



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:51 am BST

PDB ID : 3N61  
Title : Structure of neuronal nitric oxide synthase D597N/M336V mutant 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 : 1.95 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

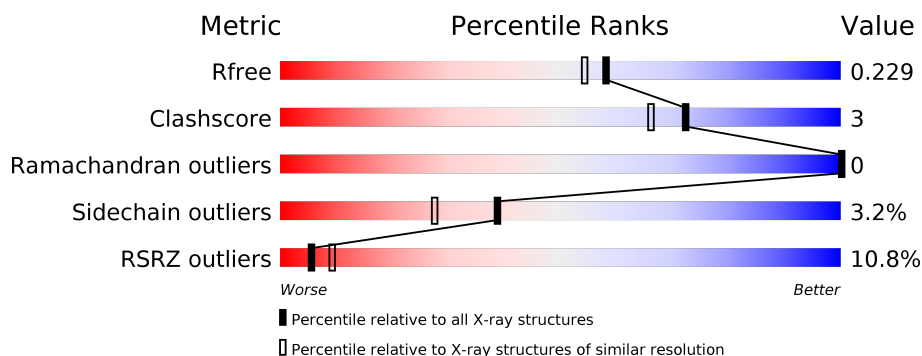
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>14%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	422	<div> <div>7%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>

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
7	CL	A	911	-	-	X	-
7	CL	B	911	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7293 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.

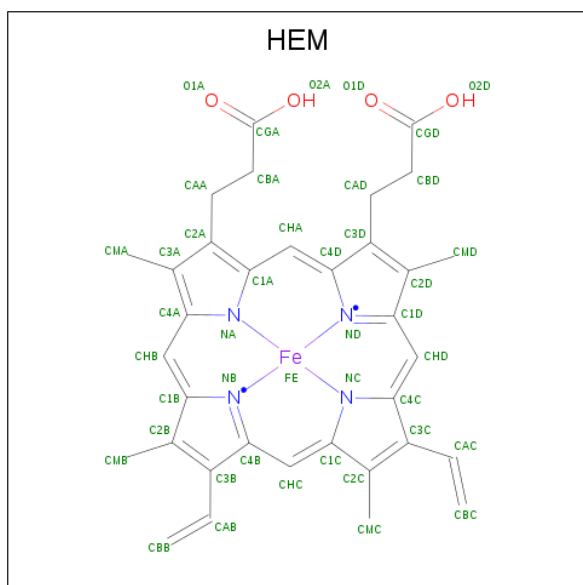
- Molecule 1 is a protein called Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	4	0
			3336	2138	568	609	21			
1	B	411	Total	C	N	O	S	0	3	0
			3362	2154	575	612	21			

There are 4 discrepancies between the modelled and reference sequences:

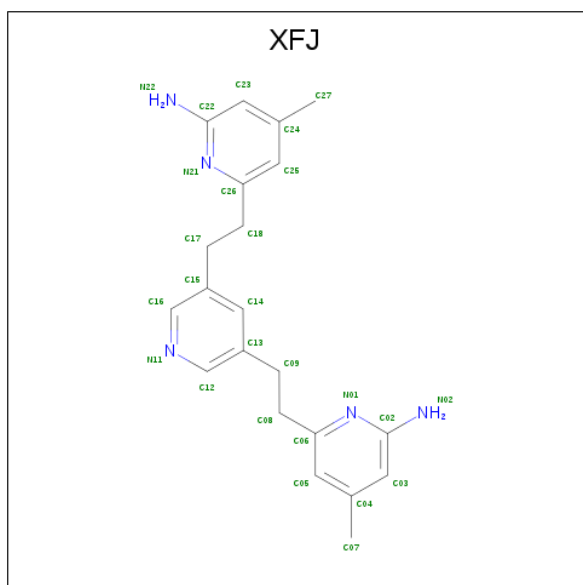
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	ENGINEERED MUTATION	UNP P29476
A	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476
B	336	VAL	MET	ENGINEERED MUTATION	UNP P29476
B	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476

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



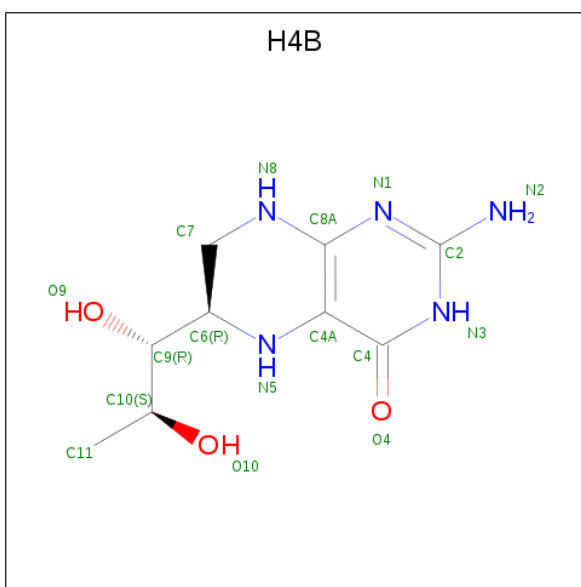
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			48	37	1	4	6	1
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 3 is 6,6'-(pyridine-3,5-diyl)diethane-2,1-diyl)bis(4-methylpyridin-2-amine) (three-letter code: XFJ) (formula: C<sub>21</sub>H<sub>25</sub>N<sub>5</sub>).



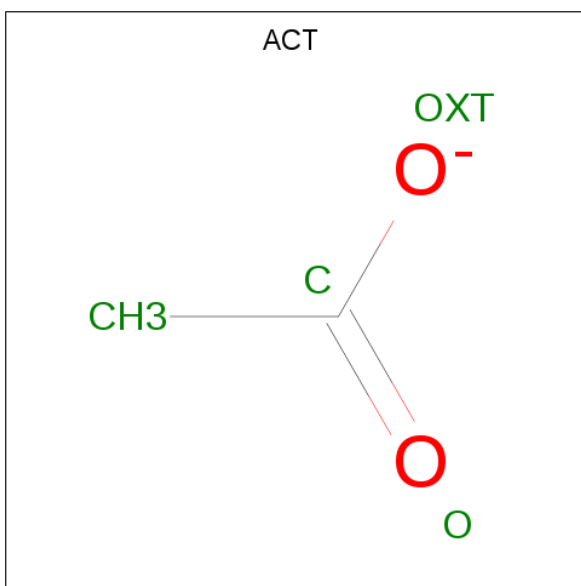
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N		
			26	21	5	0	0
3	B	1	Total	C	N		
			26	21	5	0	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>).



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Zn 1	0	0
6	A	2	Total 2	Zn 2	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total 2	Cl 2	0	0
7	A	2	Total 2	Cl 2	0	0

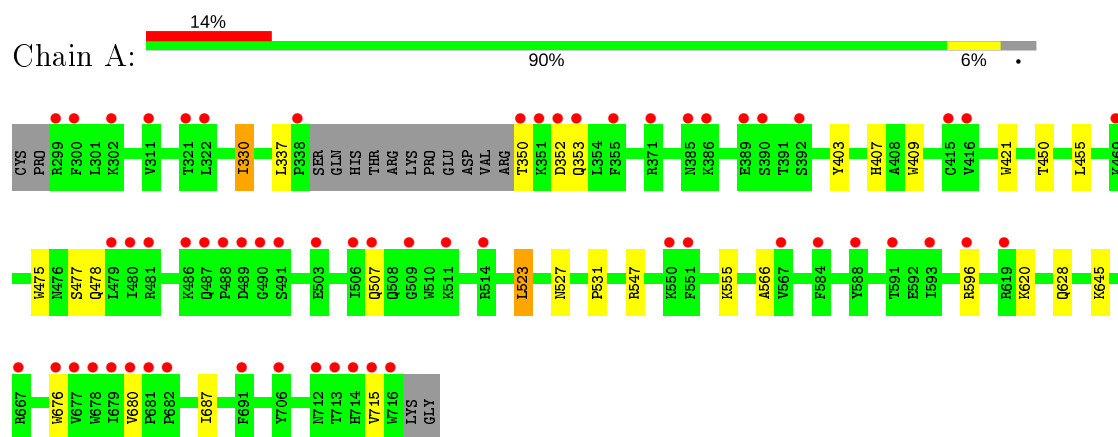
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	174	Total 174	O 174	0	0
8	B	229	Total 229	O 229	0	0

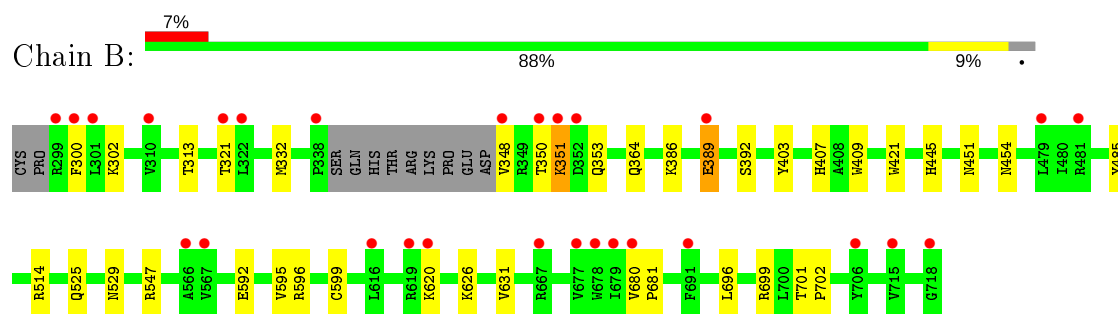
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	51.84Å 110.50Å 164.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.49 – 1.95 37.80 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.49-1.95) 99.7 (37.80-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, $R_{free}$	0.179 , 0.213 0.195 , 0.229	Depositor DCC
$R_{free}$ test set	3424 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, XFJ, H4B, CL, ACT, HEM

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	0.60	0/3439	0.64	0/4667
1	B	0.65	0/3465	0.64	0/4699
All	All	0.63	0/6904	0.64	0/9366

There are no bond length outliers.

There are no bond angle outliers.

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	3336	0	3247	15	0
1	B	3362	0	3281	19	0
2	A	48	0	8	4	0
2	B	43	0	30	7	0
3	A	26	0	25	1	0
3	B	26	0	25	3	0
4	A	17	0	15	2	0
4	B	17	0	15	0	0
5	A	4	0	3	0	0
5	B	4	0	3	1	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	2	0	0	2	0
7	B	2	0	0	3	0
8	A	174	0	0	1	0
8	B	229	0	0	3	0
All	All	7293	0	6652	43	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 3.

All (43) 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)
7:B:911:CL:CL	8:B:1231:HOH:O	2.34	0.81
2:B:750:HEM:HBB2	2:B:750:HEM:HHC	1.63	0.81
2:B:750:HEM:HBA1	3:B:800:XFJ:H08A	1.66	0.78
7:A:911:CL:CL	8:A:1087:HOH:O	2.41	0.74
1:A:596:ARG:NH1	2:A:750[B]:HEM:O2A	2.27	0.67
7:B:910:CL:CL	8:B:1231:HOH:O	2.49	0.67
2:A:750[A]:HEM:O1A	4:A:760:H4B:N3	2.27	0.62
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.85	0.59
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.83	0.59
2:A:750[B]:HEM:CGA	4:A:760:H4B:HN22	2.18	0.55
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.90	0.54
1:B:596:ARG:HB2	7:B:911:CL:CL	2.45	0.53
2:B:750:HEM:HMB3	5:B:860:ACT:H2	1.90	0.53
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.47	0.49
2:B:750:HEM:HBA1	3:B:800:XFJ:C08	2.41	0.49
1:A:337:LEU:HD21	3:A:800:XFJ:H23	1.94	0.48
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.01	0.48
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.47	0.48
1:B:592:GLU:HB3	1:B:596:ARG:NH2	2.30	0.47
1:B:386:LYS:HA	1:B:389:GLU:HG2	1.97	0.47
1:B:300:PHE:HB3	1:B:313:THR:CG2	2.48	0.45
1:B:525:GLN:HG3	1:B:529:ASN:O	2.17	0.44
1:B:364:GLN:NE2	8:B:1369:HOH:O	2.49	0.44
1:A:478:GLN:HA	1:A:566:ALA:O	2.17	0.43
1:A:450:THR:HA	1:A:455:LEU:HD22	2.00	0.42
1:B:348:VAL:HG13	1:B:348:VAL:O	2.18	0.42
1:B:351:LYS:HB3	1:B:351:LYS:HE2	1.80	0.42
1:B:445:HIS:C	1:B:445:HIS:CD2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ASN:HB3	1:B:454:ASN:O	2.20	0.42
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.49	0.42
2:B:750:HEM:CBB	2:B:750:HEM:HHC	2.42	0.42
1:B:595:VAL:O	1:B:599:CYS:HB2	2.20	0.41
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.55	0.41
1:A:596:ARG:HH12	2:A:750[B]:HEM:CGA	2.33	0.41
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.41
2:B:750:HEM:C1C	3:B:800:XFJ:H07B	2.55	0.41
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.56	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.90	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.41
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.02	0.41
1:A:687:ILE:HD12	1:B:626:LYS:HB3	2.03	0.41
1:A:596:ARG:HB2	7:A:911:CL:CL	2.58	0.40
1:A:527:ASN:HD22	1:A:527:ASN:HA	1.74	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	407/422 (96%)	395 (97%)	12 (3%)	0	100	100
1	B	410/422 (97%)	403 (98%)	7 (2%)	0	100	100
All	All	817/844 (97%)	798 (98%)	19 (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	367/377 (97%)	355 (97%)	12 (3%)	38	26
1	B	369/377 (98%)	358 (97%)	11 (3%)	41	30
All	All	736/754 (98%)	713 (97%)	23 (3%)	39	28

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	ILE
1	A	350	THR
1	A	352	ASP
1	A	353	GLN
1	A	477	SER
1	A	507	GLN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	302	LYS
1	B	321	THR
1	B	332	MET
1	B	350	THR
1	B	351	LYS
1	B	353	GLN
1	B	389	GLU
1	B	392	SER
1	B	547	ARG
1	B	620	LYS
1	B	699	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	487	GLN
1	A	527	ASN

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Mol	Chain	Res	Type
1	A	601	ASN
1	A	605	ASN
1	A	628	GLN
1	A	642	GLN
1	A	692	HIS
1	A	697	ASN
1	B	364	GLN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	601	ASN
1	B	605	ASN
1	B	697	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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[B]	-	27,50,50	2.02	6 (22%)	17,82,82	2.63	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ACT	A	860	-	1,3,3	1.58	0	0,3,3	0.00	-
4	H4B	A	760	-	16,18,18	0.89	0	11,26,26	2.92	8 (72%)
2	HEM	B	750	1	27,50,50	2.05	8 (29%)	17,82,82	2.28	6 (35%)
4	H4B	B	760	-	16,18,18	1.00	0	11,26,26	2.68	5 (45%)
5	ACT	B	860	-	1,3,3	1.91	0	0,3,3	0.00	-
3	XFJ	A	800	-	28,28,28	0.62	0	38,38,38	1.99	13 (34%)
3	XFJ	B	800	-	28,28,28	0.69	0	38,38,38	2.16	15 (39%)
2	HEM	A	750[A]	-	27,50,50	2.00	6 (22%)	17,82,82	2.76	8 (47%)

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[B]	-	-	1/6/54/54	-
4	H4B	A	760	-	-	0/8/17/17	0/2/2/2
2	HEM	B	750	1	-	1/6/54/54	-
4	H4B	B	760	-	-	2/8/17/17	0/2/2/2
3	XFJ	A	800	-	-	2/10/10/10	0/3/3/3
3	XFJ	B	800	-	-	0/10/10/10	0/3/3/3
2	HEM	A	750[A]	-	-	0/6/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750[B]	HEM	C3D-C2D	4.89	1.52	1.37
2	A	750[A]	HEM	C3D-C2D	4.89	1.52	1.37
2	B	750	HEM	C3C-C2C	-4.62	1.34	1.40
2	B	750	HEM	C3D-C2D	4.49	1.51	1.37
2	B	750	HEM	C3B-C2B	-3.86	1.35	1.40
2	A	750[B]	HEM	C3B-CAB	3.79	1.55	1.47
2	A	750[A]	HEM	C3B-CAB	3.79	1.55	1.47
2	A	750[B]	HEM	C3B-C2B	-3.73	1.35	1.40
2	A	750[A]	HEM	C3B-C2B	-3.73	1.35	1.40
2	B	750	HEM	C3C-CAC	3.29	1.54	1.47
2	B	750	HEM	C3B-CAB	3.04	1.54	1.47
2	A	750[B]	HEM	C3C-C2C	-3.02	1.36	1.40
2	A	750[A]	HEM	C3C-C2C	-3.02	1.36	1.40
2	A	750[B]	HEM	C3C-CAC	2.91	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750[A]	HEM	C3C-CAC	2.91	1.53	1.47
2	A	750[B]	HEM	CAA-C2A	2.70	1.56	1.52
2	A	750[A]	HEM	CAA-C2A	2.18	1.55	1.52
2	B	750	HEM	CMD-C2D	2.09	1.56	1.51
2	B	750	HEM	CAD-C3D	2.09	1.55	1.52
2	B	750	HEM	CMB-C2B	2.08	1.56	1.51

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750[B]	HEM	CBD-CAD-C3D	-6.77	100.00	112.48
2	A	750[A]	HEM	CBD-CAD-C3D	-6.77	100.00	112.48
2	B	750	HEM	CBD-CAD-C3D	-5.28	102.75	112.48
3	A	800	XFJ	C22-N21-C26	5.13	121.99	118.10
3	B	800	XFJ	C22-N21-C26	4.94	121.84	118.10
3	B	800	XFJ	C02-N01-C06	4.76	121.70	118.10
3	B	800	XFJ	C14-C15-C16	4.68	121.22	116.71
2	A	750[A]	HEM	CBA-CAA-C2A	-4.56	104.07	112.49
2	B	750	HEM	CBA-CAA-C2A	-4.50	104.19	112.49
4	B	760	H4B	C4-C4A-C8A	4.42	118.50	114.57
4	A	760	H4B	C4-N3-C2	4.37	122.88	115.93
4	A	760	H4B	C4-C4A-C8A	4.34	118.43	114.57
3	B	800	XFJ	C05-C06-N01	-4.26	118.39	122.90
3	A	800	XFJ	C02-N01-C06	4.04	121.16	118.10
4	A	760	H4B	N3-C2-N1	-3.98	119.17	125.42
4	B	760	H4B	C4-N3-C2	3.92	122.15	115.93
3	A	800	XFJ	C14-C15-C16	3.73	120.31	116.71
2	A	750[B]	HEM	CAA-CBA-CGA	-3.72	106.43	112.67
4	A	760	H4B	C4-C4A-N5	3.68	122.21	119.12
2	A	750[B]	HEM	C1D-C2D-C3D	-3.67	104.44	107.00
2	A	750[A]	HEM	C1D-C2D-C3D	-3.67	104.44	107.00
4	B	760	H4B	N3-C2-N1	-3.65	119.69	125.42
3	B	800	XFJ	C08-C06-N01	3.62	121.34	115.95
4	B	760	H4B	C4-C4A-N5	3.58	122.12	119.12
3	A	800	XFJ	C05-C06-N01	-3.42	119.28	122.90
2	A	750[B]	HEM	C4C-C3C-C2C	3.34	109.23	106.90
2	A	750[A]	HEM	C4C-C3C-C2C	3.34	109.23	106.90
3	A	800	XFJ	C15-C14-C13	-3.06	117.46	121.23
2	B	750	HEM	C1D-C2D-C3D	-2.98	104.92	107.00
3	B	800	XFJ	C15-C14-C13	-2.91	117.65	121.23
3	B	800	XFJ	C17-C15-C16	-2.88	117.18	121.83
2	B	750	HEM	CMA-C3A-C4A	-2.88	124.04	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	XFJ	C14-C13-C12	2.81	119.43	116.71
4	A	760	H4B	N2-C2-N3	2.78	121.58	117.25
3	A	800	XFJ	C24-C25-C26	-2.78	118.50	120.32
2	A	750[B]	HEM	CMC-C2C-C3C	2.76	129.84	124.68
2	A	750[A]	HEM	CMC-C2C-C3C	2.76	129.84	124.68
2	A	750[B]	HEM	CMA-C3A-C4A	-2.68	124.34	128.46
2	A	750[A]	HEM	CMA-C3A-C4A	-2.68	124.34	128.46
3	A	800	XFJ	C16-N11-C12	2.68	121.14	117.48
4	A	760	H4B	C2-N1-C8A	2.58	120.32	114.54
3	B	800	XFJ	C16-N11-C12	2.48	120.87	117.48
4	B	760	H4B	C2-N1-C8A	2.44	120.00	114.54
2	B	750	HEM	CMB-C2B-C3B	2.43	129.22	124.68
3	B	800	XFJ	C18-C26-N21	2.40	119.53	115.95
3	B	800	XFJ	C09-C13-C12	-2.39	117.98	121.83
4	A	760	H4B	C4A-N5-C6	-2.38	114.69	121.16
3	B	800	XFJ	C24-C25-C26	-2.32	118.80	120.32
3	A	800	XFJ	C08-C06-N01	2.31	119.40	115.95
3	A	800	XFJ	C18-C26-N21	2.30	119.38	115.95
2	A	750[A]	HEM	CAA-CBA-CGA	-2.24	108.91	112.67
3	A	800	XFJ	C17-C15-C16	-2.21	118.27	121.83
3	B	800	XFJ	C25-C26-N21	-2.10	120.67	122.90
2	B	750	HEM	C3B-C4B-NB	-2.10	106.50	109.21
4	A	760	H4B	C4A-C4-N3	-2.09	118.07	124.01
3	A	800	XFJ	N22-C22-N21	2.09	119.80	116.49
3	B	800	XFJ	C09-C13-C14	2.07	123.94	120.54
3	A	800	XFJ	C17-C18-C26	-2.06	108.36	112.99
3	B	800	XFJ	C15-C16-N11	-2.06	119.70	123.72
2	A	750[B]	HEM	C3C-C4C-NC	-2.05	107.06	110.94
2	A	750[A]	HEM	C3C-C4C-NC	-2.05	107.06	110.94
3	B	800	XFJ	N22-C22-N21	2.00	119.65	116.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

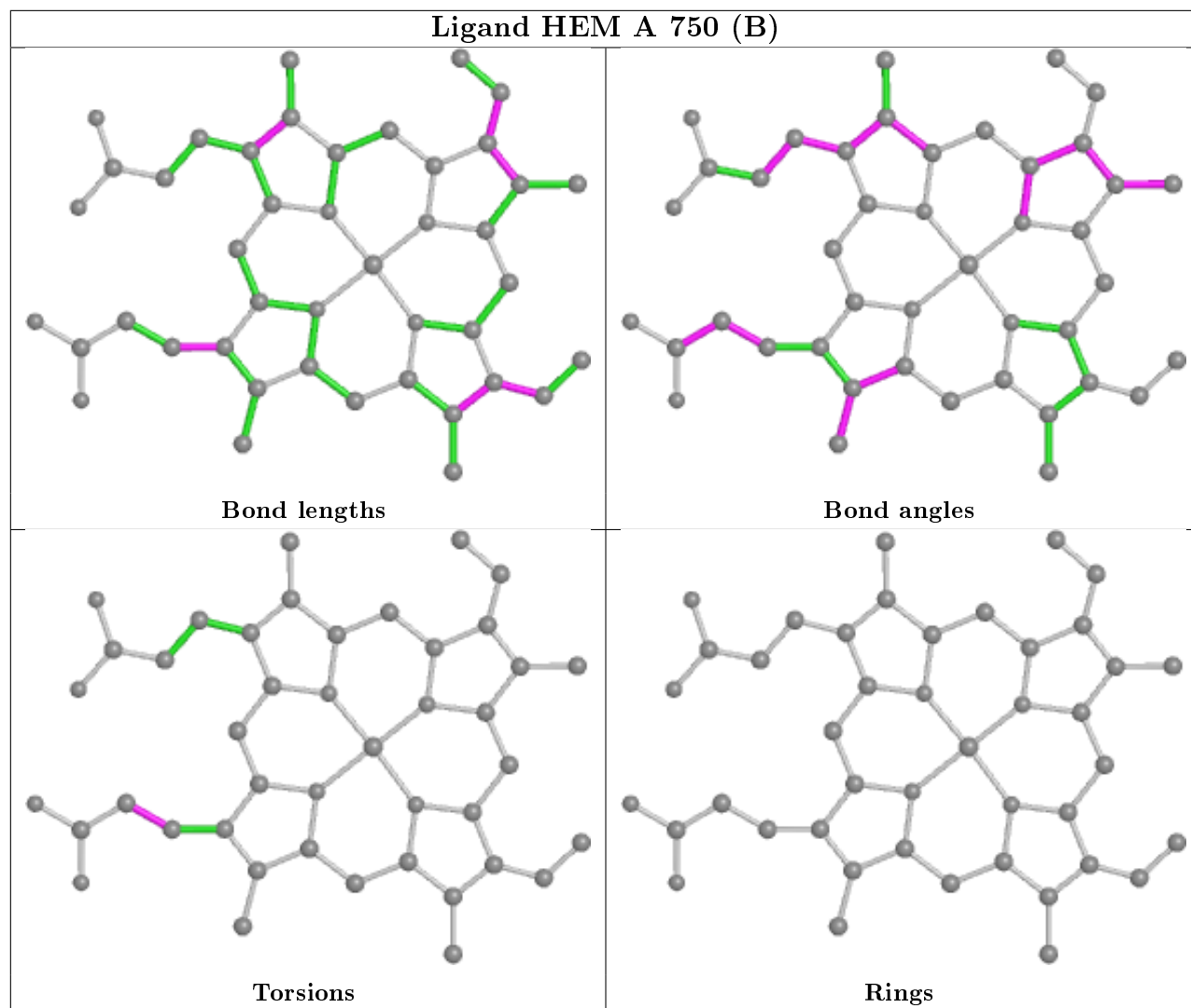
Mol	Chain	Res	Type	Atoms
2	A	750[B]	HEM	C2A-CAA-CBA-CGA
3	A	800	XFJ	C05-C06-C08-C09
2	B	750	HEM	C2A-CAA-CBA-CGA
3	A	800	XFJ	N01-C06-C08-C09
4	B	760	H4B	C7-C6-C9-C10
4	B	760	H4B	N5-C6-C9-O9

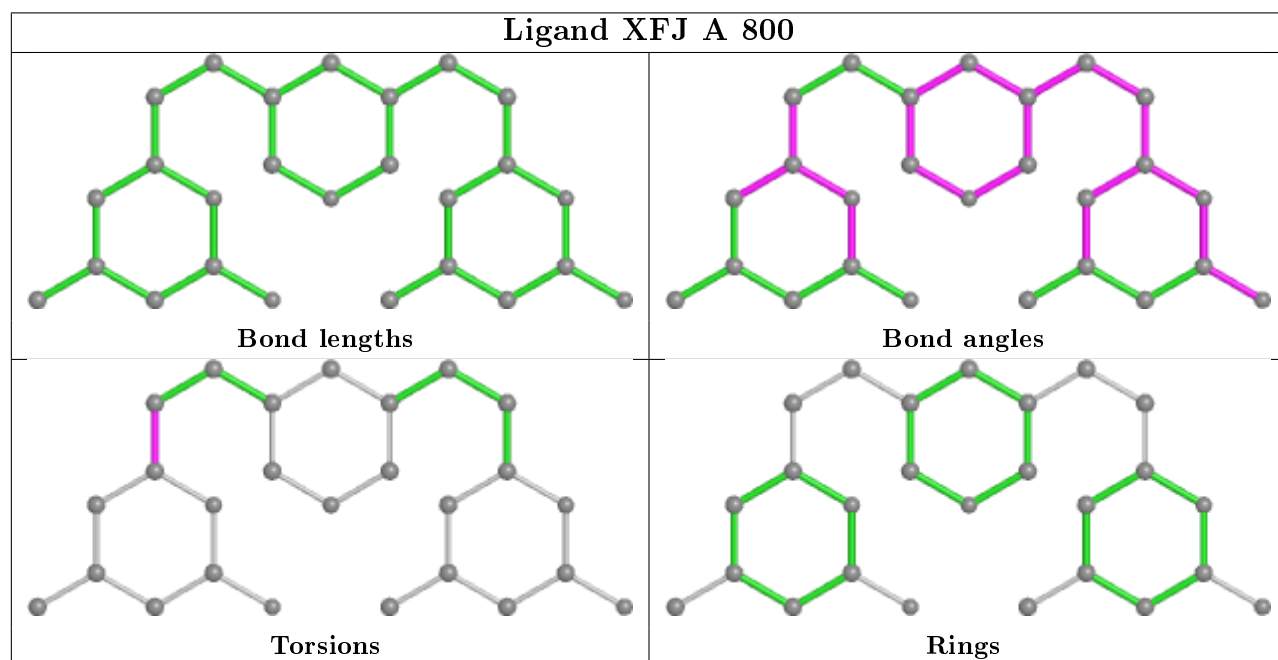
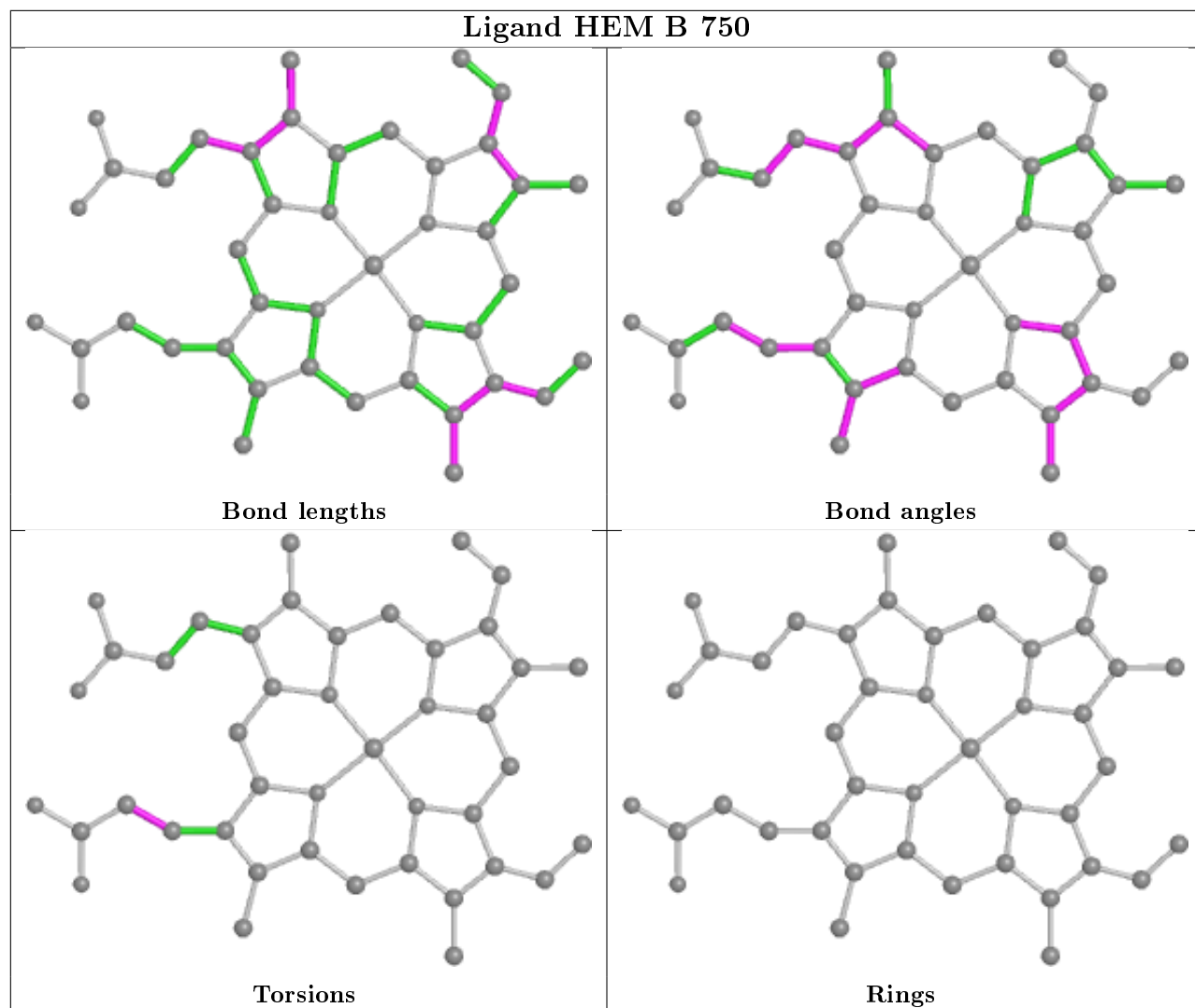
There are no ring outliers.

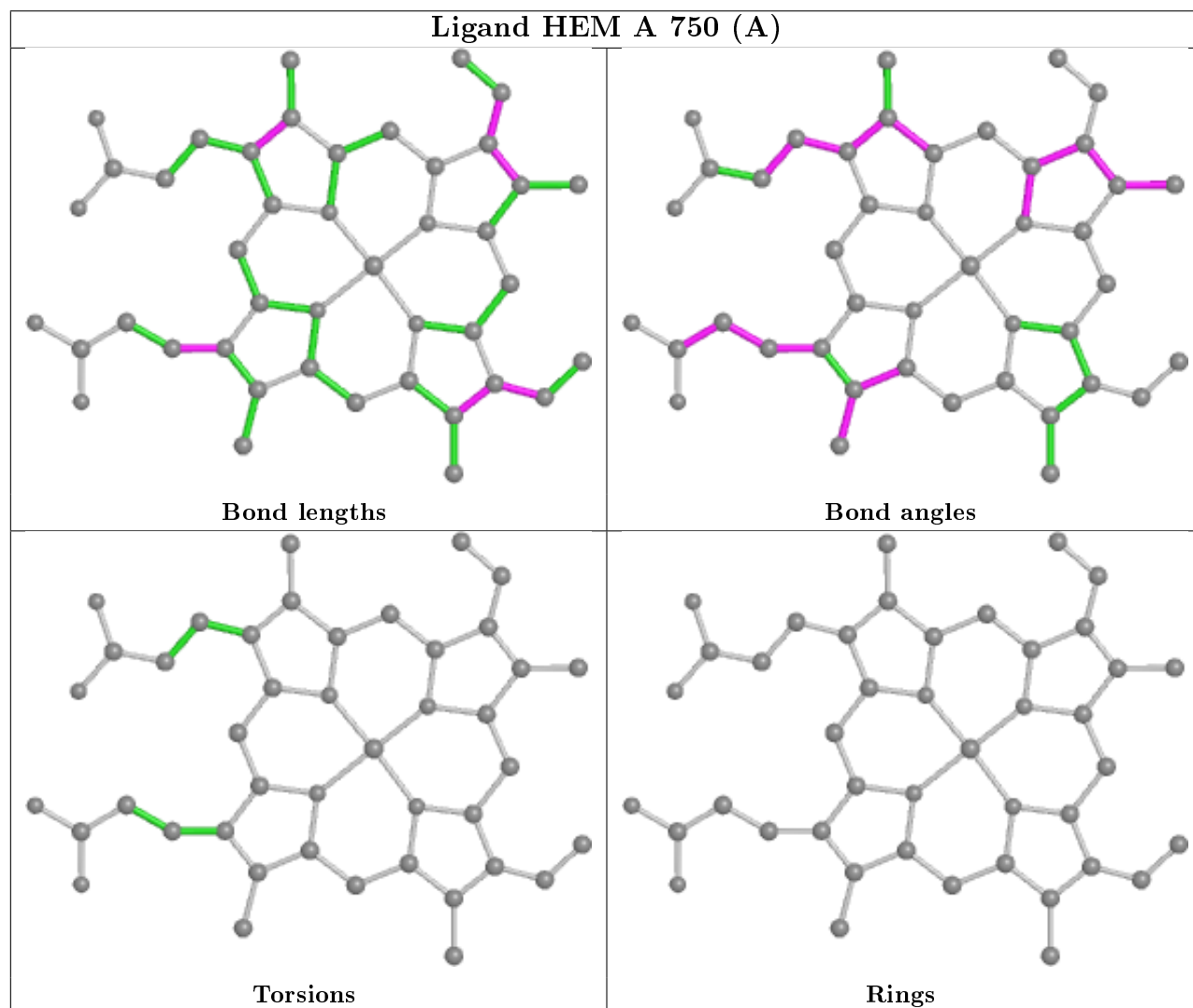
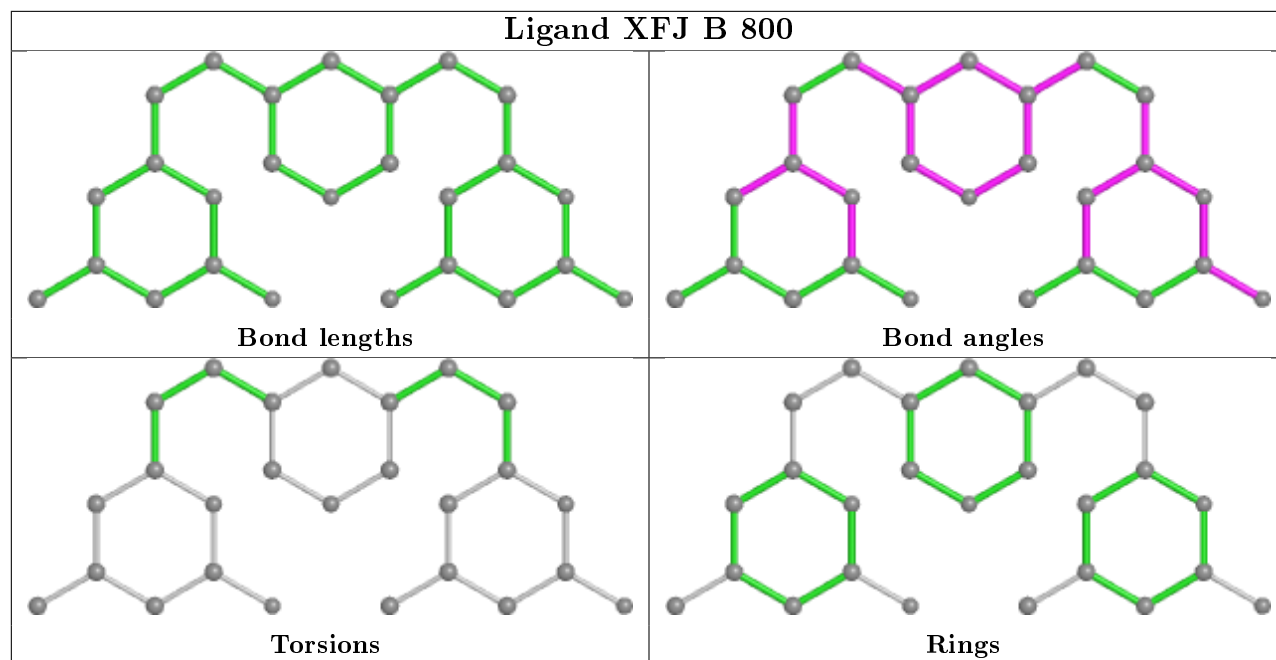
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750[B]	HEM	3	0
4	A	760	H4B	2	0
2	B	750	HEM	7	0
5	B	860	ACT	1	0
3	A	800	XFJ	1	0
3	B	800	XFJ	3	0
2	A	750[A]	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.







## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/422 (96%)	0.77	60 (14%) 2 3	24, 43, 77, 98	1 (0%)
1	B	411/422 (97%)	0.38	28 (6%) 17 25	21, 35, 59, 84	1 (0%)
All	All	818/844 (96%)	0.57	88 (10%) 5 9	21, 39, 72, 98	2 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	7.2
1	B	300	PHE	7.0
1	A	488	PRO	6.5
1	A	351	LYS	5.9
1	A	352	ASP	5.9
1	A	716	TRP	5.7
1	A	300	PHE	5.7
1	B	619	ARG	5.4
1	B	350	THR	5.1
1	A	355	PHE	5.0
1	A	350	THR	4.8
1	A	713	THR	4.8
1	A	715	VAL	4.7
1	A	481	ARG	4.6
1	B	718	GLY	4.5
1	A	486	LYS	4.2
1	A	392	SER	4.0
1	A	619	ARG	4.0
1	B	616	LEU	4.0
1	A	678	TRP	3.9
1	B	352	ASP	3.9
1	B	620	LYS	3.9
1	A	507	GLN	3.8
1	A	322	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	489	ASP	3.6
1	A	677	VAL	3.6
1	A	311	VAL	3.5
1	A	706[A]	TYR	3.4
1	B	481	ARG	3.3
1	A	667	ARG	3.2
1	A	567	VAL	3.2
1	B	567	VAL	3.2
1	B	677	VAL	3.2
1	A	680	VAL	3.1
1	B	322	LEU	3.1
1	A	321	THR	3.1
1	A	385	ASN	3.1
1	A	469	LYS	3.0
1	A	714	HIS	3.0
1	B	715	VAL	3.0
1	A	299	ARG	2.9
1	A	679	ILE	2.9
1	B	678	TRP	2.8
1	A	682	PRO	2.8
1	A	591	THR	2.8
1	B	338	PRO	2.7
1	A	386	LYS	2.7
1	A	487	GLN	2.7
1	A	551	PHE	2.7
1	A	676	TRP	2.7
1	B	351	LYS	2.6
1	A	415	CYS	2.6
1	A	712	ASN	2.6
1	B	299	ARG	2.6
1	B	691	PHE	2.6
1	B	566	ALA	2.6
1	A	550	LYS	2.5
1	A	593	ILE	2.5
1	B	680	VAL	2.5
1	A	389	GLU	2.5
1	A	371	ARG	2.5
1	A	302	LYS	2.4
1	B	321	THR	2.4
1	A	514	ARG	2.4
1	A	480	ILE	2.4
1	A	506	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	390	SER	2.3
1	A	511	LYS	2.3
1	A	416	VAL	2.3
1	B	389	GLU	2.3
1	A	338	PRO	2.3
1	A	681	PRO	2.3
1	B	479	LEU	2.3
1	A	491	SER	2.2
1	A	509	GLY	2.2
1	A	503	GLU	2.2
1	A	691	PHE	2.2
1	B	301	LEU	2.2
1	A	479	LEU	2.1
1	A	353	GLN	2.1
1	A	584	PHE	2.1
1	B	679	ILE	2.1
1	A	588	TYR	2.1
1	B	706[A]	TYR	2.1
1	A	596	ARG	2.1
1	A	490	GLY	2.1
1	B	667	ARG	2.0
1	B	310	VAL	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	XFJ	A	800	26/26	0.87	0.27	31,51,58,59	0

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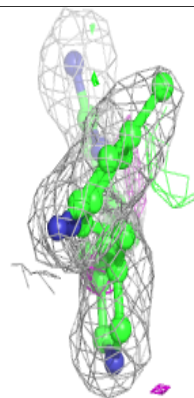
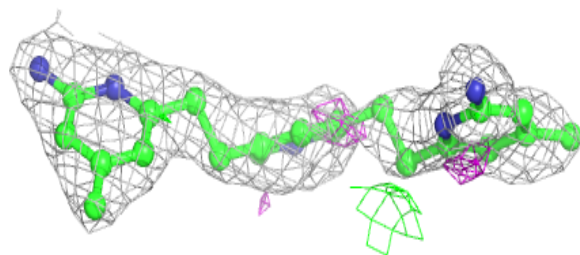
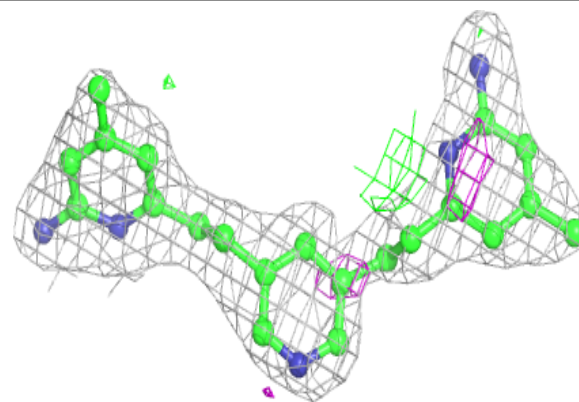
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACT	B	860	4/4	0.88	0.18	47,48,48,48	0
4	H4B	A	760	17/17	0.90	0.18	41,45,48,48	0
4	H4B	B	760	17/17	0.91	0.17	37,40,44,44	0
3	XFJ	B	800	26/26	0.91	0.18	32,45,48,48	0
5	ACT	A	860	4/4	0.92	0.18	57,58,58,59	0
7	CL	B	911	1/1	0.95	0.06	44,44,44,44	0
2	HEM	A	750[B]	43/43	0.97	0.21	24,29,42,45	5
2	HEM	B	750	43/43	0.97	0.17	23,27,44,50	0
2	HEM	A	750[A]	43/43	0.97	0.21	24,29,36,44	5
7	CL	A	911	1/1	0.98	0.09	43,43,43,43	0
6	ZN	A	901	1/1	0.99	0.06	33,33,33,33	1
7	CL	A	910	1/1	0.99	0.09	43,43,43,43	0
7	CL	B	910	1/1	0.99	0.07	48,48,48,48	0
6	ZN	B	901	1/1	0.99	0.05	38,38,38,38	1
6	ZN	A	900	1/1	0.99	0.08	32,32,32,32	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.

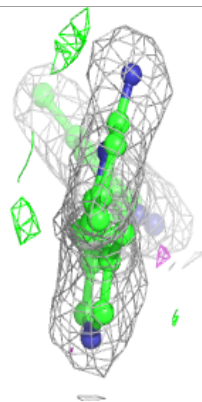
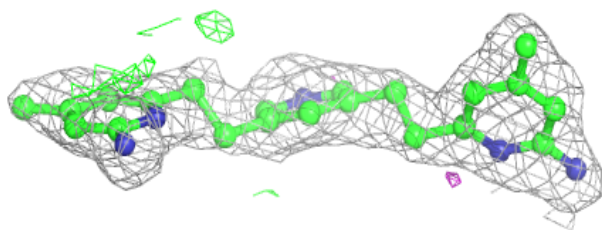
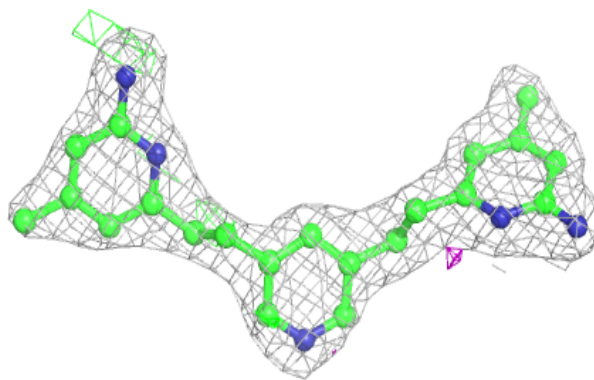
**Electron density around XFJ A 800:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



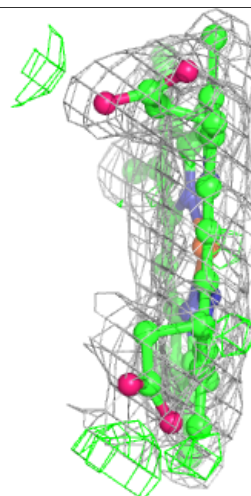
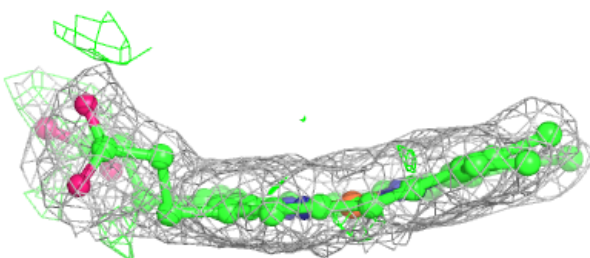
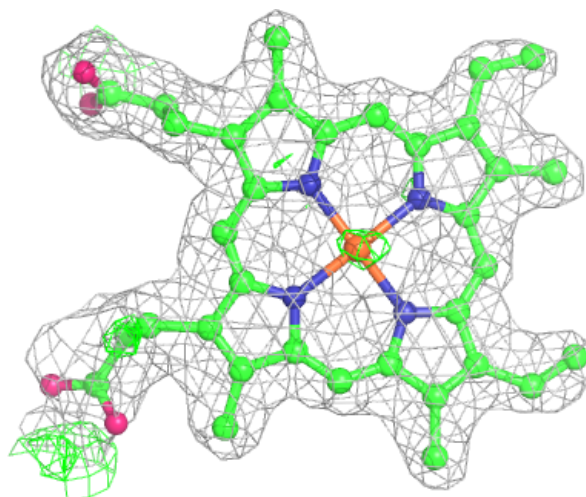
**Electron density around XFJ B 800:**

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



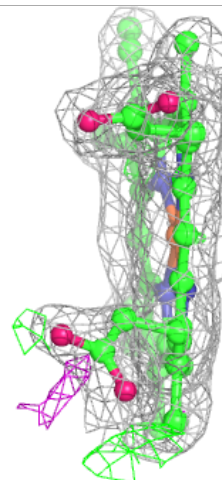
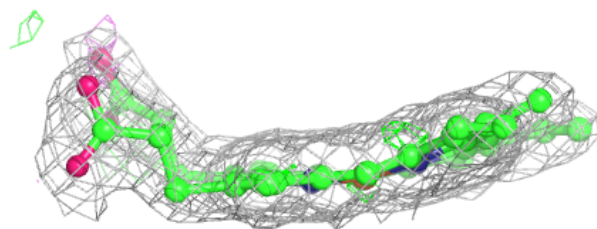
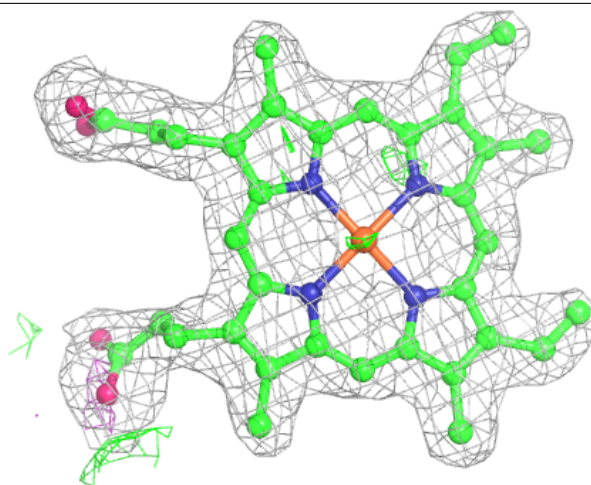
**Electron density around HEM A 750 (B):**

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and green (positive)



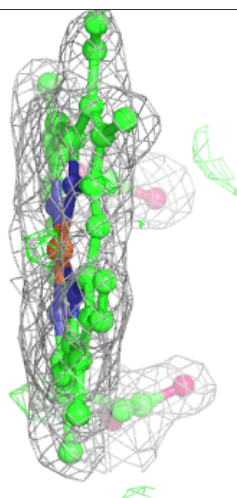
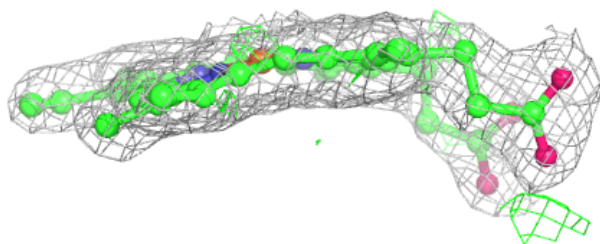
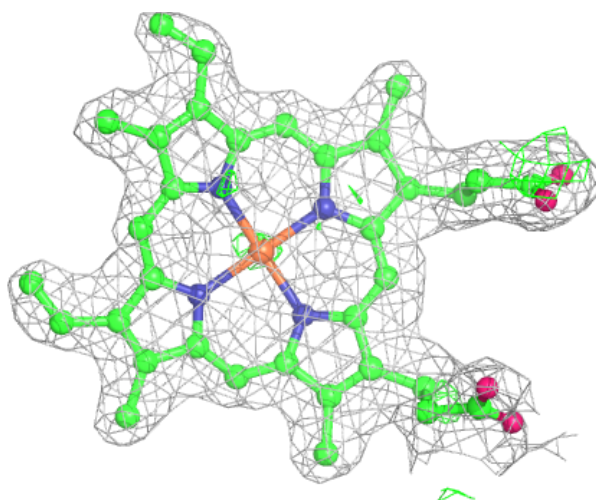
**Electron density around HEM B 750:**

$2mF_o-DF_c$  (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 (A):**

$2mF_o-DF_c$  (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.