Full wwPDB EM Validation Report ⓘ

Sep 26, 2022 – 11:20 pm BST

PDB ID	:	7Z7S
EMDB ID	:	EMD-14536
Title	:	Complex I from E. coli, LMNG-purified, under Turnover at pH 6, Closed state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2022-03-16
Resolution	:	2.40 Å(reported)
Based on initial models	:	4HEA, 3RKO

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:

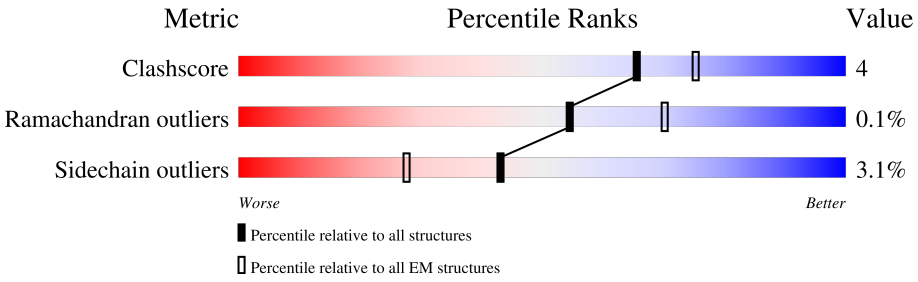
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	445	89% 10% •
2	E	166	86% 8% 6%
3	G	908	87% 12% •
4	C	596	89% 10% •
5	B	220	83% 14% •
6	I	180	88% 11% •
7	H	325	• 84% 14% ••
8	A	147	77% 10% • 11%

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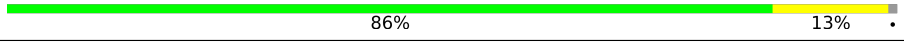
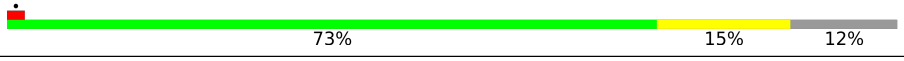
Mol	Chain	Length	Quality of chain
9	L	613	
10	M	509	
11	N	485	
12	K	100	
13	J	184	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 39208 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	7017	4388	1268	1324	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	589	4760	3049	828	859	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	213	1693	1070	295	312	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	322	Total	C	N	O	S	0	0
			2534	1702	398	416	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	131	Total	C	N	O	S	0	0
			1037	688	177	167	5		

- Molecule 9 is a protein called NADH dehydrogenase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	598	Total	C	N	O	S	0	0
			4558	3036	726	764	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	475	Total	C	N	O	S	0	0
			3601	2407	568	606	20		

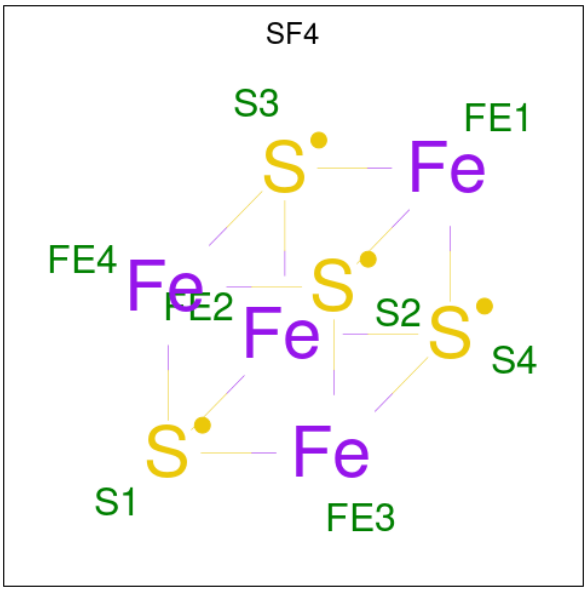
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

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.

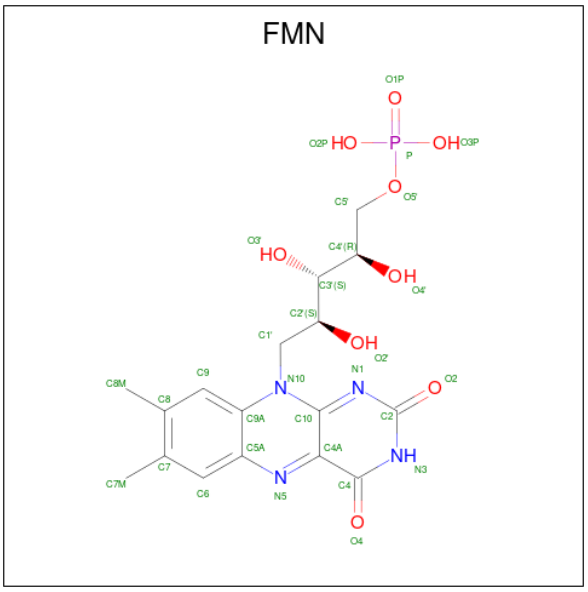
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	162	Total	C	N	O	S	0	0
			1226	824	188	207	7		

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



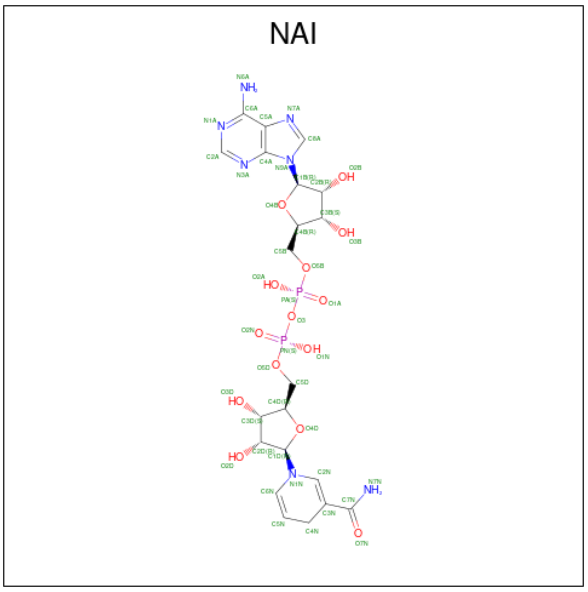
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	B	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 16 8 8	0
14	I	1	Total Fe S 16 8 8	0

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



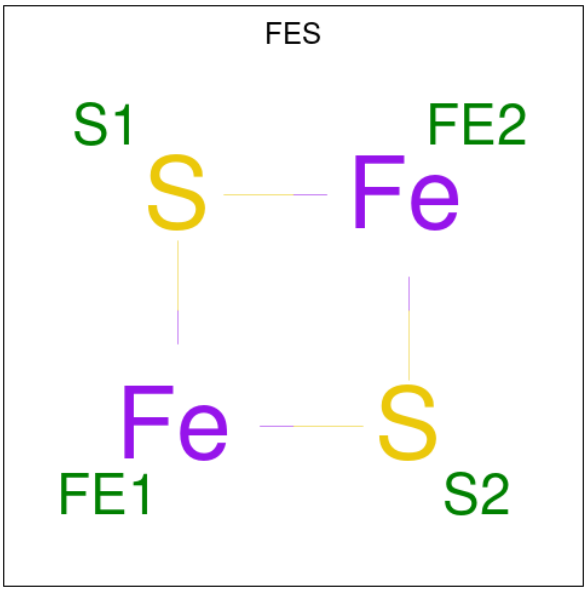
Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 16 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
16	F	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

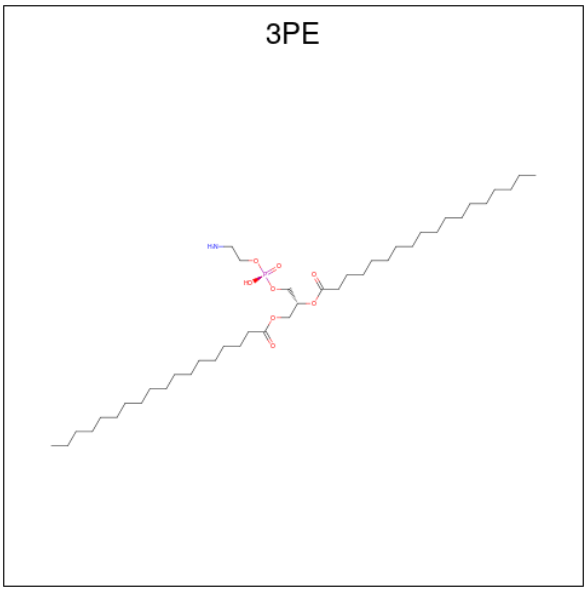


Mol	Chain	Residues	Atoms	AltConf
17	E	1	Total Fe S 4 2 2	0
17	G	1	Total Fe S 4 2 2	0

- Molecule 18 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

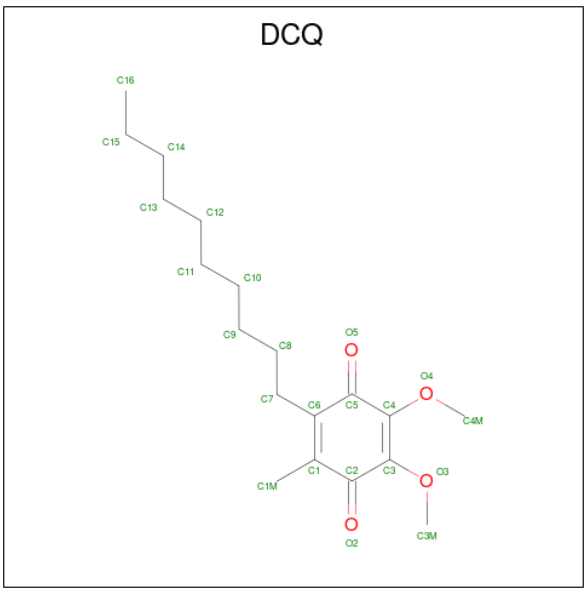
- Molecule 19 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
19	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
19	I	1	Total	C	N	O	P	0
			39	29	1	8	1	
19	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
19	L	1	Total	C	N	O	P	0
			217	167	5	40	5	
19	L	1	Total	C	N	O	P	0
			217	167	5	40	5	
19	L	1	Total	C	N	O	P	0
			217	167	5	40	5	
19	L	1	Total	C	N	O	P	0
			217	167	5	40	5	
19	L	1	Total	C	N	O	P	0
			217	167	5	40	5	
19	M	1	Total	C	N	O	P	0
			131	101	3	24	3	
19	M	1	Total	C	N	O	P	0
			131	101	3	24	3	
19	M	1	Total	C	N	O	P	0
			131	101	3	24	3	
19	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
19	J	1	Total	C	N	O	P	0
			42	32	1	8	1	

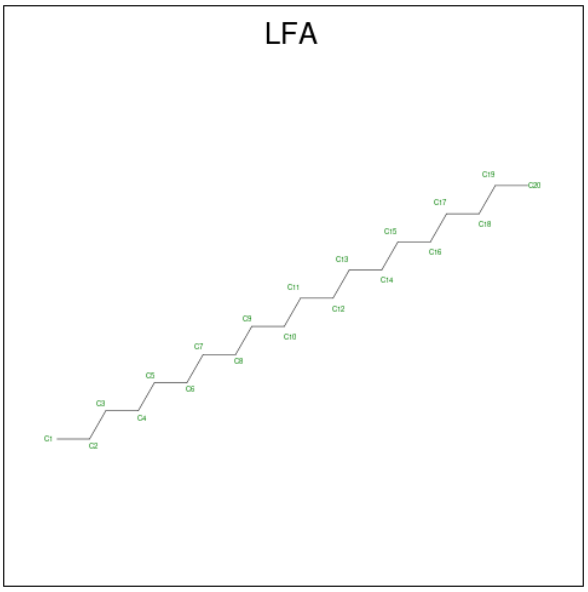
- Molecule 20 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter

code: DCQ) (formula: $C_{19}H_{30}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 21 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms	AltConf
21	H	1	Total C 20 20	0

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Mol	Chain	Residues	Atoms	AltConf
21	N	1	Total C 29 29	0
21	N	1	Total C 29 29	0
21	J	1	Total C 20 20	0

- Molecule 22 is water.

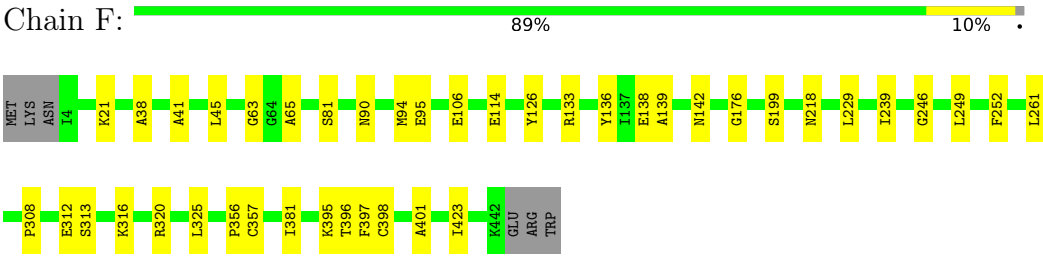
Mol	Chain	Residues	Atoms	AltConf
22	F	97	Total O 97 97	0
22	E	26	Total O 26 26	0
22	G	353	Total O 353 353	0
22	C	206	Total O 206 206	0
22	B	67	Total O 67 67	0
22	I	95	Total O 95 95	0
22	H	69	Total O 69 69	0
22	A	38	Total O 38 38	0
22	L	47	Total O 47 47	0
22	M	85	Total O 85 85	0
22	N	64	Total O 64 64	0
22	K	17	Total O 17 17	0
22	J	20	Total O 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.

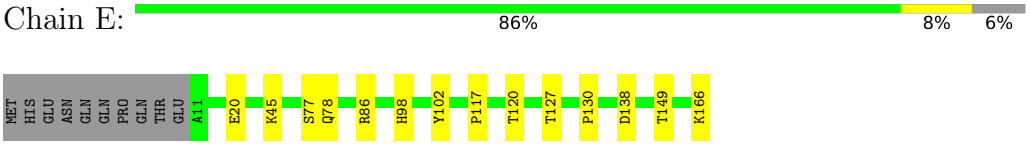
• Molecule 1: NADH-quinone oxidoreductase subunit F

Chain F:



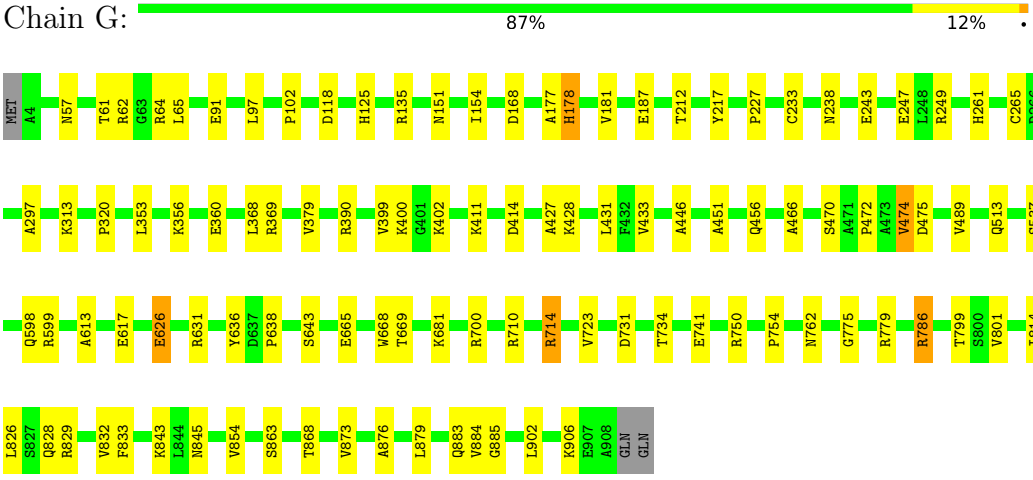
• Molecule 2: NADH dehydrogenase I subunit E

Chain E:



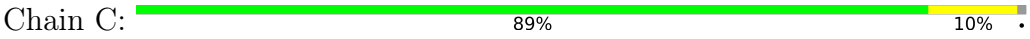
• Molecule 3: NADH-quinone oxidoreductase

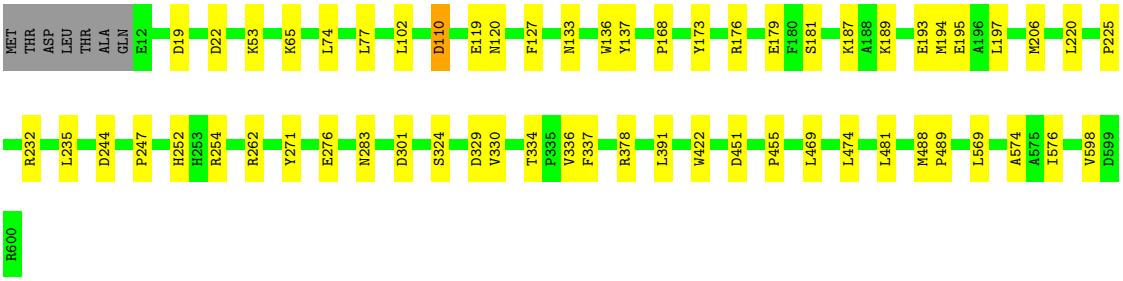
Chain G:



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

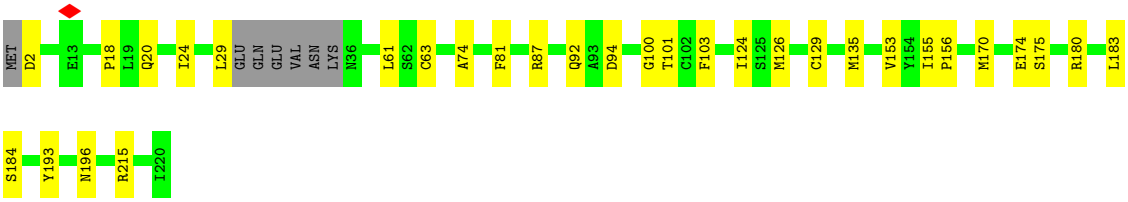
Chain C:





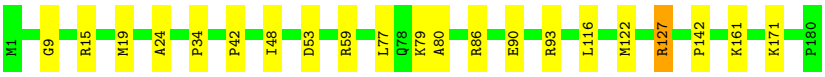
• Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:



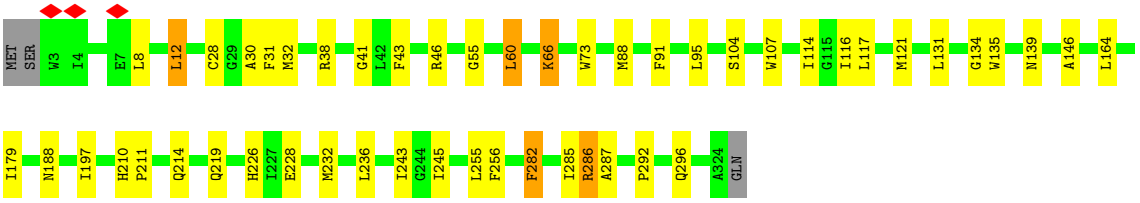
• Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:



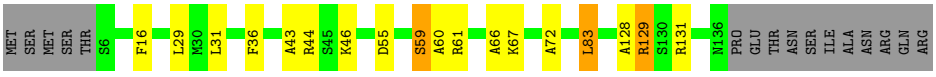
• Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:



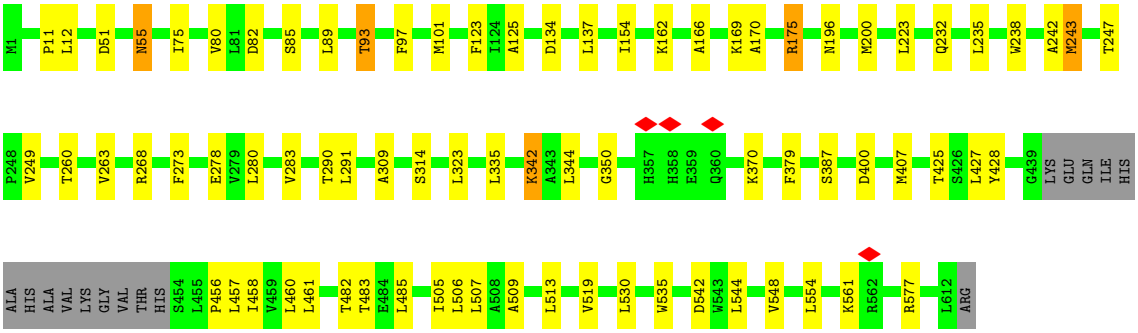
• Molecule 8: NADH-quinone oxidoreductase subunit A

Chain A:

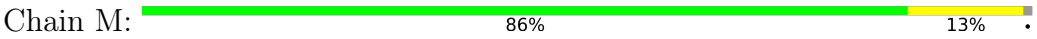


• Molecule 9: NADH dehydrogenase subunit L

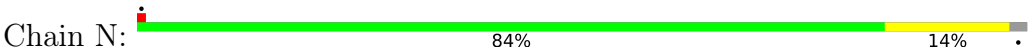
Chain L:

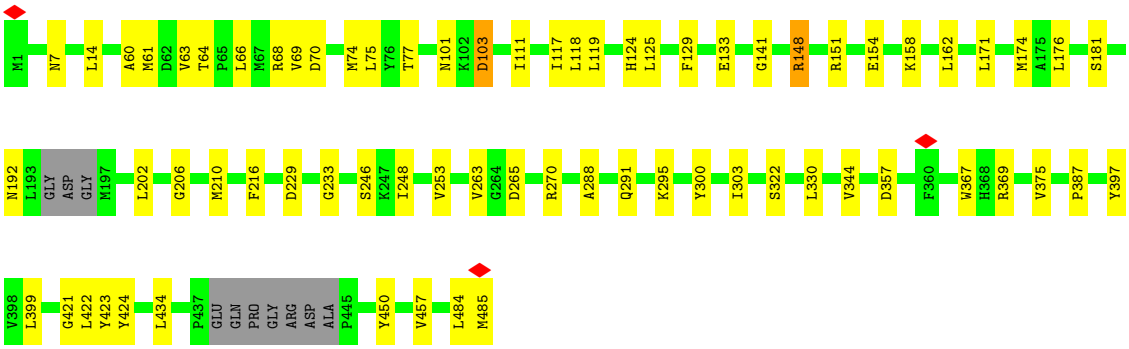


• Molecule 10: NADH dehydrogenase I subunit M

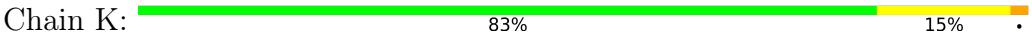


• Molecule 11: NADH-quinone oxidoreductase subunit N

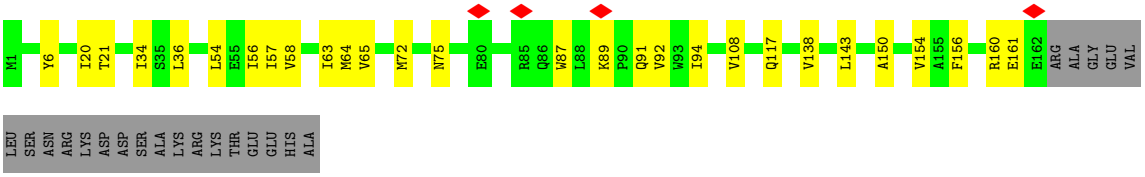




• Molecule 12: NADH-quinone oxidoreductase subunit K



• Molecule 13: NADH-quinone oxidoreductase subunit J


M1
Y6
I20
T21
I34
S35
L36
L54
E55
I56
I57
V58
I63
M64
V65
M72
N75
E80
R85
Q86
W87
L88
K89
P90
Q91
V92
W93
I94
V108
Q117
V138
L143
A150
V154
A155
F156
R160
E161
E162
ARG
ALA
GLY
GLU
VAL
LEU
SER
ASN
ARG
LYS
ASP
ASP
SER
ALA
LYS
ARG
LYS
THR
GLU
GLU
HIS
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170004	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 ($e^-/Å^2$)	80	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	0.661	Depositor
Minimum map value	-0.138	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	153.5, 214.5, 235.0	wwPDB
Map dimensions	307, 429, 470	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: NAI, CA, FMN, 3PE, DCQ, FES, LFA, SF4

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	0.35	0/3486	0.55	0/4713
2	E	0.34	0/1248	0.53	0/1691
3	G	0.36	0/7168	0.55	0/9720
4	C	0.36	0/4891	0.57	0/6637
5	B	0.37	0/1730	0.57	0/2345
6	I	0.37	0/1470	0.59	1/1985 (0.1%)
7	H	0.36	0/2610	0.56	2/3553 (0.1%)
8	A	0.35	0/1065	0.61	1/1443 (0.1%)
9	L	0.33	0/4675	0.53	1/6372 (0.0%)
10	M	0.35	0/4074	0.53	0/5546
11	N	0.34	0/3689	0.52	0/5033
12	K	0.33	0/769	0.59	2/1040 (0.2%)
13	J	0.33	0/1252	0.51	0/1708
All	All	0.35	0/38127	0.55	7/51786 (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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	83	LEU	CA-CB-CG	6.91	131.19	115.30
9	L	530	LEU	CA-CB-CG	6.04	129.19	115.30
12	K	95	VAL	CA-CB-CG1	5.80	119.60	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	53	ASP	CB-CG-OD1	5.35	123.11	118.30
12	K	81	LEU	CB-CG-CD1	-5.34	101.92	111.00
7	H	232	MET	CB-CG-SD	5.22	128.06	112.40
7	H	12	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	177	ALA	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	24	0
2	E	1220	0	1187	8	0
3	G	7017	0	6819	52	0
4	C	4760	0	4677	34	0
5	B	1693	0	1670	21	0
6	I	1436	0	1415	12	0
7	H	2534	0	2583	35	0
8	A	1037	0	1054	13	0
9	L	4558	0	4701	41	0
10	M	3953	0	4053	33	0
11	N	3601	0	3770	42	0
12	K	760	0	817	11	0
13	J	1226	0	1297	21	0
14	B	8	0	0	1	0
14	F	8	0	0	1	0
14	G	24	0	0	0	0
14	I	16	0	0	0	0
15	F	31	0	19	2	0
16	F	44	0	27	3	0
17	E	4	0	0	0	0
17	G	4	0	0	0	0
18	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	C	51	0	82	5	0
19	H	36	0	46	3	0
19	I	39	0	52	1	0
19	J	42	0	58	4	0
19	L	217	0	316	7	0
19	M	131	0	190	5	0
19	N	51	0	82	1	0
20	B	23	0	30	1	0
20	C	23	0	30	1	0
21	H	20	0	42	0	0
21	J	20	0	42	0	0
21	N	29	0	56	0	0
22	A	38	0	0	0	0
22	B	67	0	0	0	0
22	C	206	0	0	1	0
22	E	26	0	0	0	0
22	F	97	0	0	0	0
22	G	353	0	0	3	0
22	H	69	0	0	1	0
22	I	95	0	0	1	0
22	J	20	0	0	0	0
22	K	17	0	0	1	0
22	L	47	0	0	0	0
22	M	85	0	0	3	0
22	N	64	0	0	1	0
All	All	39208	0	38489	312	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 4.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:GLU:HB2	16:F:503:NAI:H42N	1.62	0.80
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.74	0.69
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.75	0.69
10:M:359:CYS:SG	10:M:369:ARG:NH1	2.67	0.68
8:A:83:LEU:HD22	13:J:54:LEU:HD13	1.77	0.65
10:M:181:SER:HB2	10:M:230:ALA:HA	1.77	0.65
19:H:602:3PE:H31	19:J:902:3PE:H11	1.80	0.64
3:G:125:HIS:ND1	22:G:1104:HOH:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:295:LYS:HD3	11:N:344:VAL:HG11	1.79	0.64
4:C:220:LEU:HD12	4:C:235:LEU:HD11	1.81	0.63
7:H:28:CYS:O	7:H:32:MET:HB2	1.98	0.63
3:G:845:ASN:ND2	3:G:879:LEU:O	2.30	0.62
7:H:210:HIS:HB3	7:H:286:ARG:HG2	1.81	0.62
19:C:701:3PE:H121	7:H:296:GLN:HE21	1.66	0.61
2:E:120:THR:HG1	2:E:127:THR:HG1	1.48	0.60
19:C:701:3PE:H231	6:I:9:GLY:HA3	1.82	0.60
19:L:801:3PE:H2I3	19:L:803:3PE:H372	1.82	0.59
3:G:599:ARG:O	3:G:829:ARG:NH2	2.35	0.59
7:H:214:GLN:NE2	7:H:292:PRO:O	2.36	0.59
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.85	0.58
3:G:843:LYS:HD2	3:G:876:ALA:HB2	1.85	0.58
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.86	0.58
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.85	0.58
12:K:1:MET:SD	12:K:1:MET:N	2.73	0.58
1:F:106:GLU:O	1:F:142:ASN:ND2	2.34	0.58
5:B:87:ARG:NH1	20:B:302:DCQ:O2	2.37	0.58
1:F:357:CYS:HB2	1:F:401:ALA:HB2	1.86	0.58
7:H:135:TRP:O	8:A:61:ARG:NH2	2.31	0.57
7:H:179:ILE:HG21	7:H:255:LEU:HD23	1.86	0.57
12:K:9:ILE:HG12	13:J:108:VAL:HG22	1.87	0.57
5:B:180:ARG:HB2	5:B:193:TYR:HB2	1.87	0.56
7:H:139:ASN:ND2	7:H:228:GLU:OE2	2.37	0.56
9:L:166:ALA:HB1	9:L:242:ALA:HA	1.85	0.56
4:C:574:ALA:O	8:A:129:ARG:NH2	2.35	0.56
7:H:134:GLY:HA3	7:H:146:ALA:HB2	1.88	0.56
8:A:83:LEU:HD23	13:J:58:VAL:HG11	1.88	0.56
11:N:369:ARG:NH2	11:N:450:TYR:OH	2.40	0.55
3:G:399:VAL:HG13	3:G:428:LYS:HB2	1.87	0.55
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.87	0.55
11:N:291:GLN:NE2	22:N:610:HOH:O	2.40	0.55
1:F:218:ASN:ND2	15:F:502:FMN:O2	2.39	0.55
4:C:254:ARG:HG3	5:B:103:PHE:HE1	1.72	0.54
19:H:602:3PE:H261	19:J:902:3PE:H271	1.88	0.54
5:B:101:THR:HA	5:B:129:CYS:HB3	1.89	0.54
11:N:118:LEU:HD22	13:J:143:LEU:HD13	1.88	0.54
11:N:68:ARG:HH11	11:N:484:LEU:HD13	1.73	0.54
5:B:92:GLN:NE2	7:H:226:HIS:O	2.41	0.54
3:G:883:GLN:NE2	22:G:1137:HOH:O	2.41	0.54
2:E:86:ARG:NH1	2:E:166:LYS:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:121:MET:HG3	13:J:57:ILE:HG13	1.90	0.54
10:M:414:SER:O	10:M:418:VAL:N	2.37	0.54
10:M:187:ILE:HD11	11:N:399:LEU:HD22	1.90	0.53
10:M:208:GLU:HA	10:M:211:LEU:HD12	1.88	0.53
13:J:91:GLN:HA	13:J:94:ILE:HG22	1.91	0.53
6:I:59:ARG:NH2	6:I:142:PRO:O	2.41	0.53
1:F:41:ALA:HA	1:F:45:LEU:HD12	1.91	0.53
12:K:85:ARG:NH1	13:J:161:GLU:OE1	2.41	0.53
4:C:262:ARG:NH2	22:C:817:HOH:O	2.38	0.53
4:C:391:LEU:HD22	4:C:474:LEU:HD22	1.91	0.53
11:N:148:ARG:O	12:K:86:ARG:NH2	2.42	0.53
11:N:171:LEU:HD23	12:K:42:SER:HB2	1.91	0.53
3:G:863:SER:HB3	3:G:868:THR:HG22	1.92	0.52
7:H:131:LEU:HD11	13:J:64:MET:HG2	1.91	0.52
9:L:175:ARG:NH2	22:M:1102:HOH:O	2.42	0.52
1:F:176:GLY:HA3	2:E:78:GLN:HG2	1.92	0.52
3:G:825:GLU:HA	3:G:828:GLN:HE21	1.74	0.52
12:K:26:ARG:NH1	13:J:87:TRP:O	2.43	0.52
3:G:626:GLU:OE1	3:G:786:ARG:NH1	2.43	0.52
9:L:457:LEU:O	9:L:461:LEU:HB2	2.09	0.52
10:M:122:TRP:CD2	10:M:149:PRO:HG3	2.45	0.52
7:H:121:MET:HG2	13:J:56:ILE:HB	1.92	0.52
9:L:154:ILE:HD13	9:L:242:ALA:HB1	1.91	0.52
9:L:247:THR:HG21	9:L:350:GLY:HA3	1.91	0.52
4:C:110:ASP:OD1	4:C:110:ASP:N	2.42	0.51
3:G:168:ASP:OD1	3:G:400:LYS:NZ	2.42	0.51
10:M:84:ASP:OD2	10:M:273:ARG:NH2	2.42	0.51
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.92	0.51
4:C:120:ASN:OD1	4:C:120:ASN:N	2.42	0.51
1:F:63:GLY:O	16:F:503:NAI:H2N	2.10	0.51
1:F:261:LEU:HD13	1:F:325:LEU:HD21	1.92	0.51
10:M:72:ILE:HB	10:M:77:ILE:HB	1.91	0.51
3:G:710:ARG:NH1	22:G:1133:HOH:O	2.39	0.51
7:H:38:ARG:NH1	7:H:55:GLY:O	2.43	0.51
9:L:535:TRP:HH2	19:L:802:3PE:H271	1.76	0.51
11:N:154:GLU:OE2	11:N:158:LYS:NZ	2.40	0.51
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.92	0.51
4:C:334:THR:OG1	7:H:287:ALA:O	2.24	0.51
12:K:43:ALA:HB1	12:K:62:TYR:HD1	1.76	0.51
3:G:247:GLU:HG3	3:G:249:ARG:HE	1.76	0.51
19:L:804:3PE:H11	11:N:423:TYR:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:66:ALA:H	13:J:72:MET:HG2	1.76	0.50
3:G:472:PRO:HG3	3:G:799:THR:HA	1.93	0.50
5:B:126:MET:HG3	5:B:155:ILE:HD12	1.94	0.50
3:G:402:LYS:HD3	3:G:427:ALA:HB1	1.93	0.50
4:C:225:PRO:HA	20:C:702:DCQ:H4M	1.94	0.50
9:L:427:LEU:HD11	9:L:507:LEU:HD12	1.93	0.50
11:N:265:ASP:HA	11:N:270:ARG:HH22	1.76	0.50
7:H:164:LEU:HD22	7:H:255:LEU:HD13	1.94	0.50
11:N:367:TRP:NE1	11:N:434:LEU:O	2.30	0.50
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.94	0.50
7:H:211:PRO:HB2	7:H:292:PRO:HD3	1.94	0.49
8:A:59:SER:OG	8:A:60:ALA:N	2.44	0.49
11:N:485:MET:SD	11:N:485:MET:N	2.85	0.49
4:C:276:GLU:O	4:C:283:ASN:ND2	2.38	0.49
9:L:85:SER:OG	9:L:268:ARG:NH2	2.46	0.49
11:N:66:LEU:HA	11:N:124:HIS:HB2	1.94	0.49
8:A:43:ALA:HB3	8:A:46:LYS:HB2	1.94	0.49
12:K:6:HIS:ND1	13:J:6:TYR:OH	2.42	0.49
9:L:519:VAL:HG13	19:L:802:3PE:H31	1.95	0.49
13:J:36:LEU:HD12	13:J:63:ILE:HD11	1.95	0.49
19:M:1002:3PE:H2C1	19:M:1002:3PE:H3F2	1.93	0.49
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.93	0.48
3:G:451:ALA:O	3:G:456:GLN:NE2	2.41	0.48
1:F:308:PRO:O	1:F:313:SER:OG	2.31	0.48
7:H:219:GLN:NE2	22:H:710:HOH:O	2.39	0.48
4:C:189:LYS:O	4:C:193:GLU:HG2	2.14	0.48
4:C:197:LEU:O	4:C:232:ARG:NH2	2.45	0.48
11:N:7:ASN:HB3	11:N:63:VAL:HG13	1.95	0.48
2:E:117:PRO:HB3	2:E:130:PRO:HD3	1.94	0.48
5:B:124:ILE:HG12	5:B:153:VAL:HB	1.94	0.48
9:L:101:MET:HG3	9:L:456:PRO:HG3	1.95	0.48
2:E:138:ASP:OD1	2:E:138:ASP:N	2.47	0.48
3:G:474:VAL:HB	3:G:801:VAL:HG11	1.94	0.48
11:N:125:LEU:HD13	11:N:174:MET:HG2	1.96	0.48
19:H:602:3PE:H341	19:J:902:3PE:H321	1.95	0.48
1:F:176:GLY:O	2:E:77:SER:OG	2.29	0.48
3:G:431:LEU:O	3:G:446:ALA:N	2.46	0.48
4:C:569:LEU:HD22	4:C:598:VAL:HG21	1.95	0.48
12:K:26:ARG:NH1	22:K:203:HOH:O	2.47	0.48
5:B:81:PHE:HZ	6:I:34:PRO:HD3	1.79	0.47
4:C:455:PRO:HB2	4:C:469:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:814:ILE:HD11	3:G:902:LEU:HD13	1.96	0.47
9:L:273:PHE:HB3	9:L:280:LEU:HD13	1.95	0.47
10:M:3:LEU:HB3	10:M:132:LEU:HD13	1.95	0.47
3:G:320:PRO:HB2	3:G:537:SER:HB2	1.97	0.47
4:C:324:SER:HB2	4:C:336:VAL:HA	1.96	0.47
5:B:156:PRO:HG2	6:I:122:MET:HB2	1.97	0.47
11:N:119:LEU:HD22	11:N:253:VAL:HG11	1.95	0.47
9:L:554:LEU:HD21	19:M:1001:3PE:H221	1.97	0.47
4:C:133:ASN:HB3	4:C:422:TRP:HA	1.97	0.47
9:L:51:ASP:O	9:L:55:ASN:ND2	2.47	0.47
3:G:466:ALA:HB3	3:G:489:VAL:HG21	1.97	0.47
11:N:129:PHE:O	11:N:133:GLU:HG2	2.15	0.47
3:G:369:ARG:NH2	3:G:775:GLY:O	2.45	0.46
7:H:41:GLY:HA2	7:H:46:ARG:HG3	1.96	0.46
11:N:421:GLY:HA2	11:N:424:TYR:CE2	2.50	0.46
8:A:128:ALA:HA	8:A:131:ARG:HG3	1.97	0.46
9:L:235:LEU:HD21	19:M:1001:3PE:H3D2	1.98	0.46
9:L:12:LEU:HD11	19:L:801:3PE:H3H1	1.97	0.46
3:G:212:THR:HG22	3:G:832:VAL:HG21	1.96	0.46
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.98	0.46
19:C:701:3PE:H262	19:C:701:3PE:H341	1.98	0.46
5:B:170:MET:O	5:B:174:GLU:HG2	2.15	0.46
9:L:89:LEU:O	9:L:93:THR:OG1	2.29	0.46
10:M:314:LEU:O	10:M:318:THR:HG23	2.15	0.46
1:F:296:GLY:O	1:F:320:ARG:NH2	2.48	0.46
3:G:217:TYR:HB3	6:I:79:LYS:HD2	1.96	0.46
9:L:243:MET:HE2	9:L:243:MET:HB3	1.79	0.46
1:F:65:ALA:HB2	16:F:503:NAI:H4D	1.98	0.46
2:E:45:LYS:HB2	2:E:45:LYS:HE2	1.73	0.46
3:G:227:PRO:HD3	3:G:754:PRO:HB3	1.98	0.46
5:B:61:LEU:HB2	5:B:100:GLY:HA3	1.97	0.46
11:N:357:ASP:OD1	11:N:357:ASP:N	2.44	0.46
3:G:313:LYS:NZ	3:G:557:GLU:OE1	2.38	0.46
4:C:206:MET:HE2	4:C:244:ASP:HB3	1.97	0.46
11:N:181:SER:HA	11:N:192:ASN:HD21	1.82	0.46
7:H:95:LEU:HG	7:H:243:ILE:HG21	1.98	0.45
10:M:31:ILE:O	10:M:35:THR:HG23	2.15	0.45
9:L:544:LEU:O	9:L:548:VAL:HB	2.16	0.45
10:M:65:SER:HB3	10:M:83:ILE:HG22	1.98	0.45
13:J:20:ILE:HG13	13:J:21:THR:HG23	1.97	0.45
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:243:GLU:HG2	3:G:636:TYR:HB3	1.98	0.45
3:G:741:GLU:OE2	4:C:176:ARG:NH1	2.39	0.45
10:M:71:TRP:HB2	10:M:79:ILE:HG13	1.97	0.45
10:M:87:SER:OG	10:M:273:ARG:NH2	2.47	0.45
12:K:57:ASP:OD1	12:K:57:ASP:N	2.48	0.45
4:C:187:LYS:HE2	8:A:44:ARG:HD2	1.98	0.45
10:M:217:SER:O	19:M:1003:3PE:N	2.45	0.45
1:F:356:PRO:HB2	1:F:396:THR:HG22	1.99	0.45
3:G:118:ASP:OD1	3:G:762:ASN:ND2	2.50	0.45
10:M:233:VAL:HG23	10:M:240:LEU:HD13	1.98	0.45
7:H:66:LYS:HE3	7:H:66:LYS:HB3	1.68	0.45
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.52	0.45
9:L:577:ARG:NH2	19:L:804:3PE:H2	2.32	0.45
11:N:288:ALA:HB2	11:N:300:TYR:HB2	1.98	0.45
7:H:114:ILE:HB	7:H:117:LEU:HB2	1.97	0.45
9:L:505:ILE:HG22	9:L:506:LEU:HD23	1.99	0.45
19:L:804:3PE:H11	11:N:423:TYR:CE2	2.52	0.45
10:M:367:HIS:ND1	22:M:1108:HOH:O	2.36	0.45
19:M:1001:3PE:H251	19:M:1001:3PE:H331	1.99	0.45
3:G:91:GLU:HG3	3:G:125:HIS:HB2	2.00	0.44
3:G:267:ARG:HA	3:G:833:PHE:HZ	1.82	0.44
5:B:29:LEU:HD13	5:B:180:ARG:HG2	1.98	0.44
6:I:80:ALA:HB2	6:I:90:GLU:HB2	1.99	0.44
11:N:176:LEU:HD22	11:N:202:LEU:HD11	1.99	0.44
3:G:843:LYS:HB2	3:G:885:GLY:HA3	1.99	0.44
7:H:88:MET:HE2	7:H:88:MET:HB3	1.74	0.44
8:A:72:ALA:HB1	13:J:65:VAL:HG22	1.98	0.44
7:H:245:ILE:HG23	7:H:282:PHE:CD2	2.52	0.44
9:L:344:LEU:HB2	9:L:460:LEU:HB3	2.00	0.44
1:F:90:ASN:ND2	15:F:502:FMN:O4'	2.49	0.44
5:B:215:ARG:HB2	6:I:42:PRO:HB3	2.00	0.44
10:M:179:GLN:HG2	11:N:422:LEU:HD11	1.99	0.44
4:C:194:MET:HG3	8:A:55:ASP:OD2	2.17	0.44
7:H:188:ASN:HB2	7:H:256:PHE:HA	2.00	0.44
9:L:170:ALA:HA	9:L:238:TRP:HB2	1.99	0.44
13:J:156:PHE:CE1	13:J:160:ARG:HD3	2.52	0.44
10:M:192:LEU:HG	10:M:210:LEU:HD22	2.00	0.44
11:N:60:ALA:HA	11:N:69:VAL:O	2.17	0.44
4:C:136:TRP:HZ2	4:C:247:PRO:HG2	1.83	0.44
7:H:8:LEU:O	7:H:12:LEU:HD22	2.18	0.44
11:N:103:ASP:OD1	11:N:103:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:164:GLY:O	10:M:168:ILE:HG12	2.18	0.43
5:B:183:LEU:HD23	5:B:183:LEU:HA	1.88	0.43
6:I:48:ILE:HG12	6:I:116:LEU:HG	2.00	0.43
1:F:395:LYS:HE3	3:G:65:LEU:HD12	2.00	0.43
3:G:97:LEU:HD22	3:G:154:ILE:HB	2.00	0.43
9:L:260:THR:HB	9:L:335:LEU:HD11	2.01	0.43
10:M:47:TRP:CG	10:M:88:LEU:HD11	2.53	0.43
4:C:19:ASP:OD1	4:C:19:ASP:N	2.39	0.43
9:L:162:LYS:HA	9:L:162:LYS:HE3	2.01	0.43
11:N:70:ASP:HB3	11:N:484:LEU:HD12	2.01	0.43
13:J:89:LYS:HB2	13:J:92:VAL:HG23	2.00	0.43
5:B:24:ILE:HD12	5:B:196:ASN:HD21	1.84	0.43
7:H:91:PHE:HB2	7:H:236:LEU:HD22	2.00	0.43
3:G:700:ARG:NH2	4:C:119:GLU:OE1	2.43	0.43
4:C:252:HIS:O	4:C:252:HIS:ND1	2.48	0.43
12:K:25:ARG:HD2	12:K:25:ARG:HA	1.71	0.43
19:C:701:3PE:H3B2	7:H:285:ILE:HG21	2.01	0.43
4:C:77:LEU:HB3	4:C:137:TYR:HB3	2.00	0.43
7:H:38:ARG:HD2	7:H:38:ARG:HA	1.77	0.43
11:N:300:TYR:HA	11:N:303:ILE:HD12	2.00	0.43
3:G:731:ASP:OD2	3:G:734:THR:OG1	2.37	0.43
3:G:102:PRO:HG3	3:G:151:ASN:HB3	1.99	0.42
9:L:263:VAL:HG13	9:L:323:LEU:HD11	2.00	0.42
10:M:192:LEU:HB2	10:M:223:LEU:HD13	2.01	0.42
3:G:353:LEU:HD21	3:G:513:GLN:HG3	2.01	0.42
3:G:356:LYS:O	3:G:360:GLU:HB2	2.19	0.42
3:G:379:VAL:HB	3:G:433:VAL:HG12	1.99	0.42
8:A:31:LEU:HD23	8:A:31:LEU:HA	1.90	0.42
9:L:169:LYS:HD3	9:L:238:TRP:HA	2.00	0.42
6:I:24:ALA:HB2	7:H:43:PHE:CD1	2.55	0.42
7:H:116:ILE:HA	7:H:116:ILE:HD12	1.77	0.42
10:M:123:ILE:HG13	10:M:149:PRO:HB2	2.01	0.42
10:M:381:MET:HB2	10:M:385:PRO:HD3	2.02	0.42
11:N:375:VAL:HG11	11:N:457:VAL:HB	2.01	0.42
9:L:342:LYS:HD3	9:L:342:LYS:HA	1.84	0.42
11:N:151:ARG:HB3	11:N:233:GLY:HA2	2.01	0.42
6:I:15:ARG:O	6:I:19:MET:HG3	2.19	0.42
3:G:278:LYS:HA	3:G:278:LYS:HD3	1.88	0.42
11:N:141:GLY:HA3	13:J:154:VAL:HG22	2.00	0.42
11:N:330:LEU:HD23	11:N:330:LEU:HA	1.90	0.42
13:J:34:ILE:HG23	19:J:902:3PE:H2D1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:ALA:HB2	1:F:114:GLU:HG3	2.01	0.42
1:F:312:GLU:O	1:F:316:LYS:HG2	2.20	0.42
3:G:178:HIS:CD2	3:G:178:HIS:H	2.36	0.42
5:B:2:ASP:N	5:B:2:ASP:OD1	2.52	0.42
9:L:425:THR:HA	9:L:428:TYR:CE2	2.55	0.42
11:N:206:GLY:O	11:N:210:MET:HG3	2.20	0.42
3:G:723:VAL:HG11	6:I:127:ARG:HG3	2.00	0.41
4:C:329:ASP:HA	7:H:219:GLN:HG2	2.01	0.41
9:L:80:VAL:HB	9:L:134:ASP:HB3	2.02	0.41
2:E:98:HIS:HA	2:E:102:TYR:HD1	1.84	0.41
3:G:854:VAL:HG11	3:G:873:VAL:HG21	2.01	0.41
9:L:75:ILE:HG21	9:L:137:LEU:HD23	2.01	0.41
4:C:337:PHE:HB3	5:B:74:ALA:HB2	2.01	0.41
5:B:18:PRO:HB2	5:B:20:GLN:HG2	2.03	0.41
9:L:458:ILE:HD13	9:L:461:LEU:HD23	2.02	0.41
10:M:384:LEU:O	10:M:388:SER:OG	2.31	0.41
1:F:397:PHE:HB3	14:F:501:SF4:S2	2.60	0.41
4:C:168:PRO:HA	4:C:173:TYR:CG	2.55	0.41
9:L:407:MET:HG2	9:L:485:LEU:HD21	2.02	0.41
9:L:509:ALA:O	9:L:513:LEU:HB2	2.21	0.41
3:G:884:VAL:HG21	3:G:902:LEU:HD22	2.02	0.41
19:I:203:3PE:H2D1	7:H:197:ILE:HD12	2.01	0.41
7:H:236:LEU:HD23	7:H:236:LEU:HA	1.89	0.41
4:C:488:MET:HE3	4:C:489:PRO:HD2	2.02	0.41
4:C:576:ILE:HD12	4:C:576:ILE:HA	1.94	0.41
9:L:82:ASP:OD1	9:L:82:ASP:N	2.53	0.41
9:L:97:PHE:O	9:L:101:MET:HG2	2.21	0.41
10:M:273:ARG:NH1	22:M:1119:HOH:O	2.44	0.41
3:G:267:ARG:HB2	3:G:820:LEU:HG	2.02	0.41
4:C:74:LEU:HA	4:C:102:LEU:HD23	2.02	0.41
19:C:701:3PE:H271	19:C:701:3PE:H361	2.02	0.41
5:B:100:GLY:HA2	14:B:301:SF4:S4	2.61	0.41
9:L:196:ASN:O	9:L:200:MET:HG3	2.21	0.41
9:L:232:GLN:HA	9:L:290:THR:HG21	2.03	0.41
10:M:225:LEU:HD23	10:M:225:LEU:HA	1.89	0.41
11:N:70:ASP:O	11:N:74:MET:HG3	2.21	0.41
11:N:162:LEU:HB3	11:N:216:PHE:CE1	2.56	0.41
1:F:381:ILE:HG13	1:F:423:ILE:HD11	2.03	0.41
6:I:93:ARG:NH2	22:I:305:HOH:O	2.35	0.41
1:F:133:ARG:HD3	1:F:136:TYR:CE1	2.56	0.40
3:G:297:ALA:HB1	3:G:668:TRP:CH2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:598:GLN:HG3	3:G:826:LEU:HD22	2.02	0.40
9:L:243:MET:SD	9:L:309:ALA:HB2	2.61	0.40
11:N:14:LEU:HD21	13:J:143:LEU:HD11	2.03	0.40
1:F:229:LEU:HD13	1:F:229:LEU:HA	1.93	0.40
4:C:481:LEU:HD23	4:C:481:LEU:HA	1.94	0.40
5:B:184:SER:OG	8:A:36:PHE:O	2.31	0.40
7:H:30:ALA:HB1	7:H:60:LEU:HD11	2.03	0.40
1:F:239:ILE:HD12	1:F:246:GLY:HA2	2.02	0.40
3:G:613:ALA:HB1	3:G:617:GLU:HB2	2.03	0.40
3:G:714:ARG:NH2	4:C:179:GLU:OE2	2.50	0.40
10:M:89:LEU:HD12	10:M:489:SER:HB3	2.02	0.40
11:N:75:LEU:HA	19:N:503:3PE:H261	2.04	0.40
3:G:411:LYS:HA	3:G:411:LYS:HD3	1.87	0.40
4:C:271:TYR:CE1	5:B:135:MET:HG3	2.57	0.40
9:L:134:ASP:OD1	9:L:134:ASP:N	2.48	0.40
10:M:127:VAL:HG11	10:M:264:LEU:HD13	2.02	0.40
10:M:144:GLU:HB2	11:N:387:PRO:HG2	2.03	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	437/445 (98%)	426 (98%)	11 (2%)	0	100	100
2	E	154/166 (93%)	150 (97%)	4 (3%)	0	100	100
3	G	903/908 (99%)	879 (97%)	21 (2%)	3 (0%)	41	55
4	C	587/596 (98%)	576 (98%)	11 (2%)	0	100	100
5	B	209/220 (95%)	196 (94%)	13 (6%)	0	100	100
6	I	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
7	H	320/325 (98%)	308 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	A	129/147 (88%)	127 (98%)	2 (2%)	0	100	100
9	L	594/613 (97%)	583 (98%)	11 (2%)	0	100	100
10	M	502/509 (99%)	492 (98%)	10 (2%)	0	100	100
11	N	469/485 (97%)	462 (98%)	6 (1%)	1 (0%)	47	62
12	K	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
13	J	160/184 (87%)	158 (99%)	2 (1%)	0	100	100
All	All	4740/4878 (97%)	4629 (98%)	107 (2%)	4 (0%)	54	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	178	HIS
3	G	261	HIS
3	G	669	THR
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	353/359 (98%)	344 (98%)	9 (2%)	47	67
2	E	129/139 (93%)	127 (98%)	2 (2%)	62	79
3	G	730/736 (99%)	704 (96%)	26 (4%)	35	54
4	C	509/515 (99%)	498 (98%)	11 (2%)	52	71
5	B	185/192 (96%)	182 (98%)	3 (2%)	62	79
6	I	154/154 (100%)	149 (97%)	5 (3%)	39	59
7	H	266/269 (99%)	260 (98%)	6 (2%)	50	70
8	A	104/119 (87%)	99 (95%)	5 (5%)	25	41
9	L	471/485 (97%)	453 (96%)	18 (4%)	33	51
10	M	413/418 (99%)	397 (96%)	16 (4%)	32	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	N	378/385 (98%)	369 (98%)	9 (2%)	49 68
12	K	79/79 (100%)	73 (92%)	6 (8%)	13 20
13	J	128/146 (88%)	125 (98%)	3 (2%)	50 70
All	All	3899/3996 (98%)	3780 (97%)	119 (3%)	43 60

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	21	LYS
1	F	81	SER
1	F	94	MET
1	F	126	TYR
1	F	138	GLU
1	F	199	SER
1	F	252	PHE
1	F	286	LYS
1	F	398	CYS
2	E	20	GLU
2	E	149	THR
3	G	57	ASN
3	G	61	THR
3	G	62	ARG
3	G	64	ARG
3	G	135	ARG
3	G	181	VAL
3	G	187	GLU
3	G	233	CYS
3	G	238	ASN
3	G	265	CYS
3	G	279	ASP
3	G	414	ASP
3	G	470	SER
3	G	474	VAL
3	G	475	ASP
3	G	593	MET
3	G	626	GLU
3	G	631	ARG
3	G	643	SER
3	G	665	GLU
3	G	681	LYS
3	G	714	ARG

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Mol	Chain	Res	Type
3	G	750	ARG
3	G	779	ARG
3	G	786	ARG
3	G	906	LYS
4	C	22	ASP
4	C	53	LYS
4	C	65	LYS
4	C	110	ASP
4	C	127	PHE
4	C	181	SER
4	C	195	GLU
4	C	301	ASP
4	C	330	VAL
4	C	378	ARG
4	C	451	ASP
5	B	63	CYS
5	B	94	ASP
5	B	175	SER
6	I	77	LEU
6	I	86	ARG
6	I	127	ARG
6	I	161	LYS
6	I	171	LYS
7	H	31	PHE
7	H	60	LEU
7	H	66	LYS
7	H	73	TRP
7	H	282	PHE
7	H	286	ARG
8	A	16	PHE
8	A	29	LEU
8	A	59	SER
8	A	67	LYS
8	A	129	ARG
9	L	55	ASN
9	L	93	THR
9	L	123	PHE
9	L	175	ARG
9	L	243	MET
9	L	249	VAL
9	L	278	GLU
9	L	291	LEU

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Mol	Chain	Res	Type
9	L	314	SER
9	L	342	LYS
9	L	370	LYS
9	L	379	PHE
9	L	387	SER
9	L	400	ASP
9	L	482	THR
9	L	483	THR
9	L	542	ASP
9	L	561	LYS
10	M	1	MET
10	M	56	GLN
10	M	74	ARG
10	M	165	LYS
10	M	166	THR
10	M	209	GLU
10	M	246	ASP
10	M	303	TRP
10	M	321	SER
10	M	332	THR
10	M	374	MET
10	M	388	SER
10	M	426	THR
10	M	433	SER
10	M	435	TYR
10	M	503	SER
11	N	61	MET
11	N	101	ASN
11	N	103	ASP
11	N	148	ARG
11	N	229	ASP
11	N	246	SER
11	N	263	VAL
11	N	322	SER
11	N	397	TYR
12	K	1	MET
12	K	29	LEU
12	K	46	PHE
12	K	51	SER
12	K	57	ASP
12	K	74	SER
13	J	75	ASN

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Mol	Chain	Res	Type
13	J	117	GLN
13	J	138	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	$\#\|Z\| > 2$
14	SF4	I	202	6	0,12,12	-	-	-		
14	SF4	I	201	6	0,12,12	-	-	-		
19	3PE	H	602	-	35,35,50	0.37	0	38,40,55	0.41	0
21	LFA	N	501	-	14,14,19	0.16	0	13,13,18	0.11	0
21	LFA	N	502	-	13,13,19	0.13	0	12,12,18	0.12	0
16	NAI	F	503	-	42,48,48	0.54	0	47,73,73	0.57	1 (2%)
14	SF4	G	1001	3	0,12,12	-	-	-		
19	3PE	J	902	-	41,41,50	0.33	0	44,46,55	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	SF4	B	301	5	0,12,12	-	-	-		
19	3PE	L	802	-	35,35,50	0.36	0	38,40,55	0.36	0
14	SF4	G	1003	3	0,12,12	-	-	-		
19	3PE	I	203	-	38,38,50	0.35	0	41,43,55	0.30	0
19	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.28	0
14	SF4	F	501	1	0,12,12	-	-	-		
19	3PE	L	805	-	38,38,50	0.34	0	41,43,55	0.35	0
17	FES	G	1004	3	0,4,4	-	-	-		
14	SF4	G	1002	3	0,12,12	-	-	-		
17	FES	E	201	2	0,4,4	-	-	-		
21	LFA	H	601	-	19,19,19	0.11	0	18,18,18	0.12	0
19	3PE	C	701	-	50,50,50	0.30	0	53,55,55	0.33	0
19	3PE	N	503	-	50,50,50	0.29	0	53,55,55	0.36	0
19	3PE	M	1001	-	46,46,50	0.31	0	49,51,55	0.34	0
20	DCQ	B	302	-	23,23,23	0.25	0	26,29,29	0.43	0
20	DCQ	C	702	-	23,23,23	0.25	0	26,29,29	0.37	0
19	3PE	M	1003	-	36,36,50	0.35	0	39,41,55	0.34	0
21	LFA	J	901	-	19,19,19	0.12	0	18,18,18	0.13	0
19	3PE	M	1002	-	46,46,50	0.30	0	49,51,55	0.29	0
19	3PE	L	804	-	50,50,50	0.30	0	53,55,55	0.31	0
19	3PE	L	803	-	39,39,50	0.34	0	42,44,55	0.34	0
15	FMN	F	502	-	33,33,33	1.12	2 (6%)	48,50,50	1.34	9 (18%)

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
14	SF4	I	202	6	-	-	0/6/5/5
19	3PE	H	602	-	-	3/39/39/54	-
21	LFA	N	501	-	-	0/12/12/17	-
14	SF4	I	201	6	-	-	0/6/5/5
21	LFA	N	502	-	-	0/11/11/17	-
16	NAI	F	503	-	-	4/25/72/72	0/5/5/5
14	SF4	G	1001	3	-	-	0/6/5/5
19	3PE	J	902	-	-	14/45/45/54	-
14	SF4	B	301	5	-	-	0/6/5/5
19	3PE	L	802	-	-	8/39/39/54	-
14	SF4	G	1003	3	-	-	0/6/5/5
19	3PE	I	203	-	-	3/42/42/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	3PE	L	801	-	-	8/54/54/54	-
14	SF4	F	501	1	-	-	0/6/5/5
19	3PE	L	805	-	-	13/42/42/54	-
17	FES	G	1004	3	-	-	0/1/1/1
14	SF4	G	1002	3	-	-	0/6/5/5
17	FES	E	201	2	-	-	0/1/1/1
21	LFA	H	601	-	-	1/17/17/17	-
19	3PE	C	701	-	-	8/54/54/54	-
19	3PE	N	503	-	-	14/54/54/54	-
19	3PE	M	1001	-	-	5/50/50/54	-
20	DCQ	B	302	-	-	4/14/38/38	0/1/1/1
20	DCQ	C	702	-	-	5/14/38/38	0/1/1/1
19	3PE	M	1003	-	-	4/40/40/54	-
21	LFA	J	901	-	-	0/17/17/17	-
19	3PE	M	1002	-	-	8/50/50/54	-
19	3PE	L	804	-	-	11/54/54/54	-
19	3PE	L	803	-	-	11/43/43/54	-
15	FMN	F	502	-	-	8/18/18/18	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.60	1.37	1.30
15	F	502	FMN	C10-N1	2.00	1.37	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4-N3-C2	-3.28	119.58	125.64
15	F	502	FMN	C4A-C10-N10	2.91	120.73	116.48
15	F	502	FMN	C4A-C4-N3	2.79	120.29	113.19
15	F	502	FMN	C10-C4A-N5	-2.45	119.67	124.86
15	F	502	FMN	C4A-C10-N1	-2.39	119.18	124.73
15	F	502	FMN	O4-C4-C4A	-2.35	120.36	126.60
16	F	503	NAI	C5A-C6A-N6A	2.30	123.84	120.35
15	F	502	FMN	O3P-P-O5'	2.14	112.44	106.73
15	F	502	FMN	C9A-C5A-N5	-2.08	120.17	122.43
15	F	502	FMN	C10-N1-C2	2.08	121.05	116.90

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	502	FMN	C5'-O5'-P-O2P
15	F	502	FMN	C5'-O5'-P-O3P
16	F	503	NAI	C5B-O5B-PA-O1A
19	C	701	3PE	C11-O13-P-O14
19	H	602	3PE	O13-C11-C12-N
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	C11-O13-P-O14
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	O13-C11-C12-N
19	L	804	3PE	C11-O13-P-O11
19	L	804	3PE	C11-O13-P-O12
19	L	804	3PE	C11-O13-P-O14
19	L	805	3PE	C1-O11-P-O12
19	L	805	3PE	C12-C11-O13-P
19	L	805	3PE	O13-C11-C12-N
19	M	1001	3PE	C1-O11-P-O13
19	M	1001	3PE	C1-O11-P-O14
19	M	1001	3PE	O13-C11-C12-N
19	M	1003	3PE	C11-O13-P-O12
19	M	1003	3PE	O13-C11-C12-N
19	N	503	3PE	C1-O11-P-O14
19	N	503	3PE	C11-O13-P-O12
19	N	503	3PE	C11-O13-P-O14
19	N	503	3PE	O13-C11-C12-N
19	J	902	3PE	C1-O11-P-O12
20	B	302	DCQ	C6-C7-C8-C9
19	I	203	3PE	C21-C22-C23-C24
19	C	701	3PE	C11-O13-P-O11
19	L	802	3PE	C1-O11-P-O13
19	L	802	3PE	C11-O13-P-O11
19	L	803	3PE	C11-O13-P-O11
19	L	805	3PE	C1-O11-P-O13
19	L	805	3PE	C11-O13-P-O11
19	M	1002	3PE	C11-O13-P-O11
19	M	1003	3PE	C11-O13-P-O11
19	N	503	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
19	N	503	3PE	C11-O13-P-O11
19	J	902	3PE	C1-O11-P-O13
19	J	902	3PE	C11-O13-P-O11
19	L	801	3PE	C2C-C2D-C2E-C2F
19	L	803	3PE	C36-C37-C38-C39
19	L	804	3PE	C3B-C3C-C3D-C3E
19	L	801	3PE	C37-C38-C39-C3A
20	C	702	DCQ	C7-C8-C9-C10
20	C	702	DCQ	C12-C13-C14-C15
19	M	1002	3PE	C3E-C3F-C3G-C3H
19	L	804	3PE	C24-C25-C26-C27
20	C	702	DCQ	C9-C10-C11-C12
19	I	203	3PE	C2A-C2B-C2C-C2D
19	L	803	3PE	C37-C38-C39-C3A
19	L	805	3PE	C21-C22-C23-C24
19	J	902	3PE	C21-C22-C23-C24
19	J	902	3PE	C24-C25-C26-C27
19	N	503	3PE	C25-C26-C27-C28
19	L	801	3PE	C23-C24-C25-C26
19	M	1002	3PE	C26-C27-C28-C29
19	M	1002	3PE	C2-C1-O11-P
15	F	502	FMN	C5'-O5'-P-O1P
21	H	601	LFA	C5-C6-C7-C8
19	C	701	3PE	C26-C27-C28-C29
19	J	902	3PE	O11-C1-C2-C3
19	J	902	3PE	O13-C11-C12-N
19	I	203	3PE	C22-C23-C24-C25
19	N	503	3PE	C2-C1-O11-P
19	L	805	3PE	C1-C2-C3-O31
19	H	602	3PE	C23-C24-C25-C26
19	M	1001	3PE	C34-C35-C36-C37
19	J	902	3PE	O11-C1-C2-O21
19	L	805	3PE	O21-C2-C3-O31
19	J	902	3PE	C2-C1-O11-P
19	L	805	3PE	O11-C1-C2-O21
16	F	503	NAI	C5B-O5B-PA-O3
19	C	701	3PE	C11-O13-P-O12
19	L	802	3PE	C11-O13-P-O12
19	L	803	3PE	C11-O13-P-O14
19	L	805	3PE	C11-O13-P-O14
19	M	1002	3PE	C1-O11-P-O12
19	M	1002	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
19	N	503	3PE	C1-O11-P-O12
19	J	902	3PE	C1-O11-P-O14
19	J	902	3PE	C11-O13-P-O14
19	L	805	3PE	O11-C1-C2-C3
19	L	804	3PE	C25-C26-C27-C28
20	B	302	DCQ	C5-C4-O4-C4M
20	B	302	DCQ	C7-C8-C9-C10
15	F	502	FMN	N10-C1'-C2'-C3'
19	L	804	3PE	O11-C1-C2-O21
19	N	503	3PE	O11-C1-C2-O21
19	L	801	3PE	C3D-C3E-C3F-C3G
19	L	803	3PE	C27-C28-C29-C2A
15	F	502	FMN	C4'-C5'-O5'-P
19	L	801	3PE	C11-O13-P-O11
16	F	503	NAI	O4D-C1D-N1N-C2N
20	C	702	DCQ	C11-C12-C13-C14
19	L	803	3PE	C2-C1-O11-P
19	L	804	3PE	C2-C1-O11-P
19	M	1001	3PE	C2-C1-O11-P
19	N	503	3PE	C3B-C3C-C3D-C3E
19	L	804	3PE	O21-C21-C22-C23
19	C	701	3PE	O13-C11-C12-N
19	M	1002	3PE	C29-C2A-C2B-C2C
15	F	502	FMN	O2'-C2'-C3'-C4'
20	C	702	DCQ	C10-C11-C12-C13
19	L	801	3PE	C29-C2A-C2B-C2C
19	J	902	3PE	C36-C37-C38-C39
19	L	804	3PE	O11-C1-C2-C3
19	L	805	3PE	O21-C21-C22-C23
19	L	803	3PE	C23-C24-C25-C26
20	B	302	DCQ	C3-C4-O4-C4M
19	N	503	3PE	C2D-C2E-C2F-C2G
19	N	503	3PE	C23-C24-C25-C26
19	C	701	3PE	C27-C28-C29-C2A
16	F	503	NAI	C2D-C1D-N1N-C2N
19	C	701	3PE	O31-C31-C32-C33
19	L	801	3PE	C31-C32-C33-C34
19	L	804	3PE	C33-C34-C35-C36
19	J	902	3PE	C23-C24-C25-C26
19	N	503	3PE	C22-C23-C24-C25
15	F	502	FMN	O2'-C2'-C3'-O3'
19	M	1003	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
19	L	802	3PE	O31-C31-C32-C33
19	C	701	3PE	O32-C31-C32-C33
19	L	802	3PE	O32-C31-C32-C33
19	M	1002	3PE	C1-O11-P-O14
19	J	902	3PE	C12-C11-O13-P
19	L	805	3PE	O31-C31-C32-C33
19	H	602	3PE	C34-C35-C36-C37
15	F	502	FMN	N10-C1'-C2'-O2'

There are no ring outliers.

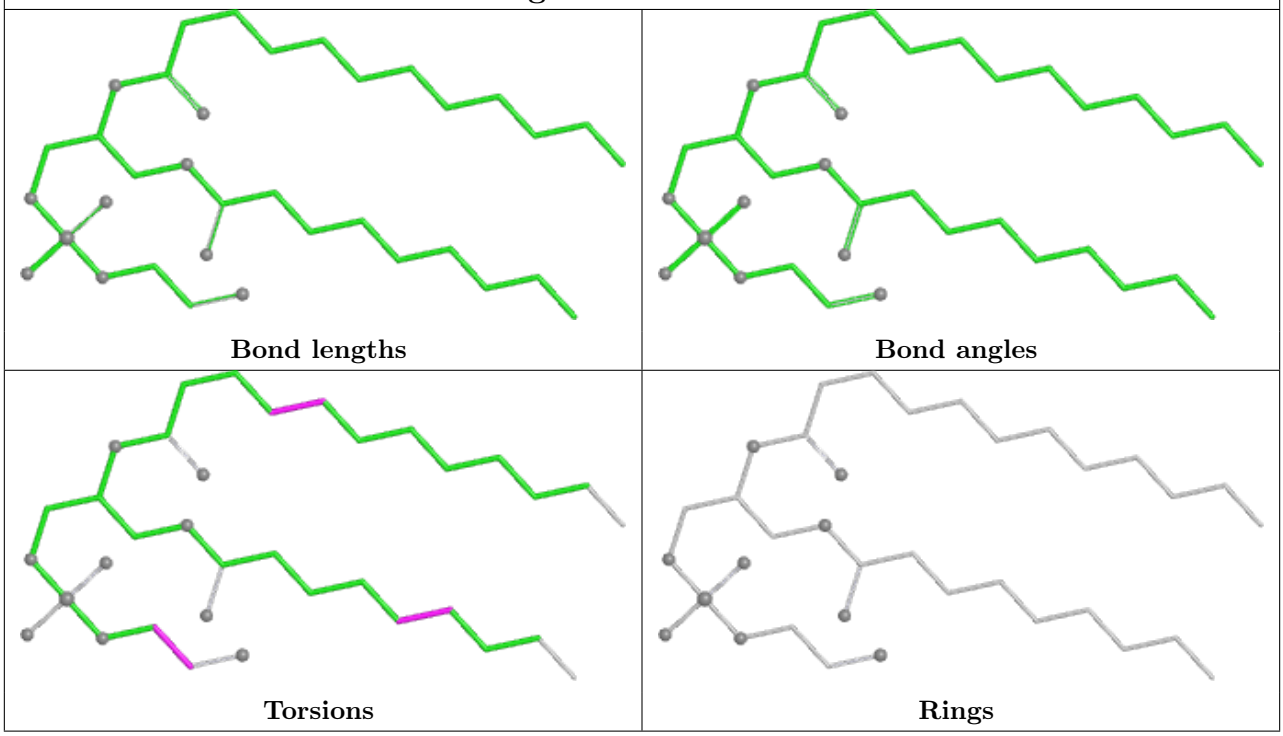
18 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	H	602	3PE	3	0
16	F	503	NAI	3	0
19	J	902	3PE	4	0
14	B	301	SF4	1	0
19	L	802	3PE	2	0
19	I	203	3PE	1	0
19	L	801	3PE	2	0
14	F	501	SF4	1	0
19	C	701	3PE	5	0
19	N	503	3PE	1	0
19	M	1001	3PE	3	0
20	B	302	DCQ	1	0
20	C	702	DCQ	1	0
19	M	1003	3PE	1	0
19	M	1002	3PE	1	0
19	L	804	3PE	3	0
19	L	803	3PE	1	0
15	F	502	FMN	2	0

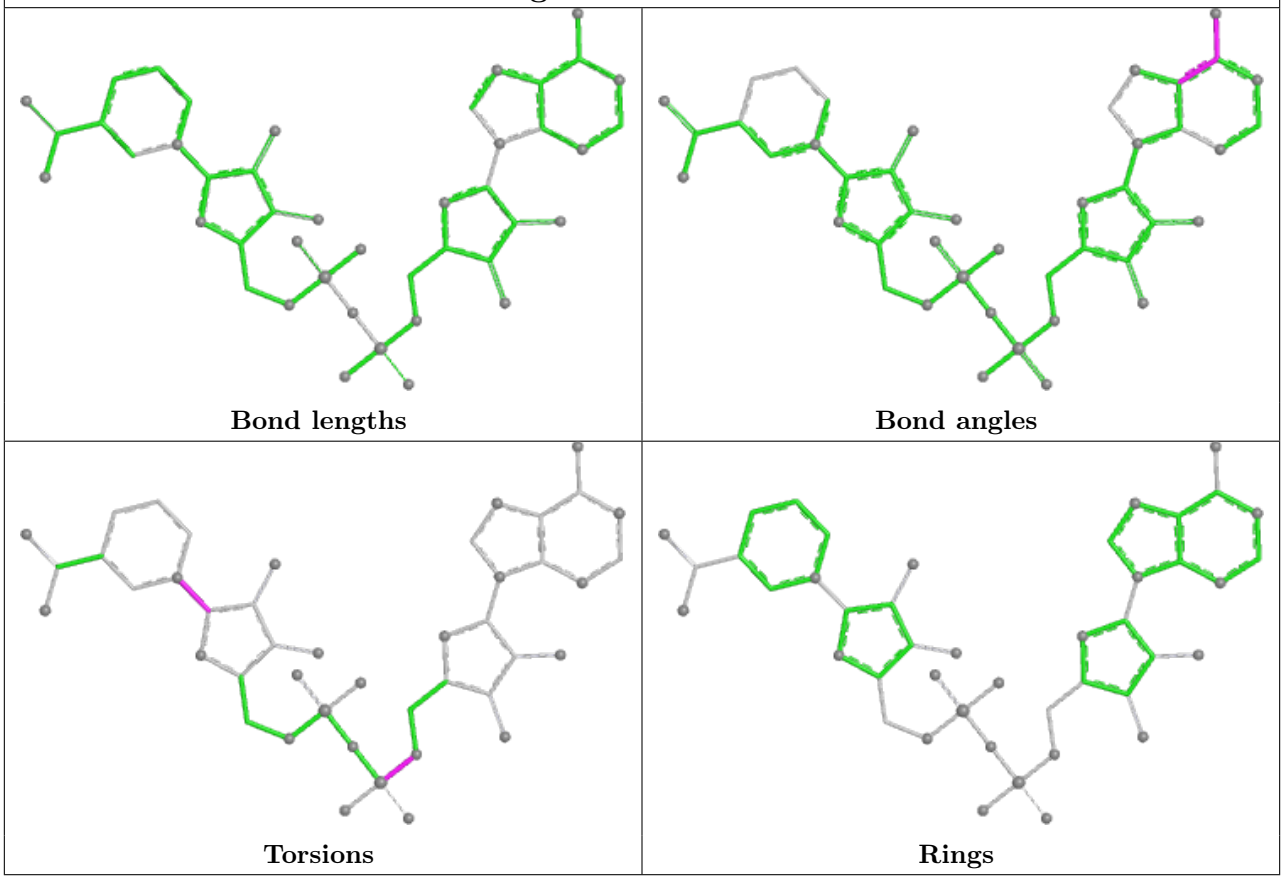
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

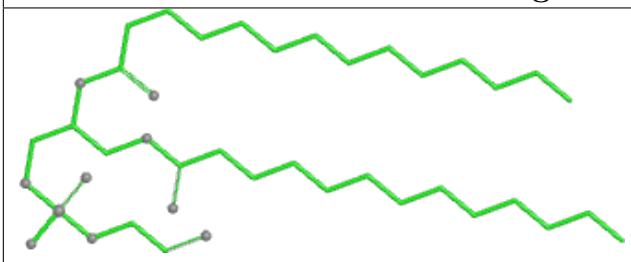
Ligand 3PE H 602



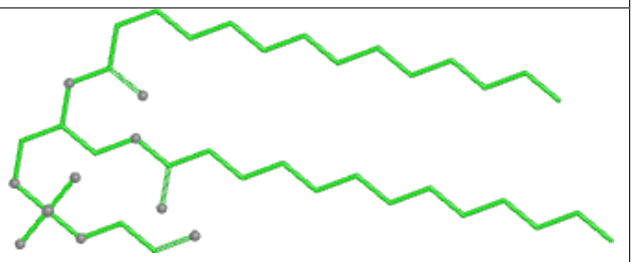
Ligand NAI F 503



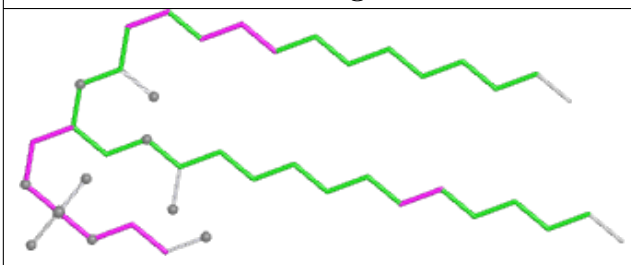
Ligand 3PE J 902



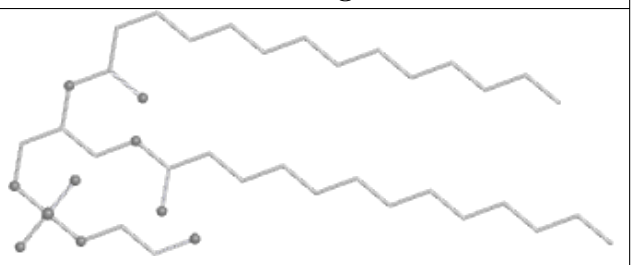
Bond lengths



Bond angles

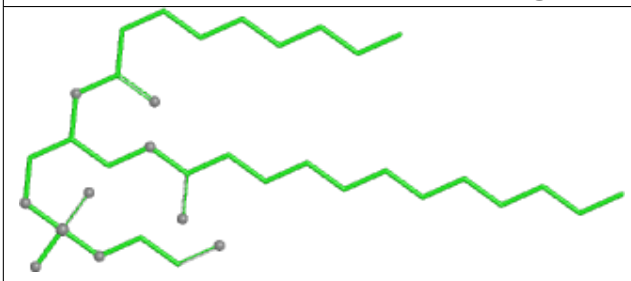


Torsions

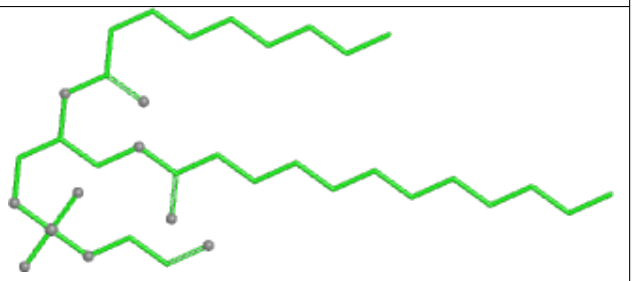


Rings

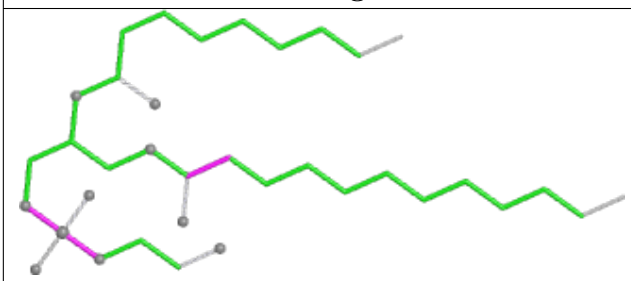
Ligand 3PE L 802



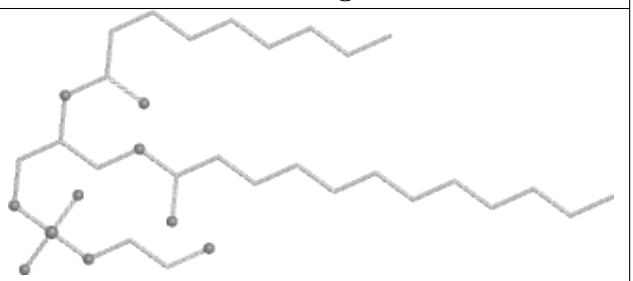
Bond lengths



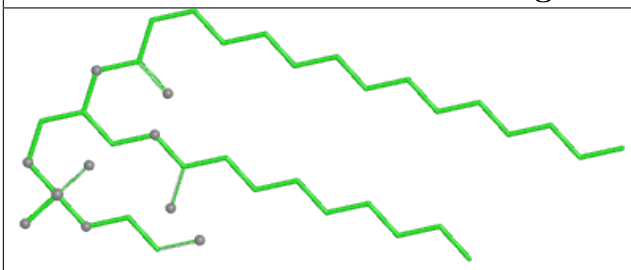
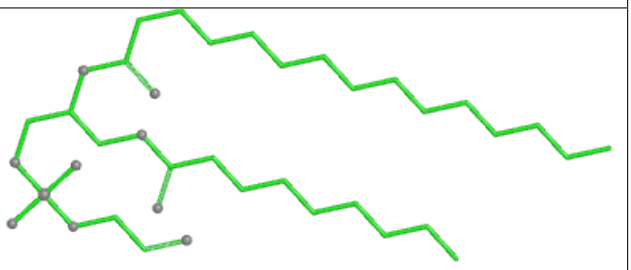
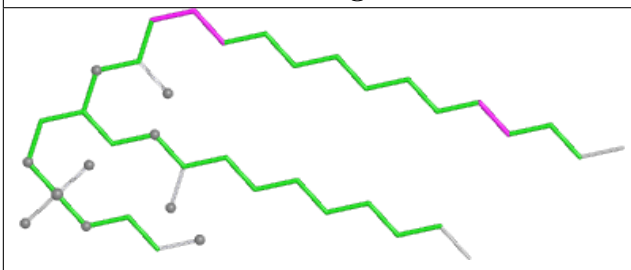
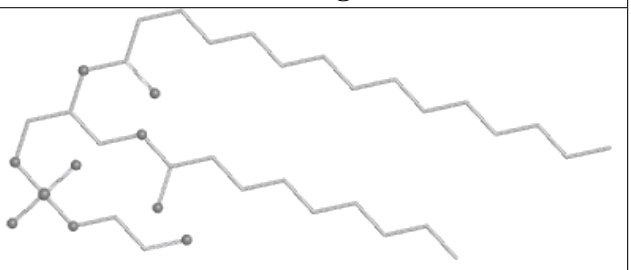
Bond angles

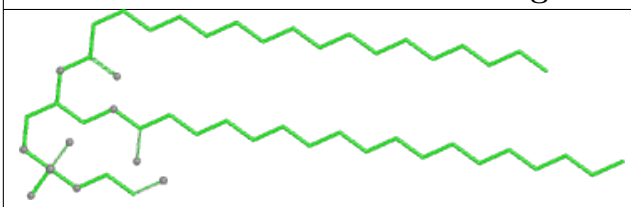
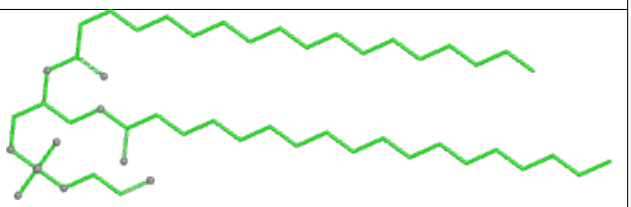
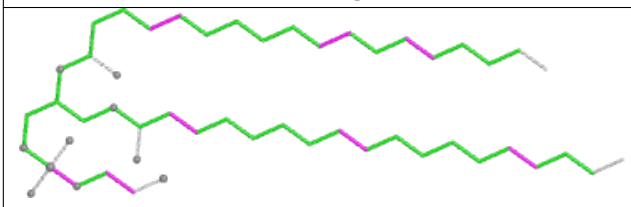
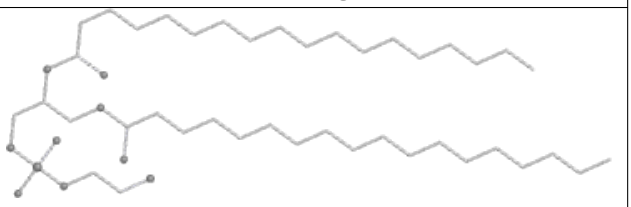


Torsions

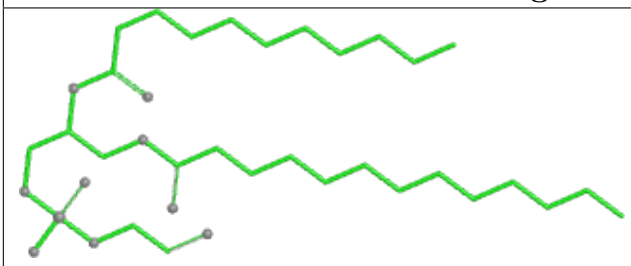


Rings

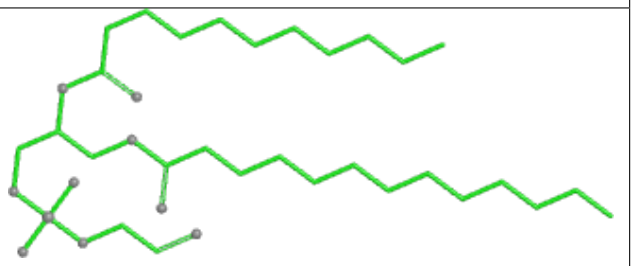
Ligand 3PE I 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

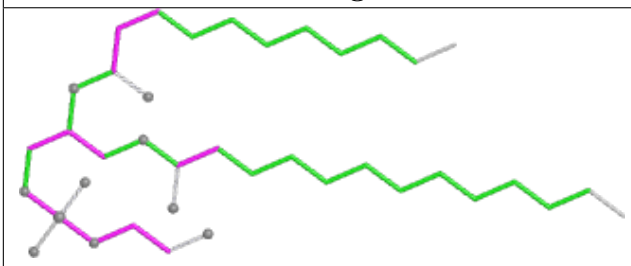
Ligand 3PE L 805



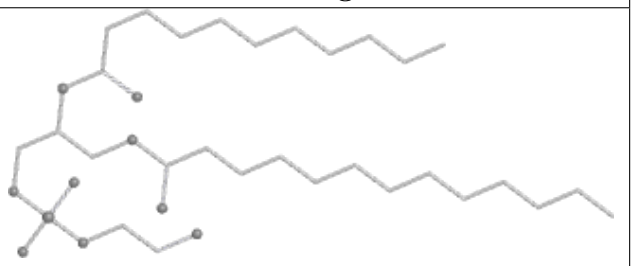
Bond lengths



Bond angles

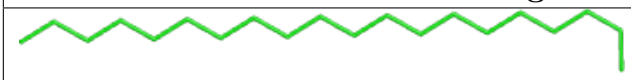


Torsions

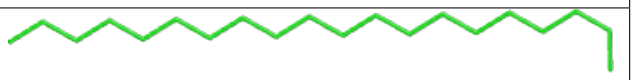


Rings

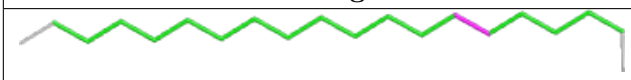
Ligand LFA H 601



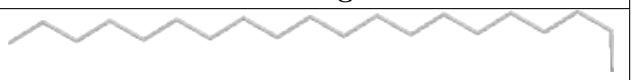
Bond lengths



Bond angles

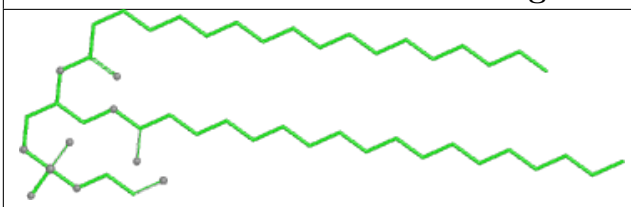


Torsions

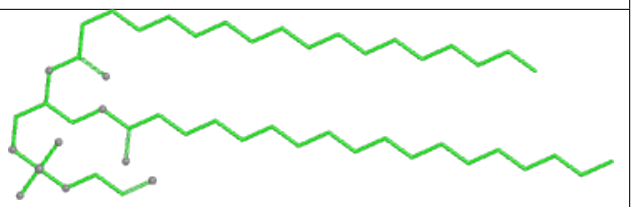


Rings

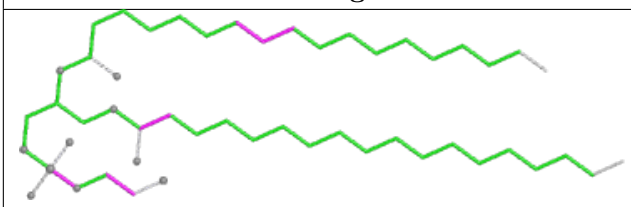
Ligand 3PE C 701



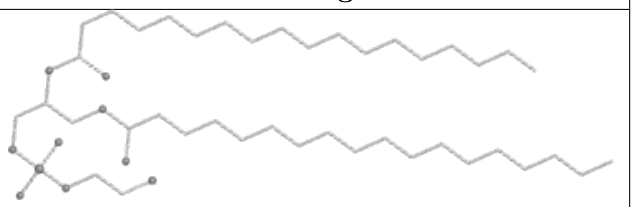
Bond lengths



Bond angles

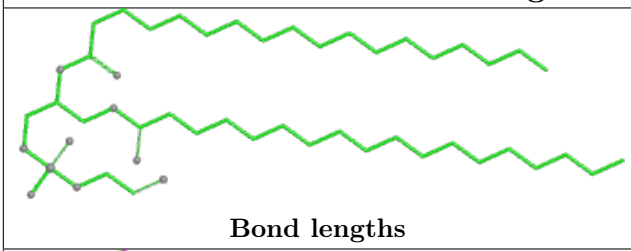


Torsions

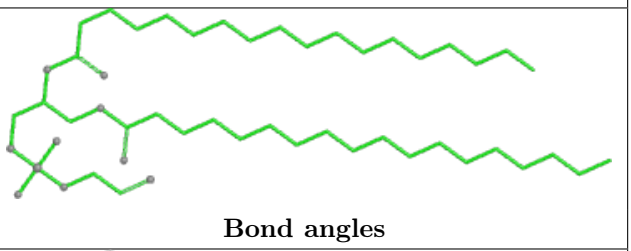


Rings

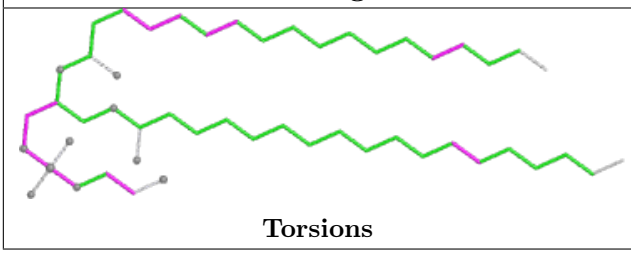
Ligand 3PE N 503



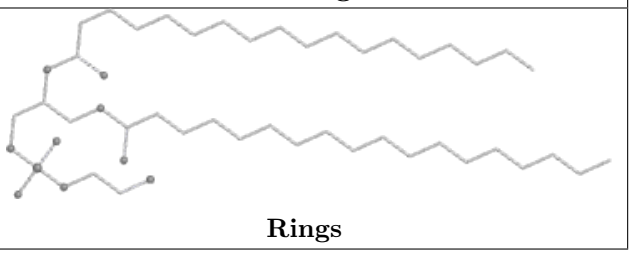
Bond lengths



Bond angles

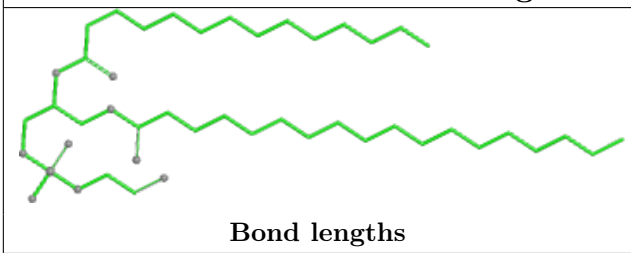


Torsions

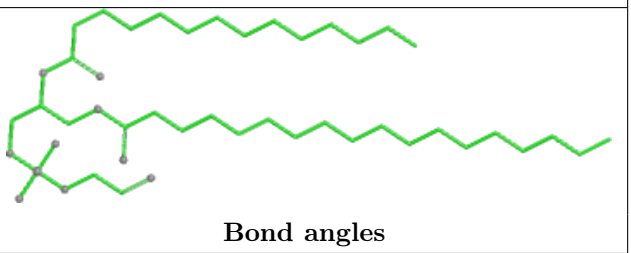


Rings

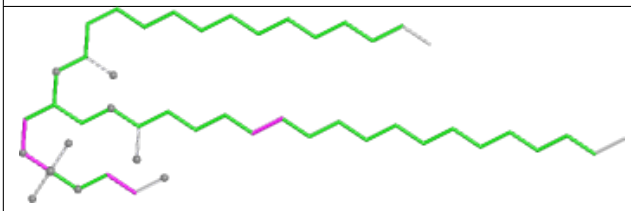
Ligand 3PE M 1001



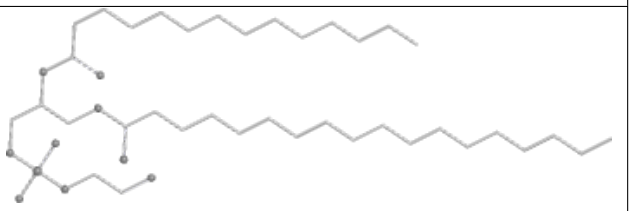
Bond lengths



Bond angles

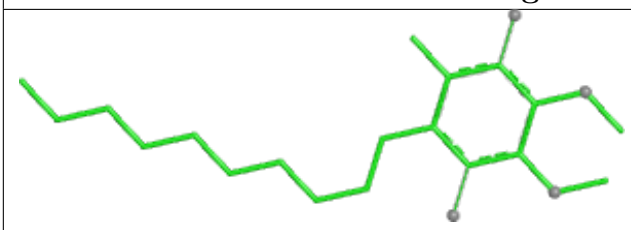


Torsions

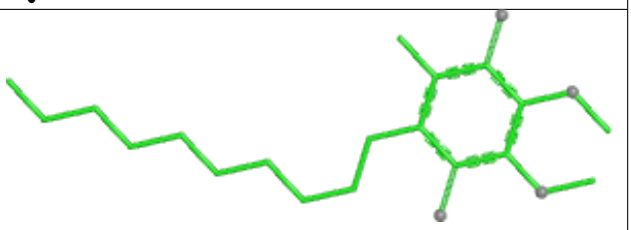


Rings

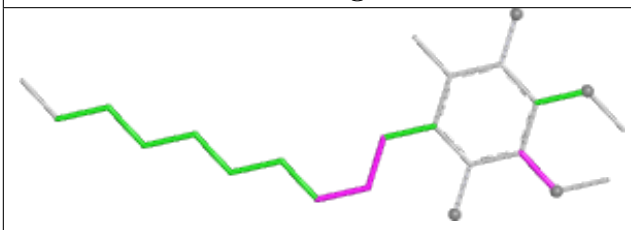
Ligand DCQ B 302



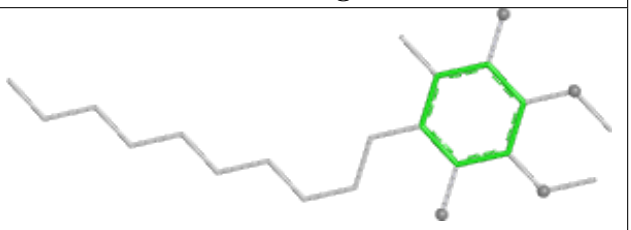
Bond lengths



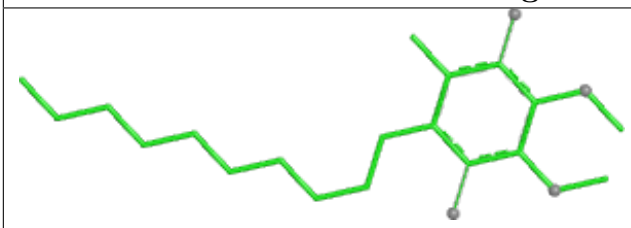
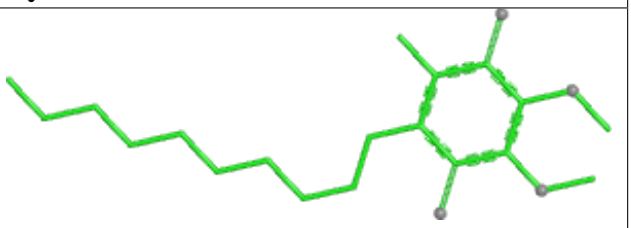
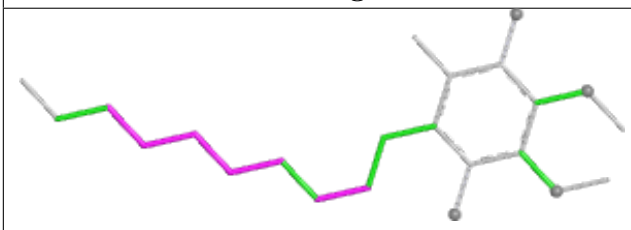
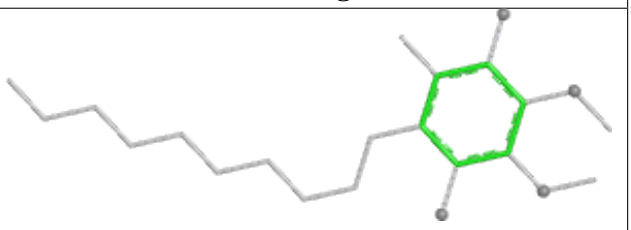
Bond angles

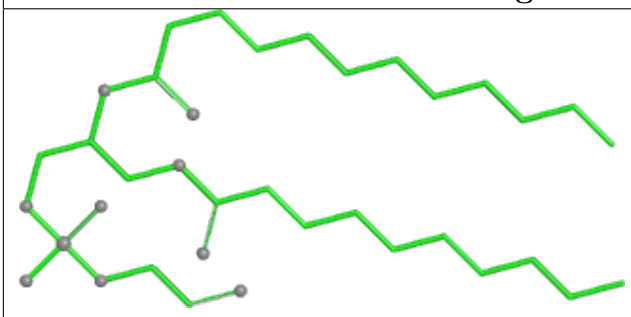
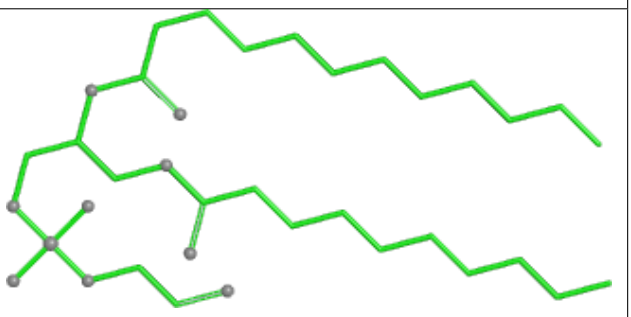
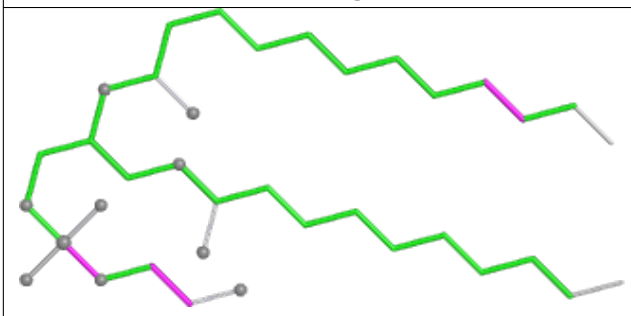
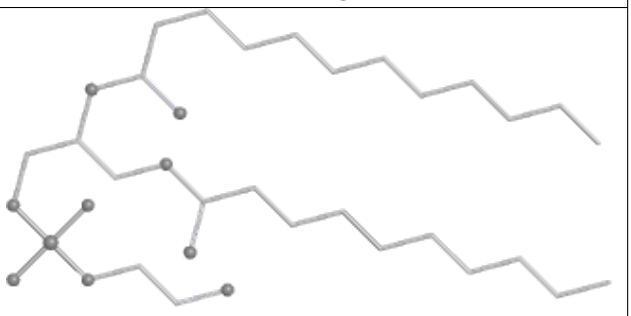


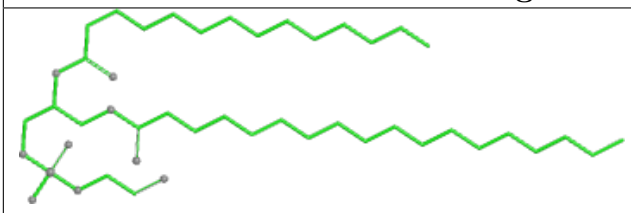
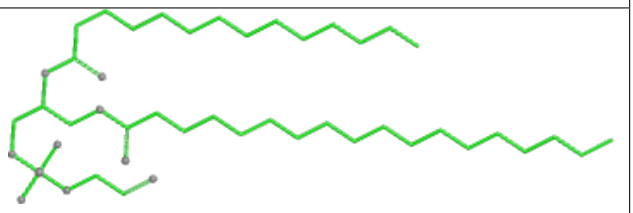
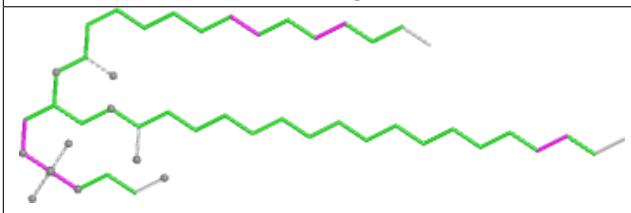
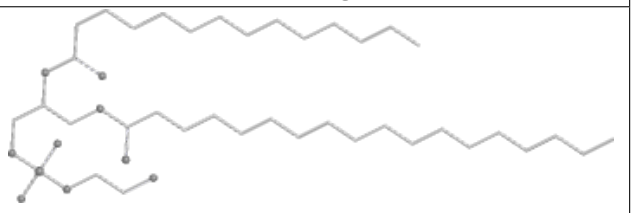
Torsions

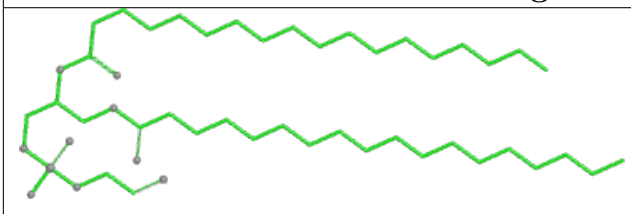
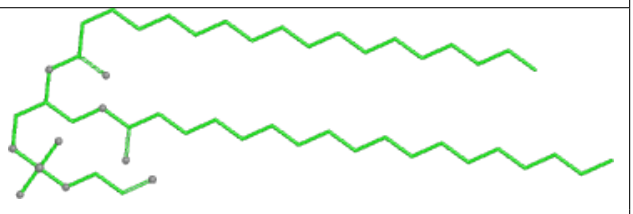
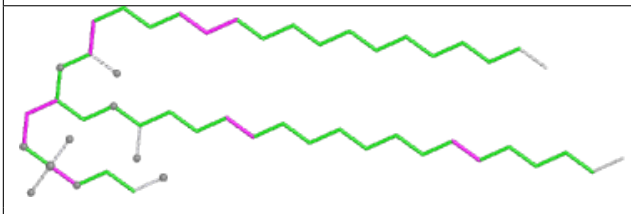
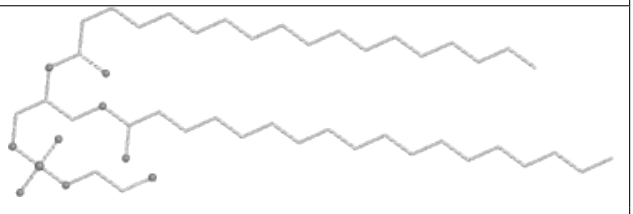


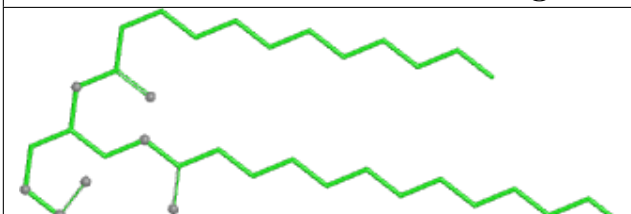
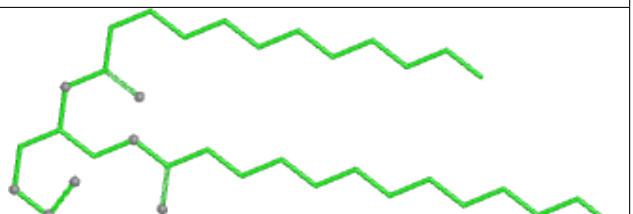
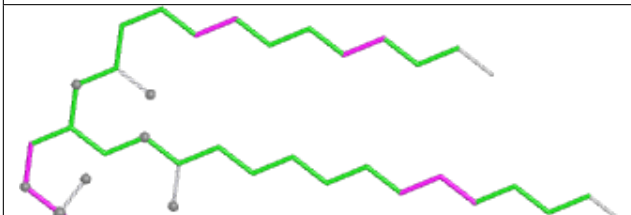
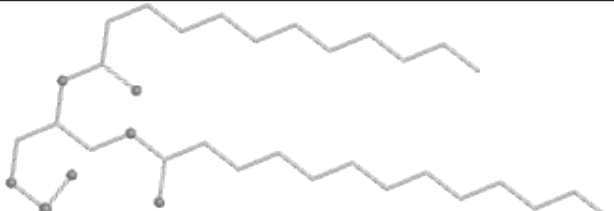
Rings

Ligand DCQ C 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

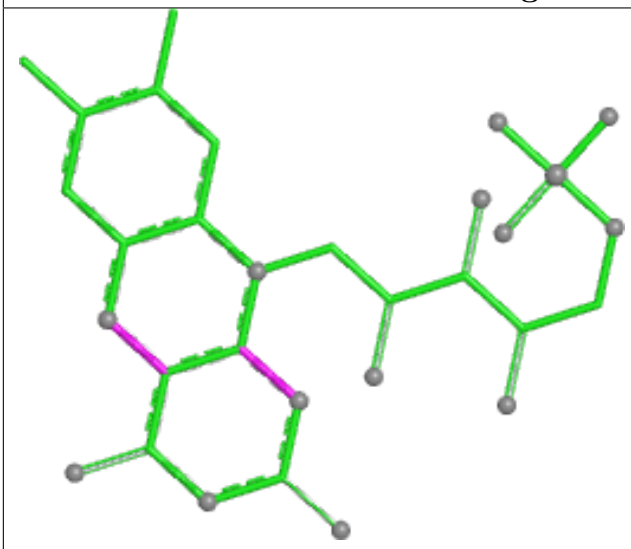
Ligand 3PE M 1003	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE M 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

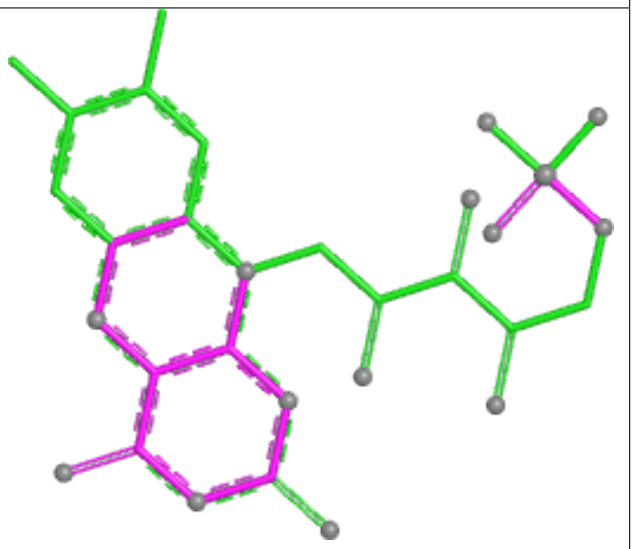
Ligand 3PE L 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

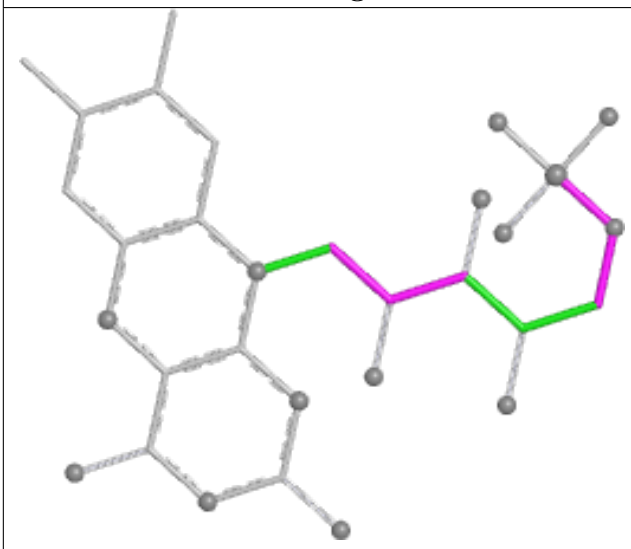
Ligand FMN F 502



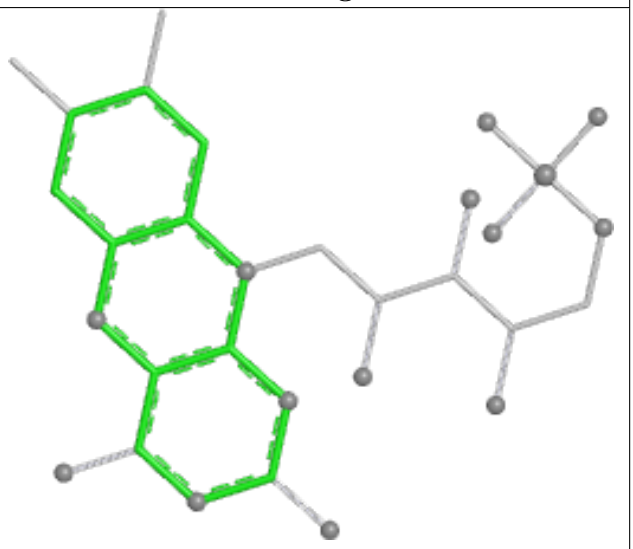
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

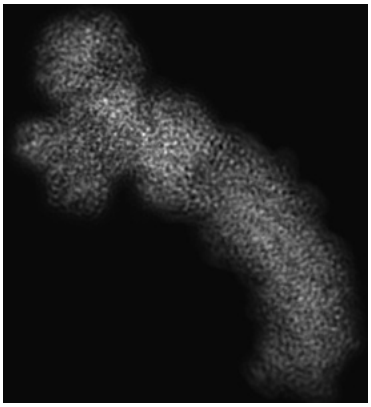
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14536. These allow visual inspection of the internal detail of the map and identification of artifacts.

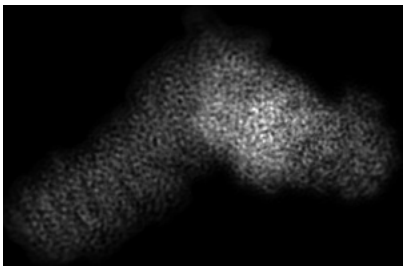
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

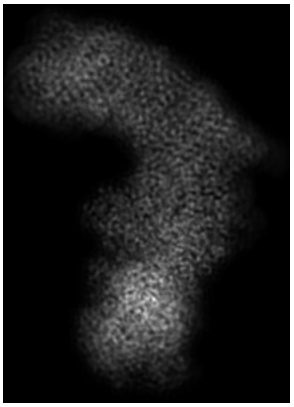
6.1.1 Primary map



X



Y



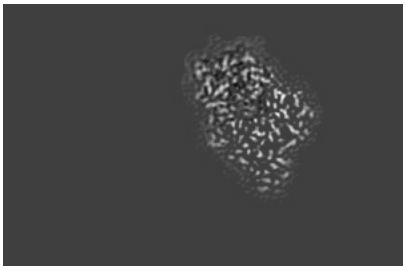
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 153



Y Index: 214

Z Index: 235

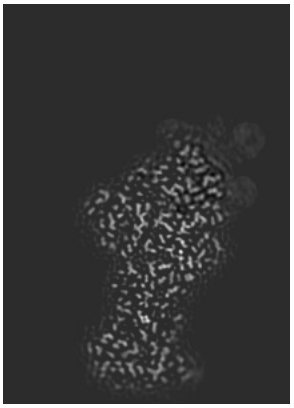
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 160

Y Index: 110



Z Index: 305

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

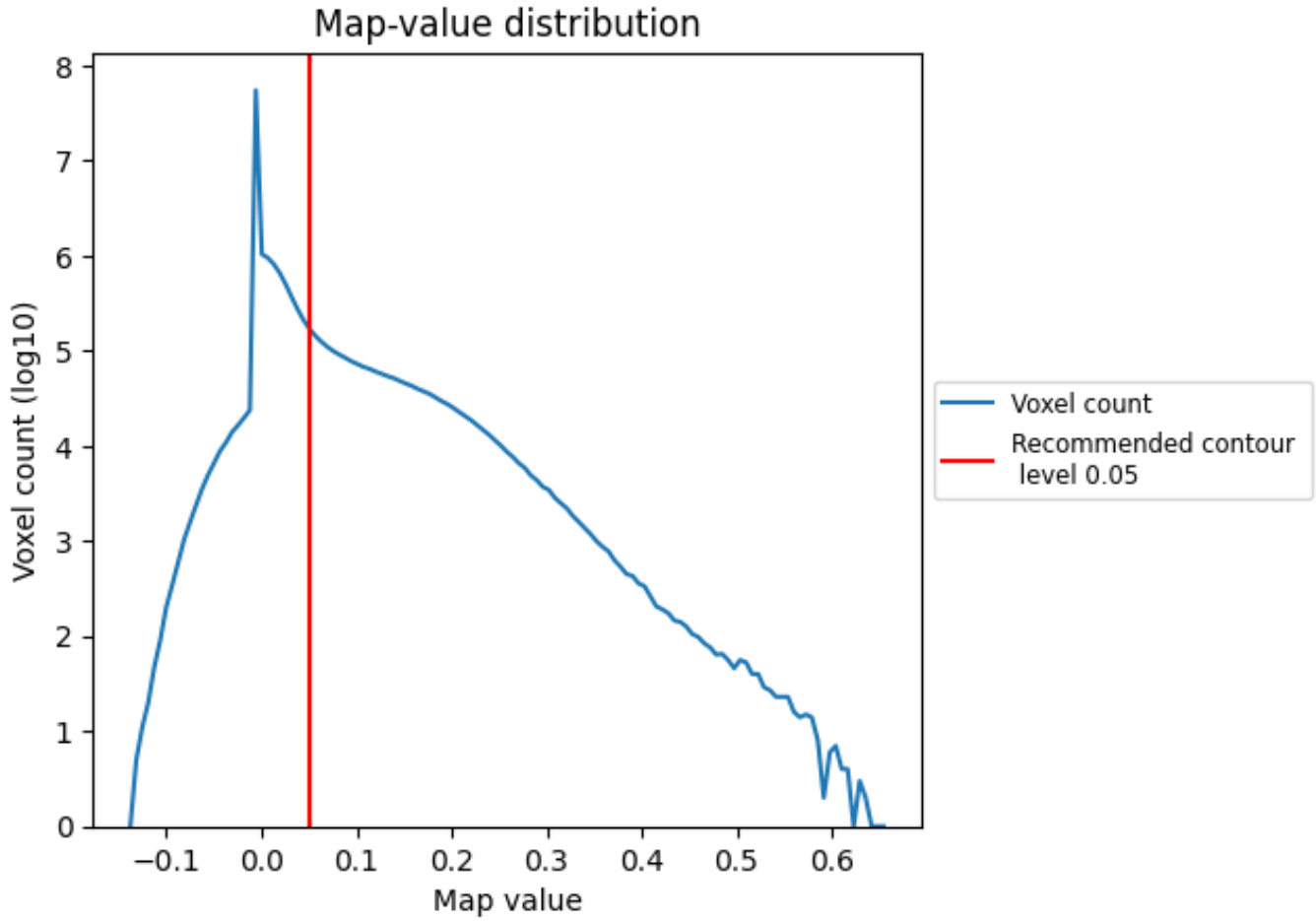
6.5 Mask visualisation (i)

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

7 Map analysis

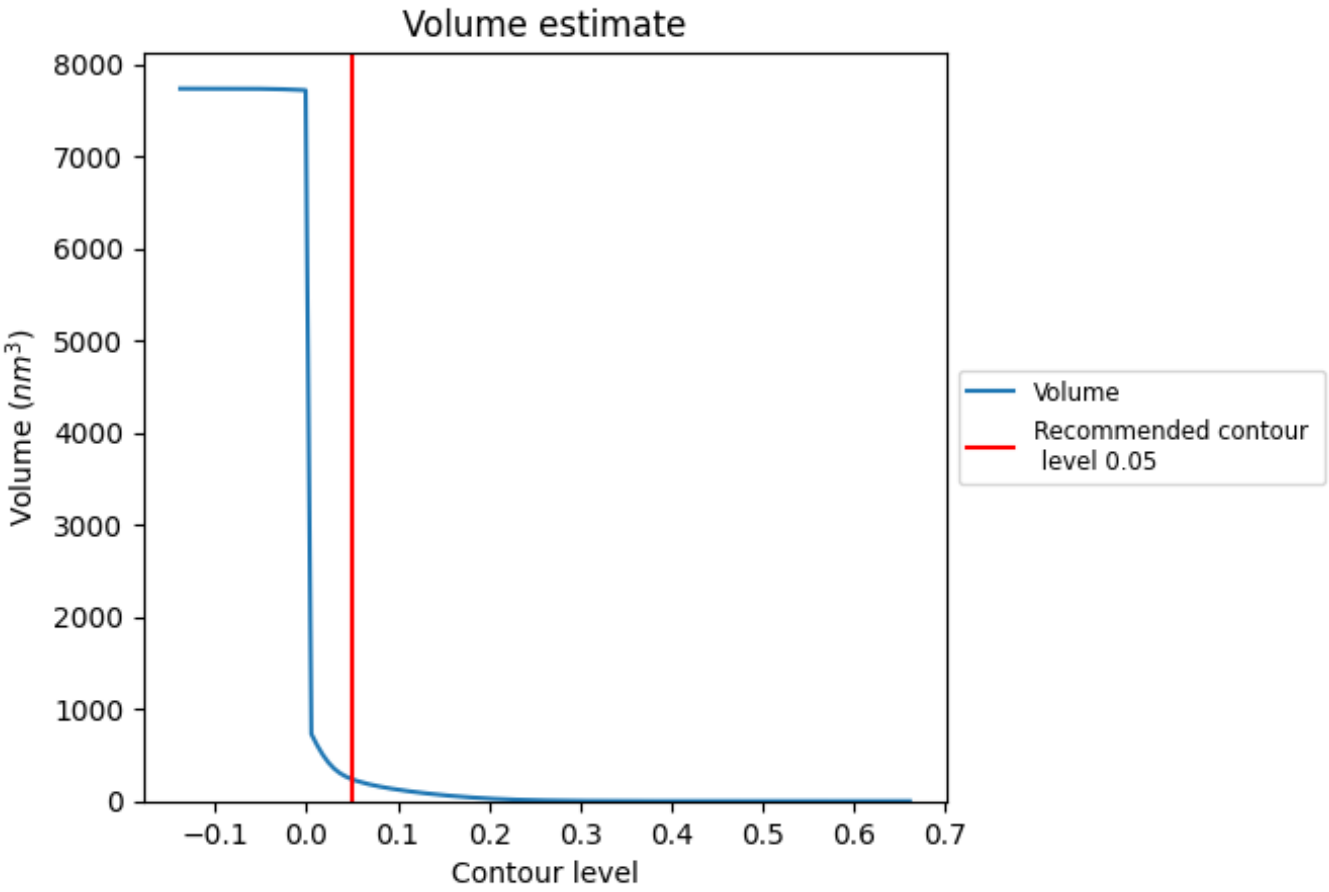
This section contains the results of statistical analysis of the map.

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 239 nm^3; this corresponds to an approximate mass of 216 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.

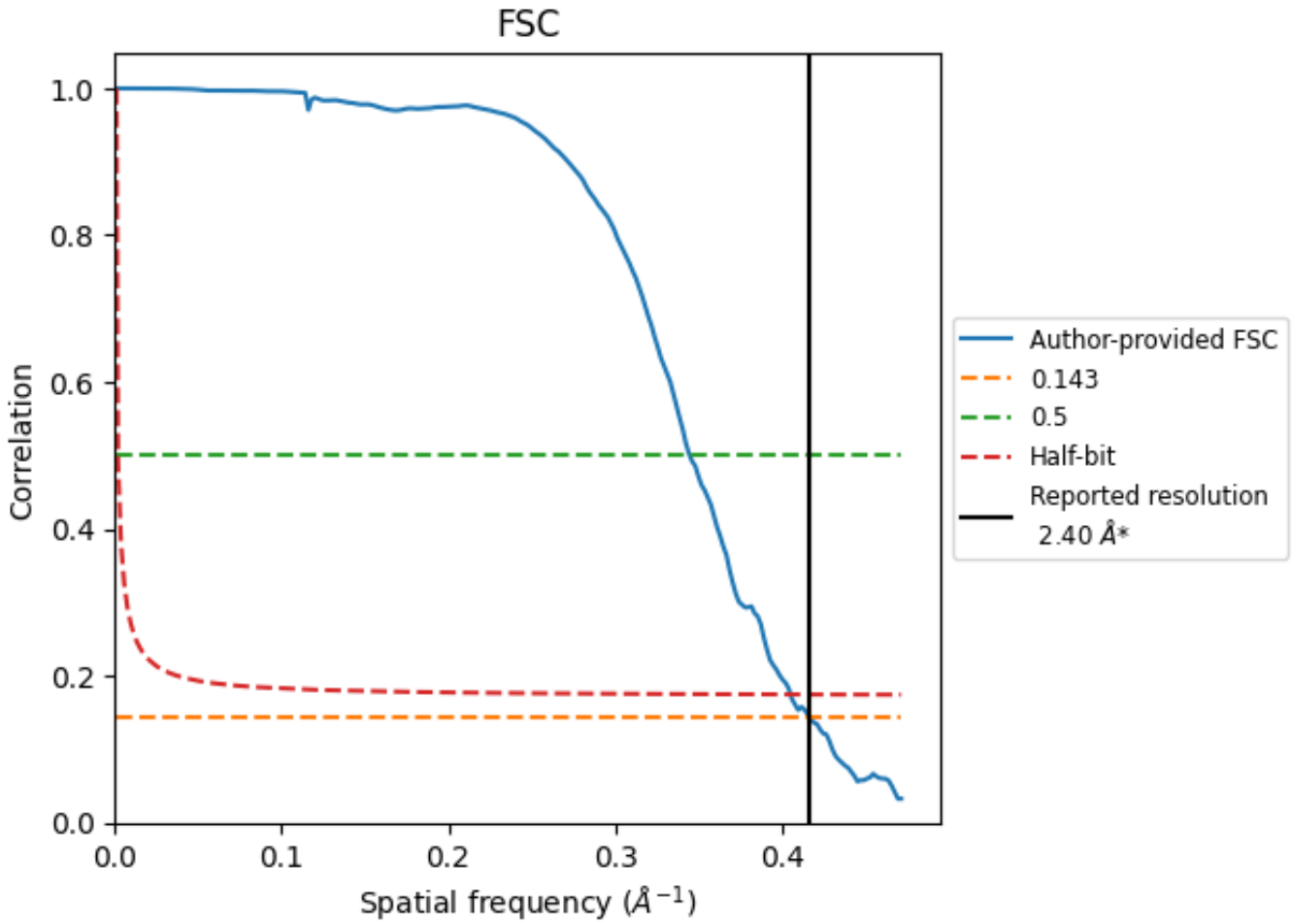
7.3 Rotationally averaged power spectrum

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 0.417 Å^{-1}

8.2 Resolution estimates (i)

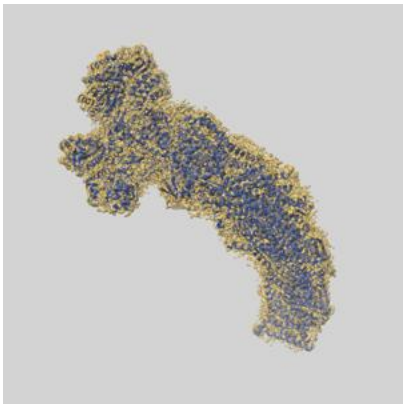
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.90	2.47
Unmasked-calculated*	-	-	-

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

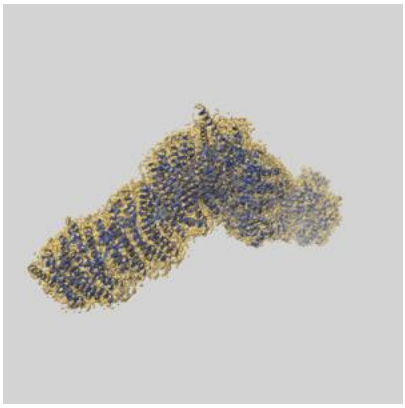
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14536 and PDB model 7Z7S. Per-residue inclusion information can be found in section 3 on page 12.

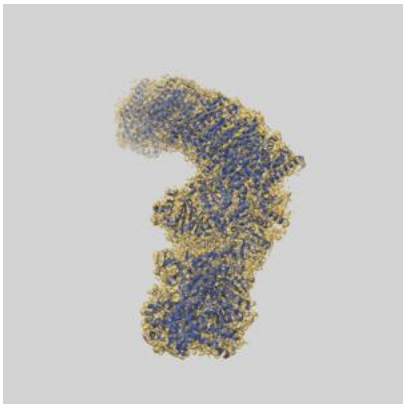
9.1 Map-model overlay



X



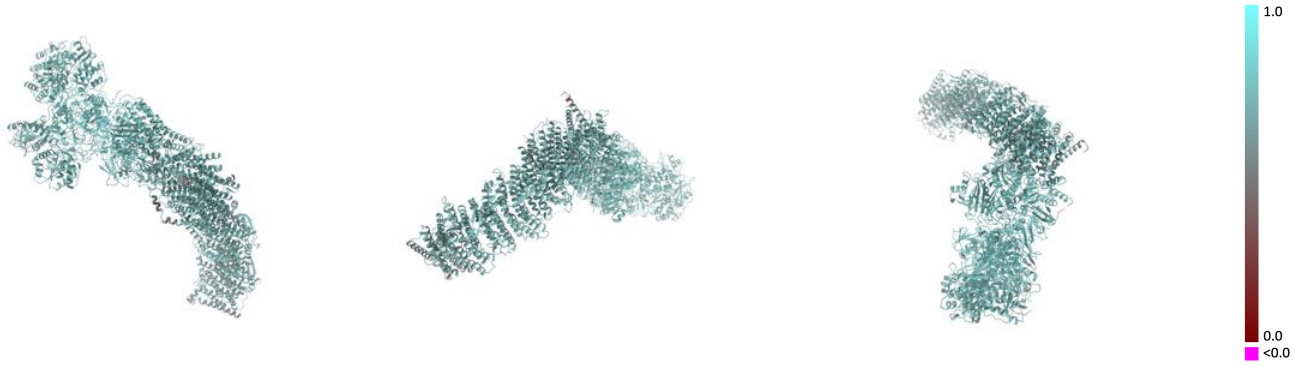
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

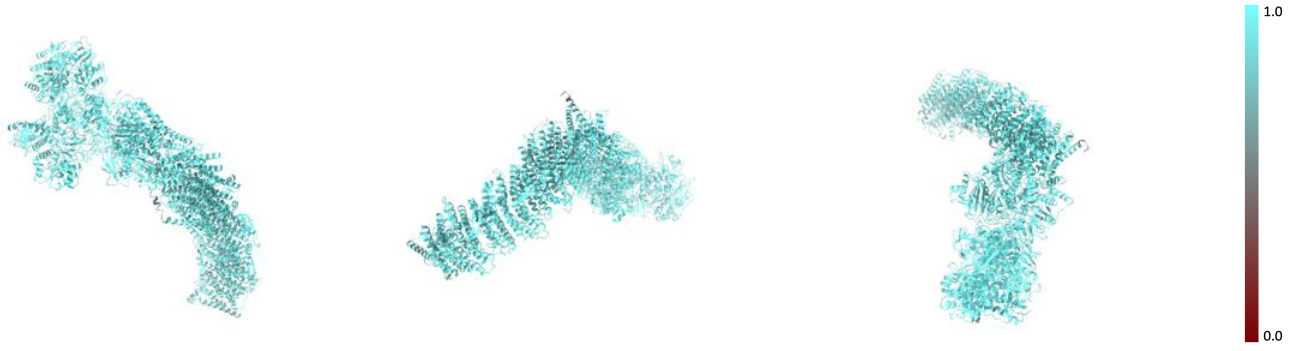
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

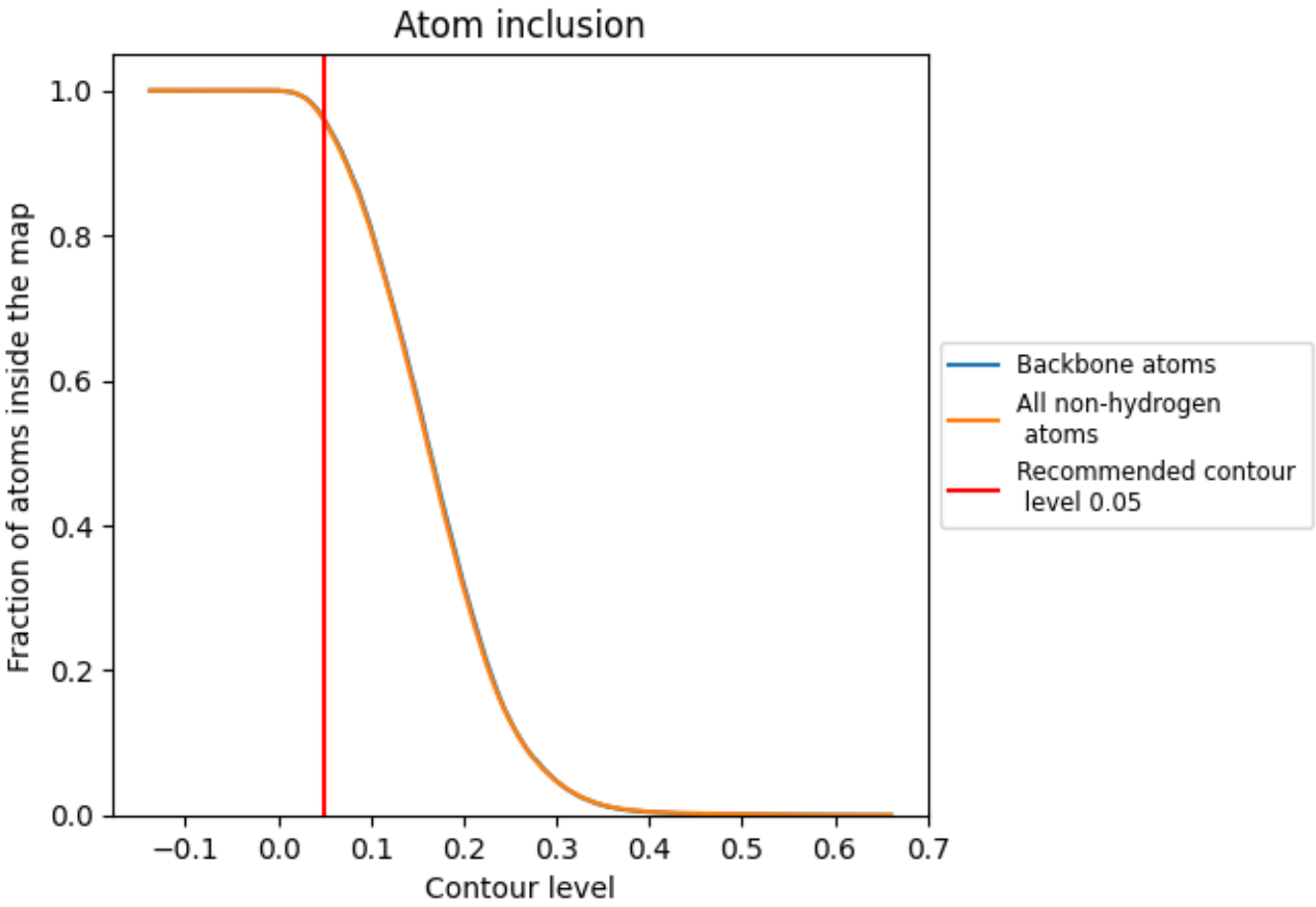
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9578	0.6900
A	0.9702	0.6740
B	0.9666	0.7120
C	0.9773	0.7270
E	0.9559	0.6890
F	0.9675	0.6980
G	0.9746	0.7190
H	0.9577	0.6650
I	0.9725	0.7330
J	0.9168	0.6480
K	0.9691	0.6860
L	0.9152	0.6320
M	0.9516	0.6690
N	0.9633	0.6820