



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:53 PM EDT

PDB ID : 3N6B / pdb_00003n6b
Title : Structure of endothelial nitric oxide synthase H373S single mutant heme domain complexed with 6,6'-(2,2'-(pyridine-3,5-diyl)bis(ethane-2,1-diyl))bis(4-methylpyridin-2-amine)
Authors : Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on : 2010-05-25
Resolution : 3.10 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

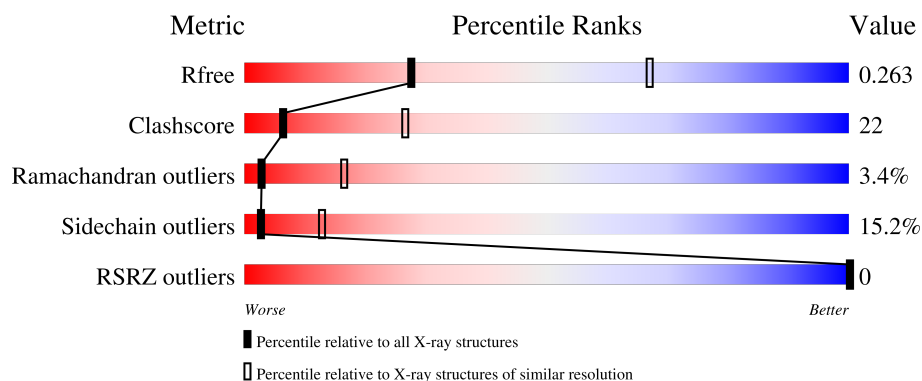
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	

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.

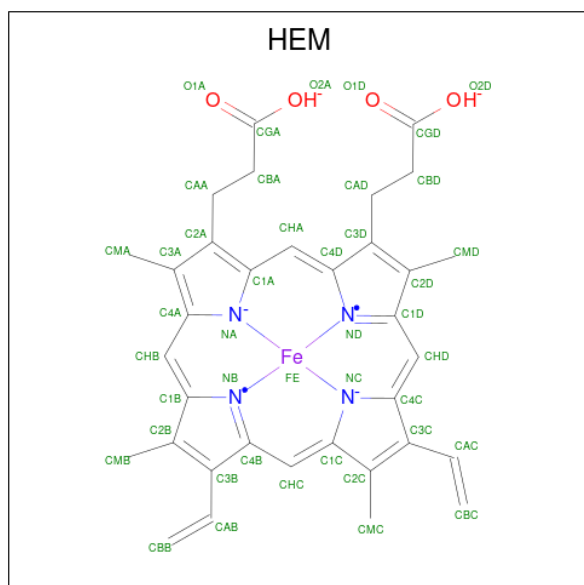
- Molecule 1 is a protein called Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total 3205	C 2038	N 562	O 589	S 16	0	0	0
1	B	402	Total 3206	C 2040	N 561	O 589	S 16	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

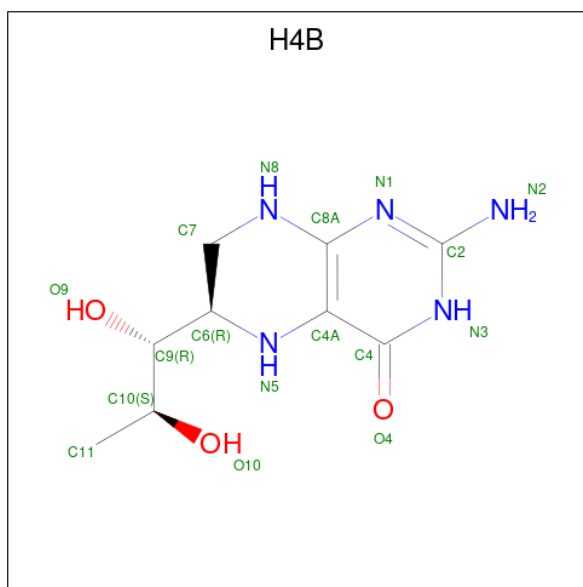
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29476
A	373	SER	HIS	engineered mutation	UNP P29476
B	100	ARG	CYS	SEE REMARK 999	UNP P29476
B	373	SER	HIS	engineered mutation	UNP P29476

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



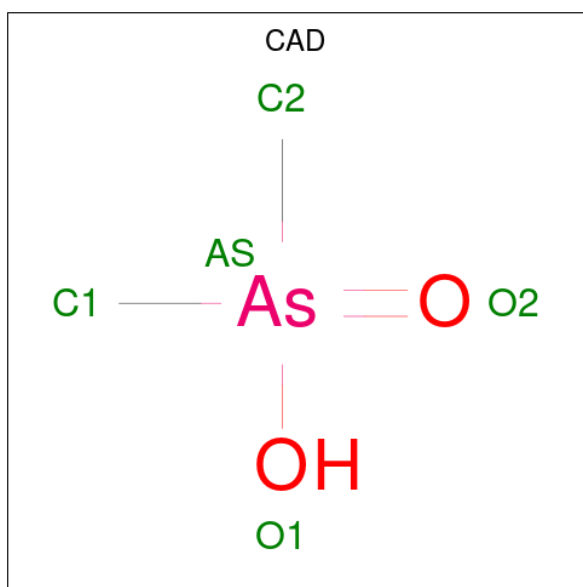
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



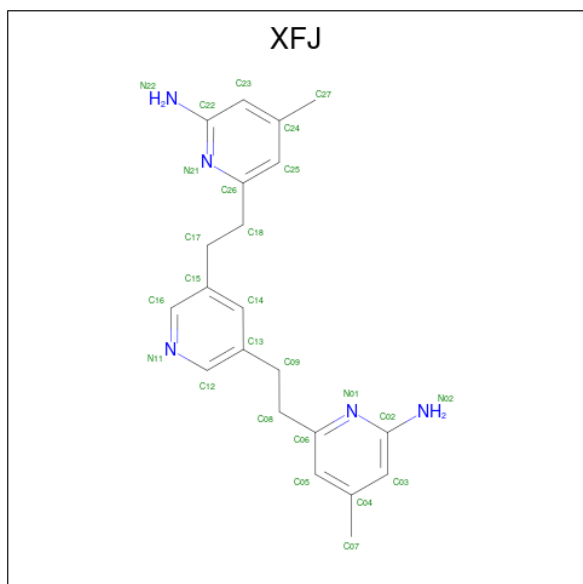
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is CACODYLIC ACID (CCD ID: CAD) (formula: $C_2H_7AsO_2$).



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

- Molecule 5 is 6,6'-(pyridine-3,5-diyl)diethane-2,1-diyl)bis(4-methylpyridin-2-amine) (CCD ID: XFJ) (formula: $C_{21}H_{25}N_5$).



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

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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

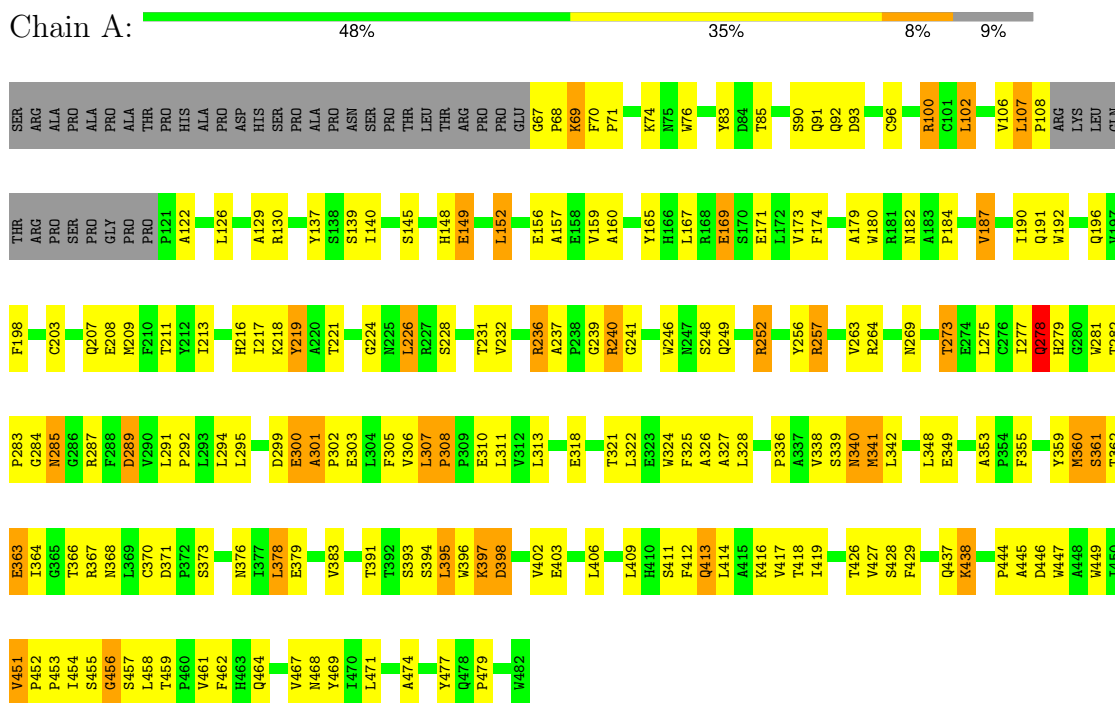
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	O	0	0
			5	5		
7	B	5	Total	O	0	0
			5	5		

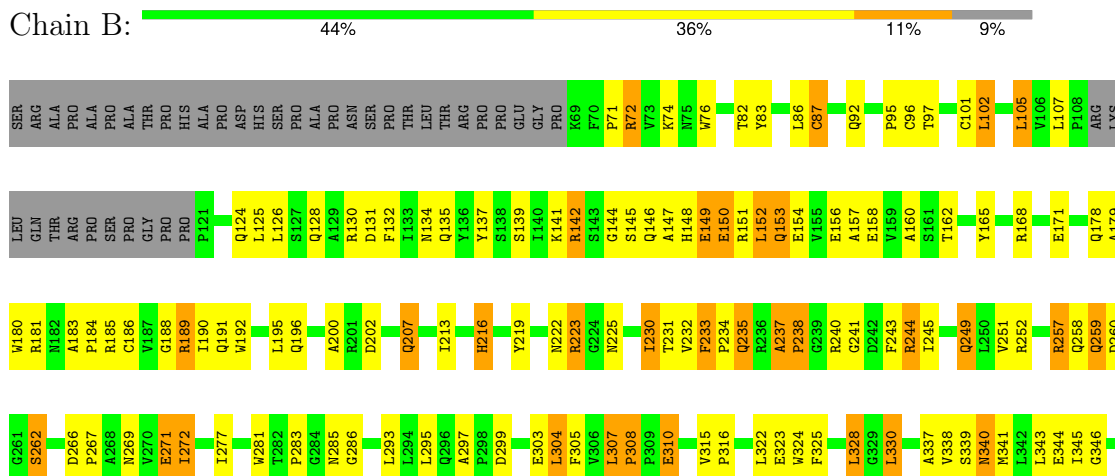
3 Residue-property plots

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



E349	F350	S351	A352		F355	S356		M360	S361	T362	E363		T366	R367	N368	L369	C370	D371	P372		N376		D380	V381		C384	M385	D386		R390	T391	T392		L395	W396	K397	D398		E403	I404	N405	L406	A407	V408	L409	H410	S411	F412	Q413	L414	A415	K416	V417		V420	D421	H422	H423
V427	S428	F429	M430	K431	H432	L433	D434	N435	E436	Q437	K438	A439	R440	G441	G442	C443	P444	A445		W449	I450	V451	P452	P453	I454	S455	G456	S457	L458	T459	P460	V461	F462	H463	Q464		V467	N468	Y469	I470	L471	S472	P473		R476	Y477	Q478		W482									

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.76Å 106.55Å 157.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.46 – 3.10 39.46 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.46-3.10) 99.3 (39.46-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.187 , 0.274 0.185 , 0.263	Depositor DCC
R_{free} test set	900 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 77.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6600	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, CAD, XFJ, H4B

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	0.93	1/3294 (0.0%)	1.21	22/4487 (0.5%)
1	B	0.91	1/3295 (0.0%)	1.24	24/4488 (0.5%)
All	All	0.92	2/6589 (0.0%)	1.22	46/8975 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	470	ILE	CA-CB	5.67	1.60	1.54
1	A	179	ALA	CA-CB	-5.14	1.45	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ALA	CA-C-N	9.92	130.54	119.83
1	A	301	ALA	C-N-CA	9.92	130.54	119.83
1	B	145	SER	N-CA-C	9.84	118.20	108.75
1	A	451	VAL	CA-C-N	9.80	130.48	120.38
1	A	451	VAL	C-N-CA	9.80	130.48	120.38
1	B	452	PRO	CA-C-N	9.73	129.49	119.56
1	B	452	PRO	C-N-CA	9.73	129.49	119.56
1	A	67	GLY	CA-C-N	8.21	130.10	119.84
1	A	67	GLY	C-N-CA	8.21	130.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	ILE	N-CA-C	-7.51	103.47	110.53
1	B	233	PHE	CA-C-N	7.37	129.05	119.84
1	B	233	PHE	C-N-CA	7.37	129.05	119.84
1	B	134	ASN	N-CA-C	-6.58	104.04	111.14
1	B	286	GLY	N-CA-C	6.55	119.02	111.36
1	A	452	PRO	CA-C-N	6.33	127.47	120.45
1	A	452	PRO	C-N-CA	6.33	127.47	120.45
1	B	297	ALA	N-CA-C	-6.18	103.03	110.13
1	B	272	ILE	N-CA-C	6.17	116.33	110.53
1	A	307	LEU	CA-C-N	6.11	126.67	120.38
1	A	307	LEU	C-N-CA	6.11	126.67	120.38
1	A	353	ALA	CA-C-N	6.04	126.54	120.14
1	A	353	ALA	C-N-CA	6.04	126.54	120.14
1	A	376	ASN	N-CA-C	5.98	119.49	111.24
1	A	182	ASN	N-CA-C	5.96	118.73	111.82
1	B	349	GLU	N-CA-C	5.91	118.08	108.26
1	A	445	ALA	N-CA-C	5.80	118.66	108.75
1	B	451	VAL	CA-C-N	5.74	126.30	120.38
1	B	451	VAL	C-N-CA	5.74	126.30	120.38
1	B	97	THR	CA-C-N	-5.60	112.83	119.05
1	B	97	THR	C-N-CA	-5.60	112.83	119.05
1	B	237	ALA	N-CA-C	5.54	118.40	109.15
1	B	366	THR	N-CA-C	5.54	117.12	111.14
1	B	232	VAL	N-CA-C	5.54	116.08	107.28
1	B	237	ALA	CA-C-N	5.50	126.72	119.84
1	B	237	ALA	C-N-CA	5.50	126.72	119.84
1	A	437	GLN	N-CA-C	-5.34	105.51	112.23
1	B	470	ILE	N-CA-C	5.31	116.35	108.23
1	A	302	PRO	N-CA-C	5.28	119.16	111.03
1	A	373	SER	CA-C-N	-5.28	117.48	123.13
1	A	373	SER	C-N-CA	-5.28	117.48	123.13
1	B	189	ARG	N-CA-C	5.26	117.92	111.82
1	A	383	VAL	N-CA-C	-5.21	105.42	110.42
1	B	471	LEU	N-CA-C	5.18	118.10	107.69
1	A	232	VAL	N-CA-C	5.16	115.29	107.80
1	B	285	ASN	N-CA-C	-5.05	105.50	113.02
1	A	226	LEU	N-CA-C	5.03	118.14	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3205	0	3113	130	0
1	B	3206	0	3112	155	0
2	A	43	0	30	6	0
2	B	43	0	30	8	0
3	A	17	0	15	3	0
3	B	17	0	15	1	0
4	A	3	0	0	0	0
4	B	3	0	0	2	0
5	A	26	0	25	0	0
5	B	26	0	25	3	0
6	A	1	0	0	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
All	All	6600	0	6365	284	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 (284) 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	1.20	1.02
1:B:260:ASP:OD1	1:B:262:SER:HB2	1.63	0.99
1:B:409:LEU:HD11	1:B:421:ASP:HB3	1.47	0.95
1:A:236:ARG:HH11	1:A:236:ARG:HB2	1.29	0.94
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.36	0.90
1:B:244:ARG:HG3	1:B:244:ARG:NH1	1.83	0.88
1:B:384:CYS:SG	4:B:950:CAD:AS	2.94	0.86
1:B:430:MET:HE1	1:B:464:GLN:HB2	1.56	0.84
1:B:328:LEU:HB3	1:B:330:LEU:HD23	1.59	0.82
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:O	1:B:156:GLU:HG2	1.77	0.82
1:B:328:LEU:HB3	1:B:330:LEU:CD2	2.10	0.82
1:B:431:LYS:HE3	1:B:435:ASN:OD1	1.82	0.80
1:B:244:ARG:HH11	1:B:244:ARG:CG	1.95	0.79
1:B:344:GLU:HG3	1:B:476:ARG:HH21	1.46	0.78
1:B:158:GLU:OE2	1:B:165:TYR:HA	1.83	0.77
1:A:196:GLN:HG2	1:A:219:TYR:OH	1.87	0.75
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.50	0.74
2:B:500:HEM:O1A	3:B:600:H4B:N3	2.20	0.73
1:B:362:THR:HA	1:B:405:ASN:HD21	1.54	0.73
1:A:203:CYS:HA	1:A:208:GLU:OE2	1.89	0.72
1:A:236:ARG:HB2	1:A:236:ARG:NH1	2.03	0.72
1:B:230:ILE:HD12	1:B:355:PHE:HB3	1.71	0.70
1:B:260:ASP:OD1	1:B:262:SER:CB	2.37	0.70
1:A:338:VAL:CG1	1:A:341:MET:HG3	2.21	0.69
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.73	0.69
1:A:398:ASP:OD1	1:A:398:ASP:N	2.19	0.69
1:A:303:GLU:HB2	1:A:305:PHE:CE1	2.28	0.69
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.76	0.68
1:B:150:GLU:O	1:B:153:GLN:HB2	1.94	0.68
1:A:273:THR:HG23	1:A:291:LEU:HD21	1.74	0.68
1:A:196:GLN:HG2	1:A:219:TYR:CZ	2.30	0.67
1:B:251:VAL:O	1:B:252:ARG:HG2	1.92	0.67
1:B:409:LEU:HD11	1:B:421:ASP:CB	2.22	0.67
1:A:426:THR:O	1:A:427:VAL:C	2.38	0.67
1:B:156:GLU:O	1:B:160:ALA:HB2	1.95	0.66
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.29	0.66
1:A:446:ASP:HB3	1:A:449:TRP:HB2	1.77	0.66
1:A:277:ILE:HG12	1:A:283:PRO:HD3	1.78	0.65
1:B:437:GLN:HA	1:B:442:GLY:H	1.61	0.65
1:A:249:GLN:HB2	1:A:252:ARG:HG3	1.79	0.65
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.79	0.65
1:A:218:LYS:HG2	1:A:311:LEU:HD11	1.78	0.65
1:A:355:PHE:CD1	2:A:500:HEM:HAC	2.32	0.65
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.78	0.64
1:A:409:LEU:O	1:A:413:GLN:HB2	1.97	0.64
1:A:207:GLN:HE21	1:A:211:THR:HG23	1.63	0.64
1:A:364:ILE:HA	1:A:368:ASN:HD22	1.63	0.64
1:A:213:ILE:O	1:A:216:HIS:HB3	1.97	0.63
1:B:186:CYS:HB2	2:B:500:HEM:ND	2.13	0.63
1:A:338:VAL:HG11	1:A:341:MET:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ALA:CB	1:B:356:SER:HB3	2.29	0.63
1:B:251:VAL:C	1:B:252:ARG:HG2	2.24	0.62
1:A:203:CYS:SG	1:A:208:GLU:HB3	2.40	0.61
1:A:303:GLU:HB2	1:A:305:PHE:HE1	1.62	0.61
1:B:340:ASN:H	1:B:340:ASN:HD22	1.47	0.61
1:B:396:TRP:CE2	1:B:397:LYS:HD2	2.35	0.61
1:A:370:CYS:SG	1:A:378:LEU:HD12	2.40	0.60
1:B:131:ASP:O	1:B:135:GLN:HG3	2.00	0.60
1:A:226:LEU:HD12	1:A:418:THR:HB	1.84	0.60
1:B:180:TRP:CZ3	1:B:192:TRP:HA	2.36	0.60
1:B:366:THR:HG21	1:B:453:PRO:HB2	1.84	0.60
1:A:318:GLU:HG2	1:A:326:ALA:HB2	1.83	0.60
1:B:207:GLN:NE2	1:B:305:PHE:HE1	2.00	0.60
1:B:72:ARG:HB3	1:B:72:ARG:HH11	1.66	0.59
1:B:281:TRP:O	1:B:283:PRO:HD3	2.02	0.59
1:A:100:ARG:HG2	1:A:100:ARG:NH1	2.13	0.59
1:A:367:ARG:NE	1:A:371:ASP:OD2	2.36	0.59
1:B:168:ARG:HH11	1:B:168:ARG:HG2	1.67	0.58
1:B:407:ALA:O	1:B:411:SER:OG	2.21	0.58
2:A:500:HEM:O1A	3:A:600:H4B:N2	2.36	0.58
1:B:237:ALA:HB3	1:B:240:ARG:HG3	1.86	0.58
1:B:423:HIS:O	1:B:427:VAL:HG23	2.03	0.58
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.38	0.58
1:A:360:MET:O	1:A:361:SER:C	2.46	0.57
1:A:371:ASP:OD1	1:B:463:HIS:CE1	2.57	0.57
1:A:257:ARG:HG3	1:A:257:ARG:NH1	2.08	0.56
1:A:139:SER:HB3	1:A:174:PHE:CE1	2.40	0.56
1:B:216:HIS:HB2	1:B:231:THR:OG1	2.06	0.56
1:A:156:GLU:O	1:A:157:ALA:C	2.49	0.55
1:A:453:PRO:HB2	1:B:457:SER:HB3	1.87	0.55
1:A:221:THR:O	1:A:226:LEU:HD23	2.05	0.55
1:A:252:ARG:HB3	1:A:269:ASN:ND2	2.22	0.55
1:B:225:ASN:C	1:B:225:ASN:HD22	2.15	0.55
1:A:360:MET:O	1:A:362:THR:N	2.40	0.55
1:B:372:PRO:HA	1:B:376:ASN:CG	2.32	0.54
1:B:396:TRP:CZ2	1:B:397:LYS:HD2	2.43	0.54
1:B:444:PRO:HG3	1:B:471:LEU:HD12	1.89	0.54
1:B:412:PHE:HD2	1:B:417:VAL:CG1	2.20	0.54
1:A:74:LYS:HD3	1:A:76:TRP:CE2	2.42	0.54
1:A:236:ARG:HH11	1:A:236:ARG:CB	2.11	0.54
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:HH11	1:B:223:ARG:CG	2.21	0.54
1:A:184:PRO:CB	1:A:468:ASN:HD21	2.20	0.53
1:A:277:ILE:C	1:A:279:HIS:H	2.17	0.53
2:A:500:HEM:O1A	3:A:600:H4B:N3	2.40	0.53
1:B:216:HIS:C	1:B:216:HIS:CD2	2.86	0.53
1:A:269:ASN:O	1:A:273:THR:OG1	2.25	0.53
1:A:378:LEU:HD21	1:A:397:LYS:HB3	1.91	0.53
1:B:381:VAL:HG12	1:B:381:VAL:O	2.08	0.53
1:B:126:LEU:O	1:B:130:ARG:HB2	2.09	0.53
1:A:209:MET:HE2	1:A:295:LEU:HD22	1.90	0.53
1:A:299:ASP:O	1:A:300:GLU:C	2.52	0.52
1:B:310:GLU:CD	1:B:310:GLU:H	2.17	0.52
1:B:363:GLU:OE1	5:B:800:XFJ:N01	2.43	0.52
1:B:428:SER:O	1:B:431:LYS:HB3	2.09	0.52
1:B:293:LEU:HB3	1:B:295:LEU:HD21	1.91	0.52
1:B:303:GLU:HB2	1:B:305:PHE:HE2	1.74	0.52
1:A:159:VAL:HG23	1:A:165:TYR:HB3	1.90	0.52
1:B:144:GLY:HA2	1:B:148:HIS:ND1	2.25	0.52
1:B:328:LEU:HB3	1:B:330:LEU:HD21	1.89	0.52
1:B:281:TRP:HB2	1:B:304:LEU:CD1	2.40	0.52
1:B:343:LEU:HB3	1:B:350:PHE:HB2	1.92	0.52
1:B:460:PRO:O	1:B:461:VAL:C	2.52	0.52
1:B:384:CYS:SG	4:B:950:CAD:C2	2.99	0.51
1:B:153:GLN:O	1:B:156:GLU:HB2	2.10	0.51
1:A:308:PRO:HB2	1:A:311:LEU:HB2	1.92	0.51
1:B:260:ASP:C	1:B:262:SER:H	2.18	0.51
1:B:445:ALA:O	1:B:468:ASN:HB2	2.11	0.51
1:A:145:SER:O	1:A:149:GLU:HG2	2.11	0.50
1:B:179:ALA:HA	1:B:473:PRO:O	2.11	0.50
1:A:224:GLY:O	1:A:417:VAL:HA	2.12	0.50
1:B:223:ARG:HH11	1:B:223:ARG:HG2	1.77	0.50
1:B:360:MET:HA	1:B:420:VAL:O	2.12	0.50
1:A:100:ARG:HH12	1:A:102:LEU:HD22	1.76	0.50
1:A:137:TYR:HA	1:A:140:ILE:HG12	1.94	0.49
1:B:430:MET:HE2	1:B:460:PRO:HB2	1.93	0.49
2:B:500:HEM:HBB2	2:B:500:HEM:CHC	2.30	0.49
1:B:267:PRO:C	1:B:269:ASN:H	2.19	0.49
1:B:384:CYS:C	1:B:386:ASP:H	2.21	0.49
1:B:240:ARG:NH1	1:B:241:GLY:O	2.45	0.49
1:A:393:SER:HB2	1:B:409:LEU:HD22	1.95	0.49
1:A:281:TRP:CG	1:A:292:PRO:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:CZ	1:B:440:ARG:HD3	2.43	0.49
1:B:192:TRP:CD1	1:B:432:HIS:HE1	2.30	0.49
1:B:433:LEU:O	1:B:434:ASP:C	2.55	0.49
1:A:277:ILE:C	1:A:279:HIS:N	2.72	0.48
1:B:237:ALA:HA	1:B:238:PRO:HD2	1.60	0.48
1:A:96:CYS:CB	1:B:96:CYS:HB3	2.41	0.48
1:A:355:PHE:CD1	2:A:500:HEM:CAC	2.95	0.48
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.48	0.48
1:B:230:ILE:O	1:B:230:ILE:HG23	2.14	0.48
1:A:165:TYR:CE2	1:A:348:LEU:HD11	2.48	0.48
2:A:500:HEM:CMC	2:A:500:HEM:HBC2	2.43	0.48
1:A:366:THR:O	1:A:370:CYS:HB2	2.14	0.48
1:A:96:CYS:HB3	1:B:96:CYS:CB	2.44	0.48
1:A:219:TYR:C	1:A:219:TYR:CD2	2.92	0.48
1:A:403:GLU:OE1	1:A:403:GLU:HA	2.13	0.48
1:A:156:GLU:O	1:A:160:ALA:N	2.45	0.48
1:A:457:SER:HA	1:A:462:PHE:CG	2.49	0.48
1:B:222:ASN:HB3	1:B:225:ASN:O	2.13	0.48
1:B:455:SER:O	1:B:458:LEU:HB2	2.14	0.47
1:A:371:ASP:OD1	1:B:463:HIS:HE1	1.97	0.47
1:B:281:TRP:HB2	1:B:304:LEU:HD11	1.96	0.47
1:A:203:CYS:HA	1:A:208:GLU:CD	2.39	0.47
1:B:125:LEU:HA	1:B:128:GLN:OE1	2.14	0.47
1:B:149:GLU:O	1:B:153:GLN:NE2	2.48	0.47
1:B:243:PHE:O	1:B:351:SER:HB2	2.14	0.47
1:A:396:TRP:CH2	1:A:397:LYS:HD3	2.49	0.47
1:A:455:SER:O	1:A:456:GLY:C	2.57	0.47
1:B:102:LEU:HB3	1:B:105:LEU:HG	1.97	0.47
1:B:196:GLN:NE2	1:B:196:GLN:HA	2.29	0.47
1:A:68:PRO:HG2	1:A:83:TYR:CE1	2.49	0.47
1:B:366:THR:O	1:B:370:CYS:HB2	2.14	0.47
1:A:289:ASP:N	1:A:289:ASP:OD1	2.48	0.46
1:B:395:LEU:HD22	1:B:398:ASP:OD2	2.15	0.46
1:A:257:ARG:NH1	1:A:257:ARG:CG	2.78	0.46
1:A:456:GLY:O	1:A:459:THR:OG1	2.33	0.46
1:A:256:TYR:CZ	1:A:284:GLY:O	2.68	0.46
1:A:190:ILE:HG23	1:A:191:GLN:HG2	1.98	0.46
1:B:341:MET:C	1:B:478:GLN:HE21	2.24	0.46
1:A:100:ARG:HD3	1:A:100:ARG:N	2.30	0.46
1:B:86:LEU:O	1:B:87:CYS:C	2.57	0.46
1:B:137:TYR:HB3	1:B:142:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ARG:HB2	1:B:171:GLU:OE2	2.16	0.46
1:B:185:ARG:HD3	1:B:449:TRP:CE3	2.50	0.46
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.51	0.46
1:A:438:LYS:HE3	1:A:438:LYS:CA	2.46	0.46
1:B:181:ARG:NH2	1:B:440:ARG:HD3	2.31	0.46
1:A:96:CYS:SG	1:B:101:CYS:HB2	2.56	0.45
1:B:186:CYS:HB2	2:B:500:HEM:C4D	2.51	0.45
1:B:235:GLN:O	1:B:235:GLN:HG2	2.15	0.45
1:B:328:LEU:CB	1:B:330:LEU:HD23	2.41	0.45
1:B:416:LYS:HD3	1:B:416:LYS:HA	1.77	0.45
1:B:457:SER:HA	1:B:462:PHE:CG	2.51	0.45
1:A:70:PHE:HB3	1:A:71:PRO:CD	2.46	0.45
1:A:273:THR:HG23	1:A:291:LEU:CD2	2.43	0.45
1:B:147:ALA:C	1:B:149:GLU:N	2.72	0.45
1:A:129:ALA:O	1:A:130:ARG:C	2.60	0.45
1:A:148:HIS:CD2	1:A:152:LEU:HD13	2.51	0.45
1:A:165:TYR:HE2	1:A:167:LEU:HD23	1.81	0.45
1:A:248:SER:C	1:A:339:SER:HG	2.24	0.45
1:B:315:VAL:HG12	1:B:316:PRO:O	2.17	0.45
1:A:69:LYS:N	1:A:69:LYS:HD2	2.32	0.45
1:A:467:VAL:HG12	1:A:469:TYR:HD1	1.82	0.45
1:B:200:ALA:C	1:B:202:ASP:H	2.24	0.45
1:B:444:PRO:HA	1:B:467:VAL:O	2.17	0.45
1:A:169:GLU:O	1:A:173:VAL:HG23	2.17	0.45
1:A:184:PRO:HB2	1:A:468:ASN:HD21	1.82	0.45
1:A:426:THR:C	1:A:428:SER:N	2.74	0.45
1:A:198:PHE:HZ	1:A:219:TYR:CD1	2.35	0.44
1:A:180:TRP:CZ3	1:A:192:TRP:HA	2.52	0.44
1:A:467:VAL:HG12	1:A:469:TYR:CD1	2.52	0.44
1:A:362:THR:O	1:A:363:GLU:C	2.60	0.44
1:A:444:PRO:HA	1:A:467:VAL:O	2.17	0.44
1:A:471:LEU:O	1:A:474:ALA:HB2	2.18	0.44
1:A:394:SER:O	1:A:395:LEU:HB2	2.18	0.44
1:B:189:ARG:C	1:B:191:GLN:H	2.26	0.44
1:B:363:GLU:O	1:B:368:ASN:HB2	2.17	0.44
1:A:252:ARG:HB3	1:A:269:ASN:HD21	1.83	0.44
1:A:139:SER:HB3	1:A:174:PHE:HE1	1.82	0.44
2:B:500:HEM:O2D	5:B:800:XFJ:H18A	2.18	0.44
1:A:275:LEU:HA	1:A:278:GLN:HE21	1.82	0.43
1:B:157:ALA:O	1:B:160:ALA:HB3	2.18	0.43
1:B:455:SER:HB3	1:B:458:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:C	1:B:153:GLN:H	2.26	0.43
1:B:219:TYR:CD2	1:B:219:TYR:C	2.95	0.43
1:A:148:HIS:HD2	1:A:152:LEU:HD13	1.83	0.43
1:A:285:ASN:HD22	1:A:285:ASN:HA	1.64	0.43
1:B:178:GLN:HB3	1:B:473:PRO:HG2	2.01	0.43
1:A:236:ARG:HG2	1:A:237:ALA:N	2.33	0.43
1:B:147:ALA:C	1:B:149:GLU:H	2.26	0.43
1:B:436:GLU:C	1:B:438:LYS:N	2.76	0.43
1:A:336:PRO:HB3	1:A:359:TYR:CZ	2.54	0.43
1:B:71:PRO:O	1:B:83:TYR:HA	2.19	0.43
1:B:267:PRO:C	1:B:269:ASN:N	2.76	0.43
1:A:412:PHE:CG	1:A:419:ILE:HD12	2.54	0.43
2:A:500:HEM:CGA	3:A:600:H4B:HN3	2.31	0.43
1:B:233:PHE:HB2	1:B:352:ALA:HB3	2.01	0.43
1:B:412:PHE:CD2	1:B:417:VAL:CG1	3.02	0.43
1:B:325:PHE:O	1:B:328:LEU:HB2	2.18	0.42
1:B:185:ARG:HD3	1:B:449:TRP:CD2	2.53	0.42
1:B:457:SER:HA	1:B:462:PHE:CD1	2.54	0.42
1:A:165:TYR:CD2	1:A:165:TYR:C	2.97	0.42
1:A:341:MET:HE2	1:A:477:TYR:HA	2.01	0.42
1:A:190:ILE:HD13	1:A:428:SER:O	2.20	0.42
1:A:447:TRP:CZ2	1:A:451:VAL:HG21	2.54	0.42
1:B:429:PHE:O	1:B:430:MET:C	2.62	0.42
1:A:217:ILE:O	1:A:218:LYS:C	2.63	0.42
1:B:223:ARG:HH11	1:B:223:ARG:CB	2.33	0.42
1:B:340:ASN:H	1:B:340:ASN:ND2	2.16	0.42
1:B:390:ARG:HB3	1:B:390:ARG:HH11	1.84	0.42
1:A:240:ARG:HD2	1:A:240:ARG:C	2.44	0.42
1:B:74:LYS:HE2	1:B:76:TRP:CD2	2.55	0.42
1:B:188:GLY:HA3	2:B:500:HEM:C2B	2.55	0.42
1:B:223:ARG:HG2	1:B:223:ARG:NH1	2.35	0.42
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.49	0.42
1:A:398:ASP:O	1:A:402:VAL:HG23	2.20	0.41
1:A:137:TYR:CD1	1:A:140:ILE:HD11	2.54	0.41
1:A:187:VAL:HG22	1:A:429:PHE:HB2	2.01	0.41
1:B:195:LEU:HG	1:B:196:GLN:N	2.33	0.41
1:B:245:ILE:HG21	1:B:339:SER:HB2	2.02	0.41
1:A:248:SER:HA	1:A:340:ASN:HB3	2.02	0.41
1:A:461:VAL:O	1:A:464:GLN:HB3	2.20	0.41
1:B:307:LEU:O	1:B:308:PRO:C	2.63	0.41
1:B:343:LEU:HD21	1:B:345:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ALA:C	1:B:202:ASP:N	2.77	0.41
1:B:266:ASP:HA	1:B:267:PRO:HD3	1.92	0.41
1:B:151:ARG:C	1:B:153:GLN:N	2.78	0.41
1:B:183:ALA:HA	1:B:184:PRO:HD3	1.81	0.41
1:B:186:CYS:HB2	2:B:500:HEM:C1D	2.56	0.41
1:A:107:LEU:HA	1:A:108:PRO:HD3	1.79	0.41
1:B:249:GLN:HB2	1:B:252:ARG:HD2	2.03	0.41
1:B:434:ASP:O	1:B:435:ASN:C	2.63	0.41
1:B:477[B]:TYR:OH	5:B:800:XFJ:N21	2.50	0.41
1:B:168:ARG:HG2	1:B:168:ARG:NH1	2.35	0.41
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.67	0.41
1:B:449:TRP:CD1	1:B:449:TRP:N	2.89	0.41
1:A:378:LEU:CD2	1:A:397:LYS:HB3	2.49	0.41
1:A:417:VAL:O	1:A:418:THR:C	2.64	0.41
1:A:447:TRP:O	1:A:449:TRP:N	2.54	0.41
1:A:455:SER:HA	1:B:454:ILE:HG22	2.03	0.41
1:B:307:LEU:HD23	1:B:308:PRO:HD2	2.01	0.41
1:A:342:LEU:HD11	1:A:349:GLU:HB3	2.02	0.41
1:B:452:PRO:HA	1:B:453:PRO:HD2	1.60	0.41
1:A:307:LEU:HA	1:A:308:PRO:HD2	1.67	0.40
1:A:240:ARG:O	1:A:241:GLY:C	2.64	0.40
1:A:106:VAL:HG13	1:A:449:TRP:HZ2	1.87	0.40
1:A:325:PHE:C	1:A:327:ALA:N	2.77	0.40
1:A:396:TRP:O	1:A:397:LYS:C	2.64	0.40
1:B:403:GLU:OE1	1:B:403:GLU:HA	2.21	0.40
1:A:367:ARG:NH2	1:A:371:ASP:OD2	2.54	0.40
1:B:132:PHE:HB2	1:B:346:GLY:HA2	2.02	0.40
1:B:151:ARG:HD2	1:B:154:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/444 (90%)	339 (85%)	51 (13%)	10 (2%)	4	21
1	B	399/444 (90%)	319 (80%)	63 (16%)	17 (4%)	2	12
All	All	799/888 (90%)	658 (82%)	114 (14%)	27 (3%)	3	16

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	257	ARG
1	A	90	SER
1	A	122	ALA
1	A	239	GLY
1	A	361	SER
1	B	142	ARG
1	B	258	GLN
1	B	259	GLN
1	A	278	GLN
1	A	363	GLU
1	A	456	GLY
1	A	479	PRO
1	B	190	ILE
1	B	380	ASP
1	B	385	MET
1	A	308	PRO
1	B	368	ASN
1	B	410	HIS
1	B	411	SER
1	B	433	LEU
1	A	240	ARG
1	B	238	PRO
1	B	271	GLU
1	B	462	PHE
1	B	230	ILE
1	B	308	PRO
1	B	95	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%)	292 (85%)	51 (15%)	3	13
1	B	343/377 (91%)	290 (84%)	53 (16%)	2	12
All	All	686/754 (91%)	582 (85%)	104 (15%)	3	13

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	85	THR
1	A	91	GLN
1	A	92	GLN
1	A	93	ASP
1	A	100	ARG
1	A	102	LEU
1	A	107	LEU
1	A	126	LEU
1	A	149	GLU
1	A	152	LEU
1	A	169	GLU
1	A	171	GLU
1	A	187	VAL
1	A	219	TYR
1	A	228	SER
1	A	231	THR
1	A	236	ARG
1	A	252	ARG
1	A	257	ARG
1	A	263	VAL
1	A	264	ARG
1	A	273	THR
1	A	278	GLN
1	A	282	THR
1	A	285	ASN
1	A	287	ARG
1	A	289	ASP
1	A	300	GLU
1	A	306	VAL
1	A	310	GLU
1	A	313	LEU
1	A	321	THR
1	A	328	LEU

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Mol	Chain	Res	Type
1	A	340	ASN
1	A	341	MET
1	A	360	MET
1	A	378	LEU
1	A	379	GLU
1	A	391	THR
1	A	395	LEU
1	A	397	LYS
1	A	398	ASP
1	A	406	LEU
1	A	411	SER
1	A	413	GLN
1	A	414	LEU
1	A	416	LYS
1	A	438	LYS
1	A	454	ILE
1	A	458	LEU
1	B	72	ARG
1	B	82	THR
1	B	87	CYS
1	B	92	GLN
1	B	102	LEU
1	B	105	LEU
1	B	107	LEU
1	B	124	GLN
1	B	139	SER
1	B	141	LYS
1	B	146	GLN
1	B	149	GLU
1	B	150	GLU
1	B	152	LEU
1	B	153	GLN
1	B	162	THR
1	B	207	GLN
1	B	213	ILE
1	B	216	HIS
1	B	223	ARG
1	B	235	GLN
1	B	244	ARG
1	B	249	GLN
1	B	257	ARG
1	B	259	GLN

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Mol	Chain	Res	Type
1	B	262	SER
1	B	271	GLU
1	B	272	ILE
1	B	277	ILE
1	B	299	ASP
1	B	304	LEU
1	B	307	LEU
1	B	310	GLU
1	B	323	GLU
1	B	328	LEU
1	B	330	LEU
1	B	338	VAL
1	B	340	ASN
1	B	351	SER
1	B	372	PRO
1	B	386	ASP
1	B	390	ARG
1	B	391	THR
1	B	392	THR
1	B	397	LYS
1	B	398	ASP
1	B	405	ASN
1	B	409	LEU
1	B	411	SER
1	B	414	LEU
1	B	430	MET
1	B	443	CYS
1	B	455	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	128	GLN
1	A	146	GLN
1	A	191	GLN
1	A	207	GLN
1	A	278	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	422	HIS

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Mol	Chain	Res	Type
1	A	468	ASN
1	B	134	ASN
1	B	146	GLN
1	B	153	GLN
1	B	166	HIS
1	B	178	GLN
1	B	191	GLN
1	B	196	GLN
1	B	207	GLN
1	B	222	ASN
1	B	225	ASN
1	B	259	GLN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN
1	B	410	HIS
1	B	463	HIS
1	B	478	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
2	HEM	B	500	-	50,50,50	1.88	14 (28%)	67,82,82	1.28	7 (10%)
3	H4B	B	600	-	17,18,18	0.88	0	14,26,26	2.22	7 (50%)
4	CAD	A	950	1	0,2,4	-	-	0,1,6	-	-
5	XFJ	A	800	-	28,28,28	0.48	0	36,38,38	1.97	12 (33%)
3	H4B	A	600	-	17,18,18	0.95	0	14,26,26	1.73	6 (42%)
5	XFJ	B	800	-	28,28,28	0.77	0	36,38,38	1.63	6 (16%)
2	HEM	A	500	1	50,50,50	1.95	10 (20%)	67,82,82	1.68	17 (25%)
4	CAD	B	950	-	0,2,4	-	-	0,1,6	-	-

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3D-C2D	6.74	1.51	1.36
2	A	500	HEM	FE-ND	6.50	2.14	1.94
2	A	500	HEM	C3D-C2D	6.13	1.50	1.36
2	A	500	HEM	FE-NB	5.19	2.10	1.94
2	B	500	HEM	FE-NB	3.34	2.05	1.94
2	A	500	HEM	C3B-C2B	-3.01	1.31	1.37
2	B	500	HEM	C3B-C2B	-2.90	1.31	1.37
2	B	500	HEM	FE-ND	2.81	2.03	1.94
2	B	500	HEM	C2A-C3A	-2.76	1.31	1.38
2	B	500	HEM	CAC-C3C	2.68	1.54	1.47
2	A	500	HEM	CMC-C2C	2.59	1.56	1.50
2	B	500	HEM	C1B-NB	-2.50	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	CMA-C3A	2.42	1.55	1.50
2	B	500	HEM	CAB-C3B	2.27	1.53	1.47
2	A	500	HEM	O1D-CGD	2.27	1.29	1.22
2	B	500	HEM	CHA-C1A	-2.23	1.34	1.39
2	A	500	HEM	CAC-C3C	2.23	1.53	1.47
2	A	500	HEM	CAB-C3B	2.22	1.53	1.47
2	B	500	HEM	C3C-C2C	-2.20	1.32	1.37
2	A	500	HEM	CHC-C4B	-2.15	1.34	1.39
2	B	500	HEM	CHD-C4C	-2.13	1.34	1.38
2	B	500	HEM	C4D-ND	-2.07	1.36	1.40
2	B	500	HEM	O1D-CGD	2.03	1.28	1.22
2	B	500	HEM	C4B-NB	-2.01	1.34	1.38

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	XFJ	C02-N01-C06	6.11	122.64	118.07
5	B	800	XFJ	C02-N01-C06	5.12	121.90	118.07
2	A	500	HEM	C4D-ND-C1D	4.42	110.44	105.21
2	A	500	HEM	CAD-C3D-C4D	3.89	131.48	124.70
5	A	800	XFJ	C14-C15-C16	3.89	120.50	116.90
3	B	600	H4B	N2-C2-N3	3.79	124.75	116.76
2	A	500	HEM	CAD-CBD-CGD	-3.75	103.72	113.67
3	B	600	H4B	C2-N1-C8A	3.58	119.68	113.36
3	B	600	H4B	O4-C4-C4A	-3.33	119.22	127.26
2	A	500	HEM	CHD-C4C-NC	3.25	127.99	124.45
2	B	500	HEM	CAD-C3D-C4D	3.16	130.20	124.70
2	A	500	HEM	CHC-C1C-NC	3.12	127.85	124.45
2	B	500	HEM	C1D-C2D-C3D	-3.08	103.75	106.98
3	A	600	H4B	C2-N1-C8A	3.07	118.77	113.36
2	A	500	HEM	CHB-C4A-NA	3.04	129.38	123.86
5	B	800	XFJ	C22-N21-C26	3.01	120.32	118.07
2	B	500	HEM	CBA-CAA-C2A	-2.95	104.36	112.53
5	B	800	XFJ	C14-C15-C16	2.95	119.63	116.90
2	A	500	HEM	CHB-C1B-NB	-2.89	120.79	124.37
5	A	800	XFJ	C14-C13-C12	2.87	119.56	116.90
2	A	500	HEM	CMB-C2B-C1B	2.81	129.43	125.03
5	A	800	XFJ	N22-C22-N21	2.73	120.98	116.59
2	A	500	HEM	CBC-CAC-C3C	-2.73	113.87	127.53
2	A	500	HEM	CHA-C4D-ND	-2.70	121.03	124.37
5	A	800	XFJ	C18-C26-N21	2.68	120.13	116.06
2	A	500	HEM	CAD-C3D-C2D	-2.68	122.86	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	XFJ	C18-C17-C15	-2.54	104.60	113.23
2	A	500	HEM	CHA-C4D-C3D	2.48	129.81	125.23
5	A	800	XFJ	C15-C14-C13	-2.46	118.14	121.20
3	A	600	H4B	O10-C10-C9	-2.45	105.72	109.77
2	B	500	HEM	CMD-C2D-C1D	2.40	128.78	125.03
5	A	800	XFJ	C22-N21-C26	2.39	119.86	118.07
5	A	800	XFJ	C18-C26-C25	-2.39	118.19	121.65
2	B	500	HEM	C2D-C1D-ND	2.39	112.66	109.90
5	A	800	XFJ	C05-C06-N01	-2.38	120.02	122.73
3	B	600	H4B	O10-C10-C9	-2.37	105.85	109.77
5	B	800	XFJ	C18-C17-C15	-2.36	105.20	113.23
3	A	600	H4B	C2-N3-C4	-2.35	120.86	125.11
2	B	500	HEM	CAA-CBA-CGA	-2.26	107.66	113.67
2	A	500	HEM	CMB-C2B-C3B	-2.23	123.04	128.43
2	A	500	HEM	C2A-C1A-NA	-2.21	107.70	110.15
3	A	600	H4B	C4A-C4-N3	2.20	118.17	112.13
2	B	500	HEM	C4D-ND-C1D	2.18	107.79	105.21
5	A	800	XFJ	C08-C06-C05	2.18	124.81	121.65
2	A	500	HEM	CMD-C2D-C1D	2.12	128.34	125.03
3	A	600	H4B	O4-C4-C4A	-2.12	122.16	127.26
5	B	800	XFJ	C14-C13-C12	2.12	118.86	116.90
3	A	600	H4B	C4-C4A-N5	2.10	121.99	116.27
5	B	800	XFJ	C15-C14-C13	-2.09	118.60	121.20
3	B	600	H4B	N2-C2-N1	-2.06	115.65	119.67
3	B	600	H4B	O4-C4-N3	2.05	123.98	120.11
2	A	500	HEM	CHA-C1A-NA	2.05	127.58	123.86
3	B	600	H4B	N3-C2-N1	-2.03	119.60	123.32
2	A	500	HEM	C1D-C2D-C3D	-2.01	104.87	106.98
5	A	800	XFJ	C16-N11-C12	2.01	120.24	117.51

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	800	XFJ	C15-C17-C18-C26
2	A	500	HEM	C3D-CAD-CBD-CGD
2	A	500	HEM	C2B-C3B-CAB-CBB
2	A	500	HEM	C4D-C3D-CAD-CBD
2	B	500	HEM	C4B-C3B-CAB-CBB
5	B	800	XFJ	C08-C09-C13-C12
2	A	500	HEM	C2D-C3D-CAD-CBD
2	A	500	HEM	CAD-CBD-CGD-O2D

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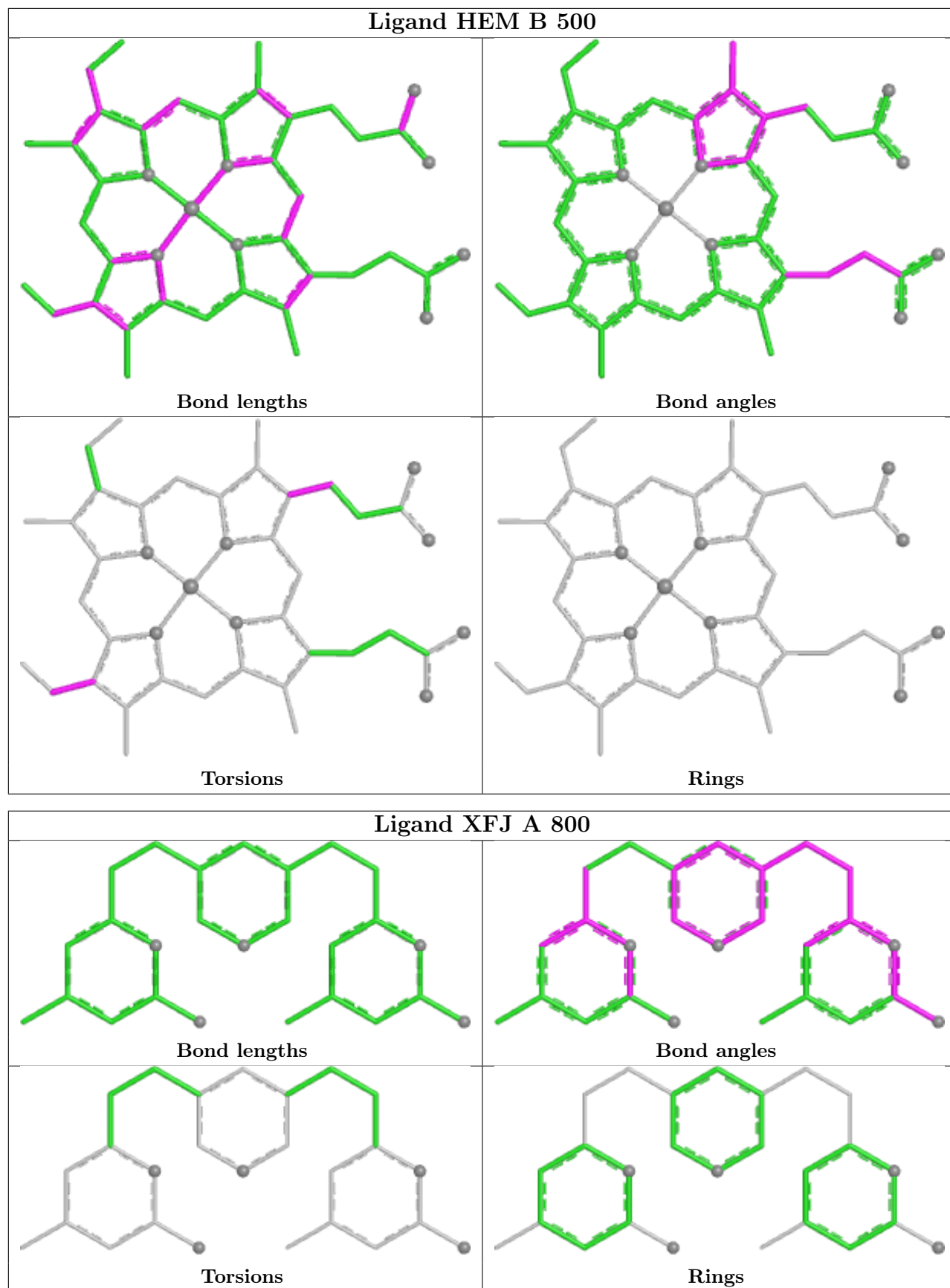
Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C4B-C3B-CAB-CBB
5	B	800	XFJ	C08-C09-C13-C14
2	A	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	C2D-C3D-CAD-CBD

There are no ring outliers.

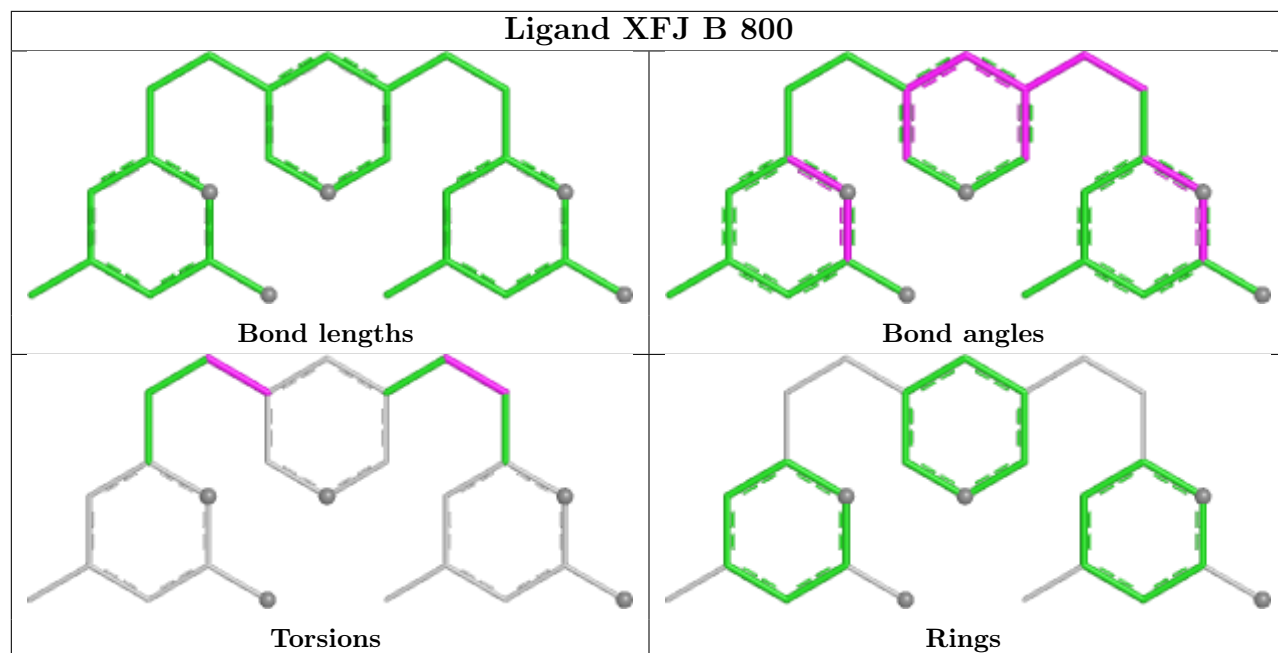
6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	HEM	8	0
3	B	600	H4B	1	0
3	A	600	H4B	3	0
5	B	800	XFJ	3	0
2	A	500	HEM	6	0
4	B	950	CAD	2	0

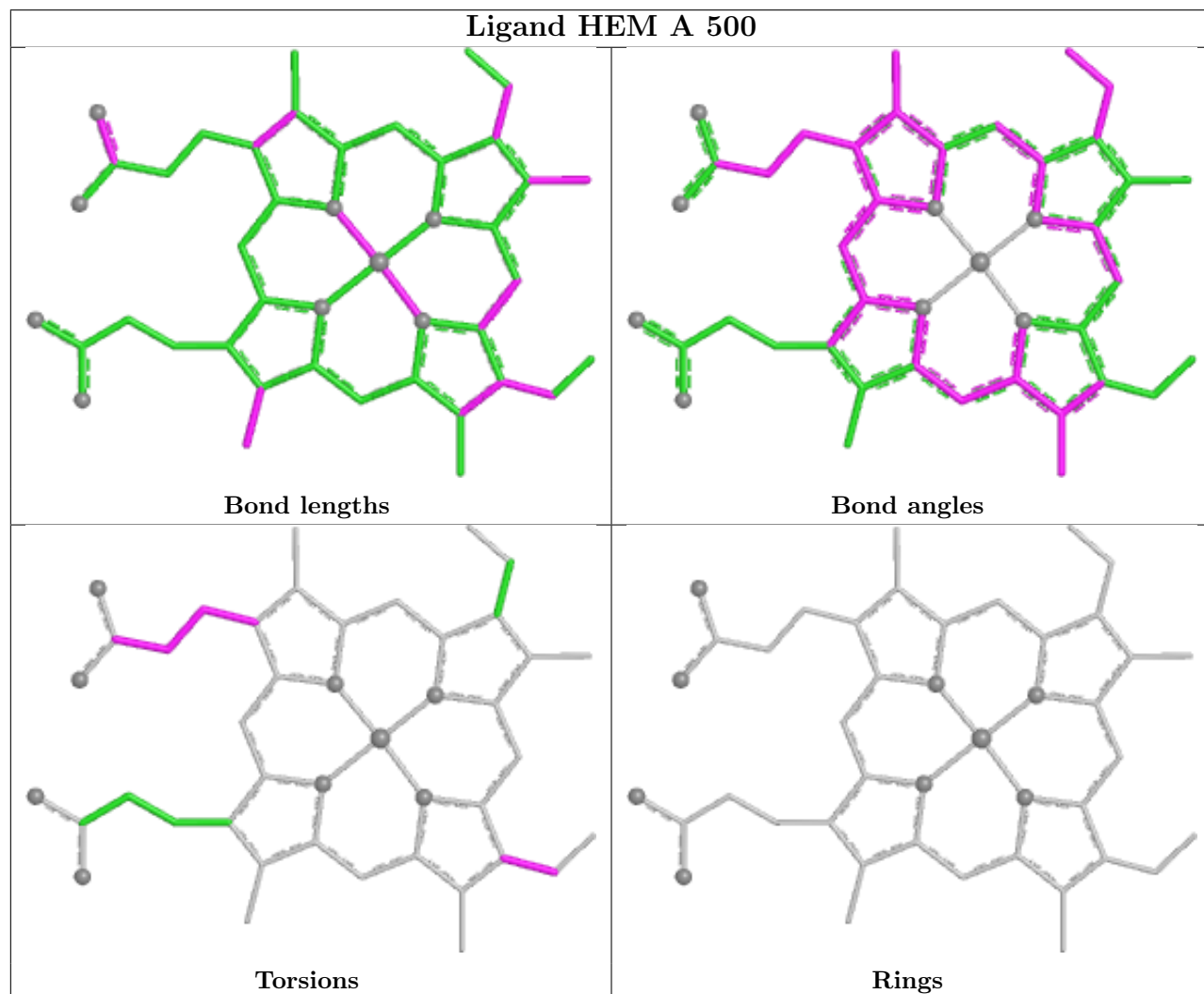
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand XFJ B 800



Ligand HEM A 500



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%)	-0.62	0 100 100	52, 77, 108, 120	0
1	B	402/444 (90%)	-0.58	0 100 100	35, 77, 114, 145	1 (0%)
All	All	806/888 (90%)	-0.60	0 100 100	35, 77, 110, 145	1 (0%)

There are no RSRZ outliers to report.

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
3	H4B	B	600	17/17	0.90	0.10	77,82,84,84	0
5	XFJ	B	800	26/26	0.91	0.13	57,89,105,106	0
4	CAD	B	950	3/5	0.94	0.17	122,122,122,124	0
3	H4B	A	600	17/17	0.94	0.08	71,73,77,79	0
5	XFJ	A	800	26/26	0.95	0.13	81,104,110,111	0
4	CAD	A	950	3/5	0.95	0.13	103,103,106,106	0
2	HEM	A	500	43/43	0.98	0.07	51,57,63,69	0

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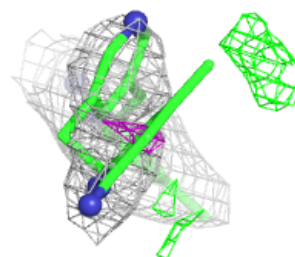
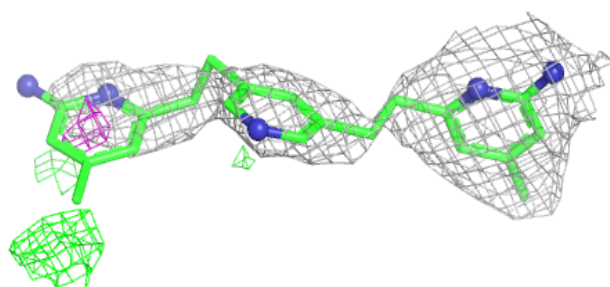
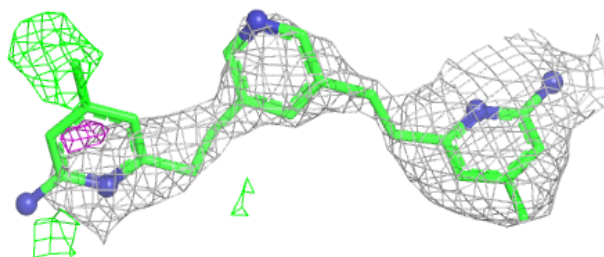
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	500	43/43	0.99	0.06	46,51,65,74	0
6	ZN	A	900	1/1	1.00	0.02	73,73,73,73	0

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.

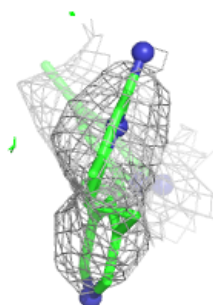
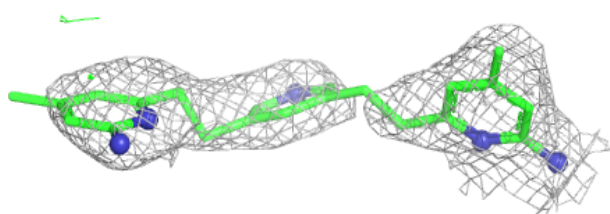
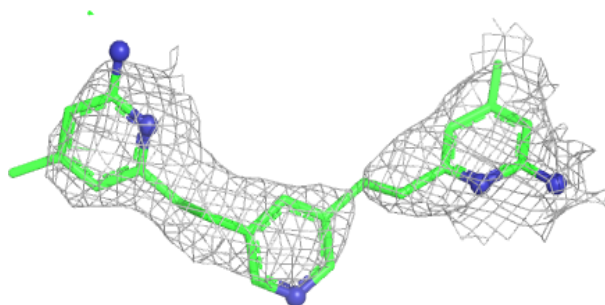
Electron density around XFJ B 800:

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



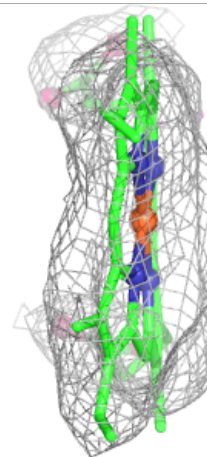
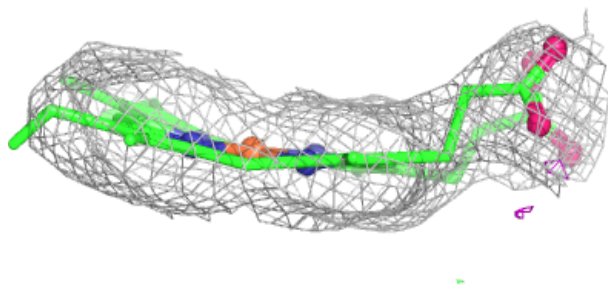
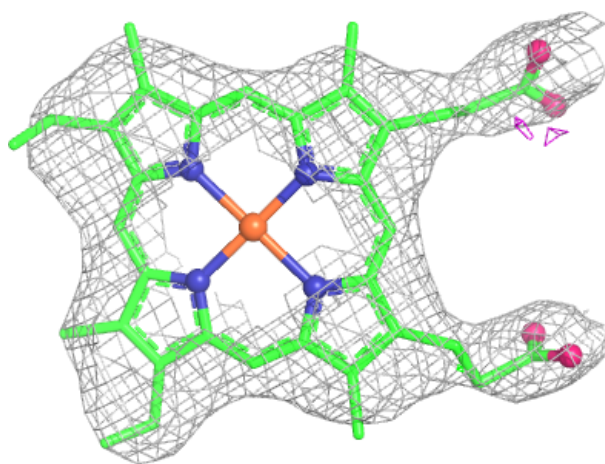
Electron density around XFJ A 800:

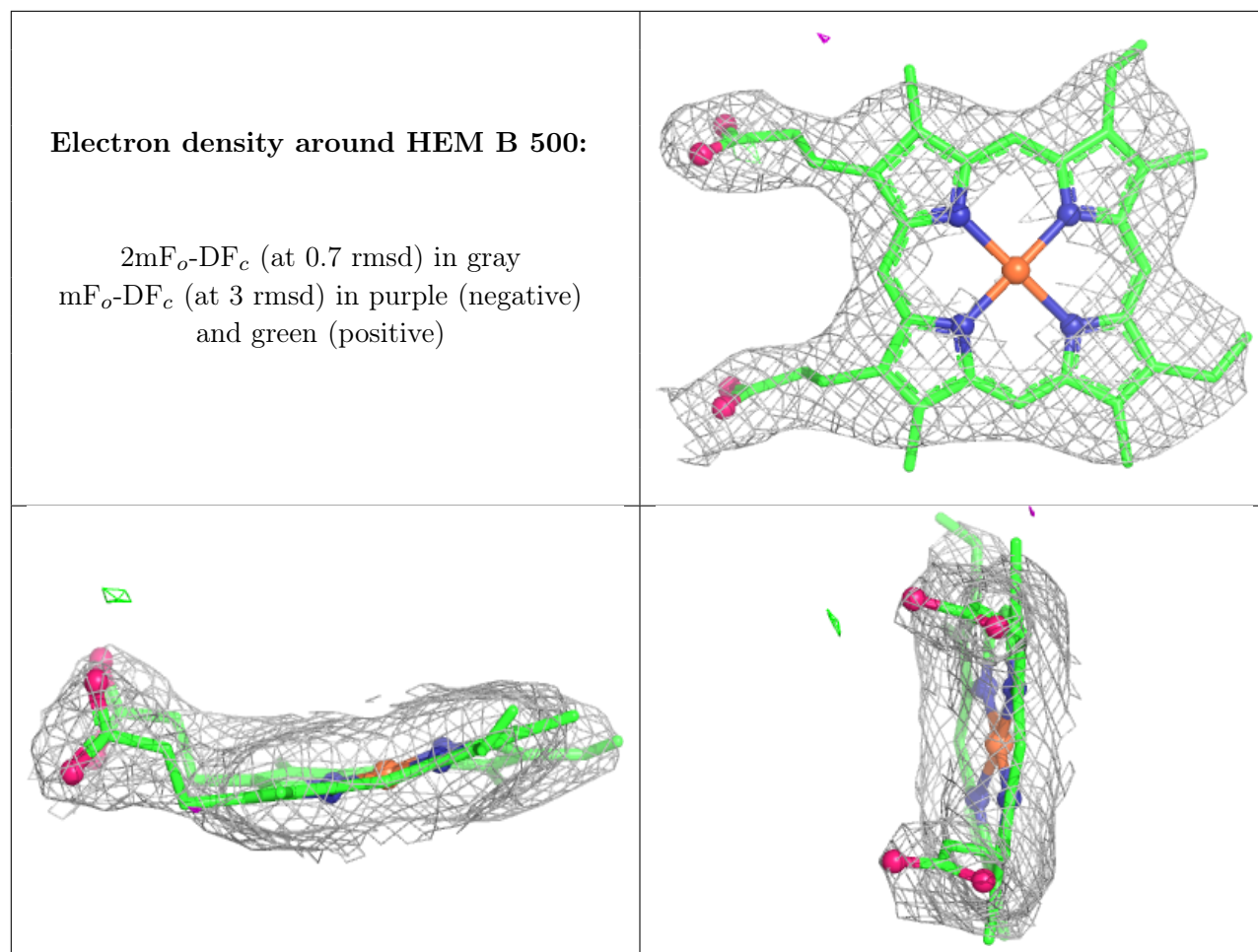
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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.