wwPDB X-ray Structure Validation Summary Report (i)

Sep 3, 2023 – 05:09 PM EDT

PDB ID	:	3SVW
Title	:	Crystal Structure of the P107V-MauG/pre-Methylamine Dehydrogenase Complex
Authors	:	Jensen, L.M.R.; Wilmot, C.M.
Deposited on	:	2011-07-12
Resolution	:	1.86 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.35
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)	:	2.35

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.
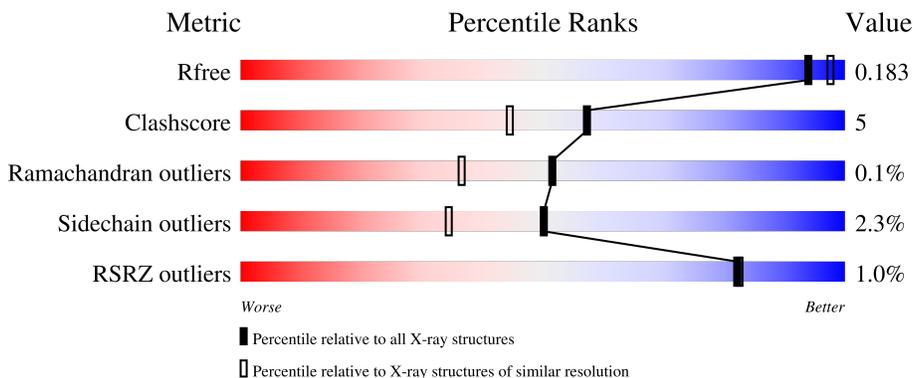
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% 83% 7% · 10%
1	B	373	% 85% 10% · 5%
2	C	137	% 80% 14% · ·
2	E	137	% 76% 13% · 9%
3	D	386	2% 89% 8% · ·
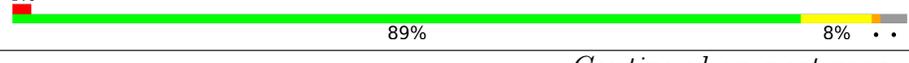
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Mol	Chain	Length	Quality of chain
3	F	386	85% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	PEG	B	376	-	-	X	-
8	PEG	F	388	-	-	X	-
9	EDO	D	387	-	-	X	-
9	EDO	F	389	-	-	X	-

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 15652 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	337	Total	C	N	O	S	0	5	0
			2648	1663	472	500	13			
1	B	355	Total	C	N	O	S	0	5	0
			2774	1733	498	531	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	VAL	PRO	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	107	VAL	PRO	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	3	0
			1027	634	179	200	14			
2	E	125	Total	C	N	O	S	0	3	0
			974	606	162	192	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 2932	C 1862	N 502	O 560	S 8	0	2	0
3	F	376	Total 2953	C 1876	N 506	O 563	S 8	0	5	0

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

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

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

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

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).
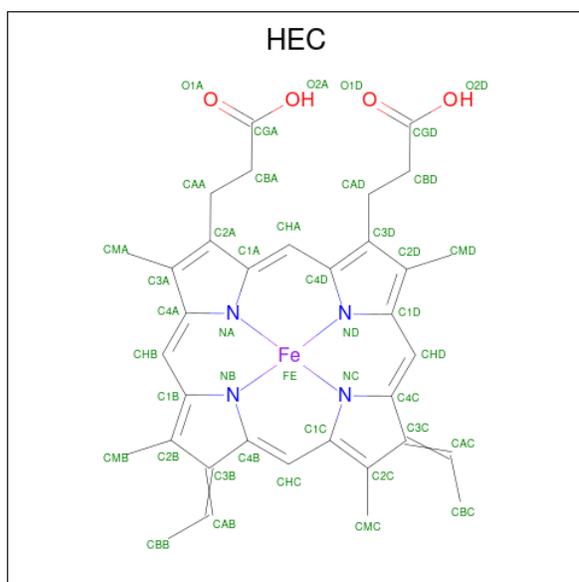
HEC

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

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

PGE
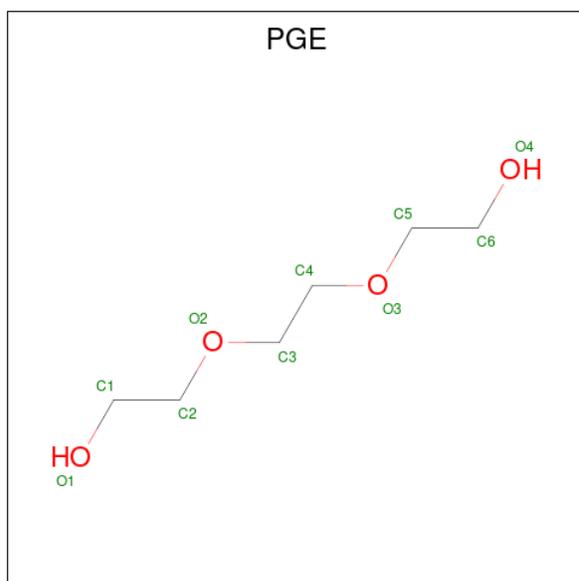
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 10	C 6	O 4	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
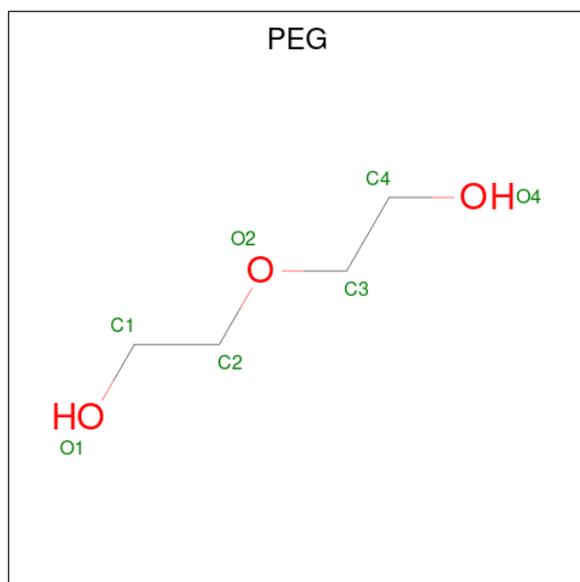
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 7	C 4	O 3	0	0
8	B	1	Total 7	C 4	O 3	0	0
8	F	1	Total 7	C 4	O 3	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1
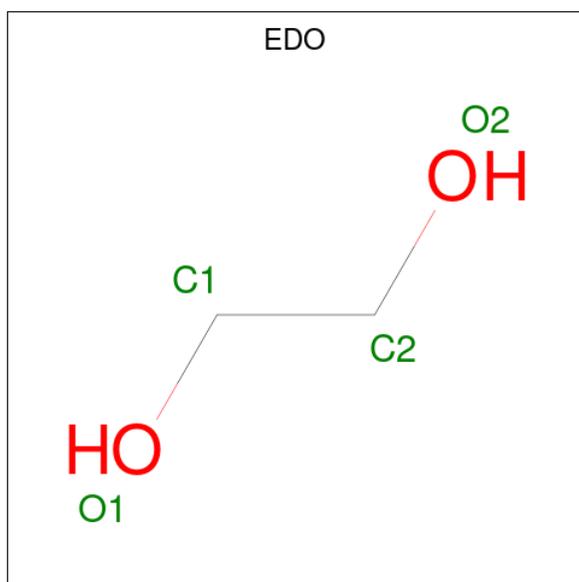
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total 4	C 2	O 2	0	0
9	D	1	Total 4	C 2	O 2	0	0
9	F	1	Total 4	C 2	O 2	0	0

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

ACT

OXT

O^-

C

CH3

O

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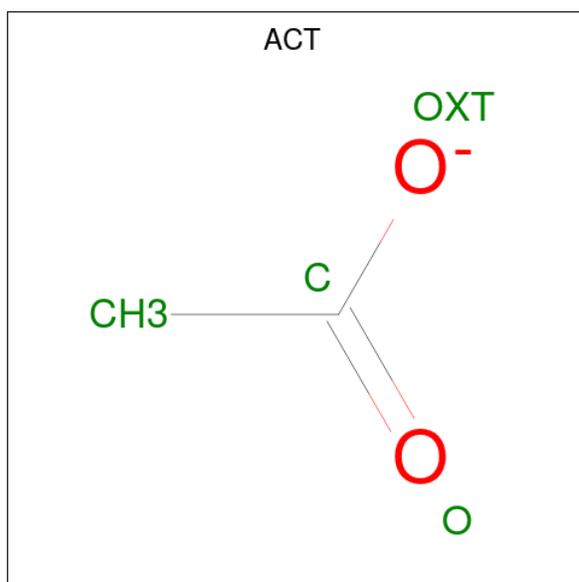
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total 4	C 2	O 2	0	0

WORLDWIDE
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PROTEIN DATA BANK

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).
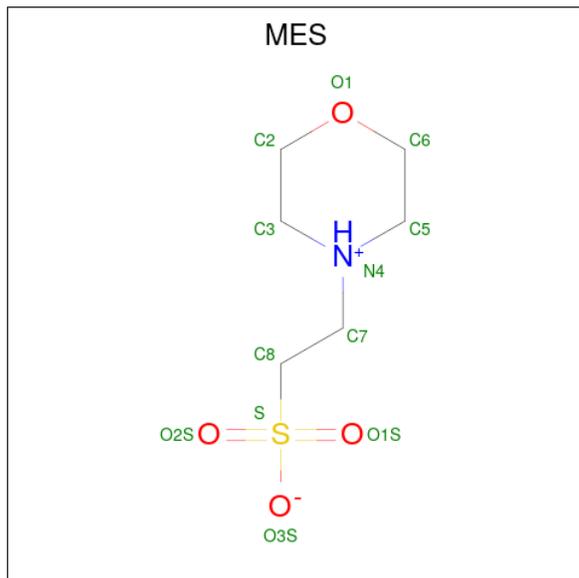
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
11	F	1	12	6	1	4	1	0	0

- Molecule 12 is water.

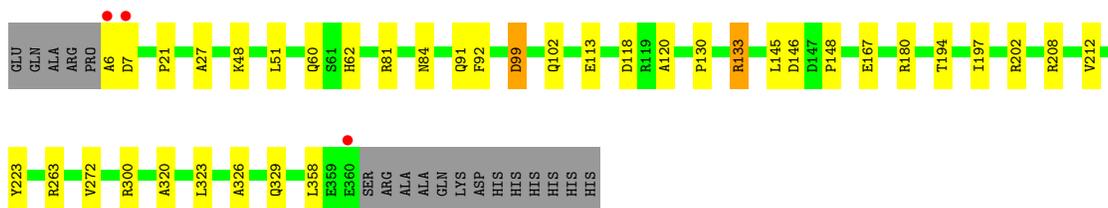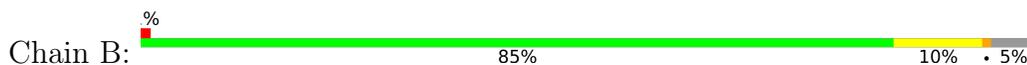| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	431	Total	O	0	0
			431	431		
12	B	438	Total	O	0	0
			438	438		
12	C	141	Total	O	0	0
			141	141		
12	D	410	Total	O	0	0
			410	410		
12	E	146	Total	O	0	0
			146	146		
12	F	541	Total	O	0	0
			541	541		

3 Residue-property plots ⓘ

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

• Molecule 1: Methylamine utilization protein MauG
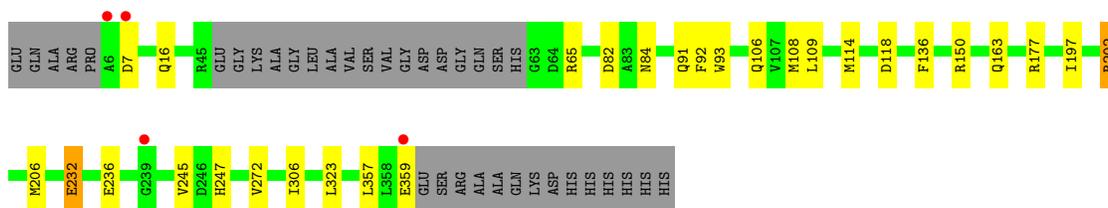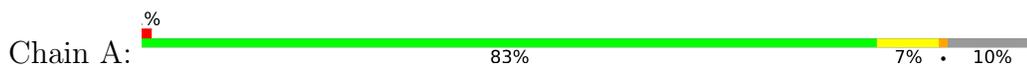
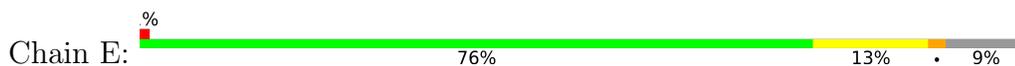Chain A:

• Molecule 1: Methylamine utilization protein MauG

Chain B:

• Molecule 2: Methylamine dehydrogenase light chain

Chain C:

• Molecule 2: Methylamine dehydrogenase light chain

Chain E:

• Molecule 3: Methylamine dehydrogenase heavy chain

Chain D:

Chain D residue map (Q11, Q14, P42, D43, D51, V63, R70, M74, I75, H94, I102, E106, P116, L119, R132, K173, R174, D177, V178, P179, D180, C181, Y182, G207, T208, E209, T215, D275, R278, W282)

R305, L316, D341, E342, K343, K354, P377, Q378, G386

• Molecule 3: Methylamine dehydrogenase heavy chain

Chain F:

Chain F residue map (Q11, I36, P42, R45, D51, P52, A53, H54, F55, A56, N82, D88, F91, H94, F99, I102, P116, F133, T142, P158, A159, P160, K170, R174, C181, Y182, D190, C196, E213)

Y233, R239, D253, D258, R273, W277, R278, R293, E303, W304, R305, L316, E322, K326, E342, K343, K354, D360, Q372, P377, T381, G386
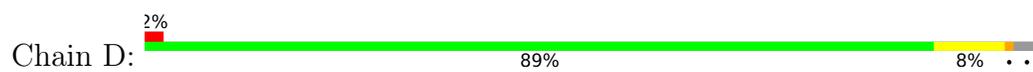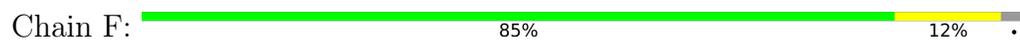
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.61Å 89.00Å 104.81Å 67.05° 79.51° 79.72°	Depositor
Resolution (Å)	33.89 – 1.86 33.89 – 1.86	Depositor EDS
% Data completeness (in resolution range)	96.2 (33.89-1.86) 96.2 (33.89-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	5.99 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.131 , 0.174 0.141 , 0.183	Depositor DCC
R_{free} test set	7327 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15652	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 0AF, PEG, NA, CA, ACT, MES, HEC, EDO, PGE

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	1/2724 (0.0%)	0.97	6/3694 (0.2%)
1	B	1.16	2/2852 (0.1%)	0.97	6/3867 (0.2%)
2	C	1.22	2/1050 (0.2%)	0.98	2/1430 (0.1%)
2	E	1.19	3/994 (0.3%)	1.05	2/1358 (0.1%)
3	D	1.10	1/3015 (0.0%)	0.97	5/4109 (0.1%)
3	F	1.27	9/3045 (0.3%)	1.06	12/4148 (0.3%)
All	All	1.18	18/13680 (0.1%)	1.00	33/18606 (0.2%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	133	PHE	CE2-CZ	6.55	1.49	1.37
2	E	88[A]	CYS	CB-SG	-6.21	1.71	1.82
2	E	88[B]	CYS	CB-SG	-6.21	1.71	1.82
1	A	136	PHE	CE2-CZ	6.11	1.49	1.37
3	F	213	GLU	CD-OE1	5.90	1.32	1.25

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	177	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	82	ASP	CB-CG-OD2	7.54	125.09	118.30
3	F	278	ARG	NE-CZ-NH1	7.26	123.93	120.30
3	F	239	ARG	NE-CZ-NH1	7.08	123.84	120.30

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	2648	0	2556	18	0
1	B	2774	0	2665	23	0
2	C	1027	0	916	21	0
2	E	974	0	880	18	0
3	D	2932	0	2828	16	0
3	F	2953	0	2857	24	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	5	0
6	B	86	0	60	3	0
7	A	10	0	14	3	0
8	B	14	0	20	12	0
8	F	7	0	10	9	0
9	B	4	0	6	0	0
9	D	4	0	6	5	0
9	F	4	0	6	6	0
10	D	4	0	3	0	0
11	F	12	0	12	0	0
12	A	431	0	0	6	0
12	B	438	0	0	5	0
12	C	141	0	0	4	0
12	D	410	0	0	6	0
12	E	146	0	0	5	0
12	F	541	0	0	13	0
All	All	15652	0	12899	129	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 5.

The worst 5 of 129 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[B]:GLN:NE2	12:F:1487:HOH:O	1.80	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:372[A]:GLN:OE1	12:F:2086:HOH:O	1.76	1.03
2:C:101[A]:GLU:HG3	12:C:2537:HOH:O	0.80	0.97
8:F:388:PEG:H22	12:F:479:HOH:O	1.68	0.91
9:D:387:EDO:H12	12:D:1241:HOH:O	1.75	0.86

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	338/373 (91%)	330 (98%)	8 (2%)	0	100	100
1	B	358/373 (96%)	350 (98%)	8 (2%)	0	100	100
2	C	131/137 (96%)	127 (97%)	4 (3%)	0	100	100
2	E	125/137 (91%)	123 (98%)	2 (2%)	0	100	100
3	D	376/386 (97%)	365 (97%)	10 (3%)	1 (0%)	41	26
3	F	379/386 (98%)	366 (97%)	12 (3%)	1 (0%)	41	26
All	All	1707/1792 (95%)	1661 (97%)	44 (3%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	102	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	270/292 (92%)	264 (98%)	6 (2%)	52	36
1	B	282/292 (97%)	277 (98%)	5 (2%)	59	45
2	C	113/112 (101%)	111 (98%)	2 (2%)	59	45
2	E	107/112 (96%)	103 (96%)	4 (4%)	34	17
3	D	306/311 (98%)	297 (97%)	9 (3%)	42	26
3	F	309/311 (99%)	304 (98%)	5 (2%)	62	49
All	All	1387/1430 (97%)	1356 (98%)	31 (2%)	50	36

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	106	GLU
3	F	94	HIS
3	D	275	ASP
3	F	316	LEU
2	E	80	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	134	HIS
2	C	136	HIS
3	F	300	GLN
3	D	30	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	0AF	E	57	2	13,16,17	1.68	3 (23%)	11,22,24	1.73	2 (18%)
2	0AF	C	57	2	13,16,17	1.61	2 (15%)	11,22,24	2.23	2 (18%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	0AF	CB-CA	-3.72	1.45	1.53
2	E	57	0AF	CZ3-CE3	2.90	1.43	1.36
2	E	57	0AF	CB-CA	-2.79	1.47	1.53
2	C	57	0AF	CZ3-CE3	2.71	1.42	1.36
2	E	57	0AF	CD1-CG	2.41	1.43	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	57	0AF	CG-CB-CA	-5.84	105.50	114.53
2	E	57	0AF	CG-CB-CA	-4.13	108.14	114.53
2	C	57	0AF	CB-CG-CD2	2.95	130.84	126.25
2	E	57	0AF	CB-CA-C	2.63	116.39	111.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	0AF	2	0
2	C	57	0AF	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
9	EDO	D	387	-	3,3,3	1.63	0	2,2,2	1.85	1 (50%)
6	HEC	A	500	1	32,50,50	1.46	5 (15%)	24,82,82	2.05	7 (29%)
6	HEC	A	600	1	32,50,50	1.44	6 (18%)	24,82,82	2.99	12 (50%)
6	HEC	B	500	1	32,50,50	1.59	8 (25%)	24,82,82	2.27	9 (37%)
9	EDO	B	375	-	3,3,3	0.35	0	2,2,2	0.24	0
8	PEG	B	376	-	6,6,6	0.29	0	5,5,5	0.97	0
7	PGE	A	374	-	9,9,9	0.39	0	8,8,8	0.94	0
6	HEC	B	600	1	32,50,50	1.60	8 (25%)	24,82,82	3.10	13 (54%)
9	EDO	F	389	-	3,3,3	0.28	0	2,2,2	1.37	0
10	ACT	D	388	-	3,3,3	1.08	0	3,3,3	1.44	0
11	MES	F	387	-	12,12,12	1.02	1 (8%)	14,16,16	2.70	4 (28%)
8	PEG	F	388	-	6,6,6	0.51	0	5,5,5	1.42	1 (20%)
8	PEG	B	374	-	6,6,6	0.57	0	5,5,5	0.91	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
9	EDO	D	387	-	-	1/1/1/1	-
6	HEC	A	500	1	-	0/10/54/54	-
6	HEC	A	600	1	-	2/10/54/54	-
6	HEC	B	500	1	-	0/10/54/54	-
9	EDO	B	375	-	-	1/1/1/1	-
8	PEG	B	376	-	-	2/4/4/4	-
7	PGE	A	374	-	-	2/7/7/7	-
6	HEC	B	600	1	-	2/10/54/54	-
9	EDO	F	389	-	-	1/1/1/1	-
11	MES	F	387	-	-	1/6/14/14	0/1/1/1
8	PEG	F	388	-	-	3/4/4/4	-
8	PEG	B	374	-	-	4/4/4/4	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	500	HEC	C3A-C4A	3.47	1.50	1.42
6	B	500	HEC	C3C-C4C	3.21	1.48	1.43
6	B	600	HEC	C1B-NB	-3.15	1.29	1.36
6	A	500	HEC	C2A-C1A	2.99	1.49	1.42
6	A	500	HEC	C3C-C4C	2.95	1.48	1.43

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	HEC	CBD-CAD-C3D	-8.09	98.81	112.62
6	A	600	HEC	CBD-CAD-C3D	-7.96	99.03	112.62
11	F	387	MES	C5-N4-C3	6.42	123.29	108.83
6	B	600	HEC	CBA-CAA-C2A	-5.71	102.98	112.60
6	A	600	HEC	CMB-C2B-C3B	5.63	132.44	125.82

There are no chirality outliers.

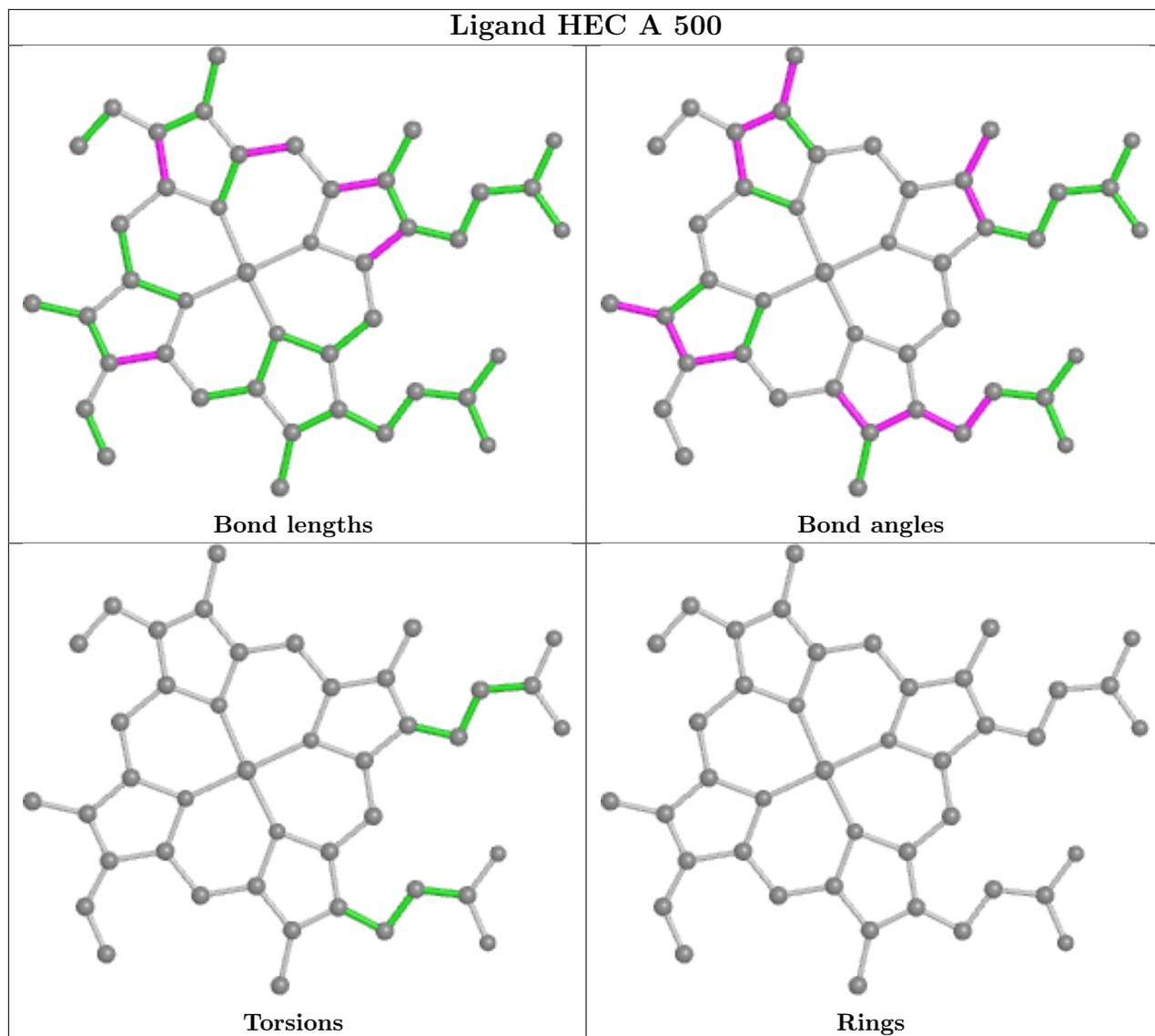5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	387	MES	C8-C7-N4-C5
8	F	388	PEG	C1-C2-O2-C3
8	F	388	PEG	O2-C3-C4-O4
8	F	388	PEG	O1-C1-C2-O2
7	A	374	PGE	C1-C2-O2-C3

There are no ring outliers.

10 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	387	EDO	5	0
6	A	500	HEC	3	0
6	A	600	HEC	2	0
6	B	500	HEC	1	0
8	B	376	PEG	11	0
7	A	374	PGE	3	0
6	B	600	HEC	2	0
9	F	389	EDO	6	0
8	F	388	PEG	9	0
8	B	374	PEG	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEC A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC B 600

Bond lengths

Bond angles

Torsions

Rings
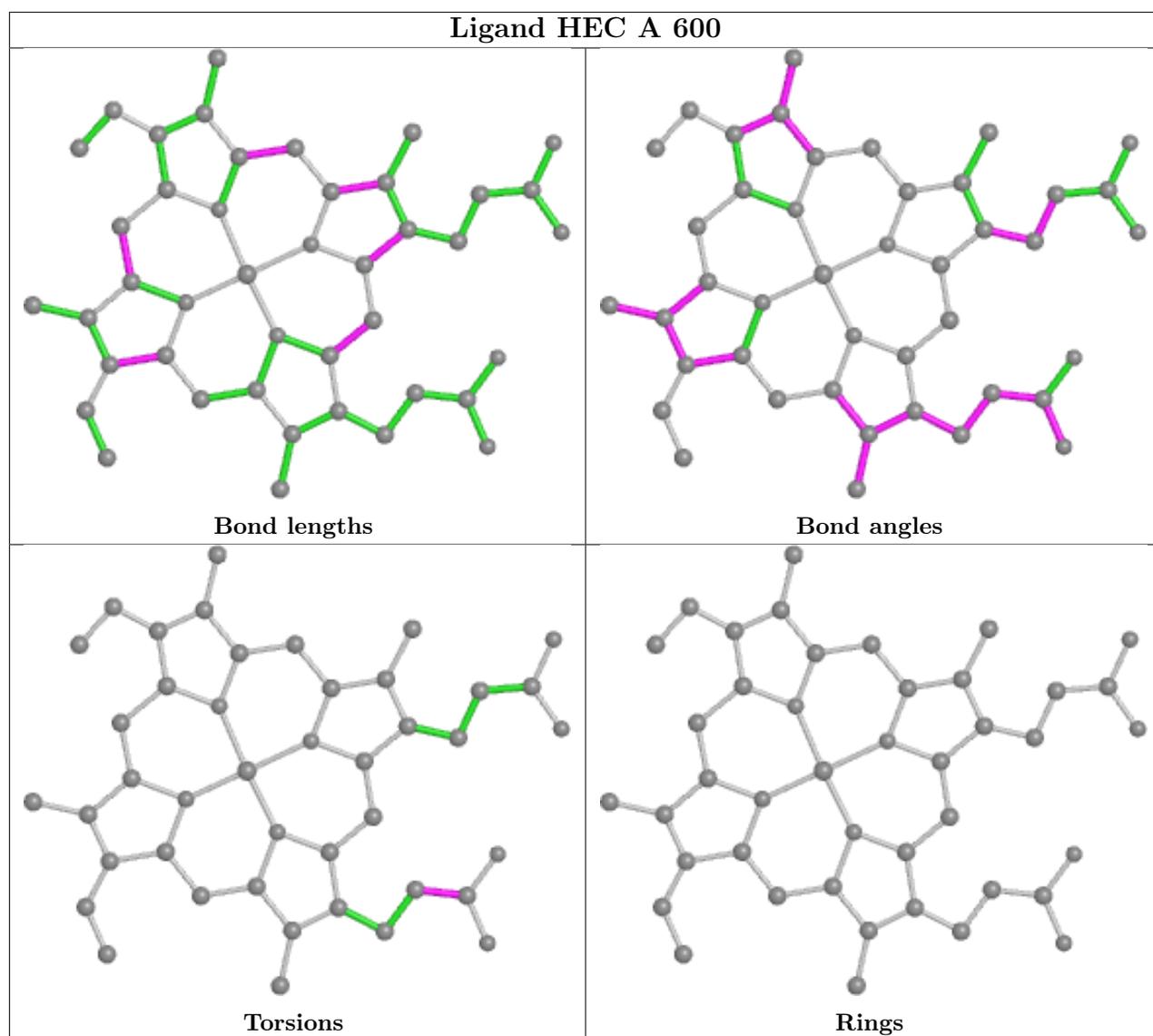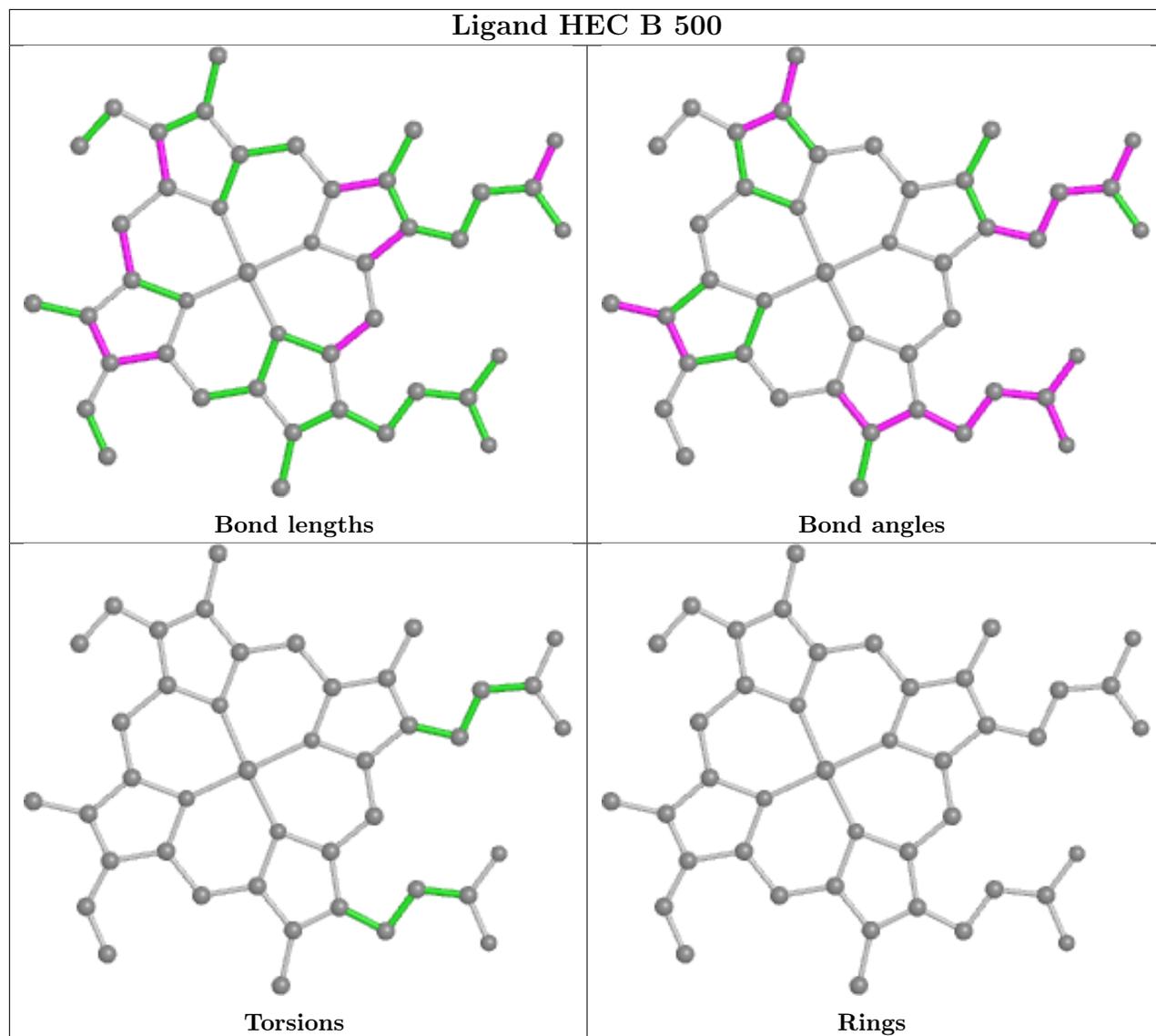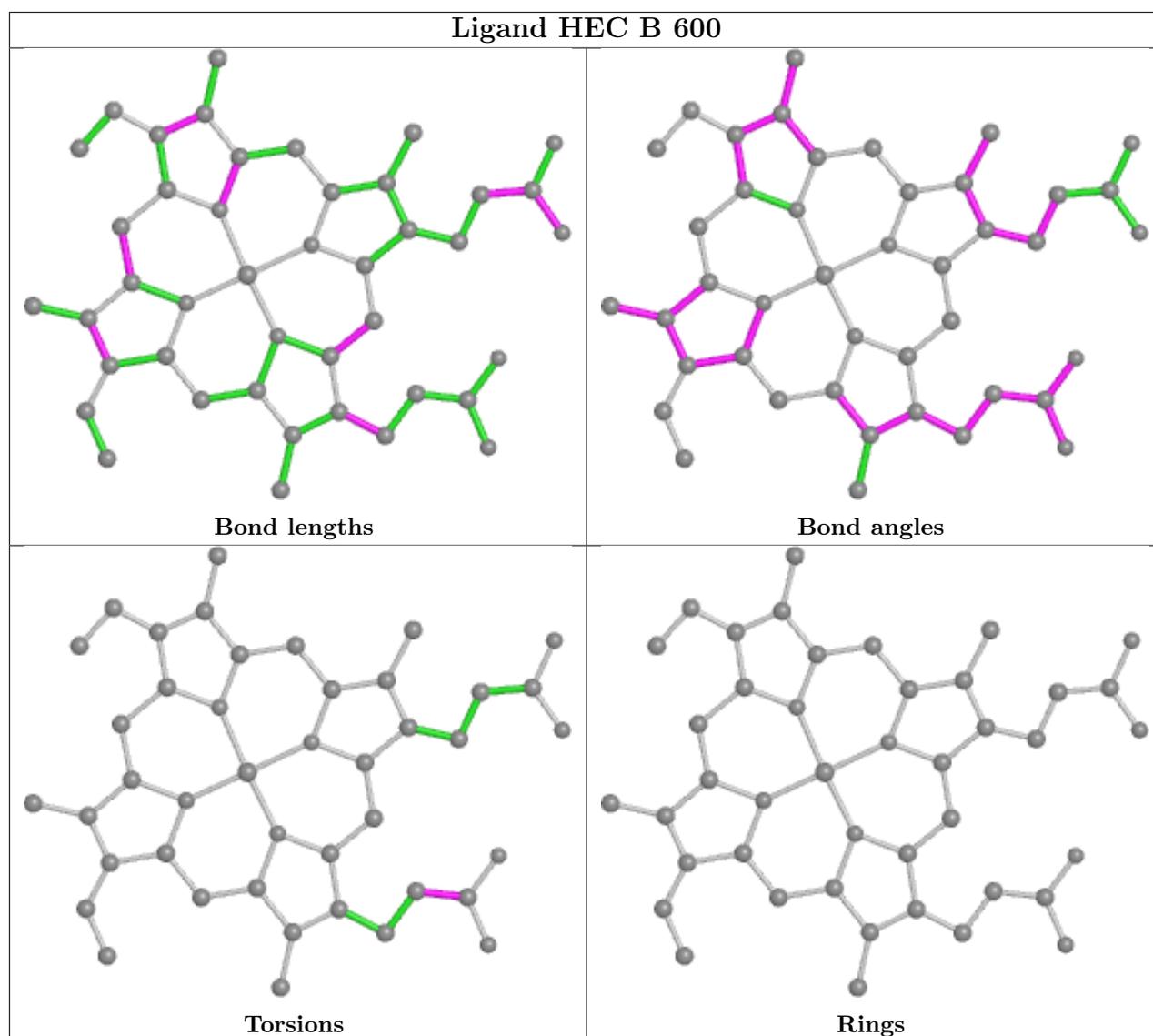
5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	337/373 (90%)	-0.57	4 (1%)	79	79	11, 19, 34, 50	0
1	B	355/373 (95%)	-0.64	3 (0%)	86	86	9, 17, 33, 56	0
2	C	130/137 (94%)	-0.61	1 (0%)	86	86	10, 16, 30, 42	0
2	E	124/137 (90%)	-0.67	2 (1%)	72	72	10, 14, 25, 52	0
3	D	376/386 (97%)	-0.38	6 (1%)	72	72	11, 21, 37, 64	0
3	F	376/386 (97%)	-0.62	1 (0%)	94	93	8, 13, 26, 49	0
All	All	1698/1792 (94%)	-0.56	17 (1%)	82	82	8, 17, 33, 64	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	5.6
1	B	6	ALA	5.6
1	B	7	ASP	3.9
3	D	208	THR	3.9
3	D	207	GLY	3.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	0AF	C	57	15/16	0.96	0.09	16,18,25,25	0
2	0AF	E	57	15/16	0.97	0.08	13,16,26,27	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PEG	B	374	7/7	0.85	0.12	39,40,42,44	0
8	PEG	F	388	7/7	0.89	0.17	31,37,39,41	0
9	EDO	B	375	4/4	0.91	0.10	28,33,35,40	0
8	PEG	B	376	7/7	0.92	0.26	25,33,43,50	0
9	EDO	D	387	4/4	0.92	0.15	26,28,31,33	0
7	PGE	A	374	10/10	0.94	0.14	34,39,44,45	0
9	EDO	F	389	4/4	0.94	0.26	27,33,38,47	0
5	NA	B	401	1/1	0.98	0.08	24,24,24,24	0
5	NA	A	401	1/1	0.98	0.15	30,30,30,30	0
10	ACT	D	388	4/4	0.98	0.07	20,21,24,25	0
11	MES	F	387	12/12	0.98	0.10	23,37,42,43	0
6	HEC	A	600	43/43	0.99	0.09	10,14,15,15	0
6	HEC	B	500	43/43	0.99	0.09	7,12,14,17	0
6	HEC	B	600	43/43	0.99	0.10	4,10,11,14	0
5	NA	A	402	1/1	0.99	0.07	22,22,22,22	0
5	NA	B	402	1/1	0.99	0.04	23,23,23,23	0
6	HEC	A	500	43/43	0.99	0.10	9,12,16,18	0
4	CA	B	400	1/1	1.00	0.07	13,13,13,13	0
4	CA	A	400	1/1	1.00	0.03	17,17,17,17	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.
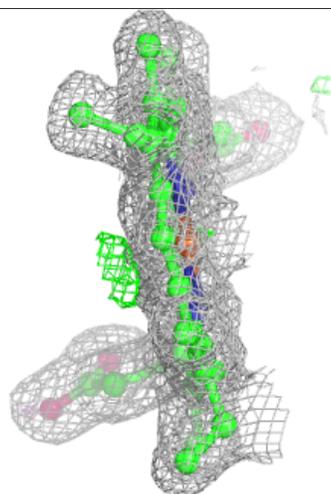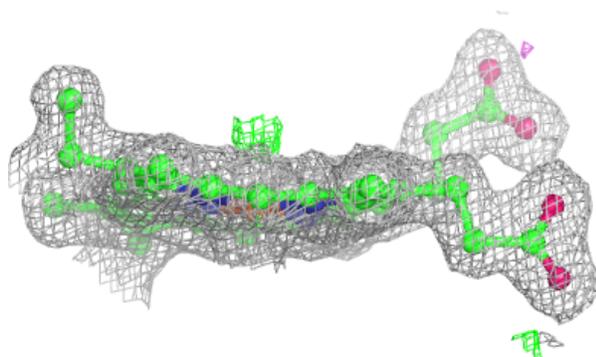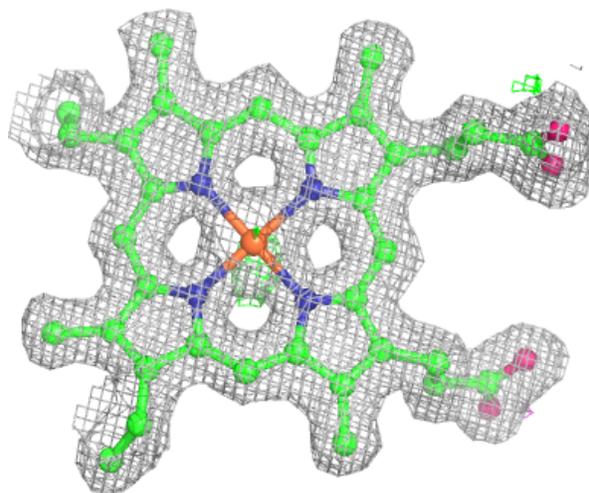
Electron density around HEC A 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
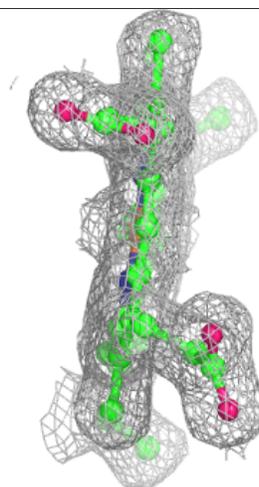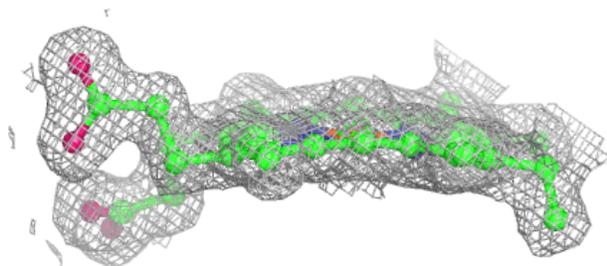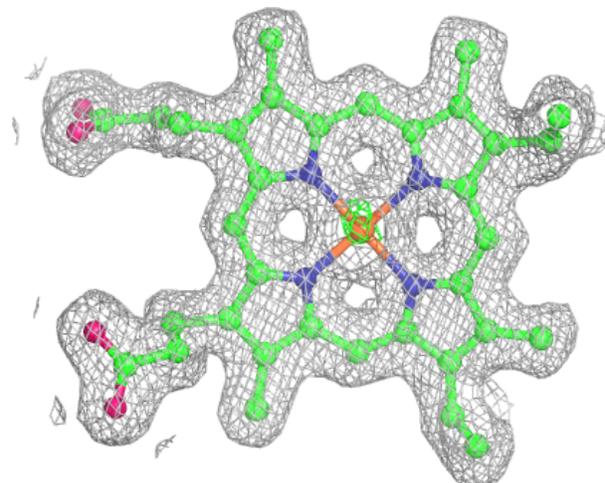mF_o-DF_c (at 3 rmsd) in purple (negative)
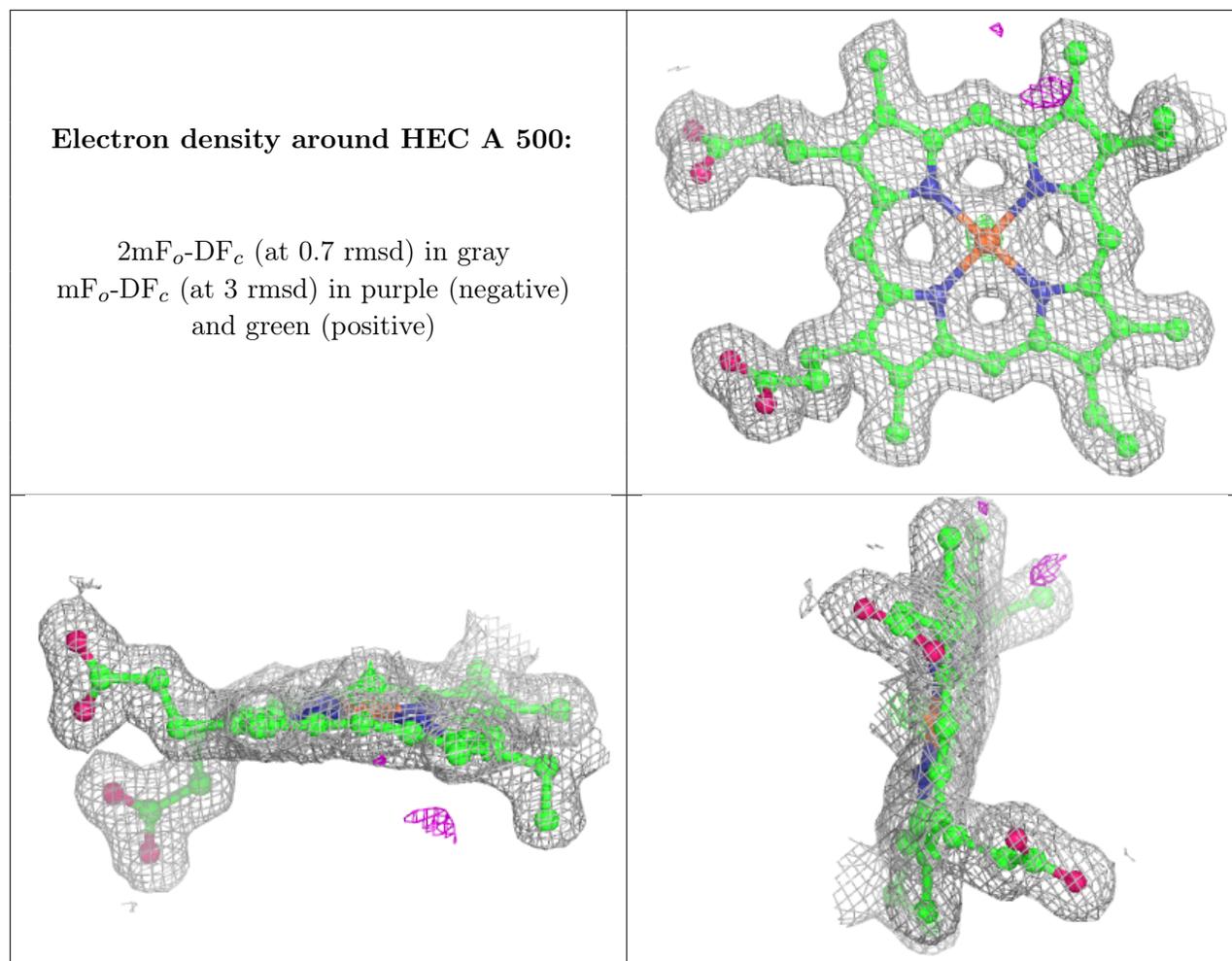and green (positive)
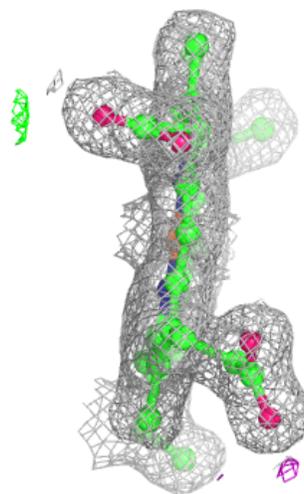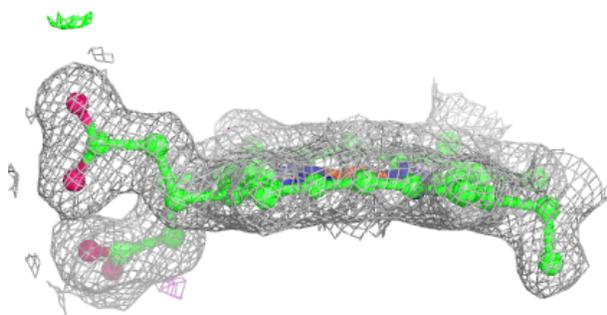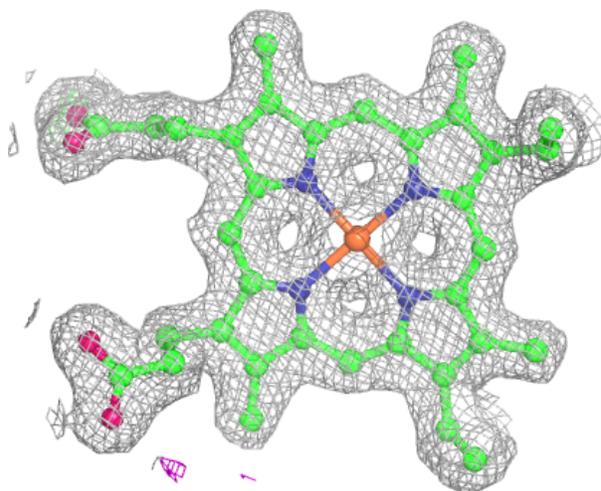
Electron density around HEC B 500:

$2mF_o$-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.