wwPDB EM Validation Summary Report (i)

Sep 9, 2026 – 03:38 am BST

PDB ID	:	7BKD / pdb_00007bkd
EMDB ID	:	EMD-12210
Title	:	Formate dehydrogenase - heterodisulfide reductase - formylmethanofuran dehydrogenase complex from Methanospirillum hungatei (heterodislfide reductase core and mobile arm in conformational state 1, 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 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:

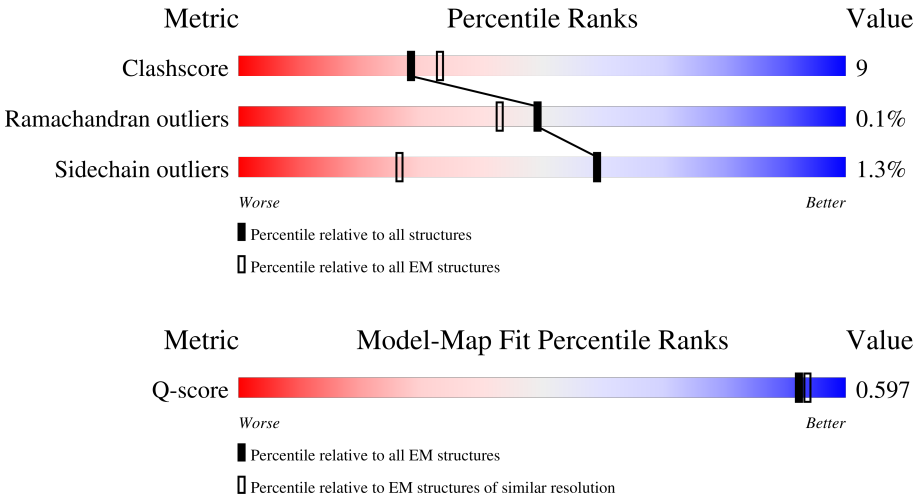
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	79% 20%
1	a	671	50% 17% 34%
2	C	191	9% 77% 20%
2	c	191	10% 80% 18%

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Mol	Chain	Length	Quality of chain
3	B	296	9% 67% 32%
3	b	296	9% 68% 31%
4	F	140	75% 23%
5	E	414	81% 19%
6	D	686	7% 64% 15% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	a	703	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 24799 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	664	Total	C	N	O	S	0	0
			5013	3168	852	937	56		
1	a	446	Total	C	N	O	S	0	0
			3368	2133	570	632	33		

- Molecule 2 is a protein called CoB–CoM heterodisulfide reductase subunit C.

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

- Molecule 3 is a protein called CoB–CoM heterodisulfide reductase subunit B.

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

- Molecule 4 is a protein called F420-non-reducing hydrogenase subunit D.

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

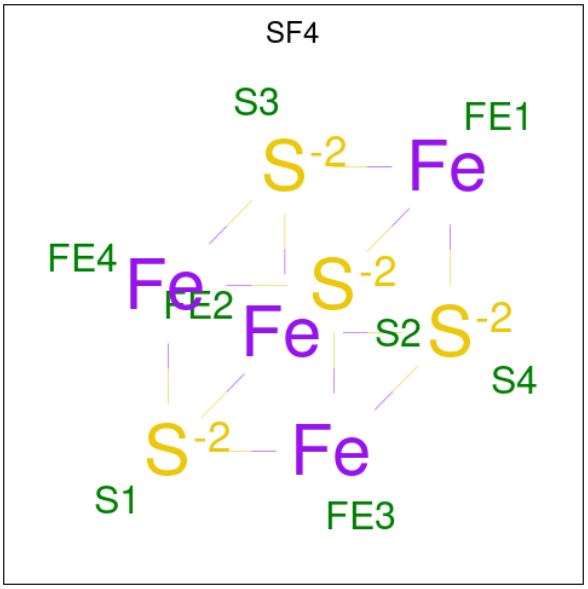
- Molecule 5 is a protein called Formate dehydrogenase, beta subunit (F420).

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

- Molecule 6 is a protein called Formate dehydrogenase.

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

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



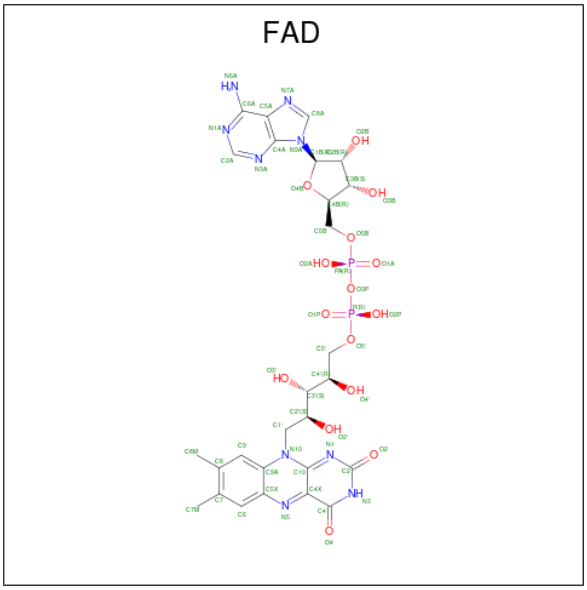
Mol	Chain	Residues	Atoms				AltConf
			Total	Fe	S		
7	A	1	8	4	4		0
7	A	1	8	4	4		0
7	A	1	8	4	4		0
7	A	1	8	4	4		0
7	A	1	8	4	4		0
7	A	1	8	4	4		0
7	C	1	8	4	4		0
7	C	1	8	4	4		0
7	a	1	8	4	4		0
7	a	1	8	4	4		0

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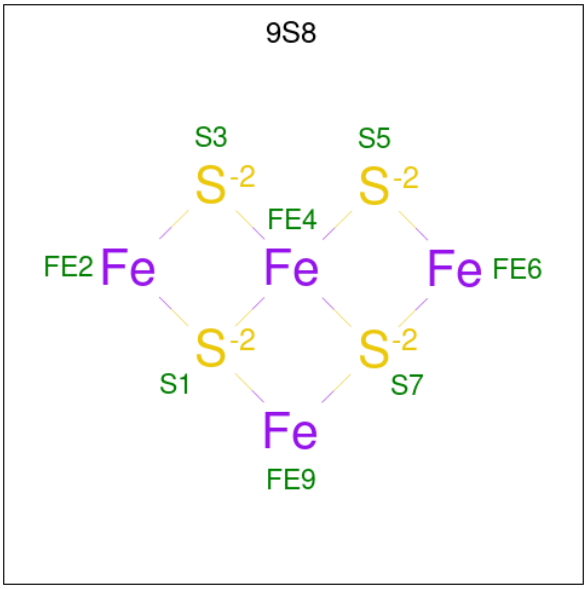
Mol	Chain	Residues	Atoms	AltConf
7	a	1	Total Fe S 8 4 4	0
7	c	1	Total Fe S 8 4 4	0
7	c	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0
7	D	1	Total Fe S 8 4 4	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



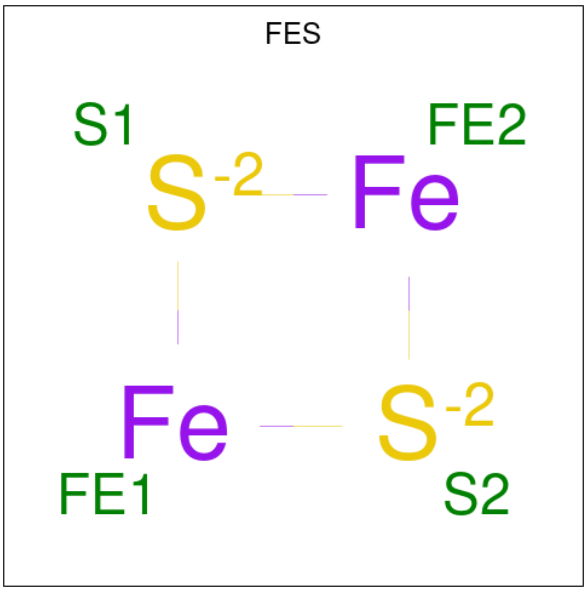
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C N O P 53 27 9 15 2	0
8	a	1	Total C N O P 53 27 9 15 2	0
8	E	1	Total C N O P 53 27 9 15 2	0

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



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

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

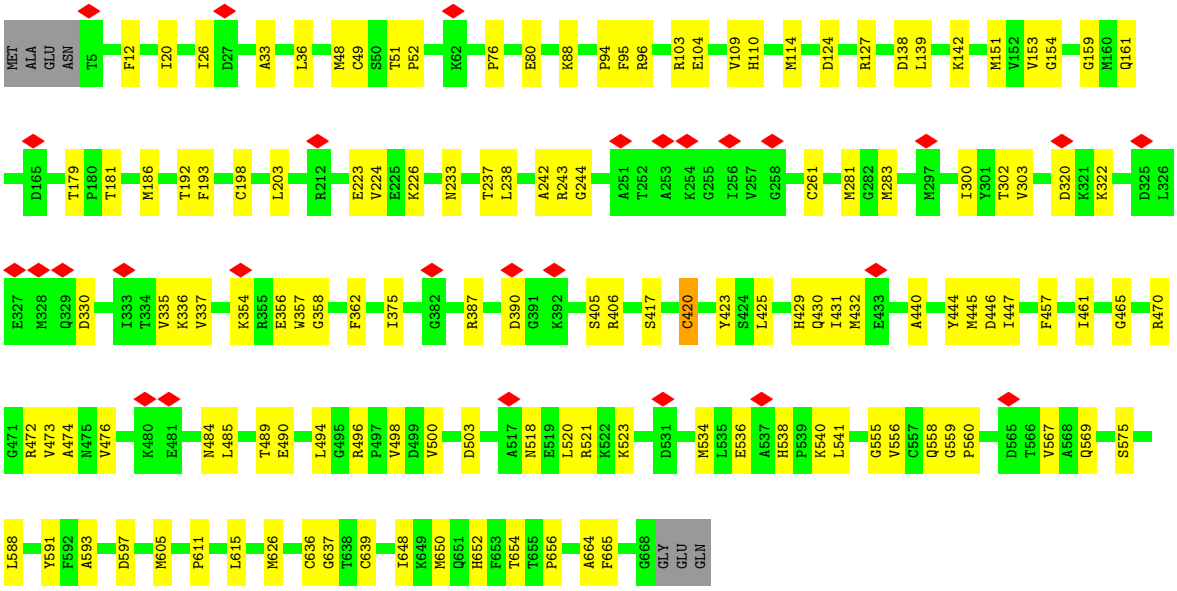
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain A:

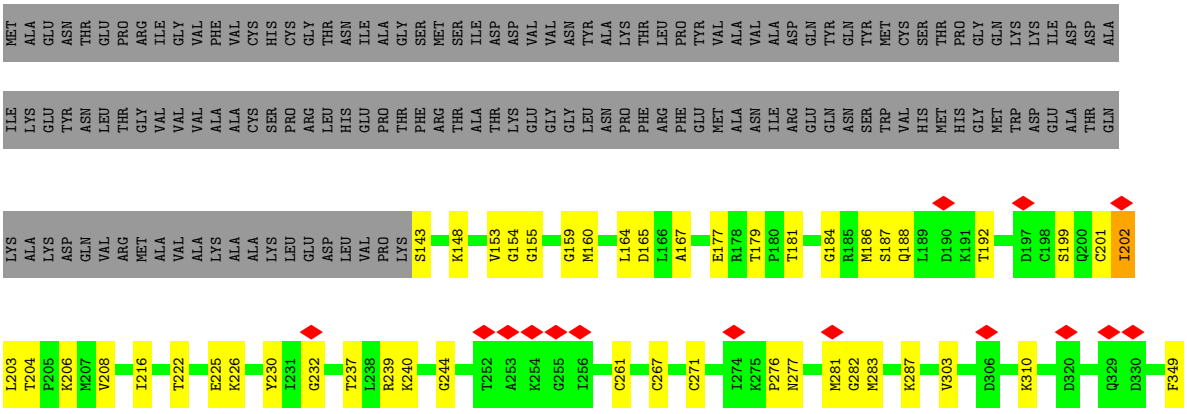


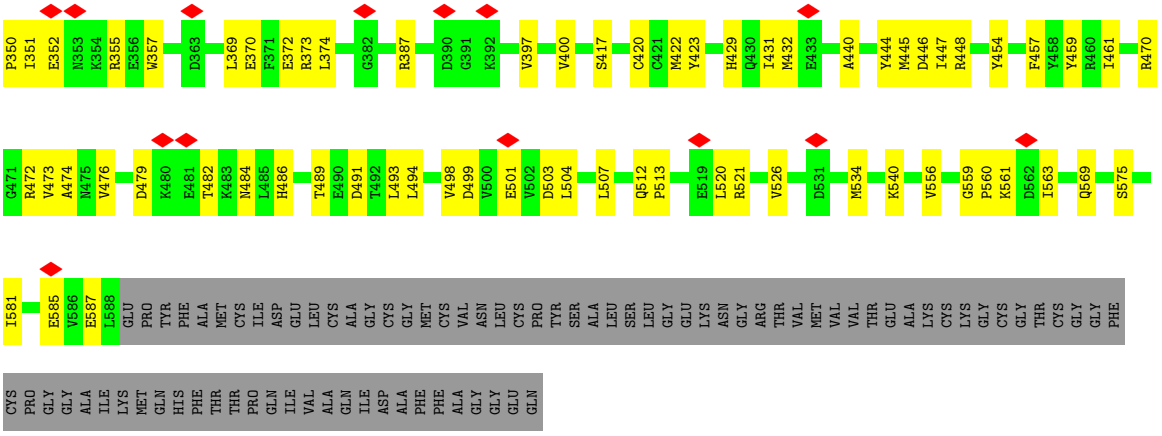


• Molecule 1: CoB–CoM heterodisulfide reductase iron-sulfur subunit A

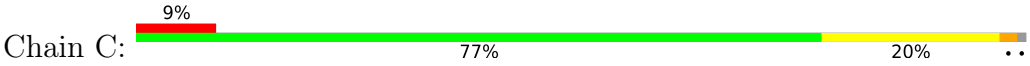
Chain a:

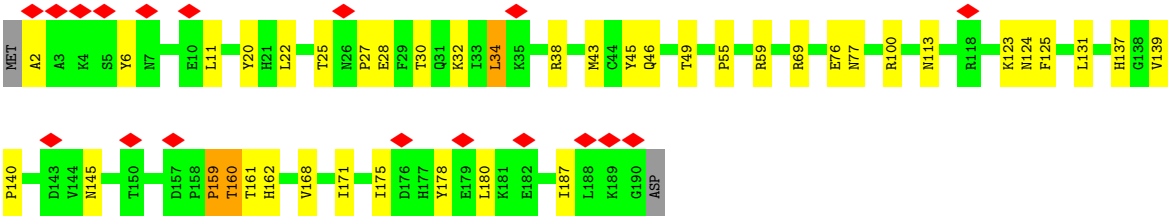




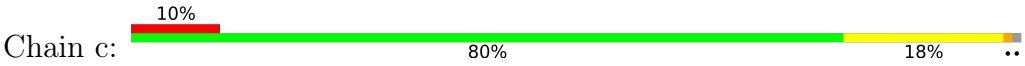


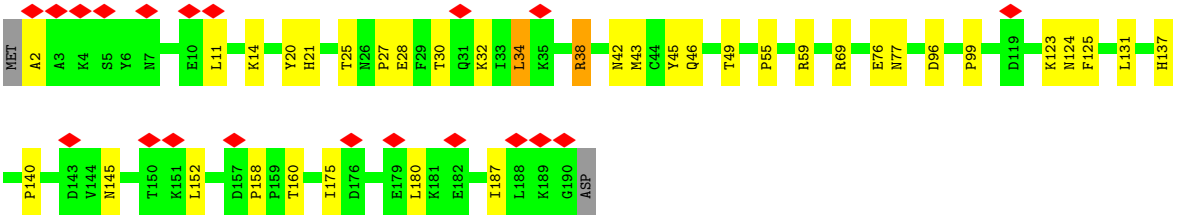
• Molecule 2: CoB–CoM heterodisulfide reductase subunit C





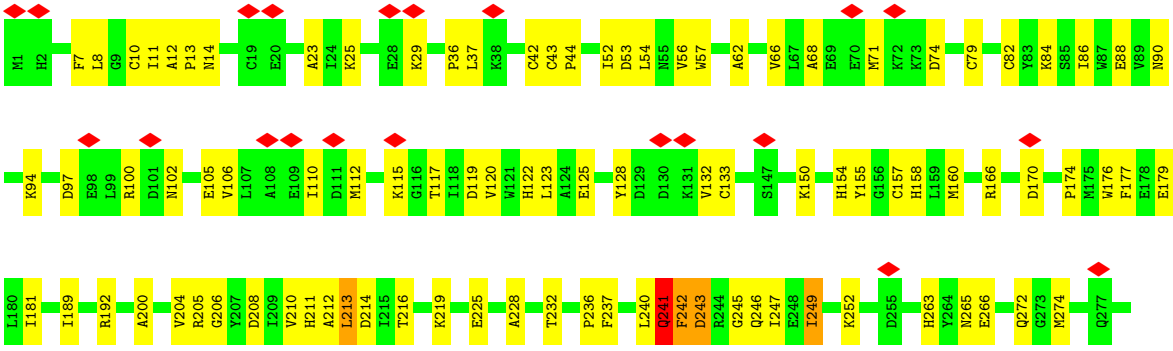
• Molecule 2: CoB–CoM heterodisulfide reductase subunit C

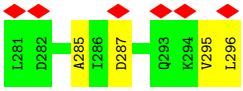




• Molecule 3: CoB–CoM heterodisulfide reductase subunit B



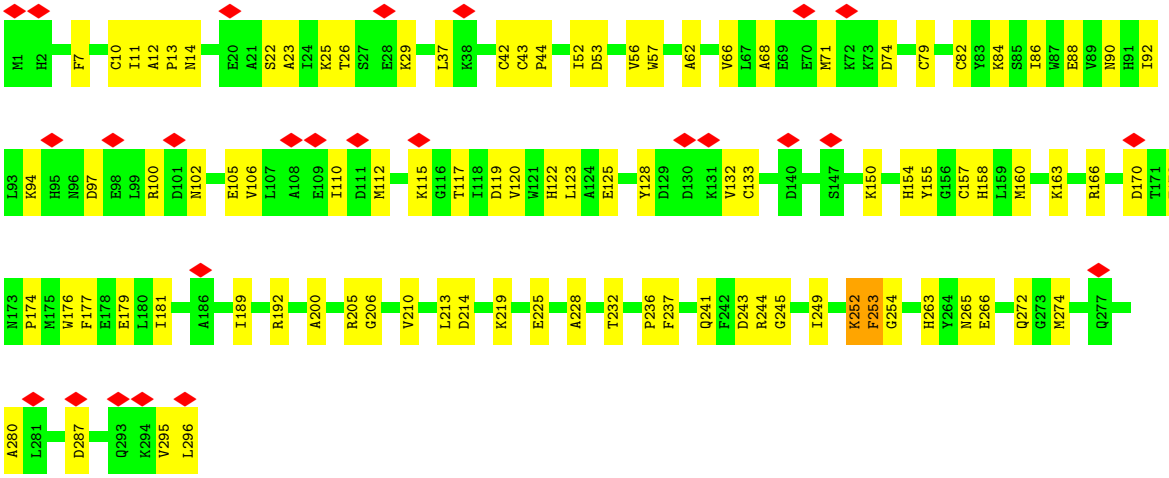




• Molecule 3: CoB–CoM heterodisulfide reductase subunit B

Chain b:

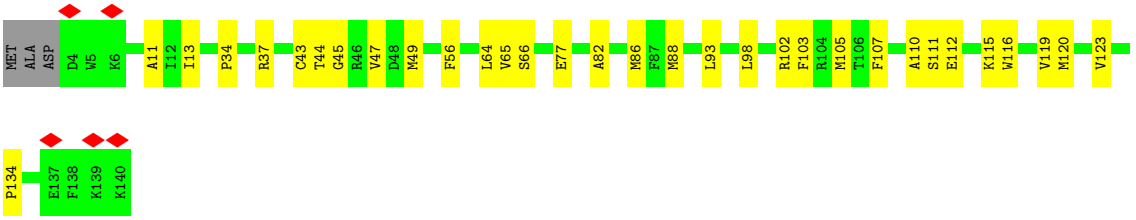




• Molecule 4: F420-non-reducing hydrogenase subunit D

Chain F:

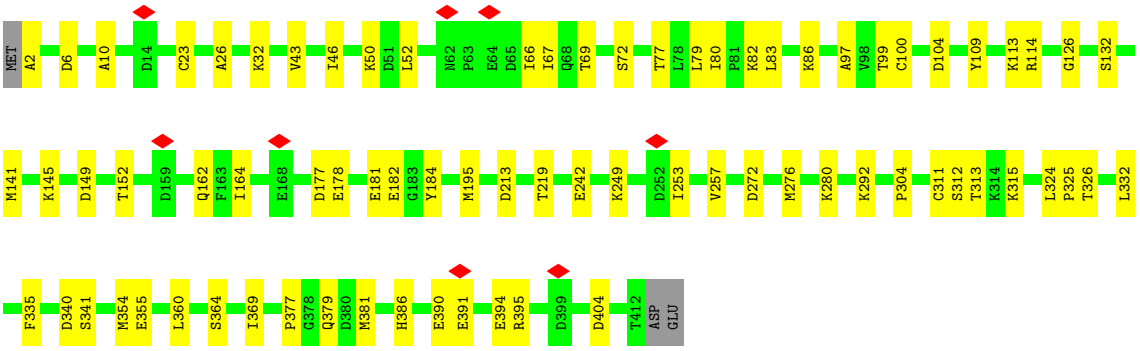




• Molecule 5: Formate dehydrogenase, beta subunit (F420)

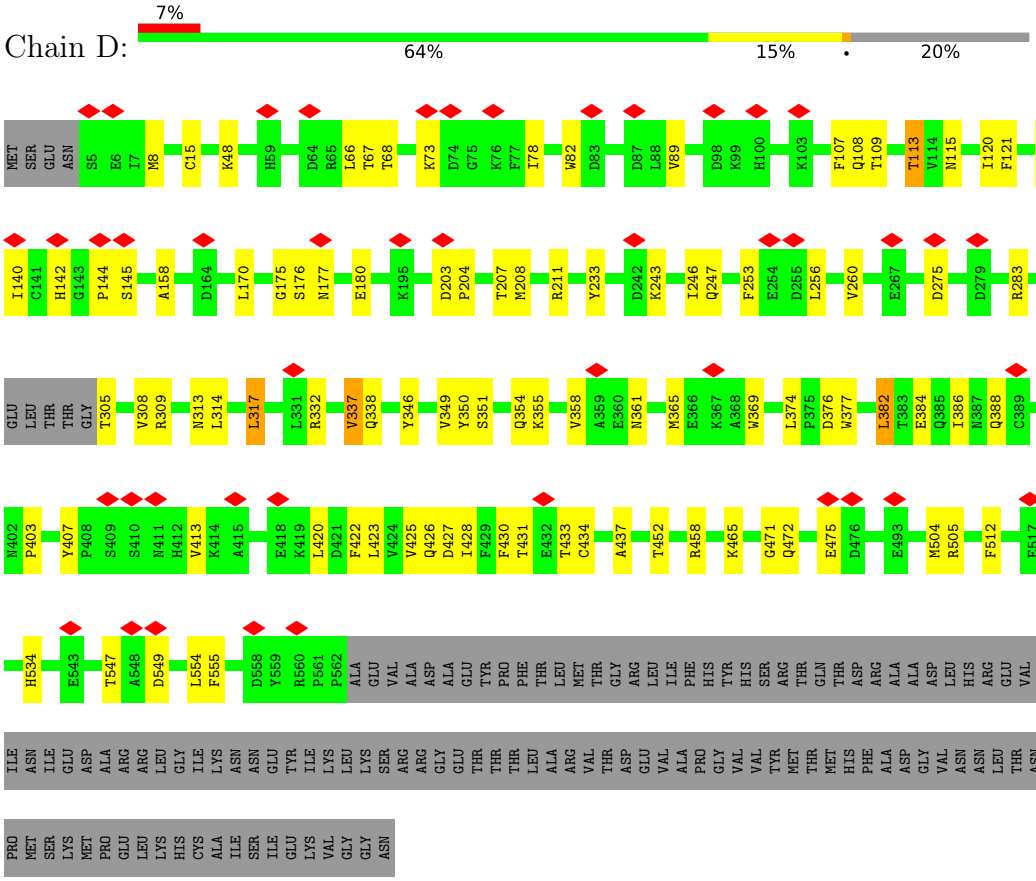
Chain E:





• Molecule 6: Formate dehydrogenase

Chain D:


7%
64%
15%
20%
MET SER GLU ASN S5 E6 T7 M8 C15 K48 H59 D64 R65 L66 T67 T68 K73 D74 G75 K76 F77 I78 W82 D83 D87 L88 V89 D98 K99 H100 K103 F107 Q108 T109 T113 Y114 N115 I120 F121 F129 K130 T131 D135 N136 C137
I140 C141 H142 G143 P144 S145 A158 D164 L170 G175 S176 N177 E180 K195 D203 P204 T207 M208 R211 Y233 D242 K243 I246 Q247 F253 E254 D255 L256 V260 E267 D275 D279 R283 K288 N289 C295 LEU GLY ILE THR
GLU LEU THR THR GLY T305 V308 R309 N313 L314 L317 L331 R332 V337 Q338 Y346 V349 Y350 S351 Q354 K355 V358 A359 E360 N361 M365 E366 K367 A368 W369 L374 P375 D376 W377 L382 T383 E384 Q385 I386 N387 Q388 C389 Y397 I398 L399 G400 L401
N402 P403 Y407 P408 S409 S410 N411 H412 V413 K414 A415 E418 K419 L420 D421 F422 L423 V424 V425 Q426 D427 I428 F429 F430 T431 E432 T433 C434 A437 T452 R458 K465 G471 Q472 E475 D476 E493 M504 R505 F512 E517 K518 P522 W527 P530
H534 E543 T547 A548 D549 L554 F555 D558 Y559 R560 P561 P562 ALA GLU VAL ALA ASP ALA GLU TYR PRO PHE THR LEU MET THR GLY ARG LEU ILE PHE HIS TYR HIS SER ARG THR GLN THR ASP ARG ALA ALA ASP LEU HIS ARG GLU VAL PRO GLU SER TYR ALA GLN
ILE ASN ILE GLU ASP ALA ARG ARG LEU GLY ILE LYS ASN ASN GLU TYR ILE LYS LEU LYS SER ARG ARG GLY GLU THR THR THR LEU ALA ARG VAL THR ASP GLU VAL ALA PRO GLY VAL VAL TYR MET THR MET HIS PHE ALA ASP GLY VAL ASN ASN LEU THR ASN THR VAL LEU ASP
PRO MET SER LYS MET PRO GLU LEU LYS HIS CYS ALA ILE SER ILE GLU LYS VAL GLY GLY ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	277450	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	101.016	Depositor
Minimum map value	-70.139	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.185	Depositor
Recommended contour level	8	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, 9S8, SF4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/5116	0.50	2/6925 (0.0%)
1	a	0.29	0/3435	0.50	0/4649
2	C	0.29	0/1529	0.53	1/2072 (0.0%)
2	c	0.19	0/1529	0.43	0/2072
3	B	0.43	3/2355 (0.1%)	0.66	5/3187 (0.2%)
3	b	0.40	3/2355 (0.1%)	0.62	2/3187 (0.1%)
4	F	0.27	0/1096	0.48	0/1474
5	E	0.24	0/3208	0.41	0/4314
6	D	0.33	0/4345	0.54	3/5889 (0.1%)
All	All	0.31	6/24968 (0.0%)	0.52	13/33769 (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
3	B	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	241	GLN	C-O	-7.47	1.15	1.24
3	B	243	ASP	C-O	6.94	1.32	1.24
3	B	241	GLN	C-O	-6.88	1.16	1.24
3	B	245	GLY	C-O	-5.88	1.16	1.23
3	b	245	GLY	C-O	-5.53	1.17	1.23

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	249	ILE	N-CA-C	-8.94	102.11	111.58
2	C	159	PRO	CB-CA-C	-7.35	103.09	113.09
1	A	591	TYR	CB-CA-C	-7.23	101.22	111.85
3	B	241	GLN	CA-C-O	-6.55	114.13	121.00
3	b	252	LYS	CA-C-N	-6.52	112.98	121.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	241	GLN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5013	0	4948	94	0
1	a	3368	0	3343	75	0
2	C	1498	0	1495	34	0
2	c	1498	0	1495	33	0
3	B	2304	0	2272	66	0
3	b	2304	0	2272	62	0
4	F	1073	0	1082	24	0
5	E	3151	0	3162	54	0
6	D	4251	0	4204	79	0
7	A	48	0	0	2	0
7	C	16	0	0	0	0
7	D	8	0	0	1	0
7	E	32	0	0	0	0
7	a	24	0	0	2	0
7	c	16	0	0	0	0
8	A	53	0	31	1	0
8	E	53	0	31	5	0
8	a	53	0	31	2	0
9	B	16	0	0	2	0
9	b	16	0	0	2	0
10	F	4	0	0	0	0
All	All	24799	0	24366	465	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 465 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:SER:HB2	1:a:575:SER:HB2	1.56	0.87
1:a:431:ILE:HD11	1:a:440:ALA:HB2	1.58	0.86
1:A:432:MET:HE3	1:A:440:ALA:H	1.46	0.78
6:D:427:ASP:OD2	6:D:428:ILE:N	2.20	0.74
5:E:355:GLU:OE2	6:D:48:LYS:NZ	2.20	0.74

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	662/671 (99%)	627 (95%)	34 (5%)	1 (0%)	43 76
1	a	444/671 (66%)	417 (94%)	27 (6%)	0	100 100
2	C	187/191 (98%)	180 (96%)	7 (4%)	0	100 100
2	c	187/191 (98%)	179 (96%)	8 (4%)	0	100 100
3	B	294/296 (99%)	280 (95%)	14 (5%)	0	100 100
3	b	294/296 (99%)	280 (95%)	13 (4%)	1 (0%)	36 70
4	F	135/140 (96%)	125 (93%)	10 (7%)	0	100 100
5	E	409/414 (99%)	393 (96%)	16 (4%)	0	100 100
6	D	545/686 (79%)	501 (92%)	44 (8%)	0	100 100
All	All	3157/3556 (89%)	2982 (94%)	173 (6%)	2 (0%)	49 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	ASP
3	b	254	GLY

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	533/543 (98%)	530 (99%)	3 (1%)	78	88
1	a	358/543 (66%)	352 (98%)	6 (2%)	53	78
2	C	168/170 (99%)	165 (98%)	3 (2%)	51	77
2	c	168/170 (99%)	166 (99%)	2 (1%)	63	82
3	B	245/245 (100%)	239 (98%)	6 (2%)	43	73
3	b	245/245 (100%)	242 (99%)	3 (1%)	63	82
4	F	112/114 (98%)	111 (99%)	1 (1%)	70	85
5	E	338/341 (99%)	338 (100%)	0	100	100
6	D	454/571 (80%)	445 (98%)	9 (2%)	48	76
All	All	2621/2942 (89%)	2588 (99%)	33 (1%)	59	81

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	374	LEU
6	D	376	ASP
6	D	527	TRP
1	a	199	SER
3	B	252	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	b	265	ASN
5	E	375	HIS
6	D	534	HIS

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Mol	Chain	Res	Type
6	D	142	HIS
5	E	128	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	9S8	B	301	3	2,10,10	1.07	0	-		
9	9S8	b	301	3	2,10,10	1.06	0	-		
7	SF4	A	706	1	0,12,12	-	-	-		
7	SF4	C	202	2	0,12,12	-	-	-		
7	SF4	E	503	5	0,12,12	-	-	-		
7	SF4	a	703	1	0,12,12	-	-	-		
7	SF4	E	504	5	0,12,12	-	-	-		
7	SF4	c	201	2	0,12,12	-	-	-		
7	SF4	A	705	1	0,12,12	-	-	-		
7	SF4	a	704	1	0,12,12	-	-	-		
7	SF4	D	701	6	0,12,12	-	-	-		
7	SF4	C	201	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	FAD	E	505	-	56,58,58	0.45	1 (1%)	81,89,89	0.37	1 (1%)
8	FAD	a	702	-	56,58,58	0.37	0	81,89,89	0.33	1 (1%)
10	FES	F	201	4	0,4,4	-	-	-		
8	FAD	A	702	-	56,58,58	0.37	0	81,89,89	0.32	1 (1%)
7	SF4	A	707	1	0,12,12	-	-	-		
7	SF4	A	704	1	0,12,12	-	-	-		
7	SF4	A	701	1	0,12,12	-	-	-		
9	9S8	b	302	3	2,10,10	1.11	0	-		
7	SF4	c	202	2	0,12,12	-	-	-		
9	9S8	B	302	3	2,10,10	1.11	0	-		
7	SF4	a	701	1	0,12,12	-	-	-		
7	SF4	E	501	5	0,12,12	-	-	-		
7	SF4	E	502	5	0,12,12	-	-	-		
7	SF4	A	703	1	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
9	9S8	B	301	3	-	-	0/3/3/3
9	9S8	b	301	3	-	-	0/3/3/3
7	SF4	A	706	1	-	-	0/6/5/5
7	SF4	C	202	2	-	-	0/6/5/5
7	SF4	E	503	5	-	-	0/6/5/5
7	SF4	E	504	5	-	-	0/6/5/5
7	SF4	c	201	2	-	-	0/6/5/5
7	SF4	A	705	1	-	-	0/6/5/5
7	SF4	a	704	1	-	-	0/6/5/5
7	SF4	D	701	6	-	-	0/6/5/5
7	SF4	C	201	2	-	-	0/6/5/5
8	FAD	E	505	-	-	15/34/50/50	0/6/6/6
8	FAD	a	702	-	-	9/34/50/50	0/6/6/6
10	FES	F	201	4	-	-	0/1/1/1
8	FAD	A	702	-	-	7/34/50/50	0/6/6/6
7	SF4	A	707	1	-	-	0/6/5/5
7	SF4	A	704	1	-	-	0/6/5/5
7	SF4	A	701	1	-	-	0/6/5/5
9	9S8	b	302	3	-	-	0/3/3/3
7	SF4	c	202	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	9S8	B	302	3	-	-	0/3/3/3
7	SF4	A	703	1	-	-	0/6/5/5
7	SF4	a	701	1	-	-	0/6/5/5
7	SF4	E	501	5	-	-	0/6/5/5
7	SF4	E	502	5	-	-	0/6/5/5
7	SF4	a	703	1	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	505	FAD	P-O2P	-2.08	1.45	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	505	FAD	P-O3P-PA	-2.40	124.60	132.83
8	a	702	FAD	P-O3P-PA	-2.04	125.82	132.83
8	A	702	FAD	P-O3P-PA	-2.03	125.86	132.83

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	702	FAD	C5B-O5B-PA-O2A
8	A	702	FAD	P-O3P-PA-O5B
8	a	702	FAD	C5B-O5B-PA-O1A
8	a	702	FAD	C5B-O5B-PA-O2A
8	a	702	FAD	P-O3P-PA-O5B

There are no ring outliers.

11 monomers are involved in 17 short contacts:

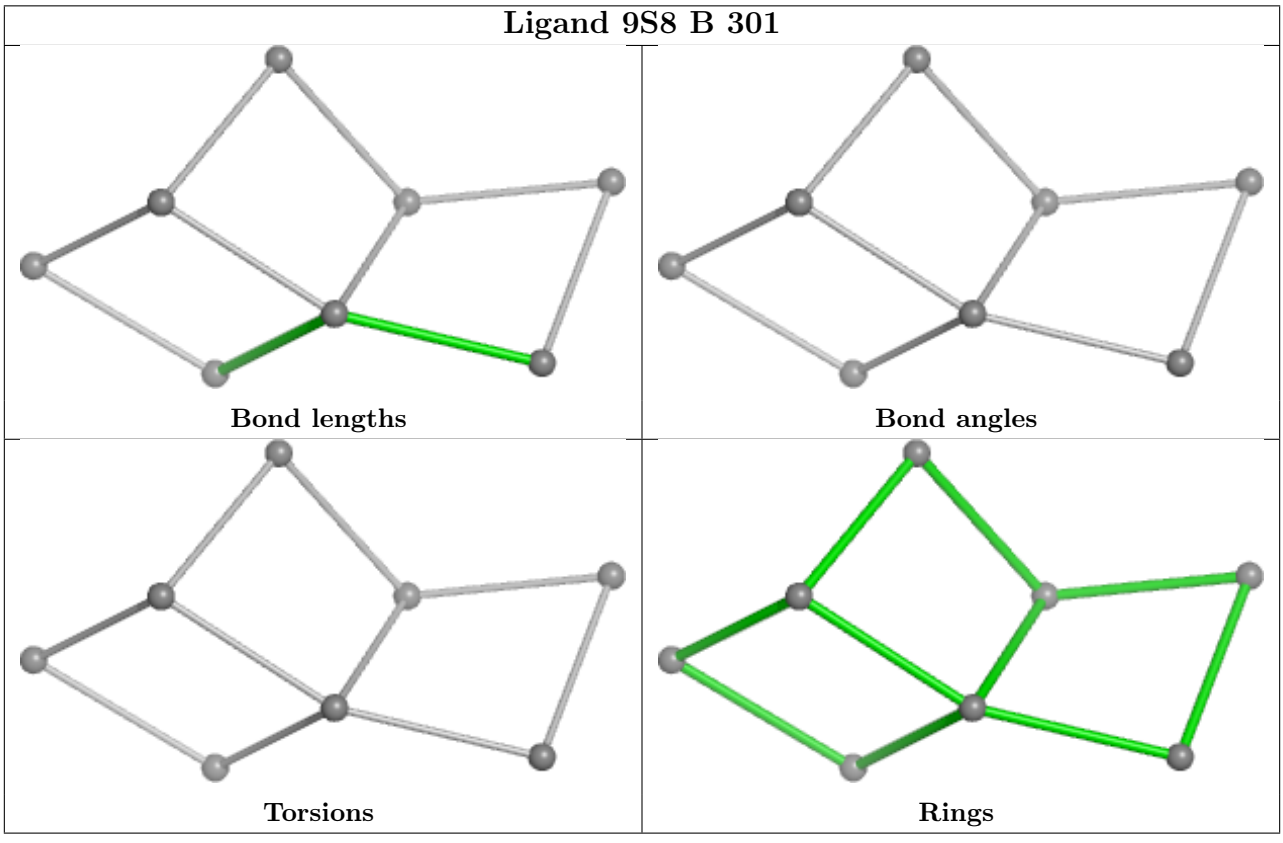
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	301	9S8	1	0
9	b	301	9S8	1	0
7	A	706	SF4	1	0
7	a	703	SF4	2	0
7	D	701	SF4	1	0
8	E	505	FAD	5	0
8	a	702	FAD	2	0
8	A	702	FAD	1	0

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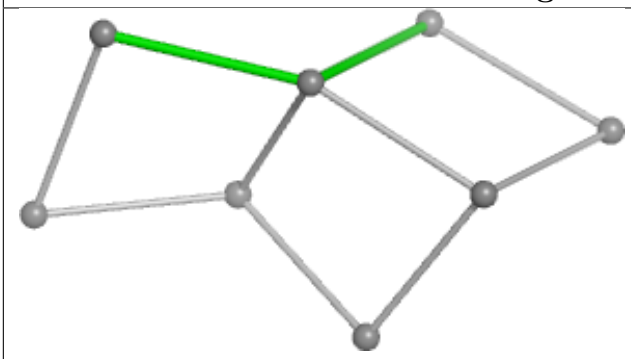
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	b	302	9S8	1	0
9	B	302	9S8	1	0
7	A	703	SF4	1	0

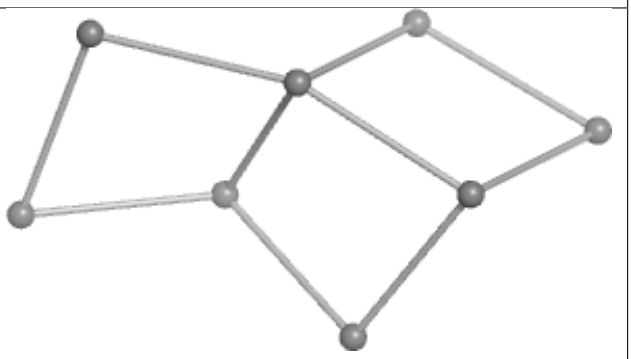
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



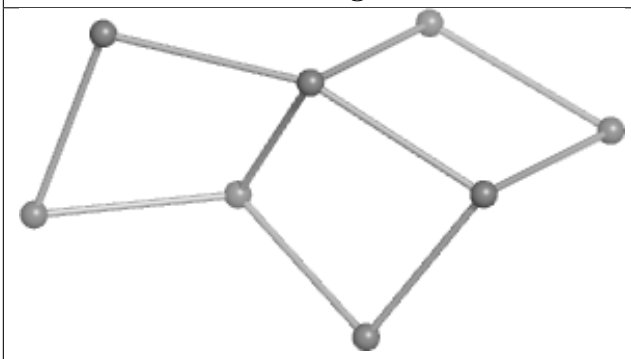
Ligand 9S8 b 301



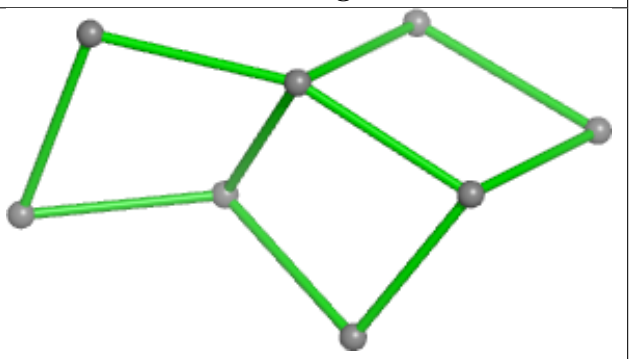
Bond lengths



Bond angles

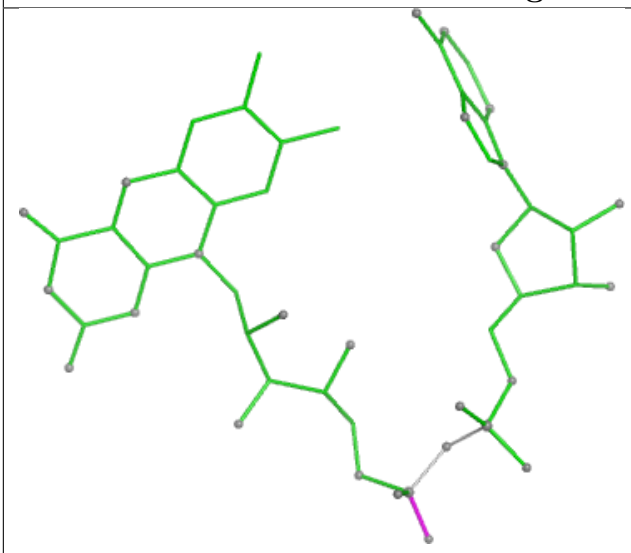


Torsions

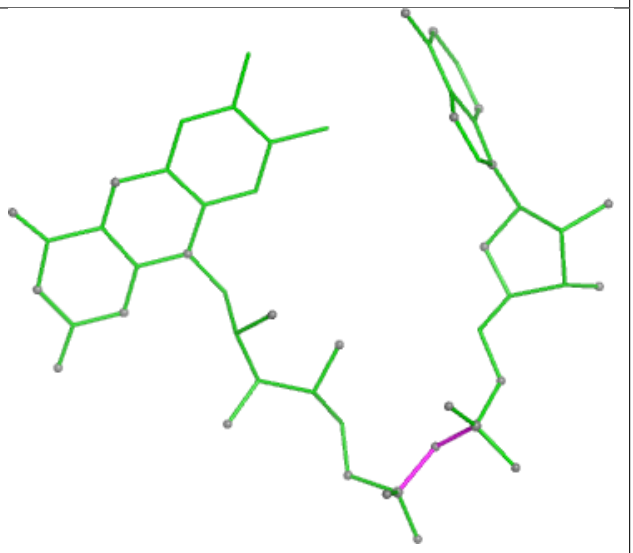


Rings

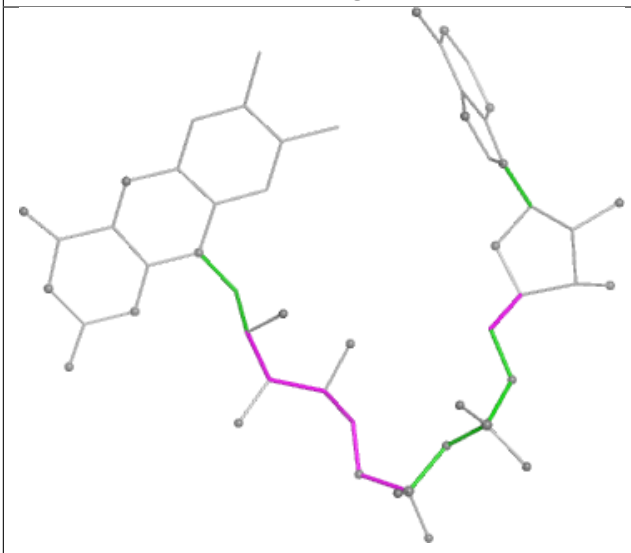
Ligand FAD E 505



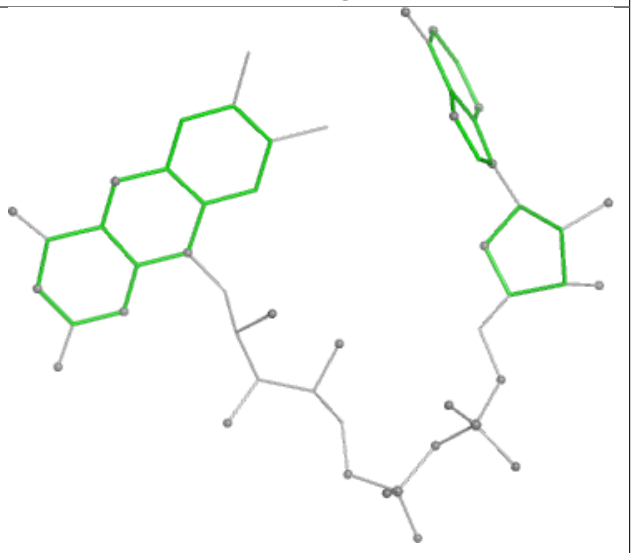
Bond lengths



Bond angles

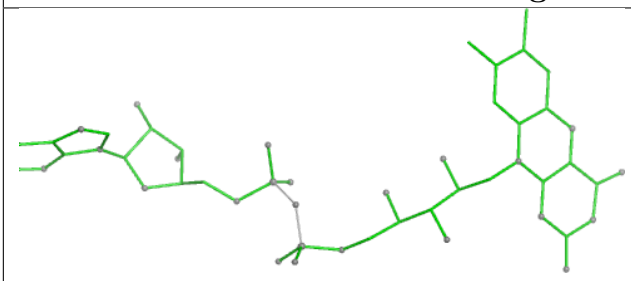


Torsions

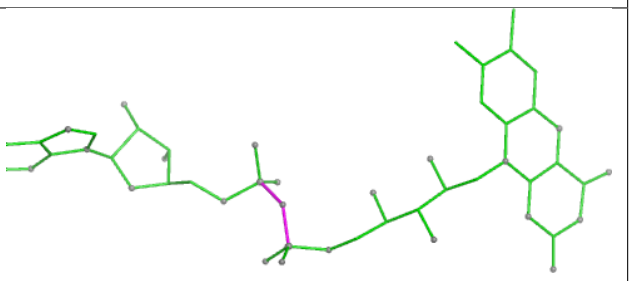


Rings

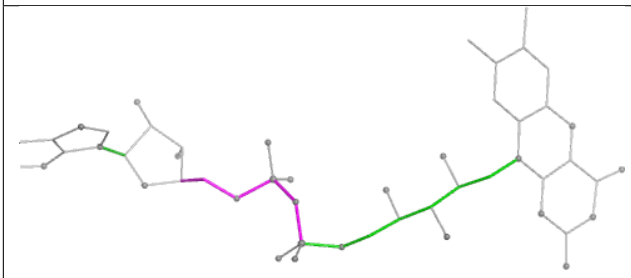
Ligand FAD a 702



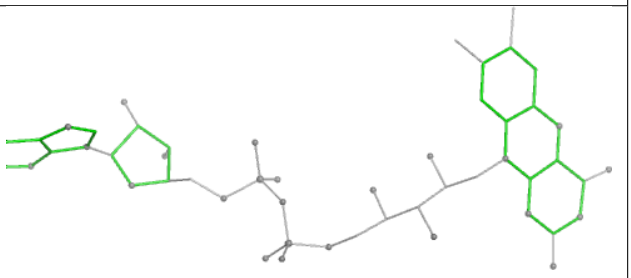
Bond lengths



Bond angles

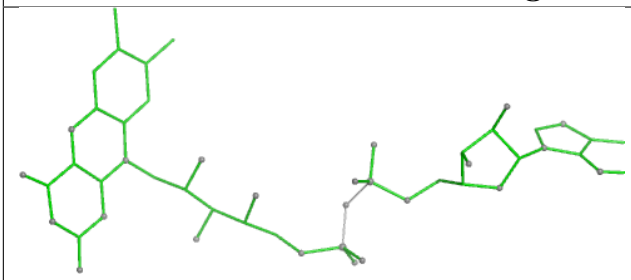


Torsions

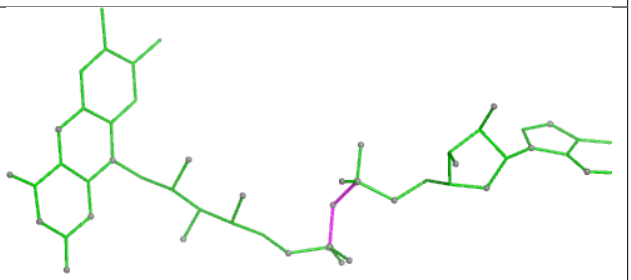


Rings

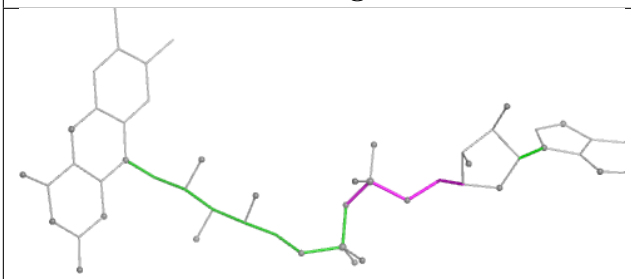
Ligand FAD A 702



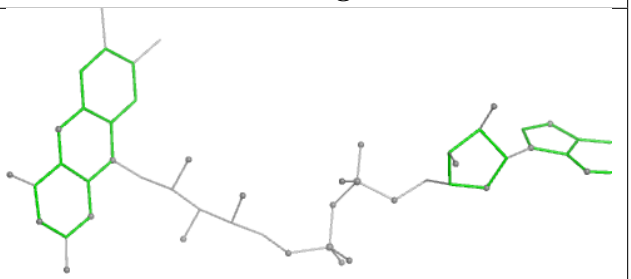
Bond lengths



Bond angles

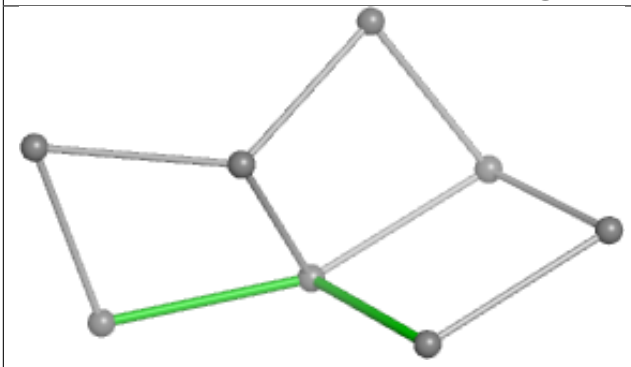


Torsions

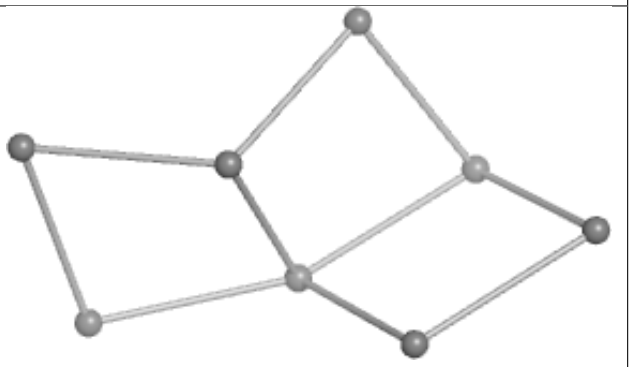


Rings

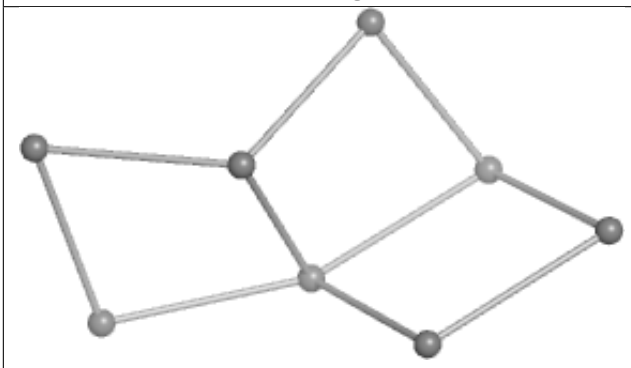
Ligand 9S8 b 302



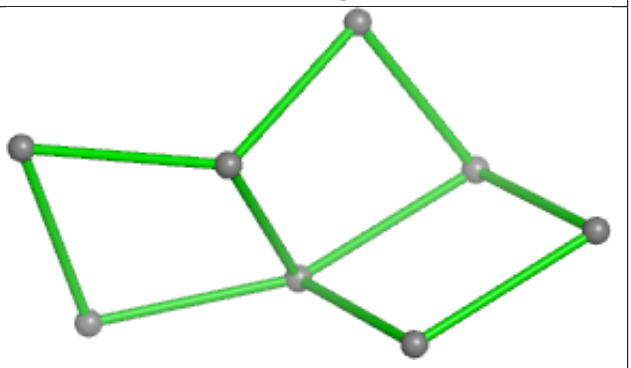
Bond lengths



Bond angles

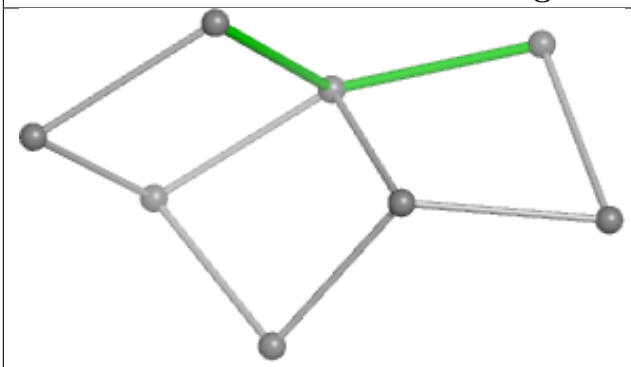


Torsions

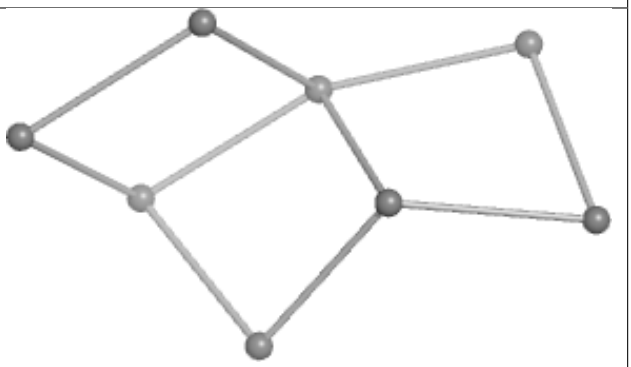


Rings

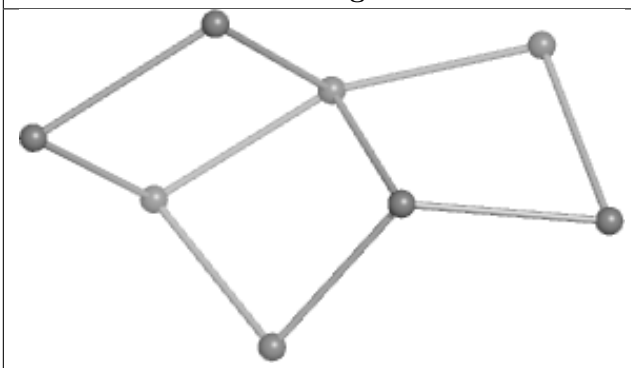
Ligand 9S8 B 302



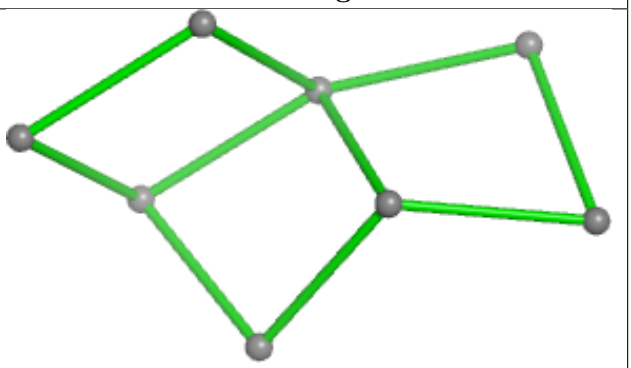
Bond lengths



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.

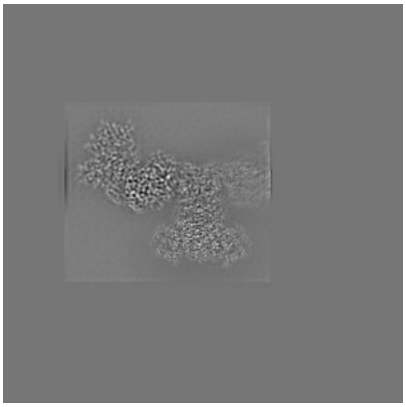
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12210. These allow visual inspection of the internal detail of the map and identification of artifacts.

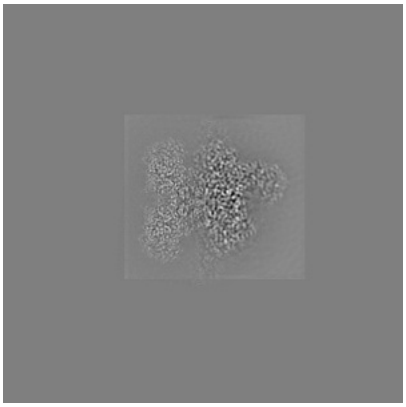
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

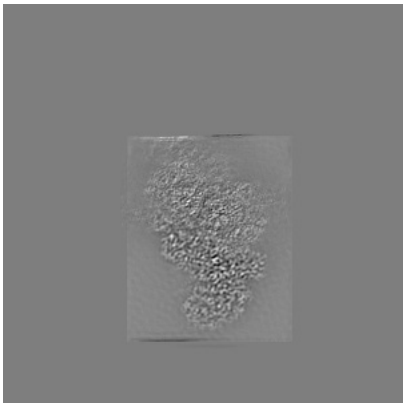
6.1.1 Primary map



X



Y

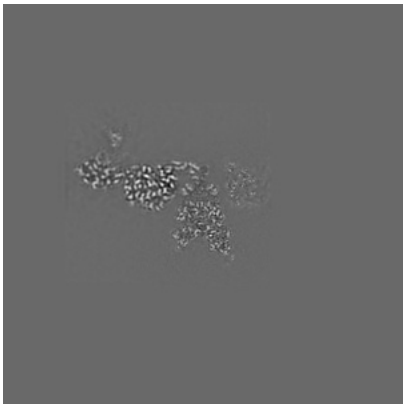


Z

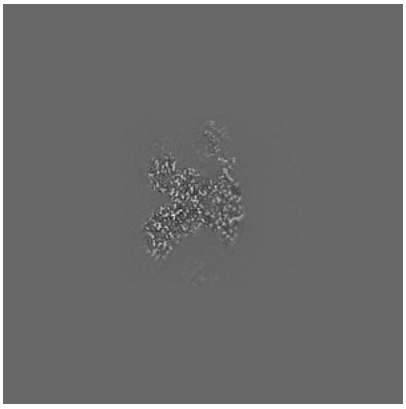
The images above show the map projected in three orthogonal directions.

6.2 Central slices

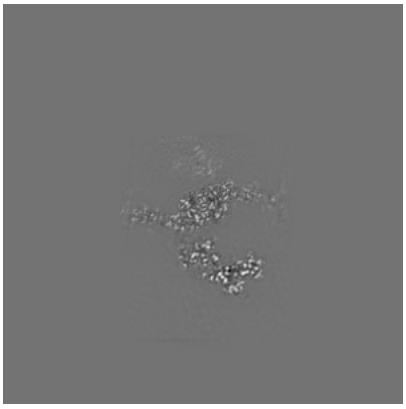
6.2.1 Primary map



X Index: 216



Y Index: 216

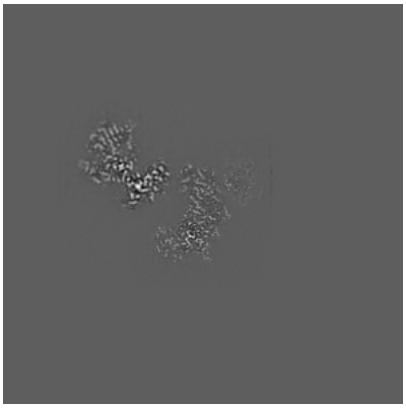


Z Index: 216

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: 141

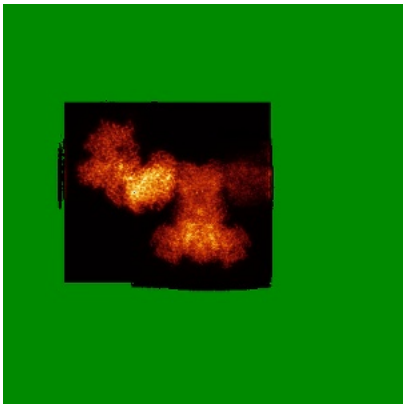


Z Index: 244

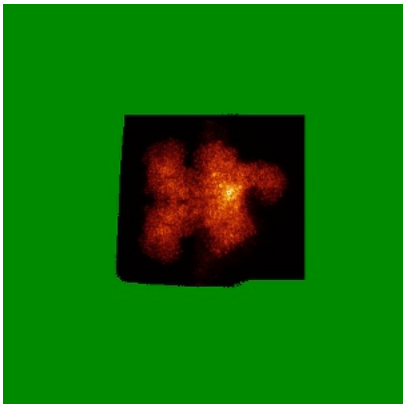
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

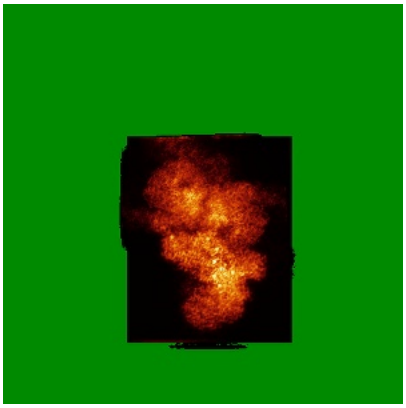
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

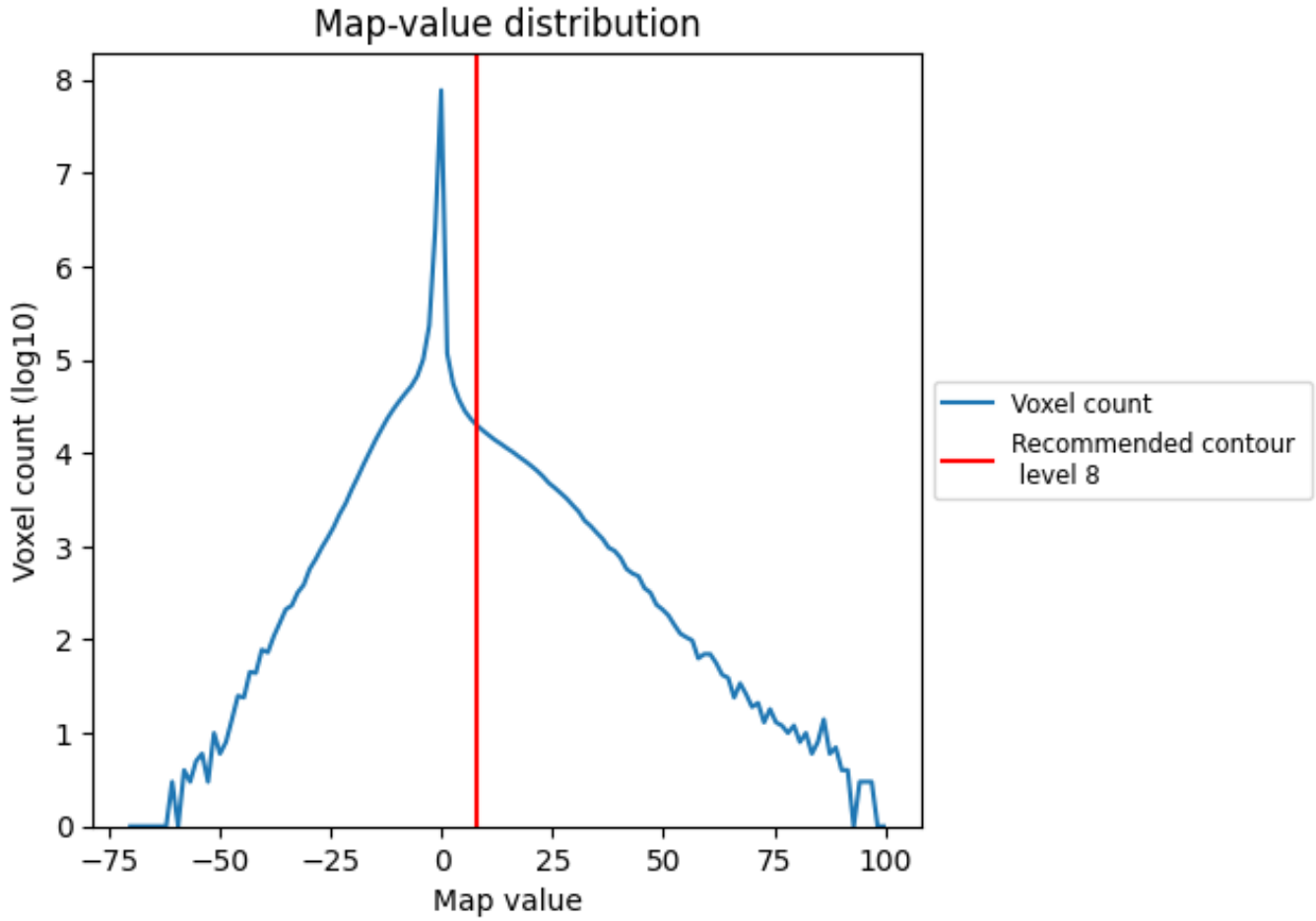
6.6 Mask visualisation (i)

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

7 Map analysis

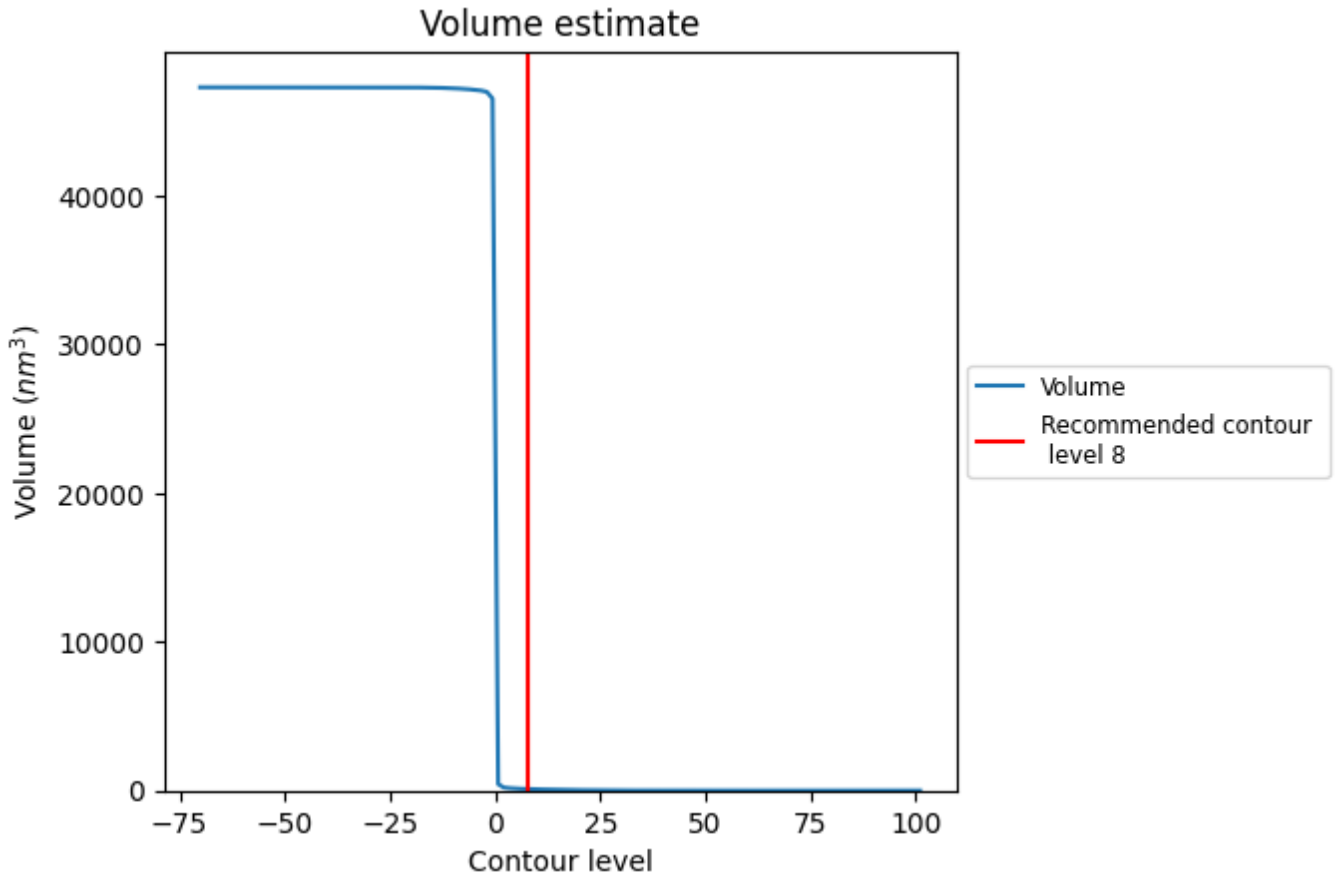
This section contains the results of statistical analysis of the map.

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.

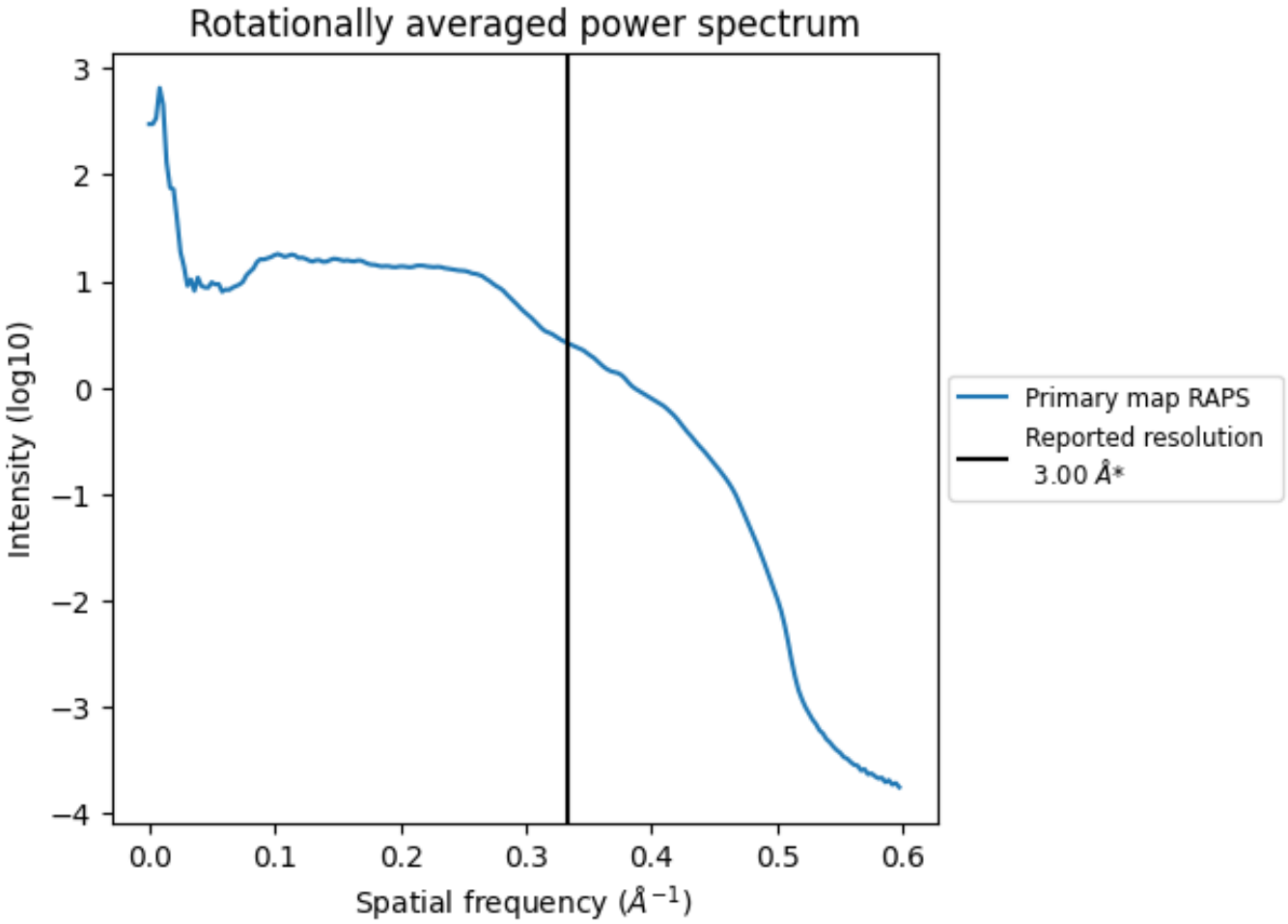
7.2 Volume estimate (i)



The volume at the recommended contour level is 101 nm^3; this corresponds to an approximate mass of 91 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}

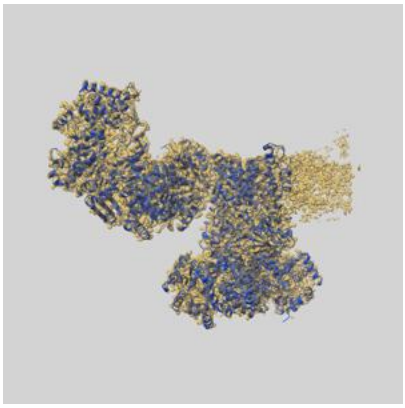
8 Fourier-Shell correlation

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

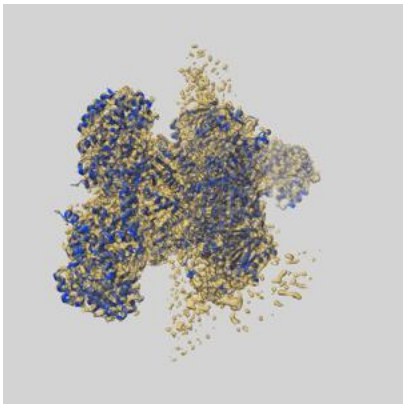
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12210 and PDB model 7BKD. Per-residue inclusion information can be found in section 3 on page 9.

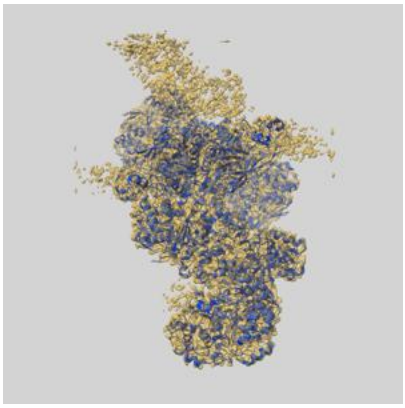
9.1 Map-model overlay



X



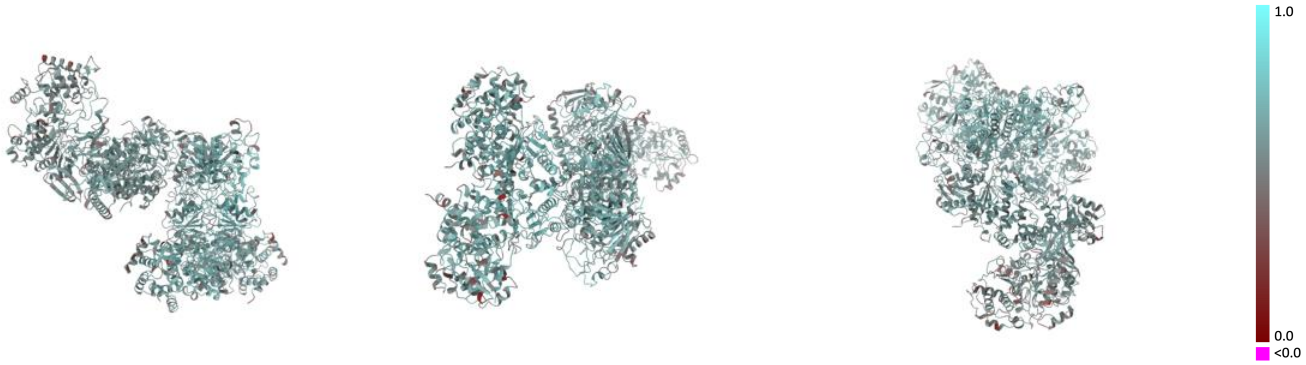
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0 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.

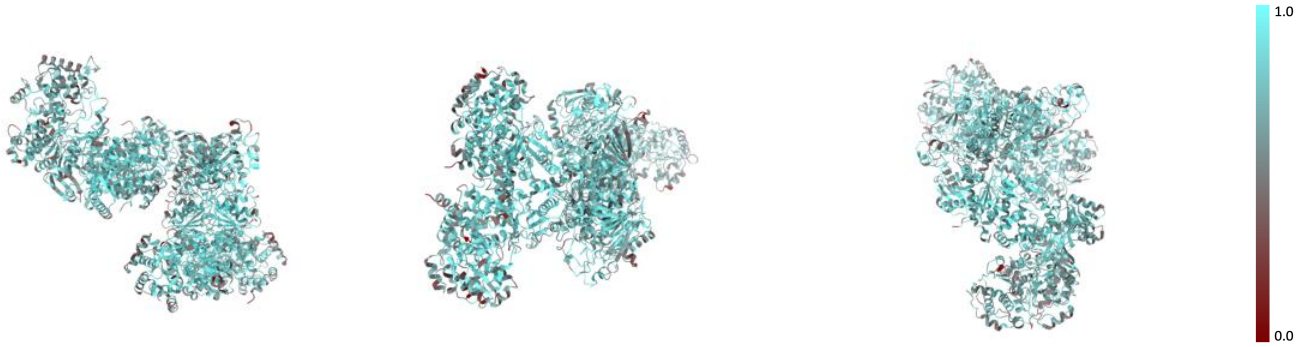
9.2 Q-score mapped to coordinate model (i)



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.

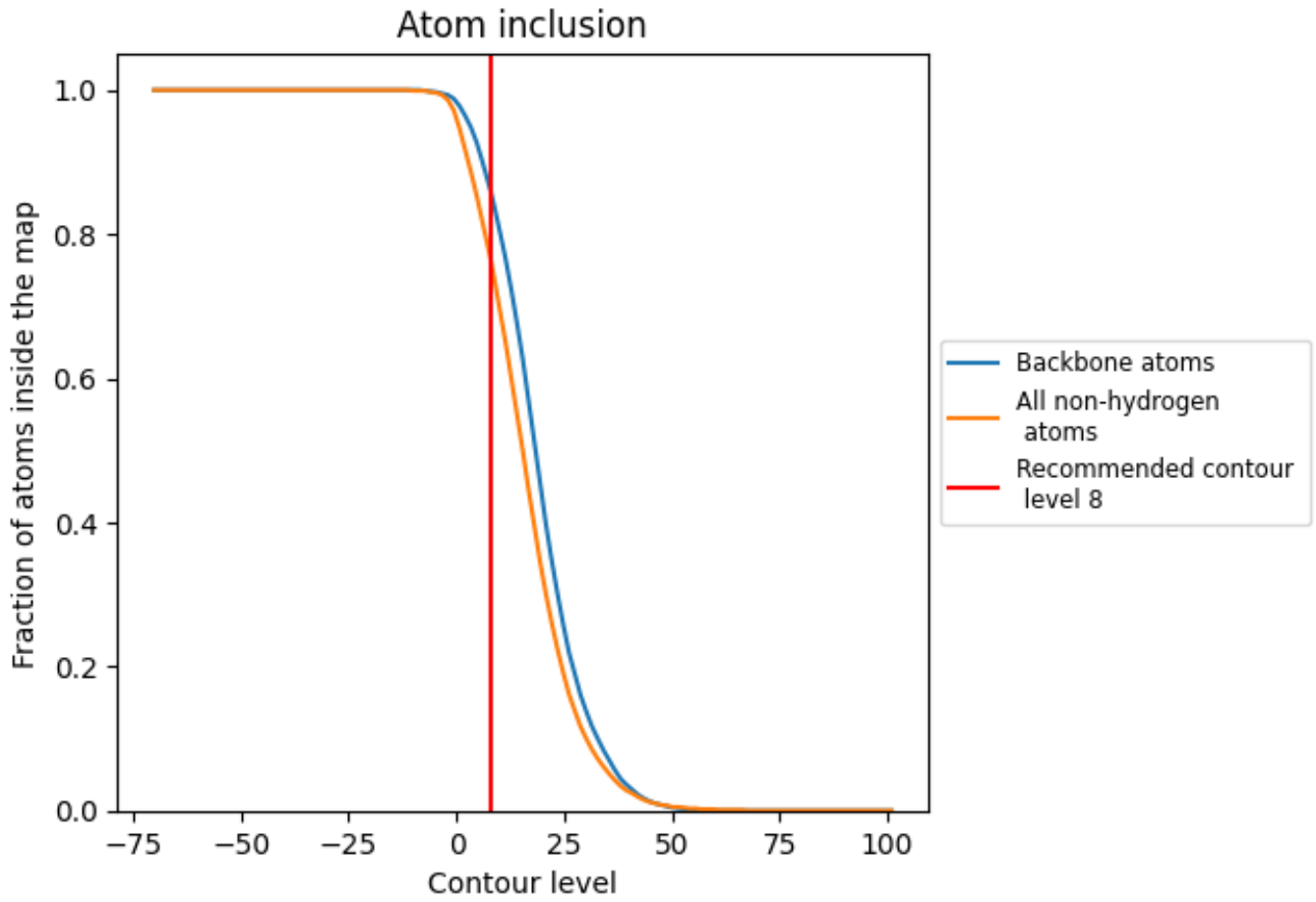
9.3 Atom inclusion mapped to coordinate model (i)



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 (8).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7640	0.5970
A	0.7970	0.6200
B	0.7660	0.6030
C	0.7650	0.6180
D	0.6870	0.5380
E	0.7930	0.5760
F	0.8020	0.5820
a	0.7690	0.6320
b	0.7660	0.6030
c	0.7620	0.6180

