



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 10:31 AM BST

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)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

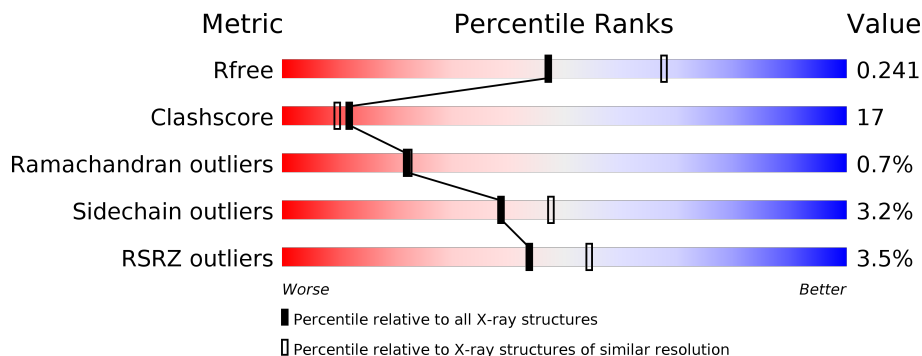
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	B	1005	-	-	-	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
			Total	C	N	O	S			
1	A	614	4736	2962	845	900	29	0	0	0

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

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

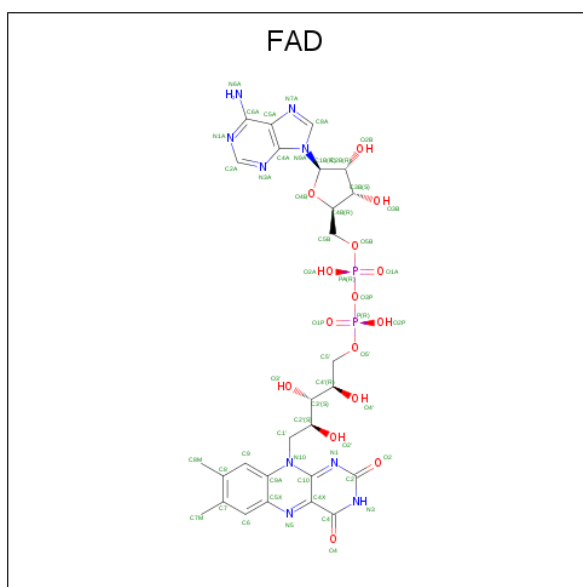
- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT.

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

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

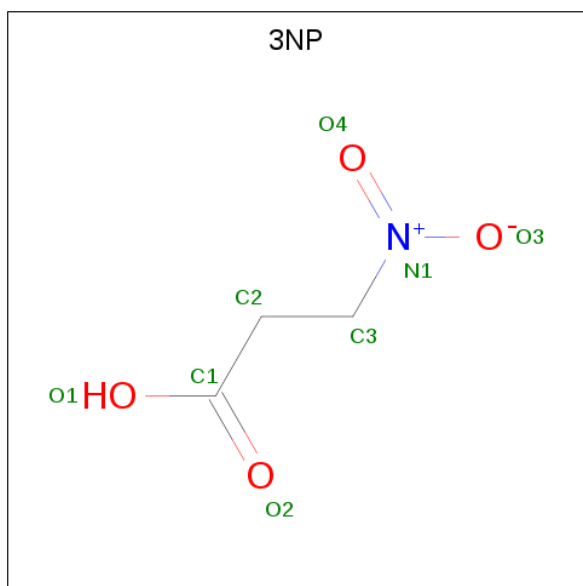
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	102	770	508	122	137	3	0	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



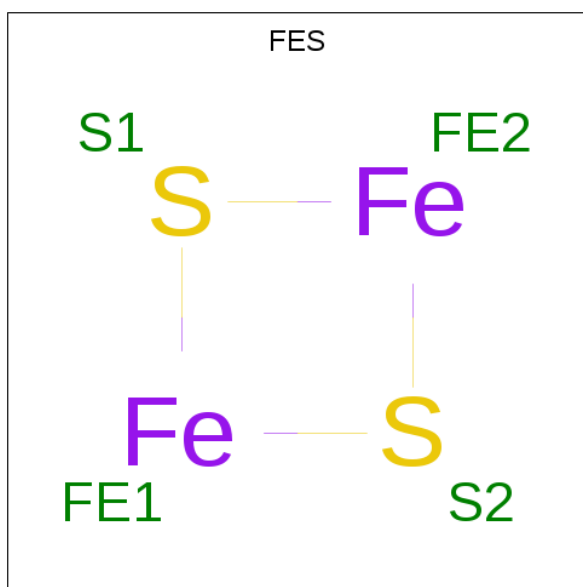
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	53	27	9	15	2	0	0

- Molecule 6 is 3-NITROPROPANOIC ACID (three-letter code: 3NP) (formula: C<sub>3</sub>H<sub>5</sub>NO<sub>4</sub>).



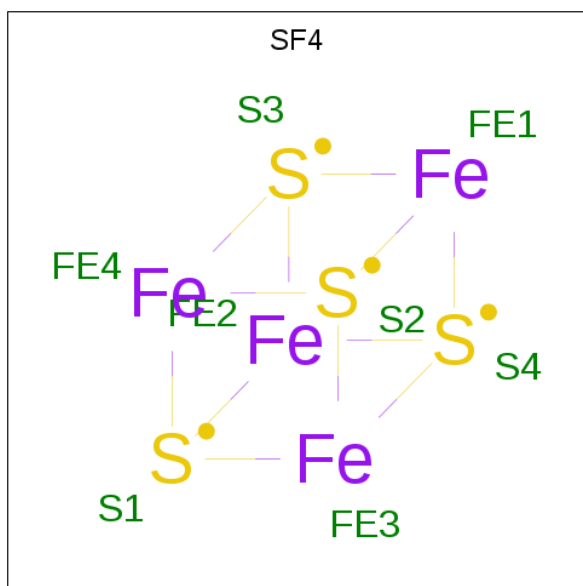
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	6	3	1	2	0	0	

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



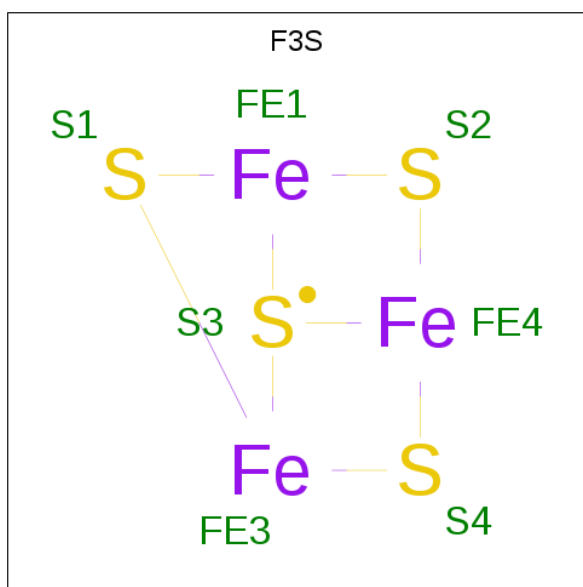
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



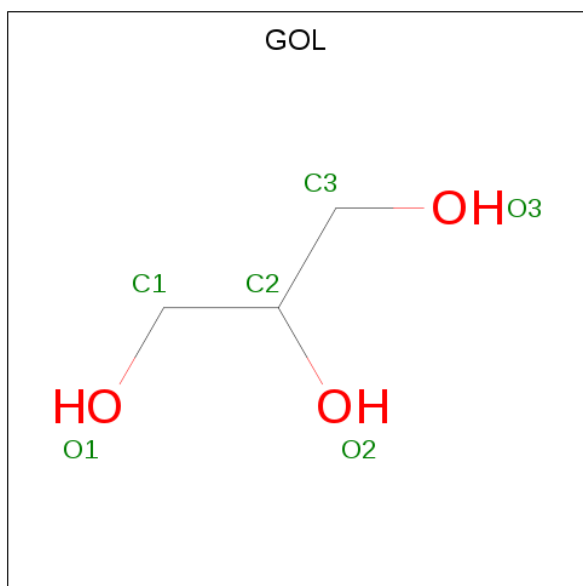
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



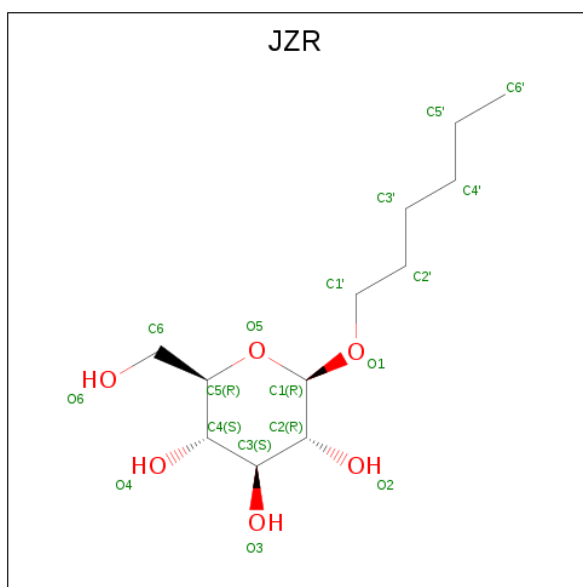
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 7 3 4	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



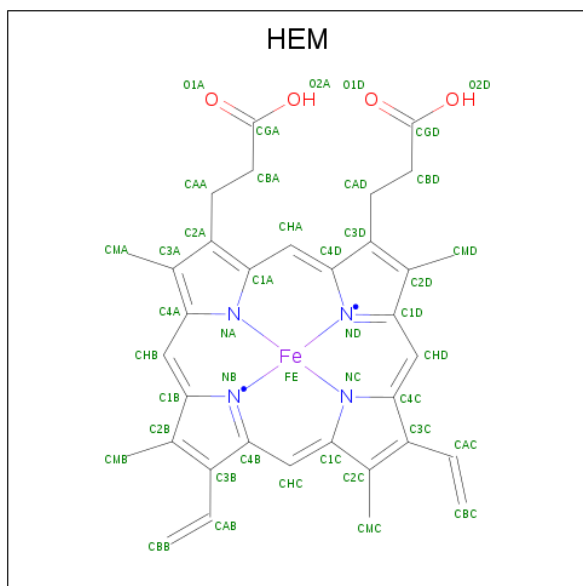
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 6 3 3	0	0

- 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	C	O			
			18	12	6	0	0	

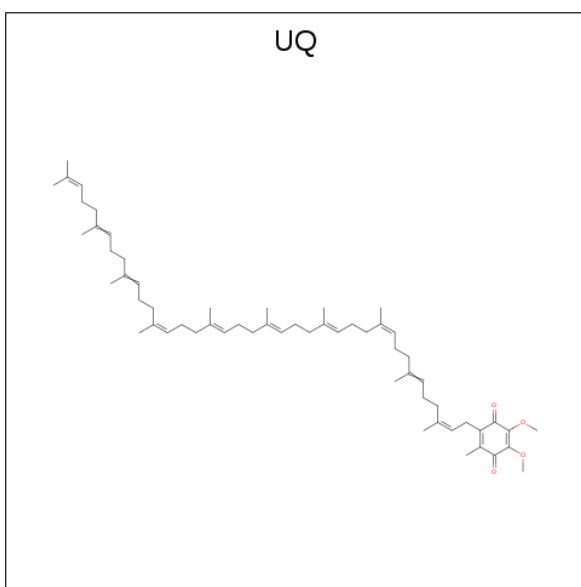
- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

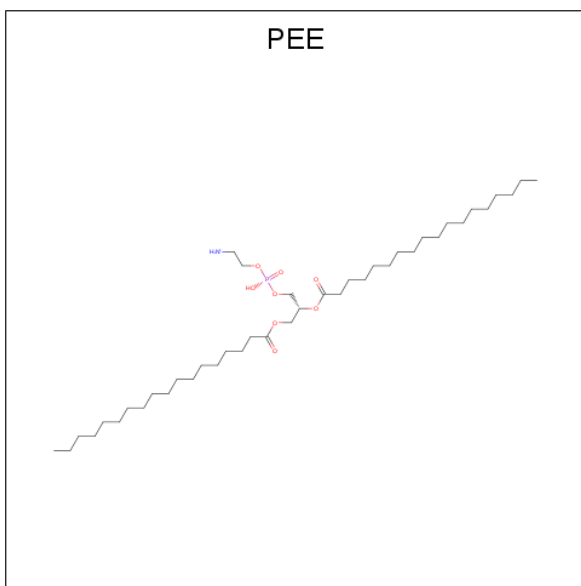
- Molecule 13 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula:  $C_{59}H_{90}O_4$ ).





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

- Molecule 14 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



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

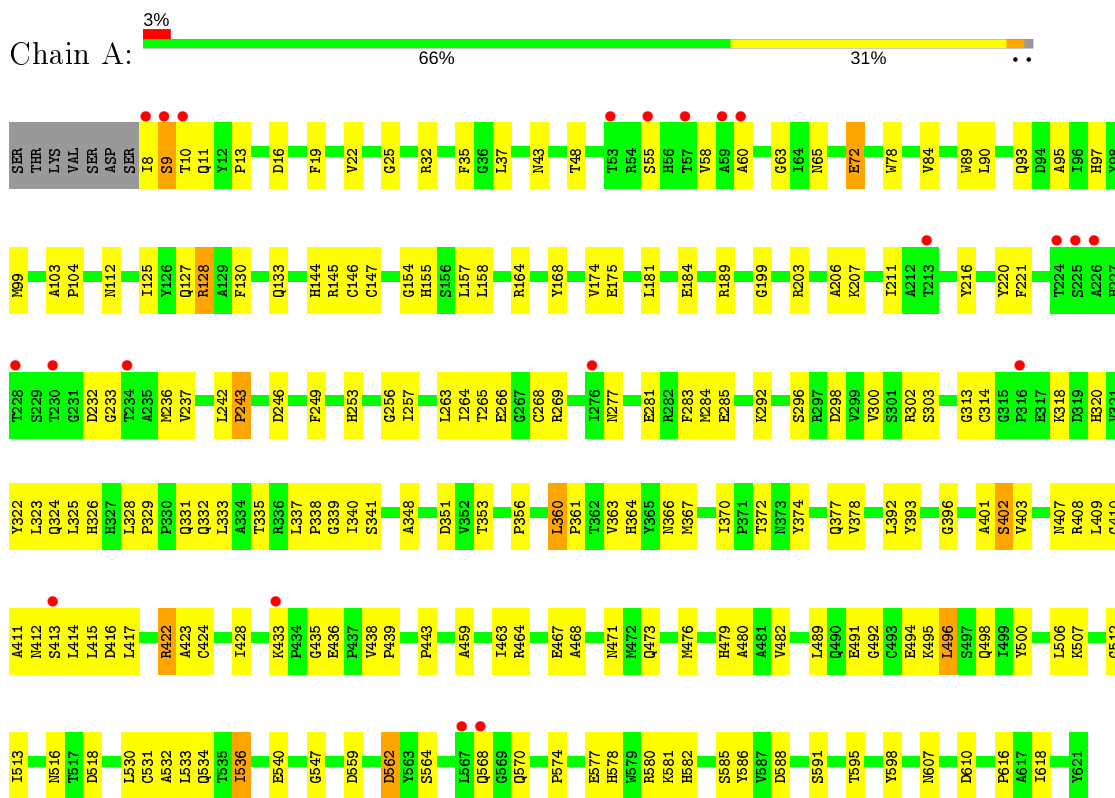
- Molecule 15 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
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

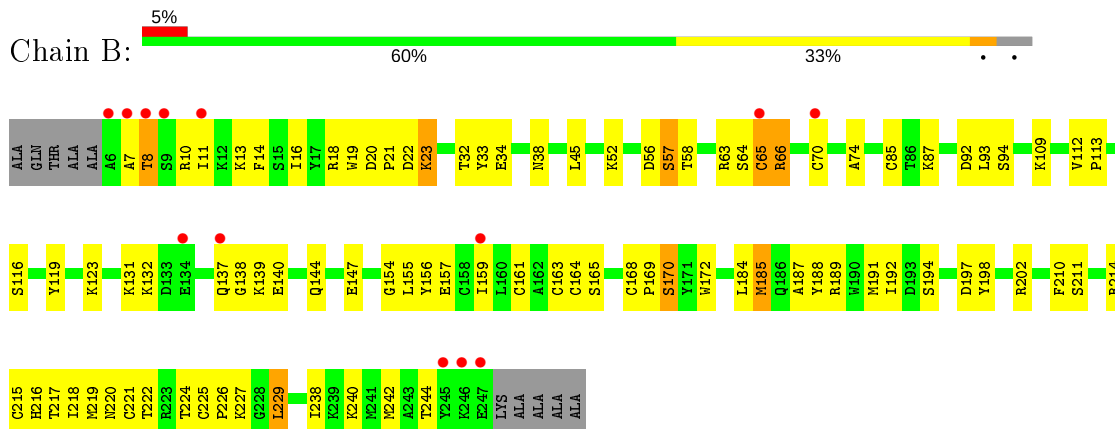
### 3 Residue-property plots [i](#)

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.

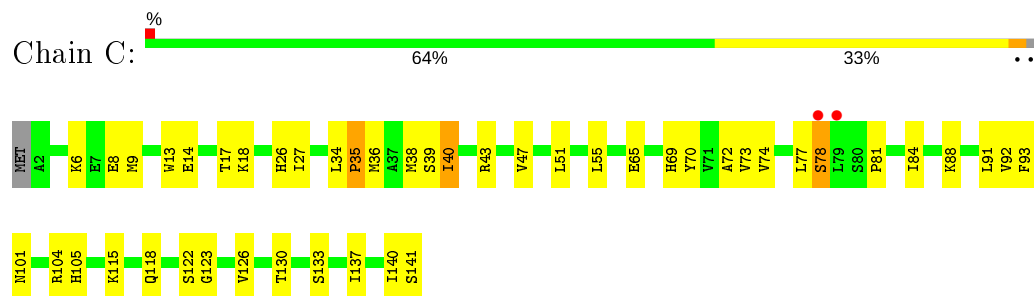
- Molecule 1: Succinate dehydrogenase flavoprotein subunit



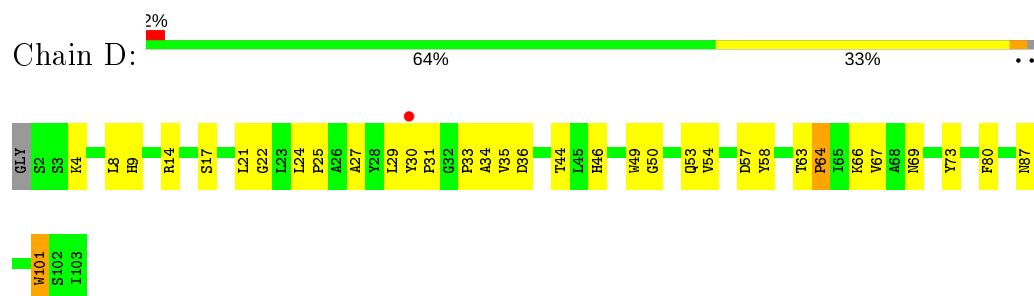
- Molecule 2: succinate dehydrogenase Ip subunit



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.252 0.195 , 0.241	Depositor DCC
$R_{free}$ test set	3830 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtrriage
Anisotropy	0.414	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9291	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SF4, UQ, F3S, FES, 3NP, PEE, HEM, JZR, 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	0.62	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(°)	Ideal(°)
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.

All (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:CE	2:B:185:MET:SD	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
1:A:32:ARG:NH2	1:A:422:ARG:HD2	1.95	0.82
2:B:214:ARG:HH22	4:D:53:GLN:HE22	1.26	0.80
1:A:112:ASN:HD22	2:B:138:GLY:H	1.28	0.79
2:B:214:ARG:HH12	4:D:53:GLN:NE2	1.80	0.79
3:C:101:ASN:HD21	3:C:104:ARG:HH11	1.31	0.78
1:A:164:ARG:HH22	2:B:137:GLN:HE22	1.31	0.78
1:A:216:TYR:H	1:A:366:ASN:ND2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:ARG:NH1	13:C:144:UQ:HM21	1.99	0.77
13:C:144:UQ:HM23	4:D:58:TYR:OH	1.86	0.76
3:C:34:LEU:HB3	3:C:35:PRO:HD3	1.67	0.75
2:B:65:CYS:HB3	2:B:70:CYS:HB3	1.68	0.75
1:A:480:ALA:HB2	1:A:536:ILE:HD12	1.69	0.75
1:A:277:ASN:ND2	1:A:281:GLU:HB3	2.01	0.75
1:A:237:VAL:HG21	1:A:370:ILE:HG12	1.69	0.74
4:D:4:LYS:O	4:D:8:LEU:HG	1.88	0.73
1:A:103:ALA:HB3	1:A:104:PRO:HD3	1.71	0.73
3:C:101:ASN:ND2	3:C:104:ARG:HH11	1.88	0.72
3:C:140:ILE:HG22	3:C:141:SER:N	2.05	0.72
2:B:66:ARG:HG2	2:B:66:ARG:O	1.87	0.72
1:A:127:GLN:NE2	1:A:145:ARG:HA	2.04	0.72
2:B:216:HIS:HB2	15:C:1006:HOH:O	1.90	0.71
1:A:313:GLY:O	1:A:318:LYS:HD3	1.91	0.70
1:A:72:GLU:OE1	1:A:144:HIS:HD2	1.74	0.70
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.73	0.70
1:A:257:ILE:HD11	1:A:348:ALA:HB2	1.75	0.69
1:A:58:VAL:HG23	1:A:155:HIS:HA	1.75	0.69
3:C:65:GLU:HB2	3:C:70:TYR:CZ	2.28	0.68
1:A:360:LEU:HD12	1:A:361:PRO:HD2	1.76	0.68
1:A:237:VAL:HG12	1:A:242:LEU:HB2	1.74	0.68
1:A:284:MET:HE3	1:A:303:SER:HB2	1.75	0.68
3:C:93:PHE:HB3	3:C:94:PRO:CD	2.24	0.68
1:A:25:GLY:HA2	5:A:1001:FAD:H1B	1.76	0.67
3:C:65:GLU:HB2	3:C:70:TYR:CE1	2.29	0.67
3:C:96:SER:HG	3:C:133:SER:HG	1.41	0.66
1:A:266:GLU:HG3	1:A:269:ARG:NH2	2.10	0.66
3:C:101:ASN:HD21	3:C:104:ARG:NH1	1.94	0.66
3:C:26:HIS:CD2	3:C:27:ILE:H	2.14	0.66
1:A:417:LEU:HD21	5:A:1001:FAD:H5'2	1.78	0.65
2:B:214:ARG:HH12	4:D:53:GLN:HE21	1.44	0.65
3:C:69:HIS:O	3:C:73:VAL:HG23	1.96	0.65
2:B:216:HIS:NE2	4:D:57:ASP:OD2	2.30	0.65
2:B:18:ARG:NH2	2:B:56:ASP:OD2	2.30	0.65
3:C:43:ARG:CZ	13:C:144:UQ:HM21	2.27	0.64
13:C:144:UQ:HM33	13:C:144:UQ:HM22	1.79	0.64
1:A:58:VAL:HB	1:A:158:LEU:HD23	1.80	0.64
1:A:284:MET:CE	1:A:303:SER:HB2	2.28	0.64
1:A:331:GLN:NE2	1:A:335:THR:OG1	2.30	0.64
2:B:188:TYR:HD1	2:B:191:MET:CE	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:OE1	1:A:144:HIS:CD2	2.50	0.63
1:A:534:GLN:NE2	1:A:585:SER:OG	2.32	0.63
3:C:47:VAL:O	3:C:51:LEU:HG	1.98	0.62
3:C:105:HIS:ND1	15:C:1107:HOH:O	2.31	0.62
2:B:187:ALA:O	2:B:191:MET:HG3	2.00	0.62
4:D:34:ALA:HB3	15:D:1470:HOH:O	2.01	0.61
1:A:479:HIS:O	1:A:489:LEU:HD23	2.01	0.60
1:A:464:ARG:HB3	1:A:507:LYS:HE3	1.82	0.60
1:A:155:HIS:HD2	15:B:1007:HOH:O	1.84	0.60
1:A:112:ASN:ND2	2:B:138:GLY:H	1.97	0.60
2:B:188:TYR:HA	2:B:191:MET:CE	2.31	0.60
1:A:396:GLY:HA2	1:A:417:LEU:HD23	1.83	0.60
3:C:43:ARG:NH1	13:C:144:UQ:CM2	2.64	0.60
1:A:243:PRO:HB3	1:A:586:TYR:CZ	2.37	0.60
2:B:188:TYR:HA	2:B:191:MET:HE2	1.82	0.60
1:A:367:MET:HE3	1:A:407:ASN:HA	1.84	0.59
4:D:4:LYS:HE2	15:D:1217:HOH:O	2.02	0.59
1:A:564:SER:HB3	1:A:618:ILE:HD11	1.85	0.59
1:A:164:ARG:HH22	2:B:137:GLN:NE2	1.98	0.59
4:D:53:GLN:HE21	4:D:53:GLN:HA	1.67	0.59
1:A:266:GLU:HG3	1:A:269:ARG:CZ	2.33	0.58
2:B:16:ILE:HD12	2:B:33:TYR:CD1	2.38	0.58
2:B:214:ARG:NH2	4:D:53:GLN:HE22	1.97	0.58
1:A:268:CYS:HB3	1:A:325:LEU:HD21	1.85	0.58
1:A:578:HIS:O	1:A:581:LYS:HE2	2.04	0.58
1:A:410:GLY:O	1:A:411:ALA:HB3	2.02	0.58
4:D:63:THR:HB	4:D:64:PRO:HD3	1.86	0.58
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.38	0.57
4:D:33:PRO:HG2	15:D:1079:HOH:O	2.03	0.57
4:D:53:GLN:NE2	4:D:53:GLN:HA	2.20	0.57
1:A:65:ASN:CG	1:A:133:GLN:HE22	2.07	0.57
1:A:401:ALA:N	1:A:402:SER:CA	2.67	0.57
2:B:219:MET:HE3	2:B:222:THR:HB	1.86	0.57
2:B:227:LYS:HB2	2:B:229:LEU:HD22	1.87	0.57
3:C:39:SER:OG	13:C:144:UQ:HM31	2.05	0.57
1:A:55:SER:O	1:A:58:VAL:HG12	2.05	0.56
1:A:328:LEU:HB2	1:A:333:LEU:HD21	1.86	0.56
2:B:21:PRO:HD2	2:B:109:LYS:HD2	1.86	0.56
2:B:10:ARG:HD3	2:B:38:ASN:HD21	1.71	0.56
2:B:147:GLU:CD	2:B:147:GLU:H	2.09	0.56
1:A:396:GLY:HA2	1:A:417:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLN:HG3	1:A:326:HIS:CE1	2.41	0.56
1:A:89:TRP:CD2	1:A:616:PRO:HA	2.40	0.56
3:C:13:TRP:O	3:C:17:THR:HG23	2.05	0.55
2:B:19:TRP:CZ3	2:B:21:PRO:HB3	2.42	0.55
2:B:154:GLY:H	2:B:157:GLU:CD	2.10	0.55
1:A:534:GLN:HG2	1:A:585:SER:HB2	1.87	0.55
1:A:367:MET:CE	1:A:407:ASN:HA	2.36	0.55
2:B:52:LYS:HG2	2:B:57:SER:HA	1.88	0.55
1:A:438:VAL:HG23	1:A:439:PRO:HD2	1.88	0.55
4:D:63:THR:O	4:D:67:VAL:HG23	2.07	0.55
1:A:16:ASP:OD1	1:A:203:ARG:HB2	2.06	0.55
3:C:74:VAL:HA	3:C:77:LEU:HD12	1.89	0.55
3:C:6:LYS:HA	3:C:9:MET:HE3	1.89	0.55
3:C:77:LEU:O	3:C:78:SER:C	2.45	0.55
1:A:559:ASP:OD2	1:A:580:ARG:HD3	2.08	0.54
2:B:191:MET:HE2	2:B:238:ILE:HG12	1.88	0.54
1:A:409:LEU:O	1:A:412:ASN:HB2	2.08	0.54
1:A:60:ALA:HA	5:A:1001:FAD:N5	2.22	0.54
2:B:16:ILE:HD12	2:B:33:TYR:HD1	1.72	0.54
3:C:34:LEU:HD23	15:C:1160:HOH:O	2.07	0.54
3:C:40:ILE:HA	13:C:144:UQ:HM32	1.89	0.54
1:A:58:VAL:O	1:A:58:VAL:HG22	2.09	0.53
2:B:92:ASP:OD1	2:B:94:SER:OG	2.23	0.53
4:D:27:ALA:HA	4:D:35:VAL:HG11	1.89	0.53
1:A:263:LEU:HB3	5:A:1001:FAD:HM73	1.91	0.53
1:A:562:ASP:C	1:A:562:ASP:OD1	2.47	0.53
1:A:339:GLY:HA3	15:A:1238:HOH:O	2.08	0.53
1:A:8:ILE:O	1:A:9:SER:HB3	2.09	0.53
1:A:60:ALA:HB3	1:A:154:GLY:CA	2.38	0.53
1:A:155:HIS:HE1	2:B:156:TYR:O	1.91	0.53
1:A:60:ALA:HA	5:A:1001:FAD:C5X	2.39	0.53
1:A:435:GLY:O	1:A:436:GLU:C	2.47	0.52
1:A:216:TYR:CD1	1:A:216:TYR:O	2.62	0.52
1:A:13:PRO:HA	15:A:1060:HOH:O	2.08	0.52
1:A:65:ASN:ND2	1:A:411:ALA:HB3	2.25	0.52
1:A:174:VAL:HG12	1:A:175:GLU:HG3	1.90	0.52
4:D:22:GLY:O	4:D:25:PRO:HG2	2.10	0.52
1:A:237:VAL:HG21	1:A:370:ILE:CG1	2.39	0.52
2:B:220:ASN:HD21	3:C:36:MET:CE	2.22	0.52
4:D:36:ASP:OD1	4:D:93:ILE:HB	2.09	0.52
1:A:10:THR:O	1:A:10:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PHE:HA	1:A:473:GLN:HB3	1.93	0.51
13:C:144:UQ:CM2	13:C:144:UQ:HM33	2.40	0.51
4:D:87:ASN:HA	4:D:92:GLY:HA2	1.92	0.51
1:A:378:VAL:HG21	1:A:392:LEU:HG	1.92	0.51
1:A:581:LYS:HD2	1:A:598:TYR:CB	2.40	0.51
3:C:26:HIS:CG	3:C:27:ILE:H	2.28	0.51
1:A:476:MET:SD	1:A:532:ALA:HB1	2.51	0.51
1:A:233:GLY:O	1:A:237:VAL:HG23	2.11	0.51
1:A:246:ASP:HB3	1:A:249:PHE:HD1	1.75	0.51
1:A:25:GLY:HA2	5:A:1001:FAD:C1B	2.41	0.50
1:A:263:LEU:HD22	1:A:364:HIS:HE1	1.76	0.50
1:A:164:ARG:NH2	2:B:137:GLN:HE22	2.05	0.50
2:B:52:LYS:CG	2:B:57:SER:HA	2.40	0.50
1:A:413:SER:O	1:A:416:ASP:HB3	2.11	0.50
3:C:140:ILE:CG2	3:C:141:SER:N	2.73	0.50
4:D:44:THR:HG21	4:D:80:PHE:HB2	1.94	0.50
2:B:119:TYR:O	2:B:123:LYS:HG3	2.11	0.50
1:A:189:ARG:HD2	1:A:439:PRO:HB2	1.94	0.50
2:B:168:CYS:SG	2:B:170:SER:HB2	2.51	0.50
1:A:464:ARG:O	1:A:467:GLU:N	2.45	0.50
2:B:198:TYR:O	2:B:202:ARG:HG3	2.11	0.50
3:C:14:GLU:O	3:C:18:LYS:HG2	2.10	0.50
1:A:574:PRO:HD2	1:A:577:GLU:HB2	1.93	0.50
1:A:58:VAL:CG2	1:A:155:HIS:HA	2.42	0.49
1:A:103:ALA:HA	1:A:415:LEU:HD11	1.94	0.49
3:C:88:LYS:HB3	4:D:101:TRP:CZ2	2.47	0.49
2:B:45:LEU:HD22	2:B:85:CYS:HB3	1.94	0.49
3:C:93:PHE:HB3	3:C:94:PRO:HD2	1.93	0.49
3:C:6:LYS:HA	3:C:9:MET:CE	2.42	0.49
1:A:500:TYR:CD1	1:A:533:LEU:HD11	2.48	0.49
1:A:351:ASP:C	1:A:351:ASP:OD1	2.52	0.48
1:A:283:PHE:CE1	1:A:284:MET:HE2	2.48	0.48
1:A:35:PHE:HB2	1:A:168:TYR:CD1	2.47	0.48
1:A:90:LEU:O	1:A:582:HIS:CE1	2.67	0.48
1:A:90:LEU:O	1:A:582:HIS:HE1	1.96	0.48
2:B:8:THR:HG22	2:B:8:THR:O	2.12	0.48
2:B:164:CYS:SG	2:B:165:SER:N	2.87	0.48
2:B:191:MET:CE	2:B:238:ILE:HG12	2.43	0.48
1:A:283:PHE:HE1	1:A:284:MET:HE2	1.78	0.48
3:C:95:LEU:HD21	14:C:145:PEE:H39	1.95	0.48
3:C:39:SER:HA	15:C:1200:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLY:O	1:A:496:LEU:HB2	2.14	0.48
4:D:24:LEU:N	4:D:25:PRO:HD2	2.29	0.48
1:A:207:LYS:HZ3	1:A:436:GLU:CD	2.18	0.47
1:A:237:VAL:CG1	1:A:242:LEU:HB2	2.40	0.47
2:B:147:GLU:CD	2:B:147:GLU:N	2.67	0.47
2:B:188:TYR:HD1	2:B:191:MET:HE3	1.78	0.47
1:A:199:GLY:HA2	1:A:513:ILE:HG13	1.95	0.47
1:A:302:ARG:HA	1:A:482:VAL:HG11	1.97	0.47
2:B:14:PHE:O	2:B:32:THR:HA	2.14	0.47
3:C:97:TYR:HA	3:C:130:THR:OG1	2.15	0.47
2:B:155:LEU:CD1	2:B:192:ILE:HD11	2.45	0.47
2:B:7:ALA:O	2:B:8:THR:HB	2.14	0.47
13:C:144:UQ:HM23	4:D:58:TYR:HH	1.79	0.47
2:B:123:LYS:HB3	15:C:1143:HOH:O	2.15	0.47
2:B:169:PRO:HA	2:B:172:TRP:CD2	2.50	0.47
3:C:72:ALA:O	3:C:73:VAL:C	2.51	0.47
1:A:37:LEU:HD21	1:A:428:ILE:HD12	1.97	0.47
1:A:125:ILE:HG21	1:A:147:CYS:HB3	1.96	0.46
2:B:221:CYS:O	2:B:224:THR:HG22	2.14	0.46
2:B:10:ARG:HD3	2:B:38:ASN:ND2	2.31	0.46
1:A:246:ASP:HB3	1:A:249:PHE:CD1	2.50	0.46
2:B:217:THR:HG22	2:B:217:THR:O	2.15	0.46
2:B:7:ALA:O	2:B:8:THR:CB	2.62	0.46
3:C:115:LYS:HB2	3:C:118:GLN:HG3	1.98	0.46
1:A:489:LEU:CD1	1:A:540:GLU:HA	2.45	0.46
1:A:65:ASN:OD1	1:A:133:GLN:NE2	2.41	0.46
2:B:23:LYS:HD2	15:B:1096:HOH:O	2.14	0.46
1:A:221:PHE:CA	1:A:473:GLN:HB3	2.46	0.46
4:D:21:LEU:O	4:D:25:PRO:HD2	2.16	0.46
2:B:139:LYS:O	2:B:140:GLU:HG2	2.16	0.46
1:A:253:HIS:O	1:A:361:PRO:HA	2.15	0.45
2:B:87:LYS:HE2	15:B:1063:HOH:O	2.15	0.45
2:B:123:LYS:HE3	3:C:8:GLU:OE1	2.16	0.45
1:A:463:ILE:O	1:A:506:LEU:HD23	2.17	0.45
2:B:225:CYS:SG	2:B:229:LEU:HB2	2.57	0.45
1:A:530:LEU:HD23	1:A:530:LEU:HA	1.75	0.45
2:B:56:ASP:C	2:B:58:THR:H	2.19	0.45
2:B:11:ILE:CG2	2:B:34:GLU:HB3	2.47	0.45
4:D:50:GLY:O	4:D:54:VAL:HG23	2.17	0.45
2:B:65:CYS:O	2:B:66:ARG:HB3	2.17	0.45
1:A:263:LEU:HD22	1:A:364:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ALA:HB1	2:B:163:CYS:SG	2.57	0.45
3:C:38:MET:HE1	3:C:123:GLY:HA2	1.98	0.45
1:A:360:LEU:HD12	1:A:361:PRO:CD	2.47	0.45
4:D:69:ASN:HD22	4:D:69:ASN:HA	1.63	0.45
1:A:322:TYR:HB3	1:A:356:PRO:HB2	1.99	0.45
1:A:377:GLN:HG2	1:A:393:TYR:CE1	2.51	0.45
1:A:468:ALA:O	1:A:471:ASN:HB2	2.16	0.45
1:A:516:ASN:OD1	1:A:518:ASP:HB3	2.17	0.45
1:A:97:HIS:C	1:A:97:HIS:CD2	2.90	0.45
1:A:263:LEU:HD23	5:A:1001:FAD:H6	2.00	0.44
1:A:329:PRO:HD2	1:A:332:GLN:OE1	2.17	0.44
1:A:340:ILE:HD12	1:A:341:SER:N	2.33	0.44
4:D:24:LEU:HA	4:D:24:LEU:HD23	1.78	0.44
4:D:9:HIS:HE1	4:D:49:TRP:CD1	2.35	0.44
1:A:401:ALA:HB3	1:A:403:VAL:HG13	2.00	0.44
1:A:459:ALA:HB1	1:A:506:LEU:O	2.16	0.44
4:D:73:TYR:HB2	15:D:1528:HOH:O	2.17	0.44
1:A:84:VAL:HG22	1:A:93:GLN:HG2	1.99	0.44
1:A:401:ALA:H	1:A:402:SER:HA	1.78	0.44
1:A:496:LEU:HD23	1:A:496:LEU:HA	1.89	0.44
2:B:159:ILE:HG13	2:B:161:CYS:HB3	1.99	0.43
2:B:225:CYS:HA	2:B:226:PRO:HD2	1.74	0.43
1:A:581:LYS:HD2	1:A:598:TYR:HB3	1.99	0.43
1:A:63:GLY:HA3	1:A:146:CYS:SG	2.58	0.43
3:C:123:GLY:O	3:C:126:VAL:HB	2.19	0.43
4:D:29:LEU:C	4:D:30:TYR:CD1	2.92	0.43
2:B:214:ARG:HD3	4:D:57:ASP:OD1	2.17	0.43
4:D:63:THR:CB	4:D:64:PRO:HD3	2.48	0.43
1:A:512:GLY:HA2	15:B:1123:HOH:O	2.17	0.43
1:A:89:TRP:CE2	1:A:616:PRO:HA	2.54	0.43
3:C:55:LEU:HA	3:C:55:LEU:HD23	1.77	0.43
1:A:340:ILE:HD12	1:A:340:ILE:C	2.39	0.43
1:A:184:GLU:HB3	1:A:189:ARG:HE	1.83	0.43
1:A:414:LEU:HA	1:A:414:LEU:HD23	1.91	0.43
1:A:424:CYS:O	1:A:428:ILE:HG13	2.19	0.43
1:A:22:VAL:HG23	1:A:206:ALA:HB2	2.01	0.42
1:A:588:ASP:OD1	1:A:591:SER:OG	2.30	0.42
1:A:372:THR:HA	1:A:377:GLN:O	2.19	0.42
4:D:30:TYR:N	4:D:31:PRO:CD	2.83	0.42
1:A:257:ILE:HD11	1:A:348:ALA:CB	2.48	0.42
2:B:13:LYS:HA	2:B:33:TYR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:ILE:HD12	3:C:27:ILE:HA	1.91	0.42
3:C:92:VAL:HG21	3:C:137:ILE:HG21	2.02	0.42
2:B:144:GLN:HG3	2:B:194:SER:OG	2.20	0.42
3:C:34:LEU:N	3:C:35:PRO:CD	2.83	0.42
1:A:128:ARG:HG2	1:A:146:CYS:HB3	2.01	0.42
1:A:264:ILE:HG21	1:A:323:LEU:HD23	2.02	0.42
1:A:351:ASP:OD1	1:A:353:THR:OG1	2.31	0.42
1:A:489:LEU:HD13	1:A:540:GLU:HA	2.02	0.42
1:A:337:LEU:N	1:A:338:PRO:CD	2.83	0.42
1:A:564:SER:CB	1:A:618:ILE:HD11	2.49	0.42
3:C:81:PRO:O	3:C:84:ILE:HB	2.20	0.42
4:D:17:SER:OG	4:D:46:HIS:CE1	2.73	0.42
1:A:491:GLU:HG2	1:A:495:LYS:HE3	2.01	0.41
3:C:122:SER:O	3:C:126:VAL:HG23	2.20	0.41
3:C:118:GLN:HG2	15:C:1337:HOH:O	2.20	0.41
1:A:422:ARG:O	1:A:423:ALA:C	2.57	0.41
1:A:494:GLU:O	1:A:495:LYS:C	2.59	0.41
1:A:157:LEU:C	1:A:157:LEU:HD23	2.40	0.41
2:B:169:PRO:HA	2:B:172:TRP:CE3	2.55	0.41
1:A:314:CYS:N	1:A:320:HIS:O	2.44	0.41
1:A:90:LEU:O	1:A:90:LEU:HG	2.21	0.41
1:A:99:MET:CE	1:A:403:VAL:HB	2.51	0.41
2:B:20:ASP:OD1	2:B:22:ASP:HB2	2.21	0.41
1:A:95:ALA:HA	1:A:374:TYR:HB2	2.03	0.41
3:C:65:GLU:O	3:C:70:TYR:HE1	2.04	0.41
1:A:232:ASP:O	1:A:236:MET:HG3	2.21	0.41
1:A:78:TRP:HB3	15:A:1028:HOH:O	2.21	0.41
1:A:607:ASN:ND2	1:A:610:ASP:HB2	2.36	0.41
2:B:238:ILE:O	2:B:242:MET:HG2	2.21	0.41
2:B:184:LEU:HA	2:B:184:LEU:HD23	1.93	0.40
2:B:132:LYS:HG2	2:B:197:ASP:HB3	2.02	0.40
2:B:93:LEU:HD23	2:B:93:LEU:HA	1.86	0.40
1:A:285:GLU:HG2	1:A:292:LYS:HD3	2.03	0.40
1:A:298:ASP:OD2	1:A:547:GLY:HA2	2.21	0.40
1:A:296:SER:O	1:A:300:VAL:HG23	2.21	0.40
1:A:19:PHE:O	1:A:206:ALA:HA	2.22	0.40
1:A:433:LYS:HA	1:A:433:LYS:HD2	1.87	0.40
1:A:586:TYR:HB2	1:A:595:THR:HB	2.03	0.40
2:B:210:PHE:O	2:B:211:SER:C	2.58	0.40
2:B:112:VAL:HA	2:B:113:PRO:HD2	1.89	0.40
2:B:218:ILE:HG12	13:C:144:UQ:O3	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%)	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

All (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
2	B	64	SER
1	A	9	SER
1	A	443	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	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

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	43	ASN
1	A	48	THR
1	A	72	GLU
1	A	128	ARG
1	A	130	PHE
1	A	243	PRO
1	A	360	LEU
1	A	402	SER
1	A	496	LEU
1	A	498	GLN
1	A	536	ILE
1	A	562	ASP
1	A	570	GLN
2	B	63	ARG
2	B	65	CYS
2	B	66	ARG
2	B	116	SER
2	B	131	LYS
2	B	170	SER
2	B	189	ARG
2	B	229	LEU
3	C	35	PRO
3	C	40	ILE
3	C	91	LEU
4	D	14	ARG
4	D	64	PRO
4	D	66	LYS
4	D	101	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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	326	HIS
1	A	331	GLN
1	A	366	ASN
1	A	383	ASN
1	A	534	GLN
2	B	121	GLN
2	B	137	GLN
3	C	26	HIS
3	C	42	HIS
3	C	101	ASN
4	D	9	HIS
4	D	53	GLN
4	D	69	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
7	FES	B	1002	2	0,4,4	0.00	-	-	-	-
8	SF4	B	1003	2	0,12,12	0.00	-	-	-	-
14	PEE	D	104	-	22,22,50	0.90	1 (4%)	20,20,55	1.01	2 (10%)
6	3NP	A	1002	1	1,5,7	1.60	0	0,5,8	0.00	-
12	HEM	C	143	3,4	26,48,50	1.92	7 (26%)	21,80,82	1.43	3 (14%)
11	JZR	C	142	-	18,18,18	2.00	3 (16%)	23,23,23	0.99	2 (8%)
10	GOL	B	1005	-	5,5,5	1.31	0	5,5,5	0.60	0
13	UQ	C	144	-	14,14,63	1.95	7 (50%)	18,20,79	0.45	0
5	FAD	A	1001	1	51,58,58	2.32	22 (43%)	60,89,89	2.05	15 (25%)
14	PEE	C	145	-	16,19,50	1.14	2 (12%)	15,19,55	1.31	4 (26%)
9	F3S	B	1004	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
7	FES	B	1002	2	-	-	0/1/1/1
14	PEE	C	145	-	-	9/15/17/54	-
14	PEE	D	104	-	-	10/18/18/54	-
6	3NP	A	1002	1	-	1/1/3/5	-
12	HEM	C	143	3,4	-	0/6/50/54	-
11	JZR	C	142	-	-	3/9/29/29	0/1/1/1
10	GOL	B	1005	-	-	3/4/4/4	-
13	UQ	C	144	-	-	2/4/28/87	0/1/1/1
5	FAD	A	1001	1	-	10/30/50/50	0/6/6/6
8	SF4	B	1003	2	-	-	0/6/5/5
9	F3S	B	1004	2	-	-	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	142	JZR	O1-C1	5.94	1.50	1.40
12	C	143	HEM	CAB-C3B	-5.35	1.40	1.51
5	A	1001	FAD	PA-O2A	-5.05	1.31	1.55
5	A	1001	FAD	C1'-N10	5.04	1.53	1.48
5	A	1001	FAD	PA-O1A	-4.77	1.34	1.50
5	A	1001	FAD	C10-N1	4.25	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	FAD	C4X-C10	3.98	1.42	1.38
5	A	1001	FAD	C4A-N3A	3.87	1.41	1.35
12	C	143	HEM	CAD-C3D	3.81	1.58	1.52
12	C	143	HEM	CAC-C3C	-3.79	1.42	1.51
5	A	1001	FAD	C4-N3	3.74	1.39	1.33
5	A	1001	FAD	C2A-N3A	3.74	1.38	1.32
5	A	1001	FAD	C5'-C4'	-3.62	1.46	1.51
5	A	1001	FAD	C9A-N10	3.01	1.42	1.38
14	C	145	PEE	C22-C21	-2.98	1.34	1.51
11	C	142	JZR	O5-C1	2.94	1.49	1.41
13	C	144	UQ	C7-C6	2.90	1.56	1.50
5	A	1001	FAD	C2'-C3'	-2.89	1.48	1.53
14	C	145	PEE	C19-C18	-2.82	1.35	1.51
5	A	1001	FAD	C9-C8	2.80	1.44	1.37
13	C	144	UQ	C6-C1	2.70	1.56	1.47
5	A	1001	FAD	C6-C7	2.70	1.44	1.37
5	A	1001	FAD	O5'-C5'	-2.69	1.34	1.44
14	D	104	PEE	C18-C17	-2.67	1.36	1.51
12	C	143	HEM	CMC-C2C	2.60	1.57	1.51
5	A	1001	FAD	C8-C7	2.60	1.47	1.40
13	C	144	UQ	O3-C3	2.57	1.43	1.36
5	A	1001	FAD	C2B-C1B	-2.46	1.50	1.53
13	C	144	UQ	C3-C4	2.45	1.55	1.48
5	A	1001	FAD	C4X-N5	2.34	1.36	1.33
5	A	1001	FAD	C9A-C5X	2.25	1.47	1.42
13	C	144	UQ	C2-C1	2.24	1.55	1.48
5	A	1001	FAD	C2A-N1A	2.23	1.38	1.33
11	C	142	JZR	O1-C1'	2.23	1.49	1.43
13	C	144	UQ	CM5-C5	2.21	1.55	1.50
5	A	1001	FAD	PA-O5B	-2.20	1.50	1.59
12	C	143	HEM	C1B-C2B	2.19	1.47	1.42
5	A	1001	FAD	C4-C4X	2.16	1.45	1.41
5	A	1001	FAD	C4'-C3'	2.11	1.57	1.53
12	C	143	HEM	C3C-C2C	-2.10	1.34	1.41
13	C	144	UQ	C5-C4	2.07	1.54	1.47
12	C	143	HEM	C1C-C2C	2.04	1.47	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	FAD	C4-N3-C2	6.89	120.96	115.14
5	A	1001	FAD	C4X-N5-C5X	6.24	123.00	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	FAD	N3A-C2A-N1A	-5.90	119.46	128.68
5	A	1001	FAD	C4-C4X-C10	-4.24	117.14	119.95
5	A	1001	FAD	C4-C4X-N5	3.69	122.81	118.60
5	A	1001	FAD	C5X-C9A-N10	-3.32	115.31	117.72
12	C	143	HEM	C1C-C2C-C3C	-3.08	104.74	106.85
14	D	104	PEE	C19-C18-C17	2.96	129.44	114.42
14	C	145	PEE	C20-C19-C18	2.84	128.84	114.42
14	D	104	PEE	C18-C17-C16	2.63	127.80	114.42
5	A	1001	FAD	C1'-C2'-C3'	2.63	117.13	109.79
5	A	1001	FAD	P-O3P-PA	2.61	141.78	132.83
12	C	143	HEM	C1D-C2D-C3D	2.61	108.81	107.00
5	A	1001	FAD	C4X-C4-N3	-2.60	119.88	123.43
12	C	143	HEM	C1B-C2B-C3B	-2.50	105.13	106.85
14	C	145	PEE	C22-C21-C20	2.48	127.04	114.42
14	C	145	PEE	C19-C18-C17	2.39	126.56	114.42
14	C	145	PEE	C23-C22-C21	2.28	125.99	114.42
5	A	1001	FAD	O3'-C3'-C2'	-2.25	103.37	108.81
5	A	1001	FAD	C1B-N9A-C4A	-2.18	122.81	126.64
5	A	1001	FAD	C4X-C10-N10	-2.15	118.09	120.30
11	C	142	JZR	O1-C1'-C2'	2.08	116.87	109.56
5	A	1001	FAD	O2'-C2'-C3'	-2.06	104.09	109.10
5	A	1001	FAD	C1'-N10-C9A	2.04	119.90	118.29
5	A	1001	FAD	C7M-C7-C6	-2.01	115.53	120.34
11	C	142	JZR	C1'-O1-C1	2.00	117.16	113.84

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	3NP	C1-C2-C3-N1
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	PA-O3P-P-O5'
14	C	145	PEE	C11-C12-C13-C14
14	C	145	PEE	C19-C20-C21-C22
14	D	104	PEE	C33-C34-C35-C36
14	C	145	PEE	C12-C13-C14-C15
14	C	145	PEE	C23-C24-C25-C26
10	B	1005	GOL	C1-C2-C3-O3
14	C	145	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
11	C	142	JZR	O1-C1'-C2'-C3'
10	B	1005	GOL	O2-C2-C3-O3
14	D	104	PEE	C32-C33-C34-C35
5	A	1001	FAD	C3'-C4'-C5'-O5'
14	D	104	PEE	C16-C17-C18-C19
14	D	104	PEE	C10-C11-C12-C13
14	D	104	PEE	C18-C19-C20-C21
14	D	104	PEE	C37-C38-C39-C40
14	D	104	PEE	C15-C16-C17-C18
14	D	104	PEE	C31-C32-C33-C34
14	C	145	PEE	C18-C19-C20-C21
14	C	145	PEE	C17-C18-C19-C20
14	D	104	PEE	C35-C36-C37-C38
13	C	144	UQ	C4-C3-O3-CM3
5	A	1001	FAD	N10-C1'-C2'-C3'
11	C	142	JZR	C2'-C3'-C4'-C5'
14	D	104	PEE	C34-C35-C36-C37
11	C	142	JZR	C3'-C4'-C5'-C6'
14	C	145	PEE	C24-C25-C26-C27
13	C	144	UQ	C2-C3-O3-CM3
5	A	1001	FAD	O4B-C4B-C5B-O5B
14	C	145	PEE	C14-C15-C16-C17
5	A	1001	FAD	C5'-O5'-P-O3P
5	A	1001	FAD	PA-O3P-P-O1P
10	B	1005	GOL	O1-C1-C2-O2

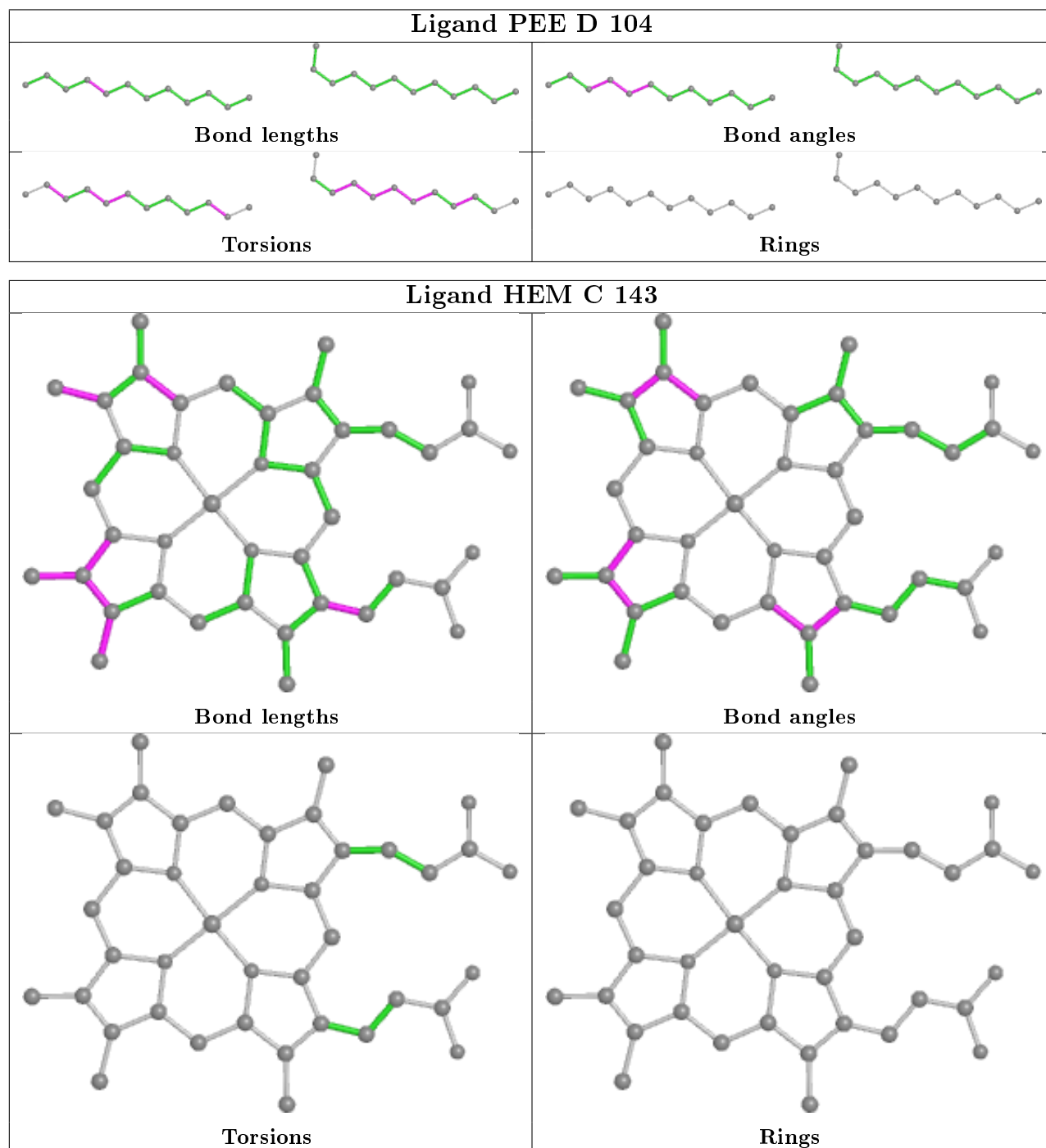
There are no ring outliers.

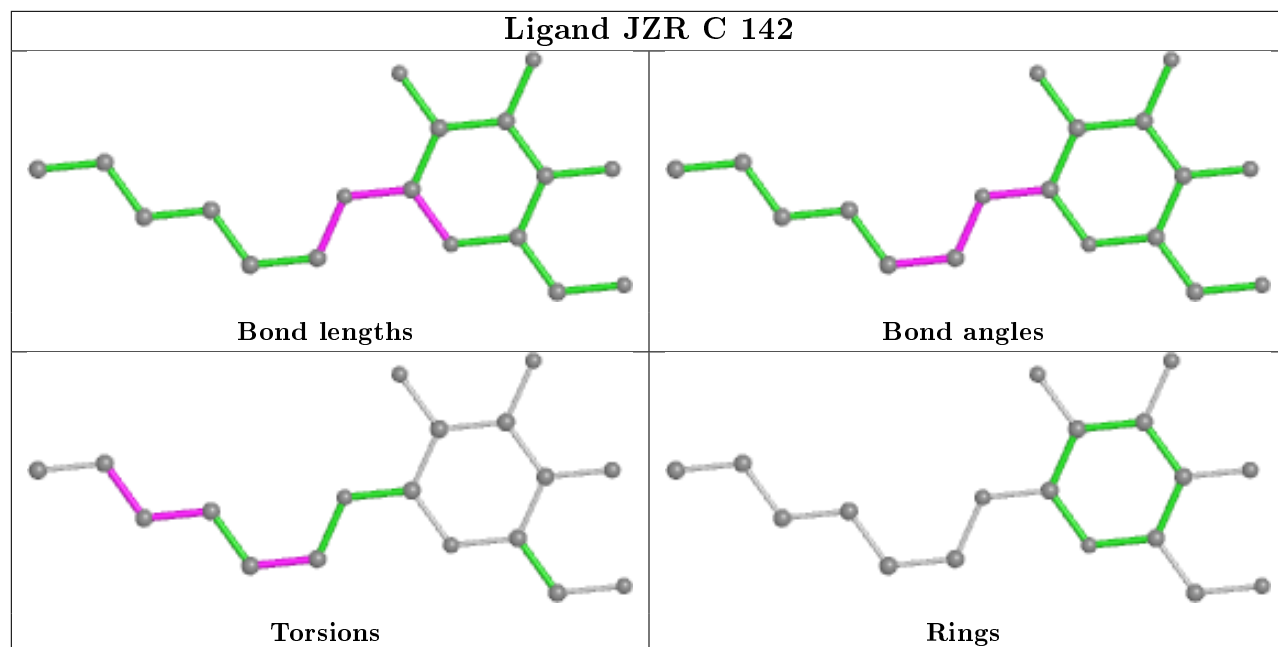
3 monomers are involved in 18 short contacts:

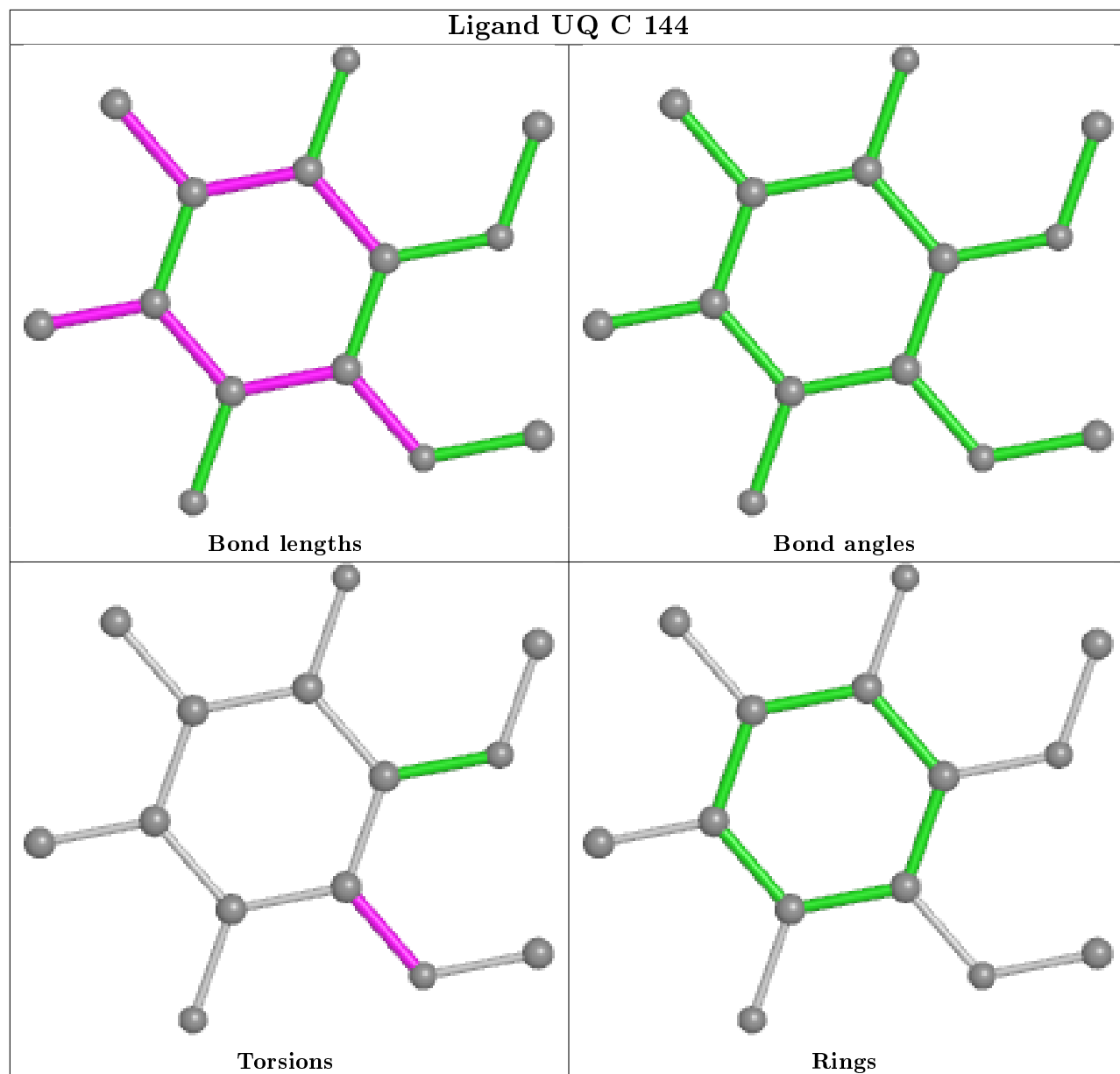
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	144	UQ	10	0
5	A	1001	FAD	7	0
14	C	145	PEE	1	0

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 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

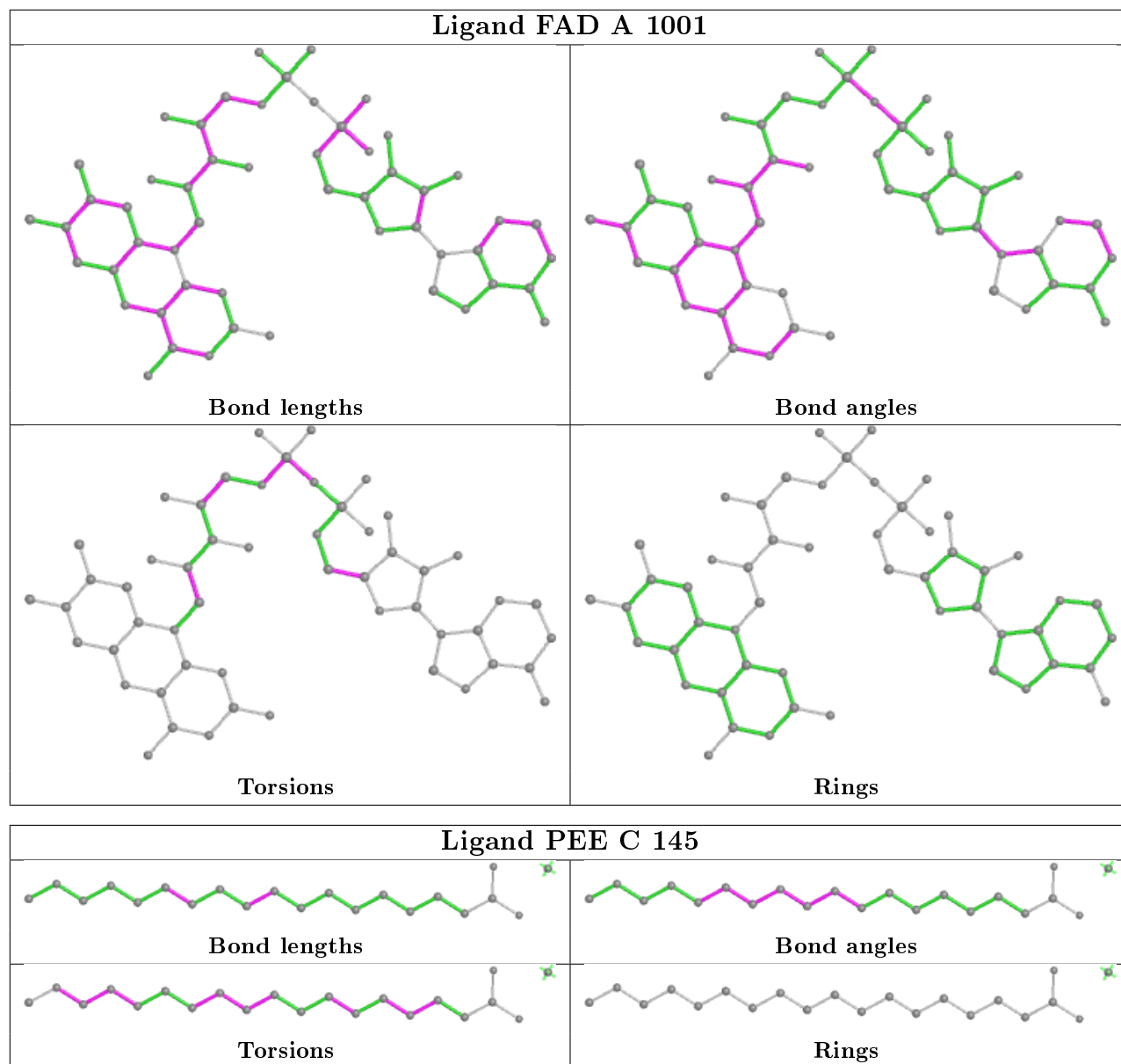
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents 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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	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

All (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
2	B	134	GLU	4.0
1	A	10	THR	3.8
1	A	59	ALA	3.6
3	C	79	LEU	3.5
1	A	228	THR	3.2
2	B	9	SER	3.2
1	A	57	THR	3.2
1	A	226	ALA	2.9
1	A	55	SER	2.9
1	A	224	THR	2.9
2	B	70	CYS	2.9
1	A	230	THR	2.8
1	A	234	THR	2.8
1	A	53	THR	2.8
1	A	316	PRO	2.7
2	B	11	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	159	ILE	2.6
1	A	225	SER	2.6
2	B	247	GLU	2.6
2	B	65	CYS	2.5
1	A	213	THR	2.4
2	B	246	LYS	2.3
1	A	276	ILE	2.3
1	A	433	LYS	2.2
4	D	30	TYR	2.2
1	A	60	ALA	2.2
4	D	97	VAL	2.1
1	A	567	LEU	2.1
3	C	78	SER	2.1
2	B	245	TYR	2.1
1	A	568	GLN	2.0
1	A	413	SER	2.0
2	B	137	GLN	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 [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

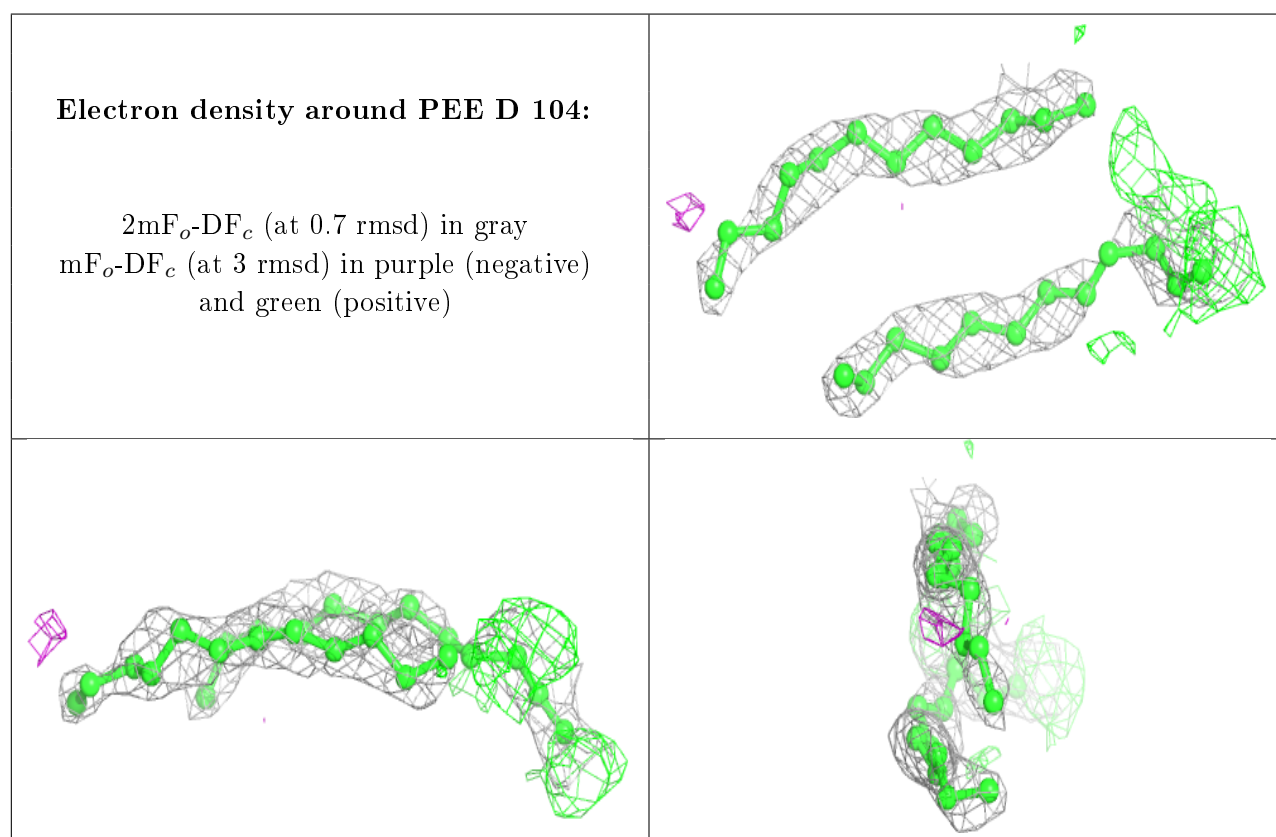
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	GOL	B	1005	6/6	0.32	0.59	156,160,161,162	0
14	PEE	D	104	24/51	0.80	0.28	53,72,98,99	0
13	UQ	C	144	14/63	0.84	0.44	90,99,109,113	0
14	PEE	C	145	21/51	0.84	0.23	45,74,88,92	0
11	JZR	C	142	18/18	0.93	0.15	38,48,61,63	0
6	3NP	A	1002	6/8	0.98	0.19	38,39,44,47	0

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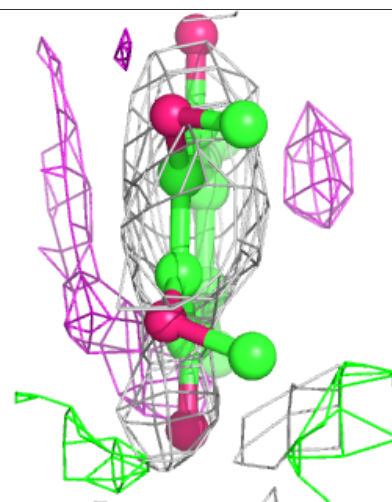
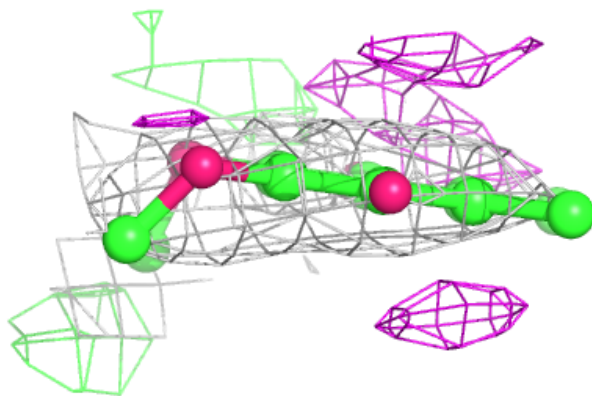
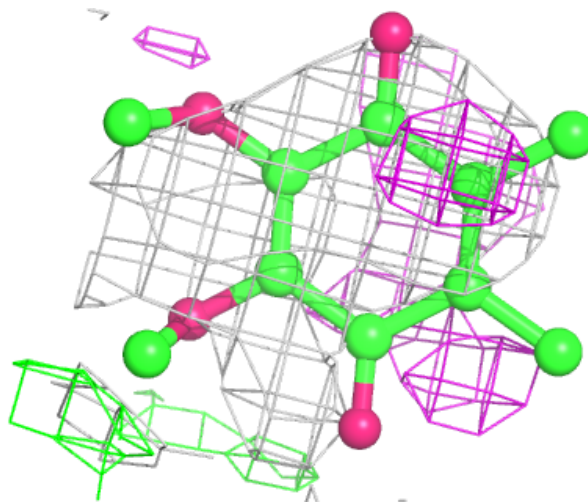
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	FAD	A	1001	53/53	0.98	0.23	18,32,43,52	0
12	HEM	C	143	41/43	0.98	0.10	29,41,65,67	0
7	FES	B	1002	4/4	0.99	0.15	30,32,34,37	0
8	SF4	B	1003	8/8	0.99	0.14	32,34,38,38	0
9	F3S	B	1004	7/7	0.99	0.11	26,27,28,30	0

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.



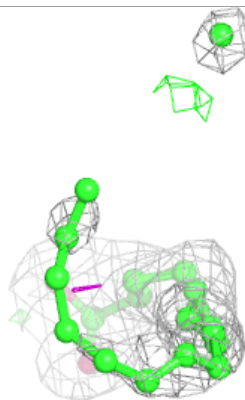
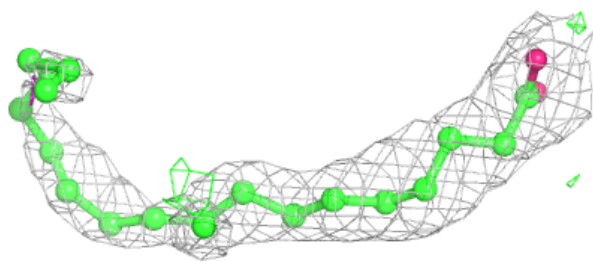
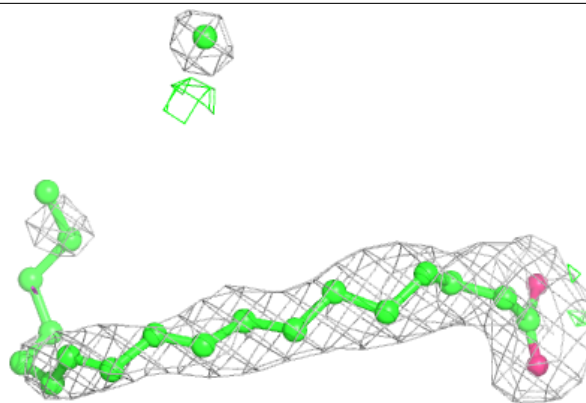
**Electron density around UQ C 144:**

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

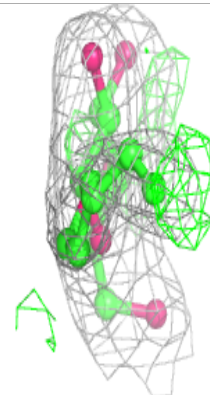
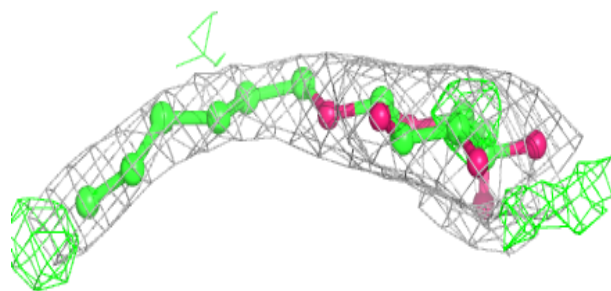
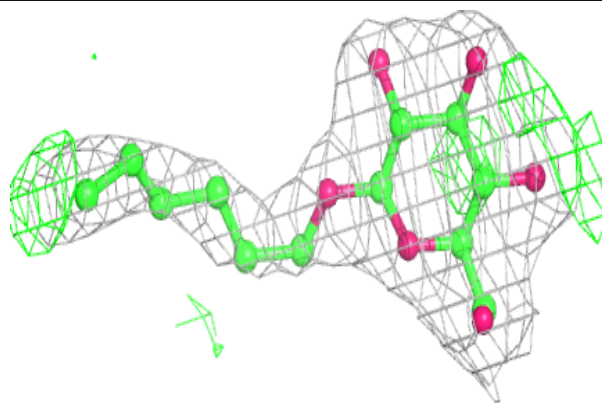


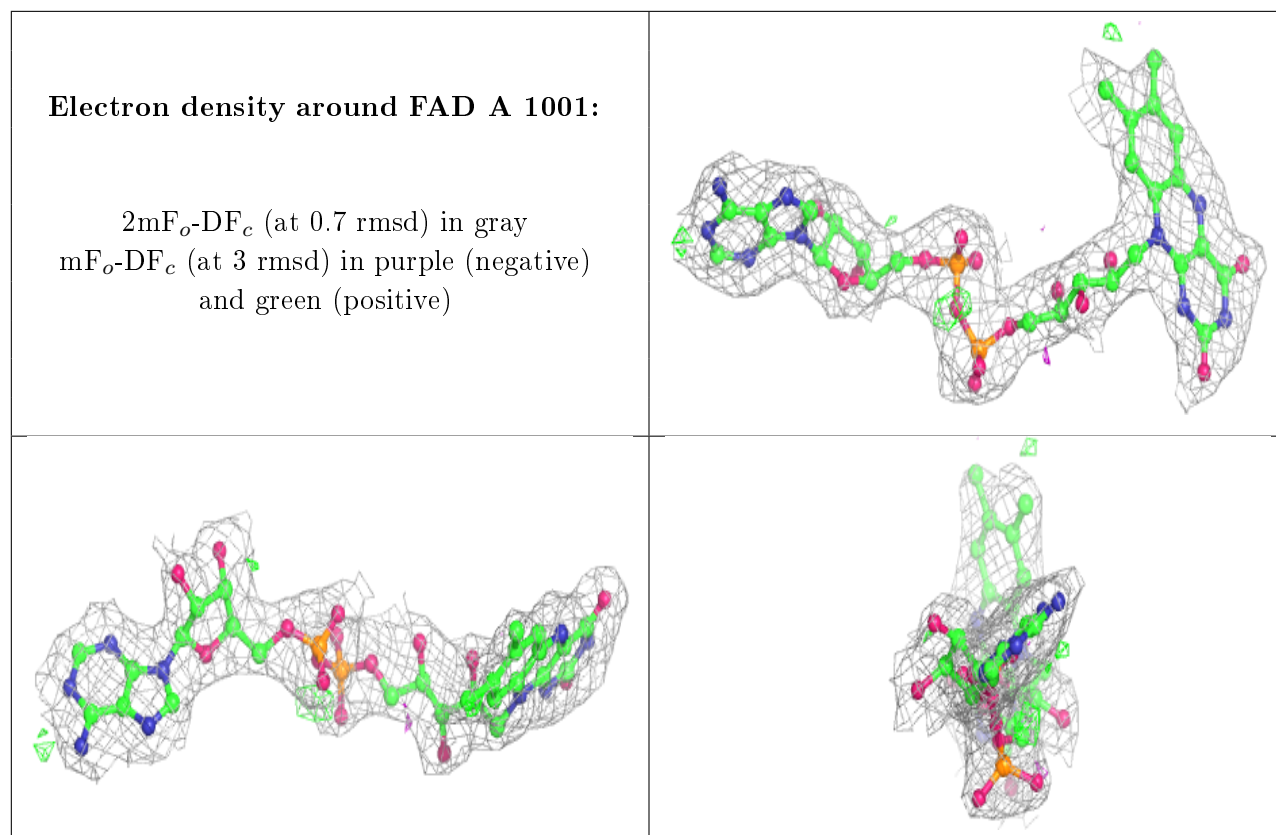
**Electron density around PEE C 145:**

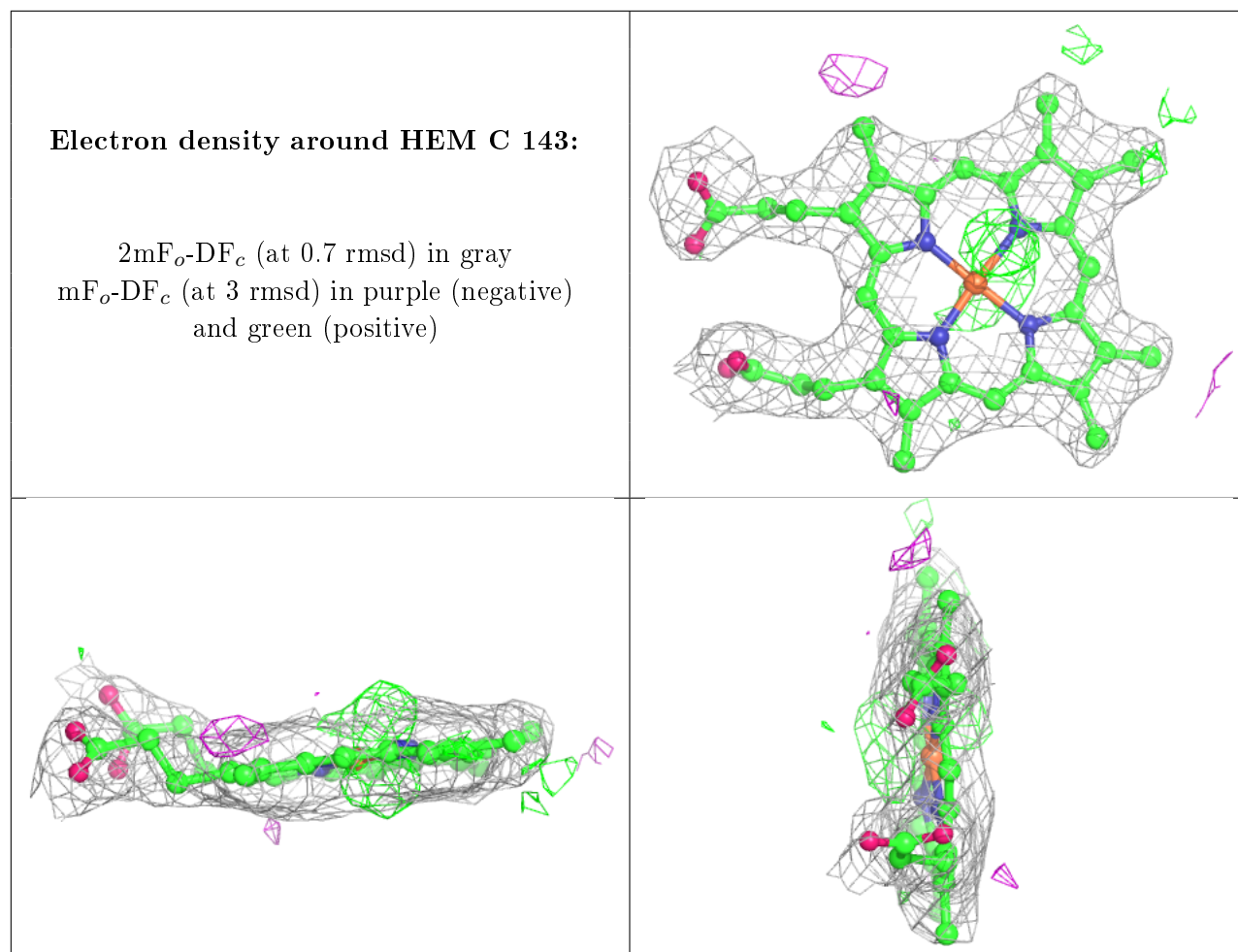
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.