Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 10:20 pm GMT

PDB ID	:	7BKC
EMDB ID	:	EMD-12209
Title	:	Formate dehydrogenase - heterodisulfide reductase - formylmethanofuran dehydrogenase complex from Methanospirillum hungatei (dimeric, composite structure)
Authors	:	Pfeil-Gardiner, O.; Watanabe, T.; Shima, S.; Murphy, B.J.
Deposited on	:	2021-01-15
Resolution	:	3.00 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:

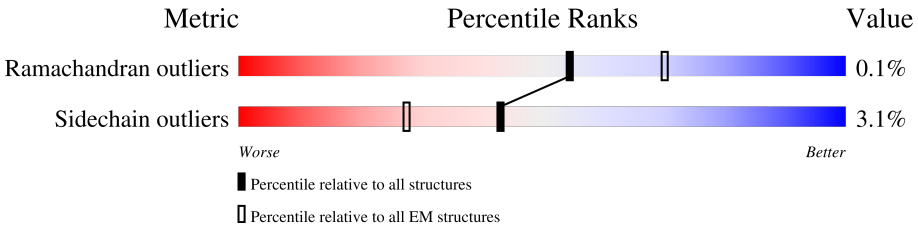
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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.



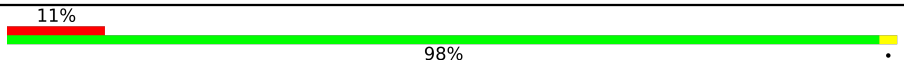
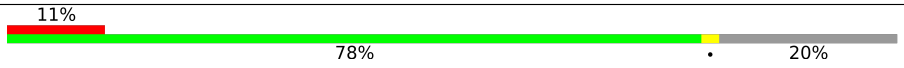
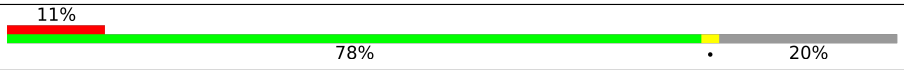
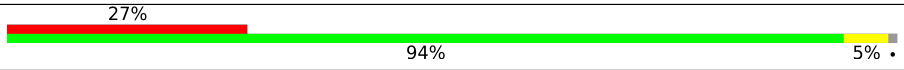
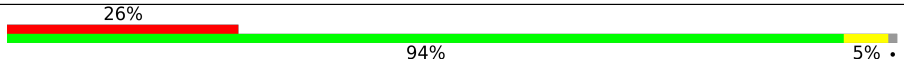
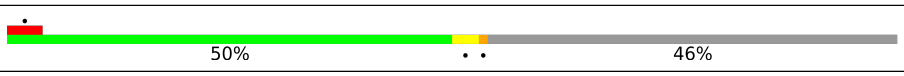
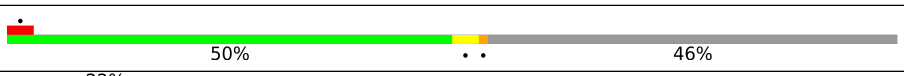
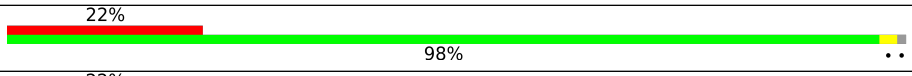
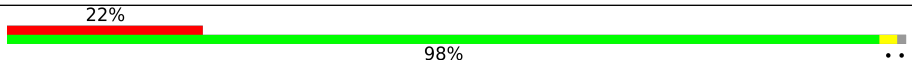
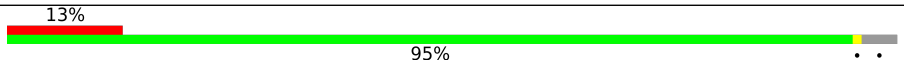
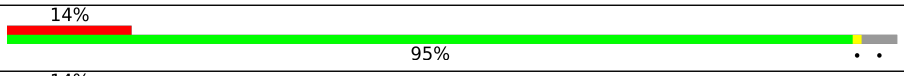
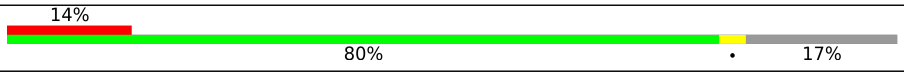
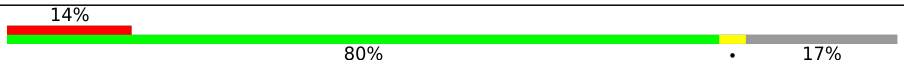
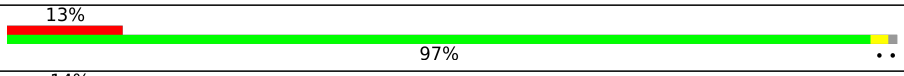
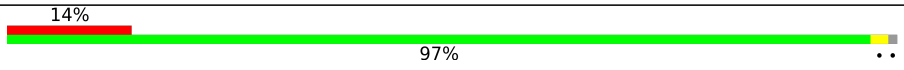
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	97%
1	a	671	97%
2	F	140	5% 95%
2	f	140	5% 95%
3	E	414	96%
3	e	414	96%
4	C	191	8% 99%
4	c	191	9% 99%
5	B	296	9% 98%

Continued on next page...

Continued from previous page...

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	M	388	
11	k	388	
11	m	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		

Continued on next page...

Continued from previous page...

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

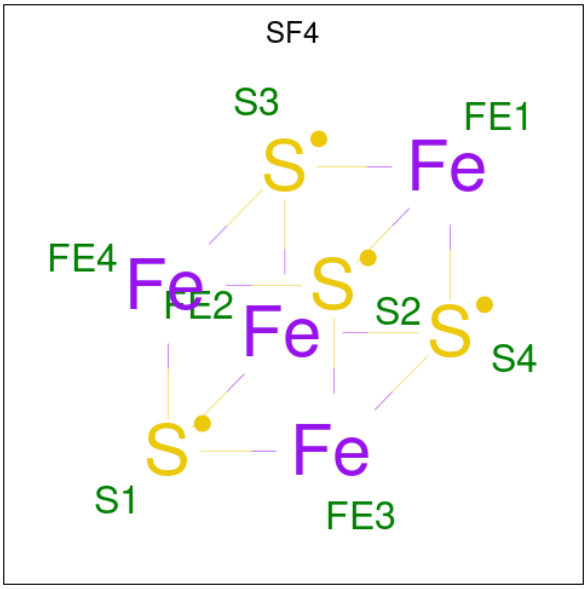
- Molecule 11 is a protein called Formylmethanofuran dehydrogenase, subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	65	Total	C	N	O	S	0	0
			487	303	77	99	8		
11	K	321	Total	C	N	O	S	0	0
			2423	1512	411	472	28		
11	m	65	Total	C	N	O	S	0	0
			487	303	77	99	8		
11	k	321	Total	C	N	O	S	0	0
			2423	1512	411	472	28		

- 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 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	M	1	Total Fe S 16 8 8	0
13	M	1	Total Fe S 16 8 8	0
13	K	1	Total Fe S 48 24 24	0
13	K	1	Total Fe S 48 24 24	0
13	K	1	Total Fe S 48 24 24	0
13	K	1	Total Fe S 48 24 24	0
13	K	1	Total Fe S 48 24 24	0

Continued on next page...

Continued from previous page...

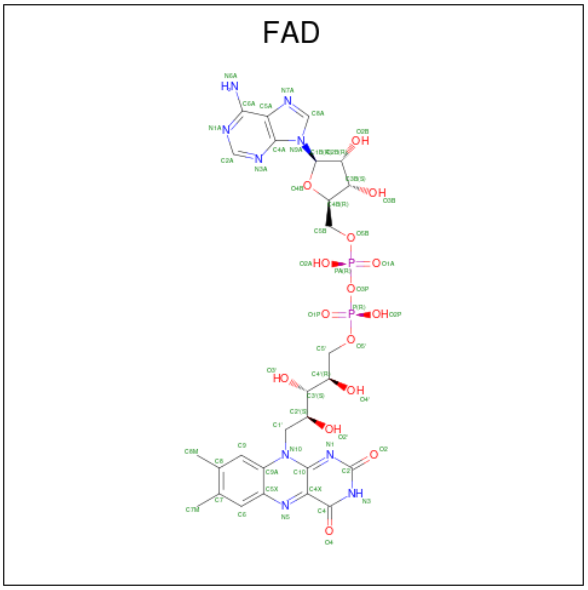
Mol	Chain	Residues	Atoms	AltConf
13	K	1	Total Fe S 48 24 24	0
13	H	1	Total Fe S 8 4 4	0
13	a	1	Total Fe S 48 24 24	0
13	a	1	Total Fe S 48 24 24	0
13	a	1	Total Fe S 48 24 24	0
13	a	1	Total Fe S 48 24 24	0
13	a	1	Total Fe S 48 24 24	0
13	a	1	Total Fe S 48 24 24	0
13	e	1	Total Fe S 32 16 16	0
13	e	1	Total 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	m	1	Total Fe S 16 8 8	0
13	m	1	Total Fe S 16 8 8	0
13	k	1	Total Fe S 48 24 24	0
13	k	1	Total Fe S 48 24 24	0

Continued on next page...

Continued from previous page...

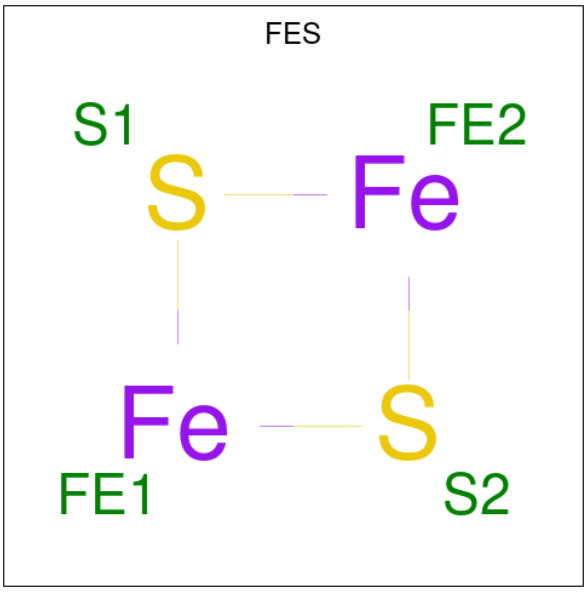
Mol	Chain	Residues	Atoms	AltConf
13	k	1	Total Fe S 48 24 24	0
13	k	1	Total Fe S 48 24 24	0
13	k	1	Total Fe S 48 24 24	0
13	k	1	Total Fe S 48 24 24	0
13	h	1	Total Fe S 8 4 4	0

- 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).



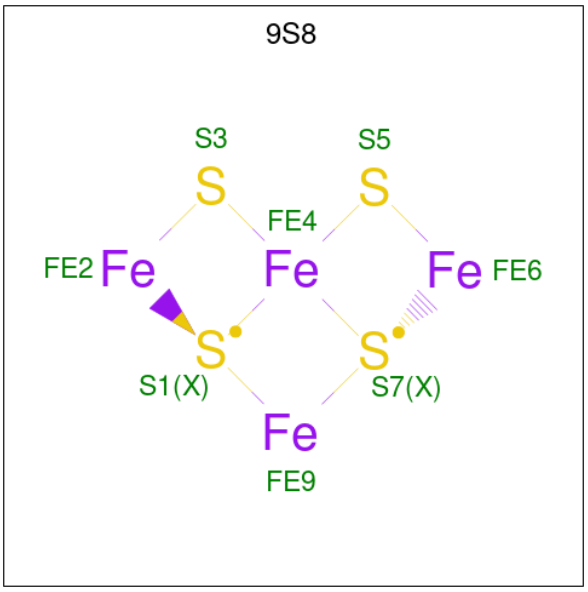
Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C N O P 53 27 9 15 2	0
14	E	1	Total C N O P 53 27 9 15 2	0
14	a	1	Total C N O P 53 27 9 15 2	0
14	e	1	Total C N O P 53 27 9 15 2	0

- 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 4 2 2	0
15	f	1	Total Fe S 4 2 2	0

- 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 16 8 8	0

Continued on next page...

Continued from previous page...

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

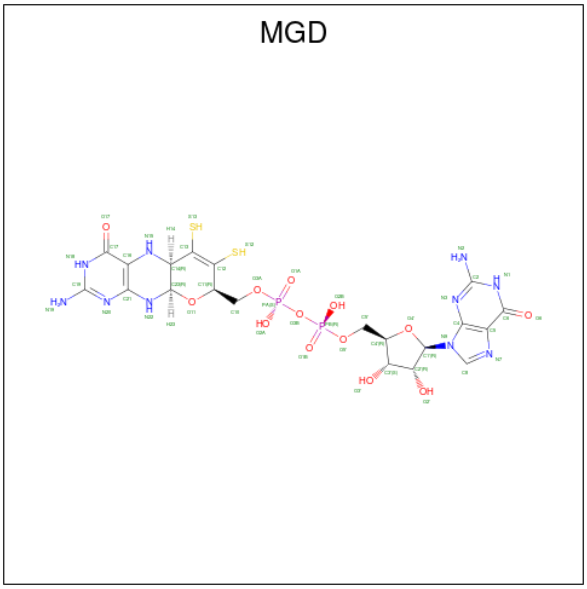
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

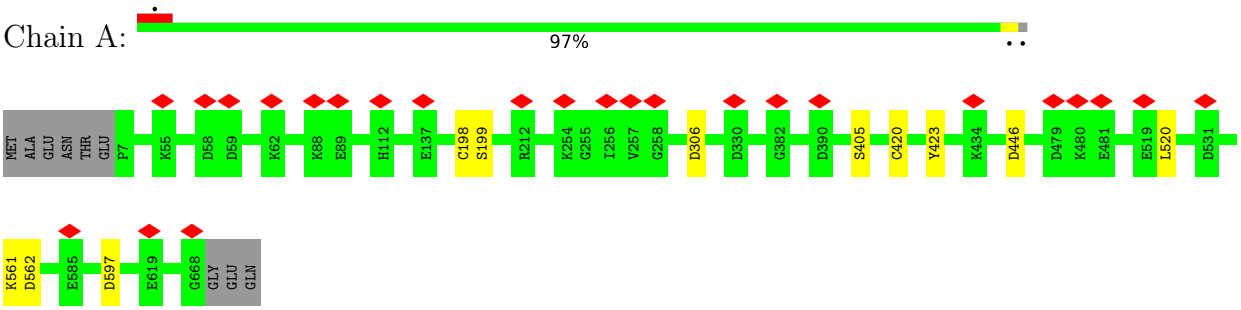


Mol	Chain	Residues	Atoms						AltConf
19	H	1	Total	C	N	O	P	S	0
			94	40	20	26	4	4	
19	H	1	Total	C	N	O	P	S	0
			94	40	20	26	4	4	
19	h	1	Total	C	N	O	P	S	0
			94	40	20	26	4	4	
19	h	1	Total	C	N	O	P	S	0
			94	40	20	26	4	4	

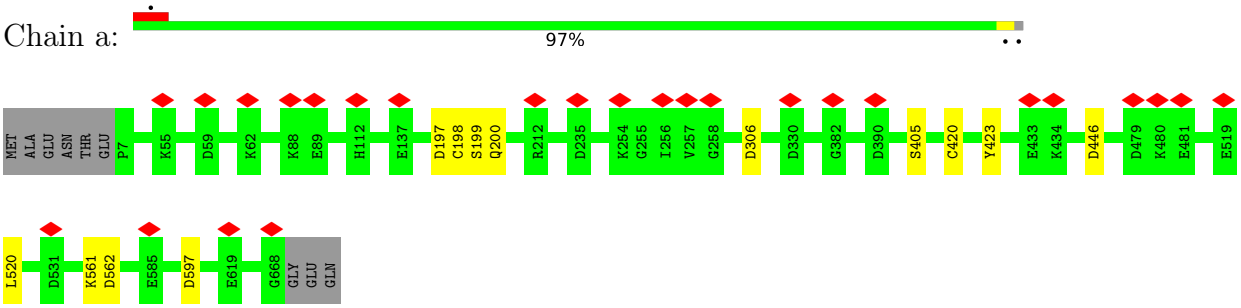
3 Residue-property plots (i)

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.

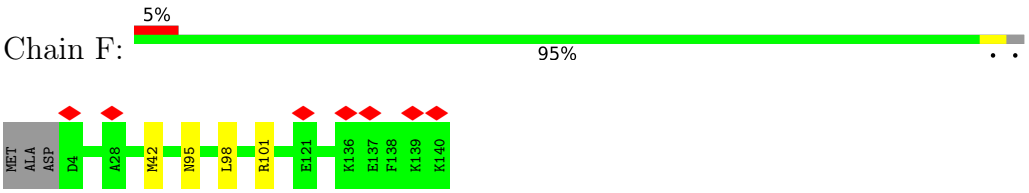
• Molecule 1: CoB–CoM heterodisulfide reductase iron-sulfur subunit A



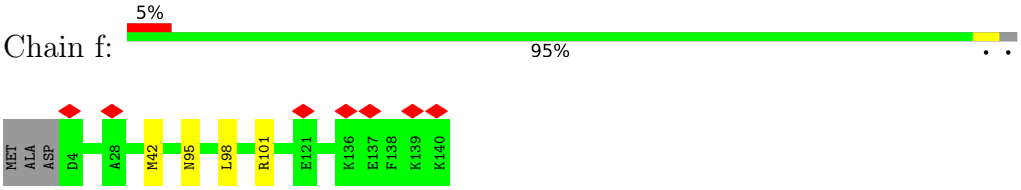
• Molecule 1: CoB–CoM heterodisulfide reductase iron-sulfur subunit A



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

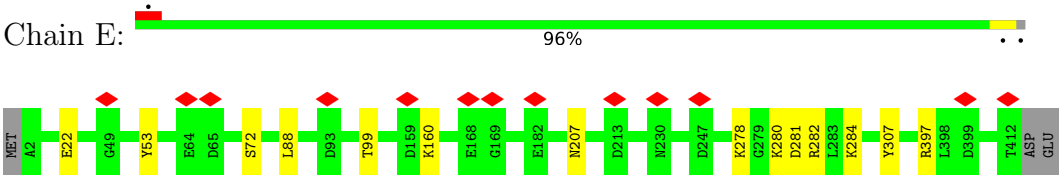


• Molecule 2: F420-non-reducing hydrogenase subunit D



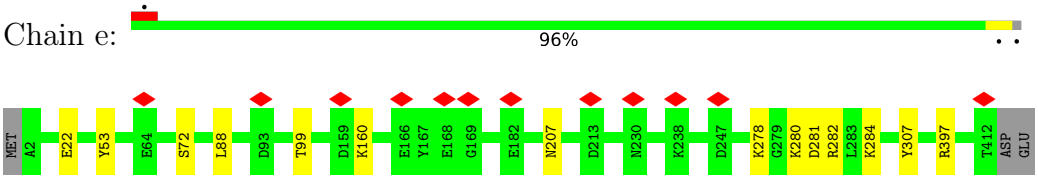
• Molecule 3: Formate dehydrogenase, beta subunit (F420)

Chain E:



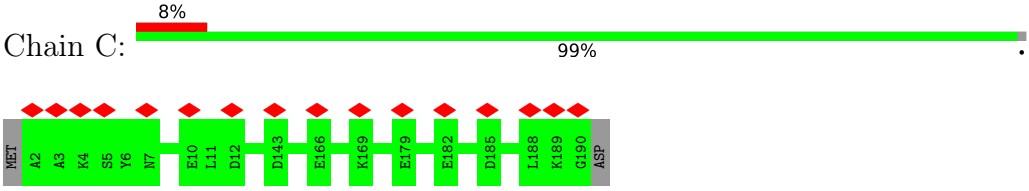
• Molecule 3: Formate dehydrogenase, beta subunit (F420)

Chain e:



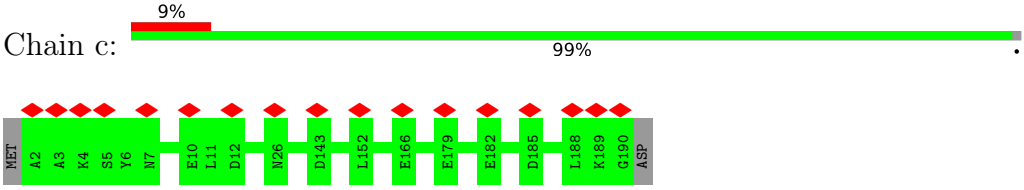
• Molecule 4: CoB–CoM heterodisulfide reductase subunit C

Chain C:



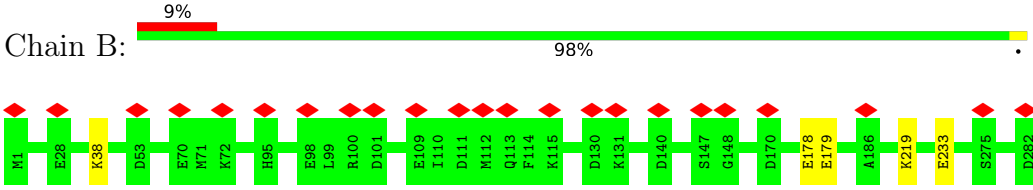
• Molecule 4: CoB–CoM heterodisulfide reductase subunit C

Chain c:



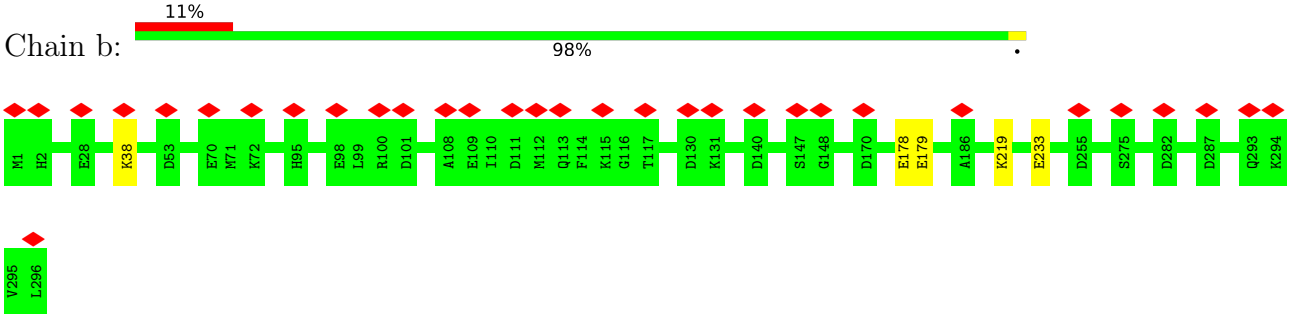
• Molecule 5: CoB–CoM heterodisulfide reductase subunit B

Chain B:

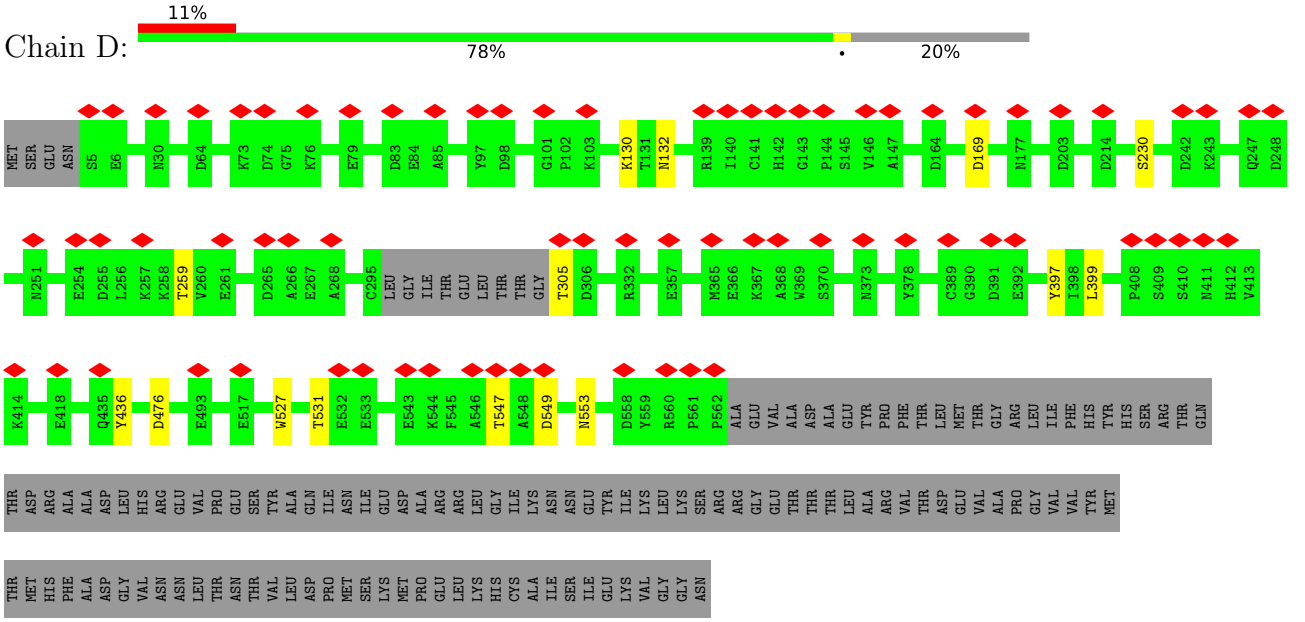


• Molecule 5: CoB–CoM heterodisulfide reductase subunit B

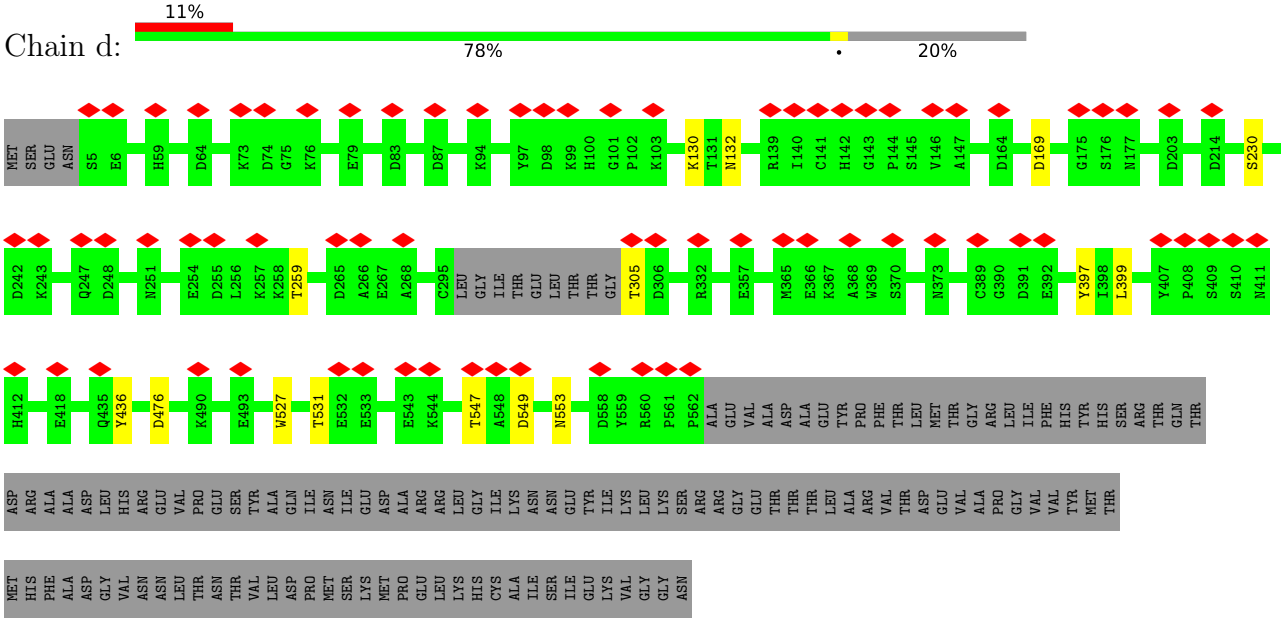
Chain b:



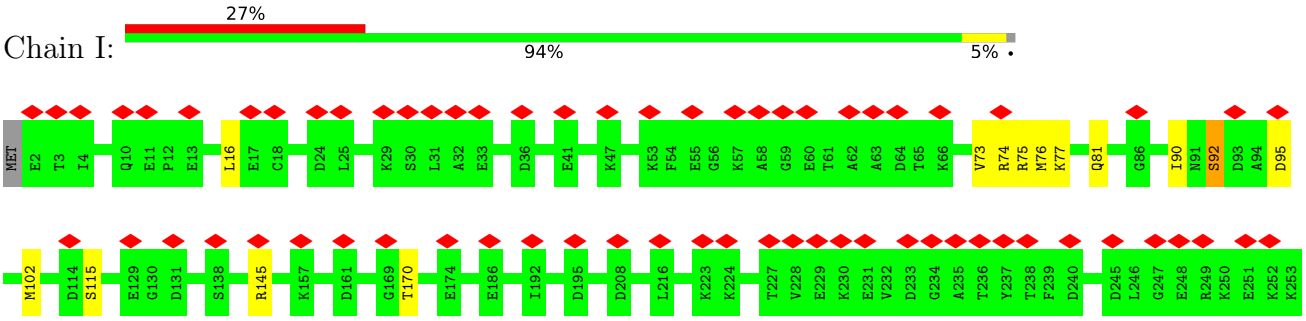
• Molecule 6: Formate dehydrogenase

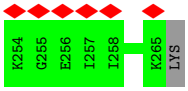


• Molecule 6: Formate dehydrogenase



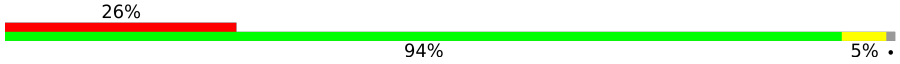
• Molecule 7: Formylmethanofuran dehydrogenase

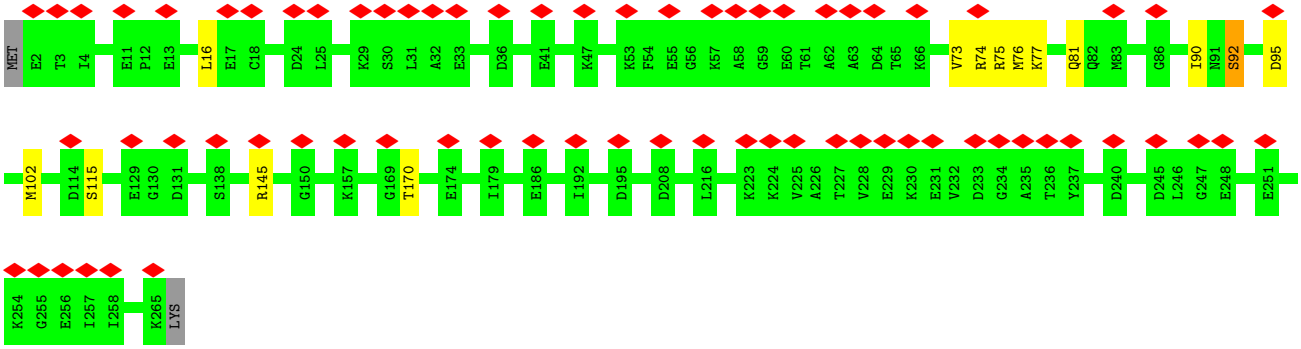




• Molecule 7: Formylmethanofuran dehydrogenase

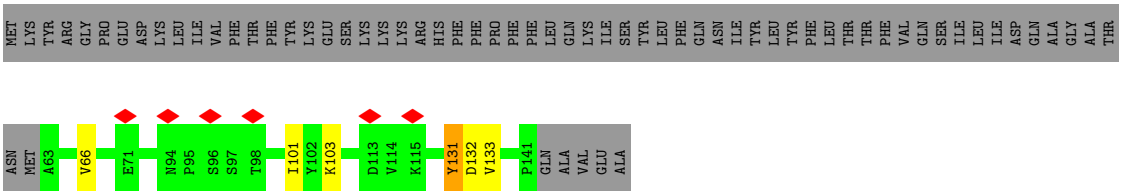
Chain i:





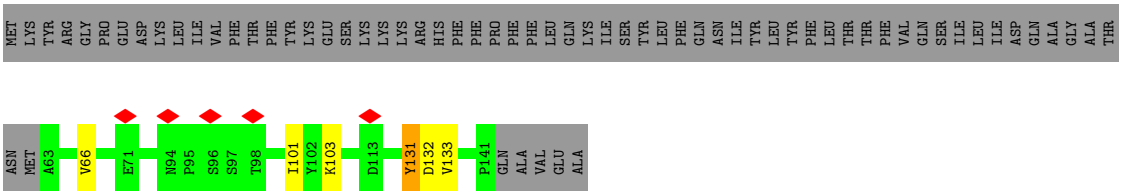
• Molecule 8: Formylmethanofuran dehydrogenase, subunit G

Chain L:



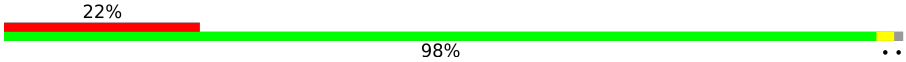
• Molecule 8: Formylmethanofuran dehydrogenase, subunit G

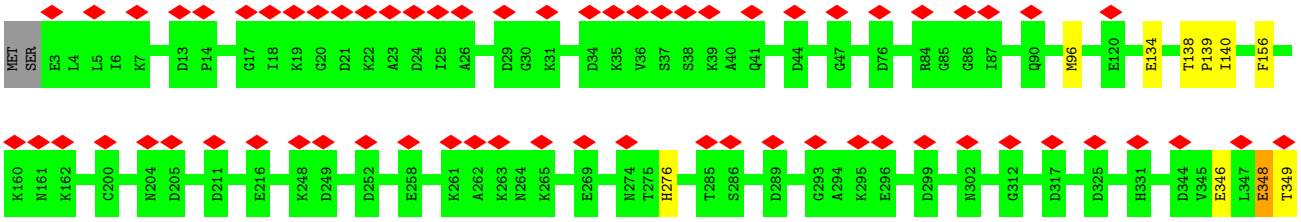
Chain l:

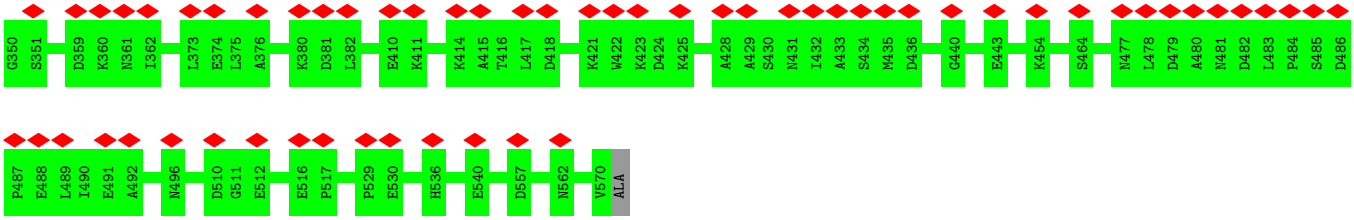


• Molecule 9: Formylmethanofuran dehydrogenase, subunit A

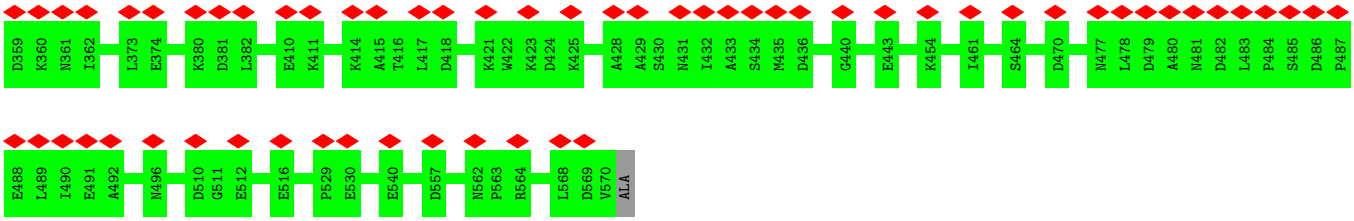
Chain G:



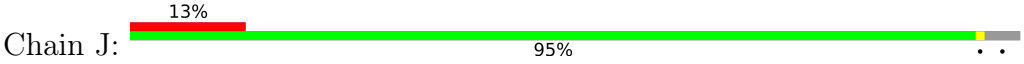




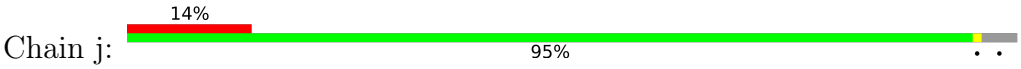
• Molecule 9: Formylmethanofuran dehydrogenase, subunit A



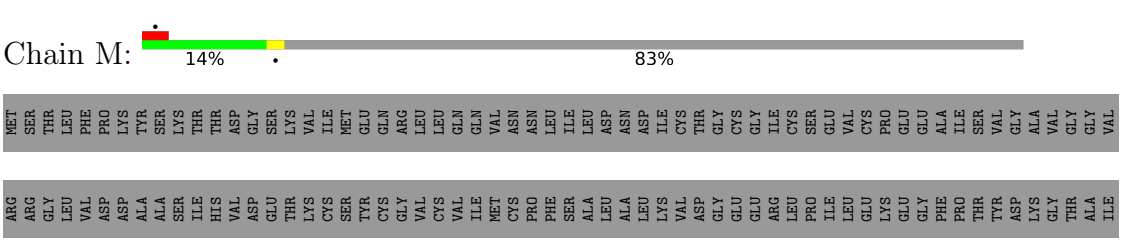
• Molecule 10: Formylmethanofuran dehydrogenase, subunit D

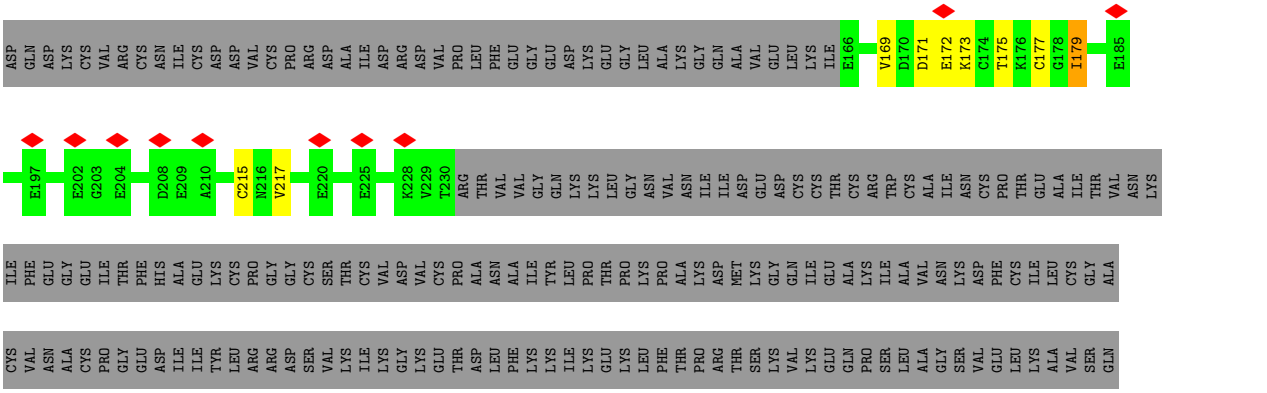


• Molecule 10: Formylmethanofuran dehydrogenase, subunit D



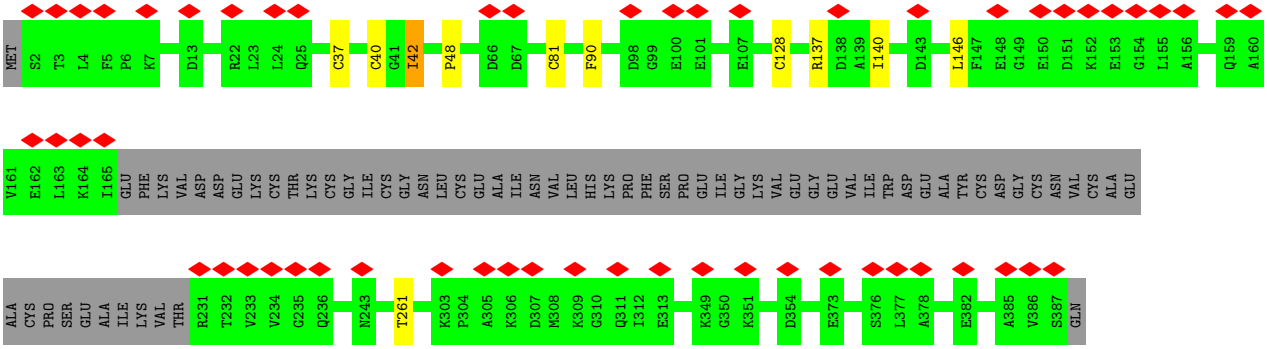
• Molecule 11: Formylmethanofuran dehydrogenase, subunit F





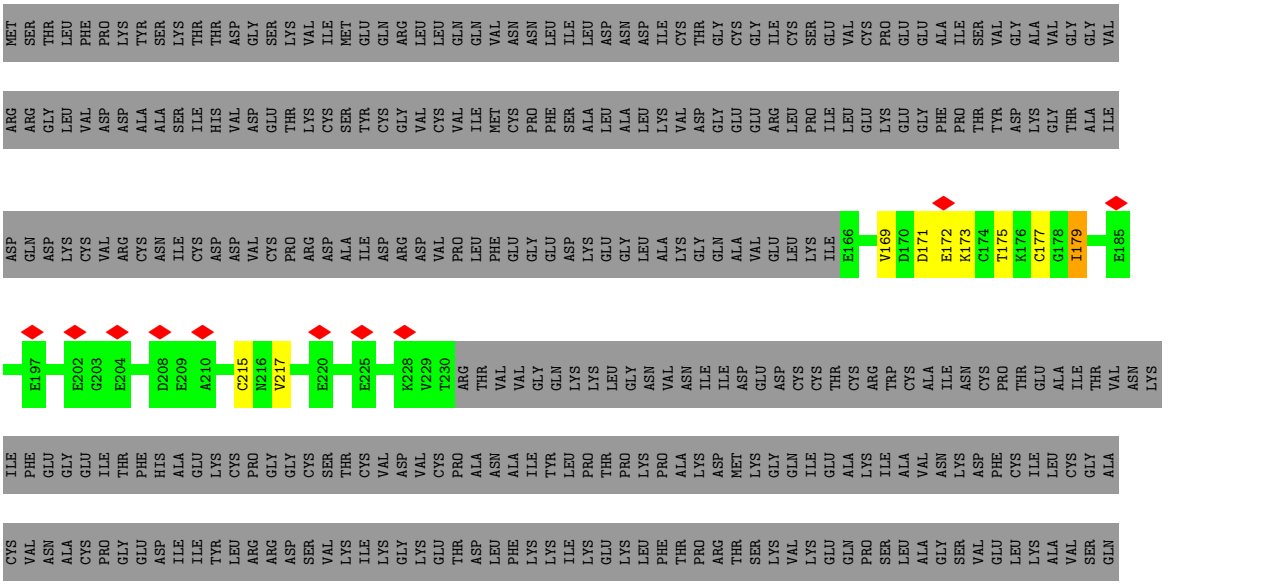
• Molecule 11: Formylmethanofuran dehydrogenase, subunit F

Chain K:



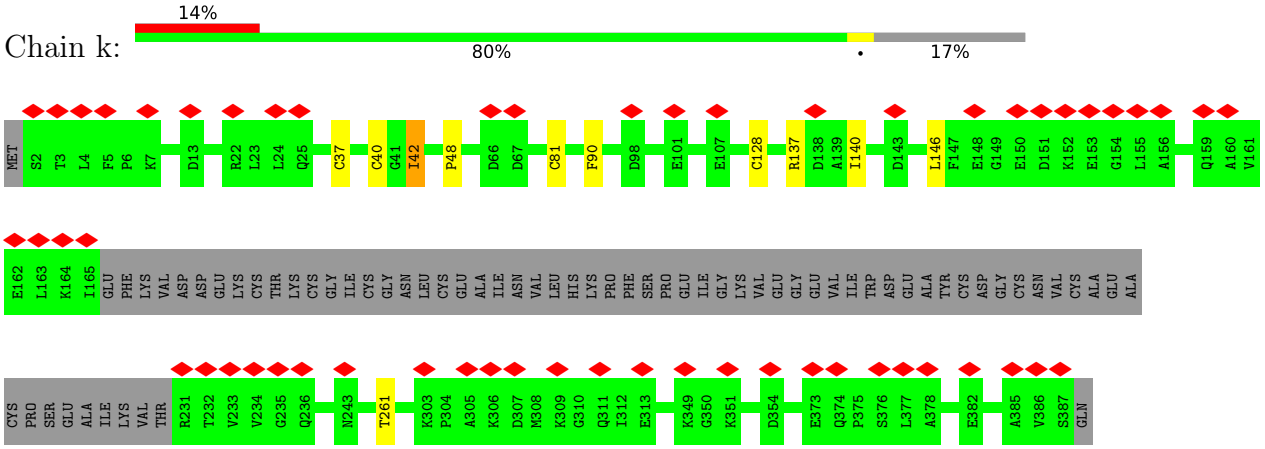
• Molecule 11: Formylmethanofuran dehydrogenase, subunit F

Chain m:



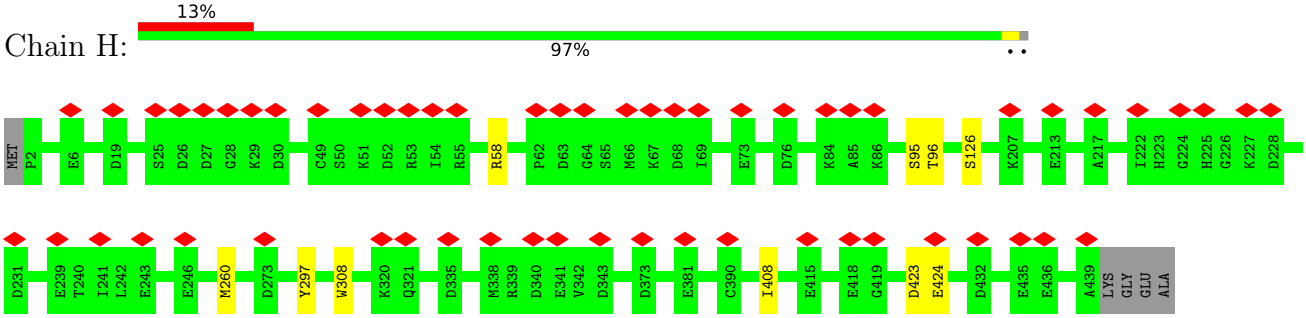
• Molecule 11: Formylmethanofuran dehydrogenase, subunit F

Chain k:



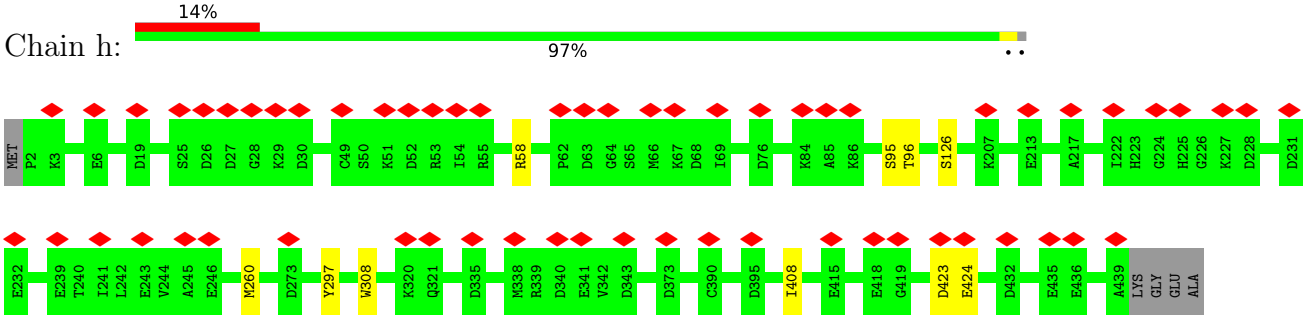
• Molecule 12: Formylmethanofuran dehydrogenase, subunit B

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, C2	Depositor
Number of particles used	1239454	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	103.221	Depositor
Minimum map value	-64.149	Depositor
Average map value	-0.069	Depositor
Map value standard deviation	1.898	Depositor
Recommended contour level	10.0	Depositor
Map size (Å)	361.584, 361.584, 361.584	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, KCX, ZN, MO, SF4, FAD, 9S8, 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	0.60	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	0.53	0/2455	0.68	0/3313
11	M	0.50	0/495	0.76	0/669
11	k	0.53	0/2455	0.68	0/3313
11	m	0.50	0/495	0.76	0/669
12	H	0.48	0/3497	0.59	0/4732
12	h	0.48	0/3497	0.59	0/4732
All	All	0.47	0/64562	0.60	6/87302 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	139	PRO	N-CA-C	6.00	127.71	112.10
9	G	139	PRO	N-CA-C	6.00	127.70	112.10
3	e	307	TYR	CB-CA-C	-5.56	99.27	110.40
3	E	307	TYR	CB-CA-C	-5.54	99.31	110.40
8	l	131	TYR	CB-CA-C	-5.24	99.92	110.40
8	L	131	TYR	CB-CA-C	-5.23	99.94	110.40

There are no chirality outliers.

There are no planarity outliers.

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%)	626 (95%)	33 (5%)	1 (0%)	47 82
1	a	660/671 (98%)	627 (95%)	32 (5%)	1 (0%)	47 82
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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	317/388 (82%)	276 (87%)	40 (13%)	1 (0%)	41 76
11	M	63/388 (16%)	55 (87%)	7 (11%)	1 (2%)	9 40
11	k	317/388 (82%)	276 (87%)	40 (13%)	1 (0%)	41 76
11	m	63/388 (16%)	55 (87%)	7 (11%)	1 (2%)	9 40
12	H	436/443 (98%)	390 (89%)	46 (11%)	0	100 100
12	h	436/443 (98%)	390 (89%)	46 (11%)	0	100 100
All	All	8158/9474 (86%)	7513 (92%)	633 (8%)	12 (0%)	54 85

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	G	276	HIS
9	g	276	HIS
1	A	446	ASP
11	K	42	ILE
1	a	446	ASP
11	k	42	ILE
7	I	92	SER
9	G	348	GLU
7	i	92	SER
9	g	348	GLU
11	M	179	ILE
11	m	179	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%)	526 (98%)	10 (2%)	57	84
1	a	536/543 (99%)	524 (98%)	12 (2%)	52	81
2	F	112/114 (98%)	108 (96%)	4 (4%)	35	70
2	f	112/114 (98%)	108 (96%)	4 (4%)	35	70
3	E	338/341 (99%)	325 (96%)	13 (4%)	33	69
3	e	338/341 (99%)	325 (96%)	13 (4%)	33	69
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	83
5	b	245/245 (100%)	240 (98%)	5 (2%)	55	83
6	D	454/571 (80%)	439 (97%)	15 (3%)	38	73
6	d	454/571 (80%)	439 (97%)	15 (3%)	38	73
7	I	202/204 (99%)	188 (93%)	14 (7%)	15	48
7	i	202/204 (99%)	188 (93%)	14 (7%)	15	48
8	L	67/128 (52%)	61 (91%)	6 (9%)	9	35
8	l	67/128 (52%)	61 (91%)	6 (9%)	9	35
9	G	472/474 (100%)	464 (98%)	8 (2%)	60	85
9	g	472/474 (100%)	464 (98%)	8 (2%)	60	85
10	J	111/116 (96%)	110 (99%)	1 (1%)	78	92
10	j	111/116 (96%)	110 (99%)	1 (1%)	78	92
11	K	275/332 (83%)	264 (96%)	11 (4%)	31	68
11	M	55/332 (17%)	46 (84%)	9 (16%)	2	11
11	k	275/332 (83%)	264 (96%)	11 (4%)	31	68
11	m	55/332 (17%)	46 (84%)	9 (16%)	2	11
12	H	370/373 (99%)	360 (97%)	10 (3%)	44	77
12	h	370/373 (99%)	360 (97%)	10 (3%)	44	77
All	All	6810/7886 (86%)	6596 (97%)	214 (3%)	43	75

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	CYS
1	A	199	SER
1	A	306	ASP
1	A	405	SER
1	A	420	CYS
1	A	423	TYR
1	A	520	LEU
1	A	561	LYS
1	A	562	ASP
1	A	597	ASP
2	F	42	MET
2	F	95	ASN
2	F	98	LEU
2	F	101	ARG
3	E	22	GLU
3	E	53	TYR
3	E	72	SER
3	E	88	LEU
3	E	99	THR
3	E	160	LYS
3	E	207	ASN
3	E	278	LYS
3	E	280	LYS
3	E	281	ASP
3	E	282	ARG
3	E	284	LYS
3	E	397	ARG
5	B	38	LYS
5	B	178	GLU
5	B	179	GLU
5	B	219	LYS
5	B	233	GLU
6	D	130	LYS
6	D	132	ASN
6	D	169	ASP
6	D	230	SER
6	D	259	THR
6	D	305	THR
6	D	397	TYR
6	D	399	LEU
6	D	436	TYR
6	D	476	ASP
6	D	527	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	531	THR
6	D	547	THR
6	D	549	ASP
6	D	553	ASN
7	I	16	LEU
7	I	73	VAL
7	I	74	ARG
7	I	75	ARG
7	I	76	MET
7	I	77	LYS
7	I	81	GLN
7	I	90	ILE
7	I	92	SER
7	I	95	ASP
7	I	102	MET
7	I	115	SER
7	I	145	ARG
7	I	170	THR
8	L	66	VAL
8	L	101	ILE
8	L	103	LYS
8	L	131	TYR
8	L	132	ASP
8	L	133	VAL
9	G	96	MET
9	G	134	GLU
9	G	138	THR
9	G	140	ILE
9	G	156	PHE
9	G	346	GLU
9	G	348	GLU
9	G	349	THR
10	J	63	GLU
11	M	169	VAL
11	M	171	ASP
11	M	172	GLU
11	M	173	LYS
11	M	175	THR
11	M	177	CYS
11	M	179	ILE
11	M	215	CYS
11	M	217	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	37	CYS
11	K	40	CYS
11	K	42	ILE
11	K	48	PRO
11	K	81	CYS
11	K	90	PHE
11	K	128	CYS
11	K	137	ARG
11	K	140	ILE
11	K	146	LEU
11	K	261	THR
12	H	58	ARG
12	H	95	SER
12	H	96	THR
12	H	126	SER
12	H	260	MET
12	H	297	TYR
12	H	308	TRP
12	H	408	ILE
12	H	423	ASP
12	H	424	GLU
1	a	197	ASP
1	a	198	CYS
1	a	199	SER
1	a	200	GLN
1	a	306	ASP
1	a	405	SER
1	a	420	CYS
1	a	423	TYR
1	a	520	LEU
1	a	561	LYS
1	a	562	ASP
1	a	597	ASP
2	f	42	MET
2	f	95	ASN
2	f	98	LEU
2	f	101	ARG
3	e	22	GLU
3	e	53	TYR
3	e	72	SER
3	e	88	LEU
3	e	99	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	e	160	LYS
3	e	207	ASN
3	e	278	LYS
3	e	280	LYS
3	e	281	ASP
3	e	282	ARG
3	e	284	LYS
3	e	397	ARG
5	b	38	LYS
5	b	178	GLU
5	b	179	GLU
5	b	219	LYS
5	b	233	GLU
6	d	130	LYS
6	d	132	ASN
6	d	169	ASP
6	d	230	SER
6	d	259	THR
6	d	305	THR
6	d	397	TYR
6	d	399	LEU
6	d	436	TYR
6	d	476	ASP
6	d	527	TRP
6	d	531	THR
6	d	547	THR
6	d	549	ASP
6	d	553	ASN
7	i	16	LEU
7	i	73	VAL
7	i	74	ARG
7	i	75	ARG
7	i	76	MET
7	i	77	LYS
7	i	81	GLN
7	i	90	ILE
7	i	92	SER
7	i	95	ASP
7	i	102	MET
7	i	115	SER
7	i	145	ARG
7	i	170	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	l	66	VAL
8	l	101	ILE
8	l	103	LYS
8	l	131	TYR
8	l	132	ASP
8	l	133	VAL
9	g	96	MET
9	g	134	GLU
9	g	138	THR
9	g	140	ILE
9	g	156	PHE
9	g	346	GLU
9	g	348	GLU
9	g	349	THR
10	j	63	GLU
11	m	169	VAL
11	m	171	ASP
11	m	172	GLU
11	m	173	LYS
11	m	175	THR
11	m	177	CYS
11	m	179	ILE
11	m	215	CYS
11	m	217	VAL
11	k	37	CYS
11	k	40	CYS
11	k	42	ILE
11	k	48	PRO
11	k	81	CYS
11	k	90	PHE
11	k	128	CYS
11	k	137	ARG
11	k	140	ILE
11	k	146	LEU
11	k	261	THR
12	h	58	ARG
12	h	95	SER
12	h	96	THR
12	h	126	SER
12	h	260	MET
12	h	297	TYR
12	h	308	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	h	408	ILE
12	h	423	ASP
12	h	424	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	31	GLN
6	D	534	HIS
9	G	152	ASN
9	G	270	GLN
9	G	273	HIS
9	G	274	ASN
10	J	73	GLN
12	H	325	HIS
1	a	200	GLN
1	a	429	HIS
2	f	31	GLN
6	d	534	HIS
9	g	152	ASN
9	g	270	GLN
9	g	273	HIS
9	g	274	ASN
9	g	331	HIS
10	j	73	GLN
12	h	156	ASN
12	h	325	HIS
12	h	386	HIS

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	17,9	9,11,12	0.35	0	5,12,14	0.51	0
9	KCX	G	184	17,9	9,11,12	0.35	0	5,12,14	0.52	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	17,9	-	3/9/10/12	-
9	KCX	G	184	17,9	-	3/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (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
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	k	403	11	0,12,12	-	-	-		
13	SF4	M	401	11	0,12,12	-	-	-		
13	SF4	c	202	4	0,12,12	-	-	-		
13	SF4	H	504	12	0,12,12	-	-	-		
15	FES	F	201	2	0,4,4	-	-	-		
13	SF4	C	202	4	0,12,12	-	-	-		
13	SF4	K	405	11	0,12,12	-	-	-		
13	SF4	k	401	11	0,12,12	-	-	-		
13	SF4	l	201	8	0,12,12	-	-	-		
13	SF4	e	501	3	0,12,12	-	-	-		
13	SF4	K	402	11	0,12,12	-	-	-		
13	SF4	E	501	3	0,12,12	-	-	-		
13	SF4	a	705	1	0,12,12	-	-	-		
13	SF4	k	402	11	0,12,12	-	-	-		
15	FES	f	201	2	0,4,4	-	-	-		
13	SF4	C	201	4	0,12,12	-	-	-		
13	SF4	A	701	1	0,12,12	-	-	-		
13	SF4	k	405	11	0,12,12	-	-	-		
13	SF4	a	701	1	0,12,12	-	-	-		
19	MGD	h	503	18	41,52,52	5.93	28 (68%)	40,81,81	1.80	10 (25%)
13	SF4	K	406	11	0,12,12	-	-	-		
13	SF4	A	707	1	0,12,12	-	-	-		
13	SF4	K	403	11	0,12,12	-	-	-		
13	SF4	M	402	11	0,12,12	-	-	-		
14	FAD	a	702	-	53,58,58	0.87	2 (3%)	68,89,89	0.59	1 (1%)
13	SF4	a	703	1	0,12,12	-	-	-		
13	SF4	e	504	3	0,12,12	-	-	-		
16	9S8	b	302	5	2,10,10	1.20	0	-		
13	SF4	E	504	3	0,12,12	-	-	-		
13	SF4	A	703	1	0,12,12	-	-	-		
13	SF4	A	704	1	0,12,12	-	-	-		
13	SF4	e	502	3	0,12,12	-	-	-		
13	SF4	L	202	8	0,12,12	-	-	-		
13	SF4	d	701	6	0,12,12	-	-	-		
16	9S8	B	301	5	2,10,10	1.13	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	SF4	L	201	8	0,12,12	-	-	-		
19	MGD	H	502	18	41,52,52	5.91	27 (65%)	40,81,81	1.92	9 (22%)
13	SF4	h	504	12	0,12,12	-	-	-		
13	SF4	e	503	3	0,12,12	-	-	-		
13	SF4	A	705	1	0,12,12	-	-	-		
13	SF4	K	404	11	0,12,12	-	-	-		
19	MGD	h	502	18	41,52,52	5.90	27 (65%)	40,81,81	1.92	9 (22%)
13	SF4	l	202	8	0,12,12	-	-	-		
13	SF4	A	706	1	0,12,12	-	-	-		
13	SF4	a	706	1	0,12,12	-	-	-		
13	SF4	c	201	4	0,12,12	-	-	-		
14	FAD	E	505	-	53,58,58	1.06	3 (5%)	68,89,89	0.60	1 (1%)
14	FAD	e	505	-	53,58,58	1.06	3 (5%)	68,89,89	0.60	1 (1%)
13	SF4	K	401	11	0,12,12	-	-	-		
19	MGD	H	503	18	41,52,52	5.93	28 (68%)	40,81,81	1.80	10 (25%)
16	9S8	B	302	5	2,10,10	1.19	0	-		
13	SF4	E	502	3	0,12,12	-	-	-		
13	SF4	D	701	6	0,12,12	-	-	-		
13	SF4	k	404	11	0,12,12	-	-	-		
13	SF4	m	402	11	0,12,12	-	-	-		
13	SF4	k	406	11	0,12,12	-	-	-		
14	FAD	A	702	-	53,58,58	0.87	2 (3%)	68,89,89	0.59	1 (1%)
13	SF4	a	707	1	0,12,12	-	-	-		
16	9S8	b	301	5	2,10,10	1.12	0	-		
13	SF4	E	503	3	0,12,12	-	-	-		
13	SF4	a	704	1	0,12,12	-	-	-		
13	SF4	m	401	11	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	k	403	11	-	-	0/6/5/5
13	SF4	M	401	11	-	-	0/6/5/5
13	SF4	c	202	4	-	-	0/6/5/5
13	SF4	H	504	12	-	-	0/6/5/5
15	FES	F	201	2	-	-	0/1/1/1
13	SF4	C	202	4	-	-	0/6/5/5
13	SF4	K	405	11	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	k	401	11	-	-	0/6/5/5
13	SF4	l	201	8	-	-	0/6/5/5
13	SF4	e	501	3	-	-	0/6/5/5
13	SF4	E	501	3	-	-	0/6/5/5
13	SF4	K	402	11	-	-	0/6/5/5
13	SF4	a	705	1	-	-	0/6/5/5
13	SF4	k	402	11	-	-	0/6/5/5
15	FES	f	201	2	-	-	0/1/1/1
13	SF4	C	201	4	-	-	0/6/5/5
13	SF4	A	701	1	-	-	0/6/5/5
13	SF4	k	405	11	-	-	0/6/5/5
13	SF4	a	701	1	-	-	0/6/5/5
19	MGD	h	503	18	-	9/18/66/66	0/6/6/6
13	SF4	K	406	11	-	-	0/6/5/5
13	SF4	A	707	1	-	-	0/6/5/5
13	SF4	K	403	11	-	-	0/6/5/5
14	FAD	a	702	-	-	2/30/50/50	0/6/6/6
13	SF4	M	402	11	-	-	0/6/5/5
13	SF4	a	703	1	-	-	0/6/5/5
13	SF4	e	504	3	-	-	0/6/5/5
16	9S8	b	302	5	-	-	0/3/3/3
13	SF4	E	504	3	-	-	0/6/5/5
13	SF4	A	703	1	-	-	0/6/5/5
13	SF4	A	704	1	-	-	0/6/5/5
13	SF4	e	502	3	-	-	0/6/5/5
13	SF4	L	202	8	-	-	0/6/5/5
13	SF4	d	701	6	-	-	0/6/5/5
16	9S8	B	301	5	-	-	0/3/3/3
19	MGD	H	502	18	-	9/18/66/66	0/6/6/6
13	SF4	L	201	8	-	-	0/6/5/5
13	SF4	h	504	12	-	-	0/6/5/5
13	SF4	e	503	3	-	-	0/6/5/5
13	SF4	A	705	1	-	-	0/6/5/5
13	SF4	K	404	11	-	-	0/6/5/5
19	MGD	h	502	18	-	9/18/66/66	0/6/6/6
13	SF4	l	202	8	-	-	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
14	FAD	e	505	-	-	13/30/50/50	0/6/6/6
19	MGD	H	503	18	-	9/18/66/66	0/6/6/6
13	SF4	a	706	1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	K	401	11	-	-	0/6/5/5
13	SF4	c	201	4	-	-	0/6/5/5
16	9S8	B	302	5	-	-	0/3/3/3
13	SF4	E	502	3	-	-	0/6/5/5
13	SF4	D	701	6	-	-	0/6/5/5
14	FAD	A	702	-	-	2/30/50/50	0/6/6/6
13	SF4	m	402	11	-	-	0/6/5/5
13	SF4	k	404	11	-	-	0/6/5/5
13	SF4	k	406	11	-	-	0/6/5/5
13	SF4	a	707	1	-	-	0/6/5/5
16	9S8	b	301	5	-	-	0/3/3/3
13	SF4	E	503	3	-	-	0/6/5/5
13	SF4	a	704	1	-	-	0/6/5/5
13	SF4	m	401	11	-	-	0/6/5/5

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	502	MGD	C2'-C1'	-19.01	1.24	1.53
19	h	502	MGD	C2'-C1'	-19.01	1.24	1.53
19	H	503	MGD	C2'-C1'	-17.92	1.26	1.53
19	h	503	MGD	C2'-C1'	-17.85	1.26	1.53
19	h	503	MGD	C16-C21	12.90	1.60	1.38
19	H	503	MGD	C16-C21	12.84	1.60	1.38
19	H	502	MGD	C16-C21	12.25	1.59	1.38
19	h	502	MGD	C16-C21	12.24	1.59	1.38
19	h	502	MGD	O11-C11	10.79	1.58	1.43
19	H	502	MGD	O11-C11	10.78	1.58	1.43
19	H	503	MGD	C14-N15	10.71	1.58	1.46
19	h	503	MGD	C14-N15	10.68	1.58	1.46
19	H	502	MGD	C14-N15	10.41	1.58	1.46
19	h	502	MGD	C14-N15	10.36	1.58	1.46
19	h	503	MGD	C3'-C4'	-10.25	1.26	1.53
19	h	502	MGD	C3'-C4'	-10.25	1.26	1.53
19	H	502	MGD	C3'-C4'	-10.25	1.26	1.53
19	H	503	MGD	C3'-C4'	-10.23	1.26	1.53
19	h	503	MGD	O11-C11	10.15	1.57	1.43
19	H	503	MGD	O4'-C1'	10.14	1.55	1.41
19	H	503	MGD	O11-C11	10.10	1.57	1.43
19	h	503	MGD	O4'-C1'	10.07	1.55	1.41
19	H	503	MGD	O11-C23	-8.85	1.31	1.43
19	h	503	MGD	O11-C23	-8.81	1.31	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	h	502	MGD	O4'-C1'	8.73	1.53	1.41
19	h	503	MGD	C23-C14	-8.71	1.46	1.53
19	H	502	MGD	O4'-C1'	8.71	1.53	1.41
19	H	503	MGD	C23-C14	-8.64	1.46	1.53
19	H	502	MGD	C23-C14	-8.60	1.46	1.53
19	h	502	MGD	C23-C14	-8.57	1.46	1.53
19	H	502	MGD	O11-C23	-7.81	1.32	1.43
19	h	502	MGD	O11-C23	-7.81	1.32	1.43
19	H	502	MGD	C23-N22	7.53	1.57	1.45
19	h	502	MGD	C23-N22	7.52	1.57	1.45
19	H	503	MGD	C23-N22	7.24	1.57	1.45
19	h	503	MGD	C23-N22	7.21	1.57	1.45
19	h	502	MGD	C19-N20	6.67	1.49	1.33
19	H	502	MGD	C19-N20	6.66	1.49	1.33
19	H	503	MGD	C19-N18	6.64	1.54	1.37
19	h	503	MGD	C19-N18	6.60	1.54	1.37
19	H	502	MGD	C19-N18	6.33	1.53	1.37
19	h	502	MGD	C19-N18	6.33	1.53	1.37
19	h	503	MGD	C19-N20	6.29	1.48	1.33
19	H	503	MGD	C19-N20	6.25	1.48	1.33
19	h	503	MGD	C2-N3	5.28	1.46	1.33
19	H	503	MGD	C2-N3	5.23	1.45	1.33
19	H	503	MGD	C17-N18	5.02	1.48	1.38
19	h	503	MGD	C17-N18	5.00	1.48	1.38
19	H	502	MGD	C17-N18	4.86	1.47	1.38
19	h	502	MGD	C17-N18	4.85	1.47	1.38
19	h	503	MGD	C4-N3	4.66	1.48	1.37
19	h	502	MGD	C21-N20	4.66	1.43	1.36
19	H	503	MGD	C4-N3	4.65	1.48	1.37
19	H	502	MGD	C21-N20	4.62	1.43	1.36
19	h	502	MGD	C2-N3	4.60	1.44	1.33
19	H	502	MGD	C2-N3	4.59	1.44	1.33
19	H	503	MGD	O4'-C4'	4.50	1.55	1.45
19	h	503	MGD	O4'-C4'	4.50	1.55	1.45
19	h	503	MGD	C2-N2	4.47	1.44	1.34
19	H	503	MGD	C2-N2	4.47	1.44	1.34
19	H	502	MGD	C4-N3	4.44	1.48	1.37
19	h	502	MGD	C4-N3	4.44	1.48	1.37
19	H	502	MGD	C2-N2	4.38	1.44	1.34
19	h	502	MGD	C2-N2	4.37	1.44	1.34
19	H	502	MGD	O4'-C4'	4.31	1.54	1.45
19	h	502	MGD	O4'-C4'	4.29	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	h	503	MGD	C19-N19	4.25	1.44	1.34
19	H	503	MGD	C19-N19	4.22	1.44	1.34
19	H	503	MGD	C2'-C3'	4.20	1.64	1.53
19	h	503	MGD	C2'-C3'	4.19	1.64	1.53
19	H	502	MGD	C19-N19	4.19	1.44	1.34
19	h	502	MGD	C19-N19	4.17	1.44	1.34
14	E	505	FAD	P-O2P	-3.98	1.36	1.55
14	e	505	FAD	P-O2P	-3.98	1.36	1.55
19	h	502	MGD	C2'-C3'	3.90	1.64	1.53
19	H	502	MGD	C2'-C3'	3.90	1.64	1.53
19	H	502	MGD	C21-N22	3.81	1.39	1.35
19	h	502	MGD	C21-N22	3.80	1.39	1.35
14	E	505	FAD	PA-O5B	-3.51	1.45	1.59
19	H	503	MGD	C21-N20	3.51	1.41	1.36
14	e	505	FAD	PA-O5B	-3.50	1.45	1.59
19	h	503	MGD	C21-N20	3.48	1.41	1.36
19	H	502	MGD	C5-C4	-3.31	1.34	1.43
19	h	502	MGD	C5-C4	-3.31	1.34	1.43
14	A	702	FAD	P-O2P	-3.18	1.40	1.55
14	a	702	FAD	P-O2P	-3.17	1.40	1.55
19	h	503	MGD	C6-N1	3.07	1.42	1.37
19	H	503	MGD	C6-N1	3.04	1.42	1.37
19	h	502	MGD	O17-C17	-2.96	1.17	1.23
19	H	502	MGD	O17-C17	-2.96	1.18	1.23
19	h	503	MGD	C5-C4	-2.92	1.35	1.43
19	H	503	MGD	C5-C4	-2.90	1.35	1.43
19	h	502	MGD	O6-C6	-2.85	1.17	1.23
19	H	502	MGD	O6-C6	-2.84	1.17	1.23
19	H	503	MGD	C5-C6	2.82	1.53	1.47
19	h	503	MGD	C5-C6	2.81	1.53	1.47
19	h	503	MGD	O17-C17	-2.76	1.18	1.23
19	H	503	MGD	O17-C17	-2.75	1.18	1.23
19	h	503	MGD	C12-C13	2.74	1.53	1.35
19	H	503	MGD	C12-C13	2.74	1.53	1.35
19	H	502	MGD	C12-C13	2.62	1.52	1.35
19	h	502	MGD	C12-C13	2.61	1.52	1.35
19	H	503	MGD	C16-C17	2.60	1.49	1.42
19	h	503	MGD	C16-C17	2.60	1.49	1.42
19	H	503	MGD	C21-N22	2.59	1.38	1.35
19	h	503	MGD	C21-N22	2.58	1.38	1.35
19	h	503	MGD	O6-C6	-2.44	1.18	1.23
19	H	503	MGD	O6-C6	-2.43	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	503	MGD	C2-N1	2.29	1.43	1.37
19	h	503	MGD	C2-N1	2.26	1.43	1.37
14	a	702	FAD	C4-N3	-2.20	1.34	1.38
14	A	702	FAD	C4-N3	-2.19	1.34	1.38
19	h	502	MGD	C6-N1	2.15	1.41	1.37
19	H	502	MGD	C6-N1	2.13	1.41	1.37
19	H	502	MGD	C10-C11	2.11	1.54	1.52
19	h	502	MGD	C10-C11	2.10	1.54	1.52
19	h	502	MGD	C16-C17	2.09	1.47	1.42
19	H	502	MGD	C16-C17	2.09	1.47	1.42
14	e	505	FAD	C8A-N7A	-2.08	1.31	1.34
14	E	505	FAD	C8A-N7A	-2.02	1.31	1.34

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	h	502	MGD	O11-C23-N22	-5.60	102.81	108.57
19	H	502	MGD	O11-C23-N22	-5.60	102.81	108.57
19	h	502	MGD	C19-N20-C21	3.90	120.47	113.43
19	H	502	MGD	C19-N20-C21	3.89	120.45	113.43
19	H	503	MGD	C19-N20-C21	3.70	120.11	113.43
19	H	503	MGD	C5-C6-N1	3.70	120.49	113.95
19	h	503	MGD	C19-N20-C21	3.69	120.09	113.43
19	h	503	MGD	C5-C6-N1	3.67	120.44	113.95
19	h	503	MGD	O4'-C1'-C2'	-3.40	101.96	106.93
19	H	502	MGD	O17-C17-C16	-3.38	119.50	127.24
19	h	502	MGD	O17-C17-C16	-3.37	119.51	127.24
19	H	503	MGD	O4'-C1'-C2'	-3.35	102.03	106.93
19	H	503	MGD	C2-N1-C6	-3.27	119.08	125.10
19	h	503	MGD	C2-N1-C6	-3.26	119.09	125.10
19	h	503	MGD	N19-C19-N18	3.24	123.61	116.71
19	H	503	MGD	N19-C19-N18	3.23	123.58	116.71
19	H	502	MGD	C5-C6-N1	3.14	119.50	113.95
19	h	502	MGD	C5-C6-N1	3.13	119.48	113.95
19	H	502	MGD	C19-N18-C17	-2.89	119.84	125.10
19	h	502	MGD	C19-N18-C17	-2.87	119.87	125.10
19	h	503	MGD	C8-N7-C5	2.72	108.18	102.99
19	H	503	MGD	C8-N7-C5	2.72	108.16	102.99
19	H	502	MGD	C16-C17-N18	2.61	120.08	112.31
19	h	502	MGD	C16-C17-N18	2.61	120.07	112.31
19	h	503	MGD	O17-C17-C16	-2.56	121.37	127.24
19	H	503	MGD	O17-C17-C16	-2.53	121.44	127.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	H	503	MGD	C19-N18-C17	-2.48	120.58	125.10
19	h	503	MGD	C19-N18-C17	-2.47	120.59	125.10
19	h	502	MGD	N1-C2-N3	-2.47	118.71	123.32
19	H	502	MGD	N1-C2-N3	-2.44	118.76	123.32
19	h	502	MGD	O4'-C1'-C2'	-2.41	103.41	106.93
19	H	502	MGD	C8-N7-C5	2.39	107.53	102.99
19	h	502	MGD	C8-N7-C5	2.38	107.52	102.99
19	H	502	MGD	O4'-C1'-C2'	-2.37	103.46	106.93
19	h	503	MGD	C16-C17-N18	2.34	119.27	112.31
19	H	503	MGD	C16-C17-N18	2.33	119.24	112.31
14	e	505	FAD	C5A-C6A-N6A	2.26	123.79	120.35
14	E	505	FAD	C5A-C6A-N6A	2.25	123.77	120.35
14	A	702	FAD	C5A-C6A-N6A	2.21	123.71	120.35
14	a	702	FAD	C5A-C6A-N6A	2.20	123.69	120.35
19	h	503	MGD	PA-O3B-PB	-2.14	125.49	132.83
19	H	503	MGD	PA-O3B-PB	-2.13	125.51	132.83

There are no chirality outliers.

All (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'
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'
19	H	502	MGD	C5'-O5'-PB-O3B
19	H	502	MGD	PB-O3B-PA-O3A
19	H	502	MGD	C10-O3A-PA-O1A
19	H	502	MGD	C10-O3A-PA-O2A
19	H	502	MGD	O3A-C10-C11-O11
19	H	502	MGD	O3A-C10-C11-C12
19	H	503	MGD	C5'-O5'-PB-O2B
19	H	503	MGD	C3'-C4'-C5'-O5'
19	h	502	MGD	C5'-O5'-PB-O3B
19	h	502	MGD	PB-O3B-PA-O3A
19	h	502	MGD	C10-O3A-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	h	502	MGD	C10-O3A-PA-O2A
19	h	502	MGD	O3A-C10-C11-O11
19	h	502	MGD	O3A-C10-C11-C12
19	h	503	MGD	C5'-O5'-PB-O2B
19	h	503	MGD	C3'-C4'-C5'-O5'
19	H	503	MGD	O4'-C4'-C5'-O5'
19	h	503	MGD	O4'-C4'-C5'-O5'
14	E	505	FAD	C5'-O5'-P-O3P
14	e	505	FAD	C5'-O5'-P-O3P
19	H	502	MGD	C10-O3A-PA-O3B
19	H	503	MGD	C5'-O5'-PB-O3B
19	H	503	MGD	C10-O3A-PA-O3B
19	h	502	MGD	C10-O3A-PA-O3B
19	h	503	MGD	C5'-O5'-PB-O3B
19	h	503	MGD	C10-O3A-PA-O3B
14	E	505	FAD	C5B-O5B-PA-O2A
14	E	505	FAD	C5'-O5'-P-O2P
14	e	505	FAD	C5B-O5B-PA-O2A
14	e	505	FAD	C5'-O5'-P-O2P
19	H	503	MGD	C5'-O5'-PB-O1B
19	H	503	MGD	C10-O3A-PA-O2A
19	h	503	MGD	C5'-O5'-PB-O1B
19	h	503	MGD	C10-O3A-PA-O2A
14	E	505	FAD	C4'-C5'-O5'-P
14	e	505	FAD	C4'-C5'-O5'-P
19	H	503	MGD	PB-O3B-PA-O2A
19	h	503	MGD	PB-O3B-PA-O2A
19	H	502	MGD	O4'-C4'-C5'-O5'
19	h	502	MGD	O4'-C4'-C5'-O5'
14	A	702	FAD	O4B-C4B-C5B-O5B
14	a	702	FAD	O4B-C4B-C5B-O5B
14	A	702	FAD	O4'-C4'-C5'-O5'
14	a	702	FAD	O4'-C4'-C5'-O5'
14	E	505	FAD	C5B-O5B-PA-O3P
14	e	505	FAD	C5B-O5B-PA-O3P
14	E	505	FAD	O4B-C4B-C5B-O5B
14	e	505	FAD	O4B-C4B-C5B-O5B
19	H	503	MGD	PB-O3B-PA-O1A
19	h	503	MGD	PB-O3B-PA-O1A
19	H	502	MGD	C5'-O5'-PB-O2B
19	h	502	MGD	C5'-O5'-PB-O2B
14	E	505	FAD	N10-C1'-C2'-O2'

Continued on next page...

Continued from previous page...

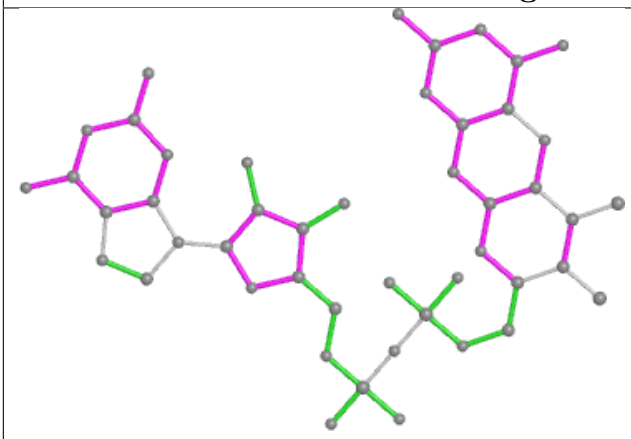
Mol	Chain	Res	Type	Atoms
14	e	505	FAD	N10-C1'-C2'-O2'
14	E	505	FAD	O4'-C4'-C5'-O5'
14	e	505	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

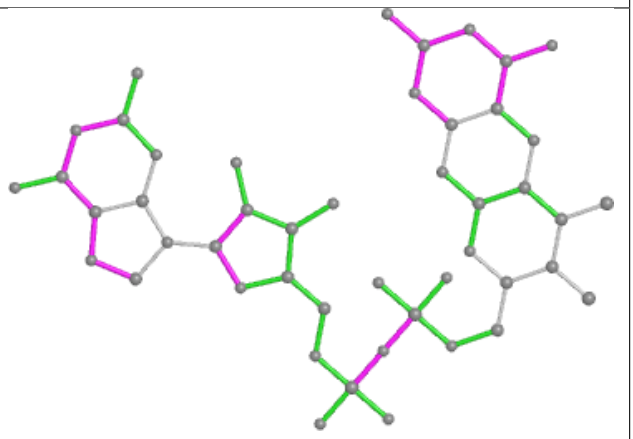
No monomer is involved in short contacts.

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.

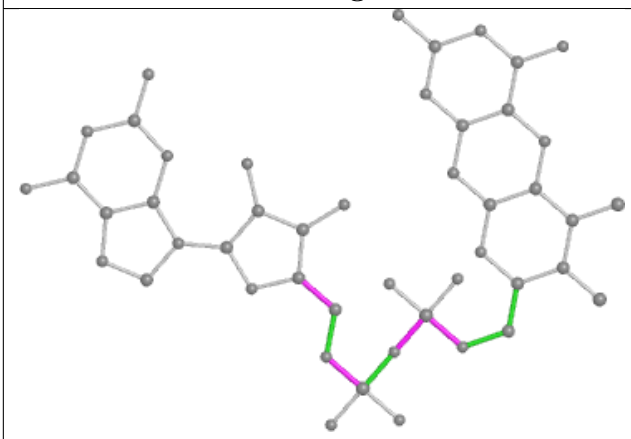
Ligand MGD h 503



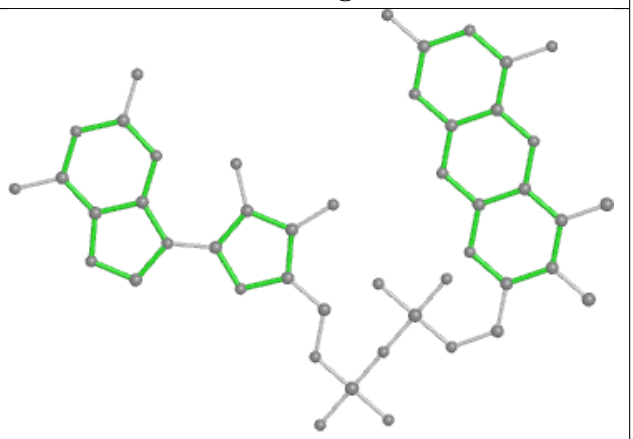
Bond lengths



Bond angles

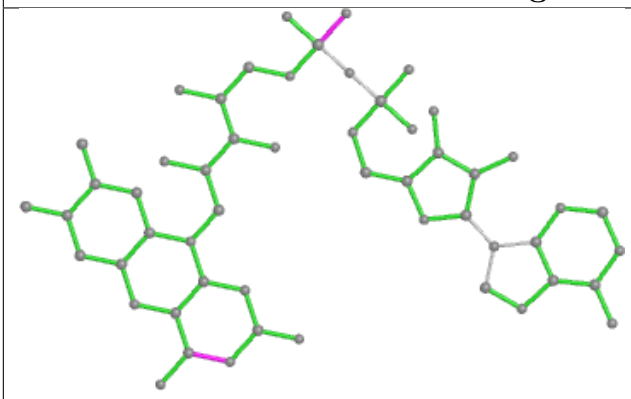


Torsions

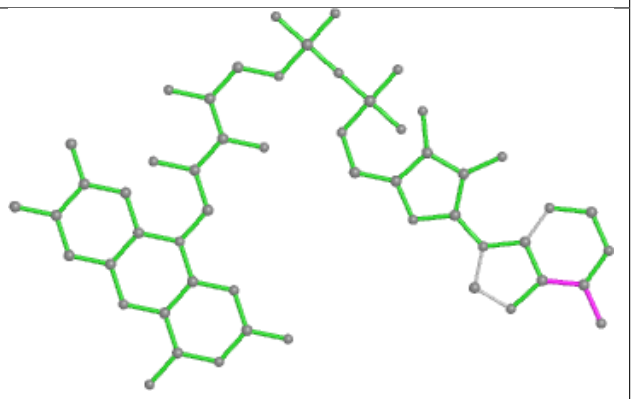


Rings

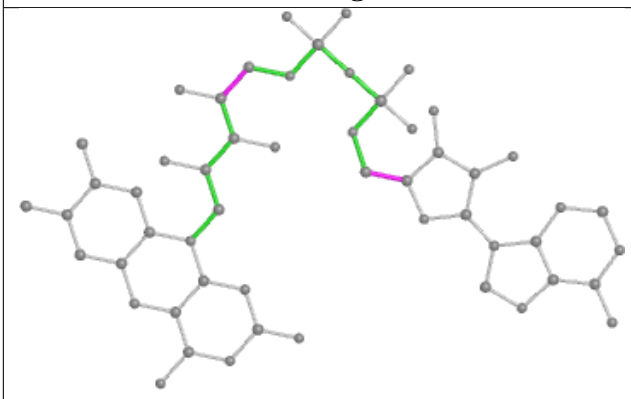
Ligand FAD a 702



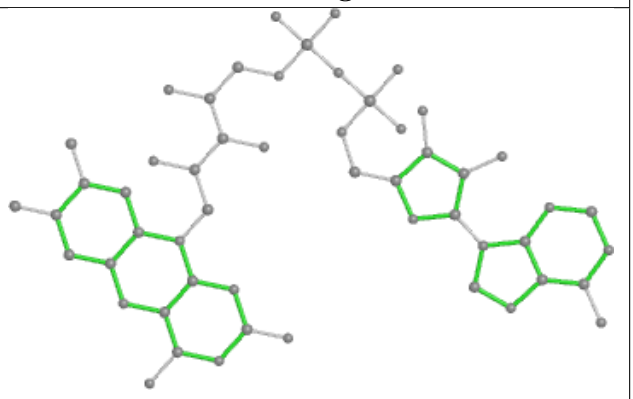
Bond lengths



Bond angles

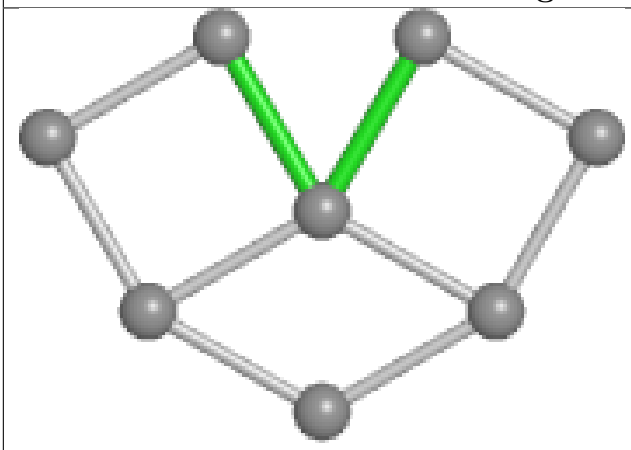


Torsions

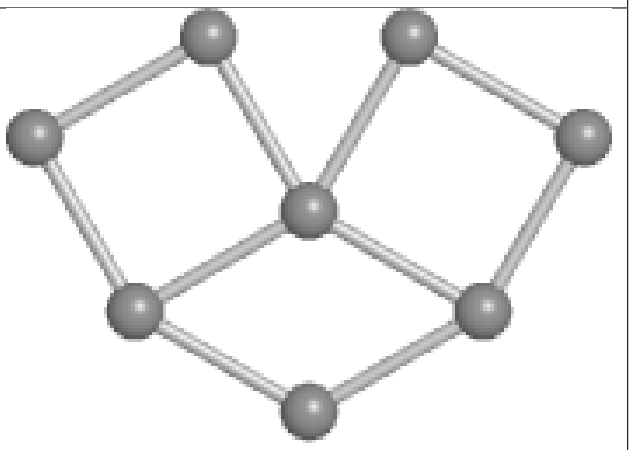


Rings

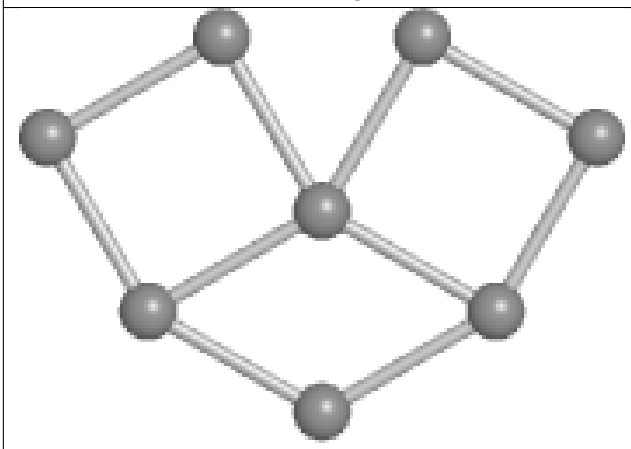
Ligand 9S8 b 302



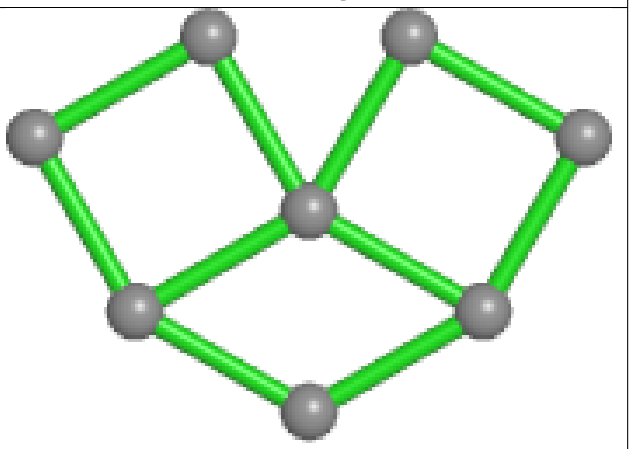
Bond lengths



Bond angles

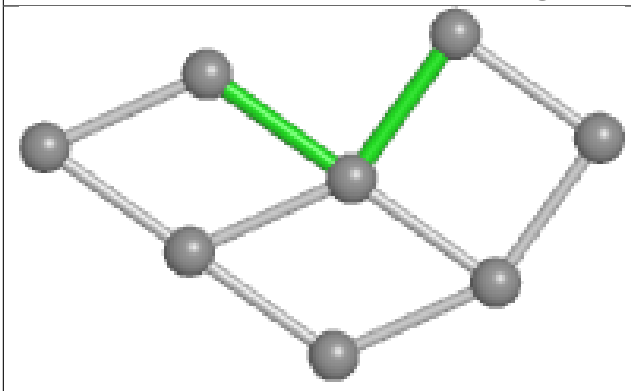


Torsions

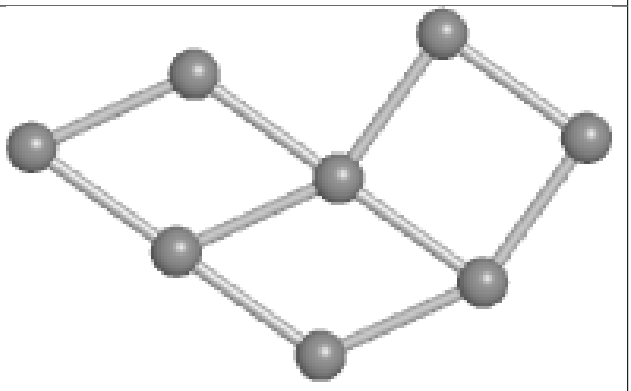


Rings

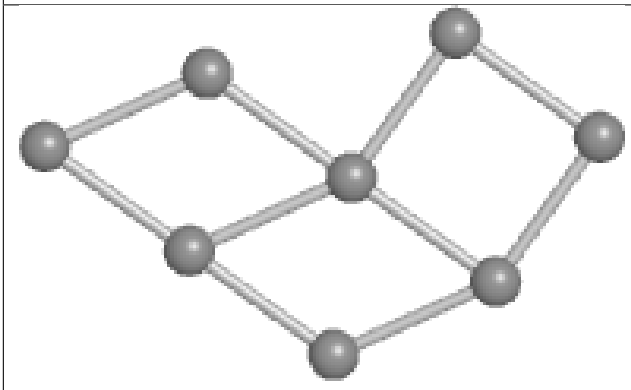
Ligand 9S8 B 301



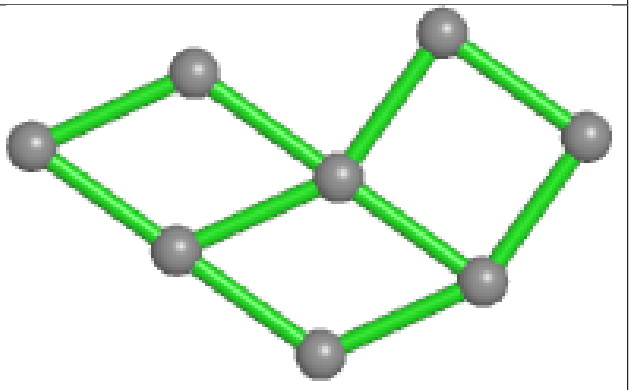
Bond lengths



Bond angles

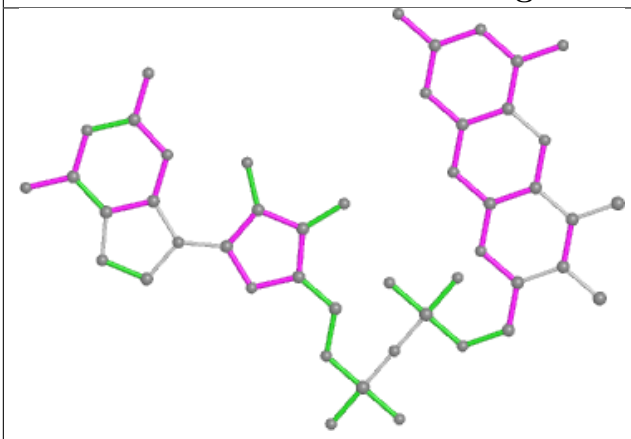


Torsions

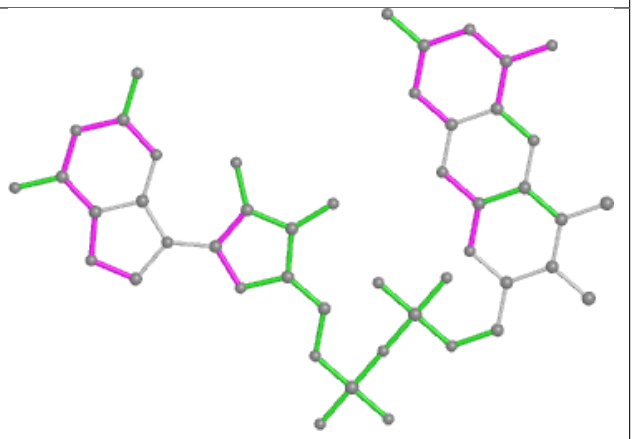


Rings

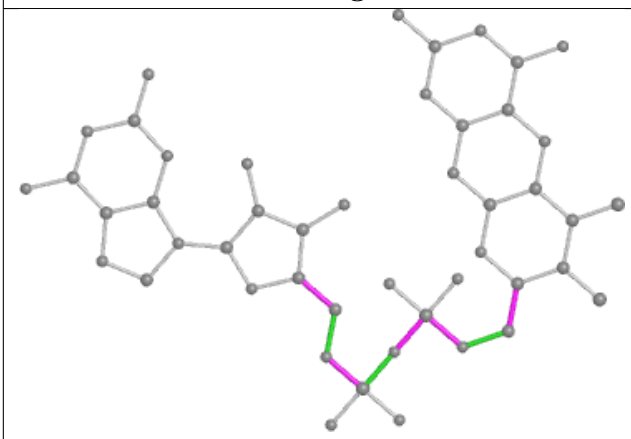
Ligand MGD H 502



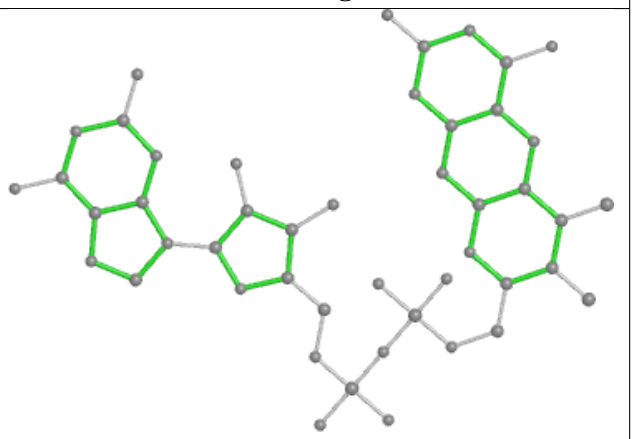
Bond lengths



Bond angles

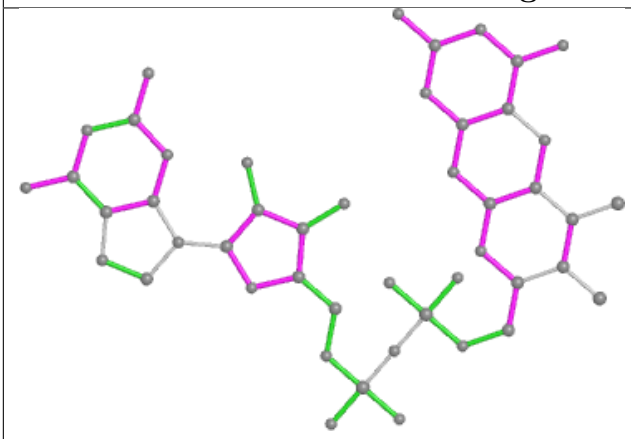


Torsions

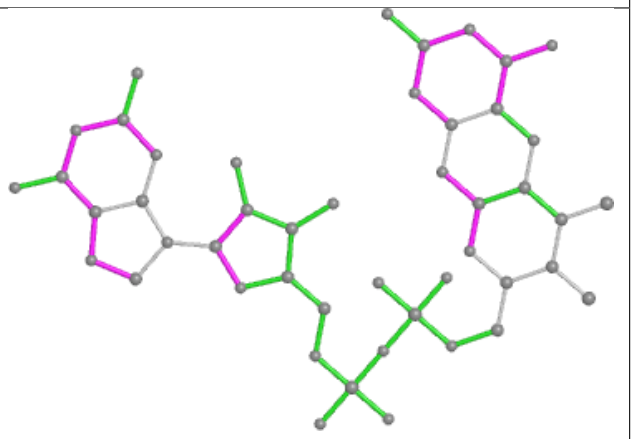


Rings

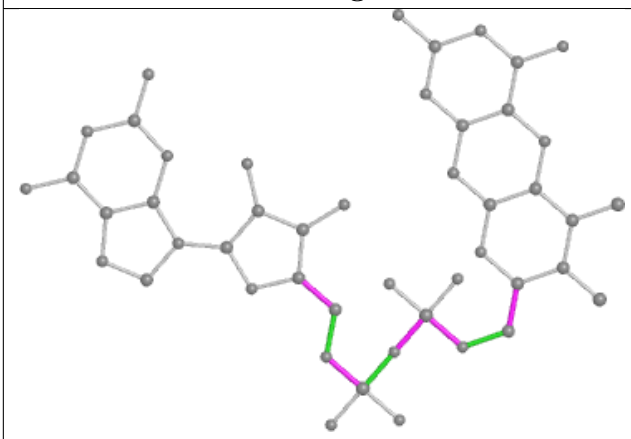
Ligand MGD h 502



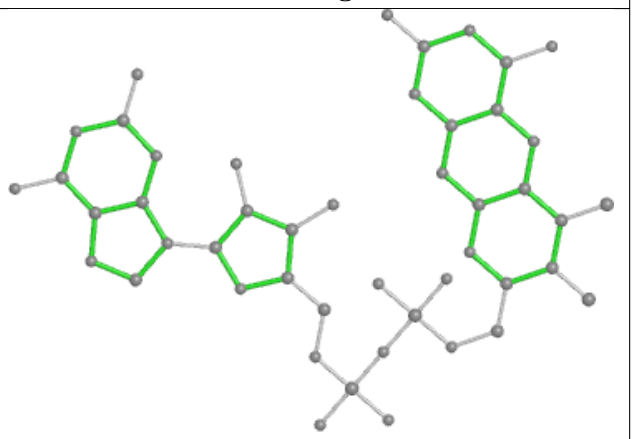
Bond lengths



Bond angles

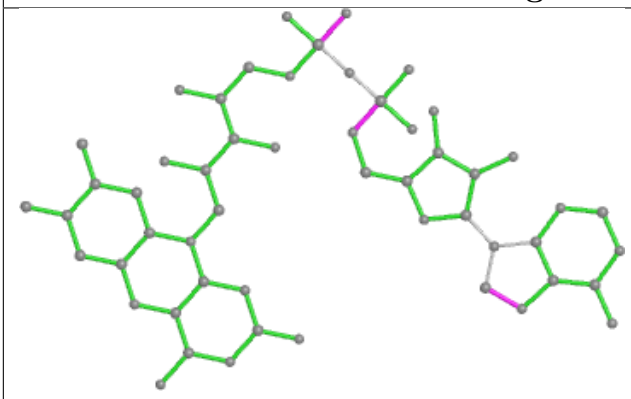


Torsions

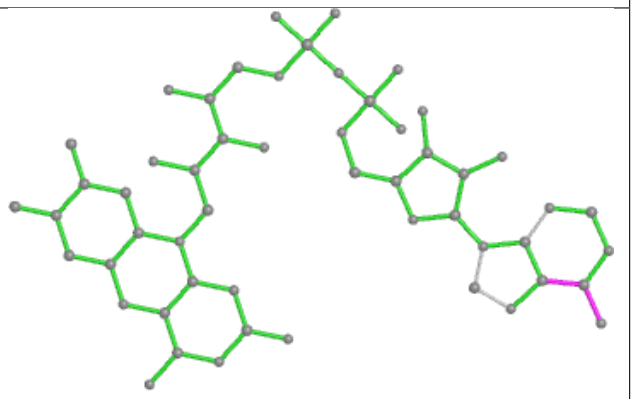


Rings

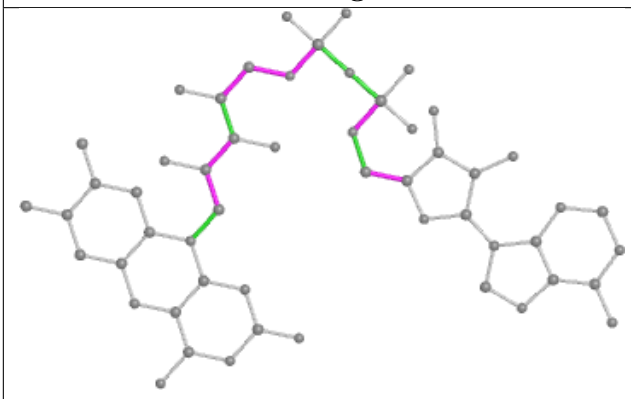
Ligand FAD E 505



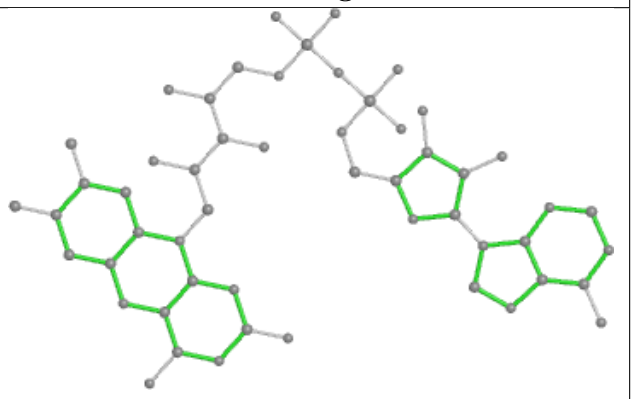
Bond lengths



Bond angles

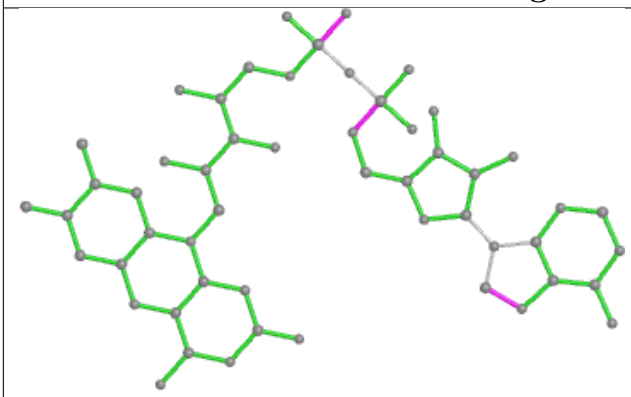


Torsions

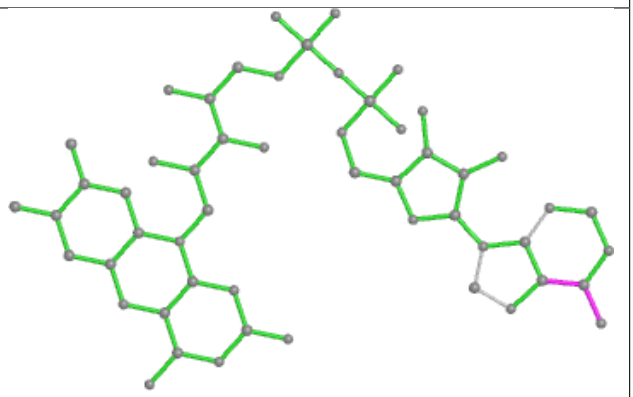


Rings

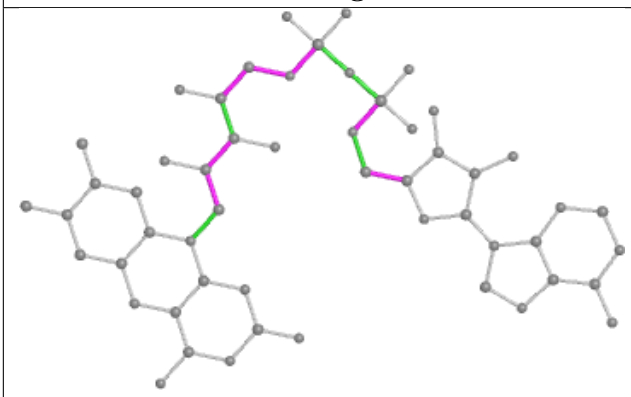
Ligand FAD e 505



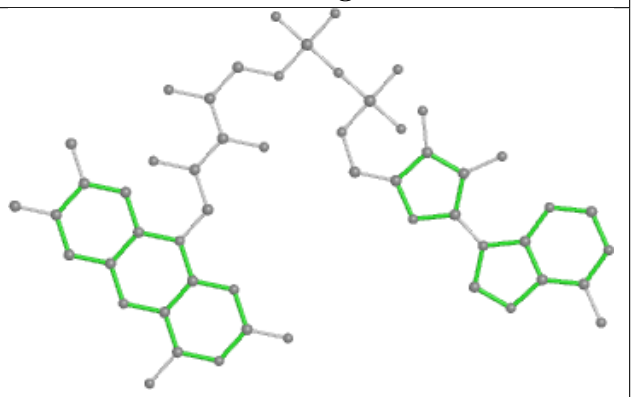
Bond lengths



Bond angles

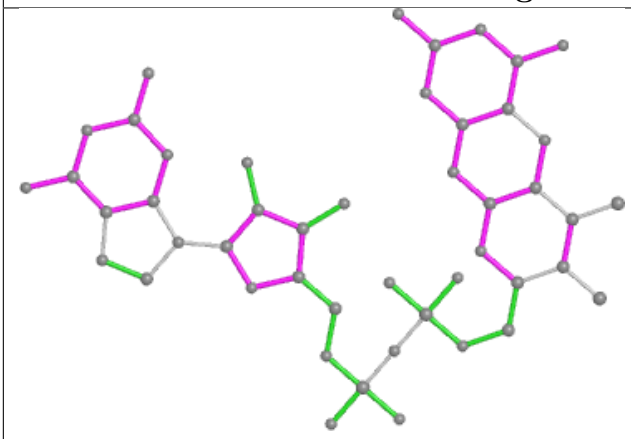


Torsions

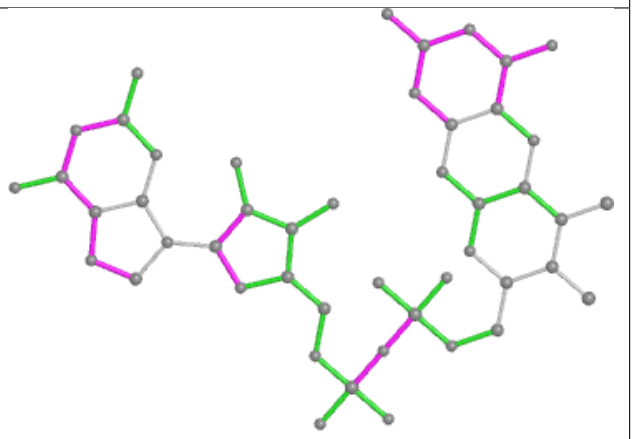


Rings

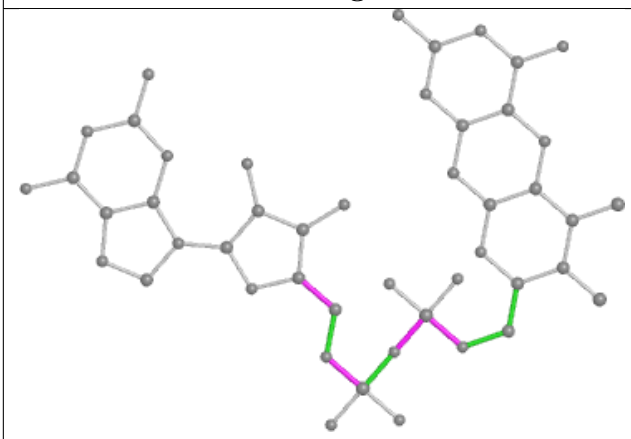
Ligand MGD H 503



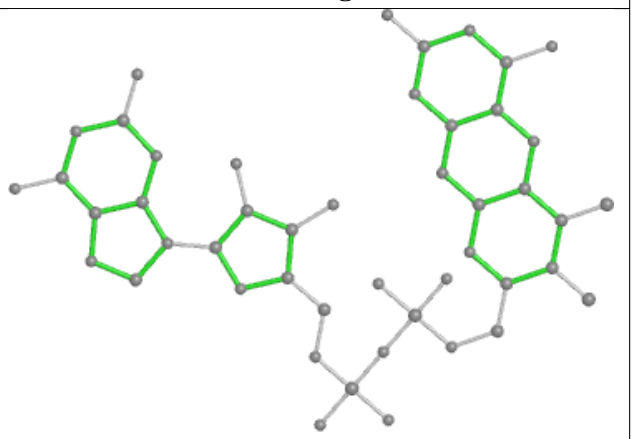
Bond lengths



Bond angles

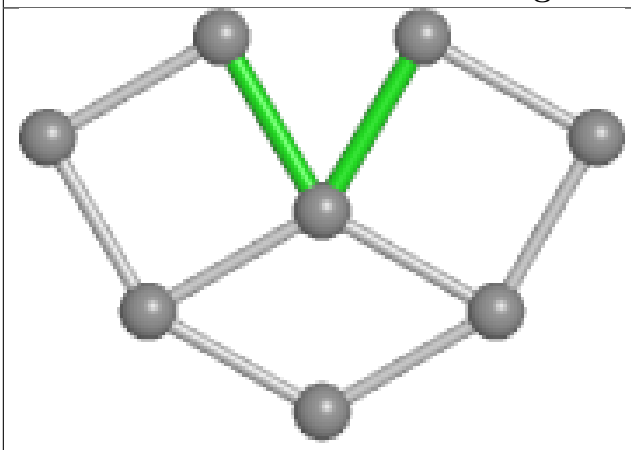


Torsions

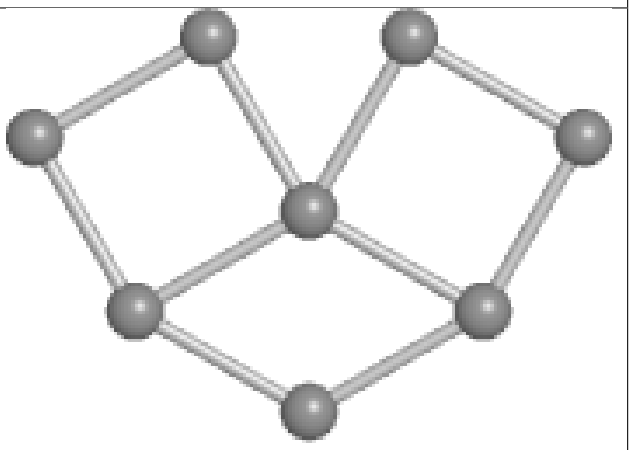


Rings

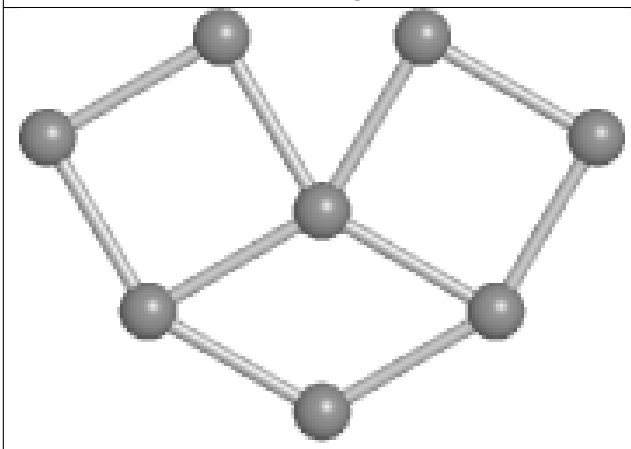
Ligand 9S8 B 302



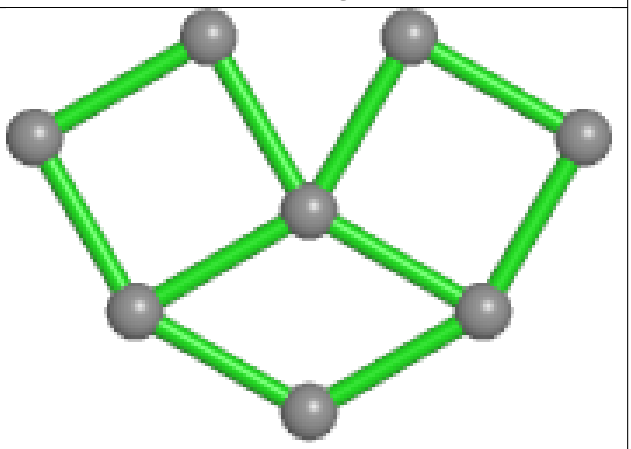
Bond lengths



Bond angles

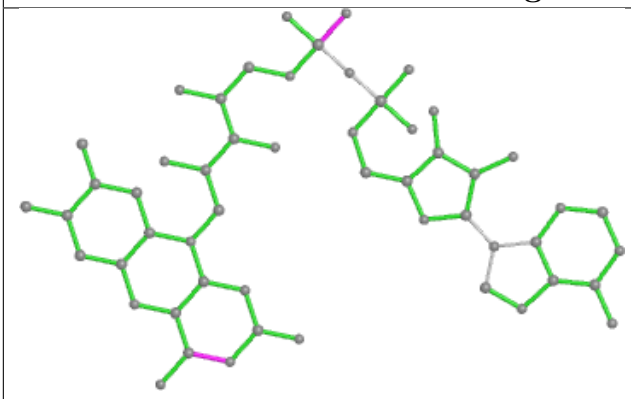


Torsions

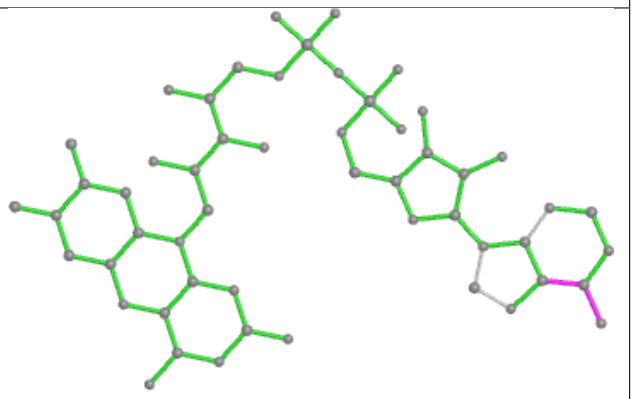


Rings

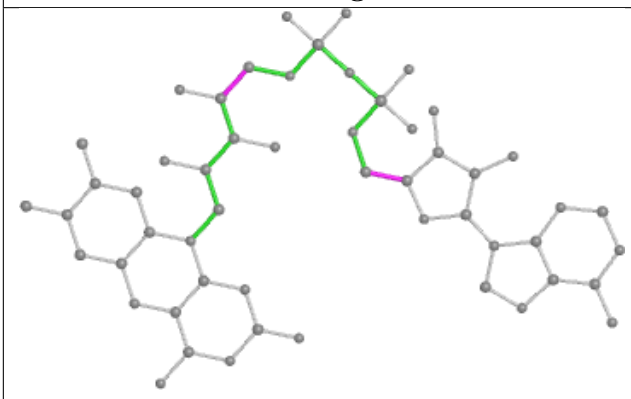
Ligand FAD A 702



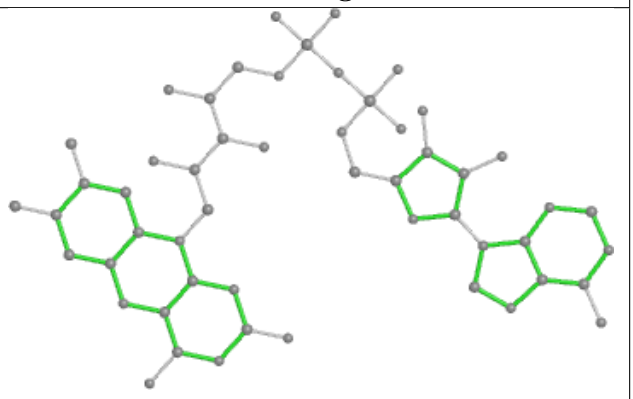
Bond lengths



Bond angles

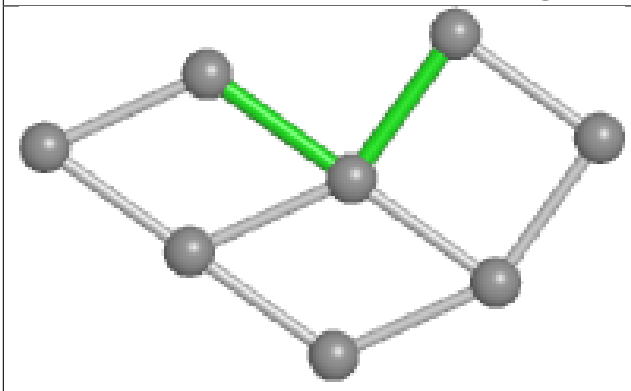


Torsions

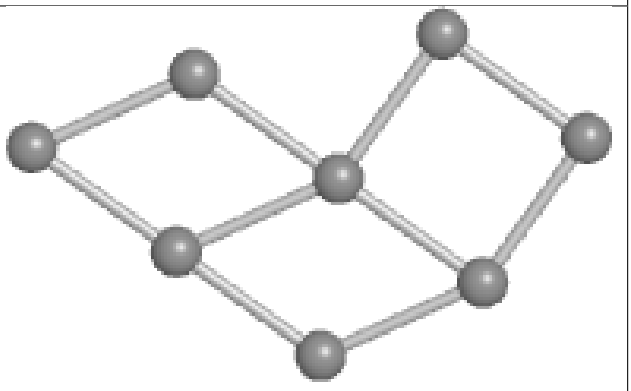


Rings

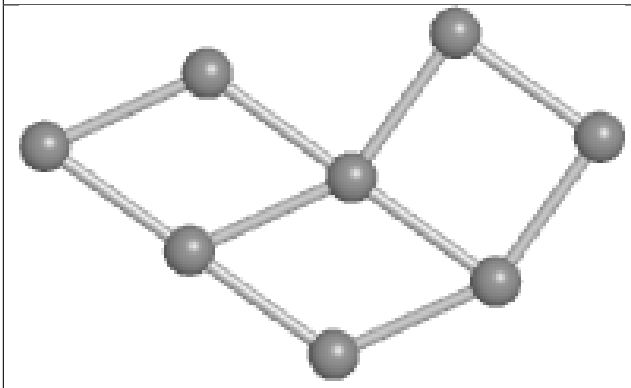
Ligand 9S8 b 301



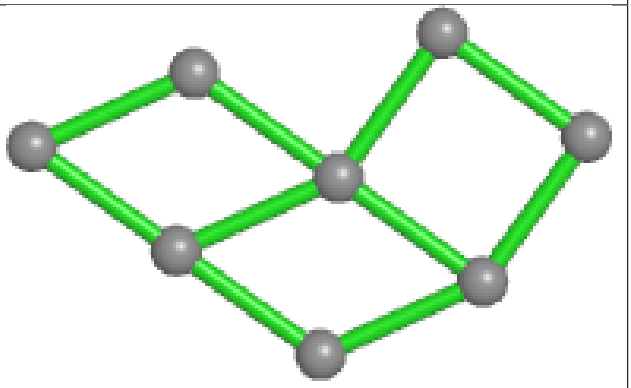
Bond lengths



Bond angles



Torsions



Rings

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.

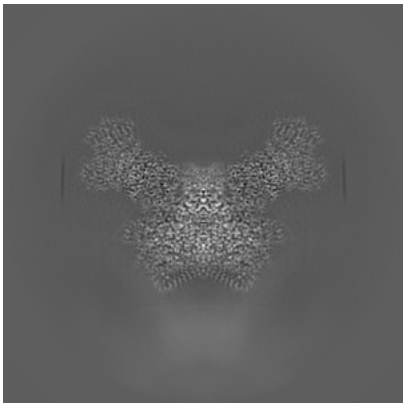
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12209. These allow visual inspection of the internal detail of the map and identification of artifacts.

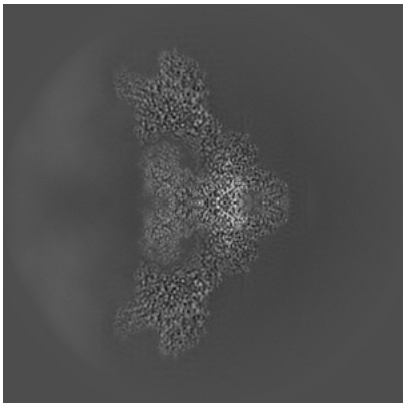
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

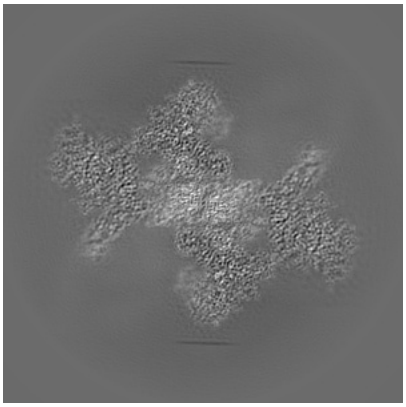
6.1.1 Primary map



X



Y

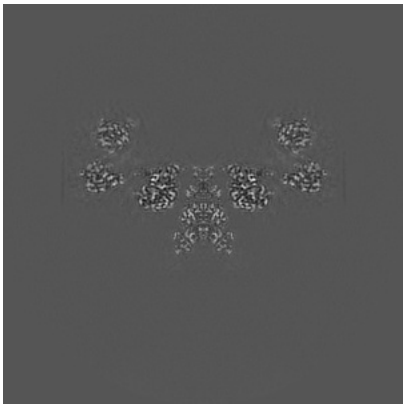


Z

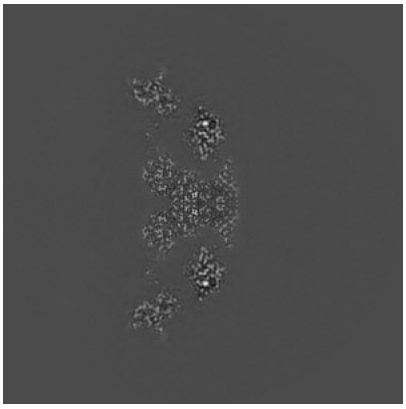
The images above show the map projected in three orthogonal directions.

6.2 Central slices

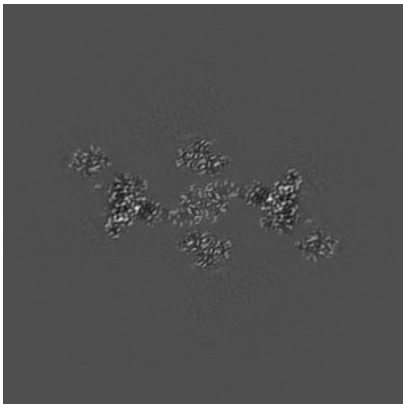
6.2.1 Primary map



X Index: 216



Y Index: 216

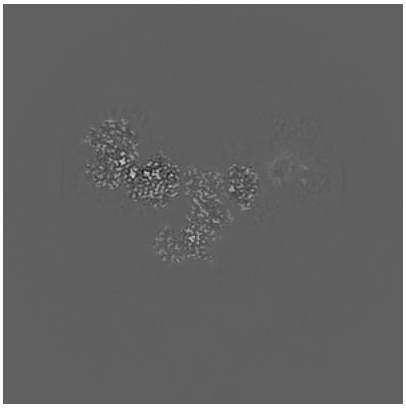


Z Index: 216

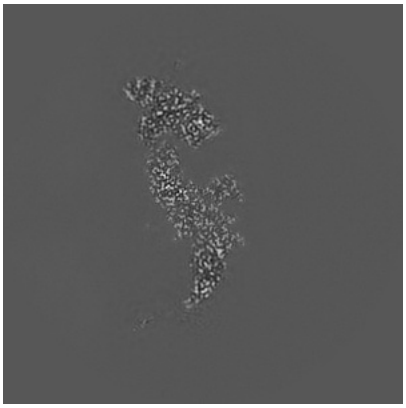
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

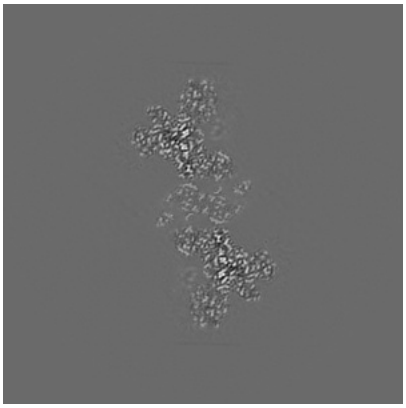
6.3.1 Primary map



X Index: 235



Y Index: 202



Z Index: 248

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 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

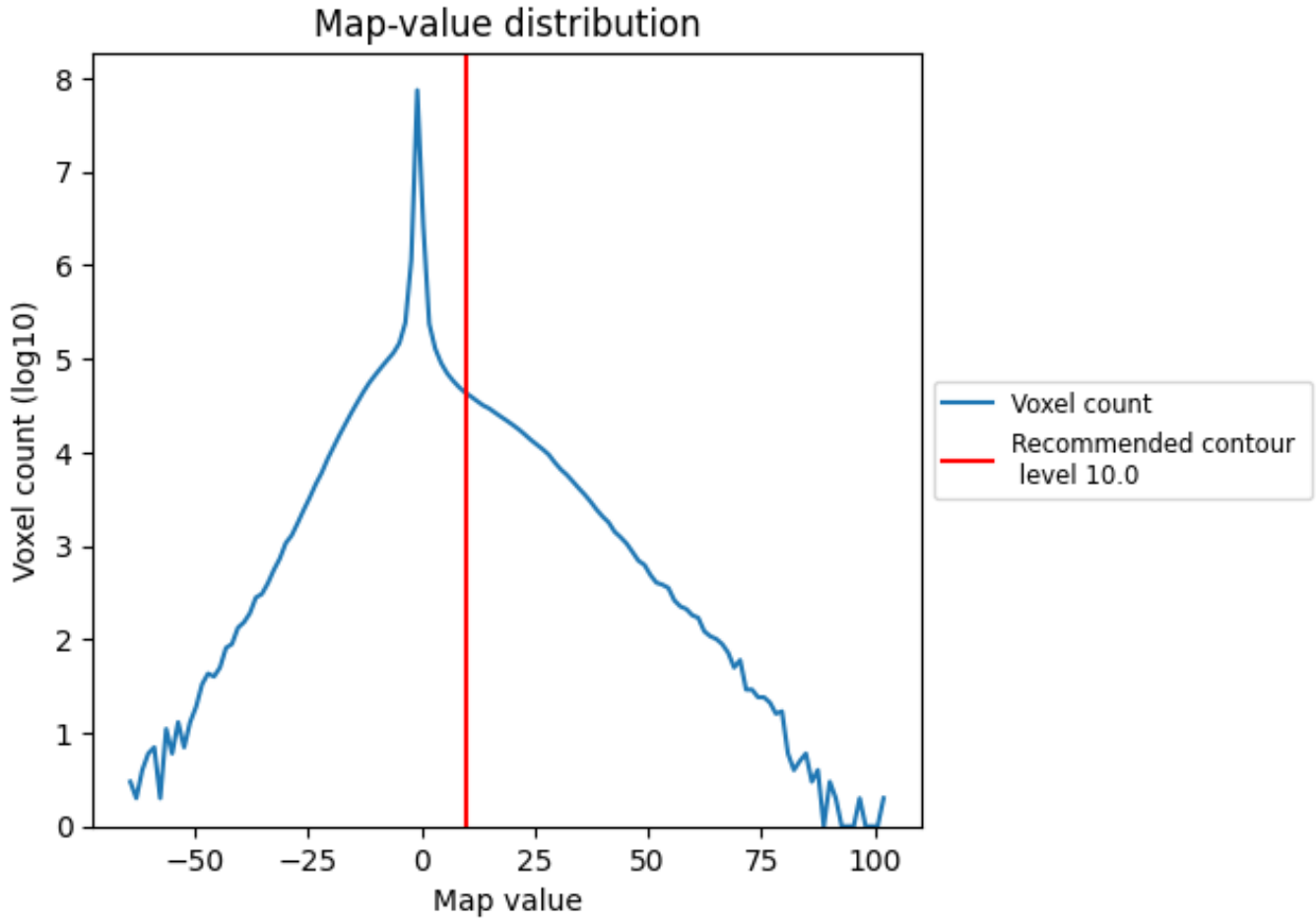
6.5 Mask visualisation (i)

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

7 Map analysis

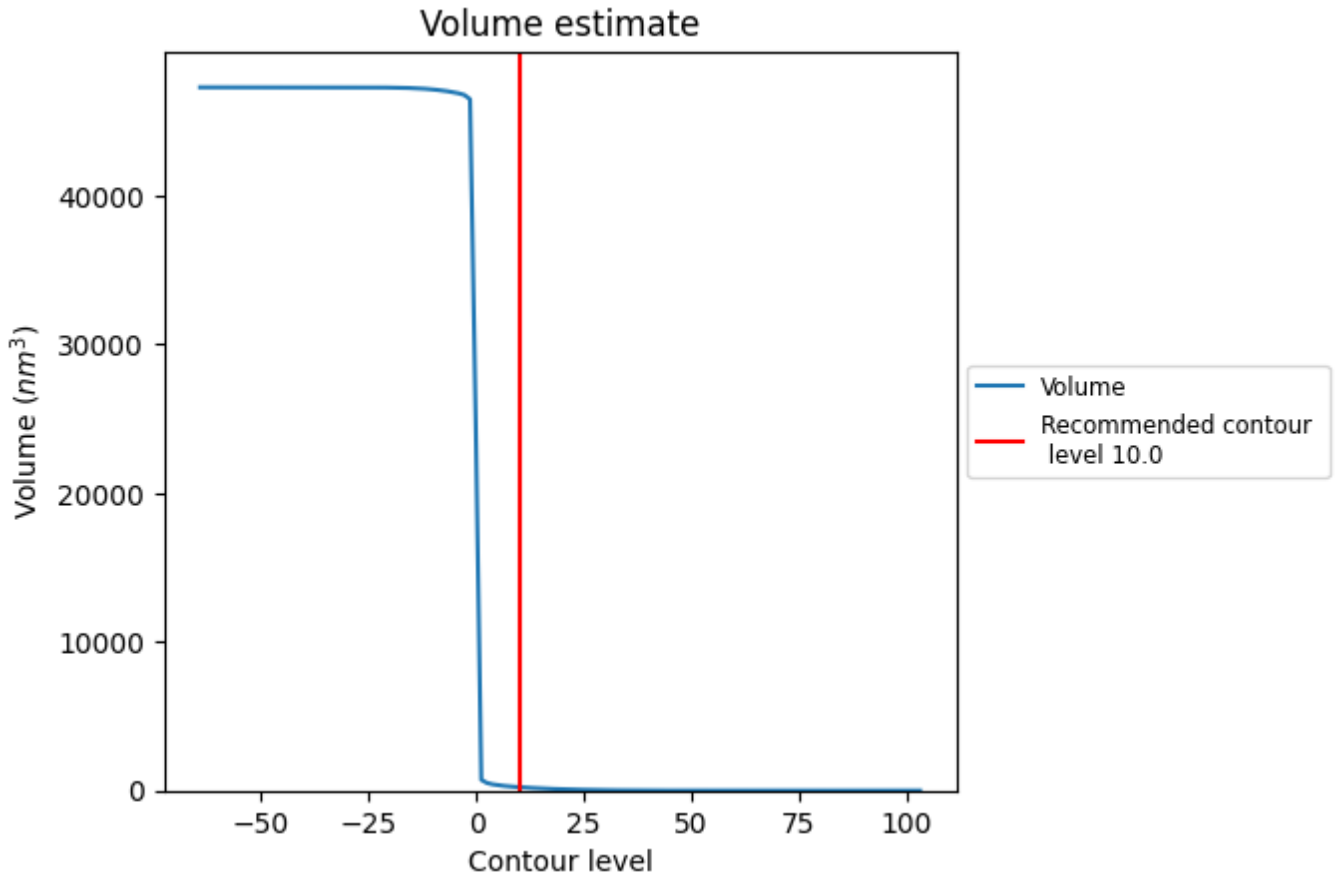
This section contains the results of statistical analysis of the map.

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.

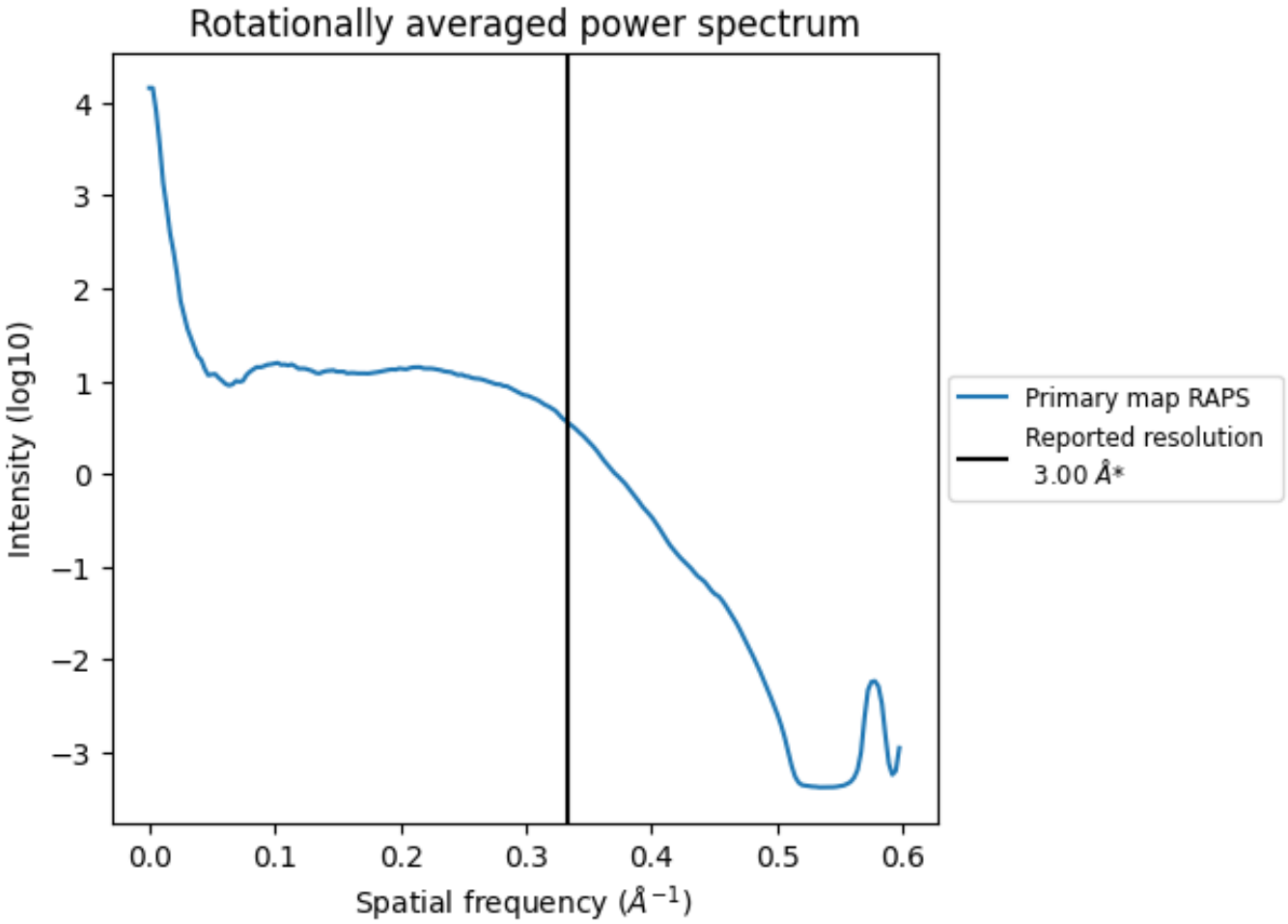
7.2 Volume estimate



The volume at the recommended contour level is 229 nm^3; this corresponds to an approximate mass of 207 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 0.333 Å^{-1}

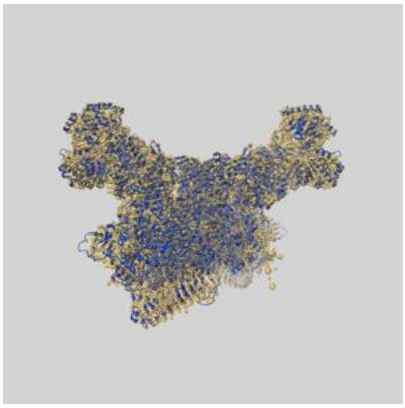
8 Fourier-Shell correlation

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

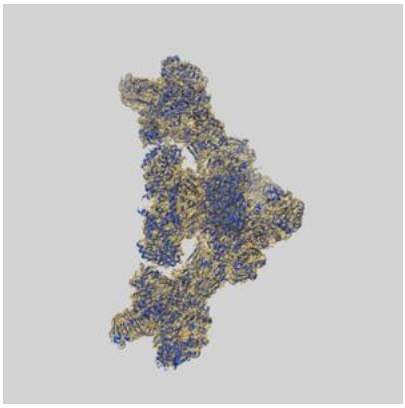
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12209 and PDB model 7BKC. Per-residue inclusion information can be found in section 3 on page 13.

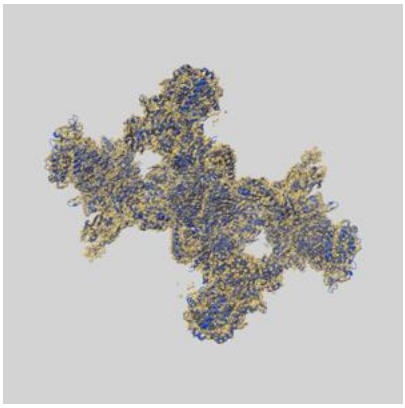
9.1 Map-model overlay



X



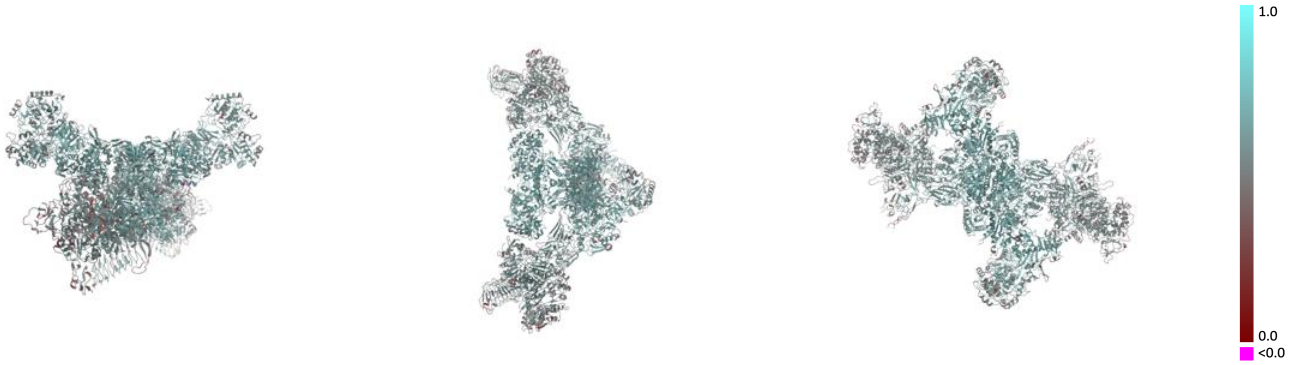
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0 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.

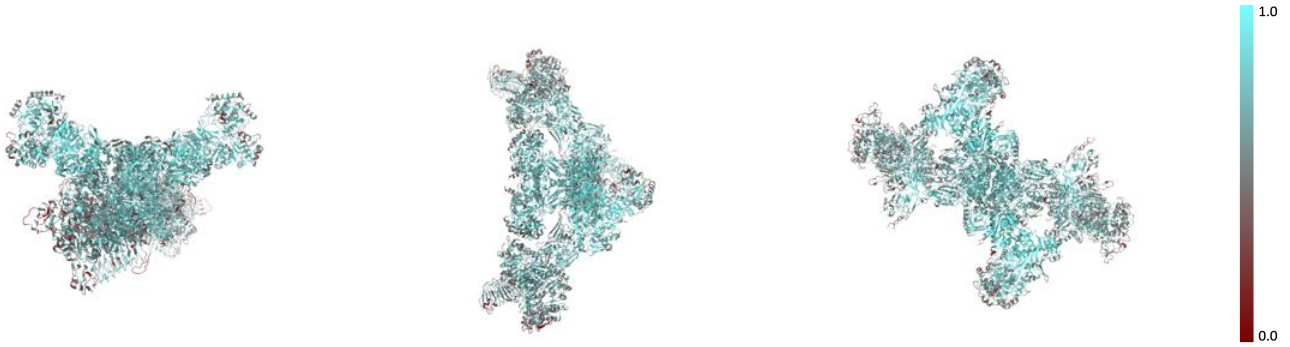
9.2 Q-score mapped to coordinate model (i)



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.

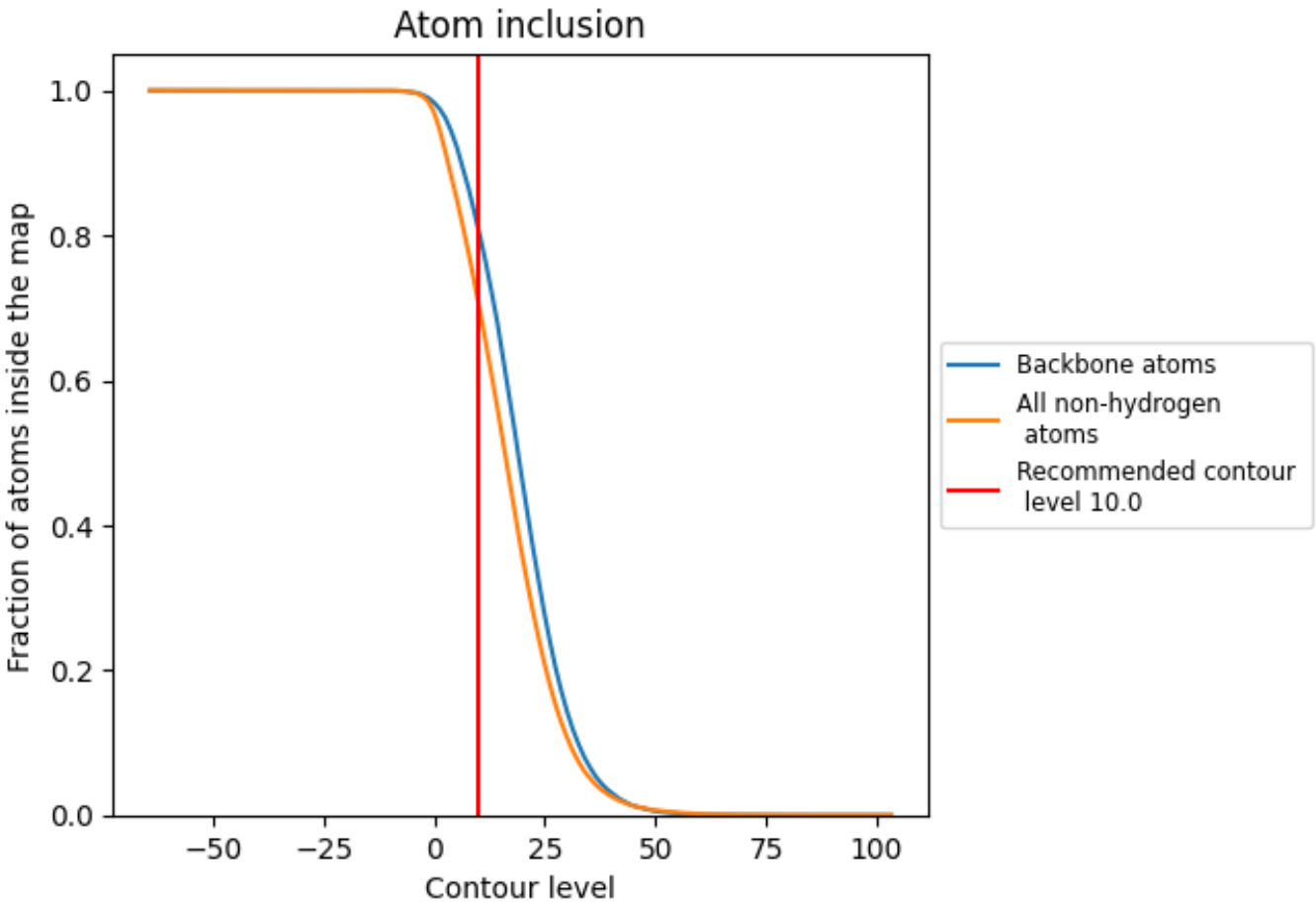
9.3 Atom inclusion mapped to coordinate model (i)



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 (10.0).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 71% 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 (10.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.5690
A	0.8178	0.6480
B	0.7455	0.6300
C	0.7512	0.6450
D	0.6950	0.5610
E	0.8237	0.6040
F	0.8432	0.6230
G	0.5785	0.4970
H	0.6909	0.5390
I	0.5376	0.4860
J	0.6326	0.5310
K	0.6604	0.5200
L	0.7415	0.5590
M	0.5988	0.4860
a	0.8190	0.6460
b	0.7438	0.6310
c	0.7471	0.6420
d	0.6931	0.5600
e	0.8231	0.6050
f	0.8460	0.6210
g	0.5741	0.4980
h	0.6958	0.5410
i	0.5371	0.4850
j	0.6336	0.5310
k	0.6624	0.5200
l	0.7466	0.5630
m	0.6048	0.4880