Full wwPDB EM Validation Report ⓘ

Sep 26, 2022 – 10:30 pm BST

PDB ID	:	7P7J
EMDB ID	:	EMD-13237
Title	:	Complex I from E. coli, DDM/LMNG-purified, with DQ, Open state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2021-07-19
Resolution	:	2.70 Å(reported)
Based on initial models	:	3RKO, 4HEA

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:

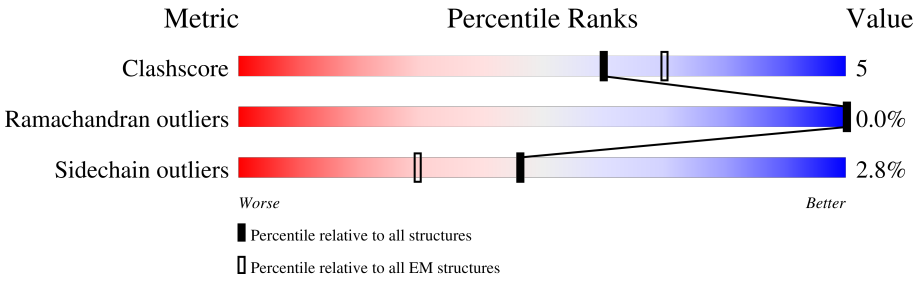
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	F	439	86% 14%
2	E	156	90% 10%
3	G	905	85% 15%
4	C	600	84% 13%
5	B	220	74% 15% 10%
6	I	180	86% 14%
7	H	325	79% 18%
8	A	147	58% 11% 31%

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Mol	Chain	Length	Quality of chain
9	L	613	
10	M	504	
11	N	485	
12	K	100	
13	J	184	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 37448 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 NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	439	3407	2162	596	629	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase I subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	156	1220	768	215	229	8	0	0

- Molecule 3 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	905	7022	4388	1269	1328	37	0	0

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	584	4712	3023	818	847	24	0	0

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	197	1553	986	268	283	16	0	0

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	180	1436	915	242	264	15	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	314	Total	C	N	O	S	0	0
			2470	1662	388	402	18		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	102	Total	C	N	O	S	0	0
			808	555	124	125	4		

- Molecule 9 is a protein called Proton-translocating NADH-quinone oxidoreductase, chain L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	598	Total	C	N	O	S	0	0
			4563	3037	725	769	32		

- Molecule 10 is a protein called NADH dehydrogenase I subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	504	Total	C	N	O	S	0	0
			3953	2661	617	646	29		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	480	Total	C	N	O	S	0	0
			3638	2428	574	616	20		

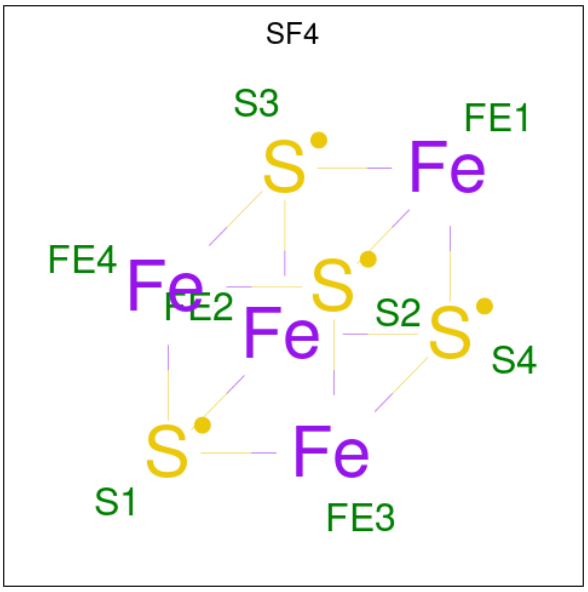
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	100	Total	C	N	O	S	0	0
			760	494	132	129	5		

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit J.

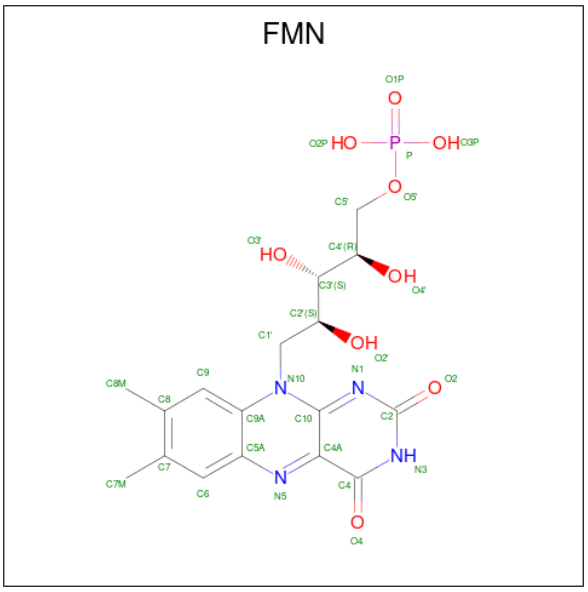
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	160	Total	C	N	O	S	0	0
			1199	809	185	198	7		

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



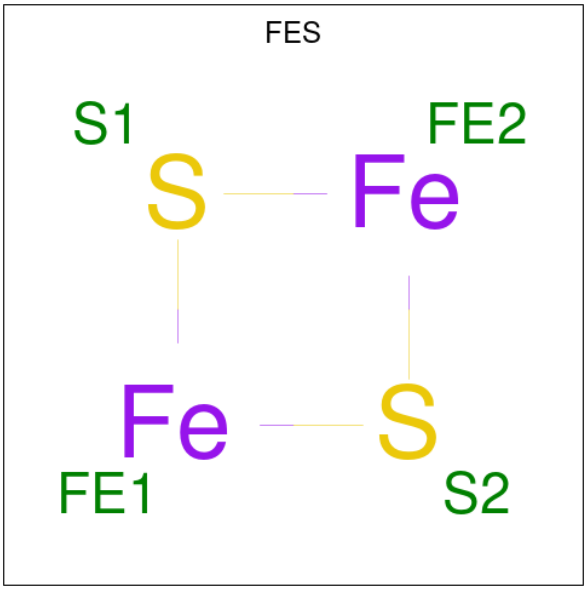
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	B	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 16 8 8	0
14	I	1	Total Fe S 16 8 8	0

- Molecule 15 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

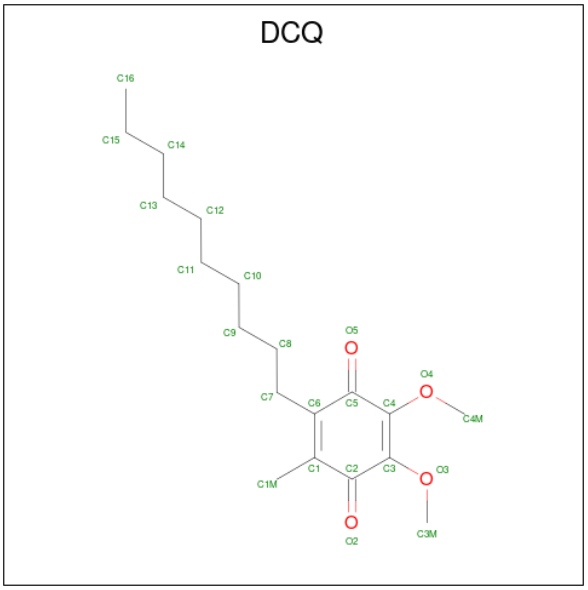


Mol	Chain	Residues	Atoms			AltConf
16	E	1	Total	Fe	S	0
			4	2	2	
16	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is CALCIUM ION (three-letter code: CA) (formula: Ca).

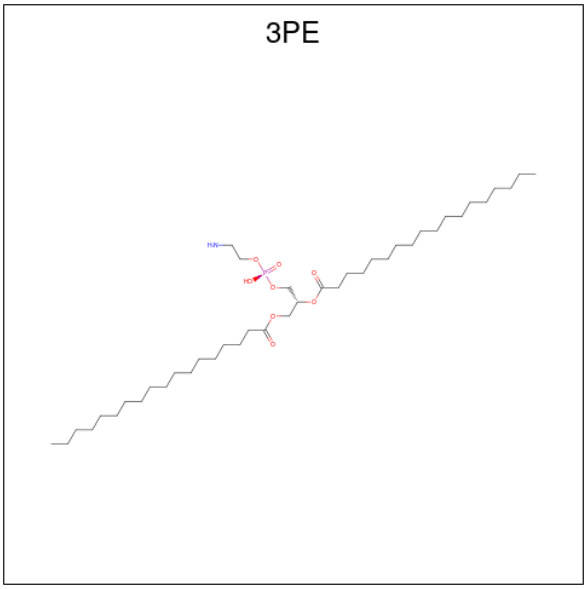
Mol	Chain	Residues	Atoms	AltConf
17	G	1	Total Ca 1 1	0

- Molecule 18 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter code: DCQ) (formula: $C_{19}H_{30}O_4$) (labeled as "Ligand of Interest" by depositor).



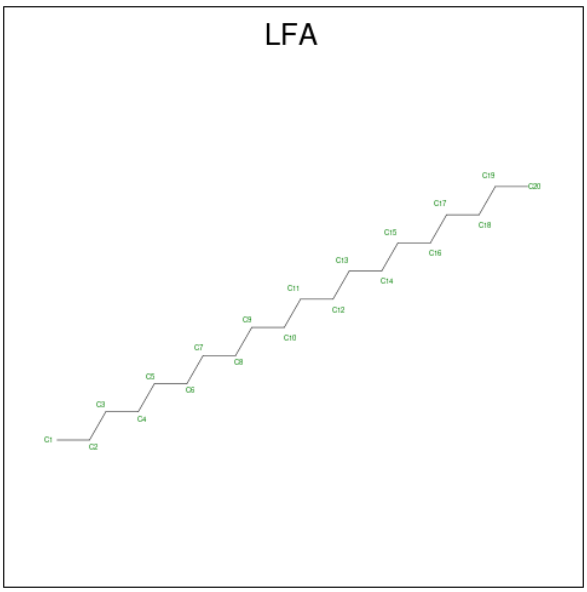
Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C O 23 19 4	0

- Molecule 19 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
19	I	1	Total	C	N	O	P	0
			33	23	1	8	1	
19	H	1	Total	C	N	O	P	0
			89	69	2	16	2	
19	H	1	Total	C	N	O	P	0
			89	69	2	16	2	
19	A	1	Total	C	N	O	P	0
			77	57	2	16	2	
19	A	1	Total	C	N	O	P	0
			77	57	2	16	2	
19	L	1	Total	C	N	O	P	0
			230	180	5	40	5	
19	L	1	Total	C	N	O	P	0
			230	180	5	40	5	
19	L	1	Total	C	N	O	P	0
			230	180	5	40	5	
19	L	1	Total	C	N	O	P	0
			230	180	5	40	5	
19	L	1	Total	C	N	O	P	0
			230	180	5	40	5	
19	M	1	Total	C	N	O	P	0
			85	65	2	16	2	
19	M	1	Total	C	N	O	P	0
			85	65	2	16	2	

- Molecule 20 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



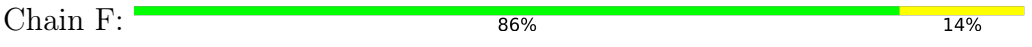
Mol	Chain	Residues	Atoms	AltConf
20	H	1	Total C 20 20	0
20	N	1	Total C 34 34	0
20	N	1	Total C 34 34	0
20	J	1	Total C 20 20	0

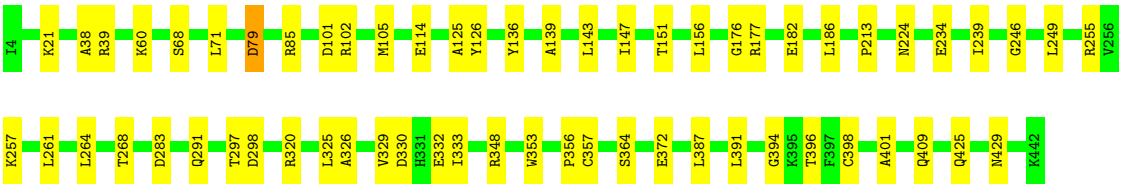
3 Residue-property plots (i)

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: NADH-quinone oxidoreductase subunit F

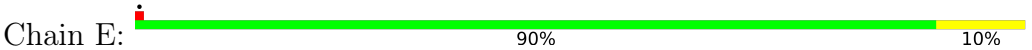
Chain F:





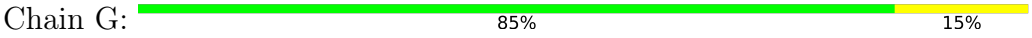
• Molecule 2: NADH dehydrogenase I subunit E

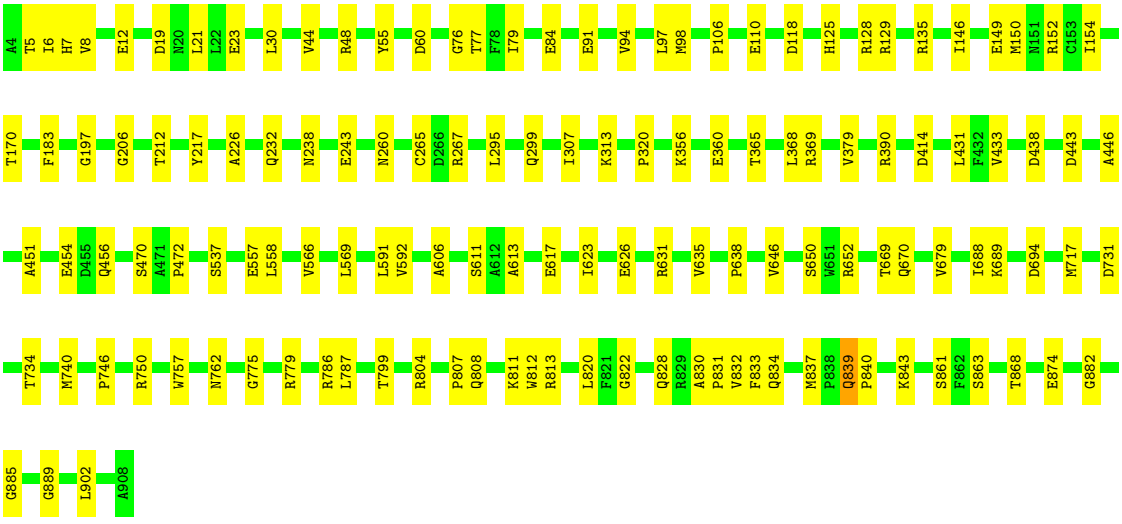
Chain E:



• Molecule 3: NADH-quinone oxidoreductase

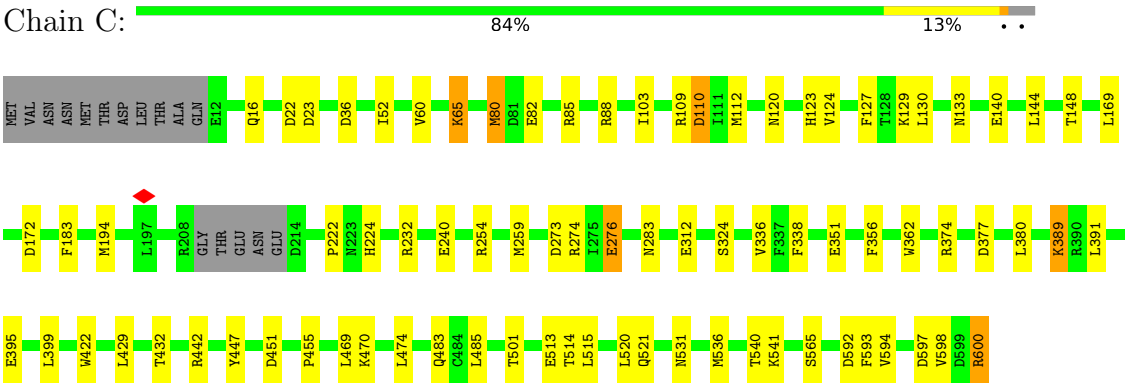
Chain G:





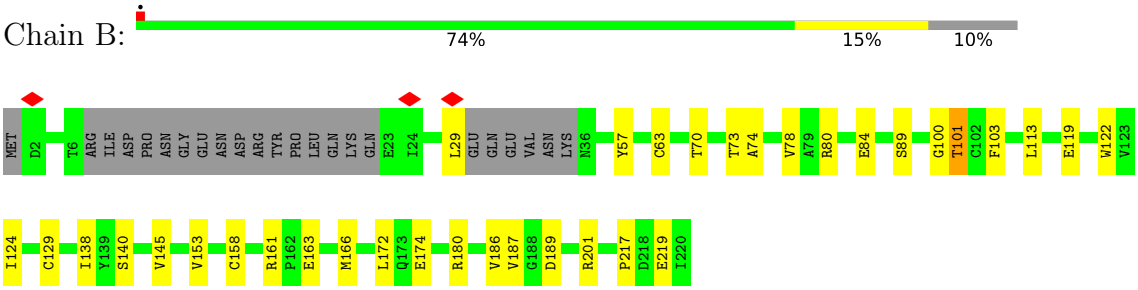
• Molecule 4: NADH-quinone oxidoreductase subunit C/D

Chain C:



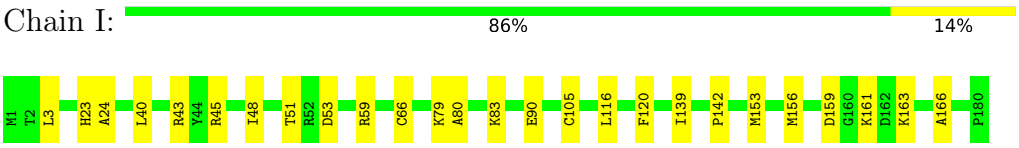
• Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:



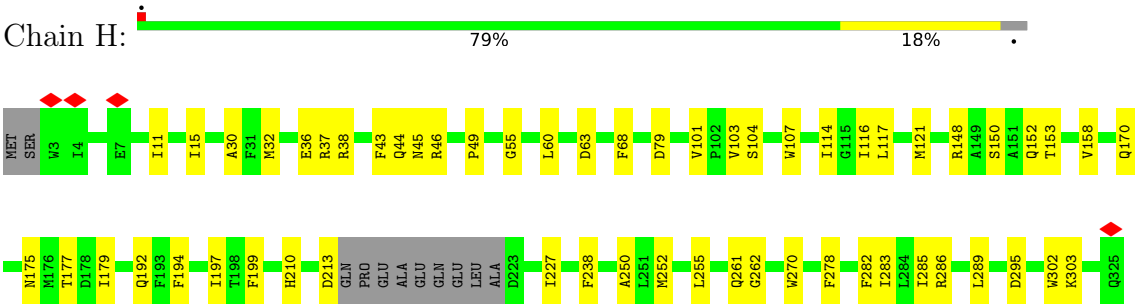
• Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:



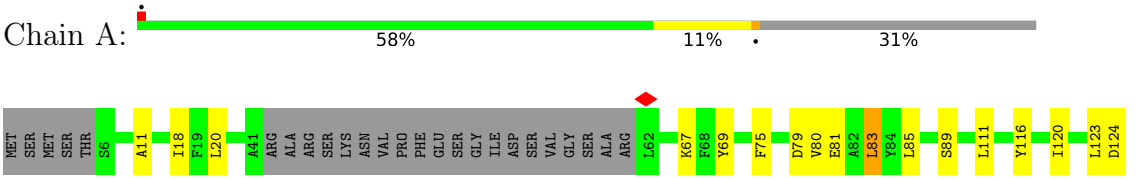
• Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:



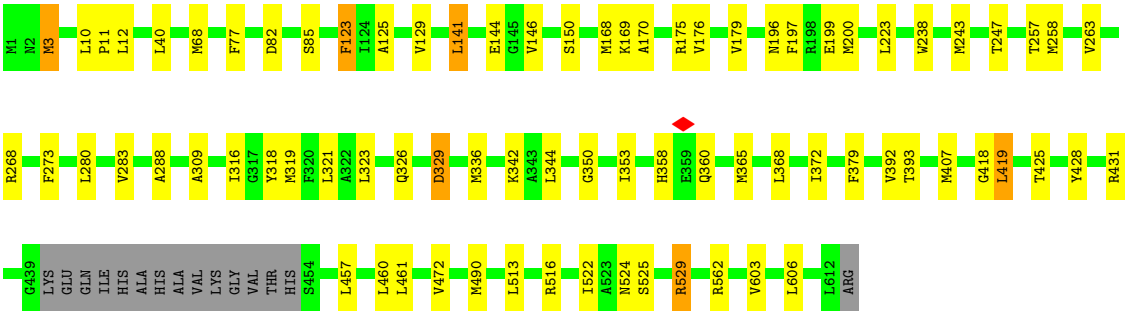
• Molecule 8: NADH-quinone oxidoreductase subunit A

Chain A:



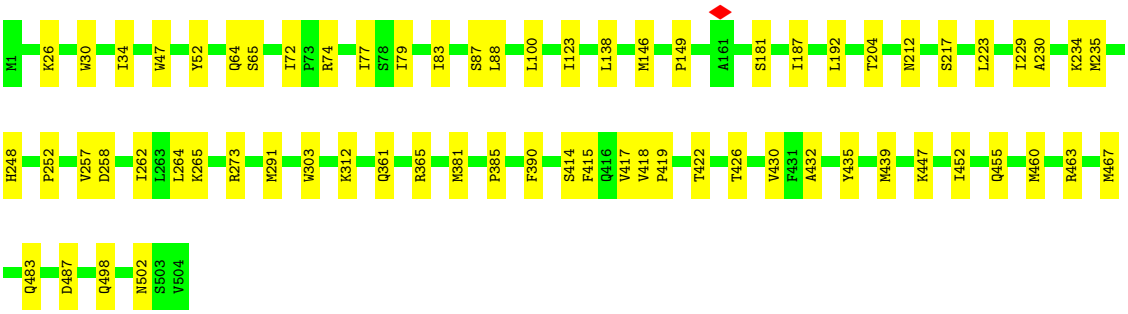
• Molecule 9: Proton-translocating NADH-quinone oxidoreductase, chain L

Chain L:



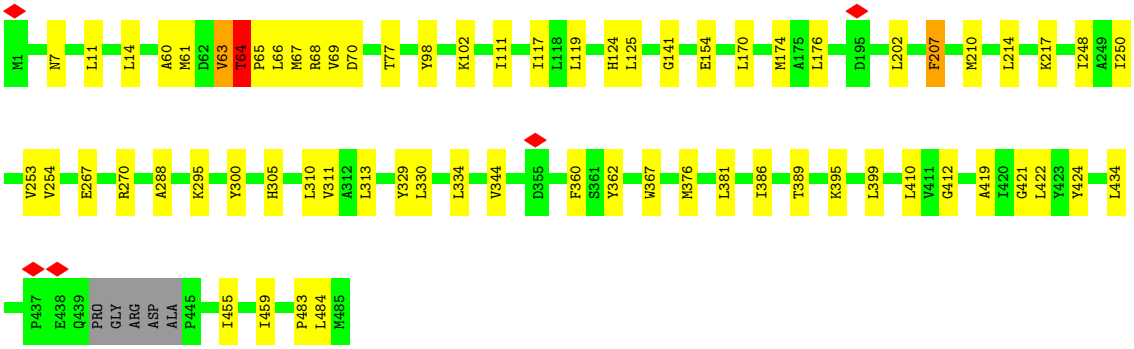
• Molecule 10: NADH dehydrogenase I subunit M

Chain M:



• Molecule 11: NADH-quinone oxidoreductase subunit N

Chain N:

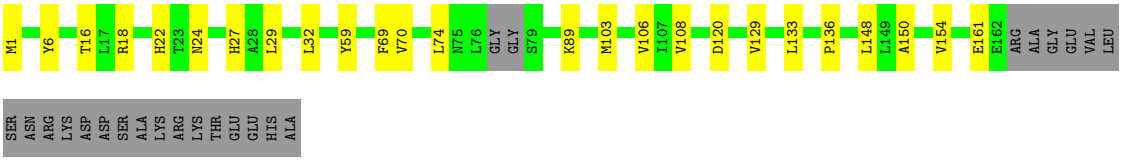


• Molecule 12: NADH-quinone oxidoreductase subunit K

Chain K:

• Molecule 13: NADH-quinone oxidoreductase subunit J

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56249	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 ($e^-/Å^2$)	78	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.498	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	153.7, 206.69998, 243.79999	wwPDB
Map dimensions	230, 195, 145	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DCQ, SF4, FMN, LFA, 3PE, CA, FES

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	F	0.28	0/3486	0.51	0/4713
2	E	0.27	0/1248	0.53	0/1691
3	G	0.31	0/7173	0.53	0/9726
4	C	0.32	0/4842	0.56	1/6572 (0.0%)
5	B	0.32	0/1586	0.55	1/2149 (0.0%)
6	I	0.32	0/1470	0.56	1/1985 (0.1%)
7	H	0.32	0/2544	0.54	0/3461
8	A	0.30	0/833	0.53	0/1134
9	L	0.28	0/4680	0.51	1/6380 (0.0%)
10	M	0.30	0/4074	0.53	1/5546 (0.0%)
11	N	0.31	0/3727	0.55	2/5085 (0.0%)
12	K	0.28	0/769	0.61	0/1040
13	J	0.31	0/1224	0.53	0/1671
All	All	0.30	0/37656	0.54	7/51153 (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	G	0	1
7	H	0	1
11	N	0	2
12	K	0	1
All	All	0	5

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	483	PRO	CA-N-CD	-8.87	99.08	111.50
4	C	36	ASP	CB-CG-OD2	6.78	124.40	118.30
5	B	189	ASP	CB-CG-OD2	6.18	123.86	118.30
6	I	53	ASP	CB-CG-OD2	5.87	123.58	118.30
10	M	262	ILE	CG1-CB-CG2	-5.35	99.63	111.40
11	N	64	THR	N-CA-C	-5.13	97.15	111.00
9	L	141	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	260	ASN	Peptide
7	H	32	MET	Peptide
12	K	86	ARG	Sidechain
11	N	63	VAL	Peptide
11	N	64	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3407	0	3374	33	0
2	E	1220	0	1187	9	0
3	G	7022	0	6824	70	0
4	C	4712	0	4626	49	0
5	B	1553	0	1536	21	0
6	I	1436	0	1415	13	0
7	H	2470	0	2517	36	0
8	A	808	0	821	14	0
9	L	4563	0	4698	40	0
10	M	3953	0	4053	34	0
11	N	3638	0	3804	40	0
12	K	760	0	817	12	0
13	J	1199	0	1263	21	0
14	B	8	0	0	1	0
14	F	8	0	0	0	0
14	G	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	I	16	0	0	0	0
15	F	31	0	19	0	0
16	E	4	0	0	0	0
16	G	4	0	0	0	0
17	G	1	0	0	0	0
18	B	23	0	30	0	0
19	A	77	0	102	3	0
19	H	89	0	132	7	0
19	I	33	0	40	0	0
19	L	230	0	354	9	0
19	M	85	0	124	2	0
20	H	20	0	42	2	0
20	J	20	0	42	0	0
20	N	34	0	69	2	0
All	All	37448	0	37889	351	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 5.

All (351) 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)
11:N:63:VAL:O	11:N:67:MET:HB2	1.71	0.91
11:N:64:THR:HB	11:N:66:LEU:H	1.46	0.79
10:M:181:SER:HB2	10:M:230:ALA:HA	1.71	0.73
7:H:36:GLU:HG3	7:H:283:ILE:HD12	1.73	0.71
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.72	0.70
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.76	0.67
11:N:125:LEU:HB3	11:N:174:MET:HE3	1.77	0.67
4:C:276:GLU:O	4:C:283:ASN:ND2	2.28	0.67
4:C:389:LYS:H	4:C:389:LYS:HE2	1.61	0.66
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.78	0.66
3:G:98:MET:HG3	4:C:513:GLU:HG3	1.79	0.65
9:L:179:VAL:HG22	10:M:426:THR:HG22	1.79	0.65
9:L:316:ILE:HA	9:L:319:MET:HG3	1.80	0.64
19:L:802:3PE:H3B2	19:L:802:3PE:H3I3	1.81	0.62
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.81	0.61
4:C:259:MET:HE2	5:B:138:ILE:HD13	1.82	0.61
3:G:451:ALA:O	3:G:456:GLN:NE2	2.34	0.60
10:M:417:VAL:HG12	10:M:418:VAL:HG13	1.83	0.60
7:H:285:ILE:HG13	19:H:401:3PE:H3E2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:414:SER:O	10:M:418:VAL:N	2.35	0.60
3:G:812:TRP:HB2	3:G:902:LEU:HB3	1.84	0.60
5:B:186:VAL:HG23	5:B:187:VAL:HG23	1.83	0.59
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.84	0.59
11:N:419:ALA:HA	11:N:422:LEU:HD12	1.84	0.59
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.85	0.58
19:L:804:3PE:H3A2	19:L:804:3PE:H2E2	1.86	0.57
11:N:386:ILE:O	11:N:389:THR:OG1	2.22	0.57
1:F:85:ARG:HG2	1:F:213:PRO:HG2	1.85	0.57
13:J:129:VAL:O	13:J:133:LEU:HB2	2.04	0.56
1:F:151:THR:HG22	1:F:156:LEU:HB2	1.86	0.56
4:C:374:ARG:NH2	5:B:219:GLU:OE1	2.39	0.56
7:H:15:ILE:HG23	8:A:18:ILE:HG21	1.87	0.56
3:G:454:GLU:OE2	3:G:813:ARG:NH1	2.33	0.56
8:A:111:LEU:HD22	19:A:201:3PE:H271	1.87	0.56
9:L:85:SER:OG	9:L:268:ARG:NH2	2.39	0.56
10:M:187:ILE:HD11	11:N:399:LEU:HD22	1.86	0.56
11:N:11:LEU:HD22	11:N:14:LEU:HD12	1.88	0.56
5:B:101:THR:HA	5:B:129:CYS:HB3	1.87	0.55
10:M:87:SER:OG	10:M:273:ARG:NH2	2.37	0.55
1:F:391:LEU:HD23	1:F:401:ALA:HB1	1.89	0.55
2:E:141:PRO:HG2	2:E:153:LEU:HB2	1.88	0.55
3:G:118:ASP:OD1	3:G:762:ASN:ND2	2.40	0.55
3:G:55:TYR:HB3	3:G:60:ASP:HB3	1.89	0.55
3:G:110:GLU:HG3	3:G:206:GLY:HA2	1.88	0.55
10:M:452:ILE:HD12	10:M:455:GLN:HE22	1.71	0.55
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.89	0.54
11:N:154:GLU:HG3	12:K:95:VAL:HB	1.89	0.54
3:G:91:GLU:HG3	3:G:125:HIS:HB2	1.88	0.54
3:G:365:THR:O	3:G:786:ARG:NH2	2.39	0.54
3:G:5:THR:O	3:G:76:GLY:N	2.40	0.54
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.89	0.54
10:M:229:ILE:HD12	19:M:702:3PE:H2F1	1.88	0.54
7:H:303:LYS:NZ	8:A:124:ASP:OD1	2.40	0.54
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.89	0.54
12:K:80:LEU:HD21	13:J:74:LEU:HD11	1.89	0.54
3:G:97:LEU:HD22	3:G:154:ILE:HB	1.90	0.54
3:G:863:SER:HB3	3:G:868:THR:HG22	1.91	0.53
6:I:48:ILE:HG12	6:I:116:LEU:HG	1.90	0.53
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.90	0.53
4:C:254:ARG:HG3	5:B:103:PHE:HE1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:451:ASP:O	4:C:483:GLN:NE2	2.38	0.53
1:F:357:CYS:HB2	1:F:401:ALA:HB2	1.90	0.53
3:G:212:THR:HG22	3:G:832:VAL:HG21	1.91	0.53
1:F:60:LYS:HA	1:F:68:SER:HA	1.91	0.53
11:N:170:LEU:O	11:N:174:MET:HG3	2.08	0.53
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.91	0.53
4:C:541:LYS:NZ	4:C:592:ASP:OD1	2.42	0.52
9:L:179:VAL:HG21	10:M:430:VAL:HG23	1.90	0.52
1:F:297:THR:HG22	1:F:320:ARG:HB2	1.91	0.52
9:L:123:PHE:HE1	9:L:146:VAL:HG13	1.74	0.52
9:L:273:PHE:HB3	9:L:280:LEU:HD13	1.91	0.52
1:F:429:ASN:ND2	3:G:128:ARG:O	2.41	0.52
3:G:369:ARG:NH2	3:G:775:GLY:O	2.43	0.52
3:G:822:GLY:O	3:G:828:GLN:NE2	2.42	0.52
4:C:65:LYS:NZ	4:C:130:LEU:O	2.43	0.52
11:N:98:TYR:O	11:N:102:LYS:NZ	2.40	0.52
3:G:106:PRO:HD3	4:C:515:LEU:HD21	1.90	0.52
4:C:240:GLU:OE2	7:H:148:ARG:NH1	2.36	0.52
9:L:329:ASP:OD1	9:L:329:ASP:N	2.43	0.52
11:N:248:ILE:HD11	11:N:334:LEU:HB2	1.91	0.52
9:L:524:ASN:HA	9:L:529:ARG:HH12	1.75	0.52
3:G:631:ARG:NH2	3:G:688:ILE:O	2.43	0.52
3:G:472:PRO:HG3	3:G:799:THR:HA	1.92	0.51
10:M:291:MET:HE1	10:M:418:VAL:HG11	1.92	0.51
8:A:80:VAL:HA	8:A:83:LEU:HD23	1.90	0.51
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.92	0.51
9:L:12:LEU:HD21	19:L:801:3PE:H3H1	1.92	0.51
4:C:222:PRO:HG3	4:C:232:ARG:HD3	1.91	0.51
7:H:38:ARG:NH1	7:H:55:GLY:O	2.43	0.51
1:F:85:ARG:HB2	1:F:125:ALA:HA	1.92	0.51
5:B:163:GLU:HA	5:B:166:MET:HG3	1.92	0.51
1:F:239:ILE:HD12	1:F:246:GLY:HA2	1.92	0.51
1:F:257:LYS:NZ	1:F:283:ASP:OD1	2.42	0.51
19:L:802:3PE:H2B2	19:L:802:3PE:H3C2	1.93	0.51
4:C:455:PRO:HB2	4:C:469:LEU:HD22	1.93	0.51
4:C:110:ASP:OD2	4:C:442:ARG:NH1	2.44	0.51
11:N:65:PRO:HG2	13:J:136:PRO:HB3	1.93	0.51
3:G:125:HIS:CD2	4:C:513:GLU:HG2	2.46	0.51
12:K:34:GLY:O	12:K:38:MET:HG3	2.11	0.51
11:N:412:GLY:HA3	20:N:502:LFA:H62	1.93	0.50
13:J:24:ASN:HB3	13:J:27:HIS:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:69:TYR:OH	12:K:74:SER:O	2.29	0.50
12:K:33:ILE:HG23	13:J:32:LEU:HD22	1.92	0.50
3:G:217:TYR:HB3	6:I:79:LYS:HD2	1.93	0.50
6:I:80:ALA:HB2	6:I:90:GLU:HB2	1.94	0.50
9:L:344:LEU:HB2	9:L:460:LEU:HB3	1.92	0.50
1:F:353:TRP:HZ2	3:G:44:VAL:HB	1.77	0.50
3:G:226:ALA:HB3	3:G:635:VAL:HG22	1.94	0.50
4:C:23:ASP:OD1	4:C:109:ARG:NH1	2.45	0.50
9:L:318:TYR:OH	9:L:418:GLY:O	2.25	0.50
6:I:24:ALA:HB2	7:H:43:PHE:HD1	1.77	0.50
4:C:395:GLU:HA	4:C:399:LEU:HB2	1.94	0.49
9:L:144:GLU:OE2	9:L:175:ARG:NH1	2.45	0.49
9:L:247:THR:HG21	9:L:350:GLY:HA3	1.93	0.49
11:N:295:LYS:HD3	11:N:344:VAL:HG11	1.94	0.49
3:G:828:GLN:O	3:G:834:GLN:NE2	2.45	0.49
4:C:380:LEU:HD23	4:C:485:LEU:HD13	1.95	0.49
19:H:403:3PE:H382	8:A:20:LEU:HD23	1.93	0.49
3:G:694:ASP:N	3:G:694:ASP:OD1	2.45	0.49
3:G:731:ASP:OD2	3:G:734:THR:OG1	2.28	0.49
9:L:263:VAL:HG13	9:L:323:LEU:HD11	1.95	0.49
9:L:358:HIS:ND1	9:L:360:GLN:OE1	2.45	0.49
10:M:123:ILE:HG13	10:M:149:PRO:HB2	1.93	0.49
11:N:64:THR:HG22	11:N:65:PRO:HD2	1.93	0.49
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.93	0.49
19:H:403:3PE:H272	8:A:20:LEU:HD21	1.93	0.49
10:M:65:SER:HB3	10:M:83:ILE:HG22	1.95	0.49
7:H:36:GLU:OE1	7:H:286:ARG:NH1	2.39	0.49
3:G:356:LYS:O	3:G:360:GLU:HB2	2.13	0.49
7:H:302:TRP:HB3	8:A:123:LEU:HD13	1.95	0.49
10:M:217:SER:O	19:M:701:3PE:N	2.45	0.49
9:L:176:VAL:HG11	19:L:802:3PE:H3B1	1.95	0.48
11:N:311:VAL:HG22	11:N:410:LEU:HD13	1.94	0.48
5:B:70:THR:O	5:B:73:THR:OG1	2.29	0.48
4:C:80:MET:HG2	4:C:82:GLU:HG2	1.94	0.48
4:C:351:GLU:OE2	5:B:161:ARG:NH1	2.32	0.48
5:B:84:GLU:OE2	7:H:37:ARG:NE	2.43	0.48
3:G:808:GLN:HG3	3:G:811:LYS:HB2	1.95	0.48
10:M:30:TRP:O	10:M:34:ILE:HD12	2.13	0.48
10:M:248:HIS:ND1	10:M:258:ASP:OD1	2.42	0.48
3:G:611:SER:OG	3:G:646:VAL:O	2.32	0.48
3:G:843:LYS:HD3	3:G:874:GLU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:455:ILE:O	11:N:459:ILE:HG12	2.14	0.48
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.87	0.48
11:N:267:GLU:OE2	11:N:270:ARG:NH1	2.47	0.48
1:F:348:ARG:NH2	2:E:93:ASP:OD1	2.47	0.47
3:G:843:LYS:HB2	3:G:885:GLY:HA3	1.96	0.47
4:C:133:ASN:HB3	4:C:422:TRP:HA	1.95	0.47
7:H:199:PHE:HE2	7:H:252:MET:HB2	1.78	0.47
7:H:44:GLN:OE1	7:H:46:ARG:NH2	2.46	0.47
11:N:207:PHE:HA	11:N:210:MET:HE2	1.95	0.47
1:F:298:ASP:OD2	1:F:409:GLN:NE2	2.47	0.47
3:G:320:PRO:HB2	3:G:537:SER:HB3	1.95	0.47
4:C:377:ASP:N	4:C:377:ASP:OD1	2.45	0.47
7:H:262:GLY:HA3	7:H:270:TRP:CD1	2.50	0.47
11:N:310:LEU:HD12	11:N:313:LEU:HD23	1.97	0.47
11:N:367:TRP:NE1	11:N:434:LEU:O	2.41	0.47
2:E:65:PRO:HB3	3:G:170:THR:HB	1.97	0.47
3:G:652:ARG:NH2	3:G:669:THR:O	2.41	0.47
9:L:603:VAL:HG22	13:J:103:MET:HB2	1.96	0.47
19:L:801:3PE:H371	10:M:390:PHE:HD1	1.79	0.47
10:M:192:LEU:HB2	10:M:223:LEU:HD13	1.95	0.47
11:N:360:PHE:CE2	11:N:362:TYR:HB3	2.49	0.47
3:G:21:LEU:HD13	3:G:79:ILE:HD13	1.95	0.47
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.49	0.47
9:L:457:LEU:O	9:L:461:LEU:HB2	2.14	0.47
19:L:801:3PE:H262	19:L:801:3PE:H322	1.97	0.47
11:N:305:HIS:ND1	11:N:329:TYR:OH	2.32	0.47
19:H:403:3PE:H351	19:A:202:3PE:H342	1.96	0.47
9:L:257:THR:OG1	9:L:258:MET:N	2.48	0.47
3:G:807:PRO:HB3	3:G:882:GLY:HA3	1.97	0.46
3:G:295:LEU:HB3	3:G:299:GLN:HG3	1.97	0.46
10:M:248:HIS:O	10:M:312:LYS:NZ	2.41	0.46
3:G:592:VAL:HB	3:G:606:ALA:HA	1.97	0.46
3:G:679:VAL:HG21	3:G:689:LYS:HB2	1.97	0.46
11:N:70:ASP:N	11:N:70:ASP:OD1	2.48	0.46
11:N:381:LEU:HD12	20:N:501:LFA:H181	1.96	0.46
1:F:102:ARG:HH22	2:E:149:THR:HG21	1.80	0.46
3:G:313:LYS:NZ	3:G:557:GLU:OE1	2.36	0.46
4:C:52:ILE:HD12	4:C:60:VAL:HG21	1.96	0.46
4:C:541:LYS:HE3	4:C:594:VAL:HG22	1.96	0.46
1:F:261:LEU:HD13	1:F:325:LEU:HD21	1.97	0.46
10:M:483:GLN:NE2	10:M:487:ASP:OD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:9:ILE:HG12	13:J:108:VAL:HG22	1.97	0.46
1:F:255:ARG:NH1	1:F:330:ASP:OD2	2.48	0.46
3:G:839:GLN:HG2	3:G:840:PRO:HD2	1.98	0.46
1:F:21:LYS:HA	1:F:21:LYS:HD3	1.85	0.46
3:G:669:THR:OG1	3:G:670:GLN:N	2.49	0.45
2:E:138:ASP:OD1	2:E:138:ASP:N	2.48	0.45
6:I:51:THR:HG22	6:I:139:ILE:HD11	1.98	0.45
7:H:101:VAL:HG11	7:H:250:ALA:HB1	1.99	0.45
11:N:176:LEU:HD22	11:N:202:LEU:HD11	1.98	0.45
3:G:828:GLN:NE2	3:G:889:GLY:O	2.50	0.45
7:H:11:ILE:HD13	8:A:11:ALA:HA	1.98	0.45
8:A:67:LYS:HA	8:A:67:LYS:HD2	1.75	0.45
9:L:3:MET:SD	9:L:3:MET:N	2.82	0.45
10:M:146:MET:SD	10:M:234:LYS:NZ	2.83	0.45
10:M:498:GLN:O	10:M:502:ASN:HB2	2.16	0.45
1:F:255:ARG:HH12	1:F:332:GLU:HB3	1.82	0.45
3:G:746:PRO:O	3:G:779:ARG:NH1	2.49	0.45
6:I:45:ARG:HG2	6:I:116:LEU:HD22	1.98	0.45
12:K:6:HIS:HD1	13:J:6:TYR:HH	1.54	0.45
1:F:101:ASP:O	1:F:105:MET:HG3	2.17	0.45
1:F:182:GLU:O	1:F:186:LEU:N	2.44	0.45
3:G:307:ILE:HG22	3:G:591:LEU:HD22	1.98	0.45
10:M:381:MET:HB2	10:M:385:PRO:HD3	1.99	0.45
11:N:119:LEU:HD22	11:N:253:VAL:HG11	1.98	0.45
3:G:146:ILE:HD11	3:G:197:GLY:HA2	1.99	0.45
3:G:569:LEU:HD11	3:G:650:SER:HB3	1.99	0.45
6:I:156:MET:O	6:I:161:LYS:NZ	2.42	0.45
5:B:100:GLY:HA2	14:B:301:SF4:S4	2.57	0.45
3:G:149:GLU:OE2	6:I:163:LYS:NZ	2.49	0.44
3:G:379:VAL:HB	3:G:433:VAL:HG12	1.98	0.44
4:C:22:ASP:OD1	4:C:22:ASP:N	2.50	0.44
7:H:179:ILE:HG21	7:H:255:LEU:HD23	1.99	0.44
9:L:10:LEU:HD13	9:L:40:LEU:HB3	1.98	0.44
4:C:144:LEU:HB3	4:C:169:LEU:HB2	1.98	0.44
4:C:312:GLU:OE2	4:C:447:TYR:OH	2.29	0.44
7:H:103:VAL:HG21	20:H:402:LFA:H81	1.98	0.44
11:N:60:ALA:HA	11:N:69:VAL:O	2.17	0.44
12:K:43:ALA:HB1	12:K:62:TYR:HD1	1.81	0.44
3:G:431:LEU:O	3:G:446:ALA:N	2.50	0.44
4:C:85:ARG:HB3	4:C:88:ARG:HD2	2.00	0.44
3:G:267:ARG:HA	3:G:833:PHE:HZ	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:565:SER:HB3	4:C:593:PHE:HB2	1.99	0.44
10:M:47:TRP:CG	10:M:88:LEU:HD11	2.53	0.44
10:M:365:ARG:HH21	10:M:460:MET:HA	1.82	0.44
1:F:394:GLY:O	3:G:48:ARG:NH2	2.51	0.44
3:G:19:ASP:HB3	3:G:23:GLU:HG3	2.00	0.44
3:G:150:MET:HE1	3:G:183:PHE:HD1	1.81	0.44
5:B:80:ARG:HA	7:H:49:PRO:HA	1.99	0.44
7:H:170:GLN:HG3	7:H:192:GLN:HE21	1.82	0.44
5:B:124:ILE:HG12	5:B:153:VAL:HB	2.00	0.44
6:I:59:ARG:NH2	6:I:142:PRO:O	2.51	0.44
7:H:175:ASN:ND2	7:H:177:THR:OG1	2.51	0.44
11:N:141:GLY:HA3	13:J:154:VAL:HG22	1.99	0.44
1:F:147:ILE:O	1:F:151:THR:HG23	2.18	0.43
4:C:123:HIS:HA	4:C:148:THR:O	2.17	0.43
4:C:140:GLU:OE2	4:C:600:ARG:NH1	2.48	0.43
10:M:52:TYR:CE2	10:M:64:GLN:HG3	2.53	0.43
2:E:22:ILE:O	2:E:26:MET:HG3	2.18	0.43
3:G:438:ASP:OD1	3:G:438:ASP:N	2.49	0.43
4:C:103:ILE:HD11	4:C:536:MET:HE1	2.00	0.43
4:C:501:THR:HG23	4:C:521:GLN:HB3	2.01	0.43
5:B:201:ARG:HE	5:B:201:ARG:HB3	1.67	0.43
7:H:103:VAL:HG11	20:H:402:LFA:H61	2.00	0.43
9:L:82:ASP:OD1	9:L:82:ASP:N	2.48	0.43
3:G:267:ARG:HB2	3:G:820:LEU:HG	1.99	0.43
7:H:194:PHE:HA	7:H:197:ILE:HG12	2.00	0.43
3:G:7:HIS:NE2	3:G:12:GLU:OE1	2.52	0.43
4:C:324:SER:HB3	4:C:336:VAL:HA	2.01	0.43
7:H:150:SER:HA	7:H:153:THR:HG22	2.00	0.43
1:F:79:ASP:OD1	1:F:79:ASP:N	2.51	0.43
11:N:68:ARG:HD3	11:N:484:LEU:HB2	1.99	0.43
12:K:37:ILE:HD13	13:J:16:THR:HG23	2.00	0.43
13:J:161:GLU:N	13:J:161:GLU:OE2	2.51	0.43
3:G:6:ILE:HG22	3:G:77:THR:HB	2.00	0.43
4:C:338:PHE:HE1	7:H:45:ASN:HB2	1.83	0.43
4:C:391:LEU:HD22	4:C:474:LEU:HD22	2.00	0.43
8:A:75:PHE:O	8:A:79:ASP:HB2	2.19	0.43
8:A:81:GLU:HG2	13:J:148:LEU:HD13	2.00	0.43
5:B:57:TYR:HE2	5:B:113:LEU:HD13	1.84	0.43
19:L:801:3PE:H2I3	19:L:804:3PE:H391	2.00	0.43
1:F:38:ALA:HB2	1:F:114:GLU:HG3	2.00	0.43
1:F:176:GLY:O	2:E:77:SER:OG	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:520:LEU:HD23	4:C:520:LEU:HA	1.88	0.43
5:B:74:ALA:HA	7:H:46:ARG:HD3	2.01	0.43
11:N:214:LEU:HD13	11:N:254:VAL:HG22	2.01	0.43
10:M:100:LEU:HD22	10:M:467:MET:HB2	2.00	0.42
1:F:364:SER:HB3	1:F:387:LEU:HD13	2.00	0.42
7:H:213:ASP:OD1	7:H:213:ASP:N	2.52	0.42
9:L:170:ALA:HA	9:L:238:TRP:HB2	2.02	0.42
9:L:522:ILE:O	9:L:525:SER:OG	2.35	0.42
13:J:120:ASP:OD2	13:J:120:ASP:N	2.51	0.42
1:F:291:GLN:O	1:F:326:ALA:HA	2.20	0.42
9:L:197:PHE:HA	9:L:200:MET:HE2	2.01	0.42
6:I:161:LYS:HE3	6:I:166:ALA:HB2	2.00	0.42
7:H:114:ILE:HB	7:H:117:LEU:HB2	2.01	0.42
7:H:278:PHE:HD1	19:H:401:3PE:H3H2	1.84	0.42
7:H:278:PHE:HB3	19:H:401:3PE:H3I1	2.01	0.42
19:H:403:3PE:H341	19:A:202:3PE:H321	2.00	0.42
3:G:558:LEU:HD21	3:G:566:VAL:HB	2.00	0.42
3:G:623:ILE:HD12	3:G:787:LEU:HD11	2.02	0.42
11:N:66:LEU:HA	11:N:124:HIS:HB2	2.00	0.42
3:G:443:ASP:OD1	3:G:443:ASP:N	2.52	0.42
5:B:217:PRO:HB3	6:I:43:ARG:HB3	2.01	0.42
9:L:196:ASN:HB3	9:L:199:GLU:HG3	2.01	0.42
11:N:7:ASN:HB3	11:N:63:VAL:HG13	2.01	0.42
12:K:43:ALA:HB1	12:K:62:TYR:CD1	2.54	0.42
1:F:177:ARG:HA	1:F:177:ARG:HD3	1.91	0.42
1:F:329:VAL:HG13	1:F:333:ILE:HD12	2.02	0.42
7:H:116:ILE:H	7:H:116:ILE:HG13	1.66	0.42
7:H:117:LEU:O	7:H:121:MET:HG3	2.20	0.42
9:L:129:VAL:HG11	9:L:141:LEU:HD22	2.02	0.42
4:C:120:ASN:OD1	4:C:120:ASN:N	2.53	0.42
4:C:470:LYS:NZ	4:C:540:THR:O	2.52	0.42
9:L:243:MET:SD	9:L:309:ALA:HB2	2.60	0.42
9:L:425:THR:HA	9:L:428:TYR:CE2	2.54	0.42
10:M:252:PRO:HD2	10:M:257:VAL:HG21	2.02	0.42
13:J:18:ARG:HH21	13:J:22:HIS:CD2	2.38	0.42
3:G:295:LEU:HA	3:G:299:GLN:HE21	1.85	0.42
6:I:66:CYS:HB2	6:I:105:CYS:HB2	2.01	0.42
9:L:368:LEU:HD23	9:L:372:ILE:HD11	2.02	0.41
7:H:79:ASP:OD2	13:J:27:HIS:NE2	2.49	0.41
9:L:353:ILE:HD12	9:L:353:ILE:HA	1.90	0.41
4:C:194:MET:N	4:C:194:MET:SD	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:288:ALA:HB2	11:N:300:TYR:HB2	2.02	0.41
13:J:89:LYS:HA	13:J:89:LYS:HD3	1.94	0.41
9:L:169:LYS:HA	19:L:802:3PE:H332	2.01	0.41
9:L:288:ALA:HB2	9:L:321:LEU:HD12	2.02	0.41
10:M:72:ILE:HB	10:M:77:ILE:HB	2.01	0.41
10:M:418:VAL:HA	10:M:419:PRO:HD3	1.93	0.41
8:A:116:TYR:O	8:A:120:ILE:HG12	2.21	0.41
2:E:26:MET:HE3	2:E:32:PRO:HB3	2.03	0.41
3:G:149:GLU:HG2	3:G:152:ARG:CZ	2.51	0.41
7:H:30:ALA:HB1	7:H:60:LEU:HD11	2.01	0.41
1:F:264:LEU:HD13	1:F:268:THR:HG21	2.01	0.41
4:C:169:LEU:HD23	4:C:169:LEU:HA	1.90	0.41
9:L:606:LEU:HB3	13:J:106:VAL:HG11	2.03	0.41
11:N:421:GLY:HA2	11:N:424:TYR:CE2	2.56	0.41
3:G:8:VAL:HG11	3:G:30:LEU:HD13	2.02	0.41
3:G:613:ALA:HB1	3:G:617:GLU:HB2	2.03	0.41
4:C:112:MET:HE2	4:C:112:MET:HB2	1.91	0.41
4:C:429:LEU:O	4:C:432:THR:OG1	2.32	0.41
4:C:598:VAL:O	4:C:600:ARG:NH2	2.54	0.41
5:B:29:LEU:HD13	5:B:180:ARG:HD2	2.03	0.41
6:I:40:LEU:HD11	6:I:120:PHE:HD1	1.85	0.41
7:H:210:HIS:NE2	7:H:289:LEU:O	2.46	0.41
10:M:361:GLN:O	10:M:365:ARG:HG2	2.20	0.41
11:N:217:LYS:HA	11:N:217:LYS:HD3	1.86	0.41
2:E:116:LYS:H	2:E:119:GLN:NE2	2.18	0.41
4:C:109:ARG:HD3	4:C:109:ARG:HA	1.81	0.41
4:C:172:ASP:OD1	4:C:172:ASP:N	2.48	0.41
8:A:85:LEU:O	8:A:89:SER:OG	2.31	0.41
3:G:757:TRP:NE1	3:G:762:ASN:OD1	2.52	0.40
4:C:110:ASP:OD1	4:C:110:ASP:N	2.54	0.40
4:C:594:VAL:HG23	4:C:597:ASP:HB2	2.02	0.40
9:L:392:VAL:HG23	9:L:393:THR:HG23	2.02	0.40
3:G:830:ALA:HA	3:G:831:PRO:HD3	1.98	0.40
9:L:342:LYS:HD3	9:L:342:LYS:HA	1.90	0.40
3:G:232:GLN:HB2	14:G:1003:SF4:S3	2.61	0.40
5:B:89:SER:HB2	7:H:227:ILE:HG22	2.04	0.40
5:B:122:TRP:HB3	5:B:172:LEU:HD11	2.02	0.40
10:M:498:GLN:OE1	10:M:502:ASN:ND2	2.53	0.40
12:K:77:LEU:HD22	13:J:70:VAL:HG11	2.04	0.40
5:B:138:ILE:HG23	5:B:140:SER:H	1.86	0.40
9:L:12:LEU:HD23	9:L:12:LEU:HA	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:419:LEU:HD13	9:L:419:LEU:HA	1.90	0.40
12:K:6:HIS:ND1	13:J:6:TYR:OH	2.41	0.40
1:F:356:PRO:HB2	1:F:396:THR:HG22	2.04	0.40
13:J:29:LEU:HD23	13:J:29:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	437/439 (100%)	429 (98%)	8 (2%)	0	100	100
2	E	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
3	G	903/905 (100%)	872 (97%)	31 (3%)	0	100	100
4	C	580/600 (97%)	567 (98%)	13 (2%)	0	100	100
5	B	191/220 (87%)	184 (96%)	7 (4%)	0	100	100
6	I	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
7	H	310/325 (95%)	305 (98%)	5 (2%)	0	100	100
8	A	98/147 (67%)	98 (100%)	0	0	100	100
9	L	594/613 (97%)	578 (97%)	16 (3%)	0	100	100
10	M	502/504 (100%)	488 (97%)	14 (3%)	0	100	100
11	N	476/485 (98%)	465 (98%)	10 (2%)	1 (0%)	47	73
12	K	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
13	J	156/184 (85%)	153 (98%)	3 (2%)	0	100	100
All	All	4677/4858 (96%)	4562 (98%)	114 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	N	64	THR

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	F	353/353 (100%)	343 (97%)	10 (3%)	43	73
2	E	129/129 (100%)	125 (97%)	4 (3%)	40	69
3	G	732/732 (100%)	715 (98%)	17 (2%)	50	78
4	C	502/519 (97%)	485 (97%)	17 (3%)	37	66
5	B	169/192 (88%)	163 (96%)	6 (4%)	35	64
6	I	154/154 (100%)	149 (97%)	5 (3%)	39	68
7	H	259/269 (96%)	251 (97%)	8 (3%)	40	69
8	A	80/119 (67%)	79 (99%)	1 (1%)	69	87
9	L	473/486 (97%)	453 (96%)	20 (4%)	30	58
10	M	413/413 (100%)	402 (97%)	11 (3%)	44	74
11	N	382/385 (99%)	378 (99%)	4 (1%)	76	91
12	K	79/79 (100%)	77 (98%)	2 (2%)	47	76
13	J	123/146 (84%)	120 (98%)	3 (2%)	49	77
All	All	3848/3976 (97%)	3740 (97%)	108 (3%)	46	73

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	39	ARG
1	F	71	LEU
1	F	79	ASP
1	F	126	TYR
1	F	143	LEU
1	F	224	ASN
1	F	234	GLU
1	F	372	GLU

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Mol	Chain	Res	Type
1	F	398	CYS
1	F	425	GLN
2	E	46	GLN
2	E	122	PHE
2	E	125	ARG
2	E	144	MET
3	G	84	GLU
3	G	94	VAL
3	G	129	ARG
3	G	135	ARG
3	G	238	ASN
3	G	243	GLU
3	G	265	CYS
3	G	414	ASP
3	G	470	SER
3	G	626	GLU
3	G	717	MET
3	G	740	MET
3	G	750	ARG
3	G	804	ARG
3	G	837	MET
3	G	839	GLN
3	G	861	SER
4	C	16	GLN
4	C	65	LYS
4	C	80	MET
4	C	110	ASP
4	C	124	VAL
4	C	127	PHE
4	C	129	LYS
4	C	183	PHE
4	C	224	HIS
4	C	273	ASP
4	C	276	GLU
4	C	356	PHE
4	C	362	TRP
4	C	389	LYS
4	C	514	THR
4	C	531	ASN
4	C	600	ARG
5	B	63	CYS
5	B	78	VAL

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Mol	Chain	Res	Type
5	B	101	THR
5	B	119	GLU
5	B	145	VAL
5	B	174	GLU
6	I	3	LEU
6	I	23	HIS
6	I	83	LYS
6	I	153	MET
6	I	159	ASP
7	H	63	ASP
7	H	68	PHE
7	H	152	GLN
7	H	158	VAL
7	H	238	PHE
7	H	261	GLN
7	H	282	PHE
7	H	295	ASP
8	A	83	LEU
9	L	3	MET
9	L	68	MET
9	L	77	PHE
9	L	123	PHE
9	L	150	SER
9	L	168	MET
9	L	326	GLN
9	L	329	ASP
9	L	336	MET
9	L	365	MET
9	L	379	PHE
9	L	407	MET
9	L	419	LEU
9	L	431	ARG
9	L	472	VAL
9	L	490	MET
9	L	513	LEU
9	L	516	ARG
9	L	529	ARG
9	L	562	ARG
10	M	26	LYS
10	M	74	ARG
10	M	204	THR
10	M	212	ASN

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Mol	Chain	Res	Type
10	M	235	MET
10	M	264	LEU
10	M	265	LYS
10	M	303	TRP
10	M	439	MET
10	M	447	LYS
10	M	463	ARG
11	N	61	MET
11	N	207	PHE
11	N	376	MET
11	N	395	LYS
12	K	1	MET
12	K	46	PHE
13	J	1	MET
13	J	59	TYR
13	J	69	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
9	L	360	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 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	$\#\|Z\| > 2$
20	LFA	J	901	-	19,19,19	0.14	0	18,18,18	0.14	0
19	3PE	A	202	-	41,41,50	0.33	0	44,46,55	0.29	0
16	FES	E	201	2	0,4,4	-	-	-		
19	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.30	0
15	FMN	F	502	-	33,33,33	1.06	2 (6%)	48,50,50	1.25	6 (12%)
14	SF4	G	1003	3	0,12,12	-	-	-		
16	FES	G	1004	3	0,4,4	-	-	-		
19	3PE	L	802	-	50,50,50	0.30	0	53,55,55	0.29	0
19	3PE	L	804	-	50,50,50	0.30	0	53,55,55	0.29	0
14	SF4	I	202	6	0,12,12	-	-	-		
19	3PE	L	803	-	25,25,50	0.41	0	28,30,55	0.39	0
14	SF4	G	1001	3	0,12,12	-	-	-		
14	SF4	B	301	5	0,12,12	-	-	-		
19	3PE	H	401	-	50,50,50	0.30	0	53,55,55	0.32	0
20	LFA	N	502	-	13,13,19	0.13	0	12,12,18	0.13	0
19	3PE	M	701	-	33,33,50	0.36	0	36,38,55	0.32	0
20	LFA	N	501	-	19,19,19	0.13	0	18,18,18	0.14	0
14	SF4	I	201	6	0,12,12	-	-	-		
14	SF4	F	501	1	0,12,12	-	-	-		
18	DCQ	B	302	-	23,23,23	0.24	0	26,29,29	0.39	0
19	3PE	I	203	-	32,32,50	0.36	0	35,37,55	0.33	0
19	3PE	H	403	-	37,37,50	0.35	0	40,42,55	0.33	0
19	3PE	A	201	-	34,34,50	0.36	0	37,39,55	0.31	0
19	3PE	L	805	-	50,50,50	0.30	0	53,55,55	0.27	0
19	3PE	M	702	-	50,50,50	0.29	0	53,55,55	0.29	0
20	LFA	H	402	-	19,19,19	0.16	0	18,18,18	0.10	0
14	SF4	G	1002	3	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
20	LFA	J	901	-	-	0/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	3PE	A	202	-	-	8/45/45/54	-
16	FES	E	201	2	-	-	0/1/1/1
19	3PE	L	801	-	-	13/54/54/54	-
15	FMN	F	502	-	-	6/18/18/18	0/3/3/3
14	SF4	G	1003	3	-	-	0/6/5/5
16	FES	G	1004	3	-	-	0/1/1/1
19	3PE	L	802	-	-	8/54/54/54	-
19	3PE	L	804	-	-	14/54/54/54	-
14	SF4	I	202	6	-	-	0/6/5/5
19	3PE	L	803	-	-	8/29/29/54	-
14	SF4	G	1001	3	-	-	0/6/5/5
14	SF4	B	301	5	-	-	0/6/5/5
19	3PE	H	401	-	-	10/54/54/54	-
20	LFA	N	502	-	-	0/11/11/17	-
19	3PE	M	701	-	-	9/37/37/54	-
20	LFA	N	501	-	-	0/17/17/17	-
14	SF4	I	201	6	-	-	0/6/5/5
14	SF4	F	501	1	-	-	0/6/5/5
18	DCQ	B	302	-	-	0/14/38/38	0/1/1/1
19	3PE	I	203	-	-	5/36/36/54	-
19	3PE	H	403	-	-	5/41/41/54	-
19	3PE	A	201	-	-	9/38/38/54	-
19	3PE	L	805	-	-	11/54/54/54	-
19	3PE	M	702	-	-	8/54/54/54	-
20	LFA	H	402	-	-	1/17/17/17	-
14	SF4	G	1002	3	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.61	1.37	1.30
15	F	502	FMN	C10-N1	2.20	1.37	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4-N3-C2	-3.26	119.61	125.64
15	F	502	FMN	C4A-C10-N10	2.92	120.75	116.48
15	F	502	FMN	C4A-C4-N3	2.67	119.98	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	O4-C4-C4A	-2.56	119.81	126.60
15	F	502	FMN	C4A-C10-N1	-2.29	119.41	124.73
15	F	502	FMN	C10-C4A-N5	-2.29	120.00	124.86

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	502	FMN	N10-C1'-C2'-O2'
15	F	502	FMN	N10-C1'-C2'-C3'
15	F	502	FMN	C5'-O5'-P-O2P
15	F	502	FMN	C5'-O5'-P-O3P
19	I	203	3PE	C1-O11-P-O13
19	I	203	3PE	O13-C11-C12-N
19	H	401	3PE	O13-C11-C12-N
19	H	403	3PE	C11-O13-P-O12
19	H	403	3PE	O13-C11-C12-N
19	A	201	3PE	C1-O11-P-O12
19	A	201	3PE	C1-O11-P-O14
19	A	201	3PE	O13-C11-C12-N
19	A	202	3PE	O13-C11-C12-N
19	L	801	3PE	C1-O11-P-O14
19	L	801	3PE	C11-O13-P-O12
19	L	801	3PE	C11-O13-P-O14
19	L	801	3PE	O13-C11-C12-N
19	L	802	3PE	C1-O11-P-O12
19	L	802	3PE	C1-O11-P-O14
19	L	802	3PE	O13-C11-C12-N
19	L	803	3PE	C1-O11-P-O12
19	L	803	3PE	C1-O11-P-O13
19	L	803	3PE	C1-O11-P-O14
19	L	803	3PE	C11-O13-P-O14
19	L	804	3PE	C1-O11-P-O14
19	L	804	3PE	C2-C1-O11-P
19	L	805	3PE	C11-O13-P-O12
19	L	805	3PE	C2-C1-O11-P
19	M	701	3PE	C11-O13-P-O11
19	M	701	3PE	C11-O13-P-O14
19	M	701	3PE	O13-C11-C12-N
19	M	702	3PE	C11-O13-P-O11
19	M	702	3PE	C11-O13-P-O12
19	M	702	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
19	M	702	3PE	O13-C11-C12-N
19	H	401	3PE	C11-O13-P-O11
19	H	403	3PE	C11-O13-P-O11
19	A	201	3PE	C1-O11-P-O13
19	A	202	3PE	C1-O11-P-O13
19	L	801	3PE	C1-O11-P-O13
19	L	801	3PE	C11-O13-P-O11
19	L	802	3PE	C1-O11-P-O13
19	L	803	3PE	C11-O13-P-O11
19	L	805	3PE	C1-O11-P-O13
19	M	701	3PE	C1-O11-P-O13
19	M	702	3PE	C26-C27-C28-C29
19	L	801	3PE	C2C-C2D-C2E-C2F
19	L	804	3PE	C31-C32-C33-C34
20	H	402	LFA	C14-C15-C16-C17
19	M	701	3PE	C24-C25-C26-C27
19	L	805	3PE	C2A-C2B-C2C-C2D
19	L	804	3PE	C39-C3A-C3B-C3C
19	L	801	3PE	C3E-C3F-C3G-C3H
19	M	702	3PE	C3C-C3D-C3E-C3F
19	A	202	3PE	C21-C22-C23-C24
19	L	802	3PE	C3E-C3F-C3G-C3H
19	H	401	3PE	C1-C2-C3-O31
15	F	502	FMN	C5'-O5'-P-O1P
19	M	702	3PE	C2-C1-O11-P
19	L	801	3PE	C23-C24-C25-C26
19	A	201	3PE	C11-O13-P-O11
19	L	805	3PE	C11-O13-P-O11
19	H	401	3PE	C3B-C3C-C3D-C3E
19	H	401	3PE	O21-C2-C3-O31
19	I	203	3PE	C2-C1-O11-P
19	A	202	3PE	C2-C1-O11-P
19	M	701	3PE	C2-C1-O11-P
19	L	804	3PE	C3E-C3F-C3G-C3H
19	A	202	3PE	C11-O13-P-O11
19	I	203	3PE	C1-O11-P-O12
19	H	401	3PE	C11-O13-P-O14
19	A	202	3PE	C1-O11-P-O12
19	A	202	3PE	C1-O11-P-O14
19	L	801	3PE	C1-O11-P-O12
19	L	803	3PE	C11-O13-P-O12
19	L	805	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
19	L	805	3PE	C1-O11-P-O14
19	L	805	3PE	C11-O13-P-O14
19	M	701	3PE	C1-O11-P-O14
19	L	804	3PE	O13-C11-C12-N
19	L	804	3PE	C3D-C3E-C3F-C3G
19	L	805	3PE	O21-C21-C22-C23
19	L	801	3PE	C37-C38-C39-C3A
19	L	801	3PE	C25-C26-C27-C28
19	L	802	3PE	C11-O13-P-O11
19	L	804	3PE	C1-O11-P-O13
19	L	804	3PE	C11-O13-P-O11
19	L	805	3PE	C25-C26-C27-C28
19	H	403	3PE	C21-C22-C23-C24
19	H	401	3PE	C3C-C3D-C3E-C3F
19	L	804	3PE	C3C-C3D-C3E-C3F
19	A	202	3PE	O21-C21-C22-C23
19	H	401	3PE	C28-C29-C2A-C2B
19	L	804	3PE	O21-C2-C3-O31
19	L	805	3PE	O21-C2-C3-O31
19	M	702	3PE	C2F-C2G-C2H-C2I
19	M	701	3PE	C23-C24-C25-C26
19	L	802	3PE	C3D-C3E-C3F-C3G
19	A	201	3PE	O31-C31-C32-C33
19	H	401	3PE	C3F-C3G-C3H-C3I
19	H	401	3PE	C25-C26-C27-C28
19	L	803	3PE	O31-C31-C32-C33
19	A	201	3PE	O21-C21-C22-C23
19	H	403	3PE	C23-C24-C25-C26
19	L	801	3PE	C34-C35-C36-C37
19	A	201	3PE	O32-C31-C32-C33
19	L	803	3PE	O32-C31-C32-C33
15	F	502	FMN	C4'-C5'-O5'-P
19	L	802	3PE	C11-O13-P-O14
19	L	804	3PE	C1-O11-P-O12
19	M	701	3PE	C12-C11-O13-P
19	A	201	3PE	O22-C21-C22-C23
19	L	804	3PE	C34-C35-C36-C37
19	I	203	3PE	O21-C21-C22-C23
19	L	804	3PE	C3F-C3G-C3H-C3I

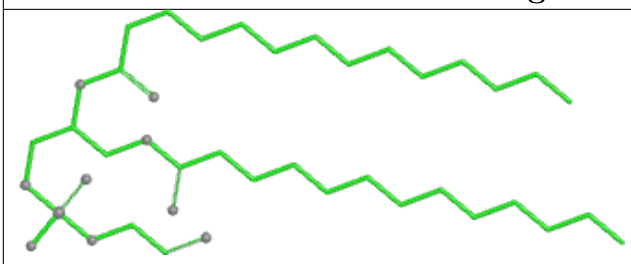
There are no ring outliers.

14 monomers are involved in 25 short contacts:

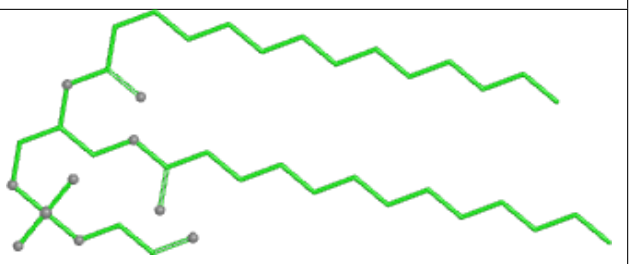
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	202	3PE	2	0
19	L	801	3PE	4	0
14	G	1003	SF4	1	0
19	L	802	3PE	4	0
19	L	804	3PE	2	0
14	B	301	SF4	1	0
19	H	401	3PE	3	0
20	N	502	LFA	1	0
19	M	701	3PE	1	0
20	N	501	LFA	1	0
19	H	403	3PE	4	0
19	A	201	3PE	1	0
19	M	702	3PE	1	0
20	H	402	LFA	2	0

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

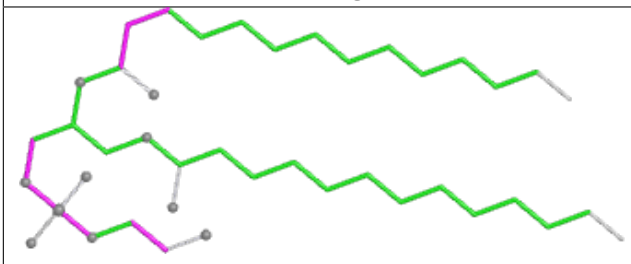
Ligand 3PE A 202



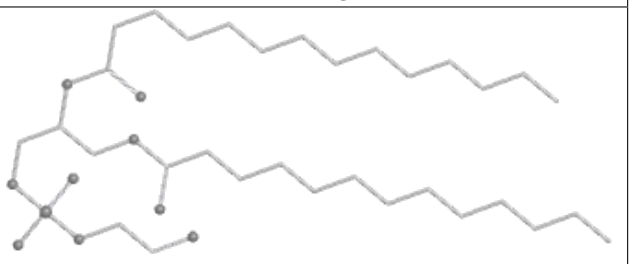
Bond lengths



Bond angles

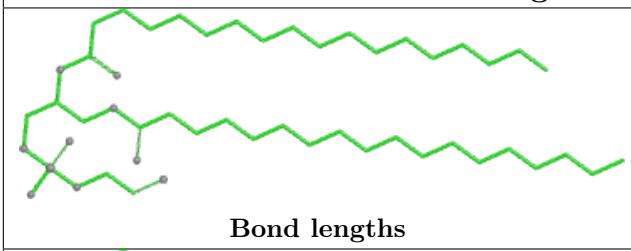


Torsions

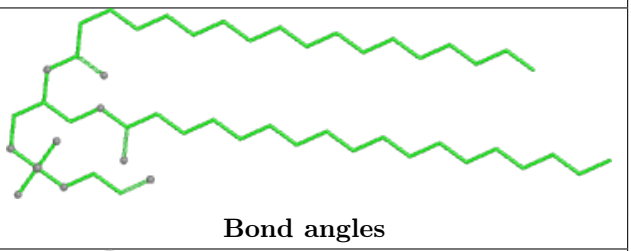


Rings

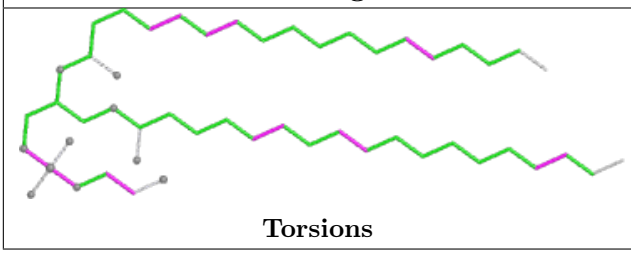
Ligand 3PE L 801



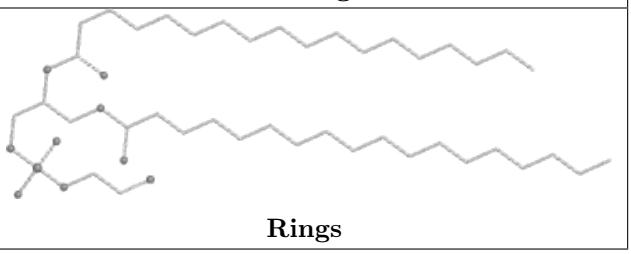
Bond lengths



Bond angles

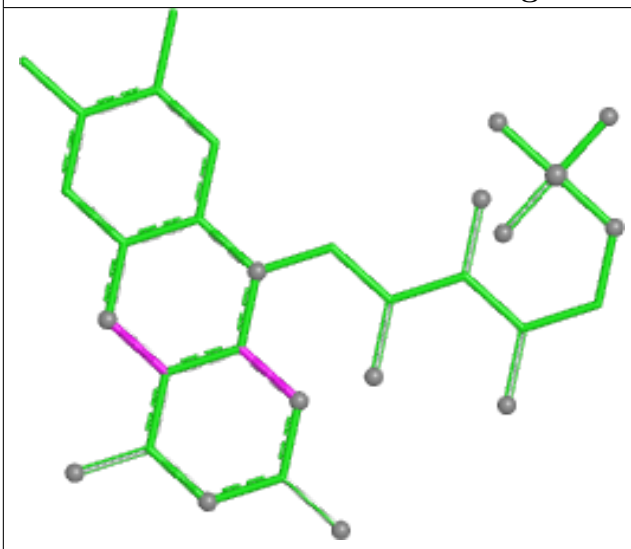


Torsions

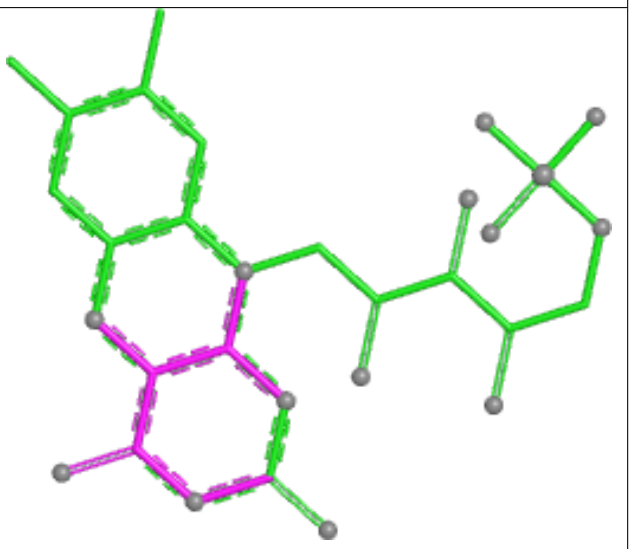


Rings

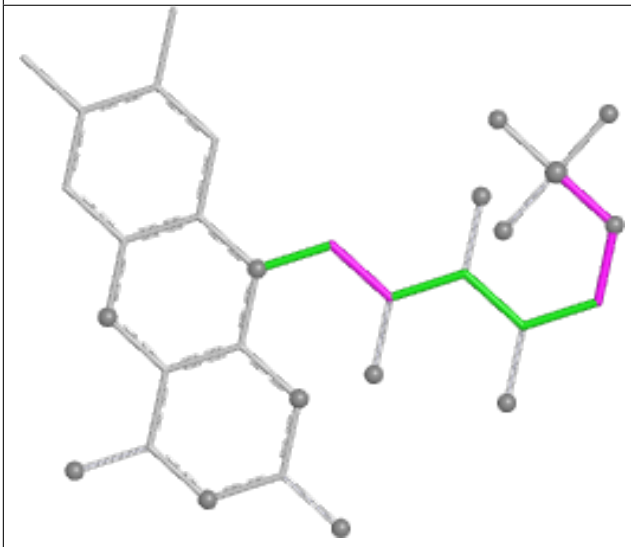
Ligand FMN F 502



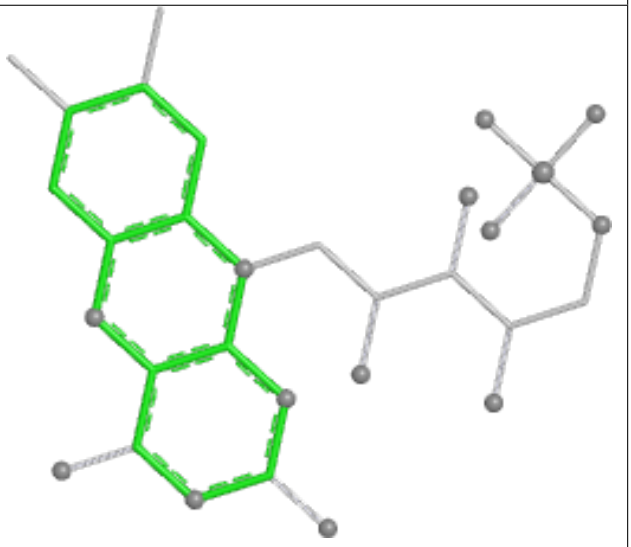
Bond lengths



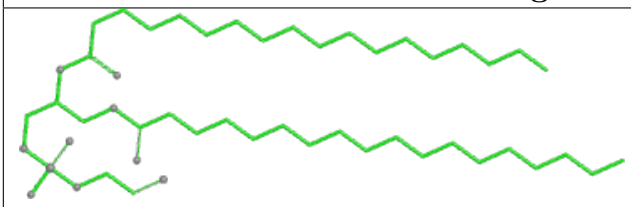
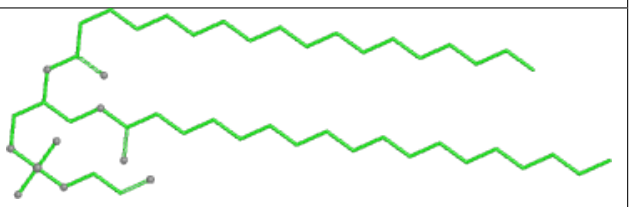
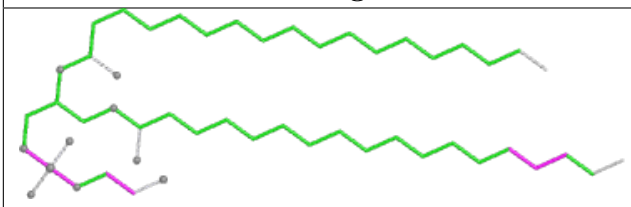
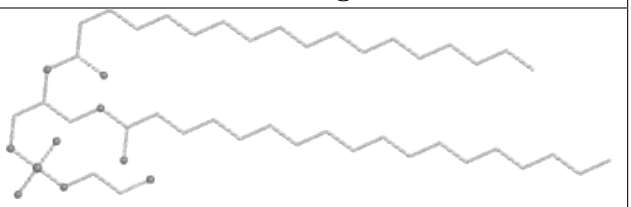
Bond angles

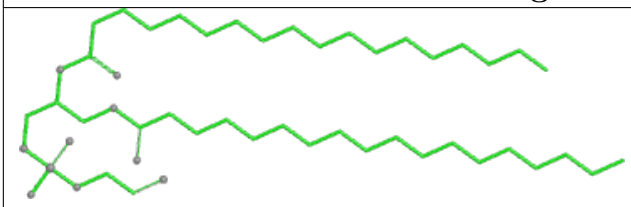
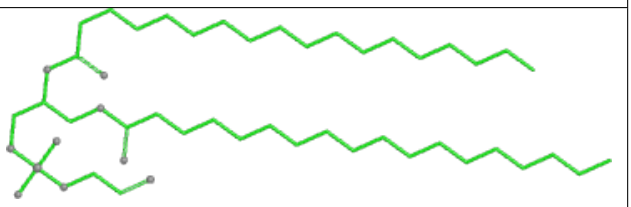
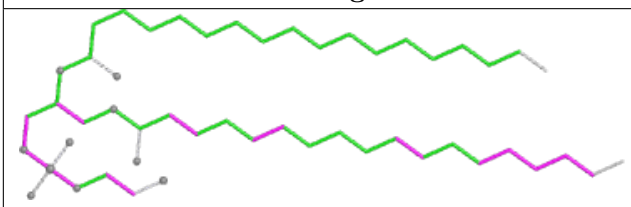
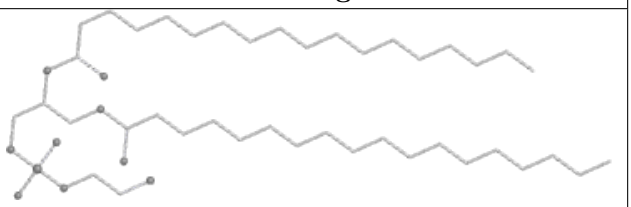


Torsions

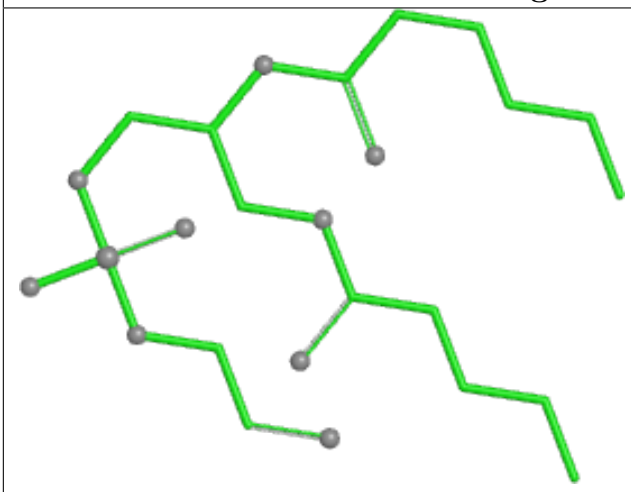


Rings

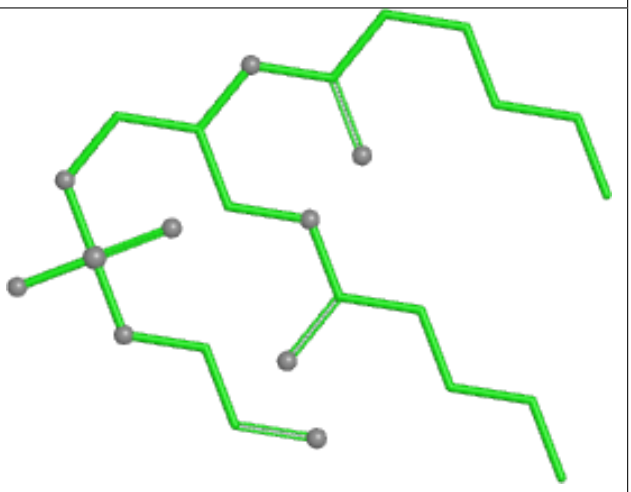
Ligand 3PE L 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

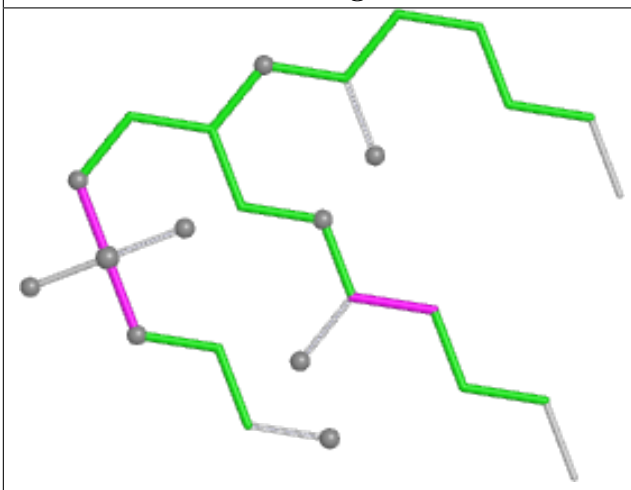
Ligand 3PE L 803



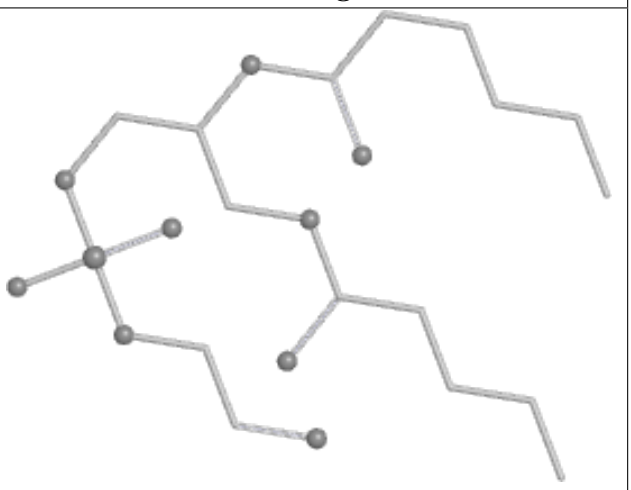
Bond lengths



Bond angles

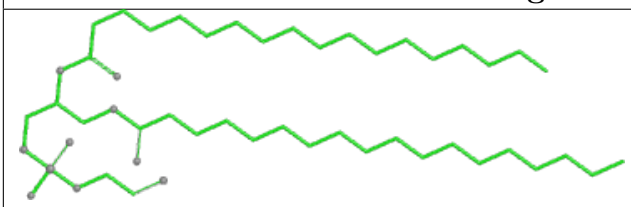


Torsions

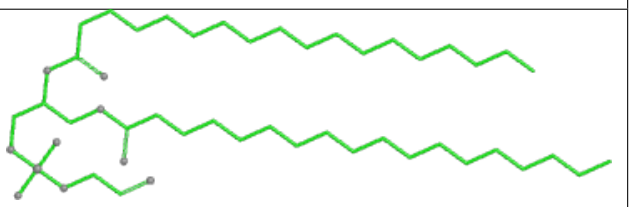


Rings

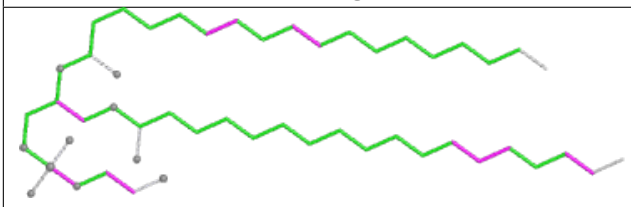
Ligand 3PE H 401



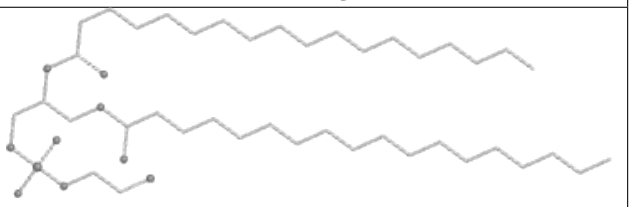
Bond lengths



Bond angles

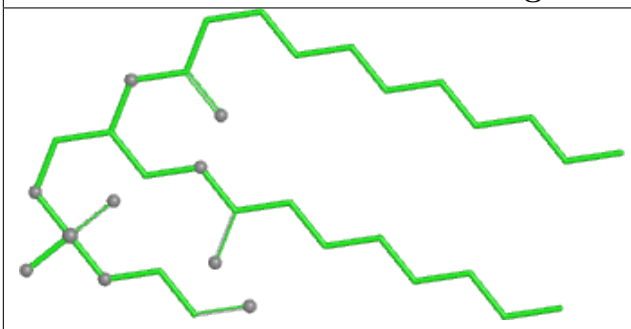


Torsions

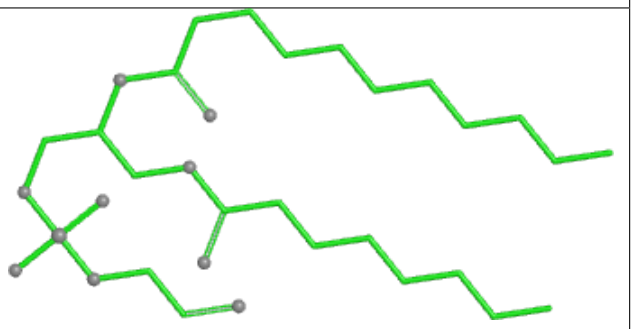


Rings

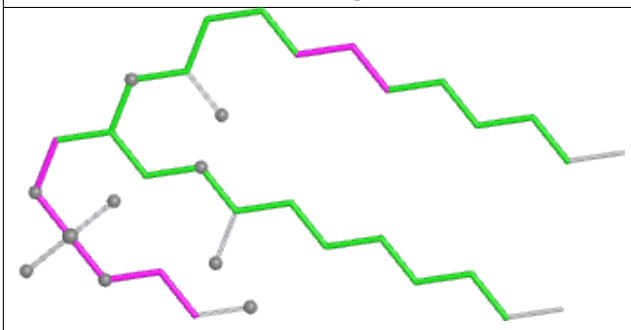
Ligand 3PE M 701



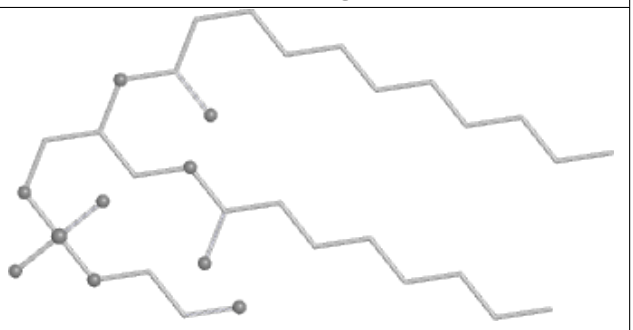
Bond lengths



Bond angles

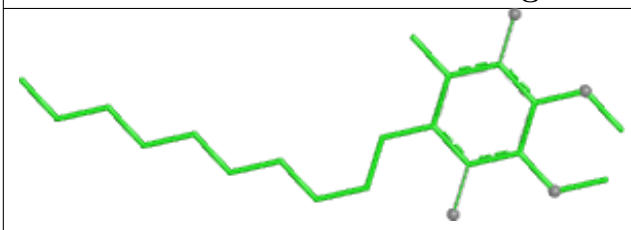


Torsions

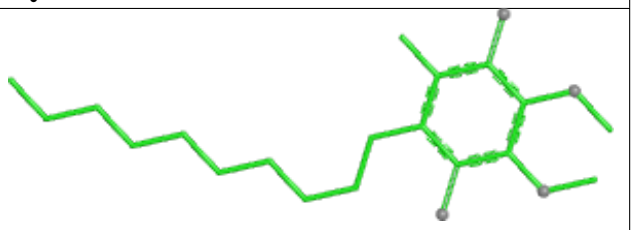


Rings

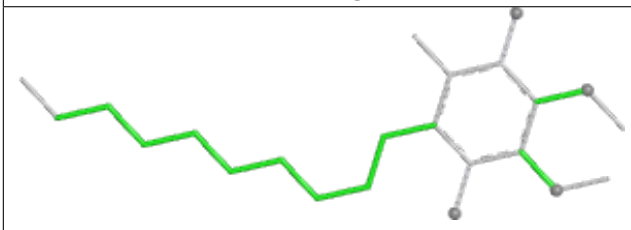
Ligand DCQ B 302



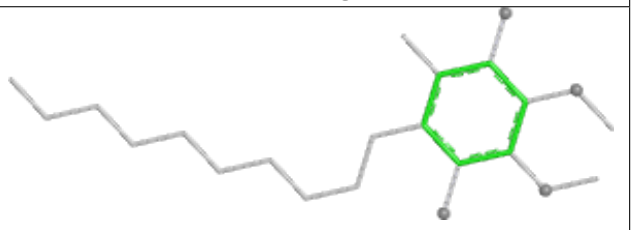
Bond lengths



Bond angles

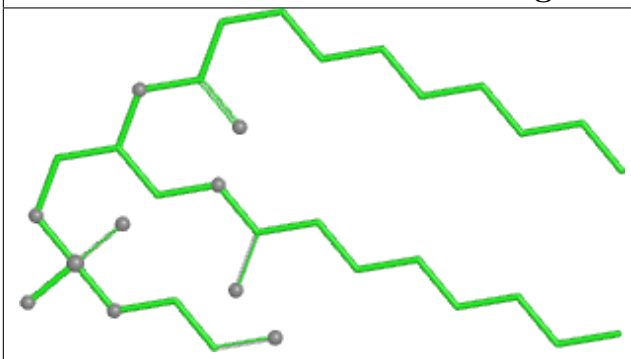


Torsions

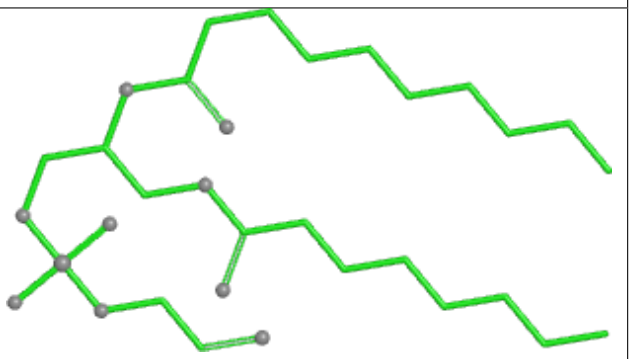


Rings

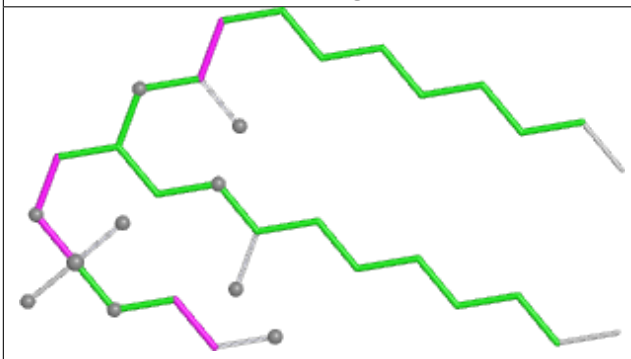
Ligand 3PE I 203



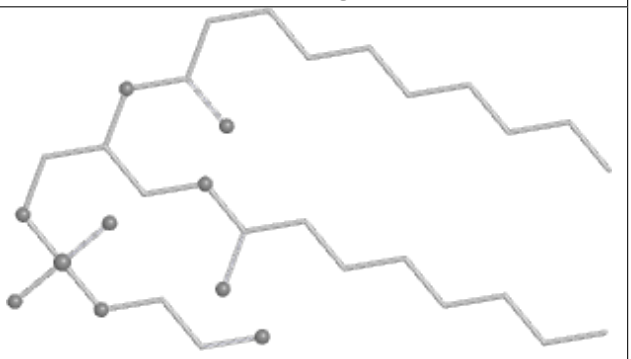
Bond lengths



Bond angles

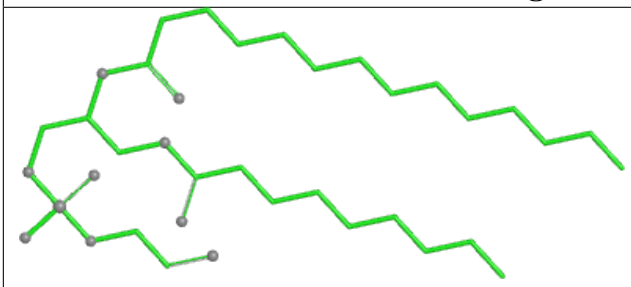


Torsions

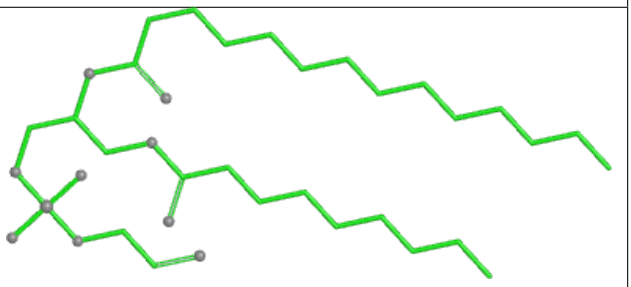


Rings

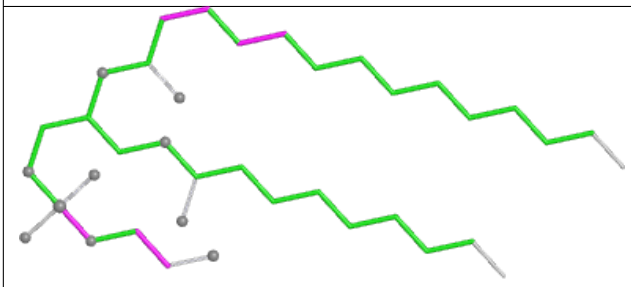
Ligand 3PE H 403



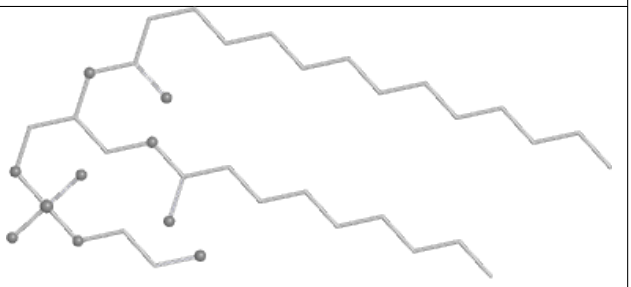
Bond lengths



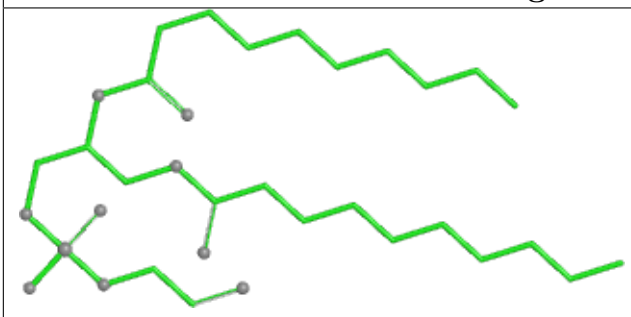
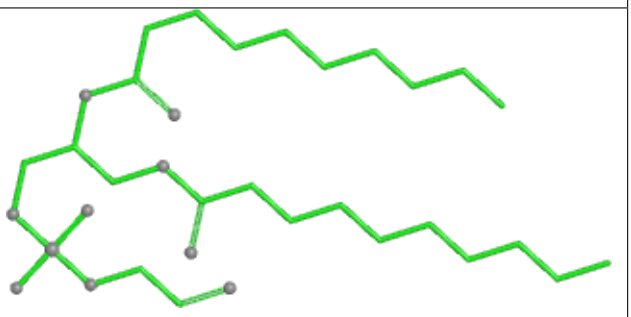
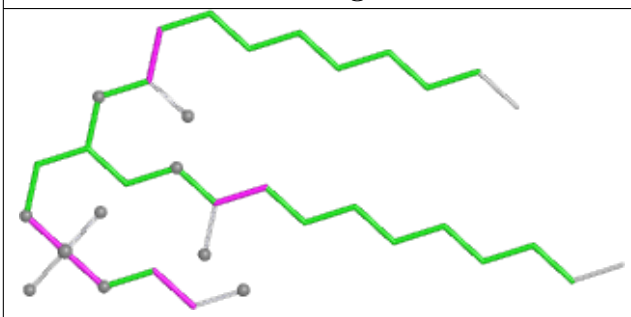
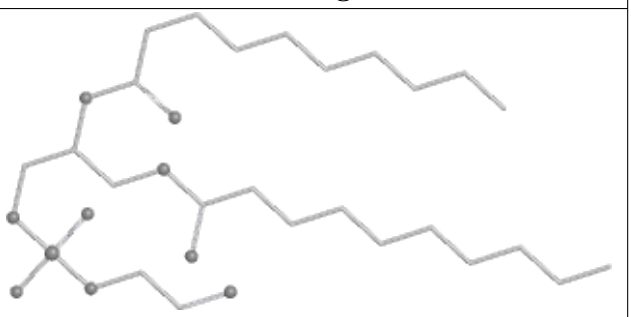
Bond angles

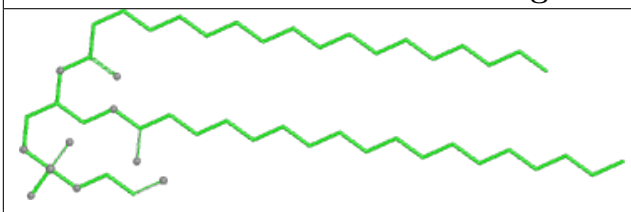
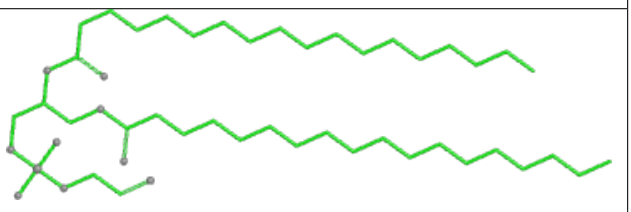
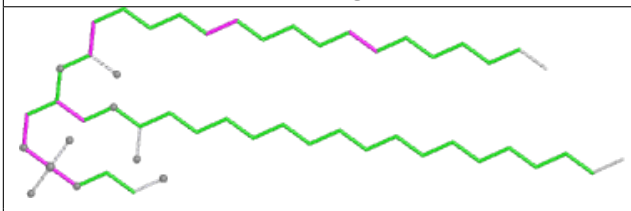
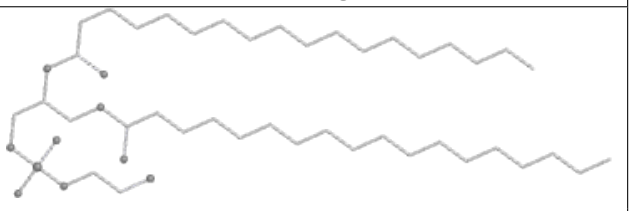


Torsions

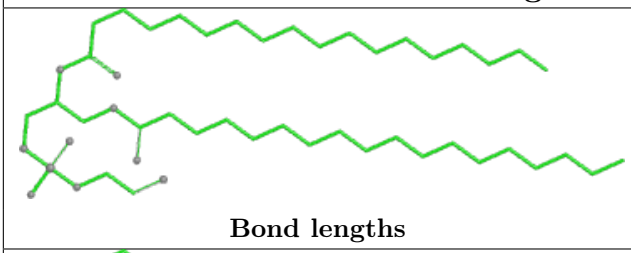


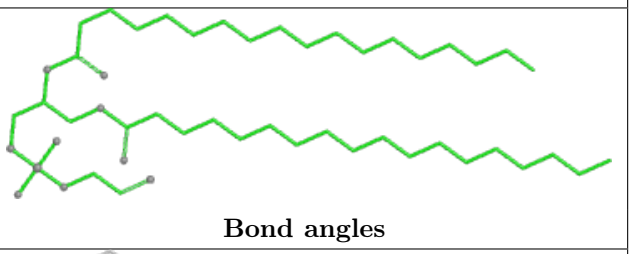
Rings

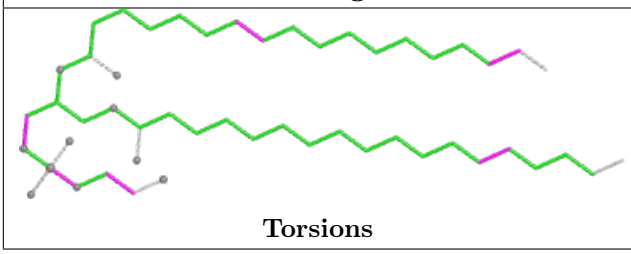
Ligand 3PE A 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

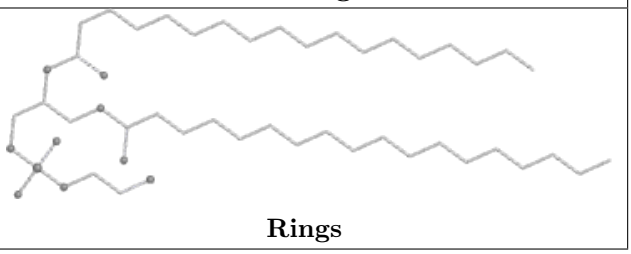
Ligand 3PE L 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE M 702

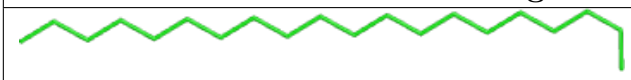

Bond lengths

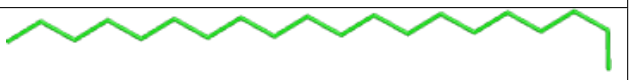

Bond angles

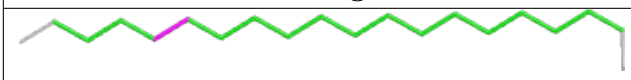

Torsions

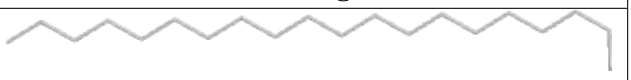

Rings

Ligand LFA H 402


Bond lengths


Bond angles


Torsions


Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

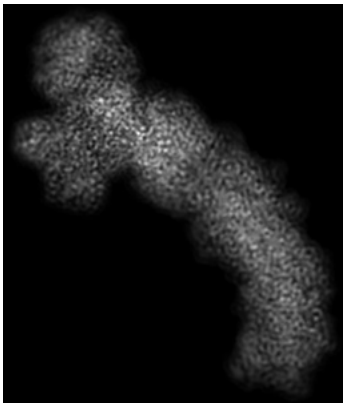
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13237. These allow visual inspection of the internal detail of the map and identification of artifacts.

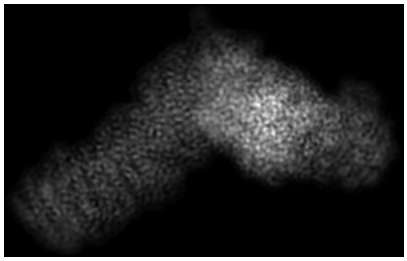
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

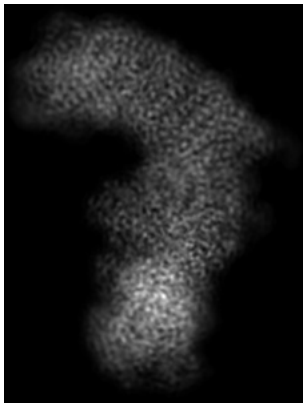
6.1.1 Primary map



X



Y

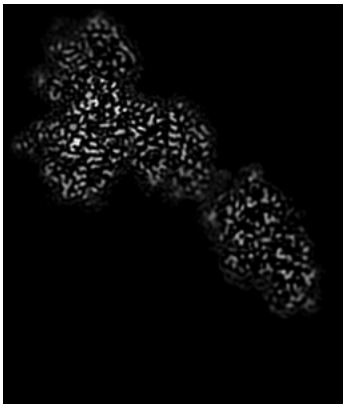


Z

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

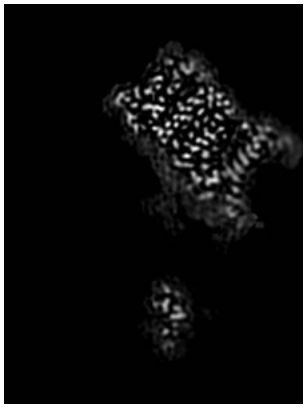
6.2 Central slices

6.2.1 Primary map



X Index: 72

Y Index: 97



Z Index: 115

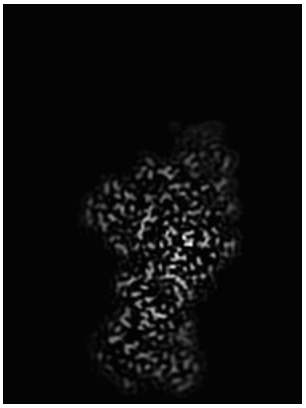
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 81

Y Index: 60



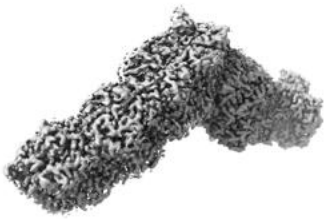
Z Index: 155

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

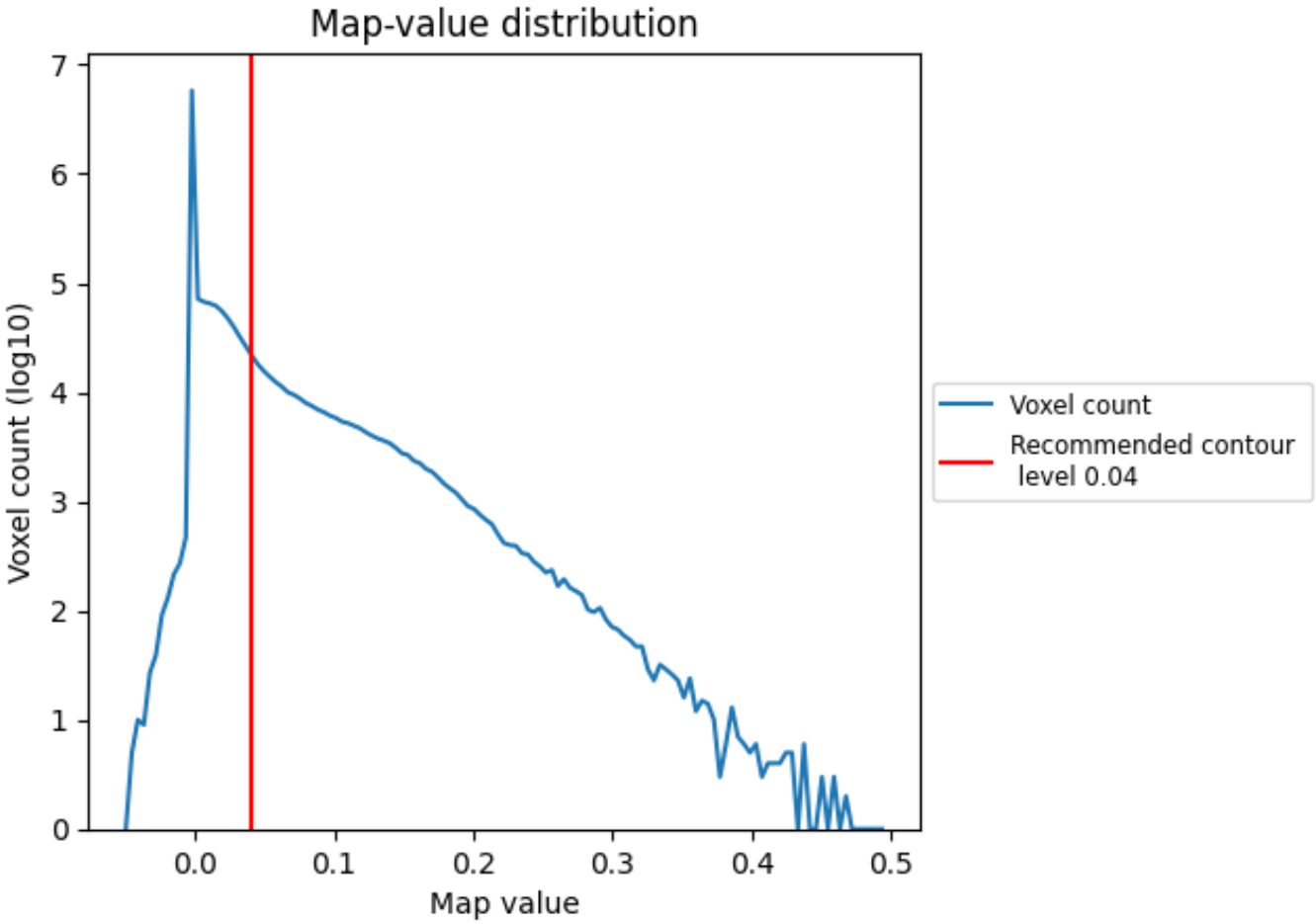
6.5 Mask visualisation (i)

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

7 Map analysis

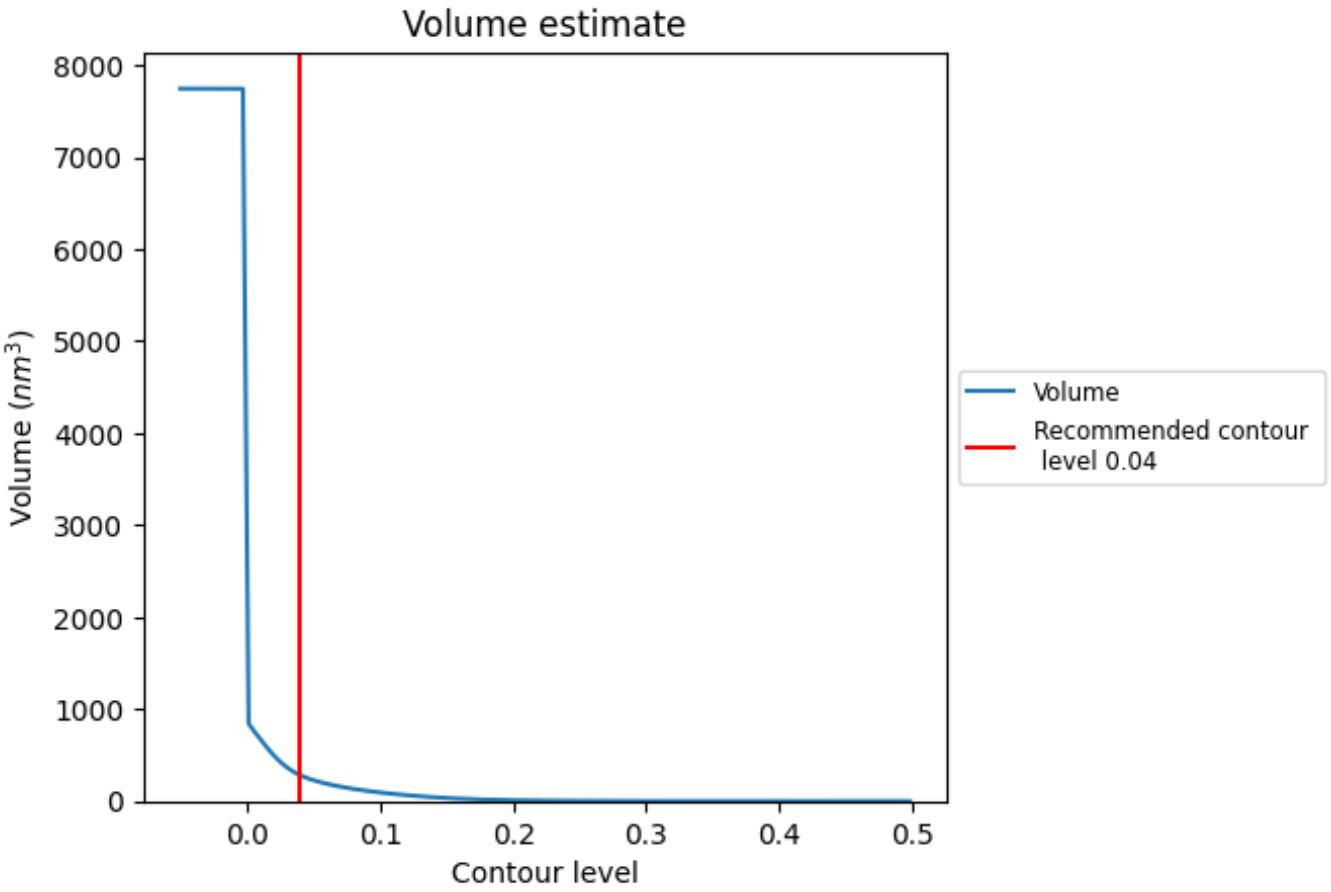
This section contains the results of statistical analysis of the map.

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 285 nm^3; this corresponds to an approximate mass of 257 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.

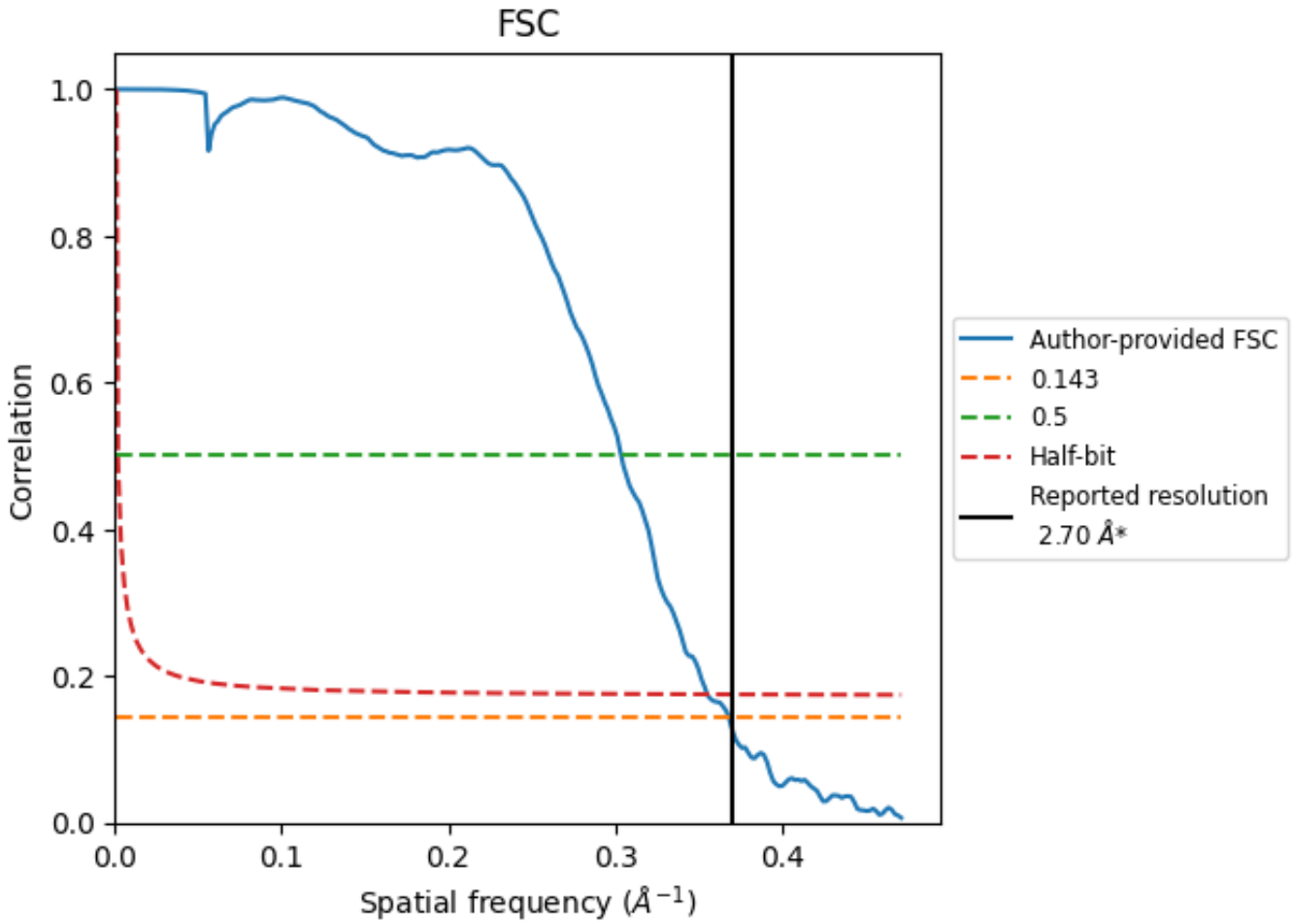
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

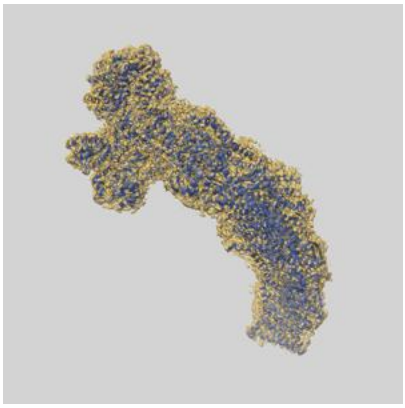
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	3.29	2.81
Unmasked-calculated*	-	-	-

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

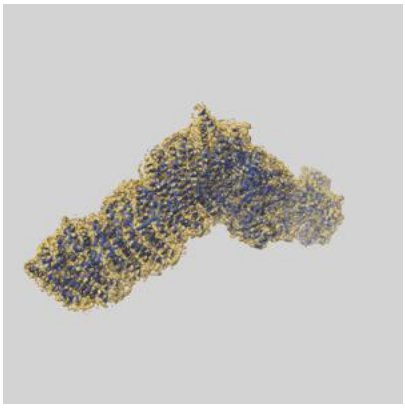
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13237 and PDB model 7P7J. Per-residue inclusion information can be found in section 3 on page 11.

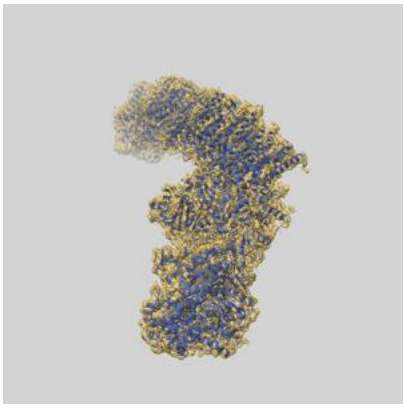
9.1 Map-model overlay



X



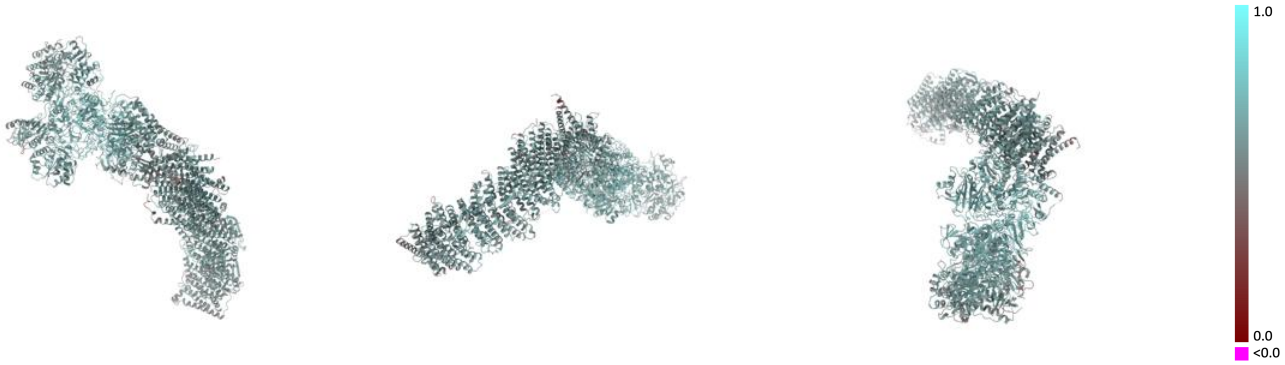
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

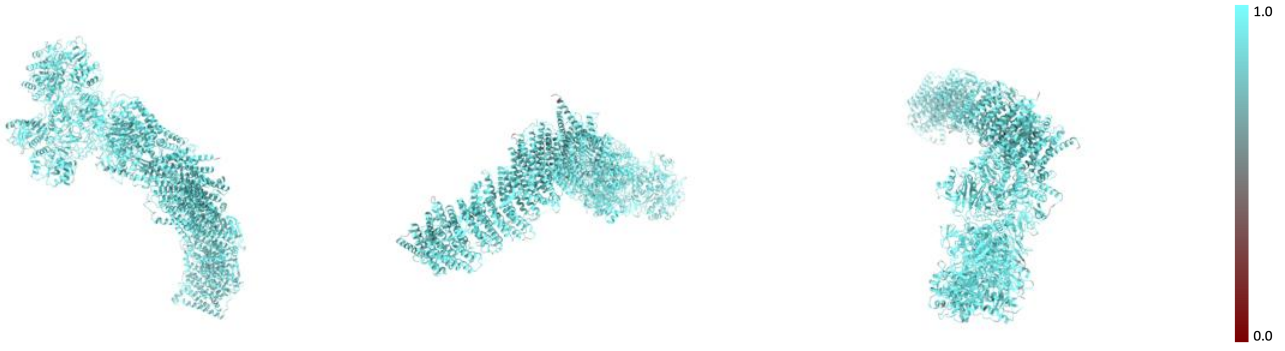
9.2 Q-score mapped to coordinate model



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.

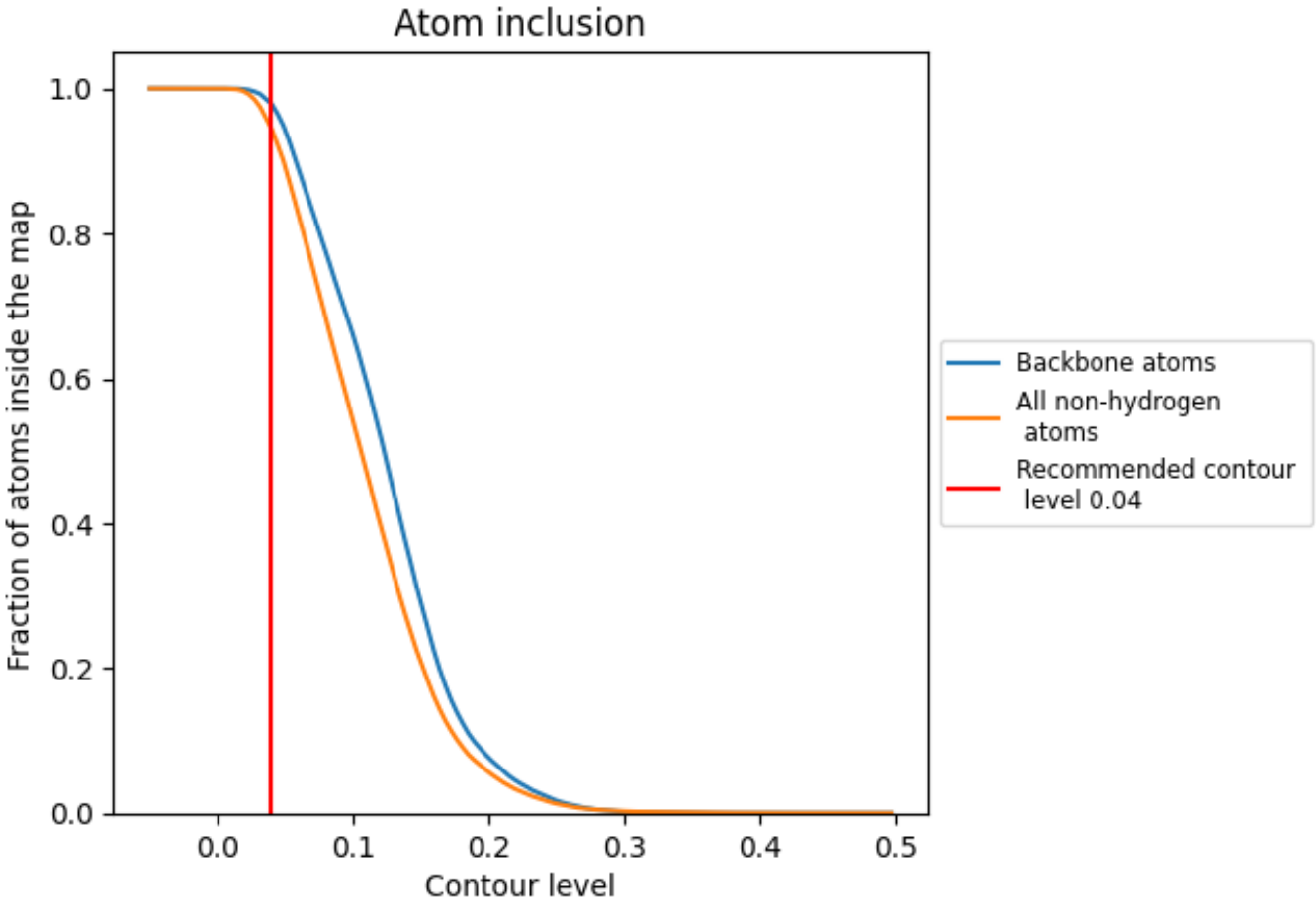
9.3 Atom inclusion mapped to coordinate model



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9447	0.6080
A	0.9264	0.5690
B	0.9540	0.6360
C	0.9591	0.6420
E	0.9226	0.5790
F	0.9410	0.5990
G	0.9657	0.6450
H	0.9208	0.5650
I	0.9482	0.6550
J	0.9386	0.5830
K	0.9745	0.6150
L	0.9108	0.5630
M	0.9450	0.5920
N	0.9527	0.6040