



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 01:03 PM BST

PDB ID : 3SWS  
Title : Crystal Structure of the Quinone Form of Methylamine Dehydrogenase in Complex with the Diferric Form of MauG  
Authors : Jensen, L.M.R.; Wilmot, C.M.  
Deposited on : 2011-07-14  
Resolution : 1.86 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 : 2.13.1  
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) : 2.13.1

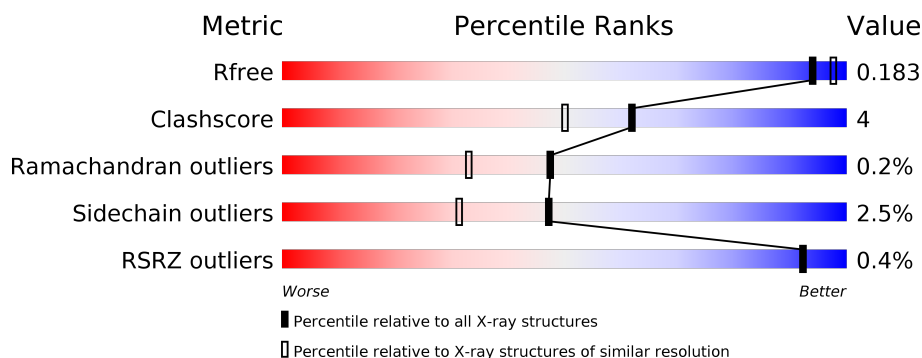
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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>83%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	373	<div> <div></div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	C	137	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>8%</div> </div> </div>
2	E	137	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>9%</div> </div> </div>
3	D	386	<div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div>
3	F	386	<div> <div></div> <div>87%</div> <div>10%</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	EDO	D	388	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 15667 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	3	0
			2753	1721	494	527	11			
1	B	354	Total	C	N	O	S	0	8	0
			2781	1740	495	534	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	126	Total	C	N	O	S	0	2	0
			979	605	167	194	13			
2	E	125	Total	C	N	O	S	0	2	0
			964	596	161	193	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	EXPRESSION TAG	UNP P22619
C	133	HIS	-	EXPRESSION TAG	UNP P22619
C	134	HIS	-	EXPRESSION TAG	UNP P22619
C	135	HIS	-	EXPRESSION TAG	UNP P22619
C	136	HIS	-	EXPRESSION TAG	UNP P22619
C	137	HIS	-	EXPRESSION TAG	UNP P22619
E	132	HIS	-	EXPRESSION TAG	UNP P22619
E	133	HIS	-	EXPRESSION TAG	UNP P22619
E	134	HIS	-	EXPRESSION TAG	UNP P22619
E	135	HIS	-	EXPRESSION TAG	UNP P22619
E	136	HIS	-	EXPRESSION TAG	UNP P22619
E	137	HIS	-	EXPRESSION TAG	UNP P22619

- 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	12	0
			2994	1904	508	574	8			
3	F	376	Total	C	N	O	S	0	5	0
			2952	1874	504	566	8			

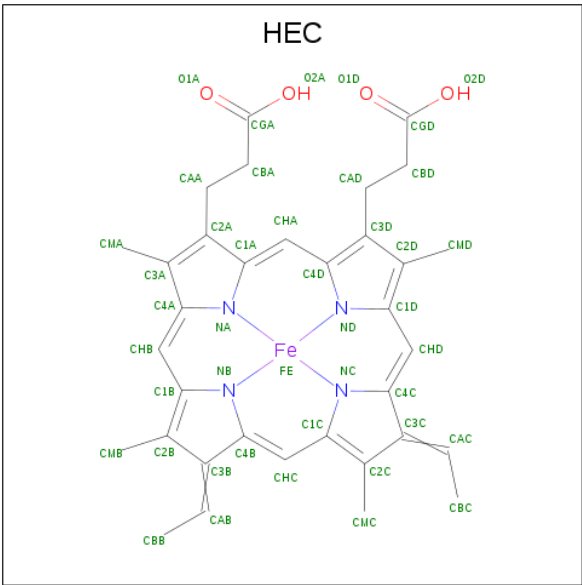
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

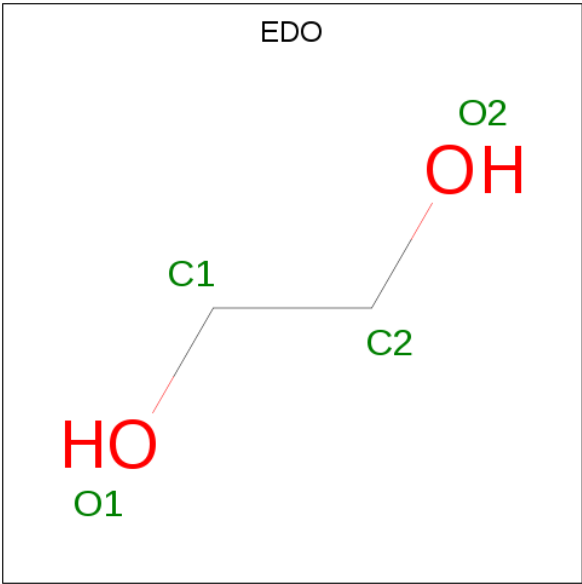
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	2	Total	Na	0	0
			2	2		

- 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>).



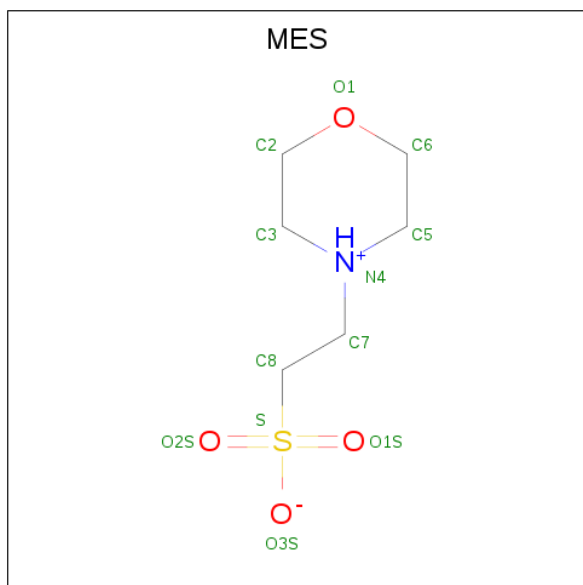
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



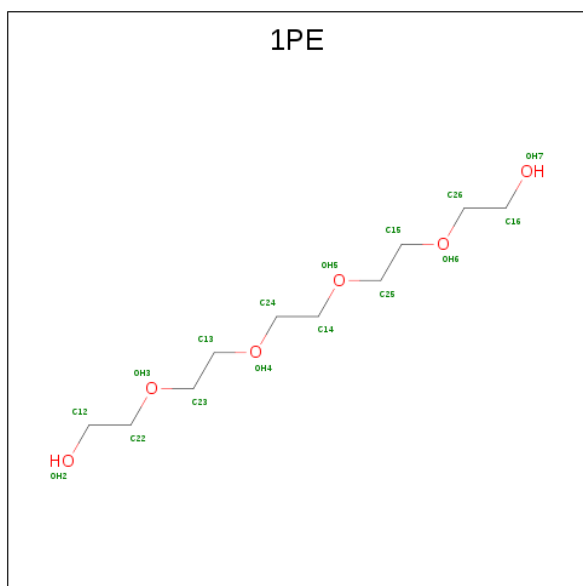
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			4	2	2		

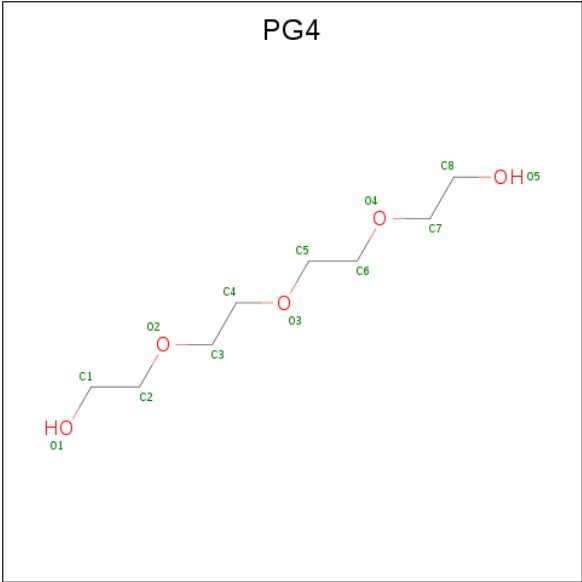
- Molecule 10 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



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

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).





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

- Molecule 12 is water.

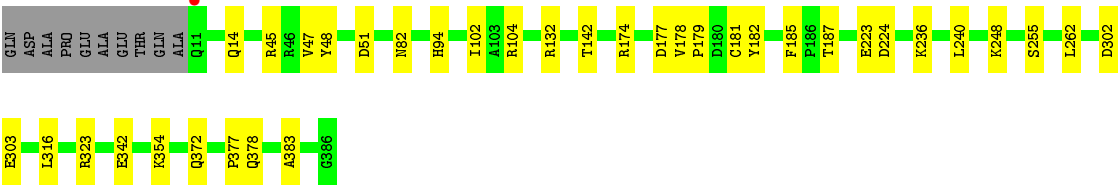
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	359	Total	O	0	0
			359	359		
12	B	415	Total	O	0	0
			415	415		
12	C	151	Total	O	0	0
			151	151		
12	D	475	Total	O	0	0
			475	475		
12	E	131	Total	O	0	0
			131	131		
12	F	478	Total	O	0	0
			478	478		



Chain D: 

88%

9%

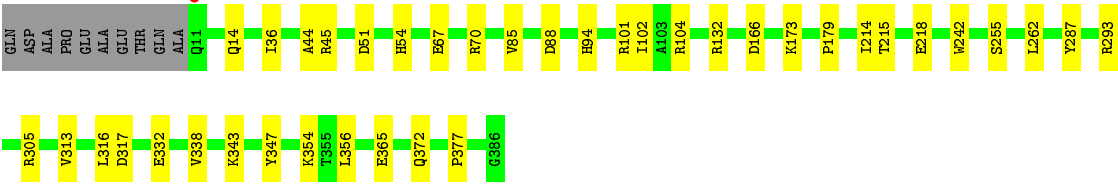


• Molecule 3: Methylamine dehydrogenase heavy chain

Chain F: 

87%

10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.22Å 99.42Å 102.83Å 64.77° 74.77° 75.14°	Depositor
Resolution (Å)	49.12 – 1.86 49.11 – 1.86	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.12-1.86) 97.1 (49.11-1.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.136 , 0.178 0.142 , 0.183	Depositor DCC
$R_{free}$ test set	7734 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,h-k,h-l 0.009 for -h,-l,-k 0.004 for -h,-h+l,-h+k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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, MES, HEC, TRQ

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	1.13	1/2826 (0.0%)	1.01	13/3834 (0.3%)
1	B	1.20	3/2869 (0.1%)	1.07	12/3891 (0.3%)
2	C	1.36	5/994 (0.5%)	1.09	3/1357 (0.2%)
2	E	1.21	2/978 (0.2%)	0.97	1/1335 (0.1%)
3	D	1.29	7/3107 (0.2%)	1.06	7/4231 (0.2%)
3	F	1.26	9/3044 (0.3%)	1.02	7/4147 (0.2%)
All	All	1.23	27/13818 (0.2%)	1.04	43/18795 (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
1	B	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	62	TYR	CD2-CE2	7.32	1.50	1.39
3	D	48	TYR	CE1-CZ	6.86	1.47	1.38
3	D	342	GLU	C-O	6.15	1.35	1.23
3	F	287	TYR	CD1-CE1	6.03	1.48	1.39
3	F	242	TRP	CE3-CZ3	5.86	1.48	1.38
1	A	265	LYS	CD-CE	5.76	1.65	1.51
2	C	25	TYR	CE1-CZ	5.72	1.46	1.38
1	B	167	GLU	CD-OE2	5.64	1.31	1.25
3	D	185	PHE	CE2-CZ	5.63	1.48	1.37
2	C	13	TRP	CZ3-CH2	5.56	1.49	1.40
1	B	30	SER	CB-OG	5.49	1.49	1.42
2	C	80	TYR	CD1-CE1	5.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	48	TYR	CD1-CE1	5.44	1.47	1.39
2	C	98	TYR	CE2-CZ	5.40	1.45	1.38
2	C	30	SER	CB-OG	5.38	1.49	1.42
3	D	48	TYR	CG-CD2	5.37	1.46	1.39
3	F	85	VAL	CB-CG2	5.30	1.64	1.52
3	F	218	GLU	CD-OE1	5.30	1.31	1.25
1	B	162	TYR	CD2-CE2	5.27	1.47	1.39
2	E	51	LYS	CD-CE	5.23	1.64	1.51
3	F	338	VAL	CB-CG2	5.22	1.63	1.52
3	F	313	VAL	CB-CG2	5.20	1.63	1.52
3	F	332	GLU	CB-CG	5.18	1.61	1.52
3	F	44	ALA	CA-CB	5.16	1.63	1.52
3	F	67	GLU	CD-OE2	-5.08	1.20	1.25
3	D	383	ALA	CA-CB	5.02	1.62	1.52
3	D	47	VAL	CB-CG1	5.02	1.63	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	B	180	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	B	118	ASP	CB-CG-OD1	7.79	125.31	118.30
3	D	224	ASP	CB-CG-OD1	7.58	125.12	118.30
3	F	104	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	127	ARG	NE-CZ-NH2	7.49	124.04	120.30
3	D	323	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	A	208	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	127	ARG	NE-CZ-NH1	-6.82	116.89	120.30
3	F	101	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	82	ASP	CB-CG-OD2	6.74	124.36	118.30
1	B	352	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	A	202[A]	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	202[B]	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	150	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	B	112	VAL	CG1-CB-CG2	6.37	121.09	110.90
3	F	132	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	202[A]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	202[B]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
3	D	302	ASP	CB-CG-OD1	-6.13	112.79	118.30
3	D	45	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	B	321	ARG	NE-CZ-NH2	-6.02	117.29	120.30
3	D	132	ARG	NE-CZ-NH2	-6.01	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	317	ASP	CB-CG-OD1	5.77	123.50	118.30
2	C	71	LEU	CB-CG-CD1	5.77	120.81	111.00
3	D	240	LEU	CB-CG-CD2	-5.72	101.27	111.00
3	D	104	ARG	NE-CZ-NH2	-5.60	117.50	120.30
3	F	305	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	243	ASP	CB-CG-OD1	5.51	123.26	118.30
2	C	24	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	99	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	147	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	203	LEU	CB-CG-CD1	-5.43	101.78	111.00
1	A	147	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	150	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	75	LEU	CA-CB-CG	-5.25	103.23	115.30
2	E	19	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	300	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	243	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	B	243	ASP	CB-CA-C	-5.12	100.17	110.40
2	C	75	ARG	NE-CZ-NH2	-5.10	117.75	120.30
3	F	88	ASP	CB-CG-OD1	5.07	122.86	118.30
3	F	215	THR	CB-CA-C	-5.01	98.06	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	358	LEU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2753	0	2639	26	0
1	B	2781	0	2672	32	0
2	C	979	0	883	10	0
2	E	964	0	868	8	0
3	D	2994	0	2906	20	0
3	F	2952	0	2847	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
6	B	86	0	60	1	0
7	A	4	0	6	0	0
7	B	4	0	6	1	0
7	D	4	0	6	9	0
8	D	12	0	12	1	0
9	D	4	0	3	0	0
10	D	16	0	22	5	0
11	F	13	0	18	6	0
12	A	359	0	0	4	0
12	B	415	0	0	9	0
12	C	151	0	0	3	0
12	D	475	0	0	7	0
12	E	131	0	0	2	0
12	F	478	0	0	9	0
All	All	15667	0	13008	117	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 4.

All (117) 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:F:372[A]:GLN:OE1	12:F:1498:HOH:O	1.62	1.17
1:B:26[A]:ASN:ND2	12:B:2258:HOH:O	1.82	1.10
1:B:46[B]:GLU:HG2	1:B:51:LEU:HD12	1.40	0.99
3:F:372[B]:GLN:NE2	12:F:1047:HOH:O	2.02	0.93
1:B:48:LYS:H	1:B:62:HIS:HE1	1.03	0.93
1:B:48:LYS:H	1:B:62:HIS:CE1	1.90	0.89
1:A:197[B]:ILE:HD12	1:A:202[B]:ARG:HD3	1.57	0.87
1:A:202[B]:ARG:HD2	1:A:206:MET:HG3	1.57	0.85
2:C:21:GLN:HE22	3:F:14[B]:GLN:HE21	1.23	0.85
1:A:48:LYS:H	1:A:62:HIS:HE1	1.25	0.82
1:B:46[B]:GLU:HG2	1:B:51:LEU:CD1	2.08	0.82
3:D:378:GLN:OE1	7:D:388:EDO:H11	1.81	0.81
1:A:202[B]:ARG:CD	1:A:206:MET:HG3	2.12	0.80
2:C:99[A]:ARG:NH2	12:C:1827:HOH:O	2.07	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LYS:HE2	12:B:872:HOH:O	1.80	0.79
1:B:84:ASN:C	1:B:84:ASN:HD22	1.85	0.77
11:F:387:PG4:H21	12:F:851:HOH:O	1.87	0.74
1:B:243:ASP:HB2	12:B:2194:HOH:O	1.88	0.72
3:F:365[B]:GLU:OE1	12:F:1090:HOH:O	2.05	0.72
1:A:197[B]:ILE:CD1	1:A:202[B]:ARG:HD3	2.20	0.71
3:D:378:GLN:OE1	7:D:388:EDO:C1	2.38	0.71
10:D:390:1PE:H132	12:D:1365:HOH:O	1.90	0.71
12:C:1655:HOH:O	3:F:36[A]:ILE:HD11	1.90	0.70
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.60	0.66
2:C:57:TRQ:HB2	2:C:108:TRP:NE1	2.10	0.66
1:B:82:ASP:OD2	1:B:84:ASN:ND2	2.29	0.66
3:D:255:SER:HA	10:D:390:1PE:H141	1.77	0.65
1:B:46[B]:GLU:CG	1:B:51:LEU:CD1	2.75	0.64
1:A:48:LYS:H	1:A:62:HIS:CE1	2.13	0.63
3:D:236[A]:LYS:NZ	12:D:976:HOH:O	2.11	0.62
1:A:107:PRO:HG3	12:A:2200:HOH:O	1.99	0.62
1:B:98:ASP:H	1:B:102[B]:GLN:HE21	1.45	0.62
2:E:57:TRQ:HB2	2:E:108:TRP:NE1	2.15	0.62
11:F:387:PG4:H72	12:F:851:HOH:O	1.99	0.61
1:B:88:LYS:CE	12:B:872:HOH:O	2.43	0.61
10:D:390:1PE:C13	12:D:1365:HOH:O	2.46	0.60
11:F:387:PG4:H51	12:F:851:HOH:O	2.02	0.60
1:B:197:ILE:O	1:B:202:ARG:HD2	2.02	0.59
6:A:600:HEC:HBC3	6:A:600:HEC:HMC1	1.83	0.59
1:A:102[A]:GLN:HG2	12:A:1802:HOH:O	2.01	0.59
1:B:48:LYS:N	1:B:62:HIS:HE1	1.87	0.58
12:E:1528:HOH:O	3:F:54:HIS:HD2	1.86	0.58
3:D:372[B]:GLN:NE2	12:D:1255:HOH:O	2.37	0.57
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.69	0.57
2:C:57:TRQ:HB2	2:C:108:TRP:HE1	1.70	0.56
1:A:353:ARG:HG2	1:A:353:ARG:HH11	1.70	0.56
1:B:98:ASP:H	1:B:102[B]:GLN:NE2	2.03	0.56
1:A:202[B]:ARG:HD2	1:A:206:MET:CG	2.34	0.55
1:A:61:SER:HB3	1:A:112:VAL:HB	1.88	0.55
3:F:51:ASP:HA	3:F:377:PRO:HA	1.88	0.55
3:D:236[B]:LYS:NZ	12:D:976:HOH:O	2.39	0.54
3:D:378:GLN:HE22	7:D:388:EDO:C1	2.21	0.54
3:D:51:ASP:HA	3:D:377:PRO:HA	1.90	0.54
1:B:84:ASN:C	1:B:84:ASN:ND2	2.60	0.53
1:B:84:ASN:HD21	1:B:86:LYS:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:372[A]:GLN:HE22	2:E:86:CYS:H	1.55	0.53
1:A:352:ARG:HD3	12:A:2029:HOH:O	2.09	0.52
2:C:86:CYS:H	3:F:372[A]:GLN:HE22	1.58	0.52
1:A:299:SER:HB2	1:A:333:MET:HG3	1.92	0.51
1:B:209:LYS:NZ	12:B:751:HOH:O	2.44	0.51
1:A:81:ARG:CZ	1:A:85:GLY:HA2	2.41	0.50
7:D:388:EDO:H21	12:D:695:HOH:O	2.10	0.50
3:D:187:THR:O	10:D:390:1PE:H241	2.11	0.50
1:A:357:LEU:C	1:A:359:GLU:H	2.15	0.50
11:F:387:PG4:H32	12:F:851:HOH:O	2.12	0.49
2:C:101[B]:GLU:HG2	2:C:102:PHE:CD2	2.47	0.49
1:B:232[B]:GLU:HG2	12:B:1486:HOH:O	2.13	0.48
10:D:390:1PE:HO7	10:D:390:1PE:HO2	1.61	0.48
3:D:378:GLN:HE22	7:D:388:EDO:H12	1.78	0.48
3:D:378:GLN:NE2	7:D:388:EDO:H12	2.28	0.47
2:E:75:ARG:HD2	12:E:394:HOH:O	2.14	0.47
1:A:60:GLN:O	1:A:62:HIS:HD2	1.98	0.47
1:B:60:GLN:O	1:B:62:HIS:HD2	1.98	0.46
1:A:163:GLN:HE22	6:A:500:HEC:HMA1	1.81	0.46
1:B:352:ARG:NH2	1:B:352:ARG:HG3	2.30	0.46
1:B:347:GLU:OE1	7:B:374:EDO:H21	2.15	0.46
3:F:347:TYR:HB3	3:F:356:LEU:HD11	1.98	0.46
1:A:25:ARG:HD3	12:A:1834:HOH:O	2.14	0.46
3:D:181:CYS:C	3:D:182:TYR:CD1	2.89	0.46
3:F:179:PRO:HD3	3:F:214:ILE:HD13	1.98	0.46
1:B:197:ILE:O	1:B:202:ARG:CD	2.64	0.45
3:D:178:VAL:HB	3:D:179:PRO:CD	2.46	0.45
3:F:14[A]:GLN:HE21	3:F:70:ARG:HH11	1.65	0.44
3:D:248:LYS:HE2	3:D:248:LYS:HB2	1.61	0.44
12:B:2119:HOH:O	2:E:127:VAL:HG12	2.16	0.44
3:F:54:HIS:HE1	12:F:618:HOH:O	1.99	0.44
1:B:352:ARG:HH21	1:B:352:ARG:HG3	1.81	0.44
3:D:372[A]:GLN:NE2	2:E:86:CYS:H	2.16	0.44
8:D:387:MES:H32	8:D:387:MES:H82	1.64	0.44
1:A:29:GLN:HG2	1:A:57:ASP:HB2	2.00	0.43
1:B:35:HIS:CE1	1:B:67:THR:HG23	2.53	0.43
3:D:82:ASN:HB3	3:D:142:THR:HB	1.99	0.43
3:D:378:GLN:NE2	7:D:388:EDO:C1	2.81	0.43
3:F:166:ASP:HB2	3:F:173:LYS:HD3	2.01	0.43
3:F:255:SER:HA	11:F:387:PG4:H32	2.00	0.43
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:255:SER:O	12:F:851:HOH:O	2.22	0.42
1:A:353:ARG:NH1	1:A:353:ARG:HG2	2.35	0.42
1:A:354:TYR:O	1:A:357:LEU:HB2	2.19	0.42
3:F:45:ARG:NH2	3:F:343:LYS:O	2.53	0.42
1:A:296:LYS:HE2	1:A:296:LYS:HB2	1.94	0.41
1:A:357:LEU:O	1:A:359:GLU:N	2.53	0.41
1:B:21:PRO:O	1:B:27:ALA:HA	2.19	0.41
2:C:99[A]:ARG:NH2	12:C:2195:HOH:O	2.50	0.41
3:F:255:SER:HA	11:F:387:PG4:C3	2.51	0.41
2:C:68:GLN:HB2	2:C:70:TYR:CE1	2.55	0.41
1:A:200:ASN:O	6:A:600:HEC:HMC3	2.21	0.41
1:B:107:PRO:HG3	12:B:407:HOH:O	2.21	0.41
1:B:327:GLU:OE2	12:B:1719:HOH:O	2.22	0.41
7:D:388:EDO:C2	12:D:695:HOH:O	2.67	0.41
1:A:197[B]:ILE:HD12	1:A:197[B]:ILE:HA	1.86	0.41
1:B:355:GLU:N	1:B:356:PRO:CD	2.85	0.40
1:B:272:VAL:HG21	6:B:600:HEC:HMA3	2.02	0.40
2:C:80:TYR:HB2	2:C:120:HIS:HB2	2.04	0.40
3:D:378:GLN:HE22	7:D:388:EDO:C2	2.34	0.40
2:E:55:ALA:HB2	2:E:110:PHE:HB2	2.04	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	355/373 (95%)	346 (98%)	8 (2%)	1 (0%)	41	26
1	B	360/373 (96%)	350 (97%)	9 (2%)	1 (0%)	41	26
2	C	125/137 (91%)	120 (96%)	5 (4%)	0	100	100
2	E	124/137 (90%)	121 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	386/386 (100%)	372 (96%)	12 (3%)	2 (0%)	29	15
3	F	379/386 (98%)	365 (96%)	13 (3%)	1 (0%)	41	26
All	All	1729/1792 (96%)	1674 (97%)	50 (3%)	5 (0%)	47	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	ASP
1	A	358	LEU
3	D	102[A]	ILE
3	D	102[B]	ILE
3	F	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	279/292 (96%)	267 (96%)	12 (4%)	29	12
1	B	284/292 (97%)	279 (98%)	5 (2%)	59	45
2	C	107/112 (96%)	105 (98%)	2 (2%)	57	43
2	E	106/112 (95%)	103 (97%)	3 (3%)	43	27
3	D	316/311 (102%)	305 (96%)	11 (4%)	36	18
3	F	309/311 (99%)	304 (98%)	5 (2%)	62	49
All	All	1401/1430 (98%)	1363 (97%)	38 (3%)	47	29

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	23	LEU
1	A	112	VAL
1	A	157	GLU
1	A	202[A]	ARG

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Mol	Chain	Res	Type
1	A	202[B]	ARG
1	A	209	LYS
1	A	219	THR
1	A	236	GLU
1	A	323	LEU
1	A	357	LEU
1	A	359	GLU
1	B	8	ASP
1	B	23	LEU
1	B	84	ASN
1	B	219	THR
1	B	359	GLU
2	C	68	GLN
2	C	71	LEU
3	D	14[A]	GLN
3	D	14[B]	GLN
3	D	94	HIS
3	D	174	ARG
3	D	177	ASP
3	D	223[A]	GLU
3	D	223[B]	GLU
3	D	303[A]	GLU
3	D	303[B]	GLU
3	D	316	LEU
3	D	354	LYS
2	E	16	GLN
2	E	71	LEU
2	E	131	SER
3	F	94	HIS
3	F	262	LEU
3	F	293	ARG
3	F	316	LEU
3	F	354	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	91	GLN
1	A	163	GLN
1	A	210	GLN
1	B	62	HIS

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Mol	Chain	Res	Type
1	B	84	ASN
1	B	210	GLN
3	F	54	HIS

### 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	TRQ	E	57	2	13,17,18	3.18	3 (23%)	14,24,26	2.80	4 (28%)
2	TRQ	C	57	2	13,17,18	3.14	6 (46%)	14,24,26	2.88	6 (42%)

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	TRQ	E	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	C	57	2	-	0/4/19/21	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	TRQ	CH2-CZ2	-8.06	1.45	1.54
2	E	57	TRQ	CZ3-CE3	7.16	1.46	1.34
2	C	57	TRQ	CH2-CZ2	-6.93	1.46	1.54
2	C	57	TRQ	CZ3-CE3	6.48	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	TRQ	O7-CZ2	3.91	1.31	1.23
2	C	57	TRQ	CE2-CZ2	-2.96	1.46	1.50
2	E	57	TRQ	O7-CZ2	2.84	1.29	1.23
2	C	57	TRQ	CB-CG	-2.26	1.48	1.51
2	C	57	TRQ	CD2-CE3	-2.19	1.40	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	TRQ	CZ2-CE2-NE1	6.59	130.46	119.94
2	C	57	TRQ	O6-CH2-CZ2	-6.12	114.34	118.51
2	C	57	TRQ	CZ2-CE2-NE1	5.69	129.02	119.94
2	E	57	TRQ	O6-CH2-CZ2	-5.39	114.84	118.51
2	E	57	TRQ	CB-CG-CD1	-4.65	122.22	127.97
2	C	57	TRQ	CB-CG-CD1	-3.82	123.24	127.97
2	C	57	TRQ	O7-CZ2-CH2	2.92	122.43	119.00
2	C	57	TRQ	CZ3-CH2-CZ2	2.51	122.15	118.72
2	C	57	TRQ	CB-CA-C	2.18	115.56	111.47
2	E	57	TRQ	O6-CH2-CZ3	2.08	125.27	121.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	1.57	4 (15%)	18,82,82	3.35	10 (55%)
6	HEC	A	500	1,12	26,50,50	1.56	7 (26%)	18,82,82	2.82	5 (27%)
11	PG4	F	387	-	12,12,12	0.37	0	11,11,11	0.55	0
6	HEC	B	600	1	26,50,50	1.44	5 (19%)	18,82,82	2.56	8 (44%)
7	EDO	A	374	-	3,3,3	0.52	0	2,2,2	0.26	0
8	MES	D	387	-	12,12,12	1.70	1 (8%)	14,16,16	3.04	7 (50%)
10	1PE	D	390	-	15,15,15	0.46	0	14,14,14	0.66	0
6	HEC	B	500	1,12	26,50,50	1.83	5 (19%)	18,82,82	2.77	8 (44%)
7	EDO	D	388	-	3,3,3	1.69	0	2,2,2	2.29	1 (50%)
9	ACT	D	389	-	1,3,3	3.76	1 (100%)	0,3,3	0.00	-
7	EDO	B	374	-	3,3,3	0.74	0	2,2,2	0.75	0

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	A	500	1,12	-	0/6/54/54	-
11	PG4	F	387	-	-	5/10/10/10	-
6	HEC	B	600	1	-	0/6/54/54	-
7	EDO	A	374	-	-	1/1/1/1	-
8	MES	D	387	-	-	2/6/14/14	0/1/1/1
10	1PE	D	390	-	-	7/13/13/13	-
6	HEC	B	500	1,12	-	0/6/54/54	-
7	EDO	D	388	-	-	0/1/1/1	-
7	EDO	B	374	-	-	1/1/1/1	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	387	MES	C8-S	-5.08	1.70	1.77
6	B	500	HEC	C4A-C3A	4.84	1.53	1.42
6	A	600	HEC	C3B-C2B	-4.75	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	389	ACT	CH3-C	3.76	1.53	1.48
6	B	500	HEC	C3C-C4C	3.76	1.49	1.43
6	B	500	HEC	C1A-C2A	3.62	1.50	1.42
6	A	500	HEC	C3C-C4C	3.53	1.49	1.43
6	B	600	HEC	C3B-C2B	-2.93	1.37	1.40
6	A	500	HEC	C1A-C2A	2.88	1.49	1.42
6	A	500	HEC	C4A-C3A	2.78	1.48	1.42
6	B	600	HEC	C3C-C4C	2.58	1.47	1.43
6	B	600	HEC	C4A-C3A	2.50	1.48	1.42
6	B	600	HEC	C1D-CHD	2.50	1.47	1.41
6	A	600	HEC	C4D-CHA	2.45	1.47	1.41
6	A	600	HEC	C4D-ND	-2.43	1.31	1.36
6	B	600	HEC	C4D-CHA	2.42	1.47	1.41
6	B	500	HEC	C3B-C2B	-2.36	1.38	1.40
6	A	500	HEC	C1D-CHD	2.31	1.47	1.41
6	A	500	HEC	C3B-C4B	2.19	1.47	1.43
6	A	500	HEC	C1C-CHC	2.17	1.47	1.41
6	B	500	HEC	C1B-CHB	2.16	1.47	1.41
6	A	600	HEC	C1C-CHC	2.14	1.47	1.41
6	A	500	HEC	C4D-CHA	2.02	1.46	1.41

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	HEC	CBD-CAD-C3D	-8.06	97.62	112.49
6	A	500	HEC	CBD-CAD-C3D	-6.41	100.67	112.49
8	D	387	MES	C5-N4-C3	6.39	123.22	108.83
8	D	387	MES	C6-C5-N4	-6.09	100.87	110.10
6	B	600	HEC	CBD-CAD-C3D	-6.01	101.39	112.49
6	A	500	HEC	CMB-C2B-C3B	5.85	132.70	125.82
6	B	500	HEC	CMB-C2B-C3B	5.76	132.59	125.82
6	B	500	HEC	CBD-CAD-C3D	-5.49	102.37	112.49
6	A	600	HEC	C1D-C2D-C3D	-5.42	103.23	107.00
6	A	600	HEC	CMC-C2C-C3C	4.90	131.58	125.82
6	B	600	HEC	CMC-C2C-C3C	4.07	130.60	125.82
6	A	600	HEC	CBA-CAA-C2A	-4.05	105.02	112.48
6	A	500	HEC	CMC-C2C-C3C	3.98	130.50	125.82
6	B	500	HEC	CMB-C2B-C1B	-3.85	122.55	128.46
6	A	600	HEC	CMD-C2D-C3D	3.85	132.20	124.94
6	B	600	HEC	CMB-C2B-C3B	3.75	130.23	125.82
6	A	500	HEC	CMB-C2B-C1B	-3.68	122.81	128.46
6	B	500	HEC	CMC-C2C-C3C	3.61	130.06	125.82

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	387	MES	O1S-S-C8	-3.53	102.66	106.92
6	B	600	HEC	CBA-CAA-C2A	-3.42	106.18	112.48
8	D	387	MES	C2-C3-N4	-3.38	104.98	110.10
7	D	388	EDO	O1-C1-C2	3.21	135.02	111.91
6	B	500	HEC	CBA-CAA-C2A	-3.15	106.67	112.48
6	A	600	HEC	CAD-CBD-CGD	-3.10	107.47	112.67
6	B	600	HEC	CMA-C3A-C2A	2.94	130.48	124.94
6	B	500	HEC	C1D-C2D-C3D	-2.90	104.98	107.00
8	D	387	MES	C7-N4-C3	2.85	118.52	111.23
6	A	600	HEC	CMC-C2C-C1C	-2.77	124.21	128.46
8	D	387	MES	C7-N4-C5	2.75	118.26	111.23
6	A	600	HEC	CMA-C3A-C2A	2.68	129.99	124.94
6	A	600	HEC	CMD-C2D-C1D	-2.64	124.41	128.46
6	A	500	HEC	C4B-C3B-C2B	-2.63	103.52	106.35
6	A	600	HEC	C4B-C3B-C2B	-2.62	103.52	106.35
6	B	600	HEC	C4C-C3C-C2C	-2.34	103.83	106.35
6	B	500	HEC	CMD-C2D-C3D	2.28	129.25	124.94
6	B	600	HEC	CMC-C2C-C1C	-2.18	125.11	128.46
6	B	600	HEC	CAA-CBA-CGA	-2.15	109.07	112.67
8	D	387	MES	C6-O1-C2	2.14	117.03	109.89
6	B	500	HEC	C4B-C3B-C2B	-2.07	104.12	106.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

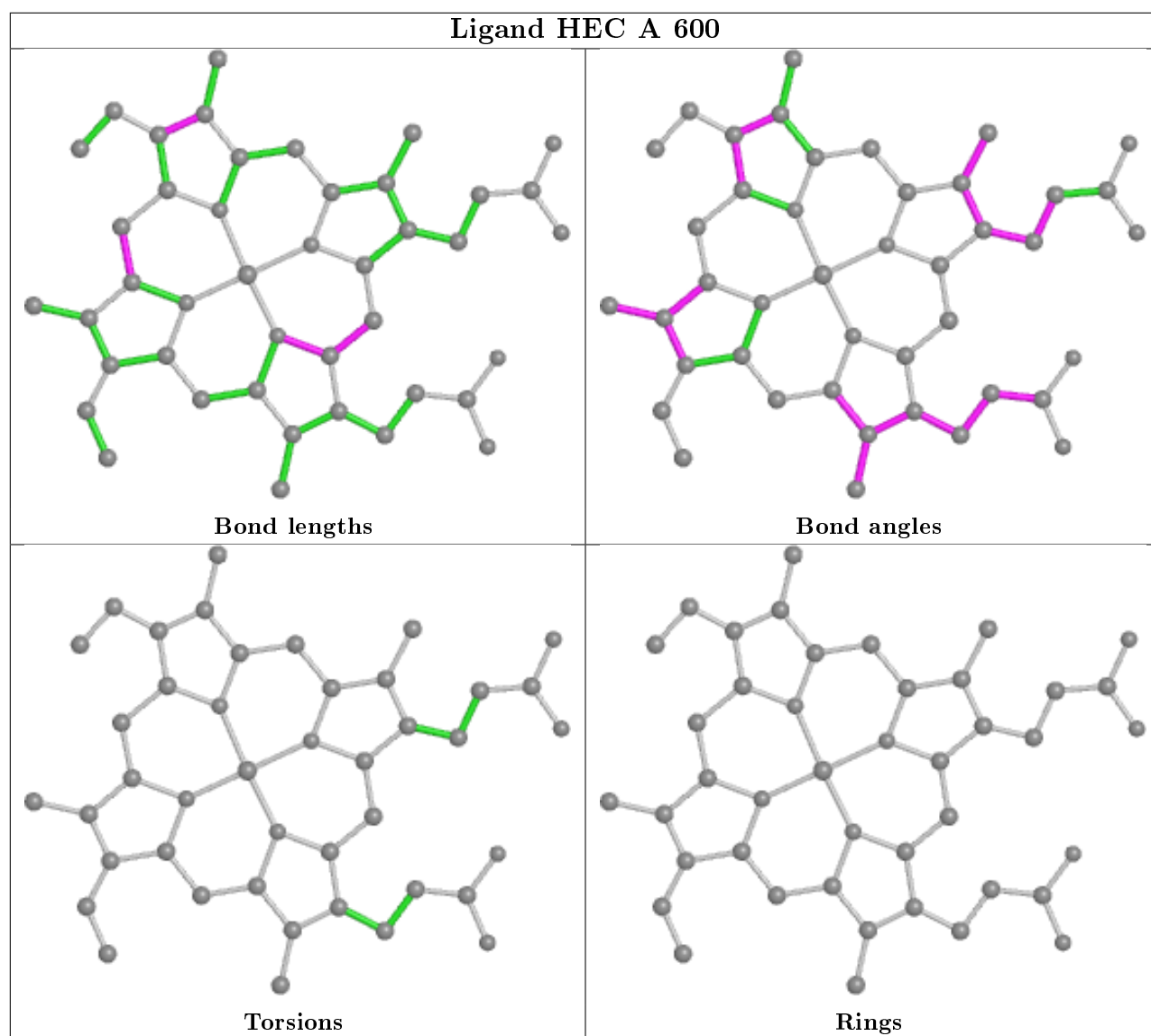
Mol	Chain	Res	Type	Atoms
8	D	387	MES	C8-C7-N4-C3
10	D	390	1PE	OH4-C13-C23-OH3
10	D	390	1PE	OH5-C14-C24-OH4
10	D	390	1PE	OH2-C12-C22-OH3
11	F	387	PG4	O2-C3-C4-O3
10	D	390	1PE	C13-C23-OH3-C22
8	D	387	MES	C8-C7-N4-C5
7	A	374	EDO	O1-C1-C2-O2
10	D	390	1PE	C12-C22-OH3-C23
10	D	390	1PE	C23-C13-OH4-C24
11	F	387	PG4	O1-C1-C2-O2
11	F	387	PG4	O3-C5-C6-O4
11	F	387	PG4	C4-C3-O2-C2
11	F	387	PG4	C3-C4-O3-C5
7	B	374	EDO	O1-C1-C2-O2
10	D	390	1PE	C14-C24-OH4-C13

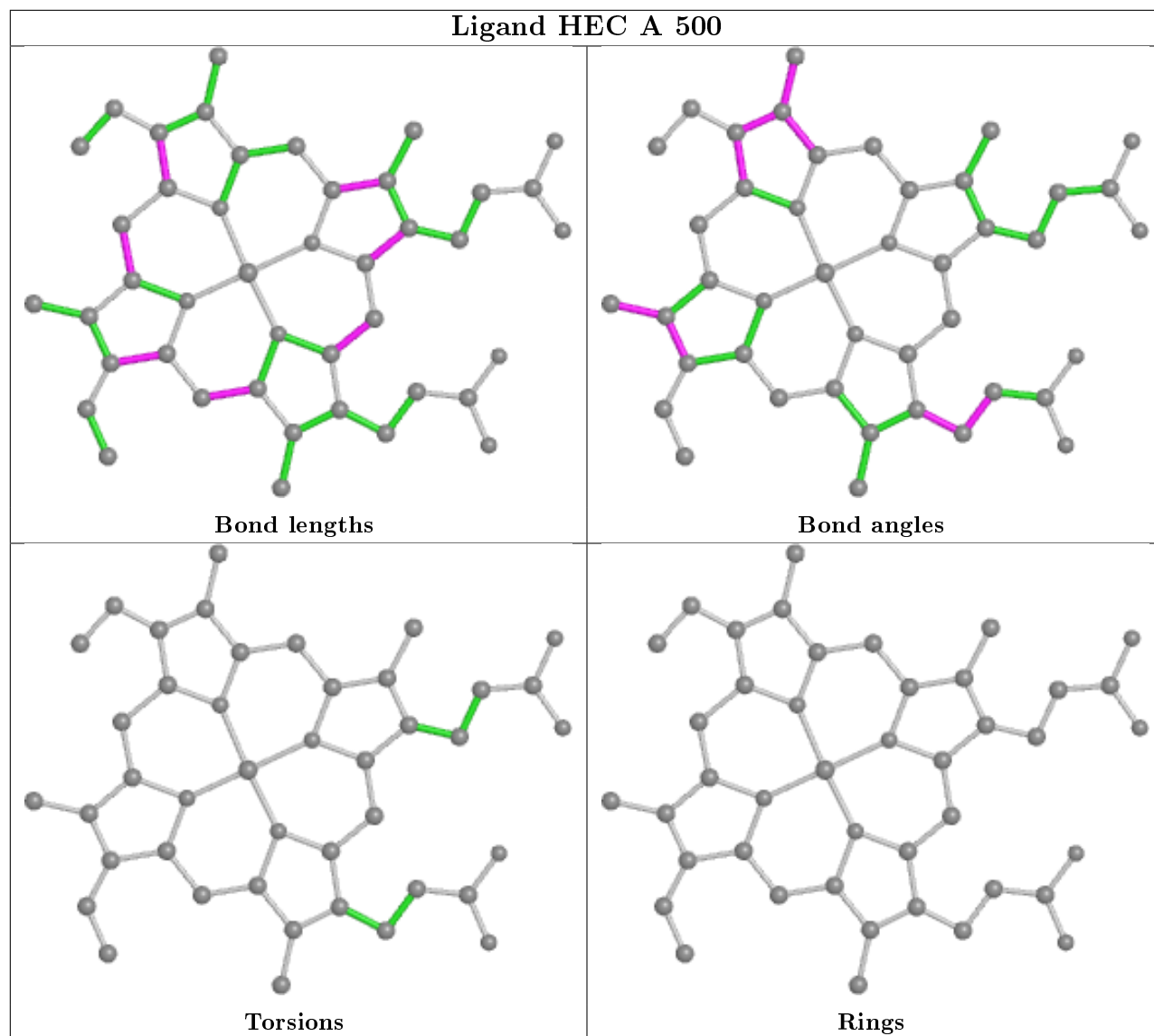
There are no ring outliers.

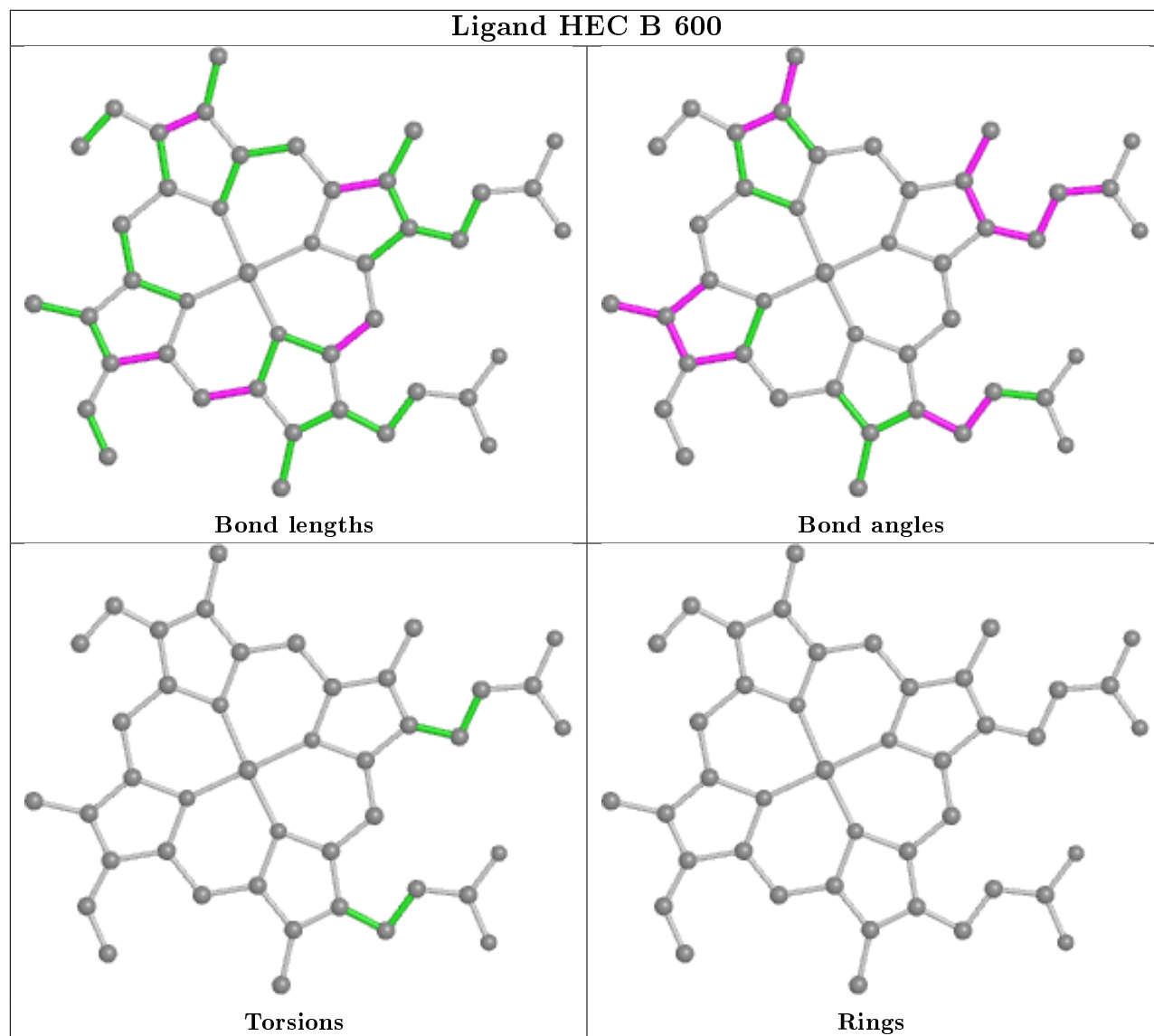
8 monomers are involved in 26 short contacts:

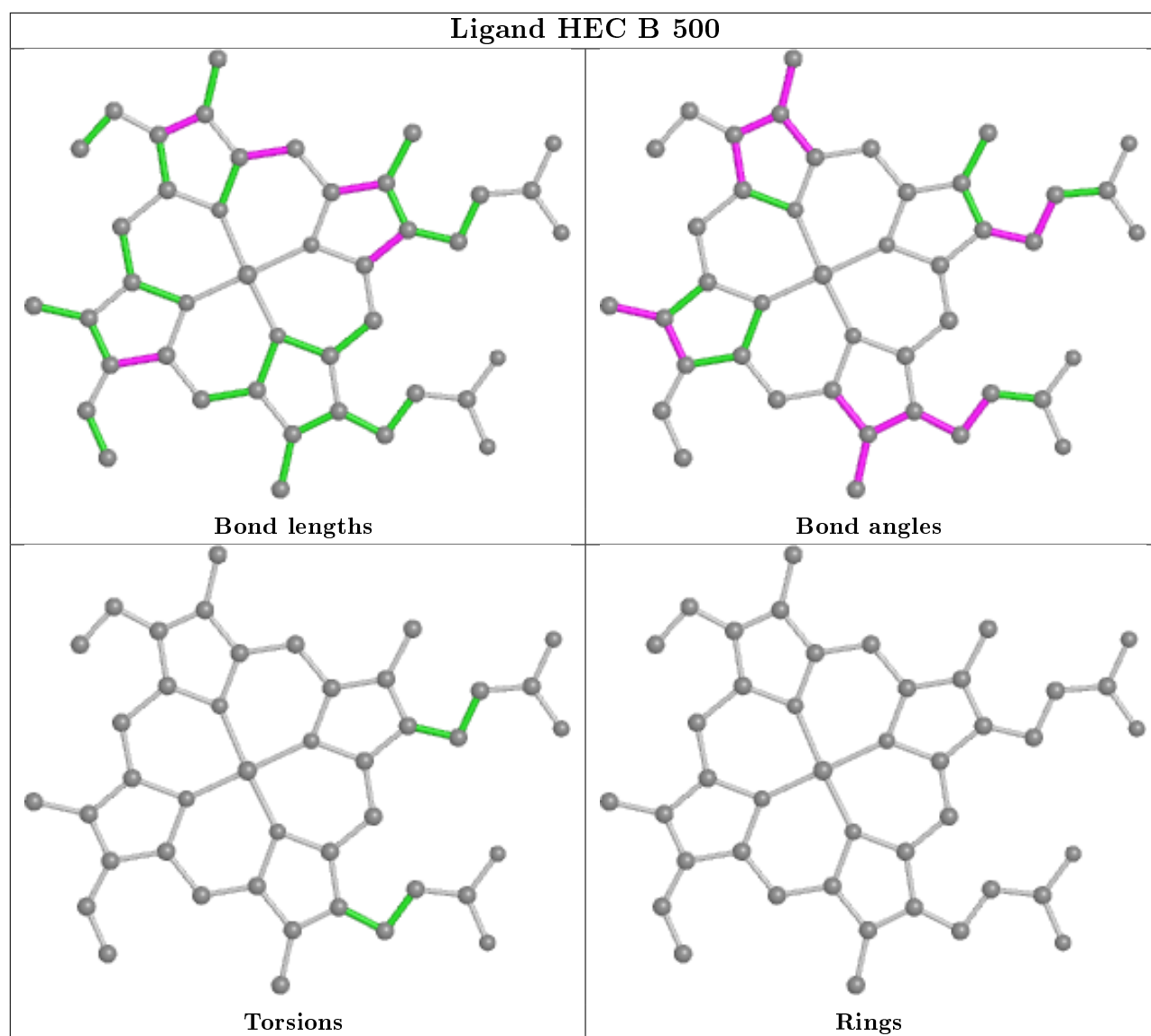
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	600	HEC	2	0
6	A	500	HEC	1	0
11	F	387	PG4	6	0
6	B	600	HEC	1	0
8	D	387	MES	1	0
10	D	390	1PE	5	0
7	D	388	EDO	9	0
7	B	374	EDO	1	0

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.58	2 (0%) 89 89	14, 23, 38, 58	0
1	B	354/373 (94%)	-0.82	1 (0%) 94 93	15, 21, 34, 56	0
2	C	125/137 (91%)	-0.36	1 (0%) 86 86	13, 15, 24, 55	0
2	E	124/137 (90%)	-0.65	1 (0%) 86 86	14, 18, 28, 56	0
3	D	376/386 (97%)	-0.62	1 (0%) 94 93	12, 17, 28, 53	0
3	F	376/386 (97%)	-0.65	1 (0%) 94 93	13, 19, 30, 55	0
All	All	1709/1792 (95%)	-0.64	7 (0%) 92 92	12, 19, 34, 58	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	132	HIS	6.2
1	A	6	ALA	5.2
3	F	11	GLN	3.2
1	A	7	ASP	3.0
3	D	11	GLN	3.0
1	B	6	ALA	2.9
2	E	131	SER	2.4

### 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(Å <sup>2</sup> )	Q<0.9
2	TRQ	E	57	16/17	0.98	0.06	17,18,25,29	0
2	TRQ	C	57	16/17	0.98	0.09	14,16,21,26	0



## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

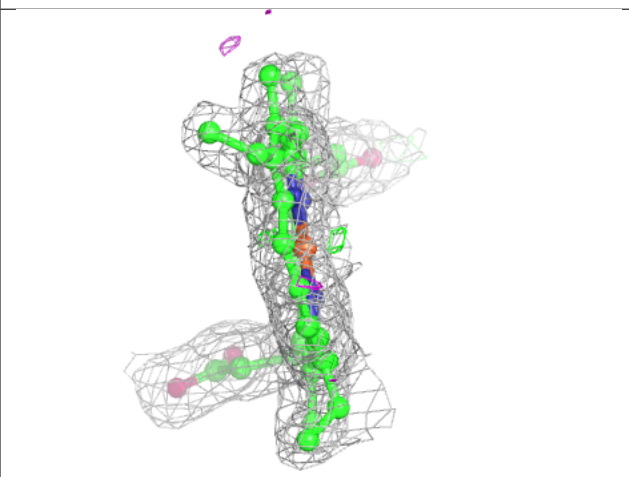
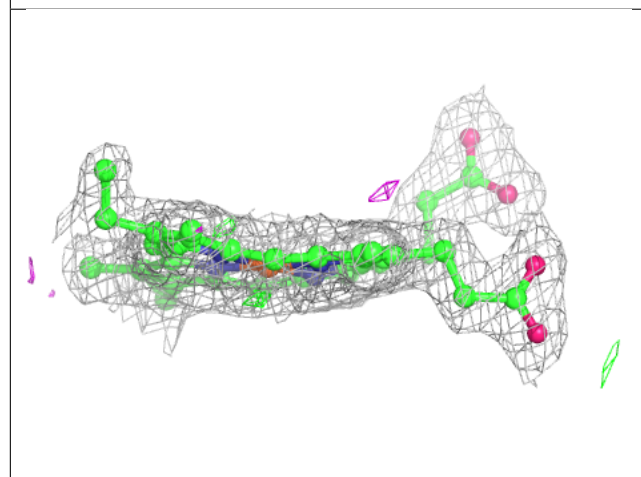
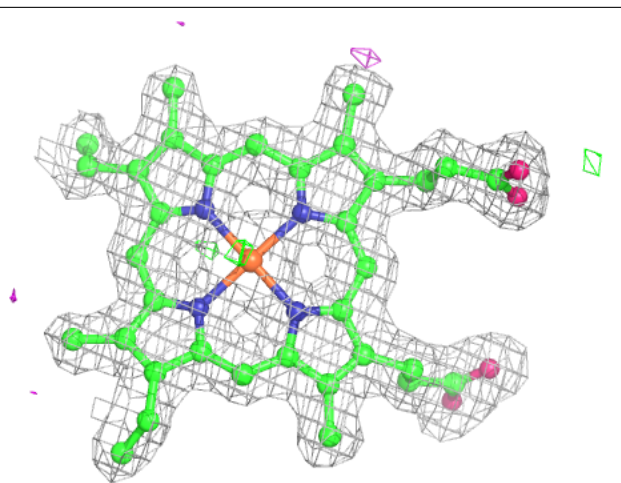
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	D	388	4/4	0.86	0.18	29,29,30,33	0
7	EDO	B	374	4/4	0.87	0.19	38,38,40,41	0
11	PG4	F	387	13/13	0.89	0.11	42,50,62,63	0
7	EDO	A	374	4/4	0.90	0.08	46,47,49,50	0
10	1PE	D	390	16/16	0.91	0.18	38,51,59,62	0
9	ACT	D	389	4/4	0.95	0.11	25,28,31,32	0
8	MES	D	387	12/12	0.96	0.15	32,52,60,62	0
5	NA	A	402	1/1	0.98	0.08	31,31,31,31	0
5	NA	A	401	1/1	0.98	0.07	24,24,24,24	0
5	NA	B	402	1/1	0.98	0.05	27,27,27,27	0
6	HEC	A	500	43/43	0.99	0.06	15,19,23,24	0
6	HEC	B	500	43/43	0.99	0.07	12,15,20,21	0
6	HEC	B	600	43/43	0.99	0.06	10,16,17,18	0
6	HEC	A	600	43/43	0.99	0.06	10,14,17,20	0
5	NA	B	401	1/1	0.99	0.04	22,22,22,22	0
4	CA	B	400	1/1	1.00	0.07	15,15,15,15	0
4	CA	A	400	1/1	1.00	0.04	19,19,19,19	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.

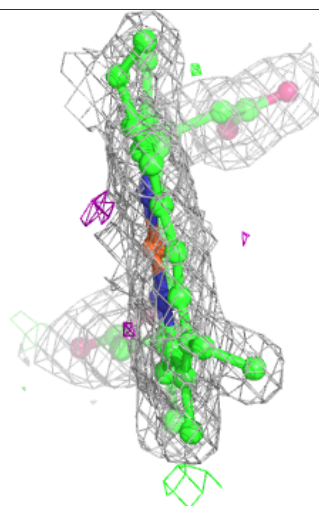
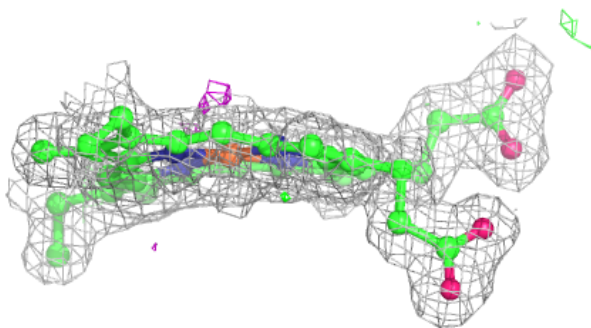
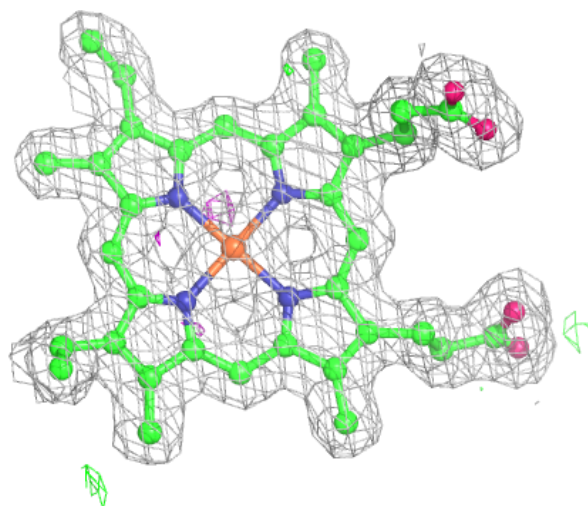
**Electron density around HEC A 500:**

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



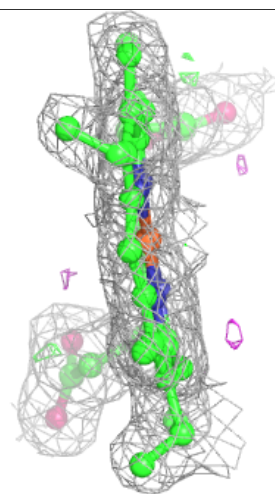
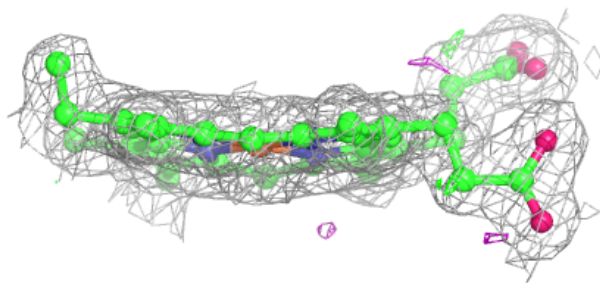
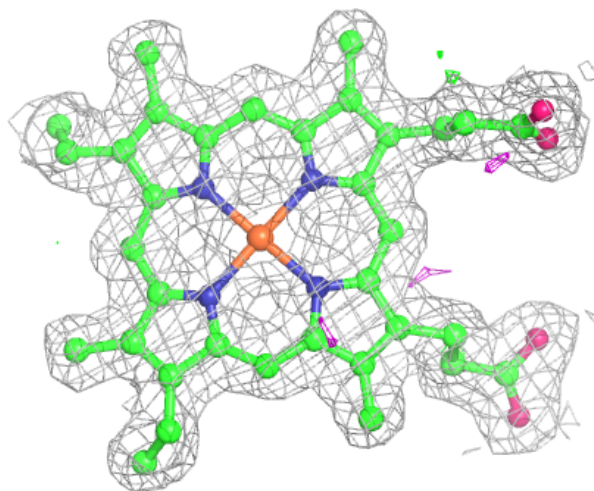
**Electron density around HEC B 500:**

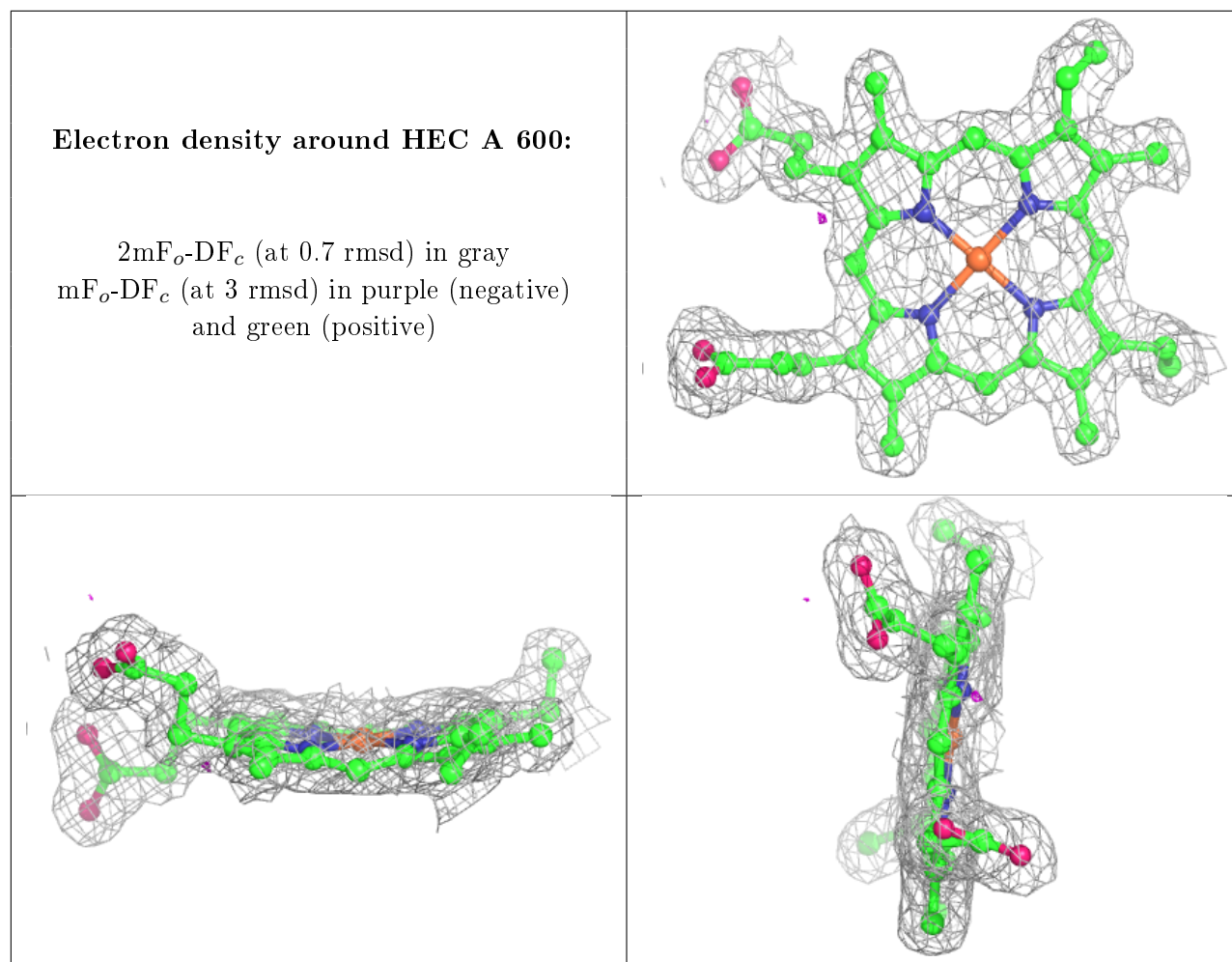
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.