



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:10 PM UTC

PDB ID : 3N5W / pdb_00003n5w
Title : Structure of neuronal nitric oxide synthase heme domain in complex with 6,6'-((2,2'-(pyridine-3,5-diyl)bis(ethane-2,1-diyl))bis(4-methylpyridin-2-amine)
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Deposited on : 2010-05-25
Resolution : 1.73 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

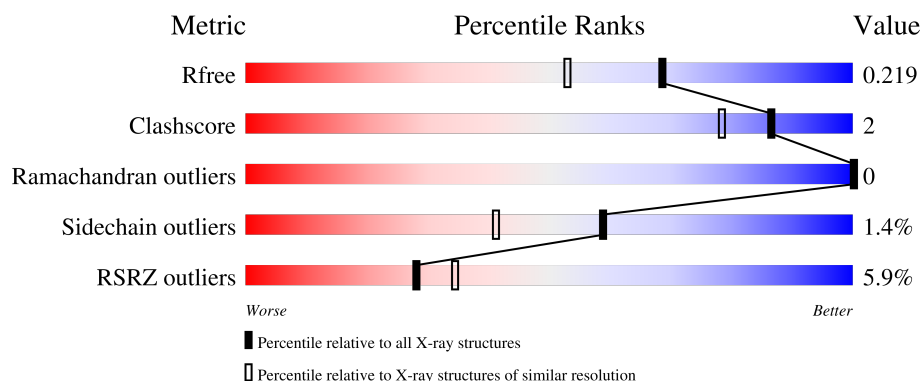
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	422	7% 92%
1	B	422	4% 91% 6%

2 Entry composition [i](#)

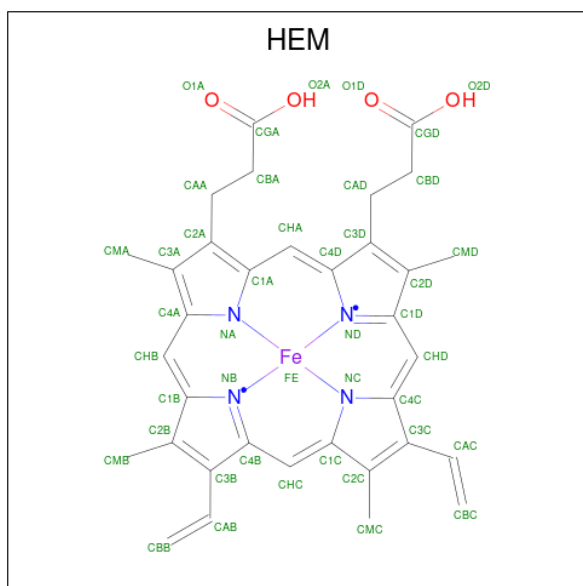
There are 7 unique types of molecules in this entry. The entry contains 7476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

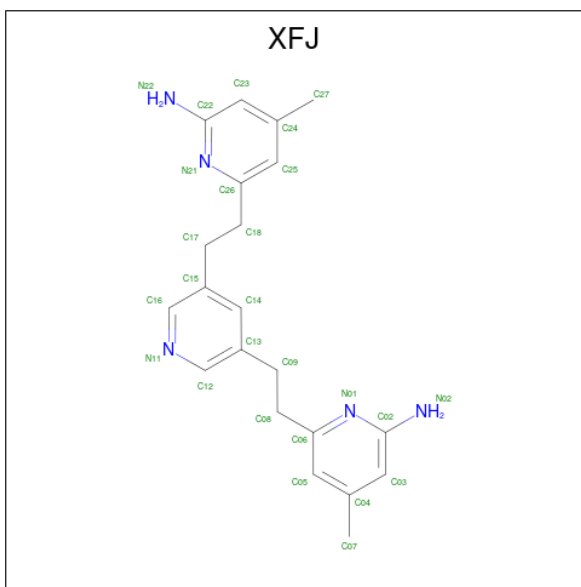
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	1	0
			3322	2129	566	606	21			
1	B	411	Total	C	N	O	S	0	2	0
			3357	2150	574	612	21			

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



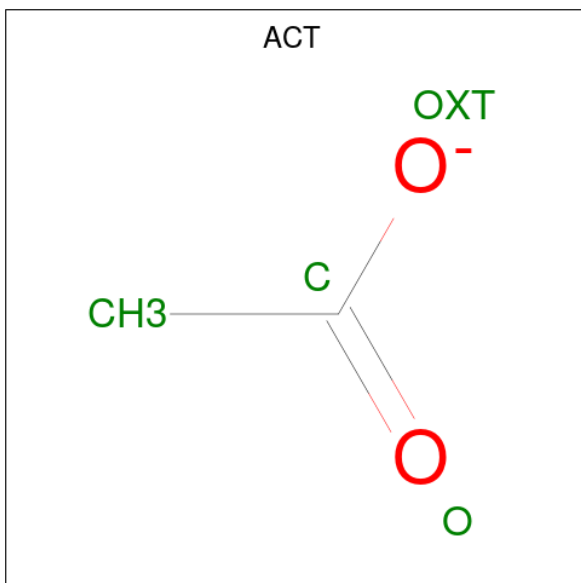
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 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
3	A	1	Total	C	N	0	0
			26	21	5		
3	A	1	Total	C	N	0	0
			26	21	5		
3	B	1	Total	C	N	0	0
			26	21	5		
3	B	1	Total	C	N	0	0
			26	21	5		

- 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 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Zn 3 3	0	0

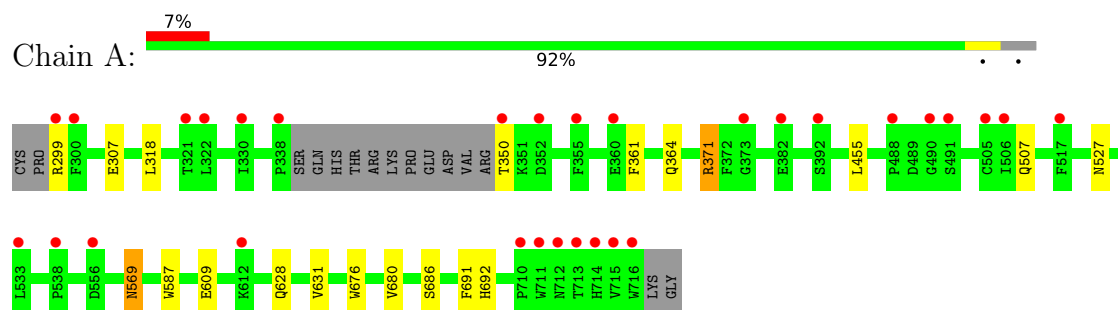
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	263	Total O 263 263	0	0
7	B	331	Total O 331 331	0	0

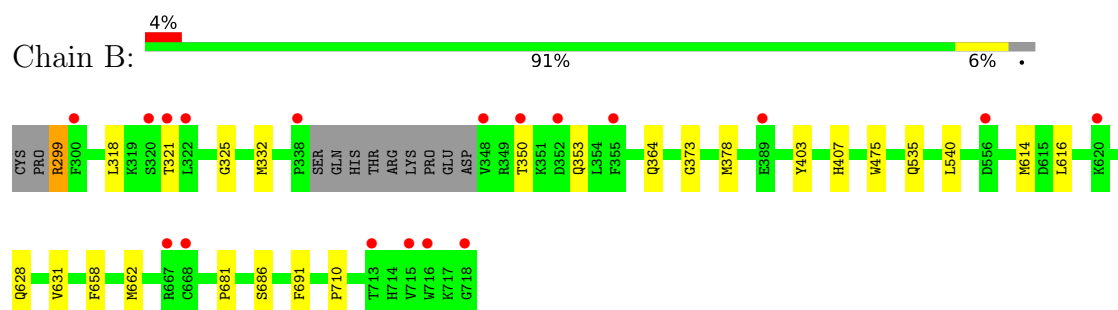
3 Residue-property plots [i](#)

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

• Molecule 1: Nitric oxide synthase



• Molecule 1: Nitric oxide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.34Å 111.21Å 164.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.11 – 1.73 38.11 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.11-1.73) 99.1 (38.11-1.73)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.182 , 0.205 0.192 , 0.219	Depositor DCC
R_{free} test set	5018 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7476	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.65	0/3419	0.79	0/4639
1	B	0.70	1/3457 (0.0%)	0.78	0/4687
All	All	0.68	1/6876 (0.0%)	0.79	0/9326

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	681	PRO	CA-C	5.29	1.54	1.51

There are no bond angle outliers.

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	3322	0	3230	16	0
1	B	3357	0	3273	12	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	52	0	50	0	0
3	B	52	0	50	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	0	0	0
7	A	263	0	0	1	0
7	B	331	0	0	2	0
All	All	7476	0	6669	28	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 2.

All (28) 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:A:299:ARG:HB3	1:A:318:LEU:HD21	1.61	0.81
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.00	0.75
1:A:609:GLU:HG3	7:A:1047:HOH:O	1.97	0.63
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.81	0.61
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.83	0.61
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.65	0.59
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.70	0.56
1:A:299:ARG:CB	1:A:318:LEU:HD21	2.35	0.55
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.91	0.53
1:A:569:ASN:HD22	1:A:569:ASN:H	1.57	0.50
1:B:364:GLN:NE2	7:B:1503:HOH:O	2.45	0.50
1:B:686:SER:HA	1:B:691:PHE:CG	2.46	0.50
1:A:371:ARG:NH2	1:A:371:ARG:HG2	2.27	0.49
1:A:371:ARG:HH21	1:A:371:ARG:HG2	1.77	0.48
1:A:686:SER:HA	1:A:691:PHE:CG	2.50	0.47
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.97	0.47
1:B:614:MET:HE2	1:B:616:LEU:HD21	1.97	0.46
1:B:325:GLY:O	1:B:332:MET:HG3	2.15	0.45
1:B:299:ARG:HB3	1:B:318:LEU:HD21	1.98	0.45
1:B:535:GLN:HG3	7:B:1440:HOH:O	2.16	0.45
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.99	0.44
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.06	0.43
1:B:373:GLY:HA2	1:B:378:MET:HE3	1.99	0.43
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.56	0.41
1:A:307:GLU:HG2	1:A:692:HIS:CG	2.56	0.41
1:B:475:TRP:CG	1:B:710:PRO:HG2	2.55	0.41
1:A:361:PHE:O	1:A:364:GLN:HG2	2.21	0.40
1:B:658:PHE:CE2	1:B:662:MET:HE3	2.56	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	404/422 (96%)	393 (97%)	11 (3%)	0	100	100
1	B	409/422 (97%)	404 (99%)	5 (1%)	0	100	100
All	All	813/844 (96%)	797 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	364/377 (97%)	359 (99%)	5 (1%)	59	41
1	B	368/377 (98%)	363 (99%)	5 (1%)	59	41
All	All	732/754 (97%)	722 (99%)	10 (1%)	59	41

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	THR
1	A	371	ARG
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN

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Mol	Chain	Res	Type
1	B	299	ARG
1	B	321	THR
1	B	350	THR
1	B	353	GLN
1	B	540	LEU

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	395	GLN
1	A	454	ASN
1	A	500	GLN
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	395	GLN
1	B	425	GLN
1	B	440	ASN
1	B	454	ASN
1	B	478	GLN
1	B	507	GLN
1	B	527	ASN
1	B	605	ASN
1	B	697	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 5 are 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	A	750	1	50,50,50	1.95	11 (22%)	67,82,82	1.34	6 (8%)
4	ACT	A	860	-	3,3,3	0.82	0	3,3,3	0.68	0
3	XFJ	A	800	-	28,28,28	0.61	0	36,38,38	2.08	10 (27%)
3	XFJ	A	805	6	28,28,28	0.63	0	36,38,38	1.77	10 (27%)
3	XFJ	B	800	-	28,28,28	0.78	0	36,38,38	1.99	11 (30%)
2	HEM	B	750	1	50,50,50	1.79	10 (20%)	67,82,82	1.26	7 (10%)
4	ACT	B	860	-	3,3,3	0.79	0	3,3,3	0.84	0
3	XFJ	B	805	6	28,28,28	0.56	0	36,38,38	1.64	9 (25%)

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	A	750	1	-	1/14/54/54	-
3	XFJ	A	800	-	-	2/10/10/10	0/3/3/3
3	XFJ	A	805	6	-	0/10/10/10	0/3/3/3
3	XFJ	B	800	-	-	0/10/10/10	0/3/3/3
2	HEM	B	750	1	-	2/14/54/54	-
3	XFJ	B	805	6	-	0/10/10/10	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	6.80	1.51	1.36
2	B	750	HEM	C3D-C2D	6.11	1.50	1.36
2	A	750	HEM	FE-NC	4.65	2.10	1.95
2	A	750	HEM	FE-NB	4.40	2.08	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	FE-NA	3.96	2.08	1.95
2	B	750	HEM	FE-NA	3.84	2.07	1.95
2	A	750	HEM	FE-ND	3.60	2.06	1.94
2	B	750	HEM	FE-NC	3.56	2.06	1.95
2	B	750	HEM	FE-NB	3.29	2.05	1.94
2	B	750	HEM	CAB-C3B	3.20	1.55	1.47
2	B	750	HEM	CAC-C3C	3.13	1.55	1.47
2	A	750	HEM	CAC-C3C	3.03	1.55	1.47
2	A	750	HEM	CMD-C2D	2.93	1.56	1.50
2	A	750	HEM	CAB-C3B	2.93	1.55	1.47
2	B	750	HEM	FE-ND	2.86	2.03	1.94
2	A	750	HEM	CMC-C2C	2.67	1.56	1.50
2	B	750	HEM	CMC-C2C	2.32	1.55	1.50
2	B	750	HEM	CMD-C2D	2.31	1.55	1.50
2	A	750	HEM	CMA-C3A	2.20	1.55	1.50
2	B	750	HEM	CMB-C2B	2.15	1.55	1.50
2	A	750	HEM	CMB-C2B	2.03	1.54	1.50

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	800	XFJ	C02-N01-C06	6.09	122.62	118.07
3	A	800	XFJ	C22-N21-C26	6.08	122.62	118.07
3	A	800	XFJ	C02-N01-C06	5.87	122.46	118.07
3	B	800	XFJ	C22-N21-C26	4.89	121.73	118.07
2	A	750	HEM	C4D-ND-C1D	4.65	110.71	105.21
3	A	805	XFJ	C02-N01-C06	4.16	121.18	118.07
3	A	805	XFJ	C22-N21-C26	4.15	121.17	118.07
2	B	750	HEM	C4D-ND-C1D	3.77	109.67	105.21
2	A	750	HEM	CBD-CAD-C3D	-3.72	102.24	112.53
3	B	805	XFJ	C22-N21-C26	3.68	120.82	118.07
3	B	800	XFJ	C14-C15-C16	3.40	120.05	116.90
3	A	800	XFJ	C05-C06-N01	-3.39	118.87	122.73
3	A	805	XFJ	C08-C06-N01	3.29	121.04	116.06
2	B	750	HEM	CBD-CAD-C3D	-3.27	103.50	112.53
3	B	805	XFJ	C08-C06-N01	3.14	120.81	116.06
3	B	800	XFJ	C05-C06-N01	-3.09	119.21	122.73
2	B	750	HEM	C3B-C2B-C1B	3.04	108.69	106.41
2	B	750	HEM	C3B-C4B-NB	-2.97	107.33	109.47
3	A	800	XFJ	C14-C13-C12	2.97	119.65	116.90
3	B	805	XFJ	C08-C06-C05	-2.91	117.44	121.65
3	A	800	XFJ	C14-C15-C16	2.89	119.58	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	805	XFJ	C14-C13-C12	2.87	119.56	116.90
3	A	800	XFJ	C15-C14-C13	-2.71	117.83	121.20
3	A	805	XFJ	C08-C06-C05	-2.71	117.73	121.65
2	A	750	HEM	C3B-C2B-C1B	2.70	108.44	106.41
3	B	805	XFJ	C14-C15-C16	2.56	119.28	116.90
2	B	750	HEM	CAD-C3D-C4D	2.56	129.16	124.70
3	B	800	XFJ	C15-C14-C13	-2.52	118.07	121.20
3	B	805	XFJ	N02-C02-N01	2.49	120.59	116.59
3	B	805	XFJ	C02-N01-C06	2.45	119.90	118.07
3	B	800	XFJ	C25-C26-N21	-2.44	119.95	122.73
3	A	805	XFJ	C25-C26-N21	-2.43	119.96	122.73
3	B	805	XFJ	C18-C26-N21	2.42	119.73	116.06
3	A	800	XFJ	C18-C26-N21	2.36	119.64	116.06
3	B	800	XFJ	C08-C06-N01	2.31	119.56	116.06
3	B	800	XFJ	C09-C08-C06	-2.29	107.91	113.01
3	A	805	XFJ	C16-N11-C12	2.28	120.60	117.51
2	B	750	HEM	C1B-NB-C4B	2.24	107.86	105.21
3	A	805	XFJ	C14-C15-C16	2.21	118.95	116.90
3	A	800	XFJ	C25-C26-N21	-2.20	120.23	122.73
2	A	750	HEM	CHC-C1C-NC	2.19	126.84	124.45
3	B	800	XFJ	C16-N11-C12	2.19	120.48	117.51
2	A	750	HEM	CAD-C3D-C4D	2.16	128.47	124.70
3	A	800	XFJ	N22-C22-N21	2.13	120.01	116.59
3	B	800	XFJ	C14-C13-C12	2.09	118.83	116.90
3	A	800	XFJ	C08-C06-N01	2.08	119.21	116.06
3	A	805	XFJ	N22-C22-N21	2.07	119.92	116.59
2	B	750	HEM	CHA-C4D-ND	2.07	126.92	124.37
3	B	800	XFJ	C09-C13-C12	-2.05	118.08	121.73
3	A	805	XFJ	C14-C13-C12	2.05	118.80	116.90
3	B	805	XFJ	C15-C14-C13	-2.04	118.66	121.20
3	A	805	XFJ	C18-C26-N21	2.03	119.13	116.06
2	A	750	HEM	CHA-C4D-ND	2.03	126.87	124.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

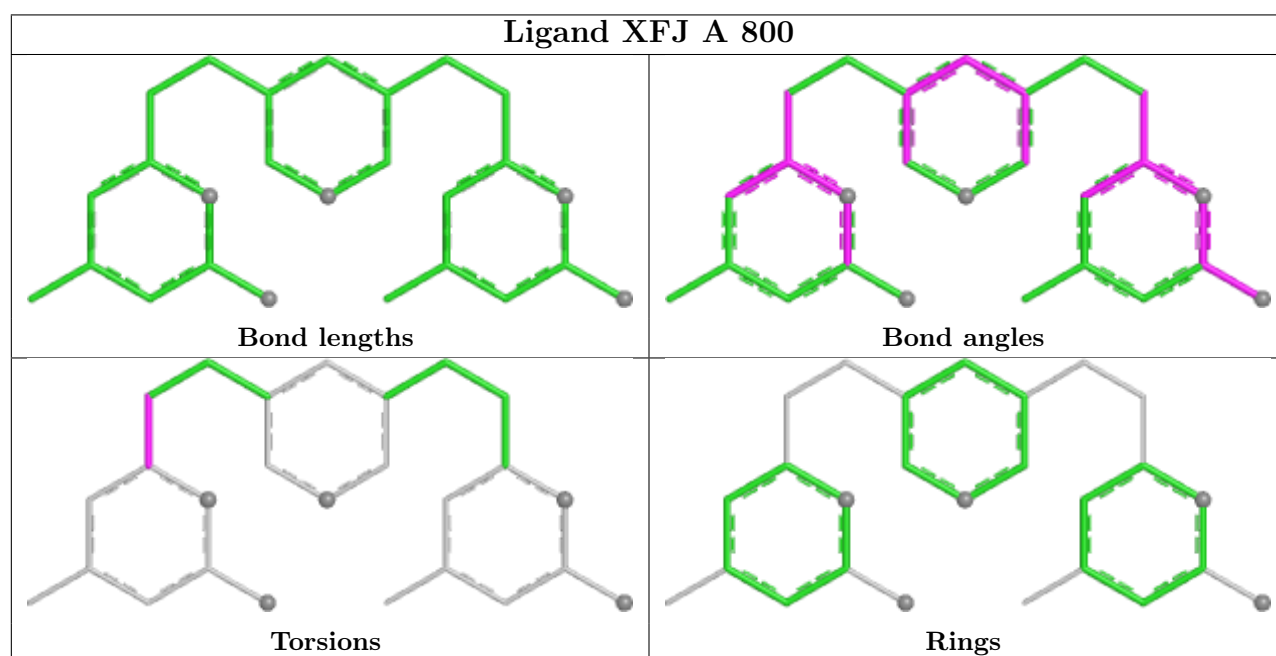
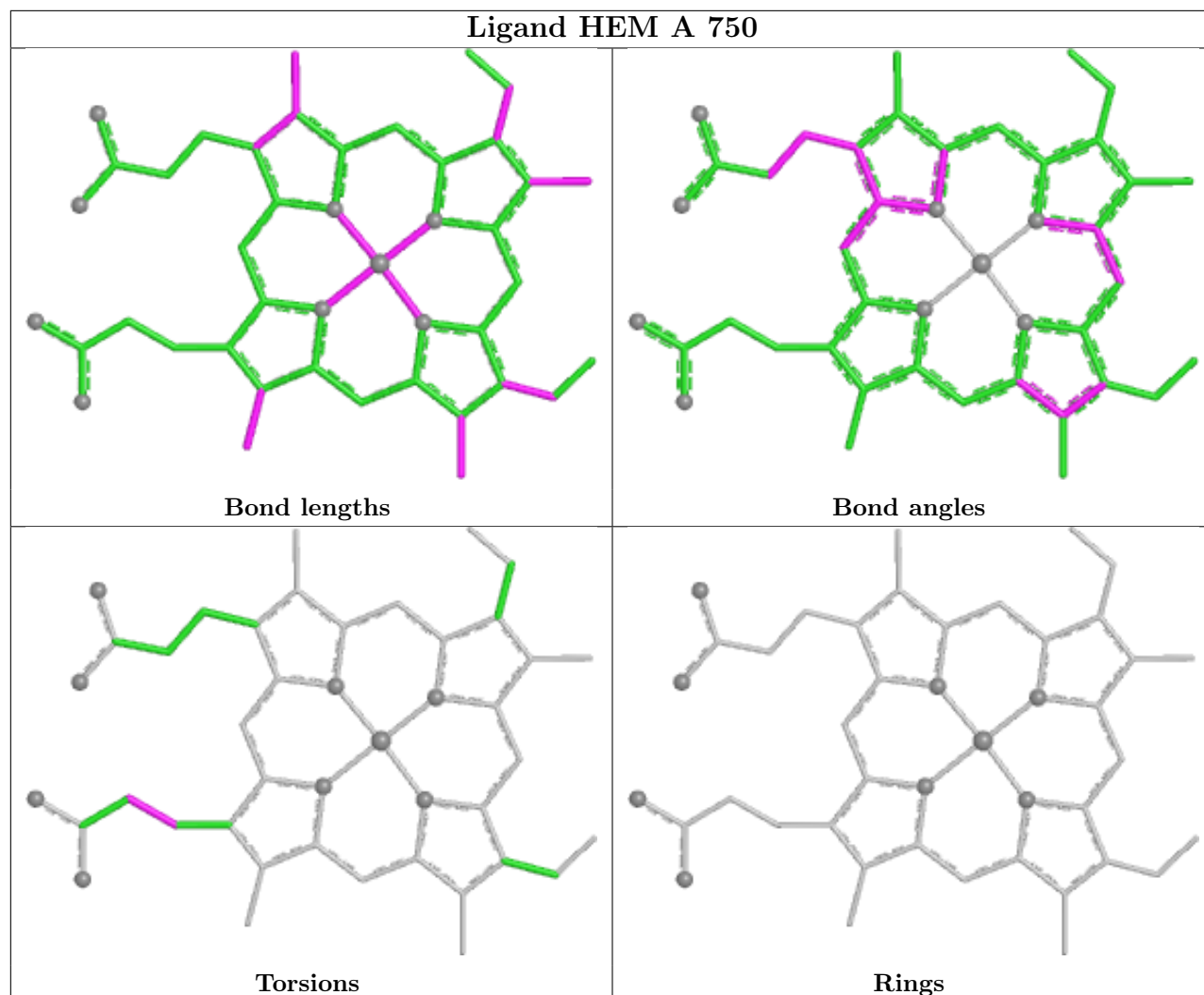
Mol	Chain	Res	Type	Atoms
2	A	750	HEM	C2A-CAA-CBA-CGA
2	B	750	HEM	C2A-CAA-CBA-CGA
2	B	750	HEM	C4B-C3B-CAB-CBB
3	A	800	XFJ	C05-C06-C08-C09
3	A	800	XFJ	N01-C06-C08-C09

There are no ring outliers.

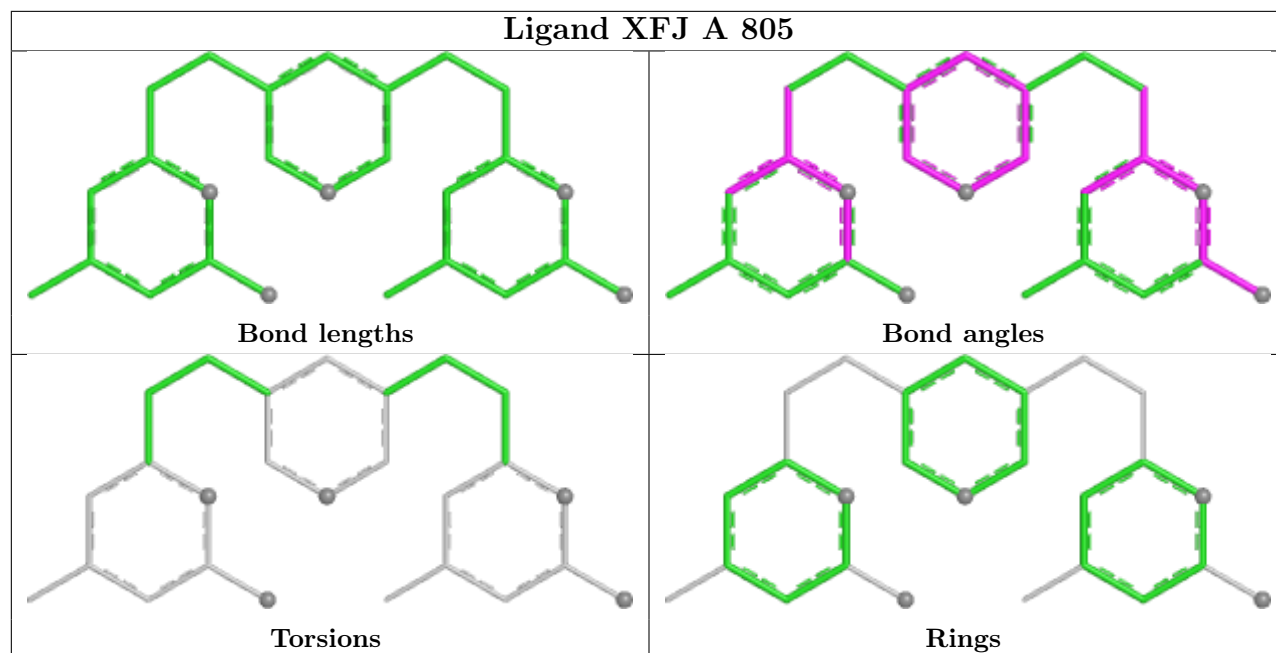
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	1	0
2	B	750	HEM	1	0

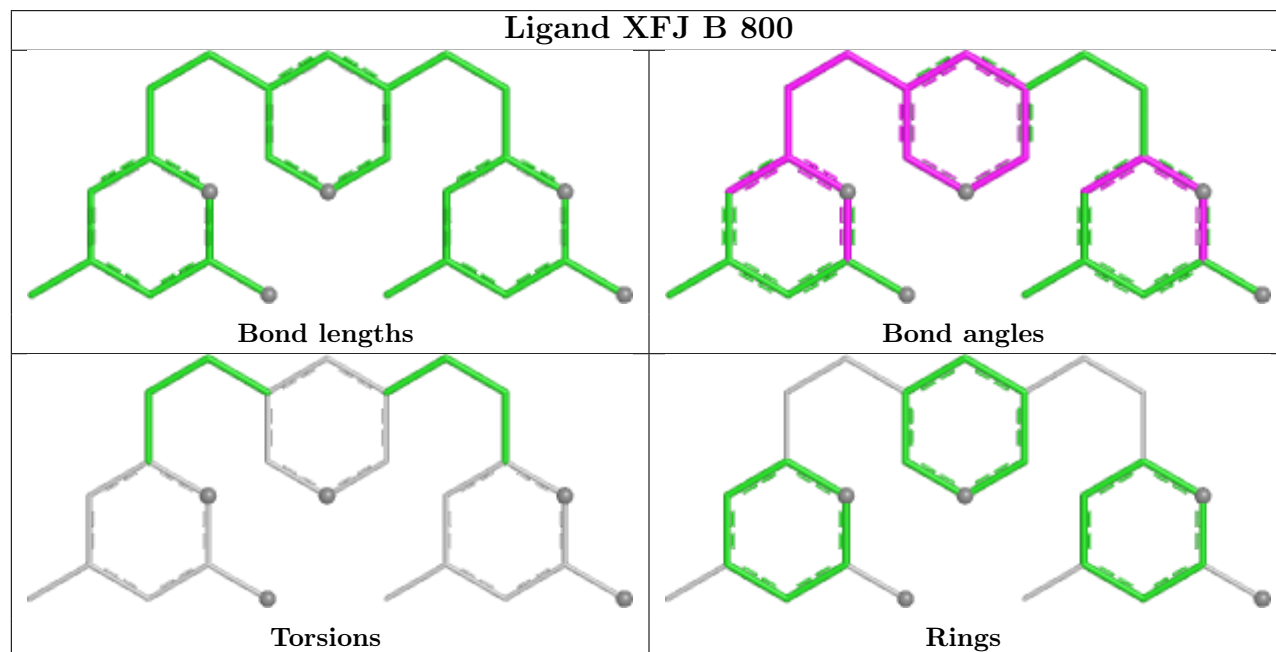
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

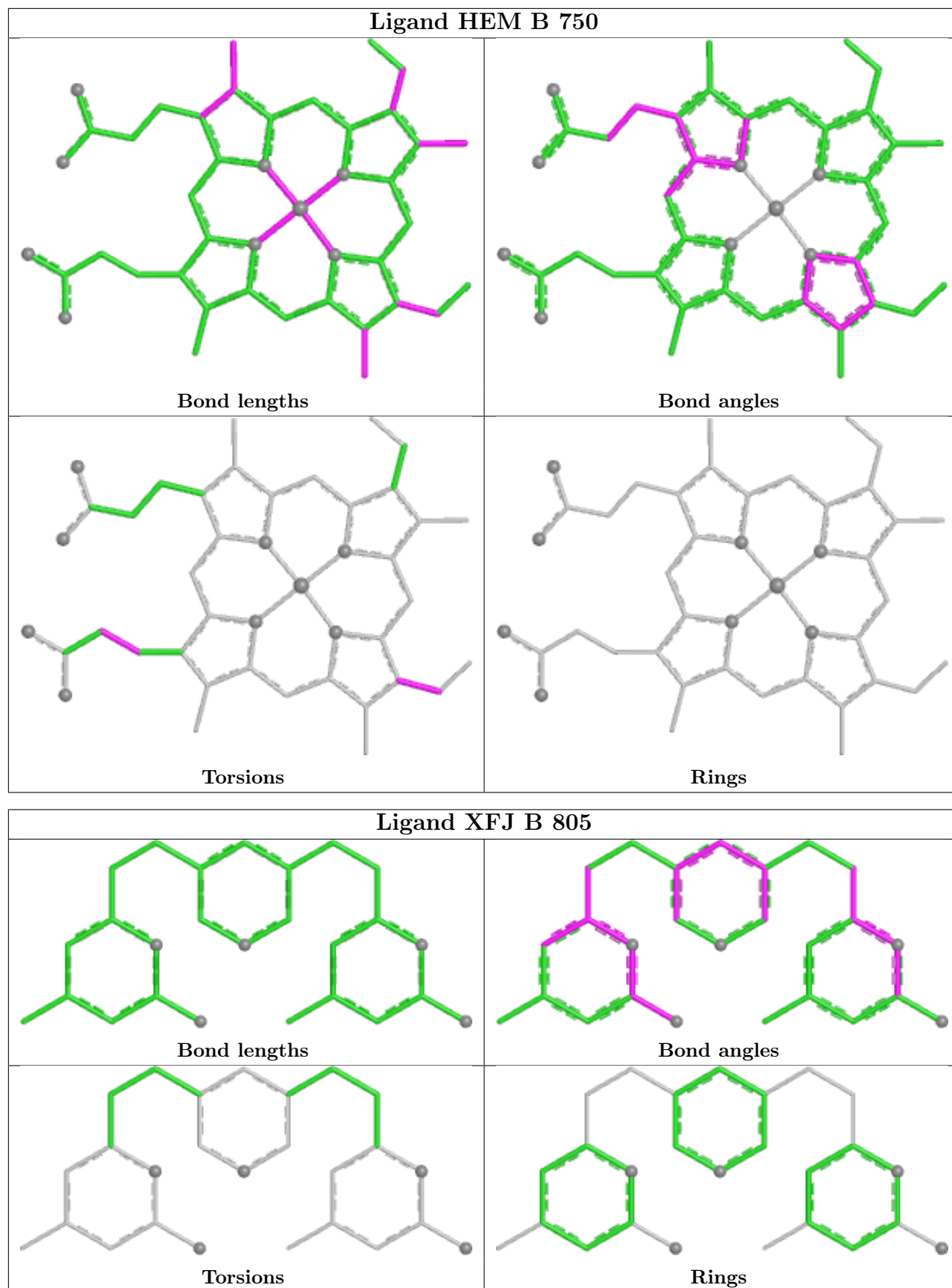


Ligand XFJ A 805



Ligand XFJ B 800





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	407/422 (96%)	0.58	30 (7%) 20 26	18, 35, 62, 78	1 (0%)
1	B	411/422 (97%)	0.21	18 (4%) 39 48	14, 28, 49, 68	2 (0%)
All	All	818/844 (96%)	0.39	48 (5%) 28 34	14, 31, 58, 78	3 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	322	LEU	5.6
1	A	322	LEU	5.4
1	B	321	THR	5.1
1	B	348	VAL	4.9
1	A	338	PRO	4.7
1	A	715	VAL	4.5
1	A	350	THR	4.2
1	B	350	THR	4.2
1	B	338	PRO	3.9
1	B	352	ASP	3.7
1	A	716	TRP	3.6
1	A	321	THR	3.5
1	A	300	PHE	3.4
1	A	488	PRO	3.3
1	A	712	ASN	3.3
1	A	490	GLY	3.2
1	A	713	THR	3.2
1	A	355	PHE	3.1
1	B	320	SER	3.1
1	A	299	ARG	3.0
1	A	373	GLY	2.9
1	B	300	PHE	2.8
1	B	389	GLU	2.7
1	B	715	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	718	GLY	2.7
1	A	505	CYS	2.7
1	A	533	LEU	2.6
1	A	382	GLU	2.6
1	A	491	SER	2.5
1	A	517	PHE	2.5
1	A	711	TRP	2.5
1	A	710	PRO	2.5
1	B	668	CYS	2.4
1	A	392	SER	2.4
1	A	330	ILE	2.4
1	A	714	HIS	2.3
1	A	352	ASP	2.3
1	B	620	LYS	2.2
1	A	506	ILE	2.2
1	B	713	THR	2.2
1	A	360	GLU	2.1
1	B	667	ARG	2.1
1	A	556	ASP	2.1
1	B	716	TRP	2.1
1	A	538	PRO	2.1
1	B	355	PHE	2.1
1	B	556	ASP	2.0
1	A	612	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

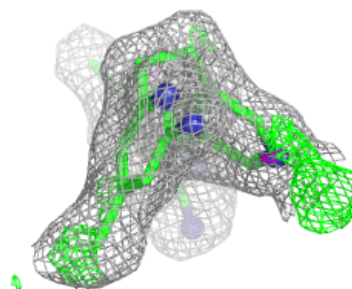
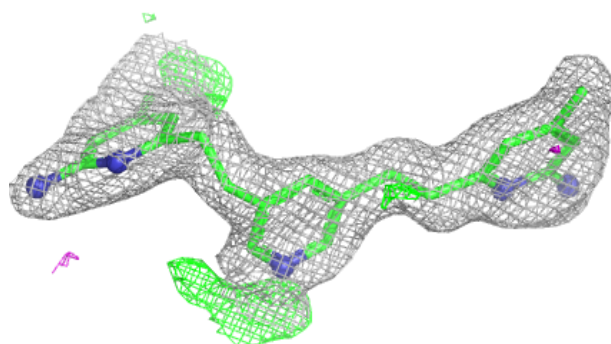
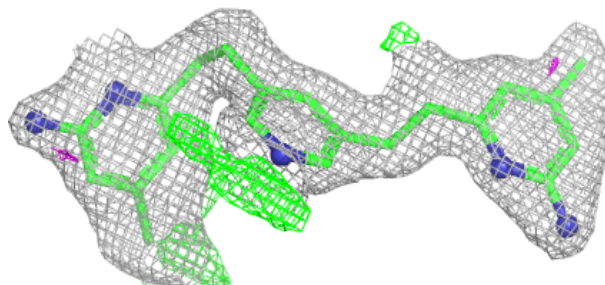
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	XFJ	B	805	26/26	0.91	0.09	25,29,37,39	0
4	ACT	A	860	4/4	0.91	0.11	40,41,42,43	0
3	XFJ	A	805	26/26	0.93	0.08	26,29,43,44	0
4	ACT	B	860	4/4	0.93	0.08	29,32,33,34	0
3	XFJ	B	800	26/26	0.96	0.06	17,23,26,29	0
3	XFJ	A	800	26/26	0.96	0.06	21,25,28,31	0
2	HEM	A	750	43/43	0.98	0.07	18,20,29,33	0
2	HEM	B	750	43/43	0.98	0.06	16,18,24,29	0
5	CL	A	910	1/1	0.98	0.06	27,27,27,27	0
5	CL	B	910	1/1	0.98	0.05	25,25,25,25	0
6	ZN	A	901	1/1	0.98	0.04	22,22,22,22	1
6	ZN	A	900	1/1	0.99	0.03	26,26,26,26	0
6	ZN	A	719	1/1	0.99	0.05	19,19,19,19	1

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.

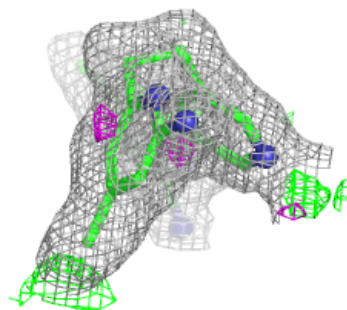
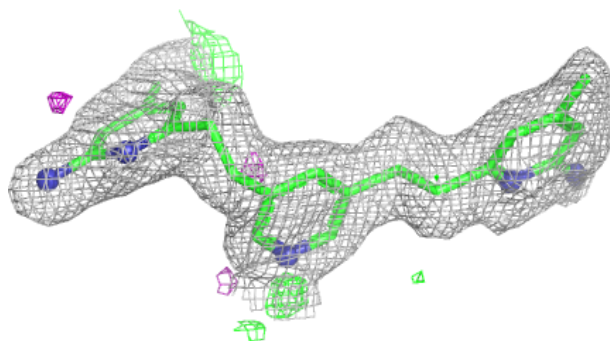
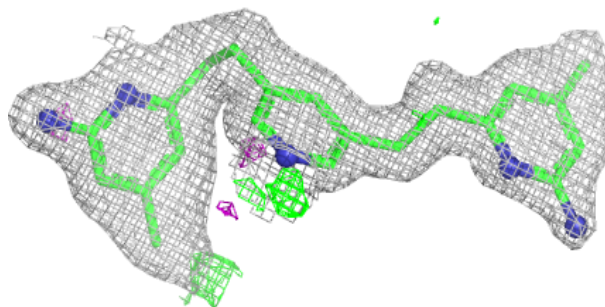
Electron density around XFJ B 805:

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

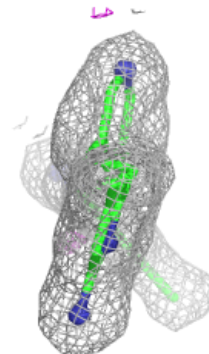
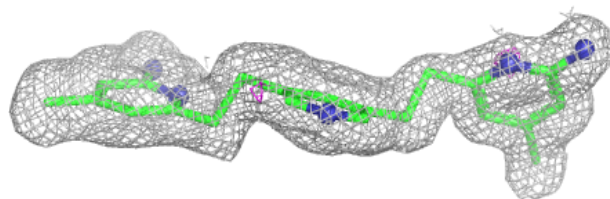
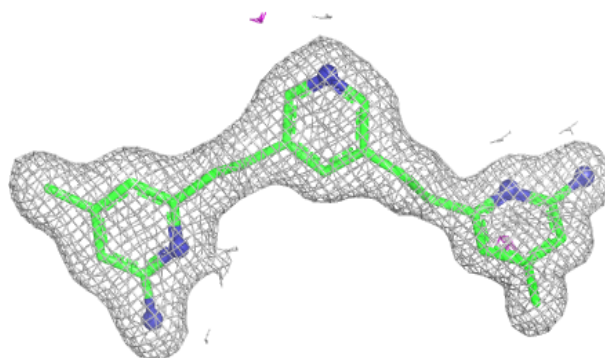


Electron density around XFJ A 805:

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

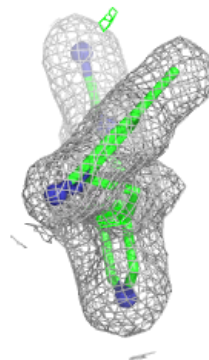
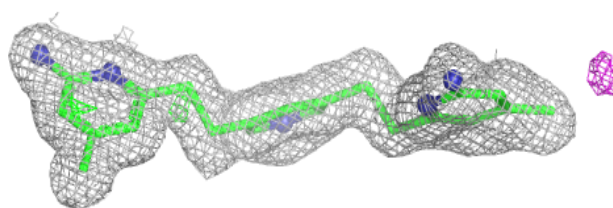
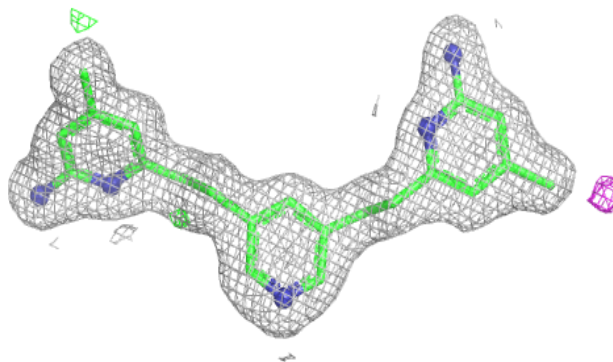
**Electron density around XFJ B 800:**

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



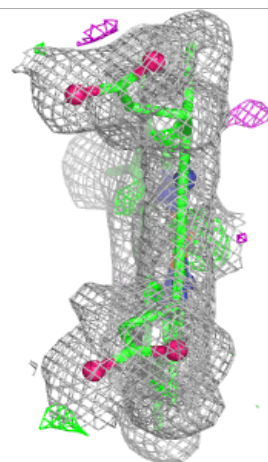
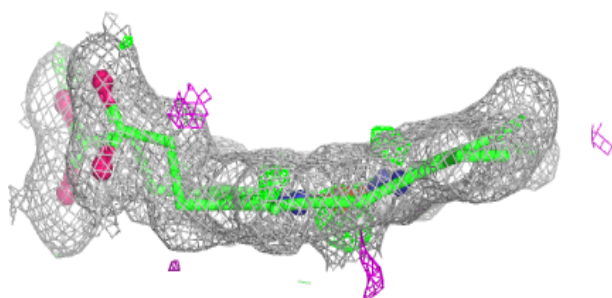
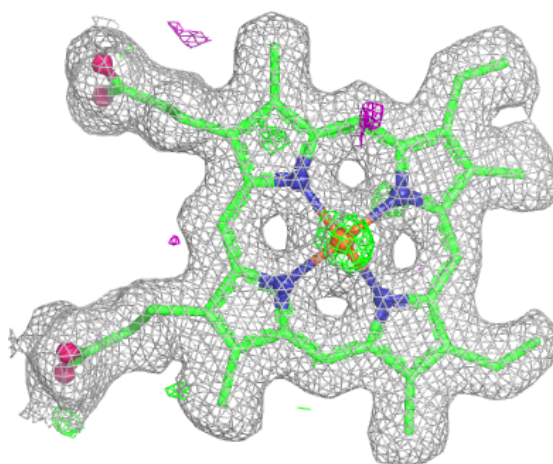
Electron density around XFJ A 800:

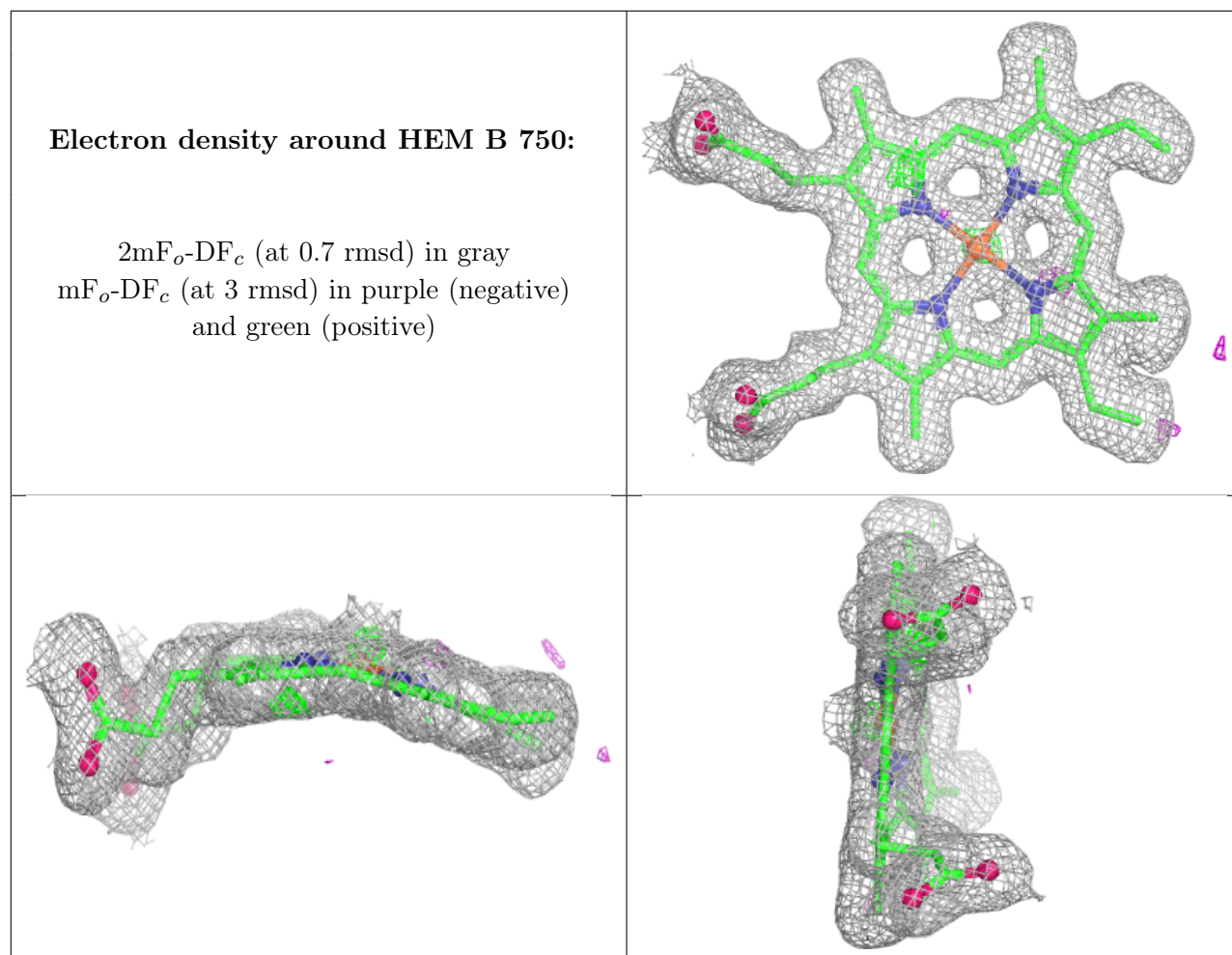
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 750:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.