Full wwPDB EM Validation Report ⓘ

Oct 1, 2022 – 10:30 am BST

PDB ID	:	7P7E
EMDB ID	:	EMD-13236
Title	:	Complex I from E. coli, DDM/LMNG-purified, Apo, Resting 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:

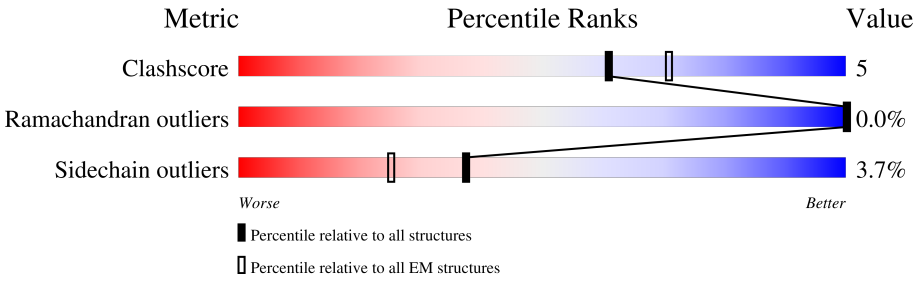
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	442	87% 13%
2	E	156	90% 10%
3	G	905	87% 13%
4	C	600	83% 10% • 6%
5	B	220	61% 13% • 25%
6	I	145	86% 14%
7	H	325	78% 12% • 8%
8	A	147	59% 10% 31%

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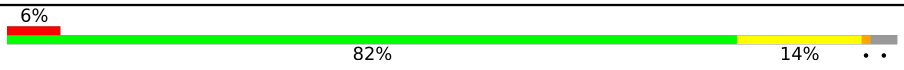
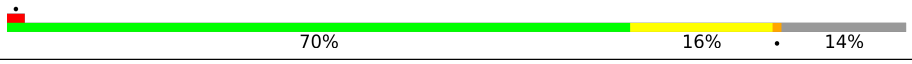
Mol	Chain	Length	Quality of chain
9	L	613	
10	M	504	
11	N	485	
12	K	100	
13	J	184	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 37326 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	442	3432	2177	601	633	21	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	565	4571	2933	795	820	23	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	166	1320	836	228	240	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	145	1149	728	192	217	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	298	Total	C	N	O	S	0	0
			2330	1570	359	383	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	101	Total	C	N	O	S	0	0
			790	544	117	125	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	592	Total	C	N	O	S	0	0
			4508	3003	714	759	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		

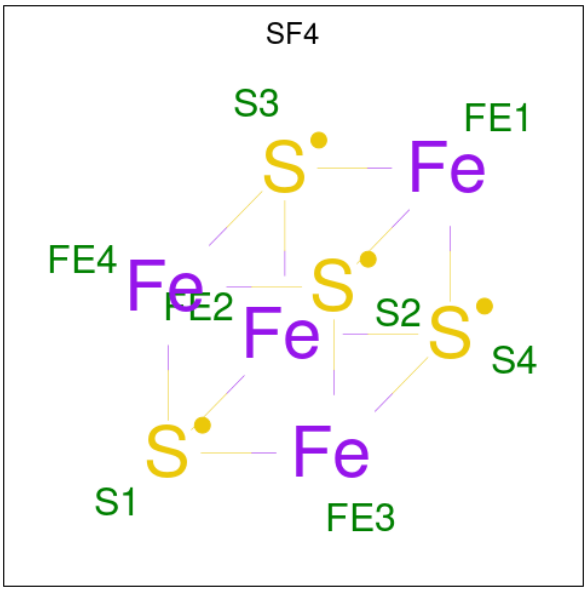
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

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.

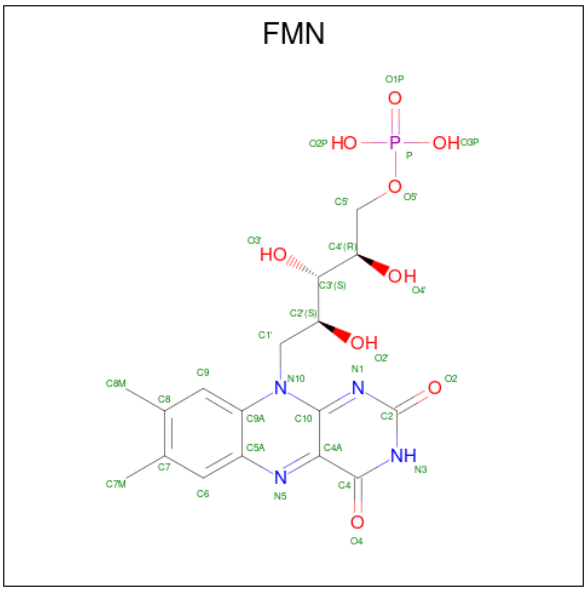
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	158	Total	C	N	O	S	0	0
			1203	812	184	200	7		

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



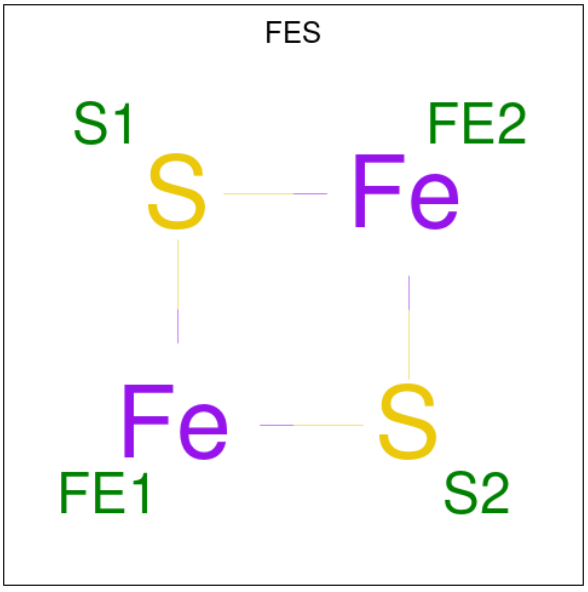
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	B	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 16 8 8	0
14	I	1	Total Fe S 16 8 8	0

- 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).

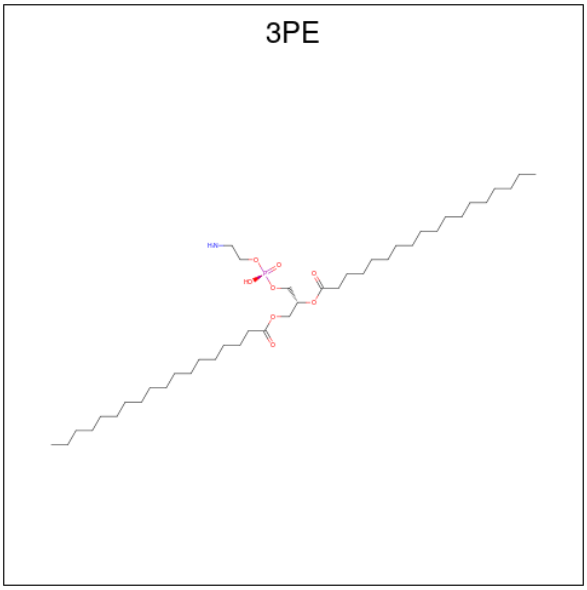


Mol	Chain	Residues	Atoms				AltConf
16	E	1	Total	Fe	S		0
			4	2	2		
16	G	1	Total	Fe	S		0
			4	2	2		

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

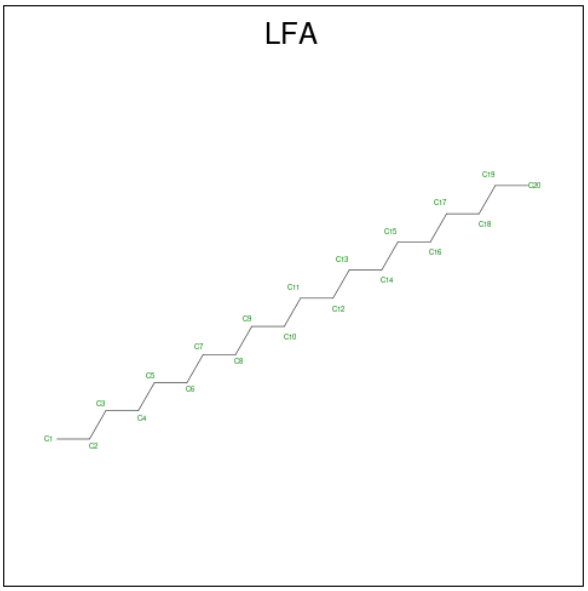
Mol	Chain	Residues	Atoms	AltConf
17	G	1	Total Ca 1 1	0

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total C N O P 51 41 1 8 1	0
18	A	1	Total C N O P 51 41 1 8 1	0
18	L	1	Total C N O P 182 142 4 32 4	0
18	L	1	Total C N O P 182 142 4 32 4	0
18	L	1	Total C N O P 182 142 4 32 4	0
18	L	1	Total C N O P 182 142 4 32 4	0
18	M	1	Total C N O P 153 123 3 24 3	0
18	M	1	Total C N O P 153 123 3 24 3	0
18	M	1	Total C N O P 153 123 3 24 3	0

- Molecule 19 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C 20 20	0
19	N	1	Total C 40 40	0
19	N	1	Total C 40 40	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	AltConf
20	F	83	Total O 83 83	0
20	E	20	Total O 20 20	0
20	G	367	Total O 367 367	0
20	C	122	Total O 122 122	0
20	B	17	Total O 17 17	0
20	I	56	Total O 56 56	0
20	H	23	Total O 23 23	0
20	A	5	Total O 5 5	0
20	L	43	Total O 43 43	0

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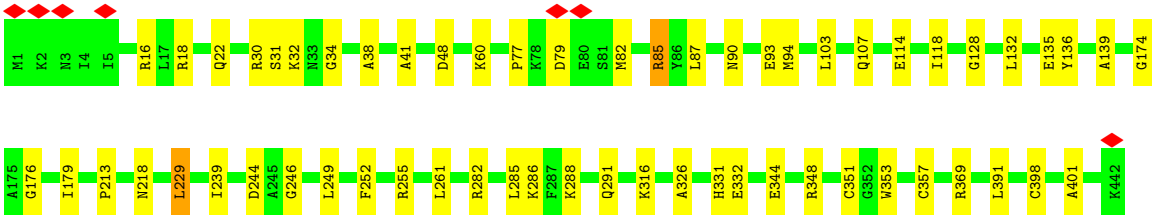
Mol	Chain	Residues	Atoms	AltConf
20	M	47	Total O 47 47	0
20	N	29	Total O 29 29	0
20	K	16	Total O 16 16	0
20	J	9	Total O 9 9	0

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:

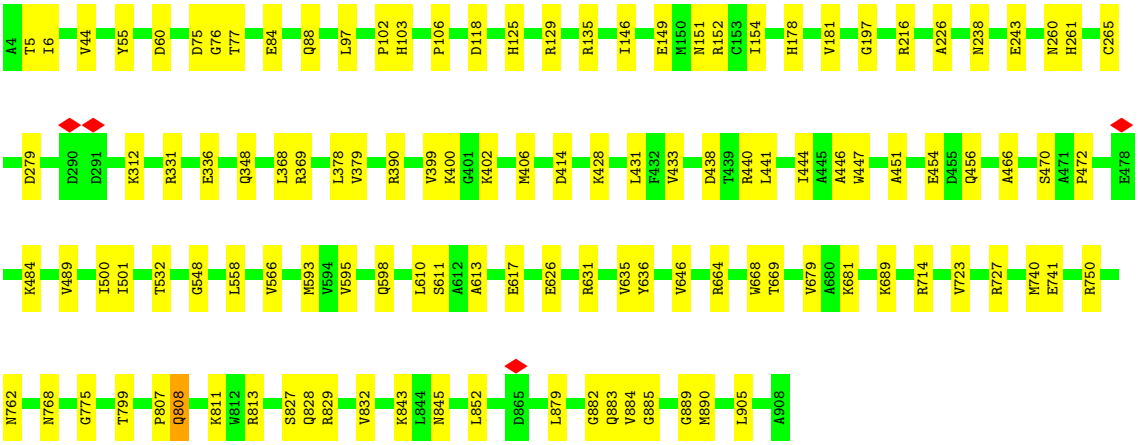


• Molecule 2: NADH dehydrogenase I subunit E

Chain E:

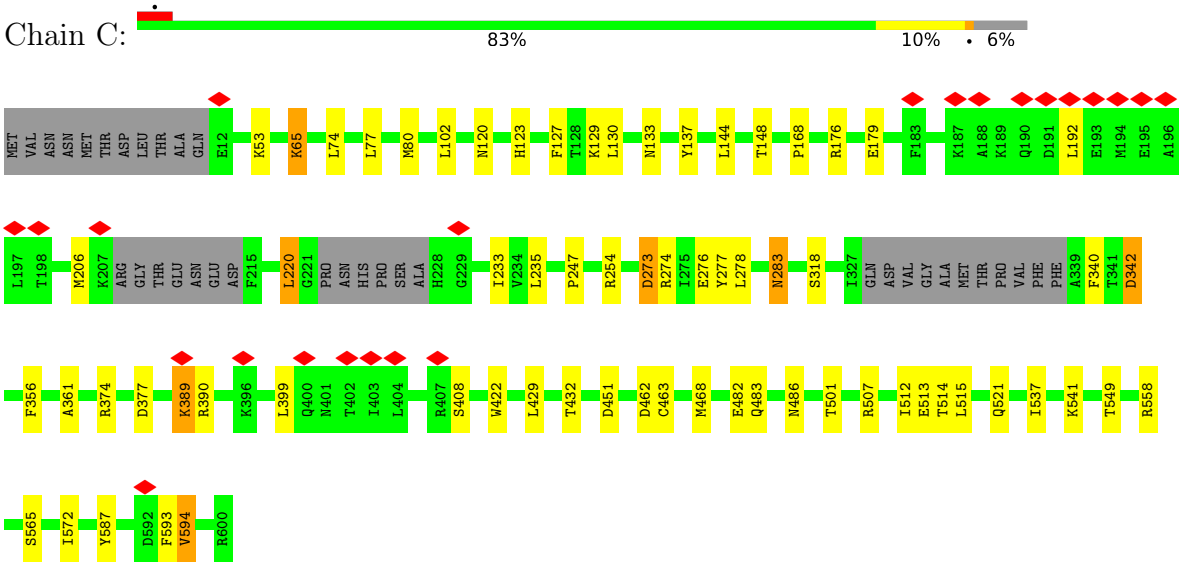
• Molecule 3: NADH-quinone oxidoreductase

Chain G:



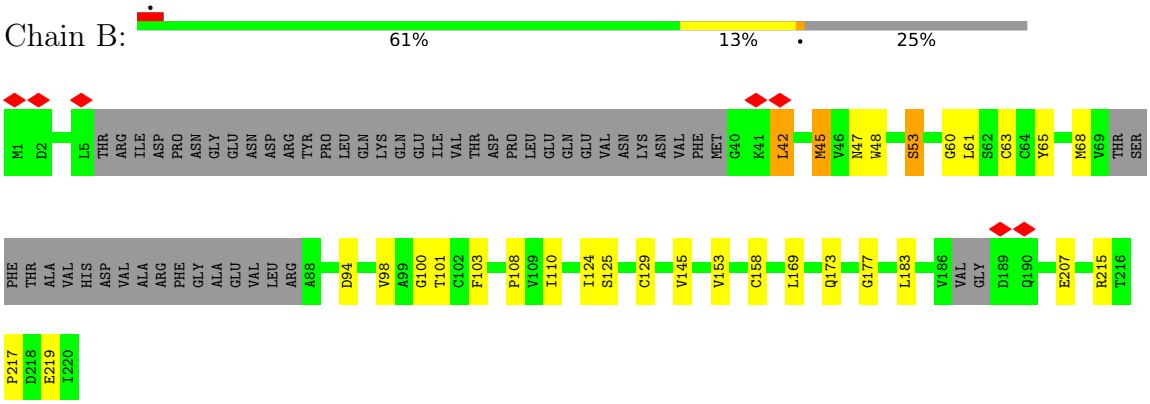
• Molecule 4: NADH-quinone oxidoreductase subunit C/D

Chain C:



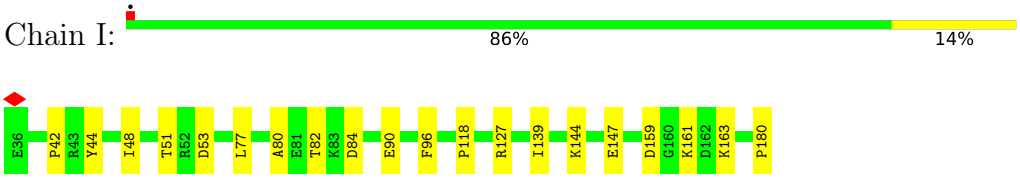
• Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:



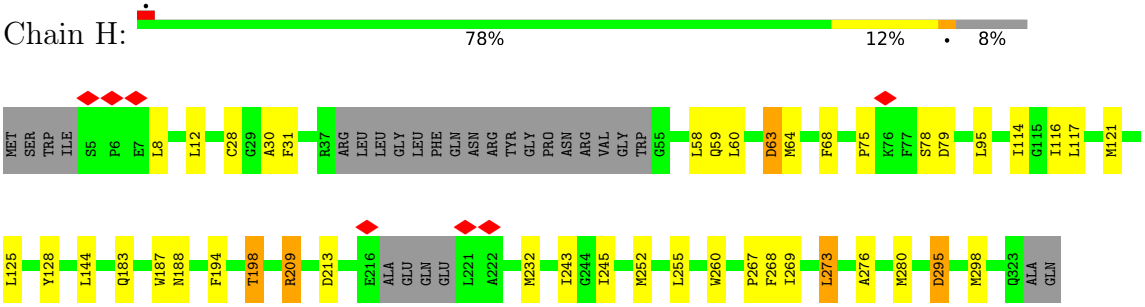
• Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:

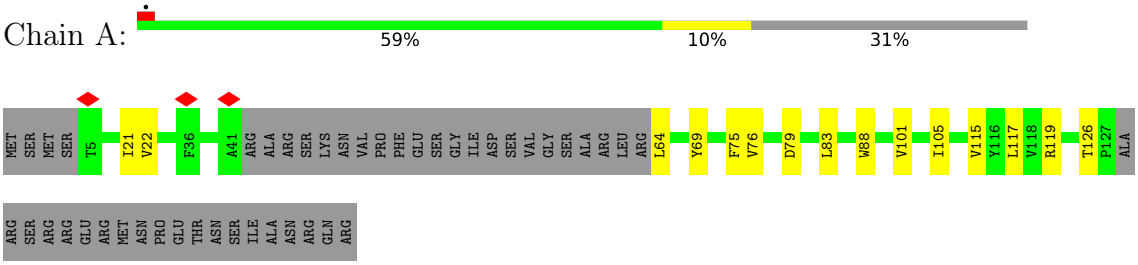


• Molecule 7: NADH-quinone oxidoreductase subunit H

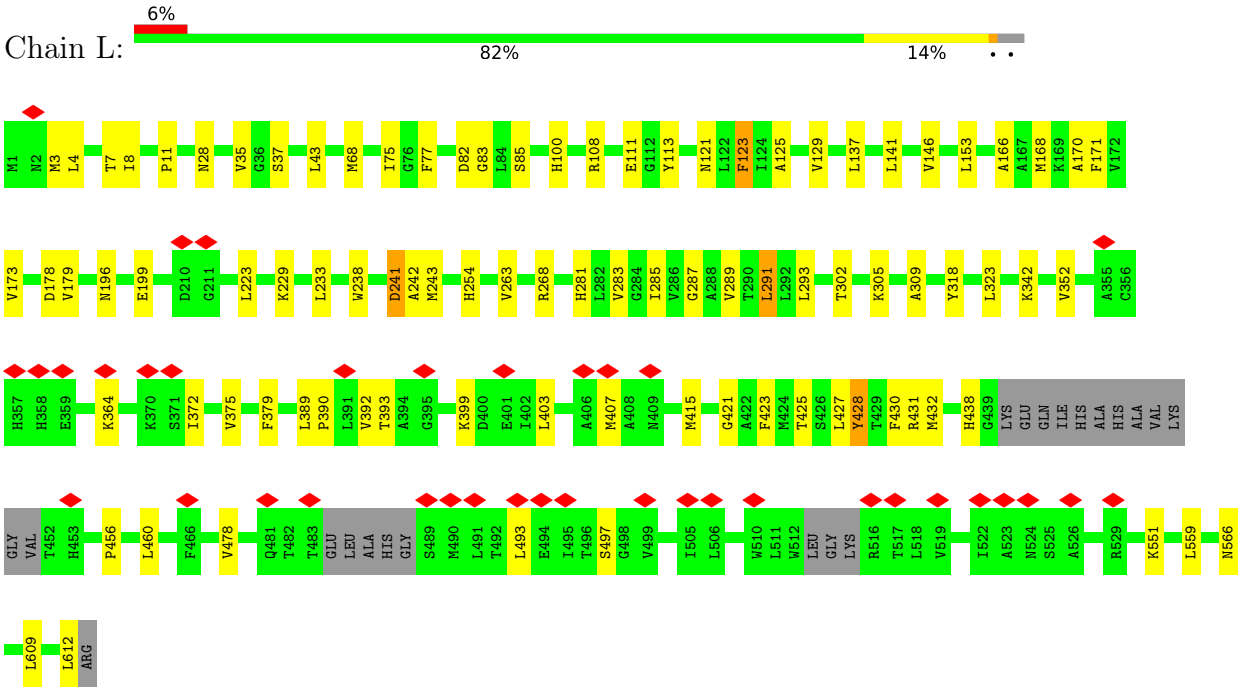
Chain H:



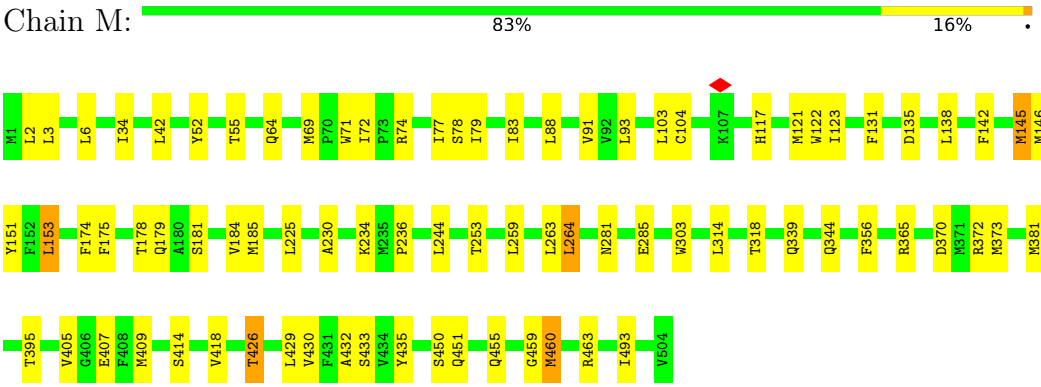
• Molecule 8: NADH-quinone oxidoreductase subunit A



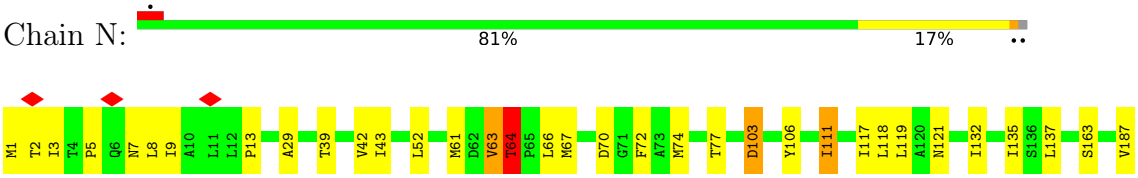
• Molecule 9: Proton-translocating NADH-quinone oxidoreductase, chain L

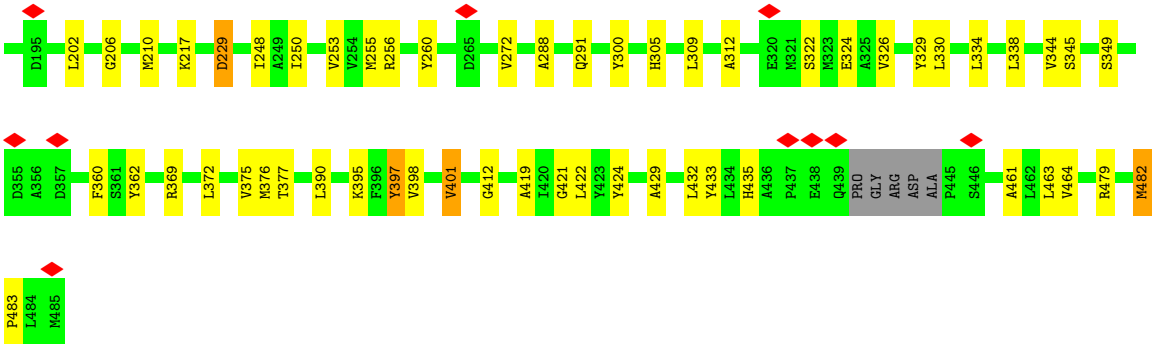


• Molecule 10: NADH dehydrogenase I subunit M



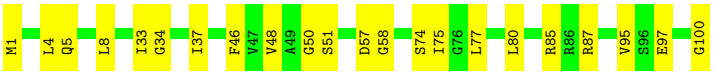
• Molecule 11: NADH-quinone oxidoreductase subunit N





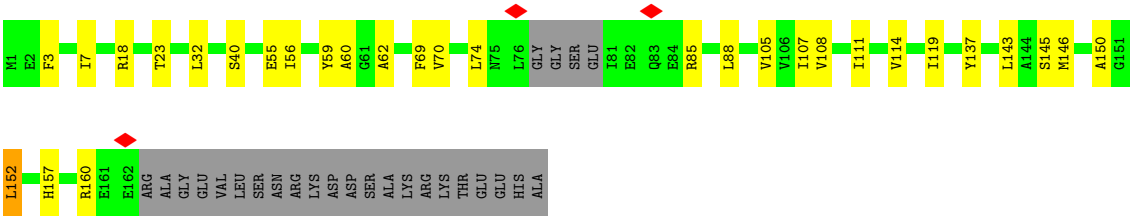
• Molecule 12: NADH-quinone oxidoreductase subunit K

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	199310	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	0.643	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	154.0, 212.5, 238.0	wwPDB
Map dimensions	476, 425, 308	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/3511	0.52	0/4745
2	E	0.29	0/1248	0.53	0/1691
3	G	0.29	0/7173	0.54	1/9726 (0.0%)
4	C	0.27	0/4693	0.52	0/6363
5	B	0.28	0/1347	0.56	0/1819
6	I	0.29	0/1176	0.55	1/1590 (0.1%)
7	H	0.32	0/2397	0.55	2/3260 (0.1%)
8	A	0.33	0/815	0.59	0/1112
9	L	0.29	0/4621	0.53	2/6299 (0.0%)
10	M	0.29	0/4074	0.53	1/5546 (0.0%)
11	N	0.31	0/3727	0.58	3/5085 (0.1%)
12	K	0.29	0/769	0.54	0/1040
13	J	0.30	0/1228	0.55	0/1675
All	All	0.29	0/36779	0.54	10/49951 (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	2
11	N	0	2
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	559	LEU	CA-CB-CG	6.37	129.95	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	279	ASP	CB-CG-OD1	6.33	124.00	118.30
6	I	53	ASP	CB-CG-OD1	6.00	123.70	118.30
7	H	79	ASP	CB-CG-OD1	5.97	123.67	118.30
11	N	8	LEU	CA-CB-CG	5.57	128.11	115.30
9	L	291	LEU	CA-CB-CG	5.53	128.01	115.30
10	M	153	LEU	CA-CB-CG	5.49	127.94	115.30
7	H	273	LEU	CA-CB-CG	5.20	127.26	115.30
11	N	64	THR	N-CA-C	-5.16	97.07	111.00
11	N	111	ILE	CG1-CB-CG2	-5.16	100.06	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	260	ASN	Peptide
3	G	668	TRP	Peptide
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	3432	0	3405	36	0
2	E	1220	0	1187	11	0
3	G	7022	0	6824	59	0
4	C	4571	0	4500	35	0
5	B	1320	0	1308	19	0
6	I	1149	0	1114	11	0
7	H	2330	0	2385	21	0
8	A	790	0	793	10	0
9	L	4508	0	4639	44	0
10	M	3953	0	4053	47	0
11	N	3638	0	3804	51	0
12	K	760	0	817	14	0
13	J	1203	0	1279	21	0
14	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	F	8	0	0	0	0
14	G	24	0	0	0	0
14	I	16	0	0	0	0
15	F	31	0	19	2	0
16	E	4	0	0	0	0
16	G	4	0	0	0	0
17	G	1	0	0	0	0
18	A	51	0	82	2	0
18	H	51	0	82	4	0
18	L	182	0	278	4	0
18	M	153	0	246	2	0
19	A	20	0	42	0	0
19	N	40	0	84	2	0
20	A	5	0	0	0	0
20	B	17	0	0	0	0
20	C	122	0	0	0	0
20	E	20	0	0	0	0
20	F	83	0	0	3	0
20	G	367	0	0	8	0
20	H	23	0	0	0	0
20	I	56	0	0	0	0
20	J	9	0	0	0	0
20	K	16	0	0	0	0
20	L	43	0	0	2	0
20	M	47	0	0	2	0
20	N	29	0	0	2	0
All	All	37326	0	36941	340	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 (340) 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	1.61	1.00
10:M:181:SER:HB2	10:M:230:ALA:HA	1.69	0.74
11:N:375:VAL:HG23	11:N:461:ALA:HB2	1.73	0.69
11:N:64:THR:HB	11:N:66:LEU:H	1.59	0.68
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.76	0.67
11:N:369:ARG:HG3	11:N:372:LEU:HB2	1.79	0.65
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:MET:HB2	2:E:153:LEU:HD11	1.80	0.63
10:M:414:SER:O	10:M:418:VAL:N	2.31	0.62
3:G:845:ASN:ND2	3:G:879:LEU:O	2.32	0.62
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.83	0.61
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.81	0.60
10:M:344:GLN:NE2	20:M:1102:HOH:O	2.33	0.60
4:C:374:ARG:NH2	5:B:219:GLU:OE2	2.34	0.60
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.83	0.59
3:G:5:THR:O	3:G:76:GLY:N	2.35	0.58
3:G:768:ASN:ND2	20:G:1115:HOH:O	2.34	0.58
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.73	0.58
1:F:77:PRO:O	1:F:85:ARG:NH2	2.35	0.58
4:C:342:ASP:OD1	4:C:342:ASP:N	2.34	0.58
9:L:129:VAL:HG11	9:L:141:LEU:HD23	1.84	0.58
4:C:408:SER:HB3	4:C:463:CYS:HB2	1.86	0.58
7:H:183:GLN:NE2	7:H:255:LEU:O	2.37	0.58
4:C:482:GLU:OE2	4:C:486:ASN:ND2	2.37	0.58
2:E:84:VAL:HB	2:E:127:THR:HG21	1.86	0.57
11:N:163:SER:HB3	11:N:217:LYS:HZ1	1.69	0.57
13:J:143:LEU:HA	13:J:146:MET:HB2	1.86	0.57
3:G:723:VAL:HG11	6:I:127:ARG:HB3	1.86	0.57
1:F:135:GLU:HG3	2:E:90:ARG:HH22	1.68	0.57
11:N:412:GLY:HA3	19:N:902:LFA:H81	1.86	0.57
1:F:90:ASN:ND2	15:F:502:FMN:O4'	2.37	0.57
3:G:55:TYR:HB3	3:G:60:ASP:HB3	1.85	0.56
4:C:276:GLU:O	4:C:283:ASN:ND2	2.35	0.56
5:B:61:LEU:HD21	5:B:110:ILE:HD11	1.86	0.56
7:H:209:ARG:HD2	7:H:245:ILE:HD11	1.88	0.56
11:N:376:MET:HG3	11:N:432:LEU:HD11	1.87	0.56
9:L:421:GLY:O	9:L:425:THR:OG1	2.17	0.56
10:M:3:LEU:HA	10:M:6:LEU:HB2	1.87	0.56
7:H:260:TRP:HB2	7:H:267:PRO:HB3	1.86	0.56
12:K:5:GLN:HG2	13:J:111:ILE:HG22	1.88	0.56
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.88	0.55
1:F:348:ARG:HD2	6:I:180:PRO:HB2	1.87	0.55
11:N:334:LEU:O	11:N:338:LEU:HB2	2.07	0.55
13:J:157:HIS:O	13:J:160:ARG:NH1	2.40	0.55
10:M:381:MET:HB2	10:M:385:PRO:HD3	1.89	0.55
1:F:218:ASN:ND2	15:F:502:FMN:O2	2.40	0.55
5:B:101:THR:HA	5:B:129:CYS:HB3	1.89	0.55
7:H:183:GLN:HG2	7:H:187:TRP:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:263:VAL:HG13	9:L:323:LEU:HD11	1.87	0.55
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.88	0.55
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.89	0.54
9:L:37:SER:OG	9:L:121:ASN:OD1	2.25	0.54
3:G:883:GLN:NE2	20:G:1137:HOH:O	2.40	0.54
7:H:95:LEU:HD13	7:H:243:ILE:HD13	1.89	0.54
3:G:118:ASP:OD1	3:G:762:ASN:ND2	2.39	0.54
18:H:401:3PE:H3E1	18:H:401:3PE:H2C1	1.89	0.54
10:M:2:LEU:HD22	10:M:42:LEU:HD21	1.90	0.54
11:N:324:GLU:OE2	11:N:397:TYR:OH	2.25	0.54
2:E:141:PRO:HG2	2:E:153:LEU:HB2	1.90	0.53
11:N:118:LEU:HD22	13:J:143:LEU:HD13	1.88	0.53
1:F:344:GLU:OE2	1:F:369:ARG:NH2	2.40	0.53
18:L:801:3PE:H2I3	18:L:803:3PE:H391	1.90	0.53
5:B:98:VAL:HG11	5:B:145:VAL:HG21	1.90	0.53
10:M:263:LEU:HD11	10:M:356:PHE:HD2	1.73	0.53
12:K:1:MET:N	13:J:119:ILE:O	2.41	0.53
7:H:75:PRO:HB2	7:H:78:SER:HB3	1.90	0.53
10:M:236:PRO:HG3	10:M:244:LEU:HD22	1.89	0.53
1:F:107:GLN:NE2	20:F:607:HOH:O	2.41	0.53
4:C:254:ARG:HG3	5:B:103:PHE:HE1	1.73	0.53
11:N:119:LEU:HD22	11:N:253:VAL:HG11	1.91	0.53
7:H:183:GLN:HE21	7:H:188:ASN:H	1.55	0.53
10:M:72:ILE:HB	10:M:77:ILE:HB	1.91	0.52
10:M:88:LEU:HA	10:M:91:VAL:HG22	1.90	0.52
7:H:114:ILE:HB	7:H:117:LEU:HB2	1.91	0.52
18:H:401:3PE:H3B1	18:A:202:3PE:H3B2	1.90	0.52
10:M:407:GLU:HG2	10:M:429:LEU:HD21	1.91	0.52
1:F:348:ARG:NH2	20:F:608:HOH:O	2.43	0.52
4:C:65:LYS:NZ	4:C:130:LEU:O	2.42	0.51
10:M:370:ASP:OD2	10:M:372:ARG:NH2	2.40	0.51
5:B:53:SER:O	5:B:53:SER:OG	2.29	0.51
11:N:429:ALA:HA	11:N:432:LEU:HD12	1.92	0.51
3:G:741:GLU:OE2	4:C:176:ARG:NH1	2.41	0.51
5:B:217:PRO:HG3	6:I:144:LYS:HD2	1.92	0.51
10:M:234:LYS:NZ	20:M:1106:HOH:O	2.42	0.51
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.93	0.51
12:K:4:LEU:HD12	12:K:48:VAL:HG12	1.92	0.51
3:G:438:ASP:OD1	3:G:438:ASP:N	2.43	0.51
3:G:226:ALA:HB3	3:G:635:VAL:HG22	1.92	0.51
1:F:357:CYS:HB2	1:F:401:ALA:HB2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:85:SER:OG	9:L:268:ARG:NH2	2.44	0.50
3:G:369:ARG:NH2	3:G:775:GLY:O	2.44	0.50
9:L:566:ASN:ND2	20:L:910:HOH:O	2.44	0.50
12:K:33:ILE:HG23	13:J:32:LEU:HD22	1.94	0.50
4:C:220:LEU:HD21	4:C:235:LEU:HD12	1.92	0.50
8:A:101:VAL:O	8:A:105:ILE:HD12	2.12	0.50
11:N:13:PRO:HB2	11:N:117:ILE:HD13	1.94	0.50
7:H:125:LEU:HD13	18:H:401:3PE:H2G1	1.94	0.50
9:L:399:LYS:NZ	20:L:911:HOH:O	2.45	0.50
3:G:125:HIS:ND1	20:G:1101:HOH:O	2.33	0.50
1:F:282:ARG:HB2	1:F:285:LEU:HD12	1.93	0.49
1:F:79:ASP:OD1	1:F:79:ASP:N	2.44	0.49
3:G:400:LYS:NZ	20:G:1159:HOH:O	2.43	0.49
3:G:451:ALA:O	3:G:456:GLN:NE2	2.43	0.49
4:C:233:ILE:HA	4:C:247:PRO:HA	1.95	0.49
8:A:76:VAL:HG22	13:J:62:ALA:HB1	1.95	0.49
1:F:16:ARG:NH1	1:F:32:LYS:O	2.45	0.49
3:G:727:ARG:HD3	4:C:179:GLU:HB2	1.95	0.49
11:N:421:GLY:HA2	11:N:424:TYR:CE2	2.48	0.49
2:E:44:GLN:NE2	2:E:78:GLN:O	2.42	0.49
4:C:277:TYR:CG	5:B:63:CYS:HB3	2.48	0.49
8:A:119:ARG:HG3	11:N:29:ALA:HB1	1.95	0.49
9:L:179:VAL:HG21	10:M:430:VAL:HG23	1.94	0.49
11:N:202:LEU:HD22	13:J:114:VAL:HG11	1.95	0.48
3:G:598:GLN:HB3	3:G:829:ARG:HH21	1.77	0.48
8:A:69:TYR:OH	12:K:74:SER:O	2.29	0.48
9:L:75:ILE:HG21	9:L:137:LEU:HD23	1.95	0.48
9:L:170:ALA:HA	9:L:238:TRP:HB2	1.96	0.48
10:M:405:VAL:O	10:M:409:MET:HB2	2.14	0.48
2:E:123:ASP:OD1	2:E:123:ASP:N	2.41	0.48
3:G:466:ALA:HB3	3:G:489:VAL:HG21	1.95	0.48
9:L:82:ASP:N	9:L:82:ASP:OD1	2.47	0.48
11:N:479:ARG:NH1	20:N:1003:HOH:O	2.46	0.48
3:G:6:ILE:HG22	3:G:77:THR:HB	1.95	0.48
11:N:7:ASN:HD22	11:N:63:VAL:HG22	1.78	0.48
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.95	0.48
7:H:30:ALA:HB1	7:H:60:LEU:HD11	1.95	0.48
1:F:82:MET:O	1:F:85:ARG:NH1	2.47	0.47
1:F:286:LYS:NZ	20:F:610:HOH:O	2.46	0.47
7:H:194:PHE:O	7:H:198:THR:OG1	2.33	0.47
4:C:462:ASP:OD1	4:C:462:ASP:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:60:GLY:HA3	5:B:65:TYR:HB2	1.95	0.47
7:H:276:ALA:O	7:H:280:MET:HG2	2.14	0.47
3:G:399:VAL:HG13	3:G:428:LYS:HB2	1.96	0.47
6:I:161:LYS:HB3	6:I:161:LYS:HE3	1.70	0.47
9:L:196:ASN:HB3	9:L:199:GLU:HB2	1.97	0.47
6:I:80:ALA:HB2	6:I:90:GLU:HB2	1.97	0.47
10:M:451:GLN:O	10:M:455:GLN:NE2	2.47	0.47
11:N:419:ALA:HA	11:N:422:LEU:HD12	1.97	0.47
1:F:348:ARG:NH2	2:E:93:ASP:OD1	2.48	0.47
2:E:105:ILE:HG21	2:E:153:LEU:HD13	1.97	0.47
5:B:61:LEU:HB2	5:B:100:GLY:HA3	1.97	0.47
10:M:451:GLN:OE1	10:M:455:GLN:NE2	2.47	0.47
11:N:312:ALA:HB2	11:N:398:VAL:HG12	1.96	0.47
10:M:314:LEU:O	10:M:318:THR:HG23	2.15	0.47
1:F:132:LEU:O	1:F:174:GLY:N	2.48	0.47
10:M:151:TYR:HB2	10:M:175:PHE:HD2	1.80	0.47
1:F:239:ILE:HD11	1:F:246:GLY:HA2	1.96	0.46
10:M:179:GLN:NE2	20:N:1005:HOH:O	2.35	0.46
12:K:50:GLY:HA3	12:K:58:GLY:HA3	1.97	0.46
3:G:679:VAL:HG11	3:G:689:LYS:HB2	1.96	0.46
4:C:541:LYS:HE2	4:C:594:VAL:HG22	1.97	0.46
9:L:243:MET:HE2	9:L:305:LYS:HB3	1.97	0.46
11:N:187:VAL:HG12	11:N:260:TYR:HB3	1.97	0.46
3:G:402:LYS:O	3:G:406:MET:HG3	2.15	0.46
8:A:117:LEU:HD11	13:J:152:LEU:HD11	1.97	0.46
9:L:281:HIS:O	9:L:285:ILE:HG13	2.15	0.46
9:L:403:LEU:HB3	9:L:493:LEU:HD21	1.98	0.46
10:M:131:PHE:HE2	10:M:264:LEU:HD13	1.81	0.46
13:J:3:PHE:O	13:J:7:ILE:HG13	2.16	0.46
3:G:216:ARG:NH2	20:G:1170:HOH:O	2.46	0.46
7:H:269:ILE:O	7:H:273:LEU:HG	2.16	0.46
10:M:103:LEU:O	10:M:463:ARG:NE	2.40	0.46
3:G:611:SER:OG	3:G:646:VAL:O	2.34	0.46
10:M:123:ILE:HG13	10:M:149:PRO:HB2	1.98	0.46
11:N:229:ASP:OD1	11:N:229:ASP:N	2.48	0.46
2:E:138:ASP:OD1	2:E:138:ASP:N	2.47	0.46
3:G:714:ARG:NH2	20:G:1153:HOH:O	2.42	0.46
6:I:82:THR:OG1	6:I:84:ASP:OD1	2.25	0.46
9:L:456:PRO:O	9:L:460:LEU:HD12	2.16	0.46
10:M:184:VAL:HG13	18:M:1003:3PE:H2B1	1.98	0.46
10:M:365:ARG:HH21	10:M:460:MET:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:77:LEU:HB3	4:C:137:TYR:HB3	1.98	0.46
3:G:261:HIS:CD2	3:G:369:ARG:HD3	2.51	0.45
4:C:74:LEU:HA	4:C:102:LEU:HD23	1.97	0.45
9:L:179:VAL:HG22	10:M:426:THR:HG22	1.97	0.45
3:G:501:ILE:HG12	3:G:532:THR:HB	1.98	0.45
11:N:5:PRO:O	11:N:9:ILE:HG12	2.17	0.45
3:G:431:LEU:O	3:G:446:ALA:N	2.50	0.45
3:G:440:ARG:NH2	20:G:1176:HOH:O	2.48	0.45
5:B:124:ILE:HG12	5:B:153:VAL:HB	1.96	0.45
7:H:121:MET:HG2	13:J:56:ILE:HB	1.99	0.45
8:A:75:PHE:O	8:A:79:ASP:HB2	2.17	0.45
11:N:103:ASP:HA	11:N:106:TYR:HD2	1.80	0.45
13:J:40:SER:HB2	13:J:55:GLU:HB3	1.99	0.45
4:C:549:THR:HB	4:C:558:ARG:HB3	1.99	0.45
1:F:85:ARG:HG2	1:F:213:PRO:HG2	1.98	0.45
3:G:472:PRO:HG3	3:G:799:THR:HA	1.99	0.45
3:G:852:LEU:HD23	3:G:905:LEU:HD12	1.98	0.45
9:L:83:GLY:H	9:L:478:VAL:HG21	1.82	0.45
4:C:565:SER:HB2	4:C:593:PHE:HB2	1.99	0.45
11:N:2:THR:OG1	11:N:3:ILE:N	2.48	0.45
1:F:176:GLY:HA3	2:E:78:GLN:HG2	1.98	0.45
9:L:8:ILE:HG21	18:L:803:3PE:H3G2	1.99	0.45
3:G:102:PRO:HG3	3:G:151:ASN:HB3	1.99	0.45
10:M:365:ARG:NH2	10:M:459:GLY:O	2.50	0.45
3:G:84:GLU:O	3:G:88:GLN:HG3	2.17	0.45
3:G:595:VAL:HG22	3:G:610:LEU:HD12	1.99	0.45
3:G:664:ARG:HE	3:G:664:ARG:HB2	1.68	0.45
10:M:71:TRP:H	10:M:78:SER:HA	1.82	0.45
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.52	0.44
11:N:206:GLY:O	11:N:210:MET:HG3	2.17	0.44
5:B:215:ARG:HB2	6:I:42:PRO:HB3	1.99	0.44
12:K:34:GLY:HA2	12:K:37:ILE:HD12	1.98	0.44
3:G:106:PRO:HD3	4:C:515:LEU:HD21	1.99	0.44
3:G:331:ARG:HH21	3:G:336:GLU:HG3	1.83	0.44
3:G:613:ALA:HB1	3:G:617:GLU:HB2	1.99	0.44
7:H:59:GLN:NE2	7:H:63:ASP:OD1	2.48	0.44
9:L:425:THR:HA	9:L:428:TYR:CE2	2.51	0.44
1:F:60:LYS:NZ	1:F:244:ASP:OD1	2.44	0.44
1:F:87:LEU:O	1:F:128:GLY:HA2	2.17	0.44
3:G:828:GLN:NE2	3:G:889:GLY:O	2.50	0.44
3:G:829:ARG:NH2	20:G:1121:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:35:VAL:HG22	9:L:100:HIS:HB3	1.98	0.44
11:N:322:SER:HA	11:N:401:VAL:HG21	2.00	0.44
3:G:843:LYS:HB2	3:G:885:GLY:HA3	2.00	0.44
10:M:135:ASP:HB3	10:M:138:LEU:HB3	1.98	0.44
10:M:142:PHE:HA	10:M:145:MET:HG3	1.99	0.44
11:N:390:LEU:HB3	11:N:464:VAL:HG23	2.00	0.44
4:C:507:ARG:HB2	4:C:514:THR:HG21	1.99	0.44
10:M:117:HIS:O	10:M:121:MET:HG2	2.18	0.44
12:K:8:LEU:HB3	13:J:111:ILE:HD12	2.00	0.44
11:N:305:HIS:ND1	11:N:329:TYR:OH	2.39	0.43
1:F:291:GLN:O	1:F:326:ALA:HA	2.17	0.43
6:I:48:ILE:HB	6:I:96:PHE:HZ	1.82	0.43
10:M:64:GLN:N	10:M:83:ILE:O	2.51	0.43
4:C:399:LEU:HD22	4:C:468:MET:HG2	2.00	0.43
8:A:115:VAL:O	8:A:119:ARG:HG2	2.19	0.43
9:L:423:PHE:O	9:L:427:LEU:HG	2.18	0.43
3:G:149:GLU:OE2	6:I:163:LYS:NZ	2.42	0.43
4:C:133:ASN:HB3	4:C:422:TRP:HA	1.99	0.43
7:H:144:LEU:HD13	8:A:64:LEU:HD22	2.00	0.43
9:L:254:HIS:HE1	9:L:309:ALA:HA	1.84	0.43
9:L:372:ILE:HD12	9:L:375:VAL:HB	2.00	0.43
4:C:429:LEU:O	4:C:432:THR:OG1	2.29	0.43
3:G:807:PRO:HB3	3:G:882:GLY:HA3	2.00	0.43
10:M:391:PHE:O	10:M:395:THR:HG23	2.19	0.43
12:K:57:ASP:OD2	13:J:137:TYR:OH	2.26	0.43
6:I:44:TYR:HD2	6:I:118:PRO:HA	1.83	0.43
9:L:233:LEU:HD21	9:L:293:LEU:HD12	2.00	0.43
10:M:225:LEU:HD23	10:M:225:LEU:HA	1.86	0.43
1:F:118:ILE:HG21	1:F:229:LEU:HD13	2.00	0.43
10:M:147:LEU:HD11	10:M:178:THR:OG1	2.18	0.43
11:N:137:LEU:HD23	12:K:75:ILE:HD12	2.01	0.43
11:N:463:LEU:HD12	11:N:463:LEU:HA	1.84	0.43
3:G:454:GLU:OE1	3:G:813:ARG:NH2	2.52	0.42
4:C:389:LYS:HD2	4:C:390:ARG:HG2	2.01	0.42
9:L:146:VAL:HG12	9:L:229:LYS:HE3	2.00	0.42
10:M:259:LEU:HD23	10:M:263:LEU:HD12	2.01	0.42
10:M:281:ASN:O	10:M:285:GLU:HG2	2.19	0.42
2:E:98:HIS:HA	2:E:102:TYR:HD1	1.84	0.42
18:L:803:3PE:H291	18:L:803:3PE:H2C2	1.91	0.42
10:M:34:ILE:HD13	10:M:34:ILE:HA	1.88	0.42
11:N:52:LEU:HD23	11:N:52:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:ARG:HE	1:F:22:GLN:HB2	1.83	0.42
1:F:41:ALA:HB2	1:F:229:LEU:HD22	2.02	0.42
4:C:572:ILE:HG12	4:C:587:TYR:HE2	1.84	0.42
8:A:21:ILE:HD12	8:A:22:VAL:HG23	2.01	0.42
9:L:108:ARG:NH2	9:L:113:TYR:OH	2.52	0.42
10:M:52:TYR:CE2	10:M:88:LEU:HD13	2.54	0.42
3:G:558:LEU:HD21	3:G:566:VAL:HB	2.02	0.42
5:B:42:LEU:HA	5:B:45:MET:HB2	2.00	0.42
5:B:48:TRP:HH2	7:H:58:LEU:HB3	1.84	0.42
7:H:295:ASP:OD2	8:A:126:THR:OG1	2.29	0.42
3:G:243:GLU:HG2	3:G:636:TYR:HB3	2.01	0.42
4:C:192:LEU:HD12	5:B:108:PRO:HB2	2.00	0.42
3:G:378:LEU:HD23	3:G:500:ILE:HD12	2.02	0.42
7:H:116:ILE:HD12	7:H:116:ILE:HA	1.76	0.42
1:F:353:TRP:HZ2	3:G:44:VAL:HB	1.84	0.42
11:N:291:GLN:NE2	12:K:100:GLY:O	2.45	0.42
11:N:344:VAL:HA	11:N:360:PHE:CE1	2.55	0.42
13:J:107:ILE:O	13:J:111:ILE:HG12	2.19	0.42
3:G:441:LEU:HD22	3:G:444:ILE:HD11	2.02	0.42
5:B:47:ASN:HB3	5:B:177:GLY:HA2	2.00	0.42
9:L:166:ALA:HB1	9:L:242:ALA:HA	2.01	0.42
9:L:241:ASP:N	9:L:241:ASP:OD1	2.52	0.42
9:L:287:GLY:O	9:L:291:LEU:HB2	2.20	0.42
11:N:330:LEU:HD23	11:N:330:LEU:HA	1.86	0.42
5:B:183:LEU:HD12	5:B:183:LEU:HA	1.89	0.42
6:I:51:THR:HG22	6:I:139:ILE:HD11	2.02	0.42
9:L:178:ASP:N	9:L:178:ASP:OD1	2.53	0.42
3:G:125:HIS:NE2	4:C:513:GLU:OE2	2.44	0.41
10:M:148:VAL:HG11	19:N:901:LFA:H182	2.01	0.41
11:N:7:ASN:HB3	11:N:63:VAL:HG13	2.02	0.41
11:N:377:THR:HG1	11:N:433:TYR:HE2	1.68	0.41
3:G:149:GLU:HG2	3:G:152:ARG:CZ	2.51	0.41
4:C:278:LEU:O	4:C:318:SER:OG	2.37	0.41
11:N:345:SER:O	11:N:349:SER:OG	2.32	0.41
11:N:482:MET:HA	11:N:483:PRO:HD3	1.94	0.41
12:K:77:LEU:HB3	13:J:70:VAL:HG21	2.02	0.41
13:J:105:VAL:HA	13:J:108:VAL:HG22	2.03	0.41
3:G:808:GLN:HG3	3:G:811:LYS:HB2	2.02	0.41
4:C:144:LEU:HA	4:C:168:PRO:HD2	2.03	0.41
4:C:451:ASP:O	4:C:483:GLN:NE2	2.42	0.41
9:L:171:PHE:HE2	10:M:433:SER:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:39:THR:O	11:N:43:ILE:HG13	2.20	0.41
4:C:123:HIS:HA	4:C:148:THR:O	2.20	0.41
9:L:123:PHE:HE1	9:L:146:VAL:HG13	1.85	0.41
12:K:77:LEU:HD22	13:J:70:VAL:HG11	2.02	0.41
1:F:288:LYS:HD2	1:F:331:HIS:HA	2.03	0.41
4:C:501:THR:HG23	4:C:521:GLN:HB3	2.02	0.41
11:N:39:THR:HA	11:N:42:VAL:HG22	2.02	0.41
11:N:288:ALA:HB2	11:N:300:TYR:HB2	2.02	0.41
1:F:30:ARG:HA	1:F:34:GLY:HA3	2.02	0.41
1:F:93:GLU:OE1	1:F:136:TYR:OH	2.30	0.41
3:G:5:THR:H	3:G:75:ASP:HA	1.86	0.41
10:M:339:GLN:HG2	10:M:493:ILE:HG21	2.03	0.41
11:N:132:ILE:O	11:N:135:ILE:HD12	2.21	0.41
12:K:87:ARG:HH22	12:K:95:VAL:HG13	1.86	0.41
3:G:447:TRP:CZ2	3:G:484:LYS:HD3	2.56	0.41
18:H:401:3PE:H351	18:A:202:3PE:H342	2.02	0.41
10:M:185:MET:HB2	10:M:230:ALA:HB2	2.02	0.41
11:N:255:MET:HG3	11:N:326:VAL:HG11	2.02	0.41
1:F:38:ALA:HB2	1:F:114:GLU:HG3	2.02	0.41
1:F:179:ILE:HG12	1:F:351:CYS:HB3	2.03	0.41
1:F:255:ARG:NH2	1:F:332:GLU:OE1	2.54	0.41
3:G:146:ILE:HD11	3:G:197:GLY:HA2	2.03	0.41
4:C:273:ASP:OD2	4:C:361:ALA:N	2.53	0.41
5:B:169:LEU:O	5:B:173:GLN:HG3	2.21	0.41
9:L:28:ASN:OD1	9:L:28:ASN:N	2.53	0.41
10:M:93:LEU:HB3	10:M:264:LEU:HD11	2.03	0.41
13:J:85:ARG:HB3	13:J:88:LEU:HD12	2.02	0.41
1:F:286:LYS:HE2	1:F:331:HIS:HB2	2.01	0.41
9:L:173:VAL:HG22	18:M:1001:3PE:H381	2.02	0.41
9:L:403:LEU:HD23	9:L:403:LEU:HA	1.88	0.41
11:N:70:ASP:O	11:N:74:MET:HG3	2.21	0.41
9:L:289:VAL:O	9:L:293:LEU:HG	2.21	0.40
1:F:391:LEU:HD23	1:F:401:ALA:HB1	2.02	0.40
3:G:103:HIS:HA	4:C:512:ILE:HD13	2.03	0.40
9:L:389:LEU:HA	9:L:390:PRO:HD3	1.96	0.40
3:G:97:LEU:HD22	3:G:154:ILE:HB	2.03	0.40
3:G:348:GLN:NE2	3:G:548:GLY:O	2.44	0.40
3:G:379:VAL:HB	3:G:433:VAL:HG12	2.02	0.40
7:H:128:TYR:OH	13:J:60:ALA:O	2.28	0.40
9:L:4:LEU:O	9:L:7:THR:OG1	2.33	0.40
11:N:360:PHE:CE2	11:N:362:TYR:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:609:LEU:HG	11:N:272:VAL:HG21	2.03	0.40
7:H:213:ASP:OD1	7:H:213:ASP:N	2.48	0.40
9:L:129:VAL:HG21	18:L:801:3PE:H3H2	2.02	0.40
9:L:392:VAL:HG13	9:L:393:THR:HG23	2.03	0.40
10:M:2:LEU:O	10:M:6:LEU:N	2.53	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	440/442 (100%)	432 (98%)	8 (2%)	0	100	100
2	E	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
3	G	903/905 (100%)	873 (97%)	29 (3%)	1 (0%)	51	78
4	C	557/600 (93%)	543 (98%)	14 (2%)	0	100	100
5	B	158/220 (72%)	152 (96%)	6 (4%)	0	100	100
6	I	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
7	H	292/325 (90%)	280 (96%)	12 (4%)	0	100	100
8	A	97/147 (66%)	95 (98%)	2 (2%)	0	100	100
9	L	584/613 (95%)	572 (98%)	12 (2%)	0	100	100
10	M	502/504 (100%)	489 (97%)	13 (3%)	0	100	100
11	N	476/485 (98%)	460 (97%)	15 (3%)	1 (0%)	47	73
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	154/184 (84%)	151 (98%)	3 (2%)	0	100	100
All	All	4558/4826 (94%)	4434 (97%)	122 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	N	64	THR
3	G	669	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	356/356 (100%)	347 (98%)	9 (2%)	47 76
2	E	129/129 (100%)	128 (99%)	1 (1%)	81 93
3	G	732/732 (100%)	712 (97%)	20 (3%)	44 74
4	C	487/519 (94%)	470 (96%)	17 (4%)	36 65
5	B	144/192 (75%)	137 (95%)	7 (5%)	25 52
6	I	124/124 (100%)	121 (98%)	3 (2%)	49 77
7	H	247/269 (92%)	233 (94%)	14 (6%)	20 44
8	A	78/119 (66%)	76 (97%)	2 (3%)	46 75
9	L	466/486 (96%)	441 (95%)	25 (5%)	22 47
10	M	413/413 (100%)	397 (96%)	16 (4%)	32 61
11	N	382/385 (99%)	369 (97%)	13 (3%)	37 66
12	K	79/79 (100%)	74 (94%)	5 (6%)	18 40
13	J	126/146 (86%)	119 (94%)	7 (6%)	21 45
All	All	3763/3949 (95%)	3624 (96%)	139 (4%)	37 63

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	31	SER
1	F	48	ASP
1	F	85	ARG
1	F	94	MET
1	F	103	LEU
1	F	229	LEU
1	F	252	PHE

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Mol	Chain	Res	Type
1	F	316	LYS
1	F	398	CYS
2	E	111	LYS
3	G	129	ARG
3	G	135	ARG
3	G	178	HIS
3	G	181	VAL
3	G	238	ASN
3	G	265	CYS
3	G	312	LYS
3	G	414	ASP
3	G	470	SER
3	G	593	MET
3	G	626	GLU
3	G	631	ARG
3	G	681	LYS
3	G	740	MET
3	G	750	ARG
3	G	808	GLN
3	G	827	SER
3	G	832	VAL
3	G	884	VAL
3	G	890	MET
4	C	53	LYS
4	C	65	LYS
4	C	80	MET
4	C	120	ASN
4	C	127	PHE
4	C	129	LYS
4	C	206	MET
4	C	220	LEU
4	C	273	ASP
4	C	283	ASN
4	C	340	PHE
4	C	342	ASP
4	C	356	PHE
4	C	377	ASP
4	C	389	LYS
4	C	537	ILE
4	C	594	VAL
5	B	42	LEU
5	B	45	MET

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Mol	Chain	Res	Type
5	B	53	SER
5	B	68	MET
5	B	94	ASP
5	B	125	SER
5	B	207	GLU
6	I	77	LEU
6	I	147	GLU
6	I	159	ASP
7	H	8	LEU
7	H	12	LEU
7	H	28	CYS
7	H	31	PHE
7	H	63	ASP
7	H	64	MET
7	H	68	PHE
7	H	198	THR
7	H	209	ARG
7	H	232	MET
7	H	252	MET
7	H	268	PHE
7	H	295	ASP
7	H	298	MET
8	A	83	LEU
8	A	88	TRP
9	L	3	MET
9	L	43	LEU
9	L	68	MET
9	L	77	PHE
9	L	111	GLU
9	L	123	PHE
9	L	153	LEU
9	L	168	MET
9	L	241	ASP
9	L	302	THR
9	L	318	TYR
9	L	342	LYS
9	L	352	VAL
9	L	364	LYS
9	L	379	PHE
9	L	407	MET
9	L	415	MET
9	L	428	TYR

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Mol	Chain	Res	Type
9	L	430	PHE
9	L	431	ARG
9	L	432	MET
9	L	438	HIS
9	L	497	SER
9	L	551	LYS
9	L	612	LEU
10	M	55	THR
10	M	69	MET
10	M	74	ARG
10	M	104	CYS
10	M	122	TRP
10	M	145	MET
10	M	146	MET
10	M	153	LEU
10	M	174	PHE
10	M	253	THR
10	M	264	LEU
10	M	303	TRP
10	M	373	MET
10	M	426	THR
10	M	450	SER
10	M	460	MET
11	N	1	MET
11	N	61	MET
11	N	72	PHE
11	N	103	ASP
11	N	121	ASN
11	N	229	ASP
11	N	256	ARG
11	N	309	LEU
11	N	395	LYS
11	N	397	TYR
11	N	401	VAL
11	N	435	HIS
11	N	482	MET
12	K	46	PHE
12	K	51	SER
12	K	80	LEU
12	K	85	ARG
12	K	97	GLU
13	J	18	ARG

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Mol	Chain	Res	Type
13	J	23	THR
13	J	59	TYR
13	J	69	PHE
13	J	74	LEU
13	J	145	SER
13	J	152	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	845	ASN
7	H	183	GLN
7	H	312	ASN
9	L	163	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	$\#\|Z\|>2$
18	3PE	M	1002	-	50,50,50	0.31	0	53,55,55	0.30	0
14	SF4	G	1001	3	0,12,12	-	-	-		
18	3PE	L	803	-	50,50,50	0.30	0	53,55,55	0.33	0
19	LFA	A	201	-	19,19,19	0.13	0	18,18,18	0.12	0
18	3PE	L	801	-	50,50,50	0.29	0	53,55,55	0.30	0
18	3PE	M	1003	-	50,50,50	0.30	0	53,55,55	0.28	0
19	LFA	N	901	-	19,19,19	0.14	0	18,18,18	0.09	0
18	3PE	H	401	-	50,50,50	0.31	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%)
18	3PE	M	1001	-	50,50,50	0.30	0	53,55,55	0.28	0
14	SF4	G	1003	3	0,12,12	-	-	-		
16	FES	G	1004	3	0,4,4	-	-	-		
16	FES	E	201	2	0,4,4	-	-	-		
18	3PE	L	804	-	50,50,50	0.30	0	53,55,55	0.29	0
19	LFA	N	902	-	19,19,19	0.13	0	18,18,18	0.13	0
14	SF4	I	201	6	0,12,12	-	-	-		
14	SF4	F	501	1	0,12,12	-	-	-		
14	SF4	B	301	5	0,12,12	-	-	-		
18	3PE	L	802	-	28,28,50	0.39	0	31,33,55	0.37	0
18	3PE	A	202	-	50,50,50	0.30	0	53,55,55	0.28	0
14	SF4	G	1002	3	0,12,12	-	-	-		
14	SF4	I	202	6	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	3PE	M	1002	-	-	10/54/54/54	-
14	SF4	G	1001	3	-	-	0/6/5/5
18	3PE	L	803	-	-	13/54/54/54	-
19	LFA	A	201	-	-	3/17/17/17	-
18	3PE	L	801	-	-	11/54/54/54	-
18	3PE	M	1003	-	-	11/54/54/54	-
19	LFA	N	901	-	-	0/17/17/17	-
18	3PE	H	401	-	-	13/54/54/54	-
15	FMN	F	502	-	-	6/18/18/18	0/3/3/3
18	3PE	M	1001	-	-	15/54/54/54	-
14	SF4	G	1003	3	-	-	0/6/5/5
16	FES	G	1004	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	FES	E	201	2	-	-	0/1/1/1
18	3PE	L	804	-	-	9/54/54/54	-
19	LFA	N	902	-	-	0/17/17/17	-
14	SF4	I	201	6	-	-	0/6/5/5
14	SF4	F	501	1	-	-	0/6/5/5
14	SF4	B	301	5	-	-	0/6/5/5
18	3PE	L	802	-	-	8/32/32/54	-
18	3PE	A	202	-	-	12/54/54/54	-
14	SF4	G	1002	3	-	-	0/6/5/5
14	SF4	I	202	6	-	-	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	2.29	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	-3.25	119.63	125.64
15	F	502	FMN	C4A-C10-N10	2.86	120.66	116.48
15	F	502	FMN	C4A-C4-N3	2.69	120.03	113.19
15	F	502	FMN	O4-C4-C4A	-2.52	119.91	126.60
15	F	502	FMN	C4A-C10-N1	-2.37	119.23	124.73
15	F	502	FMN	C10-C4A-N5	-2.27	120.03	124.86

There are no chirality outliers.

All (111) 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
18	H	401	3PE	C1-O11-P-O14
18	H	401	3PE	O13-C11-C12-N
18	A	202	3PE	C1-O11-P-O12
18	A	202	3PE	C1-O11-P-O13
18	A	202	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
18	A	202	3PE	C11-O13-P-O12
18	A	202	3PE	C11-O13-P-O14
18	A	202	3PE	O13-C11-C12-N
18	L	801	3PE	C1-O11-P-O14
18	L	801	3PE	C11-O13-P-O12
18	L	802	3PE	C1-O11-P-O12
18	L	802	3PE	C1-O11-P-O14
18	L	802	3PE	O13-C11-C12-N
18	L	803	3PE	C11-O13-P-O12
18	L	803	3PE	C2-C1-O11-P
18	L	803	3PE	O13-C11-C12-N
18	L	804	3PE	C1-O11-P-O14
18	L	804	3PE	C11-O13-P-O11
18	L	804	3PE	C11-O13-P-O14
18	M	1001	3PE	C1-O11-P-O14
18	M	1001	3PE	C11-O13-P-O12
18	M	1001	3PE	C11-O13-P-O14
18	M	1002	3PE	C11-O13-P-O11
18	M	1002	3PE	C11-O13-P-O14
18	M	1002	3PE	O13-C11-C12-N
18	M	1003	3PE	C11-O13-P-O12
18	M	1003	3PE	O13-C11-C12-N
18	L	804	3PE	O21-C2-C3-O31
18	L	803	3PE	C3C-C3D-C3E-C3F
18	H	401	3PE	C1-O11-P-O13
18	A	202	3PE	C11-O13-P-O11
18	L	801	3PE	C1-O11-P-O13
18	L	802	3PE	C1-O11-P-O13
18	L	802	3PE	C11-O13-P-O11
18	L	803	3PE	C1-O11-P-O13
18	L	803	3PE	C11-O13-P-O11
18	L	804	3PE	C1-O11-P-O13
18	M	1001	3PE	C1-O11-P-O13
18	M	1001	3PE	C11-O13-P-O11
18	M	1002	3PE	C1-O11-P-O13
18	M	1003	3PE	C11-O13-P-O11
18	L	801	3PE	C2C-C2D-C2E-C2F
18	M	1003	3PE	C3E-C3F-C3G-C3H
18	L	802	3PE	C35-C36-C37-C38
18	M	1001	3PE	O13-C11-C12-N
18	M	1003	3PE	C3C-C3D-C3E-C3F
18	L	804	3PE	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
18	M	1002	3PE	C24-C25-C26-C27
18	A	202	3PE	C21-C22-C23-C24
18	L	801	3PE	C37-C38-C39-C3A
18	L	801	3PE	C23-C24-C25-C26
15	F	502	FMN	C5'-O5'-P-O1P
18	M	1001	3PE	O21-C2-C3-O31
18	M	1002	3PE	C2-C1-O11-P
18	L	804	3PE	C1-C2-C3-O31
18	L	803	3PE	C3D-C3E-C3F-C3G
18	M	1003	3PE	C2-C1-O11-P
18	L	803	3PE	C35-C36-C37-C38
18	M	1003	3PE	C2E-C2F-C2G-C2H
18	A	202	3PE	O21-C21-C22-C23
18	A	202	3PE	C23-C24-C25-C26
18	M	1001	3PE	O31-C31-C32-C33
19	A	201	LFA	C12-C13-C14-C15
18	L	801	3PE	C11-O13-P-O11
18	A	202	3PE	C2-C1-O11-P
18	H	401	3PE	C1-O11-P-O12
18	L	801	3PE	C1-O11-P-O12
18	L	801	3PE	C11-O13-P-O14
18	L	802	3PE	C11-O13-P-O12
18	L	803	3PE	C1-O11-P-O14
18	L	804	3PE	C1-O11-P-O12
18	M	1001	3PE	C1-O11-P-O12
18	M	1002	3PE	C1-O11-P-O14
18	H	401	3PE	C21-C22-C23-C24
18	M	1001	3PE	C1-C2-C3-O31
18	M	1002	3PE	C3C-C3D-C3E-C3F
18	L	801	3PE	C25-C26-C27-C28
15	F	502	FMN	C4'-C5'-O5'-P
18	M	1002	3PE	C3B-C3C-C3D-C3E
18	M	1003	3PE	C26-C27-C28-C29
18	M	1001	3PE	C39-C3A-C3B-C3C
18	M	1003	3PE	C31-C32-C33-C34
19	A	201	LFA	C11-C12-C13-C14
18	M	1001	3PE	C3A-C3B-C3C-C3D
18	H	401	3PE	C2E-C2F-C2G-C2H
18	L	804	3PE	C25-C26-C27-C28
18	L	801	3PE	C34-C35-C36-C37
18	L	803	3PE	C32-C33-C34-C35
18	M	1003	3PE	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
18	L	803	3PE	C37-C38-C39-C3A
18	M	1003	3PE	C1-O11-P-O13
18	H	401	3PE	C26-C27-C28-C29
18	L	803	3PE	O21-C21-C22-C23
18	H	401	3PE	C33-C34-C35-C36
18	L	802	3PE	O31-C31-C32-C33
18	H	401	3PE	C34-C35-C36-C37
18	L	803	3PE	O22-C21-C22-C23
18	H	401	3PE	C3C-C3D-C3E-C3F
18	H	401	3PE	C28-C29-C2A-C2B
18	A	202	3PE	O22-C21-C22-C23
18	H	401	3PE	C12-C11-O13-P
18	M	1001	3PE	C12-C11-O13-P
18	M	1002	3PE	C12-C11-O13-P
18	M	1001	3PE	O21-C21-C22-C23
18	H	401	3PE	C2F-C2G-C2H-C2I
19	A	201	LFA	C13-C14-C15-C16
18	M	1001	3PE	O22-C21-C22-C23

There are no ring outliers.

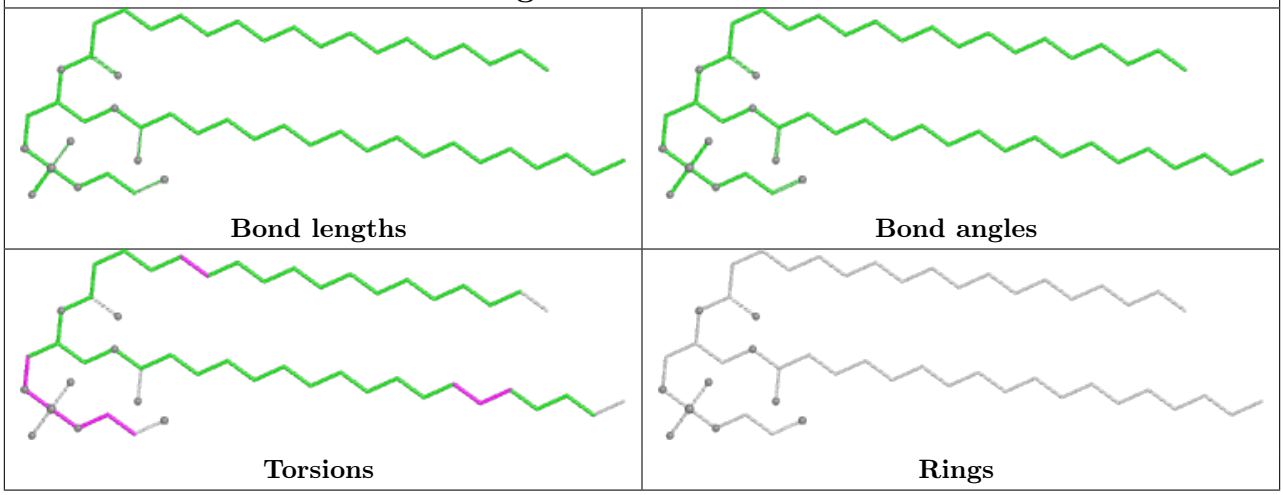
9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	803	3PE	3	0
18	L	801	3PE	2	0
18	M	1003	3PE	1	0
19	N	901	LFA	1	0
18	H	401	3PE	4	0
15	F	502	FMN	2	0
18	M	1001	3PE	1	0
19	N	902	LFA	1	0
18	A	202	3PE	2	0

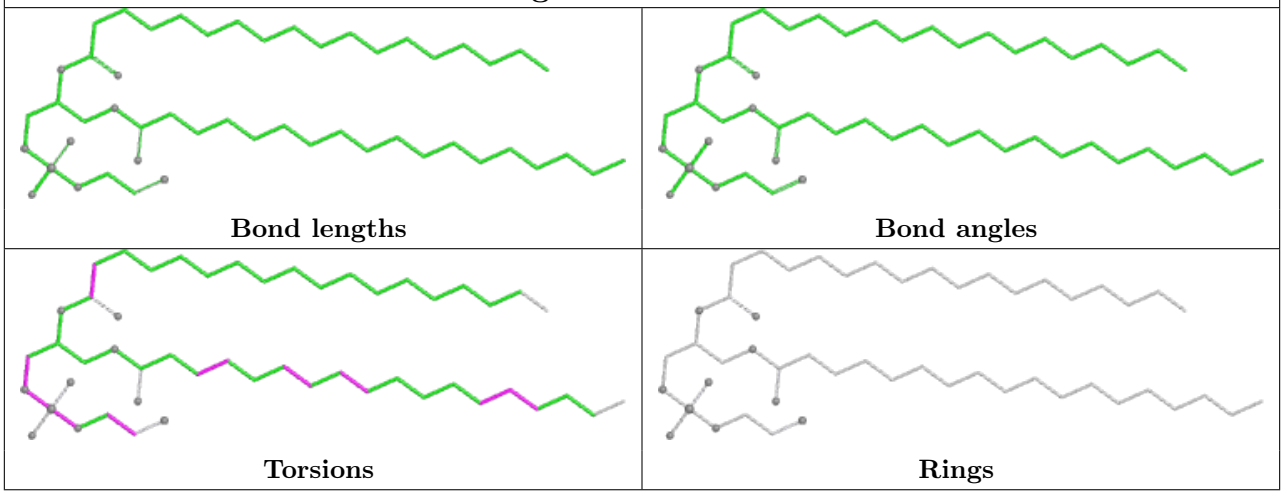
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

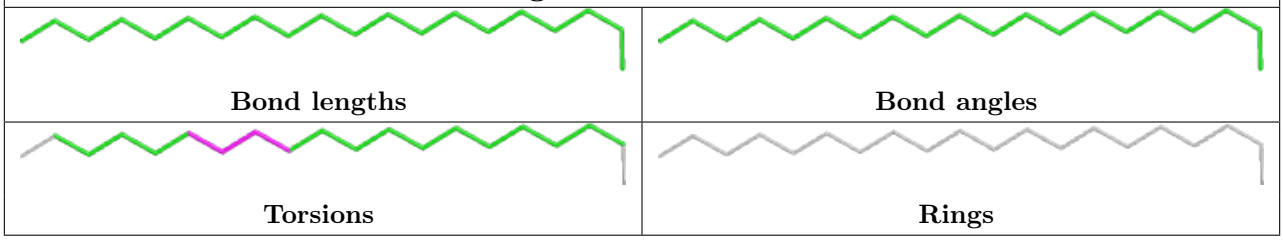
Ligand 3PE M 1002

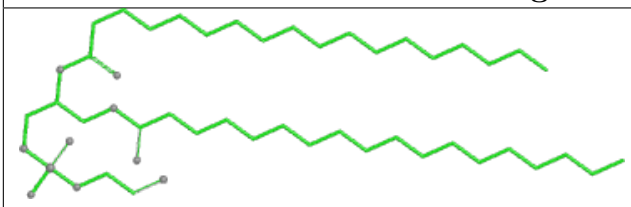
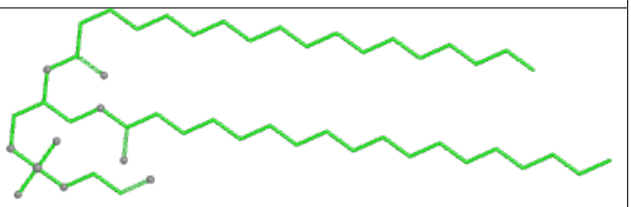
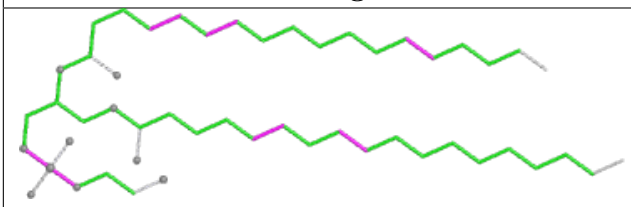
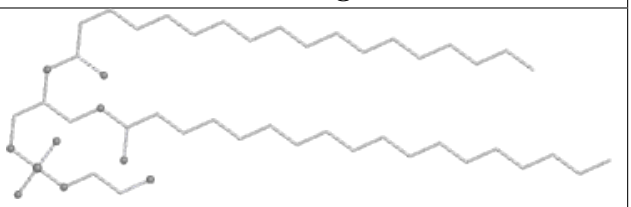


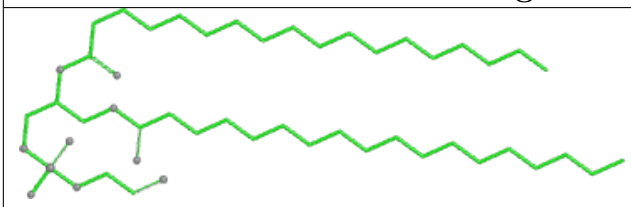
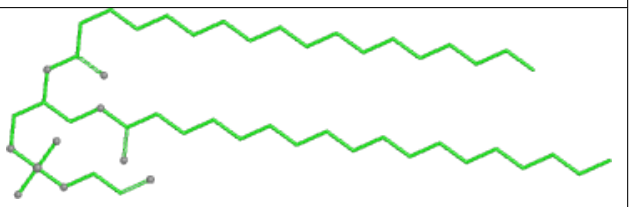
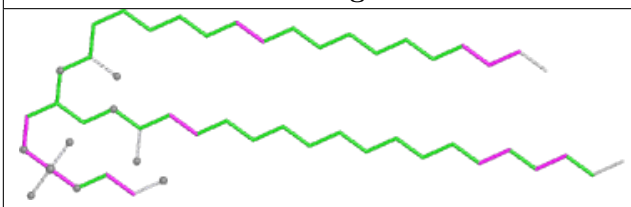
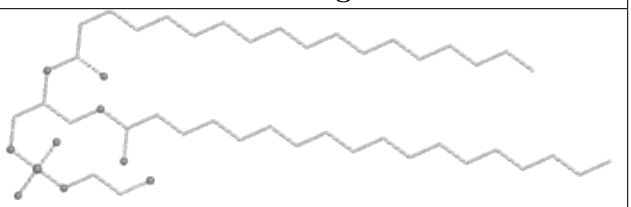
Ligand 3PE L 803

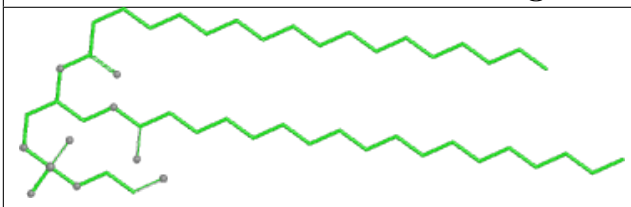
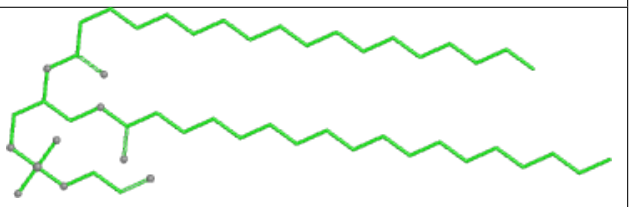
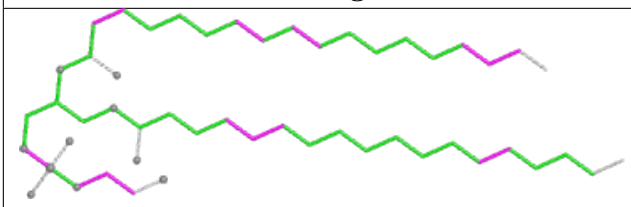
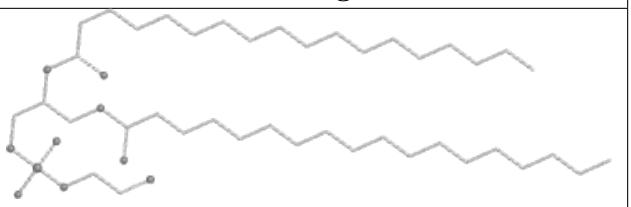


Ligand LFA A 201

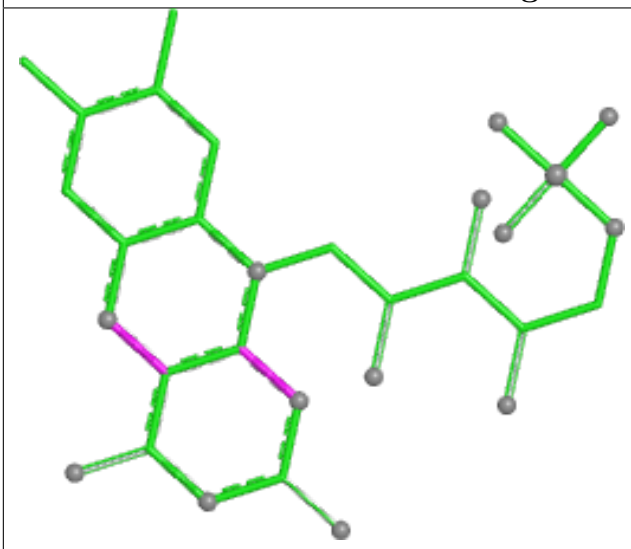


Ligand 3PE L 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

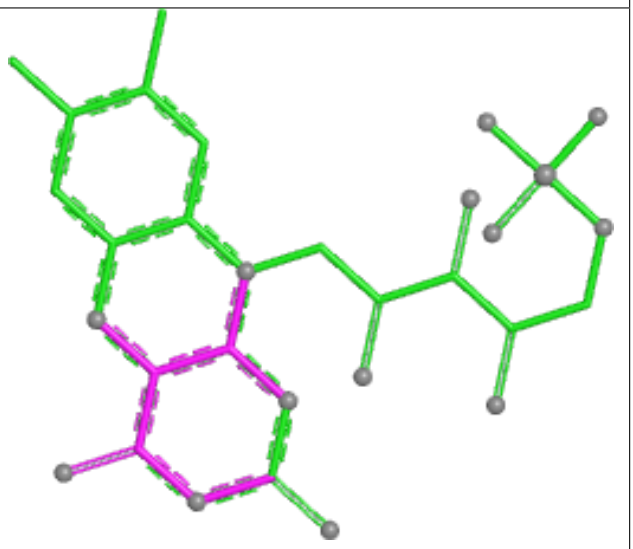
Ligand 3PE M 1003	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE H 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

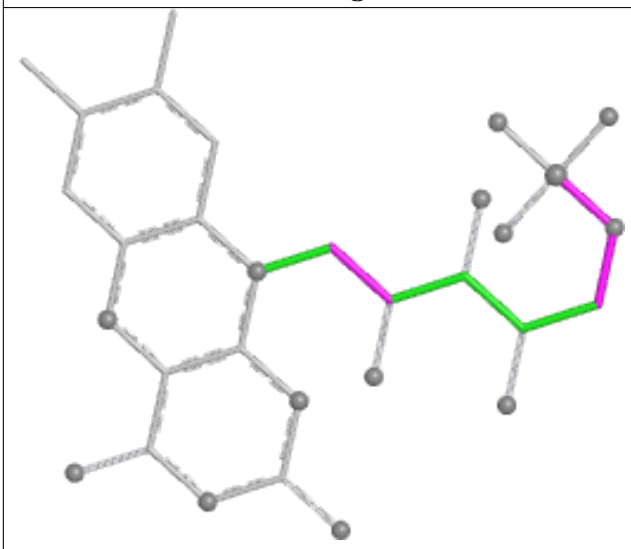
Ligand FMN F 502



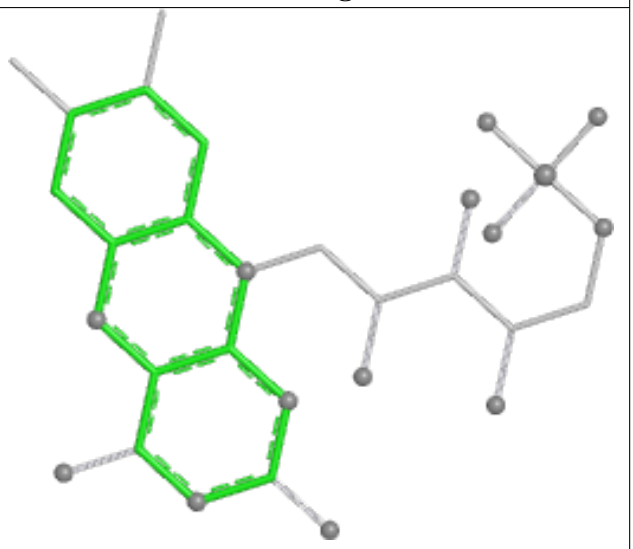
Bond lengths



Bond angles

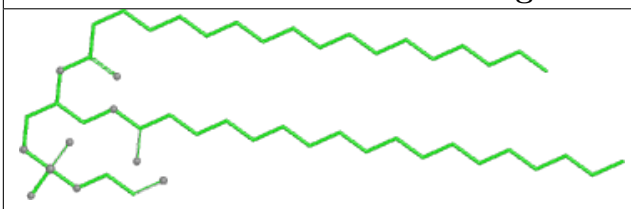


Torsions

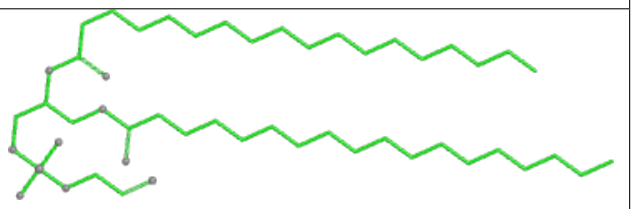


Rings

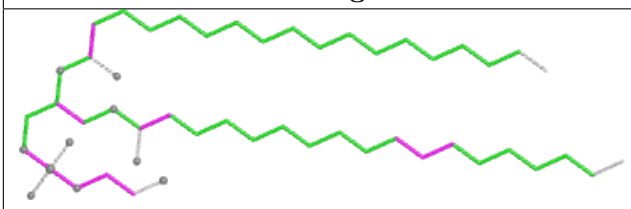
Ligand 3PE M 1001



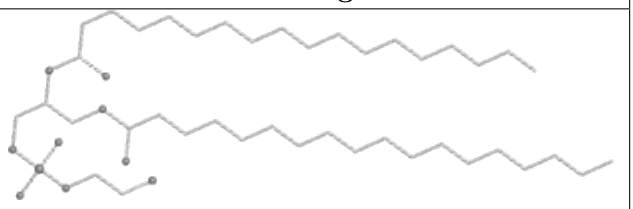
Bond lengths



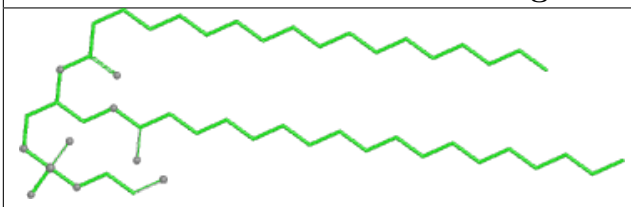
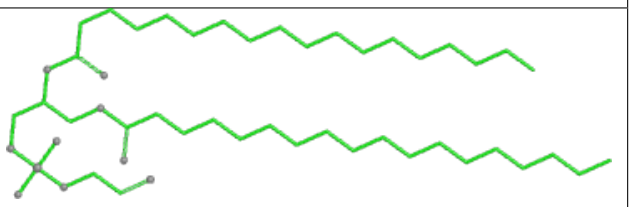
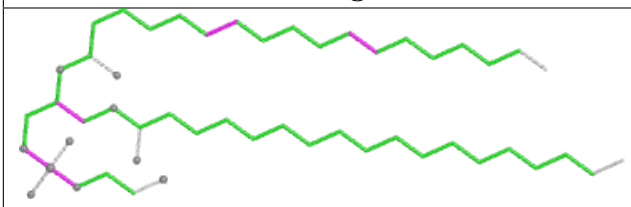
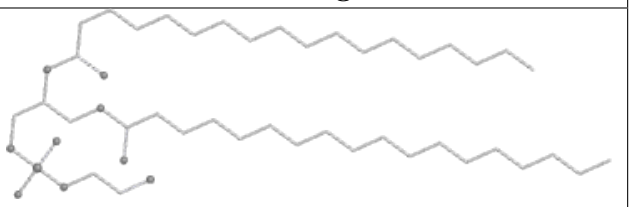
Bond angles

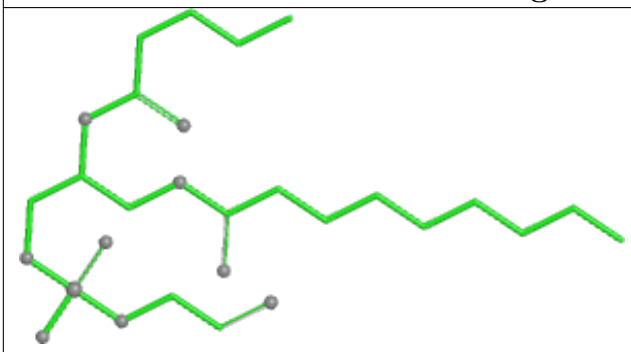
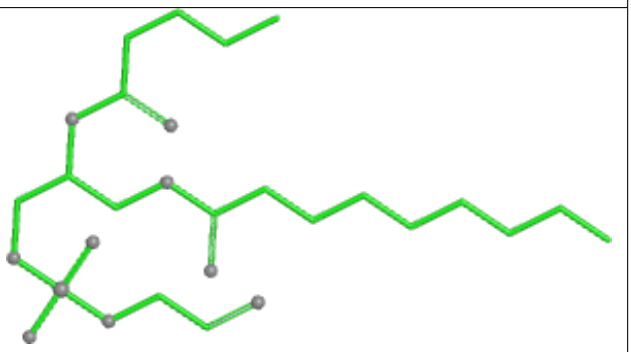
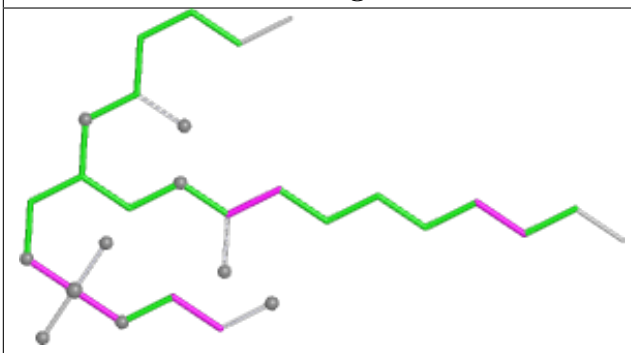
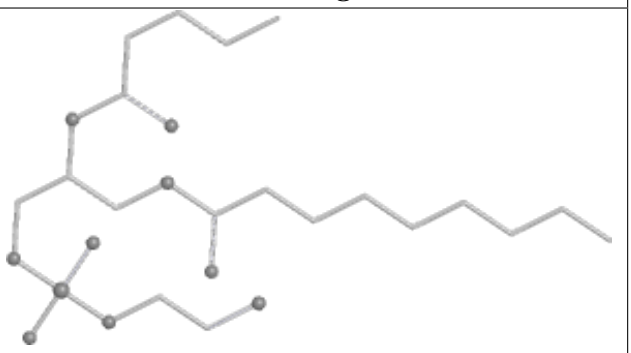


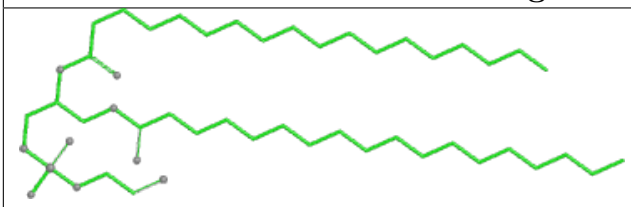
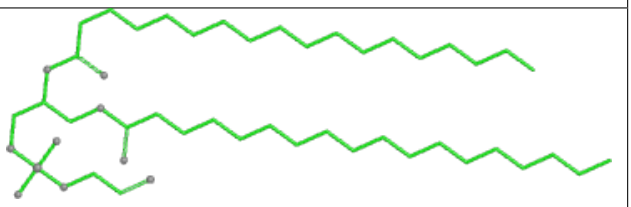
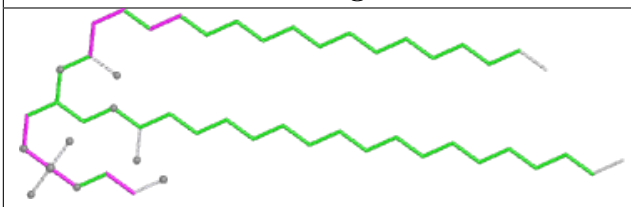
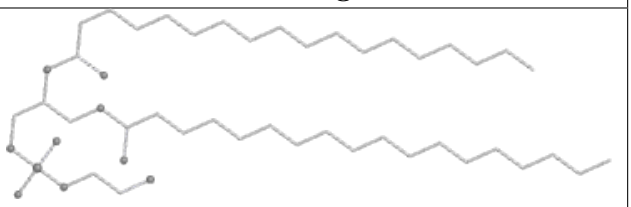
Torsions



Rings

Ligand 3PE L 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE A 202	
 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.

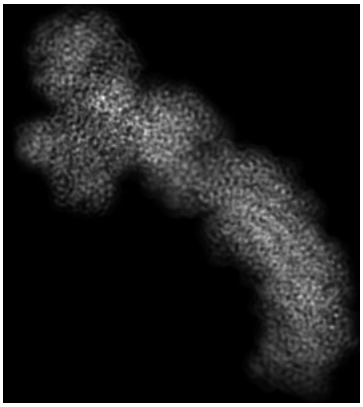
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13236. These allow visual inspection of the internal detail of the map and identification of artifacts.

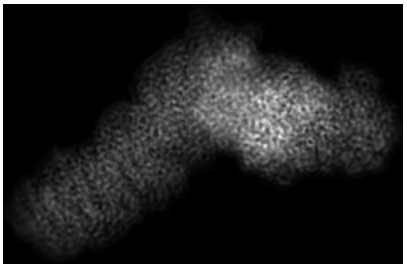
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

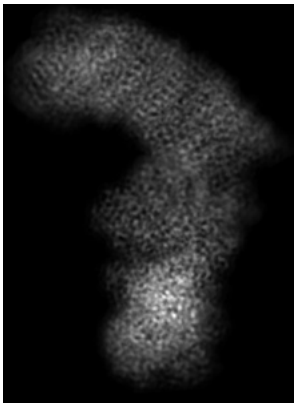
6.1.1 Primary map



X



Y

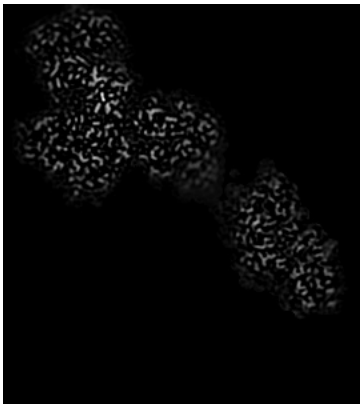


Z

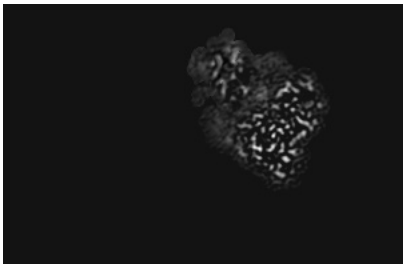
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 154



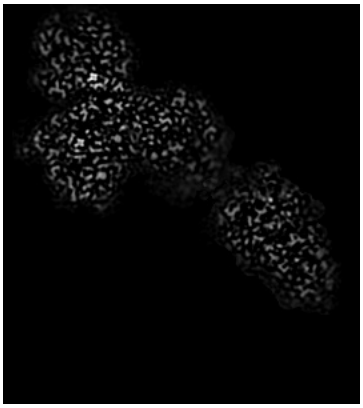
Y Index: 212

Z Index: 238

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: 166

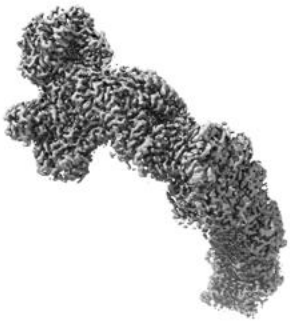
Y Index: 112

Z Index: 311

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

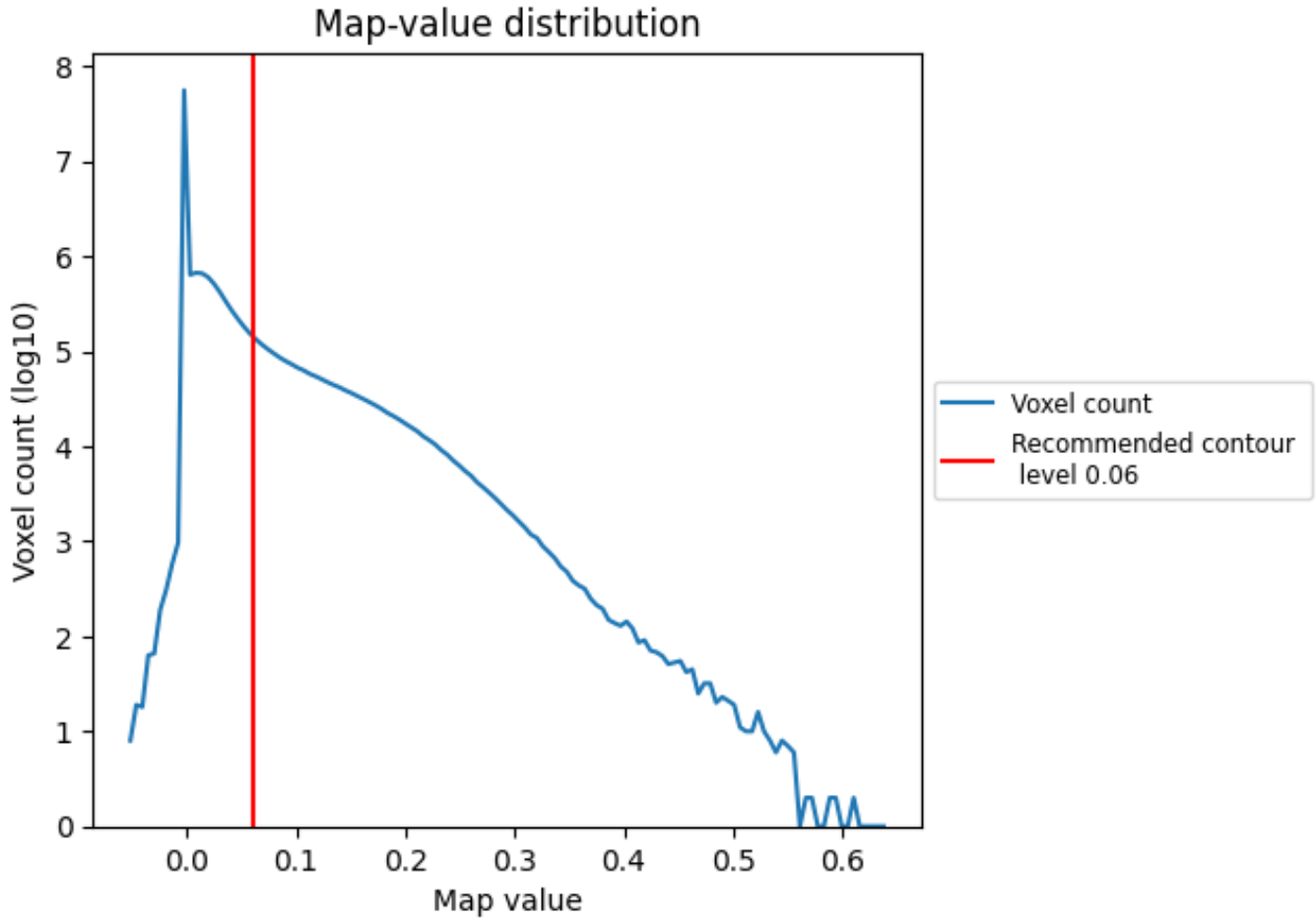
6.5 Mask visualisation (i)

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

7 Map analysis

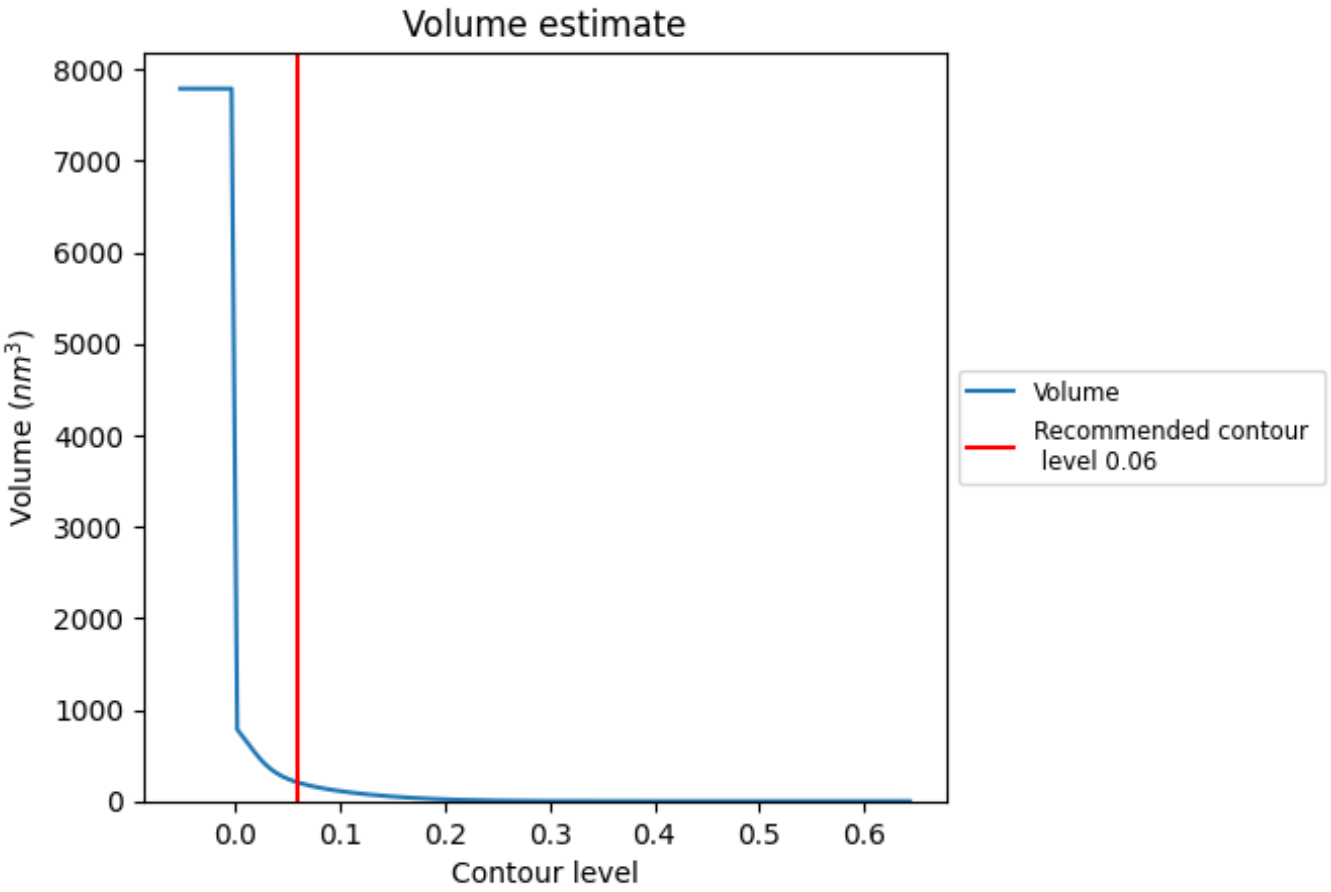
This section contains the results of statistical analysis of the map.

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 205 nm^3; this corresponds to an approximate mass of 186 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.

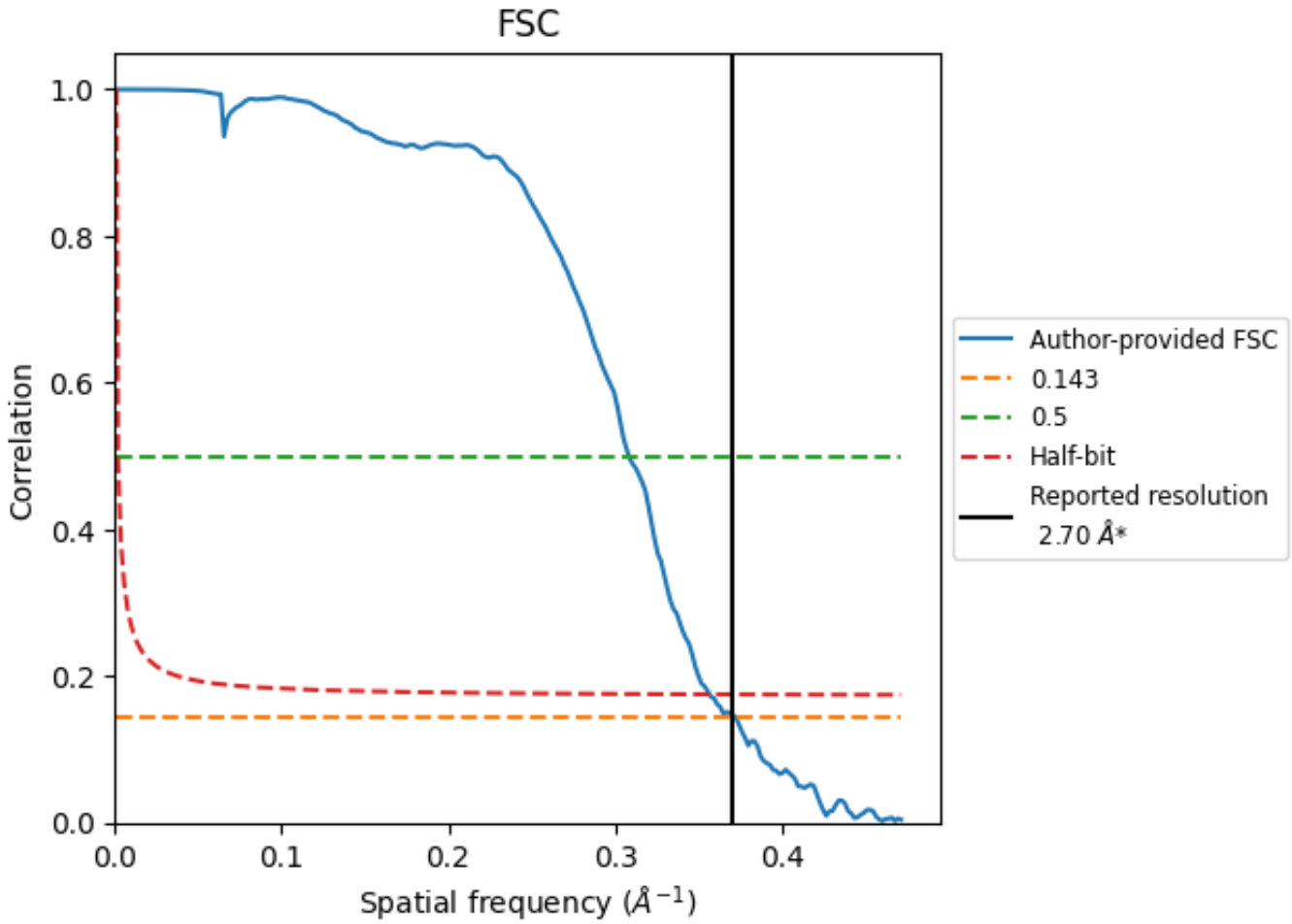
7.3 Rotationally averaged power spectrum

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)

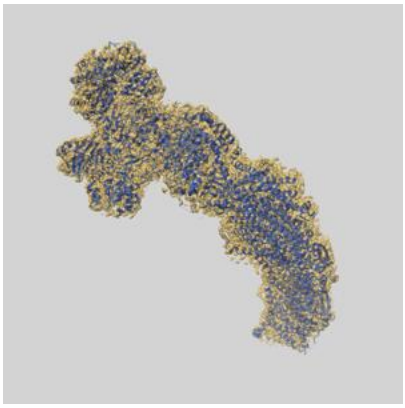
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	3.24	2.80
Unmasked-calculated*	-	-	-

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

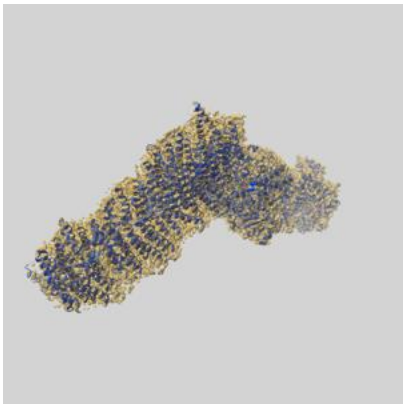
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13236 and PDB model 7P7E. Per-residue inclusion information can be found in section 3 on page 11.

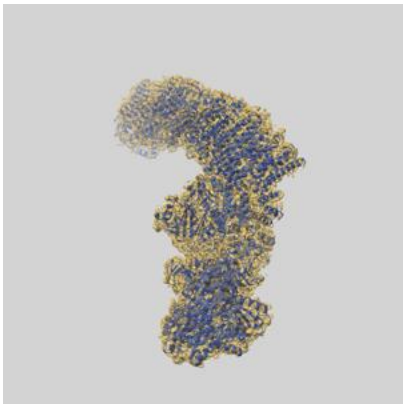
9.1 Map-model overlay



X



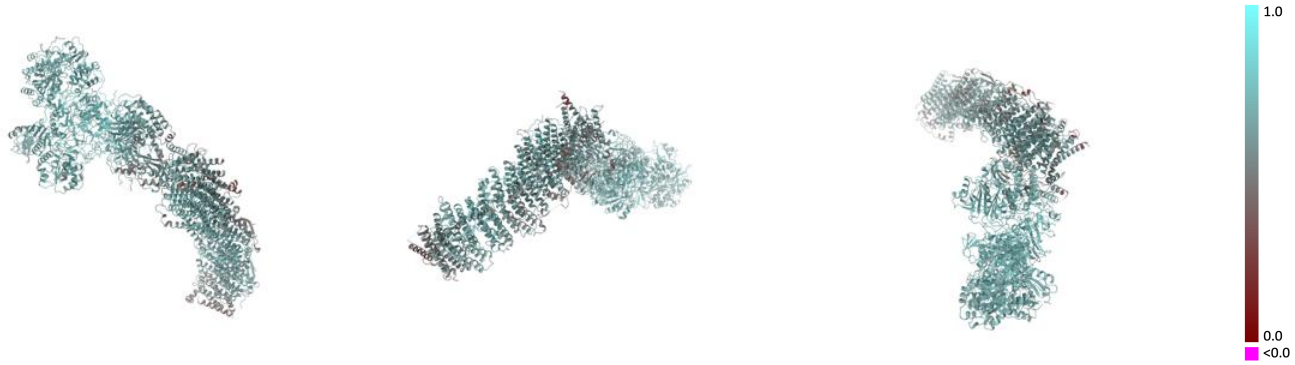
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

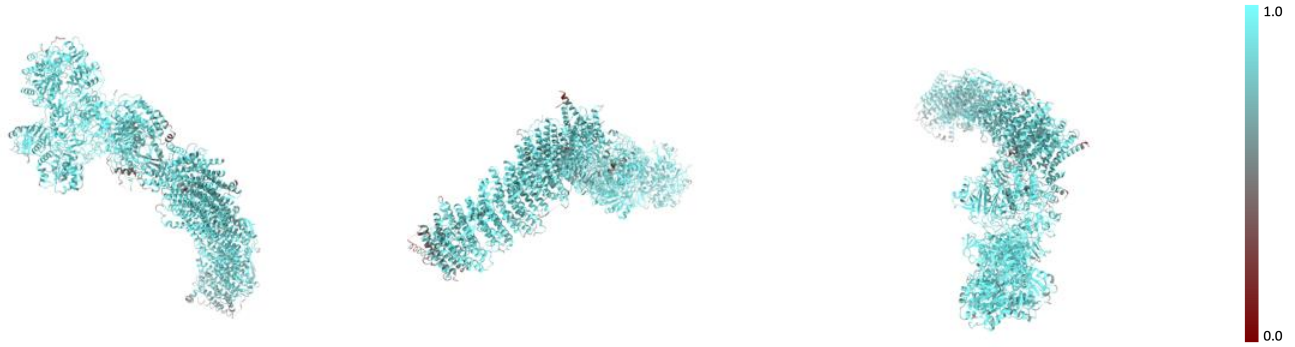
9.2 Q-score mapped to coordinate model



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.

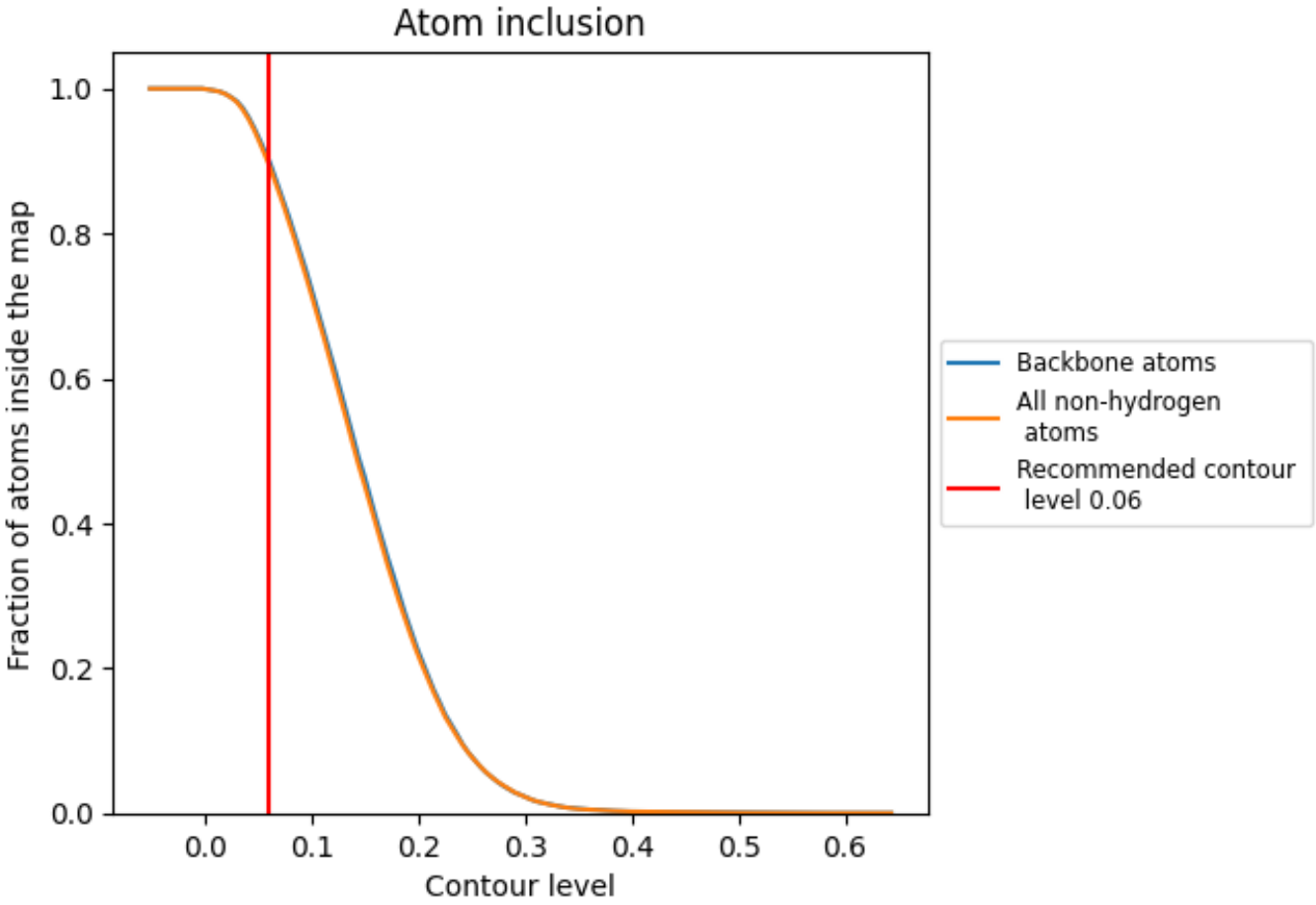
9.3 Atom inclusion mapped to coordinate model



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8935	0.6400
A	0.8477	0.5620
B	0.8575	0.6170
C	0.8974	0.6640
E	0.9160	0.6660
F	0.9179	0.6680
G	0.9439	0.6950
H	0.8574	0.5730
I	0.9454	0.7090
J	0.8991	0.6250
K	0.9651	0.6880
L	0.8084	0.5770
M	0.9053	0.6200
N	0.8945	0.6100