Full wwPDB EM Validation Report ⓘ

Oct 1, 2022 – 10:01 am BST

PDB ID	:	7ZCI
EMDB ID	:	EMD-14632
Title	:	Complex I from E. coli, LMNG-purified, under Turnover at pH 6, Resting state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2022-03-28
Resolution	:	2.69 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:

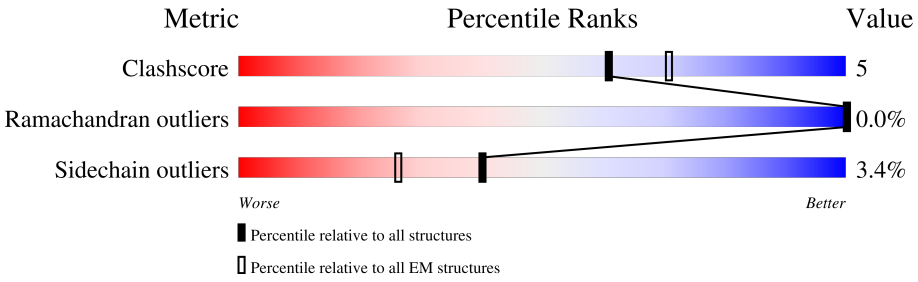
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.69 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	85% 14%
2	E	166	80% 14% 6%
3	G	908	89% 11%
4	C	596	84% 12%
5	B	220	5% 58% 17% 23%
6	I	180	71% 9% 19%
7	H	325	10% 81% 13% 5%
8	A	147	5% 60% 8% 31%

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Mol	Chain	Length	Quality of chain
9	L	613	85% 12%
10	M	509	84% 14%
11	N	485	83% 14%
12	K	100	82% 17%
13	J	184	7% 70% 18% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	SF4	B	301	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 36981 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	7027	4392	1269	1329	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	576	4628	2966	807	833	22	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	169	1339	848	231	243	17	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	309	Total	C	N	O	S	0	0
			2422	1628	375	401	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
			796	547	120	125	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	601	Total	C	N	O	S	0	0
			4593	3055	734	772	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
			3635	2427	574	614	20		

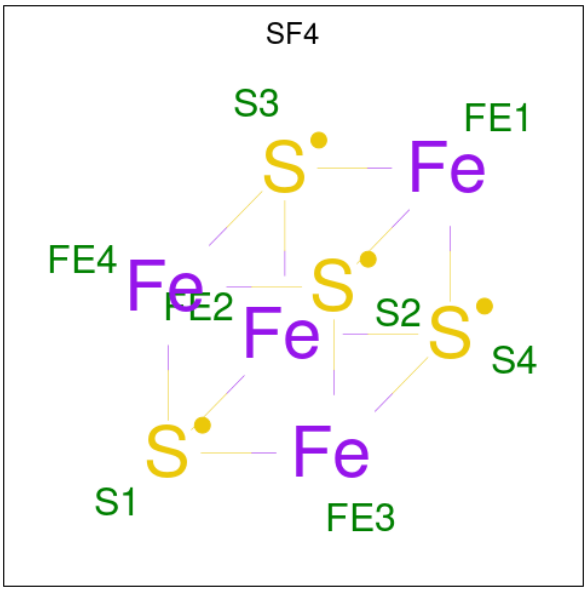
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

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.

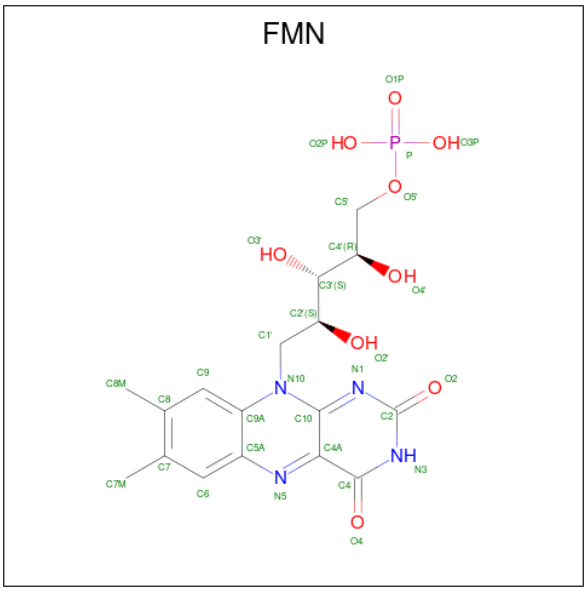
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	162	Total	C	N	O	S	0	0
			1226	824	188	207	7		

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



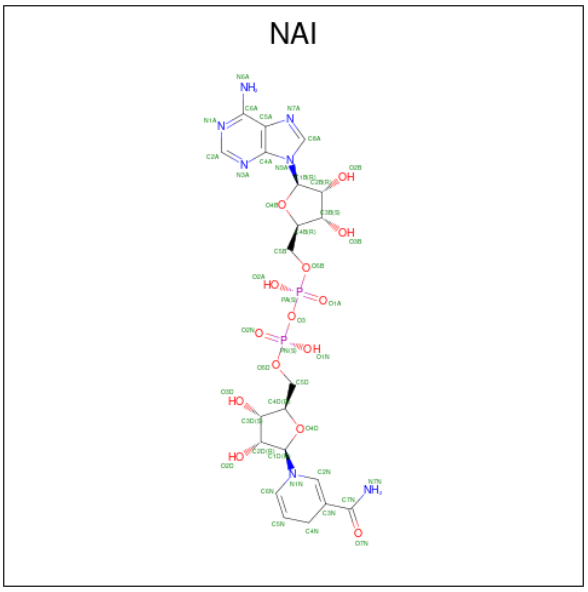
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	B	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 16 8 8	0
14	I	1	Total Fe S 16 8 8	0

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



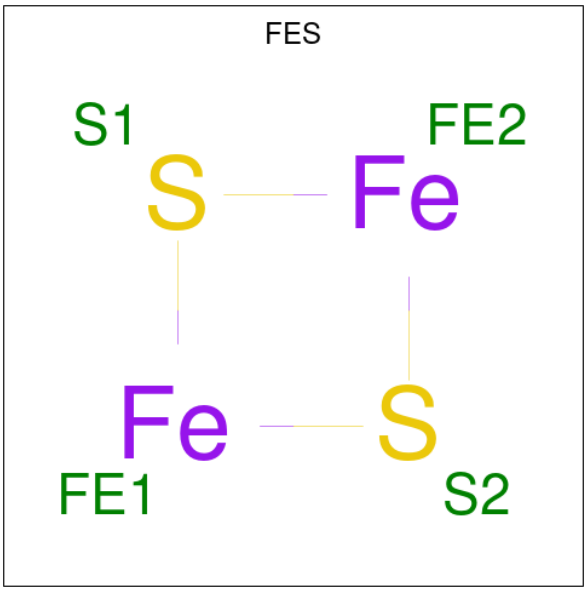
Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- 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).

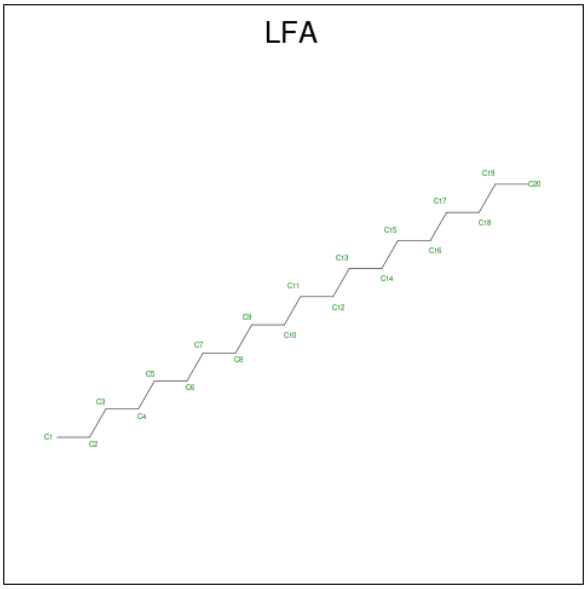


Mol	Chain	Residues	Atoms	AltConf
17	E	1	Total Fe S 4 2 2	0
17	G	1	Total Fe S 4 2 2	0

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

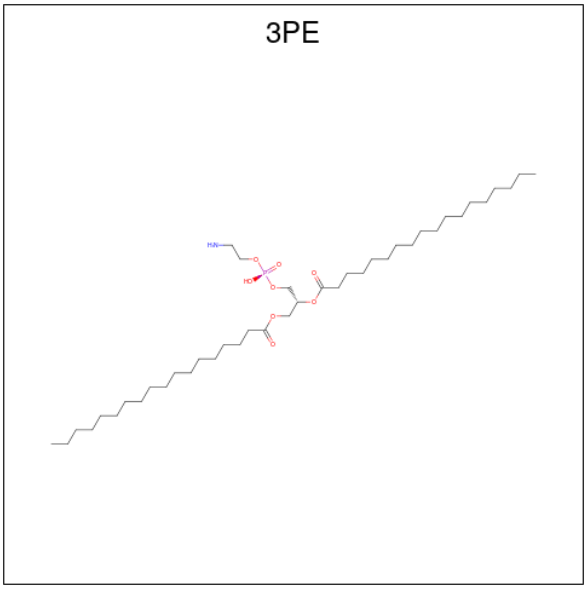
Mol	Chain	Residues	Atoms	AltConf
18	G	1	Total Ca 1 1	0

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



Mol	Chain	Residues	Atoms	AltConf
19	H	1	Total C 20 20	0
19	A	1	Total C 20 20	0
19	L	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 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
20	H	1	Total C N O P 51 41 1 8 1	0
20	L	1	Total C N O P 306 246 6 48 6	0
20	L	1	Total C N O P 306 246 6 48 6	0
20	L	1	Total C N O P 306 246 6 48 6	0
20	L	1	Total C N O P 306 246 6 48 6	0
20	L	1	Total C N O P 306 246 6 48 6	0

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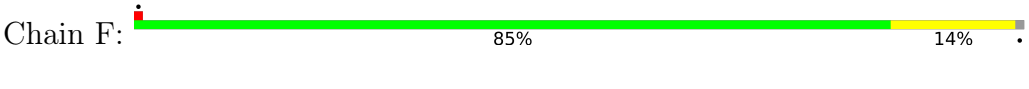
Mol	Chain	Residues	Atoms					AltConf
20	L	1	Total	C	N	O	P	0
			306	246	6	48	6	
20	M	1	Total	C	N	O	P	0
			102	82	2	16	2	
20	M	1	Total	C	N	O	P	0
			102	82	2	16	2	
20	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
20	J	1	Total	C	N	O	P	0
			51	41	1	8	1	

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.

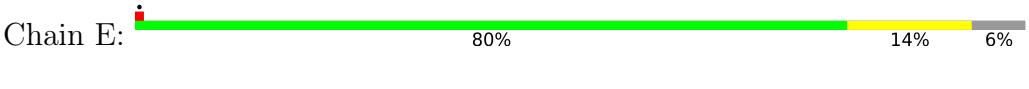
• Molecule 1: NADH-quinone oxidoreductase subunit F

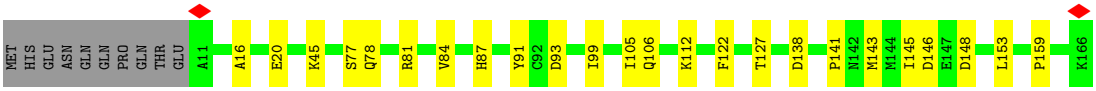
Chain F:



• Molecule 2: NADH dehydrogenase I subunit E

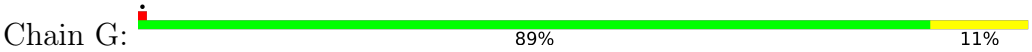
Chain E:

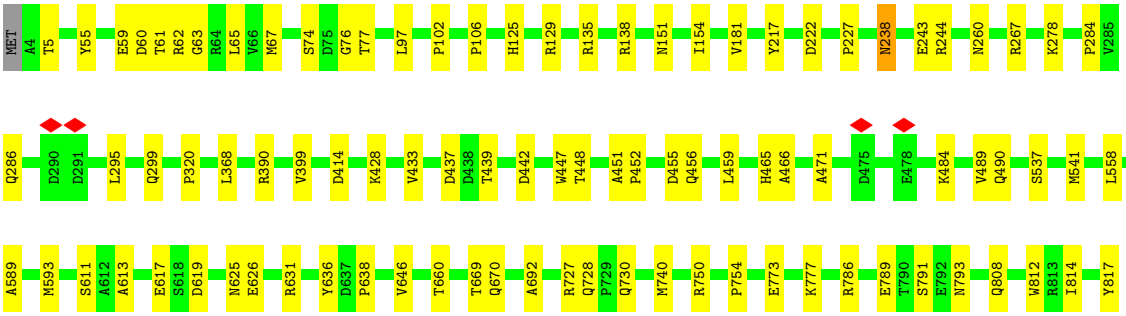


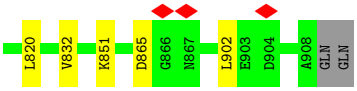


• Molecule 3: NADH-quinone oxidoreductase

Chain G:

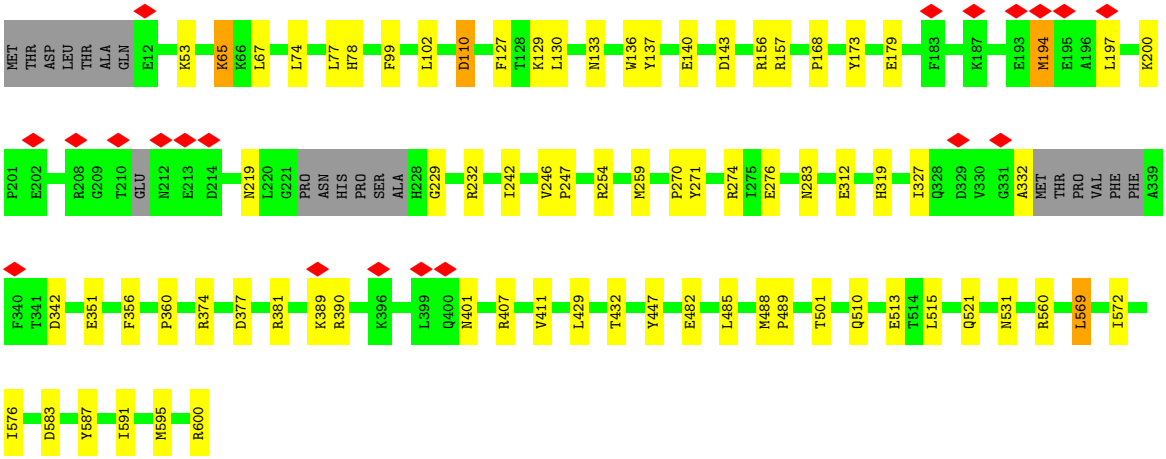






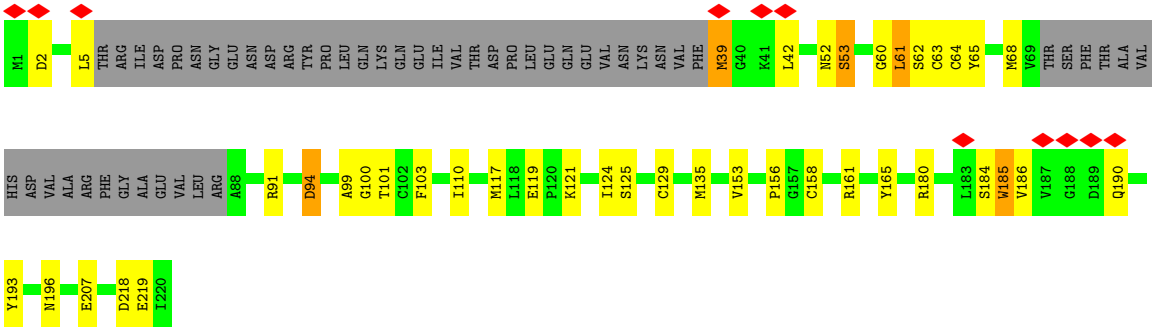
• Molecule 4: NADH-quinone oxidoreductase subunit C/D

Chain C:



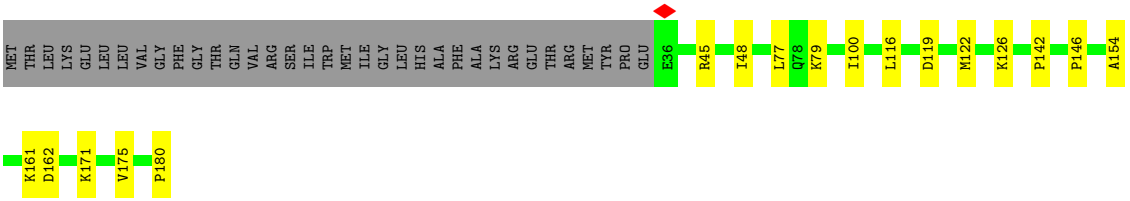
• Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:



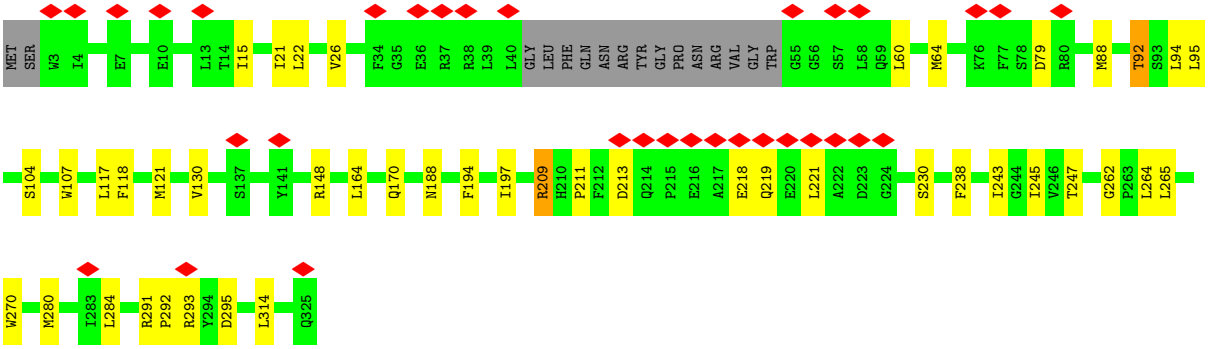
• Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:



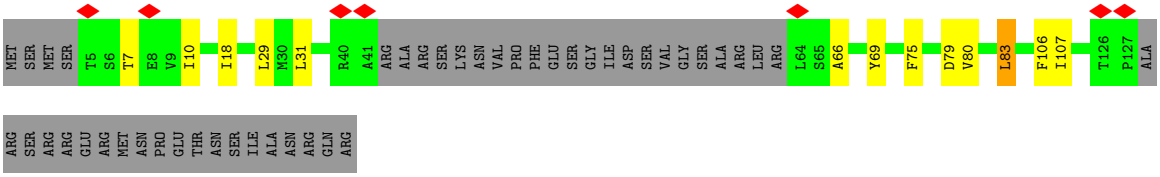
• Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:



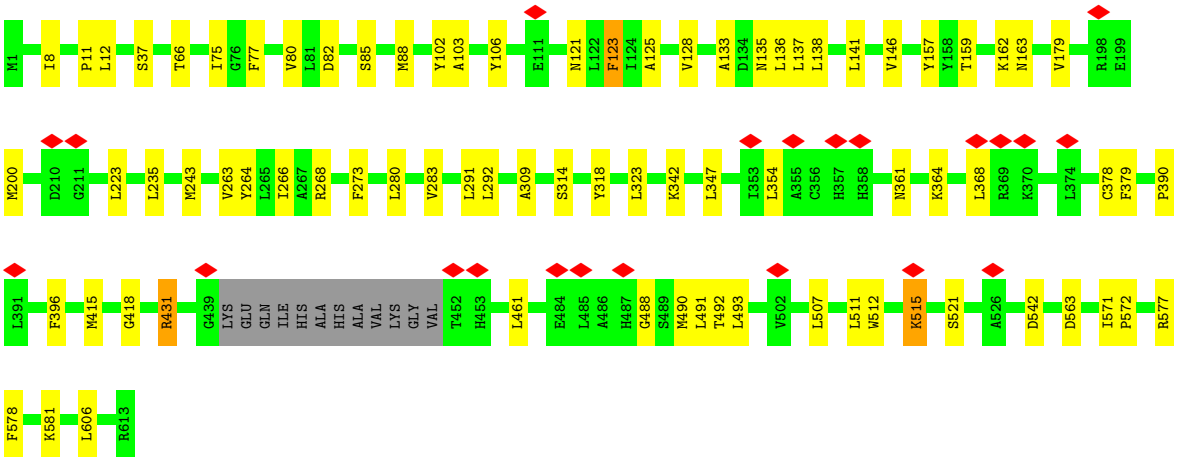
• Molecule 8: NADH-quinone oxidoreductase subunit A

Chain A:



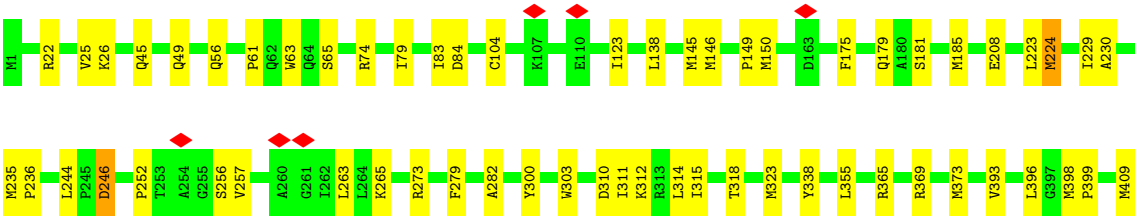
• Molecule 9: NADH dehydrogenase subunit L

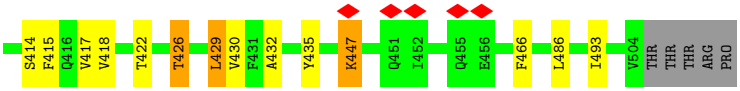
Chain L:



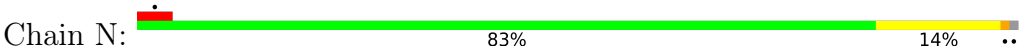
• Molecule 10: NADH dehydrogenase I subunit M

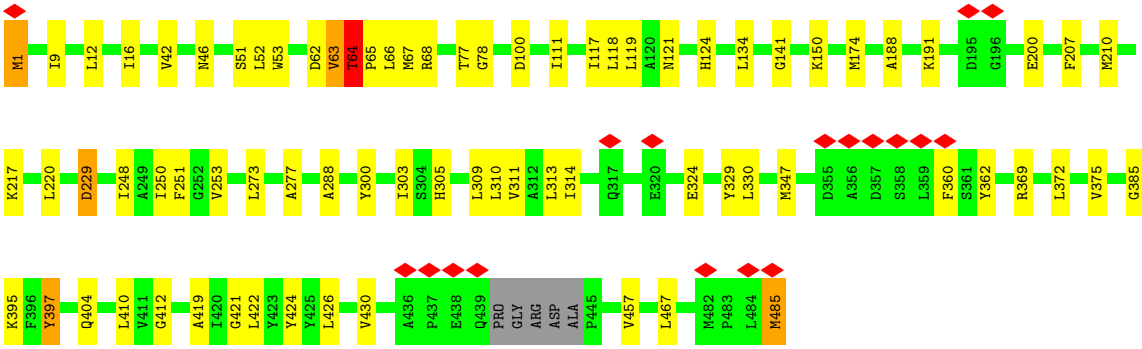
Chain M:



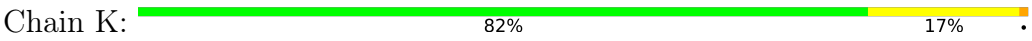


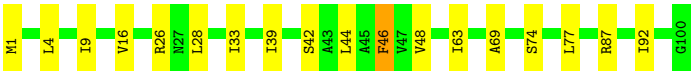
• Molecule 11: NADH-quinone oxidoreductase subunit N



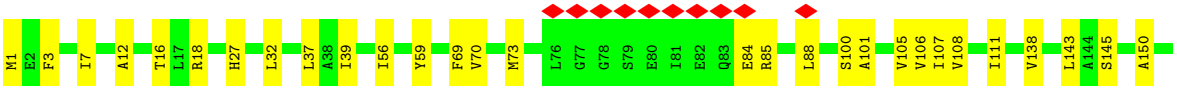


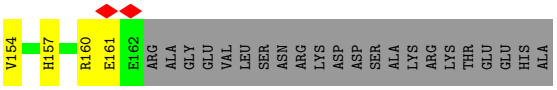
• Molecule 12: NADH-quinone oxidoreductase subunit K





• Molecule 13: NADH-quinone oxidoreductase subunit J





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	189796	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	0.538	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	152.63998, 205.63998, 244.85999	wwPDB
Map dimensions	144, 194, 231	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/3511	0.55	0/4745
2	E	0.34	0/1248	0.52	0/1691
3	G	0.37	0/7178	0.56	0/9733
4	C	0.36	0/4750	0.56	0/6442
5	B	0.37	0/1367	0.61	0/1847
6	I	0.39	0/1176	0.61	1/1590 (0.1%)
7	H	0.34	0/2492	0.57	2/3391 (0.1%)
8	A	0.33	0/821	0.54	2/1119 (0.2%)
9	L	0.32	0/4711	0.53	0/6420
10	M	0.35	0/4074	0.56	2/5546 (0.0%)
11	N	0.34	0/3724	0.55	1/5081 (0.0%)
12	K	0.34	0/769	0.53	0/1040
13	J	0.34	0/1252	0.54	0/1708
All	All	0.35	0/37073	0.56	8/50353 (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
2	E	0	1
3	G	0	1
11	N	0	2
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	429	LEU	CA-CB-CG	6.63	130.55	115.30
7	H	164	LEU	CB-CG-CD2	-6.36	100.20	111.00
10	M	263	LEU	CA-CB-CG	5.73	128.47	115.30
6	I	119	ASP	CB-CG-OD2	5.32	123.09	118.30
8	A	83	LEU	CA-CB-CG	5.31	127.52	115.30
11	N	64	THR	N-CA-C	-5.23	96.89	111.00
7	H	264	LEU	CA-CB-CG	5.06	126.95	115.30
8	A	29	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	145	ILE	Peptide
3	G	260	ASN	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	13	0
3	G	7027	0	6829	44	0
4	C	4628	0	4533	46	0
5	B	1339	0	1330	27	0
6	I	1149	0	1114	11	0
7	H	2422	0	2469	24	0
8	A	796	0	804	11	0
9	L	4593	0	4734	42	0
10	M	3953	0	4053	39	0
11	N	3635	0	3802	50	0
12	K	760	0	817	14	0
13	J	1226	0	1297	23	0
14	B	8	0	0	2	0
14	F	8	0	0	0	0
14	G	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	I	16	0	0	0	0
15	F	31	0	19	1	0
16	F	44	0	27	3	0
17	E	4	0	0	0	0
17	G	4	0	0	1	0
18	G	1	0	0	0	0
19	A	20	0	42	0	0
19	H	20	0	42	1	0
19	L	20	0	42	0	0
19	N	40	0	84	2	0
20	H	51	0	82	3	0
20	J	51	0	82	2	0
20	L	306	0	492	7	0
20	M	102	0	164	7	0
20	N	51	0	82	3	0
All	All	36981	0	37532	339	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 (339) 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	1.61	0.80
11:N:63:VAL:O	11:N:67:MET:HB2	1.85	0.77
10:M:181:SER:HB2	10:M:230:ALA:HA	1.71	0.73
11:N:64:THR:HB	11:N:66:LEU:H	1.54	0.73
3:G:238:ASN:HD22	3:G:238:ASN:N	1.86	0.72
10:M:426:THR:HA	10:M:429:LEU:HD13	1.74	0.70
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.77	0.67
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.74	0.67
12:K:16:VAL:HG13	13:J:100:SER:HB3	1.78	0.66
20:M:702:3PE:H351	19:N:903:LFA:H171	1.80	0.64
2:E:143:MET:HB2	2:E:153:LEU:HD11	1.80	0.63
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.80	0.63
4:C:194:MET:HB2	4:C:197:LEU:HB3	1.80	0.62
3:G:727:ARG:HD3	4:C:179:GLU:HB3	1.81	0.62
3:G:626:GLU:OE1	3:G:786:ARG:NH1	2.34	0.61
9:L:577:ARG:NH1	20:L:807:3PE:O22	2.32	0.60
10:M:123:ILE:HG13	10:M:149:PRO:HB2	1.84	0.60
3:G:399:VAL:HG13	3:G:428:LYS:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:117:ILE:O	11:N:121:ASN:ND2	2.36	0.59
4:C:219:ASN:OD1	4:C:232:ARG:NH1	2.35	0.59
9:L:507:LEU:O	9:L:511:LEU:HB2	2.02	0.59
5:B:61:LEU:HD21	5:B:110:ILE:HD11	1.84	0.59
9:L:85:SER:OG	9:L:268:ARG:NH2	2.36	0.58
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.84	0.58
11:N:485:MET:SD	11:N:485:MET:N	2.75	0.58
1:F:288:LYS:HD2	1:F:331:HIS:HA	1.85	0.58
9:L:571:ILE:HG13	9:L:572:PRO:HD3	1.85	0.58
11:N:347:MET:SD	11:N:369:ARG:NH1	2.75	0.58
1:F:348:ARG:HD2	6:I:180:PRO:HB2	1.86	0.57
5:B:117:MET:HB2	5:B:121:LYS:HE2	1.85	0.57
13:J:37:LEU:HD23	13:J:56:ILE:HD12	1.87	0.57
3:G:243:GLU:HG2	3:G:636:TYR:HB3	1.85	0.57
6:I:48:ILE:HG12	6:I:116:LEU:HG	1.87	0.57
8:A:69:TYR:OH	12:K:74:SER:O	2.22	0.57
1:F:85:ARG:HB2	1:F:125:ALA:HA	1.87	0.56
10:M:45:GLN:NE2	10:M:49:GLN:OE1	2.38	0.56
7:H:293:ARG:NH1	7:H:295:ASP:OD2	2.38	0.56
1:F:160:ILE:HG22	1:F:161:MET:HG3	1.86	0.56
11:N:305:HIS:ND1	11:N:329:TYR:OH	2.33	0.55
4:C:77:LEU:HB3	4:C:137:TYR:HB3	1.87	0.55
9:L:179:VAL:HG22	10:M:426:THR:HG22	1.88	0.55
1:F:357:CYS:HB2	1:F:401:ALA:HB2	1.89	0.55
1:F:56:ASP:O	1:F:237:GLN:NE2	2.39	0.55
20:L:807:3PE:H2G2	20:M:701:3PE:H3D2	1.89	0.55
1:F:239:ILE:HD11	1:F:246:GLY:HA2	1.89	0.55
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.88	0.55
3:G:814:ILE:HD11	3:G:902:LEU:HD13	1.90	0.54
13:J:157:HIS:O	13:J:160:ARG:NH1	2.40	0.54
11:N:42:VAL:O	11:N:46:ASN:ND2	2.41	0.54
4:C:276:GLU:O	4:C:283:ASN:ND2	2.37	0.54
10:M:252:PRO:HD2	10:M:257:VAL:HG21	1.89	0.54
1:F:218:ASN:ND2	15:F:502:FMN:O2	2.38	0.54
5:B:94:ASP:OD1	5:B:94:ASP:N	2.41	0.54
11:N:134:LEU:HD11	13:J:143:LEU:HB3	1.88	0.54
7:H:79:ASP:OD1	13:J:27:HIS:NE2	2.41	0.53
20:H:602:3PE:N	20:J:201:3PE:O14	2.38	0.53
1:F:386:GLN:OE1	3:G:129:ARG:NH2	2.41	0.53
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.91	0.53
4:C:351:GLU:OE2	5:B:161:ARG:NH1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.90	0.53
3:G:138:ARG:NH1	6:I:162:ASP:OD2	2.38	0.52
11:N:412:GLY:HA3	19:N:903:LFA:H81	1.90	0.52
9:L:37:SER:OG	9:L:121:ASN:OD1	2.24	0.52
10:M:229:ILE:HD12	20:M:702:3PE:H2F1	1.91	0.52
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.91	0.52
9:L:263:VAL:HG13	9:L:323:LEU:HD11	1.91	0.52
12:K:39:ILE:HD13	12:K:69:ALA:HB2	1.90	0.52
1:F:85:ARG:HG2	1:F:213:PRO:HG2	1.91	0.52
3:G:227:PRO:HD3	3:G:754:PRO:HB3	1.90	0.52
4:C:374:ARG:NH2	5:B:219:GLU:OE2	2.43	0.52
4:C:429:LEU:O	4:C:432:THR:OG1	2.24	0.52
2:E:141:PRO:HG2	2:E:153:LEU:HB2	1.92	0.51
4:C:143:ASP:OD1	4:C:157:ARG:NH1	2.43	0.51
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.92	0.51
1:F:106:GLU:O	1:F:142:ASN:ND2	2.41	0.51
4:C:381:ARG:NH2	4:C:482:GLU:OE2	2.43	0.51
3:G:106:PRO:HD3	4:C:515:LEU:HD21	1.93	0.51
7:H:170:GLN:NE2	7:H:188:ASN:OD1	2.43	0.51
10:M:338:TYR:HB3	10:M:493:ILE:HD12	1.93	0.51
4:C:374:ARG:NH1	5:B:218:ASP:OD2	2.44	0.51
4:C:488:MET:HE3	4:C:489:PRO:HD2	1.93	0.51
12:K:44:LEU:HD13	13:J:39:ILE:HG23	1.92	0.51
10:M:65:SER:HB3	10:M:83:ILE:HG22	1.93	0.50
11:N:1:MET:HG3	11:N:65:PRO:HD3	1.94	0.50
4:C:110:ASP:N	4:C:110:ASP:OD2	2.42	0.50
20:H:602:3PE:H341	20:J:201:3PE:H321	1.93	0.50
1:F:176:GLY:O	2:E:77:SER:OG	2.28	0.50
4:C:254:ARG:NH2	5:B:62:SER:OG	2.44	0.50
11:N:229:ASP:OD1	11:N:229:ASP:N	2.44	0.50
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.93	0.49
11:N:369:ARG:HG2	11:N:372:LEU:HD12	1.94	0.49
4:C:254:ARG:HG3	5:B:103:PHE:HE1	1.77	0.49
11:N:419:ALA:HA	11:N:422:LEU:HD12	1.94	0.49
1:F:291:GLN:O	1:F:326:ALA:HA	2.12	0.49
5:B:39:MET:SD	5:B:39:MET:N	2.85	0.49
10:M:396:LEU:HD22	10:M:398:MET:HG2	1.95	0.49
10:M:414:SER:O	10:M:418:VAL:N	2.38	0.49
7:H:209:ARG:HD3	7:H:245:ILE:HD11	1.93	0.49
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.92	0.49
11:N:188:ALA:HA	11:N:191:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:148:ARG:HH12	7:H:218:GLU:HB2	1.76	0.49
10:M:236:PRO:HG3	10:M:244:LEU:HD22	1.93	0.49
11:N:66:LEU:HA	11:N:124:HIS:HB2	1.95	0.49
5:B:101:THR:HA	5:B:129:CYS:HB3	1.94	0.48
11:N:53:TRP:HA	20:N:902:3PE:H242	1.94	0.48
11:N:119:LEU:HD22	11:N:253:VAL:HG11	1.94	0.48
12:K:33:ILE:HG23	13:J:32:LEU:HD22	1.95	0.48
3:G:558:LEU:HD22	3:G:589:ALA:HB2	1.95	0.48
9:L:159:THR:HB	10:M:447:LYS:HE2	1.96	0.48
20:L:804:3PE:H3D1	20:L:804:3PE:H292	1.95	0.48
11:N:310:LEU:HD12	11:N:313:LEU:HD23	1.95	0.48
11:N:360:PHE:CE2	11:N:362:TYR:HB3	2.48	0.48
3:G:217:TYR:HB3	6:I:79:LYS:HD2	1.95	0.48
1:F:297:THR:HG22	1:F:320:ARG:HG3	1.94	0.48
13:J:85:ARG:HD3	13:J:88:LEU:HD12	1.95	0.48
1:F:63:GLY:O	16:F:503:NAI:H2N	2.13	0.48
1:F:103:LEU:HD22	1:F:261:LEU:HD23	1.95	0.48
10:M:84:ASP:OD2	10:M:273:ARG:NH2	2.47	0.48
20:M:701:3PE:H322	20:M:702:3PE:H392	1.95	0.48
11:N:64:THR:HG22	11:N:65:PRO:HD2	1.94	0.48
9:L:102:TYR:CD1	9:L:347:LEU:HD22	2.48	0.48
3:G:286:GLN:HB2	3:G:295:LEU:HD11	1.95	0.48
4:C:327:ILE:HG23	4:C:332:ALA:HB3	1.95	0.48
10:M:185:MET:HB2	10:M:230:ALA:HB2	1.95	0.48
2:E:84:VAL:HB	2:E:127:THR:HG21	1.96	0.47
3:G:611:SER:OG	3:G:646:VAL:O	2.30	0.47
10:M:314:LEU:O	10:M:318:THR:HG23	2.14	0.47
1:F:434:ASN:HB3	6:I:146:PRO:HD2	1.95	0.47
3:G:466:ALA:HB3	3:G:489:VAL:HG21	1.96	0.47
20:M:702:3PE:H3C1	20:M:702:3PE:H2C2	1.96	0.47
3:G:613:ALA:HB1	3:G:617:GLU:HB2	1.97	0.47
5:B:64:CYS:HB3	5:B:99:ALA:HB1	1.96	0.47
11:N:118:LEU:HD22	13:J:143:LEU:HD13	1.96	0.47
1:F:77:PRO:O	1:F:85:ARG:NH2	2.43	0.47
10:M:393:VAL:HG13	10:M:398:MET:HG3	1.96	0.47
11:N:78:GLY:HA3	20:N:902:3PE:H392	1.96	0.47
5:B:184:SER:O	5:B:190:GLN:NE2	2.43	0.47
7:H:21:ILE:HG12	19:H:601:LFA:H62	1.97	0.47
5:B:180:ARG:HB2	5:B:193:TYR:HB2	1.97	0.46
1:F:388:CYS:HB3	1:F:409:GLN:HG3	1.97	0.46
2:E:105:ILE:HG21	2:E:153:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:385:GLY:HA3	11:N:395:LYS:HE3	1.96	0.46
7:H:95:LEU:HB2	7:H:243:ILE:HG21	1.97	0.46
9:L:266:ILE:HB	9:L:323:LEU:HD13	1.96	0.46
4:C:501:THR:HG23	4:C:521:GLN:HB3	1.98	0.46
9:L:82:ASP:N	9:L:82:ASP:OD1	2.48	0.46
10:M:104:CYS:HB3	10:M:256:SER:HB3	1.97	0.46
3:G:439:THR:OG1	3:G:442:ASP:OD1	2.30	0.46
11:N:150:LYS:HG2	12:K:87:ARG:HH12	1.81	0.46
11:N:207:PHE:HA	11:N:210:MET:HE2	1.97	0.46
11:N:311:VAL:HG22	11:N:410:LEU:HD13	1.98	0.46
7:H:22:LEU:O	7:H:26:VAL:HG23	2.16	0.46
9:L:66:THR:H	20:L:804:3PE:H122	1.81	0.46
5:B:53:SER:O	5:B:53:SER:OG	2.33	0.46
6:I:142:PRO:HB2	6:I:146:PRO:HA	1.98	0.46
9:L:179:VAL:HG21	10:M:430:VAL:HG23	1.98	0.46
7:H:194:PHE:HA	7:H:197:ILE:HG12	1.97	0.46
7:H:94:LEU:HB3	7:H:247:THR:HG21	1.98	0.45
9:L:235:LEU:HD21	20:L:802:3PE:H3D2	1.98	0.45
1:F:381:ILE:HD12	1:F:419:PHE:HB3	1.97	0.45
9:L:431:ARG:HG3	9:L:512:TRP:CE2	2.52	0.45
4:C:78:HIS:HE2	4:C:140:GLU:HG2	1.81	0.45
12:K:26:ARG:HH22	13:J:84:GLU:HG2	1.81	0.45
3:G:125:HIS:NE2	4:C:513:GLU:OE2	2.49	0.45
4:C:360:PRO:O	6:I:45:ARG:NH1	2.37	0.45
8:A:75:PHE:O	8:A:79:ASP:HB2	2.15	0.45
3:G:74:SER:O	3:G:77:THR:OG1	2.29	0.45
10:M:63:TRP:NE1	10:M:208:GLU:OE2	2.41	0.45
10:M:311:ILE:HD12	10:M:311:ILE:H	1.80	0.45
2:E:138:ASP:OD1	2:E:138:ASP:N	2.50	0.45
3:G:631:ARG:HD2	3:G:692:ALA:HB3	1.98	0.45
4:C:229:GLY:HA3	4:C:595:MET:HB2	1.98	0.45
12:K:28:LEU:HD13	12:K:92:ILE:HD13	1.99	0.45
4:C:133:ASN:OD1	4:C:133:ASN:N	2.45	0.45
11:N:9:ILE:HD12	11:N:12:LEU:HD22	1.99	0.45
7:H:262:GLY:HA3	7:H:270:TRP:CD1	2.52	0.45
9:L:291:LEU:HA	9:L:314:SER:HA	1.99	0.45
11:N:288:ALA:HB2	11:N:300:TYR:HB2	1.97	0.45
3:G:55:TYR:HB3	3:G:60:ASP:HB3	1.99	0.45
10:M:417:VAL:HG12	10:M:418:VAL:HG13	1.99	0.45
3:G:62:ARG:NH2	3:G:63:GLY:O	2.49	0.44
3:G:97:LEU:HD22	3:G:154:ILE:HB	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:175:PHE:CE1	10:M:179:GLN:HG3	2.52	0.44
4:C:242:ILE:HD13	4:C:576:ILE:HD13	1.99	0.44
9:L:133:ALA:HB1	9:L:138:LEU:HB3	1.99	0.44
9:L:378:CYS:HA	9:L:461:LEU:HD21	1.99	0.44
11:N:62:ASP:OD1	11:N:68:ARG:NE	2.50	0.44
11:N:251:PHE:CZ	11:N:309:LEU:HB3	2.52	0.44
9:L:123:PHE:HE1	9:L:146:VAL:HB	1.82	0.44
9:L:135:ASN:OD1	9:L:135:ASN:N	2.51	0.44
3:G:67:MET:HE2	17:G:1004:FES:S1	2.58	0.44
9:L:157:TYR:HB2	9:L:163:ASN:HD22	1.83	0.44
3:G:102:PRO:HG3	3:G:151:ASN:HB3	2.00	0.44
7:H:15:ILE:HG23	8:A:18:ILE:HG21	1.99	0.44
4:C:65:LYS:NZ	4:C:130:LEU:O	2.46	0.44
4:C:274:ARG:HG2	14:B:301:SF4:S2	2.58	0.44
5:B:100:GLY:HA2	14:B:301:SF4:S4	2.58	0.44
9:L:12:LEU:HD23	9:L:12:LEU:HA	1.89	0.44
11:N:324:GLU:OE2	11:N:397:TYR:OH	2.23	0.44
8:A:7:THR:HA	8:A:10:ILE:HG22	2.00	0.43
13:J:12:ALA:O	13:J:16:THR:HG22	2.18	0.43
1:F:83:ASN:OD1	1:F:83:ASN:N	2.51	0.43
9:L:354:LEU:HD23	9:L:354:LEU:HA	1.91	0.43
8:A:66:ALA:HB3	13:J:161:GLU:HB2	2.00	0.43
9:L:103:ALA:HA	9:L:106:TYR:HB3	1.99	0.43
10:M:235:MET:HG3	10:M:323:MET:HB3	1.99	0.43
10:M:315:ILE:HD13	10:M:355:LEU:HB3	2.00	0.43
3:G:669:THR:OG1	3:G:670:GLN:N	2.50	0.43
6:I:154:ALA:O	6:I:161:LYS:NZ	2.44	0.43
9:L:273:PHE:HB3	9:L:280:LEU:HD13	2.01	0.43
9:L:488:GLY:O	9:L:492:THR:HG23	2.18	0.43
11:N:141:GLY:HA3	13:J:154:VAL:HG22	1.99	0.43
1:F:255:ARG:HG3	2:E:99:ILE:HG22	2.01	0.43
2:E:87:HIS:ND1	2:E:146:ASP:OD2	2.52	0.43
5:B:124:ILE:HG12	5:B:153:VAL:HB	2.00	0.43
11:N:300:TYR:HA	11:N:303:ILE:HD12	2.00	0.43
4:C:312:GLU:OE2	4:C:447:TYR:OH	2.30	0.43
9:L:563:ASP:OD1	10:M:300:TYR:OH	2.24	0.43
4:C:381:ARG:HD2	4:C:485:LEU:HD21	2.00	0.43
5:B:185:TRP:CD1	5:B:186:VAL:HG13	2.54	0.43
6:I:45:ARG:HG2	6:I:116:LEU:HD22	2.01	0.43
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.54	0.43
20:H:602:3PE:H3D1	20:H:602:3PE:H2A1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:395:LYS:HE3	3:G:65:LEU:HD12	2.00	0.43
4:C:99:PHE:HZ	4:C:560:ARG:HG2	1.84	0.43
9:L:243:MET:SD	9:L:309:ALA:HB2	2.59	0.43
10:M:310:ASP:OD1	10:M:369:ARG:HB3	2.18	0.43
11:N:421:GLY:HA2	11:N:424:TYR:CE2	2.53	0.43
1:F:126:TYR:CZ	1:F:127:ARG:HD2	2.54	0.42
3:G:451:ALA:HB1	3:G:455:ASP:HB2	2.00	0.42
4:C:156:ARG:HH22	4:C:246:VAL:HG11	1.84	0.42
7:H:26:VAL:HG13	7:H:243:ILE:HD11	2.01	0.42
9:L:390:PRO:HA	9:L:396:PHE:CG	2.54	0.42
10:M:223:LEU:HD23	20:M:702:3PE:H281	2.00	0.42
4:C:136:TRP:HZ2	4:C:247:PRO:HG2	1.84	0.42
20:L:804:3PE:H2B1	20:L:804:3PE:H3A2	2.01	0.42
11:N:119:LEU:HD23	11:N:119:LEU:HA	1.86	0.42
11:N:311:VAL:HA	11:N:314:ILE:HD12	2.00	0.42
3:G:238:ASN:N	3:G:238:ASN:ND2	2.58	0.42
3:G:267:ARG:HB2	3:G:820:LEU:HG	2.02	0.42
4:C:572:ILE:HA	4:C:587:TYR:HE2	1.84	0.42
11:N:16:ILE:HD12	11:N:51:SER:HB3	2.01	0.42
3:G:320:PRO:HB2	3:G:537:SER:HB2	2.01	0.42
4:C:53:LYS:HA	4:C:53:LYS:HD3	1.89	0.42
1:F:178:TYR:OH	16:F:503:NAI:H5N	2.19	0.42
3:G:812:TRP:HB2	3:G:902:LEU:HB3	2.00	0.42
4:C:389:LYS:HZ3	4:C:390:ARG:HG2	1.83	0.42
10:M:246:ASP:OD1	10:M:246:ASP:N	2.53	0.42
12:K:44:LEU:HD13	13:J:39:ILE:HD12	2.00	0.42
2:E:16:ALA:O	2:E:20:GLU:HG3	2.20	0.42
5:B:60:GLY:HA2	5:B:65:TYR:CG	2.55	0.42
5:B:61:LEU:HD23	5:B:61:LEU:HA	1.89	0.42
9:L:515:LYS:HD3	9:L:515:LYS:HA	1.92	0.42
10:M:175:PHE:CD1	11:N:426:LEU:HD11	2.55	0.42
1:F:46:SER:HB3	1:F:49:GLU:HG3	2.01	0.42
1:F:282:ARG:HB2	1:F:285:LEU:HD12	2.02	0.42
4:C:270:PRO:HB2	5:B:135:MET:HE1	2.00	0.42
4:C:342:ASP:OD1	4:C:342:ASP:N	2.52	0.42
1:F:381:ILE:HG12	1:F:423:ILE:HD11	2.02	0.42
3:G:452:PRO:O	3:G:456:GLN:HG3	2.20	0.42
8:A:106:PHE:CE2	13:J:145:SER:HB2	2.55	0.42
9:L:75:ILE:HG21	9:L:137:LEU:HD23	2.02	0.42
10:M:315:ILE:O	10:M:318:THR:OG1	2.28	0.42
2:E:91:TYR:CZ	2:E:106:GLN:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:368:LEU:HD21	3:G:390:ARG:HB3	2.02	0.42
7:H:314:LEU:HG	8:A:107:ILE:HD13	2.02	0.42
20:M:701:3PE:H12	20:M:702:3PE:H352	2.01	0.42
5:B:91:ARG:HB3	7:H:230:SER:HB3	2.02	0.41
7:H:88:MET:O	7:H:92:THR:OG1	2.29	0.41
7:H:117:LEU:O	7:H:121:MET:HG3	2.20	0.41
8:A:31:LEU:HD23	8:A:31:LEU:HA	1.80	0.41
8:A:69:TYR:HB2	13:J:73:MET:HE1	2.02	0.41
9:L:361:ASN:HB3	9:L:364:LYS:HG2	2.02	0.41
10:M:224:MET:HE2	10:M:282:ALA:HB1	2.02	0.41
11:N:52:LEU:HD12	11:N:52:LEU:HA	1.90	0.41
1:F:269:THR:HA	1:F:308:PRO:HA	2.02	0.41
3:G:777:LYS:HE3	3:G:777:LYS:HB3	1.76	0.41
4:C:136:TRP:CZ2	4:C:247:PRO:HG2	2.55	0.41
4:C:332:ALA:HB1	4:C:401:ASN:HD22	1.85	0.41
5:B:65:TYR:HA	5:B:68:MET:HG2	2.02	0.41
7:H:280:MET:O	7:H:284:LEU:HG	2.19	0.41
3:G:465:HIS:HA	3:G:471:ALA:HB3	2.01	0.41
7:H:211:PRO:HB2	7:H:292:PRO:HD3	2.01	0.41
9:L:141:LEU:HD12	10:M:399:PRO:HB2	2.03	0.41
11:N:12:LEU:HG	11:N:51:SER:HB2	2.01	0.41
13:J:107:ILE:O	13:J:111:ILE:HG12	2.20	0.41
1:F:176:GLY:HA3	2:E:78:GLN:HG2	2.02	0.41
7:H:118:PHE:HA	7:H:121:MET:SD	2.60	0.41
12:K:9:ILE:HG12	13:J:108:VAL:HG22	2.02	0.41
13:J:101:ALA:O	13:J:105:VAL:HG23	2.21	0.41
1:F:16:ARG:NH1	1:F:32:LYS:O	2.53	0.41
1:F:93:GLU:OE1	1:F:136:TYR:OH	2.27	0.41
20:L:804:3PE:H32	20:L:804:3PE:H121	2.03	0.41
11:N:273:LEU:HD22	11:N:310:LEU:HD11	2.02	0.41
12:K:4:LEU:HD12	12:K:48:VAL:HG12	2.03	0.41
4:C:569:LEU:HD13	4:C:572:ILE:HD12	2.02	0.41
9:L:88:MET:HG3	9:L:264:TYR:HD2	1.84	0.41
5:B:2:ASP:HB3	5:B:196:ASN:HD22	1.86	0.41
2:E:112:LYS:HE2	2:E:159:PRO:HB3	2.03	0.41
9:L:318:TYR:OH	9:L:418:GLY:O	2.29	0.41
9:L:368:LEU:HD23	9:L:368:LEU:HA	1.91	0.41
11:N:277:ALA:HB1	11:N:311:VAL:HG23	2.03	0.41
2:E:81:ARG:HD2	2:E:81:ARG:HA	1.86	0.41
3:G:447:TRP:CZ2	3:G:484:LYS:HD3	2.56	0.41
4:C:67:LEU:HD23	4:C:67:LEU:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:156:PRO:HG2	6:I:122:MET:HB2	2.03	0.41
10:M:61:PRO:HB3	10:M:208:GLU:HG2	2.02	0.41
11:N:174:MET:HB3	12:K:46:PHE:CZ	2.56	0.41
3:G:5:THR:O	3:G:76:GLY:N	2.54	0.41
3:G:433:VAL:HG23	3:G:448:THR:HG23	2.03	0.41
4:C:74:LEU:HA	4:C:102:LEU:HD23	2.03	0.41
7:H:213:ASP:HB2	7:H:291:ARG:HE	1.85	0.41
7:H:265:LEU:HB2	7:H:270:TRP:CD1	2.55	0.41
9:L:8:ILE:HG12	9:L:128:VAL:HG12	2.03	0.41
9:L:292:LEU:HD23	9:L:292:LEU:HA	1.95	0.41
3:G:222:ASP:O	3:G:244:ARG:HD3	2.21	0.40
1:F:431:HIS:O	4:C:510:GLN:NE2	2.40	0.40
3:G:437:ASP:OD2	3:G:817:TYR:OH	2.32	0.40
7:H:219:GLN:HG2	7:H:221:LEU:H	1.85	0.40
8:A:80:VAL:O	8:A:83:LEU:HG	2.21	0.40
9:L:162:LYS:HE2	9:L:162:LYS:HB3	1.81	0.40
9:L:606:LEU:HB3	13:J:106:VAL:HG11	2.04	0.40
11:N:220:LEU:HD13	11:N:310:LEU:HD22	2.03	0.40
4:C:168:PRO:HA	4:C:173:TYR:CG	2.56	0.40
4:C:259:MET:HG2	4:C:271:TYR:CE1	2.55	0.40
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.85	0.40
4:C:587:TYR:CZ	4:C:591:ILE:HD11	2.56	0.40
5:B:135:MET:HB3	6:I:100:ILE:HG21	2.03	0.40
11:N:375:VAL:HG11	11:N:457:VAL:HB	2.04	0.40
11:N:467:LEU:HD11	20:N:902:3PE:H3G2	2.02	0.40
3:G:541:MET:HG3	3:G:625:ASN:HA	2.03	0.40
8:A:83:LEU:HD11	12:K:63:ILE:HG23	2.03	0.40
1:F:222:LEU:O	1:F:226:PRO:HD3	2.21	0.40
3:G:284:PRO:HD3	3:G:646:VAL:HB	2.04	0.40
5:B:101:THR:HB	5:B:103:PHE:CZ	2.56	0.40
10:M:409:MET:HE1	10:M:486:LEU:HD21	2.04	0.40
10:M:493:ILE:HD13	10:M:493:ILE:HA	1.91	0.40
12:K:77:LEU:HB3	13:J:70:VAL:HG21	2.04	0.40
13:J:3:PHE:O	13:J:7:ILE:HG12	2.21	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	440/445 (99%)	430 (98%)	10 (2%)	0	100	100
2	E	154/166 (93%)	150 (97%)	4 (3%)	0	100	100
3	G	903/908 (99%)	879 (97%)	24 (3%)	0	100	100
4	C	568/596 (95%)	559 (98%)	9 (2%)	0	100	100
5	B	163/220 (74%)	156 (96%)	6 (4%)	1 (1%)	25	50
6	I	143/180 (79%)	140 (98%)	3 (2%)	0	100	100
7	H	305/325 (94%)	293 (96%)	12 (4%)	0	100	100
8	A	97/147 (66%)	97 (100%)	0	0	100	100
9	L	597/613 (97%)	579 (97%)	18 (3%)	0	100	100
10	M	502/509 (99%)	487 (97%)	15 (3%)	0	100	100
11	N	476/485 (98%)	465 (98%)	10 (2%)	1 (0%)	47	73
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	160/184 (87%)	155 (97%)	5 (3%)	0	100	100
All	All	4606/4878 (94%)	4486 (97%)	118 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	N	64	THR
5	B	61	LEU

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	356/359 (99%)	344 (97%)	12 (3%)	37	66
2	E	129/139 (93%)	125 (97%)	4 (3%)	40	69
3	G	733/736 (100%)	708 (97%)	25 (3%)	37	66
4	C	489/515 (95%)	474 (97%)	15 (3%)	40	69
5	B	146/192 (76%)	134 (92%)	12 (8%)	11	26
6	I	124/154 (80%)	120 (97%)	4 (3%)	39	68
7	H	255/269 (95%)	249 (98%)	6 (2%)	49	77
8	A	79/119 (66%)	79 (100%)	0	100	100
9	L	476/485 (98%)	459 (96%)	17 (4%)	35	64
10	M	413/418 (99%)	394 (95%)	19 (5%)	27	54
11	N	381/385 (99%)	373 (98%)	8 (2%)	53	80
12	K	79/79 (100%)	76 (96%)	3 (4%)	33	62
13	J	128/146 (88%)	123 (96%)	5 (4%)	32	61
All	All	3788/3996 (95%)	3658 (97%)	130 (3%)	40	66

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	21	LYS
1	F	48	ASP
1	F	126	TYR
1	F	152	GLU
1	F	221	THR
1	F	241	LYS
1	F	252	PHE
1	F	255	ARG
1	F	286	LYS
1	F	298	ASP
1	F	302	GLU
1	F	398	CYS
2	E	45	LYS
2	E	93	ASP
2	E	122	PHE
2	E	148	ASP
3	G	59	GLU
3	G	61	THR
3	G	135	ARG
3	G	181	VAL

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Mol	Chain	Res	Type
3	G	238	ASN
3	G	278	LYS
3	G	299	GLN
3	G	414	ASP
3	G	459	LEU
3	G	490	GLN
3	G	593	MET
3	G	619	ASP
3	G	660	THR
3	G	728	GLN
3	G	730	GLN
3	G	740	MET
3	G	750	ARG
3	G	773	GLU
3	G	789	GLU
3	G	791	SER
3	G	793	ASN
3	G	808	GLN
3	G	832	VAL
3	G	851	LYS
3	G	865	ASP
4	C	65	LYS
4	C	110	ASP
4	C	127	PHE
4	C	129	LYS
4	C	194	MET
4	C	200	LYS
4	C	319	HIS
4	C	356	PHE
4	C	377	ASP
4	C	407	ARG
4	C	411	VAL
4	C	531	ASN
4	C	569	LEU
4	C	583	ASP
4	C	600	ARG
5	B	5	LEU
5	B	39	MET
5	B	42	LEU
5	B	52	ASN
5	B	53	SER
5	B	63	CYS

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Mol	Chain	Res	Type
5	B	94	ASP
5	B	119	GLU
5	B	125	SER
5	B	165	TYR
5	B	185	TRP
5	B	207	GLU
6	I	77	LEU
6	I	126	LYS
6	I	171	LYS
6	I	175	VAL
7	H	60	LEU
7	H	64	MET
7	H	92	THR
7	H	130	VAL
7	H	209	ARG
7	H	238	PHE
9	L	77	PHE
9	L	80	VAL
9	L	123	PHE
9	L	136	LEU
9	L	200	MET
9	L	342	LYS
9	L	379	PHE
9	L	415	MET
9	L	431	ARG
9	L	490	MET
9	L	491	LEU
9	L	493	LEU
9	L	515	LYS
9	L	521	SER
9	L	542	ASP
9	L	578	PHE
9	L	581	LYS
10	M	22	ARG
10	M	25	VAL
10	M	26	LYS
10	M	56	GLN
10	M	74	ARG
10	M	145	MET
10	M	146	MET
10	M	150	MET
10	M	224	MET

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Mol	Chain	Res	Type
10	M	246	ASP
10	M	265	LYS
10	M	279	PHE
10	M	303	TRP
10	M	312	LYS
10	M	365	ARG
10	M	373	MET
10	M	426	THR
10	M	447	LYS
10	M	466	PHE
11	N	1	MET
11	N	100	ASP
11	N	200	GLU
11	N	229	ASP
11	N	397	TYR
11	N	404	GLN
11	N	430	VAL
11	N	485	MET
12	K	1	MET
12	K	42	SER
12	K	46	PHE
13	J	1	MET
13	J	18	ARG
13	J	59	TYR
13	J	69	PHE
13	J	138	VAL

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

Mol	Chain	Res	Type
5	B	196	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 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	3PE	M	701	-	50,50,50	0.30	0	53,55,55	0.27	0
20	3PE	H	602	-	50,50,50	0.31	0	53,55,55	0.35	0
14	SF4	F	501	1	0,12,12	-	-	-		
16	NAI	F	503	-	42,48,48	0.54	0	47,73,73	0.58	1 (2%)
19	LFA	H	601	-	19,19,19	0.14	0	18,18,18	0.13	0
19	LFA	N	901	-	19,19,19	0.14	0	18,18,18	0.18	0
20	3PE	L	803	-	50,50,50	0.31	0	53,55,55	0.30	0
20	3PE	J	201	-	50,50,50	0.30	0	53,55,55	0.28	0
20	3PE	M	702	-	50,50,50	0.29	0	53,55,55	0.28	0
14	SF4	G	1001	3	0,12,12	-	-	-		
19	LFA	N	903	-	19,19,19	0.09	0	18,18,18	0.16	0
14	SF4	G	1003	3	0,12,12	-	-	-		
19	LFA	L	805	-	19,19,19	0.15	0	18,18,18	0.13	0
20	3PE	L	806	-	50,50,50	0.30	0	53,55,55	0.31	0
20	3PE	L	802	-	50,50,50	0.30	0	53,55,55	0.29	0
14	SF4	G	1002	3	0,12,12	-	-	-		
20	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.30	0
17	FES	E	201	2	0,4,4	-	-	-		
20	3PE	N	902	-	50,50,50	0.30	0	53,55,55	0.28	0
14	SF4	B	301	5	0,12,12	-	-	-		
14	SF4	I	201	6	0,12,12	-	-	-		
20	3PE	L	807	-	50,50,50	0.30	0	53,55,55	0.29	0
19	LFA	A	201	-	19,19,19	0.12	0	18,18,18	0.23	0
15	FMN	F	502	-	33,33,33	1.13	2 (6%)	48,50,50	1.29	8 (16%)
17	FES	G	1004	3	0,4,4	-	-	-		
14	SF4	I	202	6	0,12,12	-	-	-		
20	3PE	L	804	-	50,50,50	0.30	0	53,55,55	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	3PE	M	701	-	-	9/54/54/54	-
20	3PE	H	602	-	-	6/54/54/54	-
16	NAI	F	503	-	-	5/25/72/72	0/5/5/5
19	LFA	H	601	-	-	2/17/17/17	-
19	LFA	N	901	-	-	3/17/17/17	-
14	SF4	F	501	1	-	-	0/6/5/5
20	3PE	L	803	-	-	13/54/54/54	-
20	3PE	J	201	-	-	11/54/54/54	-
20	3PE	M	702	-	-	6/54/54/54	-
14	SF4	G	1001	3	-	-	0/6/5/5
19	LFA	N	903	-	-	0/17/17/17	-
19	LFA	L	805	-	-	1/17/17/17	-
20	3PE	L	806	-	-	13/54/54/54	-
14	SF4	G	1003	3	-	-	0/6/5/5
20	3PE	L	802	-	-	10/54/54/54	-
14	SF4	G	1002	3	-	-	0/6/5/5
20	3PE	L	801	-	-	8/54/54/54	-
17	FES	E	201	2	-	-	0/1/1/1
20	3PE	N	902	-	-	12/54/54/54	-
14	SF4	B	301	5	-	-	0/6/5/5
20	3PE	L	807	-	-	14/54/54/54	-
14	SF4	I	201	6	-	-	0/6/5/5
19	LFA	A	201	-	-	1/17/17/17	-
15	FMN	F	502	-	-	10/18/18/18	0/3/3/3
17	FES	G	1004	3	-	-	0/1/1/1
14	SF4	I	202	6	-	-	0/6/5/5
20	3PE	L	804	-	-	16/54/54/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.55	1.37	1.30
15	F	502	FMN	C10-N1	2.14	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4-N3-C2	-3.20	119.73	125.64
15	F	502	FMN	C4A-C4-N3	2.67	119.98	113.19
15	F	502	FMN	C4A-C10-N10	2.63	120.33	116.48
15	F	502	FMN	O4-C4-C4A	-2.54	119.86	126.60
15	F	502	FMN	C4A-C10-N1	-2.38	119.22	124.73
15	F	502	FMN	C10-C4A-N5	-2.36	119.84	124.86
16	F	503	NAI	C5A-C6A-N6A	2.30	123.85	120.35
15	F	502	FMN	C9A-C5A-N5	-2.24	120.00	122.43
15	F	502	FMN	C4-C4A-C10	2.05	120.23	116.79

There are no chirality outliers.

All (140) 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
16	F	503	NAI	C5B-O5B-PA-O1A
16	F	503	NAI	C5B-O5B-PA-O3
20	H	602	3PE	O13-C11-C12-N
20	L	801	3PE	O13-C11-C12-N
20	L	802	3PE	C1-O11-P-O12
20	L	802	3PE	C11-O13-P-O12
20	L	802	3PE	O13-C11-C12-N
20	L	803	3PE	C1-O11-P-O12
20	L	803	3PE	C1-O11-P-O14
20	L	803	3PE	C11-O13-P-O14
20	L	803	3PE	O13-C11-C12-N
20	L	804	3PE	C1-O11-P-O14
20	L	804	3PE	C11-O13-P-O12
20	L	804	3PE	C11-O13-P-O14
20	L	804	3PE	O13-C11-C12-N
20	L	806	3PE	O13-C11-C12-N
20	L	807	3PE	C1-O11-P-O14
20	L	807	3PE	C11-O13-P-O11
20	M	701	3PE	C1-O11-P-O14
20	M	701	3PE	O13-C11-C12-N
20	M	702	3PE	C11-O13-P-O12
20	M	702	3PE	C11-O13-P-O14
20	N	902	3PE	C1-O11-P-O12
20	N	902	3PE	C1-O11-P-O13
20	N	902	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
20	J	201	3PE	C1-O11-P-O12
20	J	201	3PE	C1-O11-P-O13
20	L	804	3PE	C31-C32-C33-C34
20	L	806	3PE	C21-C22-C23-C24
15	F	502	FMN	O3'-C3'-C4'-C5'
20	L	802	3PE	C1-O11-P-O13
20	L	802	3PE	C11-O13-P-O11
20	L	803	3PE	C1-O11-P-O13
20	L	803	3PE	C11-O13-P-O11
20	L	804	3PE	C11-O13-P-O11
20	L	806	3PE	C11-O13-P-O11
20	L	807	3PE	C1-O11-P-O13
20	M	702	3PE	C11-O13-P-O11
20	N	902	3PE	C11-O13-P-O11
20	L	803	3PE	C35-C36-C37-C38
20	L	806	3PE	C35-C36-C37-C38
20	L	806	3PE	C37-C38-C39-C3A
19	L	805	LFA	C6-C7-C8-C9
20	M	701	3PE	C24-C25-C26-C27
20	H	602	3PE	C21-C22-C23-C24
20	L	801	3PE	C2C-C2D-C2E-C2F
19	H	601	LFA	C14-C15-C16-C17
20	L	801	3PE	C23-C24-C25-C26
20	L	801	3PE	C3E-C3F-C3G-C3H
20	L	806	3PE	C25-C26-C27-C28
20	L	807	3PE	O21-C2-C3-O31
15	F	502	FMN	C2'-C3'-C4'-O4'
20	L	804	3PE	C1-O11-P-O13
20	L	804	3PE	C3C-C3D-C3E-C3F
20	H	602	3PE	C28-C29-C2A-C2B
20	L	807	3PE	C1-C2-C3-O31
15	F	502	FMN	C5'-O5'-P-O1P
20	N	902	3PE	C2D-C2E-C2F-C2G
19	N	901	LFA	C13-C14-C15-C16
20	L	804	3PE	O11-C1-C2-C3
15	F	502	FMN	C2'-C3'-C4'-C5'
20	M	702	3PE	C29-C2A-C2B-C2C
15	F	502	FMN	O3'-C3'-C4'-O4'
20	L	807	3PE	C2-C1-O11-P
20	L	804	3PE	C39-C3A-C3B-C3C
20	M	702	3PE	C2-C1-O11-P
20	L	804	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
20	J	201	3PE	C23-C24-C25-C26
20	L	801	3PE	C25-C26-C27-C28
20	L	804	3PE	C3D-C3E-C3F-C3G
16	F	503	NAI	PN-O3-PA-O2A
16	F	503	NAI	O4D-C1D-N1N-C2N
20	M	701	3PE	C1-O11-P-O13
20	L	804	3PE	C2-C1-O11-P
20	J	201	3PE	C2-C1-O11-P
20	H	602	3PE	C3C-C3D-C3E-C3F
16	F	503	NAI	C5B-O5B-PA-O2A
20	L	802	3PE	C1-O11-P-O14
20	L	803	3PE	C11-O13-P-O12
20	L	804	3PE	C1-O11-P-O12
20	L	806	3PE	C11-O13-P-O14
20	L	807	3PE	C1-O11-P-O12
20	L	807	3PE	C11-O13-P-O12
20	N	902	3PE	C1-O11-P-O14
20	N	902	3PE	C11-O13-P-O14
20	J	201	3PE	C1-O11-P-O14
20	J	201	3PE	O11-C1-C2-C3
20	N	902	3PE	C12-C11-O13-P
20	M	702	3PE	C28-C29-C2A-C2B
20	M	701	3PE	C2-C1-O11-P
19	A	201	LFA	C12-C13-C14-C15
20	N	902	3PE	C2B-C2C-C2D-C2E
20	L	807	3PE	C31-C32-C33-C34
19	N	901	LFA	C15-C16-C17-C18
20	L	804	3PE	C32-C33-C34-C35
20	J	201	3PE	O21-C21-C22-C23
20	J	201	3PE	O11-C1-C2-O21
20	L	807	3PE	C2D-C2E-C2F-C2G
20	L	806	3PE	C1-O11-P-O13
20	M	701	3PE	C11-O13-P-O11
20	J	201	3PE	C11-O13-P-O11
20	H	602	3PE	C3B-C3C-C3D-C3E
15	F	502	FMN	C4'-C5'-O5'-P
20	L	801	3PE	C39-C3A-C3B-C3C
20	L	807	3PE	C25-C26-C27-C28
20	H	602	3PE	C2F-C2G-C2H-C2I
20	L	802	3PE	C36-C37-C38-C39
20	N	902	3PE	C38-C39-C3A-C3B
20	J	201	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	L	807	3PE	C29-C2A-C2B-C2C
20	N	902	3PE	C2C-C2D-C2E-C2F
20	M	701	3PE	C2F-C2G-C2H-C2I
19	N	901	LFA	C11-C12-C13-C14
20	L	802	3PE	C37-C38-C39-C3A
20	M	701	3PE	C35-C36-C37-C38
19	H	601	LFA	C7-C8-C9-C10
20	L	804	3PE	C3E-C3F-C3G-C3H
20	L	807	3PE	O11-C1-C2-C3
20	L	802	3PE	O31-C31-C32-C33
20	L	803	3PE	O21-C21-C22-C23
20	L	803	3PE	O31-C31-C32-C33
20	L	806	3PE	C2F-C2G-C2H-C2I
20	L	807	3PE	C23-C24-C25-C26
20	L	801	3PE	C1-O11-P-O14
20	M	701	3PE	C11-O13-P-O14
20	J	201	3PE	C11-O13-P-O14
20	L	803	3PE	O32-C31-C32-C33
20	L	806	3PE	O21-C21-C22-C23
20	L	801	3PE	C2F-C2G-C2H-C2I
20	N	902	3PE	O31-C31-C32-C33
20	L	803	3PE	C12-C11-O13-P
20	L	806	3PE	C12-C11-O13-P
20	L	802	3PE	O32-C31-C32-C33
20	L	803	3PE	C2-C1-O11-P
20	L	806	3PE	O22-C21-C22-C23
20	L	806	3PE	C27-C28-C29-C2A

There are no ring outliers.

14 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	M	701	3PE	3	0
20	H	602	3PE	3	0
16	F	503	NAI	3	0
19	H	601	LFA	1	0
20	J	201	3PE	2	0
20	M	702	3PE	6	0
19	N	903	LFA	2	0
20	L	802	3PE	1	0
20	N	902	3PE	3	0
14	B	301	SF4	2	0

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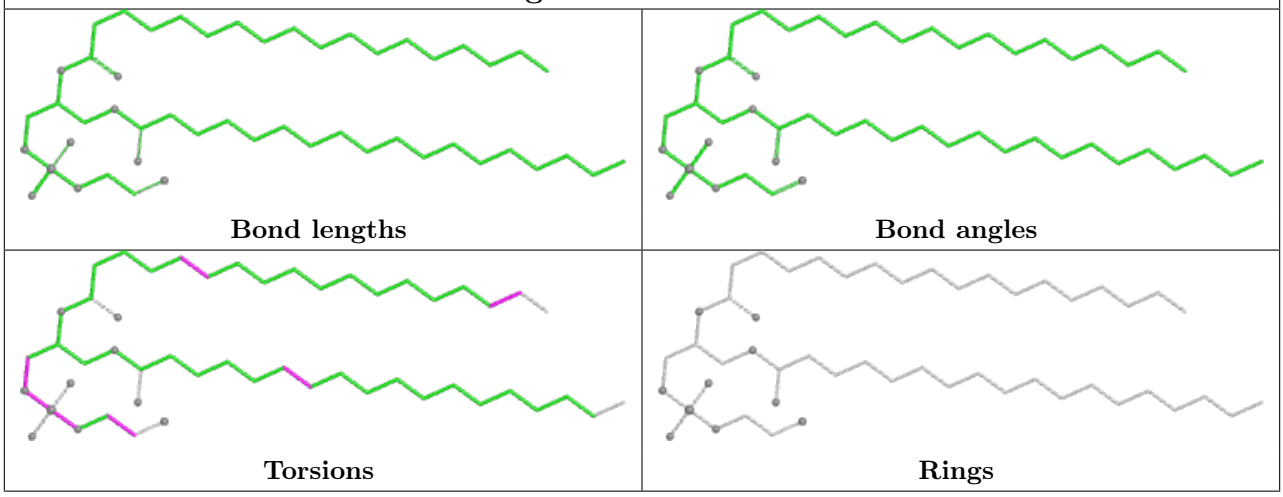
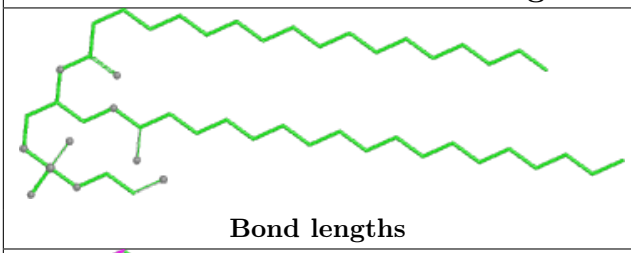
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	L	807	3PE	2	0
15	F	502	FMN	1	0
17	G	1004	FES	1	0
20	L	804	3PE	4	0

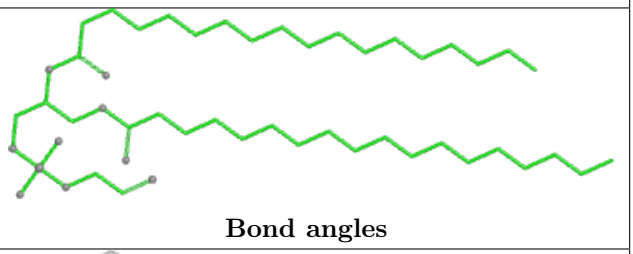
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

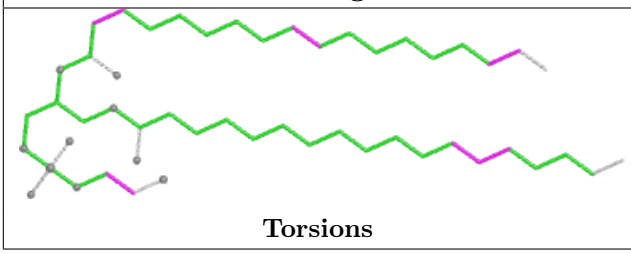
Ligand 3PE M 701

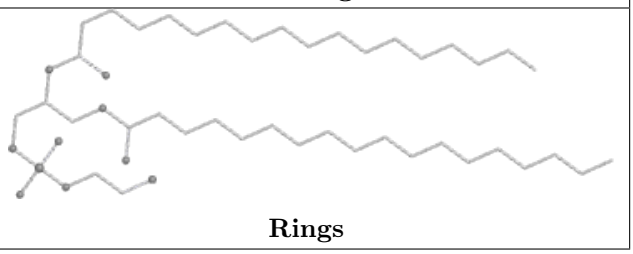


Ligand 3PE H 602

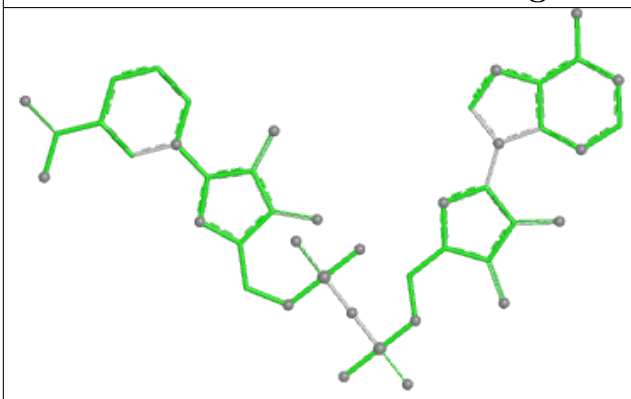

Bond lengths

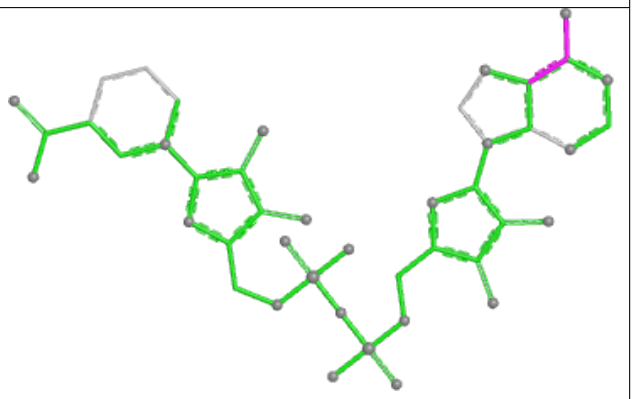

Bond angles

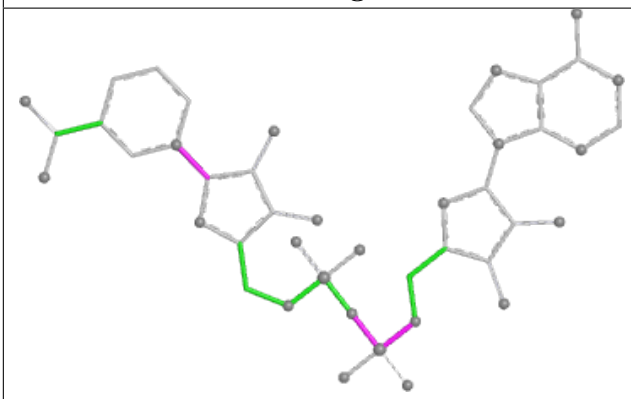

Torsions


Rings

Ligand NAI F 503


Bond lengths


Bond angles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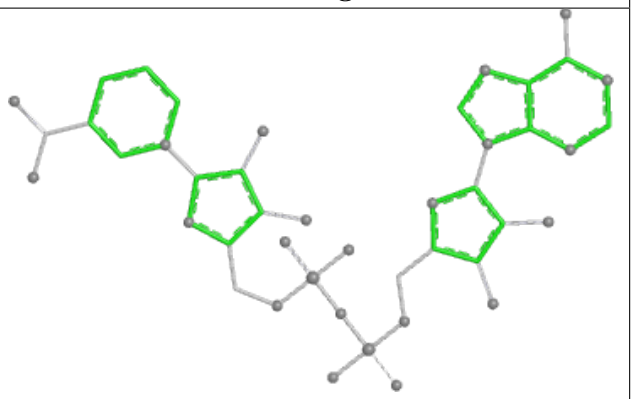
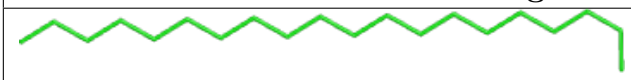
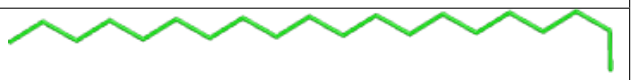
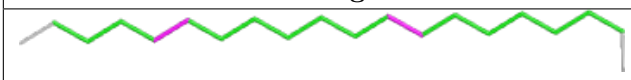
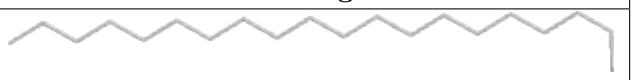

Rings

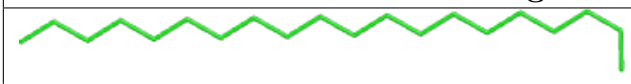
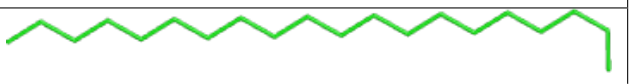
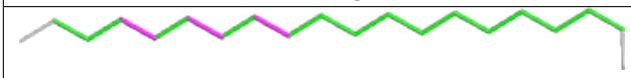
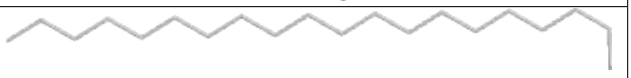
Ligand LFA H 601

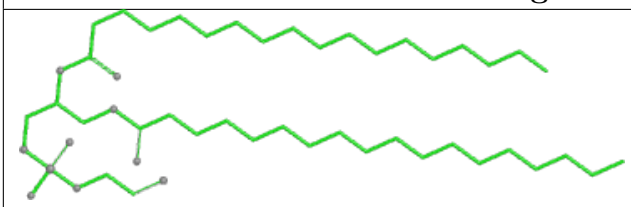
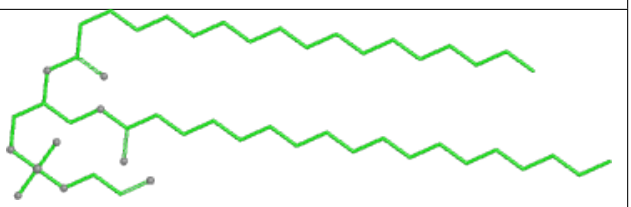
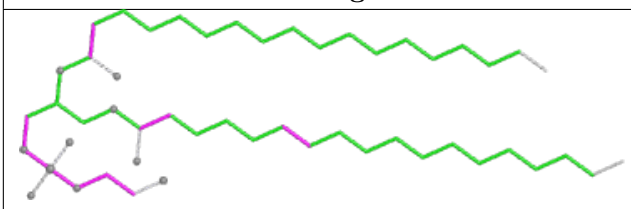
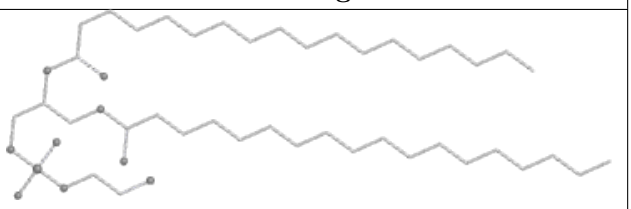

Bond lengths


Bond angles


Torsions


Rings

Ligand LFA N 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

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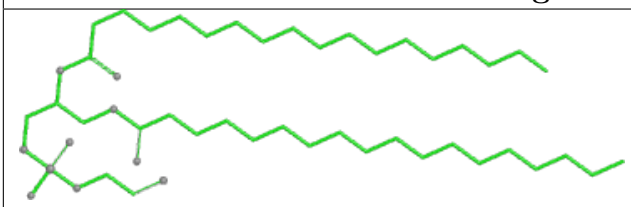
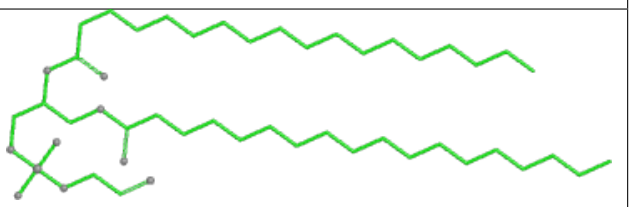
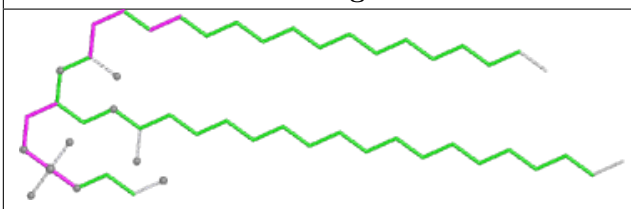
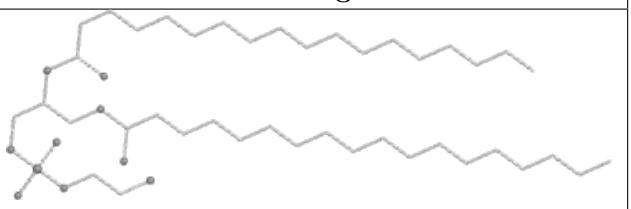
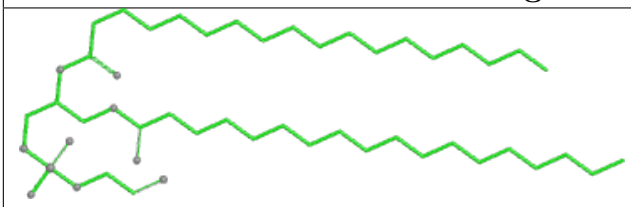
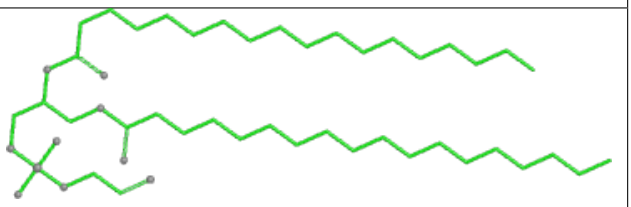
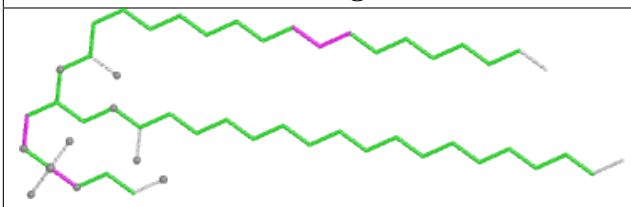
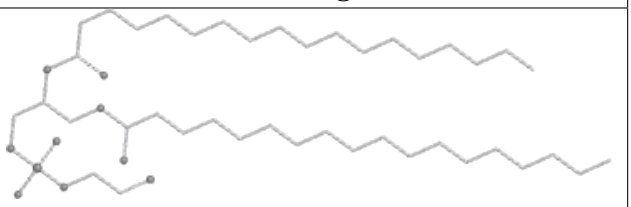
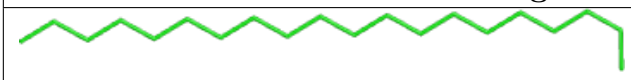
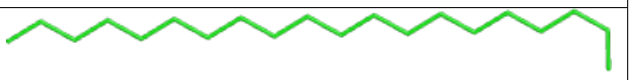
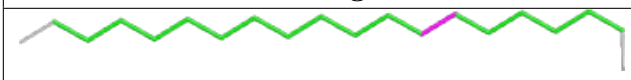
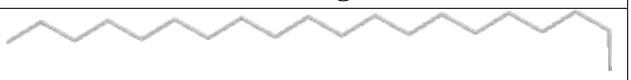
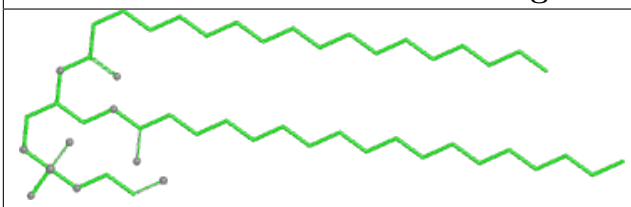
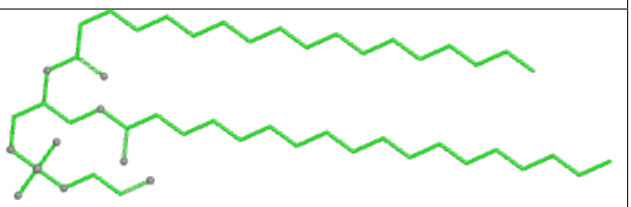
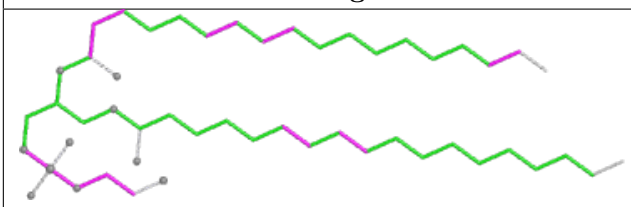
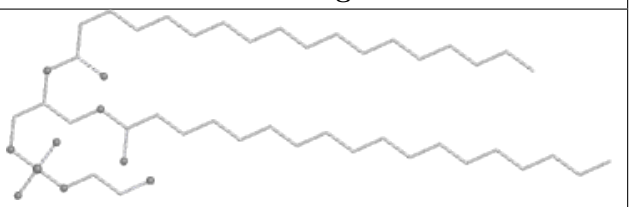
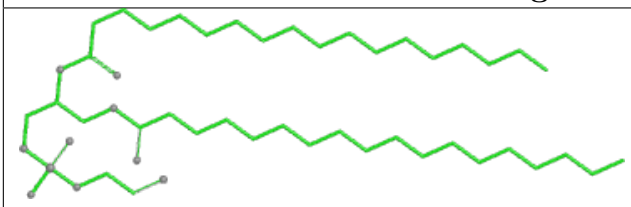
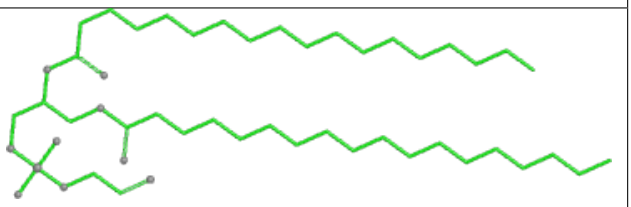
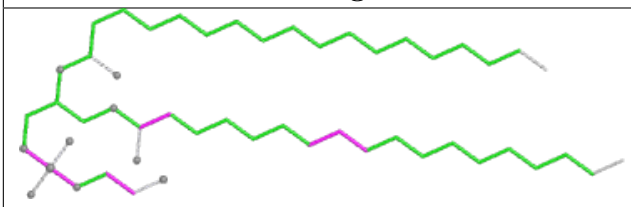
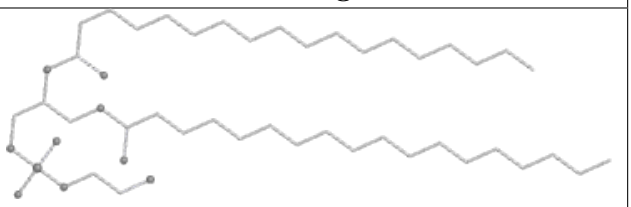
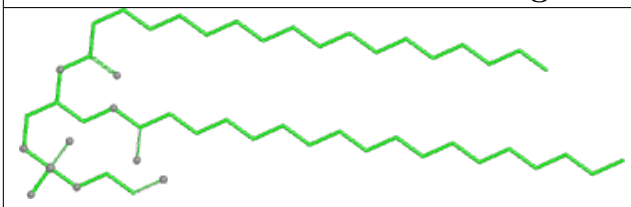
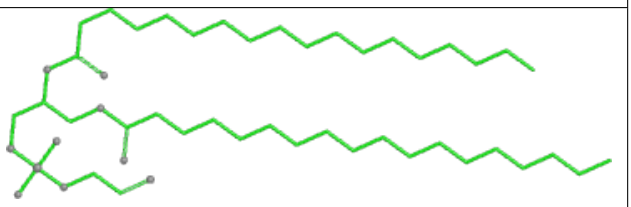
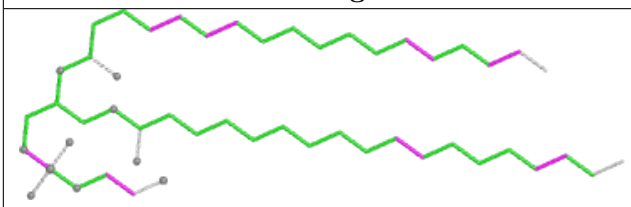
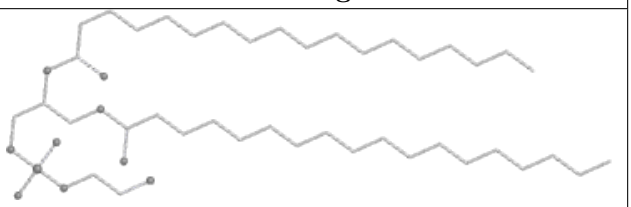
 Bond lengths	 Bond angles
 Torsions	 Rings

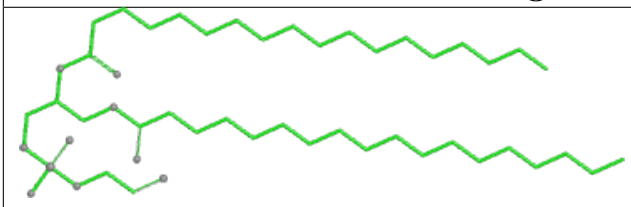
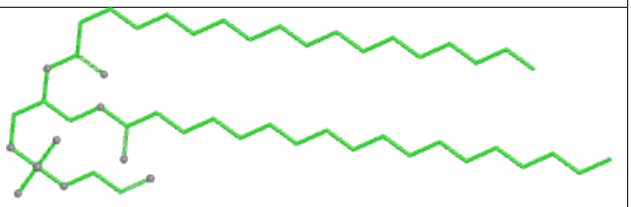
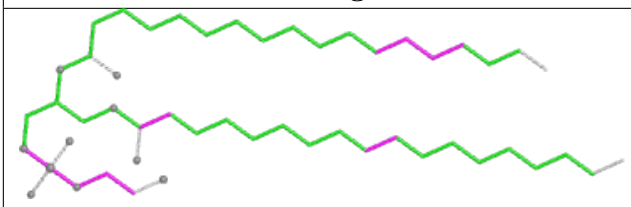
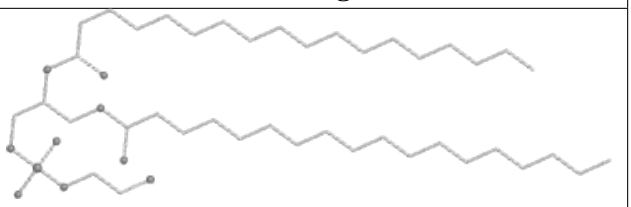
Ligand 3PE M 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LFA L 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

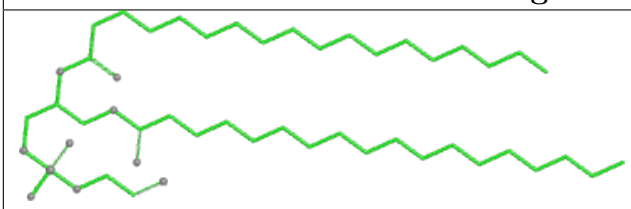
Ligand 3PE L 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

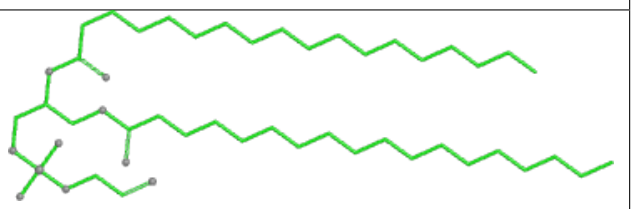
Ligand 3PE L 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE N 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

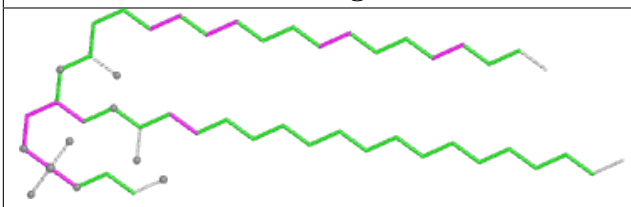
Ligand 3PE L 807



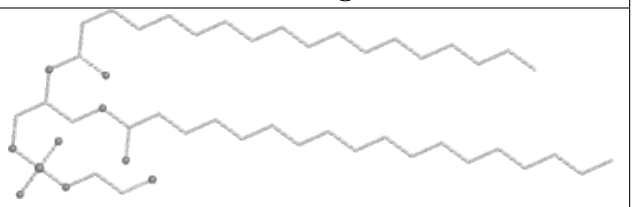
Bond lengths



Bond angles

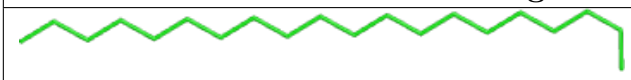


Torsions

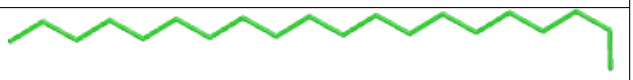


Rings

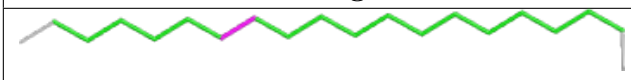
Ligand LFA A 201



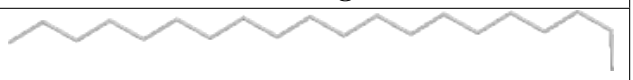
Bond lengths



Bond angles

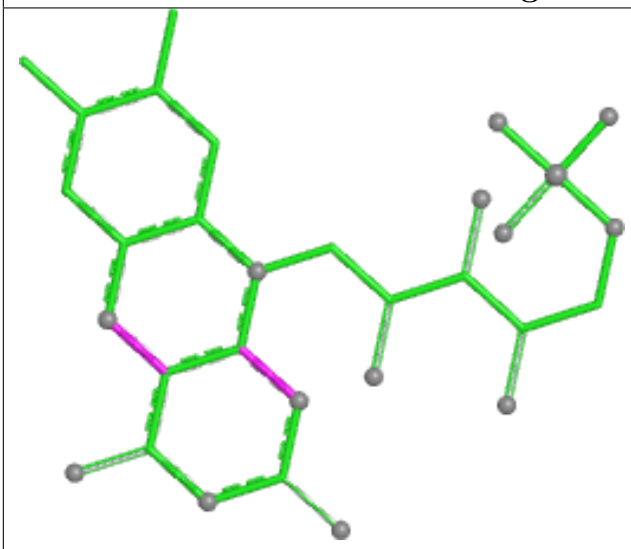


Torsions

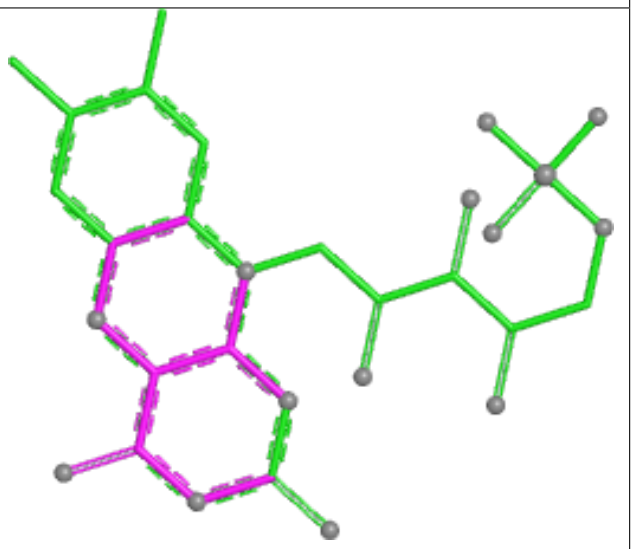


Rings

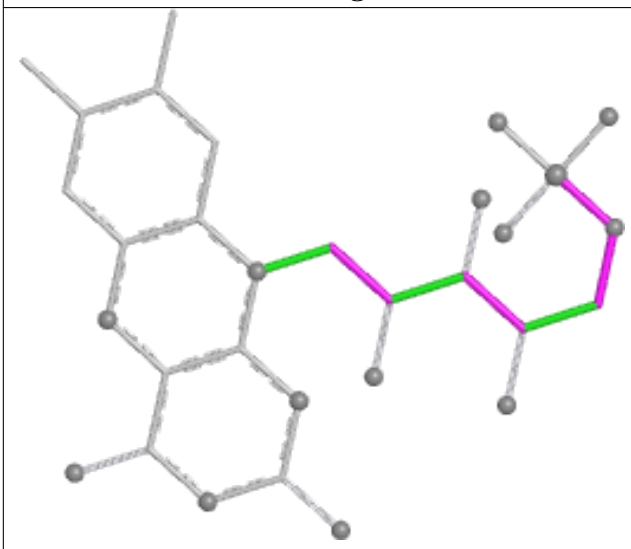
Ligand FMN F 502



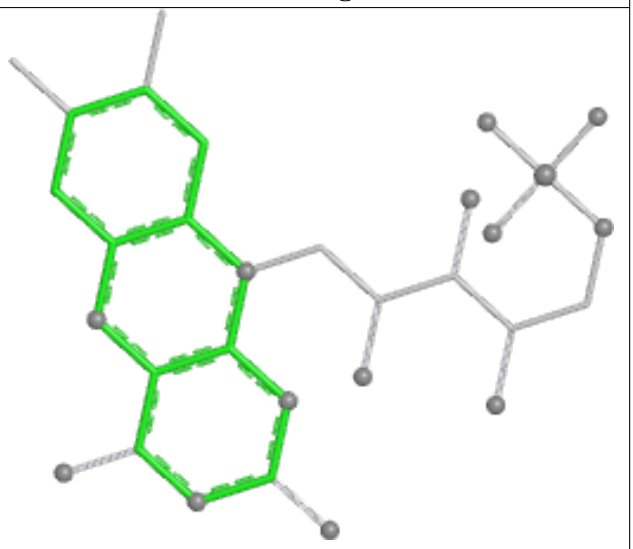
Bond lengths



Bond angles

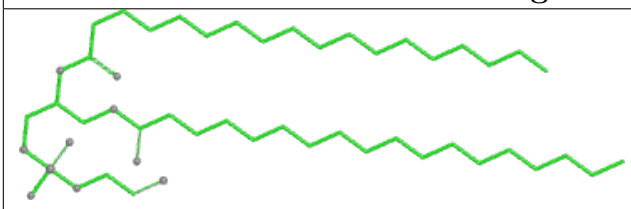


Torsions

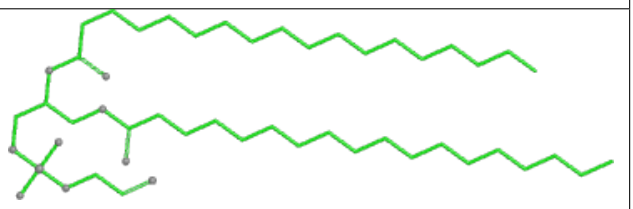


Rings

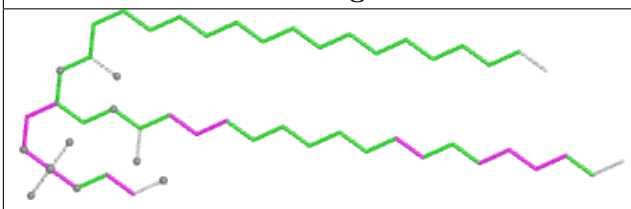
Ligand 3PE L 804



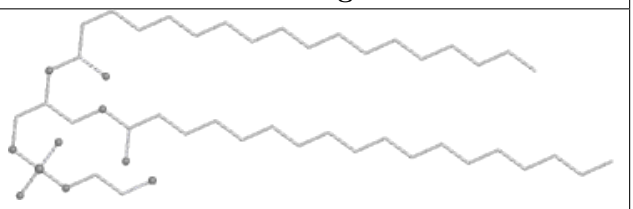
Bond lengths



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.

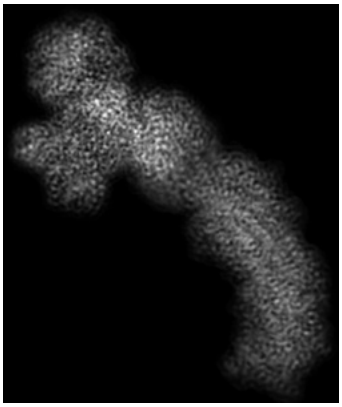
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14632. These allow visual inspection of the internal detail of the map and identification of artifacts.

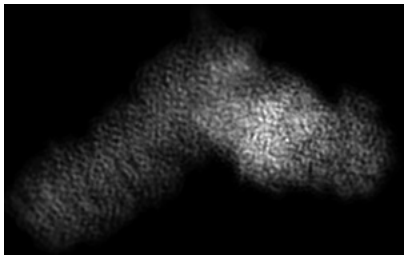
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

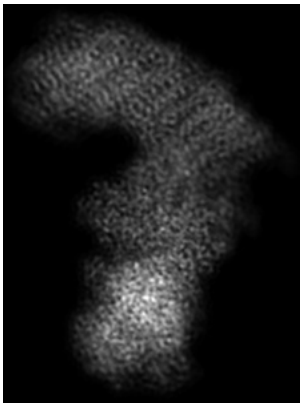
6.1.1 Primary map



X



Y



Z

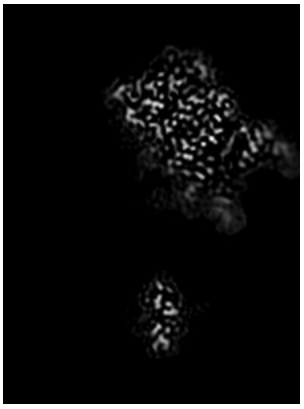
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 72

Y Index: 97



Z Index: 115

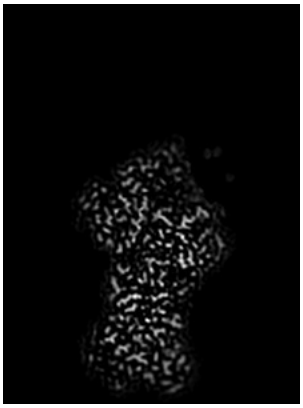
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 77

Y Index: 50



Z Index: 152

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

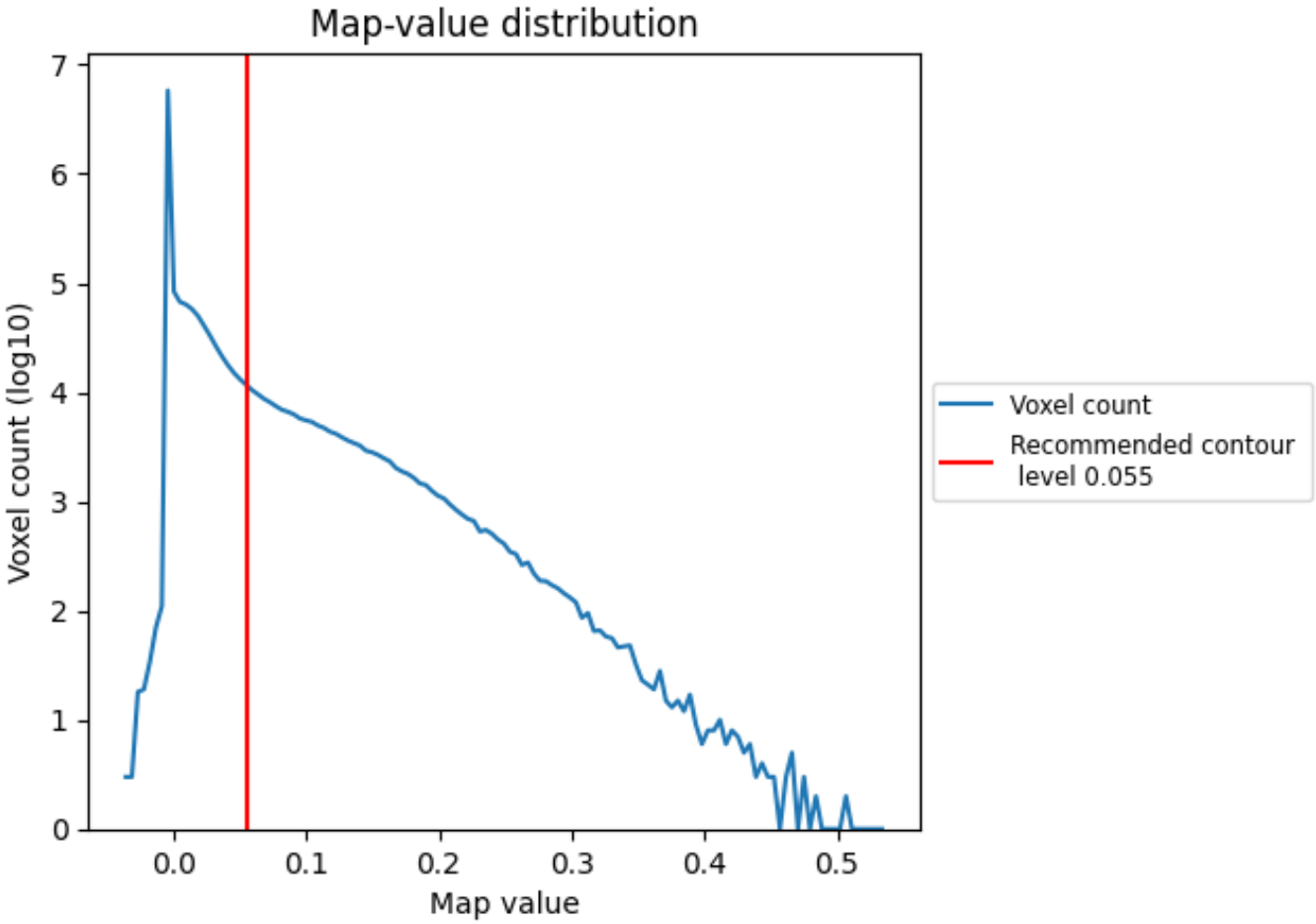
6.5 Mask visualisation (i)

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

7 Map analysis

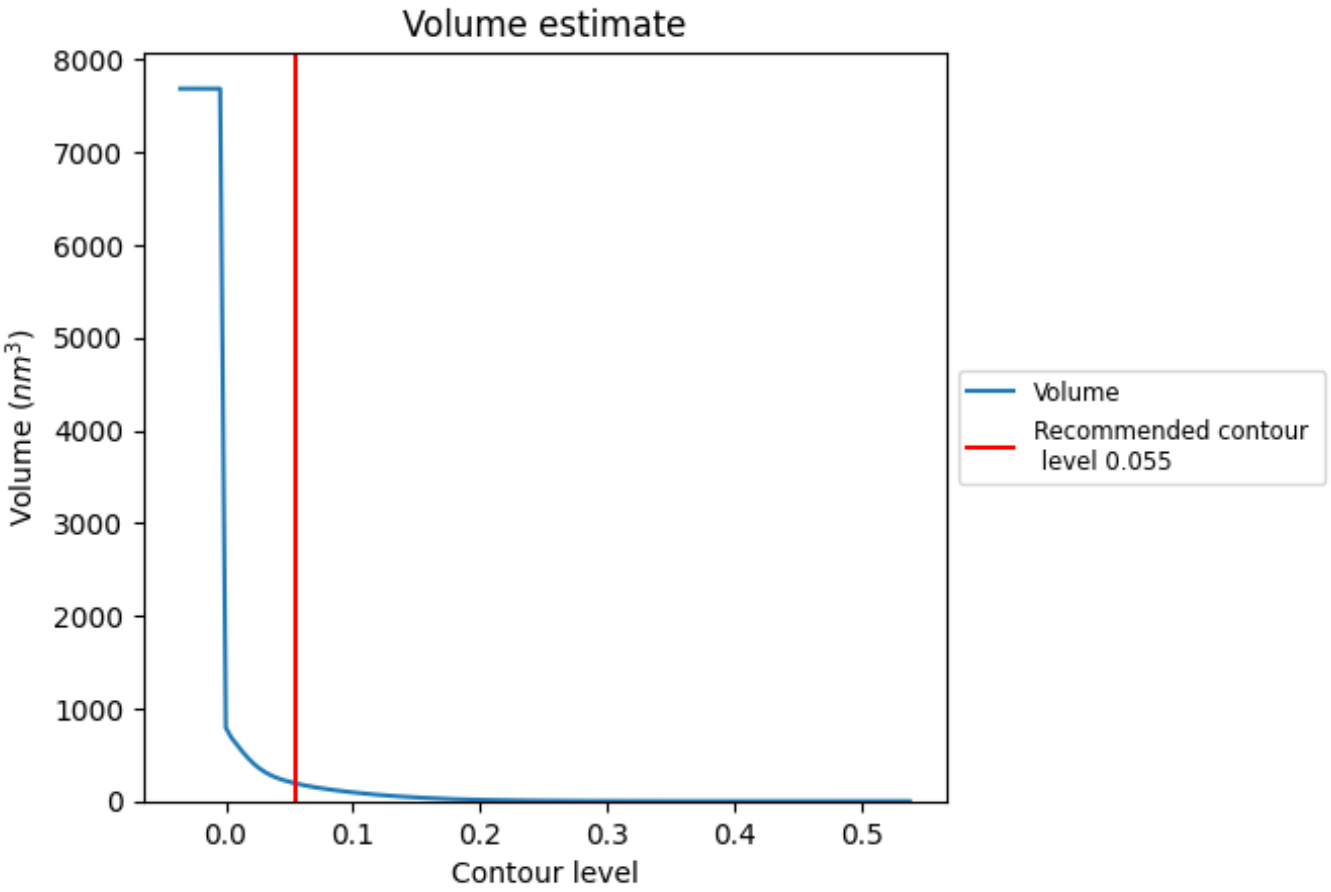
This section contains the results of statistical analysis of the map.

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 191 nm^3; this corresponds to an approximate mass of 173 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.

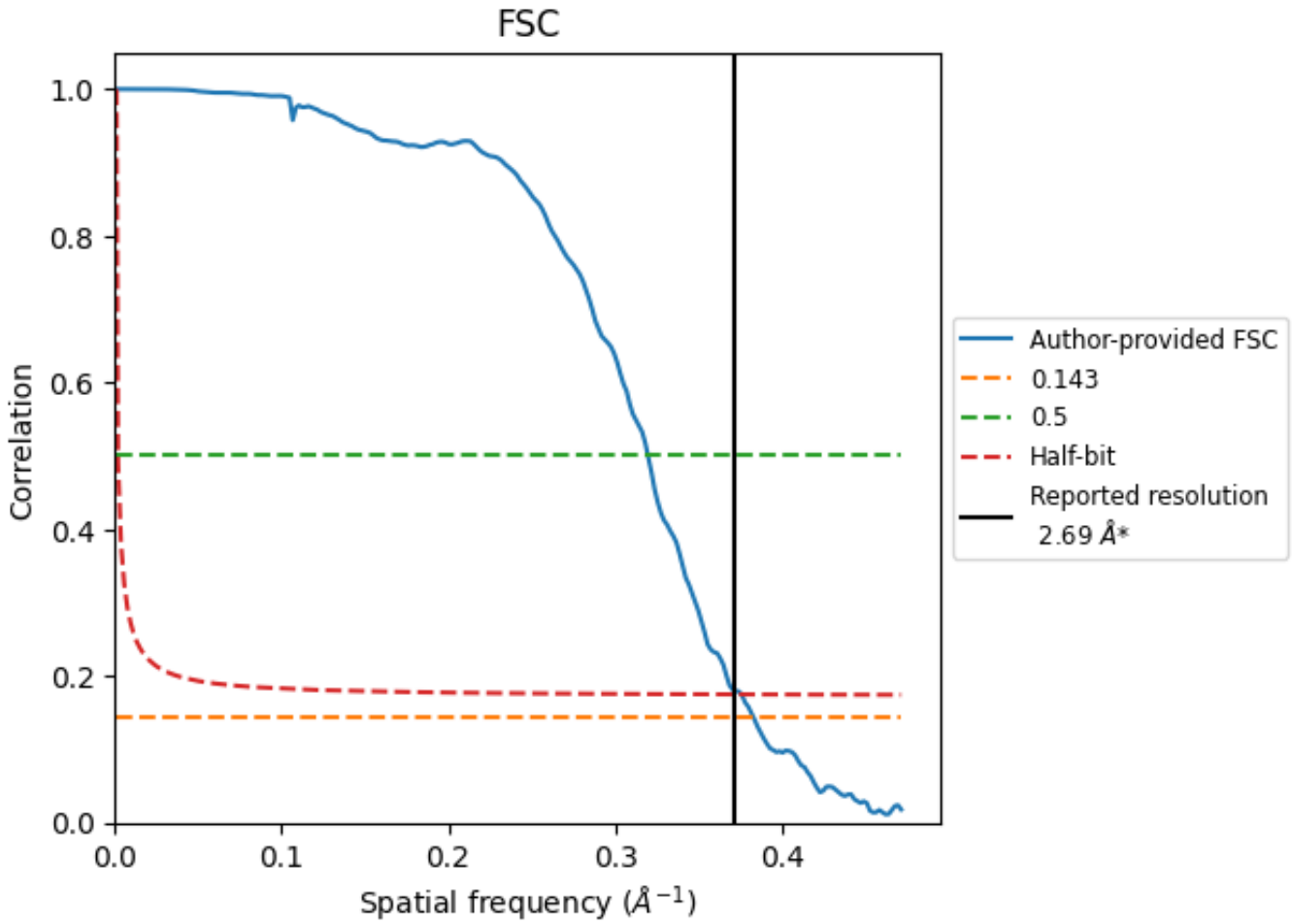
7.3 Rotationally averaged power spectrum

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 0.372 Å^{-1}

8.2 Resolution estimates (i)

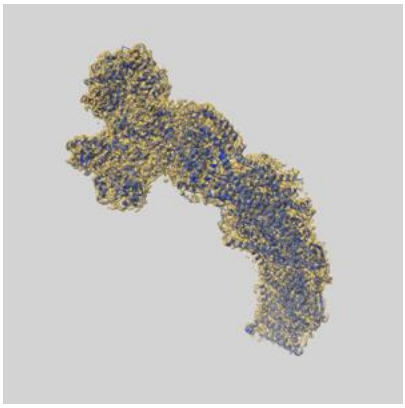
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.61	3.13	2.66
Unmasked-calculated*	-	-	-

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

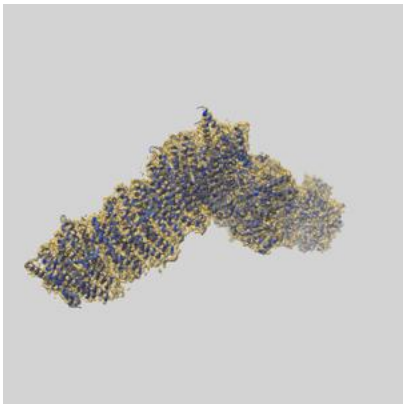
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14632 and PDB model 7ZCI. Per-residue inclusion information can be found in section 3 on page 11.

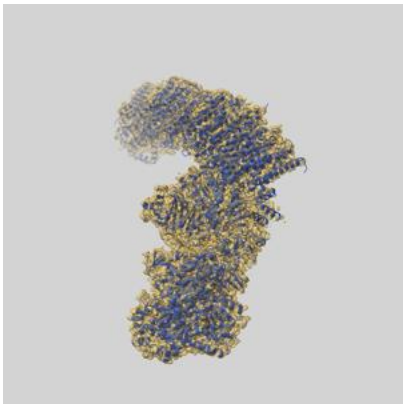
9.1 Map-model overlay



X



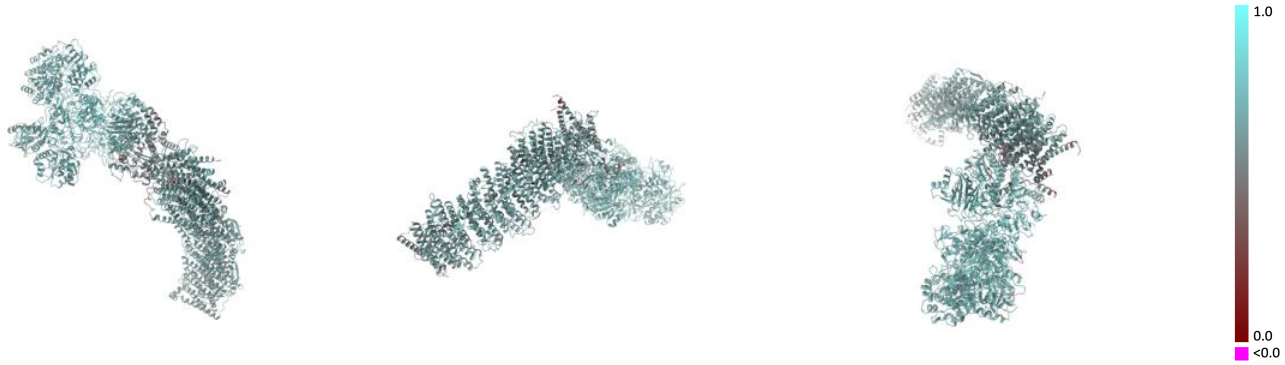
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 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.

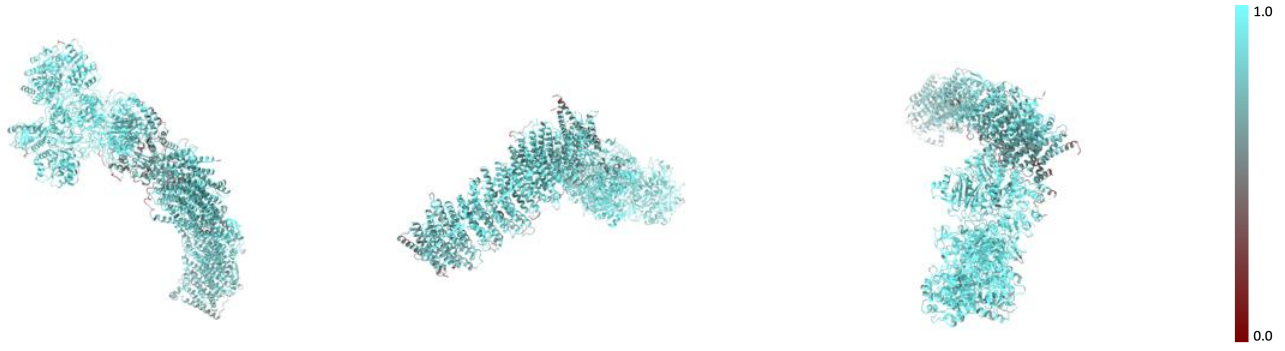
9.2 Q-score mapped to coordinate model (i)



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.

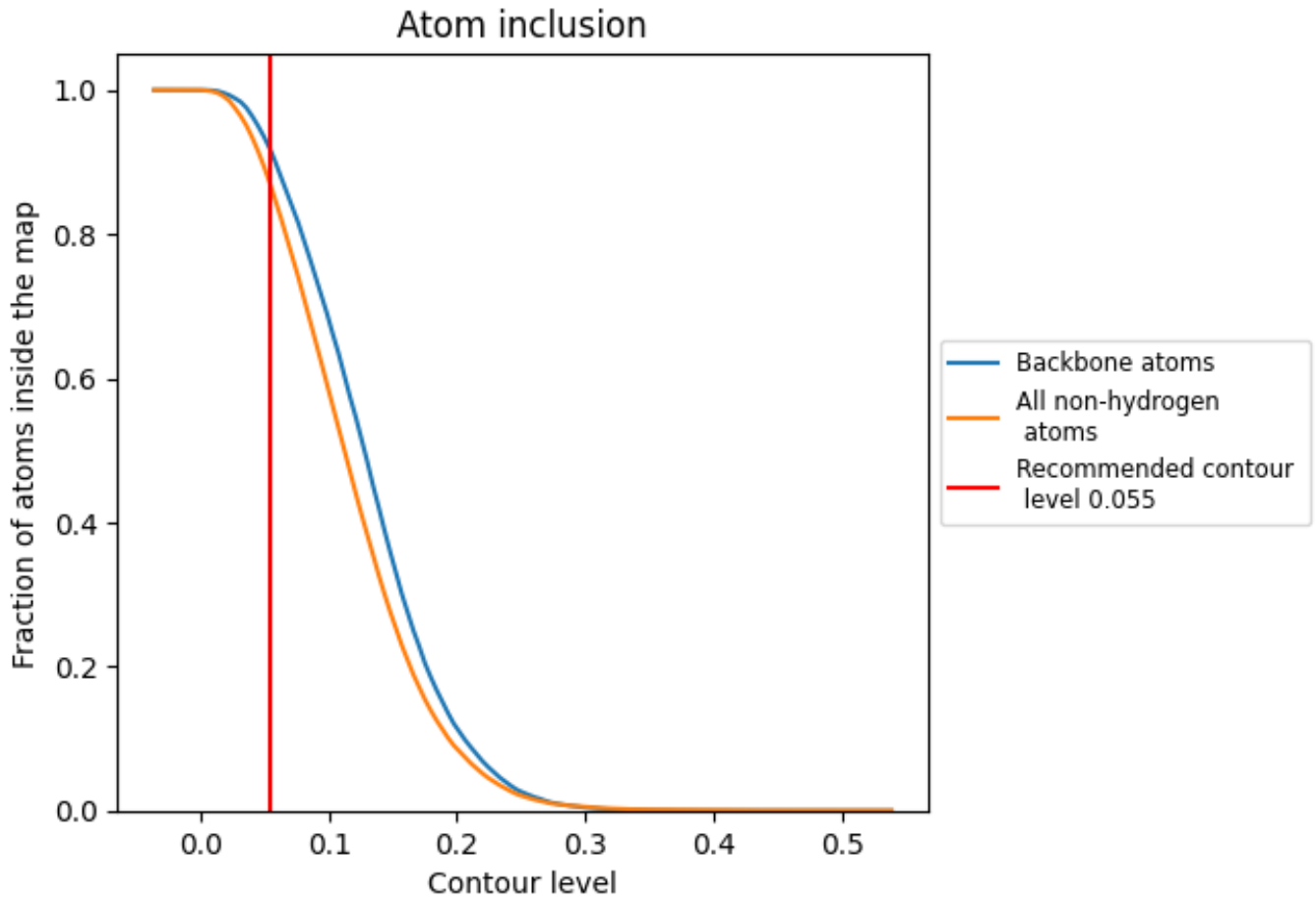
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.055).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8669	0.6370
A	0.7743	0.5920
B	0.8588	0.6180
C	0.9031	0.6600
E	0.9085	0.6640
F	0.9265	0.6650
G	0.9428	0.6880
H	0.7235	0.5550
I	0.9525	0.7040
J	0.8002	0.5940
K	0.9114	0.6410
L	0.7694	0.5900
M	0.8506	0.6210
N	0.8637	0.6250