wwPDB EM Validation Summary Report (i)

Dec 19, 2022 – 01:08 am GMT

PDB ID	:	7BKB
EMDB ID	:	EMD-12206
Title	:	Formate dehydrogenase - heterodisulfide reductase - formylmethanofuran dehydrogenase complex from Methanospirillum hungatei (hexameric, composite structure)
Authors	:	Pfeil-Gardiner, O.; Watanabe, T.; Shima, S.; Murphy, B.J.
Deposited on	:	2021-01-15
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

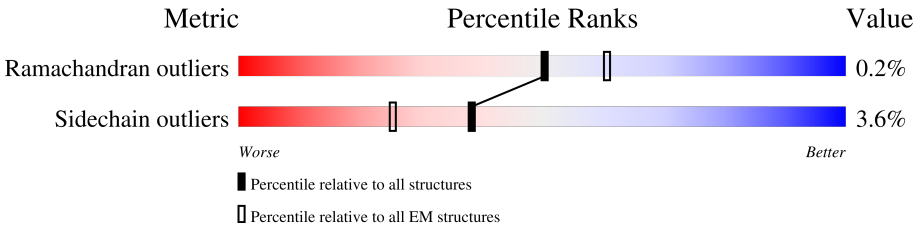
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 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)
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	671	8% 97%
1	a	671	5% 97%
2	F	140	5% 95%
2	f	140	95%
3	E	414	96%
3	e	414	96%
4	C	191	43% 99%
4	c	191	54% 99%
5	B	296	59% 98%

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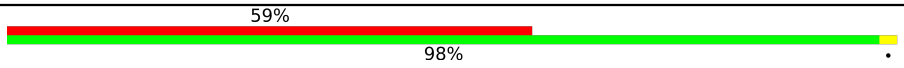
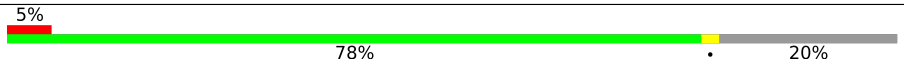
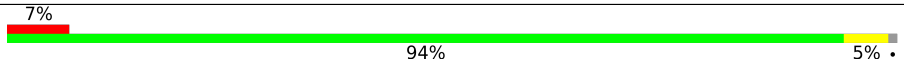
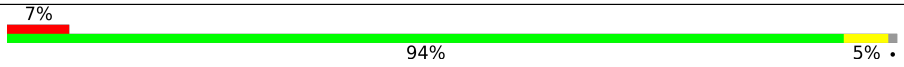
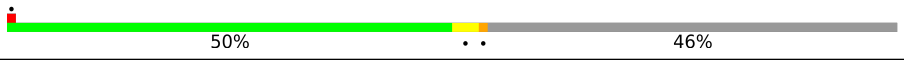
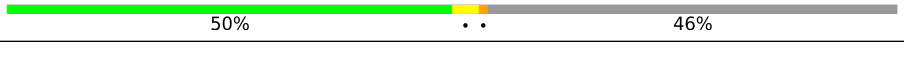
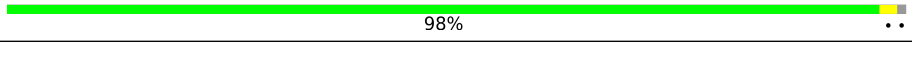
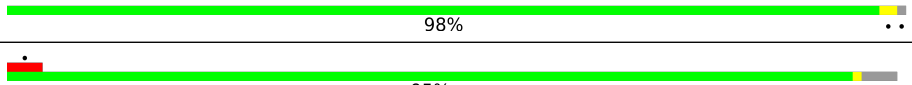
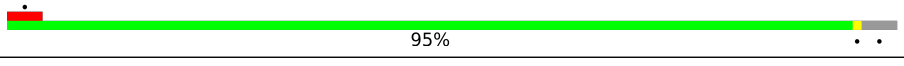
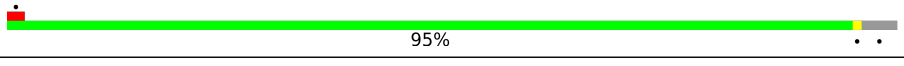
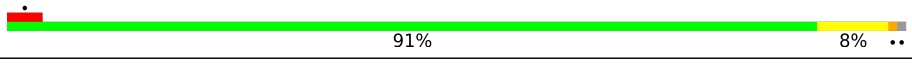
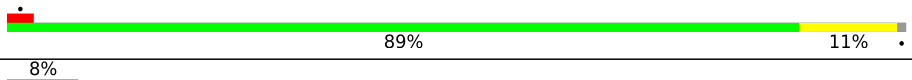
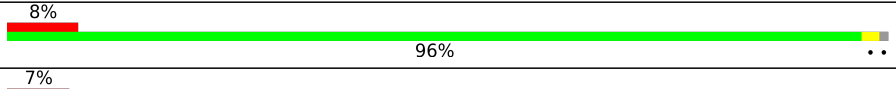
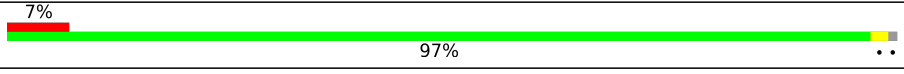
Mol	Chain	Length	Quality of chain
5	b	296	
6	D	686	
6	d	686	
7	I	266	
7	i	266	
8	L	146	
8	l	146	
9	G	571	
9	g	571	
10	J	137	
10	j	137	
11	K	388	
11	k	388	
12	H	443	
12	h	443	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 64126 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 CoB–CoM heterodisulfide reductase iron-sulfur subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	662	Total	C	N	O	S	0	0
			5011	3168	851	935	57		
1	a	662	Total	C	N	O	S	0	0
			5011	3168	851	935	57		

- Molecule 2 is a protein called F420-non-reducing hydrogenase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	137	Total	C	N	O	S	0	0
			1073	687	188	186	12		
2	f	137	Total	C	N	O	S	0	0
			1073	687	188	186	12		

- Molecule 3 is a protein called Formate dehydrogenase, beta subunit (F420).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	411	Total	C	N	O	S	0	0
			3151	1985	542	589	35		
3	e	411	Total	C	N	O	S	0	0
			3151	1985	542	589	35		

- Molecule 4 is a protein called CoB–CoM heterodisulfide reductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	189	Total	C	N	O	S	0	0
			1498	936	271	278	13		
4	c	189	Total	C	N	O	S	0	0
			1498	936	271	278	13		

- Molecule 5 is a protein called CoB–CoM heterodisulfide reductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	296	Total	C	N	O	S	0	0
			2304	1470	387	426	21		
5	b	296	Total	C	N	O	S	0	0
			2304	1470	387	426	21		

- Molecule 6 is a protein called Formate dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	549	Total	C	N	O	S	0	0
			4251	2691	737	795	28		
6	d	549	Total	C	N	O	S	0	0
			4251	2691	737	795	28		

- Molecule 7 is a protein called Formylmethanofuran dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	264	Total	C	N	O	S	0	0
			1996	1270	336	380	10		
7	i	264	Total	C	N	O	S	0	0
			1996	1270	336	380	10		

- Molecule 8 is a protein called Formylmethanofuran dehydrogenase, subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	79	Total	C	N	O	S	0	0
			576	357	98	112	9		
8	l	79	Total	C	N	O	S	0	0
			576	357	98	112	9		

- Molecule 9 is a protein called Formylmethanofuran dehydrogenase, subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	568	Total	C	N	O	S	0	0
			4455	2840	751	841	23		
9	g	568	Total	C	N	O	S	0	0
			4455	2840	751	841	23		

- Molecule 10 is a protein called Formylmethanofuran dehydrogenase, subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	131	Total	C	N	O	S	0	0
			1007	629	179	190	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	131	Total	C	N	O	S	0	0
			1007	629	179	190	9		

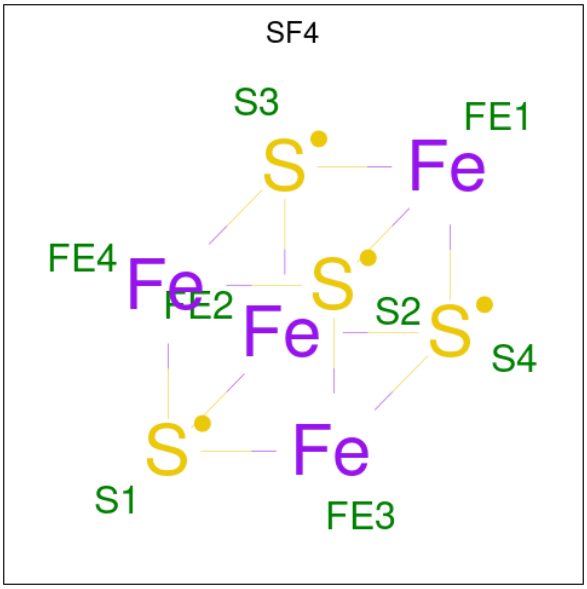
- Molecule 11 is a protein called Formylmethanofuran dehydrogenase, subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	386	Total	C	N	O	S	0	0
			2910	1815	488	571	36		
11	k	386	Total	C	N	O	S	0	0
			2910	1815	488	571	36		

- Molecule 12 is a protein called Formylmethanofuran dehydrogenase, subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	438	Total	C	N	O	S	0	0
			3416	2155	600	629	32		
12	h	438	Total	C	N	O	S	0	0
			3416	2155	600	629	32		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	Fe	S	0
			48	24	24	
13	A	1	Total	Fe	S	0
			48	24	24	

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Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total Fe S 48 24 24	0
13	A	1	Total Fe S 48 24 24	0
13	A	1	Total Fe S 48 24 24	0
13	A	1	Total Fe S 48 24 24	0
13	E	1	Total Fe S 32 16 16	0
13	E	1	Total Fe S 32 16 16	0
13	E	1	Total Fe S 32 16 16	0
13	E	1	Total Fe S 32 16 16	0
13	C	1	Total Fe S 16 8 8	0
13	C	1	Total Fe S 16 8 8	0
13	D	1	Total Fe S 8 4 4	0
13	L	1	Total Fe S 16 8 8	0
13	L	1	Total Fe S 16 8 8	0
13	K	1	Total Fe S 64 32 32	0
13	K	1	Total Fe S 64 32 32	0
13	K	1	Total Fe S 64 32 32	0
13	K	1	Total Fe S 64 32 32	0
13	K	1	Total Fe S 64 32 32	0
13	K	1	Total Fe S 64 32 32	0
13	K	1	Total Fe S 64 32 32	0

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Mol	Chain	Residues	Atoms	AltConf
13	H	1	Total Fe S 8 4 4	0
13	a	1	Total Fe S 48 24 24	0
13	a	1	Total Fe S 48 24 24	0
13	a	1	Total Fe S 48 24 24	0
13	a	1	Total Fe S 48 24 24	0
13	a	1	Total Fe S 48 24 24	0
13	a	1	Total Fe S 48 24 24	0
13	e	1	Total Fe S 32 16 16	0
13	e	1	Total Fe S 32 16 16	0
13	e	1	Total Fe S 32 16 16	0
13	e	1	Total Fe S 32 16 16	0
13	c	1	Total Fe S 16 8 8	0
13	c	1	Total Fe S 16 8 8	0
13	d	1	Total Fe S 8 4 4	0
13	l	1	Total Fe S 16 8 8	0
13	l	1	Total Fe S 16 8 8	0
13	k	1	Total Fe S 64 32 32	0
13	k	1	Total Fe S 64 32 32	0
13	k	1	Total Fe S 64 32 32	0
13	k	1	Total Fe S 64 32 32	0
13	k	1	Total Fe S 64 32 32	0

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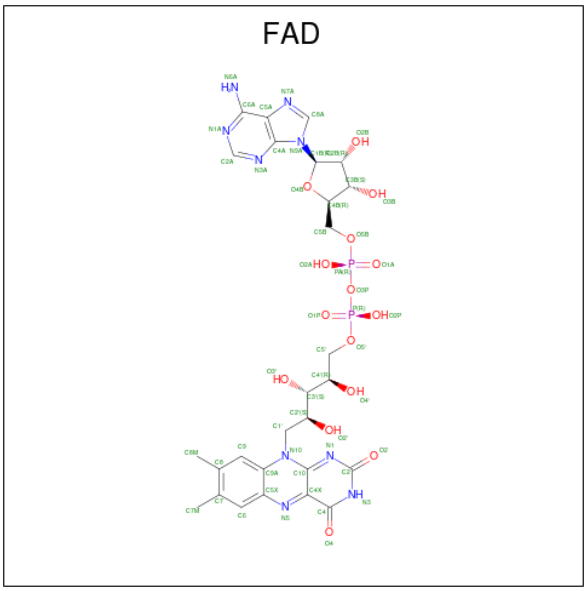
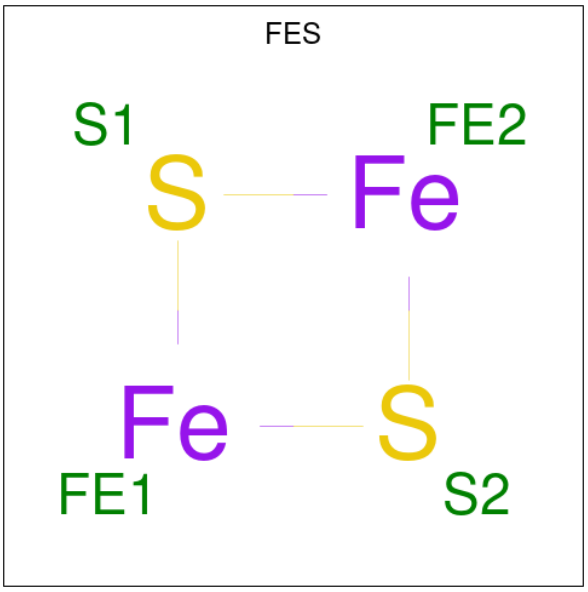
Mol	Chain	Residues	Atoms	AltConf
13	k	1	Total Fe S 64 32 32	0
13	k	1	Total Fe S 64 32 32	0
13	k	1	Total Fe S 64 32 32	0
13	h	1	Total Fe S 8 4 4	0

- Molecule 14 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).



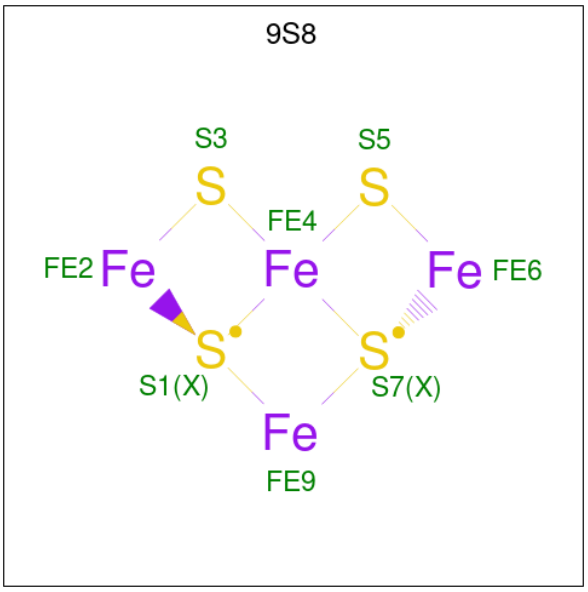
Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C N O P 53 27 9 15 2	0
14	E	1	Total C N O P 53 27 9 15 2	0
14	a	1	Total C N O P 53 27 9 15 2	0
14	e	1	Total C N O P 53 27 9 15 2	0

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
15	F	1	Total	Fe	S	0
			4	2	2	
15	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 16 is Non-cubane [4Fe-4S]-cluster (three-letter code: 9S8) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	Fe	S	0
			16	8	8	

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Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total Fe S 16 8 8	0
16	b	1	Total Fe S 16 8 8	0
16	b	1	Total Fe S 16 8 8	0

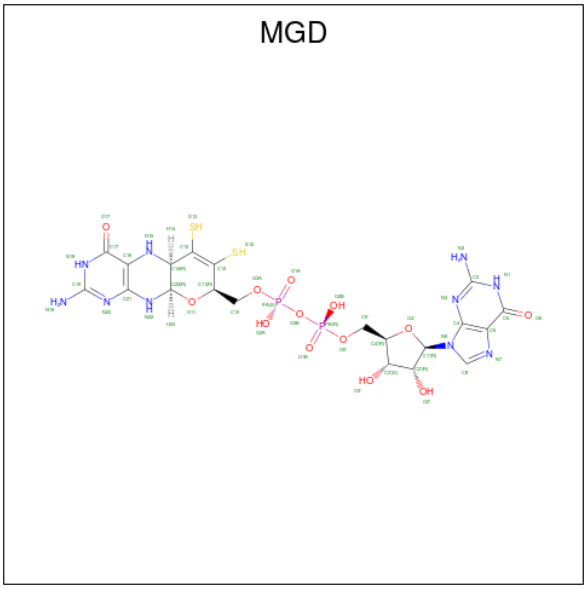
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
17	G	2	Total Zn 2 2	0
17	g	2	Total Zn 2 2	0

- Molecule 18 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total Mo 1 1	0
18	h	1	Total Mo 1 1	0

- Molecule 19 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO -8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).

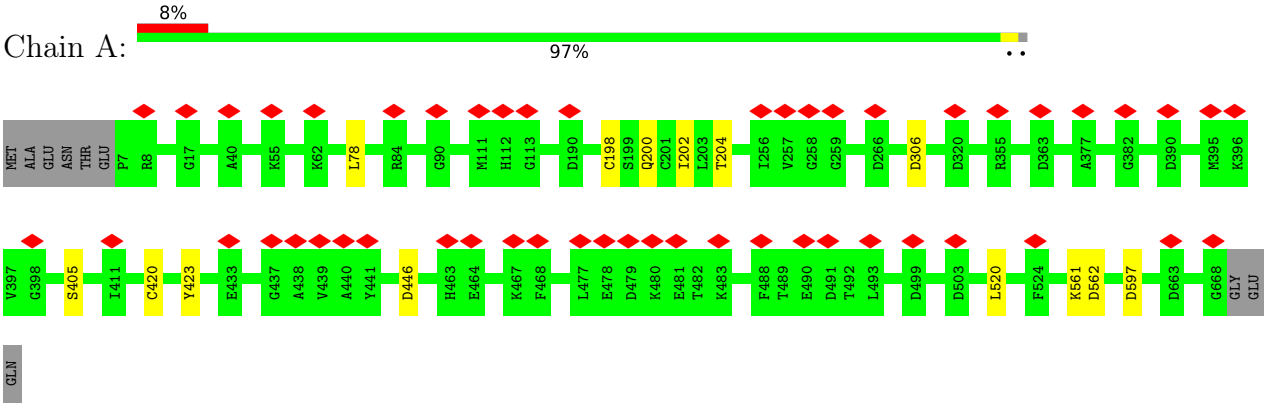


Mol	Chain	Residues	Atoms						AltConf
19	H	1	Total	C	N	O	P	S	0
			94	40	20	26	4	4	
19	H	1	Total	C	N	O	P	S	0
			94	40	20	26	4	4	
19	h	1	Total	C	N	O	P	S	0
			94	40	20	26	4	4	
19	h	1	Total	C	N	O	P	S	0
			94	40	20	26	4	4	

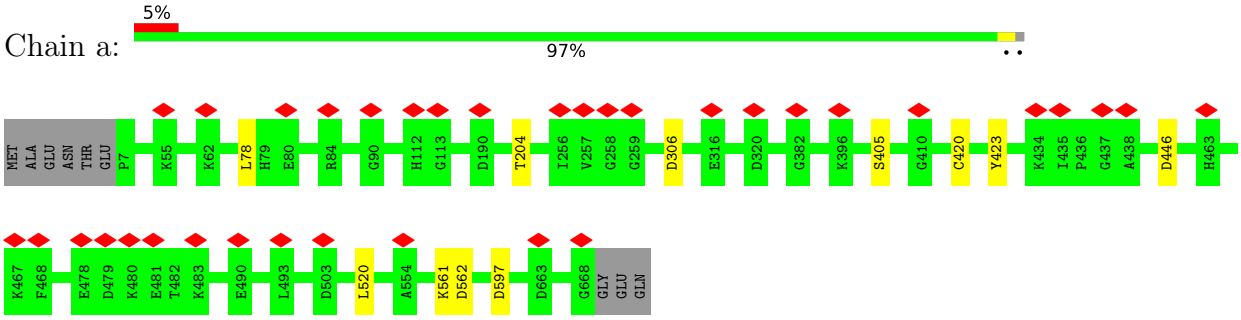
3 Residue-property plots (i)

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.

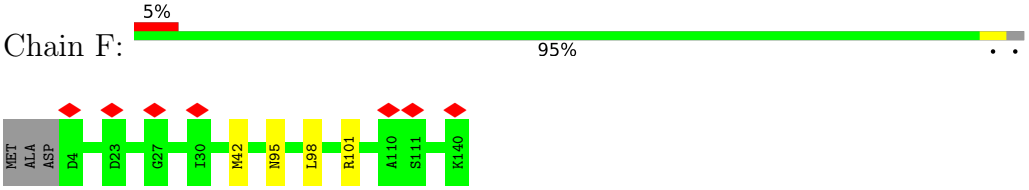
• Molecule 1: CoB–CoM heterodisulfide reductase iron-sulfur subunit A



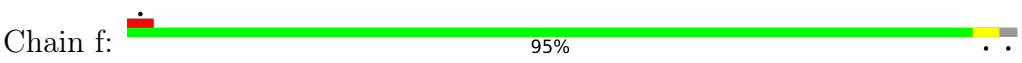
• Molecule 1: CoB–CoM heterodisulfide reductase iron-sulfur subunit A

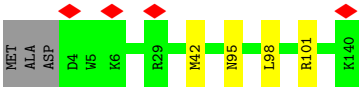


• Molecule 2: F420-non-reducing hydrogenase subunit D



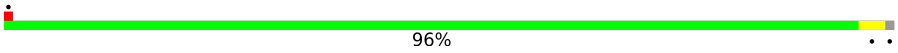
• Molecule 2: F420-non-reducing hydrogenase subunit D

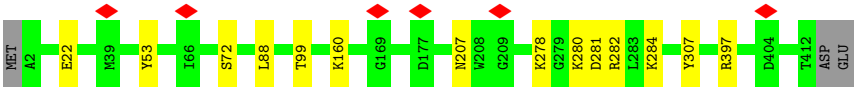




• Molecule 3: Formate dehydrogenase, beta subunit (F420)

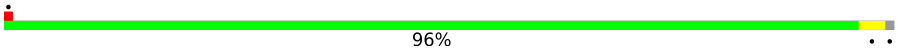
Chain E:

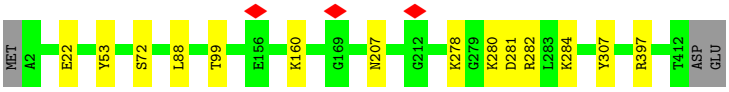




• Molecule 3: Formate dehydrogenase, beta subunit (F420)

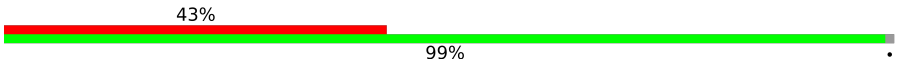
Chain e:

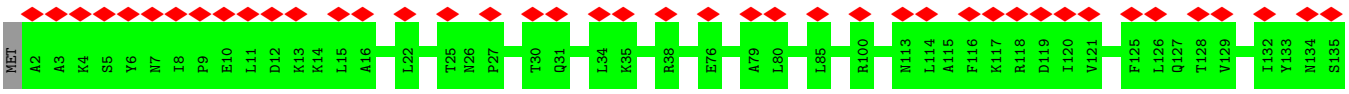


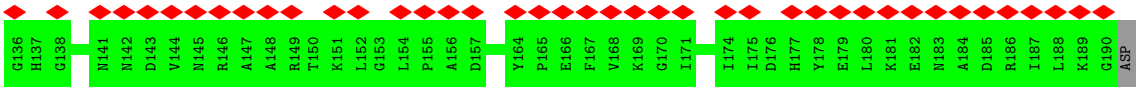


• Molecule 4: CoB–CoM heterodisulfide reductase subunit C

Chain C:

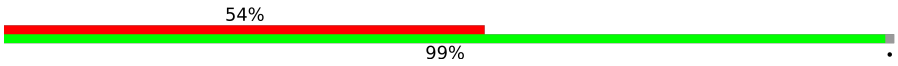


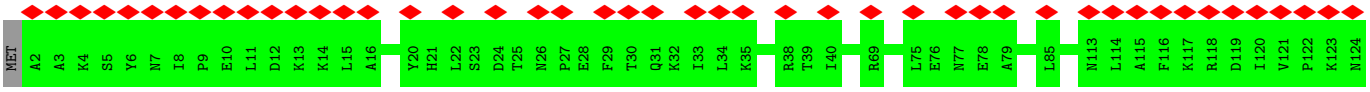


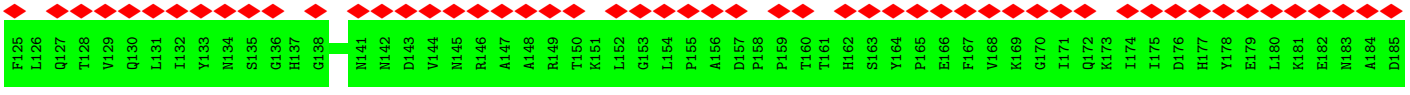


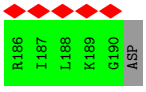
• Molecule 4: CoB–CoM heterodisulfide reductase subunit C

Chain c:



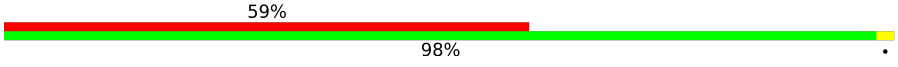


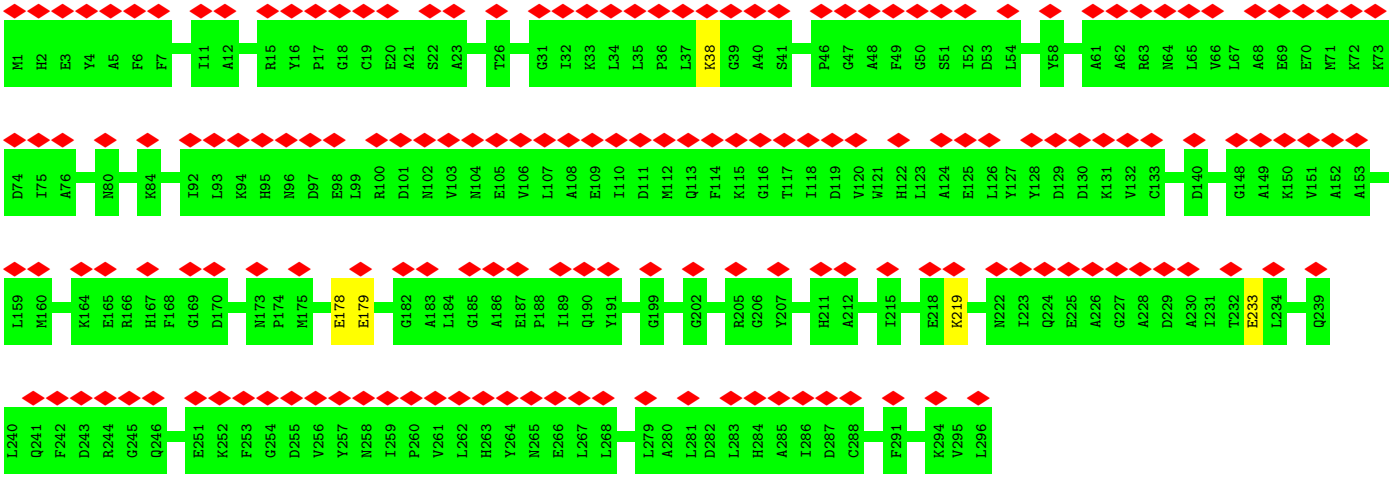




• Molecule 5: CoB–CoM heterodisulfide reductase subunit B

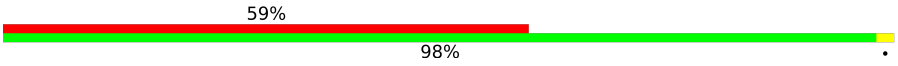
Chain B:

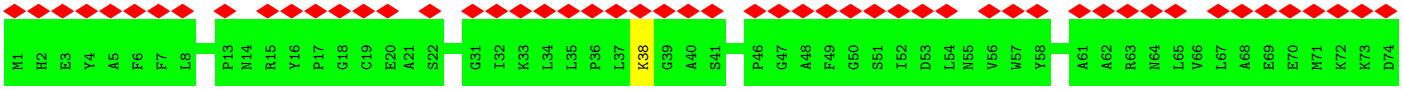


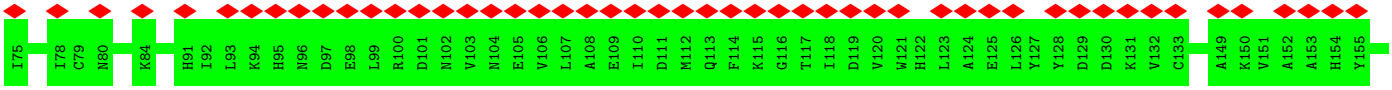


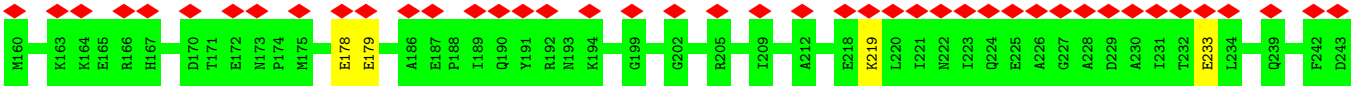
• Molecule 5: CoB–CoM heterodisulfide reductase subunit B

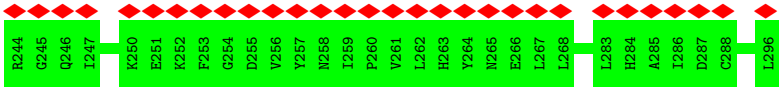
Chain b:





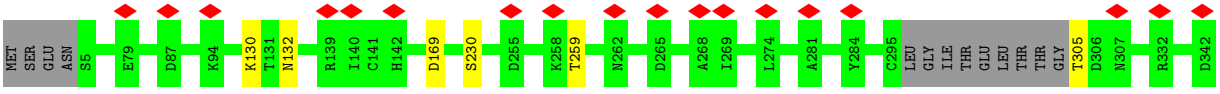


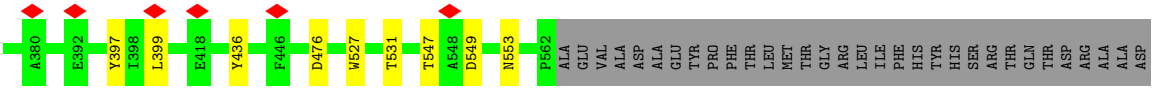


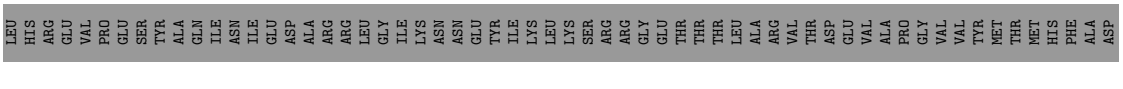


• Molecule 6: Formate dehydrogenase

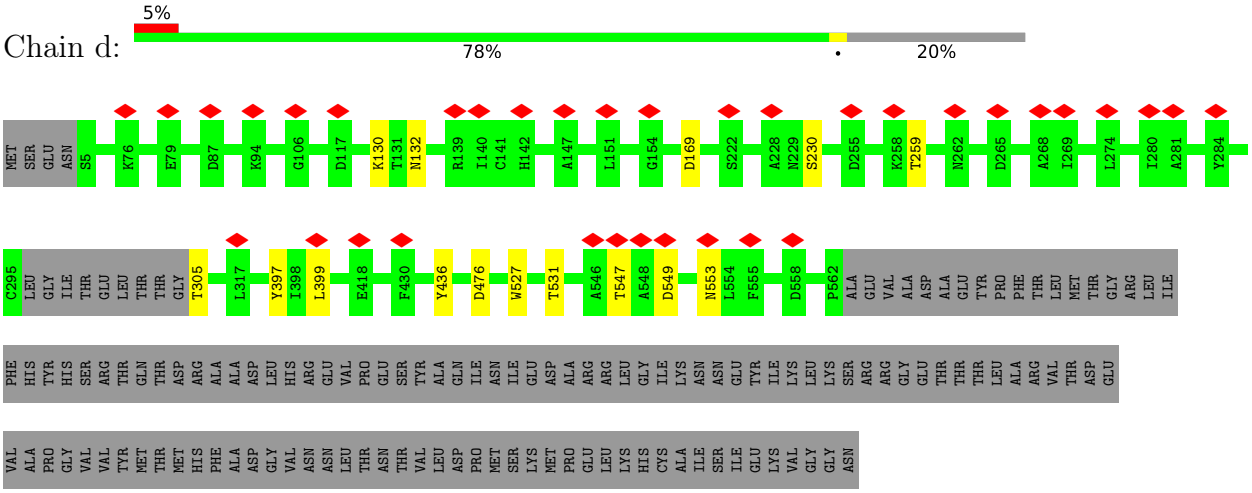
Chain D:



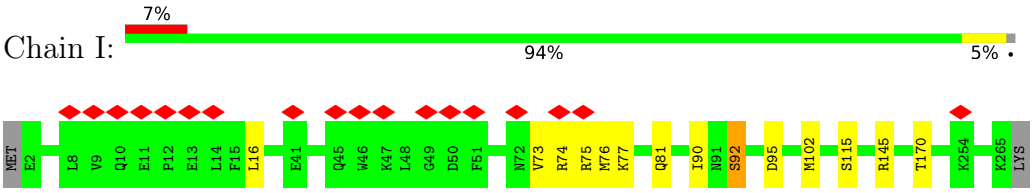




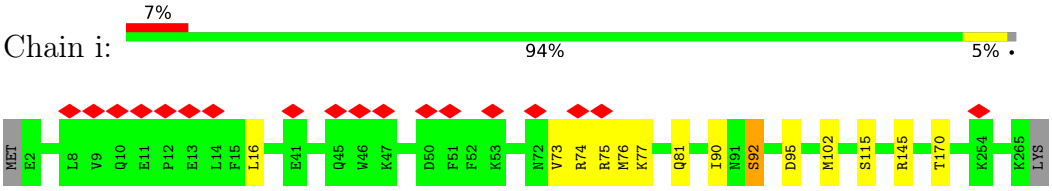
• Molecule 6: Formate dehydrogenase



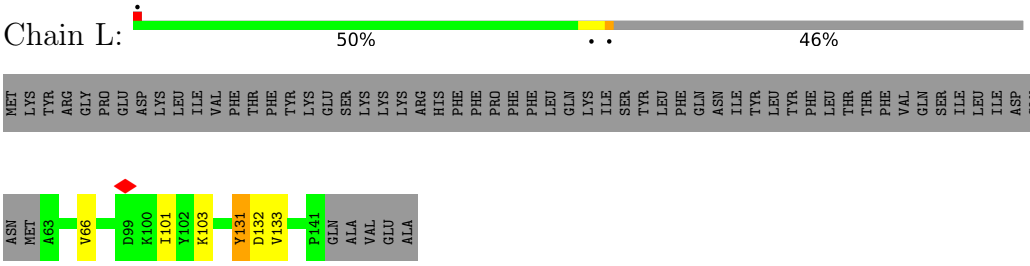
• Molecule 7: Formylmethanofuran dehydrogenase



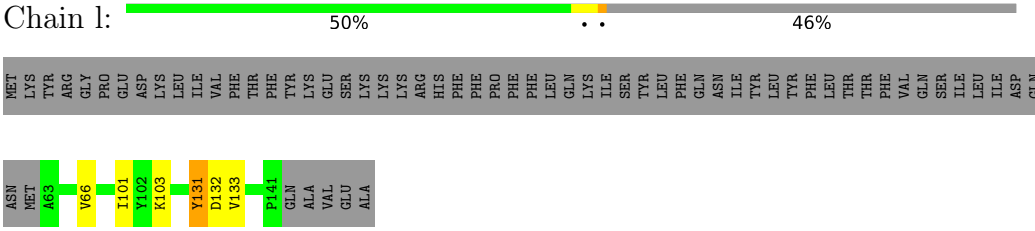
• Molecule 7: Formylmethanofuran dehydrogenase



• Molecule 8: Formylmethanofuran dehydrogenase, subunit G

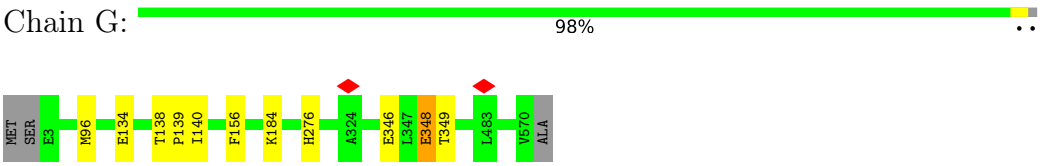


• Molecule 8: Formylmethanofuran dehydrogenase, subunit G



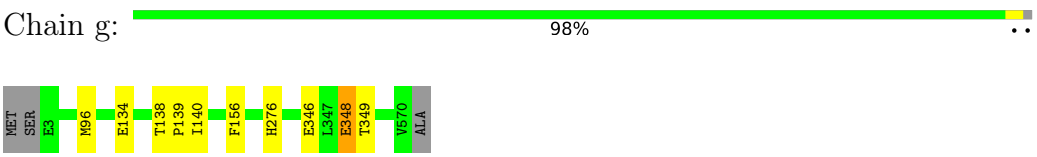
• Molecule 9: Formylmethanofuran dehydrogenase, subunit A

Chain G:



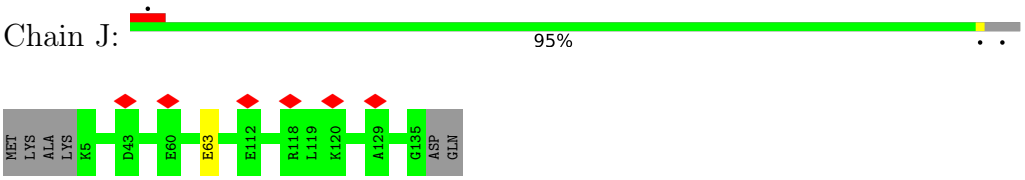
• Molecule 9: Formylmethanofuran dehydrogenase, subunit A

Chain g:



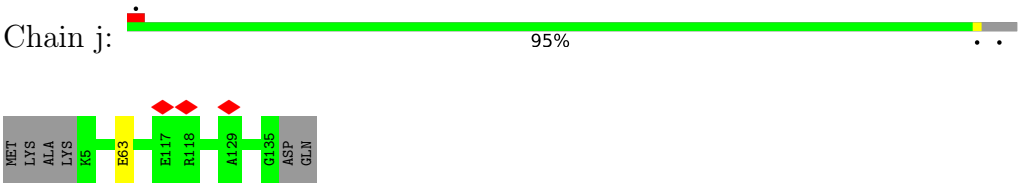
• Molecule 10: Formylmethanofuran dehydrogenase, subunit D

Chain J:



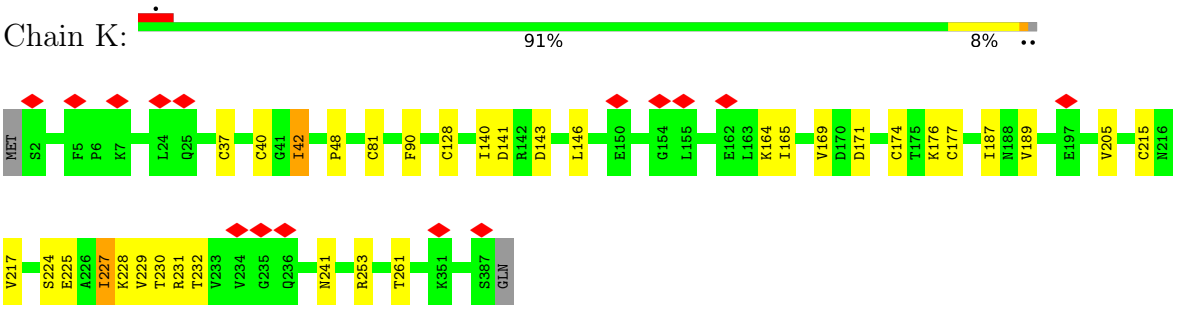
• Molecule 10: Formylmethanofuran dehydrogenase, subunit D

Chain j:



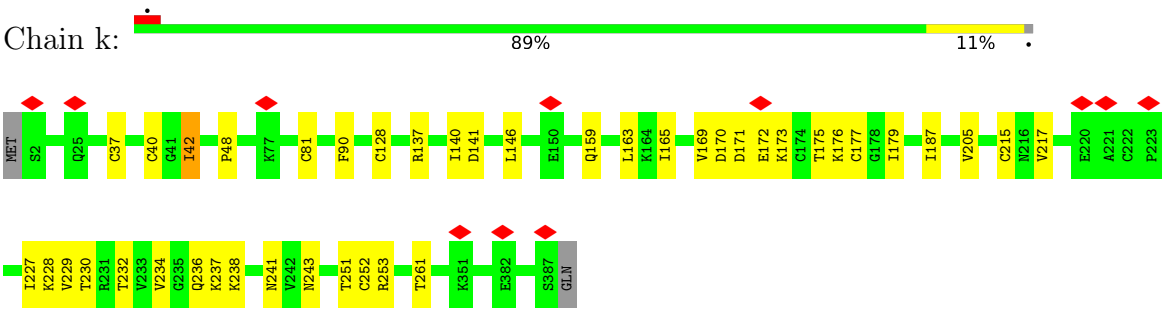
• Molecule 11: Formylmethanofuran dehydrogenase, subunit F

Chain K:



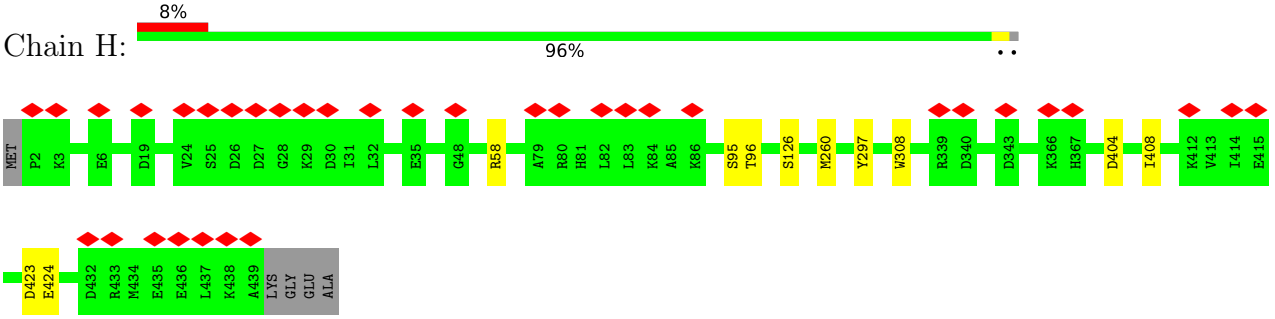
• Molecule 11: Formylmethanofuran dehydrogenase, subunit F

Chain k:



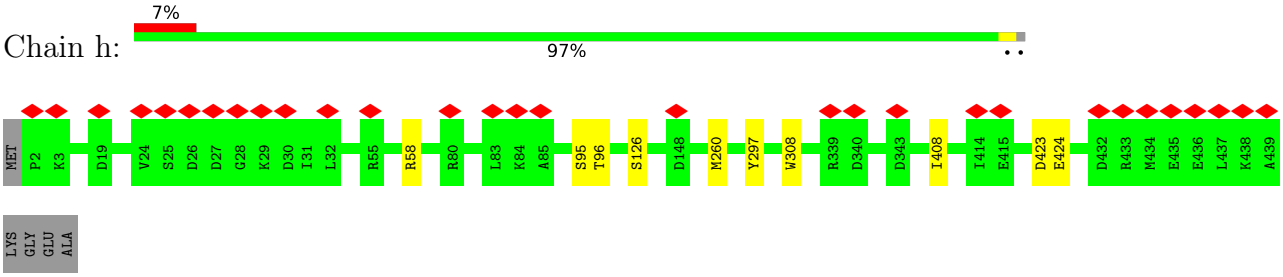
• Molecule 12: Formylmethanofuran dehydrogenase, subunit B

Chain H:



• Molecule 12: Formylmethanofuran dehydrogenase, subunit B

Chain h:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	203264	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	84.060	Depositor
Minimum map value	-31.762	Depositor
Average map value	0.047	Depositor
Map value standard deviation	1.829	Depositor
Recommended contour level	7.0	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.68, 1.68, 1.68	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FAD, 9S8, ZN, FES, KCX, MO, MGD

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	0.46	0/5115	0.57	0/6920
1	a	0.46	0/5115	0.57	0/6920
2	F	0.51	0/1096	0.59	0/1474
2	f	0.51	0/1096	0.59	0/1474
3	E	0.54	0/3208	0.61	1/4314 (0.0%)
3	e	0.54	0/3208	0.61	1/4314 (0.0%)
4	C	0.39	0/1529	0.48	0/2072
4	c	0.39	0/1529	0.48	0/2072
5	B	0.42	0/2355	0.55	0/3187
5	b	0.42	0/2355	0.55	0/3187
6	D	0.48	0/4345	0.60	0/5889
6	d	0.48	0/4345	0.61	0/5889
7	I	0.42	0/2029	0.62	0/2724
7	i	0.42	0/2029	0.62	0/2724
8	L	0.55	0/585	0.81	1/800 (0.1%)
8	l	0.55	0/585	0.81	1/800 (0.1%)
9	G	0.41	0/4549	0.57	1/6174 (0.0%)
9	g	0.41	0/4549	0.57	1/6174 (0.0%)
10	J	0.44	0/1023	0.57	0/1383
10	j	0.44	0/1023	0.57	0/1383
11	K	0.54	0/2952	0.73	0/3988
11	k	0.54	0/2952	0.73	0/3988
12	H	0.48	0/3497	0.59	0/4732
12	h	0.48	0/3497	0.59	0/4732
All	All	0.47	0/64566	0.60	6/87314 (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
11	k	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	139	PRO	N-CA-C	5.99	127.67	112.10
9	G	139	PRO	N-CA-C	5.97	127.62	112.10
3	E	307	TYR	CB-CA-C	-5.57	99.26	110.40
3	e	307	TYR	CB-CA-C	-5.55	99.29	110.40
8	l	131	TYR	CB-CA-C	-5.25	99.90	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	k	159	GLN	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	660/671 (98%)	625 (95%)	34 (5%)	1 (0%)	47 81
1	a	660/671 (98%)	625 (95%)	34 (5%)	1 (0%)	47 81
2	F	135/140 (96%)	126 (93%)	9 (7%)	0	100 100
2	f	135/140 (96%)	126 (93%)	9 (7%)	0	100 100
3	E	409/414 (99%)	389 (95%)	20 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	e	409/414 (99%)	389 (95%)	20 (5%)	0	100	100
4	C	187/191 (98%)	179 (96%)	8 (4%)	0	100	100
4	c	187/191 (98%)	179 (96%)	8 (4%)	0	100	100
5	B	294/296 (99%)	279 (95%)	15 (5%)	0	100	100
5	b	294/296 (99%)	279 (95%)	15 (5%)	0	100	100
6	D	545/686 (79%)	506 (93%)	39 (7%)	0	100	100
6	d	545/686 (79%)	506 (93%)	39 (7%)	0	100	100
7	I	262/266 (98%)	226 (86%)	35 (13%)	1 (0%)	34	72
7	i	262/266 (98%)	226 (86%)	35 (13%)	1 (0%)	34	72
8	L	77/146 (53%)	72 (94%)	5 (6%)	0	100	100
8	l	77/146 (53%)	72 (94%)	5 (6%)	0	100	100
9	G	565/571 (99%)	514 (91%)	49 (9%)	2 (0%)	34	72
9	g	565/571 (99%)	514 (91%)	49 (9%)	2 (0%)	34	72
10	J	129/137 (94%)	118 (92%)	11 (8%)	0	100	100
10	j	129/137 (94%)	118 (92%)	11 (8%)	0	100	100
11	K	384/388 (99%)	337 (88%)	44 (12%)	3 (1%)	19	58
11	k	384/388 (99%)	340 (88%)	41 (11%)	3 (1%)	19	58
12	H	436/443 (98%)	389 (89%)	47 (11%)	0	100	100
12	h	436/443 (98%)	389 (89%)	47 (11%)	0	100	100
All	All	8166/8698 (94%)	7523 (92%)	629 (8%)	14 (0%)	50	81

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	G	276	HIS
9	g	276	HIS
11	k	251	THR
1	A	446	ASP
11	K	42	ILE

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	536/543 (99%)	523 (98%)	13 (2%)	49	76
1	a	536/543 (99%)	526 (98%)	10 (2%)	57	80
2	F	112/114 (98%)	108 (96%)	4 (4%)	35	66
2	f	112/114 (98%)	108 (96%)	4 (4%)	35	66
3	E	338/341 (99%)	325 (96%)	13 (4%)	33	65
3	e	338/341 (99%)	325 (96%)	13 (4%)	33	65
4	C	168/170 (99%)	168 (100%)	0	100	100
4	c	168/170 (99%)	168 (100%)	0	100	100
5	B	245/245 (100%)	240 (98%)	5 (2%)	55	79
5	b	245/245 (100%)	240 (98%)	5 (2%)	55	79
6	D	454/571 (80%)	439 (97%)	15 (3%)	38	68
6	d	454/571 (80%)	439 (97%)	15 (3%)	38	68
7	I	202/204 (99%)	188 (93%)	14 (7%)	15	47
7	i	202/204 (99%)	188 (93%)	14 (7%)	15	47
8	L	67/128 (52%)	61 (91%)	6 (9%)	9	37
8	l	67/128 (52%)	61 (91%)	6 (9%)	9	37
9	G	472/474 (100%)	464 (98%)	8 (2%)	60	82
9	g	472/474 (100%)	464 (98%)	8 (2%)	60	82
10	J	111/116 (96%)	110 (99%)	1 (1%)	78	90
10	j	111/116 (96%)	110 (99%)	1 (1%)	78	90
11	K	330/332 (99%)	297 (90%)	33 (10%)	7	32
11	k	330/332 (99%)	291 (88%)	39 (12%)	5	25
12	H	370/373 (99%)	359 (97%)	11 (3%)	41	71
12	h	370/373 (99%)	360 (97%)	10 (3%)	44	73
All	All	6810/7222 (94%)	6562 (96%)	248 (4%)	38	66

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	H	126	SER
11	k	187	ILE
3	e	207	ASN

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Mol	Chain	Res	Type
11	k	177	CYS
11	k	253	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
9	g	273	HIS
10	j	73	GLN
12	h	386	HIS
12	h	325	HIS
9	G	274	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
9	KCX	G	184	9,17	9,11,12	2.05	1 (11%)	5,12,14	3.05	1 (20%)
9	KCX	g	184	9,17	9,11,12	0.35	0	5,12,14	0.51	0

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
9	KCX	G	184	9,17	-	3/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	KCX	g	184	9,17	-	3/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	184	KCX	OQ1-CX	6.08	1.32	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	184	KCX	OQ1-CX-NZ	-6.77	114.47	124.96

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	g	184	KCX	OQ1-CX-NZ-CE
9	G	184	KCX	OQ1-CX-NZ-CE
9	G	184	KCX	OQ2-CX-NZ-CE
9	g	184	KCX	OQ2-CX-NZ-CE
9	G	184	KCX	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 68 ligands modelled in this entry, 6 are monoatomic - leaving 62 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	SF4	a	703	1	0,12,12	-	-	-		
13	SF4	k	403	11	0,12,12	-	-	-		
13	SF4	L	201	8	0,12,12	-	-	-		
13	SF4	K	401	11	0,12,12	-	-	-		
13	SF4	A	703	1	0,12,12	-	-	-		
13	SF4	A	707	1	0,12,12	-	-	-		
13	SF4	a	707	1	0,12,12	-	-	-		
16	9S8	B	301	5	2,10,10	1.15	0	-		
13	SF4	K	402	11	0,12,12	-	-	-		
13	SF4	a	705	1	0,12,12	-	-	-		
13	SF4	A	701	1	0,12,12	-	-	-		
13	SF4	l	201	8	0,12,12	-	-	-		
13	SF4	h	504	12	0,12,12	-	-	-		
13	SF4	k	401	11	0,12,12	-	-	-		
13	SF4	K	408	11	0,12,12	-	-	-		
13	SF4	L	202	8	0,12,12	-	-	-		
13	SF4	K	406	11	0,12,12	-	-	-		
13	SF4	A	705	1	0,12,12	-	-	-		
13	SF4	k	408	11	0,12,12	-	-	-		
14	FAD	e	505	-	53,58,58	1.06	3 (5%)	68,89,89	0.60	1 (1%)
14	FAD	a	702	-	53,58,58	0.86	2 (3%)	68,89,89	0.59	1 (1%)
19	MGD	h	503	18	41,52,52	5.92	28 (68%)	40,81,81	1.80	10 (25%)
13	SF4	k	406	11	0,12,12	-	-	-		
13	SF4	E	504	3	0,12,12	-	-	-		
13	SF4	c	201	4	0,12,12	-	-	-		
19	MGD	h	502	18	41,52,52	5.90	27 (65%)	40,81,81	1.92	9 (22%)
15	FES	F	201	2	0,4,4	-	-	-		
16	9S8	B	302	5	2,10,10	1.22	0	-		
13	SF4	d	701	6	0,12,12	-	-	-		
19	MGD	H	503	18	41,52,52	5.93	28 (68%)	40,81,81	1.80	10 (25%)
13	SF4	a	706	1	0,12,12	-	-	-		
13	SF4	c	202	4	0,12,12	-	-	-		
13	SF4	e	503	3	0,12,12	-	-	-		
13	SF4	A	706	1	0,12,12	-	-	-		
14	FAD	E	505	-	53,58,58	1.06	3 (5%)	68,89,89	0.60	1 (1%)
13	SF4	C	202	4	0,12,12	-	-	-		
13	SF4	k	407	11	0,12,12	-	-	-		
13	SF4	E	503	3	0,12,12	-	-	-		
13	SF4	k	405	11	0,12,12	-	-	-		
16	9S8	b	302	5	2,10,10	1.19	0	-		
13	SF4	e	501	3	0,12,12	-	-	-		
13	SF4	E	501	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	SF4	E	502	3	0,12,12	-	-	-		
13	SF4	C	201	4	0,12,12	-	-	-		
14	FAD	A	702	-	53,58,58	0.87	2 (3%)	68,89,89	0.59	1 (1%)
13	SF4	K	403	11	0,12,12	-	-	-		
13	SF4	k	402	11	0,12,12	-	-	-		
16	9S8	b	301	5	2,10,10	1.10	0	-		
13	SF4	A	704	1	0,12,12	-	-	-		
13	SF4	a	704	1	0,12,12	-	-	-		
13	SF4	a	701	1	0,12,12	-	-	-		
13	SF4	K	407	11	0,12,12	-	-	-		
13	SF4	e	504	3	0,12,12	-	-	-		
13	SF4	k	404	11	0,12,12	-	-	-		
13	SF4	H	504	12	0,12,12	-	-	-		
13	SF4	K	404	11	0,12,12	-	-	-		
19	MGD	H	502	18	41,52,52	5.91	27 (65%)	40,81,81	1.92	9 (22%)
13	SF4	l	202	8	0,12,12	-	-	-		
13	SF4	e	502	3	0,12,12	-	-	-		
15	FES	f	201	2	0,4,4	-	-	-		
13	SF4	K	405	11	0,12,12	-	-	-		
13	SF4	D	701	6	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	a	703	1	-	-	0/6/5/5
13	SF4	k	403	11	-	-	0/6/5/5
13	SF4	L	201	8	-	-	0/6/5/5
13	SF4	K	401	11	-	-	0/6/5/5
13	SF4	A	703	1	-	-	0/6/5/5
13	SF4	A	707	1	-	-	0/6/5/5
13	SF4	a	707	1	-	-	0/6/5/5
16	9S8	B	301	5	-	-	0/3/3/3
13	SF4	K	402	11	-	-	0/6/5/5
13	SF4	a	705	1	-	-	0/6/5/5
13	SF4	A	701	1	-	-	0/6/5/5
13	SF4	l	201	8	-	-	0/6/5/5
13	SF4	h	504	12	-	-	0/6/5/5
13	SF4	k	401	11	-	-	0/6/5/5
13	SF4	K	408	11	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	L	202	8	-	-	0/6/5/5
13	SF4	K	406	11	-	-	0/6/5/5
13	SF4	A	705	1	-	-	0/6/5/5
13	SF4	k	408	11	-	-	0/6/5/5
14	FAD	e	505	-	-	13/30/50/50	0/6/6/6
14	FAD	a	702	-	-	2/30/50/50	0/6/6/6
19	MGD	h	503	18	-	9/18/66/66	0/6/6/6
13	SF4	k	406	11	-	-	0/6/5/5
13	SF4	E	504	3	-	-	0/6/5/5
19	MGD	h	502	18	-	9/18/66/66	0/6/6/6
13	SF4	c	201	4	-	-	0/6/5/5
15	FES	F	201	2	-	-	0/1/1/1
16	9S8	B	302	5	-	-	0/3/3/3
19	MGD	H	503	18	-	9/18/66/66	0/6/6/6
13	SF4	d	701	6	-	-	0/6/5/5
13	SF4	a	706	1	-	-	0/6/5/5
13	SF4	c	202	4	-	-	0/6/5/5
13	SF4	e	503	3	-	-	0/6/5/5
13	SF4	A	706	1	-	-	0/6/5/5
14	FAD	E	505	-	-	13/30/50/50	0/6/6/6
13	SF4	C	202	4	-	-	0/6/5/5
13	SF4	k	407	11	-	-	0/6/5/5
13	SF4	E	503	3	-	-	0/6/5/5
13	SF4	k	405	11	-	-	0/6/5/5
16	9S8	b	302	5	-	-	0/3/3/3
13	SF4	e	501	3	-	-	0/6/5/5
13	SF4	E	501	3	-	-	0/6/5/5
13	SF4	E	502	3	-	-	0/6/5/5
13	SF4	C	201	4	-	-	0/6/5/5
14	FAD	A	702	-	-	2/30/50/50	0/6/6/6
13	SF4	K	403	11	-	-	0/6/5/5
13	SF4	k	402	11	-	-	0/6/5/5
16	9S8	b	301	5	-	-	0/3/3/3
13	SF4	A	704	1	-	-	0/6/5/5
13	SF4	a	704	1	-	-	0/6/5/5
13	SF4	a	701	1	-	-	0/6/5/5
13	SF4	K	407	11	-	-	0/6/5/5
13	SF4	e	504	3	-	-	0/6/5/5
13	SF4	k	404	11	-	-	0/6/5/5
13	SF4	H	504	12	-	-	0/6/5/5
13	SF4	K	404	11	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	MGD	H	502	18	-	9/18/66/66	0/6/6/6
13	SF4	l	202	8	-	-	0/6/5/5
13	SF4	e	502	3	-	-	0/6/5/5
15	FES	f	201	2	-	-	0/1/1/1
13	SF4	K	405	11	-	-	0/6/5/5
13	SF4	D	701	6	-	-	0/6/5/5

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	h	502	MGD	C2'-C1'	-19.00	1.24	1.53
19	H	502	MGD	C2'-C1'	-18.98	1.25	1.53
19	H	503	MGD	C2'-C1'	-17.96	1.26	1.53
19	h	503	MGD	C2'-C1'	-17.78	1.26	1.53
19	H	503	MGD	C16-C21	12.87	1.60	1.38

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	H	502	MGD	O11-C23-N22	-5.62	102.79	108.57
19	h	502	MGD	O11-C23-N22	-5.60	102.81	108.57
19	h	502	MGD	C19-N20-C21	3.92	120.50	113.43
19	H	502	MGD	C19-N20-C21	3.89	120.45	113.43
19	H	503	MGD	C19-N20-C21	3.71	120.13	113.43

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	E	505	FAD	C5B-O5B-PA-O1A
14	E	505	FAD	C1'-C2'-C3'-O3'
14	E	505	FAD	C1'-C2'-C3'-C4'
14	E	505	FAD	O2'-C2'-C3'-O3'
14	E	505	FAD	O2'-C2'-C3'-C4'

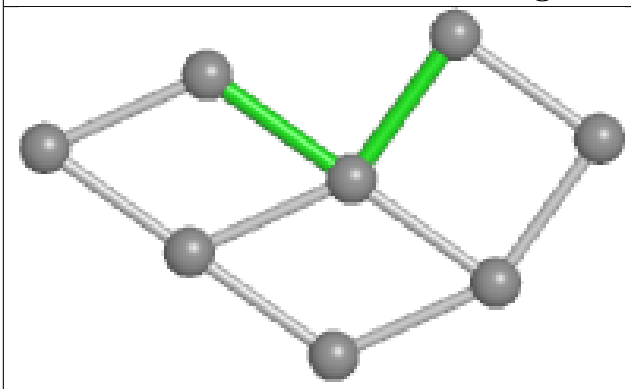
There are no ring outliers.

No monomer is involved in short contacts.

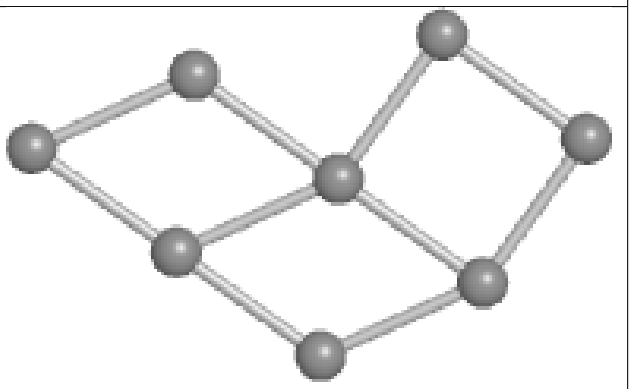
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

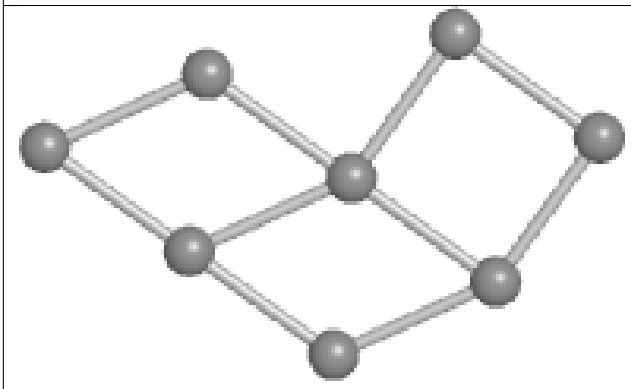
Ligand 9S8 B 301



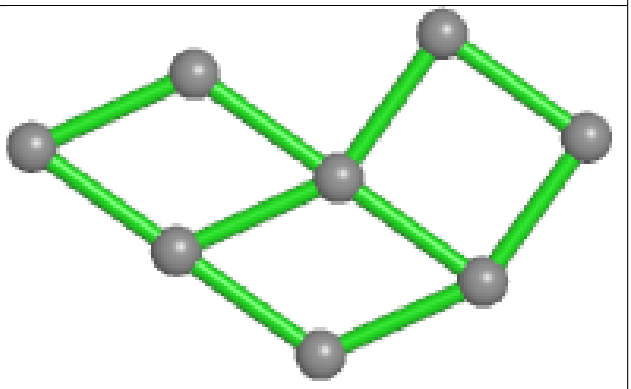
Bond lengths



Bond angles

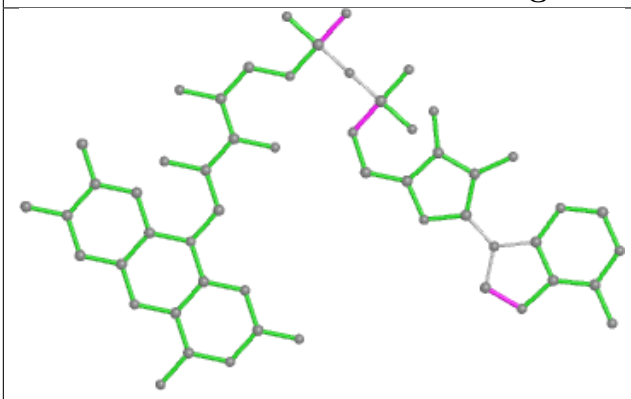


Torsions

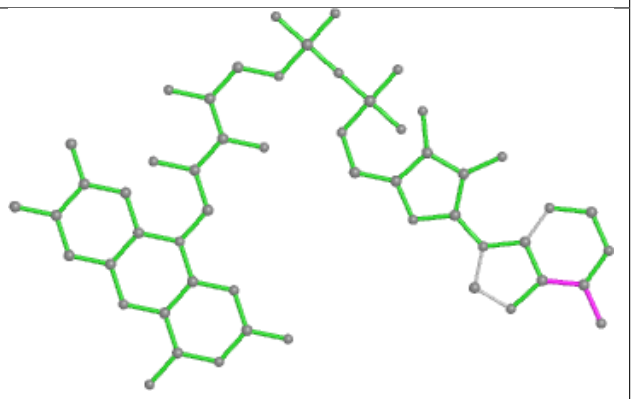


Rings

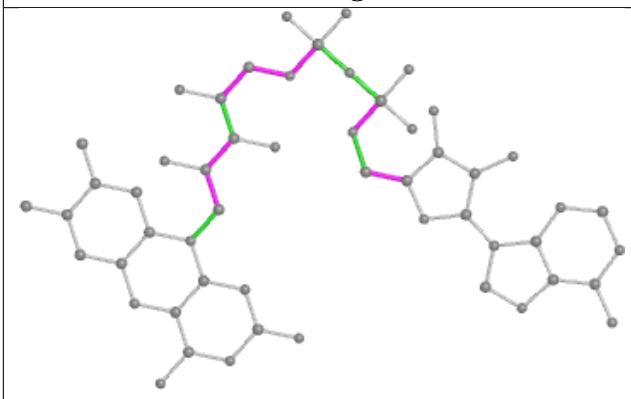
Ligand FAD e 505



Bond lengths



Bond angles



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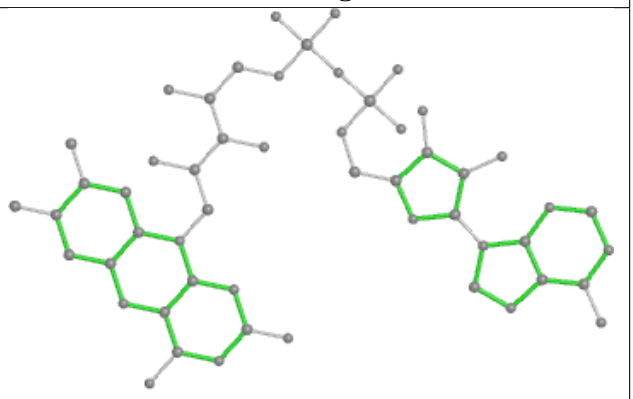
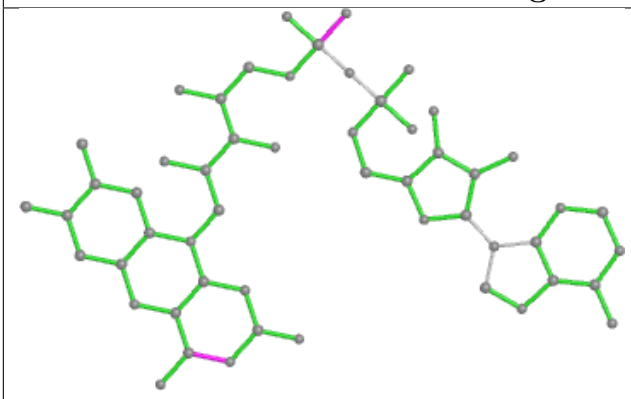
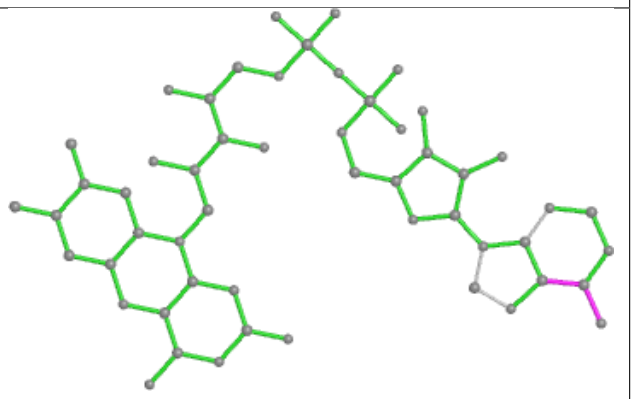


Rings

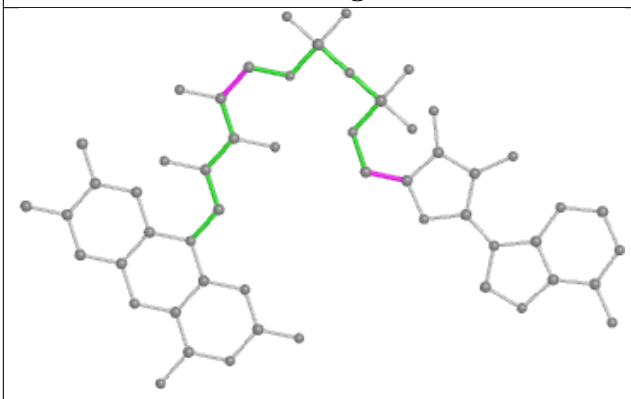
Ligand FAD a 702



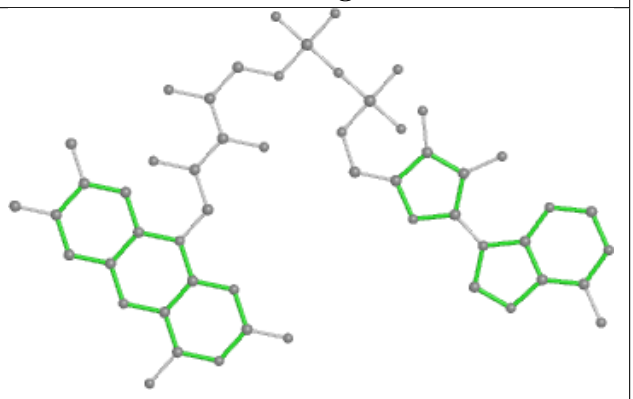
Bond lengths



Bond angles

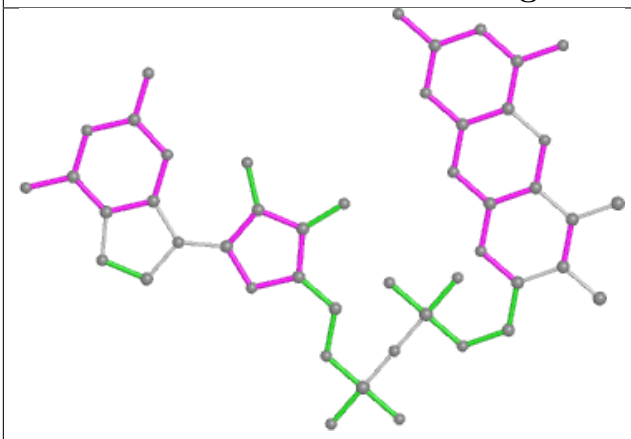


Torsions

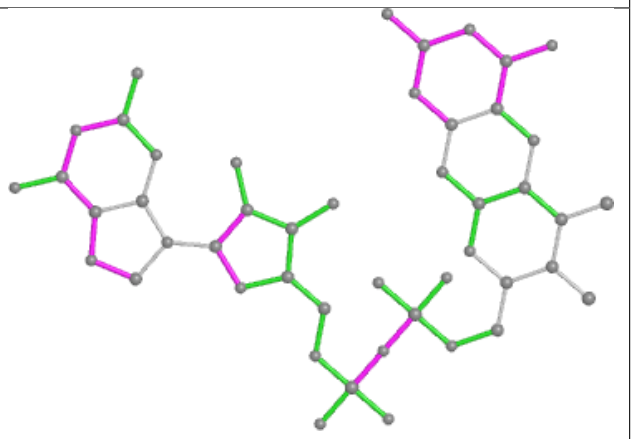


Rings

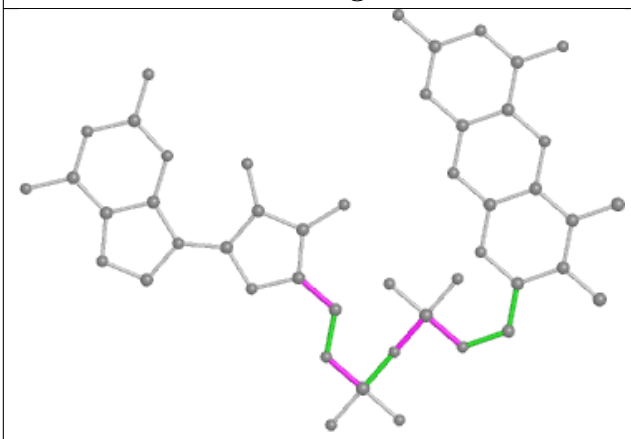
Ligand MGD h 503



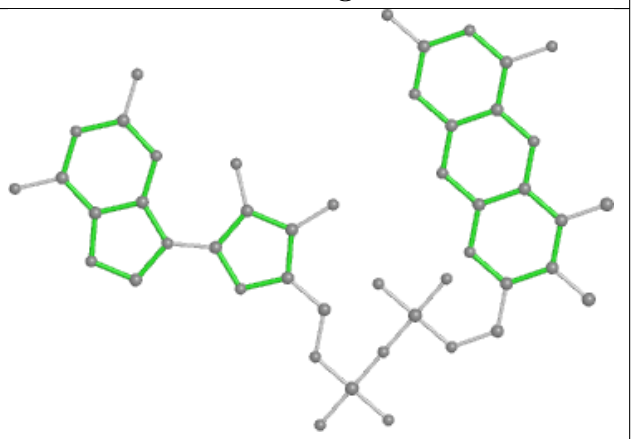
Bond lengths



Bond angles

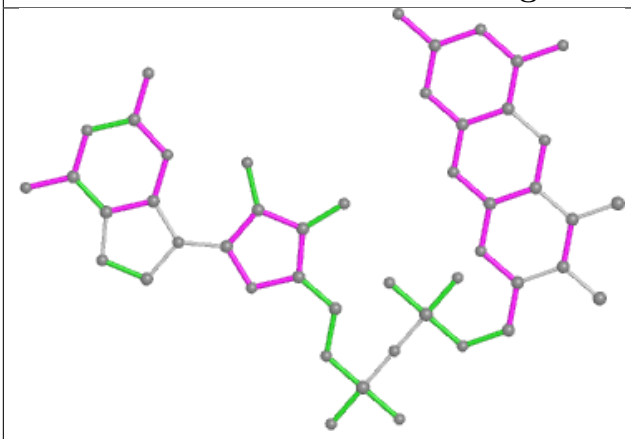


Torsions

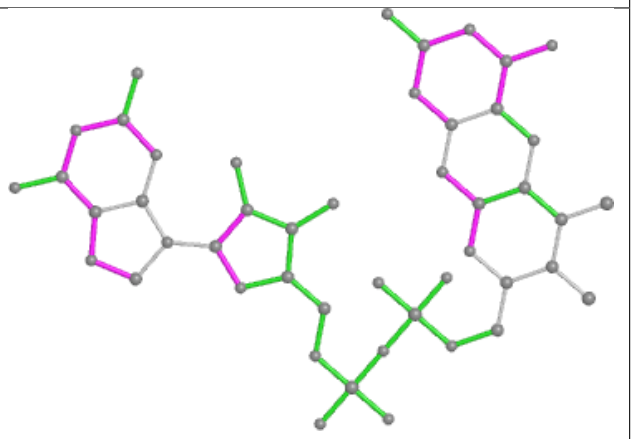


Rings

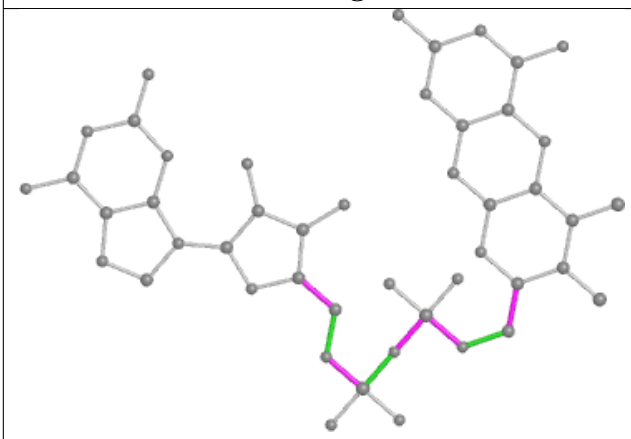
Ligand MGD h 502



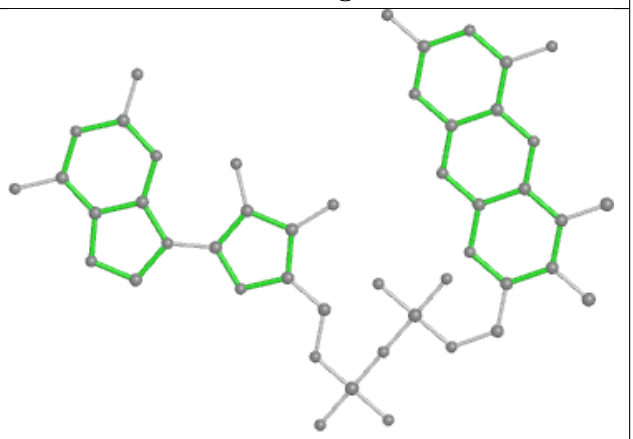
Bond lengths



Bond angles

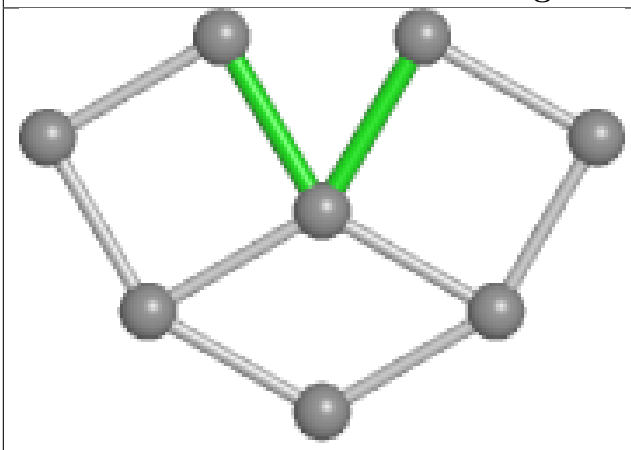


Torsions

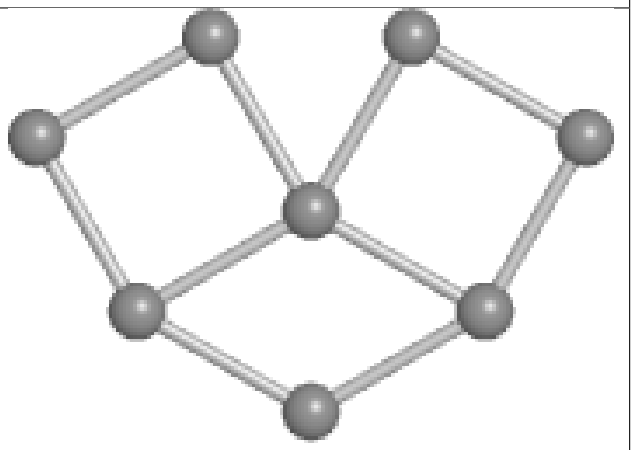


Rings

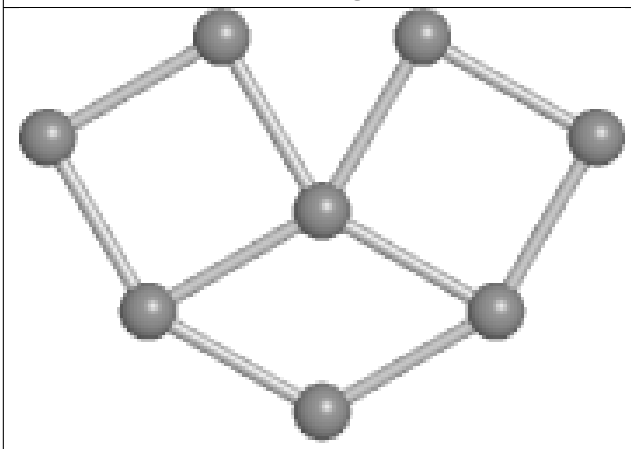
Ligand 9S8 B 302



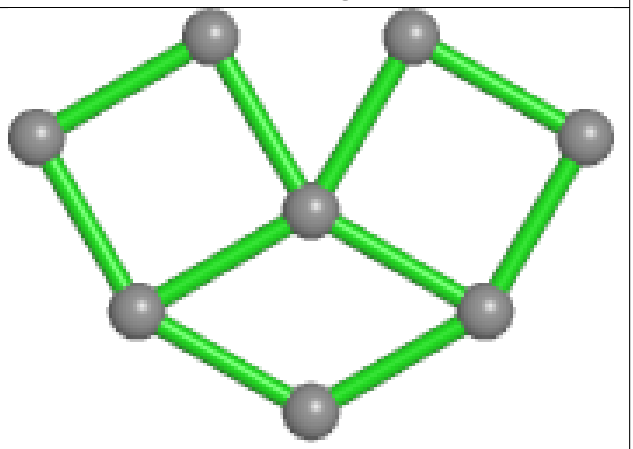
Bond lengths



Bond angles

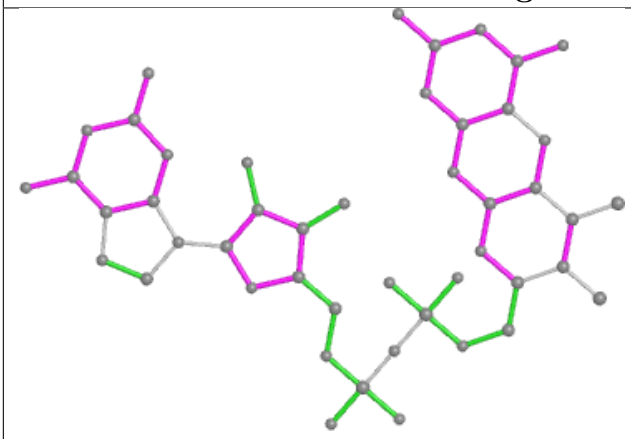


Torsions

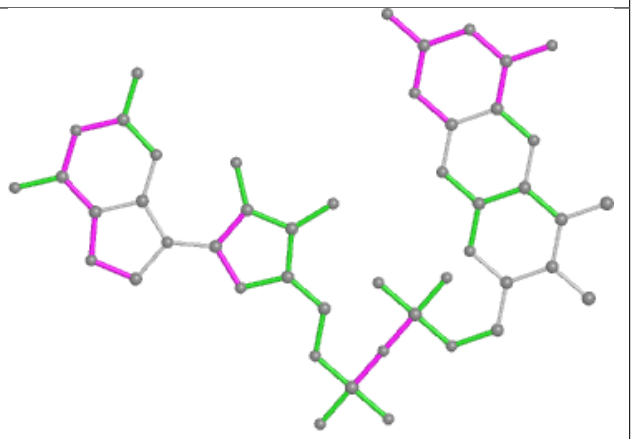


Rings

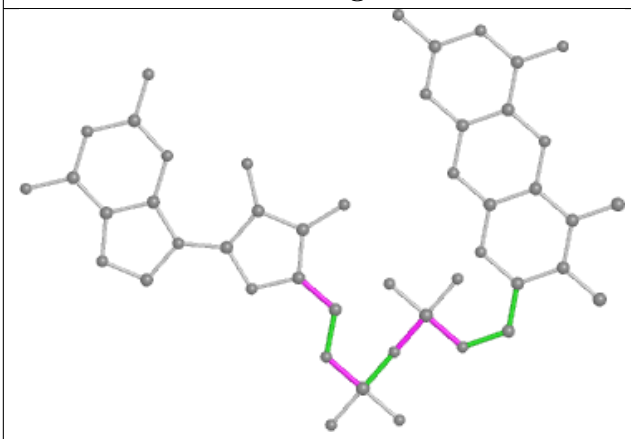
Ligand MGD H 503



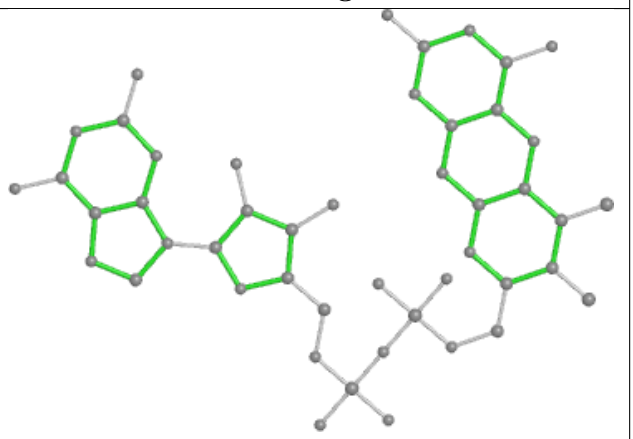
Bond lengths



Bond angles

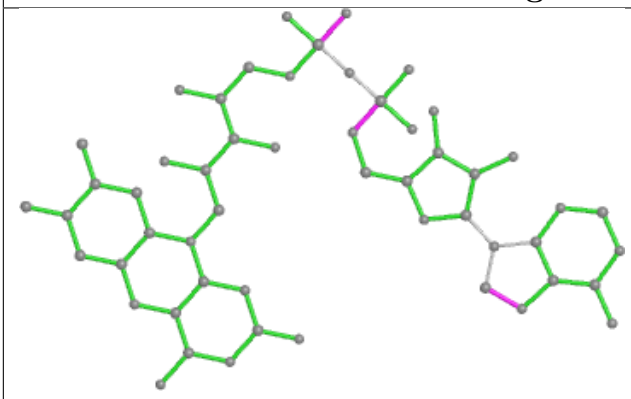


Torsions

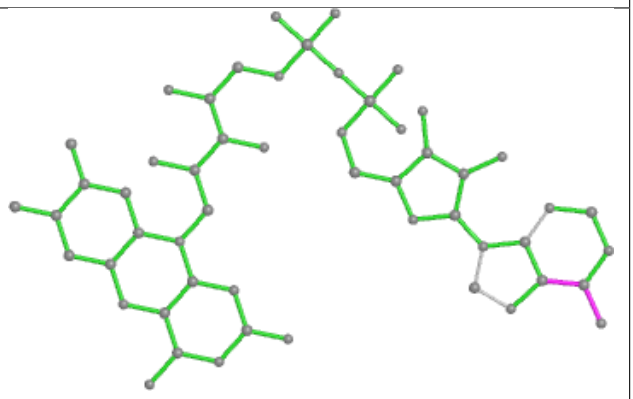


Rings

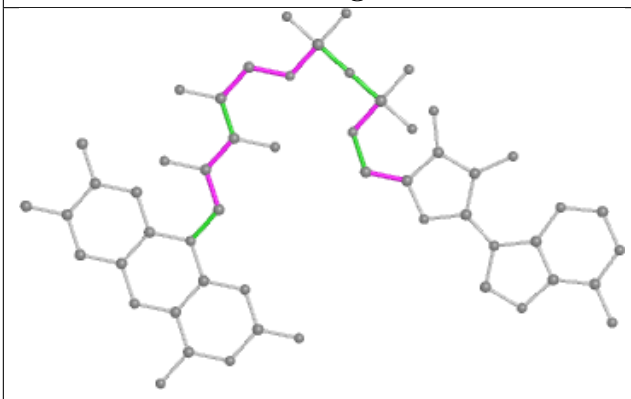
Ligand FAD E 505



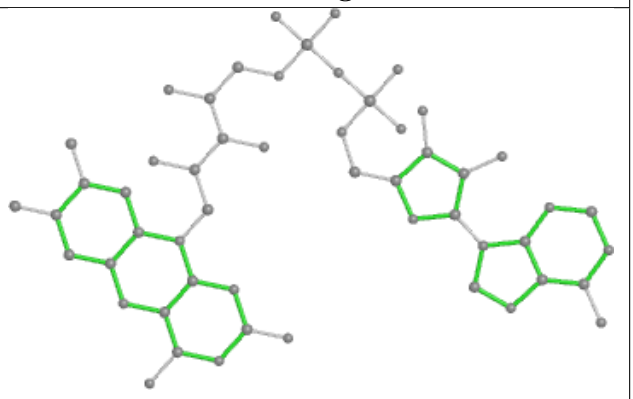
Bond lengths



Bond angles

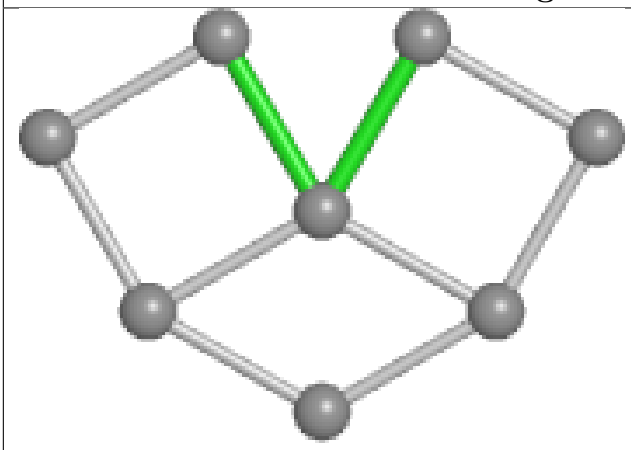


Torsions

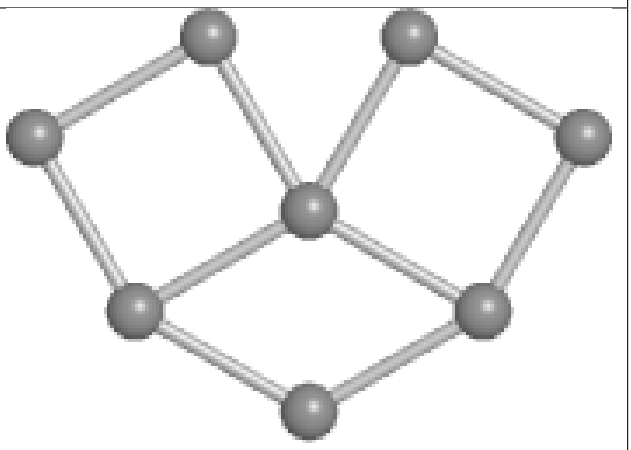


Rings

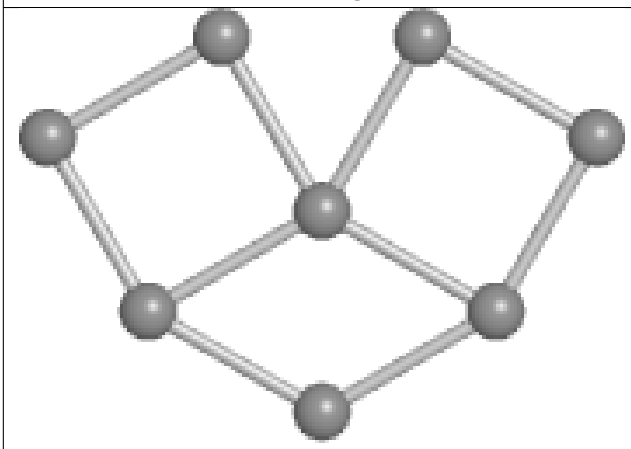
Ligand 9S8 b 302



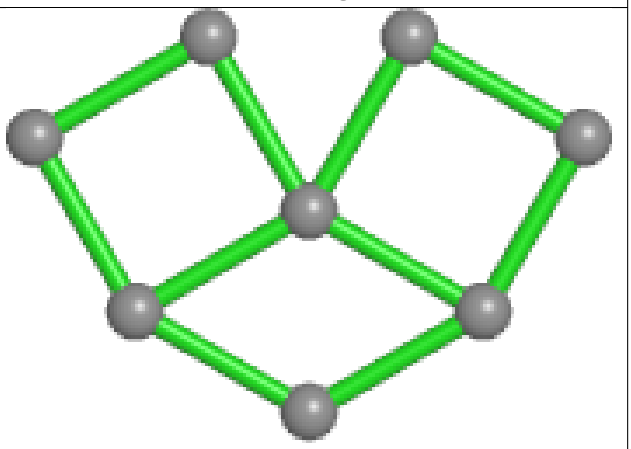
Bond lengths



Bond angles

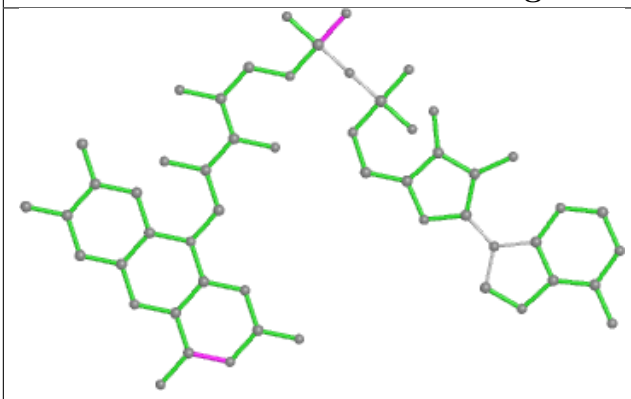


Torsions

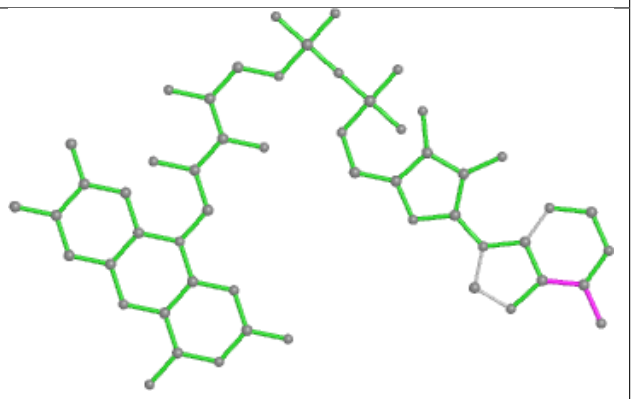


Rings

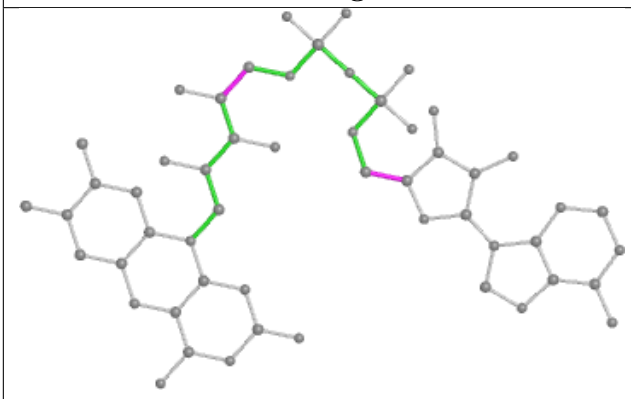
Ligand FAD A 702



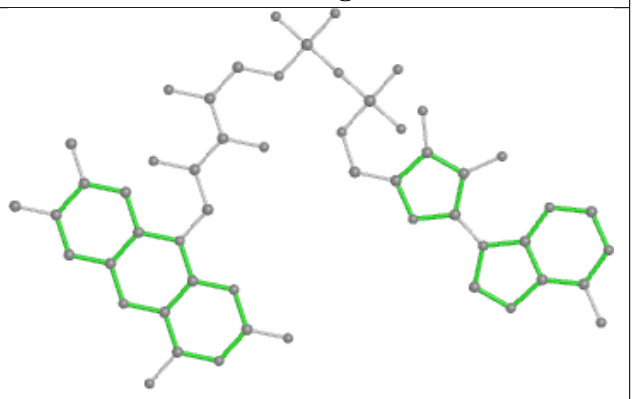
Bond lengths



Bond angles

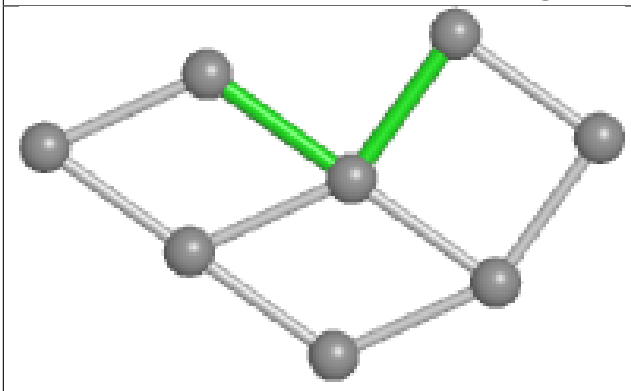


Torsions

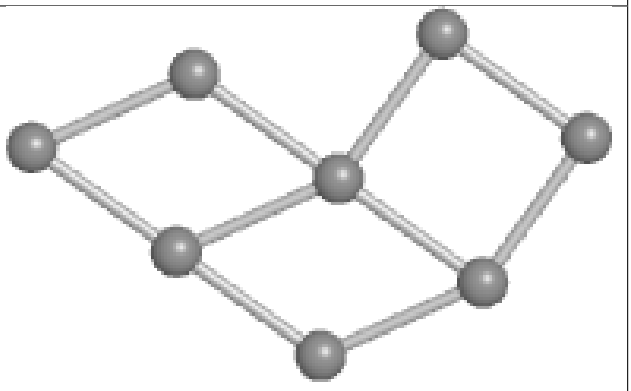


Rings

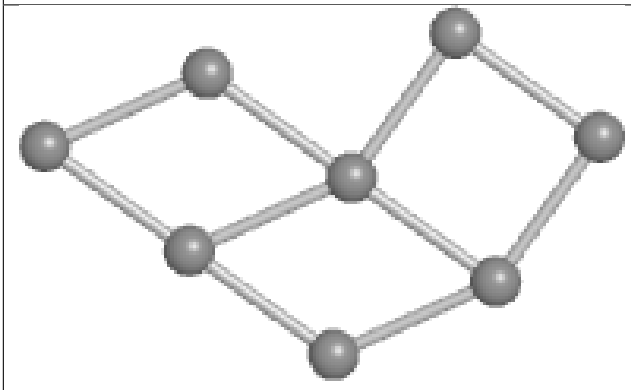
Ligand 9S8 b 301



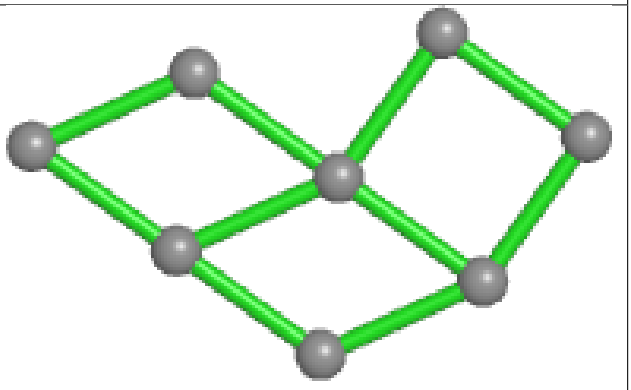
Bond lengths



Bond angles

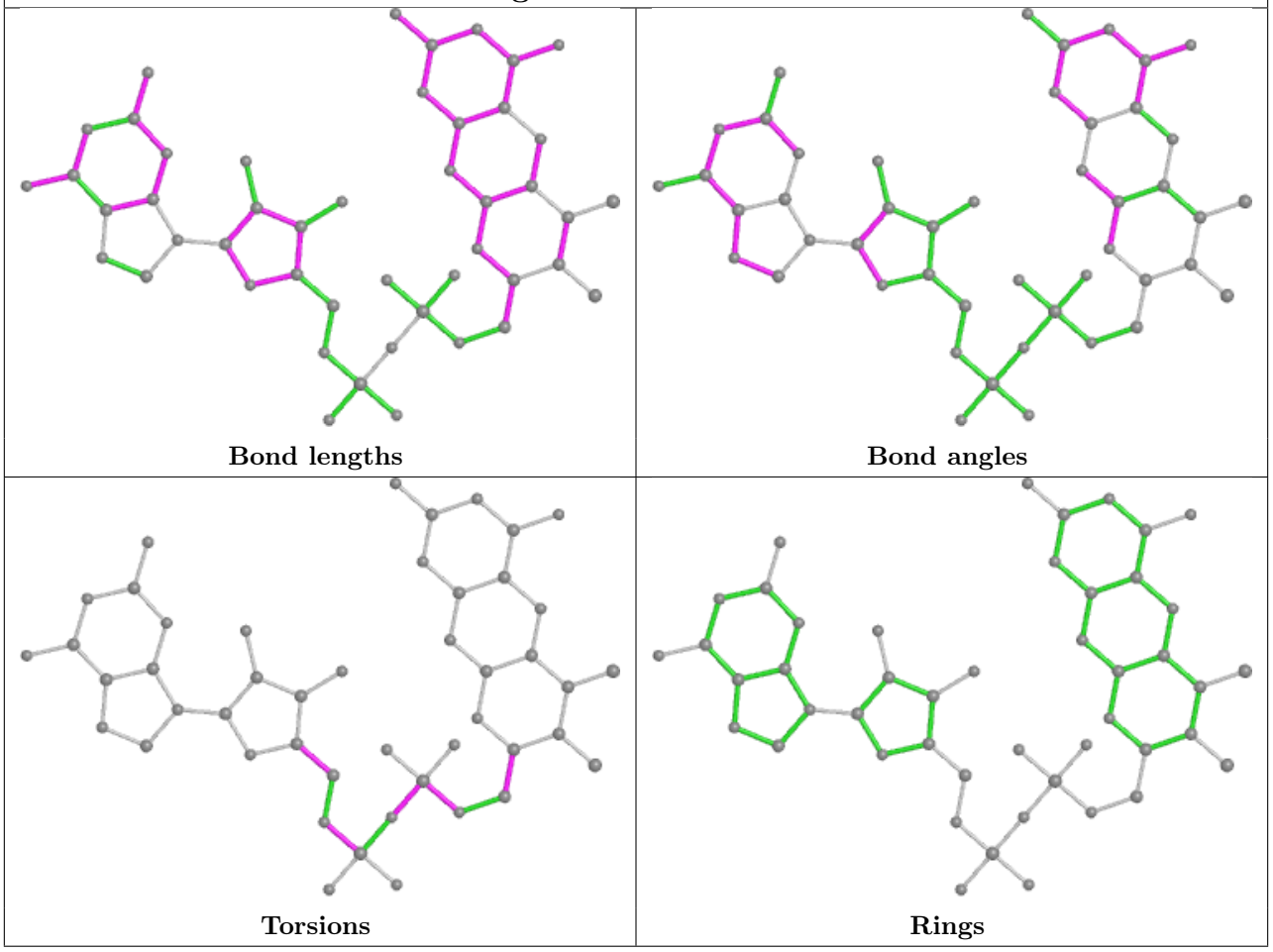


Torsions



Rings

Ligand MGD H 502



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.

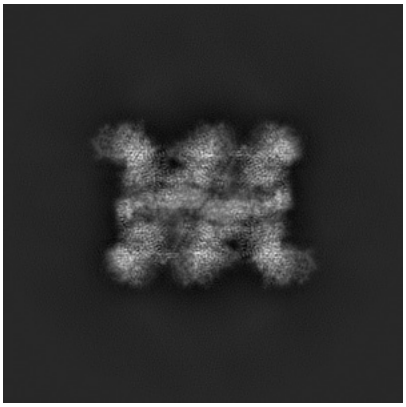
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12206. These allow visual inspection of the internal detail of the map and identification of artifacts.

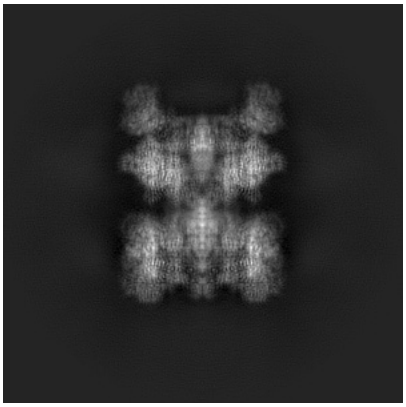
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

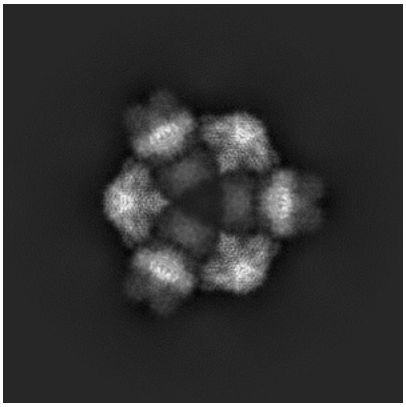
6.1.1 Primary map



X



Y

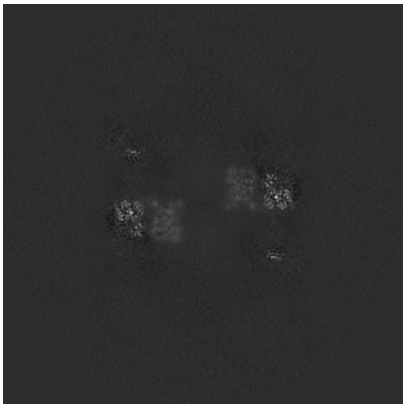


Z

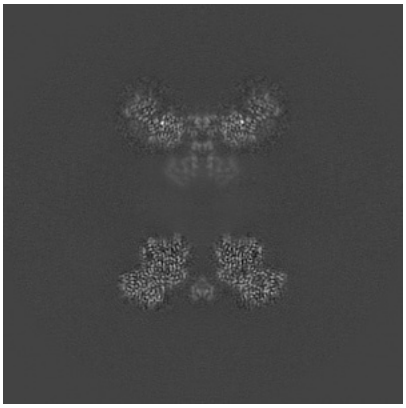
The images above show the map projected in three orthogonal directions.

6.2 Central slices

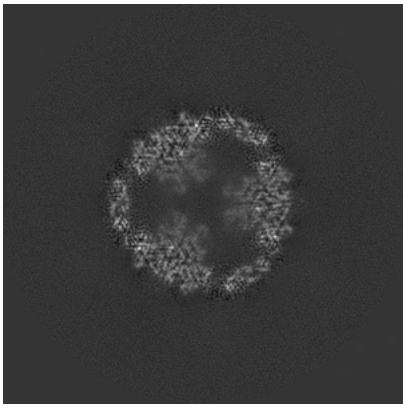
6.2.1 Primary map



X Index: 160



Y Index: 160

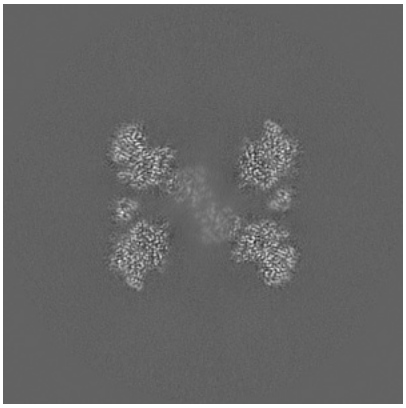


Z Index: 160

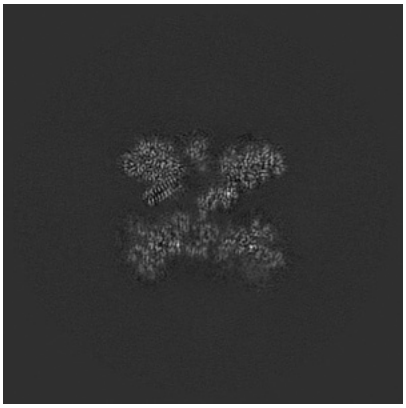
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

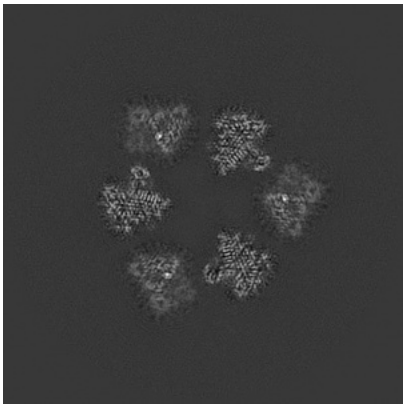
6.3.1 Primary map



X Index: 187



Y Index: 214

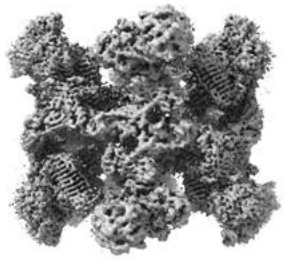


Z Index: 198

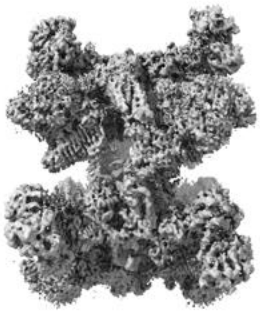
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

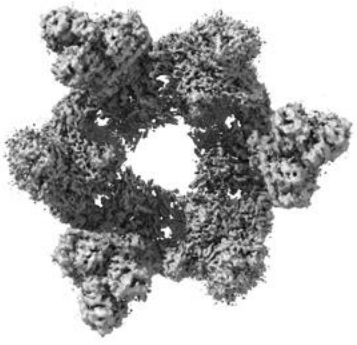
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

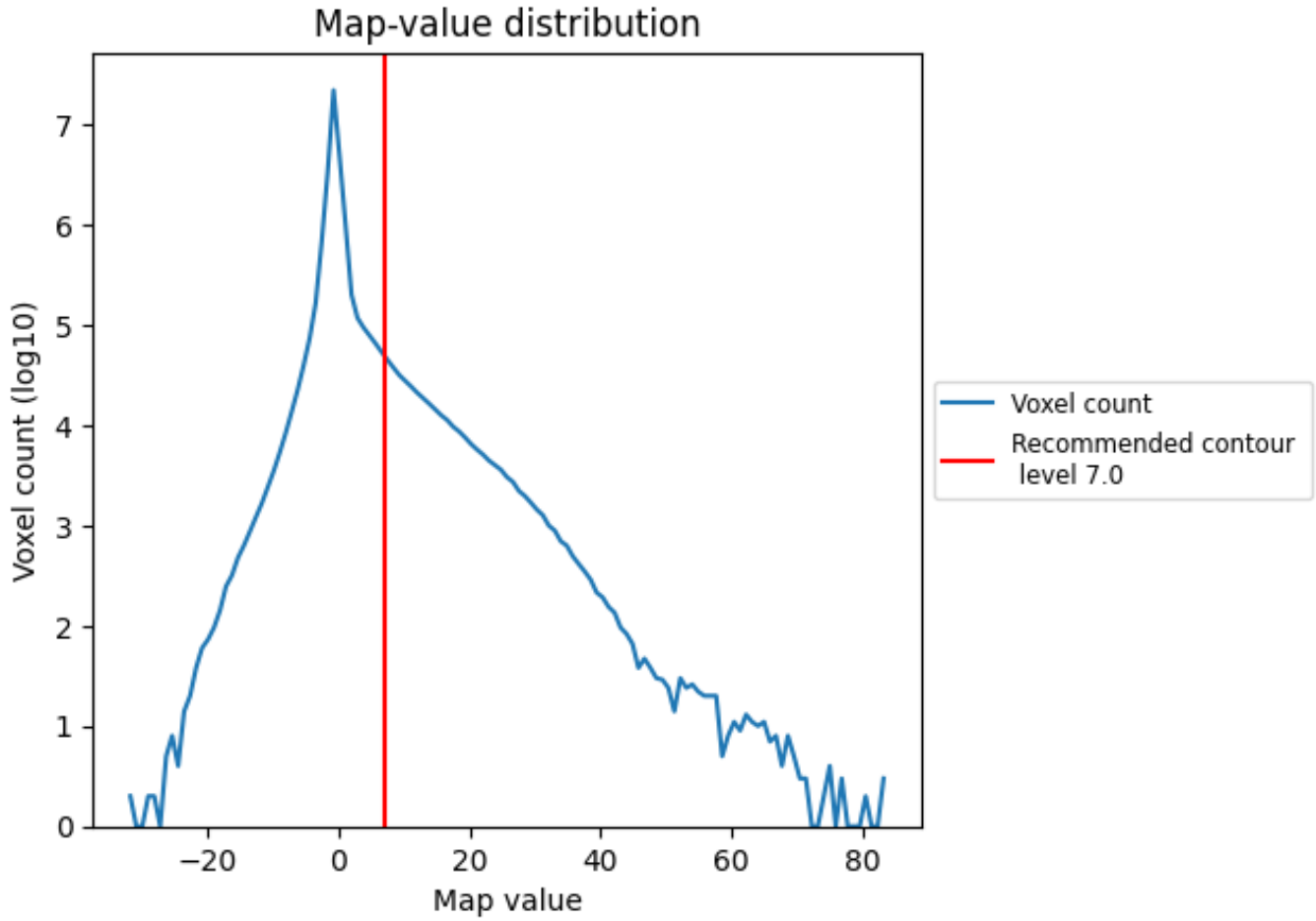
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

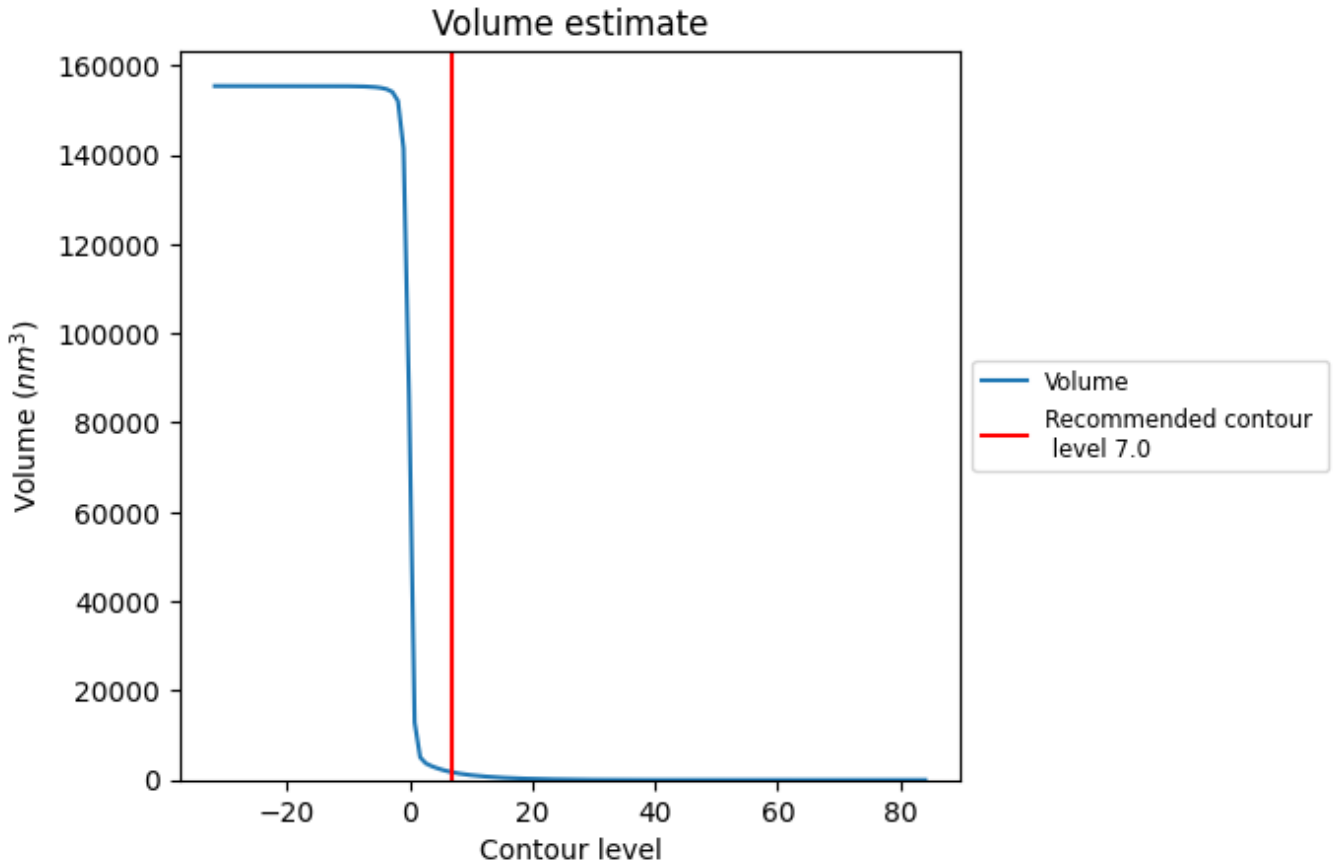
This section contains the results of statistical analysis of the map.

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.

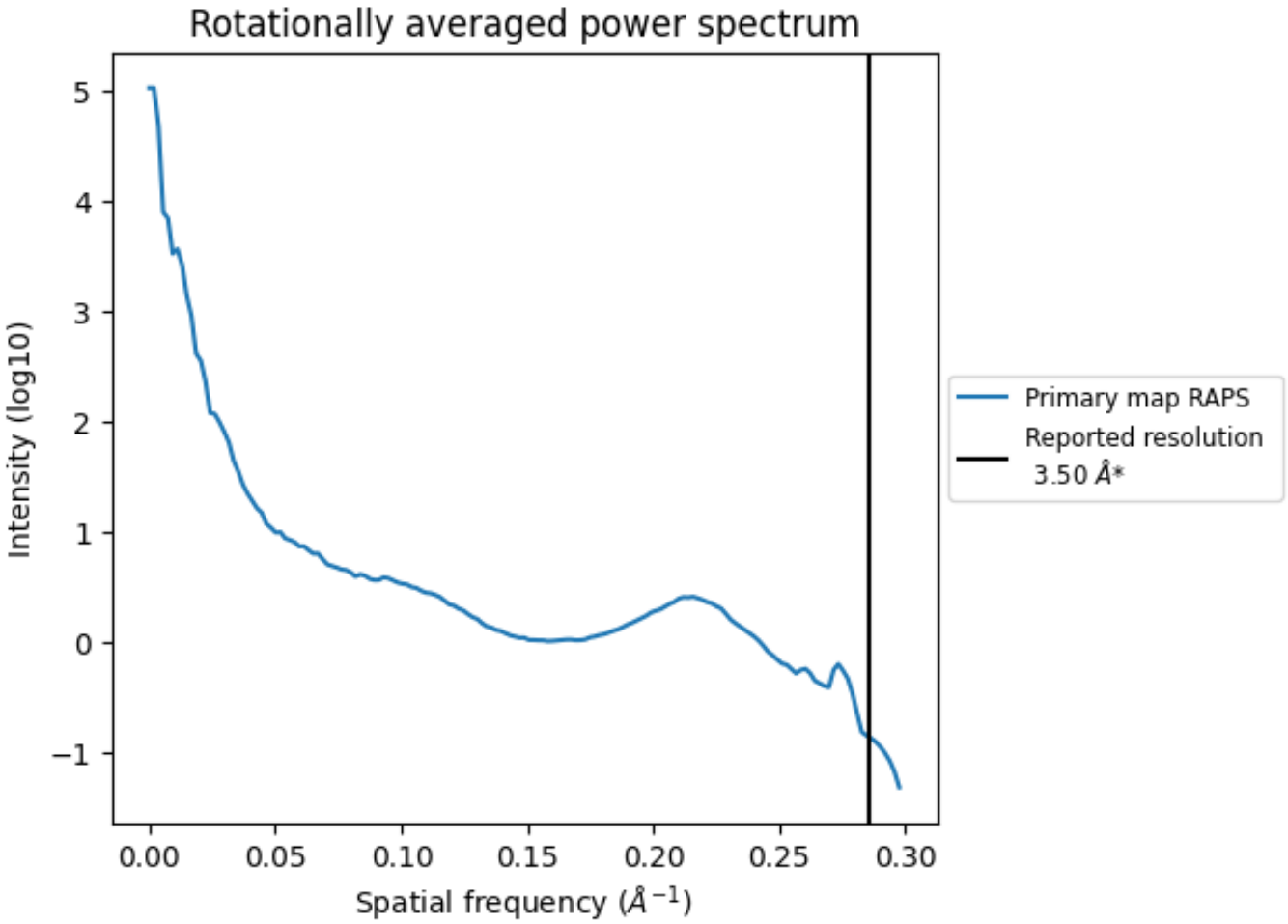
7.2 Volume estimate (i)



The volume at the recommended contour level is 1712 nm^3; this corresponds to an approximate mass of 1547 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 0.286 Å^{-1}

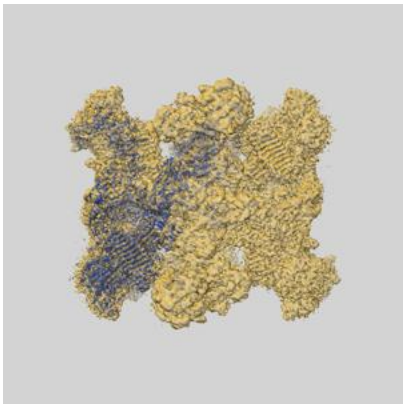
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

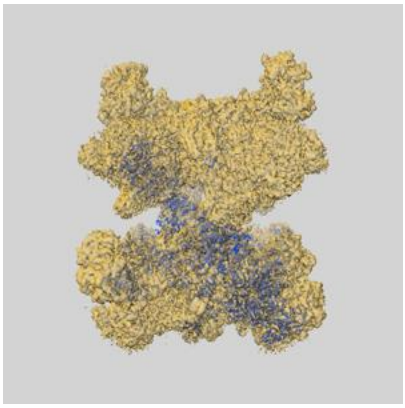
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12206 and PDB model 7BKB. Per-residue inclusion information can be found in section 3 on page 13.

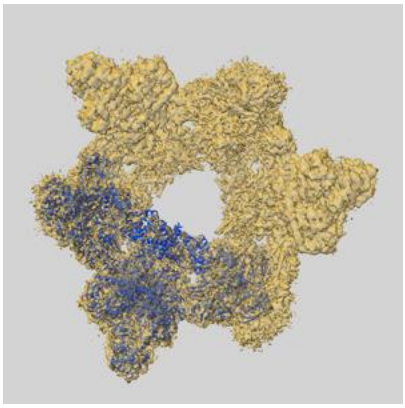
9.1 Map-model overlay



X



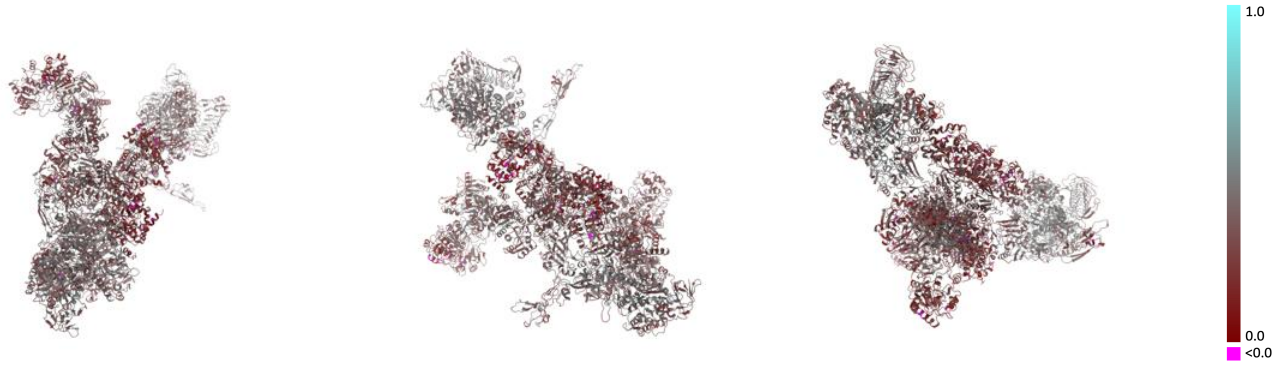
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.0 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.

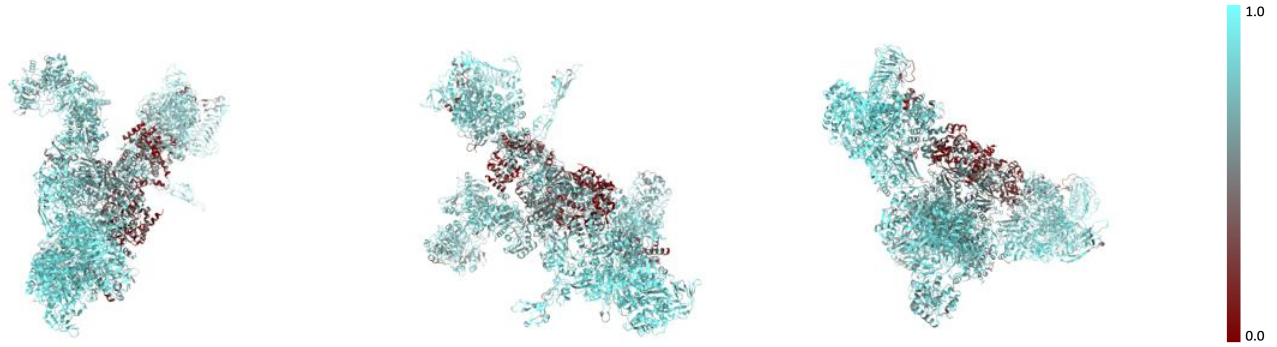
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

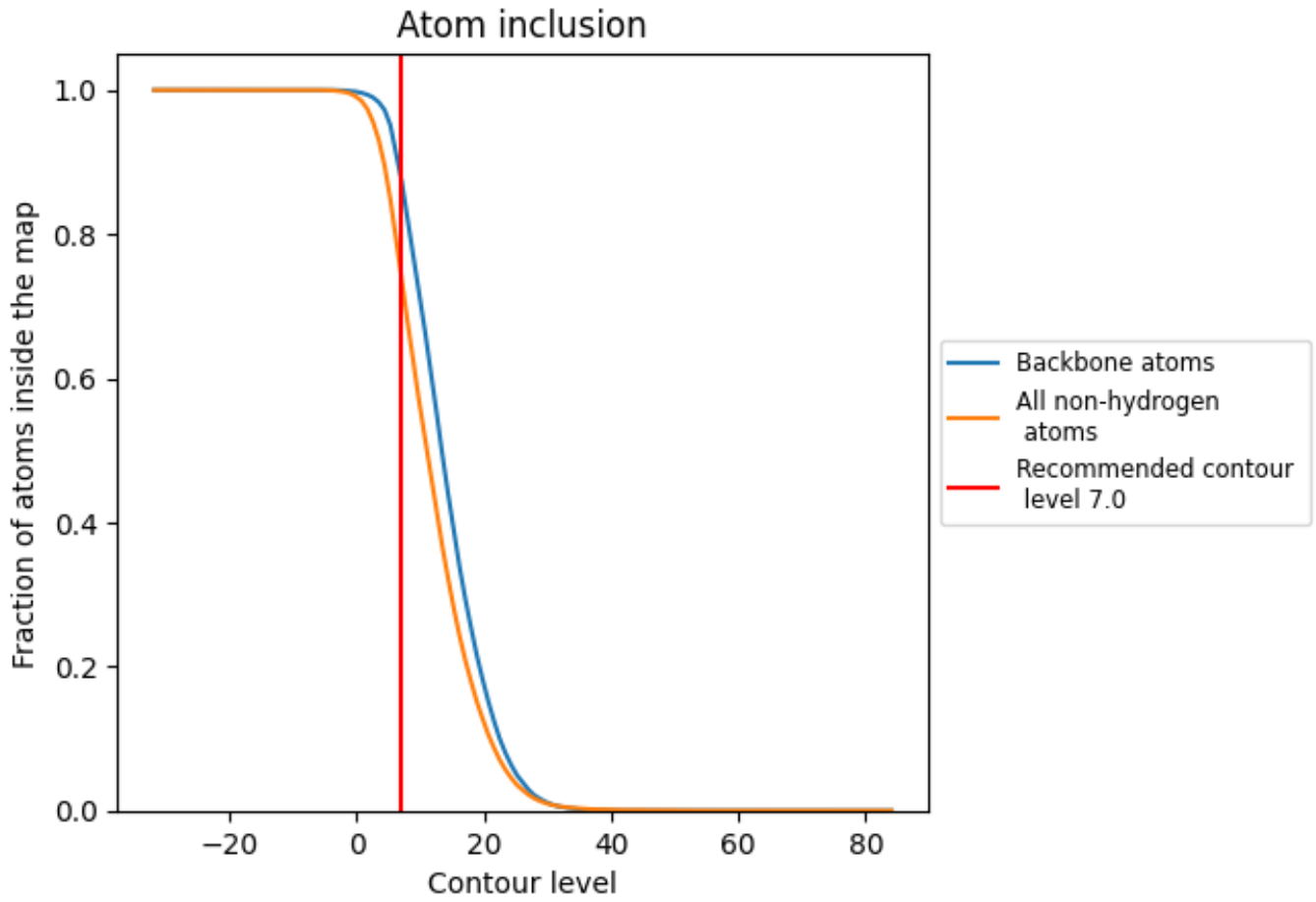
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.0).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (7.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7451	0.3480
A	0.7277	0.3440
B	0.3645	0.2380
C	0.4529	0.2320
D	0.7426	0.2900
E	0.8190	0.3260
F	0.7842	0.3330
G	0.8866	0.4040
H	0.7944	0.3980
I	0.7812	0.3820
J	0.7399	0.3440
K	0.8168	0.3900
L	0.8316	0.4130
a	0.7489	0.3490
b	0.3370	0.2670
c	0.3946	0.2370
d	0.7189	0.2690
e	0.8222	0.3380
f	0.8061	0.3480
g	0.8946	0.4200
h	0.8088	0.4260
i	0.7964	0.4090
j	0.7692	0.3960
k	0.8151	0.3760
l	0.7976	0.3730