Full wwPDB EM Validation Report

Jun 26, 2022 – 07:16 am BST

PDB ID	:	7QH2
EMDB ID	:	EMD-13960
Title	:	Cryo-EM structure of Ldh-EtfAB complex from Acetobacterium woodii
Authors	:	Kayastha, K.; Ermler, U.
Deposited on	:	2021-12-10
Resolution	:	2.43 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

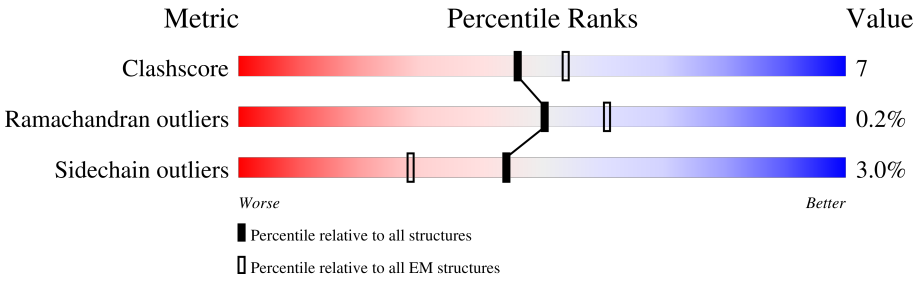
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.43 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	418	69% 12% 19%
1	D	418	71% 9% 19%
2	B	265	82% 15%
2	E	265	81% 14% 5%
3	C	467	90% 10%
3	F	467	91% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16808 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Lactate dehydrogenase (NAD(+),ferredoxin) subunit LctC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	337	Total	C	N	O	S	0	0
			2604	1666	435	488	15		
1	D	337	Total	C	N	O	S	0	0
			2604	1666	435	488	15		

- Molecule 2 is a protein called Lactate dehydrogenase (NAD(+),ferredoxin) subunit LctB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	265	Total	C	N	O	S	0	0
			2041	1295	330	403	13		
2	E	265	Total	C	N	O	S	0	0
			2041	1295	330	403	13		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP H6LBB0
B	2	SER	-	expression tag	UNP H6LBB0
E	1	MET	-	initiating methionine	UNP H6LBB0
E	2	SER	-	expression tag	UNP H6LBB0

- Molecule 3 is a protein called Lactate dehydrogenase (NAD(+),ferredoxin) subunit LctD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	467	Total	C	N	O	S	1	0
			3603	2299	587	696	21		
3	F	467	Total	C	N	O	S	0	0
			3593	2293	584	695	21		

There are 2 discrepancies between the modelled and reference sequences:

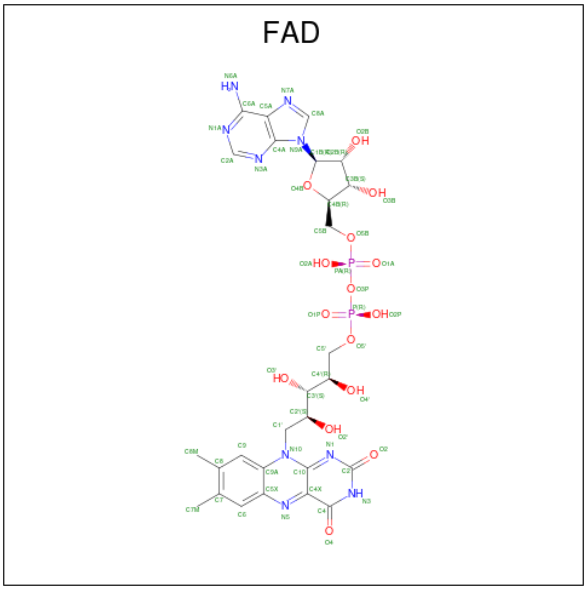
Chain	Residue	Modelled	Actual	Comment	Reference
C	467	ALA	-	expression tag	UNP H6LBS1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	467	ALA	-	expression tag	UNP H6LBS1

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	B	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	C	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	D	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	E	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	F	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Fe	0
			1	1	
5	F	1	Total	Fe	0
			1	1	

- Molecule 6 is water.

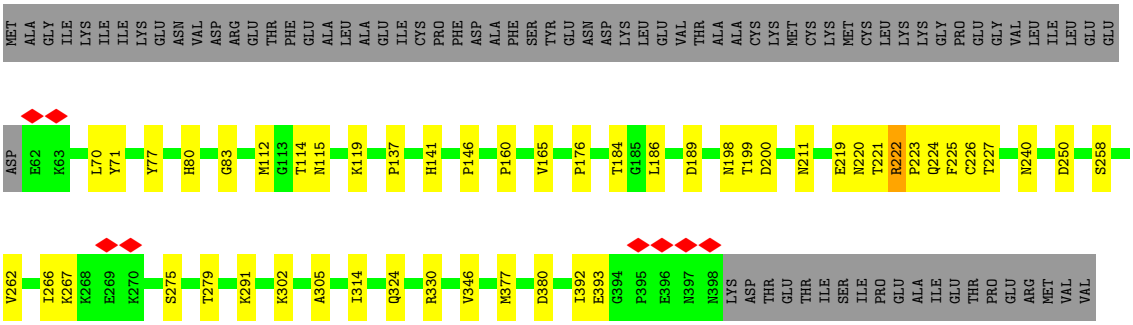
Mol	Chain	Residues	Atoms	AltConf
6	C	1	Total O 1 1	0
6	F	1	Total O 1 1	0

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

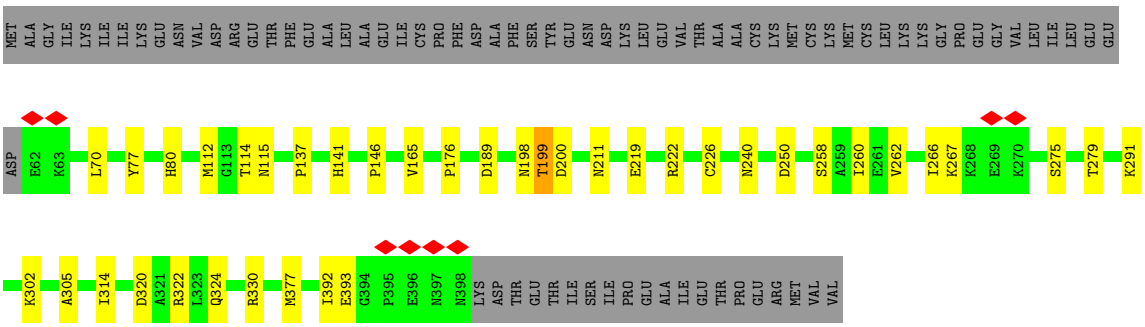
• Molecule 1: Lactate dehydrogenase (NAD(+),ferredoxin) subunit LctC

Chain A:



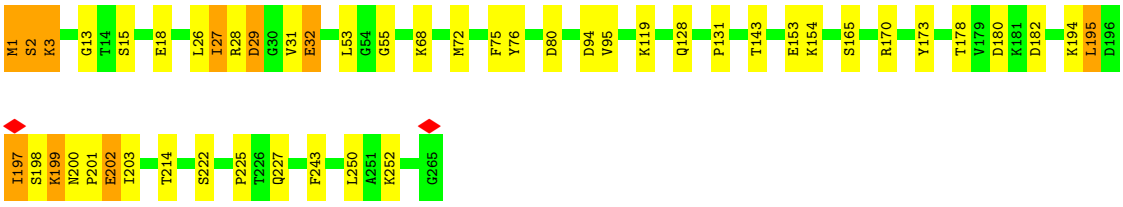
• Molecule 1: Lactate dehydrogenase (NAD(+),ferredoxin) subunit LctC

Chain D:



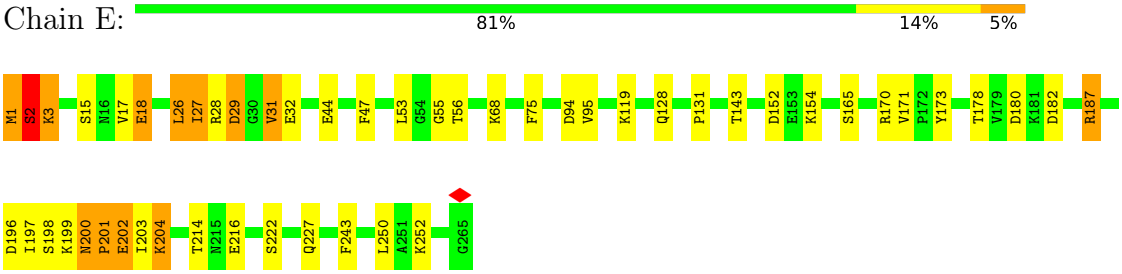
• Molecule 2: Lactate dehydrogenase (NAD(+),ferredoxin) subunit LctB

Chain B:



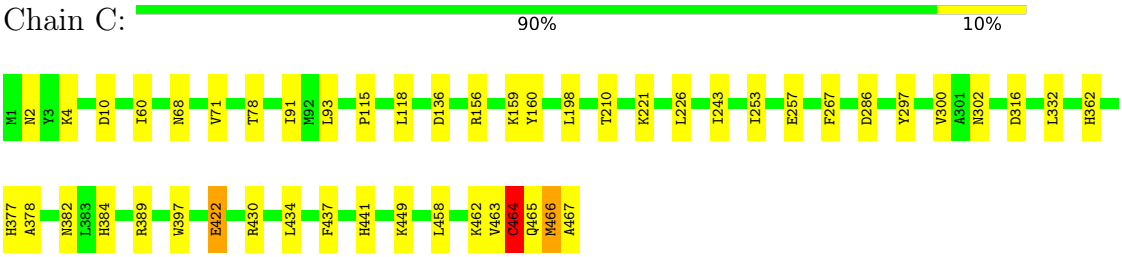
• Molecule 2: Lactate dehydrogenase (NAD(+),ferredoxin) subunit LctB

Chain E:



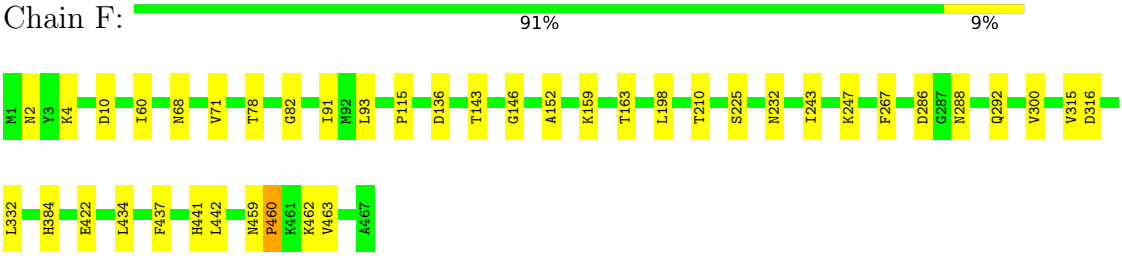
• Molecule 3: Lactate dehydrogenase (NAD(+),ferredoxin) subunit LctD

Chain C:



• Molecule 3: Lactate dehydrogenase (NAD(+),ferredoxin) subunit LctD

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	674283	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	106.17	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.136	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0102	Depositor
Map size (Å)	267.84, 267.84, 267.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 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	0.28	0/2650	0.51	1/3589 (0.0%)
1	D	0.28	0/2650	0.52	1/3589 (0.0%)
2	B	0.34	0/2072	0.55	0/2795
2	E	0.46	2/2072 (0.1%)	0.61	1/2795 (0.0%)
3	C	0.32	0/3666	0.54	2/4961 (0.0%)
3	F	0.38	2/3655 (0.1%)	0.51	1/4946 (0.0%)
All	All	0.34	4/16765 (0.0%)	0.54	6/22675 (0.0%)

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
2	E	0	2
3	C	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	PRO	N-CA	13.58	1.70	1.47
3	F	460	PRO	N-CA	12.09	1.67	1.47
2	E	200	ASN	C-N	5.99	1.45	1.34
3	F	459	ASN	C-N	5.09	1.44	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	464	CYS	O-C-N	-10.79	105.44	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	201	PRO	CA-N-CD	-9.71	97.90	111.50
3	F	460	PRO	CA-N-CD	-5.97	103.15	111.50
3	C	422	GLU	O-C-N	5.46	131.43	122.70
1	D	189	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	189	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	464	CYS	Mainchain
2	E	197	ILE	Peptide
2	E	198	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2604	0	2662	41	0
1	D	2604	0	2662	21	0
2	B	2041	0	2091	57	0
2	E	2041	0	2091	49	0
3	C	3603	0	3639	34	0
3	F	3593	0	3633	28	0
4	A	53	0	31	2	0
4	B	53	0	31	1	0
4	C	53	0	31	6	0
4	D	53	0	31	2	0
4	E	53	0	31	1	0
4	F	53	0	31	7	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
All	All	16808	0	16964	223	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 7.

All (223) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:460:PRO:N	3:F:460:PRO:CA	1.67	1.48
2:E:201:PRO:N	2:E:201:PRO:CA	1.70	1.31
1:A:71:TYR:HB2	1:A:222:ARG:HD2	1.16	1.09
2:E:27:ILE:O	2:E:27:ILE:HG23	1.51	1.09
1:A:71:TYR:CB	1:A:222:ARG:HD2	1.84	1.06
2:B:27:ILE:CG2	2:B:27:ILE:O	2.00	1.03
2:B:27:ILE:O	2:B:27:ILE:HG23	1.59	1.03
2:B:68:LYS:HG2	2:B:203:ILE:HD13	1.39	1.03
2:E:27:ILE:O	2:E:27:ILE:CG2	2.06	1.02
2:B:72:MET:HE3	2:B:199:LYS:HG2	1.39	1.01
3:F:78:THR:HB	4:F:501:FAD:O2P	1.60	1.01
3:C:78:THR:HB	4:C:501:FAD:O2P	1.68	0.94
2:E:18:GLU:O	2:E:27:ILE:HG22	1.71	0.91
2:E:2:SER:HA	2:E:55:GLY:HA3	1.51	0.91
1:A:222:ARG:HB2	1:A:222:ARG:CZ	2.01	0.90
3:C:384:HIS:HE1	3:C:422:GLU:OE1	1.55	0.89
2:E:68:LYS:HG2	2:E:203:ILE:HD13	1.55	0.88
2:B:26:LEU:HD12	2:B:26:LEU:H	1.39	0.87
3:C:464:CYS:O	3:C:465:GLN:HG2	1.72	0.87
3:C:466:MET:O	3:C:467:ALA:O	1.93	0.87
1:A:71:TYR:CD2	1:A:222:ARG:HG2	2.10	0.86
2:E:18:GLU:O	2:E:27:ILE:CG2	2.25	0.85
2:B:72:MET:CE	2:B:199:LYS:HG2	2.07	0.85
2:E:17:VAL:HG11	2:E:26:LEU:HD23	1.58	0.84
2:B:75:PHE:CD2	2:B:199:LYS:HG3	2.14	0.82
2:B:199:LYS:CE	2:B:199:LYS:HA	2.08	0.82
2:B:199:LYS:HA	2:B:199:LYS:HE3	1.63	0.80
1:A:71:TYR:HB2	1:A:222:ARG:CD	2.07	0.79
2:B:68:LYS:CG	2:B:203:ILE:HD13	2.11	0.79
2:B:202:GLU:HA	2:B:202:GLU:OE1	1.82	0.78
3:F:384:HIS:HE1	3:F:422:GLU:OE1	1.67	0.77
1:A:71:TYR:CB	1:A:222:ARG:CD	2.64	0.76
4:F:501:FAD:N1	4:F:501:FAD:H2'	2.02	0.75
2:B:27:ILE:O	2:B:27:ILE:HG22	1.86	0.74
2:B:26:LEU:HD12	2:B:26:LEU:N	2.02	0.74
4:C:501:FAD:H2'	4:C:501:FAD:N1	2.02	0.73
1:A:71:TYR:CG	1:A:222:ARG:HG2	2.24	0.72
2:B:1:MET:HB2	2:B:173:TYR:CE2	2.24	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:18:GLU:O	2:E:27:ILE:CB	2.37	0.71
2:E:18:GLU:O	2:E:27:ILE:HB	1.91	0.71
2:B:1:MET:HG3	2:B:153:GLU:HA	1.73	0.70
2:B:75:PHE:HD2	2:B:199:LYS:HG3	1.56	0.70
2:B:194:LYS:O	2:B:194:LYS:HG2	1.93	0.69
2:B:26:LEU:H	2:B:26:LEU:CD1	2.05	0.69
2:E:29:ASP:OD1	2:E:29:ASP:N	2.27	0.68
2:E:200:ASN:N	2:E:201:PRO:HD2	2.08	0.68
1:A:221:THR:OG1	2:B:225:PRO:HB3	1.94	0.67
2:B:199:LYS:HE3	2:B:199:LYS:CA	2.24	0.66
1:A:222:ARG:HB2	1:A:222:ARG:NH1	2.10	0.66
2:E:17:VAL:CG1	2:E:26:LEU:HD23	2.24	0.66
2:E:68:LYS:CG	2:E:203:ILE:HD13	2.26	0.66
2:E:75:PHE:HB3	2:E:199:LYS:HG2	1.78	0.66
2:E:2:SER:CA	2:E:55:GLY:HA3	2.25	0.65
2:B:29:ASP:OD1	2:B:29:ASP:N	2.30	0.64
2:E:44:GLU:OE1	2:E:187:ARG:HD2	1.98	0.64
2:E:95:VAL:HG11	2:E:128:GLN:HG3	1.79	0.64
2:B:95:VAL:HG11	2:B:128:GLN:HG3	1.79	0.64
1:A:222:ARG:HH12	1:A:224:GLN:HG3	1.63	0.63
2:E:2:SER:HA	2:E:55:GLY:CA	2.26	0.62
1:A:71:TYR:CG	1:A:222:ARG:HD2	2.34	0.62
3:F:460:PRO:N	3:F:460:PRO:C	2.52	0.62
2:B:1:MET:CB	2:B:173:TYR:CE2	2.82	0.61
2:B:80:ASP:O	2:B:201:PRO:HG3	2.01	0.61
2:B:31:VAL:HG12	2:B:31:VAL:O	2.02	0.60
3:C:332:LEU:HD23	4:C:501:FAD:HM72	1.84	0.60
2:E:2:SER:O	2:E:56:THR:N	2.33	0.60
2:E:18:GLU:OE1	2:E:27:ILE:HG21	2.02	0.60
2:E:47:PHE:CD2	2:E:187:ARG:HD3	2.37	0.60
2:B:1:MET:HG2	2:B:53:LEU:HD13	1.83	0.59
1:D:176:PRO:HB2	2:E:131:PRO:HB2	1.83	0.59
2:E:31:VAL:O	2:E:31:VAL:HG22	2.00	0.59
1:A:176:PRO:HB2	2:B:131:PRO:HB2	1.82	0.59
2:B:154:LYS:O	2:B:170:ARG:NH1	2.35	0.59
3:C:389:ARG:HB2	3:C:397:TRP:CD2	2.38	0.59
3:F:288:ASN:H	3:F:292:GLN:HE21	1.50	0.59
3:C:464:CYS:O	3:C:464:CYS:SG	2.61	0.59
3:F:332:LEU:HD23	4:F:501:FAD:HM72	1.85	0.58
1:D:199:THR:O	1:D:222:ARG:NH2	2.38	0.57
2:B:76:TYR:CD1	2:B:194:LYS:HB2	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:THR:HA	1:A:221:THR:HG21	1.88	0.56
2:B:1:MET:HA	2:B:53:LEU:HD13	1.86	0.56
3:F:78:THR:CB	4:F:501:FAD:O2P	2.47	0.56
3:C:430:ARG:HB3	3:C:467:ALA:HA	1.86	0.56
3:F:332:LEU:CD2	4:F:501:FAD:HM72	2.36	0.55
3:C:221:LYS:HE2	3:F:247:LYS:HE2	1.88	0.55
1:A:71:TYR:CG	1:A:222:ARG:CG	2.90	0.55
2:B:1:MET:CG	2:B:53:LEU:HD13	2.36	0.54
3:C:332:LEU:CD2	4:C:501:FAD:HM72	2.37	0.54
2:B:72:MET:HE1	2:B:199:LYS:HB2	1.88	0.54
1:A:314:ILE:HG13	1:A:324:GLN:HE21	1.72	0.53
1:D:314:ILE:HG13	1:D:324:GLN:HE21	1.72	0.53
1:A:211:ASN:ND2	2:B:15:SER:O	2.42	0.53
2:B:80:ASP:O	2:B:201:PRO:HB3	2.09	0.53
3:C:60:ILE:HG21	3:C:93:LEU:HD21	1.90	0.53
3:F:136:ASP:N	3:F:136:ASP:OD1	2.42	0.53
1:D:377:MET:HG2	2:E:243:PHE:HB2	1.92	0.52
2:E:204:LYS:HG2	2:E:204:LYS:O	2.08	0.52
3:F:60:ILE:HG21	3:F:93:LEU:HD21	1.90	0.52
3:C:136:ASP:N	3:C:136:ASP:OD1	2.43	0.52
3:C:466:MET:O	3:C:467:ALA:C	2.48	0.52
1:A:114:THR:HG22	1:A:115:ASN:HD22	1.74	0.51
1:A:330:ARG:NH1	3:C:267:PHE:O	2.36	0.51
1:A:219:GLU:OE2	2:B:227:GLN:NE2	2.42	0.51
2:E:199:LYS:HG3	2:E:201:PRO:HD2	1.93	0.51
1:D:114:THR:HG22	1:D:115:ASN:HD22	1.74	0.51
2:B:119:LYS:HB2	2:B:180:ASP:HA	1.93	0.51
3:C:4:LYS:NZ	3:C:10:ASP:OD2	2.41	0.51
2:E:143:THR:HA	2:E:178:THR:HB	1.93	0.51
2:B:2:SER:HA	2:B:55:GLY:HA3	1.92	0.50
2:B:143:THR:HA	2:B:178:THR:HB	1.93	0.50
1:A:114:THR:HG23	1:A:137:PRO:HA	1.93	0.50
2:E:18:GLU:H	2:E:27:ILE:HG22	1.77	0.50
1:A:222:ARG:NH1	1:A:222:ARG:CB	2.74	0.50
3:F:4:LYS:NZ	3:F:10:ASP:OD2	2.42	0.50
3:C:226:LEU:HD11	3:C:297:TYR:HB2	1.94	0.50
3:F:71:VAL:HG22	3:F:91:ILE:HB	1.94	0.50
3:C:115:PRO:HG3	3:C:210:THR:HA	1.93	0.50
2:E:119:LYS:HB2	2:E:180:ASP:HA	1.93	0.50
1:D:330:ARG:NH1	3:F:267:PHE:O	2.39	0.50
3:C:434:LEU:HB2	3:C:467:ALA:HB1	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:501:FAD:O4'	4:A:501:FAD:O2'	2.26	0.50
3:C:316:ASP:OD1	3:C:316:ASP:N	2.45	0.50
3:F:2:ASN:OD1	3:F:68:ASN:ND2	2.38	0.50
1:D:114:THR:HG23	1:D:137:PRO:HA	1.93	0.49
3:C:449:LYS:NZ	3:C:458:LEU:O	2.46	0.49
1:A:160:PRO:O	1:A:223:PRO:HB3	2.13	0.49
3:C:389:ARG:HB2	3:C:397:TRP:CE3	2.48	0.49
1:D:211:ASN:ND2	2:E:15:SER:O	2.46	0.49
1:A:250:ASP:OD1	1:A:250:ASP:N	2.47	0.48
2:B:13:GLY:HA3	2:B:32:GLU:O	2.13	0.48
3:C:2:ASN:O	3:C:68:ASN:ND2	2.47	0.48
2:E:202:GLU:OE1	2:E:202:GLU:HA	2.12	0.48
1:A:184:THR:HA	1:A:221:THR:CG2	2.43	0.48
2:E:27:ILE:O	2:E:27:ILE:HG22	2.06	0.48
3:F:434:LEU:HD13	3:F:442:LEU:HD22	1.95	0.48
2:B:200:ASN:HB2	2:B:201:PRO:HD3	1.96	0.48
4:D:501:FAD:O4'	4:D:501:FAD:O2'	2.27	0.47
1:A:240:ASN:OD1	1:A:240:ASN:N	2.46	0.47
1:D:322:ARG:NH1	1:D:322:ARG:HG3	2.29	0.47
2:E:94:ASP:HA	4:E:301:FAD:H1'2	1.96	0.47
3:F:115:PRO:HG3	3:F:210:THR:HA	1.94	0.47
1:A:186:LEU:HA	1:A:225:PHE:O	2.15	0.47
1:A:377:MET:HG2	2:B:243:PHE:HB2	1.96	0.47
1:D:250:ASP:N	1:D:250:ASP:OD1	2.47	0.47
2:E:17:VAL:HG11	2:E:26:LEU:CD2	2.37	0.47
3:C:159:LYS:NZ	3:C:286:ASP:OD1	2.46	0.47
3:F:152:ALA:O	3:F:163:THR:OG1	2.30	0.47
1:A:198:ASN:ND2	1:A:200:ASP:OD2	2.48	0.47
2:E:154:LYS:O	2:E:170:ARG:NH1	2.48	0.47
3:F:159:LYS:NZ	3:F:286:ASP:OD1	2.48	0.47
1:D:320:ASP:OD2	1:D:322:ARG:NH1	2.49	0.46
1:A:80:HIS:NE2	1:A:112:MET:O	2.36	0.46
1:A:222:ARG:HH11	1:A:223:PRO:HA	1.80	0.46
2:B:94:ASP:HA	4:B:301:FAD:H1'2	1.96	0.46
3:C:71:VAL:HG22	3:C:91:ILE:HB	1.98	0.46
1:D:279:THR:HG23	1:D:305:ALA:HA	1.98	0.46
2:B:1:MET:HB2	2:B:173:TYR:CZ	2.49	0.46
1:A:279:THR:HG23	1:A:305:ALA:HA	1.97	0.46
4:D:501:FAD:HO2'	4:D:501:FAD:HO4'	1.64	0.46
3:F:2:ASN:O	3:F:68:ASN:ND2	2.49	0.45
2:B:2:SER:HB3	2:B:3:LYS:H	1.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:TYR:HB3	1:D:165:VAL:HG12	1.99	0.45
2:E:152:ASP:HB3	2:E:170:ARG:HH12	1.81	0.45
4:F:501:FAD:H9	4:F:501:FAD:H1'2	1.78	0.45
2:E:196:ASP:OD2	2:E:199:LYS:NZ	2.47	0.45
2:E:47:PHE:HD2	2:E:187:ARG:HD3	1.79	0.45
2:B:76:TYR:CE1	2:B:194:LYS:HB2	2.51	0.45
2:B:195:LEU:HD11	3:C:302:ASN:OD1	2.17	0.45
1:A:77:TYR:HB3	1:A:165:VAL:HG12	1.99	0.45
3:C:198:LEU:HD11	3:F:198:LEU:HD11	1.99	0.45
4:C:501:FAD:N1	4:C:501:FAD:C2'	2.72	0.45
4:C:501:FAD:H9	4:C:501:FAD:H1'2	1.78	0.44
1:D:198:ASN:ND2	1:D:200:ASP:OD2	2.48	0.44
2:B:18:GLU:O	2:B:27:ILE:HB	2.17	0.44
1:A:83:GLY:O	1:A:119:LYS:NZ	2.39	0.44
1:A:146:PRO:HD3	1:A:258:SER:HB2	2.00	0.44
2:B:72:MET:CE	2:B:199:LYS:HB2	2.48	0.44
4:F:501:FAD:O4'	4:F:501:FAD:O2'	2.30	0.44
1:D:219:GLU:OE2	2:E:227:GLN:NE2	2.49	0.44
3:C:377:HIS:HD2	3:C:382:ASN:HB3	1.83	0.44
2:B:1:MET:CB	2:B:53:LEU:HD13	2.48	0.44
2:B:243:PHE:HB3	2:B:250:LEU:HD22	2.00	0.44
2:B:199:LYS:HE3	2:B:200:ASN:N	2.32	0.43
2:B:1:MET:HA	2:B:53:LEU:CD1	2.48	0.43
1:A:119:LYS:HB3	1:A:119:LYS:HE2	1.83	0.43
2:B:72:MET:CE	2:B:199:LYS:CG	2.90	0.43
2:B:80:ASP:O	2:B:201:PRO:CB	2.66	0.43
1:A:71:TYR:CG	1:A:222:ARG:CD	3.00	0.43
1:D:240:ASN:OD1	1:D:240:ASN:N	2.46	0.43
1:A:346:VAL:HG11	3:C:118:LEU:HD21	2.01	0.43
3:C:437:PHE:HB3	3:C:441:HIS:HB3	1.99	0.43
2:E:27:ILE:HD13	2:E:27:ILE:HA	1.70	0.43
3:F:143:THR:HG22	3:F:146:GLY:H	1.82	0.43
2:E:1:MET:HB2	2:E:173:TYR:CE2	2.54	0.43
3:F:82:GLY:O	3:F:462:LYS:HE2	2.19	0.43
1:A:302:LYS:HG3	1:A:392:ILE:HD13	2.01	0.42
3:C:253:ILE:HG22	3:C:378:ALA:HB3	2.01	0.42
1:D:146:PRO:HD3	1:D:258:SER:HB2	2.00	0.42
1:D:302:LYS:HG3	1:D:392:ILE:HD13	2.01	0.42
2:E:1:MET:CB	2:E:173:TYR:CE2	3.02	0.42
2:E:2:SER:HB3	2:E:3:LYS:H	1.77	0.42
2:E:3:LYS:HE2	2:E:3:LYS:HB3	1.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:CA	2:B:53:LEU:HD13	2.48	0.42
3:F:316:ASP:OD1	3:F:316:ASP:N	2.49	0.42
2:E:243:PHE:HB3	2:E:250:LEU:HD22	2.00	0.42
1:D:80:HIS:NE2	1:D:112:MET:O	2.36	0.42
3:F:437:PHE:HB3	3:F:441:HIS:HB3	2.02	0.42
1:A:186:LEU:HD11	1:A:227:THR:HG23	2.02	0.41
2:B:3:LYS:HE2	2:B:3:LYS:HB3	1.57	0.41
2:E:44:GLU:OE1	2:E:187:ARG:CD	2.66	0.41
3:C:257:GLU:OE1	3:C:362:HIS:NE2	2.42	0.41
3:F:225:SER:HB2	3:F:315:VAL:HB	2.03	0.41
2:B:199:LYS:HE3	2:B:200:ASN:H	1.84	0.41
3:C:156:ARG:HB3	3:C:160:TYR:HD2	1.86	0.41
1:A:380:ASP:OD1	4:A:501:FAD:N6A	2.53	0.41
3:F:232:ASN:N	3:F:232:ASN:OD1	2.54	0.41
3:F:243:ILE:HG12	3:F:300:VAL:HG13	2.03	0.41
3:C:464:CYS:O	3:C:465:GLN:CG	2.57	0.41
1:A:141:HIS:HB2	1:A:262:VAL:HG21	2.03	0.41
1:D:260:ILE:HG12	2:E:171:VAL:HG23	2.03	0.40
1:D:141:HIS:HB2	1:D:262:VAL:HG21	2.03	0.40
2:E:1:MET:HA	2:E:53:LEU:HD13	2.03	0.40
3:C:243:ILE:HG12	3:C:300:VAL:HG13	2.03	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 PDB entries followed by that with respect to all EM entries.

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	335/418 (80%)	327 (98%)	8 (2%)	0	100	100
1	D	335/418 (80%)	328 (98%)	7 (2%)	0	100	100
2	B	263/265 (99%)	245 (93%)	16 (6%)	2 (1%)	19	22
2	E	263/265 (99%)	242 (92%)	20 (8%)	1 (0%)	34	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	466/467 (100%)	456 (98%)	9 (2%)	1 (0%)	47 57
3	F	465/467 (100%)	453 (97%)	11 (2%)	1 (0%)	47 57
All	All	2127/2300 (92%)	2051 (96%)	71 (3%)	5 (0%)	50 57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	197	ILE
2	B	198	SER
3	C	463	VAL
3	F	463	VAL
2	E	2	SER

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 PDB entries followed by that with respect to all EM entries.

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	280/351 (80%)	270 (96%)	10 (4%)	35 46
1	D	280/351 (80%)	272 (97%)	8 (3%)	42 54
2	B	230/230 (100%)	214 (93%)	16 (7%)	15 18
2	E	230/230 (100%)	211 (92%)	19 (8%)	11 12
3	C	393/392 (100%)	391 (100%)	2 (0%)	88 93
3	F	392/392 (100%)	392 (100%)	0	100 100
All	All	1805/1946 (93%)	1750 (97%)	55 (3%)	44 53

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	199	THR
1	A	220	ASN
1	A	222	ARG
1	A	226	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	266	ILE
1	A	267	LYS
1	A	275	SER
1	A	291	LYS
1	A	393	GLU
2	B	1	MET
2	B	2	SER
2	B	3	LYS
2	B	27	ILE
2	B	28	ARG
2	B	29	ASP
2	B	32	GLU
2	B	165	SER
2	B	182	ASP
2	B	195	LEU
2	B	197	ILE
2	B	199	LYS
2	B	202	GLU
2	B	214	THR
2	B	222	SER
2	B	252	LYS
3	C	462	LYS
3	C	466	MET
1	D	70	LEU
1	D	199	THR
1	D	226	CYS
1	D	266	ILE
1	D	267	LYS
1	D	275	SER
1	D	291	LYS
1	D	393	GLU
2	E	1	MET
2	E	2	SER
2	E	3	LYS
2	E	18	GLU
2	E	26	LEU
2	E	27	ILE
2	E	28	ARG
2	E	29	ASP
2	E	31	VAL
2	E	32	GLU
2	E	165	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	182	ASP
2	E	187	ARG
2	E	202	GLU
2	E	204	LYS
2	E	214	THR
2	E	216	GLU
2	E	222	SER
2	E	252	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	324	GLN
1	A	354	ASN
1	A	397	ASN
2	B	16	ASN
2	B	159	GLN
2	B	200	ASN
1	D	115	ASN
1	D	324	GLN
1	D	354	ASN
1	D	397	ASN
2	E	16	ASN
2	E	66	GLN
2	E	159	GLN
3	F	292	GLN
3	F	382	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	FAD	E	301	-	53,58,58	0.50	0	68,89,89	0.51	2 (2%)
4	FAD	F	501	-	53,58,58	1.94	20 (37%)	68,89,89	1.34	12 (17%)
4	FAD	A	501	-	53,58,58	0.48	0	68,89,89	0.52	2 (2%)
4	FAD	C	501	-	53,58,58	1.94	20 (37%)	68,89,89	1.34	12 (17%)
4	FAD	B	301	-	53,58,58	0.50	0	68,89,89	0.51	2 (2%)
4	FAD	D	501	-	53,58,58	0.48	0	68,89,89	0.52	2 (2%)

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
4	FAD	E	301	-	-	18/30/50/50	0/6/6/6
4	FAD	F	501	-	-	10/30/50/50	0/6/6/6
4	FAD	A	501	-	-	17/30/50/50	0/6/6/6
4	FAD	C	501	-	-	10/30/50/50	0/6/6/6
4	FAD	B	301	-	-	18/30/50/50	0/6/6/6
4	FAD	D	501	-	-	17/30/50/50	0/6/6/6

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	FAD	C2-N3	-5.43	1.26	1.39
4	F	501	FAD	C2-N3	-5.39	1.26	1.39
4	F	501	FAD	O2-C2	-4.76	1.15	1.24
4	C	501	FAD	O2-C2	-4.71	1.15	1.24
4	F	501	FAD	C1'-C2'	-3.56	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	FAD	C1'-C2'	-3.52	1.47	1.52
4	C	501	FAD	C9-C8	-3.48	1.34	1.39
4	F	501	FAD	C9-C8	-3.48	1.34	1.39
4	F	501	FAD	C2-N1	-3.31	1.28	1.36
4	C	501	FAD	C2-N1	-3.28	1.28	1.36
4	F	501	FAD	O2'-C2'	-2.88	1.37	1.43
4	C	501	FAD	O2'-C2'	-2.85	1.37	1.43
4	C	501	FAD	C8A-N7A	-2.60	1.30	1.34
4	F	501	FAD	C8A-N7A	-2.59	1.30	1.34
4	C	501	FAD	C4X-C4	-2.41	1.35	1.44
4	F	501	FAD	C4X-C4	-2.41	1.35	1.44
4	C	501	FAD	C4-N3	-2.36	1.34	1.38
4	F	501	FAD	C4-N3	-2.36	1.34	1.38
4	F	501	FAD	PA-O2A	-2.35	1.44	1.55
4	C	501	FAD	PA-O2A	-2.35	1.44	1.55
4	C	501	FAD	O3'-C3'	-2.24	1.37	1.43
4	F	501	FAD	O3'-C3'	-2.24	1.37	1.43
4	F	501	FAD	P-O2P	-2.19	1.45	1.55
4	C	501	FAD	P-O2P	-2.19	1.45	1.55
4	C	501	FAD	C5A-C4A	-2.15	1.35	1.40
4	F	501	FAD	C5A-C4A	-2.15	1.35	1.40
4	C	501	FAD	C2B-C1B	-2.13	1.50	1.53
4	C	501	FAD	O4-C4	-2.12	1.19	1.23
4	F	501	FAD	O4-C4	-2.12	1.19	1.23
4	F	501	FAD	C2B-C1B	-2.11	1.50	1.53
4	C	501	FAD	C2'-C3'	-2.09	1.49	1.53
4	C	501	FAD	P-O1P	-2.09	1.43	1.50
4	C	501	FAD	C4A-N3A	-2.08	1.32	1.35
4	F	501	FAD	C4A-N3A	-2.08	1.32	1.35
4	F	501	FAD	P-O1P	-2.08	1.43	1.50
4	F	501	FAD	C2'-C3'	-2.06	1.49	1.53
4	C	501	FAD	PA-O1A	-2.05	1.43	1.50
4	F	501	FAD	PA-O1A	-2.05	1.43	1.50
4	C	501	FAD	C5X-N5	-2.00	1.35	1.39
4	F	501	FAD	C5X-N5	-2.00	1.35	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	501	FAD	O2'-C2'-C3'	-3.75	99.99	109.10
4	C	501	FAD	O2'-C2'-C3'	-3.73	100.04	109.10
4	C	501	FAD	P-O3P-PA	3.14	143.60	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	501	FAD	P-O3P-PA	3.14	143.59	132.83
4	C	501	FAD	C5A-C6A-N6A	2.94	124.82	120.35
4	F	501	FAD	C5A-C6A-N6A	2.93	124.81	120.35
4	C	501	FAD	N3-C2-N1	2.88	125.03	119.38
4	F	501	FAD	N3-C2-N1	2.86	125.00	119.38
4	F	501	FAD	C4-N3-C2	-2.56	120.91	125.64
4	C	501	FAD	C4-N3-C2	-2.56	120.91	125.64
4	C	501	FAD	O3B-C3B-C4B	-2.37	104.19	111.05
4	E	301	FAD	P-O3P-PA	-2.37	124.69	132.83
4	B	301	FAD	P-O3P-PA	-2.37	124.69	132.83
4	F	501	FAD	O3B-C3B-C4B	-2.36	104.23	111.05
4	C	501	FAD	O3'-C3'-C2'	-2.31	103.23	108.81
4	F	501	FAD	O3'-C3'-C2'	-2.30	103.24	108.81
4	E	301	FAD	C5A-C6A-N6A	2.30	123.85	120.35
4	A	501	FAD	C5A-C6A-N6A	2.29	123.83	120.35
4	B	301	FAD	C5A-C6A-N6A	2.28	123.82	120.35
4	D	501	FAD	C5A-C6A-N6A	2.27	123.80	120.35
4	F	501	FAD	O4B-C1B-C2B	-2.25	103.64	106.93
4	C	501	FAD	O4B-C1B-C2B	-2.22	103.68	106.93
4	C	501	FAD	C4X-C4-N3	2.17	118.70	113.19
4	F	501	FAD	C4X-C4-N3	2.17	118.70	113.19
4	A	501	FAD	P-O3P-PA	-2.11	125.57	132.83
4	C	501	FAD	O3B-C3B-C2B	-2.09	105.06	111.82
4	D	501	FAD	P-O3P-PA	-2.09	125.66	132.83
4	C	501	FAD	O3'-C3'-C4'	2.09	113.85	108.81
4	F	501	FAD	O3'-C3'-C4'	2.08	113.84	108.81
4	F	501	FAD	O3B-C3B-C2B	-2.07	105.13	111.82
4	C	501	FAD	O2P-P-O5'	-2.01	98.40	107.75
4	F	501	FAD	O2P-P-O5'	-2.00	98.44	107.75

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	FAD	C5B-O5B-PA-O1A
4	A	501	FAD	C3B-C4B-C5B-O5B
4	A	501	FAD	N10-C1'-C2'-O2'
4	A	501	FAD	N10-C1'-C2'-C3'
4	A	501	FAD	C1'-C2'-C3'-O3'
4	A	501	FAD	C1'-C2'-C3'-C4'
4	A	501	FAD	O2'-C2'-C3'-O3'
4	A	501	FAD	O2'-C2'-C3'-C4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	501	FAD	C5'-O5'-P-O1P
4	A	501	FAD	C5'-O5'-P-O2P
4	A	501	FAD	C5'-O5'-P-O3P
4	B	301	FAD	C5B-O5B-PA-O1A
4	B	301	FAD	C5B-O5B-PA-O2A
4	B	301	FAD	N10-C1'-C2'-O2'
4	B	301	FAD	N10-C1'-C2'-C3'
4	B	301	FAD	C1'-C2'-C3'-O3'
4	B	301	FAD	C1'-C2'-C3'-C4'
4	B	301	FAD	O2'-C2'-C3'-O3'
4	B	301	FAD	O2'-C2'-C3'-C4'
4	B	301	FAD	C5'-O5'-P-O1P
4	B	301	FAD	C5'-O5'-P-O2P
4	C	501	FAD	C2'-C1'-N10-C10
4	C	501	FAD	N10-C1'-C2'-O2'
4	C	501	FAD	N10-C1'-C2'-C3'
4	C	501	FAD	C2'-C3'-C4'-O4'
4	C	501	FAD	O3'-C3'-C4'-O4'
4	C	501	FAD	C3'-C4'-C5'-O5'
4	C	501	FAD	O4'-C4'-C5'-O5'
4	D	501	FAD	C5B-O5B-PA-O1A
4	D	501	FAD	C3B-C4B-C5B-O5B
4	D	501	FAD	N10-C1'-C2'-O2'
4	D	501	FAD	N10-C1'-C2'-C3'
4	D	501	FAD	C1'-C2'-C3'-O3'
4	D	501	FAD	C1'-C2'-C3'-C4'
4	D	501	FAD	O2'-C2'-C3'-O3'
4	D	501	FAD	O2'-C2'-C3'-C4'
4	D	501	FAD	C5'-O5'-P-O1P
4	D	501	FAD	C5'-O5'-P-O2P
4	D	501	FAD	C5'-O5'-P-O3P
4	E	301	FAD	C5B-O5B-PA-O1A
4	E	301	FAD	C5B-O5B-PA-O2A
4	E	301	FAD	N10-C1'-C2'-O2'
4	E	301	FAD	N10-C1'-C2'-C3'
4	E	301	FAD	C1'-C2'-C3'-O3'
4	E	301	FAD	C1'-C2'-C3'-C4'
4	E	301	FAD	O2'-C2'-C3'-O3'
4	E	301	FAD	O2'-C2'-C3'-C4'
4	E	301	FAD	C5'-O5'-P-O1P
4	E	301	FAD	C5'-O5'-P-O2P
4	F	501	FAD	C2'-C1'-N10-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	F	501	FAD	N10-C1'-C2'-O2'
4	F	501	FAD	N10-C1'-C2'-C3'
4	F	501	FAD	C2'-C3'-C4'-O4'
4	F	501	FAD	O3'-C3'-C4'-O4'
4	F	501	FAD	C3'-C4'-C5'-O5'
4	F	501	FAD	O4'-C4'-C5'-O5'
4	B	301	FAD	C2'-C3'-C4'-O4'
4	E	301	FAD	C2'-C3'-C4'-O4'
4	B	301	FAD	O3'-C3'-C4'-C5'
4	C	501	FAD	O3'-C3'-C4'-C5'
4	E	301	FAD	O3'-C3'-C4'-C5'
4	F	501	FAD	O3'-C3'-C4'-C5'
4	B	301	FAD	C2'-C3'-C4'-C5'
4	C	501	FAD	C2'-C3'-C4'-C5'
4	E	301	FAD	C2'-C3'-C4'-C5'
4	F	501	FAD	C2'-C3'-C4'-C5'
4	A	501	FAD	C2'-C3'-C4'-O4'
4	D	501	FAD	C2'-C3'-C4'-O4'
4	A	501	FAD	C2'-C3'-C4'-C5'
4	D	501	FAD	C2'-C3'-C4'-C5'
4	B	301	FAD	O3'-C3'-C4'-O4'
4	E	301	FAD	O3'-C3'-C4'-O4'
4	A	501	FAD	O4B-C4B-C5B-O5B
4	D	501	FAD	O4B-C4B-C5B-O5B
4	A	501	FAD	O3'-C3'-C4'-C5'
4	D	501	FAD	O3'-C3'-C4'-C5'
4	A	501	FAD	O3'-C3'-C4'-O4'
4	D	501	FAD	O3'-C3'-C4'-O4'
4	B	301	FAD	O4'-C4'-C5'-O5'
4	A	501	FAD	PA-O3P-P-O1P
4	D	501	FAD	PA-O3P-P-O1P
4	B	301	FAD	C3'-C4'-C5'-O5'
4	E	301	FAD	C3'-C4'-C5'-O5'
4	E	301	FAD	O4'-C4'-C5'-O5'
4	B	301	FAD	C5B-O5B-PA-O3P
4	B	301	FAD	C5'-O5'-P-O3P
4	E	301	FAD	C5B-O5B-PA-O3P
4	E	301	FAD	C5'-O5'-P-O3P
4	C	501	FAD	PA-O3P-P-O1P
4	F	501	FAD	PA-O3P-P-O1P

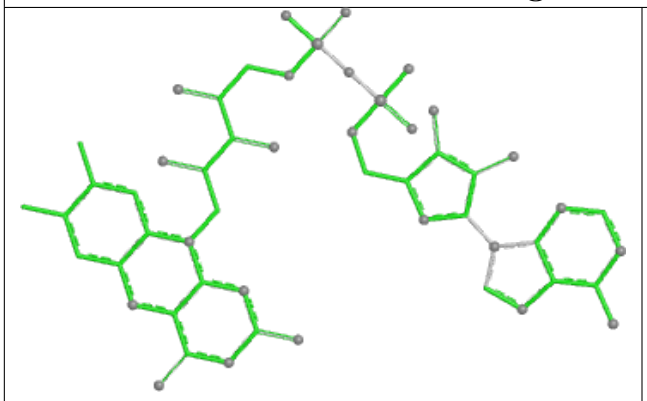
There are no ring outliers.

6 monomers are involved in 19 short contacts:

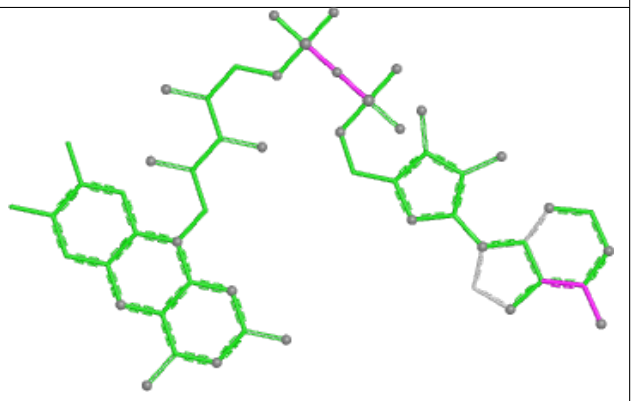
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	301	FAD	1	0
4	F	501	FAD	7	0
4	A	501	FAD	2	0
4	C	501	FAD	6	0
4	B	301	FAD	1	0
4	D	501	FAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

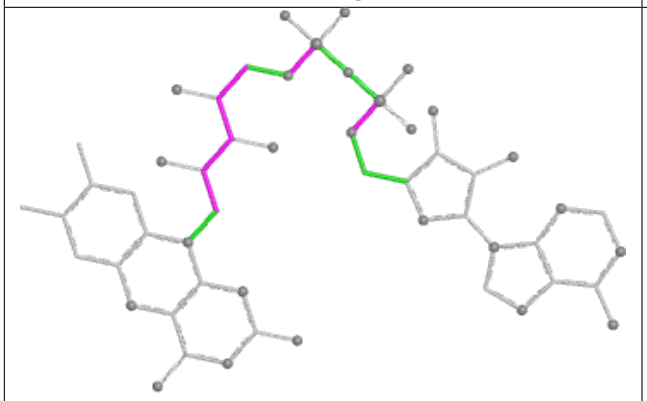
Ligand FAD E 301



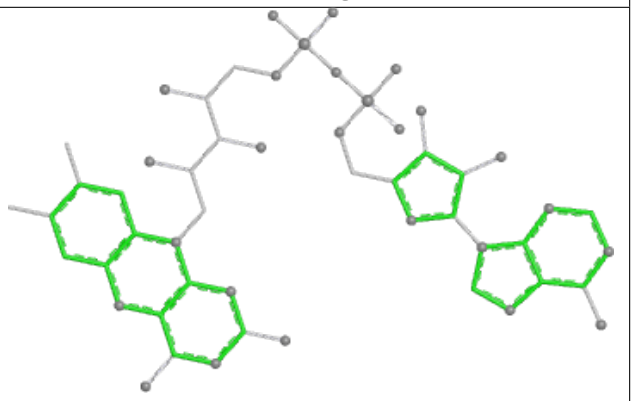
Bond lengths



Bond angles

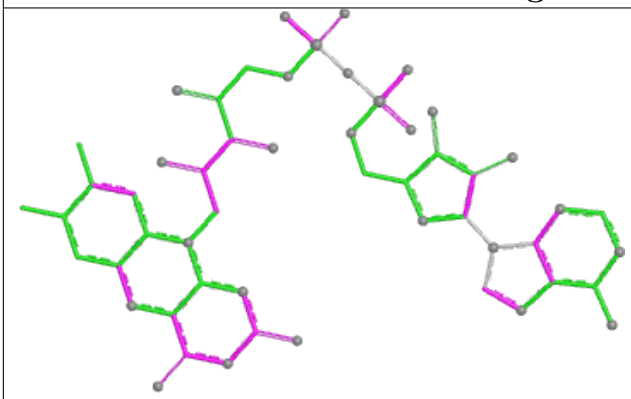


Torsions

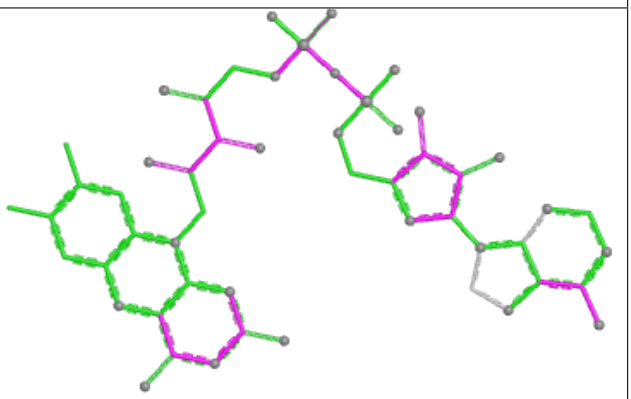


Rings

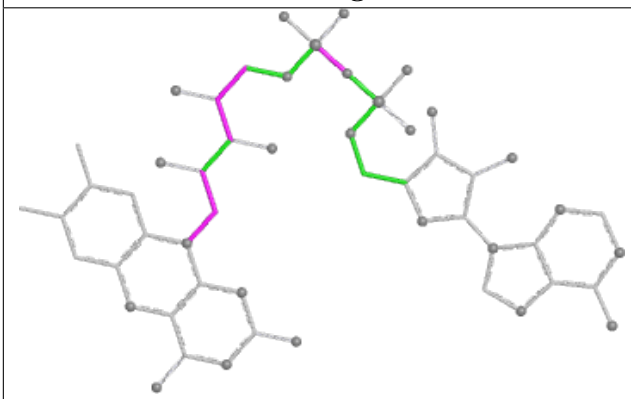
Ligand FAD F 501



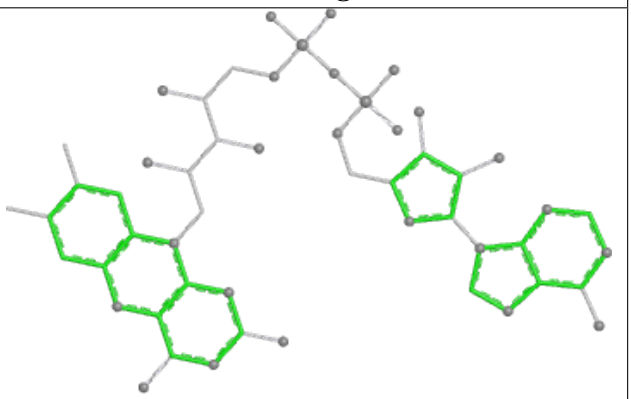
Bond lengths



Bond angles

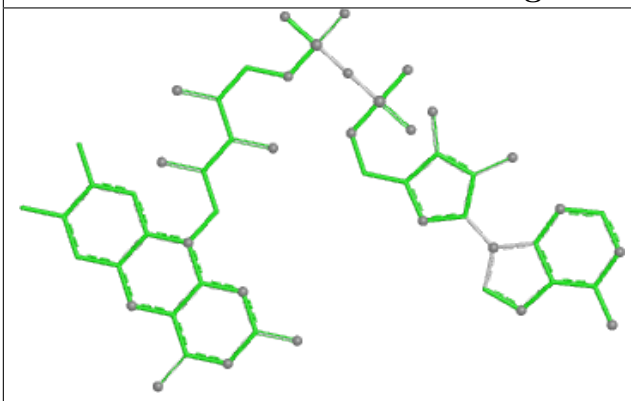


Torsions

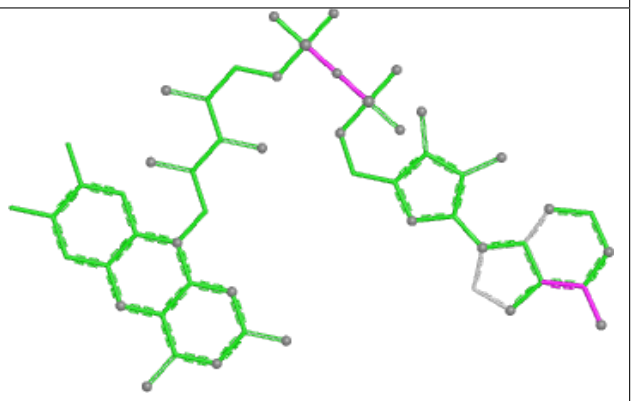


Rings

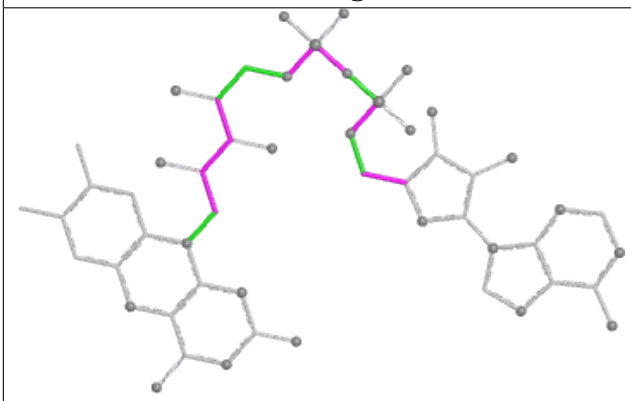
Ligand FAD A 501



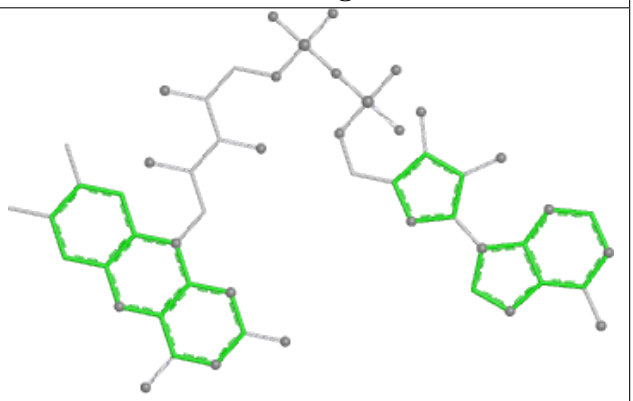
Bond lengths



Bond angles

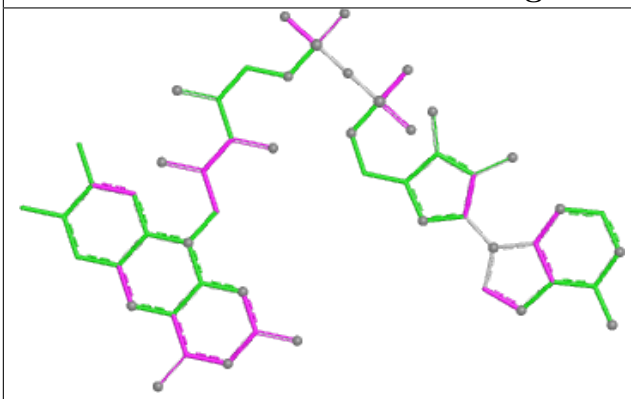


Torsions

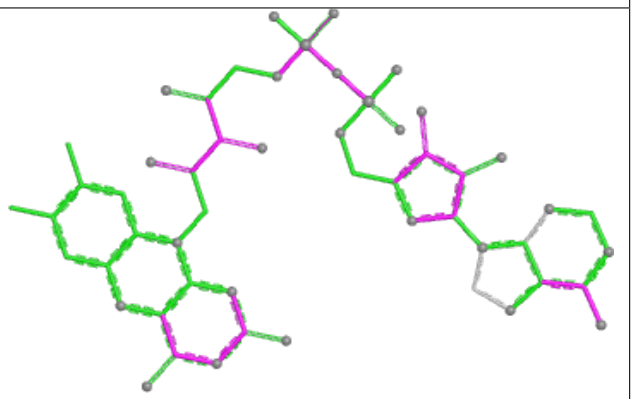


Rings

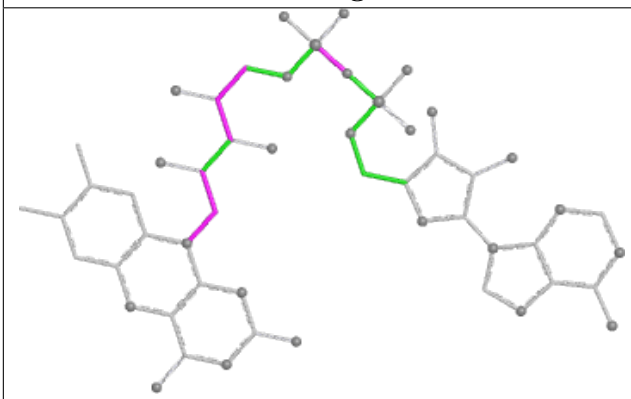
Ligand FAD C 501



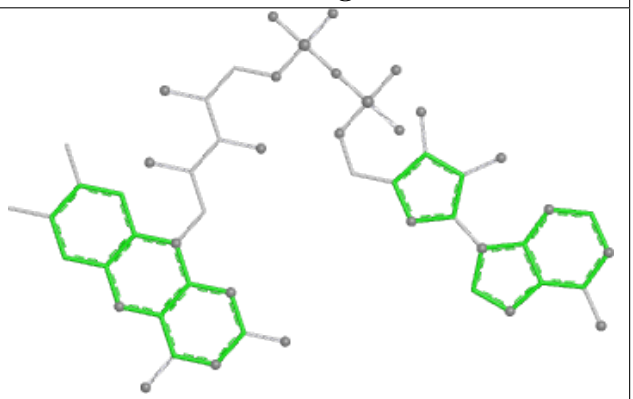
Bond lengths



Bond angles

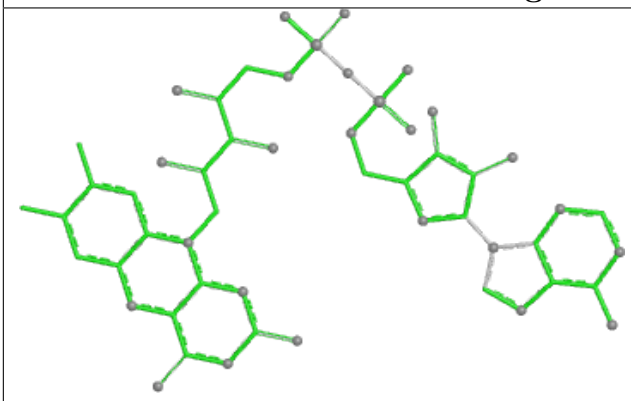


Torsions

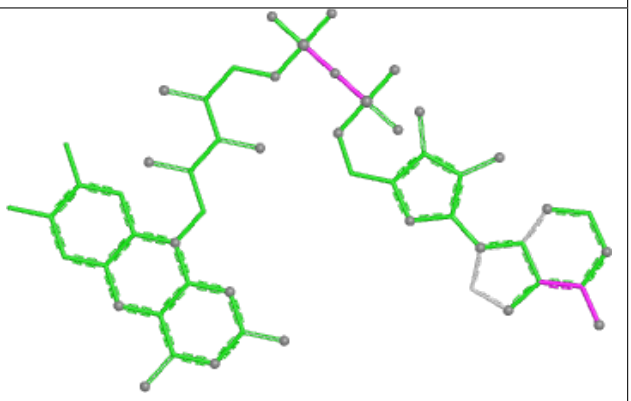


Rings

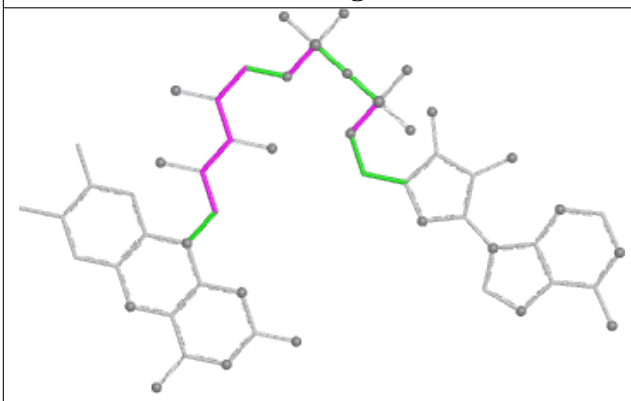
Ligand FAD B 301



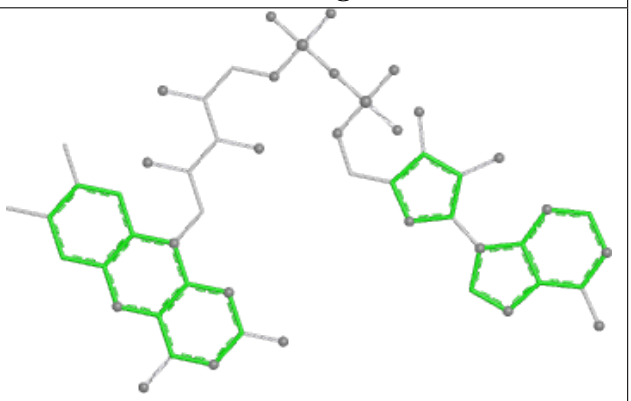
Bond lengths



Bond angles

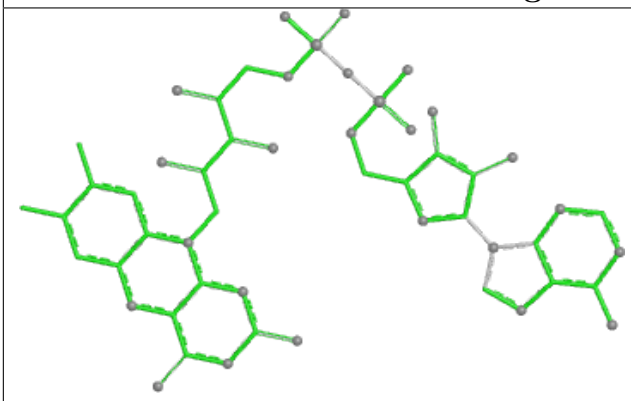


Torsions

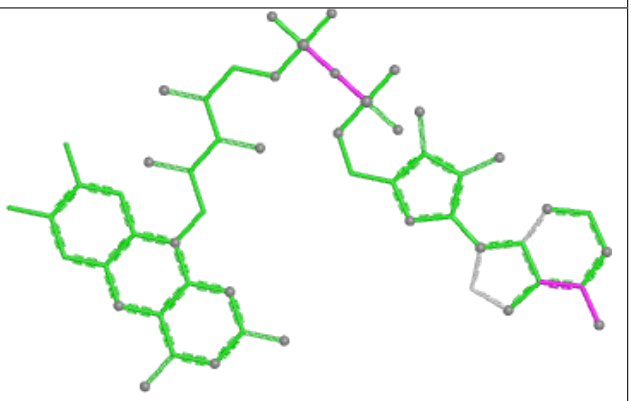


Rings

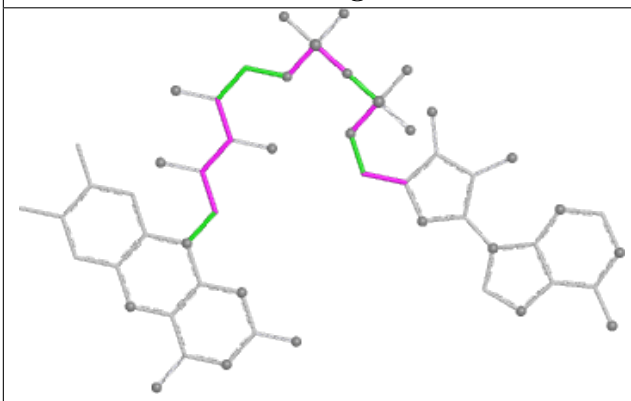
Ligand FAD D 501



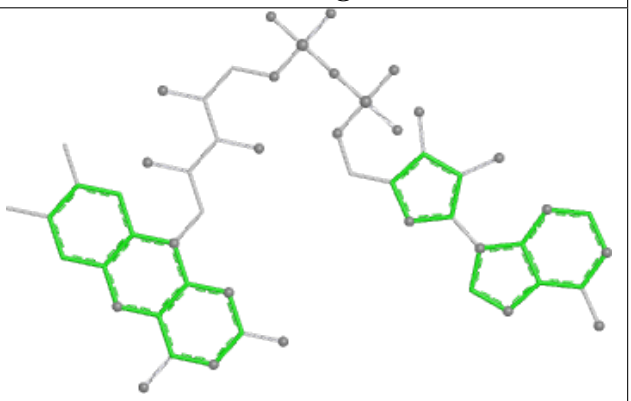
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

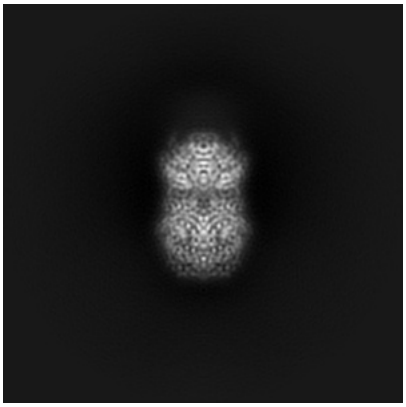
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13960. These allow visual inspection of the internal detail of the map and identification of artifacts.

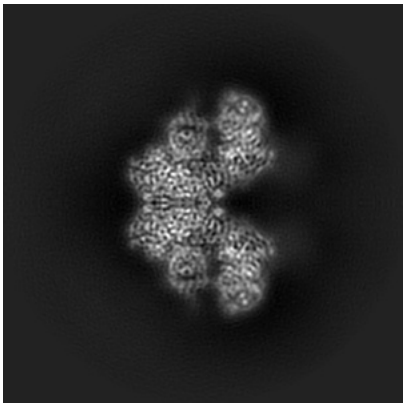
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

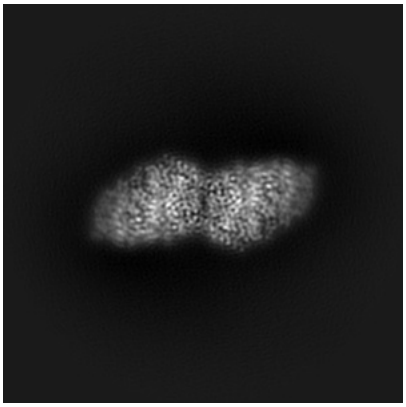
6.1.1 Primary map



X



Y

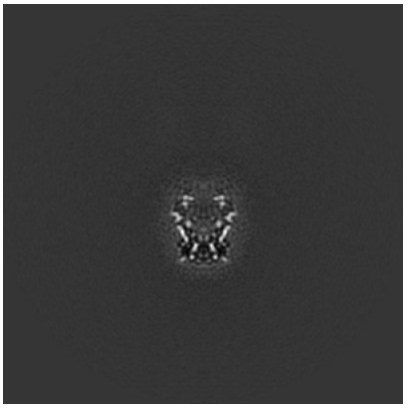


Z

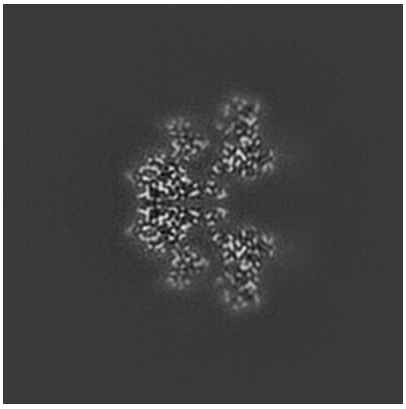
The images above show the map projected in three orthogonal directions.

6.2 Central slices

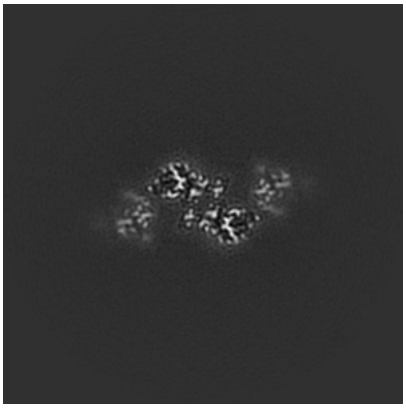
6.2.1 Primary map



X Index: 144



Y Index: 144

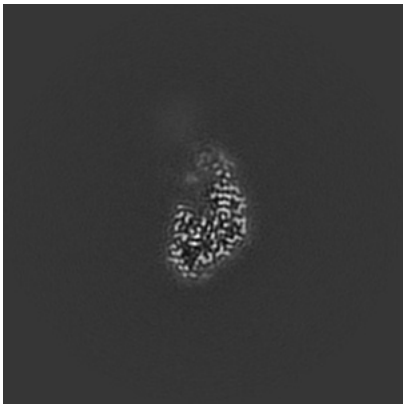


Z Index: 144

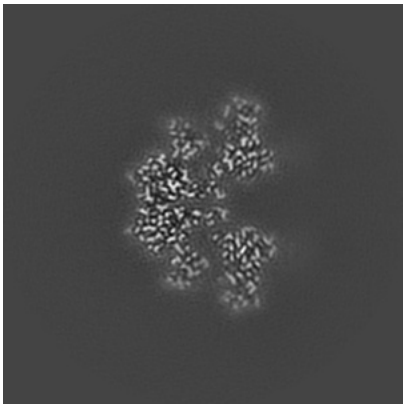
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

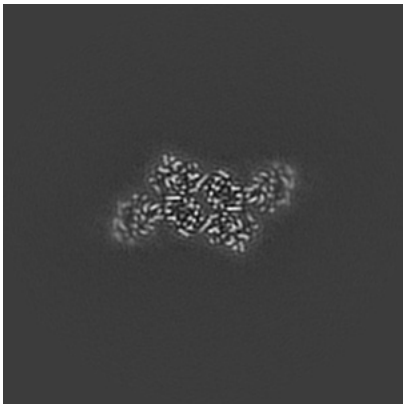
6.3.1 Primary map



X Index: 127



Y Index: 143

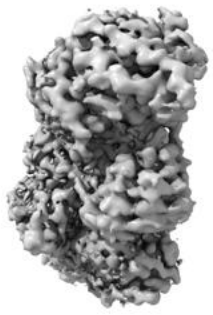


Z Index: 127

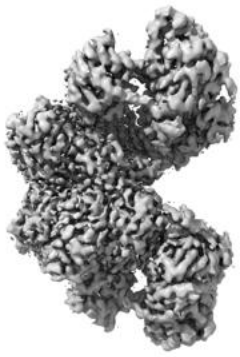
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

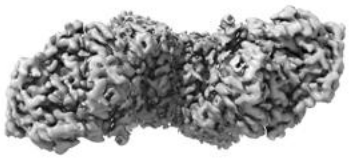
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0102. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

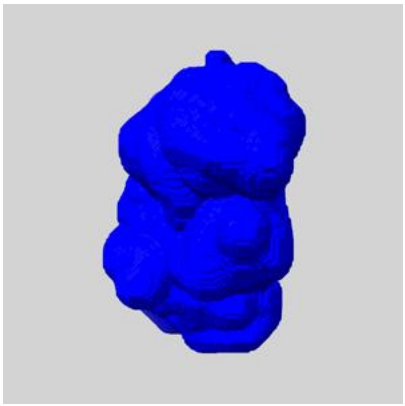
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

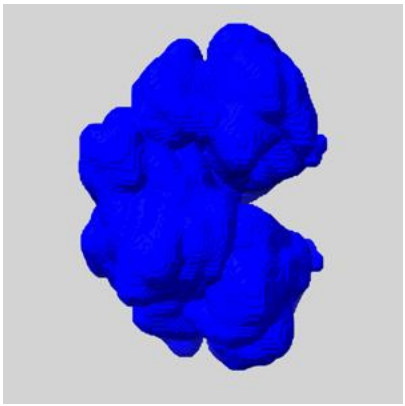
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

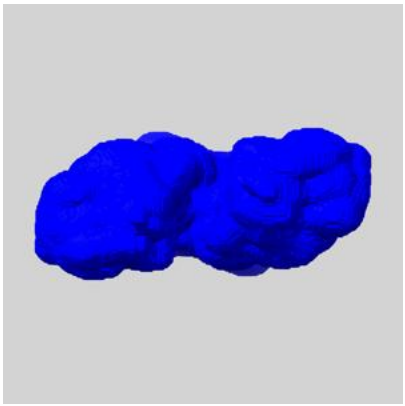
6.5.1 emd_13960_msk_1.map (i)



X



Y

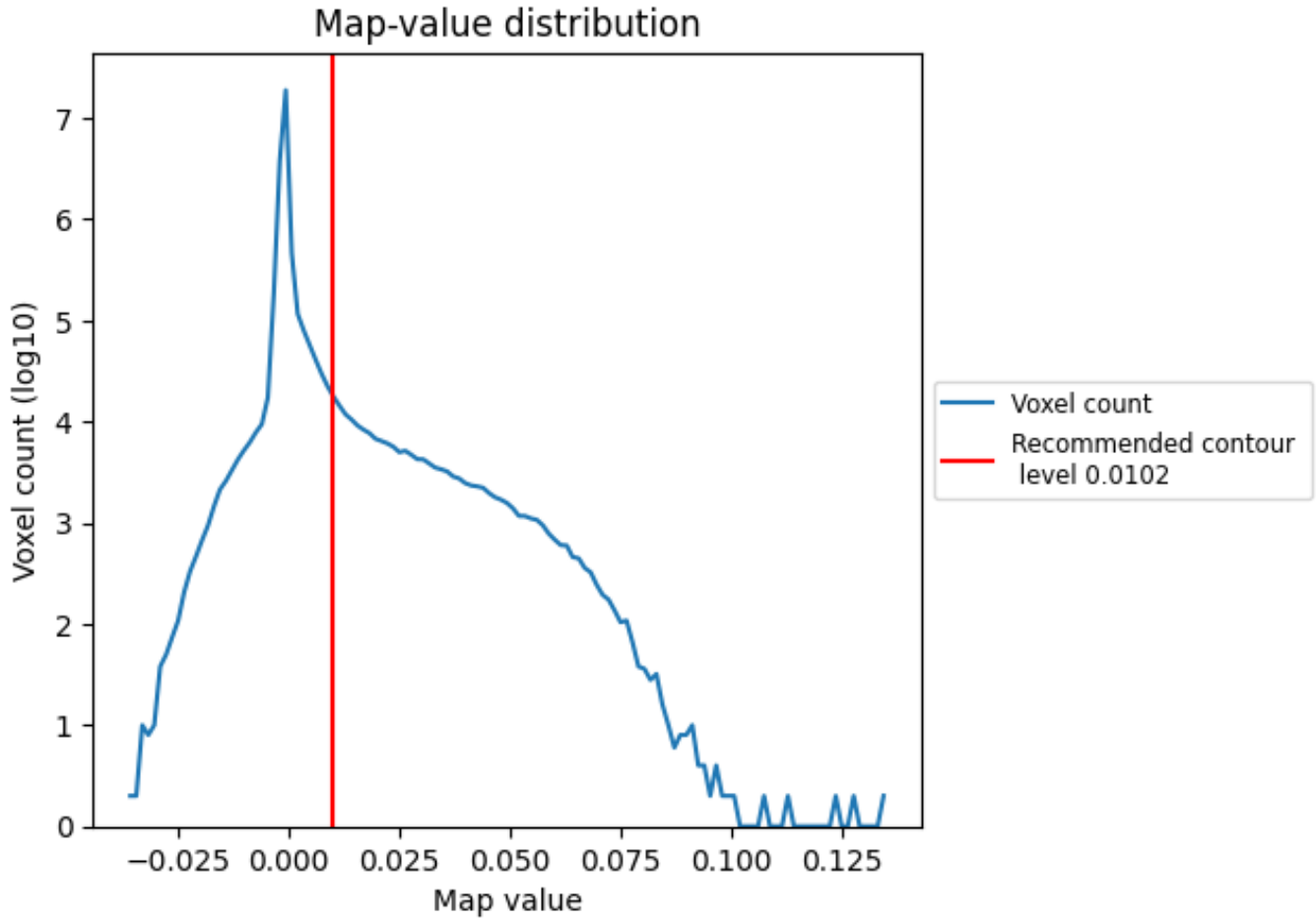


Z

7 Map analysis

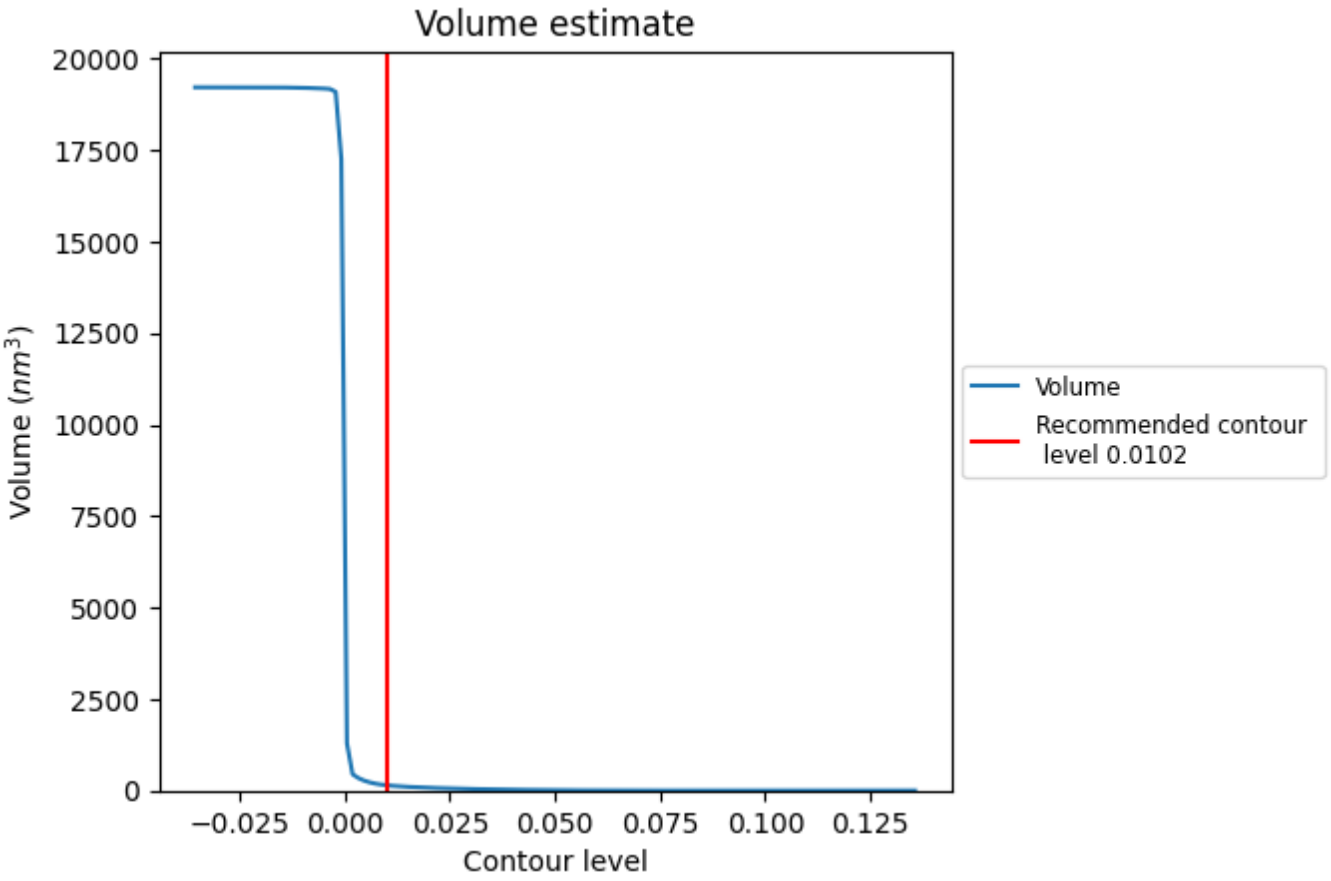
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

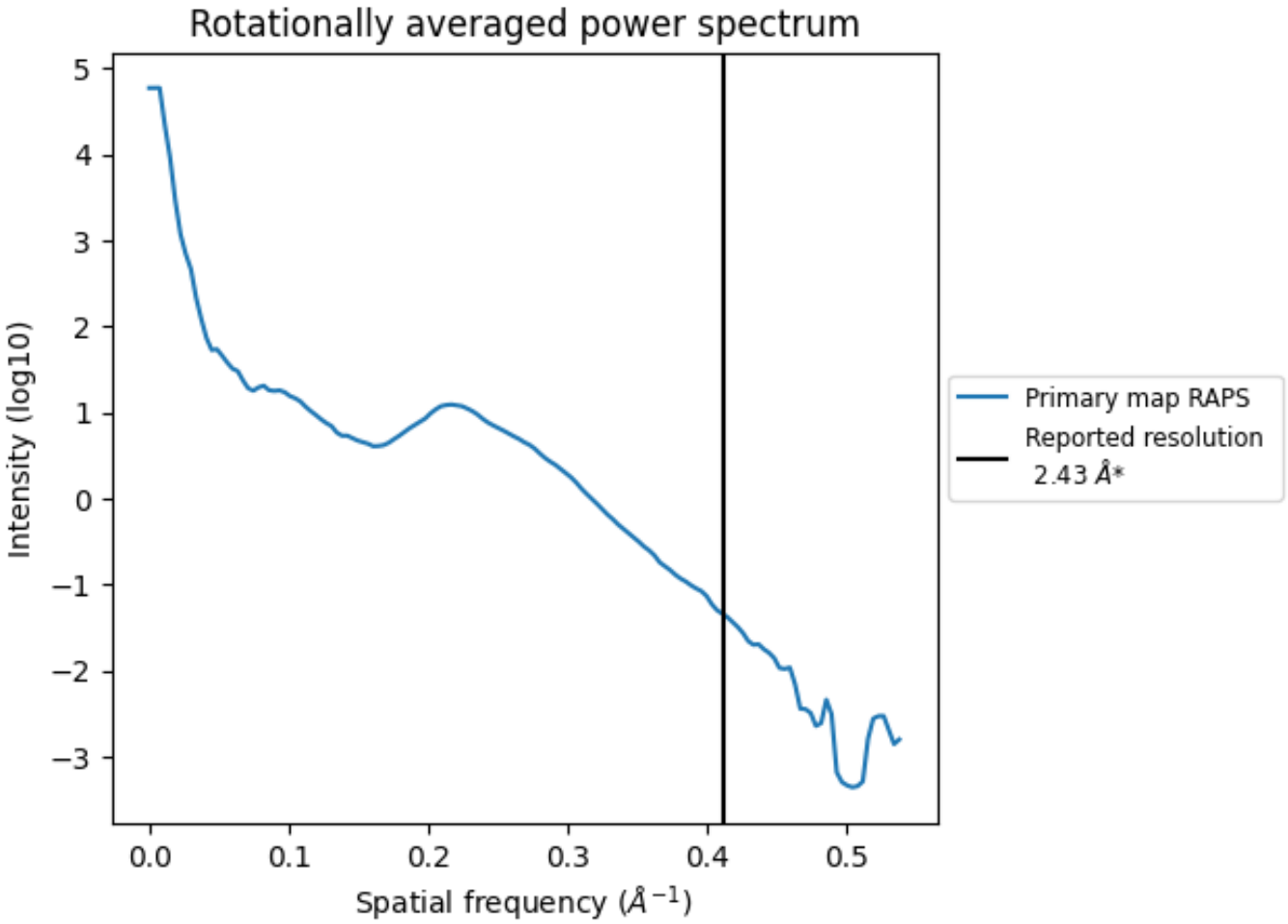
7.2 Volume estimate



The volume at the recommended contour level is 142 nm^3; this corresponds to an approximate mass of 128 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

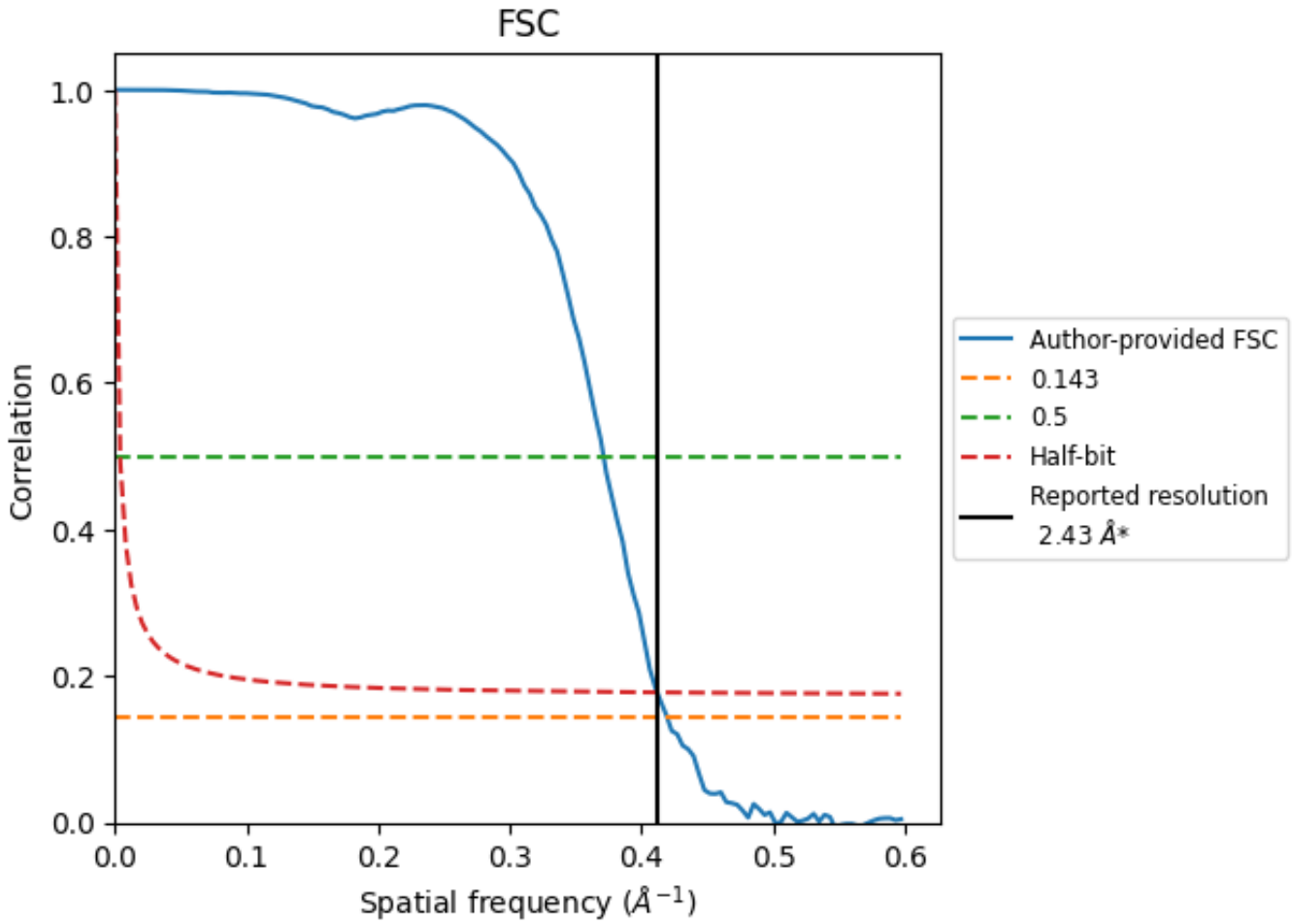


*Reported resolution corresponds to spatial frequency of 0.412 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.412 Å^{-1}

8.2 Resolution estimates (i)

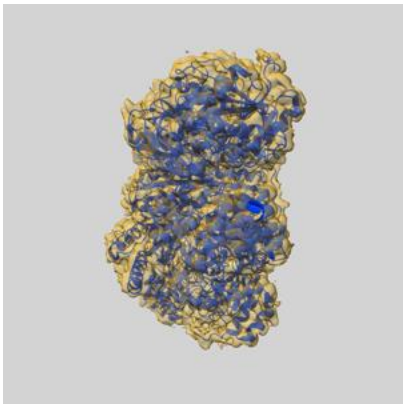
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.38	2.69	2.43
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

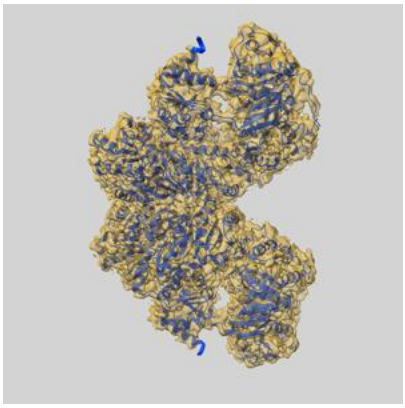
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13960 and PDB model 7QH2. Per-residue inclusion information can be found in section 3 on page 6.

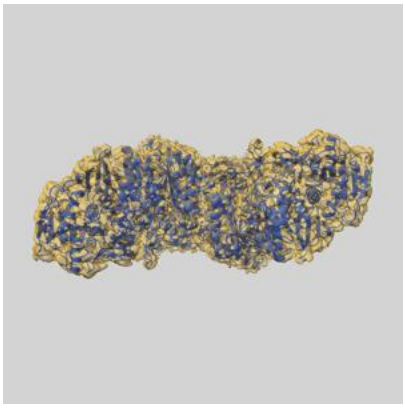
9.1 Map-model overlay



X



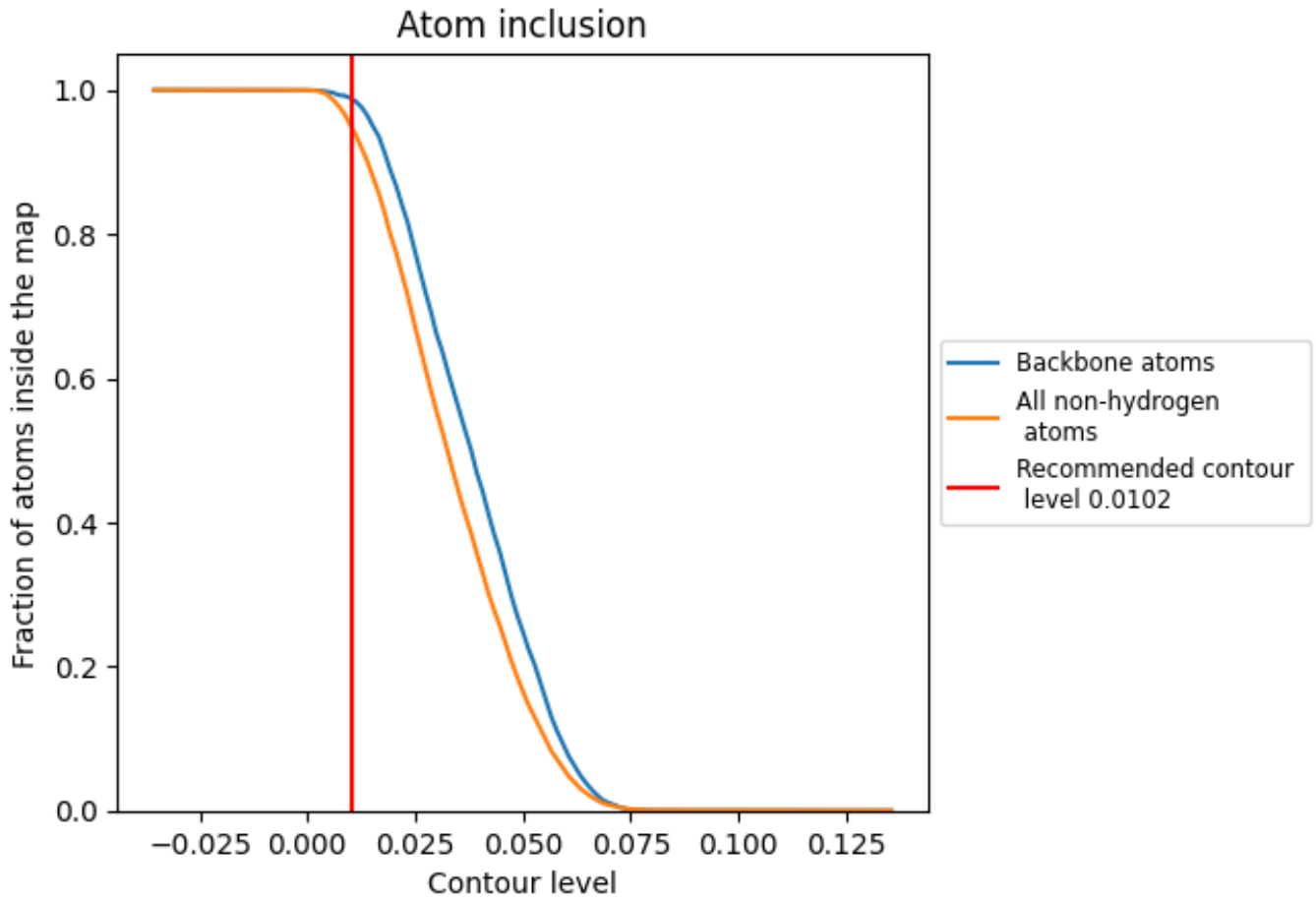
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0102 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.