



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:54 am BST

PDB ID : 3RN1  
Title : Crystal Structure of the W199E-MauG/pre-Methylamine Dehydrogenase Complex  
Authors : Jensen, L.M.R.; Wilmot, C.M.  
Deposited on : 2011-04-21  
Resolution : 1.93 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

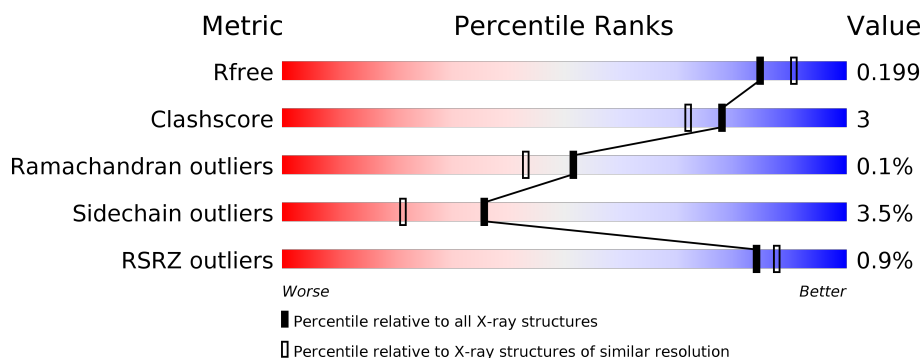
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	373	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	373	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
2	C	137	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div></div> </div> </div>
2	E	137	<div> <div></div> <div> <div>82%</div> <div>8%</div> <div>9%</div> </div> </div>
3	D	386	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> </div>
3	F	386	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>10%</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
2	0AF	C	57	X	-	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14914 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 Methylamine utilization protein MauG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	1	0
			2735	1705	490	529	11			
1	B	355	Total	C	N	O	S	0	0	0
			2738	1706	490	531	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLU	TRP	ENGINEERED MUTATION	UNP Q51658
A	368	HIS	-	EXPRESSION TAG	UNP Q51658
A	369	HIS	-	EXPRESSION TAG	UNP Q51658
A	370	HIS	-	EXPRESSION TAG	UNP Q51658
A	371	HIS	-	EXPRESSION TAG	UNP Q51658
A	372	HIS	-	EXPRESSION TAG	UNP Q51658
A	373	HIS	-	EXPRESSION TAG	UNP Q51658
B	199	GLU	TRP	ENGINEERED MUTATION	UNP Q51658
B	368	HIS	-	EXPRESSION TAG	UNP Q51658
B	369	HIS	-	EXPRESSION TAG	UNP Q51658
B	370	HIS	-	EXPRESSION TAG	UNP Q51658
B	371	HIS	-	EXPRESSION TAG	UNP Q51658
B	372	HIS	-	EXPRESSION TAG	UNP Q51658
B	373	HIS	-	EXPRESSION TAG	UNP Q51658

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	131	Total	C	N	O	S	0	2	0
			1021	630	179	198	14			
2	E	124	Total	C	N	O	S	0	1	0
			951	589	160	188	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	133	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	134	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	135	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	136	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	137	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	132	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	133	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	134	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	135	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	136	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	137	HIS	-	EXPRESSION TAG	UNP A1BBA0

- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	2	0
			2932	1859	503	561	9			
3	F	376	Total	C	N	O	S	0	2	0
			2932	1859	503	561	9			

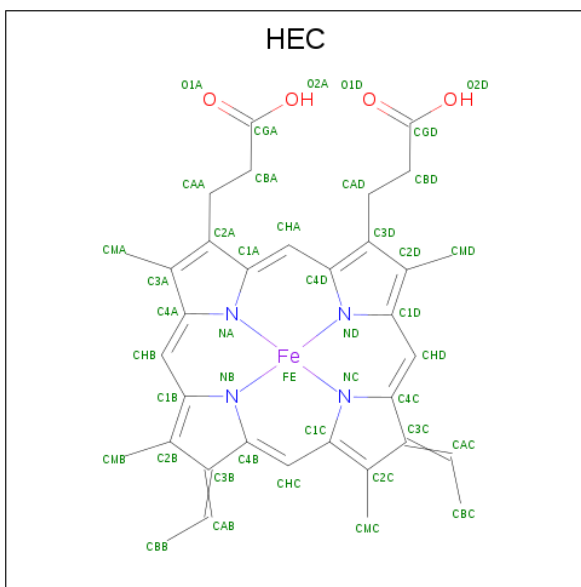
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

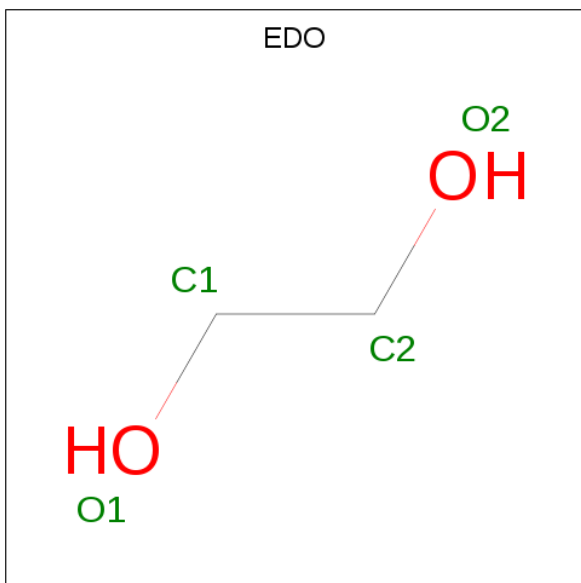
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



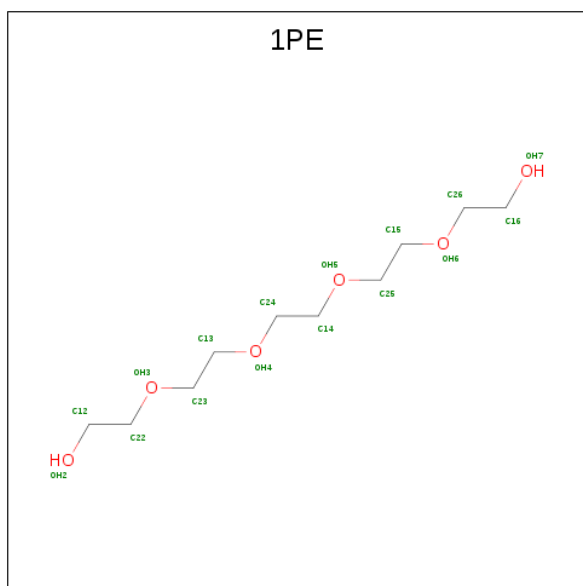
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



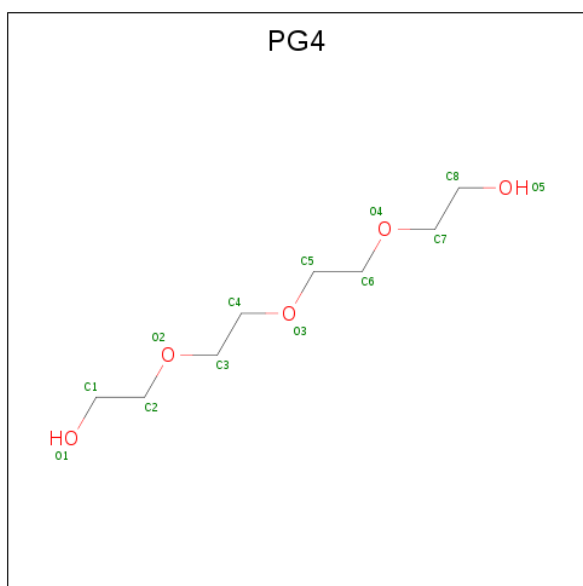
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



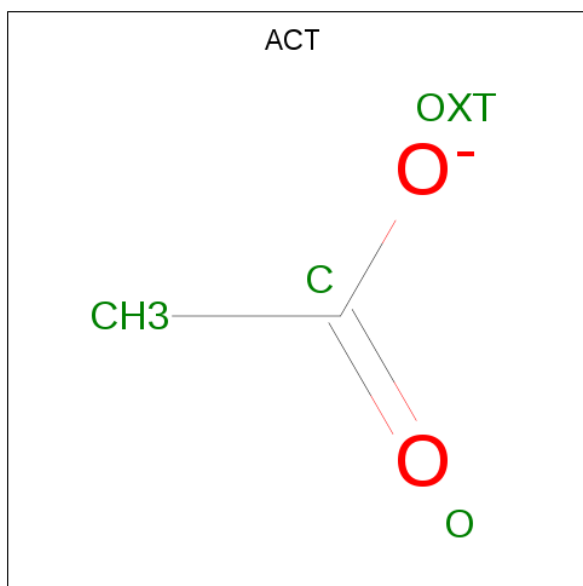
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			16	10	6		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



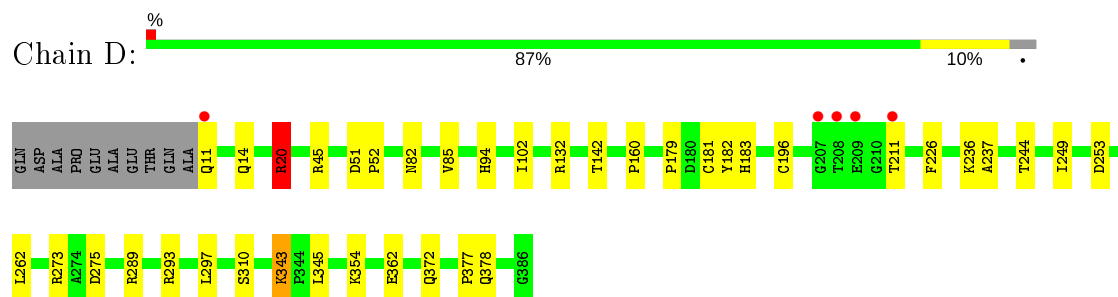
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

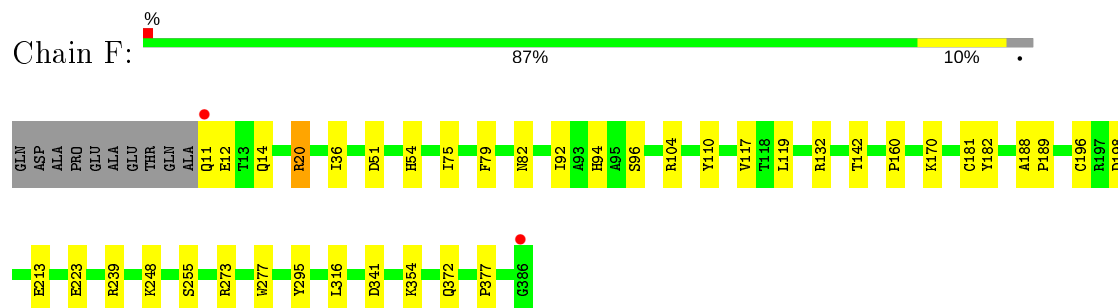
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	285	Total	O	0	0
			285	285		
11	B	277	Total	O	0	0
			277	277		
11	C	98	Total	O	0	0
			98	98		
11	D	280	Total	O	0	0
			280	280		
11	E	101	Total	O	0	0
			101	101		
11	F	349	Total	O	0	0
			349	349		







• Molecule 3: Methylamine dehydrogenase heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	43.46 – 1.93 43.46 – 1.93	Depositor EDS
% Data completeness (in resolution range)	96.8 (43.46-1.93) 96.9 (43.46-1.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.00 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.144 , 0.192 0.150 , 0.199	Depositor DCC
$R_{free}$ test set	6302 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: NA, CA, ACT, EDO, 1PE, PG4, 0AF, HEC

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	1.11	2/2800 (0.1%)	0.96	5/3798 (0.1%)
1	B	1.07	3/2800 (0.1%)	0.98	12/3798 (0.3%)
2	C	1.06	0/1041	0.91	1/1418 (0.1%)
2	E	1.19	1/963 (0.1%)	0.98	4/1315 (0.3%)
3	D	1.10	1/3015 (0.0%)	0.95	5/4108 (0.1%)
3	F	1.20	3/3015 (0.1%)	0.99	8/4108 (0.2%)
All	All	1.12	10/13634 (0.1%)	0.97	35/18545 (0.2%)

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
2	C	1	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	75	ARG	CG-CD	-6.44	1.35	1.51
3	F	79	PHE	CE1-CZ	6.01	1.48	1.37
3	F	277	TRP	CZ3-CH2	5.57	1.49	1.40
1	B	79	PHE	CE1-CZ	5.55	1.48	1.37
1	A	232	GLU	CB-CG	-5.30	1.42	1.52
1	B	303	GLU	CD-OE1	5.27	1.31	1.25
1	B	93	TRP	CB-CG	5.14	1.59	1.50
1	A	212	VAL	CB-CG2	5.11	1.63	1.52
3	D	85	VAL	CB-CG2	5.04	1.63	1.52
3	F	213	GLU	CD-OE1	5.02	1.31	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ARG	NE-CZ-NH1	-12.20	114.20	120.30
1	A	208	ARG	NE-CZ-NH2	-10.22	115.19	120.30
3	D	20	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	208	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	B	180	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	B	127	ARG	NE-CZ-NH2	-7.59	116.50	120.30
2	E	75	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	B	202	ARG	NE-CZ-NH2	7.48	124.04	120.30
2	C	8	ASP	CB-CG-OD1	6.75	124.38	118.30
3	F	198	ASP	CB-CG-OD1	6.68	124.31	118.30
3	F	273	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	206	MET	CG-SD-CE	-6.57	89.69	100.20
1	B	118	ASP	CB-CG-OD1	6.52	124.17	118.30
3	D	20	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	177	ARG	NE-CZ-NH1	6.13	123.36	120.30
3	F	239	ARG	NE-CZ-NH2	-6.07	117.27	120.30
3	F	104	ARG	CG-CD-NE	-5.97	99.26	111.80
3	F	341	ASP	CB-CG-OD1	5.78	123.50	118.30
2	E	75	ARG	CA-CB-CG	-5.72	100.81	113.40
3	D	273	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	B	36	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	36	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	257	ASP	CB-CG-OD2	-5.42	113.42	118.30
3	D	132	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	202	ARG	CG-CD-NE	-5.36	100.55	111.80
1	B	127	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	E	8	ASP	CB-CG-OD1	5.31	123.08	118.30
3	F	170	LYS	CD-CE-NZ	-5.28	99.55	111.70
1	A	82	ASP	CB-CG-OD2	5.20	122.98	118.30
3	F	20	ARG	CG-CD-NE	-5.20	100.88	111.80
3	F	132	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	180	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	E	8	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	B	351	ASP	CB-CG-OD1	5.06	122.86	118.30
3	D	253	ASP	CB-CG-OD1	5.06	122.85	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	57	0AF	CA

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	2735	0	2610	16	0
1	B	2738	0	2610	14	0
2	C	1021	0	910	14	0
2	E	951	0	859	8	0
3	D	2932	0	2821	18	0
3	F	2932	0	2821	15	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	86	0	60	0	0
6	B	86	0	60	3	0
7	B	4	0	6	0	0
8	F	16	0	22	0	0
9	F	13	0	18	2	0
10	F	4	0	3	0	0
11	A	285	0	0	1	0
11	B	277	0	0	3	0
11	C	98	0	0	3	0
11	D	280	0	0	3	0
11	E	101	0	0	1	0
11	F	349	0	0	3	0
All	All	14914	0	12800	77	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 (77) 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)
3:D:372[B]:GLN:NE2	11:D:1225:HOH:O	1.77	1.15
2:C:127:VAL:HG23	2:C:127:VAL:O	1.62	0.94
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.49	0.77
2:C:127:VAL:CG2	2:C:127:VAL:O	2.34	0.75
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:135:HIS:HE1	11:C:696:HOH:O	1.78	0.66
3:F:255:SER:HA	9:F:388:PG4:H32	1.77	0.66
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.78	0.65
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.43	0.64
2:C:129:LYS:O	2:C:130:ALA:CB	2.47	0.62
3:D:20:ARG:NH2	2:E:17:ASP:O	2.28	0.62
2:C:135:HIS:HD2	11:C:348:HOH:O	1.83	0.61
1:B:194:THR:HG22	2:E:101:GLU:HG2	1.83	0.60
3:F:51:ASP:HA	3:F:377:PRO:HA	1.83	0.60
3:F:12:GLU:OE2	3:F:20:ARG:NH1	2.33	0.60
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.85	0.59
1:B:86:LYS:HD2	11:B:700:HOH:O	2.04	0.58
3:F:181[B]:CYS:HB3	3:F:196:CYS:SG	2.46	0.56
3:D:181[B]:CYS:HB3	3:D:196:CYS:SG	2.46	0.56
3:D:51:ASP:HA	3:D:377:PRO:HA	1.89	0.55
1:A:202:ARG:HB2	1:A:206:MET:HG3	1.88	0.55
3:F:96:SER:HB3	3:F:110:TYR:CZ	2.44	0.53
1:B:163:GLN:HE22	6:B:500:HEC:HMA1	1.75	0.52
2:E:101:GLU:HA	11:E:845:HOH:O	2.10	0.52
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.74	0.52
2:C:129:LYS:O	2:C:130:ALA:HB2	2.09	0.52
1:B:88:LYS:HD3	11:B:860:HOH:O	2.10	0.51
1:B:81:ARG:HD3	1:B:85:GLY:HA2	1.91	0.51
1:A:190:GLU:O	1:A:194:THR:HG23	2.11	0.50
3:D:236:LYS:HD3	3:D:289:ARG:NH1	2.26	0.50
6:B:600:HEC:HMC1	6:B:600:HEC:HBC3	1.94	0.49
1:A:228:LEU:HD13	1:A:279:MET:HB3	1.95	0.49
1:A:197:ILE:O	1:A:202:ARG:HD2	2.12	0.49
1:A:210:GLN:NE2	2:C:44:THR:HG21	2.24	0.48
9:F:388:PG4:H12	11:F:1039:HOH:O	2.14	0.48
1:A:48:LYS:H	1:A:62:HIS:HE1	1.62	0.47
1:B:272:VAL:HG21	6:B:600:HEC:HMA3	1.94	0.47
1:B:305:LYS:HE2	11:B:609:HOH:O	2.14	0.47
2:C:57:0AF:CE3	2:C:108:TRP:CD1	2.97	0.47
3:F:75:ILE:HD11	3:F:119:LEU:HB3	1.97	0.46
11:C:1271:HOH:O	3:F:36:ILE:HD11	2.15	0.46
3:D:82:ASN:HB3	3:D:142:THR:HB	1.97	0.46
1:B:193:TYR:O	1:B:197:ILE:HG12	2.15	0.46
3:D:236:LYS:NZ	11:D:959:HOH:O	2.42	0.46
3:F:248:LYS:CE	11:F:949:HOH:O	2.64	0.46
3:D:45:ARG:NH2	3:D:343:LYS:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:ARG:HD3	3:D:345:LEU:HD11	1.99	0.45
3:D:179:PRO:HD2	3:D:181[B]:CYS:SG	2.57	0.45
1:A:39:ARG:HD2	1:A:44:PRO:HB3	2.00	0.44
1:B:360:GLU:HG2	1:B:360:GLU:H	1.43	0.44
2:C:86:CYS:H	3:F:372[A]:GLN:HE22	1.66	0.44
3:D:52:PRO:HG2	3:D:378:GLN:OE1	2.17	0.44
3:F:188:ALA:HB1	3:F:189:PRO:HD2	1.99	0.43
3:D:236:LYS:HB3	3:D:289:ARG:HH11	1.83	0.43
3:F:82:ASN:HB3	3:F:142:THR:HB	2.00	0.43
2:E:94:GLU:HG2	2:E:102:PHE:O	2.18	0.43
1:B:355:GLU:N	1:B:356:PRO:CD	2.82	0.43
1:A:48:LYS:H	1:A:62:HIS:CE1	2.37	0.42
1:B:285:THR:HG22	1:B:286:ASP:OD1	2.19	0.42
1:A:203:LEU:HD11	2:C:54:THR:HB	2.01	0.42
1:A:81:ARG:CZ	1:A:85:GLY:HA2	2.50	0.42
1:A:55:VAL:HG22	1:A:62:HIS:CE1	2.55	0.41
2:C:94:GLU:HG2	2:C:102:PHE:O	2.20	0.41
1:A:21:PRO:O	1:A:27:ALA:HA	2.20	0.41
1:A:183:GLU:HB2	11:A:1301:HOH:O	2.18	0.41
1:A:288:ARG:NH1	1:A:340:ASP:OD1	2.49	0.41
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.87	0.41
2:C:103:ALA:HB1	11:D:404:HOH:O	2.20	0.41
3:D:182:TYR:O	3:D:183:HIS:HB2	2.21	0.41
3:D:226:PHE:O	3:D:244:THR:HA	2.21	0.40
2:E:74:TYR:C	2:E:75:ARG:HG3	2.42	0.40
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.35	0.40
1:B:171:PHE:CZ	1:B:215:ARG:HB3	2.57	0.40
3:F:295:TYR:CD1	3:F:295:TYR:N	2.90	0.40
3:F:54:HIS:HE1	11:F:613:HOH:O	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/373 (95%)	344 (98%)	9 (2%)	0	100	100
1	B	353/373 (95%)	345 (98%)	8 (2%)	0	100	100
2	C	130/137 (95%)	125 (96%)	4 (3%)	1 (1%)	19	9
2	E	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
3	D	376/386 (97%)	364 (97%)	11 (3%)	1 (0%)	41	32
3	F	376/386 (97%)	363 (96%)	13 (4%)	0	100	100
All	All	1710/1792 (95%)	1660 (97%)	48 (3%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	130	ALA
3	D	102	ILE

### 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	277/292 (95%)	266 (96%)	11 (4%)	31	16
1	B	277/292 (95%)	264 (95%)	13 (5%)	26	11
2	C	112/112 (100%)	111 (99%)	1 (1%)	78	75
2	E	104/112 (93%)	101 (97%)	3 (3%)	42	28
3	D	306/311 (98%)	294 (96%)	12 (4%)	32	17
3	F	306/311 (98%)	298 (97%)	8 (3%)	46	32
All	All	1382/1430 (97%)	1334 (96%)	48 (4%)	36	21

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	23	LEU
1	A	84	ASN

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Mol	Chain	Res	Type
1	A	112	VAL
1	A	167	GLU
1	A	202	ARG
1	A	206	MET
1	A	209	LYS
1	A	219	THR
1	A	232	GLU
1	A	296	LYS
1	B	60	GLN
1	B	81	ARG
1	B	84	ASN
1	B	112	VAL
1	B	167	GLU
1	B	187	PRO
1	B	202	ARG
1	B	219	THR
1	B	300	ARG
1	B	321	ARG
1	B	352	ARG
1	B	358	LEU
1	B	360	GLU
2	C	7	THR
3	D	11	GLN
3	D	20	ARG
3	D	94	HIS
3	D	160	PRO
3	D	211	THR
3	D	249	ILE
3	D	262	LEU
3	D	275	ASP
3	D	293	ARG
3	D	343	LYS
3	D	354	LYS
3	D	362	GLU
2	E	16	GLN
2	E	30	SER
2	E	71	LEU
3	F	11	GLN
3	F	92	ILE
3	F	94	HIS
3	F	117	VAL
3	F	160	PRO

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Mol	Chain	Res	Type
3	F	223	GLU
3	F	316	LEU
3	F	354	LYS

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	26	ASN
1	A	62	HIS
1	A	91	GLN
1	A	210	GLN
1	B	16	GLN
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
2	C	135	HIS
3	D	14	GLN
3	F	11	GLN
3	F	14	GLN
3	F	30	GLN
3	F	54	HIS
3	F	60	GLN
3	F	300	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	0AF	C	57	2	13,16,17	1.60	2 (15%)	11,22,24	3.54	5 (45%)
2	0AF	E	57	2	13,16,17	1.44	2 (15%)	11,22,24	3.13	6 (54%)

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	0AF	C	57	2	1/1/1/2	1/4/6/8	0/2/2/2
2	0AF	E	57	2	-	1/4/6/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CZ3-CE3	3.08	1.43	1.36
2	C	57	0AF	CZ3-CE3	2.95	1.43	1.36
2	C	57	0AF	CZ2-CE2	-2.47	1.38	1.42
2	E	57	0AF	CH2-CZ2	2.28	1.42	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	0AF	CG-CB-CA	-9.40	100.00	114.53
2	E	57	0AF	CG-CB-CA	-7.69	102.64	114.53
2	C	57	0AF	CB-CA-C	4.10	119.16	111.47
2	E	57	0AF	CB-CA-C	3.74	118.48	111.47
2	E	57	0AF	CH2-CZ2-CE2	3.35	124.12	120.12
2	C	57	0AF	CB-CG-CD1	-3.26	123.94	127.97
2	E	57	0AF	CZ3-CH2-CZ2	-2.96	116.54	120.28
2	C	57	0AF	CB-CG-CD2	2.72	130.49	126.25
2	C	57	0AF	CE3-CZ3-CH2	-2.51	116.99	120.99
2	E	57	0AF	CB-CG-CD1	-2.29	125.13	127.97
2	E	57	0AF	CB-CG-CD2	2.10	129.52	126.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	57	0AF	CA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	57	0AF	N-CA-CB-CG
2	E	57	0AF	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	57	0AF	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 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
6	HEC	A	600	1	26,50,50	1.55	6 (23%)	18,82,82	3.56	10 (55%)
6	HEC	B	500	1	26,50,50	1.67	6 (23%)	18,82,82	2.65	10 (55%)
8	1PE	F	387	-	15,15,15	0.59	0	14,14,14	0.59	0
10	ACT	F	389	-	1,3,3	0.77	0	0,3,3	0.00	-
6	HEC	B	600	1	26,50,50	1.29	3 (11%)	18,82,82	3.12	11 (61%)
7	EDO	B	374	-	3,3,3	0.58	0	2,2,2	0.33	0
9	PG4	F	388	-	12,12,12	0.54	0	11,11,11	0.47	0
6	HEC	A	500	1	26,50,50	1.70	6 (23%)	18,82,82	2.55	8 (44%)

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
6	HEC	A	600	1	-	0/6/54/54	-
6	HEC	B	500	1	-	0/6/54/54	-
7	EDO	B	374	-	-	1/1/1/1	-
6	HEC	B	600	1	-	0/6/54/54	-
8	1PE	F	387	-	-	3/13/13/13	-
9	PG4	F	388	-	-	8/10/10/10	-
6	HEC	A	500	1	-	0/6/54/54	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	500	HEC	C4A-C3A	3.74	1.51	1.42
6	A	500	HEC	C3B-C4B	3.71	1.49	1.43
6	A	500	HEC	C1D-CHD	3.39	1.50	1.41
6	B	500	HEC	C3C-C4C	3.30	1.49	1.43
6	B	500	HEC	C4A-C3A	3.20	1.49	1.42
6	A	600	HEC	C3B-C4B	3.17	1.48	1.43
6	B	500	HEC	C1A-C2A	3.16	1.49	1.42
6	A	500	HEC	C1A-C2A	3.11	1.49	1.42
6	B	500	HEC	C1C-CHC	3.10	1.49	1.41
6	A	600	HEC	C1A-C2A	3.00	1.49	1.42
6	B	600	HEC	C4A-C3A	2.85	1.49	1.42
6	B	500	HEC	C3B-C4B	2.85	1.48	1.43
6	A	500	HEC	C1C-CHC	2.56	1.48	1.41
6	B	500	HEC	C1B-CHB	2.49	1.47	1.41
6	A	600	HEC	C1D-CHD	2.47	1.47	1.41
6	B	600	HEC	C1A-C2A	2.43	1.48	1.42
6	A	600	HEC	C1C-CHC	2.42	1.47	1.41
6	B	600	HEC	C1D-CHD	2.33	1.47	1.41
6	A	500	HEC	C3C-C4C	2.30	1.47	1.43
6	A	600	HEC	C3C-C4C	2.23	1.47	1.43
6	A	600	HEC	C3B-C2B	-2.14	1.38	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	HEC	CBD-CAD-C3D	-7.08	99.43	112.49
6	A	600	HEC	CMC-C2C-C3C	7.05	134.11	125.82
6	B	600	HEC	CBD-CAD-C3D	-6.58	100.35	112.49
6	A	600	HEC	C1D-C2D-C3D	-6.16	102.71	107.00
6	B	600	HEC	C1D-C2D-C3D	-6.03	102.80	107.00
6	B	600	HEC	CMB-C2B-C3B	5.11	131.83	125.82
6	B	500	HEC	CBD-CAD-C3D	-4.97	103.31	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	500	HEC	C4B-C3B-C2B	-4.69	101.29	106.35
6	A	500	HEC	CMB-C2B-C3B	4.40	131.00	125.82
6	B	600	HEC	CBA-CAA-C2A	-4.24	104.67	112.48
6	B	500	HEC	CMB-C2B-C3B	4.18	130.73	125.82
6	A	500	HEC	CMC-C2C-C3C	4.09	130.63	125.82
6	A	500	HEC	CBD-CAD-C3D	-4.03	105.05	112.49
6	A	600	HEC	CMC-C2C-C1C	-3.94	122.41	128.46
6	A	600	HEC	CAD-CBD-CGD	-3.91	106.10	112.67
6	A	600	HEC	CBA-CAA-C2A	-3.89	105.32	112.48
6	B	500	HEC	CMC-C2C-C3C	3.79	130.28	125.82
6	A	600	HEC	CMB-C2B-C3B	3.70	130.17	125.82
6	B	500	HEC	CMA-C3A-C2A	3.56	131.66	124.94
6	A	600	HEC	CMD-C2D-C3D	3.33	131.22	124.94
6	B	600	HEC	CMA-C3A-C2A	3.21	130.99	124.94
6	B	500	HEC	C1D-C2D-C3D	-3.14	104.81	107.00
6	B	600	HEC	CAA-CBA-CGA	-2.99	107.65	112.67
6	A	500	HEC	C3B-C4B-NB	2.98	116.56	110.94
6	A	500	HEC	C1D-C2D-C3D	-2.93	104.96	107.00
6	B	500	HEC	CMD-C2D-C3D	2.89	130.40	124.94
6	A	500	HEC	CMB-C2B-C1B	-2.83	124.11	128.46
6	B	600	HEC	C4C-C3C-C2C	-2.74	103.39	106.35
6	B	500	HEC	C4C-C3C-C2C	-2.63	103.52	106.35
6	B	500	HEC	CMD-C2D-C1D	-2.41	124.76	128.46
6	B	600	HEC	CMC-C2C-C3C	2.33	128.56	125.82
6	A	500	HEC	CMC-C2C-C1C	-2.27	124.97	128.46
6	A	600	HEC	CMA-C3A-C2A	2.25	129.18	124.94
6	B	500	HEC	CMB-C2B-C1B	-2.18	125.11	128.46
6	B	500	HEC	CBA-CAA-C2A	-2.18	108.46	112.48
6	A	600	HEC	C4C-C3C-C2C	-2.12	104.06	106.35
6	B	600	HEC	CMD-C2D-C3D	2.09	128.89	124.94
6	B	600	HEC	C3C-C4C-NC	2.09	114.89	110.94
6	B	600	HEC	CAD-CBD-CGD	-2.00	109.31	112.67

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	387	1PE	OH4-C13-C23-OH3
9	F	388	PG4	O4-C7-C8-O5
9	F	388	PG4	O3-C5-C6-O4
8	F	387	1PE	OH2-C12-C22-OH3
9	F	388	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	B	374	EDO	O1-C1-C2-O2
9	F	388	PG4	C1-C2-O2-C3
8	F	387	1PE	C24-C14-OH5-C25
9	F	388	PG4	C4-C3-O2-C2
9	F	388	PG4	C6-C5-O3-C4
9	F	388	PG4	O2-C3-C4-O3
9	F	388	PG4	C8-C7-O4-C6

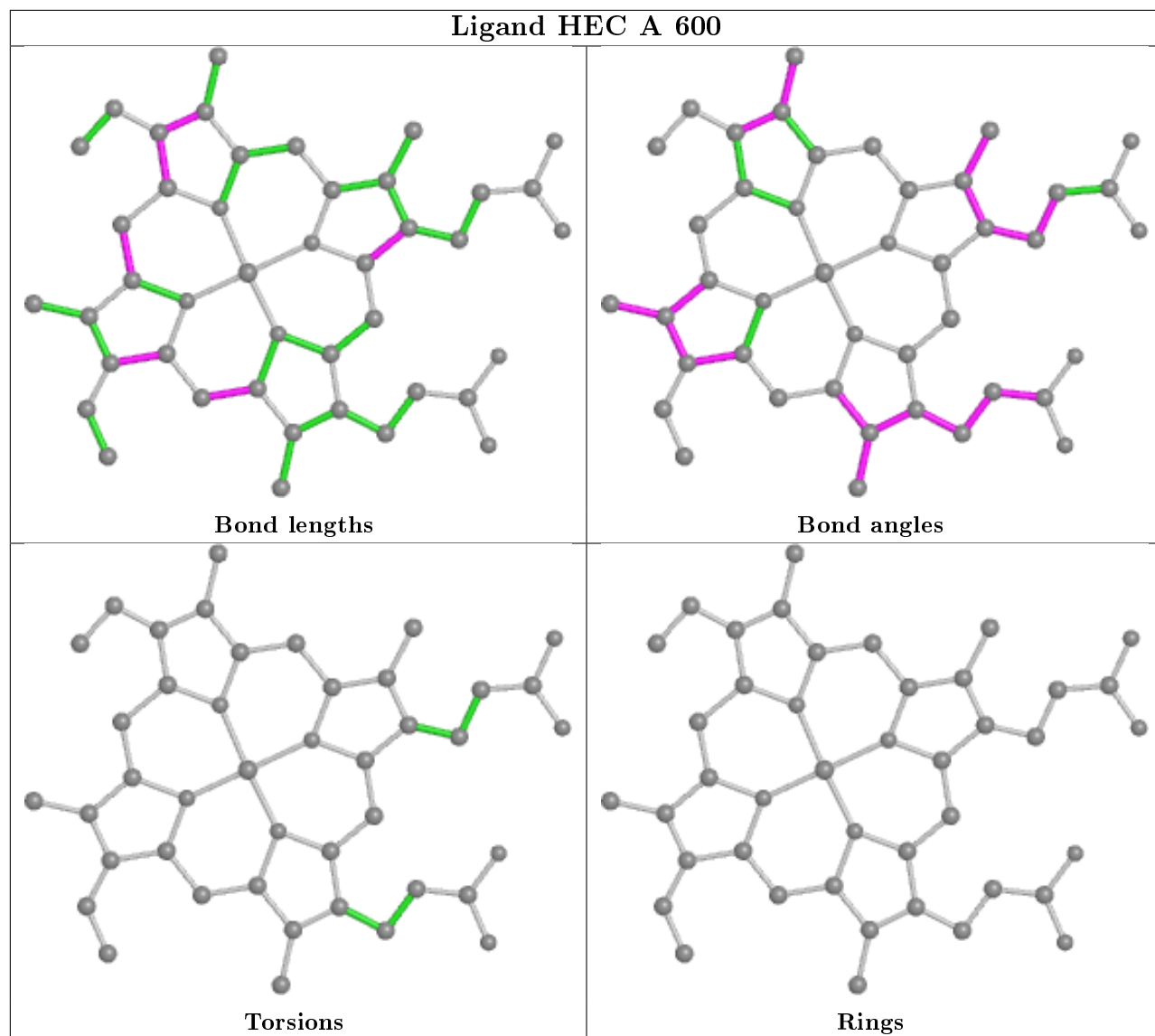
There are no ring outliers.

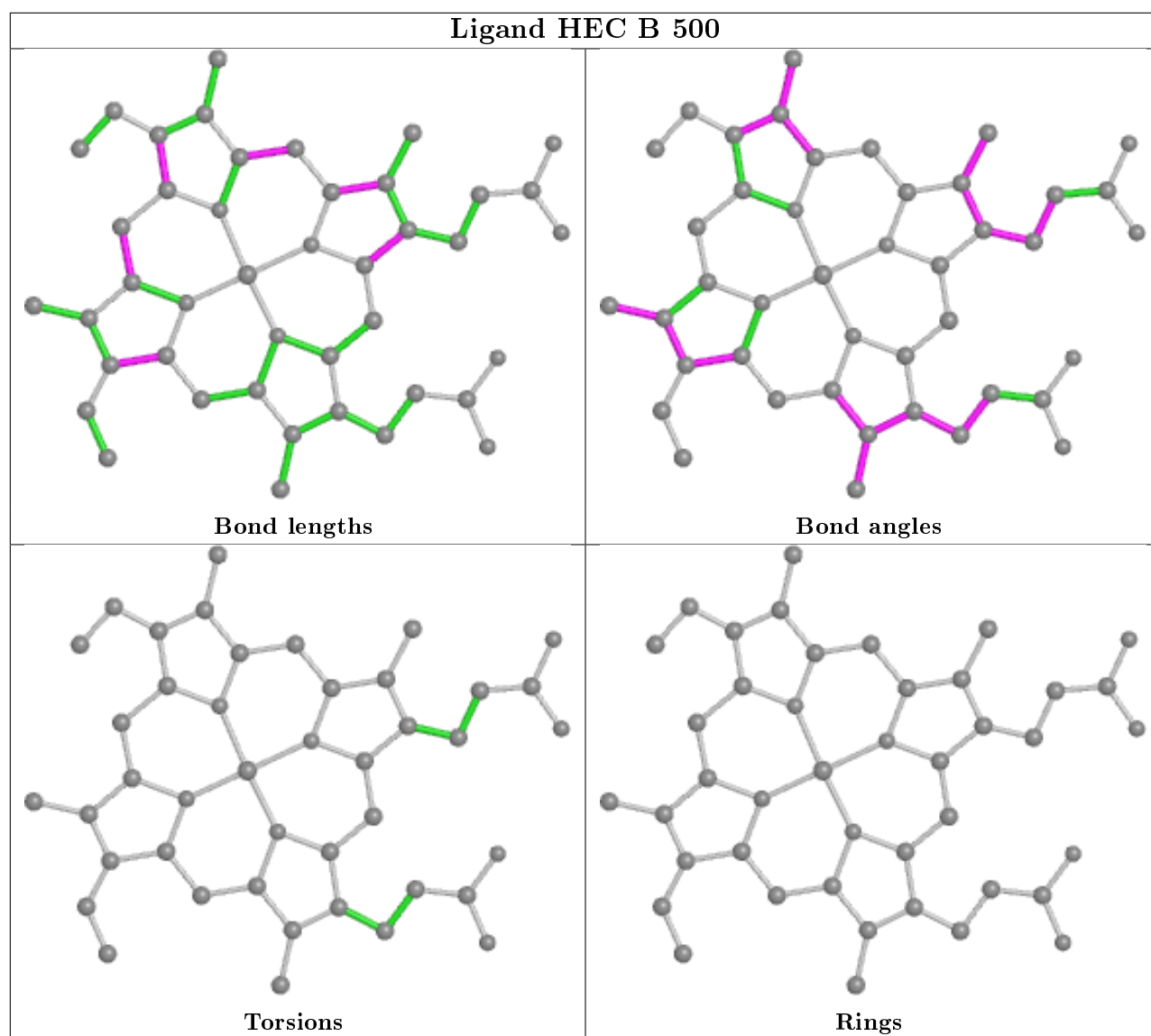
3 monomers are involved in 5 short contacts:

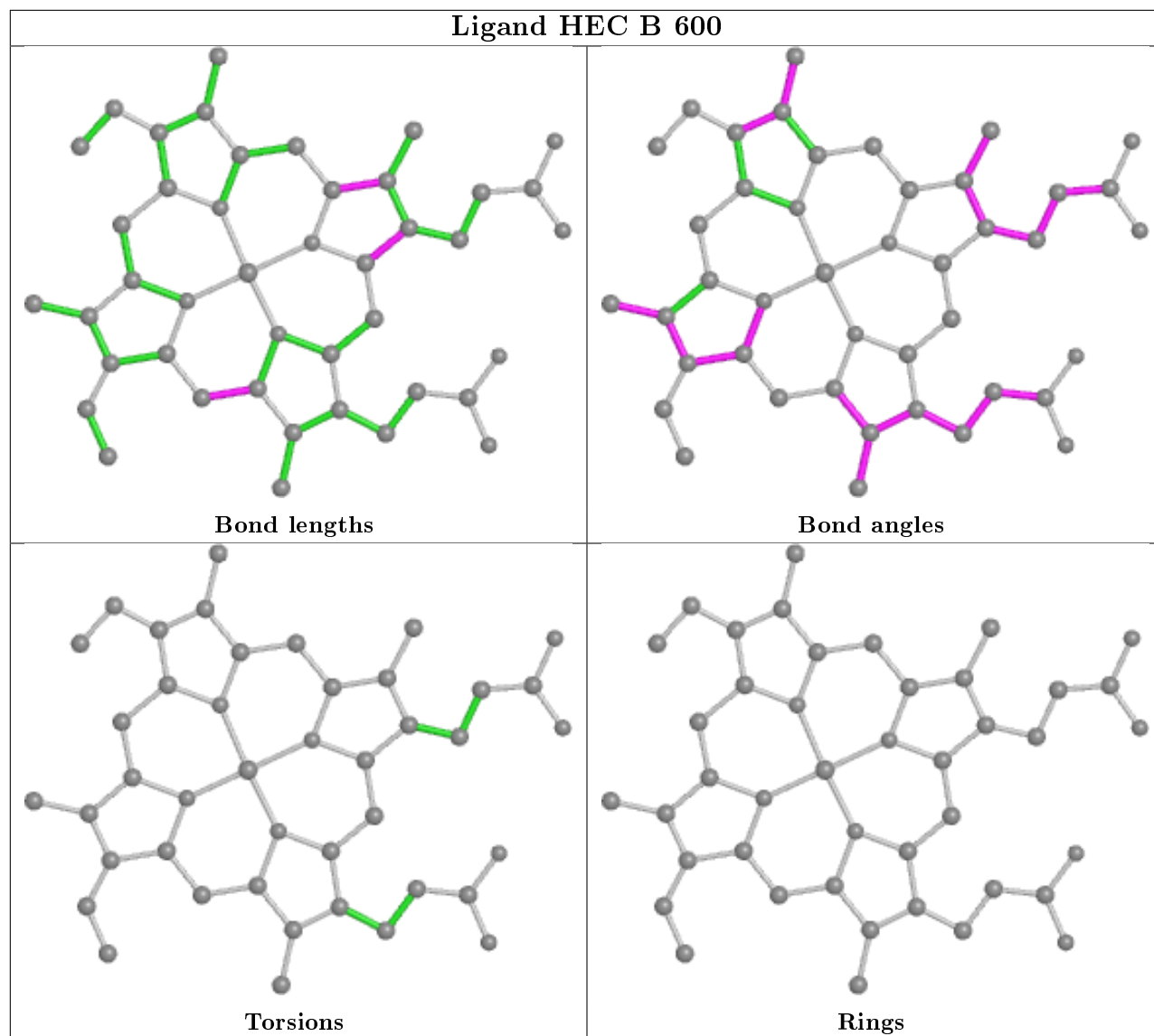
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	500	HEC	1	0
6	B	600	HEC	2	0
9	F	388	PG4	2	0

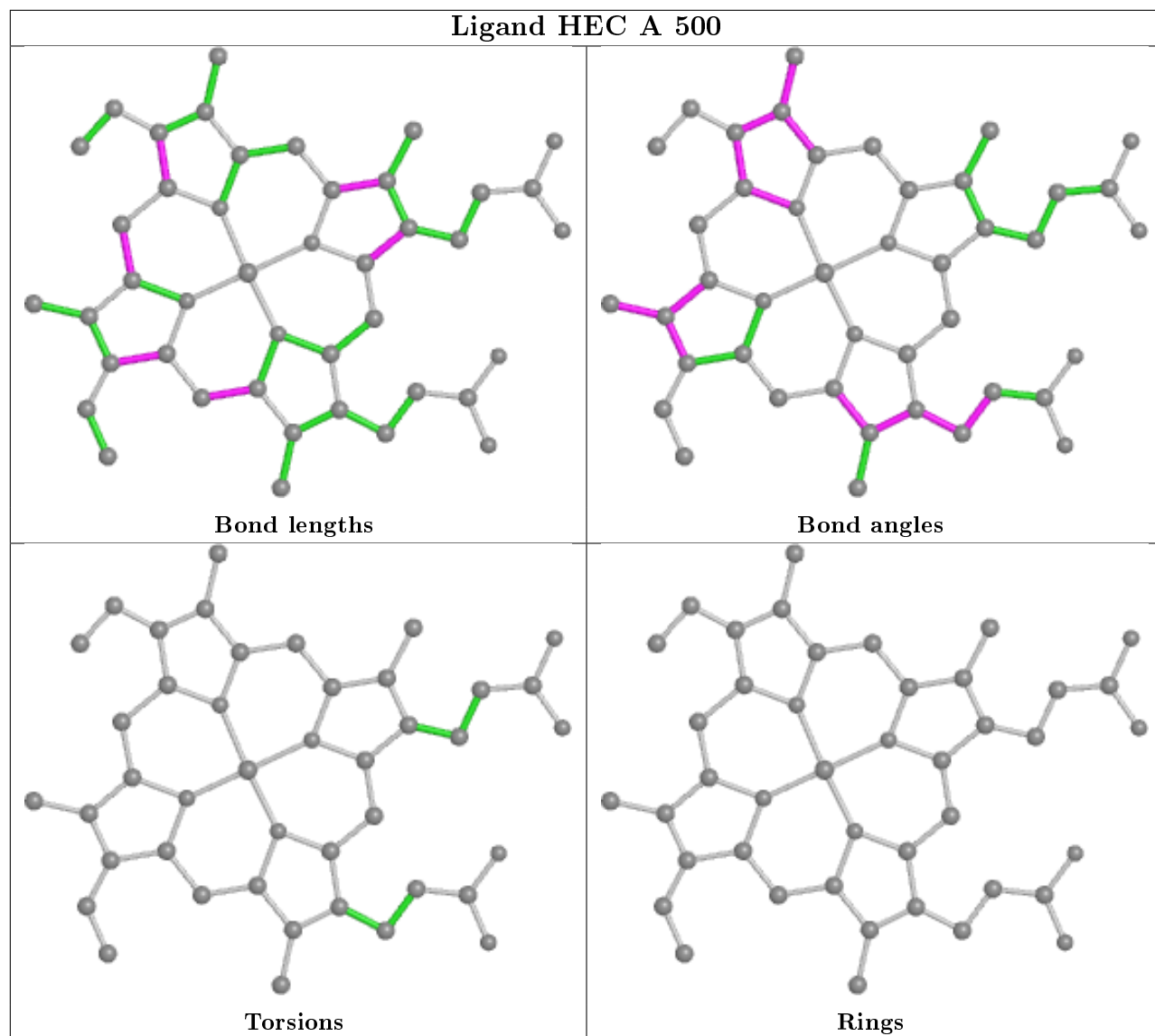
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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, 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	354/373 (94%)	-0.59	3 (0%) 86 89	8, 17, 31, 49	0
1	B	355/373 (95%)	-0.50	5 (1%) 75 80	9, 19, 34, 59	0
2	C	130/137 (94%)	-0.24	1 (0%) 86 89	9, 13, 38, 54	0
2	E	123/137 (89%)	-0.42	0 100 100	8, 12, 23, 37	0
3	D	376/386 (97%)	-0.46	5 (1%) 77 81	9, 16, 31, 55	0
3	F	376/386 (97%)	-0.57	2 (0%) 91 93	7, 13, 25, 47	0
All	All	1714/1792 (95%)	-0.50	16 (0%) 84 87	7, 16, 32, 59	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ASP	5.2
1	A	6	ALA	5.0
3	D	209	GLU	4.6
1	B	7	ASP	4.6
3	D	207	GLY	4.0
1	B	6	ALA	3.4
3	D	211	THR	3.3
3	F	386	GLY	3.3
3	D	11	GLN	3.3
3	D	208	THR	3.2
2	C	137	HIS	2.9
3	F	11	GLN	2.7
1	B	83	ALA	2.4
1	A	8	ASP	2.2
1	B	360	GLU	2.2
1	B	300	ARG	2.2

## 6.2 Non-standard residues in protein, DNA, RNA chains [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( $\text{\AA}^2$ )	Q<0.9
2	0AF	C	57	15/16	0.98	0.12	12,14,17,17	0
2	0AF	E	57	15/16	0.98	0.13	10,12,14,17	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

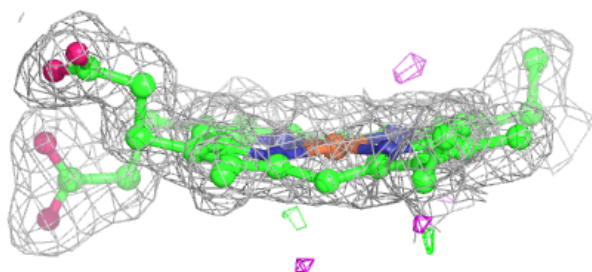
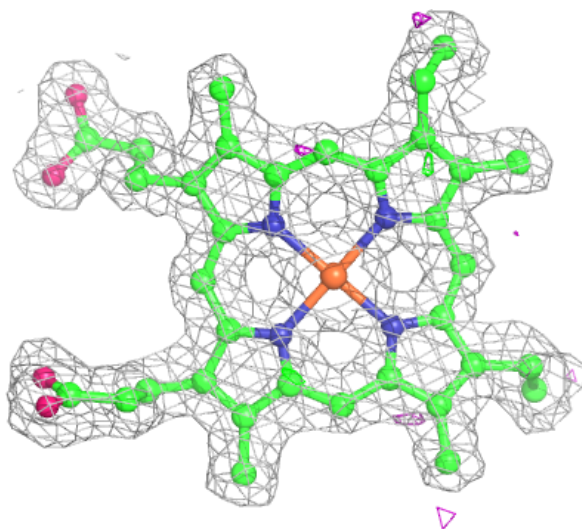
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	B	374	4/4	0.89	0.12	33,37,39,41	0
9	PG4	F	388	13/13	0.89	0.13	41,47,56,57	0
8	1PE	F	387	16/16	0.91	0.12	22,34,45,47	0
10	ACT	F	389	4/4	0.97	0.13	23,25,28,28	0
5	NA	B	401	1/1	0.97	0.12	36,36,36,36	0
5	NA	B	402	1/1	0.98	0.08	24,24,24,24	0
5	NA	A	402	1/1	0.98	0.04	29,29,29,29	0
5	NA	A	401	1/1	0.99	0.07	23,23,23,23	0
6	HEC	A	600	43/43	0.99	0.07	8,10,12,15	0
6	HEC	B	500	43/43	0.99	0.07	7,12,16,18	0
6	HEC	B	600	43/43	0.99	0.08	4,8,11,14	0
6	HEC	A	500	43/43	0.99	0.07	7,12,16,19	0
4	CA	B	400	1/1	1.00	0.06	10,10,10,10	0
4	CA	A	400	1/1	1.00	0.07	11,11,11,11	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.

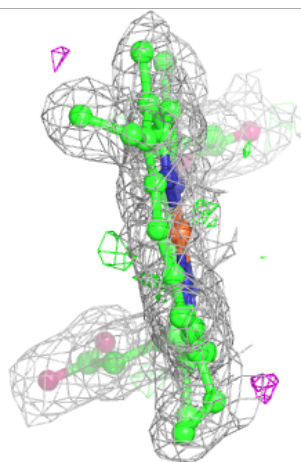
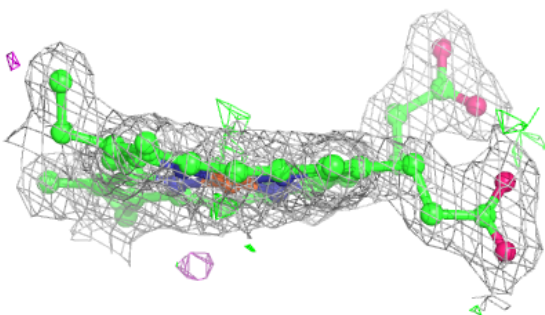
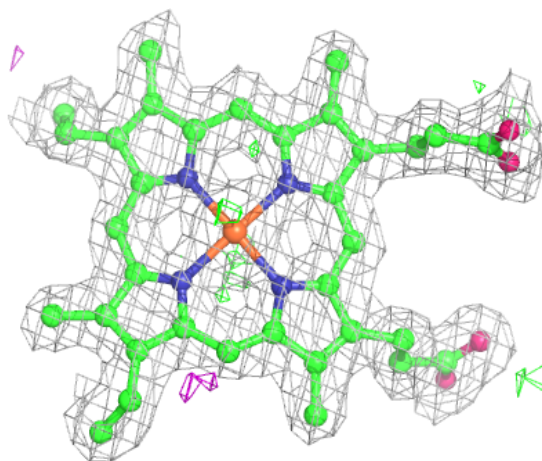
**Electron density around HEC A 600:**

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



**Electron density around HEC B 500:**

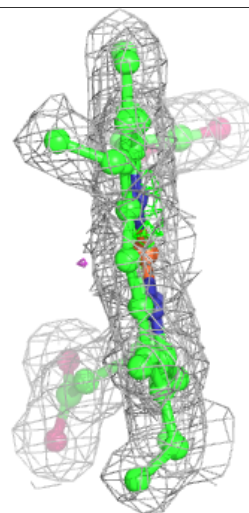
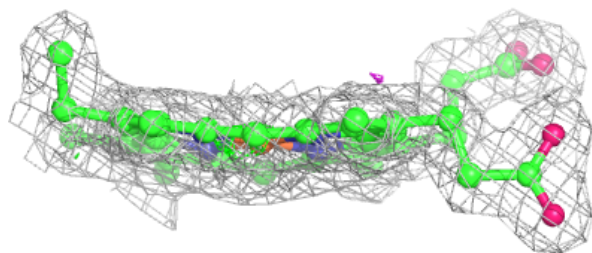
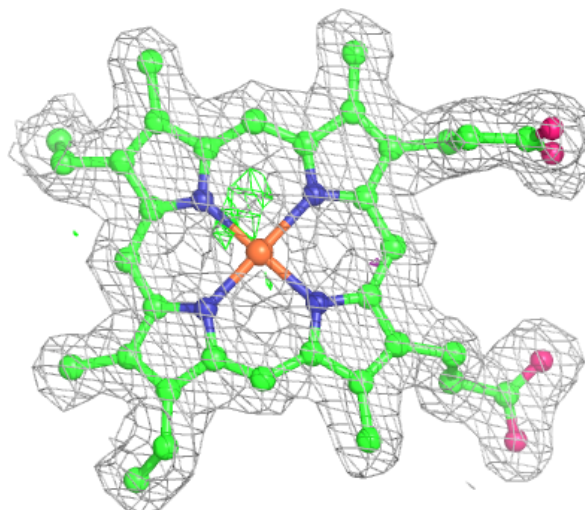
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





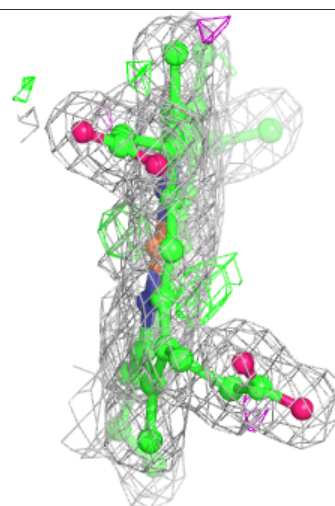
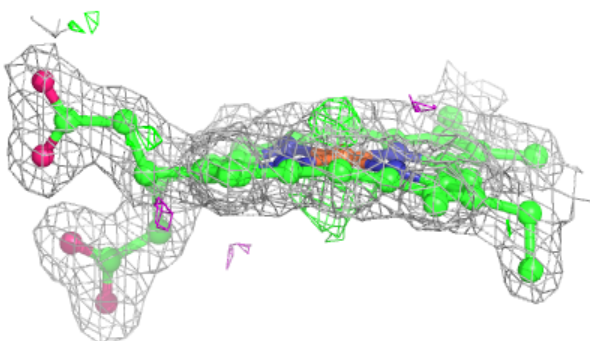
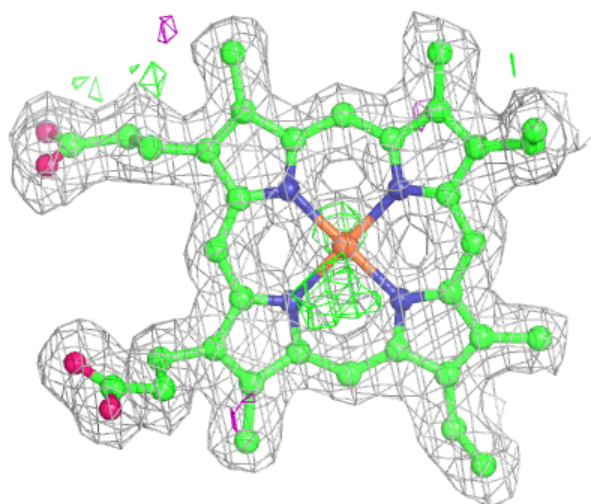
**Electron density around HEC B 600:**

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



**Electron density around HEC 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 ⓘ

There are no such residues in this entry.