WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 09:49 PM EST

PDB ID	:	3N6C
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
Authors	:	Delker, S.L.; Li, H.; Poulos, T.L.
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:

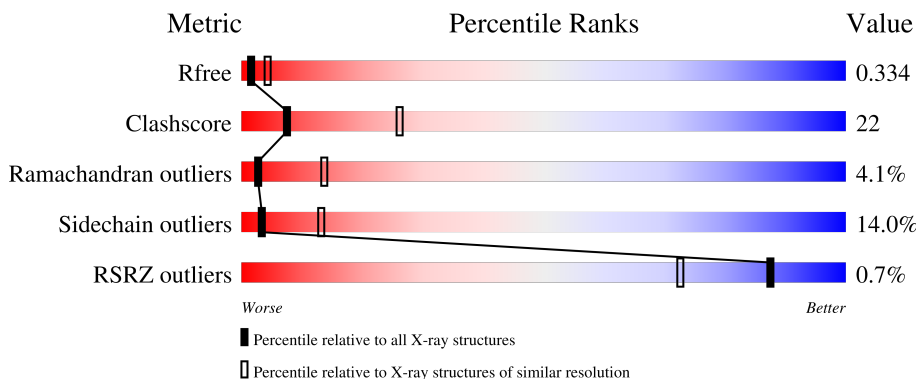|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1　Overall quality at a glance　ⓘ

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

The reported resolution of this entry is 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	Percentile Ranks	Value
Rfree		0.334
Clashscore		22
Ramachandran outliers		4.1%
Sidechain outliers		14.0%
RSRZ outliers		0.7%

Worse　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (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 <=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	%　56%　29%　5%　9%
1	B	444	43%　36%　10%　·　10%

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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).
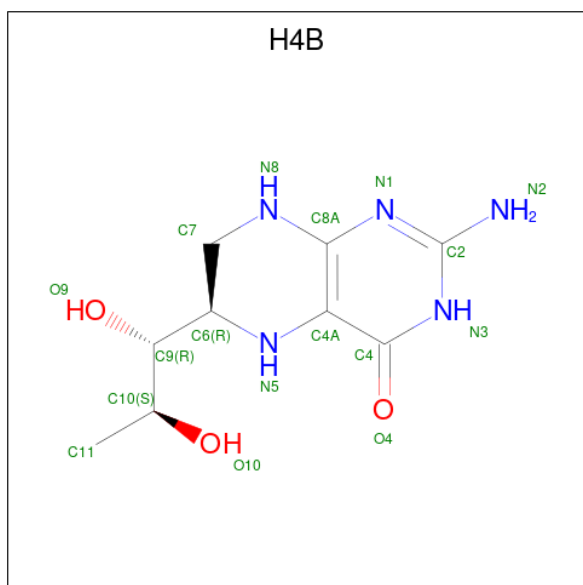
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O$^-$

C

CH3

O

O

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

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1   C2

HO

O1

OH

O2

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

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

- Molecule 6 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).
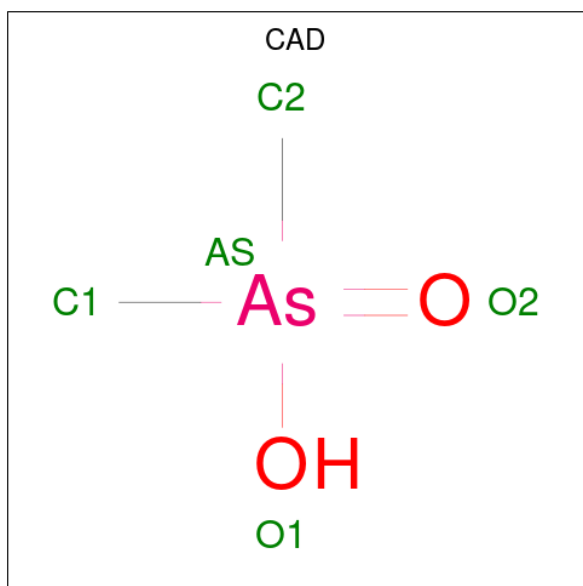
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 3	As 1	C 2	0	0
6	B	1	Total 3	As 1	C 2	0	0

- Molecule 7 is 6-(2-{6-[2-(2-amino-6-methylpyridin-4-yl)ethyl]pyridin-2-yl}ethyl)-4-methylpyridin-2-amine (three-letter code: XFM) (formula: $C_{21}H_{25}N_5$).
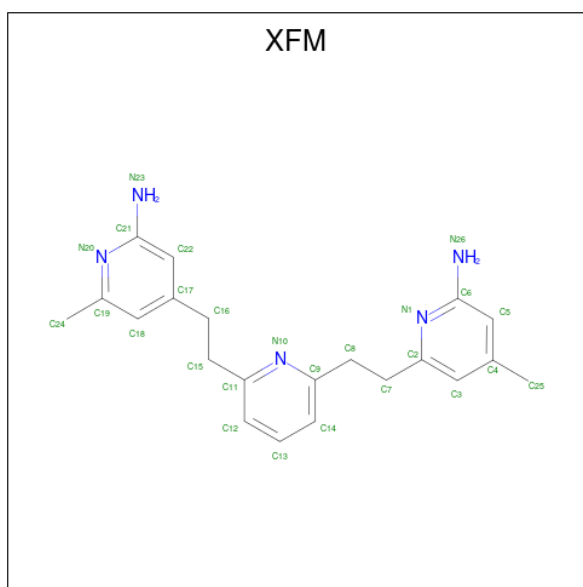
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 26	C 21	N 5	0	0
7	B	1	Total 26	C 21	N 5	0	0

• Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

• Molecule 9 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Nitric oxide synthase

• Molecule 1: Nitric oxide synthase

S356 G357 W358 Y359 M360 S361 T362 E363 I364 G365 T366 L369 C370 D371 P372 S373 R374 Y375 N376 I377 L378 E379 D380 V381 A382 V383 C384 M385 D386 T389 R390 T391 T392 S393 S394 L395 W396 K397 D398 K399 N405 L406 A407 V408 L409 H410 S411 F412 Q413 L414 A415 K416 I419 V420 D421

T426 M430 L433 C443 P444 A445 D446 W447 A448 W449 I450 V451 I454 S455 G456 S457 L458 T459 P460 V461 F462 H463 Q464 E465 M466 V467 N468 Y469 I470 L471 S472 P473 Y477 Q478 P479 D480 P481 W482

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) 97.5 (39.80-3.06)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [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 (4.92%)	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)	0.30 , 58.8	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, XFM, CAD, HEM, H4B, ZN, 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	0.56	0/3294	0.71	0/4487
1	B	0.59	0/3274	0.71	1/4459 (0.0%)
All	All	0.58	0/6568	0.71	1/8946 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	72	ARG	NE-CZ-NH1	5.68	123.14	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	3205	0	3113	122	0
1	B	3187	0	3097	173	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
8	B	1	0	0	2	0
9	A	13	0	0	0	0
9	B	13	0	0	1	0
All	All	6621	0	6375	287	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 22.

All (287) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:472:SER:HA	1:B:473:PRO:C	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:207:GLN:HE21	1:A:207:GLN:C	2.09	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:A:472:SER:HA	1:A:473:PRO:C	2.25	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: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:B:270:VAL:O	1:B:273:THR:HG22	2.07	0.54
1:B:246:TRP:HE1	1:B:296:GLN:NE2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:86:LEU:O	1:A:89:GLN:HB2	2.09	0.53
1:A:137:TYR:C	1:A:139:SER:H	2.13	0.52
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: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:B:189:ARG:C	1:B:191:GLN:H	2.15	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:325:PHE:CD1	1:B:325:PHE:C	2.86	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: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:B:372:PRO:C	1:B:374:ARG:H	2.17	0.48
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: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: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:B:445:ALA:C	1:B:468:ASN:HB2	2.36	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:465:GLU:CD	1:B:105:LEU:HD13	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:THR:O	1:B:222:ASN:C	2.54	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:A:220:ALA:O	1:A:226:LEU:HA	2.16	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: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: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: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:137:TYR:CD1	1:A:148:HIS:HB2	2.53	0.44
1:B:380:ASP:O	1:B:381:VAL:C	2.56	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
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:430:MET:CE	1:B:460:PRO:HB2	2.48	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:477:TYR:CD1	7:B:800:XFM:H24A	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:189:ARG:C	1:B:191:GLN:N	2.73	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:A:398:ASP:OD2	1:B:455:SER:OG	2.33	0.42
1:B:325:PHE:HD1	1:B:326:ALA:HA	1.84	0.42
1:B:414:LEU:C	1:B:416:LYS:H	2.21	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: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:OE1	1:A:146:GLN:N	2.45	0.42
1:A:360:MET:HA	1:A:420:VAL:O	2.19	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
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: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:375:TYR:O	1:A:376:ASN:C	2.59	0.41
1:A:447:TRP:O	1:A:451:VAL:HG23	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:249:GLN:O	1:B:250:LEU:C	2.59	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:342:LEU:C	1:A:342:LEU:HD23	2.42	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:464:GLN:HE21	1:A:465:GLU:N	2.19	0.40
1:B:97:THR:O	1:B:98:PRO:C	2.57	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%)	6	24
1	B	397/444 (89%)	302 (76%)	71 (18%)	24 (6%)	1	7
All	All	797/888 (90%)	631 (79%)	133 (17%)	33 (4%)	3	14

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	LYS

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Mol	Chain	Res	Type
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%)	306 (89%)	37 (11%)	6	22
1	B	341/377 (90%)	282 (83%)	59 (17%)	2	7
All	All	684/754 (91%)	588 (86%)	96 (14%)	3	13

All (96) 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	162	THR
1	A	178	GLN
1	A	187	VAL
1	A	191	GLN
1	A	194	LYS
1	A	196	GLN
1	A	207	GLN
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
1	A	340	ASN
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

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Mol	Chain	Res	Type
1	A	458	LEU
1	A	468	ASN
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	146	GLN
1	B	152	LEU
1	B	153	GLN
1	B	161	SER
1	B	172	LEU
1	B	181	ARG
1	B	204	SER
1	B	205	SER
1	B	207	GLN
1	B	223	ARG
1	B	228	SER
1	B	236	ARG
1	B	240	ARG
1	B	244	ARG
1	B	252	ARG
1	B	258	GLN
1	B	271	GLU
1	B	272	ILE
1	B	282	THR
1	B	287	ARG
1	B	288	PHE
1	B	294	LEU
1	B	296	GLN
1	B	311	LEU
1	B	323	GLU
1	B	330	LEU
1	B	331	ARG
1	B	340	ASN
1	B	348	LEU
1	B	351	SER
1	B	366	THR
1	B	370	CYS

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Mol	Chain	Res	Type
1	B	376	ASN
1	B	378	LEU
1	B	386	ASP
1	B	391	THR
1	B	393	SER
1	B	394	SER
1	B	395	LEU
1	B	398	ASP
1	B	405	ASN
1	B	411	SER
1	B	412	PHE
1	B	414	LEU
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	191	GLN
1	A	196	GLN
1	A	278	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	464	GLN
1	A	468	ASN
1	B	191	GLN
1	B	207	GLN
1	B	225	ASN
1	B	269	ASN
1	B	296	GLN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN
1	B	478	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	860	-	3,3,3	0.75	0	3,3,3	0.91	0
3	H4B	A	600	-	16,18,18	0.92	0	11,26,26	2.76	6 (54%)
6	CAD	A	950	-	0,2,4	-	-	0,1,6	-	-
7	XFM	B	800	-	28,28,28	0.54	0	38,38,38	1.85	11 (28%)
2	HEM	B	500	-	41,50,50	1.90	6 (14%)	45,82,82	1.57	7 (15%)
3	H4B	B	600	-	16,18,18	0.98	1 (6%)	11,26,26	2.52	5 (45%)
4	ACT	B	850	-	3,3,3	0.84	0	3,3,3	0.87	0
4	ACT	B	860	-	3,3,3	0.82	0	3,3,3	0.48	0
5	GOL	B	880	-	5,5,5	0.35	0	5,5,5	0.28	0
7	XFM	A	800	-	28,28,28	0.55	0	38,38,38	1.88	11 (28%)
5	GOL	A	880	-	5,5,5	0.41	0	5,5,5	0.18	0
6	CAD	B	950	-	0,2,4	-	-	0,1,6	-	-
2	HEM	A	500	1	41,50,50	2.04	9 (21%)	45,82,82	1.66	10 (22%)

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
7	XFM	B	800	-	-	0/10/10/10	0/3/3/3
2	HEM	B	500	-	-	6/12/54/54	-
3	H4B	B	600	-	-	3/8/17/17	0/2/2/2
5	GOL	B	880	-	-	4/4/4/4	-
7	XFM	A	800	-	-	1/10/10/10	0/3/3/3
5	GOL	A	880	-	-	4/4/4/4	-
2	HEM	A	500	1	-	8/12/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3D-C2D	7.98	1.53	1.36
2	B	500	HEM	C3D-C2D	7.09	1.51	1.36
2	A	500	HEM	C3C-C2C	-5.47	1.32	1.40
2	B	500	HEM	C3C-C2C	-4.67	1.33	1.40
2	B	500	HEM	C3C-CAC	3.69	1.55	1.47
2	A	500	HEM	FE-NB	2.79	2.10	1.96
2	A	500	HEM	CAB-C3B	2.77	1.55	1.47
2	A	500	HEM	FE-ND	2.52	2.09	1.96
2	A	500	HEM	C3C-CAC	2.51	1.53	1.47
2	B	500	HEM	CAB-C3B	2.51	1.54	1.47
2	A	500	HEM	CMD-C2D	2.36	1.55	1.50
2	B	500	HEM	C3B-C2B	-2.32	1.32	1.37
2	A	500	HEM	CAA-C2A	2.23	1.55	1.52
2	B	500	HEM	C1B-NB	-2.11	1.36	1.40
3	B	600	H4B	C4-N3	2.06	1.36	1.33
2	A	500	HEM	C3B-C2B	-2.02	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	C4D-ND-C1D	5.47	110.73	105.07
3	A	600	H4B	C8A-C4A-C4	5.30	119.27	114.57
7	B	800	XFM	C6-N1-C2	5.23	122.06	118.10
3	B	600	H4B	C8A-C4A-C4	4.90	118.92	114.57
2	B	500	HEM	C4D-ND-C1D	4.78	110.01	105.07
7	A	800	XFM	C6-N1-C2	4.65	121.63	118.10
2	B	500	HEM	CBA-CAA-C2A	-4.54	104.88	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	800	XFM	C15-C11-N10	4.07	122.02	115.95
7	B	800	XFM	C7-C2-N1	3.93	121.80	115.95
3	A	600	H4B	C4-C4A-N5	3.67	122.20	119.12
7	B	800	XFM	C3-C2-N1	-3.64	119.04	122.90
2	A	500	HEM	C4B-CHC-C1C	3.62	127.34	122.56
7	A	800	XFM	C7-C2-N1	3.53	121.20	115.95
3	A	600	H4B	C2-N3-C4	3.51	121.51	115.93
2	B	500	HEM	CAD-C3D-C4D	3.38	130.56	124.66
3	B	600	H4B	N1-C2-N3	-3.37	120.14	125.42
7	A	800	XFM	C8-C9-N10	3.24	120.77	115.95
7	A	800	XFM	C3-C2-N1	-3.23	119.47	122.90
2	A	500	HEM	CMA-C3A-C4A	-3.20	123.55	128.46
3	B	600	H4B	C2-N3-C4	3.19	121.00	115.93
3	A	600	H4B	N1-C2-N3	-3.14	120.50	125.42
7	B	800	XFM	C15-C11-N10	2.94	120.34	115.95
2	A	500	HEM	CBA-CAA-C2A	-2.89	107.69	112.62
3	B	600	H4B	C4-C4A-N5	2.87	121.53	119.12
3	B	600	H4B	C2-N1-C8A	2.65	120.47	114.54
7	A	800	XFM	C11-N10-C9	2.62	121.34	118.16
7	A	800	XFM	N26-C6-N1	2.60	120.60	116.49
7	B	800	XFM	C8-C9-N10	2.57	119.77	115.95
2	A	500	HEM	CAD-CBD-CGD	-2.48	108.26	113.60
7	A	800	XFM	C17-C22-C21	2.43	119.82	117.97
3	A	600	H4B	C2-N1-C8A	2.42	119.96	114.54
7	B	800	XFM	C24-C19-N20	2.41	120.41	116.56
2	B	500	HEM	C4B-CHC-C1C	2.41	125.74	122.56
7	B	800	XFM	C11-N10-C9	2.37	121.05	118.16
2	A	500	HEM	CMD-C2D-C1D	2.31	128.56	125.04
3	A	600	H4B	C4A-N5-C6	-2.26	115.01	121.16
2	A	500	HEM	C2C-C3C-C4C	2.23	108.46	106.90
2	A	500	HEM	C1D-C2D-C3D	-2.20	104.64	106.96
2	A	500	HEM	C4C-CHD-C1D	2.17	125.43	122.56
2	A	500	HEM	CHC-C4B-C3B	2.16	127.88	124.57
7	A	800	XFM	N23-C21-N20	2.15	119.89	116.49
7	A	800	XFM	C12-C11-N10	-2.14	119.69	122.41
7	B	800	XFM	N26-C6-N1	2.14	119.87	116.49
7	B	800	XFM	C7-C8-C9	-2.14	108.19	112.99
7	B	800	XFM	N23-C21-N20	2.13	119.86	116.49
7	A	800	XFM	C24-C19-N20	2.06	119.85	116.56
2	B	500	HEM	CMD-C2D-C1D	2.04	128.15	125.04
2	B	500	HEM	CHD-C1D-ND	2.01	126.62	124.43
7	B	800	XFM	C17-C22-C21	2.01	119.50	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HEM	C4C-CHD-C1D	2.01	125.21	122.56

There are no chirality outliers.
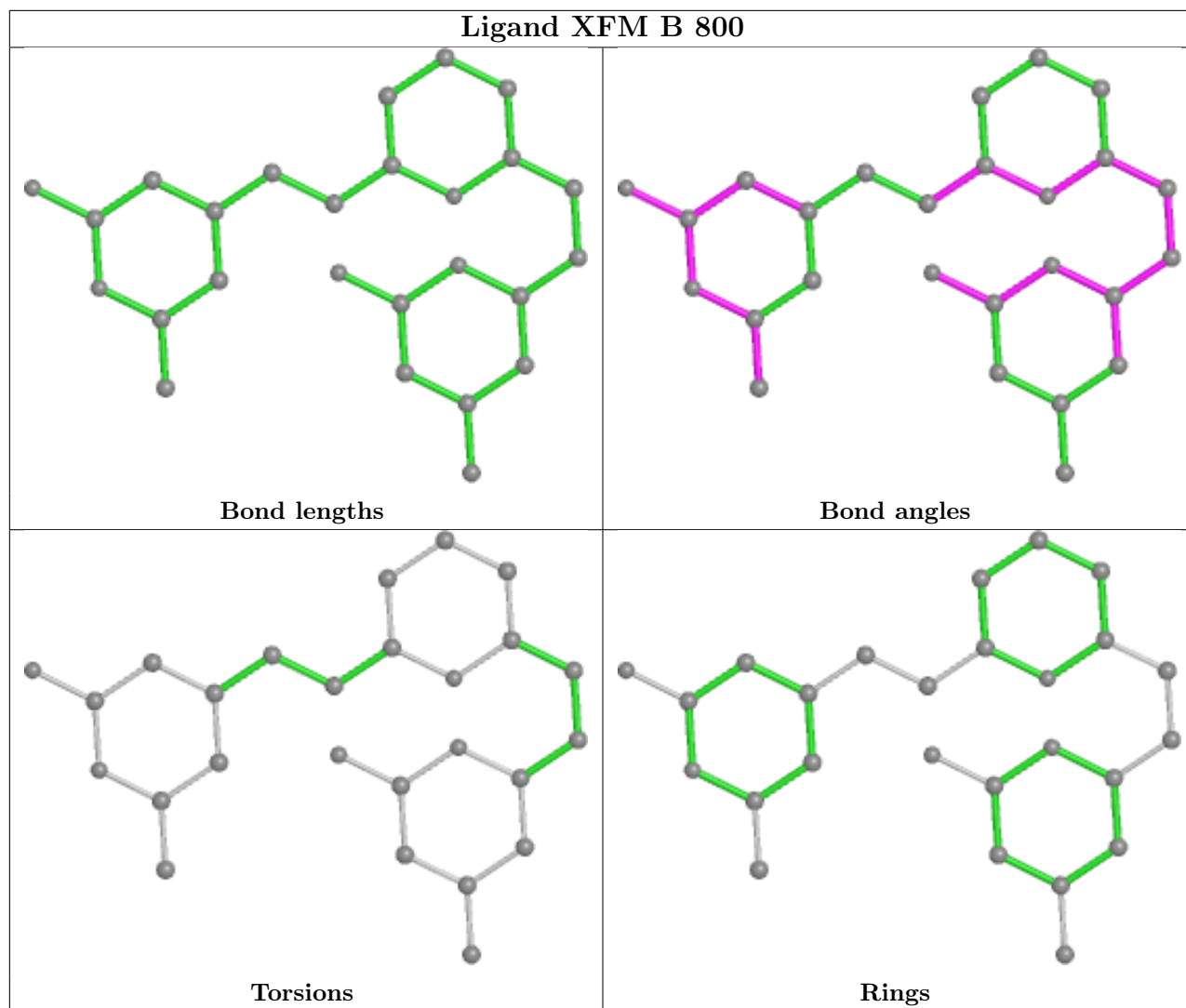
All (30) torsion outliers are listed below:

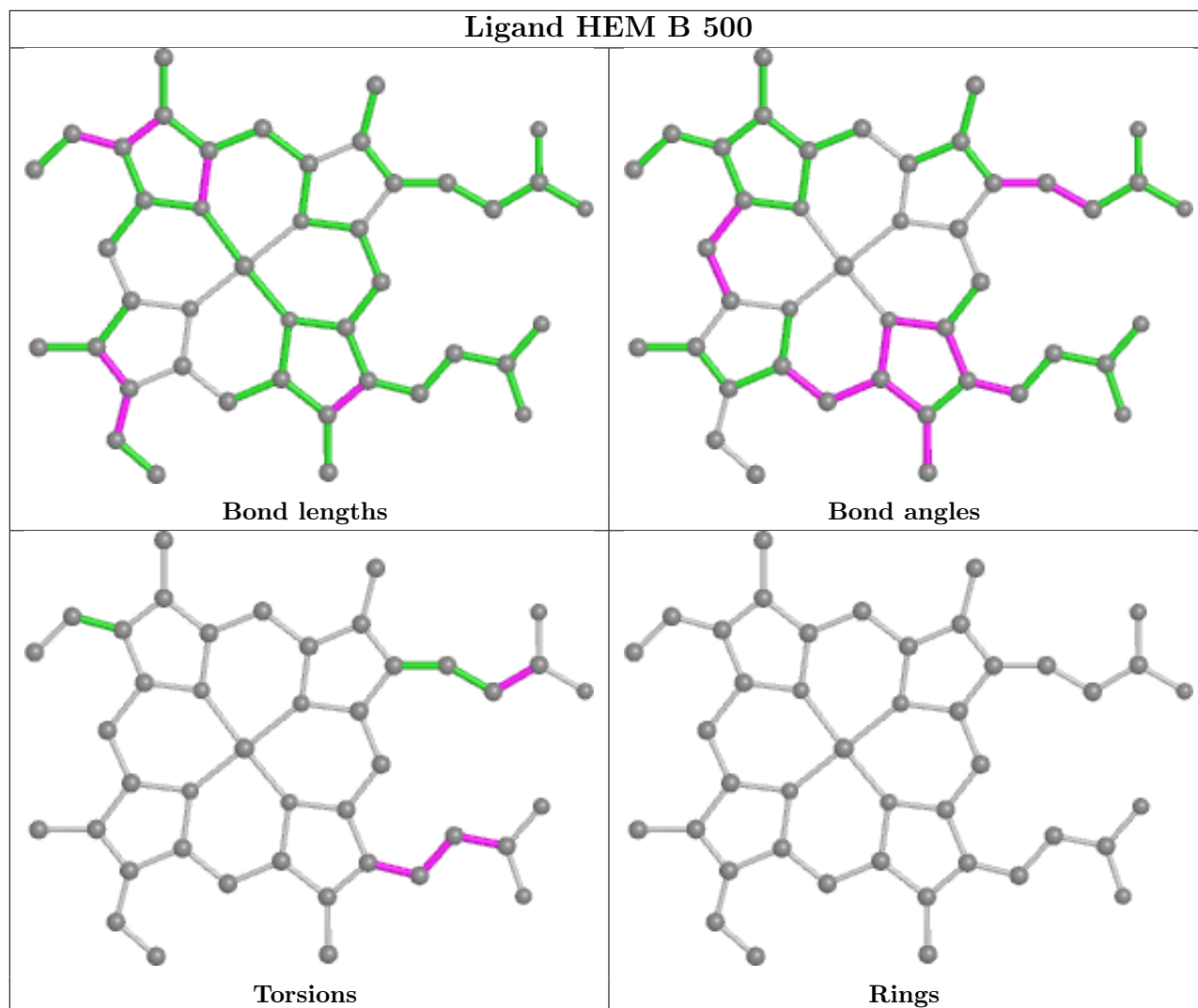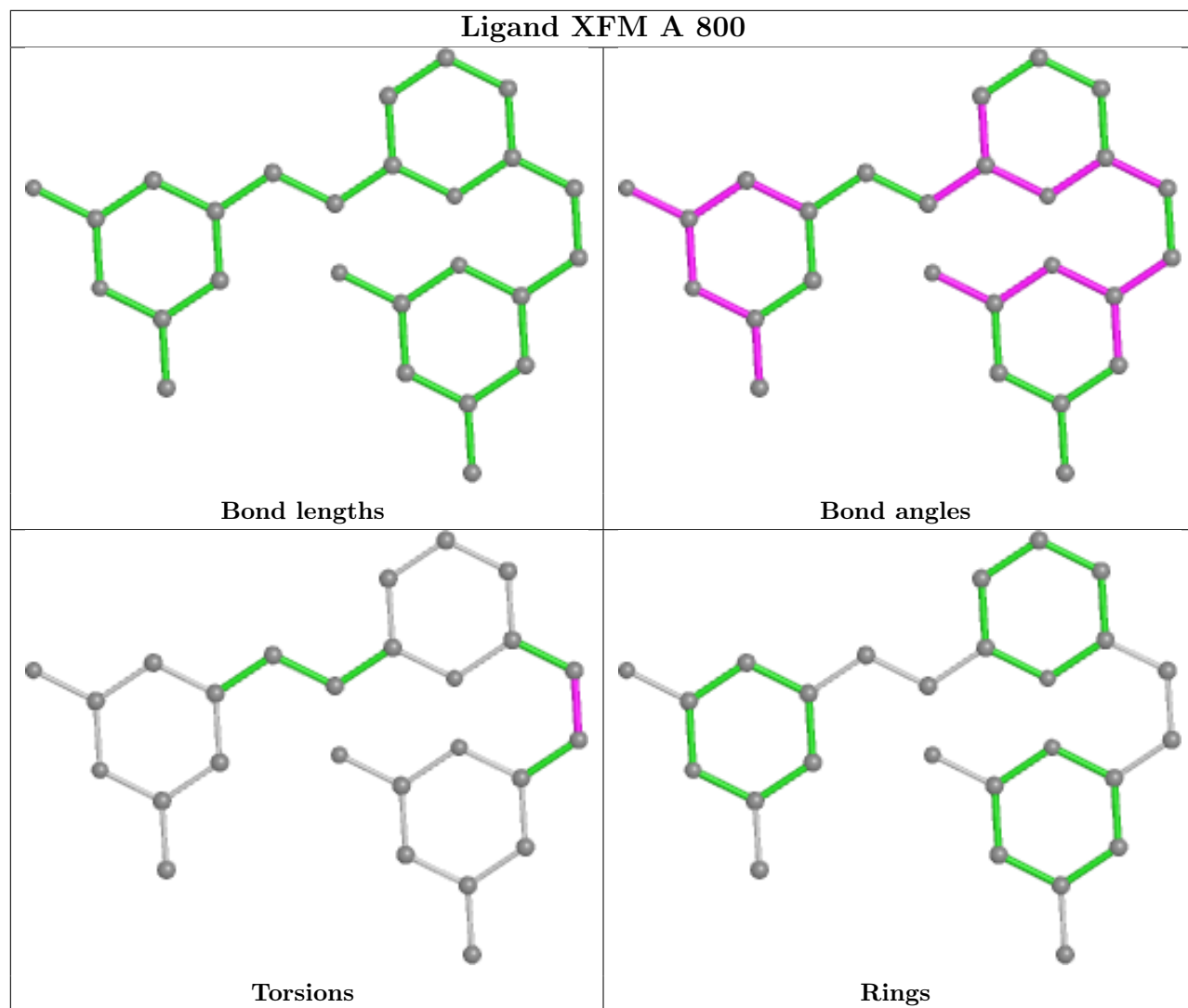| Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2D-C3D-CAD-CBD
2	A	500	HEM	C4D-C3D-CAD-CBD
3	A	600	H4B	N5-C6-C9-O9
3	A	600	H4B	N5-C6-C9-C10
3	A	600	H4B	C7-C6-C9-O9
3	A	600	H4B	C7-C6-C9-C10
3	B	600	H4B	C7-C6-C9-O9
3	B	600	H4B	C7-C6-C9-C10
5	A	880	GOL	C1-C2-C3-O3
5	B	880	GOL	O1-C1-C2-O2
5	B	880	GOL	O1-C1-C2-C3
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
2	A	500	HEM	C2B-C3B-CAB-CBB
2	B	500	HEM	C2D-C3D-CAD-CBD
2	A	500	HEM	C4B-C3B-CAB-CBB
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	CAD-CBD-CGD-O2D
2	B	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A
7	A	800	XFM	C2-C7-C8-C9
2	B	500	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

6 monomers are involved in 19 short contacts:

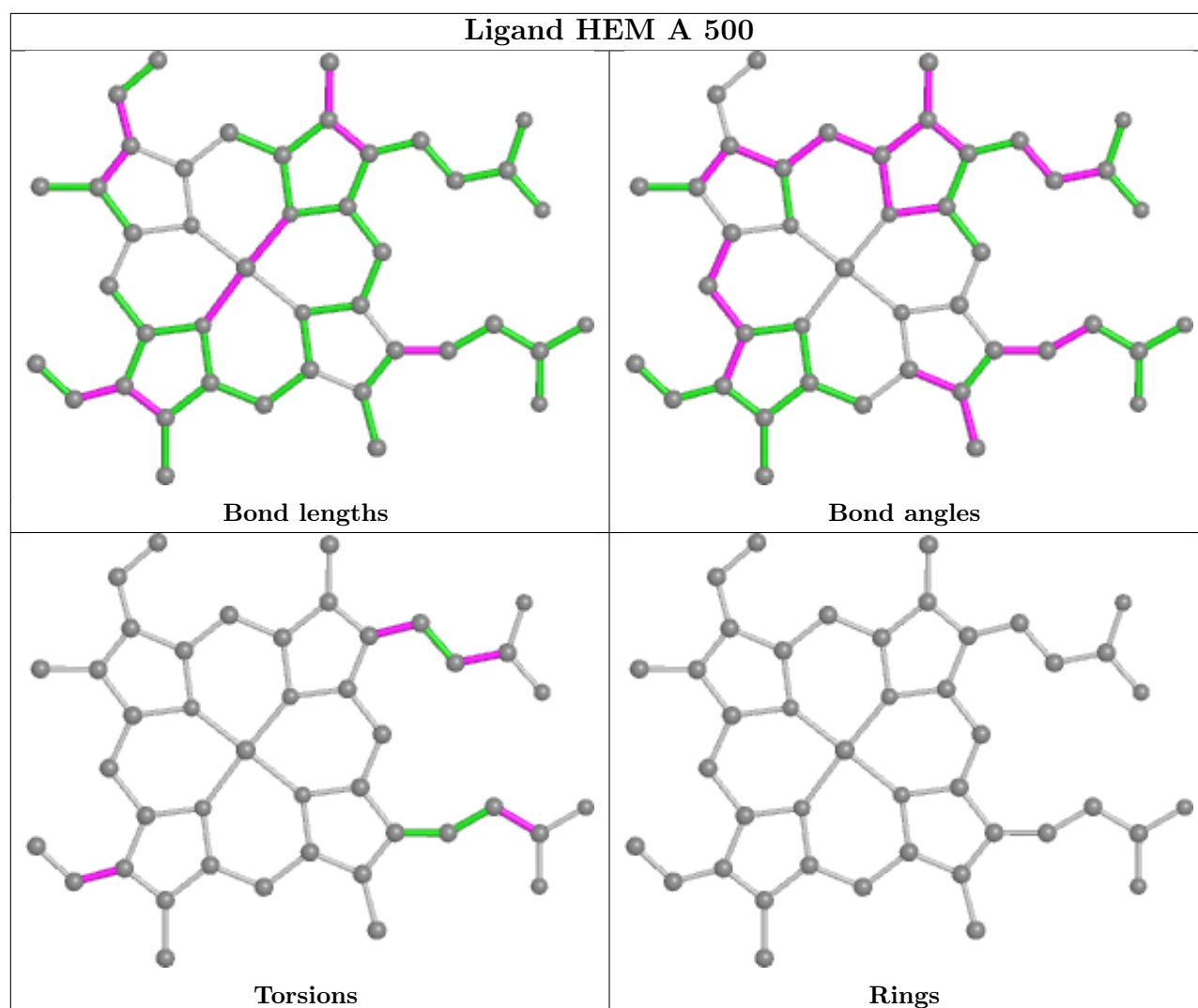| Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	950	CAD	1	0
7	B	800	XFM	2	0
2	B	500	HEM	5	0
7	A	800	XFM	4	0
6	B	950	CAD	1	0
2	A	500	HEM	8	0

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 XFM B 800

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand XFM A 800

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 500

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	404/444 (90%)	-0.36	6 (1%)	73	51	39, 55, 77, 92	0
1	B	401/444 (90%)	-0.41	0	100	100	45, 56, 71, 84	0
All	All	805/888 (90%)	-0.38	6 (0%)	87	72	39, 56, 73, 92	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	PRO	3.1
1	A	121	PRO	2.4
1	A	124	GLN	2.3
1	A	261	GLY	2.2
1	A	67	GLY	2.0
1	A	259	GLN	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.
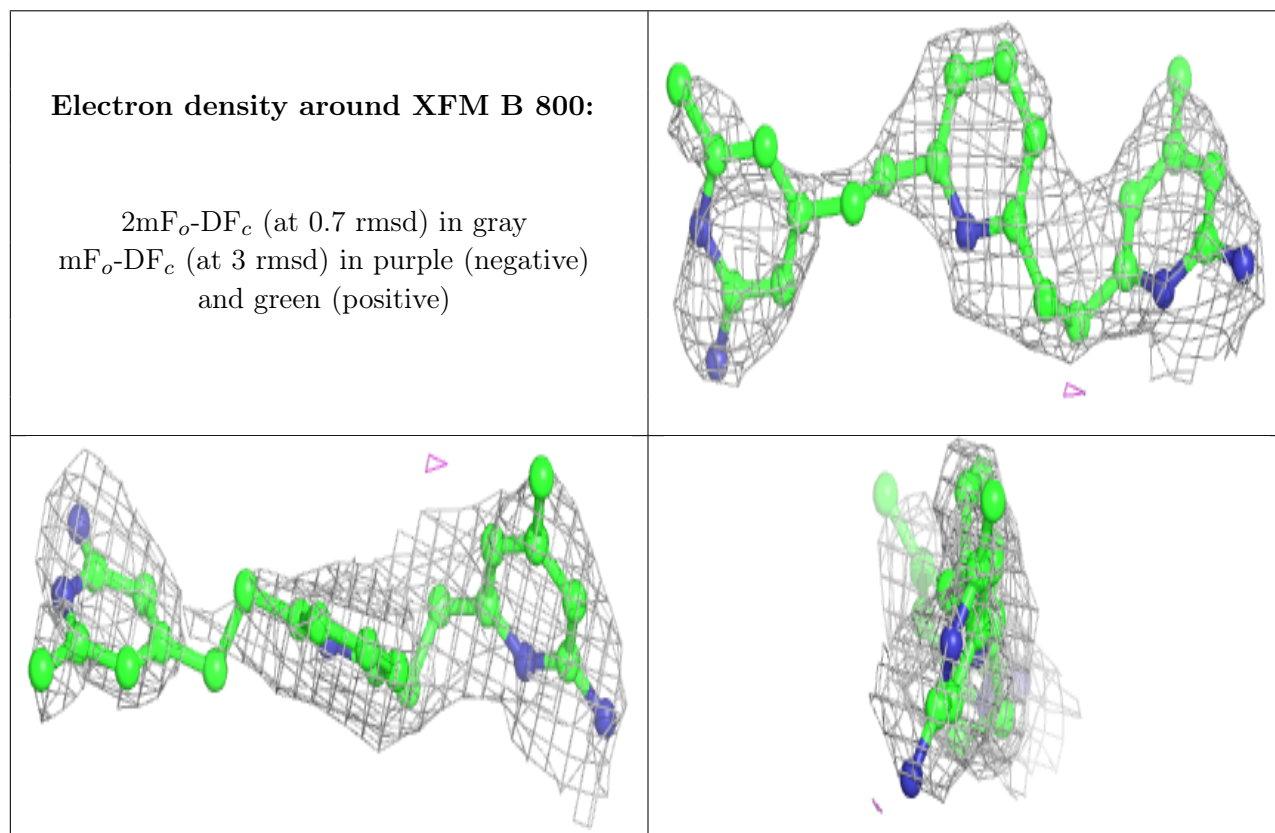
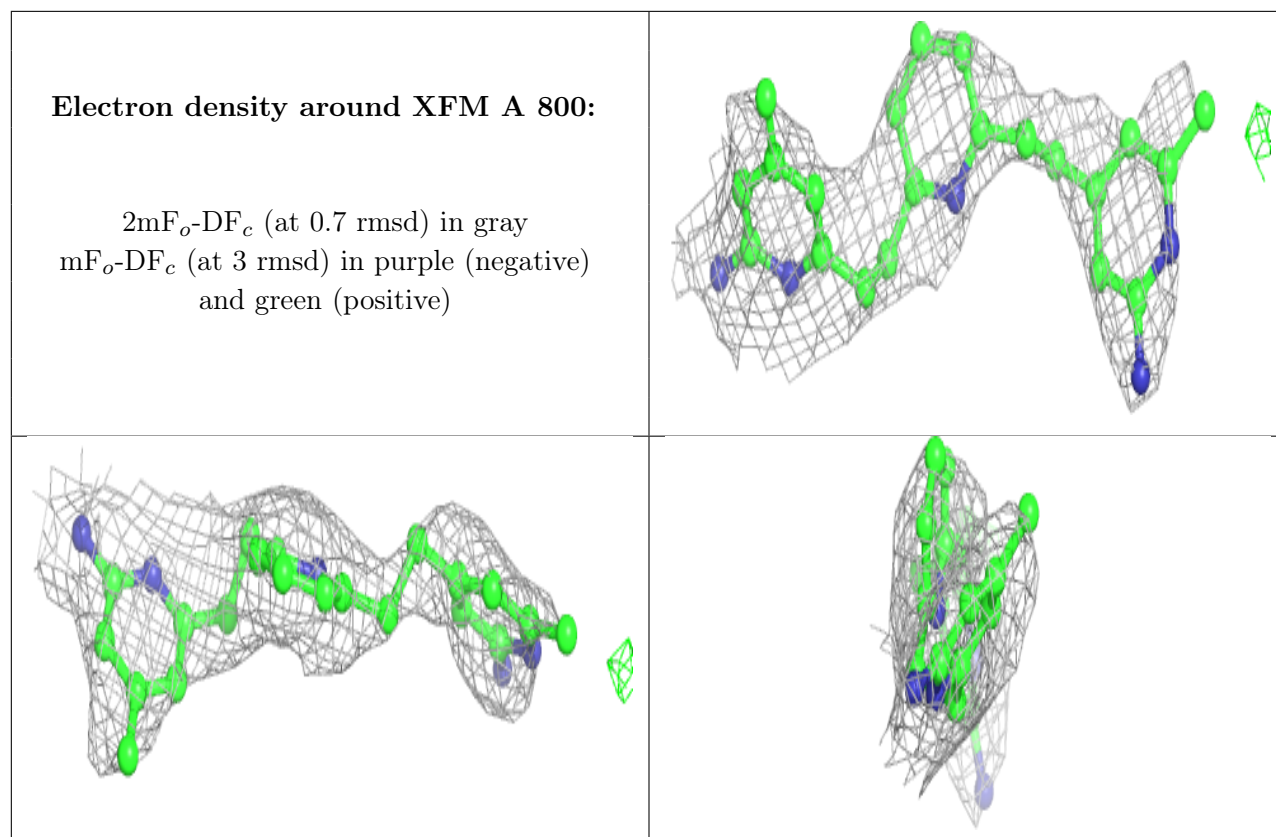## 6.3 Carbohydrates (i)

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.

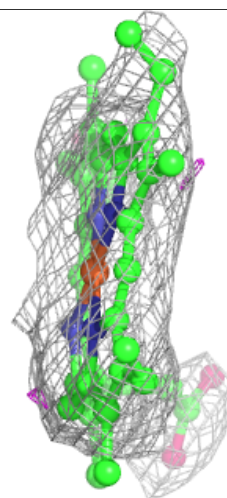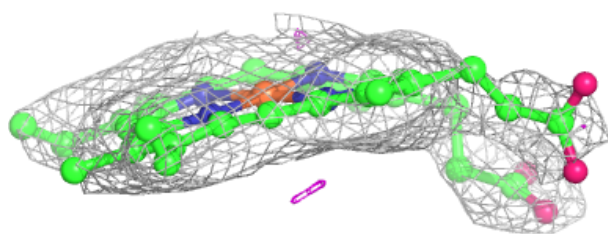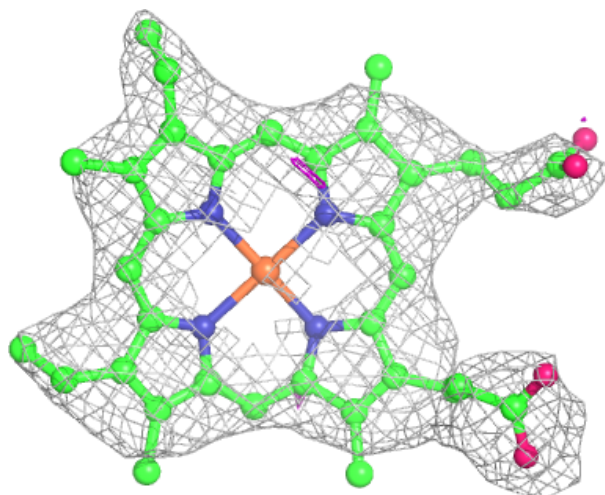| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
4	ACT	A	860	4/4	0.87	0.32	66,66,67,67	0
5	GOL	B	880	6/6	0.87	0.31	54,55,57,57	0
6	CAD	A	950	3/5	0.87	0.19	120,120,120,121	0
3	H4B	A	600	17/17	0.88	0.27	94,96,97,97	0
4	ACT	B	860	4/4	0.88	0.31	58,59,59,60	0
4	ACT	B	850	4/4	0.89	0.27	41,41,42,42	0
7	XFM	B	800	26/26	0.90	0.27	68,78,83,83	0
5	GOL	A	880	6/6	0.91	0.39	69,71,72,72	0
3	H4B	B	600	17/17	0.91	0.23	82,85,86,86	0
7	XFM	A	800	26/26	0.92	0.30	61,74,85,85	0
6	CAD	B	950	3/5	0.94	0.16	118,118,118,118	0
2	HEM	B	500	43/43	0.96	0.20	45,48,59,62	0
2	HEM	A	500	43/43	0.96	0.21	44,48,57,59	0
8	ZN	B	900	1/1	0.98	0.10	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:

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

Electron density around XFM A 800:

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

Electron density around HEM B 500:

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

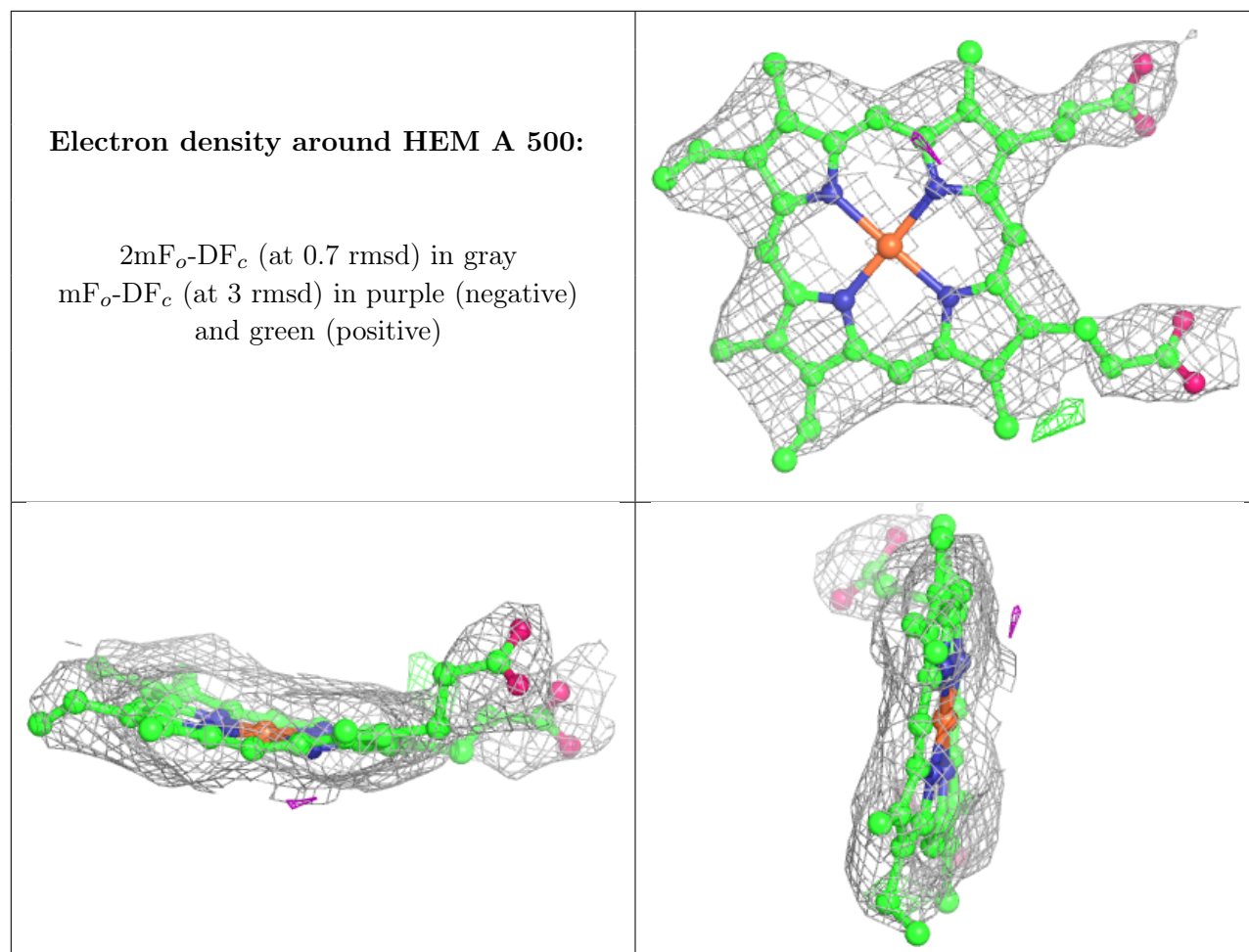**Electron density around HEM A 500:**

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

6.5 Other polymers (i)

There are no such residues in this entry.