



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:40 PM UTC

PDB ID : 1YQ3 / pdb_00001yq3
Title : Avian respiratory complex ii with oxaloacetate and ubiquinone
Authors : Huang, L.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : 2005-02-01
Resolution : 2.20 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

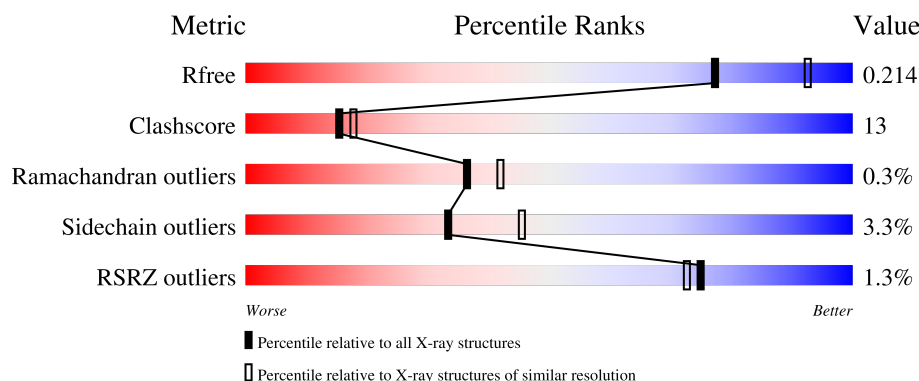
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	621	0% 64% 30% ..
2	B	252	3% 68% 20% 7% .
3	C	141	0% 57% 34% 8% .
4	D	103	2% 64% 30% ..

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
6	TEO	A	1002	X	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 9576 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
			1930	1220	327	361	22			

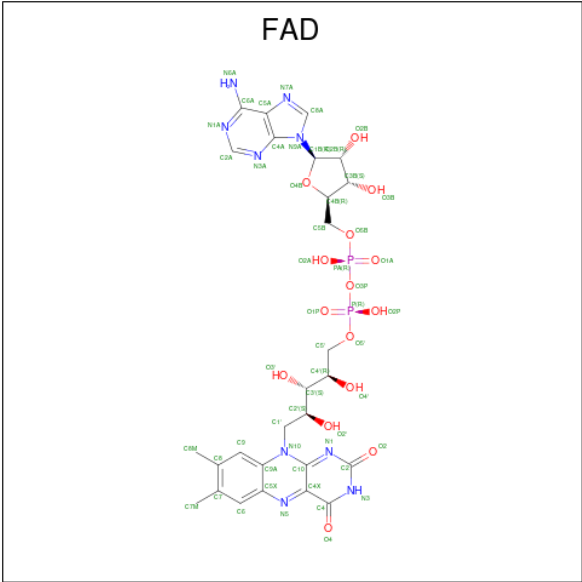
- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	140	Total	C	N	O	S	0	0	1
			1071	703	179	185	4			

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

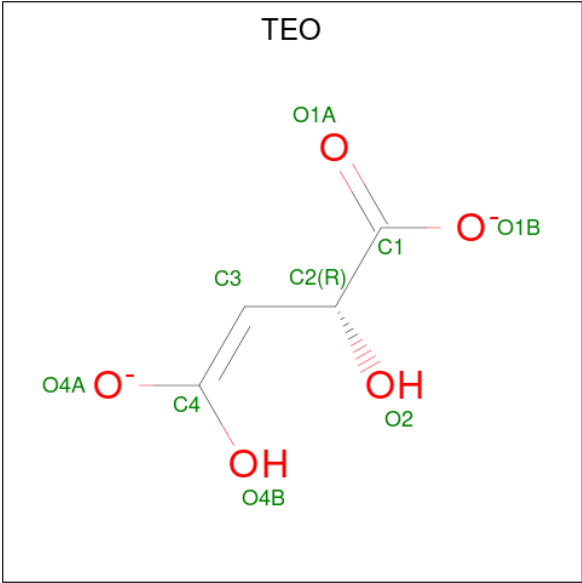
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			770	508	122	137	3			

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



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

- Molecule 6 is MALATE LIKE INTERMEDIATE (CCD ID: TEO) (formula: C₄H₄O₅).

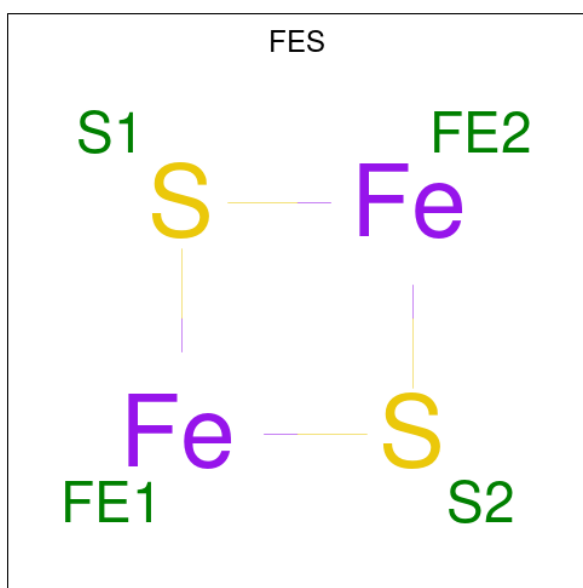


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 7 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

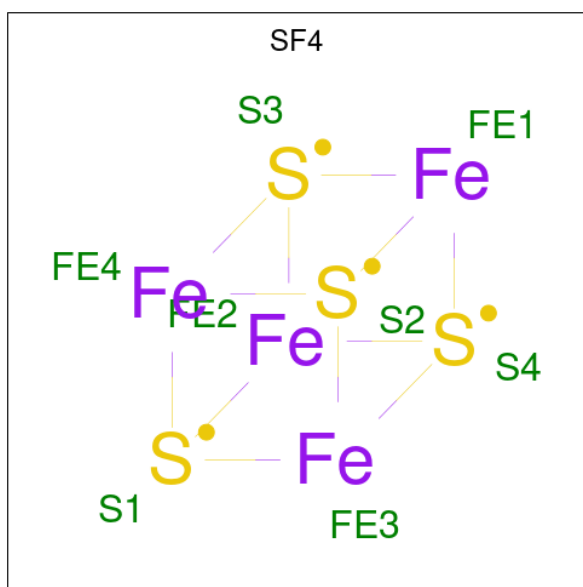
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	15	Total	O	0	0
			15	15		
7	B	6	Total	O	0	0
			6	6		
7	C	4	Total	O	0	0
			4	4		
7	D	5	Total	O	0	0
			5	5		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



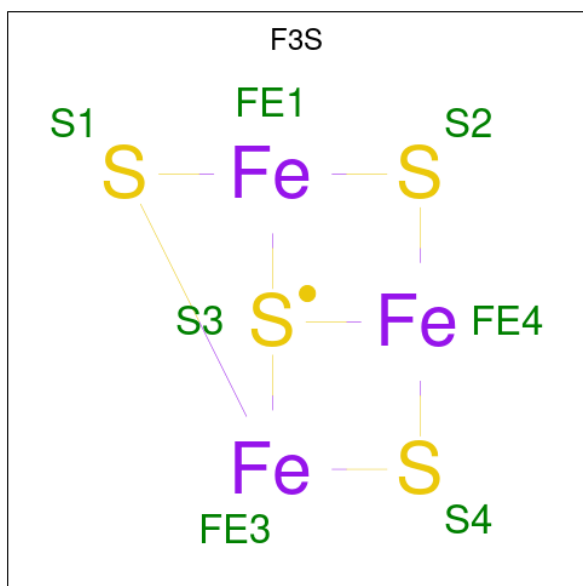
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



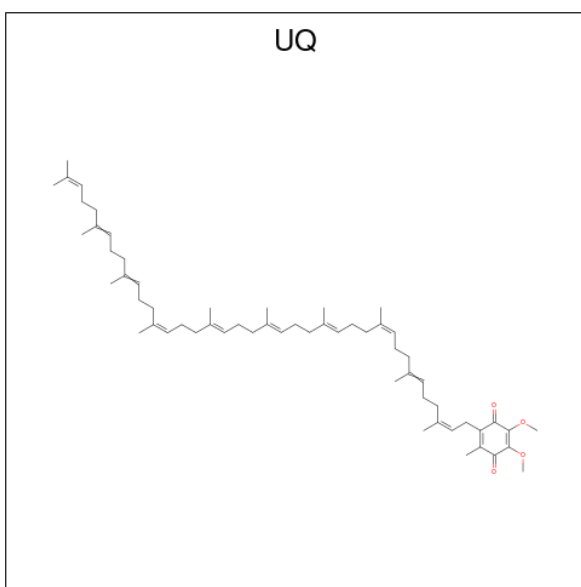
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



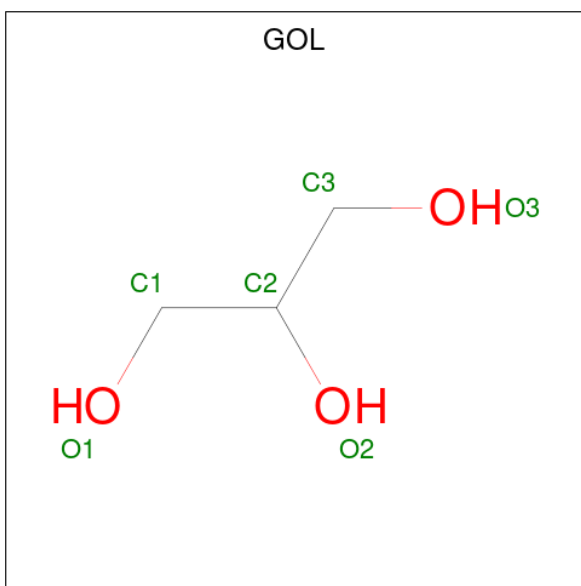
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 11 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $\text{C}_{59}\text{H}_{90}\text{O}_4$).



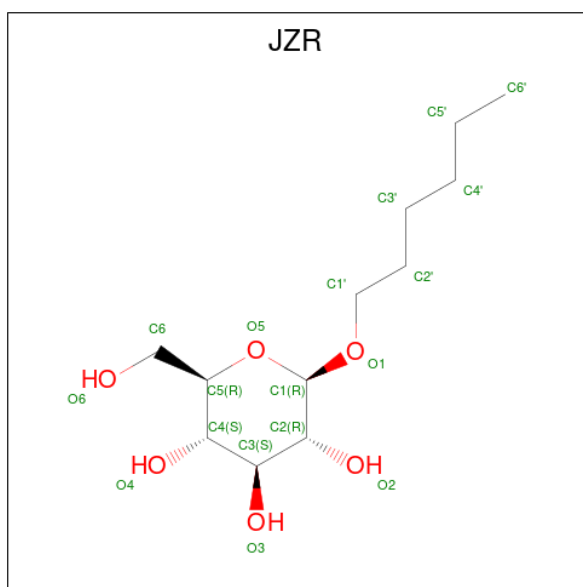
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			14	10	4		

- Molecule 12 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



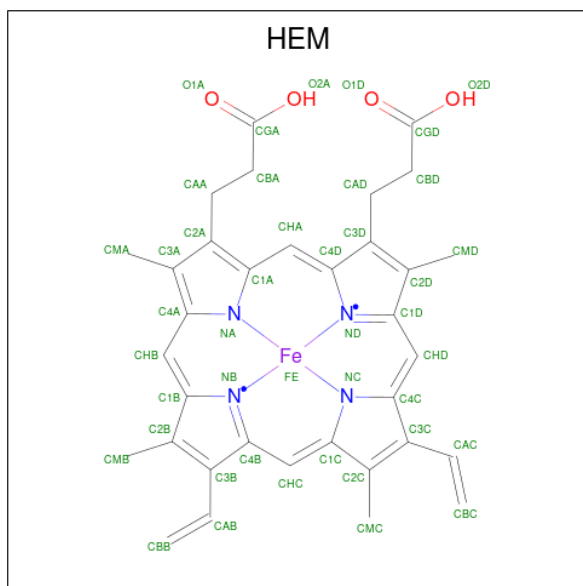
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 13 is hexyl beta-D-glucopyranoside (CCD ID: JZR) (formula: $C_{12}H_{24}O_6$).



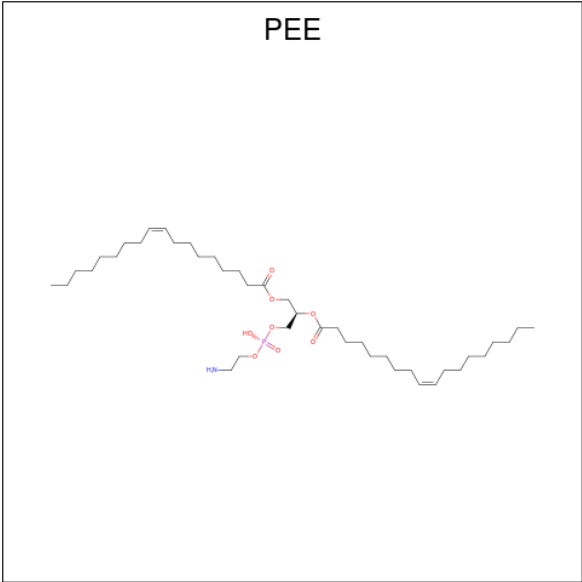
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	O		0	0
			18	12	6			

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 15 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



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

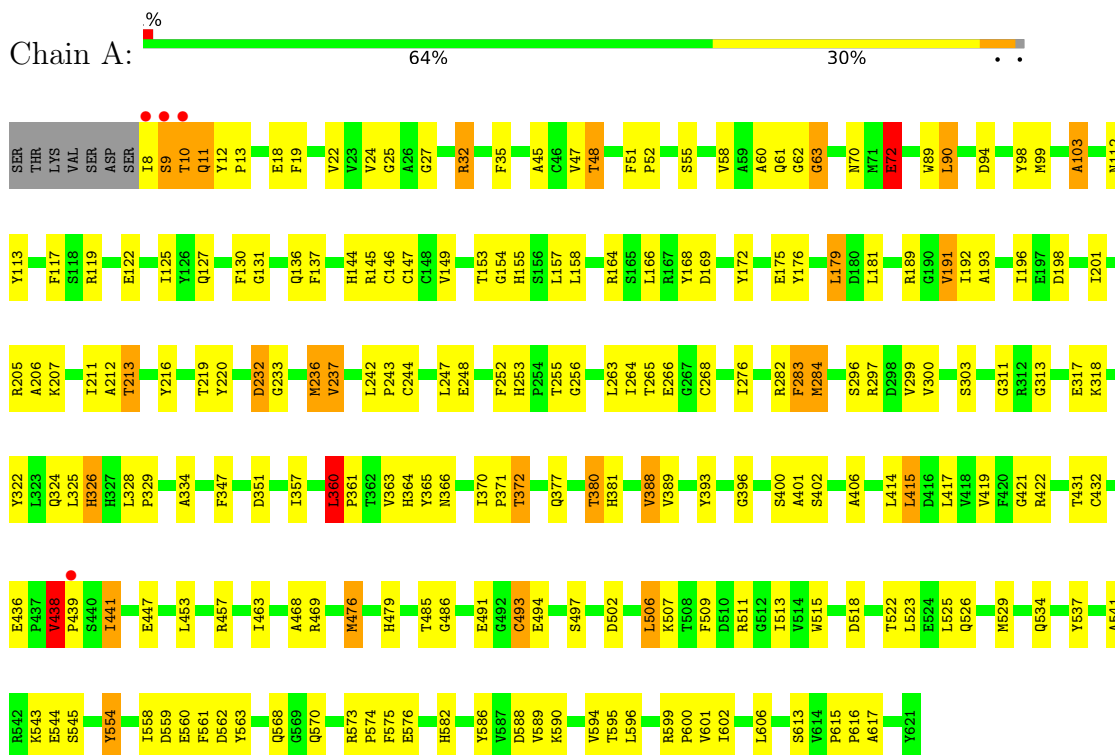
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	440	Total	O	0	0
			440	440		
16	B	213	Total	O	0	0
			213	213		
16	C	96	Total	O	0	0
			96	96		
16	D	85	Total	O	0	0
			85	85		

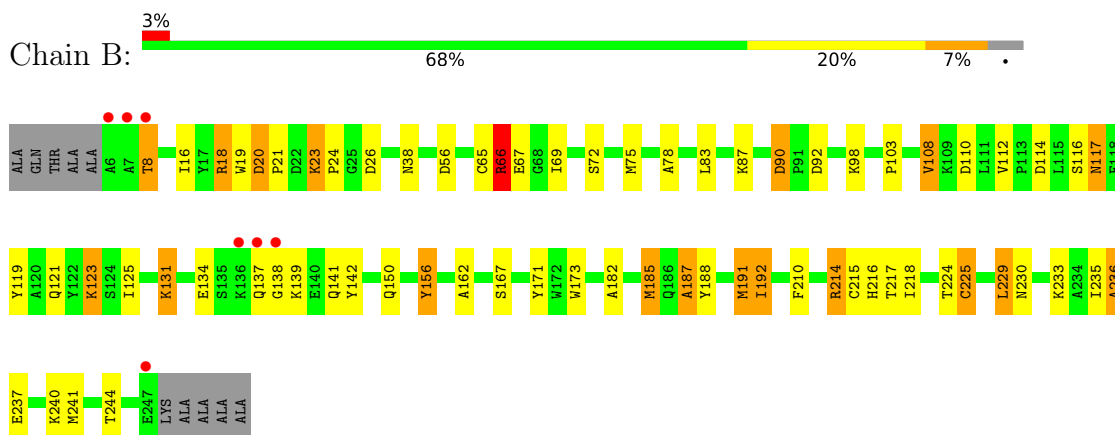
3 Residue-property plots

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.

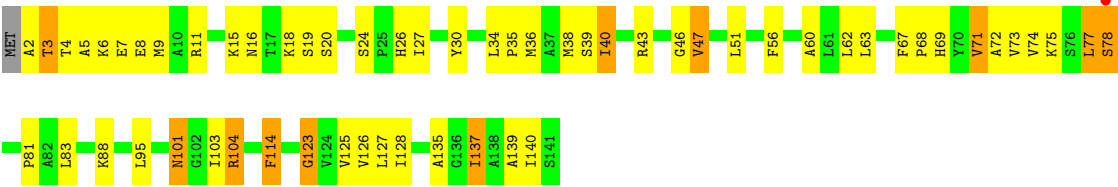
- Molecule 1: Succinate dehydrogenase flavoprotein subunit



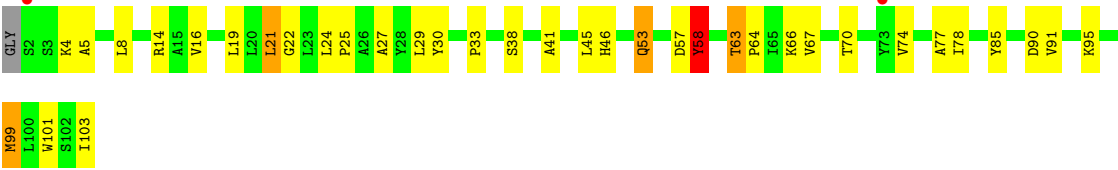
- Molecule 2: succinate dehydrogenase Ip subunit



- 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	70.01Å 84.40Å 289.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.66 – 2.20 38.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.2 (38.66-2.20) 89.3 (38.66-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.175 , 0.223 0.168 , 0.214	Depositor DCC
R_{free} test set	3842 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9576	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES, JZR, TEO, F3S, GOL, PEE, FAD, UQ, HEM, UNL

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	1.57	40/4837 (0.8%)	1.53	64/6550 (1.0%)
2	B	1.71	23/1972 (1.2%)	1.54	28/2661 (1.1%)
3	C	1.70	12/1100 (1.1%)	1.50	16/1497 (1.1%)
4	D	1.66	10/793 (1.3%)	1.42	6/1089 (0.6%)
All	All	1.63	85/8702 (1.0%)	1.52	114/11797 (1.0%)

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	A	0	5
3	C	0	1
4	D	0	1
All	All	0	7

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	191	MET	SD-CE	-19.22	1.31	1.79
3	C	36	MET	SD-CE	-17.70	1.35	1.79
2	B	241	MET	SD-CE	-11.90	1.49	1.79
1	A	284	MET	SD-CE	-11.47	1.50	1.79
3	C	126	VAL	CA-CB	11.16	1.68	1.54
1	A	236	MET	SD-CE	-10.37	1.53	1.79
1	A	103	ALA	CA-CB	10.00	1.66	1.53
1	A	476	MET	SD-CE	8.93	2.01	1.79
2	B	185	MET	SD-CE	8.86	2.01	1.79
2	B	69	ILE	CA-CB	8.47	1.65	1.54
1	A	299	VAL	CA-CB	7.53	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	PRO	CA-C	7.45	1.55	1.51
1	A	179	LEU	N-CA	7.44	1.55	1.46
2	B	235	ILE	CA-CB	-7.42	1.44	1.54
2	B	67	GLU	CA-C	7.42	1.62	1.52
2	B	69	ILE	N-CA	-7.28	1.39	1.46
2	B	66	ARG	CA-C	7.17	1.62	1.52
1	A	153	THR	C-O	7.10	1.32	1.24
1	A	175	GLU	CA-C	7.01	1.62	1.53
1	A	415	LEU	C-O	6.92	1.32	1.24
3	C	40	ILE	N-CA	-6.92	1.37	1.46
2	B	112	VAL	CA-CB	6.62	1.60	1.53
2	B	123	LYS	N-CA	6.54	1.54	1.46
4	D	41	ALA	CA-C	6.44	1.60	1.52
2	B	123	LYS	CE-NZ	6.36	1.68	1.49
3	C	60	ALA	CA-C	6.26	1.60	1.52
3	C	103	ILE	CA-CB	6.23	1.62	1.54
1	A	529	MET	SD-CE	6.19	1.95	1.79
4	D	99	MET	CA-C	-6.16	1.44	1.52
1	A	589	VAL	CA-CB	6.15	1.63	1.54
2	B	162	ALA	CA-CB	6.07	1.61	1.53
2	B	78	ALA	CA-CB	6.04	1.62	1.53
2	B	187	ALA	CA-CB	6.03	1.62	1.53
1	A	357	ILE	CA-CB	6.02	1.61	1.54
1	A	371	PRO	C-O	5.99	1.30	1.23
1	A	360	LEU	CA-C	5.96	1.59	1.52
1	A	522	THR	CA-CB	5.96	1.62	1.53
2	B	218	ILE	CA-C	5.86	1.60	1.52
3	C	123	GLY	C-O	5.86	1.30	1.23
2	B	236	ALA	CA-CB	5.82	1.62	1.53
1	A	48	THR	CA-CB	5.75	1.66	1.54
4	D	74	VAL	C-O	5.74	1.30	1.24
1	A	541	ALA	CA-CB	5.74	1.62	1.53
1	A	191	VAL	CA-CB	5.74	1.63	1.55
4	D	16	VAL	CA-CB	5.71	1.62	1.54
1	A	617	ALA	CA-CB	5.70	1.63	1.53
4	D	78	ILE	CA-CB	5.62	1.61	1.54
1	A	192	ILE	CA-CB	5.61	1.62	1.54
3	C	128	ILE	CA-CB	5.61	1.62	1.54
3	C	56	PHE	C-O	-5.57	1.17	1.24
4	D	77	ALA	CA-CB	5.56	1.61	1.53
1	A	10	THR	CA-CB	5.55	1.60	1.52
2	B	214	ARG	CA-C	5.55	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	38	SER	C-O	-5.52	1.17	1.24
1	A	389	VAL	CA-CB	-5.52	1.48	1.53
1	A	32	ARG	C-O	5.49	1.30	1.24
4	D	85	TYR	CA-C	5.45	1.59	1.52
1	A	212	ALA	CA-CB	5.43	1.61	1.53
3	C	104	ARG	N-CA	5.42	1.52	1.46
2	B	187	ALA	CA-C	5.40	1.59	1.52
2	B	83	LEU	CA-C	5.38	1.59	1.52
4	D	85	TYR	C-O	5.37	1.30	1.24
3	C	125	VAL	CA-C	5.33	1.59	1.52
1	A	602	ILE	C-O	-5.31	1.17	1.23
3	C	135	ALA	CA-CB	-5.29	1.44	1.53
1	A	388	VAL	CA-CB	5.28	1.60	1.54
2	B	230	ASN	CA-C	5.21	1.58	1.52
1	A	22	VAL	CB-CG2	-5.20	1.35	1.52
3	C	5	ALA	CA-CB	5.19	1.61	1.53
2	B	182	ALA	CA-CB	5.18	1.61	1.53
1	A	494	GLU	CG-CD	5.15	1.65	1.52
1	A	24	VAL	CA-CB	5.15	1.59	1.53
2	B	75	MET	CG-SD	5.13	1.93	1.80
1	A	493	CYS	C-O	5.12	1.30	1.24
1	A	248	GLU	CA-CB	5.11	1.62	1.53
1	A	372	THR	CA-CB	5.09	1.62	1.53
1	A	334	ALA	CA-CB	5.09	1.61	1.53
4	D	70	THR	CA-CB	5.08	1.61	1.53
1	A	497	SER	C-O	5.07	1.30	1.24
1	A	381	HIS	CA-C	5.07	1.58	1.52
1	A	351	ASP	C-O	5.03	1.29	1.23
1	A	406	ALA	CA-CB	5.03	1.62	1.53
1	A	70	ASN	CA-C	5.02	1.59	1.52
2	B	114	ASP	CA-C	5.02	1.59	1.52
1	A	45	ALA	C-O	-5.00	1.17	1.24

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	THR	N-CA-C	14.20	128.56	108.54
1	A	11	GLN	N-CA-C	-10.20	100.84	113.18
1	A	219	THR	N-CA-C	-10.07	100.99	113.18
2	B	210	PHE	N-CA-C	9.44	125.32	113.43
1	A	51	PHE	N-CA-C	-9.36	97.94	109.83
4	D	8	LEU	N-CA-C	-9.17	100.67	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	53	GLN	N-CA-C	-8.44	101.31	111.69
1	A	131	GLY	N-CA-C	8.33	122.70	111.03
1	A	256	GLY	N-CA-C	-8.22	100.87	112.37
1	A	265	THR	N-CA-C	8.20	120.90	110.24
3	C	16	ASN	N-CA-C	8.13	120.14	111.28
2	B	18	ARG	NE-CZ-NH2	-8.05	111.95	119.20
1	A	613	SER	N-CA-C	-8.05	98.37	110.28
1	A	61	GLN	N-CA-C	7.85	122.64	112.12
3	C	20	SER	N-CA-C	-7.76	103.12	112.59
1	A	526	GLN	N-CA-C	-7.38	102.92	110.97
2	B	20	ASP	CA-C-N	-7.35	112.29	120.45
2	B	20	ASP	C-N-CA	-7.35	112.29	120.45
1	A	22	VAL	CB-CA-C	-7.26	99.73	110.33
1	A	421	GLY	N-CA-C	-7.17	103.59	112.77
2	B	103	PRO	N-CA-C	7.15	122.41	111.19
3	C	63	LEU	CA-C-N	6.87	126.57	119.56
3	C	63	LEU	C-N-CA	6.87	126.57	119.56
2	B	192	ILE	CB-CG1-CD1	-6.86	99.39	113.80
1	A	62	GLY	N-CA-C	6.83	120.92	112.73
1	A	90	LEU	N-CA-C	-6.79	104.20	113.30
3	C	137	ILE	N-CA-C	6.79	117.54	110.62
2	B	18	ARG	CG-CD-NE	-6.78	97.09	112.00
1	A	594	VAL	N-CA-C	6.71	117.95	108.36
2	B	72	SER	N-CA-C	6.62	118.50	111.28
1	A	311	GLY	N-CA-C	6.59	123.79	115.42
1	A	380	THR	N-CA-C	-6.59	99.72	109.81
1	A	282	ARG	N-CA-C	-6.55	99.79	109.62
2	B	108	VAL	N-CA-C	-6.55	104.47	110.82
1	A	573	ARG	CA-C-N	6.55	126.52	119.78
1	A	573	ARG	C-N-CA	6.55	126.52	119.78
1	A	266	GLU	N-CA-C	-6.52	105.19	113.01
1	A	244	CYS	N-CA-C	-6.33	100.83	110.14
1	A	588	ASP	N-CA-C	-6.31	98.25	108.41
2	B	69	ILE	N-CA-C	-6.30	107.36	113.53
3	C	3	THR	N-CA-C	-6.30	99.13	109.40
1	A	103	ALA	N-CA-C	6.27	121.28	112.75
2	B	112	VAL	CA-C-N	6.25	128.39	120.51
2	B	112	VAL	C-N-CA	6.25	128.39	120.51
3	C	77	LEU	N-CA-C	-6.25	104.92	113.30
1	A	329	PRO	CA-C-N	-6.22	112.44	119.28
1	A	329	PRO	C-N-CA	-6.22	112.44	119.28
2	B	90	ASP	CA-C-N	6.20	126.10	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	90	ASP	C-N-CA	6.20	126.10	119.28
1	A	232	ASP	N-CA-C	6.19	118.03	111.28
1	A	213	THR	N-CA-C	6.08	120.39	113.15
1	A	119	ARG	NE-CZ-NH1	-6.07	115.43	121.50
1	A	176	TYR	N-CA-C	-6.06	99.02	108.90
1	A	438	VAL	CA-C-N	6.05	126.37	119.83
1	A	438	VAL	C-N-CA	6.05	126.37	119.83
2	B	156	TYR	N-CA-C	6.01	120.22	113.01
1	A	299	VAL	N-CA-C	6.00	116.17	110.53
2	B	192	ILE	N-CA-C	6.00	117.93	112.29
1	A	518	ASP	N-CA-C	-5.96	104.69	111.07
2	B	191	MET	CG-SD-CE	-5.94	87.83	100.90
2	B	192	ILE	CB-CA-C	-5.94	103.75	111.88
1	A	544	GLU	N-CA-C	-5.88	99.59	107.88
1	A	52	PRO	N-CA-C	5.87	124.57	112.47
2	B	142	TYR	N-CA-C	-5.87	101.79	110.48
2	B	187	ALA	N-CA-C	-5.79	104.96	111.28
1	A	502	ASP	N-CA-C	5.75	119.82	112.34
3	C	62	LEU	N-CA-C	5.75	121.73	114.31
3	C	101	ASN	N-CA-C	-5.74	105.16	111.82
1	A	347	PHE	N-CA-C	5.73	120.39	113.17
2	B	191	MET	CA-C-N	-5.70	114.18	122.28
2	B	191	MET	C-N-CA	-5.70	114.18	122.28
1	A	506	LEU	N-CA-C	5.68	118.57	110.10
2	B	116	SER	N-CA-C	5.68	119.47	112.54
1	A	193	ALA	N-CA-C	5.68	117.81	109.24
2	B	16	ILE	N-CA-C	5.67	116.65	108.48
2	B	167	SER	N-CA-C	-5.64	106.57	113.50
4	D	21	LEU	N-CA-C	-5.62	105.06	111.07
1	A	364	HIS	N-CA-C	5.59	120.61	113.18
1	A	283	PHE	N-CA-C	5.59	119.60	112.34
2	B	215	CYS	CB-CA-C	-5.58	101.13	110.29
1	A	328	LEU	CA-C-N	-5.57	115.59	119.66
1	A	328	LEU	C-N-CA	-5.57	115.59	119.66
1	A	558	ILE	N-CA-C	5.55	115.59	107.37
1	A	554	TYR	N-CA-C	-5.55	98.98	110.80
3	C	114	PHE	N-CA-C	5.54	119.76	112.89
3	C	127	LEU	CA-C-N	-5.54	111.69	120.55
3	C	127	LEU	C-N-CA	-5.54	111.69	120.55
1	A	27	GLY	N-CA-C	-5.53	102.81	112.55
4	D	70	THR	N-CA-C	-5.44	104.76	111.40
4	D	58	TYR	CA-C-N	-5.32	116.22	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	58	TYR	C-N-CA	-5.32	116.22	122.93
3	C	19	SER	CA-C-N	-5.29	114.26	122.67
3	C	19	SER	C-N-CA	-5.29	114.26	122.67
3	C	47	VAL	N-CA-C	-5.25	105.60	110.53
1	A	360	LEU	CA-C-N	5.23	125.53	119.93
1	A	360	LEU	C-N-CA	5.23	125.53	119.93
1	A	601	VAL	N-CA-C	-5.20	102.37	109.55
1	A	615	PRO	O-C-N	5.20	123.59	121.15
1	A	196	ILE	N-CA-C	5.19	117.54	111.05
1	A	326	HIS	N-CA-C	5.18	119.09	112.87
1	A	606	LEU	N-CA-C	-5.17	106.93	113.18
1	A	570	GLN	N-CA-C	-5.16	100.63	109.24
1	A	94	ASP	N-CA-C	-5.14	105.59	111.14
2	B	225	CYS	N-CA-C	5.13	118.55	109.58
1	A	506	LEU	CA-C-N	-5.10	115.80	122.99
1	A	506	LEU	C-N-CA	-5.10	115.80	122.99
1	A	47	VAL	CA-C-N	-5.08	113.91	122.29
1	A	47	VAL	C-N-CA	-5.08	113.91	122.29
1	A	237	VAL	N-CA-C	-5.04	105.58	110.42
3	C	71	VAL	N-CA-C	-5.01	105.44	110.30
2	B	117	ASN	N-CA-C	-5.01	105.53	111.69
1	A	63	GLY	N-CA-C	5.00	117.49	110.38
1	A	523	LEU	N-CA-C	-5.00	105.83	111.28
1	A	72	GLU	N-CA-C	-5.00	100.72	108.42

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	172	TYR	Sidechain
1	A	322	TYR	Sidechain
1	A	365	TYR	Sidechain
1	A	98	TYR	Sidechain
3	C	30	TYR	Sidechain
4	D	58	TYR	Sidechain

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	4616	116	0
2	B	1930	0	1916	55	0
3	C	1071	0	1106	44	0
4	D	770	0	763	32	0
5	A	53	0	29	5	0
6	A	9	0	2	4	0
7	A	15	0	0	0	0
7	B	6	0	0	0	0
7	C	4	0	0	0	0
7	D	5	0	0	1	0
8	B	4	0	0	0	0
9	B	8	0	0	0	0
10	B	7	0	0	0	0
11	B	14	0	9	13	0
12	B	6	0	8	0	0
13	C	18	0	24	1	0
14	C	41	0	24	2	0
15	C	21	0	35	3	0
15	D	24	0	40	4	0
16	A	440	0	0	18	0
16	B	213	0	0	8	0
16	C	96	0	0	7	0
16	D	85	0	0	2	0
All	All	9576	0	8572	233	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 13.

All (233) 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:123:LYS:CE	2:B:123:LYS:NZ	1.68	1.51
1:A:476:MET:CE	1:A:476:MET:SD	2.01	1.48
2:B:185:MET:SD	2:B:185:MET:CE	2.01	1.47
1:A:284:MET:HE1	1:A:303:SER:HB2	1.40	0.99
2:B:123:LYS:HE3	3:C:8:GLU:OE1	1.62	0.98
1:A:164:ARG:HH22	2:B:137:GLN:HE22	1.03	0.94
1:A:216:TYR:H	1:A:366:ASN:ND2	1.68	0.90
2:B:134:GLU:O	2:B:137:GLN:HG3	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:VAL:HG23	1:A:439:PRO:HD2	1.53	0.88
1:A:112:ASN:HD22	2:B:138:GLY:H	1.23	0.86
1:A:233:GLY:HA2	1:A:236:MET:HE3	1.59	0.83
2:B:214:ARG:HH22	4:D:53:GLN:HE22	1.22	0.81
1:A:297:ARG:HH22	6:A:1002:TEO:C3	1.94	0.81
1:A:181:LEU:HD21	1:A:211:ILE:HD11	1.64	0.79
11:B:1005:UQ:HM21	3:C:43:ARG:CZ	2.13	0.78
1:A:164:ARG:HH22	2:B:137:GLN:NE2	1.81	0.77
1:A:284:MET:HE1	1:A:303:SER:CB	2.14	0.76
3:C:18:LYS:HB3	16:C:1673:HOH:O	1.84	0.76
16:A:1254:HOH:O	2:B:123:LYS:HG2	1.85	0.76
3:C:101:ASN:HD21	3:C:104:ARG:HH11	1.34	0.75
1:A:284:MET:CE	1:A:303:SER:HB2	2.17	0.74
1:A:13:PRO:HA	16:A:1370:HOH:O	1.88	0.73
1:A:72:GLU:OE1	1:A:144:HIS:HD2	1.71	0.73
3:C:26:HIS:CD2	3:C:27:ILE:H	2.06	0.73
1:A:207:LYS:NZ	1:A:436:GLU:OE2	2.18	0.72
1:A:122:GLU:HG3	16:A:1087:HOH:O	1.90	0.71
2:B:123:LYS:NZ	2:B:123:LYS:CD	2.54	0.69
1:A:469:ARG:HD2	16:A:1050:HOH:O	1.93	0.69
1:A:401:ALA:N	1:A:402:SER:HA	2.09	0.68
2:B:150:GLN:NE2	16:B:1152:HOH:O	2.27	0.67
3:C:74:VAL:HA	3:C:77:LEU:HD12	1.77	0.67
1:A:576:GLU:H	1:A:576:GLU:CD	2.03	0.66
1:A:563:TYR:HE1	16:A:1351:HOH:O	1.77	0.66
4:D:29:LEU:C	4:D:30:TYR:CD1	2.74	0.66
1:A:237:VAL:HG21	1:A:370:ILE:HG12	1.78	0.65
11:B:1005:UQ:CM2	3:C:43:ARG:NH1	2.60	0.64
1:A:479:HIS:CE1	1:A:491:GLU:HG2	2.33	0.64
4:D:95:LYS:HE3	4:D:99:MET:HG3	1.79	0.63
2:B:18:ARG:NH2	2:B:56:ASP:OD2	2.31	0.62
1:A:568:GLN:HA	1:A:568:GLN:OE1	1.99	0.62
16:A:1254:HOH:O	2:B:123:LYS:CG	2.44	0.62
3:C:77:LEU:O	3:C:78:SER:C	2.42	0.62
1:A:112:ASN:HD22	2:B:138:GLY:N	1.94	0.62
1:A:297:ARG:HH22	6:A:1002:TEO:C2	2.13	0.62
3:C:140:ILE:CB	16:C:1187:HOH:O	2.47	0.62
1:A:485:THR:HG22	1:A:486:GLY:N	2.15	0.61
2:B:117:ASN:O	2:B:121:GLN:HG3	1.99	0.61
3:C:83:LEU:O	3:C:83:LEU:HD12	2.00	0.61
2:B:139:LYS:HE3	16:B:1176:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:HIS:HB2	16:B:1077:HOH:O	2.00	0.61
2:B:8:THR:O	2:B:38:ASN:ND2	2.34	0.61
1:A:32:ARG:NH2	1:A:422:ARG:HD2	2.16	0.60
1:A:543:LYS:HG2	1:A:554:TYR:CE1	2.35	0.60
1:A:568:GLN:HB3	16:A:1264:HOH:O	2.00	0.60
11:B:1005:UQ:CM2	3:C:43:ARG:CZ	2.80	0.60
1:A:438:VAL:CG2	1:A:439:PRO:HD2	2.28	0.59
1:A:507:LYS:HE3	16:A:1427:HOH:O	2.02	0.59
3:C:74:VAL:HG11	4:D:103:ILE:HD13	1.84	0.58
1:A:72:GLU:OE1	1:A:144:HIS:CD2	2.55	0.57
11:B:1005:UQ:HM23	3:C:43:ARG:NH1	2.20	0.57
1:A:252:PHE:CE2	1:A:363:VAL:HG23	2.39	0.57
3:C:69:HIS:O	3:C:73:VAL:HG23	2.05	0.57
1:A:324:GLN:HG3	1:A:326:HIS:CE1	2.38	0.57
1:A:10:THR:HG23	1:A:10:THR:O	2.04	0.57
1:A:25:GLY:HA2	5:A:1001:FAD:H1B	1.85	0.57
1:A:155:HIS:HE1	2:B:156:TYR:O	1.87	0.57
1:A:216:TYR:H	1:A:366:ASN:HD22	1.52	0.57
11:B:1005:UQ:CM2	11:B:1005:UQ:HM33	2.34	0.57
3:C:77:LEU:HB3	16:C:1621:HOH:O	2.04	0.56
4:D:33:PRO:HG2	7:D:205:UNL:O1	2.05	0.56
2:B:121:GLN:NE2	2:B:171:TYR:OH	2.38	0.56
2:B:24:PRO:HA	16:B:1131:HOH:O	2.04	0.56
2:B:131:LYS:O	2:B:134:GLU:HG3	2.06	0.56
3:C:26:HIS:CG	3:C:27:ILE:H	2.23	0.56
4:D:63:THR:O	4:D:67:VAL:HG23	2.06	0.55
1:A:263:LEU:HB3	5:A:1001:FAD:HM73	1.87	0.55
4:D:30:TYR:CD1	4:D:30:TYR:N	2.75	0.55
1:A:117:PHE:HA	1:A:149:VAL:HG22	1.89	0.55
2:B:240:LYS:O	2:B:244:THR:HG23	2.05	0.55
1:A:360:LEU:HD12	1:A:361:PRO:HD2	1.89	0.55
1:A:155:HIS:HD2	16:A:1309:HOH:O	1.89	0.54
2:B:65:CYS:O	2:B:66:ARG:HB3	2.06	0.54
1:A:247:LEU:HD12	1:A:534:GLN:CB	2.37	0.54
11:B:1005:UQ:HM31	3:C:39:SER:OG	2.08	0.54
3:C:88:LYS:HB3	4:D:101:TRP:CZ2	2.43	0.54
1:A:247:LEU:HD12	1:A:534:GLN:HB2	1.89	0.54
1:A:283:PHE:CE1	1:A:284:MET:HE2	2.42	0.53
3:C:4:THR:OG1	3:C:7:GLU:HG3	2.09	0.53
4:D:21:LEU:O	4:D:25:PRO:HD2	2.09	0.53
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1005:UQ:HM23	4:D:58:TYR:OH	2.08	0.53
1:A:297:ARG:HH22	6:A:1002:TEO:C4	2.21	0.53
1:A:595:THR:O	1:A:596:LEU:HD23	2.09	0.53
1:A:562:ASP:OD1	1:A:562:ASP:C	2.52	0.52
2:B:119:TYR:O	2:B:123:LYS:HG3	2.10	0.52
13:C:142:JZR:H5'A	16:C:1519:HOH:O	2.09	0.52
4:D:4:LYS:HE2	16:D:1614:HOH:O	2.09	0.52
4:D:29:LEU:HB3	4:D:30:TYR:CE1	2.44	0.52
3:C:95:LEU:HD23	15:C:144:PEE:H38	1.91	0.51
4:D:53:GLN:HA	4:D:53:GLN:NE2	2.25	0.51
1:A:396:GLY:HA2	1:A:417:LEU:HD23	1.92	0.51
2:B:214:ARG:HH12	4:D:53:GLN:NE2	2.09	0.51
11:B:1005:UQ:HM33	11:B:1005:UQ:O2	2.11	0.51
3:C:6:LYS:HA	3:C:9:MET:HE2	1.92	0.51
1:A:10:THR:OG1	1:A:12:TYR:O	2.27	0.51
1:A:283:PHE:HE1	1:A:284:MET:HE2	1.74	0.51
3:C:72:ALA:O	3:C:73:VAL:C	2.54	0.51
1:A:559:ASP:HB2	16:A:1351:HOH:O	2.11	0.51
2:B:141:GLN:HG3	16:B:1094:HOH:O	2.11	0.51
4:D:101:TRP:CD1	15:D:104:PEE:H26	2.46	0.50
1:A:463:ILE:O	1:A:506:LEU:HA	2.11	0.50
11:B:1005:UQ:HM21	3:C:43:ARG:NH1	2.22	0.50
1:A:559:ASP:CB	16:A:1351:HOH:O	2.59	0.50
1:A:485:THR:CG2	1:A:486:GLY:N	2.74	0.50
1:A:169:ASP:HA	3:C:2:ALA:HB2	1.93	0.50
1:A:205:ARG:HD2	1:A:441:ILE:HD11	1.92	0.50
1:A:179:LEU:HA	16:A:1136:HOH:O	2.11	0.49
1:A:561:PHE:N	16:A:1351:HOH:O	2.24	0.49
2:B:123:LYS:NZ	16:B:1177:HOH:O	2.46	0.49
3:C:67:PHE:HB3	3:C:68:PRO:HD3	1.94	0.49
1:A:55:SER:O	1:A:58:VAL:HG12	2.12	0.49
1:A:457:ARG:O	1:A:511:ARG:NH1	2.41	0.49
2:B:214:ARG:NH2	4:D:53:GLN:HE22	2.01	0.49
3:C:95:LEU:CD2	15:C:144:PEE:H38	2.43	0.49
2:B:23:LYS:HB3	2:B:26:ASP:HB2	1.95	0.49
1:A:125:ILE:HG21	1:A:147:CYS:HB3	1.94	0.48
2:B:188:TYR:HA	2:B:191:MET:HE2	1.95	0.48
1:A:574:PRO:O	1:A:575:PHE:C	2.56	0.48
2:B:19:TRP:CZ3	2:B:21:PRO:HB3	2.47	0.48
1:A:112:ASN:ND2	2:B:138:GLY:H	2.03	0.48
3:C:137:ILE:C	3:C:139:ALA:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLY:O	1:A:318:LYS:HD3	2.13	0.48
3:C:34:LEU:N	3:C:35:PRO:CD	2.76	0.48
1:A:243:PRO:HB3	1:A:586:TYR:CZ	2.48	0.48
1:A:431:THR:HG22	1:A:432:CYS:SG	2.54	0.48
1:A:157:LEU:HD23	1:A:157:LEU:C	2.39	0.47
2:B:214:ARG:HH12	4:D:53:GLN:HE21	1.62	0.47
4:D:90:ASP:OD1	4:D:91:VAL:N	2.38	0.47
1:A:58:VAL:HB	1:A:158:LEU:HD23	1.96	0.47
1:A:103:ALA:HB2	1:A:415:LEU:HD21	1.96	0.47
1:A:99:MET:HA	1:A:419:VAL:HG11	1.96	0.47
3:C:101:ASN:HD21	3:C:104:ARG:NH1	2.09	0.47
1:A:166:LEU:HD22	2:B:123:LYS:HD3	1.97	0.47
1:A:263:LEU:HG	1:A:264:ILE:N	2.27	0.47
1:A:268:CYS:HB3	1:A:325:LEU:HD21	1.97	0.47
2:B:185:MET:CE	2:B:185:MET:CG	2.90	0.47
2:B:87:LYS:HE2	16:B:1115:HOH:O	2.15	0.47
1:A:89:TRP:CD2	1:A:616:PRO:HA	2.50	0.46
4:D:25:PRO:HB2	16:D:1805:HOH:O	2.15	0.46
4:D:63:THR:HB	4:D:64:PRO:HD3	1.98	0.46
1:A:372:THR:HA	1:A:377:GLN:O	2.16	0.46
1:A:560:GLU:N	16:A:1351:HOH:O	2.48	0.46
1:A:563:TYR:CE1	16:A:1351:HOH:O	2.55	0.46
1:A:253:HIS:O	1:A:361:PRO:HA	2.15	0.46
1:A:297:ARG:HH12	6:A:1002:TEO:C4	2.29	0.46
2:B:173:TRP:HZ2	11:B:1005:UQ:C7	2.29	0.46
1:A:63:GLY:HA3	1:A:146:CYS:SG	2.55	0.45
4:D:101:TRP:CG	15:D:104:PEE:H26	2.51	0.45
1:A:515:TRP:CD1	2:B:108:VAL:HG11	2.51	0.45
2:B:150:GLN:NE2	16:B:1114:HOH:O	2.38	0.45
3:C:46:GLY:C	14:C:143:HEM:HMA3	2.42	0.45
1:A:284:MET:HE3	1:A:300:VAL:HG13	1.98	0.45
2:B:90:ASP:OD1	2:B:90:ASP:C	2.60	0.45
2:B:216:HIS:NE2	4:D:57:ASP:OD2	2.48	0.45
3:C:101:ASN:ND2	3:C:104:ARG:HH11	2.06	0.45
3:C:83:LEU:HD12	3:C:83:LEU:C	2.40	0.45
1:A:8:ILE:O	1:A:9:SER:CB	2.65	0.45
4:D:29:LEU:CB	4:D:30:TYR:CD1	3.00	0.45
1:A:127:GLN:NE2	1:A:145:ARG:HA	2.32	0.45
3:C:11:ARG:NH2	16:C:1803:HOH:O	2.50	0.45
3:C:47:VAL:O	3:C:51:LEU:HG	2.17	0.45
3:C:75:LYS:C	3:C:77:LEU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:O	1:A:206:ALA:HA	2.17	0.44
1:A:318:LYS:NZ	16:A:1029:HOH:O	2.50	0.44
14:C:143:HEM:ND	4:D:46:HIS:CE1	2.84	0.44
1:A:89:TRP:CE2	1:A:616:PRO:HA	2.53	0.44
1:A:213:THR:OG1	1:A:233:GLY:HA3	2.18	0.44
3:C:34:LEU:HB3	3:C:35:PRO:HD3	1.99	0.44
1:A:576:GLU:CD	1:A:576:GLU:N	2.74	0.44
2:B:134:GLU:HB3	2:B:137:GLN:OE1	2.18	0.44
1:A:189:ARG:HD2	1:A:439:PRO:HB2	1.98	0.44
2:B:192:ILE:HD13	2:B:192:ILE:HG21	1.61	0.44
2:B:233:LYS:NZ	2:B:237:GLU:OE2	2.50	0.44
3:C:15:LYS:NZ	16:C:1733:HOH:O	2.50	0.44
2:B:20:ASP:OD2	2:B:23:LYS:HE3	2.18	0.43
1:A:136:GLN:O	1:A:137:PHE:C	2.60	0.43
1:A:493:CYS:HB3	1:A:537:TYR:CZ	2.54	0.43
1:A:468:ALA:HB3	1:A:525:LEU:HD21	1.99	0.43
1:A:60:ALA:HA	5:A:1001:FAD:C5X	2.49	0.43
3:C:71:VAL:HG21	4:D:99:MET:HE2	2.01	0.43
1:A:232:ASP:O	1:A:236:MET:HG3	2.18	0.43
1:A:296:SER:O	1:A:300:VAL:HG23	2.19	0.43
2:B:187:ALA:O	2:B:191:MET:HG3	2.18	0.43
2:B:236:ALA:HB2	3:C:114:PHE:CZ	2.54	0.43
15:C:144:PEE:H39	4:D:24:LEU:HD13	2.00	0.43
2:B:66:ARG:HB3	2:B:66:ARG:HE	1.28	0.43
3:C:137:ILE:C	3:C:139:ALA:N	2.75	0.43
5:A:1001:FAD:H9	5:A:1001:FAD:H1'1	1.84	0.42
2:B:131:LYS:HB2	2:B:134:GLU:HG2	2.00	0.42
11:B:1005:UQ:HM22	3:C:43:ARG:HD2	2.01	0.42
2:B:92:ASP:OD1	2:B:92:ASP:C	2.60	0.42
4:D:27:ALA:HB1	15:D:104:PEE:H60	2.01	0.42
1:A:35:PHE:HB2	1:A:168:TYR:CD1	2.55	0.42
3:C:74:VAL:O	3:C:77:LEU:HD12	2.19	0.42
16:A:1342:HOH:O	2:B:66:ARG:HG3	2.20	0.42
4:D:53:GLN:HA	4:D:53:GLN:HE21	1.85	0.42
1:A:377:GLN:HG2	1:A:393:TYR:CE1	2.55	0.41
1:A:90:LEU:O	1:A:90:LEU:HG	2.21	0.41
1:A:509:PHE:CD1	1:A:509:PHE:N	2.88	0.41
4:D:45:LEU:HD12	4:D:45:LEU:HA	1.88	0.41
1:A:400:SER:OG	1:A:402:SER:HB2	2.21	0.41
4:D:22:GLY:O	4:D:25:PRO:HG2	2.21	0.41
1:A:201:ILE:HD12	1:A:201:ILE:HG23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:HE2	1:A:432:CYS:SG	2.61	0.41
1:A:453:LEU:C	1:A:453:LEU:HD23	2.46	0.41
2:B:173:TRP:CZ2	11:B:1005:UQ:C7	3.04	0.41
1:A:317:GLU:O	1:A:318:LYS:C	2.63	0.41
1:A:599:ARG:HA	1:A:600:PRO:HD3	1.85	0.41
3:C:38:MET:HE1	3:C:123:GLY:O	2.20	0.41
2:B:225:CYS:SG	2:B:229:LEU:HB2	2.61	0.41
4:D:4:LYS:O	4:D:5:ALA:C	2.62	0.41
4:D:27:ALA:CB	15:D:104:PEE:H60	2.50	0.41
1:A:220:TYR:CD2	1:A:363:VAL:HG21	2.56	0.41
1:A:63:GLY:O	1:A:414:LEU:HD12	2.21	0.40
1:A:198:ASP:C	1:A:198:ASP:OD2	2.63	0.40
3:C:24:SER:HB2	16:C:1427:HOH:O	2.22	0.40
1:A:90:LEU:O	1:A:582:HIS:HE1	2.03	0.40
2:B:18:ARG:HD2	2:B:110:ASP:OD1	2.21	0.40
1:A:60:ALA:HA	5:A:1001:FAD:C6	2.51	0.40
1:A:252:PHE:CE2	1:A:363:VAL:CG2	3.04	0.40
11:B:1005:UQ:HM33	11:B:1005:UQ:HM22	2.02	0.40
1:A:18:GLU:CG	1:A:205:ARG:NH1	2.84	0.40
1:A:242:LEU:HB3	16:A:1068:HOH:O	2.21	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	612/621 (99%)	583 (95%)	28 (5%)	1 (0%)	43	51
2	B	240/252 (95%)	227 (95%)	12 (5%)	1 (0%)	30	34
3	C	138/141 (98%)	132 (96%)	5 (4%)	1 (1%)	18	19
4	D	100/103 (97%)	97 (97%)	3 (3%)	0	100	100
All	All	1090/1117 (98%)	1039 (95%)	48 (4%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	THR
1	A	9	SER
3	C	78	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%)	483 (97%)	15 (3%)	36	49
2	B	214/219 (98%)	206 (96%)	8 (4%)	30	41
3	C	116/119 (98%)	113 (97%)	3 (3%)	40	55
4	D	78/79 (99%)	74 (95%)	4 (5%)	21	27
All	All	906/923 (98%)	876 (97%)	30 (3%)	33	45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	48	THR
1	A	72	GLU
1	A	130	PHE
1	A	191	VAL
1	A	276	ILE
1	A	360	LEU
1	A	380	THR
1	A	388	VAL
1	A	438	VAL
1	A	441	ILE
1	A	447	GLU
1	A	513	ILE
1	A	545	SER
1	A	590	LYS
2	B	23	LYS
2	B	66	ARG

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Mol	Chain	Res	Type
2	B	98	LYS
2	B	125	ILE
2	B	131	LYS
2	B	217	THR
2	B	224	THR
2	B	229	LEU
3	C	3	THR
3	C	40	ILE
3	C	81	PRO
4	D	14	ARG
4	D	19	LEU
4	D	63	THR
4	D	66	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	43	ASN
1	A	112	ASN
1	A	144	HIS
1	A	155	HIS
1	A	185	ASN
1	A	320	HIS
1	A	324	GLN
1	A	326	HIS
1	A	331	GLN
1	A	366	ASN
1	A	383	ASN
1	A	534	GLN
2	B	104	HIS
2	B	121	GLN
2	B	137	GLN
2	B	144	GLN
3	C	26	HIS
3	C	42	HIS
3	C	101	ASN
4	D	9	HIS
4	D	53	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 30 are unknown - 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$
13	JZR	C	142	-	18,18,18	2.21	7 (38%)	23,23,23	1.50	4 (17%)
14	HEM	C	143	3,4	48,48,50	3.14	24 (50%)	66,80,82	3.20	30 (45%)
8	FES	B	1002	2	0,4,4	-	-	-		
10	F3S	B	1004	2	0,9,9	-	-	-		
9	SF4	B	1003	2	0,12,12	-	-	-		
6	TEO	A	1002	-	5,8,8	1.73	2 (40%)	4,10,10	2.24	2 (50%)
11	UQ	B	1005	-	14,14,63	2.29	8 (57%)	20,20,79	1.04	0
15	PEE	C	144	-	19,19,50	2.10	4 (21%)	19,19,55	0.87	2 (10%)
5	FAD	A	1001	1	58,58,58	2.83	27 (46%)	85,89,89	1.99	24 (28%)
12	GOL	B	1012	-	5,5,5	1.78	2 (40%)	5,5,5	0.90	0
15	PEE	D	104	-	22,22,50	1.63	4 (18%)	20,20,55	1.25	4 (20%)

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
13	JZR	C	142	-	-	2/9/29/29	0/1/1/1
14	HEM	C	143	3,4	-	1/10/50/54	-
8	FES	B	1002	2	-	-	0/1/1/1
10	F3S	B	1004	2	-	-	0/3/3/3
9	SF4	B	1003	2	-	-	0/6/5/5
6	TEO	A	1002	-	1/1/3/4	4/6/8/8	-
11	UQ	B	1005	-	-	1/4/28/87	0/1/1/1
15	PEE	C	144	-	-	12/17/17/54	-
5	FAD	A	1001	1	-	9/34/50/50	0/6/6/6
12	GOL	B	1012	-	-	3/4/4/4	-
15	PEE	D	104	-	-	8/18/18/54	-

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	FAD	PA-O3P	-12.03	1.46	1.59
14	C	143	HEM	CMC-C2C	8.83	1.68	1.50
14	C	143	HEM	C1B-NB	8.48	1.54	1.40
14	C	143	HEM	CMB-C2B	7.74	1.66	1.50
5	A	1001	FAD	C10-N10	6.82	1.52	1.37
13	C	142	JZR	O1-C1	6.71	1.51	1.40
14	C	143	HEM	CHA-C4D	5.75	1.50	1.38
15	C	144	PEE	O2-C10	5.59	1.49	1.30
14	C	143	HEM	C1D-ND	5.33	1.49	1.38
14	C	143	HEM	C4B-C3B	4.96	1.54	1.44
11	B	1005	UQ	C6-C1	4.82	1.63	1.47
15	C	144	PEE	C11-C10	4.76	1.61	1.50
5	A	1001	FAD	C9-C8	4.70	1.46	1.39
5	A	1001	FAD	C1'-C2'	4.21	1.58	1.52
5	A	1001	FAD	P-O3P	4.18	1.64	1.59
15	D	104	PEE	C39-C38	4.16	1.55	1.31
15	D	104	PEE	C18-C19	3.95	1.54	1.31
14	C	143	HEM	C1C-C2C	3.86	1.53	1.45
5	A	1001	FAD	C6-C7	3.65	1.44	1.39
5	A	1001	FAD	C2'-C3'	-3.56	1.47	1.53
5	A	1001	FAD	C4'-C3'	3.53	1.59	1.53
15	C	144	PEE	C21-C22	-3.51	1.34	1.51
5	A	1001	FAD	PA-O2A	-3.51	1.39	1.55
5	A	1001	FAD	C4A-N9A	-3.29	1.30	1.37
11	B	1005	UQ	O1-C1	3.29	1.30	1.23
14	C	143	HEM	C4C-C3C	3.26	1.51	1.45
14	C	143	HEM	CHD-C4C	3.25	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	143	HEM	FE-NC	3.22	2.05	1.95
14	C	143	HEM	FE-NB	-3.19	1.85	1.94
14	C	143	HEM	CAA-C2A	3.10	1.59	1.51
5	A	1001	FAD	PA-O1A	-3.08	1.40	1.50
5	A	1001	FAD	C9A-C5X	3.05	1.46	1.41
5	A	1001	FAD	C8A-N9A	-3.05	1.32	1.37
14	C	143	HEM	C1C-NC	-3.02	1.33	1.39
14	C	143	HEM	C1A-C2A	-3.02	1.38	1.44
14	C	143	HEM	CAD-C3D	2.94	1.58	1.51
11	B	1005	UQ	C7-C6	2.93	1.56	1.50
5	A	1001	FAD	C5X-N5	2.92	1.44	1.39
14	C	143	HEM	CHB-C1B	2.88	1.44	1.38
11	B	1005	UQ	C3-C4	2.84	1.57	1.48
14	C	143	HEM	C2A-C3A	-2.84	1.31	1.38
5	A	1001	FAD	C8-C7	2.84	1.47	1.40
6	A	1002	TEO	C2-C1	-2.77	1.48	1.54
13	C	142	JZR	O1-C1'	2.76	1.50	1.43
5	A	1001	FAD	O2B-C2B	2.75	1.49	1.43
14	C	143	HEM	C4B-NB	2.68	1.44	1.38
14	C	143	HEM	FE-NA	2.53	2.03	1.95
13	C	142	JZR	O4-C4	2.53	1.49	1.43
11	B	1005	UQ	C2-C1	2.50	1.56	1.48
15	D	104	PEE	C17-C18	-2.42	1.36	1.50
5	A	1001	FAD	C1B-N9A	2.40	1.53	1.46
5	A	1001	FAD	C2A-N1A	2.39	1.38	1.33
11	B	1005	UQ	O3-C3	2.38	1.42	1.36
13	C	142	JZR	C2'-C1'	2.35	1.60	1.51
5	A	1001	FAD	P-O1P	-2.34	1.42	1.50
14	C	143	HEM	CHB-C4A	2.32	1.44	1.39
14	C	143	HEM	CBD-CGD	2.31	1.55	1.50
5	A	1001	FAD	C4A-N3A	2.30	1.38	1.34
14	C	143	HEM	CMA-C3A	2.30	1.55	1.50
15	C	144	PEE	O4-C10	2.29	1.29	1.22
5	A	1001	FAD	C2A-N3A	2.28	1.38	1.33
5	A	1001	FAD	C9A-N10	-2.27	1.37	1.41
5	A	1001	FAD	C9-C9A	2.26	1.43	1.39
15	D	104	PEE	C21-C20	-2.25	1.34	1.49
12	B	1012	GOL	O2-C2	2.19	1.49	1.43
14	C	143	HEM	O2A-CGA	-2.14	1.23	1.30
12	B	1012	GOL	C1-C2	2.09	1.59	1.51
5	A	1001	FAD	O5'-C5'	-2.08	1.36	1.44
13	C	142	JZR	C4-C3	2.08	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	FAD	C8A-N7A	2.07	1.35	1.31
11	B	1005	UQ	CM5-C5	2.07	1.55	1.50
13	C	142	JZR	O5-C5	2.06	1.49	1.44
5	A	1001	FAD	P-O2P	-2.06	1.45	1.55
11	B	1005	UQ	O2-C2	2.03	1.41	1.36
13	C	142	JZR	C4'-C3'	2.02	1.61	1.51
14	C	143	HEM	C4D-C3D	2.02	1.48	1.45
5	A	1001	FAD	C2B-C3B	2.02	1.58	1.53
6	A	1002	TEO	O1A-C1	2.01	1.28	1.22

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	143	HEM	C4D-ND-C1D	-9.37	94.11	105.21
14	C	143	HEM	C1B-NB-C4B	-8.79	94.79	105.21
14	C	143	HEM	CHC-C1C-NC	-8.44	115.27	124.45
14	C	143	HEM	C2B-C1B-NB	7.44	118.39	109.84
5	A	1001	FAD	N3A-C2A-N1A	-6.75	118.37	128.58
14	C	143	HEM	CHA-C4D-ND	-6.47	116.36	124.37
14	C	143	HEM	C1C-C2C-C3C	-6.31	99.93	107.22
14	C	143	HEM	CMB-C2B-C1B	5.47	133.59	125.03
14	C	143	HEM	CAB-C3B-C4B	5.06	132.94	125.03
5	A	1001	FAD	C4A-N9A-C8A	4.85	110.83	105.74
14	C	143	HEM	C2C-C1C-NC	4.77	118.46	109.64
14	C	143	HEM	CAB-C3B-C2B	-4.21	118.00	126.75
13	C	142	JZR	C1'-O1-C1	4.11	120.70	113.68
14	C	143	HEM	C1B-C2B-C3B	-3.94	103.42	107.09
14	C	143	HEM	C4C-NC-C1C	-3.79	99.65	105.82
5	A	1001	FAD	C4-N3-C2	-3.74	119.00	125.64
14	C	143	HEM	C3A-C4A-NA	-3.72	104.17	110.14
5	A	1001	FAD	C4-C4X-N5	3.69	123.31	118.21
14	C	143	HEM	C4A-CHB-C1B	-3.63	117.72	126.25
5	A	1001	FAD	C2A-N3A-C4A	3.62	120.67	111.83
5	A	1001	FAD	C10-N1-C2	3.61	124.67	116.85
5	A	1001	FAD	O2P-P-O3P	3.40	116.46	107.27
5	A	1001	FAD	C4A-N9A-C1B	-3.40	118.69	126.63
5	A	1001	FAD	C5X-N5-C4X	3.38	123.56	118.09
5	A	1001	FAD	C1'-C2'-C3'	3.15	118.20	109.66
15	D	104	PEE	C21-C20-C19	3.13	127.79	112.96
14	C	143	HEM	C1C-CHC-C4B	3.10	132.60	126.02
6	A	1002	TEO	O2-C2-C1	3.07	117.38	109.54
14	C	143	HEM	CAD-C3D-C4D	3.03	129.98	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	FAD	O2'-C2'-C3'	-3.02	102.18	109.25
5	A	1001	FAD	C5X-C9A-N10	-3.01	115.25	117.97
5	A	1001	FAD	C10-C4X-N5	-3.00	118.68	124.81
14	C	143	HEM	CAD-C3D-C2D	-2.99	122.27	127.87
5	A	1001	FAD	C7M-C7-C6	-2.89	114.48	119.57
15	D	104	PEE	C16-C17-C18	2.82	128.38	112.60
14	C	143	HEM	CHB-C1B-NB	-2.74	120.97	124.37
14	C	143	HEM	CHD-C1D-ND	-2.70	121.52	124.42
6	A	1002	TEO	O1B-C1-C2	2.68	119.27	113.00
14	C	143	HEM	CMC-C2C-C1C	2.66	129.42	124.73
5	A	1001	FAD	N3A-C4A-N9A	2.66	131.68	127.17
5	A	1001	FAD	C4'-C3'-C2'	-2.61	109.23	113.57
14	C	143	HEM	C4A-C3A-C2A	2.60	109.80	106.82
13	C	142	JZR	C3-C4-C5	-2.59	105.54	110.23
5	A	1001	FAD	C4X-C4-N3	2.54	119.72	113.25
14	C	143	HEM	CHB-C4A-NA	2.52	128.43	123.86
15	C	144	PEE	C22-C21-C20	2.52	125.98	113.86
15	C	144	PEE	C21-C22-C23	2.48	126.89	114.37
14	C	143	HEM	C3B-C4B-NB	2.46	112.75	109.90
14	C	143	HEM	CBD-CAD-C3D	-2.45	105.75	112.53
5	A	1001	FAD	C7M-C7-C8	2.45	125.76	120.76
5	A	1001	FAD	C6A-C5A-C4A	-2.44	113.85	117.18
5	A	1001	FAD	C5A-C4A-N3A	-2.41	123.40	126.72
14	C	143	HEM	CHB-C1B-C2B	-2.38	120.19	126.95
5	A	1001	FAD	O3'-C3'-C2'	-2.37	103.55	108.93
5	A	1001	FAD	C8M-C8-C7	2.35	125.56	120.76
14	C	143	HEM	C2D-C1D-ND	2.28	112.54	109.90
13	C	142	JZR	O5-C1-O1	2.24	115.35	110.04
5	A	1001	FAD	C6A-C5A-N7A	2.23	136.39	132.09
13	C	142	JZR	O5-C1-C2	-2.23	105.79	110.37
15	D	104	PEE	C20-C19-C18	-2.20	113.21	126.42
15	D	104	PEE	C40-C39-C38	-2.17	113.39	126.42
14	C	143	HEM	CHC-C4B-NB	-2.16	122.09	124.42
5	A	1001	FAD	C4X-C10-N1	-2.15	119.33	124.59
14	C	143	HEM	CAA-C2A-C1A	-2.10	120.83	124.94
14	C	143	HEM	C4B-C3B-C2B	2.09	109.03	107.09
14	C	143	HEM	C3D-C4D-ND	2.04	112.41	110.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1002	TEO	C2

All (40) torsion outliers are listed below:

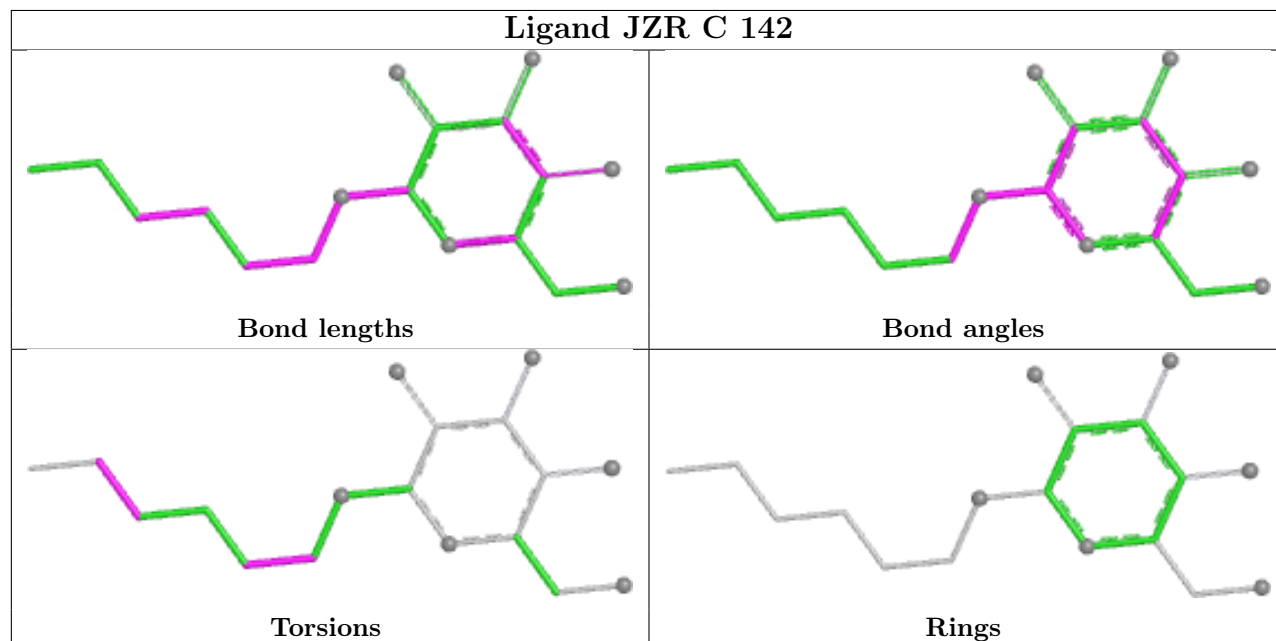
Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	N10-C1'-C2'-O2'
5	A	1001	FAD	N10-C1'-C2'-C3'
5	A	1001	FAD	O4'-C4'-C5'-O5'
5	A	1001	FAD	C5'-O5'-P-O2P
5	A	1001	FAD	C5'-O5'-P-O3P
6	A	1002	TEO	C1-C2-C3-C4
6	A	1002	TEO	O2-C2-C3-C4
12	B	1012	GOL	C1-C2-C3-O3
12	B	1012	GOL	O2-C2-C3-O3
15	D	104	PEE	C17-C18-C19-C20
6	A	1002	TEO	O1A-C1-C2-O2
6	A	1002	TEO	O1B-C1-C2-O2
15	C	144	PEE	C17-C18-C19-C20
13	C	142	JZR	O1-C1'-C2'-C3'
15	C	144	PEE	C12-C13-C14-C15
15	C	144	PEE	C11-C12-C13-C14
15	D	104	PEE	C32-C33-C34-C35
15	D	104	PEE	C12-C13-C14-C15
15	D	104	PEE	C15-C16-C17-C18
5	A	1001	FAD	C3'-C4'-C5'-O5'
15	D	104	PEE	C35-C36-C37-C38
15	D	104	PEE	C31-C32-C33-C34
15	C	144	PEE	C20-C21-C22-C23
15	C	144	PEE	C14-C15-C16-C17
15	C	144	PEE	C22-C23-C24-C25
15	C	144	PEE	C19-C20-C21-C22
12	B	1012	GOL	O1-C1-C2-O2
15	D	104	PEE	C34-C35-C36-C37
5	A	1001	FAD	PA-O3P-P-O5'
5	A	1001	FAD	C5'-O5'-P-O1P
15	C	144	PEE	C24-C25-C26-C27
14	C	143	HEM	C2A-CAA-CBA-CGA
11	B	1005	UQ	C4-C3-O3-CM3
15	C	144	PEE	O2-C10-C11-C12
15	C	144	PEE	O4-C10-C11-C12
15	D	104	PEE	C33-C34-C35-C36
15	C	144	PEE	C16-C17-C18-C19
15	C	144	PEE	C18-C19-C20-C21
13	C	142	JZR	C3'-C4'-C5'-C6'
5	A	1001	FAD	PA-O3P-P-O2P

There are no ring outliers.

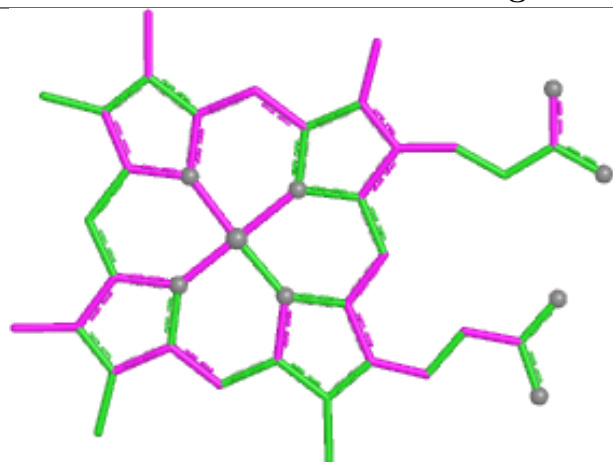
7 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	142	JZR	1	0
14	C	143	HEM	2	0
6	A	1002	TEO	4	0
11	B	1005	UQ	13	0
15	C	144	PEE	3	0
5	A	1001	FAD	5	0
15	D	104	PEE	4	0

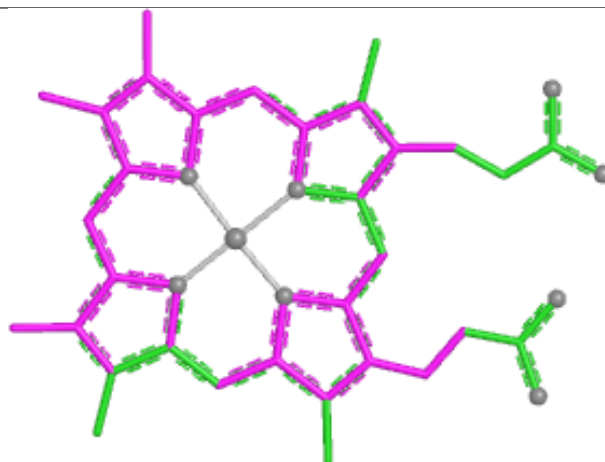
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



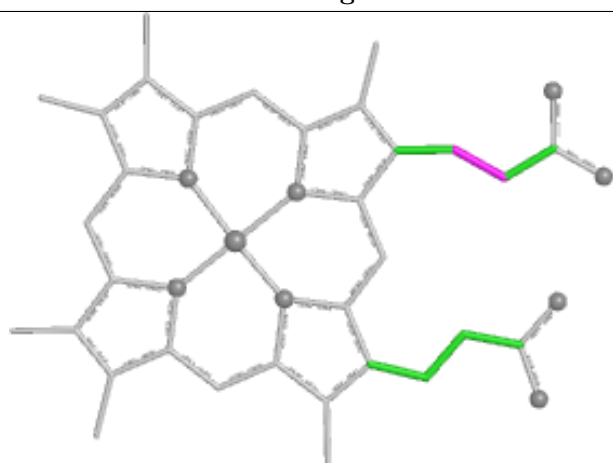
Ligand HEM C 143



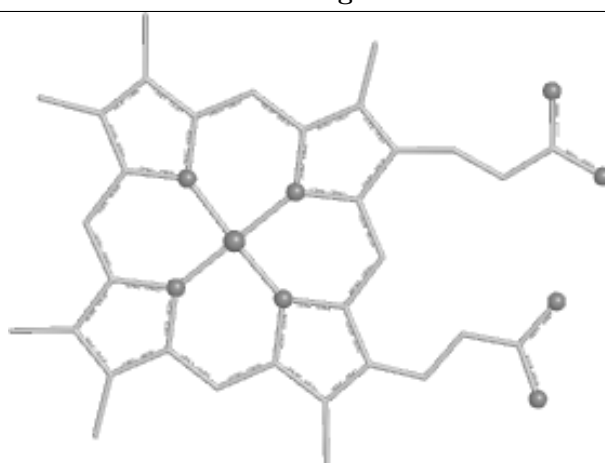
Bond lengths



Bond angles

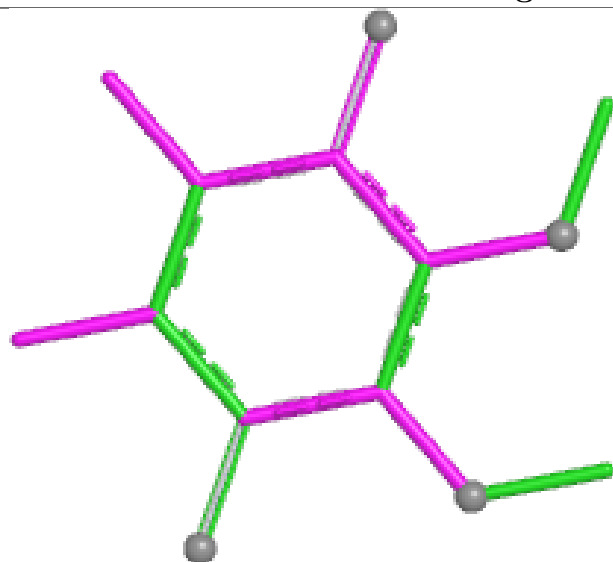


Torsions

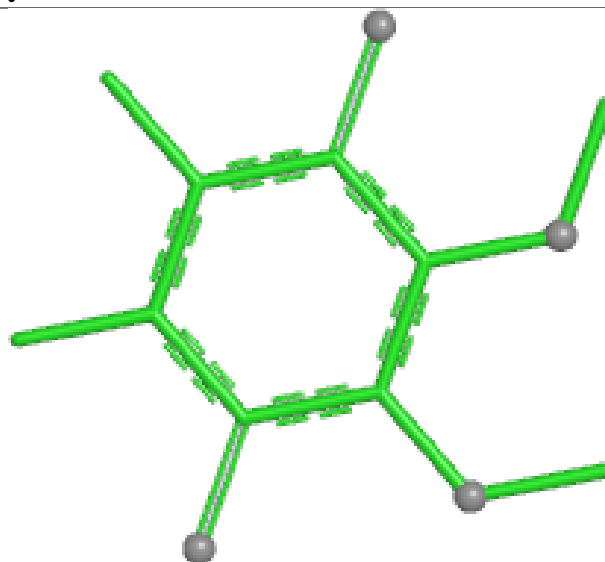


Rings

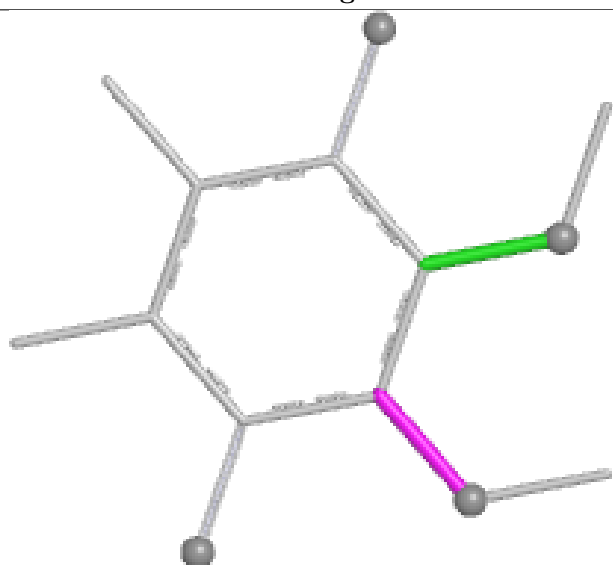
Ligand UQ B 1005



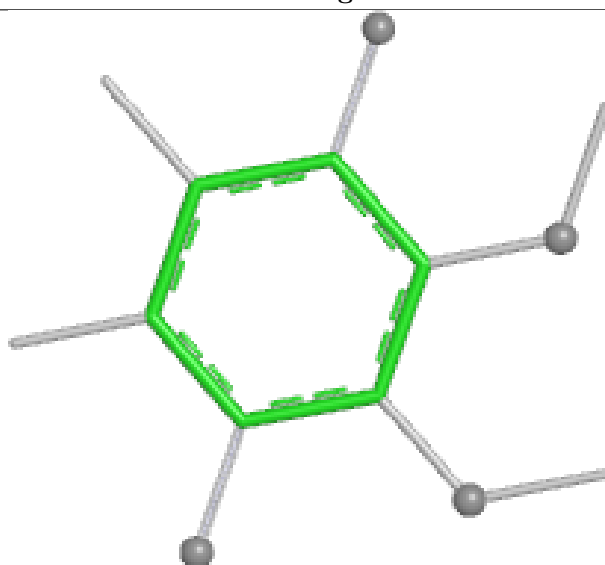
Bond lengths



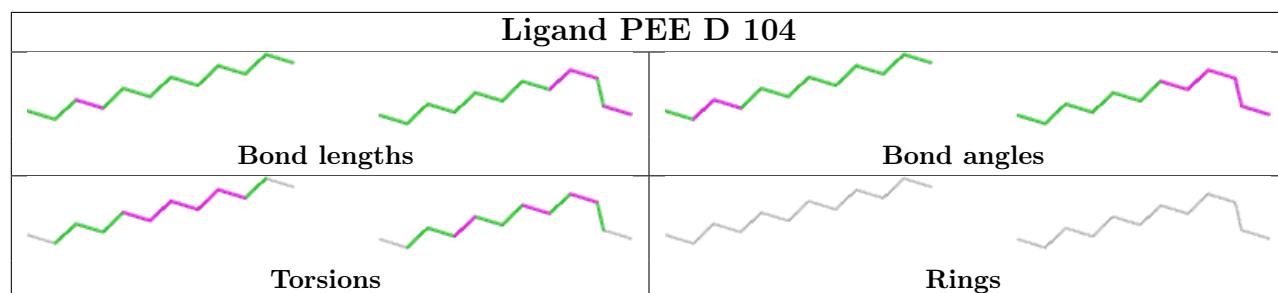
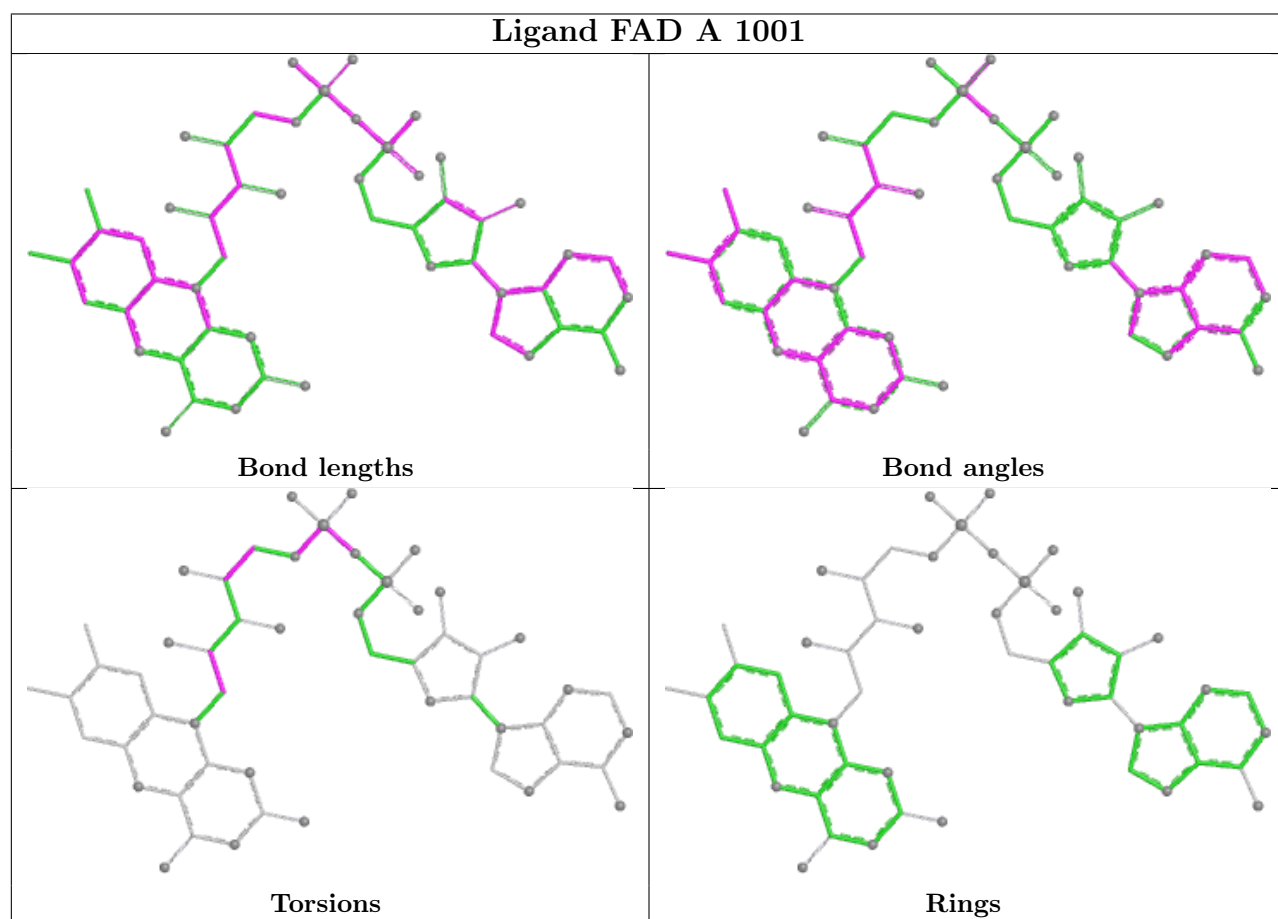
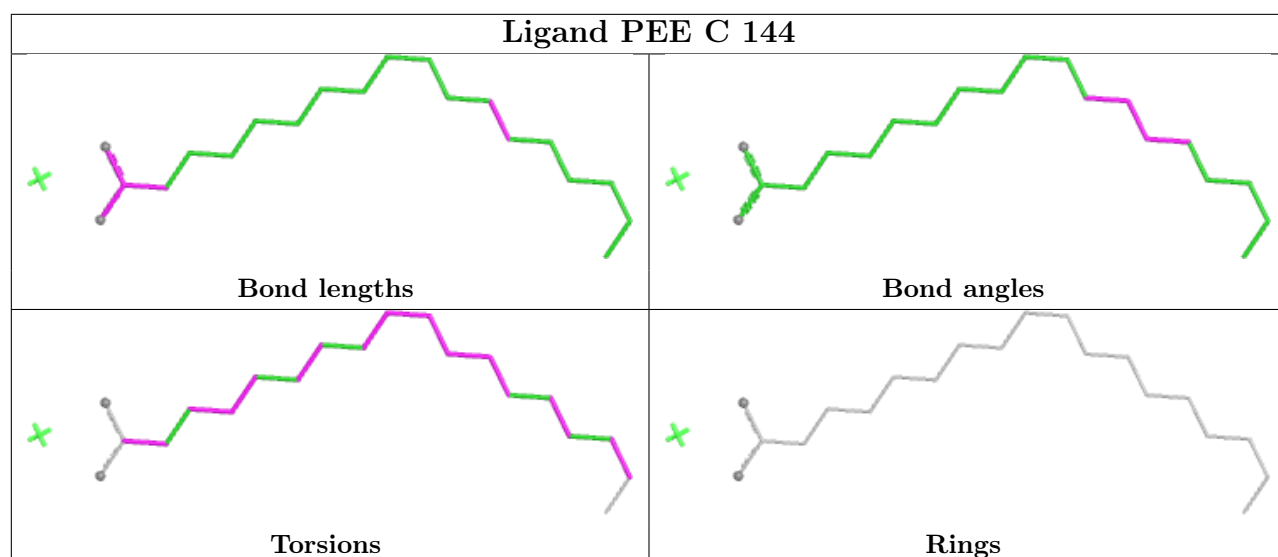
Bond angles



Torsions



Rings



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	614/621 (98%)	-0.42	4 (0%) 84 82	27, 42, 64, 130	0
2	B	242/252 (96%)	-0.49	7 (2%) 53 50	25, 37, 66, 105	0
3	C	140/141 (99%)	-0.30	1 (0%) 84 82	28, 42, 69, 80	0
4	D	102/103 (99%)	-0.41	2 (1%) 65 62	33, 40, 61, 72	0
All	All	1098/1117 (98%)	-0.42	14 (1%) 75 73	25, 41, 66, 130	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	138	GLY	5.2
2	B	6	ALA	4.0
2	B	7	ALA	3.9
1	A	8	ILE	3.5
1	A	9	SER	2.9
4	D	73	TYR	2.3
3	C	78	SER	2.3
4	D	2	SER	2.3
1	A	10	THR	2.3
2	B	8	THR	2.2
2	B	136	LYS	2.2
2	B	137	GLN	2.1
1	A	439	PRO	2.1
2	B	247	GLU	2.0

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 ⓘ

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
7	UNL	B	1007	1/-	0.71	0.30	63,63,63,63	0
12	GOL	B	1012	6/6	0.77	0.18	112,113,114,114	0
7	UNL	A	1007	1/-	0.79	0.12	66,66,66,66	0
7	UNL	D	205	1/-	0.80	0.12	59,59,59,59	0
7	UNL	A	1015	1/-	0.82	0.12	76,76,76,76	0
7	UNL	B	1010	1/-	0.82	0.21	75,75,75,75	0
7	UNL	D	228	1/-	0.83	0.12	59,59,59,59	0
15	PEE	D	104	24/51	0.84	0.22	47,62,73,77	0
11	UQ	B	1005	14/63	0.85	0.23	59,72,82,86	0
7	UNL	A	1013	1/-	0.85	0.17	77,77,77,77	0
7	UNL	A	1004	1/-	0.85	0.14	63,63,63,63	0
15	PEE	C	144	21/51	0.86	0.17	56,64,74,77	0
7	UNL	A	1016	1/-	0.87	0.12	63,63,63,63	0
7	UNL	A	1017	1/-	0.87	0.12	66,66,66,66	0
7	UNL	A	1009	1/-	0.89	0.07	65,65,65,65	0
7	UNL	C	203	1/-	0.89	0.22	61,61,61,61	0
13	JZR	C	142	18/18	0.91	0.12	41,47,63,67	0
7	UNL	C	212	1/-	0.92	0.28	76,76,76,76	0
7	UNL	C	226	1/-	0.92	0.09	56,56,56,56	0
7	UNL	D	204	1/-	0.92	0.17	65,65,65,65	0
7	UNL	A	1010	1/-	0.92	0.11	58,58,58,58	0
7	UNL	B	1008	1/-	0.92	0.15	59,59,59,59	0
7	UNL	B	1006	1/-	0.93	0.09	57,57,57,57	0
7	UNL	A	1008	1/-	0.93	0.07	58,58,58,58	0
7	UNL	A	1005	1/-	0.93	0.14	64,64,64,64	0
7	UNL	A	1003	1/-	0.93	0.20	65,65,65,65	0
7	UNL	A	1012	1/-	0.93	0.28	63,63,63,63	0
7	UNL	B	1009	1/-	0.94	0.21	60,60,60,60	0
7	UNL	A	1006	1/-	0.94	0.10	47,47,47,47	0
7	UNL	D	209	1/-	0.94	0.16	61,61,61,61	0
7	UNL	D	218	1/-	0.94	0.10	47,47,47,47	0
7	UNL	B	1011	1/-	0.94	0.10	50,50,50,50	0

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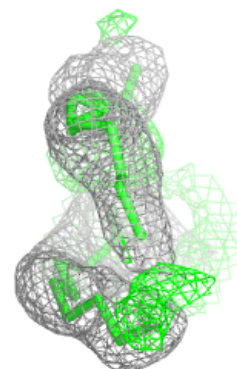
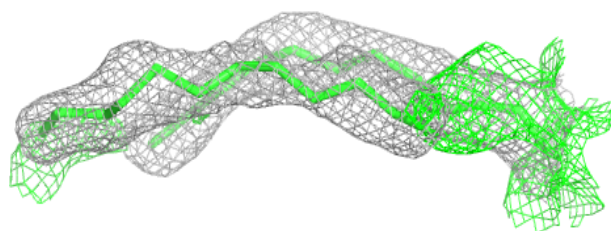
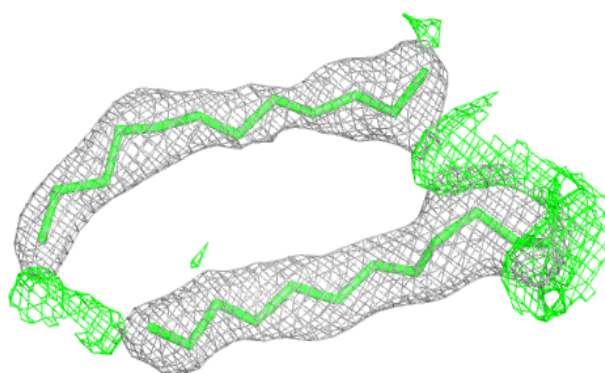
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	UNL	C	211	1/-	0.95	0.10	68,68,68,68	0
7	UNL	A	1014	1/-	0.96	0.07	59,59,59,59	0
6	TEO	A	1002	9/9	0.96	0.06	35,37,38,42	0
7	UNL	A	1011	1/-	0.96	0.11	54,54,54,54	0
5	FAD	A	1001	53/53	0.98	0.05	23,32,37,37	0
14	HEM	C	143	41/43	0.98	0.06	32,36,44,49	0
9	SF4	B	1003	8/8	0.99	0.02	31,32,35,36	0
8	FES	B	1002	4/4	1.00	0.02	31,33,34,34	0
10	F3S	B	1004	7/7	1.00	0.03	28,29,31,31	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.

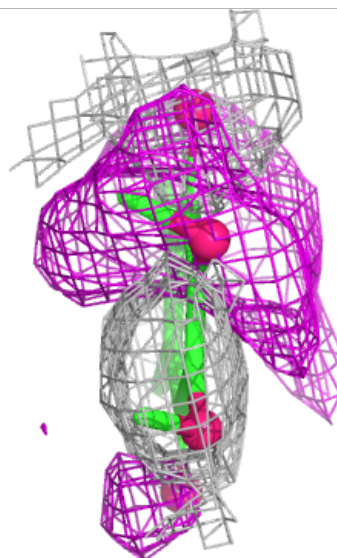
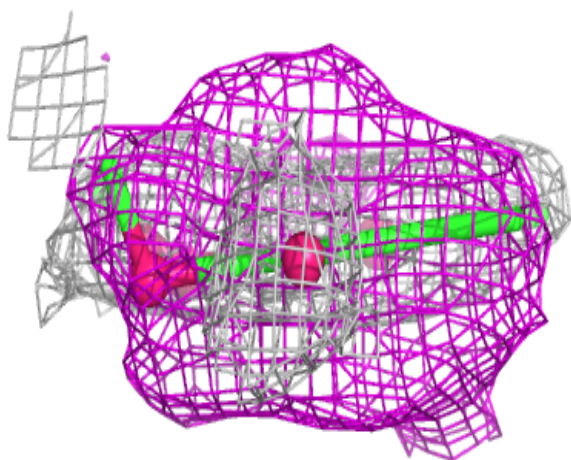
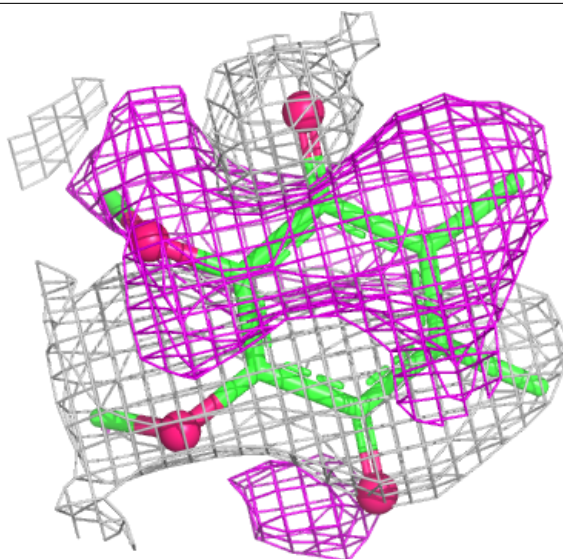
Electron density around PEE D 104:

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



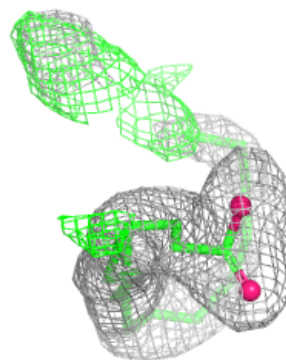
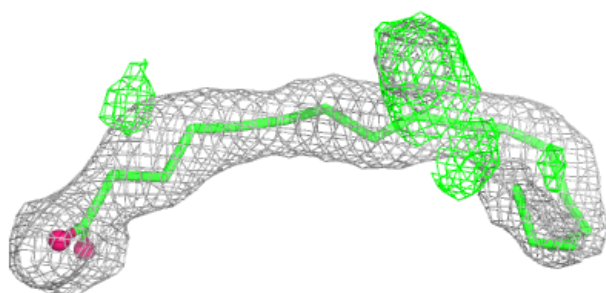
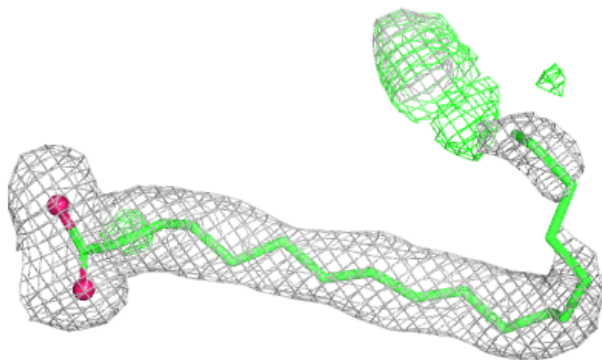
Electron density around UQ B 1005:

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

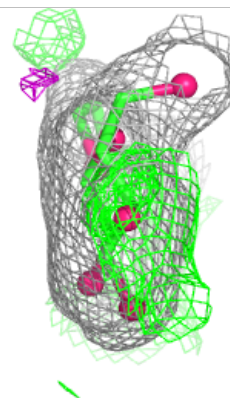
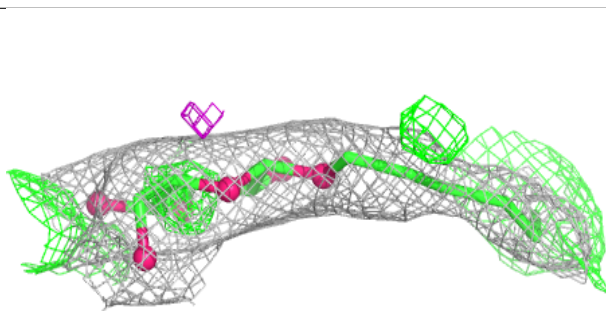
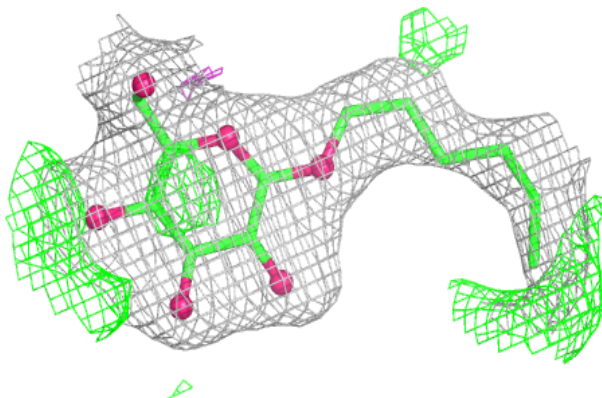


Electron density around PEE C 144:

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

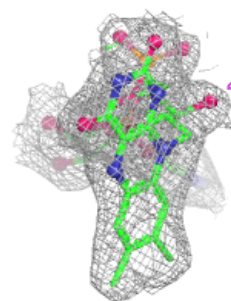
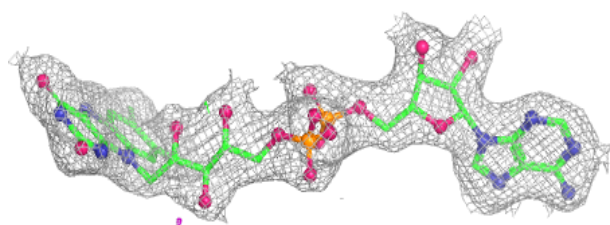
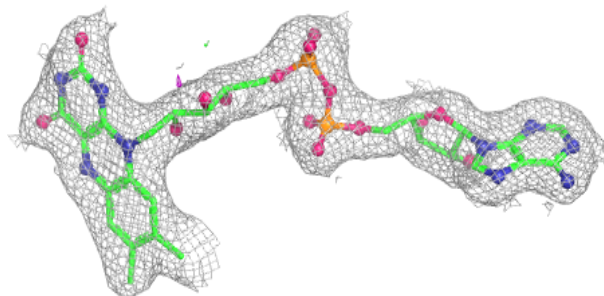
**Electron density around JZR C 142:**

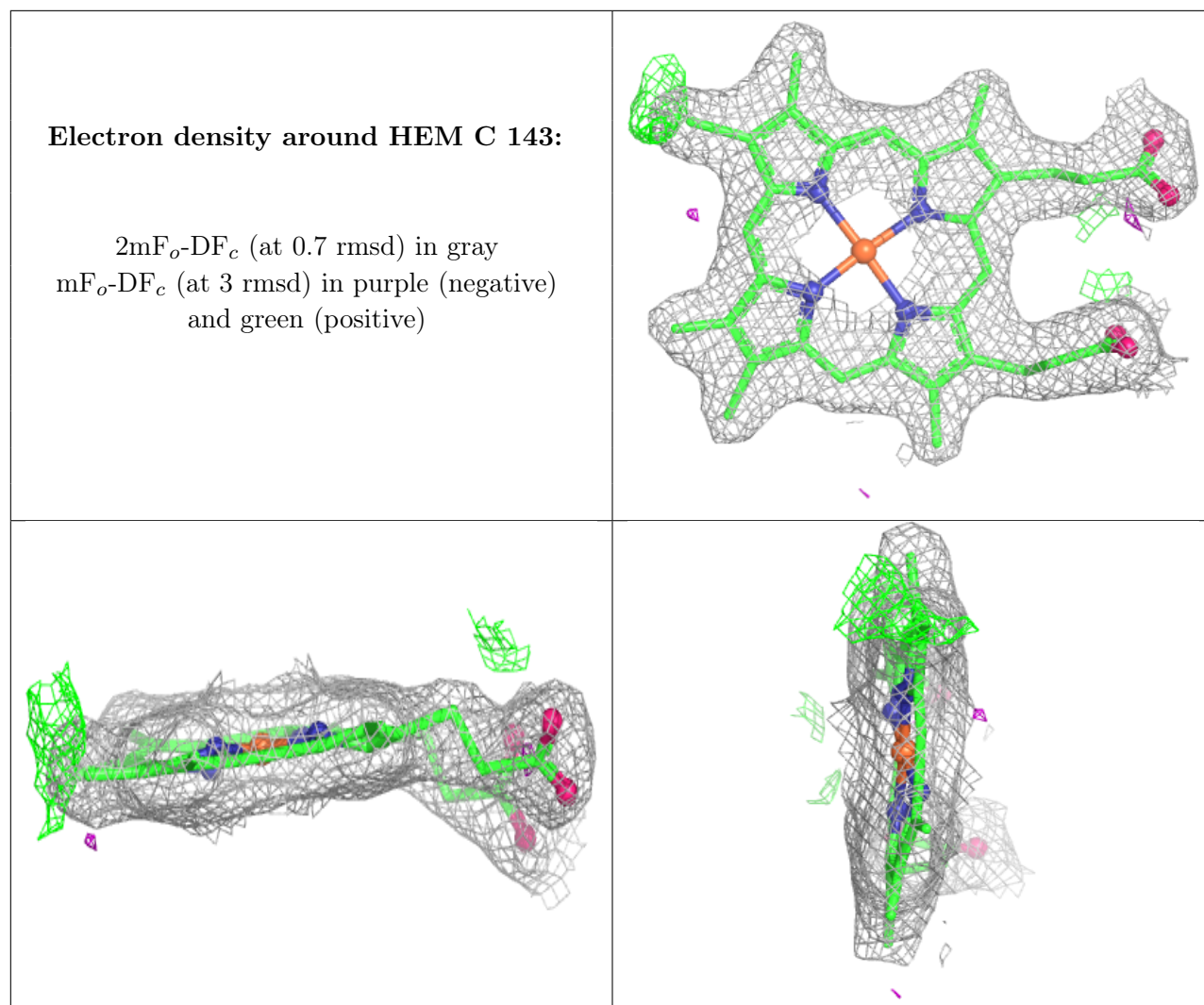
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FAD A 1001:

$2mF_o - DF_c$ (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.