



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 10:39 am BST

PDB ID : 2ACZ
Title : Complex II (Succinate Dehydrogenase) From E. Coli with Atpenin A5 inhibitor co-crystallized at the ubiquinone binding site
Authors : Horsefield, R.; Yankovskaya, V.; Sexton, G.; Whittingham, W.; Shiomi, K.; Omura, S.; Byrne, B.; Cecchini, G.; Iwata, S.
Deposited on : 2005-07-19
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

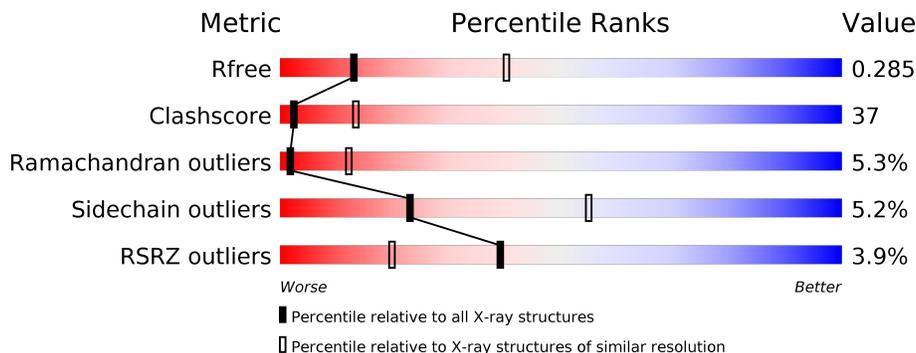
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 ≥ 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	588	
2	B	238	
3	C	129	
4	D	115	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CDN	C	132	X	-	-	X
5	OAA	A	589	-	-	X	-
9	F3S	B	304	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8521 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 Succinate dehydrogenase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	588	4522	2812	821	861	28	91	0	0

- Molecule 2 is a protein called Succinate dehydrogenase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	238	1869	1172	329	348	20	0	0	0

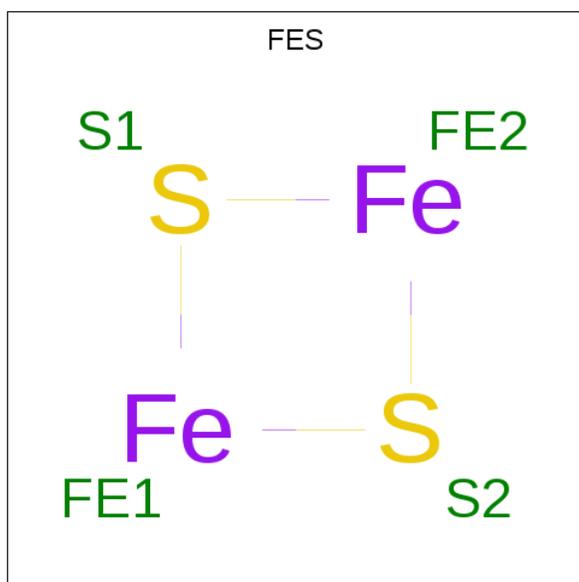
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b556 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	129	1008	668	166	168	6	0	0	0

- Molecule 4 is a protein called Succinate dehydrogenase hydrophobic membrane anchor protein.

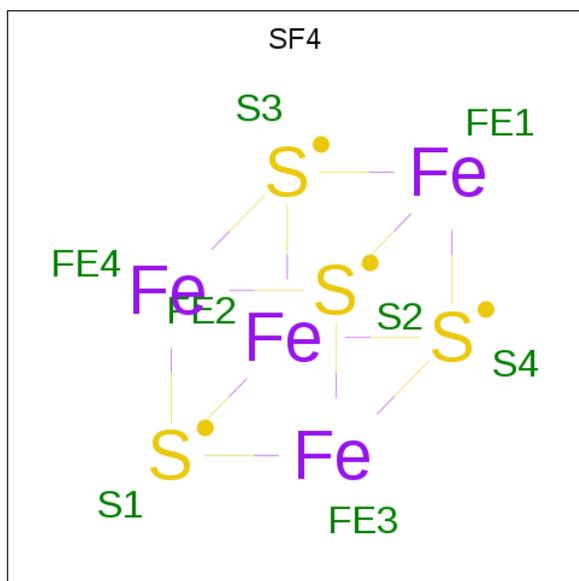
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	113	898	615	136	144	3	0	0	0

- Molecule 5 is OXALOACETATE ION (three-letter code: OAA) (formula: C₄H₃O₅).



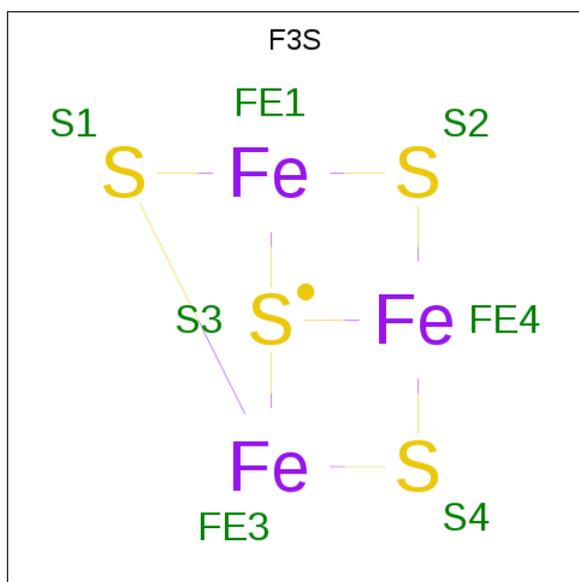
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	4	2	2	0	0

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



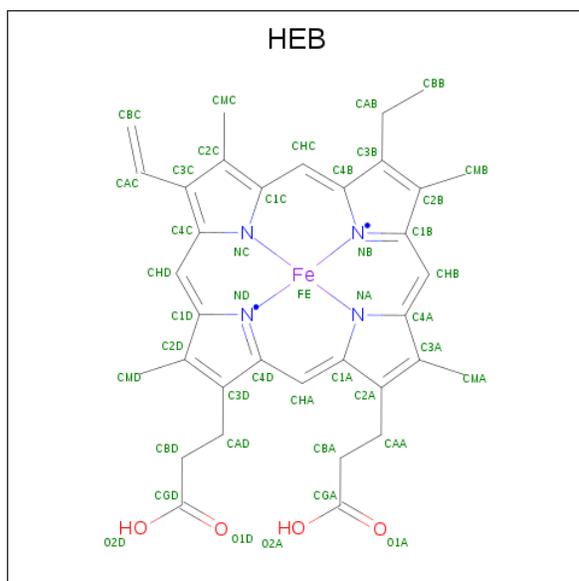
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	8	4	4	0	0

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



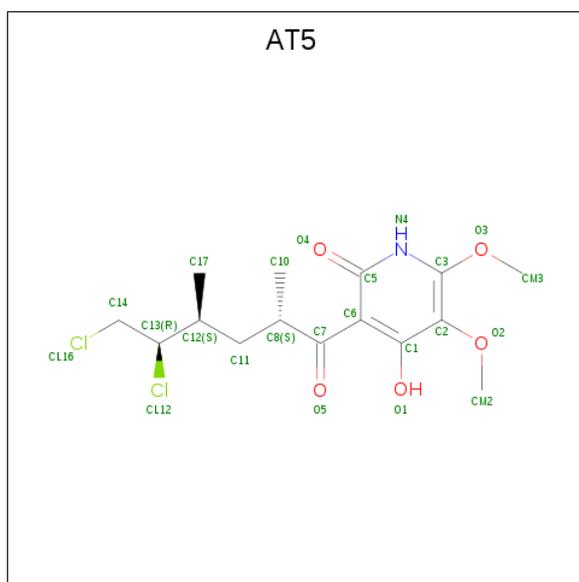
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	Fe	S			
			7	3	4	0	0	

- Molecule 10 is HEME B/C (three-letter code: HEB) (formula: $C_{34}H_{34}FeN_4O_4$).



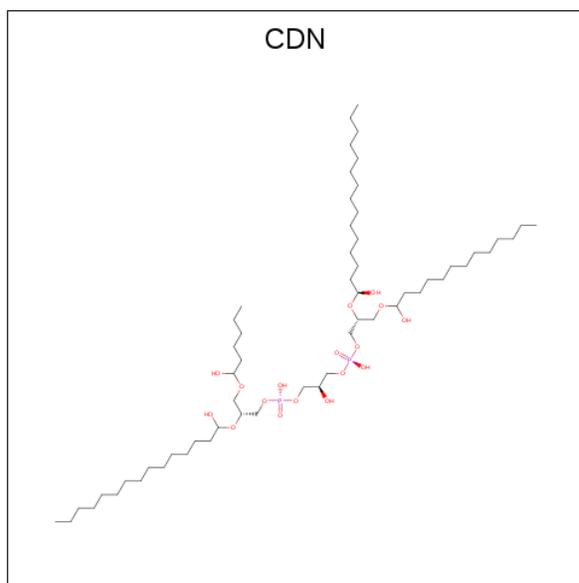
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
10	C	1	Total	C	Fe	N	O		
			43	34	1	4	4	0	0

- Molecule 11 is 3-[(2S,4S,5R)-5,6-DICHLORO-2,4-DIMETHYL-1-OXOHEXYL]-4-HYDROXY-5,6-DIMETHOXY-2(1H)-PYRIDINONE (three-letter code: AT5) (formula: $C_{15}H_{21}Cl_2NO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
11	C	1	23	15	2	1	5	0	0

- Molecule 12 is CARDIOLIPIN (three-letter code: CDN) (formula: $C_{58}H_{120}O_{17}P_2$).

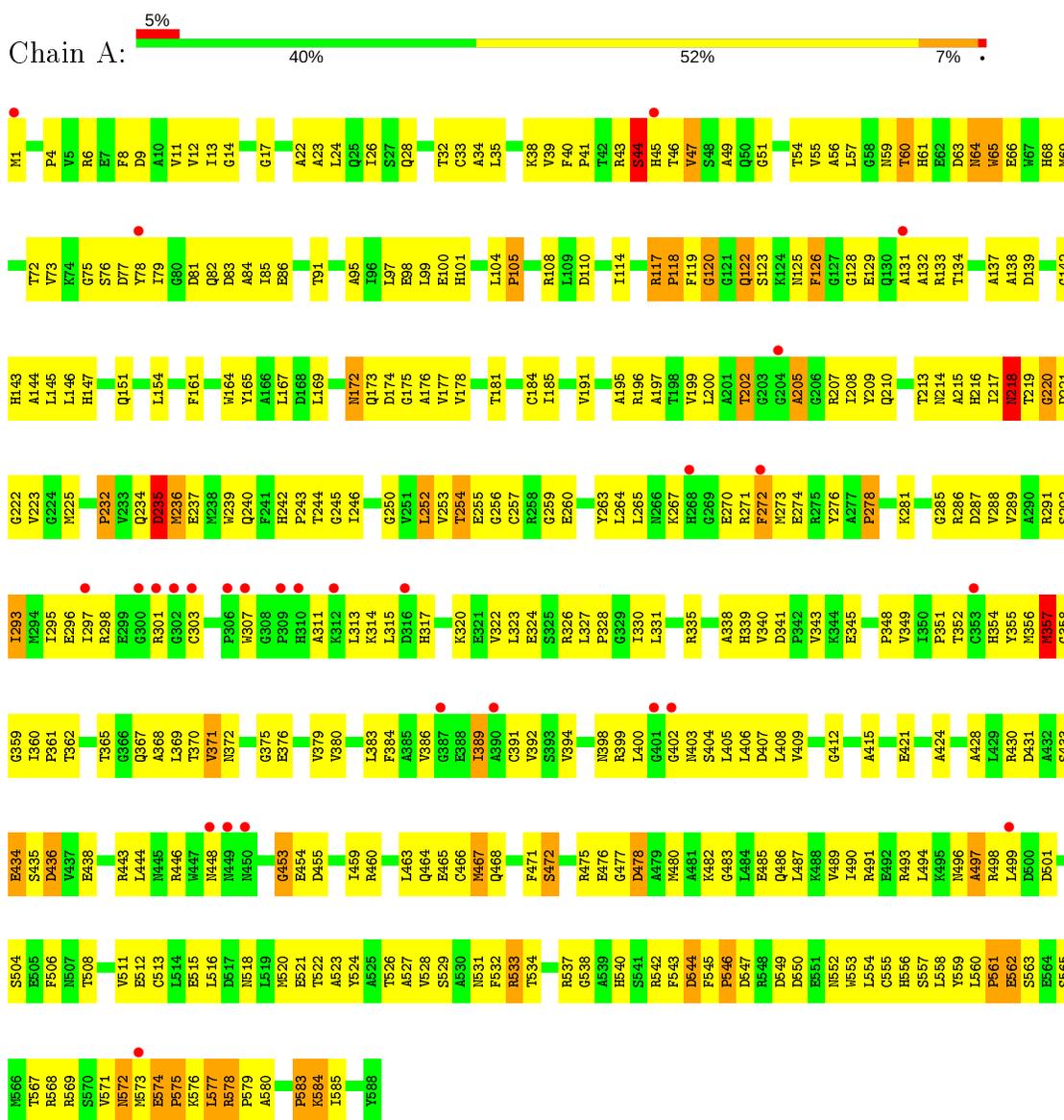


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
12	C	1	77	58	17	2	0	0

3 Residue-property plots

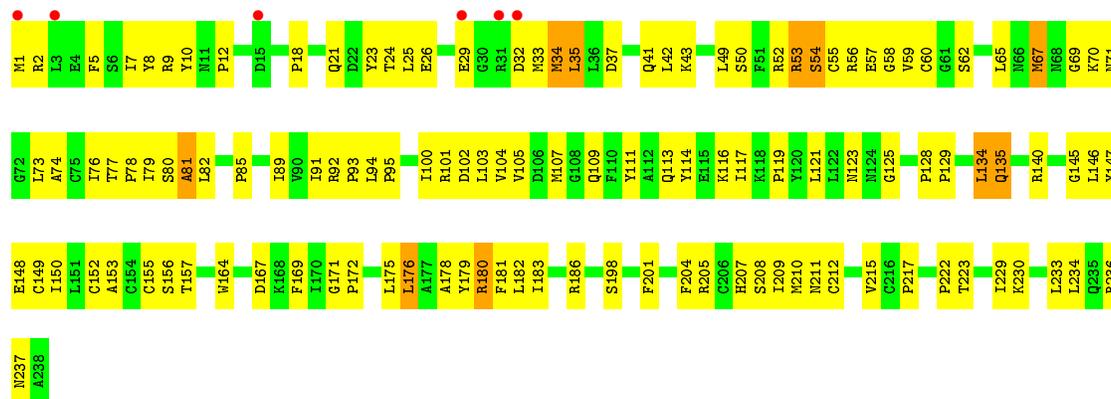
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Succinate dehydrogenase flavoprotein subunit

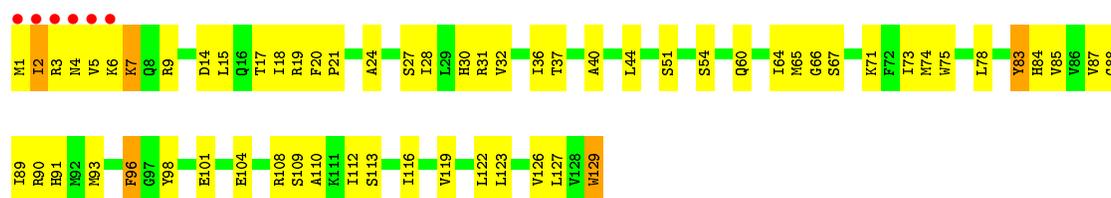


- Molecule 2: Succinate dehydrogenase iron-sulfur protein

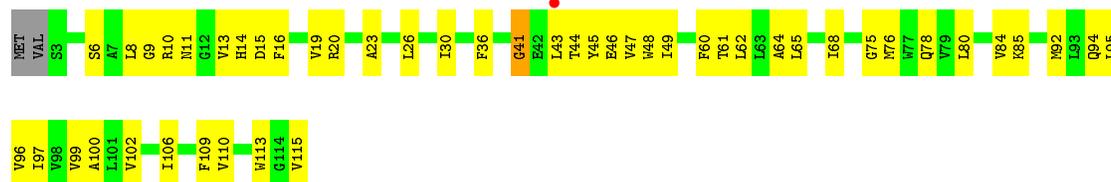




- Molecule 3: Succinate dehydrogenase cytochrome b556 subunit



- Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	138.76Å 138.76Å 521.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.10 39.40 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.10) 97.9 (39.40-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.12Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.308 0.244 , 0.285	Depositor DCC
R_{free} test set	966 reflections (2.76%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtrriage
Anisotropy	0.544	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8521	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OAA, CDN, F3S, AT5, FES, HEB, SF4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	1/4611 (0.0%)	0.68	0/6237
2	B	0.46	0/1908	0.72	0/2578
3	C	0.51	0/1030	0.68	0/1394
4	D	0.56	0/923	0.65	0/1262
All	All	0.47	1/8472 (0.0%)	0.68	0/11471

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	SER	C-N	10.51	1.58	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4522	0	4426	390	0
2	B	1869	0	1850	142	0
3	C	1008	0	1066	78	0
4	D	898	0	936	45	0
5	A	9	0	2	5	0
6	A	53	0	29	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	4	0	0	1	0
8	B	8	0	0	0	0
9	B	7	0	0	4	0
10	C	43	0	32	10	0
11	C	23	0	20	4	0
12	C	77	0	112	19	0
All	All	8521	0	8473	630	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 37.

The worst 5 of 630 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)
10:C:130:HEB:HBB1	12:C:132:CDN:C24	1.84	1.07
3:C:6:LYS:HE3	3:C:7:LYS:HG3	1.33	1.06
1:A:577:LEU:HD21	1:A:580:ALA:HA	1.38	1.04
2:B:180:ARG:HH11	2:B:180:ARG:HG2	1.23	1.02
1:A:578:ARG:HB3	1:A:579:PRO:HD3	1.39	1.00

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	586/588 (100%)	461 (79%)	81 (14%)	44 (8%)	1 6
2	B	236/238 (99%)	205 (87%)	25 (11%)	6 (2%)	5 27
3	C	127/129 (98%)	111 (87%)	11 (9%)	5 (4%)	3 18
4	D	111/115 (96%)	100 (90%)	10 (9%)	1 (1%)	17 52
All	All	1060/1070 (99%)	877 (83%)	127 (12%)	56 (5%)	2 12

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	118	PRO
1	A	220	GLY
1	A	235	ASP
1	A	546	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	473/473 (100%)	444 (94%)	29 (6%)	18	49
2	B	208/208 (100%)	197 (95%)	11 (5%)	22	54
3	C	109/109 (100%)	105 (96%)	4 (4%)	34	66
4	D	94/96 (98%)	92 (98%)	2 (2%)	53	79
All	All	884/886 (100%)	838 (95%)	46 (5%)	23	55

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	436	ASP
1	A	544	ASP
3	C	101	GLU
1	A	478	ASP
1	A	506	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	403	ASN
1	A	470	ASN
4	D	14	HIS
1	A	420	GLN
1	A	540	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands 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
10	HEB	C	130	3,4	33,50,50	5.14	18 (54%)	22,82,82	4.33	12 (54%)
6	FAD	A	601	1	51,58,58	2.86	15 (29%)	60,89,89	2.93	13 (21%)
11	AT5	C	131	-	20,23,23	2.47	9 (45%)	24,32,32	2.44	8 (33%)
12	CDN	C	132	-	76,76,76	2.21	10 (13%)	78,88,88	2.06	10 (12%)
5	OAA	A	589	-	2,8,8	2.96	2 (100%)	2,10,10	3.91	2 (100%)
7	FES	B	302	2	0,4,4	0.00	-	-		
8	SF4	B	303	2	0,12,12	0.00	-	-		
9	F3S	B	304	2	0,9,9	0.00	-	-		

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
10	HEB	C	130	3,4	-	0/8/94/94	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FAD	A	601	1	-	3/30/50/50	0/6/6/6
11	AT5	C	131	-	-	11/22/22/22	0/1/1/1
12	CDN	C	132	-	3/3/9/9	26/87/87/87	-
5	OAA	A	589	-	-	0/2/8/8	-
7	FES	B	302	2	-	-	0/1/1/1
8	SF4	B	303	2	-	-	0/6/5/5
9	F3S	B	304	2	-	-	0/3/3/3

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	130	HEB	C4B-NB	-10.23	1.35	1.49
6	A	601	FAD	C4X-N5	9.59	1.47	1.33
10	C	130	HEB	C4D-ND	-9.35	1.37	1.49
10	C	130	HEB	CHC-C4B	-9.13	1.37	1.53
10	C	130	HEB	CHA-C4D	-8.80	1.38	1.53

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	FAD	C4-N3-C2	12.49	125.68	115.14
6	A	601	FAD	O2A-PA-O5B	-9.31	64.50	107.75
10	C	130	HEB	CHC-C4B-NB	9.08	127.87	110.75
10	C	130	HEB	CHD-C1D-ND	8.76	127.27	110.75
12	C	132	CDN	OB9-CB7-C71	8.70	125.23	109.12

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	132	CDN	CB5
12	C	132	CDN	CB7
12	C	132	CDN	CA7

5 of 40 torsion outliers are listed below:

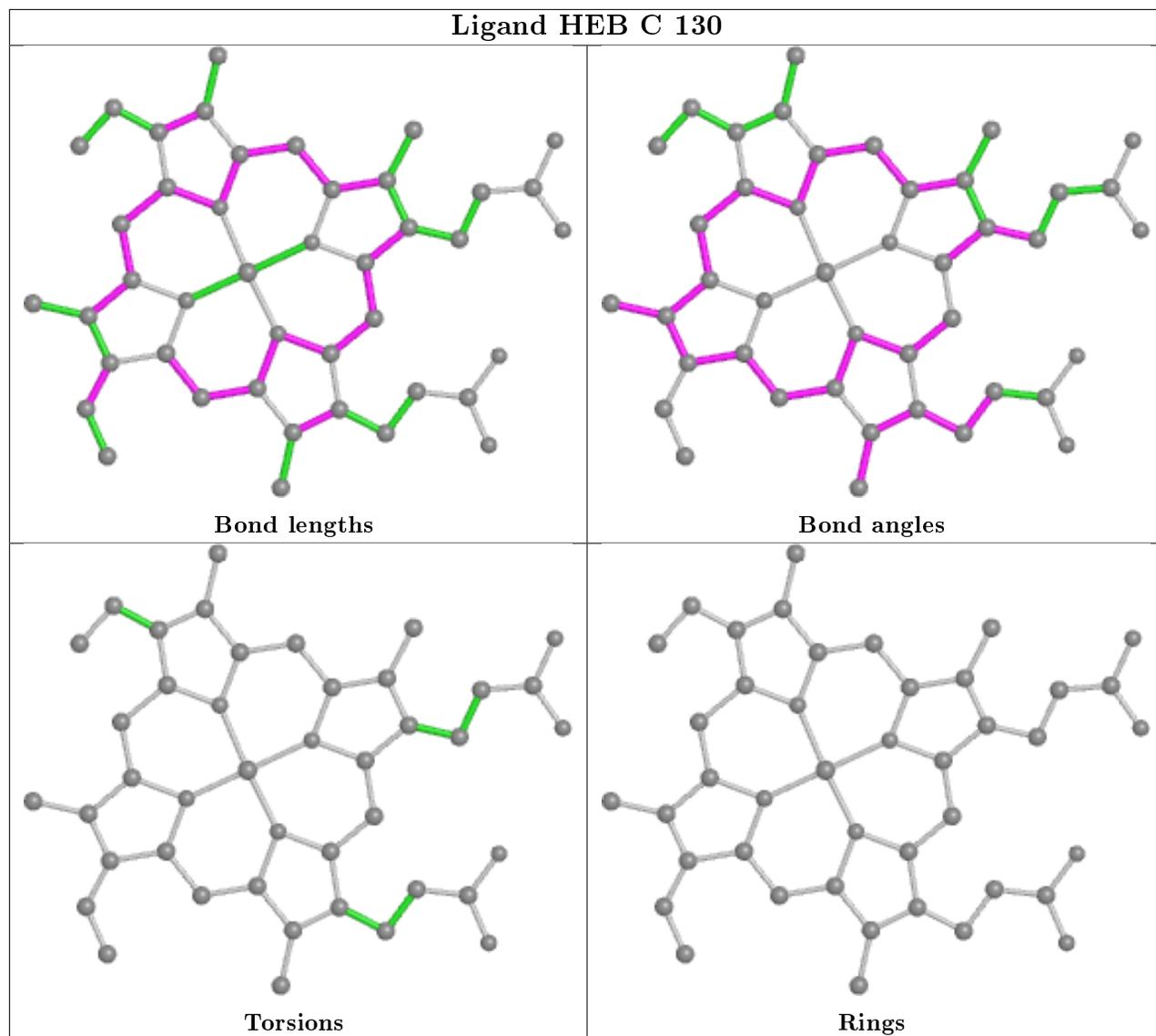
Mol	Chain	Res	Type	Atoms
11	C	131	AT5	C12-C13-C14-CL16
11	C	131	AT5	N4-C3-O3-CM3
11	C	131	AT5	C2-C3-O3-CM3
12	C	132	CDN	CB2-OB2-PB2-OB3
12	C	132	CDN	CB2-OB2-PB2-OB4

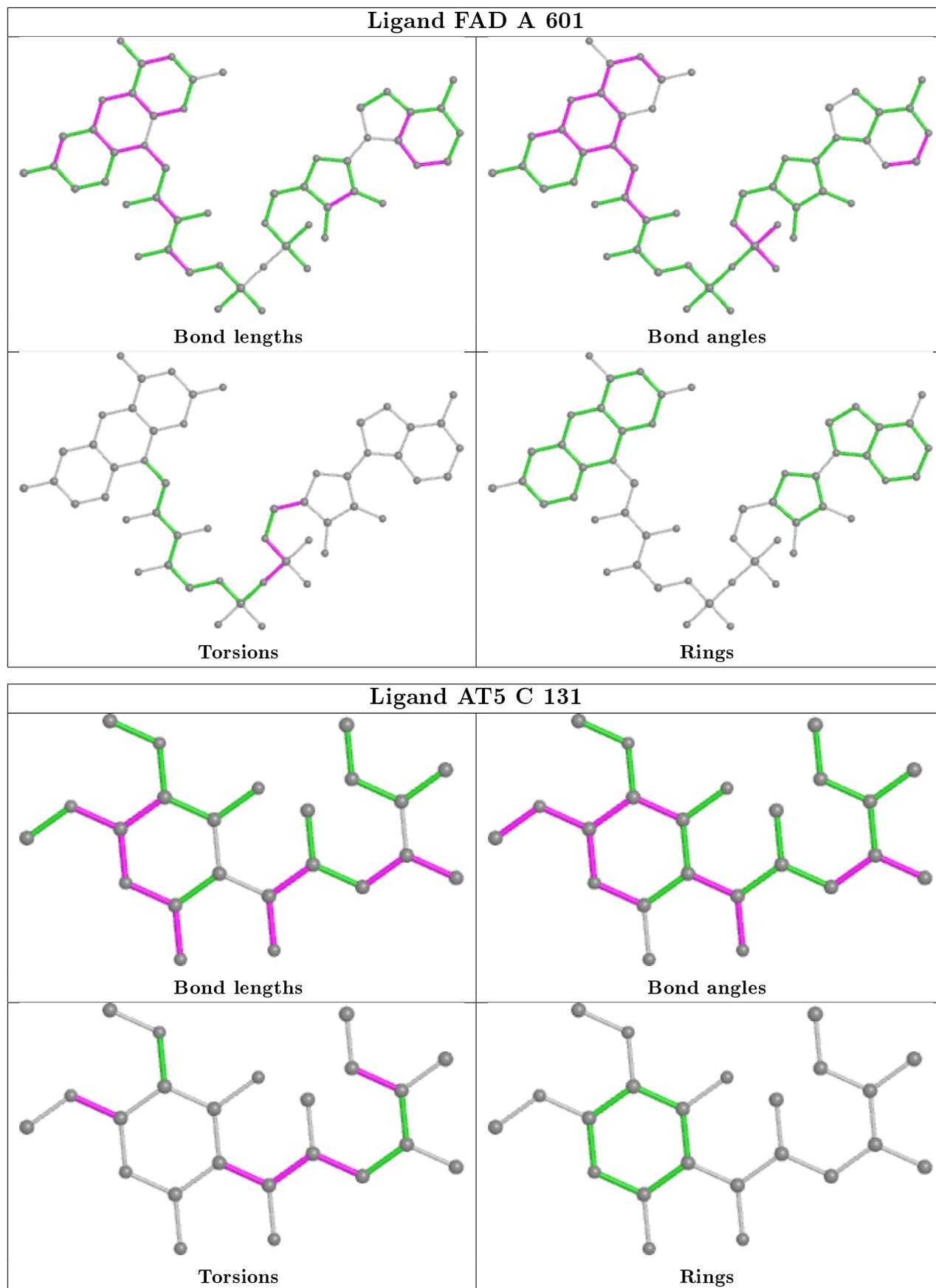
There are no ring outliers.

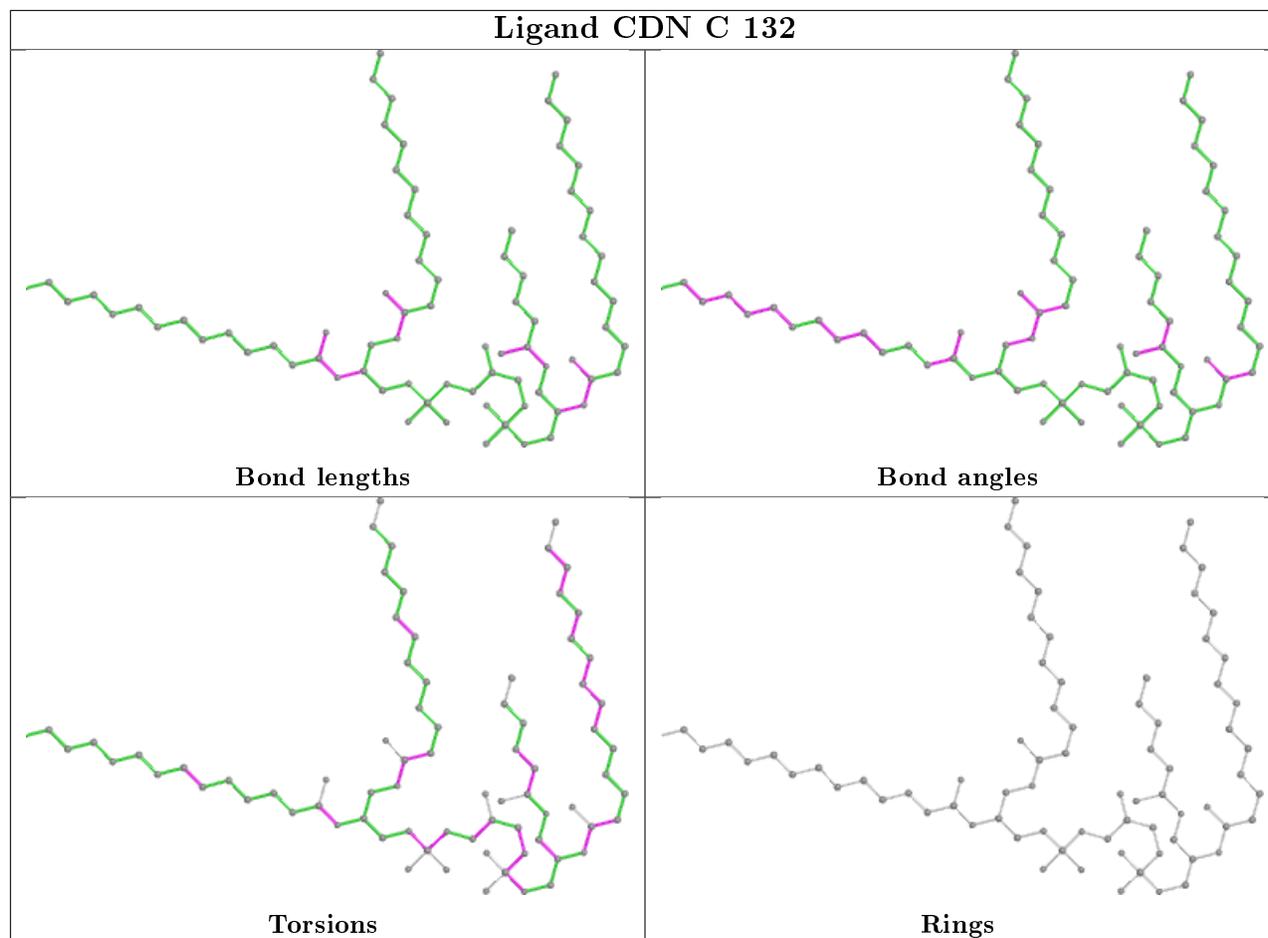
7 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	130	HEB	10	0
6	A	601	FAD	9	0
11	C	131	AT5	4	0
12	C	132	CDN	19	0
5	A	589	OAA	5	0
7	B	302	FES	1	0
9	B	304	F3S	4	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	577/588 (98%)	0.30	28 (4%) 29 14	41, 86, 112, 123	1 (0%)
2	B	238/238 (100%)	-0.08	6 (2%) 57 34	37, 57, 99, 118	0
3	C	129/129 (100%)	-0.09	6 (4%) 31 15	32, 60, 100, 132	0
4	D	113/115 (98%)	-0.19	1 (0%) 84 69	28, 44, 91, 100	0
All	All	1057/1070 (98%)	0.11	41 (3%) 39 20	28, 72, 109, 132	1 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	4	ASN	8.2
3	C	5	VAL	4.6
2	B	1	MET	4.5
3	C	1	MET	4.3
1	A	306	PRO	4.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

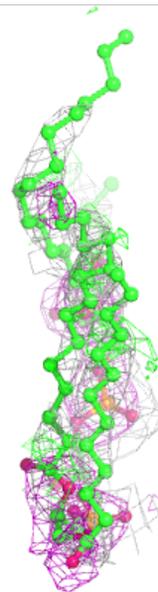
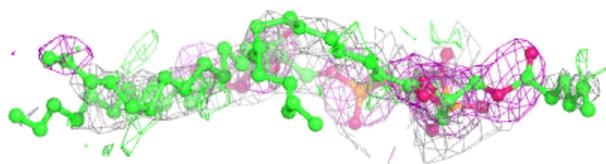
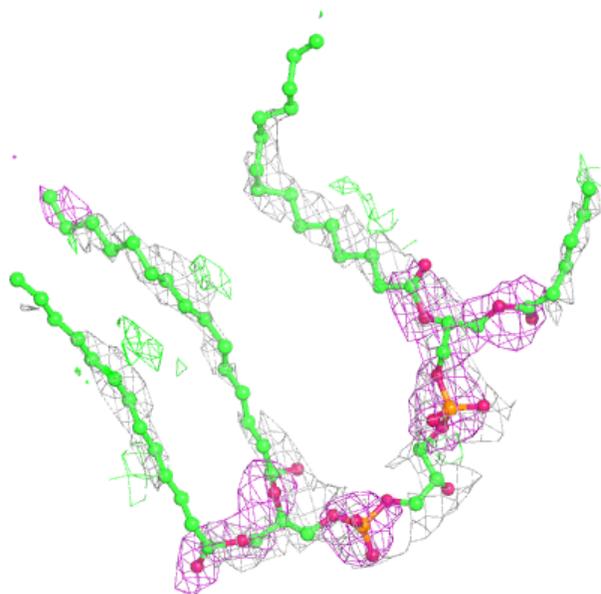
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	CDN	C	132	77/77	0.77	0.60	32,55,88,91	0
11	AT5	C	131	23/23	0.83	0.33	74,78,84,85	0
5	OAA	A	589	9/9	0.86	0.49	94,95,96,96	0
6	FAD	A	601	53/53	0.89	0.38	65,79,83,86	0
10	HEB	C	130	43/43	0.97	0.22	22,28,42,46	0
7	FES	B	302	4/4	0.99	0.20	53,57,58,60	0
8	SF4	B	303	8/8	0.99	0.20	42,46,49,49	0
9	F3S	B	304	7/7	0.99	0.16	33,39,41,42	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.

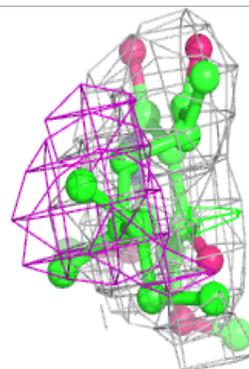
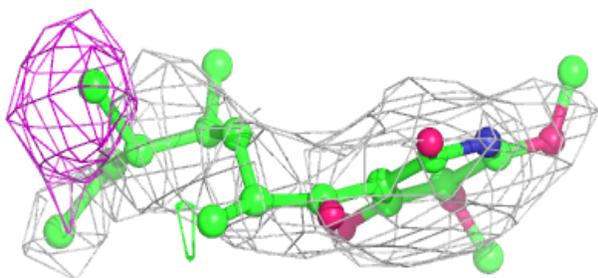
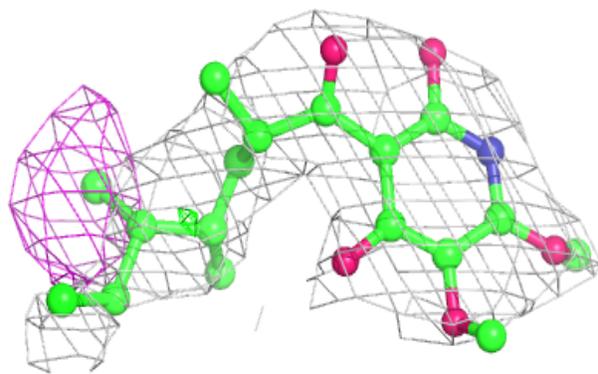
Electron density around CDN C 132:

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

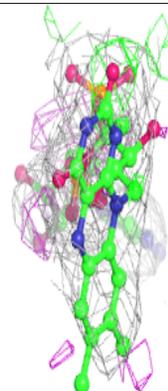
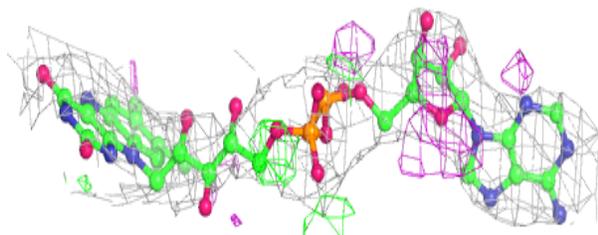
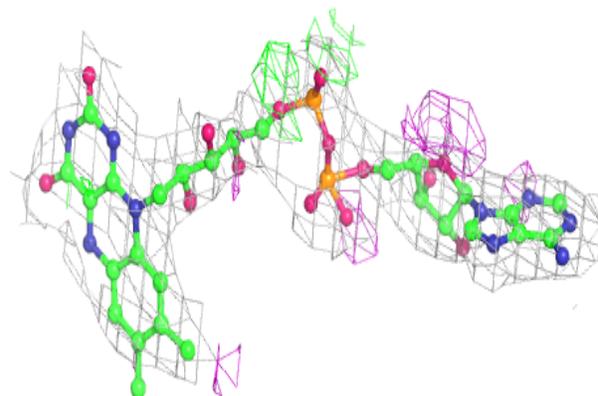


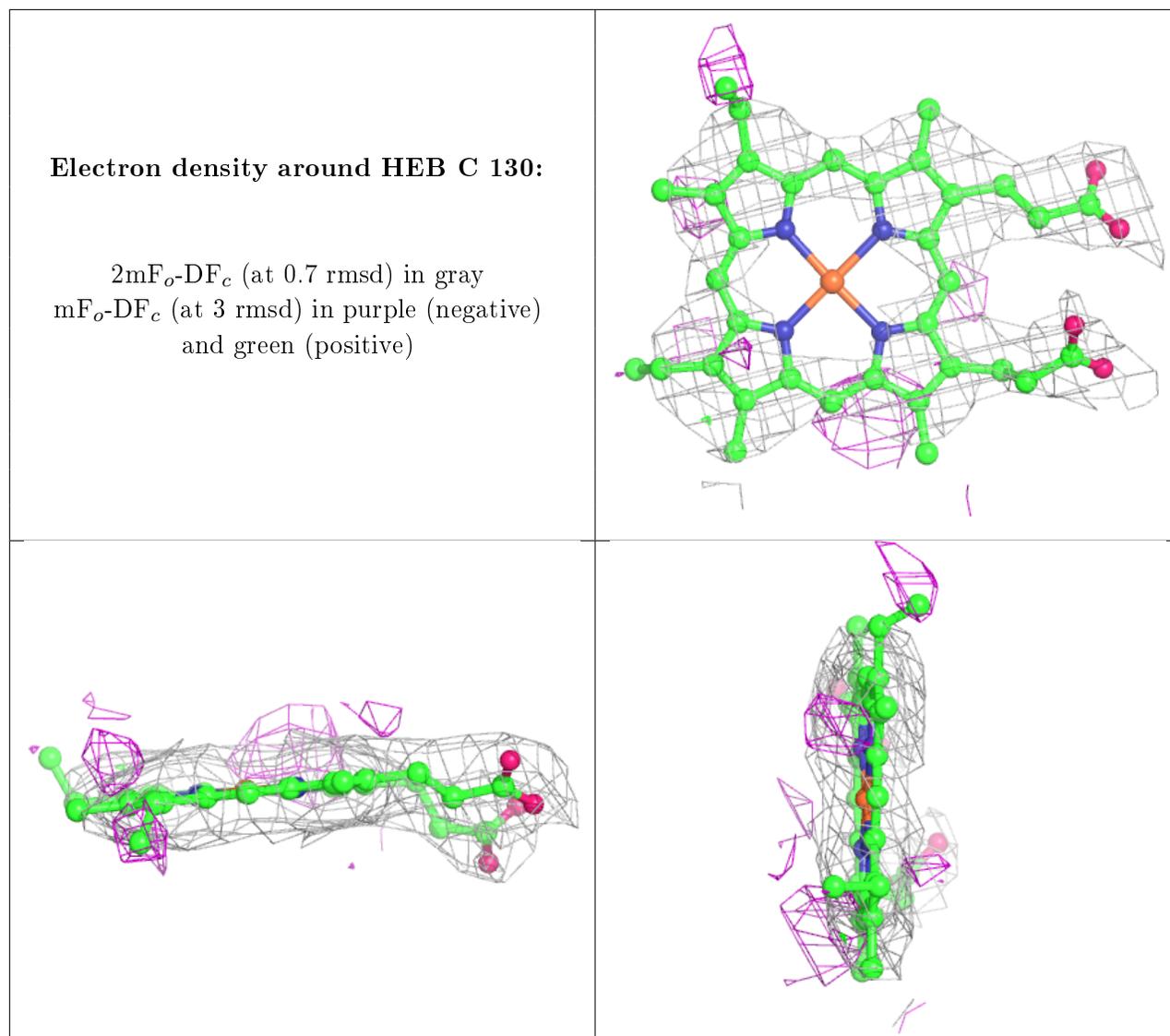
Electron density around AT5 C 131:

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

**Electron density around FAD A 601:**

$2mF_o-DF_c$ (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.