Full wwPDB EM Validation Report ⓘ

Sep 26, 2022 – 11:52 pm BST

PDB ID	:	7P7K
EMDB ID	:	EMD-13238
Title	:	Complex I from E. coli, DDM/LMNG-purified, with DQ, Resting state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2021-07-19
Resolution	:	3.10 Å(reported)
Based on initial models	:	3RKO, 4HEA

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

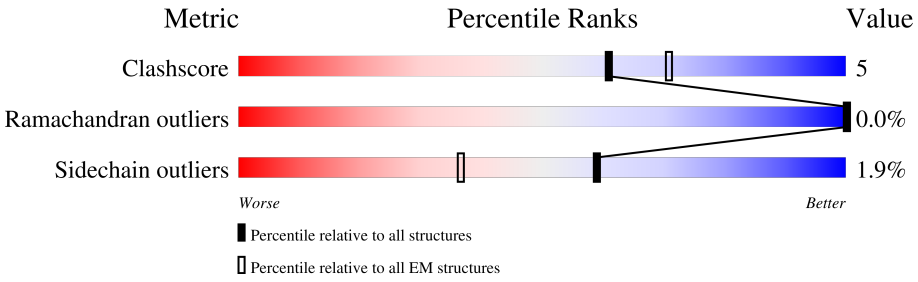
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	F	439	90% 10%
2	E	156	89% 10%
3	G	905	86% 13%
4	C	600	83% 11% 5%
5	B	220	62% 14% 24%
6	I	149	82% 18%
7	H	325	79% 13% 8%
8	A	147	60% 8% 31%

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Mol	Chain	Length	Quality of chain
9	L	613	
10	M	504	
11	N	485	
12	K	100	
13	J	162	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 36531 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-quinone oxidoreductase subunit F.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	568	4575	2934	796	823	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	168	1330	843	231	240	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	149	1185	752	196	224	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	300	Total	C	N	O	S	0	0
			2334	1572	361	383	18		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	599	Total	C	N	O	S	0	0
			4548	3027	722	767	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	478	Total	C	N	O	S	0	0
			3620	2418	571	611	20		

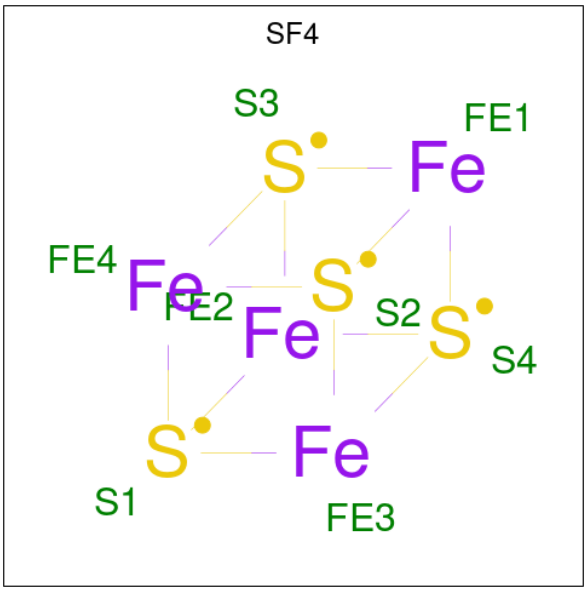
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

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.

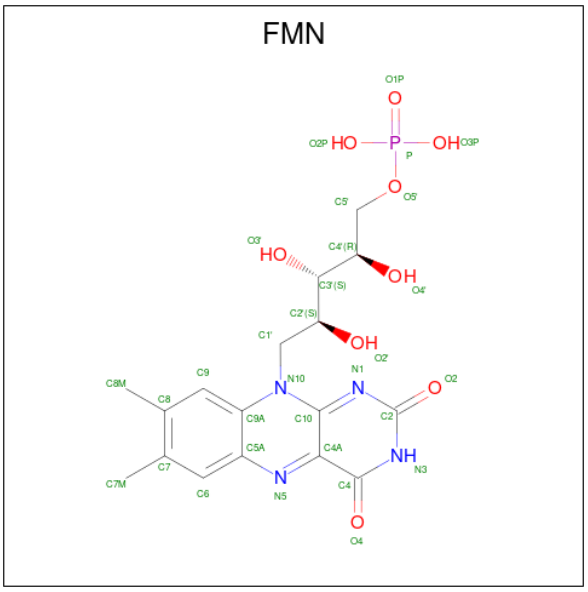
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	162	Total	C	N	O	S	0	0
			1210	815	187	201	7		

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



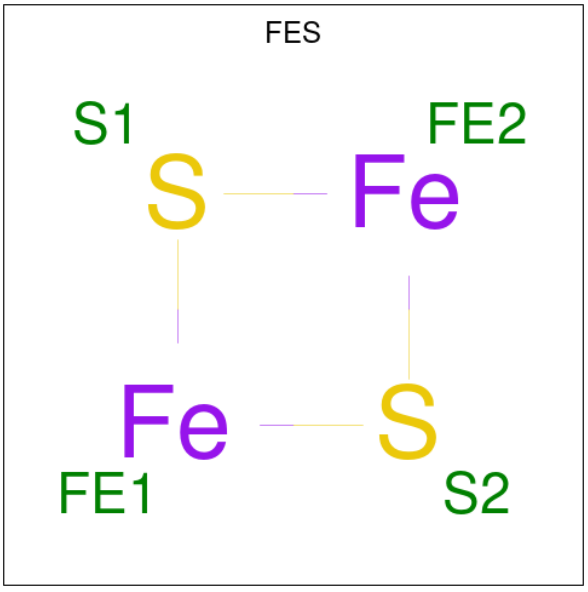
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	B	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 16 8 8	0
14	I	1	Total Fe S 16 8 8	0

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



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

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

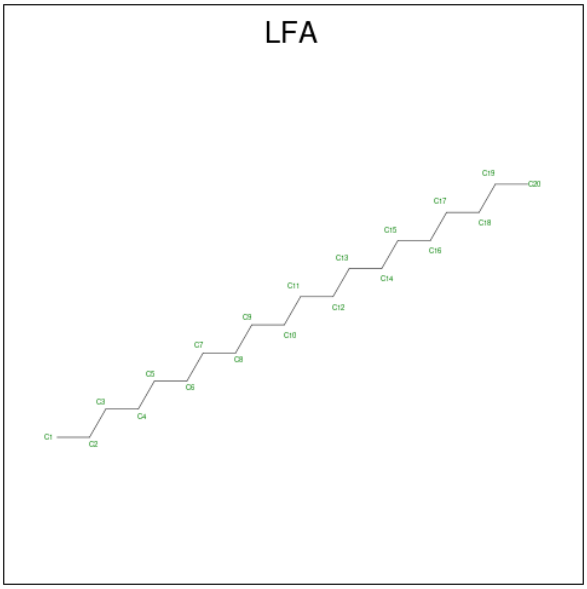


Mol	Chain	Residues	Atoms			AltConf
16	E	1	Total	Fe	S	0
			4	2	2	
16	G	1	Total	Fe	S	0
			4	2	2	

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

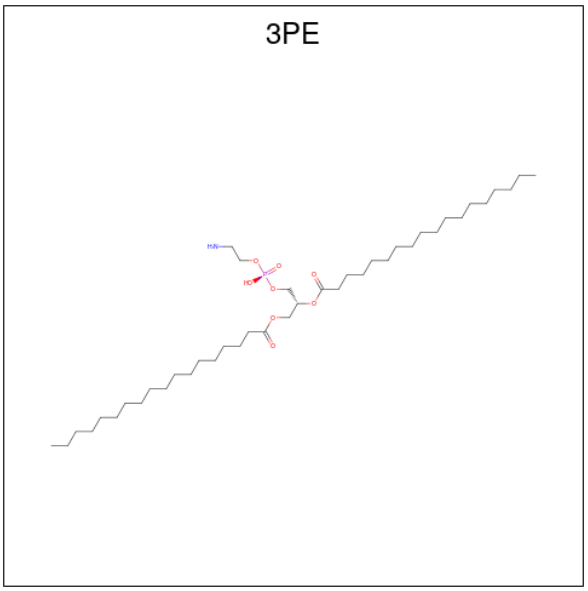
Mol	Chain	Residues	Atoms	AltConf
17	G	1	Total Ca 1 1	0

- Molecule 18 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total C 20 20	0
18	L	1	Total C 14 14	0
18	N	1	Total C 34 34	0
18	N	1	Total C 34 34	0

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

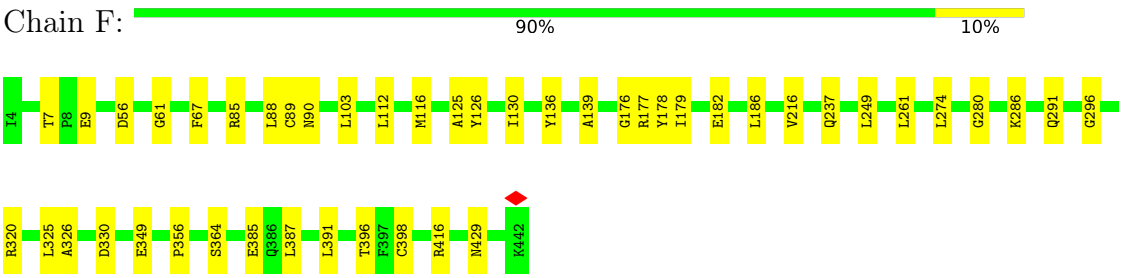


Mol	Chain	Residues	Atoms					AltConf
19	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
19	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
19	L	1	Total	C	N	O	P	0
			145	115	3	24	3	
19	L	1	Total	C	N	O	P	0
			145	115	3	24	3	
19	L	1	Total	C	N	O	P	0
			145	115	3	24	3	
19	M	1	Total	C	N	O	P	0
			153	123	3	24	3	
19	M	1	Total	C	N	O	P	0
			153	123	3	24	3	
19	M	1	Total	C	N	O	P	0
			153	123	3	24	3	

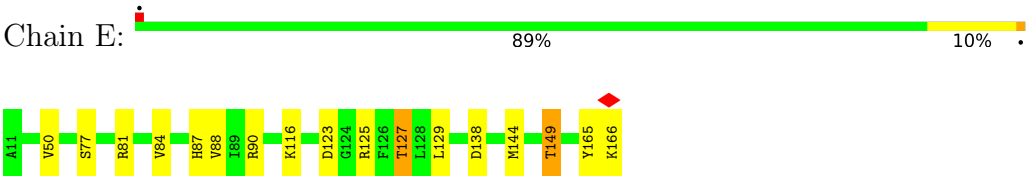
3 Residue-property plots (i)

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.

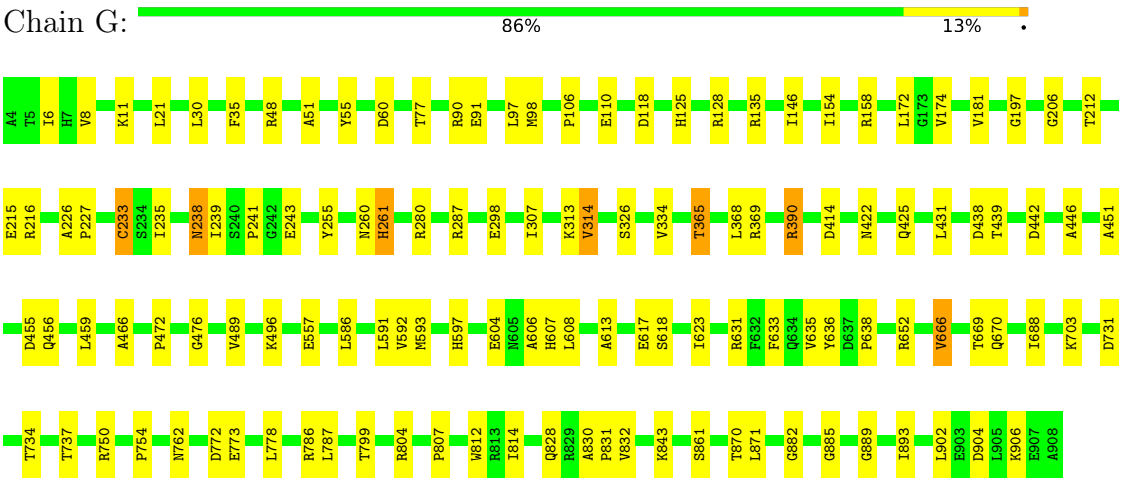
• Molecule 1: NADH-quinone oxidoreductase subunit F



• Molecule 2: NADH dehydrogenase I subunit E

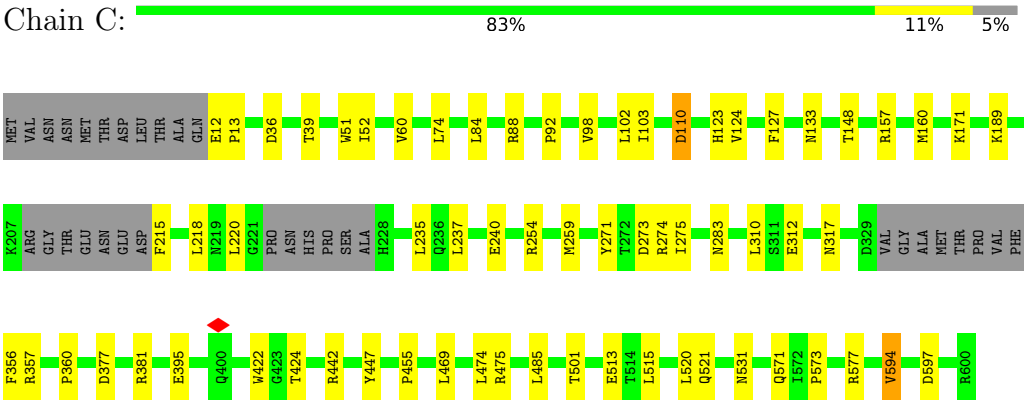


• Molecule 3: NADH-quinone oxidoreductase



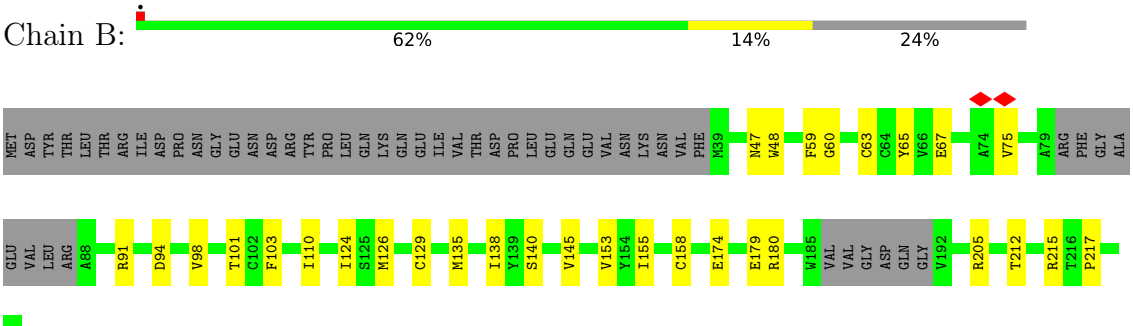
• Molecule 4: NADH-quinone oxidoreductase subunit C/D

Chain C:



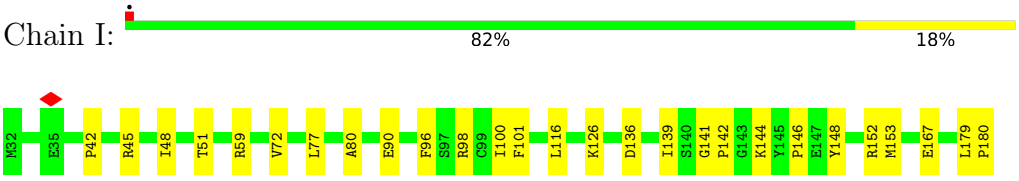
• Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:



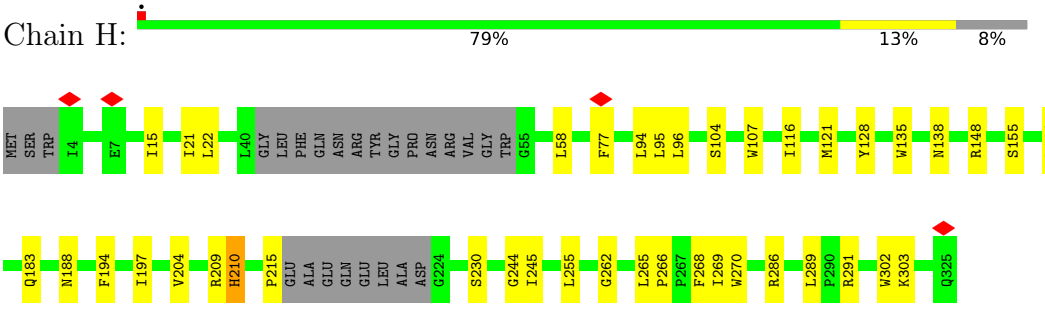
• Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:



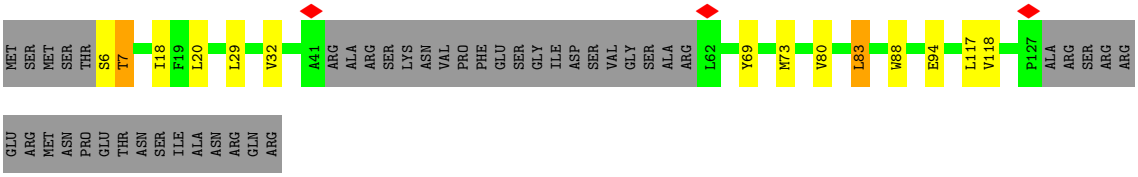
• Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:

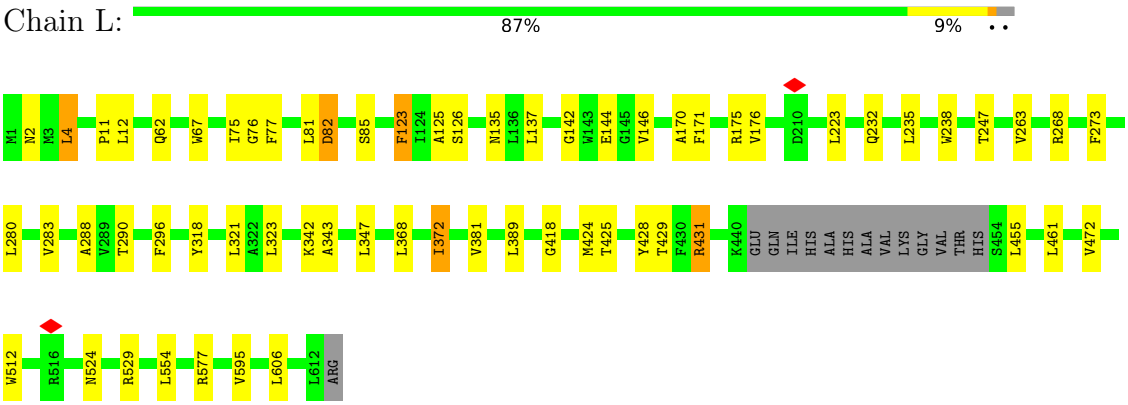


• Molecule 8: NADH-quinone oxidoreductase subunit A

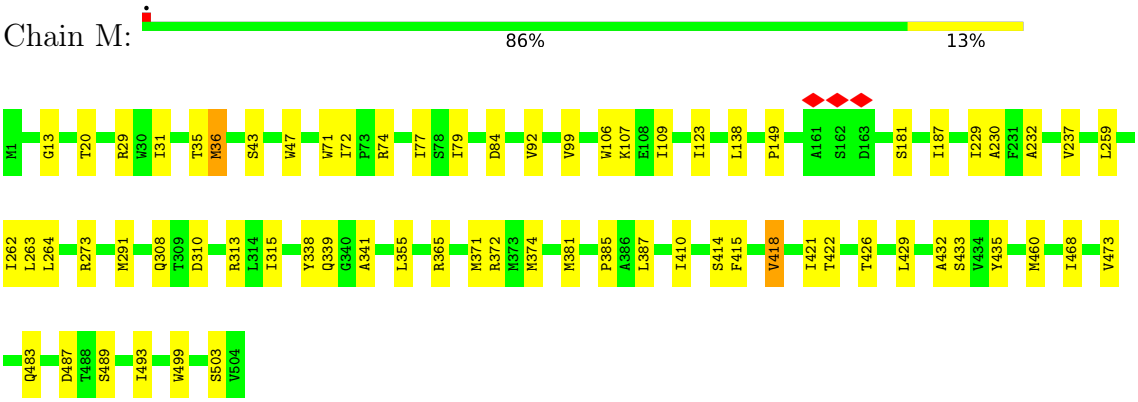
Chain A:



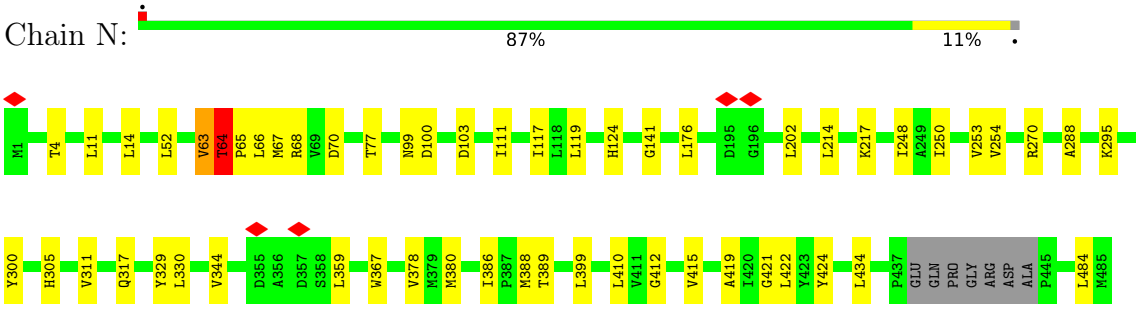
• Molecule 9: Proton-translocating NADH-quinone oxidoreductase, chain L



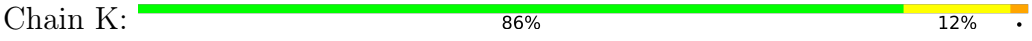
• Molecule 10: NADH dehydrogenase I subunit M

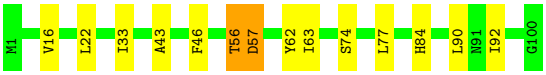


• Molecule 11: NADH-quinone oxidoreductase subunit N

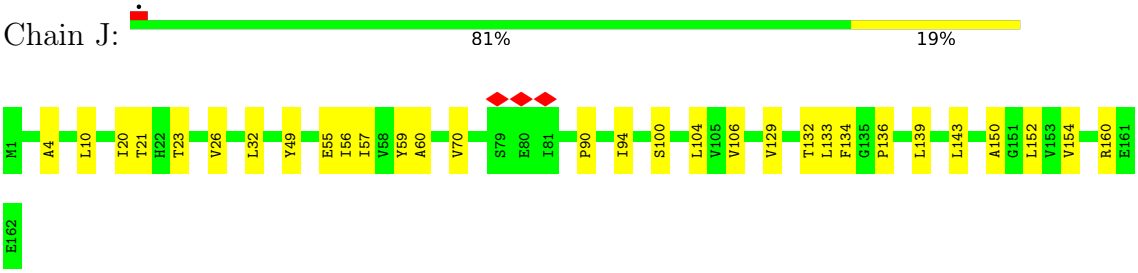


• Molecule 12: NADH-quinone oxidoreductase subunit K





• Molecule 13: NADH-quinone oxidoreductase subunit J



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66814	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	78	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.450	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	151.57999, 203.51999, 248.04	wwPDB
Map dimensions	234, 192, 143	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: FES, CA, LFA, SF4, FMN, 3PE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	F	0.32	0/3486	0.52	0/4713
2	E	0.31	0/1248	0.51	0/1691
3	G	0.38	0/7173	0.54	0/9726
4	C	0.34	0/4698	0.53	0/6374
5	B	0.32	0/1359	0.54	0/1838
6	I	0.40	0/1214	0.56	0/1642
7	H	0.32	0/2400	0.49	0/3265
8	A	0.31	0/833	0.50	0/1134
9	L	0.31	0/4663	0.48	1/6357 (0.0%)
10	M	0.33	0/4074	0.49	0/5546
11	N	0.33	0/3709	0.51	0/5061
12	K	0.31	0/769	0.51	0/1040
13	J	0.32	0/1236	0.47	0/1688
All	All	0.34	0/36862	0.51	1/50075 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1
7	H	0	1
11	N	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	455	LEU	CA-CB-CG	5.47	127.89	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	260	ASN	Peptide
7	H	210	HIS	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	3407	0	3374	25	0
2	E	1220	0	1187	10	0
3	G	7022	0	6824	72	0
4	C	4575	0	4466	40	0
5	B	1330	0	1318	24	0
6	I	1185	0	1145	20	0
7	H	2334	0	2389	31	0
8	A	808	0	821	12	0
9	L	4548	0	4673	35	0
10	M	3953	0	4053	36	0
11	N	3620	0	3790	35	0
12	K	760	0	817	13	0
13	J	1210	0	1271	24	0
14	B	8	0	0	0	0
14	F	8	0	0	0	0
14	G	24	0	0	0	0
14	I	16	0	0	0	0
15	F	31	0	19	1	0
16	E	4	0	0	0	0
16	G	4	0	0	0	0
17	G	1	0	0	0	0
18	H	20	0	42	2	0
18	L	14	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	34	0	69	2	0
19	A	46	0	69	2	0
19	H	51	0	82	3	0
19	L	145	0	227	6	0
19	M	153	0	246	8	0
All	All	36531	0	36909	336	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 (336) 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)
5:B:126:MET:HG2	5:B:155:ILE:HD12	1.68	0.74
11:N:63:VAL:O	11:N:67:MET:HB2	1.89	0.73
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.73	0.70
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.75	0.67
10:M:181:SER:HB2	10:M:230:ALA:HA	1.76	0.67
3:G:238:ASN:HD22	3:G:238:ASN:N	1.93	0.66
13:J:129:VAL:O	13:J:133:LEU:HB2	1.95	0.65
6:I:45:ARG:NH1	6:I:101:PHE:O	2.29	0.65
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.78	0.64
7:H:180:VAL:HA	7:H:183:GLN:HE21	1.63	0.64
3:G:125:HIS:CE1	4:C:513:GLU:HG2	2.32	0.64
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.78	0.64
11:N:65:PRO:HG2	13:J:136:PRO:HB3	1.81	0.62
7:H:15:ILE:HG23	8:A:18:ILE:HG21	1.81	0.61
11:N:419:ALA:HA	11:N:422:LEU:HD12	1.81	0.61
7:H:204:VAL:HG13	7:H:209:ARG:HB3	1.82	0.61
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.72	0.60
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.83	0.60
9:L:85:SER:OG	9:L:268:ARG:NH2	2.35	0.60
5:B:60:GLY:HA3	5:B:65:TYR:HB2	1.83	0.60
9:L:381:VAL:HG21	9:L:461:LEU:HG	1.84	0.60
7:H:121:MET:HG2	13:J:56:ILE:HB	1.85	0.59
3:G:451:ALA:O	3:G:456:GLN:NE2	2.34	0.58
4:C:218:LEU:HD13	4:C:237:LEU:HD13	1.85	0.58
4:C:110:ASP:OD1	4:C:110:ASP:N	2.37	0.58
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.84	0.58
19:L:804:3PE:H2G2	19:M:1002:3PE:H3D2	1.86	0.57
7:H:289:LEU:O	7:H:291:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:554:LEU:HD21	19:M:1001:3PE:H221	1.85	0.57
5:B:47:ASN:ND2	5:B:179:GLU:O	2.38	0.57
3:G:814:ILE:HD11	3:G:902:LEU:HD13	1.87	0.56
11:N:305:HIS:ND1	11:N:329:TYR:OH	2.34	0.56
4:C:395:GLU:OE2	4:C:475:ARG:NH2	2.38	0.56
4:C:360:PRO:O	6:I:45:ARG:NH2	2.37	0.56
19:L:801:3PE:H2F1	10:M:473:VAL:HG22	1.87	0.56
12:K:56:THR:HB	13:J:132:THR:HG21	1.88	0.56
6:I:152:ARG:NH1	6:I:167:GLU:OE2	2.39	0.56
10:M:308:GLN:HG2	10:M:313:ARG:HB2	1.87	0.56
3:G:55:TYR:HB3	3:G:60:ASP:HB3	1.88	0.55
4:C:344:GLN:HG3	5:B:75:VAL:HG11	1.87	0.55
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.87	0.55
4:C:215:PHE:HA	4:C:237:LEU:O	2.06	0.55
1:F:429:ASN:ND2	3:G:128:ARG:O	2.40	0.55
3:G:6:ILE:HG22	3:G:77:THR:HB	1.87	0.55
9:L:273:PHE:HB3	9:L:280:LEU:HD13	1.89	0.55
3:G:593:MET:HG3	3:G:608:LEU:HB3	1.88	0.54
9:L:263:VAL:HG13	9:L:323:LEU:HD11	1.89	0.54
6:I:80:ALA:HB2	6:I:90:GLU:HB2	1.89	0.54
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.90	0.54
9:L:82:ASP:OD1	9:L:82:ASP:N	2.36	0.54
4:C:88:ARG:NH2	4:C:92:PRO:O	2.41	0.54
2:E:84:VAL:HB	2:E:127:THR:HG21	1.90	0.54
10:M:483:GLN:NE2	10:M:487:ASP:OD1	2.39	0.54
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.90	0.54
11:N:386:ILE:O	11:N:389:THR:OG1	2.24	0.54
9:L:524:ASN:O	9:L:529:ARG:NH1	2.40	0.54
3:G:472:PRO:HG3	3:G:799:THR:HA	1.90	0.54
4:C:501:THR:HG23	4:C:521:GLN:HB3	1.90	0.53
5:B:101:THR:HA	5:B:129:CYS:HB3	1.90	0.53
11:N:295:LYS:HD3	11:N:344:VAL:HG11	1.89	0.53
11:N:367:TRP:NE1	11:N:434:LEU:O	2.39	0.53
13:J:90:PRO:O	13:J:94:ILE:HB	2.08	0.53
1:F:356:PRO:HB2	1:F:396:THR:HG22	1.90	0.53
11:N:11:LEU:HD21	13:J:139:LEU:HD21	1.89	0.53
3:G:828:GLN:NE2	3:G:889:GLY:O	2.42	0.52
7:H:148:ARG:HH11	7:H:215:PRO:HB2	1.74	0.52
3:G:476:GLY:O	3:G:804:ARG:NH2	2.42	0.52
9:L:606:LEU:HB3	13:J:106:VAL:HG11	1.91	0.52
4:C:254:ARG:HG3	5:B:103:PHE:HE1	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:170:GLN:NE2	7:H:188:ASN:OD1	2.42	0.52
7:H:266:PRO:HD2	7:H:269:ILE:HD12	1.92	0.52
2:E:88:VAL:HA	2:E:127:THR:HG23	1.91	0.52
3:G:51:ALA:O	3:G:90:ARG:NH1	2.41	0.52
3:G:110:GLU:HG3	3:G:206:GLY:HA2	1.91	0.52
3:G:91:GLU:HG3	3:G:125:HIS:HB2	1.92	0.52
3:G:365:THR:O	3:G:786:ARG:NH2	2.41	0.52
4:C:357:ARG:NH1	5:B:67:GLU:OE1	2.43	0.52
5:B:94:ASP:OD1	5:B:94:ASP:N	2.40	0.52
9:L:318:TYR:OH	9:L:418:GLY:O	2.25	0.52
5:B:217:PRO:HD3	6:I:144:LYS:HB3	1.92	0.51
8:A:6:SER:OG	8:A:7:THR:N	2.43	0.51
3:G:807:PRO:HB3	3:G:882:GLY:HA3	1.91	0.51
6:I:48:ILE:HG12	6:I:116:LEU:HG	1.92	0.51
7:H:155:SER:OG	7:H:302:TRP:NE1	2.42	0.51
11:N:270:ARG:HE	11:N:317:GLN:HE21	1.58	0.51
19:H:602:3PE:H261	19:A:201:3PE:H271	1.91	0.51
3:G:631:ARG:NH2	3:G:688:ILE:O	2.43	0.51
11:N:14:LEU:HD21	13:J:143:LEU:HD11	1.92	0.51
3:G:287:ARG:NH2	3:G:604:GLU:O	2.43	0.51
7:H:164:LEU:HD22	7:H:255:LEU:HD13	1.93	0.51
12:K:84:HIS:HB2	12:K:90:LEU:HD21	1.93	0.51
7:H:210:HIS:O	7:H:291:ARG:NH2	2.45	0.50
10:M:365:ARG:HH21	10:M:460:MET:HA	1.76	0.50
8:A:80:VAL:HA	8:A:83:LEU:HD23	1.92	0.50
3:G:118:ASP:OD1	3:G:762:ASN:ND2	2.44	0.50
9:L:235:LEU:HD21	19:M:1001:3PE:H3E2	1.92	0.50
10:M:187:ILE:HD11	11:N:399:LEU:HD22	1.92	0.50
3:G:313:LYS:NZ	3:G:557:GLU:OE1	2.43	0.50
5:B:217:PRO:HG3	6:I:144:LYS:HD2	1.94	0.50
3:G:298:GLU:HG3	3:G:666:VAL:HG21	1.93	0.50
5:B:48:TRP:HH2	7:H:58:LEU:HB2	1.76	0.50
7:H:21:ILE:HG12	18:H:601:LFA:H62	1.93	0.50
3:G:98:MET:O	3:G:128:ARG:NH1	2.43	0.50
4:C:133:ASN:HB3	4:C:422:TRP:HA	1.93	0.50
9:L:176:VAL:HG21	19:M:1001:3PE:H3B1	1.94	0.50
19:M:1002:3PE:H12	19:M:1003:3PE:H352	1.94	0.50
3:G:422:ASN:O	3:G:425:GLN:NE2	2.43	0.49
1:F:88:LEU:HB2	1:F:216:VAL:HG22	1.95	0.49
1:F:364:SER:HB3	1:F:387:LEU:HD22	1.94	0.49
3:G:226:ALA:HB3	3:G:635:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:135:ASN:N	9:L:135:ASN:OD1	2.43	0.49
11:N:119:LEU:HD22	11:N:253:VAL:HG11	1.93	0.49
9:L:126:SER:OG	9:L:142:GLY:O	2.31	0.49
10:M:20:THR:HG21	10:M:31:ILE:HD13	1.93	0.49
10:M:499:TRP:O	10:M:503:SER:OG	2.29	0.49
11:N:100:ASP:OD2	13:J:160:ARG:NH2	2.40	0.49
5:B:91:ARG:HG3	7:H:230:SER:HB3	1.95	0.49
5:B:135:MET:HA	6:I:72:VAL:HG13	1.95	0.49
8:A:69:TYR:OH	12:K:74:SER:O	2.30	0.49
10:M:43:SER:HB3	10:M:92:VAL:HG22	1.94	0.49
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.47	0.49
19:L:804:3PE:H271	19:L:804:3PE:H341	1.95	0.49
19:H:602:3PE:N	13:J:49:TYR:OH	2.45	0.49
10:M:308:GLN:HG3	10:M:310:ASP:H	1.78	0.49
1:F:330:ASP:OD1	1:F:330:ASP:N	2.39	0.48
3:G:843:LYS:HB2	3:G:885:GLY:HA3	1.93	0.48
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.94	0.48
10:M:84:ASP:OD1	10:M:273:ARG:NH2	2.39	0.48
12:K:33:ILE:HG23	13:J:32:LEU:HD22	1.95	0.48
3:G:146:ILE:HD11	3:G:197:GLY:HA2	1.94	0.48
3:G:414:ASP:OD1	3:G:414:ASP:N	2.44	0.48
4:C:275:ILE:O	4:C:283:ASN:ND2	2.47	0.48
11:N:378:VAL:HG22	18:N:501:LFA:H182	1.96	0.48
3:G:613:ALA:HB1	3:G:617:GLU:HB2	1.95	0.48
19:M:1001:3PE:H331	19:M:1001:3PE:H231	1.95	0.48
3:G:261:HIS:CD2	3:G:369:ARG:HG3	2.48	0.48
3:G:812:TRP:HB2	3:G:902:LEU:HB3	1.95	0.48
3:G:390:ARG:HD2	3:G:390:ARG:HA	1.63	0.47
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.96	0.47
6:I:59:ARG:NH2	6:I:142:PRO:O	2.48	0.47
1:F:176:GLY:O	2:E:77:SER:OG	2.32	0.47
5:B:98:VAL:HG11	5:B:145:VAL:HG21	1.96	0.47
7:H:96:LEU:HD22	8:A:20:LEU:HD23	1.96	0.47
1:F:7:THR:OG1	1:F:9:GLU:OE1	2.30	0.47
5:B:205:ARG:NH2	6:I:136:ASP:OD1	2.42	0.47
11:N:99:ASN:OD1	11:N:99:ASN:N	2.46	0.47
12:K:16:VAL:HG21	13:J:104:LEU:HB2	1.97	0.47
3:G:731:ASP:OD2	3:G:734:THR:OG1	2.33	0.47
11:N:70:ASP:N	11:N:70:ASP:OD1	2.48	0.47
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.96	0.47
9:L:288:ALA:HB2	9:L:321:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:57:ASP:OD1	12:K:57:ASP:N	2.48	0.47
1:F:387:LEU:HG	1:F:391:LEU:HD13	1.97	0.47
7:H:268:PHE:HD2	18:H:601:LFA:H203	1.80	0.47
8:A:83:LEU:HD11	12:K:63:ILE:HG23	1.97	0.47
4:C:110:ASP:OD2	4:C:442:ARG:NH1	2.49	0.46
4:C:220:LEU:HD13	4:C:235:LEU:HD13	1.98	0.46
6:I:142:PRO:HB2	6:I:146:PRO:HA	1.95	0.46
9:L:67:TRP:H	9:L:76:GLY:HA2	1.79	0.46
11:N:68:ARG:HD3	11:N:484:LEU:HD13	1.97	0.46
8:A:94:GLU:N	8:A:94:GLU:OE1	2.47	0.46
3:G:97:LEU:HD22	3:G:154:ILE:HB	1.97	0.46
1:F:85:ARG:HB2	1:F:125:ALA:HA	1.97	0.46
3:G:255:TYR:HD2	3:G:778:LEU:HD13	1.81	0.46
11:N:176:LEU:HD22	11:N:202:LEU:HD11	1.96	0.46
3:G:216:ARG:NH1	6:I:90:GLU:OE1	2.46	0.46
7:H:209:ARG:HD3	7:H:245:ILE:HD11	1.97	0.46
9:L:368:LEU:HD23	9:L:372:ILE:HD11	1.97	0.46
1:F:296:GLY:O	1:F:320:ARG:NH2	2.49	0.46
4:C:573:PRO:O	4:C:577:ARG:NE	2.48	0.46
19:H:602:3PE:H391	8:A:20:LEU:HD13	1.98	0.46
3:G:592:VAL:HB	3:G:606:ALA:HA	1.96	0.46
4:C:377:ASP:N	4:C:377:ASP:OD1	2.48	0.46
7:H:210:HIS:HB3	7:H:286:ARG:HG3	1.98	0.46
7:H:265:LEU:HB2	7:H:270:TRP:CD1	2.51	0.46
11:N:66:LEU:HA	11:N:124:HIS:HB2	1.98	0.46
11:N:288:ALA:HB2	11:N:300:TYR:HB2	1.97	0.46
2:E:144:MET:HE2	2:E:149:THR:HB	1.98	0.45
12:K:62:TYR:OH	13:J:55:GLU:OE1	2.30	0.45
4:C:455:PRO:HB2	4:C:469:LEU:HD22	1.96	0.45
9:L:2:ASN:O	9:L:62:GLN:NE2	2.46	0.45
3:G:238:ASN:N	3:G:238:ASN:ND2	2.64	0.45
9:L:171:PHE:HE2	10:M:433:SER:HB2	1.82	0.45
5:B:59:PHE:HE2	5:B:110:ILE:HG12	1.81	0.45
10:M:387:LEU:HD13	10:M:468:ILE:HG21	1.99	0.45
10:M:414:SER:O	10:M:418:VAL:N	2.39	0.45
19:M:1003:3PE:H3H2	11:N:415:VAL:HG11	1.98	0.45
10:M:338:TYR:HB3	10:M:493:ILE:HD12	1.99	0.45
4:C:157:ARG:HD3	4:C:160:MET:HB2	1.99	0.45
6:I:59:ARG:NH1	6:I:148:TYR:O	2.47	0.45
7:H:94:LEU:HD13	7:H:244:GLY:HA3	1.99	0.45
10:M:339:GLN:OE1	10:M:489:SER:OG	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:77:LEU:HB3	13:J:70:VAL:HG21	1.98	0.45
3:G:871:LEU:HD11	3:G:893:ILE:HD11	1.99	0.45
3:G:904:ASP:OD1	3:G:906:LYS:NZ	2.44	0.45
5:B:135:MET:HB3	6:I:100:ILE:HG21	1.98	0.45
8:A:117:LEU:HD11	13:J:152:LEU:HD21	1.99	0.45
1:F:56:ASP:O	1:F:237:GLN:NE2	2.45	0.44
3:G:243:GLU:HG2	3:G:636:TYR:HB3	1.98	0.44
7:H:121:MET:HG3	13:J:57:ILE:HG13	1.99	0.44
1:F:291:GLN:O	1:F:326:ALA:HA	2.17	0.44
3:G:438:ASP:OD1	3:G:438:ASP:N	2.49	0.44
4:C:123:HIS:HA	4:C:148:THR:O	2.17	0.44
3:G:703:LYS:HE3	3:G:737:THR:HB	2.00	0.44
10:M:381:MET:HB2	10:M:385:PRO:HD3	1.99	0.44
1:F:90:ASN:ND2	15:F:502:FMN:O4'	2.50	0.44
4:C:84:LEU:HD22	4:C:171:LYS:HB3	1.99	0.44
4:C:424:THR:OG1	4:C:571:GLN:OE1	2.30	0.44
10:M:493:ILE:HD13	10:M:493:ILE:HA	1.85	0.44
3:G:239:ILE:HG13	3:G:241:PRO:HD3	1.99	0.44
3:G:431:LEU:O	3:G:446:ALA:N	2.50	0.44
11:N:270:ARG:HH21	11:N:317:GLN:HG3	1.83	0.44
3:G:212:THR:HG22	3:G:832:VAL:HG21	1.99	0.43
3:G:227:PRO:HG2	3:G:633:PHE:CD1	2.53	0.43
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.99	0.43
3:G:451:ALA:HB1	3:G:455:ASP:HB2	1.98	0.43
1:F:112:LEU:O	1:F:116:MET:HG2	2.18	0.43
9:L:577:ARG:NH1	19:L:804:3PE:O22	2.48	0.43
3:G:280:ARG:HH21	3:G:597:HIS:HB2	1.83	0.43
9:L:75:ILE:HG21	9:L:137:LEU:HD23	1.98	0.43
9:L:232:GLN:HA	9:L:290:THR:HG21	1.99	0.43
7:H:128:TYR:OH	13:J:60:ALA:O	2.30	0.43
2:E:125:ARG:NH2	2:E:165:TYR:O	2.51	0.43
4:C:317:ASN:OD1	4:C:343:ARG:NH1	2.51	0.43
7:H:209:ARG:HD2	7:H:209:ARG:HA	1.78	0.43
9:L:123:PHE:HE1	9:L:146:VAL:HG13	1.84	0.43
4:C:310:LEU:HD23	4:C:310:LEU:HA	1.75	0.43
7:H:303:LYS:HE3	8:A:118:VAL:HG13	1.99	0.43
10:M:47:TRP:HE1	10:M:92:VAL:HG11	1.82	0.43
11:N:141:GLY:HA3	13:J:154:VAL:HG22	2.00	0.43
3:G:439:THR:OG1	3:G:442:ASP:OD1	2.37	0.43
7:H:262:GLY:HA3	7:H:270:TRP:CD1	2.54	0.43
10:M:71:TRP:HB2	10:M:79:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:123:ILE:HG13	10:M:149:PRO:HB2	2.00	0.43
3:G:466:ALA:HB3	3:G:489:VAL:HG21	2.00	0.43
10:M:72:ILE:HB	10:M:77:ILE:HB	2.01	0.43
10:M:315:ILE:HD13	10:M:355:LEU:HB3	2.01	0.43
11:N:330:LEU:HD23	11:N:330:LEU:HA	1.82	0.43
1:F:61:GLY:N	1:F:67:PHE:O	2.45	0.43
7:H:77:PHE:O	7:H:138:ASN:ND2	2.52	0.43
7:H:194:PHE:HA	7:H:197:ILE:HG12	1.99	0.43
9:L:12:LEU:HD11	19:L:801:3PE:H3H1	2.00	0.43
3:G:652:ARG:NH2	3:G:669:THR:O	2.43	0.42
4:C:52:ILE:HD12	4:C:60:VAL:HG21	2.01	0.42
9:L:343:ALA:O	9:L:347:LEU:HG	2.19	0.42
11:N:311:VAL:HG22	11:N:410:LEU:HD22	2.01	0.42
4:C:381:ARG:HD2	4:C:485:LEU:HD21	2.00	0.42
9:L:144:GLU:OE1	9:L:175:ARG:NH1	2.53	0.42
10:M:291:MET:HB3	10:M:421:ILE:HD13	2.01	0.42
4:C:39:THR:HB	4:C:51:TRP:HB2	2.00	0.42
4:C:103:ILE:HG12	4:C:110:ASP:HB3	2.02	0.42
10:M:13:GLY:HA3	10:M:35:THR:HG21	2.02	0.42
1:F:177:ARG:HG3	1:F:179:ILE:HG22	2.01	0.42
6:I:48:ILE:HB	6:I:96:PHE:HZ	1.84	0.42
3:G:35:PHE:O	3:G:158:ARG:HD2	2.20	0.42
3:G:772:ASP:OD1	3:G:773:GLU:N	2.50	0.42
4:C:259:MET:HG2	4:C:271:TYR:CE1	2.54	0.42
4:C:312:GLU:OE2	4:C:447:TYR:OH	2.30	0.42
9:L:296:PHE:CG	9:L:424:MET:HE1	2.55	0.42
11:N:421:GLY:HA2	11:N:424:TYR:CE2	2.55	0.42
2:E:50:VAL:O	2:E:81:ARG:NH1	2.50	0.42
2:E:138:ASP:OD1	2:E:138:ASP:N	2.52	0.42
4:C:12:GLU:HA	4:C:13:PRO:HD3	1.92	0.42
4:C:237:LEU:HD23	4:C:240:GLU:HA	2.00	0.42
1:F:274:LEU:O	1:F:280:GLY:N	2.48	0.42
1:F:385:GLU:OE2	1:F:416:ARG:NH1	2.38	0.42
3:G:8:VAL:HG11	3:G:30:LEU:HD13	2.02	0.42
4:C:74:LEU:HA	4:C:102:LEU:HD23	2.01	0.42
11:N:4:THR:H	11:N:4:THR:HG1	1.62	0.42
2:E:116:LYS:HD3	2:E:116:LYS:HA	1.82	0.42
3:G:11:LYS:HE3	3:G:11:LYS:HB2	1.89	0.42
5:B:124:ILE:HG12	5:B:153:VAL:HB	2.01	0.42
13:J:20:ILE:HG13	13:J:21:THR:HG23	2.02	0.42
5:B:138:ILE:HG23	5:B:140:SER:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:170:ALA:HA	9:L:238:TRP:HB2	2.01	0.42
9:L:425:THR:O	9:L:429:THR:OG1	2.29	0.42
1:F:325:LEU:HD23	1:F:325:LEU:HA	1.84	0.41
3:G:106:PRO:HD3	4:C:515:LEU:HD21	2.02	0.41
3:G:227:PRO:HD3	3:G:754:PRO:HB3	2.02	0.41
3:G:287:ARG:HG2	3:G:607:HIS:HA	2.01	0.41
5:B:212:THR:HA	6:I:141:GLY:HA3	2.02	0.41
7:H:22:LEU:HD11	7:H:95:LEU:HD21	2.02	0.41
10:M:229:ILE:HD12	19:M:1003:3PE:H2F1	2.02	0.41
2:E:87:HIS:NE2	2:E:166:LYS:OXT	2.52	0.41
3:G:307:ILE:HG22	3:G:591:LEU:HD22	2.02	0.41
10:M:107:LYS:HD3	10:M:107:LYS:HA	1.79	0.41
3:G:861:SER:HB2	3:G:870:THR:HG22	2.01	0.41
8:A:88:TRP:HB2	13:J:134:PHE:CE1	2.55	0.41
19:L:801:3PE:H381	19:L:801:3PE:H291	2.02	0.41
12:K:92:ILE:HD12	12:K:92:ILE:HA	1.87	0.41
4:C:254:ARG:HG3	5:B:103:PHE:CE1	2.55	0.41
9:L:4:LEU:HD11	9:L:81:LEU:HB2	2.02	0.41
11:N:412:GLY:HA3	18:N:502:LFA:H42	2.02	0.41
4:C:189:LYS:O	4:C:193:GLU:HB2	2.20	0.41
5:B:101:THR:OG1	5:B:129:CYS:SG	2.68	0.41
10:M:36:MET:HB3	10:M:99:VAL:HG22	2.02	0.41
11:N:388:MET:HE3	11:N:388:MET:HB2	1.97	0.41
3:G:623:ILE:HD12	3:G:787:LEU:HD11	2.02	0.41
3:G:669:THR:OG1	3:G:670:GLN:N	2.54	0.41
4:C:594:VAL:HG23	4:C:597:ASP:HB2	2.03	0.41
12:K:43:ALA:HB1	12:K:62:TYR:CD1	2.56	0.41
1:F:178:TYR:HB3	1:F:349:GLU:HB3	2.02	0.41
3:G:496:LYS:HA	3:G:496:LYS:HD3	1.86	0.41
9:L:342:LYS:HA	9:L:342:LYS:HD3	1.90	0.41
9:L:431:ARG:HG3	9:L:512:TRP:CE2	2.56	0.41
3:G:613:ALA:HB3	3:G:618:SER:HB3	2.02	0.41
6:I:126:LYS:HE2	6:I:126:LYS:HB2	1.86	0.41
7:H:116:ILE:HD12	7:H:116:ILE:HA	1.83	0.41
19:A:201:3PE:H242	13:J:4:ALA:HB1	2.01	0.41
10:M:47:TRP:NE1	10:M:92:VAL:HG21	2.35	0.41
4:C:98:VAL:HG21	4:C:124:VAL:HG21	2.03	0.41
6:I:51:THR:HG22	6:I:139:ILE:HD11	2.03	0.41
8:A:29:LEU:HA	8:A:32:VAL:HB	2.02	0.41
9:L:425:THR:HA	9:L:428:TYR:CE2	2.56	0.41
10:M:29:ARG:NH1	10:M:106:TRP:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:371:MET:HA	10:M:374:MET:HG2	2.02	0.41
1:F:286:LYS:HB3	1:F:286:LYS:HE3	1.86	0.41
2:E:90:ARG:HA	2:E:129:LEU:O	2.20	0.41
3:G:48:ARG:HA	3:G:48:ARG:HD2	1.98	0.41
3:G:314:VAL:HG22	3:G:334:VAL:HG12	2.03	0.40
3:G:830:ALA:HA	3:G:831:PRO:HD3	1.98	0.40
10:M:232:ALA:HB1	10:M:237:VAL:HB	2.03	0.40
4:C:520:LEU:HD23	4:C:520:LEU:HA	1.80	0.40
7:H:135:TRP:CE2	13:J:26:VAL:HG21	2.57	0.40
9:L:595:VAL:HG11	12:K:22:LEU:HG	2.03	0.40
3:G:233:CYS:SG	3:G:235:ILE:HG12	2.62	0.40
11:N:52:LEU:HD23	11:N:52:LEU:HA	1.89	0.40
1:F:89:CYS:HB3	1:F:130:ILE:HA	2.04	0.40
1:F:182:GLU:O	1:F:186:LEU:N	2.49	0.40
3:G:902:LEU:HD12	3:G:902:LEU:HA	1.96	0.40
6:I:179:LEU:HA	6:I:180:PRO:HD3	1.94	0.40
10:M:341:ALA:HA	10:M:410:ILE:HD11	2.03	0.40
11:N:214:LEU:HD13	11:N:254:VAL:HG22	2.04	0.40
12:K:77:LEU:HD22	13:J:70:VAL:HG11	2.02	0.40
3:G:261:HIS:HD2	3:G:369:ARG:HG3	1.87	0.40
5:B:215:ARG:HB2	6:I:42:PRO:HB3	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	437/439 (100%)	430 (98%)	7 (2%)	0	100	100
2	E	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
3	G	903/905 (100%)	871 (96%)	32 (4%)	0	100	100
4	C	560/600 (93%)	545 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	162/220 (74%)	158 (98%)	4 (2%)	0	100	100
6	I	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
7	H	294/325 (90%)	286 (97%)	8 (3%)	0	100	100
8	A	98/147 (67%)	97 (99%)	1 (1%)	0	100	100
9	L	595/613 (97%)	581 (98%)	14 (2%)	0	100	100
10	M	502/504 (100%)	489 (97%)	13 (3%)	0	100	100
11	N	474/485 (98%)	462 (98%)	11 (2%)	1 (0%)	47	79
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
All	All	4584/4805 (95%)	4468 (98%)	115 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	N	64	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	353/353 (100%)	350 (99%)	3 (1%)	81	92
2	E	129/129 (100%)	126 (98%)	3 (2%)	50	77
3	G	732/732 (100%)	715 (98%)	17 (2%)	50	77
4	C	483/519 (93%)	475 (98%)	8 (2%)	60	83
5	B	145/192 (76%)	142 (98%)	3 (2%)	53	79
6	I	128/128 (100%)	125 (98%)	3 (2%)	50	77
7	H	246/269 (91%)	246 (100%)	0	100	100
8	A	80/119 (67%)	77 (96%)	3 (4%)	33	66
9	L	468/486 (96%)	459 (98%)	9 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	M	413/413 (100%)	402 (97%)	11 (3%)	44 74
11	N	380/385 (99%)	376 (99%)	4 (1%)	73 89
12	K	79/79 (100%)	76 (96%)	3 (4%)	33 66
13	J	123/128 (96%)	119 (97%)	4 (3%)	38 69
All	All	3759/3932 (96%)	3688 (98%)	71 (2%)	59 81

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	103	LEU
1	F	126	TYR
1	F	398	CYS
2	E	123	ASP
2	E	127	THR
2	E	149	THR
3	G	21	LEU
3	G	135	ARG
3	G	172	LEU
3	G	174	VAL
3	G	181	VAL
3	G	215	GLU
3	G	233	CYS
3	G	238	ASN
3	G	261	HIS
3	G	314	VAL
3	G	326	SER
3	G	365	THR
3	G	390	ARG
3	G	459	LEU
3	G	586	LEU
3	G	666	VAL
3	G	750	ARG
4	C	36	ASP
4	C	110	ASP
4	C	127	PHE
4	C	273	ASP
4	C	356	PHE
4	C	474	LEU
4	C	531	ASN
4	C	594	VAL
5	B	63	CYS

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Mol	Chain	Res	Type
5	B	174	GLU
5	B	180	ARG
6	I	77	LEU
6	I	98	ARG
6	I	153	MET
8	A	7	THR
8	A	73	MET
8	A	83	LEU
9	L	4	LEU
9	L	77	PHE
9	L	82	ASP
9	L	123	PHE
9	L	247	THR
9	L	372	ILE
9	L	389	LEU
9	L	431	ARG
9	L	472	VAL
10	M	36	MET
10	M	74	ARG
10	M	109	ILE
10	M	259	LEU
10	M	262	ILE
10	M	263	LEU
10	M	264	LEU
10	M	372	ARG
10	M	418	VAL
10	M	426	THR
10	M	429	LEU
11	N	64	THR
11	N	103	ASP
11	N	359	LEU
11	N	380	MET
12	K	46	PHE
12	K	56	THR
12	K	57	ASP
13	J	10	LEU
13	J	23	THR
13	J	59	TYR
13	J	100	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	20	ASN
9	L	281	HIS

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 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	3PE	M	1001	-	50,50,50	0.30	0	53,55,55	0.30	0
18	LFA	N	502	-	13,13,19	0.14	0	12,12,18	0.13	0
16	FES	G	1004	3	0,4,4	-	-	-		
19	3PE	A	201	-	45,45,50	0.31	0	48,50,55	0.30	0
19	3PE	H	602	-	50,50,50	0.31	0	53,55,55	0.32	0
14	SF4	G	1002	3	0,12,12	-	-	-		
19	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.30	0
19	3PE	L	803	-	42,42,50	0.33	0	45,47,55	0.34	0
14	SF4	F	501	1	0,12,12	-	-	-		
14	SF4	I	201	6	0,12,12	-	-	-		
19	3PE	M	1002	-	50,50,50	0.31	0	53,55,55	0.29	0
18	LFA	L	802	-	13,13,19	0.17	0	12,12,18	0.16	0
19	3PE	M	1003	-	50,50,50	0.29	0	53,55,55	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	SF4	G	1001	3	0,12,12	-	-	-		
16	FES	E	201	2	0,4,4	-	-	-		
14	SF4	I	202	6	0,12,12	-	-	-		
14	SF4	G	1003	3	0,12,12	-	-	-		
18	LFA	H	601	-	19,19,19	0.14	0	18,18,18	0.11	0
14	SF4	B	301	5	0,12,12	-	-	-		
18	LFA	N	501	-	19,19,19	0.09	0	18,18,18	0.15	0
15	FMN	F	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.26	7 (14%)
19	3PE	L	804	-	50,50,50	0.29	0	53,55,55	0.30	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
19	3PE	M	1001	-	-	12/54/54/54	-
18	LFA	N	502	-	-	0/11/11/17	-
16	FES	G	1004	3	-	-	0/1/1/1
19	3PE	A	201	-	-	11/49/49/54	-
19	3PE	H	602	-	-	12/54/54/54	-
14	SF4	G	1002	3	-	-	0/6/5/5
19	3PE	L	801	-	-	14/54/54/54	-
19	3PE	L	803	-	-	7/46/46/54	-
14	SF4	F	501	1	-	-	0/6/5/5
14	SF4	I	201	6	-	-	0/6/5/5
19	3PE	M	1002	-	-	9/54/54/54	-
18	LFA	L	802	-	-	0/11/11/17	-
19	3PE	M	1003	-	-	12/54/54/54	-
14	SF4	G	1001	3	-	-	0/6/5/5
16	FES	E	201	2	-	-	0/1/1/1
14	SF4	I	202	6	-	-	0/6/5/5
18	LFA	H	601	-	-	1/17/17/17	-
14	SF4	G	1003	3	-	-	0/6/5/5
14	SF4	B	301	5	-	-	0/6/5/5
18	LFA	N	501	-	-	1/17/17/17	-
15	FMN	F	502	-	-	6/18/18/18	0/3/3/3
19	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	3.51	1.37	1.30
15	F	502	FMN	C10-N1	2.11	1.37	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4-N3-C2	-3.39	119.38	125.64
15	F	502	FMN	C4A-C10-N10	2.87	120.68	116.48
15	F	502	FMN	C4A-C4-N3	2.69	120.03	113.19
15	F	502	FMN	O4-C4-C4A	-2.62	119.64	126.60
15	F	502	FMN	C4A-C10-N1	-2.39	119.19	124.73
15	F	502	FMN	C10-C4A-N5	-2.22	120.14	124.86
15	F	502	FMN	C4-C4A-C10	2.10	120.32	116.79

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	502	FMN	N10-C1'-C2'-O2'
15	F	502	FMN	N10-C1'-C2'-C3'
15	F	502	FMN	C5'-O5'-P-O2P
15	F	502	FMN	C5'-O5'-P-O3P
19	H	602	3PE	C1-O11-P-O12
19	H	602	3PE	C1-O11-P-O13
19	H	602	3PE	C1-O11-P-O14
19	A	201	3PE	C1-O11-P-O12
19	A	201	3PE	C1-O11-P-O14
19	A	201	3PE	O13-C11-C12-N
19	L	801	3PE	C1-O11-P-O14
19	L	801	3PE	C11-O13-P-O11
19	L	801	3PE	C11-O13-P-O12
19	L	801	3PE	C11-O13-P-O14
19	L	801	3PE	O13-C11-C12-N
19	L	803	3PE	C1-O11-P-O12
19	L	803	3PE	C1-O11-P-O13
19	L	803	3PE	C1-O11-P-O14
19	L	803	3PE	C11-O13-P-O14
19	L	804	3PE	C1-O11-P-O14
19	L	804	3PE	C11-O13-P-O11
19	L	804	3PE	O13-C11-C12-N
19	M	1001	3PE	C1-O11-P-O14
19	M	1001	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
19	M	1001	3PE	C11-O13-P-O14
19	M	1002	3PE	C11-O13-P-O11
19	M	1002	3PE	C11-O13-P-O14
19	M	1002	3PE	O13-C11-C12-N
19	M	1003	3PE	C1-O11-P-O12
19	M	1003	3PE	O13-C11-C12-N
19	A	201	3PE	C1-O11-P-O13
19	A	201	3PE	C11-O13-P-O11
19	L	801	3PE	C1-O11-P-O13
19	L	803	3PE	C11-O13-P-O11
19	L	804	3PE	C1-O11-P-O13
19	M	1001	3PE	C1-O11-P-O13
19	M	1001	3PE	C11-O13-P-O11
19	M	1002	3PE	C1-O11-P-O13
19	M	1003	3PE	C11-O13-P-O11
19	L	804	3PE	C3B-C3C-C3D-C3E
18	H	601	LFA	C14-C15-C16-C17
19	H	602	3PE	O13-C11-C12-N
19	L	804	3PE	C1-C2-C3-O31
19	M	1002	3PE	C24-C25-C26-C27
19	L	801	3PE	C37-C38-C39-C3A
19	M	1003	3PE	C2-C1-O11-P
19	L	801	3PE	C33-C34-C35-C36
19	M	1001	3PE	C37-C38-C39-C3A
19	L	801	3PE	C2C-C2D-C2E-C2F
15	F	502	FMN	C5'-O5'-P-O1P
19	A	201	3PE	C21-C22-C23-C24
19	L	804	3PE	O21-C2-C3-O31
19	H	602	3PE	C21-C22-C23-C24
19	M	1001	3PE	C3B-C3C-C3D-C3E
19	H	602	3PE	O11-C1-C2-C3
19	A	201	3PE	C2-C1-O11-P
19	M	1003	3PE	C26-C27-C28-C29
19	M	1002	3PE	C2-C1-O11-P
19	M	1003	3PE	C3E-C3F-C3G-C3H
19	L	803	3PE	C37-C38-C39-C3A
19	A	201	3PE	C23-C24-C25-C26
19	H	602	3PE	C11-O13-P-O14
19	A	201	3PE	C11-O13-P-O14
19	L	801	3PE	C1-O11-P-O12
19	L	803	3PE	C11-O13-P-O12
19	L	804	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
19	L	804	3PE	C11-O13-P-O12
19	M	1001	3PE	C1-O11-P-O12
19	M	1002	3PE	C1-O11-P-O14
19	M	1003	3PE	C1-O11-P-O14
19	M	1003	3PE	C11-O13-P-O14
19	L	804	3PE	O11-C1-C2-C3
19	L	801	3PE	C12-C11-O13-P
19	H	602	3PE	O11-C1-C2-O21
19	L	804	3PE	O11-C1-C2-O21
19	L	801	3PE	C21-C22-C23-C24
19	L	804	3PE	C2-C1-O11-P
19	L	804	3PE	C35-C36-C37-C38
19	M	1003	3PE	C3C-C3D-C3E-C3F
19	L	804	3PE	C29-C2A-C2B-C2C
15	F	502	FMN	C4'-C5'-O5'-P
19	M	1001	3PE	C3A-C3B-C3C-C3D
19	H	602	3PE	C2F-C2G-C2H-C2I
19	H	602	3PE	C3A-C3B-C3C-C3D
19	M	1003	3PE	C1-O11-P-O13
19	M	1002	3PE	C35-C36-C37-C38
19	L	804	3PE	C25-C26-C27-C28
19	M	1001	3PE	C3C-C3D-C3E-C3F
19	A	201	3PE	O21-C21-C22-C23
19	L	801	3PE	C2D-C2E-C2F-C2G
19	M	1003	3PE	C2E-C2F-C2G-C2H
19	M	1003	3PE	C2F-C2G-C2H-C2I
18	N	501	LFA	C14-C15-C16-C17
19	H	602	3PE	C39-C3A-C3B-C3C
19	M	1001	3PE	O21-C21-C22-C23
19	L	804	3PE	O21-C21-C22-C23
19	H	602	3PE	C12-C11-O13-P
19	A	201	3PE	C12-C11-O13-P
19	M	1002	3PE	C12-C11-O13-P
19	L	801	3PE	C2F-C2G-C2H-C2I
19	M	1001	3PE	O22-C21-C22-C23

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	M	1001	3PE	4	0
18	N	502	LFA	1	0

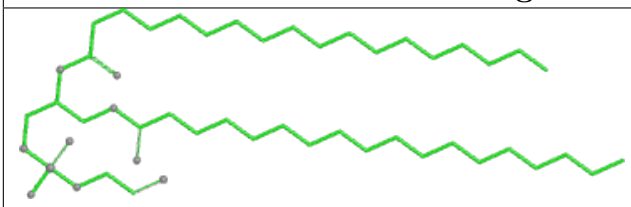
Continued on next page...

Continued from previous page...

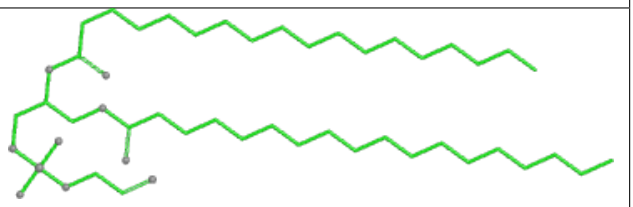
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	201	3PE	2	0
19	H	602	3PE	3	0
19	L	801	3PE	3	0
19	M	1002	3PE	2	0
19	M	1003	3PE	3	0
18	H	601	LFA	2	0
18	N	501	LFA	1	0
15	F	502	FMN	1	0
19	L	804	3PE	3	0

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.

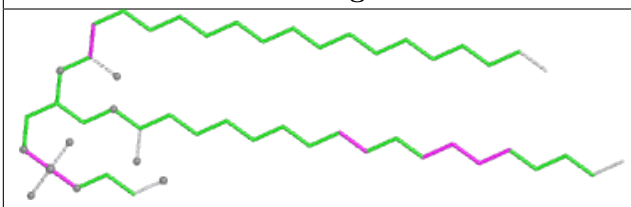
Ligand 3PE M 1001



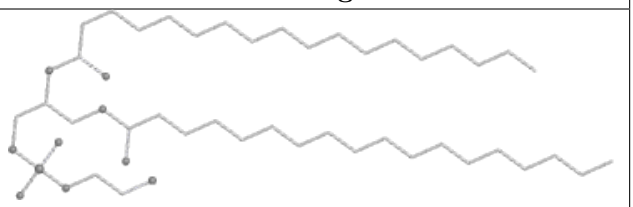
Bond lengths



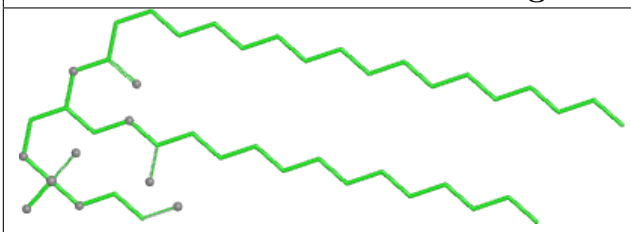
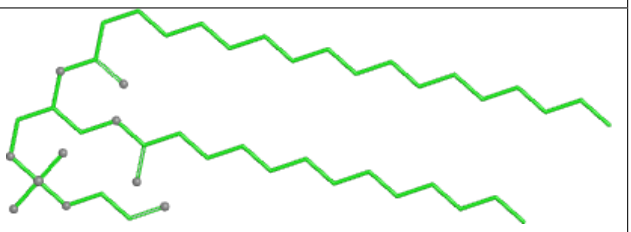
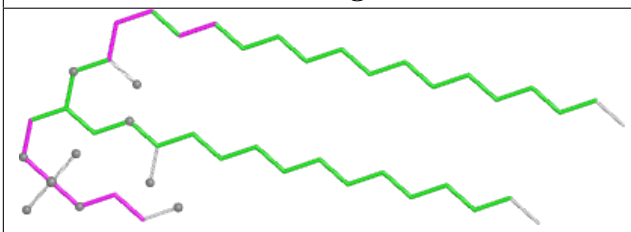
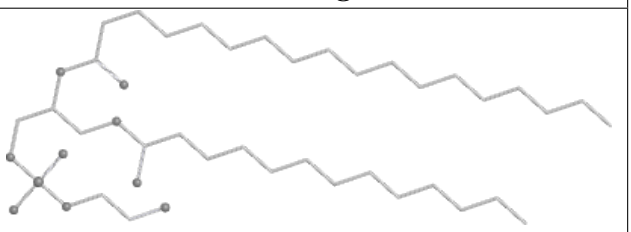
Bond angles

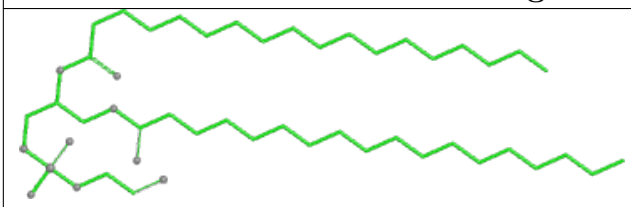
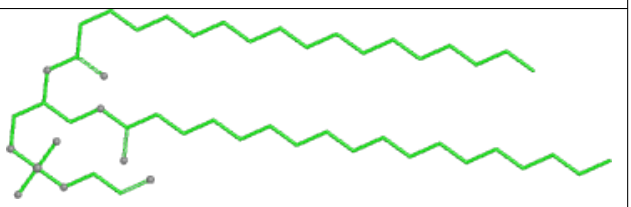
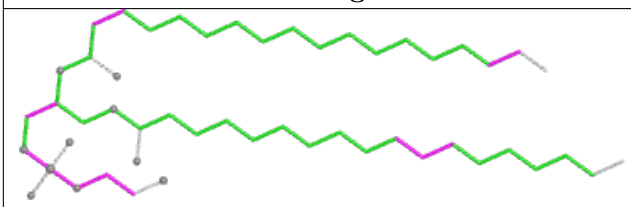
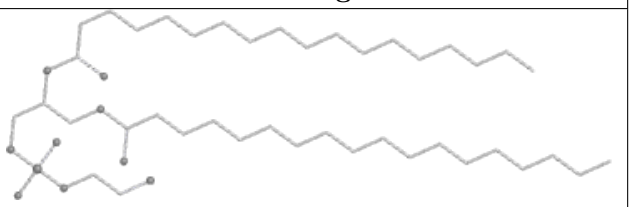


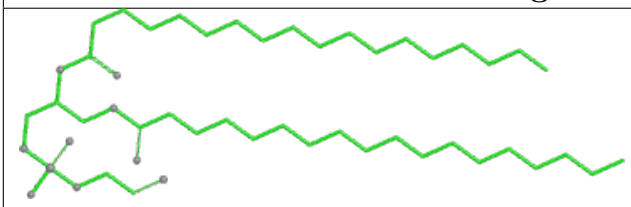
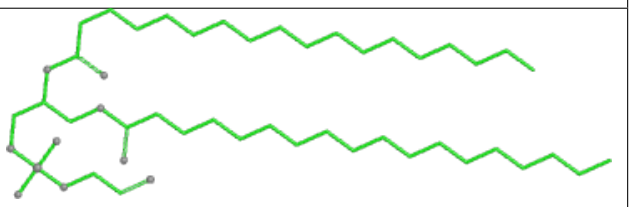
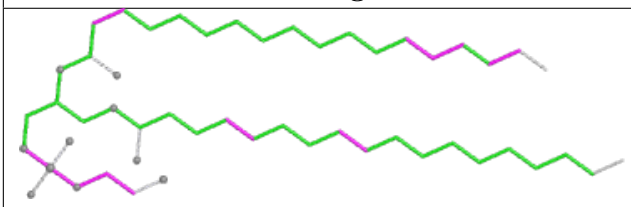
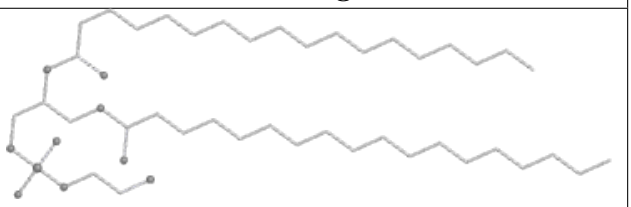
Torsions

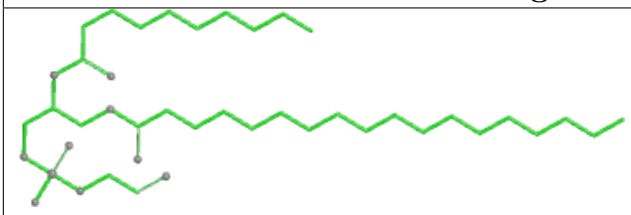
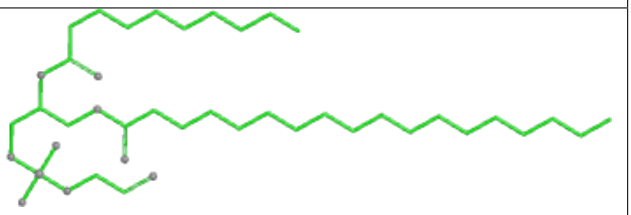
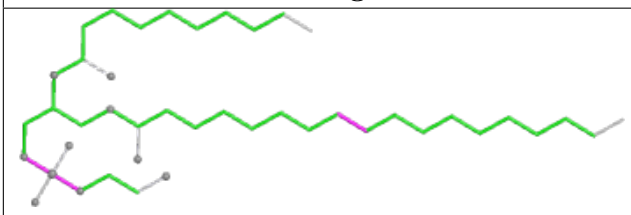
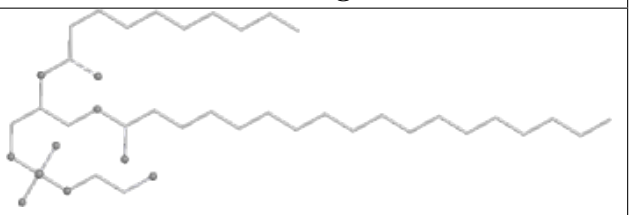


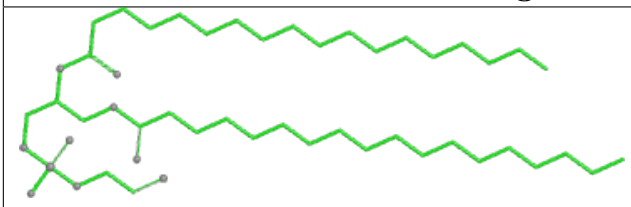
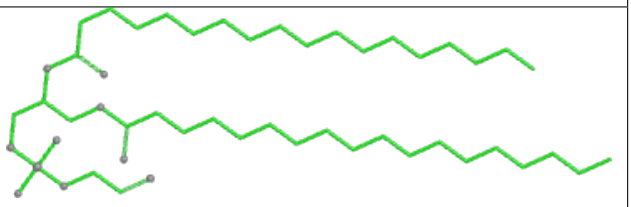
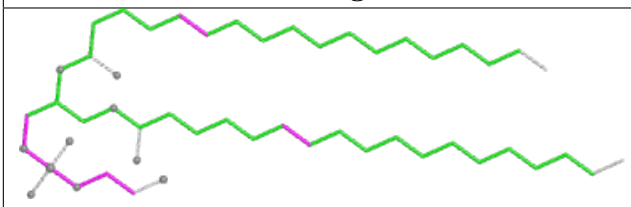
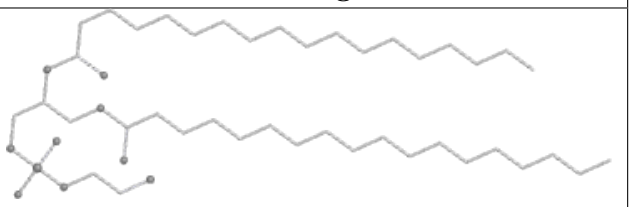
Rings

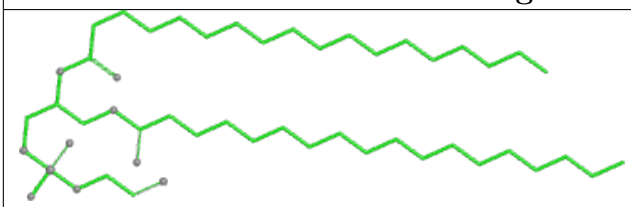
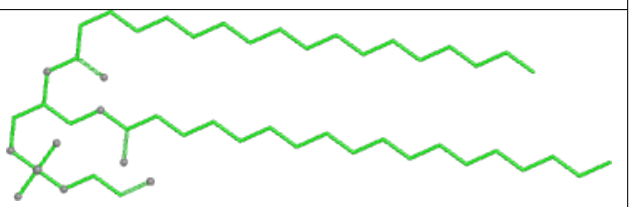
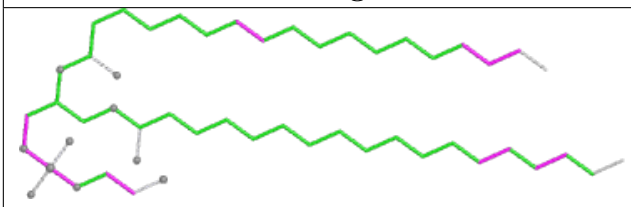
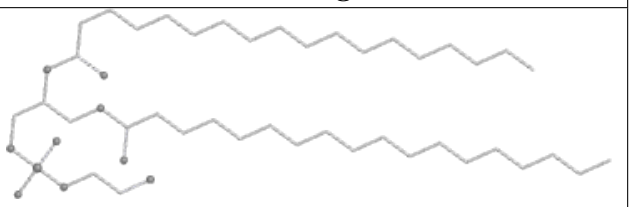
Ligand 3PE A 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE H 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

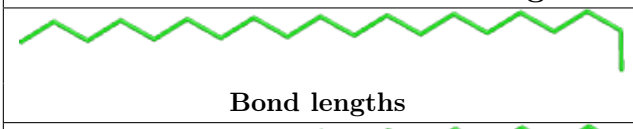
Ligand 3PE L 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

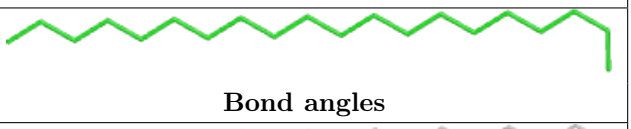
Ligand 3PE M 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE M 1003	
 Bond lengths	 Bond angles
 Torsions	 Rings

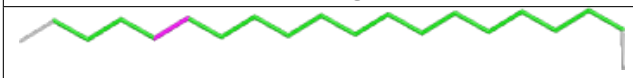
Ligand LFA H 601



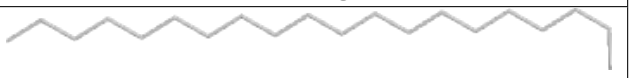
Bond lengths



Bond angles

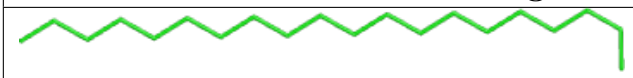


Torsions

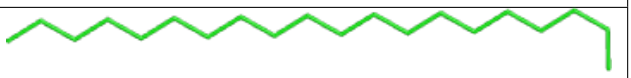


Rings

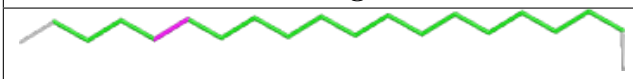
Ligand LFA N 501



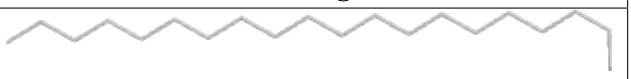
Bond lengths



Bond angles

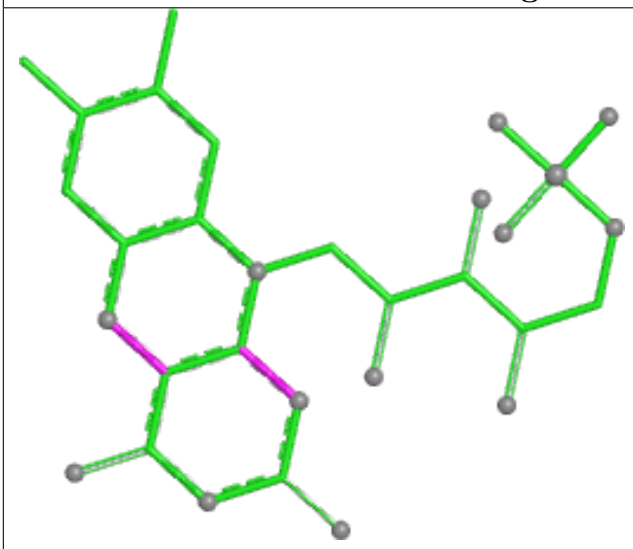


Torsions

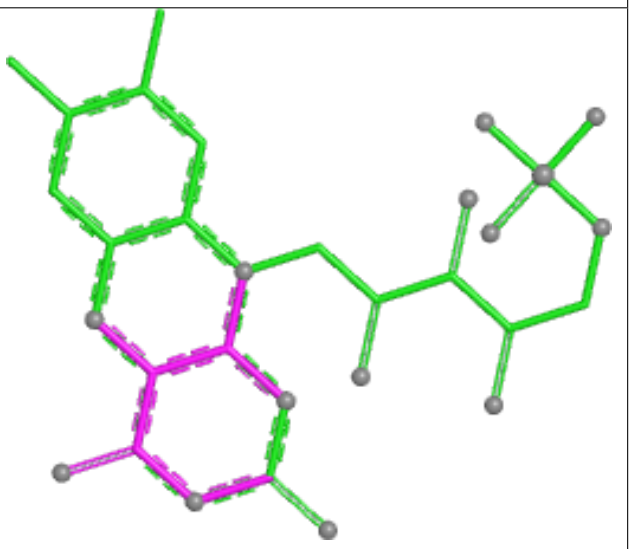


Rings

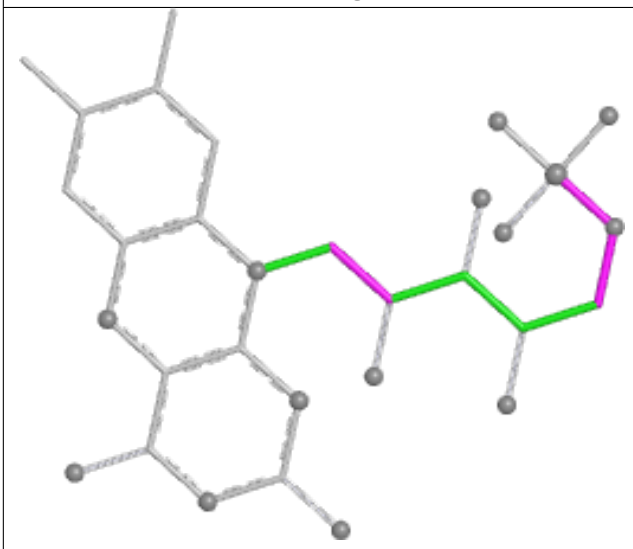
Ligand FMN F 502



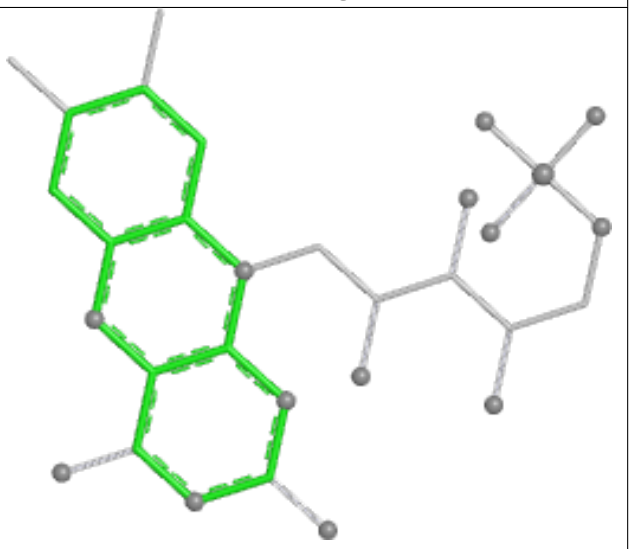
Bond lengths



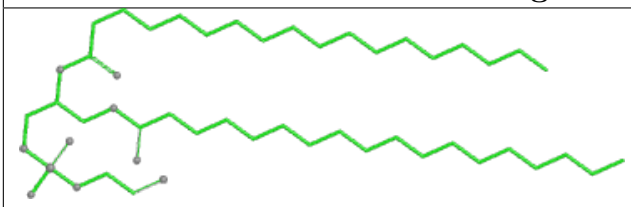
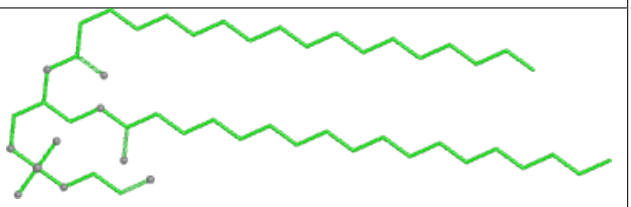
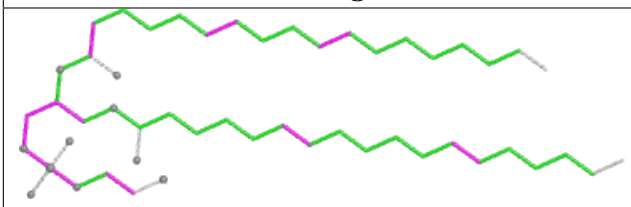
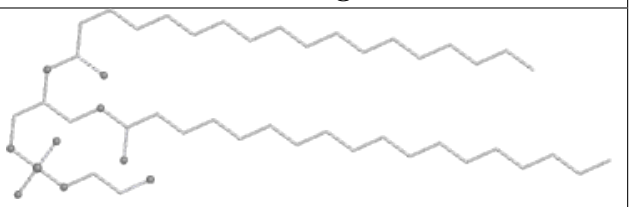
Bond angles



Torsions



Rings

Ligand 3PE L 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

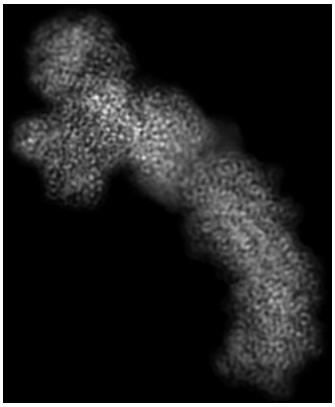
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13238. These allow visual inspection of the internal detail of the map and identification of artifacts.

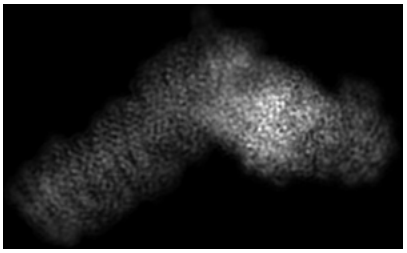
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

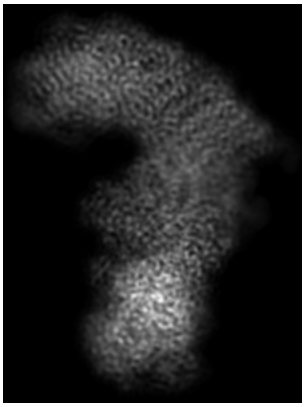
6.1.1 Primary map



X



Y

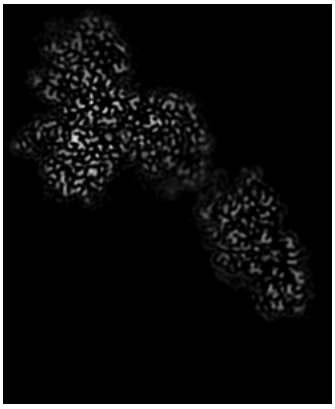


Z

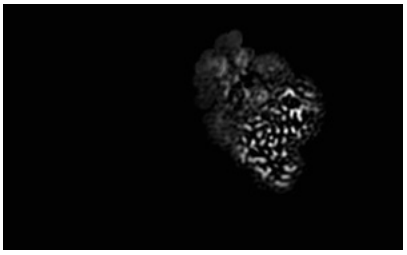
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 71



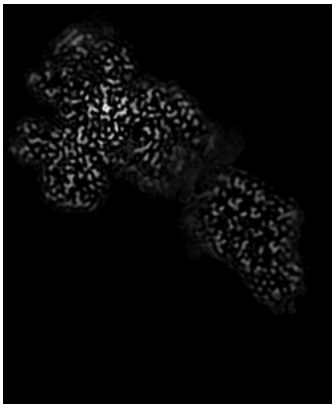
Y Index: 96

Z Index: 117

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: 79

Y Index: 51

Z Index: 160

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

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

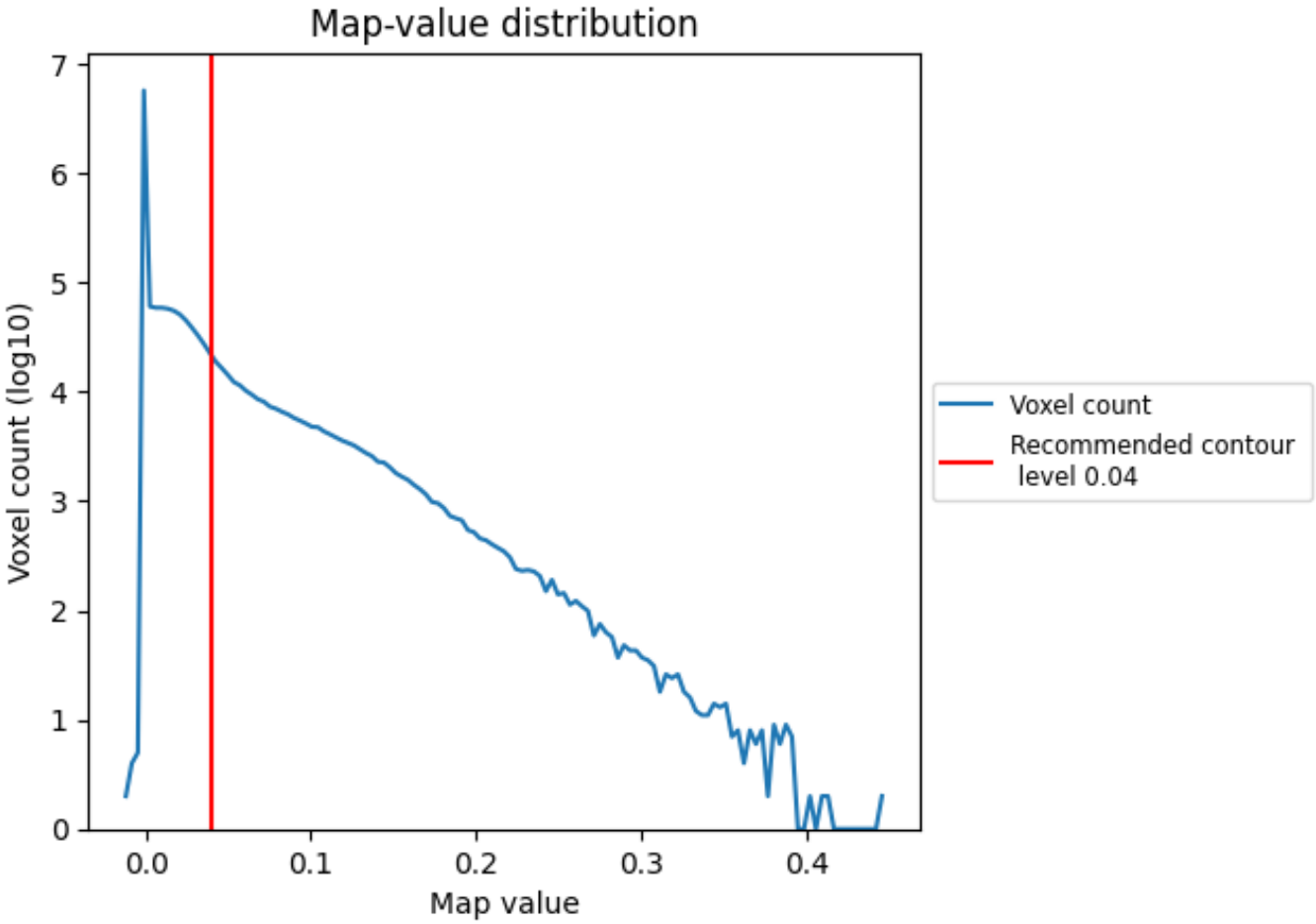
6.5 Mask visualisation (i)

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

7 Map analysis

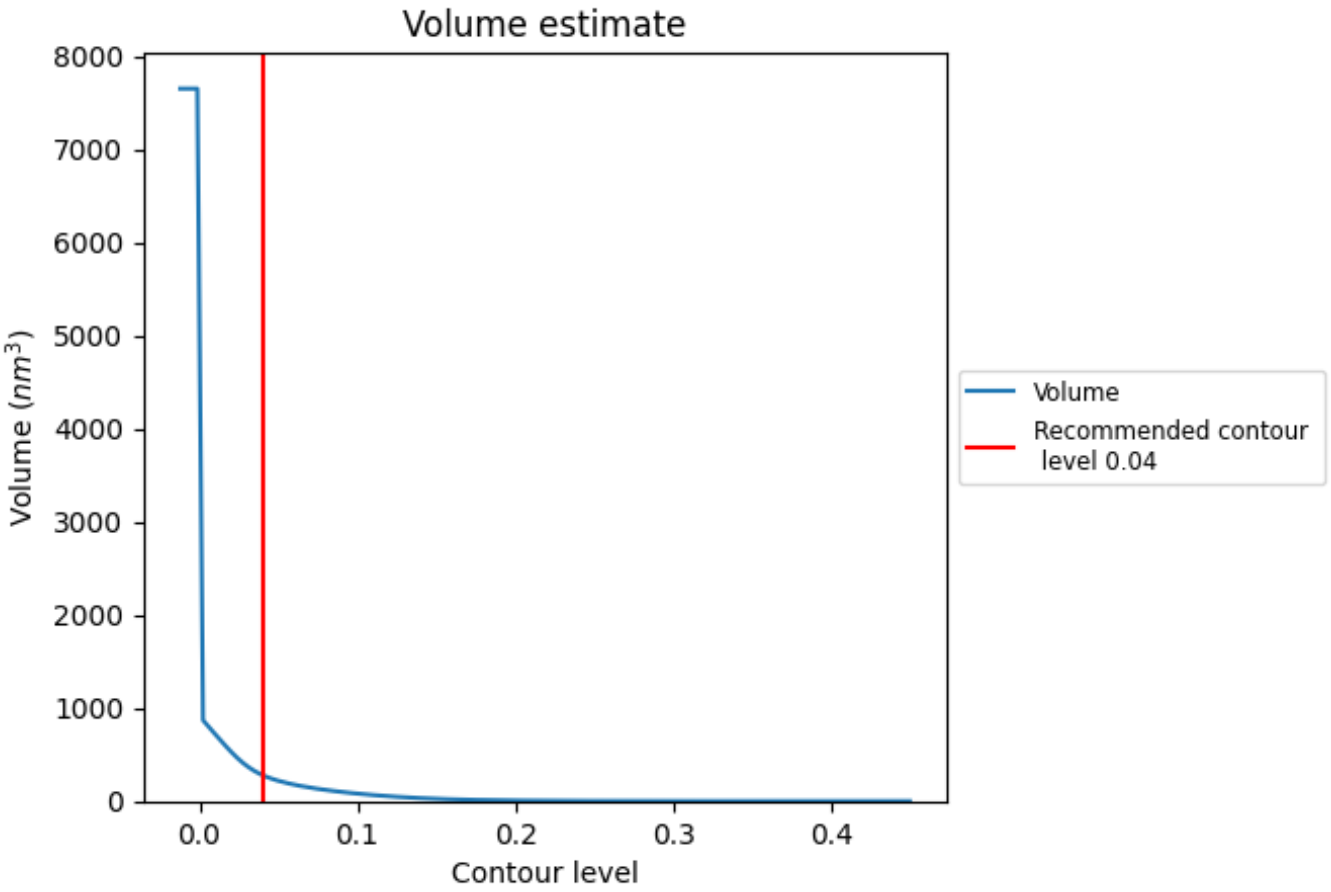
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate



The volume at the recommended contour level is 280 nm^3; this corresponds to an approximate mass of 253 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.

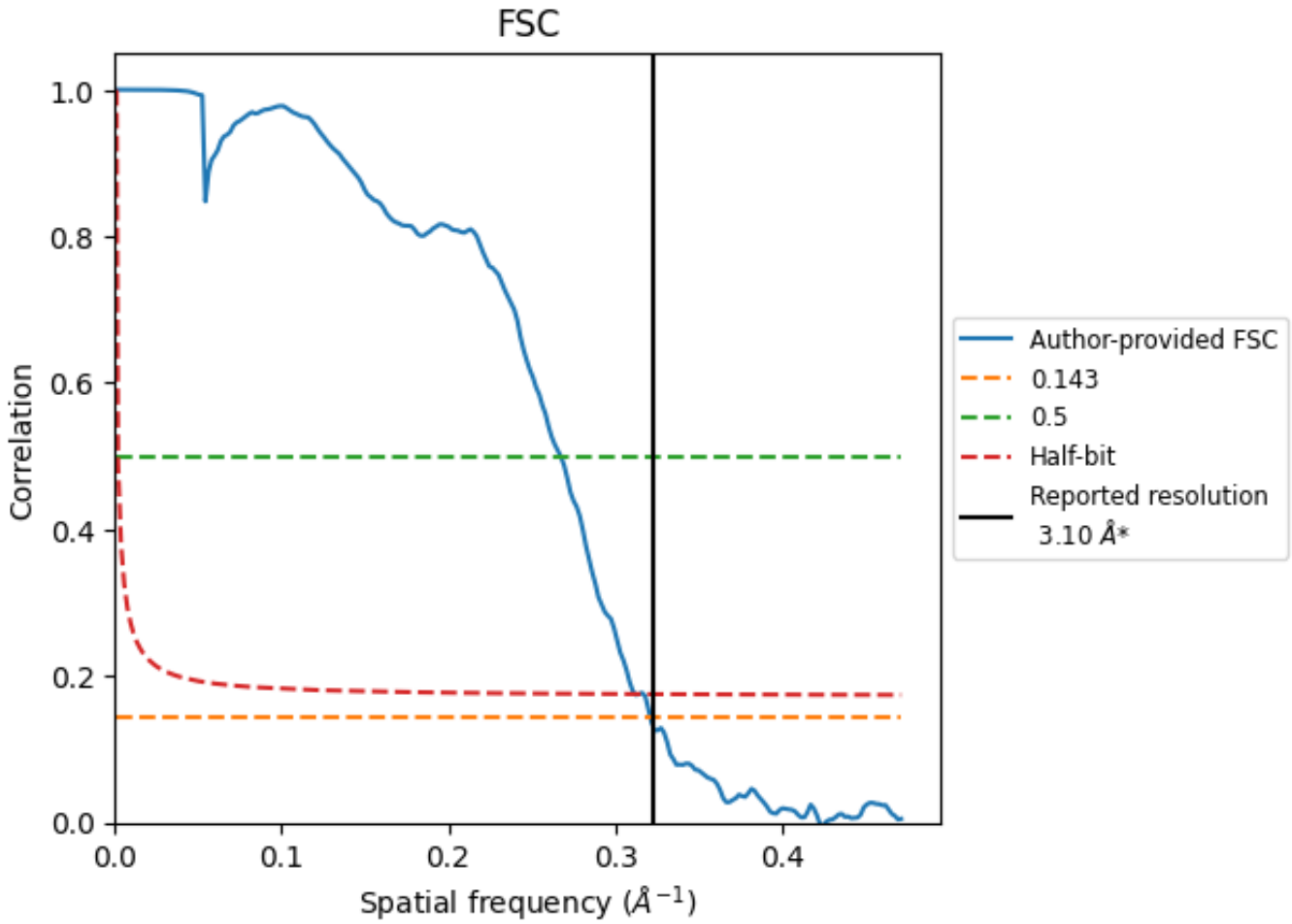
7.3 Rotationally averaged power spectrum

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

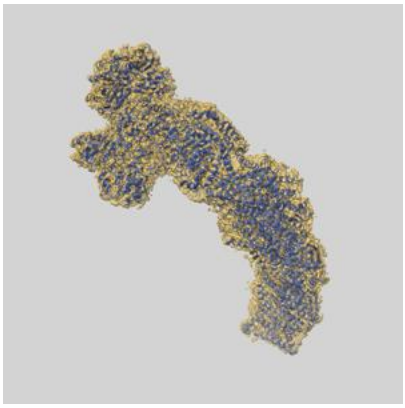
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.74	3.20
Unmasked-calculated*	-	-	-

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

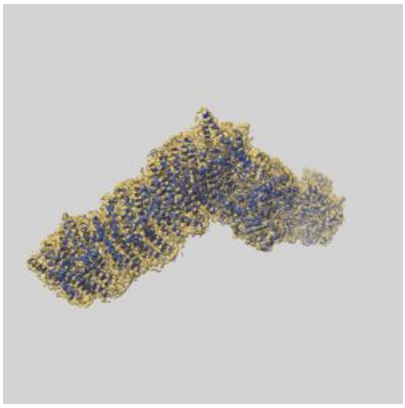
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13238 and PDB model 7P7K. Per-residue inclusion information can be found in section 3 on page 10.

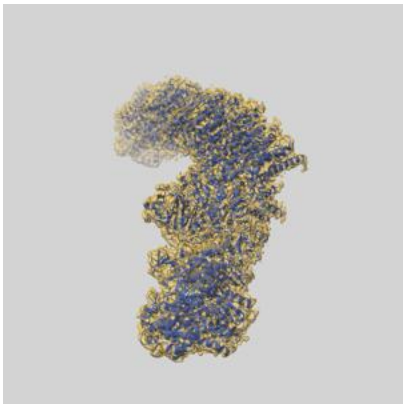
9.1 Map-model overlay



X



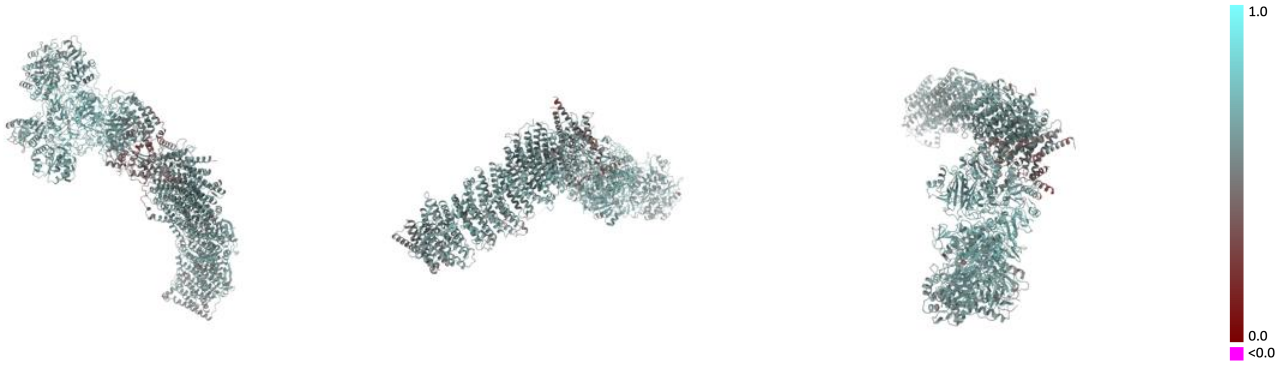
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

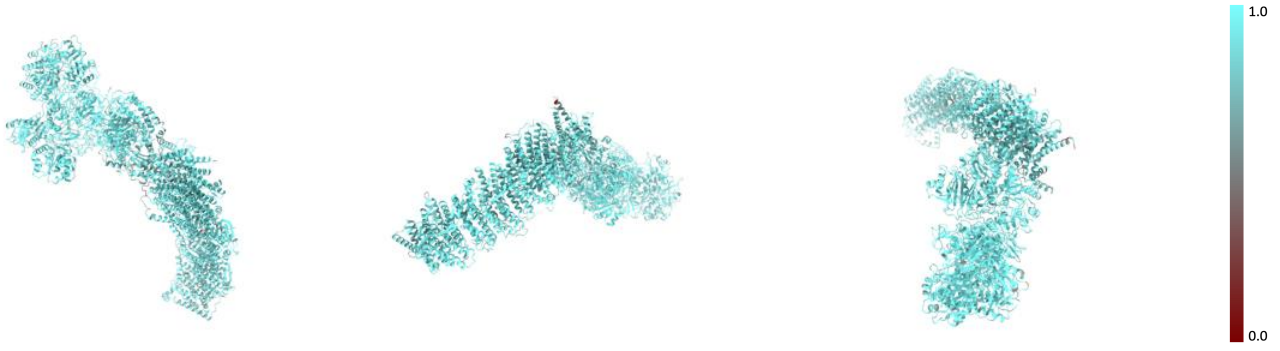
9.2 Q-score mapped to coordinate model



X Y Z

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

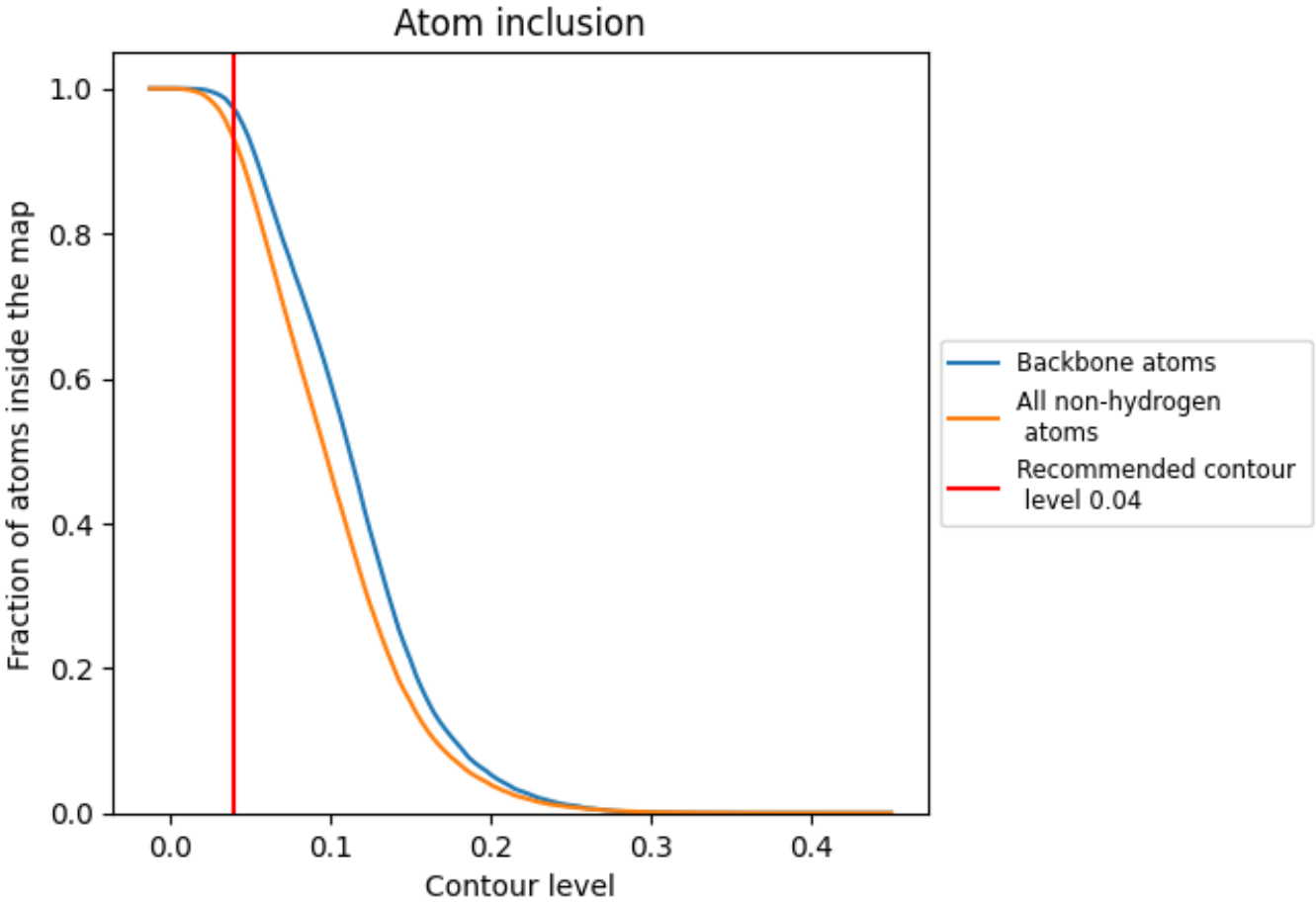
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9308	0.5890
A	0.8841	0.5330
B	0.9186	0.5410
C	0.9352	0.5980
E	0.9334	0.5930
F	0.9315	0.5910
G	0.9662	0.6400
H	0.8585	0.4960
I	0.9607	0.6520
J	0.9097	0.5640
K	0.9597	0.5950
L	0.9101	0.5640
M	0.9244	0.5810
N	0.9447	0.5910