WORLDWIDE wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 01:03 PM EDT

PDB ID	:	1YQ4
Title	:	Avian respiratory complex ii with 3-nitropropionate and ubiquinone
Authors	:	Huang, L.; Sun, G.; Cobessi, D.; Wang, A.; Shen, J.T.; Tung, E.Y.; Anderson, V.E.; Berry, E.A.
Deposited on	:	2005-02-01
Resolution	:	2.33 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

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 2.33 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.
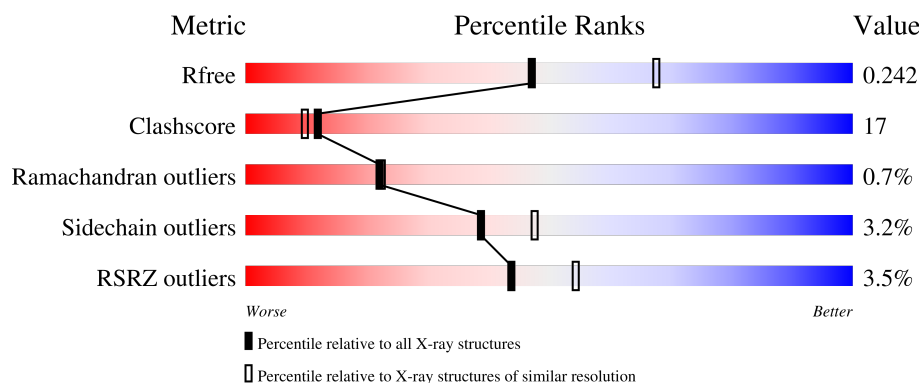
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	621	3% / 66% / 31% / · ·
2	B	252	5% / 60% / 33% / · ·
3	C	141	% / 64% / 33% / · ·
4	D	103	2% / 64% / 33% / · ·

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
10	GOL	B	1005	-	-	-	X
6	3NP	A	1002	-	X	-	-

2 Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 9291 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
1	A	614	Total	C	N	O	S	0	0	0
			4736	2962	845	900	29			

- Molecule 2 is a protein called succinate dehydrogenase Ip subunit.

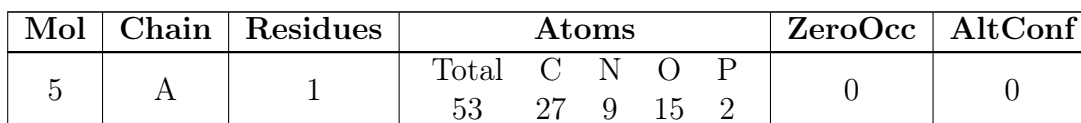| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1934	1222	327	363	22			

- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	140	Total	C	N	O	S	0	0	1
			1074	706	179	185	4			

- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			770	508	122	137	3			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	53	27	9	15	2	0	0

- Molecule 6 is 3-NITROPROPANOIC ACID (three-letter code: 3NP) (formula: $C_3H_5NO_4$).

3NP

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	6	3	1	2	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

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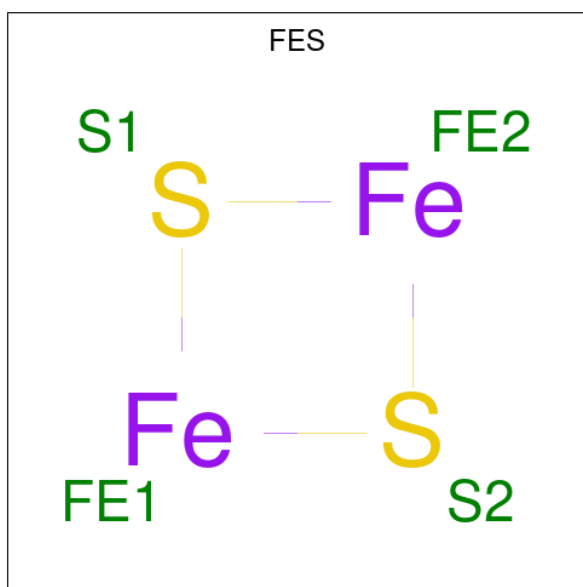
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 4	Fe 2	S 2	0	0

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

SF4
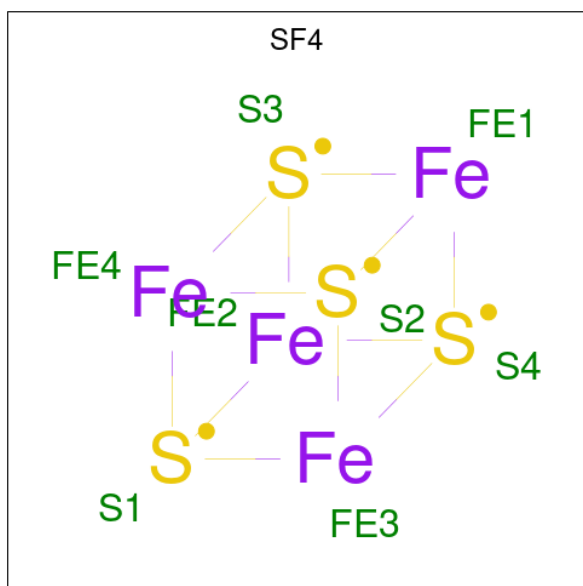
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 8	Fe 4	S 4	0	0

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).
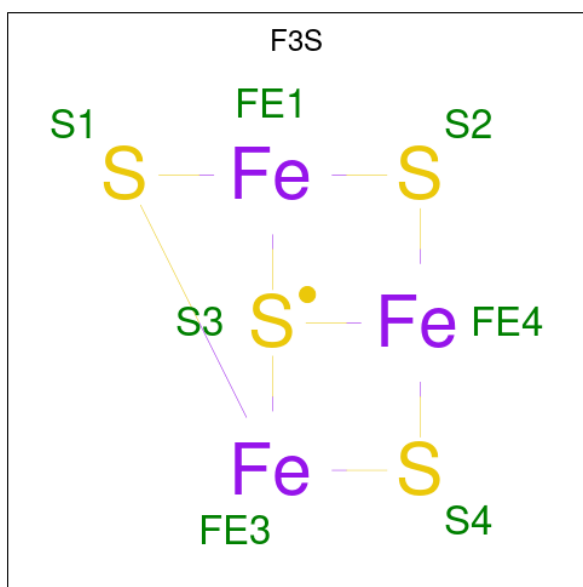
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	7	3	4	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
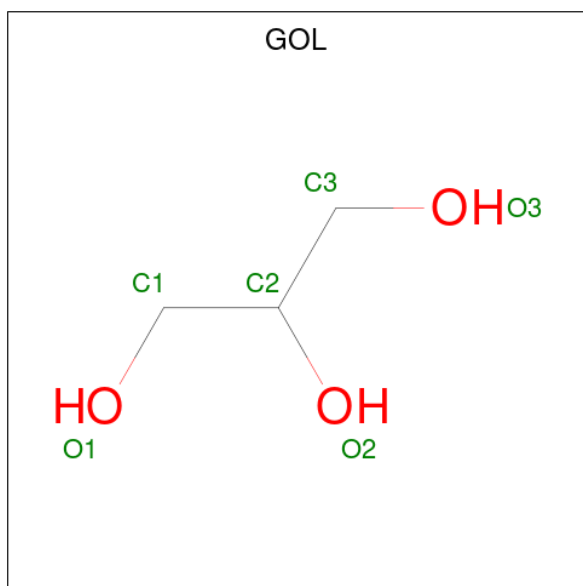
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	B	1	6	3	3	0	0

- Molecule 11 is hexyl beta-D-glucopyranoside (three-letter code: JZR) (formula: $C_{12}H_{24}O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total 18	C 12	O 6	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 41	C 32	Fe 1	N 4	O 4	0	0

- Molecule 13 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).

UQ
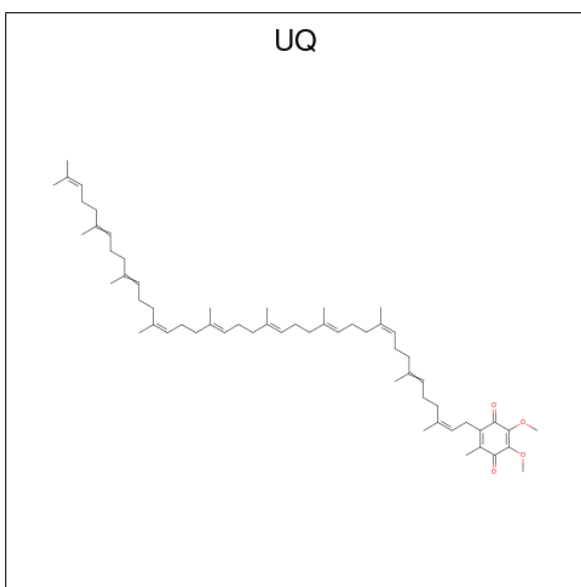
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total 14	C 10	O 4	0	0

- Molecule 14 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).

PEE
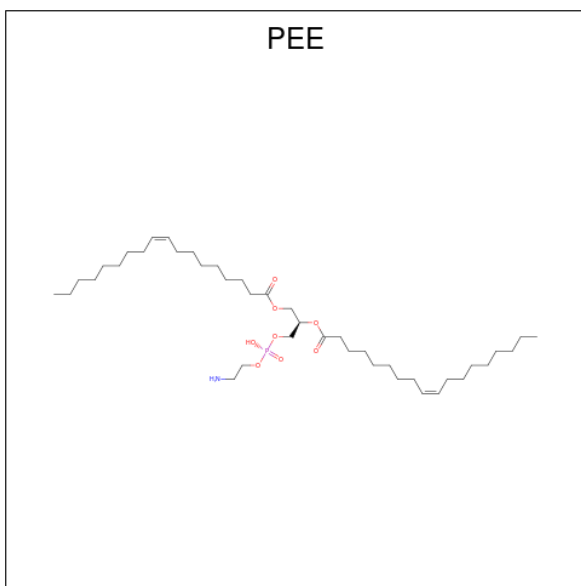
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total 21	C 19	O 2	0	0
14	D	1	Total 24	C 24		0	0

- Molecule 15 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	280	Total 280	O 280	0	0
15	B	159	Total 159	O 159	0	0
15	C	72	Total 72	O 72	0	0
15	D	64	Total 64	O 64	0	0

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.
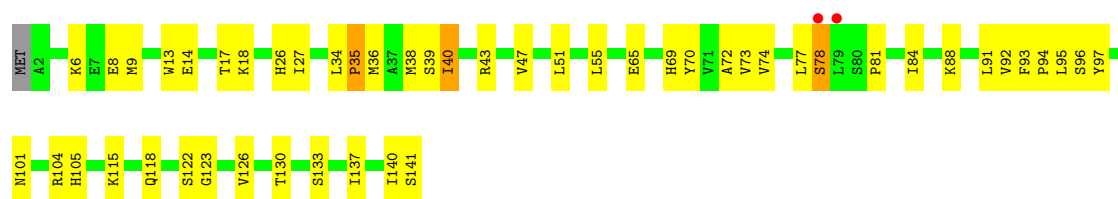
• Molecule 1: Succinate dehydrogenase flavoprotein subunit
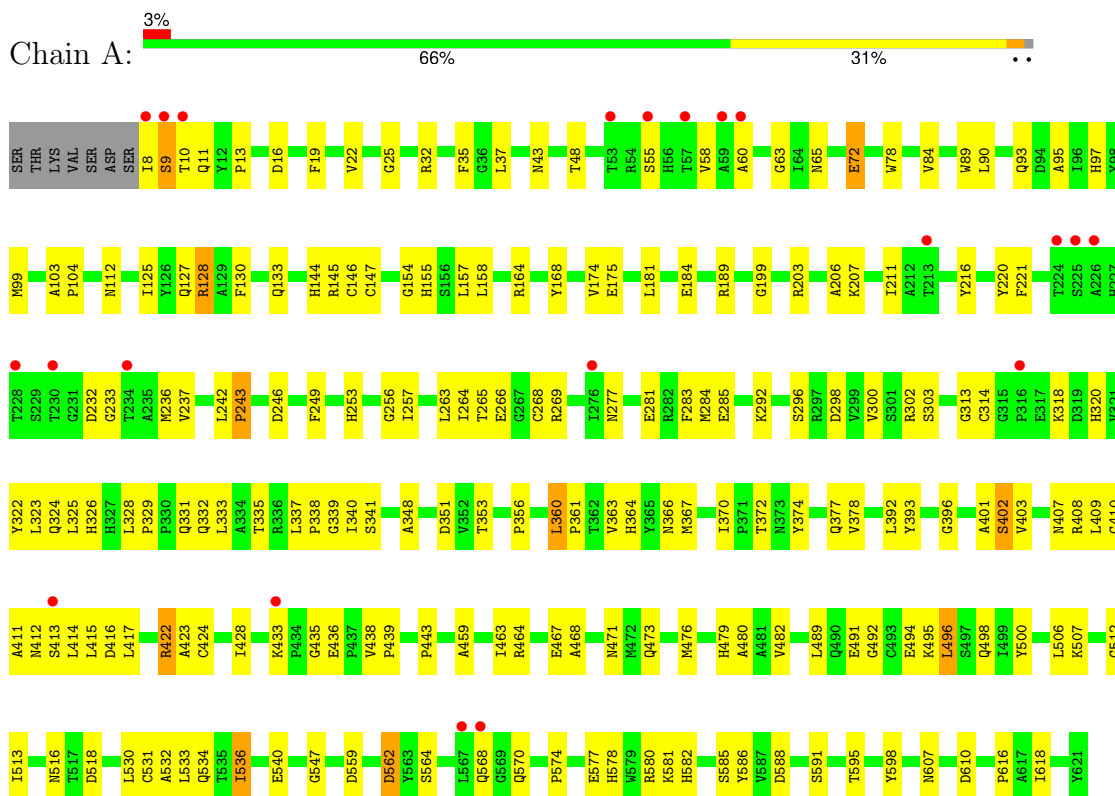
• Molecule 2: succinate dehydrogenase Ip subunit
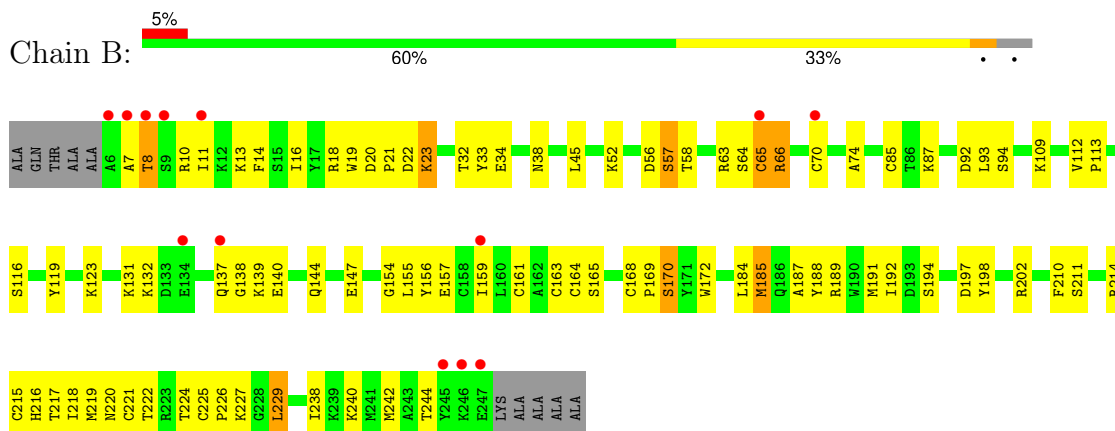
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT

• Molecule 4: SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.59Å 83.49Å 288.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.38 – 2.33 47.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	79.4 (56.38-2.33) 90.1 (47.48-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.252 0.196 , 0.242	Depositor DCC
R_{free} test set	3830 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 54.8	EDS
L-test for twinning[2]	$< |L| > = 0.41, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9291	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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: GOL, FAD, HEM, UQ, 3NP, FES, F3S, JZR, PEE, SF4

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	0.62	1/4837 (0.0%)	0.83	4/6550 (0.1%)
2	B	0.73	2/1976 (0.1%)	0.83	1/2666 (0.0%)
3	C	0.69	0/1103	0.76	0/1501
4	D	0.67	0/793	0.73	0/1089
All	All	0.66	3/8709 (0.0%)	0.81	5/11806 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	185	MET	SD-CE	6.00	2.11	1.77
1	A	531	CYS	CB-SG	-5.84	1.72	1.81
2	B	215	CYS	CB-SG	5.37	1.91	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	422	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	256	GLY	N-CA-C	-5.86	98.46	113.10
1	A	422	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	B	23	LYS	N-CA-C	-5.21	96.93	111.00
1	A	408	ARG	NE-CZ-NH2	-5.03	117.78	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	4736	0	4614	157	0
2	B	1934	0	1920	76	0
3	C	1074	0	1115	46	0
4	D	770	0	763	33	0
5	A	53	0	29	7	0
6	A	6	0	0	0	0
7	B	4	0	0	0	0
8	B	8	0	0	0	0
9	B	7	0	0	0	0
10	B	6	0	8	0	0
11	C	18	0	24	0	0
12	C	41	0	24	0	0
13	C	14	0	9	10	0
14	C	21	0	35	1	0
14	D	24	0	40	0	0
15	A	280	0	0	3	0
15	B	159	0	0	4	0
15	C	72	0	0	6	0
15	D	64	0	0	4	0
All	All	9291	0	8581	299	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 17.

The worst 5 of 299 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)
2:B:185:MET:SD	2:B:185:MET:CE	2.11	1.39
2:B:240:LYS:O	2:B:244:THR:HG23	1.71	0.88
1:A:277:ASN:HD21	1:A:281:GLU:HB3	1.39	0.85
1:A:401:ALA:N	1:A:402:SER:HA	1.91	0.85
1:A:181:LEU:HD21	1:A:211:ILE:HD11	1.57	0.84

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	612/621 (99%)	569 (93%)	39 (6%)	4 (1%)	22	22
2	B	240/252 (95%)	227 (95%)	10 (4%)	3 (1%)	12	9
3	C	138/141 (98%)	130 (94%)	7 (5%)	1 (1%)	22	22
4	D	100/103 (97%)	94 (94%)	6 (6%)	0	100	100
All	All	1090/1117 (98%)	1020 (94%)	62 (6%)	8 (1%)	22	22

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	THR
2	B	8	THR
3	C	78	SER
1	A	568	GLN
2	B	57	SER

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	498/506 (98%)	484 (97%)	14 (3%)	43	53
2	B	215/219 (98%)	207 (96%)	8 (4%)	34	43
3	C	117/119 (98%)	114 (97%)	3 (3%)	46	56
4	D	78/79 (99%)	74 (95%)	4 (5%)	24	29
All	All	908/923 (98%)	879 (97%)	29 (3%)	39	47

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	63	ARG
4	D	66	LYS
2	B	116	SER
3	C	91	LEU
2	B	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	101	ASN
4	D	69	ASN
4	D	53	GLN
1	A	383	ASN
3	C	42	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

11 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
8	SF4	B	1003	2	0,12,12	-	-	-		
7	FES	B	1002	2	0,4,4	-	-	-		
11	JZR	C	142	-	18,18,18	2.03	3 (16%)	23,23,23	1.01	2 (8%)
6	3NP	A	1002	1	5,5,7	3.73	3 (60%)	5,5,8	4.21	2 (40%)
9	F3S	B	1004	2	0,9,9	-	-	-		
10	GOL	B	1005	-	5,5,5	1.36	0	5,5,5	0.61	0
13	UQ	C	144	-	14,14,63	2.00	8 (57%)	20,20,79	0.45	0
14	PEE	D	104	-	22,22,50	1.55	4 (18%)	20,20,55	1.17	2 (10%)
12	HEM	C	143	3,4	40,48,50	1.61	7 (17%)	46,80,82	2.19	14 (30%)
5	FAD	A	1001	1	54,58,58	2.79	23 (42%)	71,89,89	1.71	18 (25%)
14	PEE	C	145	-	19,19,50	1.39	3 (15%)	19,19,55	0.85	2 (10%)

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
8	SF4	B	1003	2	-	-	0/6/5/5
7	FES	B	1002	2	-	-	0/1/1/1
11	JZR	C	142	-	-	3/9/29/29	0/1/1/1
6	3NP	A	1002	1	-	3/3/3/5	-
14	PEE	D	104	-	-	11/18/18/54	-
10	GOL	B	1005	-	-	3/4/4/4	-
13	UQ	C	144	-	-	2/4/28/87	0/1/1/1
9	F3S	B	1004	2	-	-	0/3/3/3
12	HEM	C	143	3,4	-	4/10/50/54	-
5	FAD	A	1001	1	-	11/30/50/50	0/6/6/6
14	PEE	C	145	-	-	11/17/17/54	-

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	FAD	PA-O3P	-11.25	1.47	1.59
5	A	1001	FAD	P-O3P	6.63	1.66	1.59
11	C	142	JZR	O1-C1	6.09	1.50	1.40
6	A	1002	3NP	C2-C1	-5.82	1.37	1.50
5	A	1001	FAD	PA-O2A	-5.12	1.31	1.55

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1002	3NP	C3-C2-C1	8.65	131.71	112.98
5	A	1001	FAD	N3A-C2A-N1A	-6.78	119.46	128.67
12	C	143	HEM	C4B-CHC-C1C	6.52	131.17	122.56
12	C	143	HEM	C3D-C4D-ND	4.54	115.15	110.17
12	C	143	HEM	C4C-CHD-C1D	4.03	127.88	122.56

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	N10-C1'-C2'-O2'
5	A	1001	FAD	O4'-C4'-C5'-O5'
5	A	1001	FAD	C5'-O5'-P-O1P
5	A	1001	FAD	C5'-O5'-P-O2P
5	A	1001	FAD	C5'-O5'-P-O3P

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	144	UQ	10	0
5	A	1001	FAD	7	0
14	C	145	PEE	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.
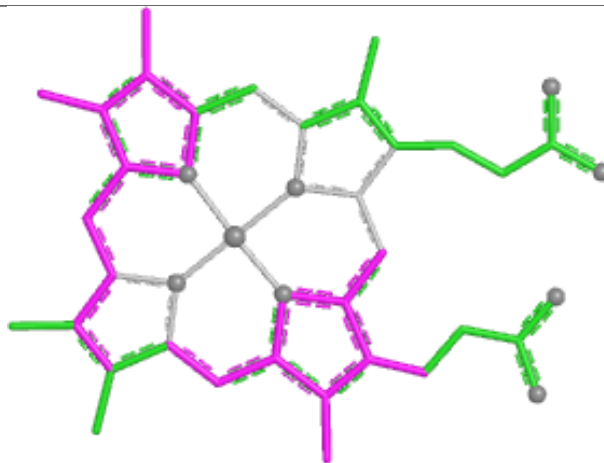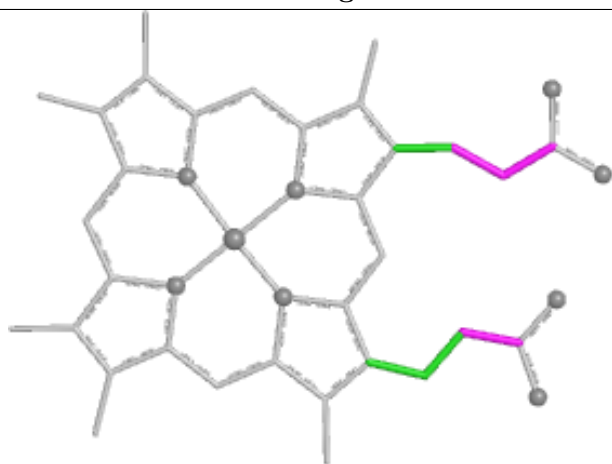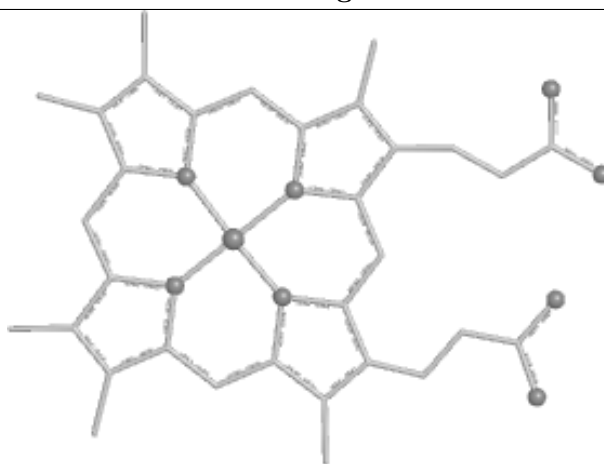
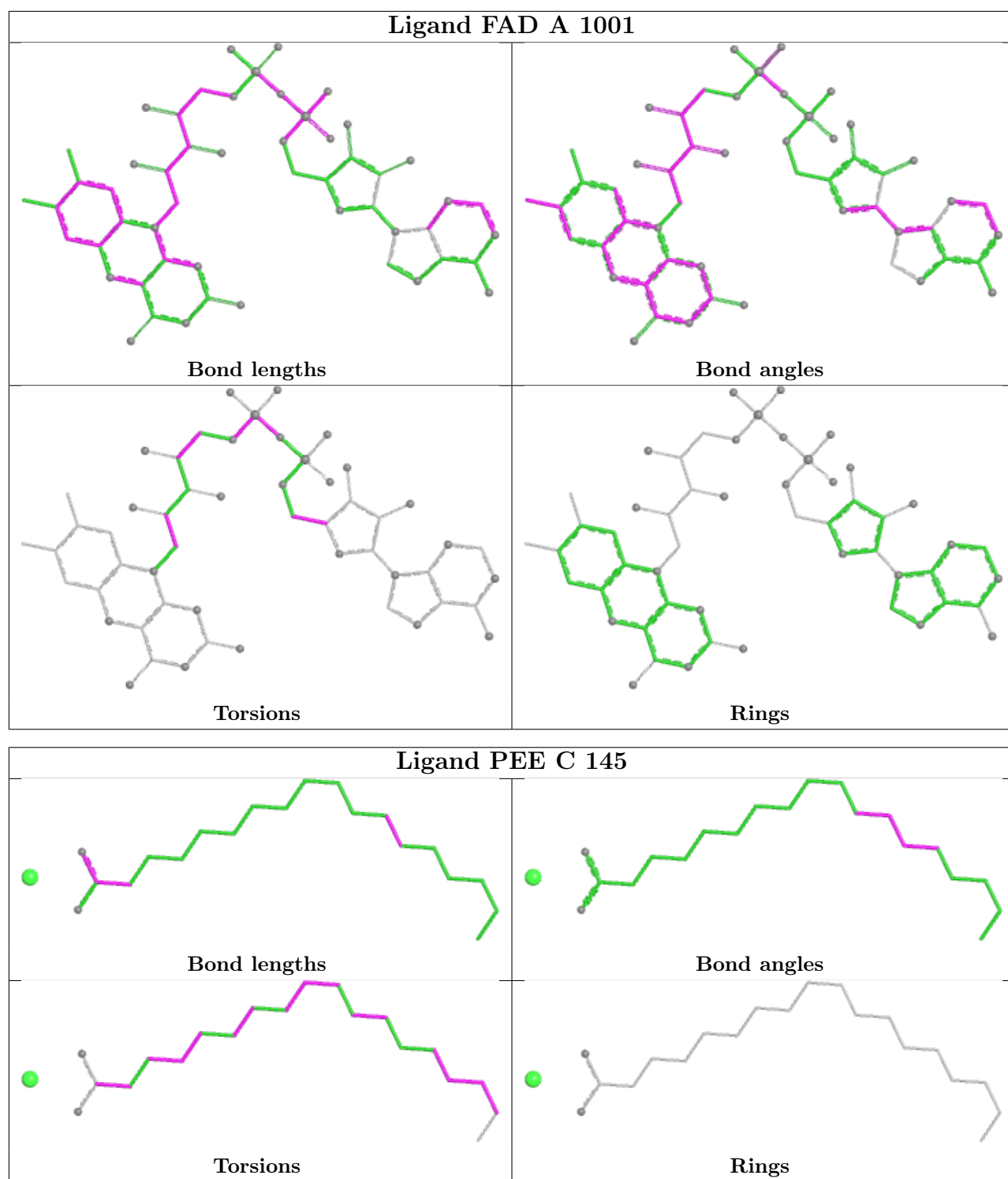## Ligand JZR C 142

Bond lengths

Bond angles

Torsions

Rings

Ligand UQ C 144

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE D 104

Bond lengths

Bond angles
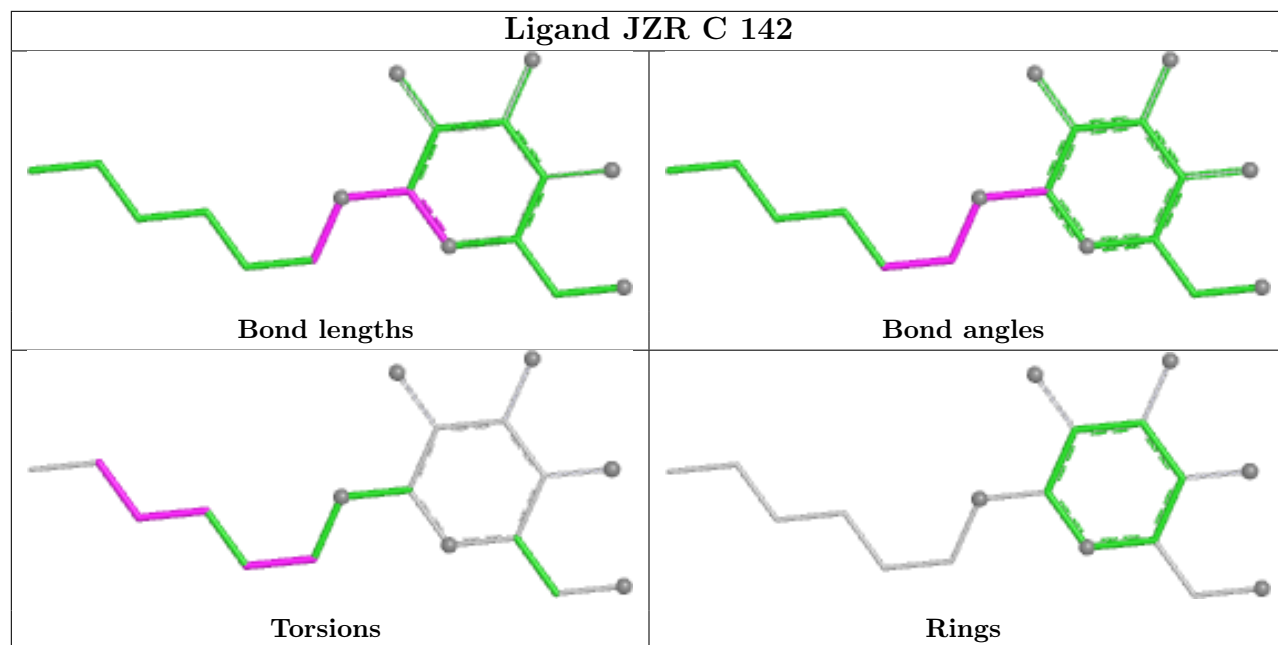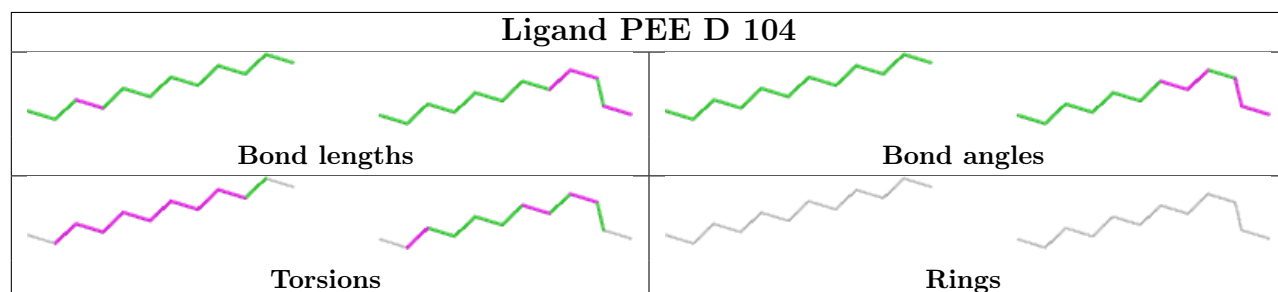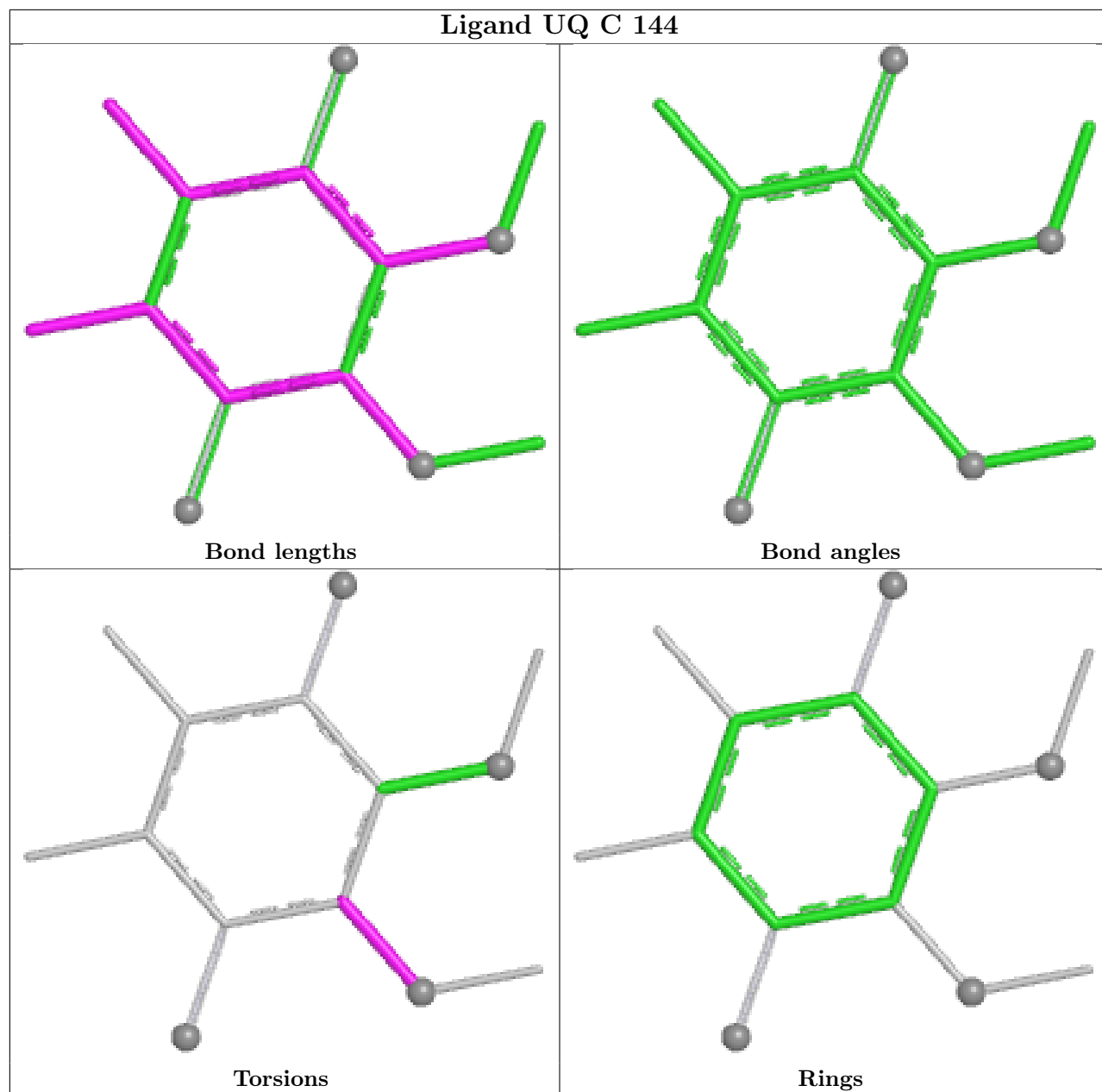
Torsions

Rings

Ligand HEM C 143

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE C 145
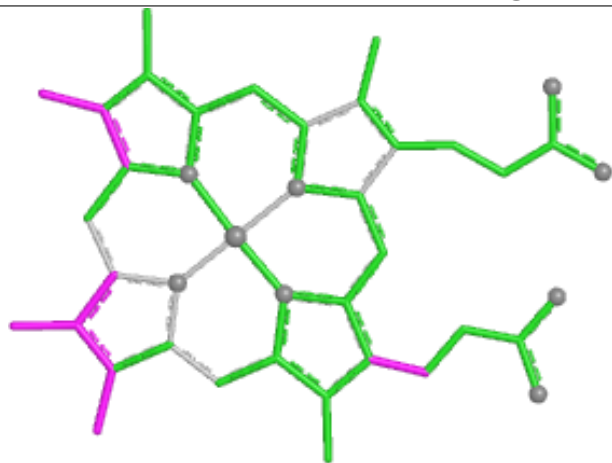
Bond lengths

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	614/621 (98%)	-0.13	21 (3%)	45	55	26, 47, 74, 152	0
2	B	242/252 (96%)	-0.09	13 (5%)	25	36	24, 40, 84, 124	0
3	C	140/141 (99%)	-0.48	2 (1%)	75	82	25, 45, 76, 91	0
4	D	102/103 (99%)	-0.46	2 (1%)	65	74	29, 42, 68, 84	0
All	All	1098/1117 (98%)	-0.20	38 (3%)	44	54	24, 45, 75, 152	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	7	ALA	6.4
1	A	8	ILE	5.7
2	B	6	ALA	5.6
1	A	9	SER	5.5
2	B	8	THR	5.1

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

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

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, 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
10	GOL	B	1005	6/6	0.31	0.59	156,160,161,162	0
14	PEE	D	104	24/51	0.80	0.28	53,72,98,99	0
14	PEE	C	145	21/51	0.84	0.23	45,74,88,92	0
13	UQ	C	144	14/63	0.84	0.44	90,99,109,113	0
11	JZR	C	142	18/18	0.93	0.15	38,48,61,63	0
5	FAD	A	1001	53/53	0.98	0.23	18,32,43,52	0
6	3NP	A	1002	6/8	0.98	0.19	38,39,44,47	0
12	HEM	C	143	41/43	0.98	0.10	29,41,65,67	0
8	SF4	B	1003	8/8	0.99	0.14	32,34,38,38	0
9	F3S	B	1004	7/7	0.99	0.11	26,27,28,30	0
7	FES	B	1002	4/4	1.00	0.15	30,32,34,37	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 PEE D 104:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
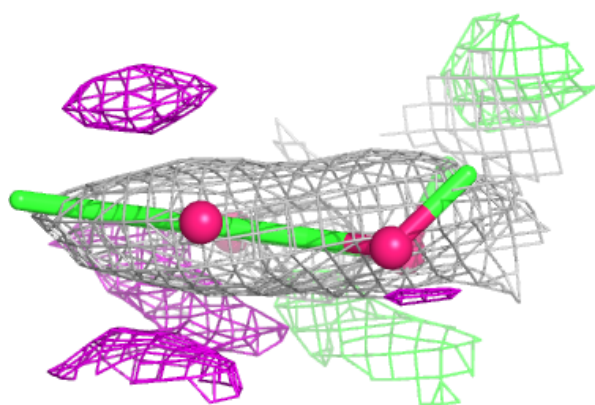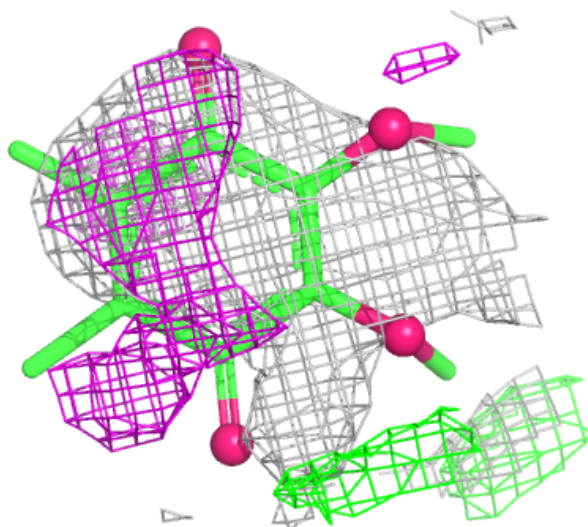mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
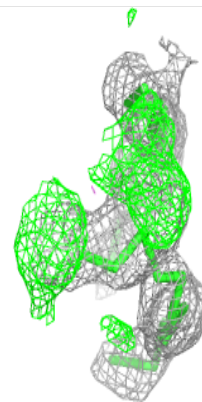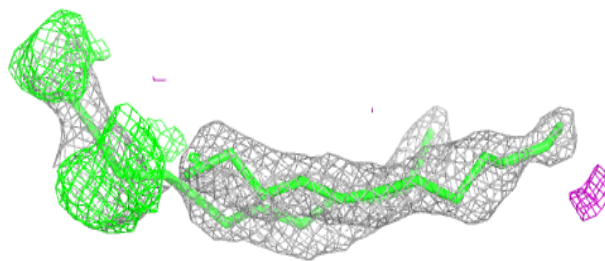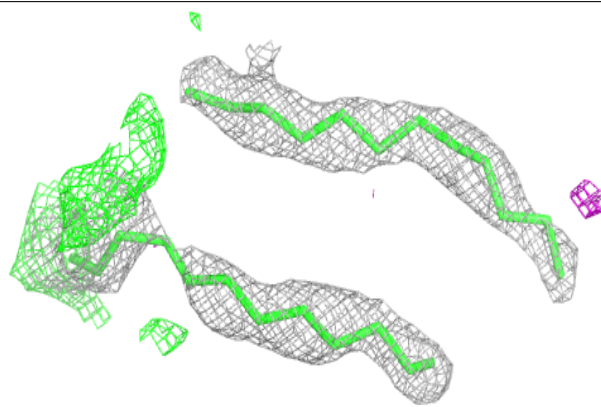
Electron density around PEE C 145:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
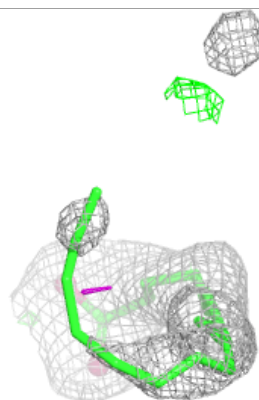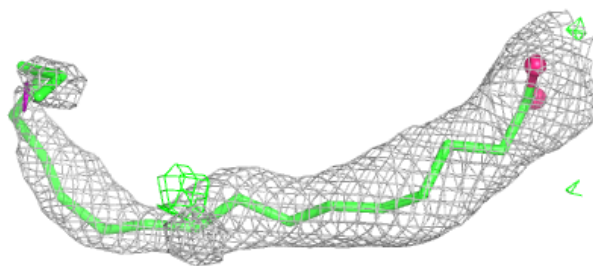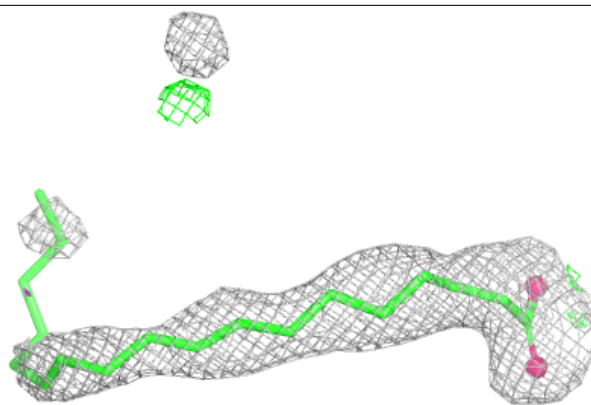
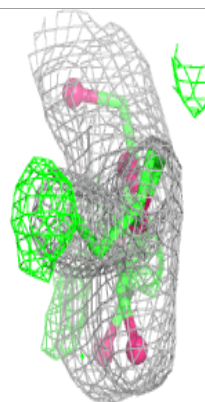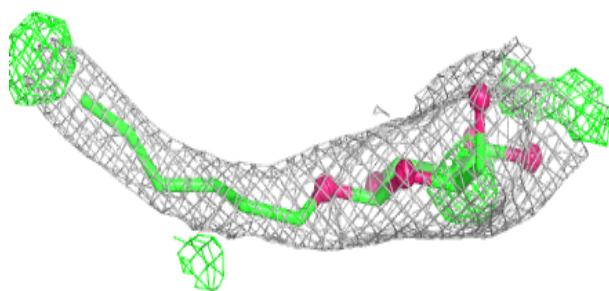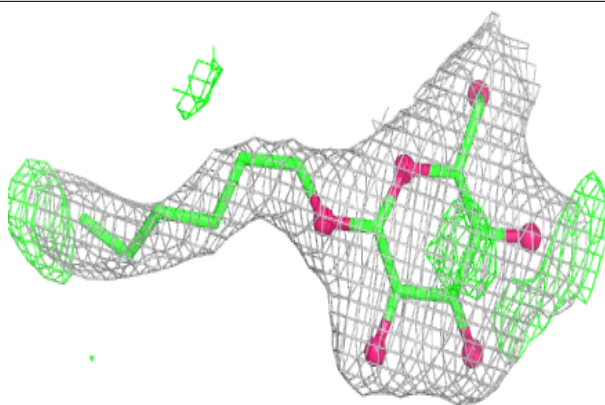**Electron density around UQ C 144:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
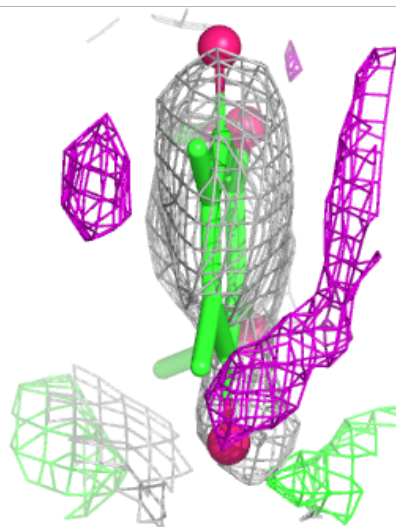
Electron density around JZR C 142:

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

Electron density around FAD A 1001:

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

Electron density around HEM C 143:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
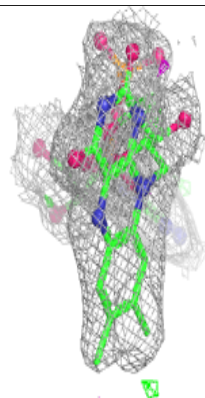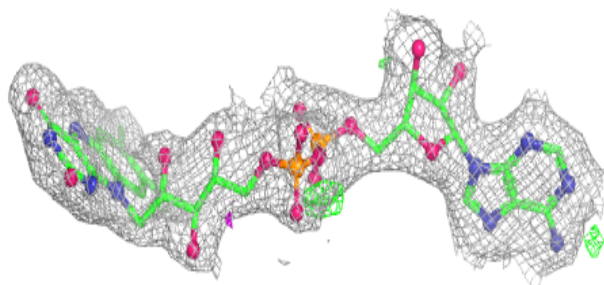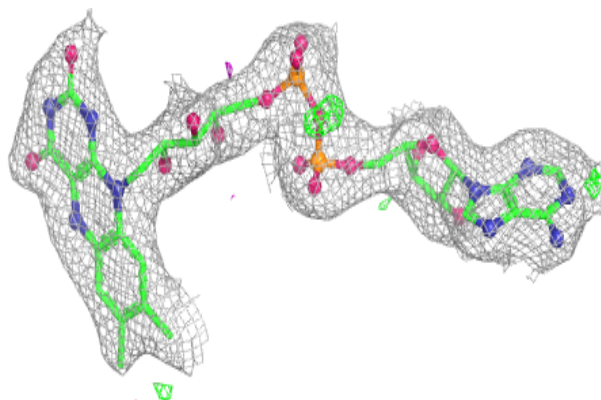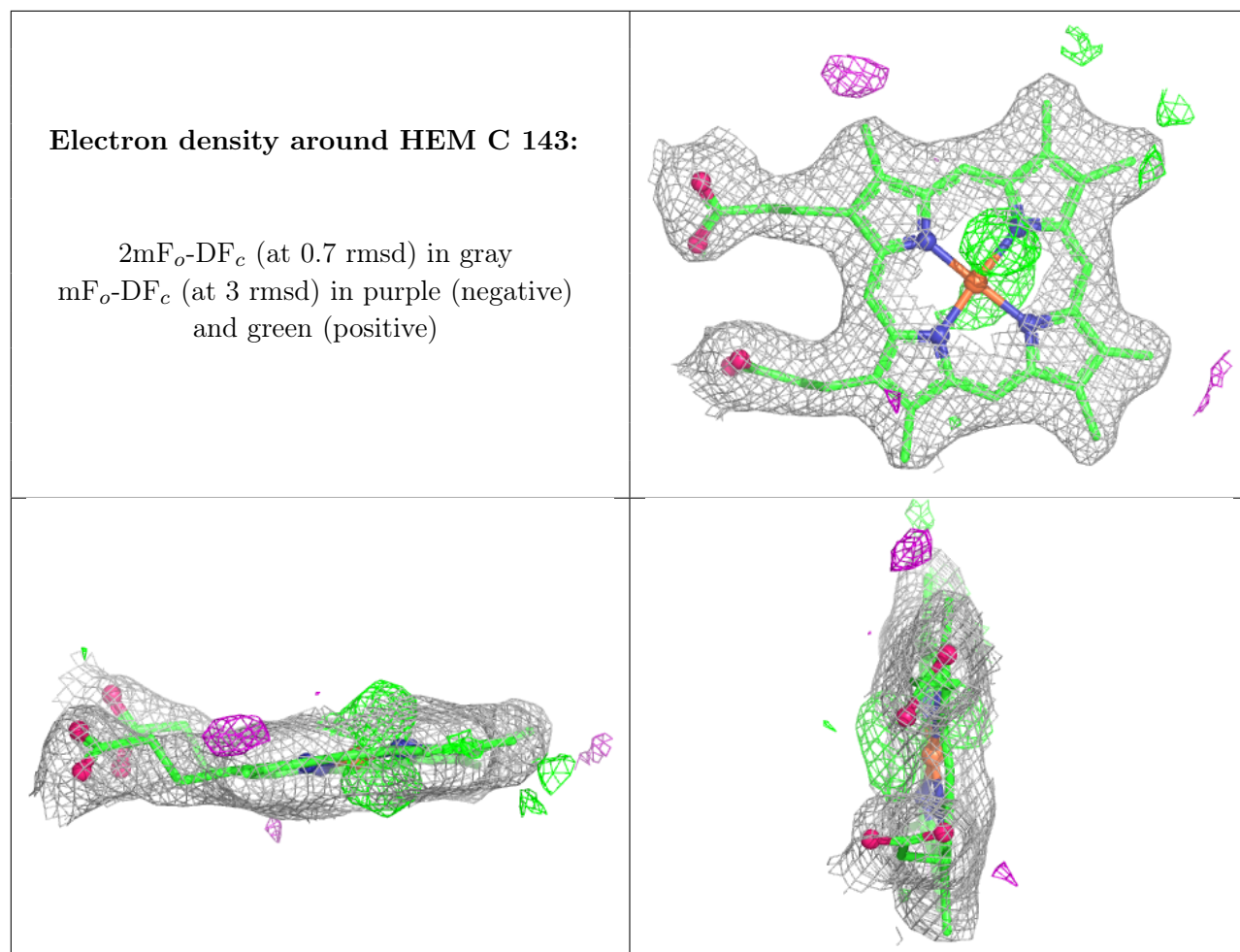
6.5 Other polymers (i)

There are no such residues in this entry.