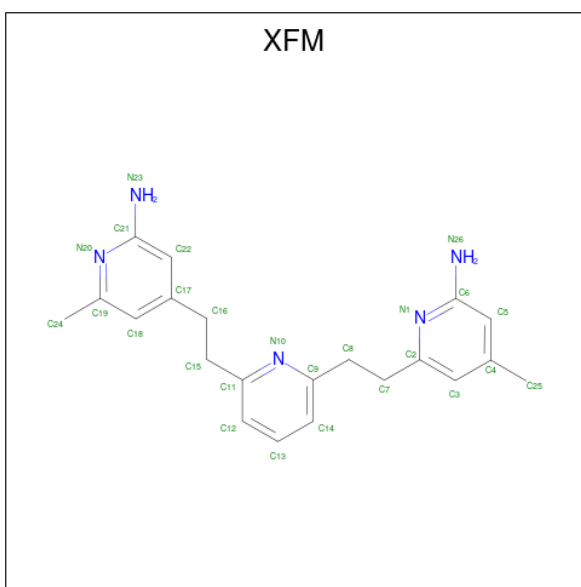
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CACODYLIC ACID (CCD ID: CAD) (formula: $C_2H_7AsO_2$).



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

- Molecule 7 is 6-(2-{6-[2-(2-amino-6-methylpyridin-4-yl)ethyl]pyridin-2-yl}ethyl)-4-methylpyridin-2-amine (CCD ID: XFM) (formula: $C_{21}H_{25}N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			26	21	5		
7	B	1	Total	C	N	0	0
			26	21	5		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Zn	0	0
			1	1		

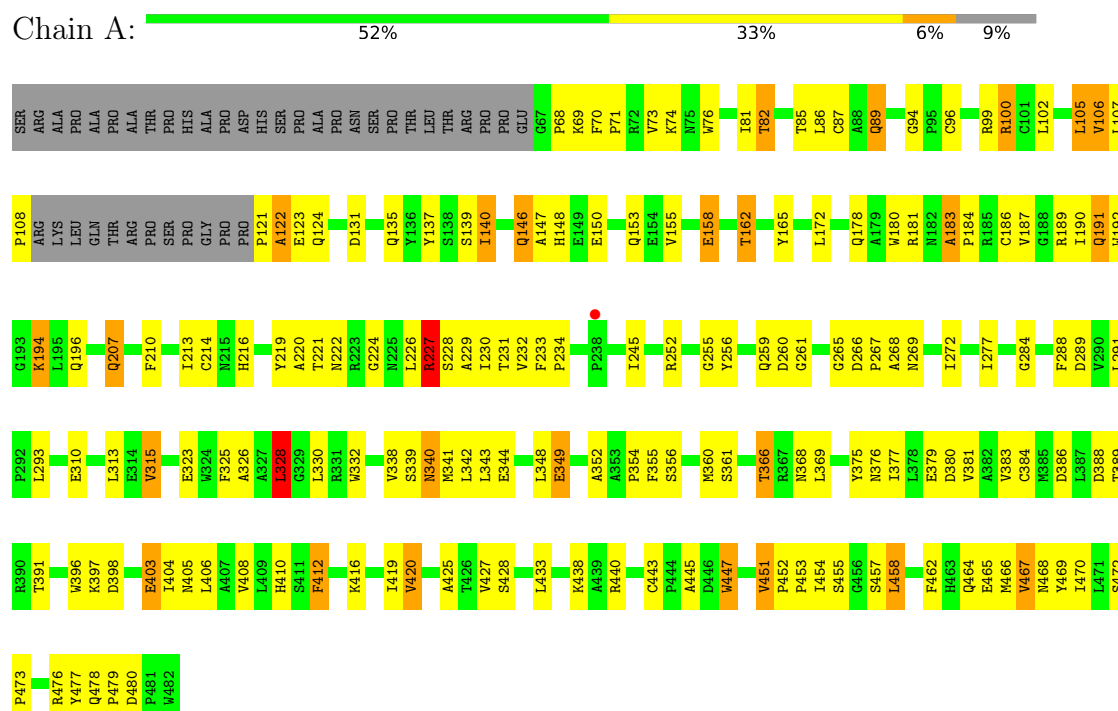
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	13	Total	O	0	0
			13	13		
9	B	13	Total	O	0	0
			13	13		

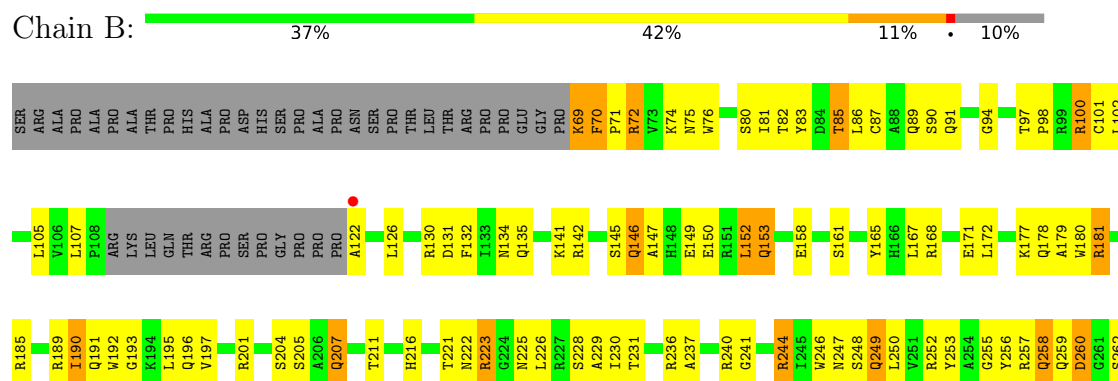
3 Residue-property plots

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: Nitric oxide synthase



• Molecule 1: Nitric oxide synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.14Å 105.69Å 159.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.80 – 3.06 39.80 – 3.06	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.80-3.06) 97.4 (39.80-3.06)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.233 , 0.332 0.233 , 0.334	Depositor DCC
R_{free} test set	917 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.982	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6621	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: CAD, H4B, HEM, XFM, ZN, ACT, GOL

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	0.69	0/3294	1.09	17/4487 (0.4%)
1	B	0.72	1/3274 (0.0%)	1.06	15/4459 (0.3%)
All	All	0.70	1/6568 (0.0%)	1.08	32/8946 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	315	VAL	CA-CB	5.06	1.59	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	VAL	CA-C-N	11.68	132.41	120.38
1	A	451	VAL	C-N-CA	11.68	132.41	120.38
1	A	284	GLY	N-CA-C	-7.15	101.66	112.60
1	A	480	ASP	CA-C-N	6.72	126.23	119.24
1	A	480	ASP	C-N-CA	6.72	126.23	119.24
1	B	94	GLY	CA-C-N	6.67	126.36	119.56
1	B	94	GLY	C-N-CA	6.67	126.36	119.56
1	B	70	PHE	CA-C-N	6.56	128.04	119.84
1	B	70	PHE	C-N-CA	6.56	128.04	119.84
1	B	331	ARG	N-CA-C	6.30	116.76	107.88
1	B	370	CYS	N-CA-C	6.24	124.09	110.80
1	B	480	ASP	CA-C-N	6.11	127.48	119.84
1	B	480	ASP	C-N-CA	6.11	127.48	119.84
1	A	467	VAL	N-CA-C	6.05	115.06	106.53
1	A	183	ALA	N-CA-C	6.05	118.37	109.42
1	A	73	VAL	N-CA-C	5.88	115.19	106.85
1	B	452	PRO	CA-C-N	5.53	125.20	119.56
1	B	452	PRO	C-N-CA	5.53	125.20	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	SER	N-CA-C	5.47	117.01	107.49
1	A	155	VAL	N-CA-C	-5.47	105.20	110.72
1	B	459	THR	CA-C-N	5.44	125.53	119.32
1	B	459	THR	C-N-CA	5.44	125.53	119.32
1	A	183	ALA	CA-C-N	5.41	125.02	119.56
1	A	183	ALA	C-N-CA	5.41	125.02	119.56
1	A	427	VAL	N-CA-C	-5.29	106.53	111.45
1	B	81	ILE	N-CA-C	5.24	114.29	106.85
1	A	85	THR	N-CA-C	-5.23	107.44	113.88
1	A	94	GLY	CA-C-N	5.21	124.83	119.05
1	A	94	GLY	C-N-CA	5.21	124.83	119.05
1	B	263	VAL	N-CA-C	5.11	115.32	108.17
1	A	227	ARG	N-CA-C	-5.11	102.50	110.42
1	A	470	ILE	N-CA-C	5.02	114.99	107.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3205	0	3113	132	0
1	B	3187	0	3097	184	0
2	A	43	0	30	8	0
2	B	43	0	30	5	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	4	0	3	0	0
4	B	8	0	6	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	3	0	0	1	0
6	B	3	0	0	1	0
7	A	26	0	25	4	0
7	B	26	0	25	1	0
8	B	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	13	0	0	0	0
9	B	13	0	0	1	0
All	All	6621	0	6375	308	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (308) 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:244:ARG:HG3	1:B:244:ARG:HH11	0.95	1.10
1:B:100:ARG:HG2	1:B:100:ARG:HH11	1.21	1.02
1:B:252:ARG:HB3	1:B:269:ASN:ND2	1.77	1.00
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.28	0.98
1:A:384:CYS:SG	6:A:950:CAD:AS	2.84	0.95
1:B:244:ARG:HG3	1:B:244:ARG:NH1	1.75	0.95
1:B:355:PHE:CD1	2:B:500:HEM:HAC	2.02	0.94
1:B:100:ARG:HH11	1:B:100:ARG:CG	1.81	0.94
1:B:299:ASP:O	1:B:300:GLU:HG2	1.69	0.92
1:B:385:MET:O	1:B:386:ASP:HB2	1.64	0.92
1:A:181:ARG:NH2	1:A:440:ARG:HG3	1.86	0.91
1:A:477:TYR:HE1	7:A:800:XFM:H18	1.39	0.88
1:A:404:ILE:O	1:A:408:VAL:HG23	1.74	0.88
1:A:181:ARG:HH21	1:A:440:ARG:HG3	1.39	0.86
1:B:222:ASN:HB3	1:B:225:ASN:O	1.76	0.85
1:B:168:ARG:HB2	1:B:171:GLU:HG3	1.57	0.84
1:A:100:ARG:HG2	1:A:100:ARG:NH1	1.90	0.81
1:B:240:ARG:HD2	1:B:241:GLY:O	1.80	0.81
1:A:477:TYR:CE1	7:A:800:XFM:H18	2.17	0.79
1:B:430:MET:HE2	1:B:460:PRO:HB2	1.64	0.79
1:A:455:SER:HA	1:B:454:ILE:HG22	1.65	0.78
1:B:69:LYS:N	1:B:69:LYS:HE2	1.98	0.78
1:B:284:GLY:HA3	1:B:289:ASP:OD2	1.84	0.77
1:A:181:ARG:HD2	1:A:192:TRP:CZ2	2.19	0.77
1:A:355:PHE:CD1	2:A:500:HEM:HAC	2.20	0.75
1:B:101:CYS:SG	8:B:900:ZN:ZN	1.74	0.75
1:B:150:GLU:HA	1:B:153:GLN:HB2	1.68	0.74
1:A:194:LYS:HE3	1:A:194:LYS:HA	1.70	0.74
1:B:362:THR:HA	1:B:405:ASN:HD21	1.52	0.74
1:B:471:LEU:O	1:B:472:SER:HB2	1.86	0.73
1:B:297:ALA:HB1	1:B:298:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:GLN:HB2	1:B:479:PRO:HD2	1.71	0.72
1:B:100:ARG:HG2	1:B:100:ARG:NH1	2.00	0.72
1:B:249:GLN:HA	1:B:337:ALA:O	1.89	0.72
1:B:365:GLY:HA2	1:B:369:LEU:HD12	1.72	0.71
1:B:101:CYS:HG	8:B:900:ZN:ZN	1.03	0.71
1:A:328:LEU:HB3	1:A:330:LEU:HG	1.73	0.71
1:B:165:TYR:CE2	1:B:348:LEU:HD11	2.26	0.71
1:B:180:TRP:CZ3	1:B:192:TRP:HA	2.26	0.70
1:B:249:GLN:HB2	1:B:252:ARG:HD2	1.74	0.70
1:A:106:VAL:HG21	1:B:76:TRP:NE1	2.06	0.70
1:A:366:THR:OG1	1:A:405:ASN:ND2	2.21	0.70
1:B:472:SER:HA	1:B:473:PRO:C	2.15	0.70
1:B:291:LEU:HB3	1:B:292:PRO:HD2	1.74	0.69
1:B:370:CYS:HA	1:B:377:ILE:H	1.56	0.69
1:B:244:ARG:HH11	1:B:244:ARG:CG	1.88	0.69
1:A:457:SER:HA	1:A:462:PHE:CD1	2.27	0.69
1:B:370:CYS:HB2	1:B:378:LEU:HD22	1.73	0.69
1:B:179:ALA:HA	1:B:473:PRO:O	1.93	0.67
1:B:280:GLY:O	1:B:304:LEU:HD22	1.94	0.67
1:A:369:LEU:O	1:A:377:ILE:HG12	1.94	0.66
1:A:420:VAL:HG22	1:A:425:ALA:HB2	1.77	0.66
1:B:395:LEU:HD22	1:B:398:ASP:OD1	1.95	0.66
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.30	0.66
1:A:455:SER:HB3	1:A:458:LEU:HB2	1.77	0.66
1:A:181:ARG:NH2	1:A:440:ARG:CG	2.59	0.66
1:B:189:ARG:O	1:B:192:TRP:HD1	1.78	0.65
1:A:230:ILE:HG13	1:A:355:PHE:HB3	1.77	0.65
1:B:255:GLY:O	1:B:273:THR:HG21	1.96	0.64
1:B:455:SER:O	1:B:458:LEU:HB2	1.96	0.64
1:A:196:GLN:HE21	1:A:196:GLN:HA	1.61	0.64
1:A:355:PHE:CG	2:A:500:HEM:HAC	2.32	0.64
1:B:319:HIS:HD2	1:B:407:ALA:HB2	1.64	0.63
1:A:181:ARG:HD2	1:A:192:TRP:CH2	2.34	0.63
1:A:377:ILE:O	1:A:381:VAL:HG23	1.99	0.63
1:A:100:ARG:HH11	1:A:100:ARG:CG	2.08	0.62
1:B:246:TRP:HB2	1:B:294:LEU:HB3	1.80	0.62
1:B:185:ARG:HG2	1:B:449:TRP:CD2	2.35	0.62
1:A:420:VAL:CG2	1:A:425:ALA:HB2	2.29	0.62
1:B:72:ARG:HB2	1:B:83:TYR:CE2	2.35	0.61
1:B:389:THR:HG22	1:B:389:THR:O	2.00	0.61
1:A:207:GLN:HE21	1:A:207:GLN:C	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:PHE:O	1:B:135:GLN:HB2	2.01	0.61
1:B:102:LEU:HG	1:B:105:LEU:HD23	1.83	0.60
1:A:403:GLU:OE1	1:A:406:LEU:HD23	2.00	0.60
1:B:165:TYR:CZ	1:B:348:LEU:HD11	2.36	0.60
1:B:379:GLU:O	1:B:383:VAL:HG23	2.02	0.59
1:B:444:PRO:HA	1:B:467:VAL:O	2.02	0.59
1:B:258:GLN:O	1:B:260:ASP:N	2.35	0.59
1:A:472:SER:HA	1:A:473:PRO:C	2.25	0.59
1:B:100:ARG:CG	1:B:100:ARG:NH1	2.50	0.59
1:B:185:ARG:HG2	1:B:449:TRP:CG	2.37	0.59
1:A:102:LEU:HD21	1:B:71:PRO:HB3	1.85	0.59
1:B:370:CYS:HB3	1:B:378:LEU:HD13	1.84	0.58
1:A:377:ILE:HD11	1:A:404:ILE:HG21	1.84	0.58
1:A:468:ASN:HD22	1:A:469:TYR:H	1.52	0.58
1:A:196:GLN:HA	1:A:196:GLN:NE2	2.18	0.58
1:B:407:ALA:O	1:B:411:SER:OG	2.21	0.58
1:A:189:ARG:O	1:A:192:TRP:HB3	2.04	0.58
1:B:267:PRO:HA	1:B:270:VAL:HG23	1.86	0.58
1:B:389:THR:HG23	1:B:396:TRP:CZ2	2.38	0.58
1:B:75:ASN:HB3	1:B:80:SER:HB2	1.85	0.57
1:A:137:TYR:C	1:A:139:SER:H	2.13	0.57
1:B:252:ARG:HB3	1:B:269:ASN:HD22	1.69	0.57
1:A:158:GLU:OE1	1:A:165:TYR:HA	2.05	0.57
1:B:299:ASP:O	1:B:300:GLU:CG	2.50	0.57
1:B:343:LEU:HD12	1:B:344:GLU:N	2.20	0.57
1:A:465:GLU:HG2	1:B:105:LEU:HA	1.86	0.56
1:A:340:ASN:HD22	1:A:340:ASN:H	1.52	0.56
1:B:216:HIS:CE1	1:B:231:THR:H	2.24	0.56
1:B:337:ALA:HA	1:B:356:SER:HB3	1.87	0.56
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.88	0.55
1:B:180:TRP:CG	2:B:500:HEM:HBC2	2.41	0.55
1:B:256:TYR:O	1:B:258:GLN:HG3	2.06	0.55
1:B:189:ARG:C	1:B:191:GLN:H	2.15	0.55
1:A:403:GLU:OE2	1:B:399:LYS:HE3	2.06	0.55
1:B:481:PRO:HD2	1:B:482:TRP:CZ3	2.42	0.55
1:A:341:MET:HE2	1:A:476:ARG:O	2.08	0.54
1:B:270:VAL:O	1:B:273:THR:HG22	2.07	0.54
1:B:325:PHE:CD1	1:B:325:PHE:C	2.86	0.54
1:B:246:TRP:HE1	1:B:296:GLN:NE2	2.06	0.54
1:A:68:PRO:O	1:A:70:PHE:N	2.41	0.54
1:B:359:TYR:CD2	1:B:364:ILE:HD11	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ILE:O	1:B:230:ILE:HG23	2.08	0.54
1:B:412:PHE:HB3	1:B:419:ILE:HG21	1.90	0.54
1:B:281:TRP:CZ3	1:B:283:PRO:HA	2.43	0.53
1:A:191:GLN:HE22	1:A:194:LYS:HD2	1.72	0.53
1:B:372:PRO:C	1:B:374:ARG:H	2.17	0.53
1:A:86:LEU:O	1:A:89:GLN:HB2	2.09	0.53
1:B:252:ARG:HB3	1:B:269:ASN:HD21	1.69	0.52
1:B:324:TRP:CE3	1:B:325:PHE:HA	2.43	0.52
1:A:181:ARG:HD2	1:A:192:TRP:CE2	2.44	0.52
1:B:322:LEU:HD22	1:B:324:TRP:HE1	1.74	0.52
1:B:89:GLN:O	1:B:91:GLN:HG2	2.10	0.52
1:A:338:VAL:HG23	7:A:800:XFM:H3	1.92	0.52
2:A:500:HEM:HBA2	7:A:800:XFM:H8	1.92	0.52
1:B:177:LYS:HG3	1:B:195:LEU:HD23	1.92	0.51
1:B:447:TRP:CH2	1:B:451:VAL:HG21	2.45	0.51
1:B:231:THR:O	1:B:354:PRO:HD2	2.11	0.51
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.46	0.51
1:B:291:LEU:HB3	1:B:292:PRO:CD	2.40	0.51
1:B:445:ALA:C	1:B:468:ASN:HB2	2.36	0.51
1:A:398:ASP:OD2	1:B:455:SER:CB	2.59	0.51
1:B:478:GLN:CB	1:B:479:PRO:HD2	2.40	0.50
1:A:256:TYR:OH	1:A:289:ASP:OD2	2.28	0.50
1:B:122:ALA:N	9:B:1019:HOH:O	2.44	0.50
1:A:252:ARG:CB	1:A:291:LEU:HD12	2.41	0.50
1:A:190:ILE:HG21	1:A:428:SER:HB2	1.93	0.50
1:A:465:GLU:CD	1:B:105:LEU:HD13	2.37	0.50
1:B:480:ASP:O	1:B:482:TRP:N	2.45	0.50
1:A:339:SER:HB3	1:A:354:PRO:HB3	1.93	0.50
1:A:410:HIS:O	1:A:410:HIS:CG	2.65	0.49
1:B:221:THR:O	1:B:222:ASN:C	2.54	0.49
1:B:317:LEU:HG	1:B:331:ARG:HA	1.94	0.49
1:B:389:THR:HA	1:B:396:TRP:NE1	2.28	0.49
1:B:391:THR:HG23	1:B:394:SER:HB3	1.95	0.49
1:B:361:SER:HB3	1:B:409:LEU:HD21	1.93	0.49
1:B:389:THR:O	1:B:389:THR:CG2	2.60	0.49
1:A:245:ILE:CD1	1:A:354:PRO:HG3	2.42	0.48
1:A:213:ILE:O	1:A:216:HIS:HB3	2.12	0.48
1:B:380:ASP:O	1:B:381:VAL:C	2.56	0.48
1:A:379:GLU:O	1:A:383:VAL:HG23	2.13	0.48
1:B:90:SER:OG	1:B:470:ILE:O	2.23	0.48
1:B:332:TRP:CD1	1:B:364:ILE:HG12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASN:HD22	1:A:469:TYR:N	2.11	0.48
1:A:477:TYR:OH	2:A:500:HEM:O2D	2.29	0.48
1:B:180:TRP:HB2	2:B:500:HEM:HBC2	1.94	0.48
1:A:342:LEU:HD21	1:A:349:GLU:HG3	1.95	0.48
1:A:377:ILE:HD12	1:A:381:VAL:HG21	1.96	0.48
1:A:228:SER:O	1:A:229:ALA:HB2	2.13	0.48
1:A:403:GLU:OE1	1:A:403:GLU:HA	2.13	0.48
1:B:247:ASN:O	1:B:339:SER:OG	2.20	0.48
1:B:464:GLN:HG3	1:B:465:GLU:O	2.14	0.48
1:B:102:LEU:HG	1:B:105:LEU:CD2	2.44	0.47
1:B:74:LYS:HD3	1:B:76:TRP:CE2	2.49	0.47
1:A:396:TRP:CZ2	1:A:397:LYS:HE2	2.50	0.47
1:B:266:ASP:OD2	1:B:374:ARG:NH2	2.43	0.47
1:B:86:LEU:HB3	1:B:469:TYR:OH	2.14	0.47
1:B:265:GLY:HA2	1:B:287:ARG:O	2.15	0.47
1:B:370:CYS:CB	1:B:378:LEU:HD13	2.44	0.47
1:B:177:LYS:HE2	1:B:193:GLY:O	2.14	0.47
1:A:388:ASP:OD2	1:A:391:THR:HG22	2.15	0.47
1:B:189:ARG:O	1:B:191:GLN:N	2.47	0.47
1:B:319:HIS:CD2	1:B:407:ALA:HB2	2.48	0.47
1:B:414:LEU:C	1:B:416:LYS:H	2.21	0.47
1:A:106:VAL:CG2	1:B:76:TRP:NE1	2.78	0.47
1:B:237:ALA:H	1:B:240:ARG:NH1	2.13	0.47
1:B:360:MET:HE3	1:B:362:THR:OG1	2.15	0.47
1:B:467:VAL:HG12	1:B:469:TYR:HD1	1.78	0.47
1:A:369:LEU:HA	1:A:375:TYR:HB2	1.97	0.46
1:A:180:TRP:CG	2:A:500:HEM:HBC2	2.50	0.46
1:B:250:LEU:HB2	1:B:337:ALA:HB3	1.98	0.46
1:B:260:ASP:HB2	1:B:262:SER:OG	2.16	0.46
1:A:180:TRP:HB2	2:A:500:HEM:HBC2	1.97	0.46
1:A:252:ARG:HB3	1:A:291:LEU:HD12	1.97	0.46
1:B:223:ARG:HH11	1:B:223:ARG:HB2	1.80	0.46
1:A:445:ALA:HB1	1:A:466:MET:SD	2.55	0.46
1:A:478:GLN:HA	1:A:479:PRO:HD3	1.88	0.46
1:A:355:PHE:CD1	2:A:500:HEM:CAC	2.95	0.46
1:A:146:GLN:NE2	1:A:147:ALA:H	2.14	0.46
1:A:375:TYR:O	1:A:376:ASN:C	2.59	0.46
1:B:142:ARG:O	1:B:145:SER:OG	2.31	0.46
1:B:189:ARG:C	1:B:191:GLN:N	2.73	0.46
1:A:186:CYS:HB2	2:A:500:HEM:C4D	2.52	0.45
1:A:377:ILE:HD11	1:A:404:ILE:CG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PHE:CZ	1:A:214:CYS:SG	3.09	0.45
1:A:332:TRP:CZ2	1:A:368:ASN:ND2	2.84	0.45
1:B:240:ARG:HD3	1:B:298:PRO:HB2	1.98	0.45
1:B:131:ASP:HA	1:B:134:ASN:HD22	1.80	0.45
1:B:360:MET:HA	1:B:420:VAL:O	2.16	0.45
1:A:233:PHE:HB3	1:A:234:PRO:CD	2.47	0.45
1:B:249:GLN:O	1:B:250:LEU:C	2.59	0.45
1:B:341:MET:HE2	1:B:475:PHE:HB3	1.98	0.45
1:A:220:ALA:O	1:A:226:LEU:HA	2.16	0.45
1:A:342:LEU:C	1:A:342:LEU:HD23	2.42	0.45
1:B:447:TRP:HD1	1:B:466:MET:HG3	1.82	0.45
1:A:107:LEU:HA	1:A:108:PRO:HD3	1.75	0.45
1:A:146:GLN:H	1:A:146:GLN:CD	2.25	0.45
1:A:172:LEU:HD21	1:A:232:VAL:HG21	1.98	0.45
1:B:246:TRP:HB2	1:B:294:LEU:CB	2.47	0.45
1:B:294:LEU:HD23	1:B:302:PRO:HB2	1.99	0.45
1:B:335:LEU:HA	1:B:336:PRO:HD3	1.89	0.45
1:B:167:LEU:O	1:B:201:ARG:NH1	2.36	0.45
1:B:207:GLN:HA	1:B:207:GLN:HE21	1.82	0.45
1:A:150:GLU:HA	1:A:153:GLN:HB2	1.97	0.45
1:B:100:ARG:NH1	1:B:102:LEU:HD13	2.32	0.45
1:B:248:SER:HA	1:B:340:ASN:HB3	1.99	0.45
1:A:123:GLU:HB2	1:A:124:GLN:OE1	2.17	0.45
1:A:219:TYR:O	1:A:227:ARG:NH2	2.47	0.45
1:A:266:ASP:CB	1:A:375:TYR:HE1	2.30	0.45
1:B:97:THR:O	1:B:98:PRO:C	2.57	0.45
1:B:456:GLY:C	1:B:458:LEU:H	2.25	0.45
1:B:382:ALA:HA	1:B:385:MET:HB2	1.99	0.44
1:A:288:PHE:CE1	1:A:375:TYR:HE2	2.34	0.44
1:B:360:MET:O	1:B:361:SER:C	2.60	0.44
1:A:102:LEU:O	1:A:105:LEU:HB2	2.16	0.44
1:B:253:TYR:CD1	1:B:288:PHE:HB3	2.52	0.44
1:A:121:PRO:O	1:A:122:ALA:CB	2.65	0.44
1:A:81:ILE:HG22	1:A:82:THR:N	2.33	0.44
1:B:358:TRP:H	2:B:500:HEM:HAB	1.82	0.44
1:A:360:MET:O	1:A:361:SER:C	2.60	0.44
1:A:146:GLN:CD	1:A:146:GLN:N	2.75	0.44
1:A:137:TYR:CD1	1:A:148:HIS:HB2	2.53	0.44
1:B:326:ALA:C	1:B:328:LEU:N	2.75	0.44
1:A:219:TYR:CZ	1:A:227:ARG:HD2	2.52	0.43
1:B:216:HIS:HE1	1:B:231:THR:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:ALA:O	1:B:386:ASP:N	2.48	0.43
1:B:391:THR:HG23	1:B:394:SER:CB	2.49	0.43
1:B:70:PHE:CD1	1:B:85:THR:HA	2.54	0.43
1:B:288:PHE:N	1:B:288:PHE:CD2	2.86	0.43
1:B:467:VAL:HG12	1:B:469:TYR:CD1	2.53	0.43
1:B:372:PRO:C	1:B:374:ARG:N	2.77	0.43
1:B:406:LEU:C	1:B:408:VAL:N	2.77	0.43
1:A:259:GLN:C	1:A:261:GLY:H	2.26	0.43
1:A:389:THR:HG22	1:A:396:TRP:CD2	2.54	0.43
1:B:72:ARG:HB2	1:B:83:TYR:HE2	1.82	0.43
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.67	0.43
1:B:146:GLN:O	1:B:147:ALA:C	2.62	0.43
1:B:286:GLY:O	1:B:287:ARG:C	2.62	0.43
1:A:315:VAL:HG21	1:A:412:PHE:CZ	2.54	0.43
1:B:130:ARG:HG2	1:B:152:LEU:HD21	2.01	0.43
1:B:181:ARG:HG3	1:B:192:TRP:CD2	2.54	0.42
1:B:360:MET:O	1:B:362:THR:N	2.52	0.42
1:A:438:LYS:HD2	1:A:438:LYS:HA	1.74	0.42
1:A:135:GLN:O	1:A:139:SER:HB3	2.18	0.42
1:A:344:GLU:HG2	1:A:348:LEU:O	2.19	0.42
1:A:452:PRO:HA	1:A:453:PRO:HD3	1.69	0.42
1:B:178:GLN:HG2	1:B:473:PRO:HD2	2.01	0.42
1:B:457:SER:HA	1:B:462:PHE:CD1	2.53	0.42
1:A:74:LYS:HG3	1:A:81:ILE:HD13	2.00	0.42
1:A:100:ARG:NH1	1:A:100:ARG:O	2.52	0.42
1:A:266:ASP:O	1:A:268:ALA:N	2.53	0.42
1:A:81:ILE:O	1:A:82:THR:HG23	2.19	0.42
1:A:96:CYS:SG	1:B:101:CYS:SG	3.17	0.42
1:B:325:PHE:HD1	1:B:326:ALA:HA	1.84	0.42
1:B:317:LEU:HD23	1:B:317:LEU:HA	1.78	0.42
1:B:325:PHE:HD1	1:B:326:ALA:N	2.17	0.42
1:A:222:ASN:HB2	1:A:227:ARG:HH21	1.85	0.42
1:A:325:PHE:O	1:A:326:ALA:C	2.61	0.42
1:B:158:GLU:OE2	1:B:165:TYR:HA	2.19	0.42
1:B:196:GLN:HB3	1:B:229:ALA:HB2	2.02	0.42
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.54	0.42
1:A:146:GLN:N	1:A:146:GLN:OE1	2.45	0.42
1:A:360:MET:HA	1:A:420:VAL:O	2.19	0.42
1:A:398:ASP:OD2	1:B:455:SER:OG	2.33	0.42
1:B:301:ALA:HA	1:B:302:PRO:HD2	1.80	0.42
1:B:433:LEU:HD22	1:B:433:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLN:HE21	1:A:196:GLN:CA	2.29	0.42
1:A:158:GLU:O	1:A:162:THR:HG23	2.20	0.41
1:B:266:ASP:CG	1:B:374:ARG:HH21	2.26	0.41
1:B:366:THR:OG1	1:B:405:ASN:OD1	2.28	0.41
1:B:381:VAL:O	1:B:385:MET:HG3	2.20	0.41
1:A:184:PRO:CB	1:A:468:ASN:HD21	2.34	0.41
1:B:178:GLN:HB3	1:B:473:PRO:HD2	2.02	0.41
1:A:131:ASP:O	1:A:135:GLN:NE2	2.49	0.41
1:A:146:GLN:O	1:A:147:ALA:C	2.63	0.41
1:A:447:TRP:O	1:A:451:VAL:HG23	2.20	0.41
1:A:87:CYS:C	1:A:89:GLN:H	2.28	0.41
1:A:255:GLY:HA2	1:A:265:GLY:HA3	2.01	0.41
1:A:412:PHE:HD1	1:A:412:PHE:N	2.19	0.41
1:B:165:TYR:O	1:B:348:LEU:HD21	2.21	0.41
1:B:319:HIS:CD2	1:B:320:PRO:HD2	2.56	0.41
1:A:433:LEU:HD23	1:A:443:CYS:HB3	2.04	0.41
1:B:70:PHE:CE1	1:B:85:THR:HG22	2.56	0.41
1:B:149:GLU:O	1:B:153:GLN:N	2.53	0.41
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.36	0.40
1:B:382:ALA:O	1:B:383:VAL:C	2.64	0.40
1:B:471:LEU:HB3	1:B:472:SER:H	1.70	0.40
2:B:500:HEM:HBD2	7:B:800:XFM:C13	2.51	0.40
1:A:222:ASN:C	1:A:224:GLY:H	2.28	0.40
1:B:384:CYS:SG	6:B:950:CAD:AS	3.40	0.40
1:A:137:TYR:O	1:A:140:ILE:HG13	2.21	0.40
1:A:384:CYS:C	1:A:386:ASP:H	2.29	0.40
1:A:464:GLN:HE21	1:A:465:GLU:N	2.19	0.40
1:B:412:PHE:CD2	1:B:419:ILE:HB	2.56	0.40
1:A:245:ILE:HG13	1:A:352:ALA:HB1	2.04	0.40
1:A:252:ARG:HB2	1:A:291:LEU:HD12	2.02	0.40
1:A:340:ASN:O	1:A:478:GLN:HG2	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	400/444 (90%)	329 (82%)	62 (16%)	9 (2%)	5	19
1	B	397/444 (89%)	302 (76%)	71 (18%)	24 (6%)	1	6
All	All	797/888 (90%)	631 (79%)	133 (17%)	33 (4%)	2	10

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	122	ALA
1	B	249	GLN
1	B	259	GLN
1	B	300	GLU
1	B	361	SER
1	B	378	LEU
1	B	386	ASP
1	A	260	ASP
1	B	260	ASP
1	B	285	ASN
1	B	299	ASP
1	B	370	CYS
1	B	373	SER
1	B	381	VAL
1	B	457	SER
1	B	472	SER
1	A	76	TRP
1	B	292	PRO
1	B	325	PHE
1	B	327	ALA
1	B	407	ALA
1	B	481	PRO
1	B	190	ILE
1	B	376	ASN
1	A	267	PRO
1	A	328	LEU
1	A	447	TRP
1	B	433	LEU
1	A	419	ILE
1	B	280	GLY
1	B	298	PRO
1	A	71	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/377 (91%)	303 (88%)	40 (12%)	5	19
1	B	341/377 (90%)	273 (80%)	68 (20%)	1	5
All	All	684/754 (91%)	576 (84%)	108 (16%)	2	10

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	THR
1	A	89	GLN
1	A	99	ARG
1	A	100	ARG
1	A	105	LEU
1	A	106	VAL
1	A	140	ILE
1	A	146	GLN
1	A	158	GLU
1	A	162	THR
1	A	178	GLN
1	A	187	VAL
1	A	191	GLN
1	A	194	LYS
1	A	207	GLN
1	A	221	THR
1	A	227	ARG
1	A	231	THR
1	A	269	ASN
1	A	272	ILE
1	A	277	ILE
1	A	293	LEU
1	A	310	GLU
1	A	313	LEU
1	A	315	VAL
1	A	323	GLU
1	A	328	LEU

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Mol	Chain	Res	Type
1	A	340	ASN
1	A	343	LEU
1	A	349	GLU
1	A	356	SER
1	A	366	THR
1	A	380	ASP
1	A	403	GLU
1	A	412	PHE
1	A	416	LYS
1	A	420	VAL
1	A	454	ILE
1	A	458	LEU
1	A	467	VAL
1	B	69	LYS
1	B	72	ARG
1	B	82	THR
1	B	85	THR
1	B	87	CYS
1	B	100	ARG
1	B	107	LEU
1	B	126	LEU
1	B	141	LYS
1	B	146	GLN
1	B	152	LEU
1	B	153	GLN
1	B	161	SER
1	B	172	LEU
1	B	181	ARG
1	B	190	ILE
1	B	197	VAL
1	B	204	SER
1	B	205	SER
1	B	207	GLN
1	B	211	THR
1	B	223	ARG
1	B	226	LEU
1	B	228	SER
1	B	236	ARG
1	B	244	ARG
1	B	257	ARG
1	B	258	GLN
1	B	271	GLU

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Mol	Chain	Res	Type
1	B	272	ILE
1	B	274	GLU
1	B	277	ILE
1	B	282	THR
1	B	287	ARG
1	B	288	PHE
1	B	294	LEU
1	B	296	GLN
1	B	306	VAL
1	B	311	LEU
1	B	317	LEU
1	B	323	GLU
1	B	330	LEU
1	B	331	ARG
1	B	338	VAL
1	B	340	ASN
1	B	348	LEU
1	B	351	SER
1	B	366	THR
1	B	378	LEU
1	B	386	ASP
1	B	387	LEU
1	B	391	THR
1	B	393	SER
1	B	394	SER
1	B	395	LEU
1	B	402	VAL
1	B	405	ASN
1	B	408	VAL
1	B	411	SER
1	B	414	LEU
1	B	420	VAL
1	B	421	ASP
1	B	426	THR
1	B	433	LEU
1	B	443	CYS
1	B	455	SER
1	B	457	SER
1	B	466	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	91	GLN
1	A	92	GLN
1	A	178	GLN
1	A	191	GLN
1	A	196	GLN
1	A	249	GLN
1	A	278	GLN
1	A	340	ASN
1	A	368	ASN
1	A	376	ASN
1	A	413	GLN
1	A	464	GLN
1	A	468	ASN
1	B	128	GLN
1	B	191	GLN
1	B	207	GLN
1	B	225	ASN
1	B	249	GLN
1	B	296	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\# Z > 2$
4	ACT	B	850	-	3,3,3	0.89	0	3,3,3	0.87	0
3	H4B	A	600	-	17,18,18	0.80	0	14,26,26	1.73	4 (28%)
6	CAD	A	950	-	0,2,4	-	-	0,1,6	-	-
4	ACT	A	860	-	3,3,3	0.79	0	3,3,3	0.91	0
5	GOL	A	880	-	5,5,5	0.42	0	5,5,5	0.19	0
3	H4B	B	600	-	17,18,18	0.74	0	14,26,26	1.87	4 (28%)
2	HEM	A	500	1	50,50,50	1.91	8 (16%)	67,82,82	1.22	5 (7%)
6	CAD	B	950	-	0,2,4	-	-	0,1,6	-	-
5	GOL	B	880	-	5,5,5	0.35	0	5,5,5	0.30	0
7	XFM	B	800	-	28,28,28	0.54	0	37,38,38	1.86	11 (29%)
7	XFM	A	800	-	28,28,28	0.55	0	37,38,38	1.88	11 (29%)
4	ACT	B	860	-	3,3,3	0.87	0	3,3,3	0.50	0
2	HEM	B	500	-	50,50,50	1.74	10 (20%)	67,82,82	1.21	4 (5%)

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	H4B	A	600	-	-	4/8/17/17	0/2/2/2
5	GOL	A	880	-	-	4/4/4/4	-
3	H4B	B	600	-	-	3/8/17/17	0/2/2/2
2	HEM	A	500	1	-	10/14/54/54	-
5	GOL	B	880	-	-	4/4/4/4	-
7	XFM	B	800	-	-	0/10/10/10	0/3/3/3
7	XFM	A	800	-	-	0/10/10/10	0/3/3/3
2	HEM	B	500	-	-	8/14/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3D-C2D	7.85	1.53	1.36
2	B	500	HEM	C3D-C2D	6.97	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	FE-NB	5.12	2.10	1.94
2	A	500	HEM	FE-ND	4.69	2.09	1.94
2	B	500	HEM	FE-NB	3.62	2.06	1.94
2	B	500	HEM	CAC-C3C	2.99	1.55	1.47
2	B	500	HEM	FE-ND	2.98	2.04	1.94
2	A	500	HEM	CAB-C3B	2.85	1.55	1.47
2	B	500	HEM	C2A-C3A	-2.59	1.32	1.38
2	B	500	HEM	CAB-C3B	2.58	1.54	1.47
2	A	500	HEM	FE-NA	2.50	2.03	1.95
2	A	500	HEM	CMD-C2D	2.45	1.55	1.50
2	B	500	HEM	C3B-C2B	-2.25	1.32	1.37
2	A	500	HEM	C3C-C2C	-2.16	1.32	1.37
2	A	500	HEM	CAC-C3C	2.09	1.53	1.47
2	B	500	HEM	CMC-C2C	2.08	1.55	1.50
2	B	500	HEM	C1B-NB	-2.06	1.36	1.40
2	B	500	HEM	CMB-C2B	2.03	1.54	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	800	XFM	C6-N1-C2	5.34	122.06	118.07
7	A	800	XFM	C6-N1-C2	4.75	121.63	118.07
2	A	500	HEM	C4D-ND-C1D	4.66	110.73	105.21
2	B	500	HEM	C4D-ND-C1D	4.06	110.01	105.21
3	B	600	H4B	C2-N1-C8A	4.03	120.47	113.36
7	A	800	XFM	C15-C11-N10	3.93	122.02	116.06
7	B	800	XFM	C7-C2-N1	3.79	121.80	116.06
3	A	600	H4B	C2-N1-C8A	3.74	119.96	113.36
7	A	800	XFM	C7-C2-N1	3.39	121.20	116.06
2	B	500	HEM	CAD-C3D-C4D	3.36	130.56	124.70
7	B	800	XFM	C3-C2-N1	-3.24	119.04	122.73
7	A	800	XFM	C8-C9-N10	3.11	120.77	116.06
3	B	600	H4B	O4-C4-C4A	-3.09	119.80	127.26
2	A	500	HEM	CHC-C1C-NC	2.96	127.67	124.45
7	A	800	XFM	C3-C2-N1	-2.86	119.47	122.73
7	B	800	XFM	C15-C11-N10	2.82	120.34	116.06
2	B	500	HEM	CBA-CAA-C2A	-2.77	104.88	112.53
3	B	600	H4B	C4A-C4-N3	2.67	119.47	112.13
3	A	600	H4B	O4-C4-C4A	-2.65	120.86	127.26
7	A	800	XFM	C17-C22-C21	2.64	119.82	117.86
7	A	800	XFM	C11-N10-C9	2.62	121.34	118.17
7	B	800	XFM	C24-C19-N20	2.55	120.41	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	800	XFM	N26-C6-N1	2.50	120.60	116.59
7	B	800	XFM	C8-C9-N10	2.45	119.77	116.06
7	B	800	XFM	C11-N10-C9	2.37	121.05	118.17
3	A	600	H4B	C4A-C4-N3	2.35	118.58	112.13
3	B	600	H4B	C2-N3-C4	-2.26	121.00	125.11
2	A	500	HEM	CMD-C2D-C1D	2.25	128.56	125.03
2	A	500	HEM	C1D-C2D-C3D	-2.22	104.64	106.98
7	B	800	XFM	C17-C22-C21	2.21	119.50	117.86
7	A	800	XFM	C24-C19-N20	2.18	119.85	116.56
3	A	600	H4B	C4-C4A-N5	2.18	122.20	116.27
7	B	800	XFM	C7-C8-C9	-2.17	108.19	113.01
7	A	800	XFM	C12-C11-N10	-2.14	119.69	122.40
7	A	800	XFM	N23-C21-N20	2.06	119.89	116.59
7	B	800	XFM	N26-C6-N1	2.04	119.87	116.59
2	B	500	HEM	CHD-C1D-ND	2.04	126.62	124.42
2	A	500	HEM	CAD-CBD-CGD	-2.04	108.26	113.67
7	B	800	XFM	N23-C21-N20	2.03	119.86	116.59

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2C-C3C-CAC-CBC
2	A	500	HEM	C4C-C3C-CAC-CBC
2	A	500	HEM	C2D-C3D-CAD-CBD
2	A	500	HEM	C4D-C3D-CAD-CBD
2	B	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC
3	A	600	H4B	N5-C6-C9-O9
3	A	600	H4B	N5-C6-C9-C10
3	A	600	H4B	C7-C6-C9-O9
3	A	600	H4B	C7-C6-C9-C10
3	B	600	H4B	C7-C6-C9-O9
3	B	600	H4B	C7-C6-C9-C10
5	A	880	GOL	C1-C2-C3-O3
5	B	880	GOL	O1-C1-C2-O2
5	B	880	GOL	O1-C1-C2-C3
5	A	880	GOL	O2-C2-C3-O3
5	A	880	GOL	O1-C1-C2-C3
5	B	880	GOL	C1-C2-C3-O3
5	A	880	GOL	O1-C1-C2-O2
2	B	500	HEM	C4D-C3D-CAD-CBD

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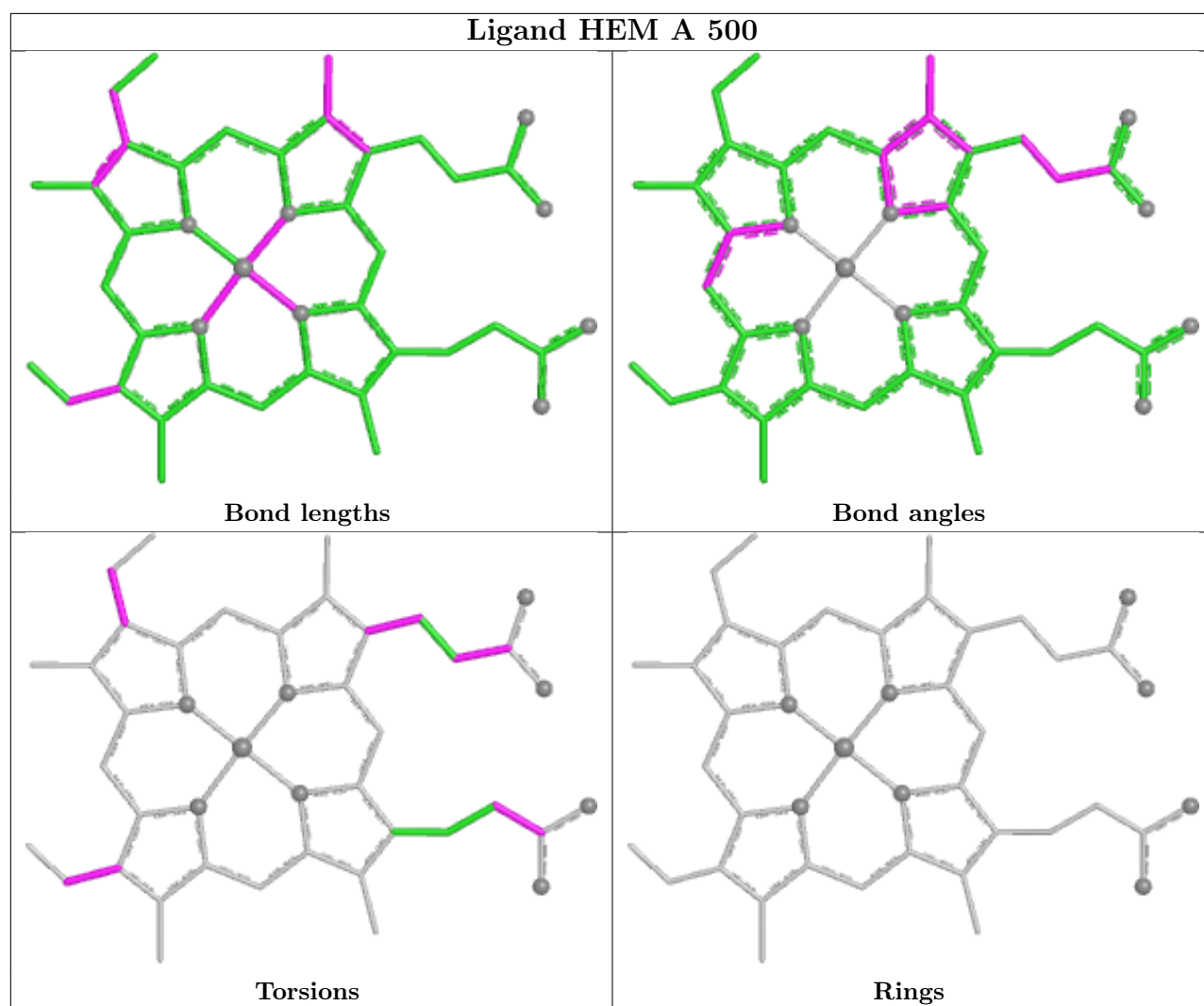
Mol	Chain	Res	Type	Atoms
2	B	500	HEM	C2D-C3D-CAD-CBD
3	B	600	H4B	N5-C6-C9-O9
2	B	500	HEM	C3D-CAD-CBD-CGD
5	B	880	GOL	O2-C2-C3-O3
2	A	500	HEM	C2B-C3B-CAB-CBB
2	A	500	HEM	C4B-C3B-CAB-CBB
2	A	500	HEM	CAD-CBD-CGD-O2D
2	B	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAD-CBD-CGD-O1D
2	A	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAD-CBD-CGD-O2D

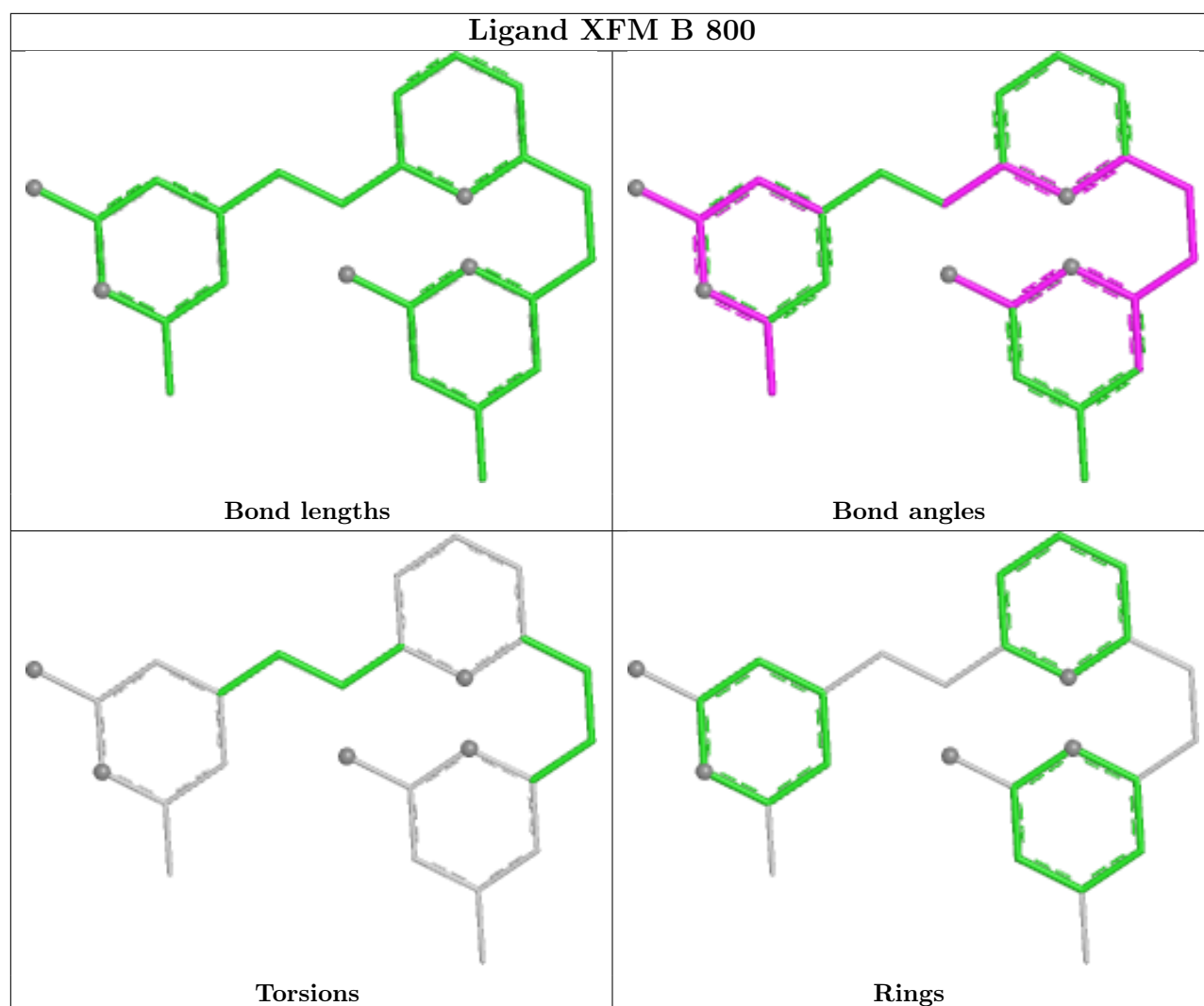
There are no ring outliers.

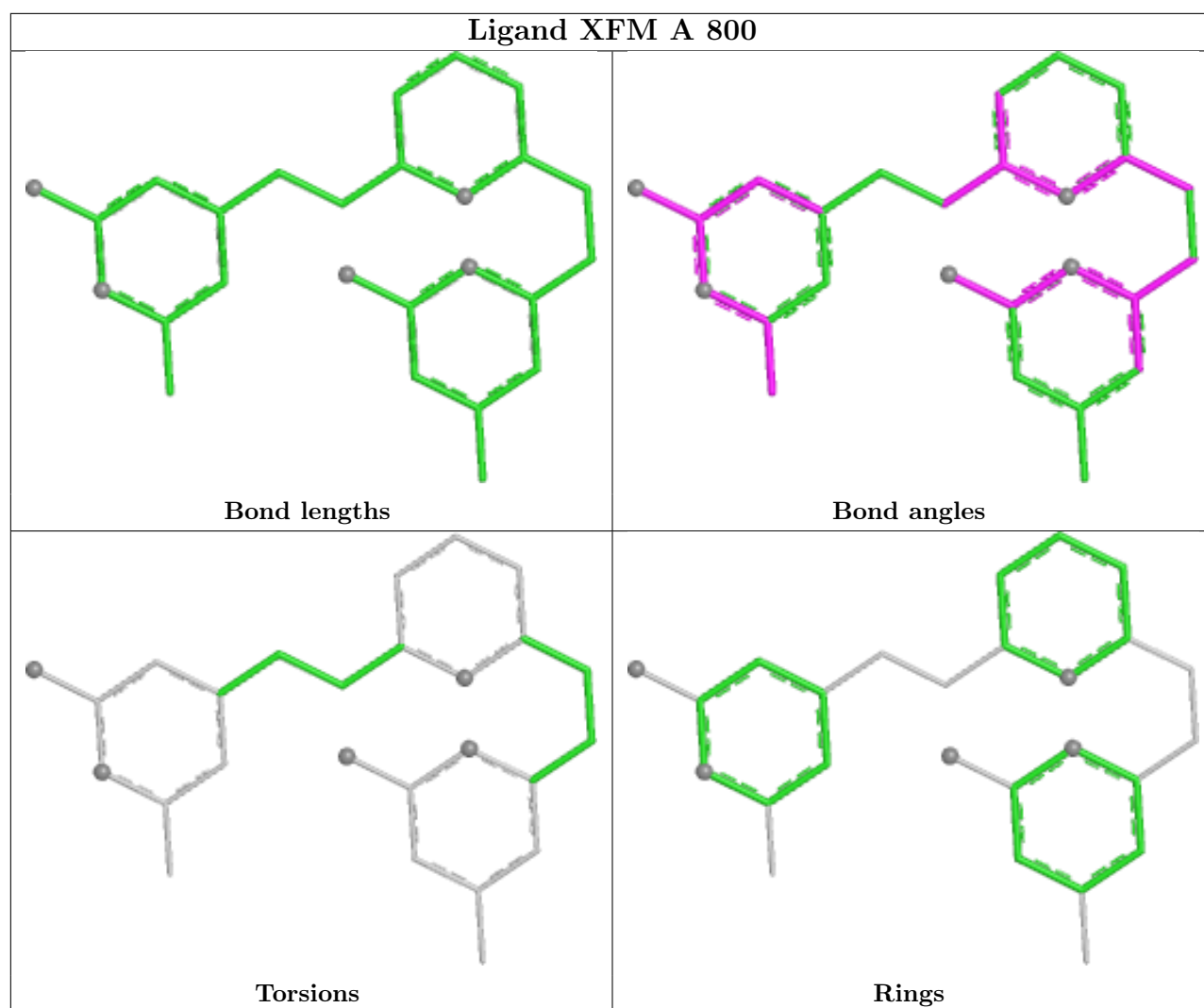
6 monomers are involved in 18 short contacts:

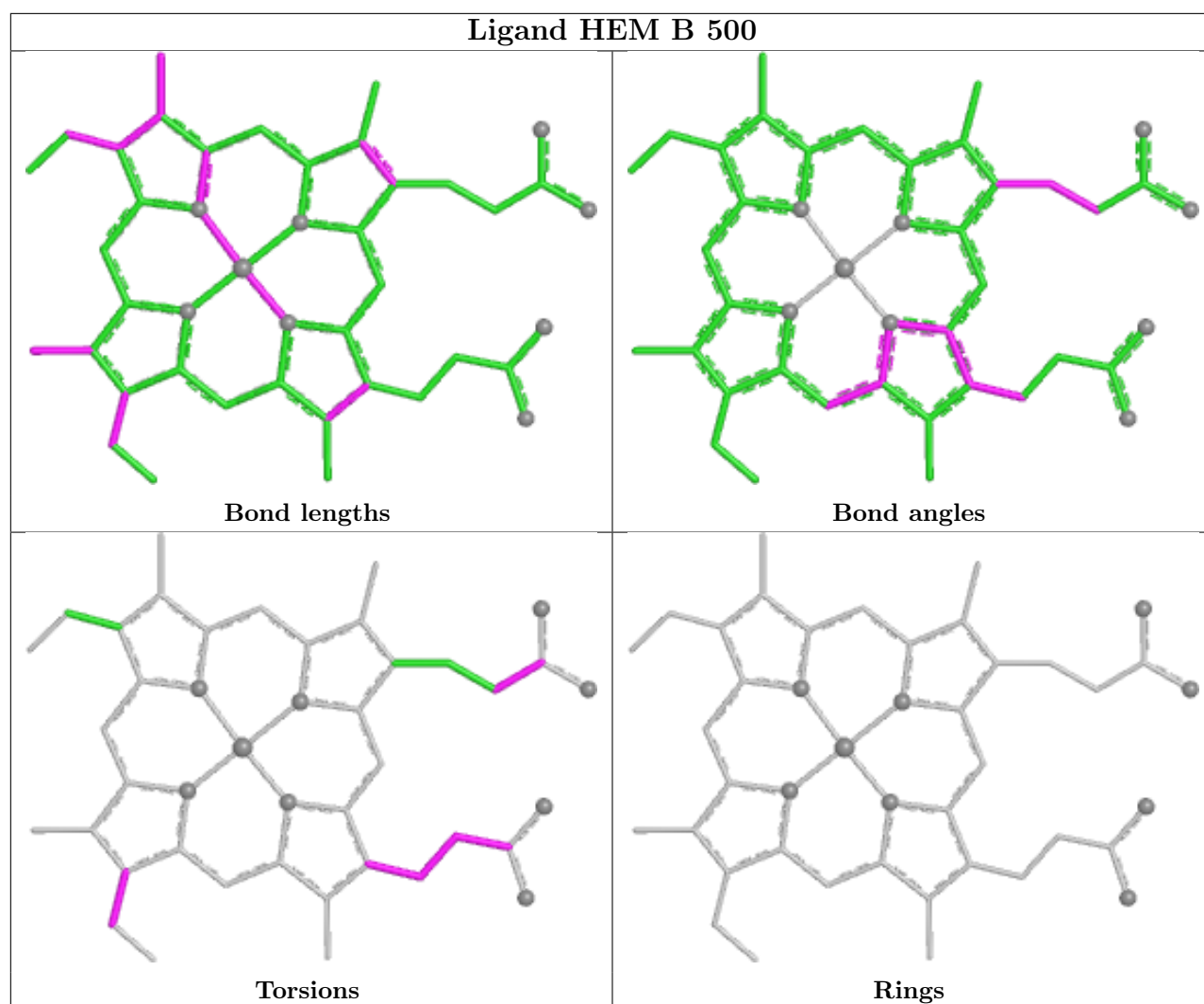
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	950	CAD	1	0
2	A	500	HEM	8	0
6	B	950	CAD	1	0
7	B	800	XFM	1	0
7	A	800	XFM	4	0
2	B	500	HEM	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	404/444 (90%)	-0.04	1 (0%) 91 83	39, 55, 77, 92	0
1	B	401/444 (90%)	0.01	1 (0%) 91 83	45, 56, 71, 84	0
All	All	805/888 (90%)	-0.01	2 (0%) 91 83	39, 56, 73, 92	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	ALA	2.1
1	A	238	PRO	2.1

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 oligosaccharides 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.

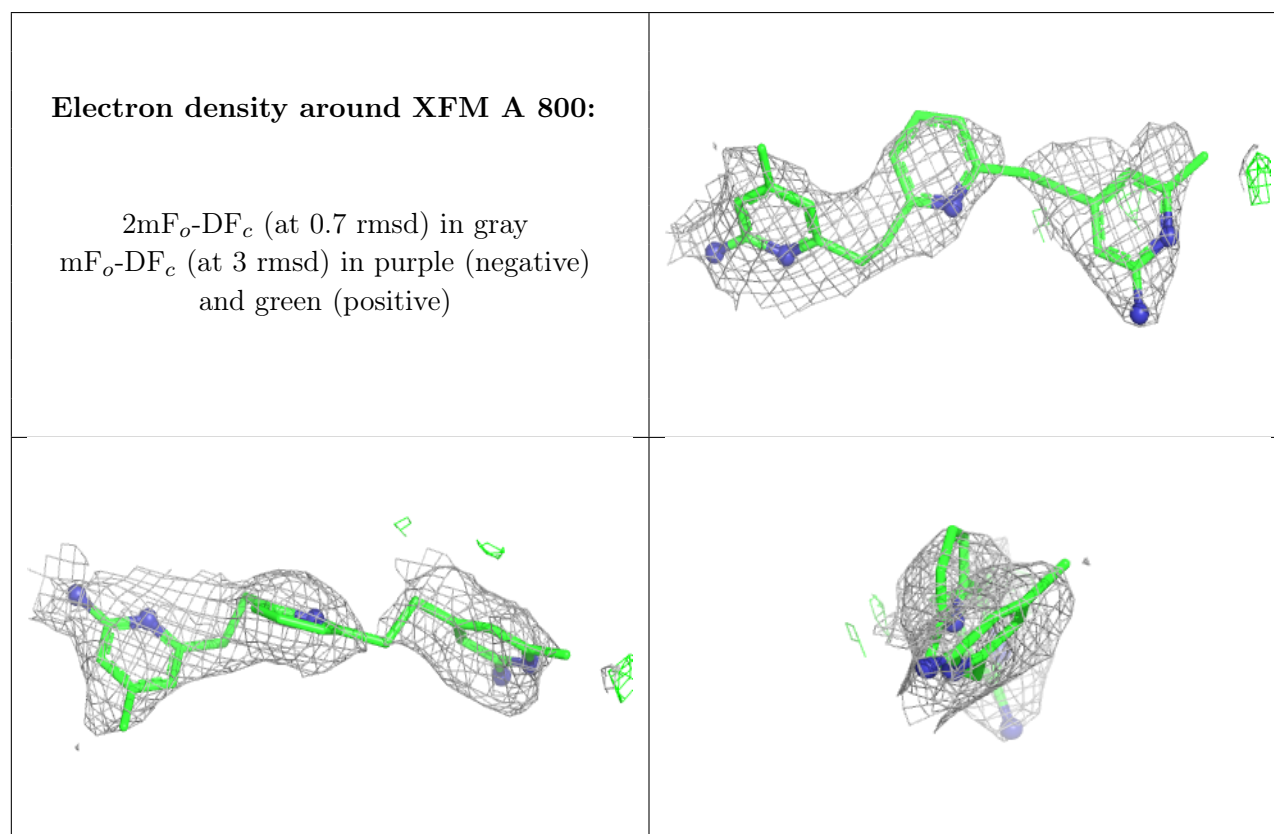
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	880	6/6	0.75	0.21	69,71,72,72	0
4	ACT	B	850	4/4	0.78	0.16	41,41,42,42	0
6	CAD	A	950	3/5	0.82	0.22	120,120,120,121	0

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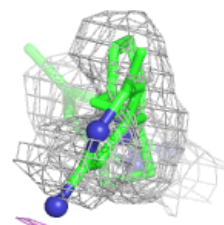
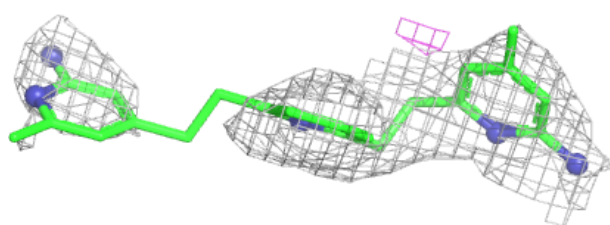
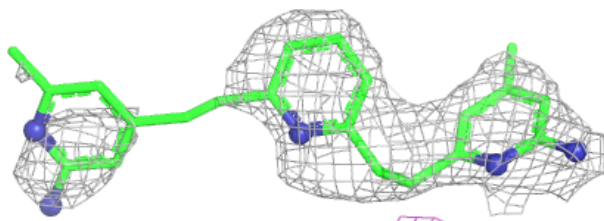
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CAD	B	950	3/5	0.84	0.21	118,118,118,118	0
3	H4B	A	600	17/17	0.86	0.18	94,96,97,97	0
4	ACT	A	860	4/4	0.87	0.17	66,66,67,67	0
4	ACT	B	860	4/4	0.88	0.22	58,59,59,60	0
3	H4B	B	600	17/17	0.88	0.17	82,85,86,86	0
7	XFM	A	800	26/26	0.88	0.16	61,74,85,85	0
7	XFM	B	800	26/26	0.88	0.16	68,78,83,83	0
5	GOL	B	880	6/6	0.89	0.12	54,55,57,57	0
2	HEM	A	500	43/43	0.95	0.12	44,48,57,59	0
2	HEM	B	500	43/43	0.96	0.12	45,48,59,62	0
8	ZN	B	900	1/1	0.99	0.03	58,58,58,58	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.

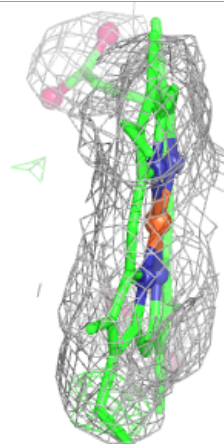
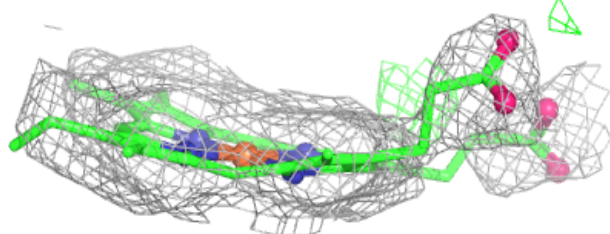
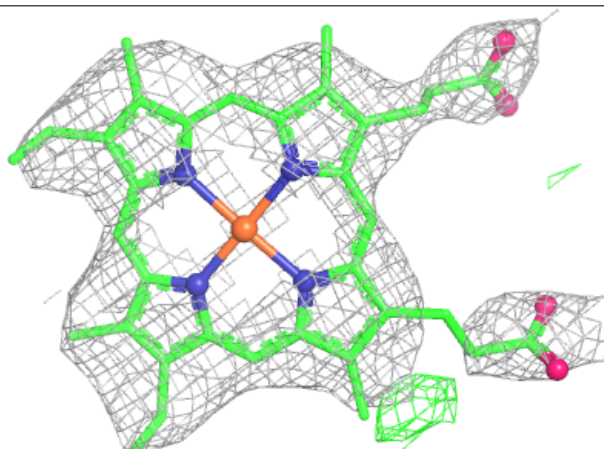


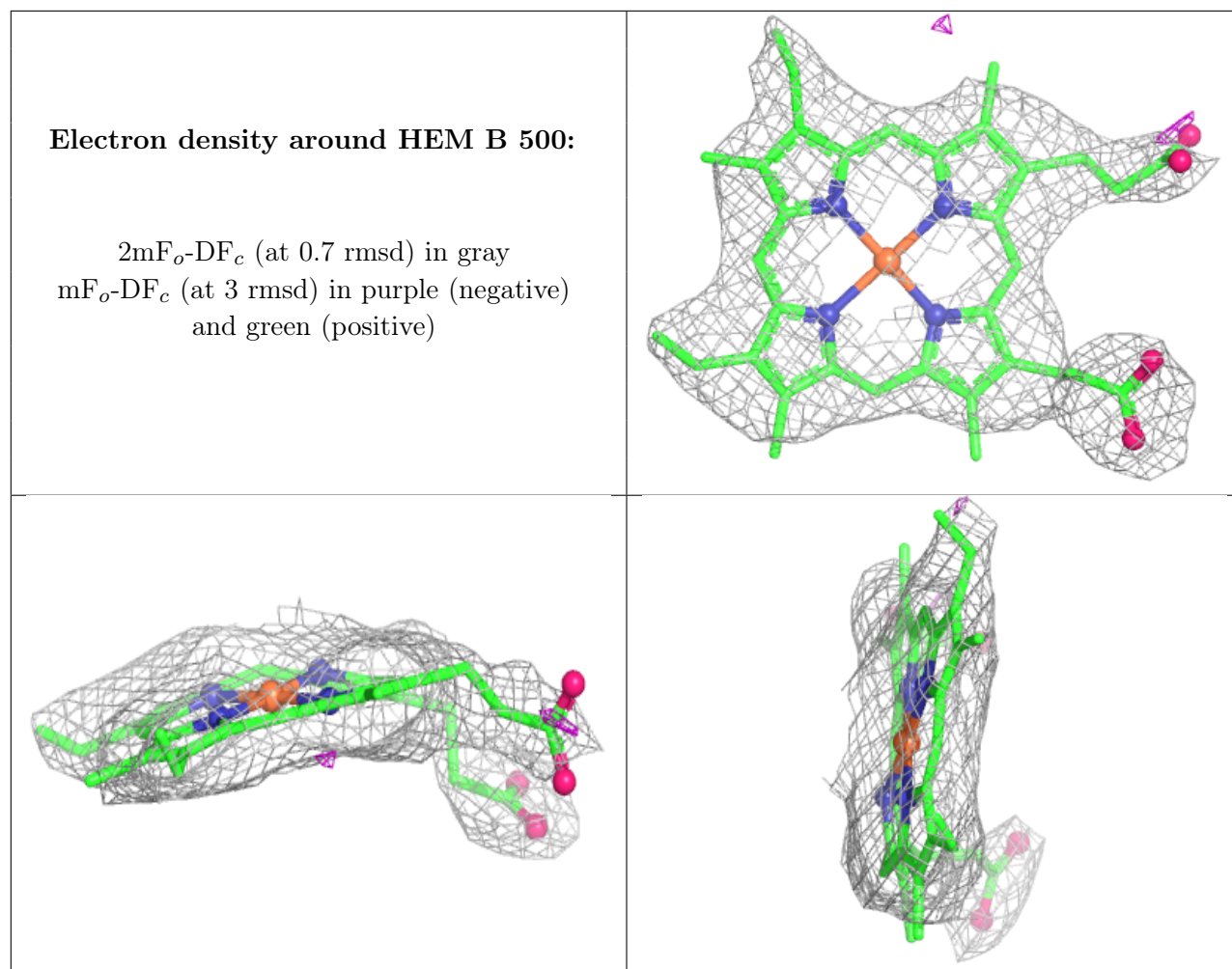
Electron density around XFM B 800:

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

**Electron density around 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.