



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:22 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
Authors : Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on : 2010-05-25
Resolution : 3.06 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

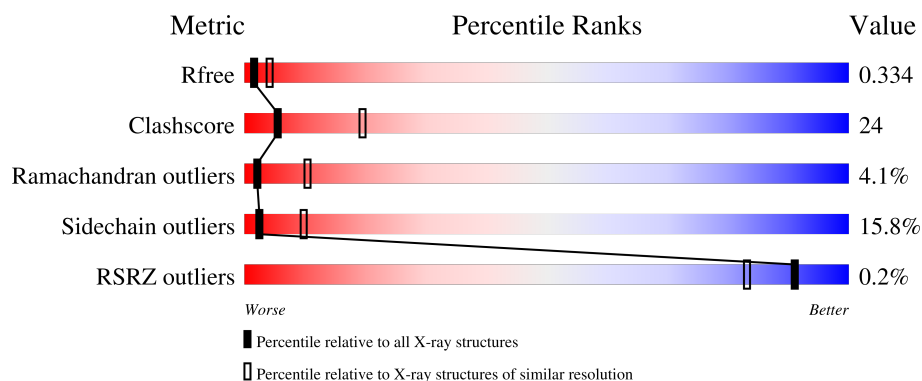
1 Overall quality at a glance

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.

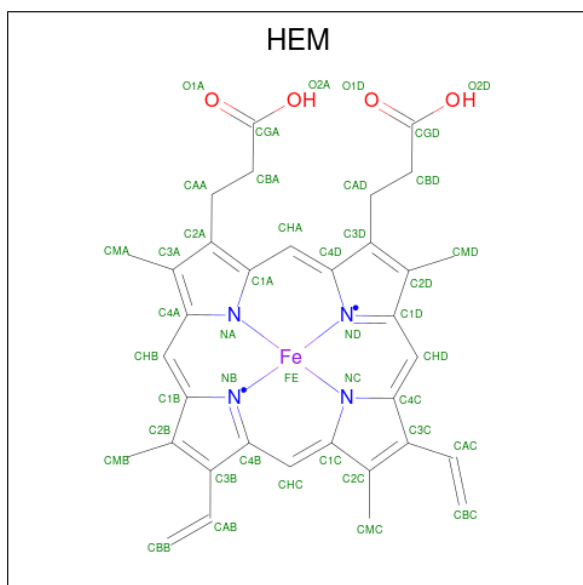
- Molecule 1 is a protein called Nitric oxide synthase.

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:

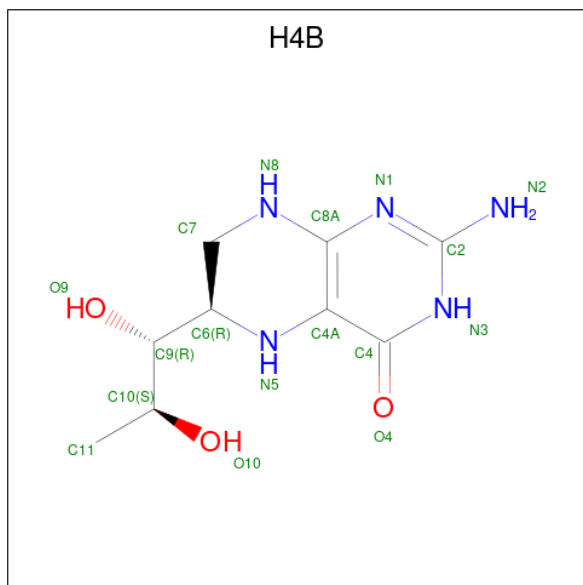
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29476
A	373	SER	HIS	engineered mutation	UNP P29476
B	100	ARG	CYS	SEE REMARK 999	UNP P29476
B	373	SER	HIS	engineered mutation	UNP P29476

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



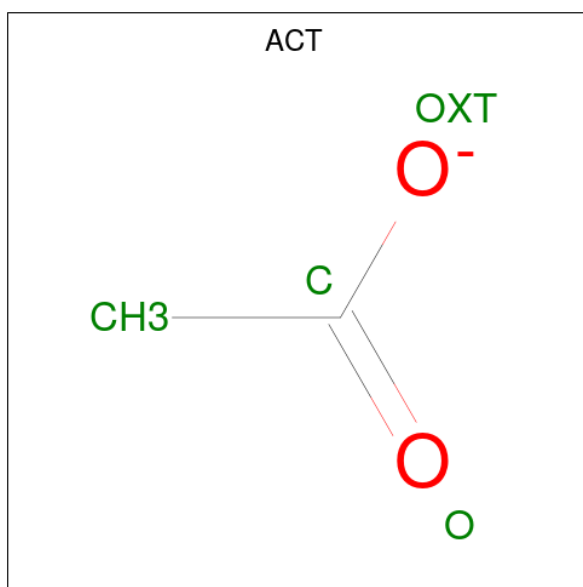
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



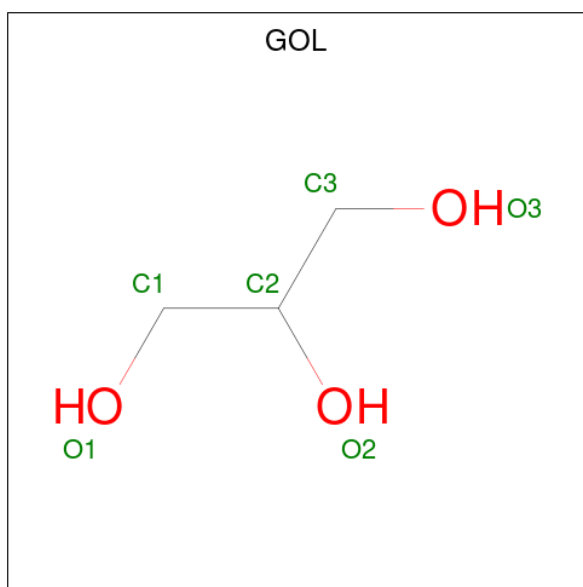
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- 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: $C_3H_8O_3$).



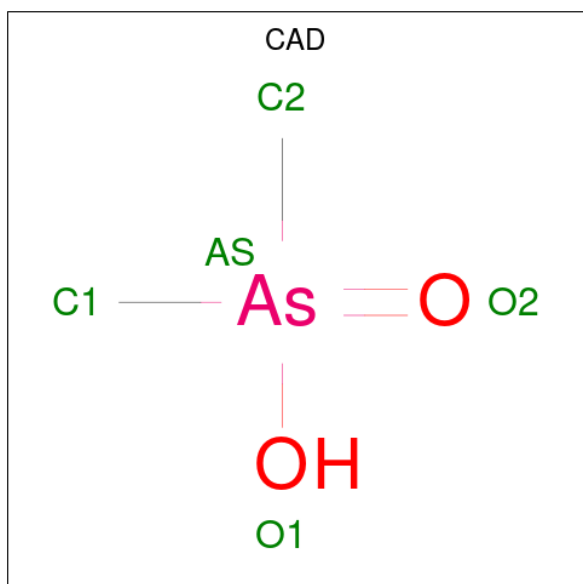
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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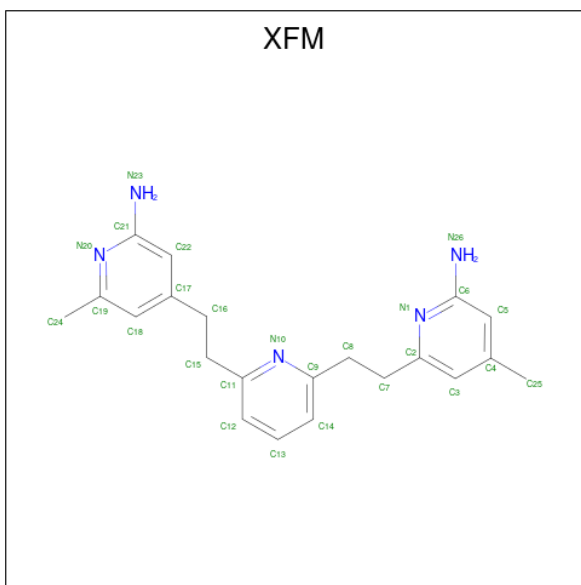
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- 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		

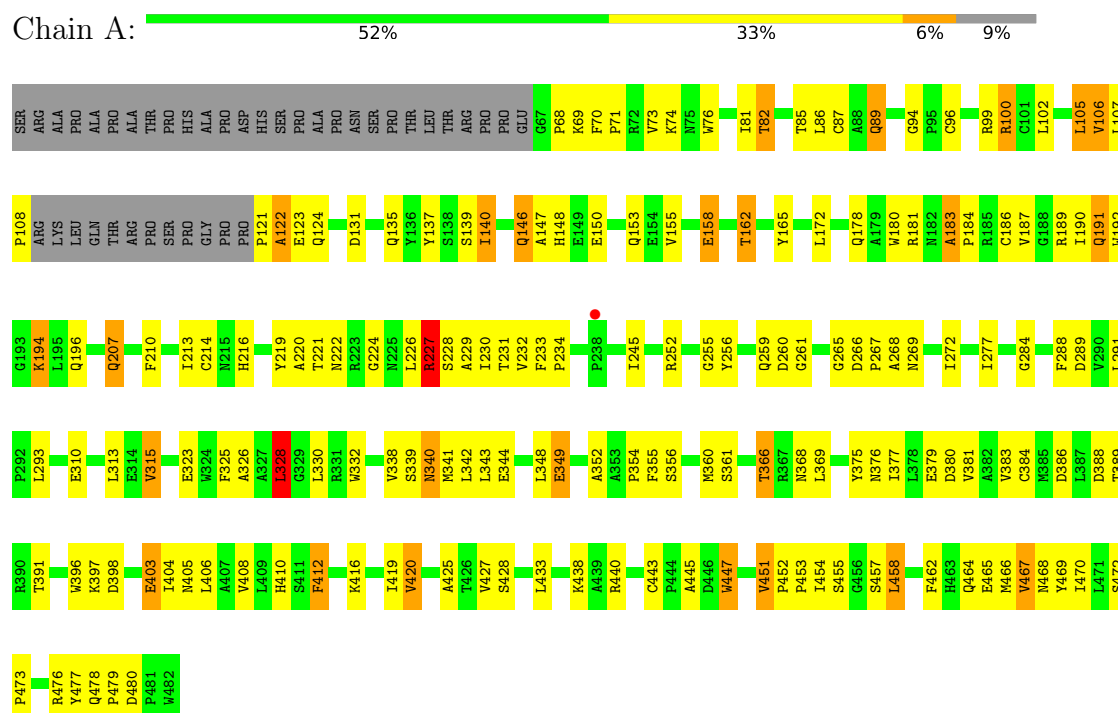
- Molecule 9 is water.

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

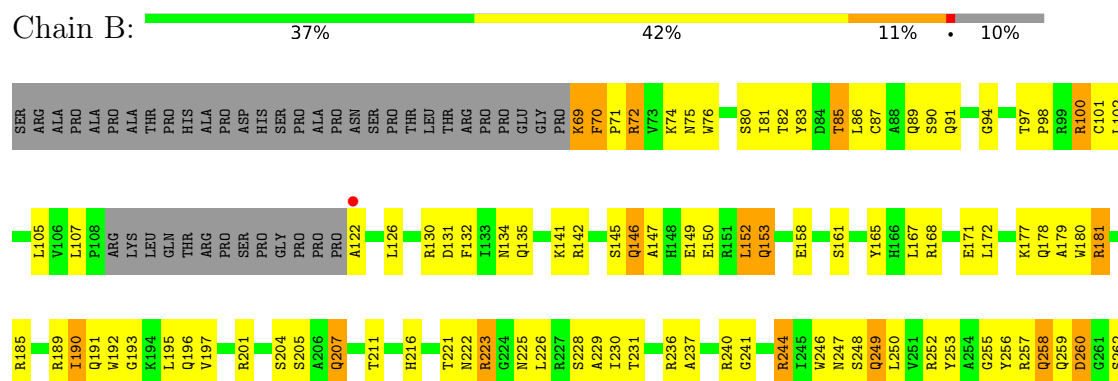
3 Residue-property plots

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



P473	P474	P475	P476	P477	P478	P479	P480	P481	P482	P483	P484	P485	P486	P487	P488	P489	P490	P491	P492	P493	P494	P495	P496	P497	P498	P499	P500	P501	P502	P503	P504	P505	P506	P507	P508	P509	P510	P511	P512	P513	P514	P515	P516	P517	P518	P519	P520	P521	P522	P523	P524	P525	P526	P527	P528	P529	P530	P531	P532	P533	P534	P535	P536	P537	P538	P539	P540	P541	P542	P543	P544	P545	P546	P547	P548	P549	P550	P551	P552	P553	P554	P555	P556	P557	P558	P559	P560	P561	P562	P563	P564	P565	P566	P567	P568	P569	P570	P571	P572	P573	P574	P575	P576	P577	P578	P579	P580	P581	P582	P583	P584	P585	P586	P587	P588	P589	P590	P591	P592	P593	P594	P595	P596	P597	P598	P599	P600	P601	P602	P603	P604	P605	P606	P607	P608	P609	P610	P611	P612	P613	P614	P615	P616	P617	P618	P619	P620	P621	P622	P623	P624	P625	P626	P627	P628	P629	P630	P631	P632	P633	P634	P635	P636	P637	P638	P639	P640	P641	P642	P643	P644	P645	P646	P647	P648	P649	P650	P651	P652	P653	P654	P655	P656	P657	P658	P659	P660	P661	P662	P663	P664	P665	P666	P667	P668	P669	P670	P671	P672	P673	P674	P675	P676	P677	P678	P679	P680	P681	P682	P683	P684	P685	P686	P687	P688	P689	P690	P691	P692	P693	P694	P695	P696	P697	P698	P699	P700	P701	P702	P703	P704	P705	P706	P707	P708	P709	P710	P711	P712	P713	P714	P715	P716	P717	P718	P719	P720	P721	P722	P723	P724	P725	P726	P727	P728	P729	P730	P731	P732	P733	P734	P735	P736	P737	P738	P739	P740	P741	P742	P743	P744	P745	P746	P747	P748	P749	P750	P751	P752	P753	P754	P755	P756	P757	P758	P759	P760	P761	P762	P763	P764	P765	P766	P767	P768	P769	P770	P771	P772	P773	P774	P775	P776	P777	P778	P779	P780	P781	P782	P783	P784	P785	P786	P787	P788	P789	P790	P791	P792	P793	P794	P795	P796	P797	P798	P799	P800	P801	P802	P803	P804	P805	P806	P807	P808	P809	P810	P811	P812	P813	P814	P815	P816	P817	P818	P819	P820	P821	P822	P823	P824	P825	P826	P827	P828	P829	P830	P831	P832	P833	P834	P835	P836	P837	P838	P839	P840	P841	P842	P843	P844	P845	P846	P847	P848	P849	P850	P851	P852	P853	P854	P855	P856	P857	P858	P859	P860	P861	P862	P863	P864	P865	P866	P867	P868	P869	P870	P871	P872	P873	P874	P875	P876	P877	P878	P879	P880	P881	P882	P883	P884	P885	P886	P887	P888	P889	P890	P891	P892	P893	P894	P895	P896	P897	P898	P899	P900	P901	P902	P903	P904	P905	P906	P907	P908	P909	P910	P911	P912	P913	P914	P915	P916	P917	P918	P919	P920	P921	P922	P923	P924	P925	P926	P927	P928	P929	P930	P931	P932	P933	P934	P935	P936	P937	P938	P939	P940	P941	P942	P943	P944	P945	P946	P947	P948	P949	P950	P951	P952	P953	P954	P955	P956	P957	P958	P959	P960	P961	P962	P963	P964	P965	P966	P967	P968	P969	P970	P971	P972	P973	P974	P975	P976	P977	P978	P979	P980	P981	P982	P983	P984	P985	P986	P987	P988	P989	P990	P991	P992	P993	P994	P995	P996	P997	P998	P999	P1000
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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 ⓘ

5.1 Standard geometry ⓘ

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

The worst 5 of 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

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
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.

The worst 5 of 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

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%)	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

5 of 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

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

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	204	SER
1	B	277	ILE
1	B	414	LEU
1	B	207	GLN
1	B	244	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	GLN
1	B	225	ASN
1	B	207	GLN
1	B	249	GLN
1	A	249	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 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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-

The worst 5 of 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
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

The worst 5 of 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

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

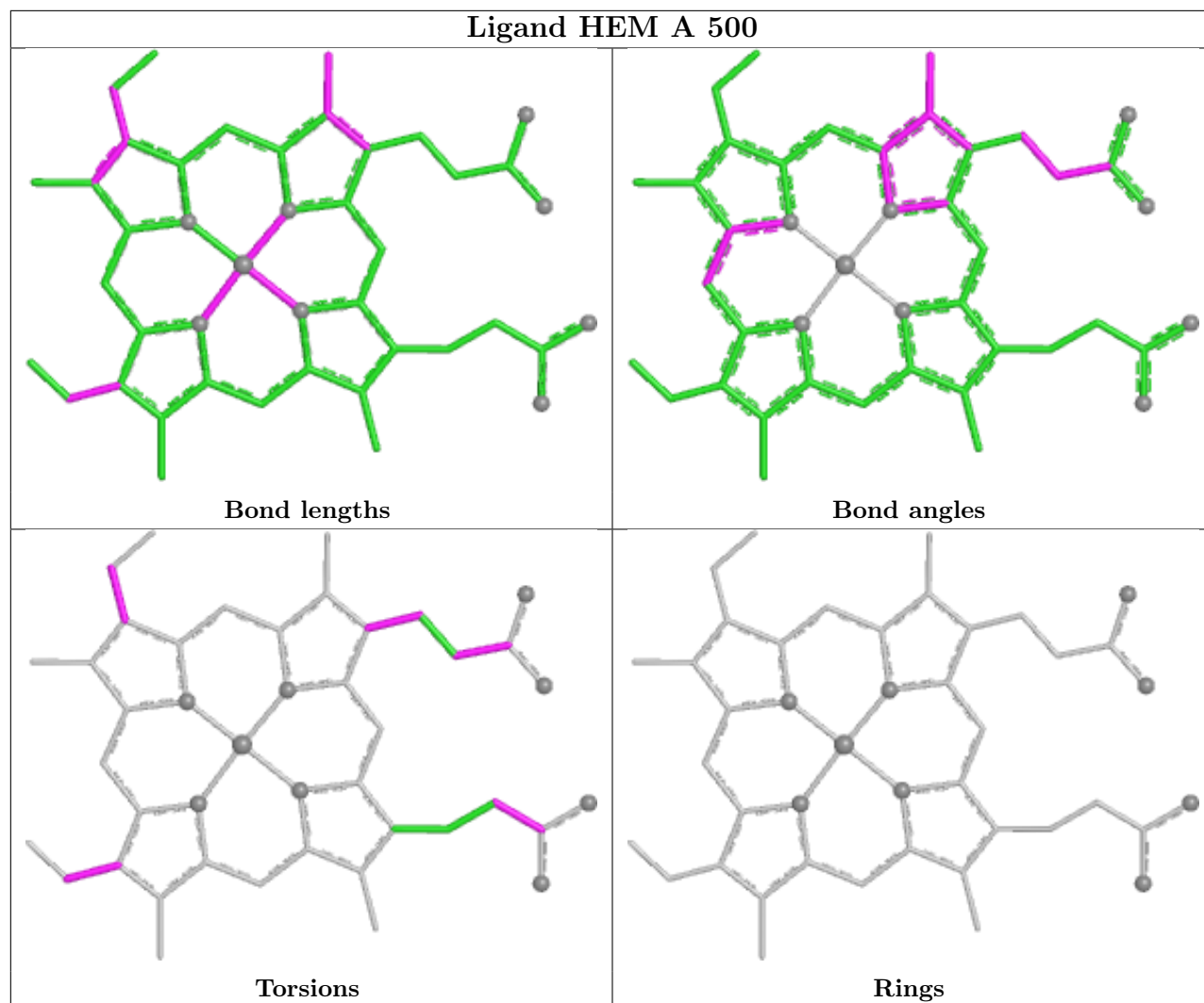
Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2C-C3C-CAC-CBC
2	A	500	HEM	C4C-C3C-CAC-CBC
2	A	500	HEM	C2D-C3D-CAD-CBD
2	A	500	HEM	C4D-C3D-CAD-CBD
2	B	500	HEM	C2C-C3C-CAC-CBC

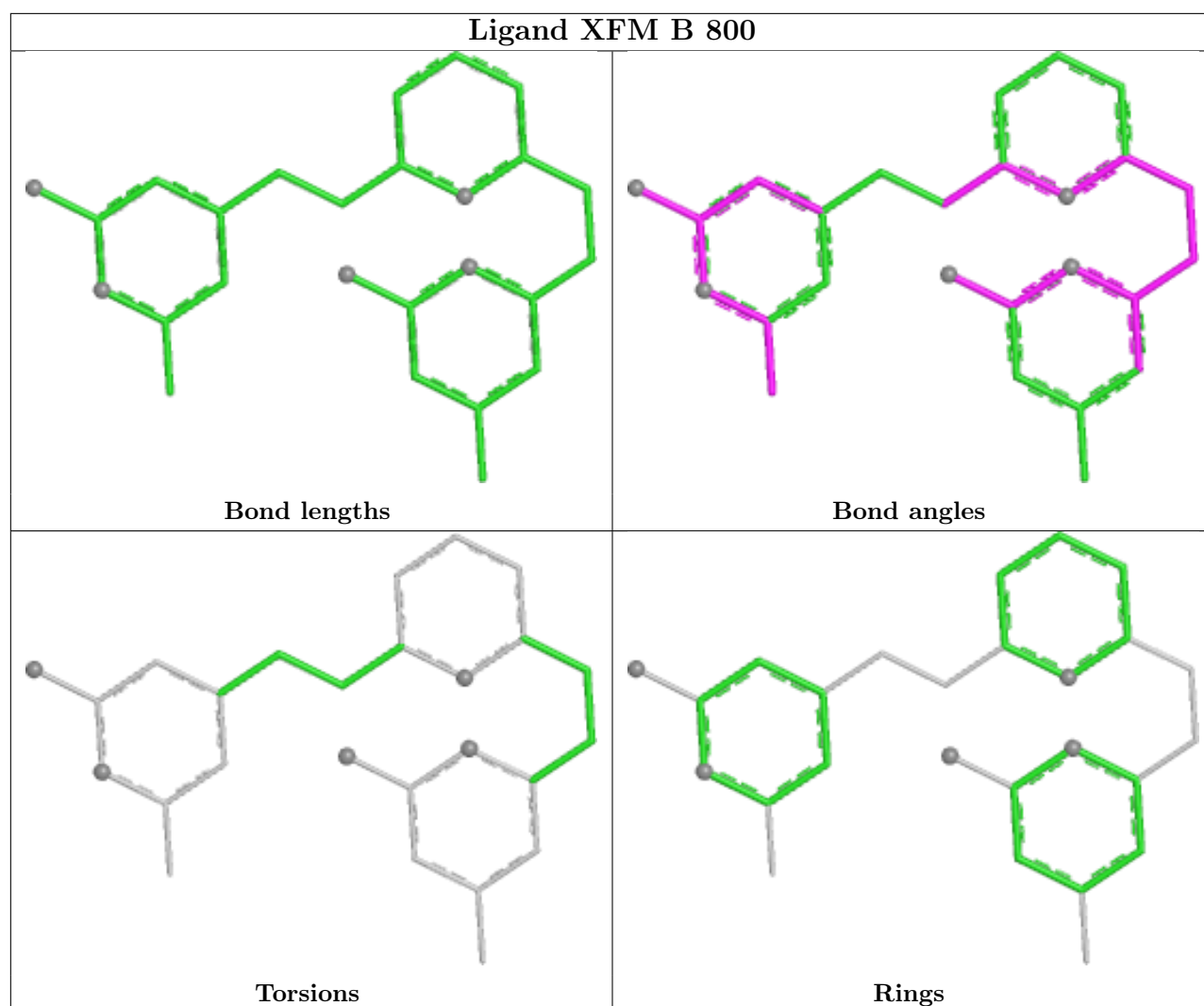
There are no ring outliers.

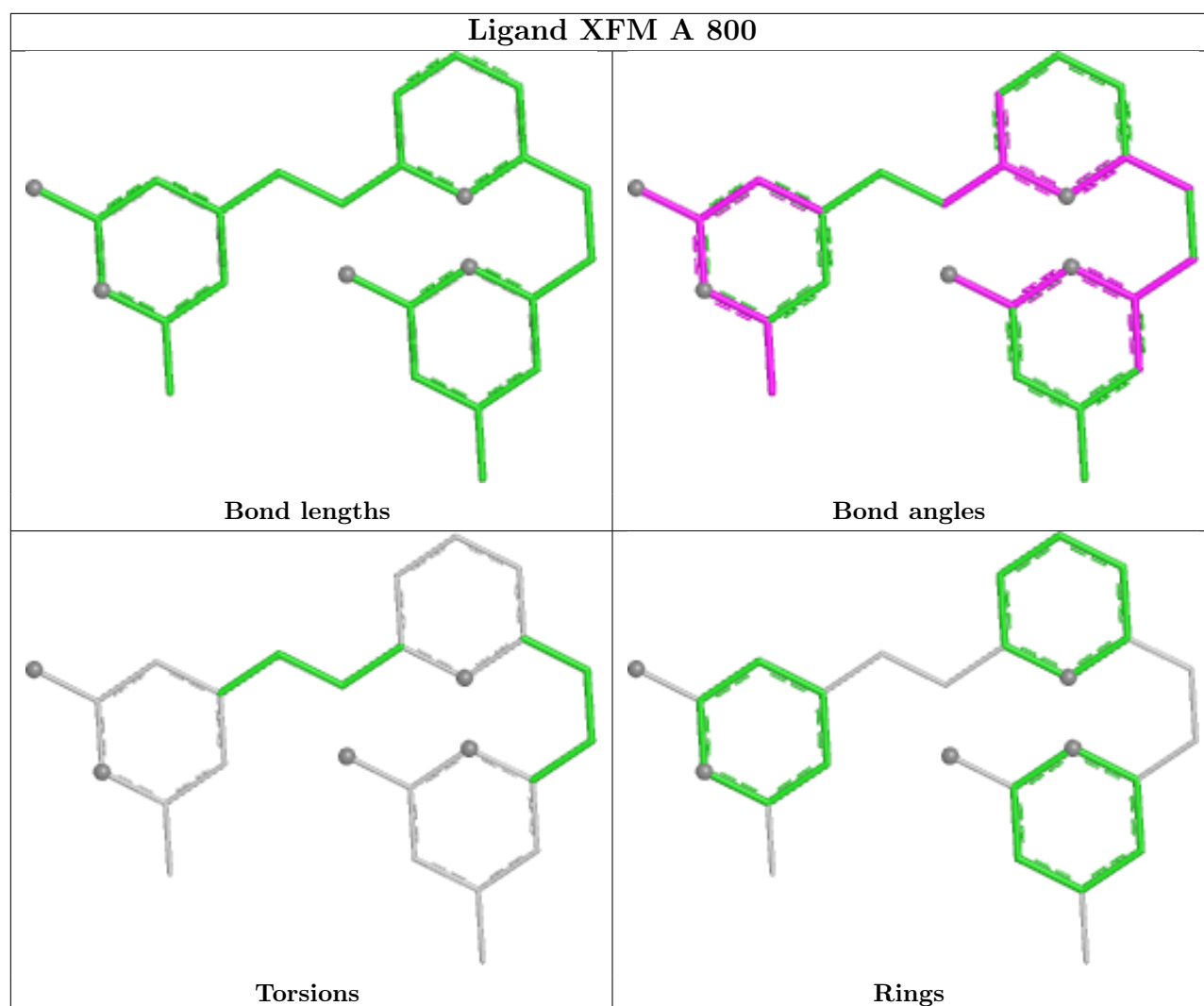
6 monomers are involved in 18 short contacts:

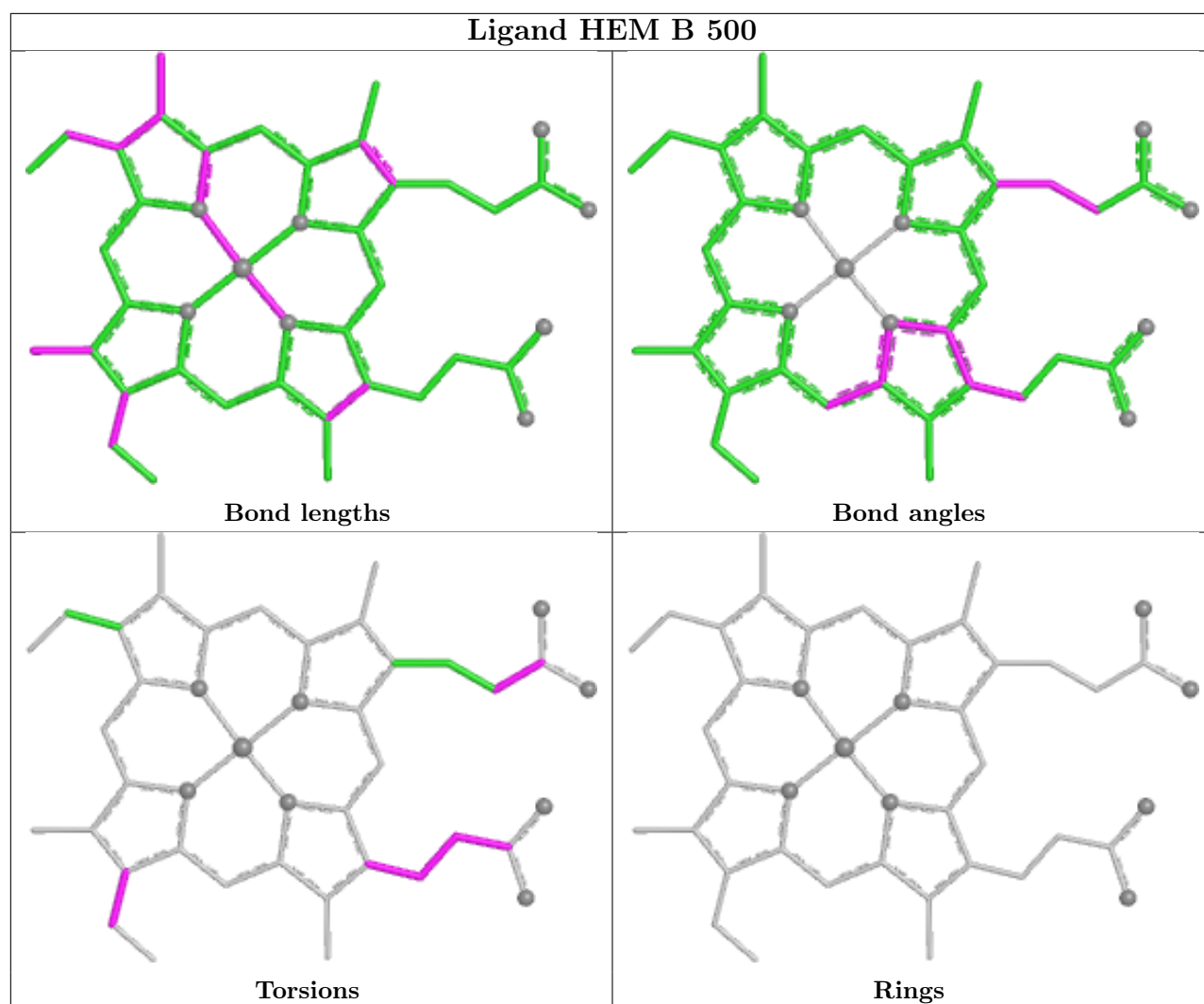
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	950	CAD	1	0
2	A	500	HEM	8	0
6	B	950	CAD	1	0
7	B	800	XFM	1	0
7	A	800	XFM	4	0
2	B	500	HEM	5	0

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.

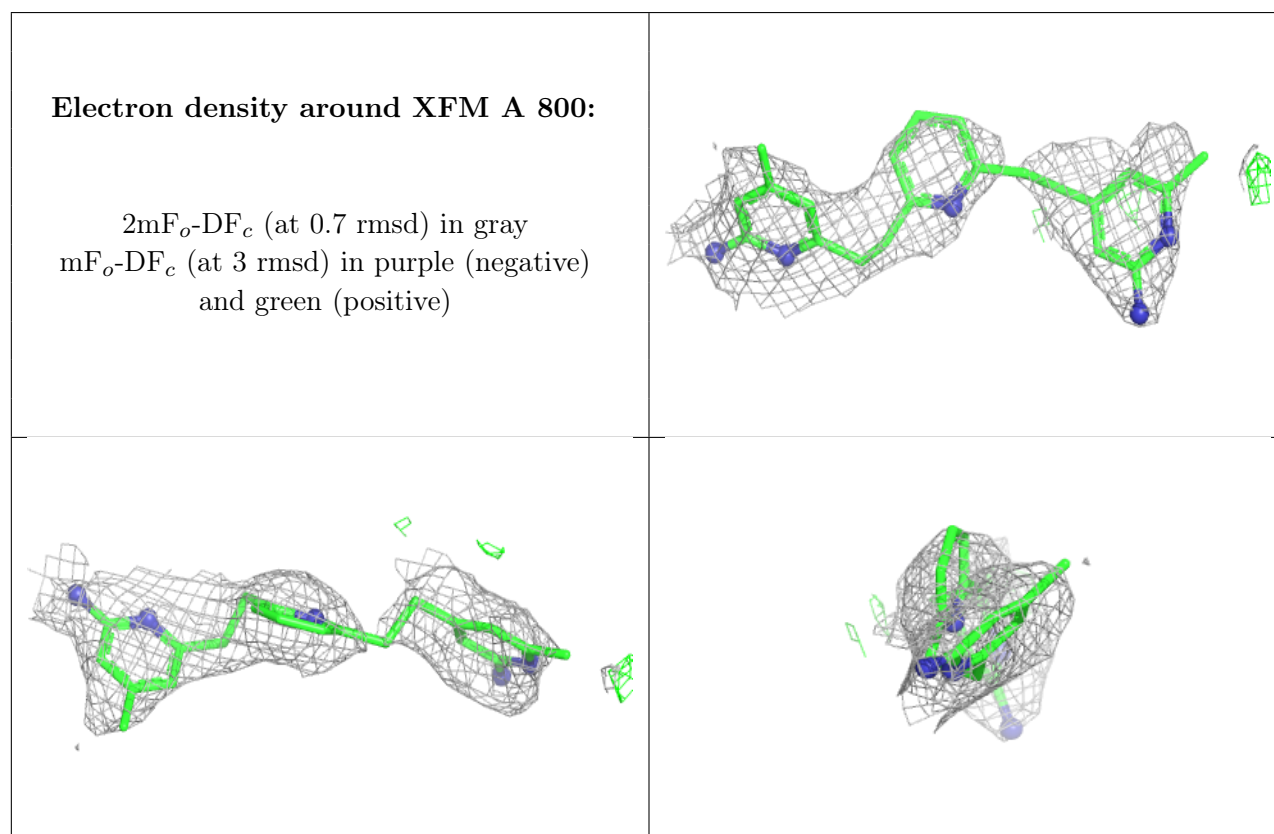
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	880	6/6	0.75	0.21	69,71,72,72	0
4	ACT	B	850	4/4	0.78	0.16	41,41,42,42	0
6	CAD	A	950	3/5	0.82	0.22	120,120,120,121	0

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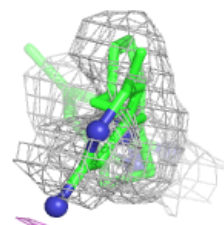
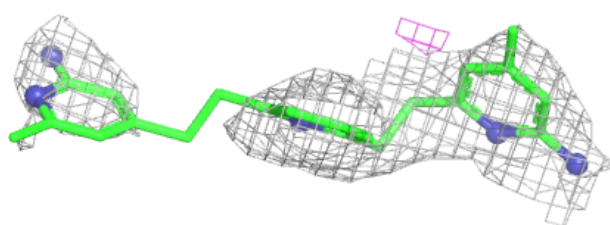
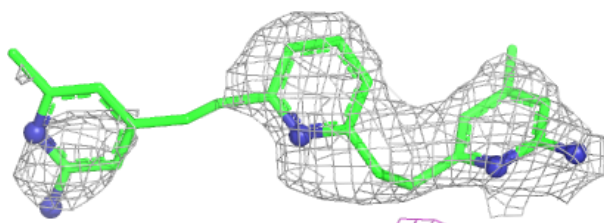
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CAD	B	950	3/5	0.84	0.21	118,118,118,118	0
3	H4B	A	600	17/17	0.86	0.18	94,96,97,97	0
4	ACT	A	860	4/4	0.87	0.17	66,66,67,67	0
4	ACT	B	860	4/4	0.88	0.22	58,59,59,60	0
3	H4B	B	600	17/17	0.88	0.17	82,85,86,86	0
7	XFM	A	800	26/26	0.88	0.16	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.

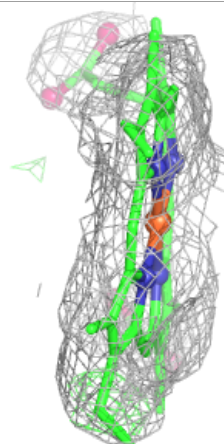
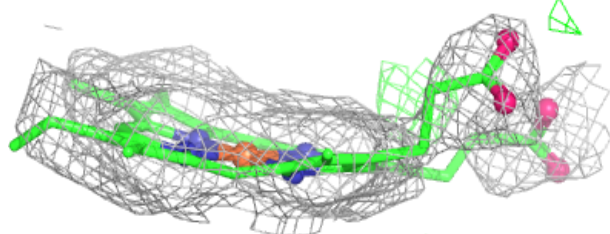
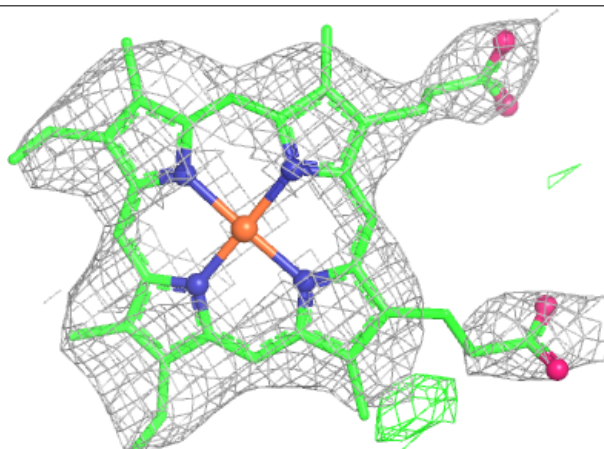


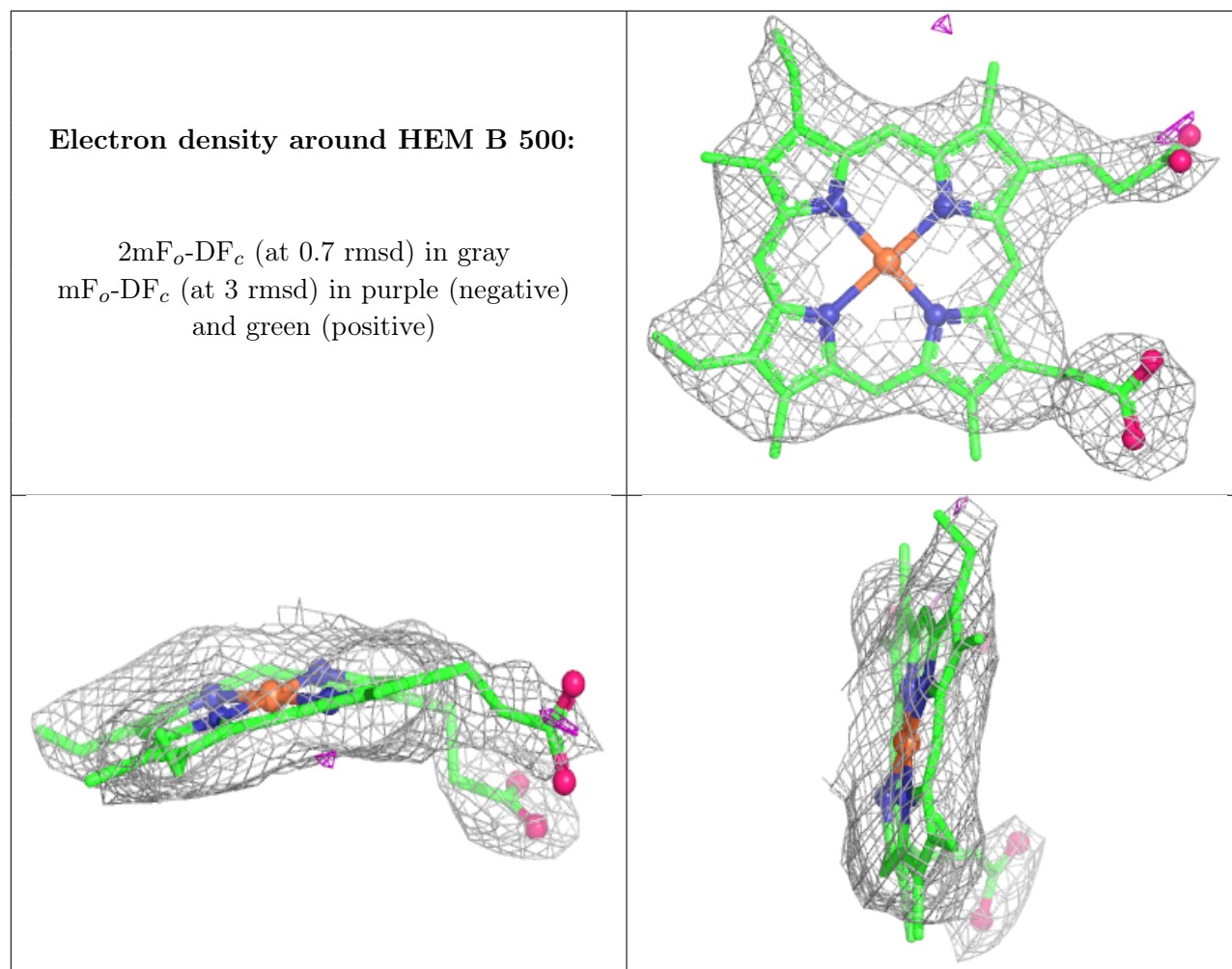
Electron density around XFM B 800:

$2mF_o-DF_c$ (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.