Full wwPDB EM Validation Report ⓘ

Sep 26, 2022 – 10:30 pm BST

PDB ID	:	7ZC5
EMDB ID	:	EMD-14620
Title	:	Complex I from E. coli, DDM/LMNG-purified, under Turnover at pH 8, Resting state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2022-03-25
Resolution	:	3.00 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:

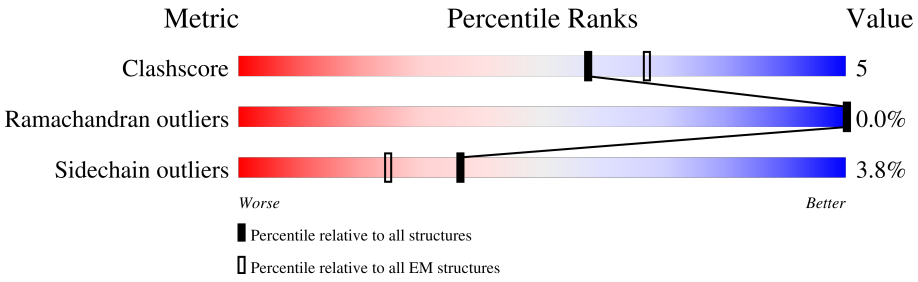
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	86% 13% •
2	E	166	83% 11% 6%
3	G	908	87% 12% •
4	C	600	• 82% 13% • 5%
5	B	220	61% 14% • 23%
6	I	180	68% 12% 19%
7	H	325	6% 78% 15% • 5%
8	A	147	• 58% 10% • 31%

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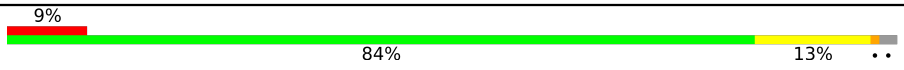
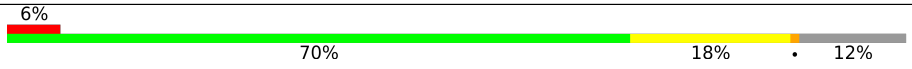
Mol	Chain	Length	Quality of chain
9	L	613	
10	M	509	
11	N	485	
12	K	100	
13	J	184	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 36692 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	442	3432	2177	601	633	21	0	0

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

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

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

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

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit CD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	571	4597	2948	801	826	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-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	601	Total	C	N	O	S	0	0
			4595	3056	734	773	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		

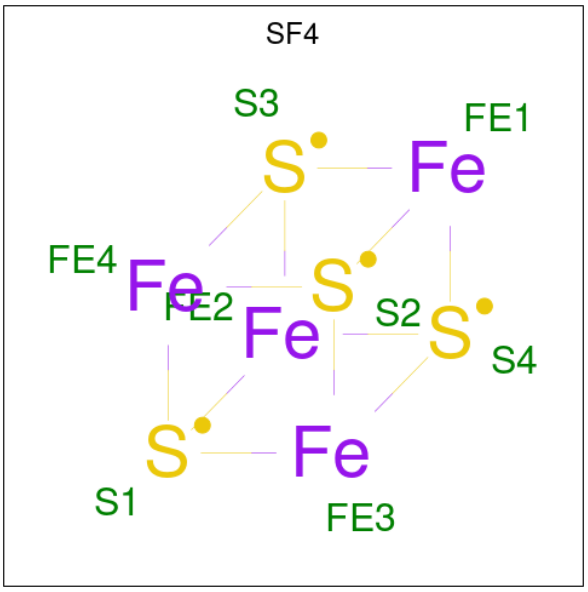
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

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.

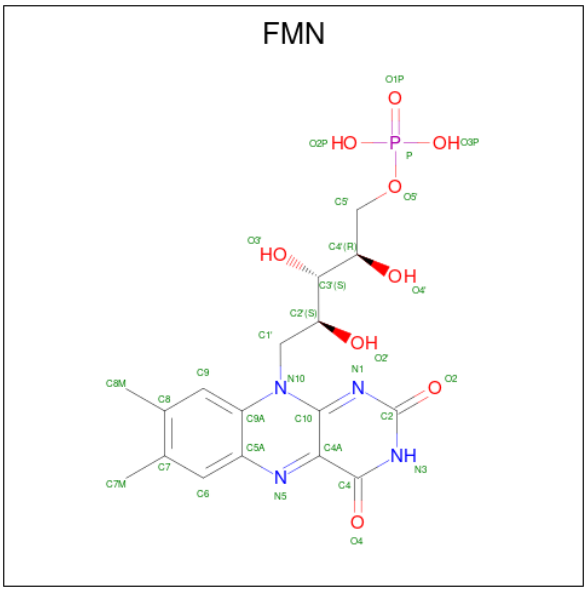
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	162	Total	C	N	O	S	0	0
			1226	824	188	207	7		

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



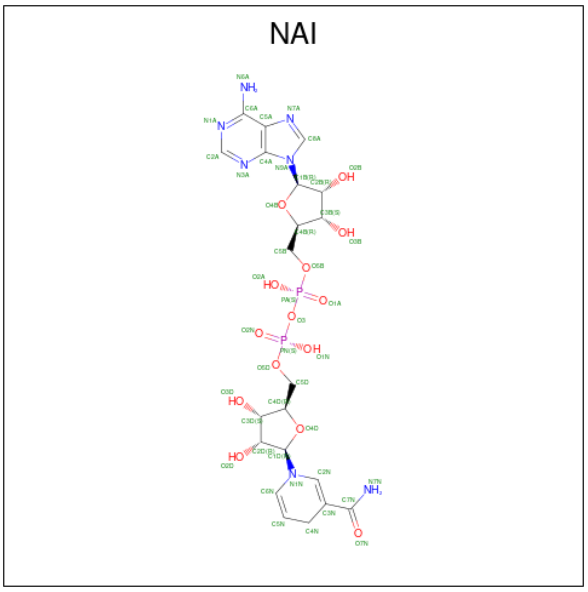
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	B	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 16 8 8	0
14	I	1	Total Fe S 16 8 8	0

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



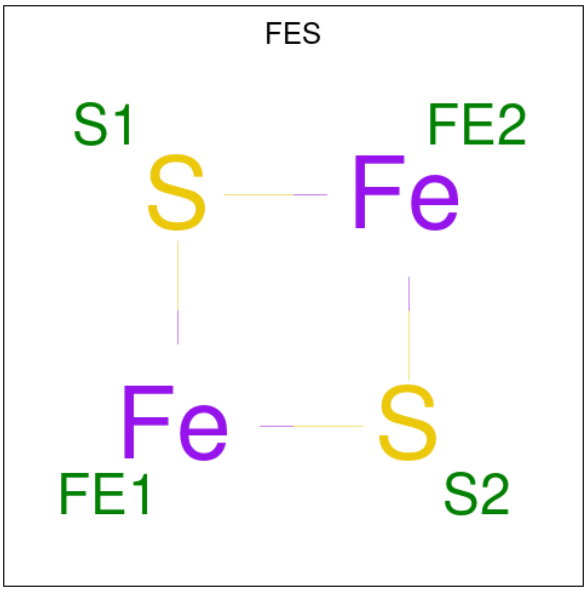
Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- 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).

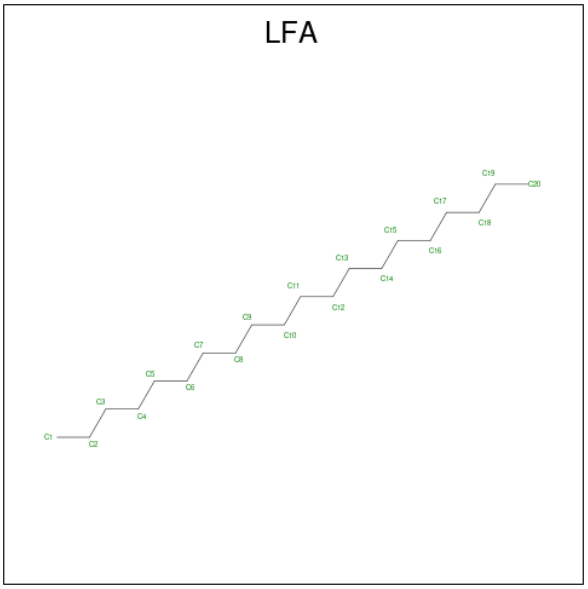


Mol	Chain	Residues	Atoms	AltConf
17	E	1	Total Fe S 4 2 2	0
17	G	1	Total Fe S 4 2 2	0

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

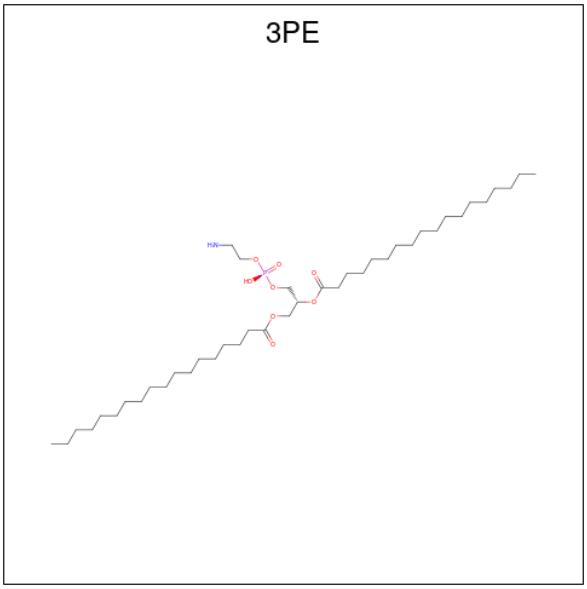
Mol	Chain	Residues	Atoms	AltConf
18	G	1	Total Ca 1 1	0

- 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	M	1	Total C 20 20	0
19	N	1	Total C 20 20	0

- Molecule 20 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



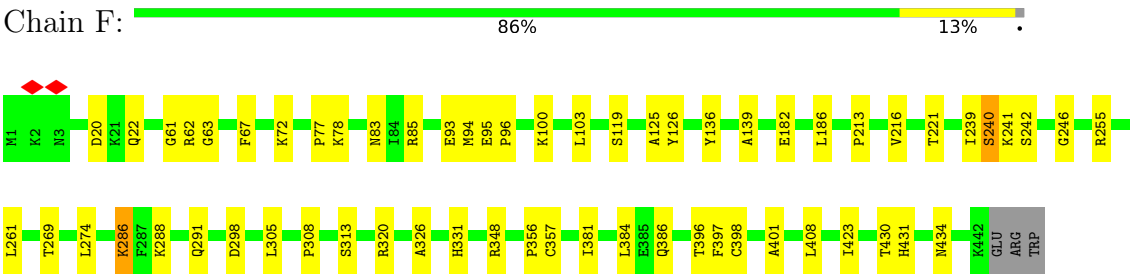
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total C N O P 51 41 1 8 1	0
20	L	1	Total C N O P 153 123 3 24 3	0
20	L	1	Total C N O P 153 123 3 24 3	0
20	L	1	Total C N O P 153 123 3 24 3	0
20	M	1	Total C N O P 51 41 1 8 1	0
20	J	1	Total C N O P 51 41 1 8 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

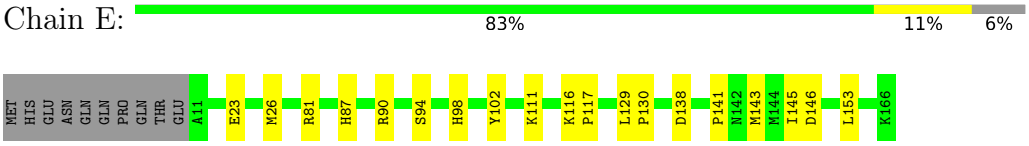
• Molecule 1: NADH-quinone oxidoreductase subunit F

Chain F:



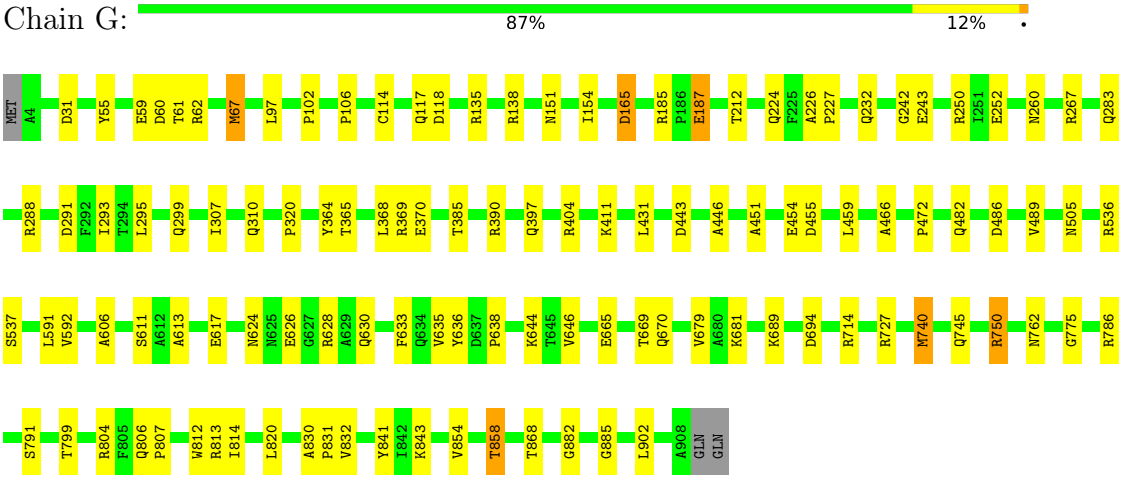
• Molecule 2: NADH dehydrogenase I subunit E

Chain E:



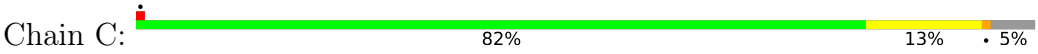
• Molecule 3: NADH-quinone oxidoreductase

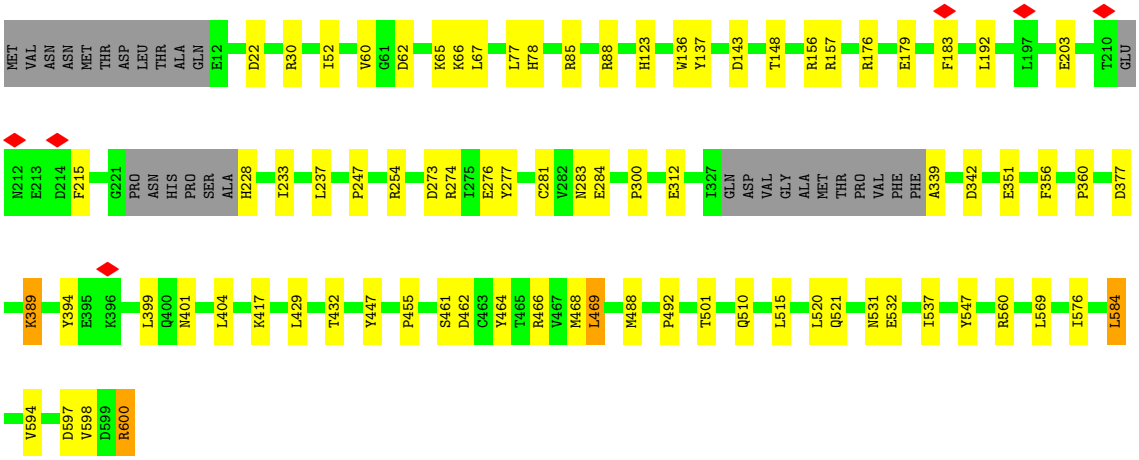
Chain G:



• Molecule 4: NADH-quinone oxidoreductase subunit CD

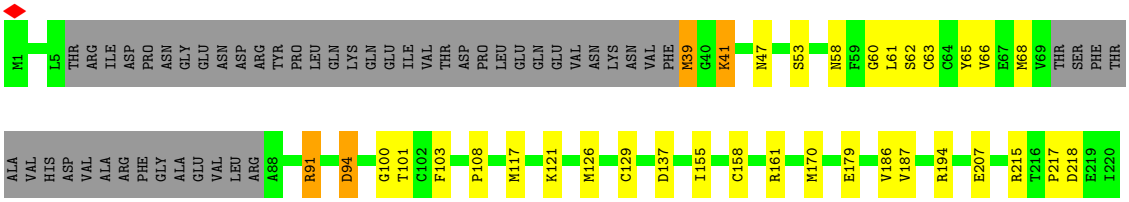
Chain C:





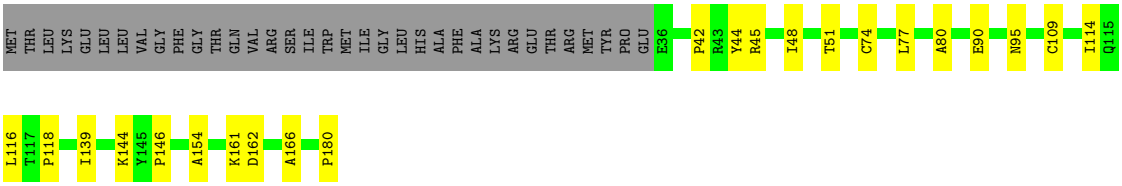
• Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:



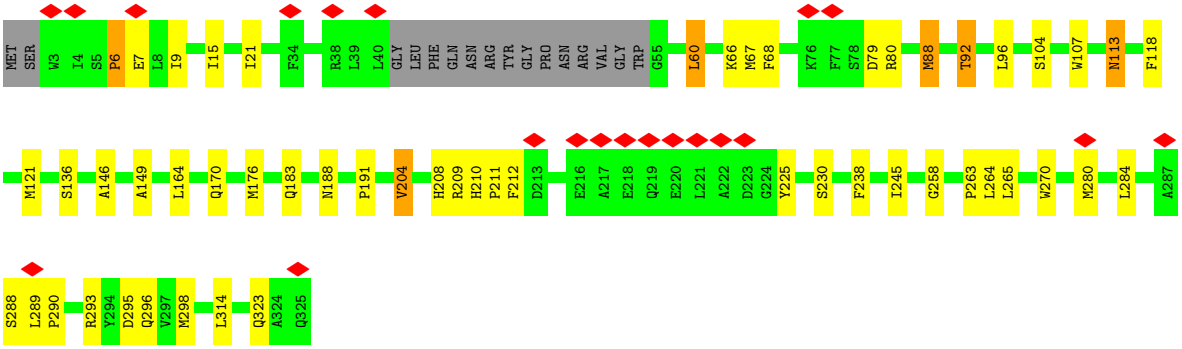
• Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:



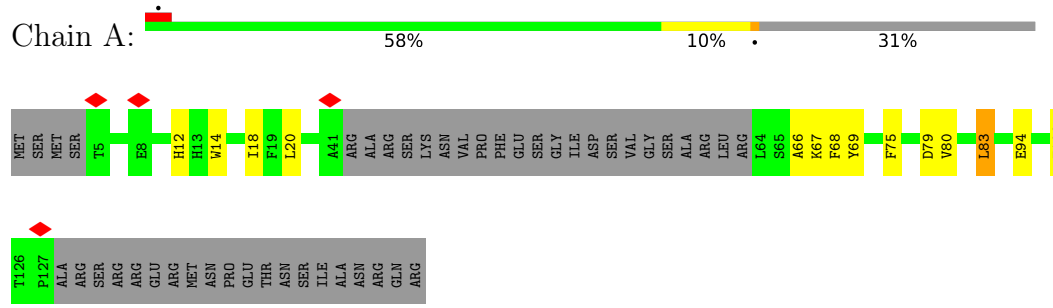
• Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:



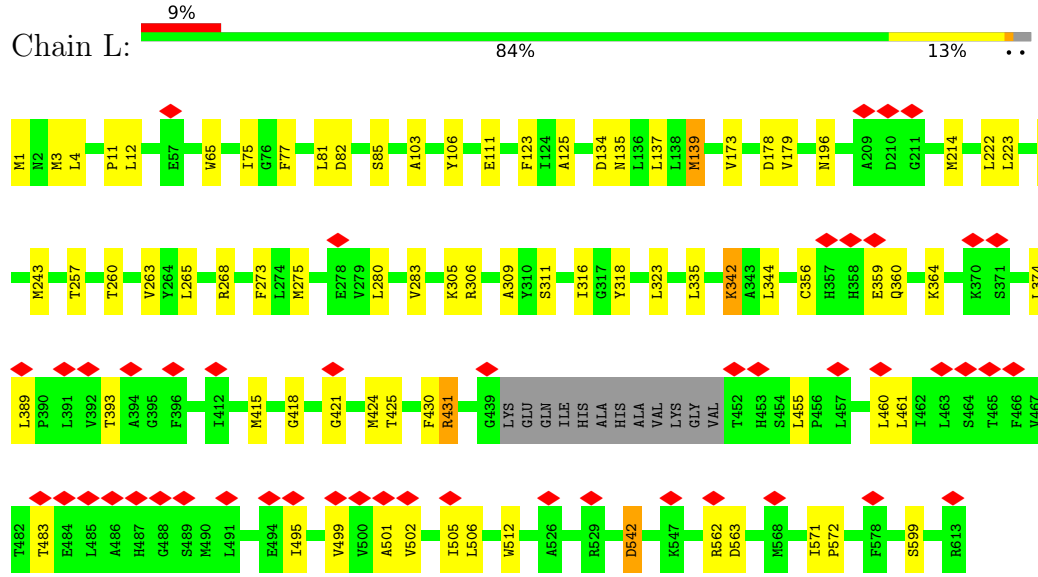
• Molecule 8: NADH-quinone oxidoreductase subunit A

Chain A:



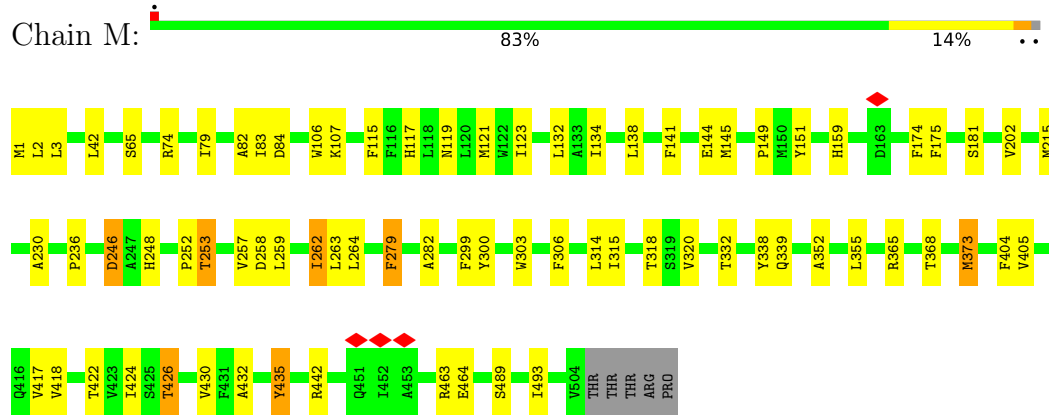
• Molecule 9: NADH-quinone oxidoreductase subunit L

Chain L:



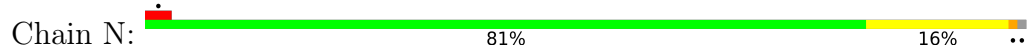
• Molecule 10: NADH dehydrogenase I subunit M

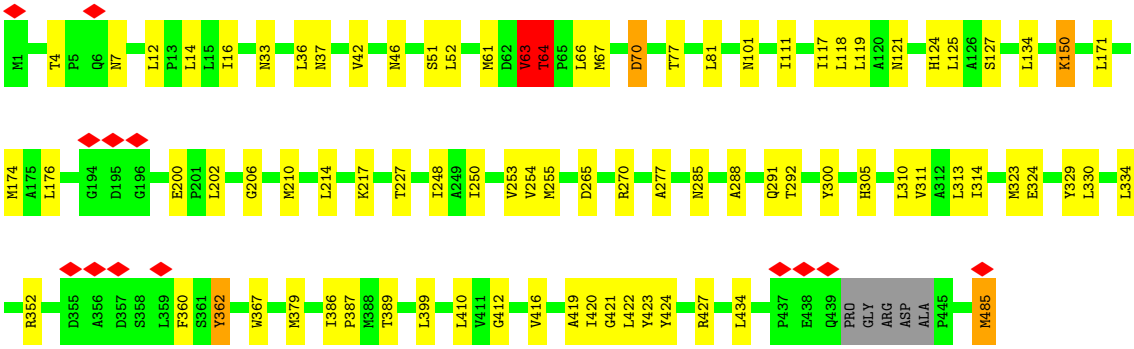
Chain M:



• Molecule 11: NADH-quinone oxidoreductase subunit N

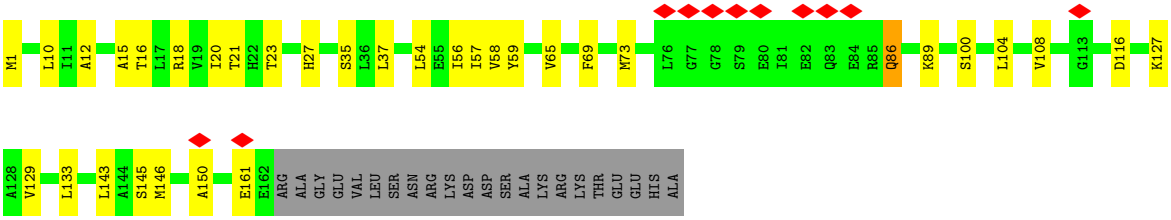
Chain N:





• Molecule 12: NADH-quinone oxidoreductase subunit K

• 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	82734	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	0.358	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	151.57999, 207.76, 248.04	wwPDB
Map dimensions	143, 196, 234	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: NAI, FMN, LFA, CA, FES, SF4, 3PE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	F	0.38	0/3511	0.56	0/4745
2	E	0.36	0/1248	0.55	0/1691
3	G	0.39	0/7173	0.56	1/9726 (0.0%)
4	C	0.39	0/4719	0.58	1/6400 (0.0%)
5	B	0.40	0/1367	0.60	0/1847
6	I	0.47	0/1176	0.58	0/1590
7	H	0.34	0/2492	0.62	2/3391 (0.1%)
8	A	0.31	0/821	0.57	0/1119
9	L	0.29	0/4713	0.53	2/6423 (0.0%)
10	M	0.32	0/4074	0.54	0/5546
11	N	0.33	0/3724	0.55	2/5081 (0.0%)
12	K	0.34	0/769	0.57	0/1040
13	J	0.35	0/1252	0.57	1/1708 (0.1%)
All	All	0.36	0/37039	0.56	9/50307 (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
9	L	0	1
11	N	0	2
All	All	0	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	6	PRO	CA-N-CD	-8.63	99.42	111.50
3	G	67	MET	CB-CG-SD	-7.01	91.36	112.40
4	C	399	LEU	CA-CB-CG	6.18	129.50	115.30
7	H	284	LEU	CA-CB-CG	5.66	128.32	115.30
9	L	214	MET	CB-CG-SD	5.46	128.78	112.40
9	L	455	LEU	CA-CB-CG	5.28	127.45	115.30
11	N	379	MET	CB-CG-SD	5.28	128.23	112.40
11	N	64	THR	N-CA-C	-5.25	96.82	111.00
13	J	10	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	145	ILE	Peptide
3	G	260	ASN	Peptide
9	L	257	THR	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	34	0
2	E	1220	0	1187	11	0
3	G	7022	0	6824	57	0
4	C	4597	0	4506	46	0
5	B	1339	0	1330	27	0
6	I	1149	0	1114	15	0
7	H	2422	0	2469	29	0
8	A	796	0	804	15	0
9	L	4595	0	4736	43	0
10	M	3953	0	4053	44	0
11	N	3635	0	3802	49	0
12	K	760	0	817	17	0
13	J	1226	0	1297	24	0
14	B	8	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	F	8	0	0	1	0
14	G	24	0	0	1	0
14	I	16	0	0	0	0
15	F	31	0	19	0	0
16	F	44	0	27	3	0
17	E	4	0	0	0	0
17	G	4	0	0	0	0
18	G	1	0	0	0	0
19	A	20	0	42	0	0
19	H	20	0	42	1	0
19	L	20	0	42	0	0
19	M	20	0	42	1	0
19	N	20	0	42	1	0
20	A	51	0	82	1	0
20	J	51	0	82	4	0
20	L	153	0	246	5	0
20	M	51	0	82	3	0
All	All	36692	0	37092	372	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 (372) 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)
9:L:243:MET:HE1	9:L:309:ALA:HB2	1.65	0.78
1:F:95:GLU:HB2	16:F:503:NAI:H42N	1.66	0.78
11:N:63:VAL:O	11:N:67:MET:HB2	1.82	0.78
9:L:356:CYS:HB3	9:L:360:GLN:HE22	1.49	0.77
2:E:143:MET:HB2	2:E:153:LEU:HD11	1.68	0.75
8:A:69:TYR:HB2	13:J:73:MET:HE1	1.72	0.72
7:H:289:LEU:HD22	7:H:290:PRO:HD2	1.72	0.70
10:M:181:SER:HB2	10:M:230:ALA:HA	1.72	0.70
11:N:255:MET:HG2	11:N:313:LEU:HD13	1.75	0.68
5:B:126:MET:HG2	5:B:155:ILE:HD13	1.76	0.67
7:H:209:ARG:HD3	7:H:245:ILE:HG21	1.76	0.67
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.75	0.66
5:B:186:VAL:HG23	5:B:187:VAL:HG23	1.77	0.66
11:N:277:ALA:HB2	11:N:310:LEU:HD12	1.78	0.66
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.78	0.65
9:L:65:TRP:HB2	20:L:802:3PE:H122	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:243:MET:HG2	9:L:305:LYS:HB3	1.80	0.63
4:C:360:PRO:O	6:I:45:ARG:NH1	2.29	0.62
4:C:560:ARG:HH12	4:C:600:ARG:HH21	1.46	0.62
12:K:85:ARG:HH12	13:J:161:GLU:HA	1.66	0.61
11:N:419:ALA:HA	11:N:422:LEU:HD12	1.82	0.60
9:L:4:LEU:HD21	9:L:81:LEU:HD22	1.82	0.60
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.83	0.60
11:N:33:ASN:O	11:N:37:ASN:ND2	2.34	0.60
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.84	0.59
4:C:351:GLU:OE2	5:B:161:ARG:NH1	2.36	0.59
11:N:117:ILE:O	11:N:121:ASN:ND2	2.36	0.59
4:C:176:ARG:HH11	5:B:137:ASP:HB3	1.67	0.59
8:A:68:PHE:HB3	13:J:69:PHE:HE2	1.67	0.59
11:N:64:THR:HB	11:N:66:LEU:H	1.68	0.59
6:I:48:ILE:HG12	6:I:116:LEU:HG	1.84	0.58
7:H:15:ILE:HG23	8:A:18:ILE:HG21	1.85	0.58
9:L:571:ILE:HG13	9:L:572:PRO:HD3	1.86	0.58
9:L:85:SER:OG	9:L:268:ARG:NH2	2.37	0.58
1:F:357:CYS:HB2	1:F:401:ALA:HB2	1.86	0.57
1:F:77:PRO:O	1:F:85:ARG:NH2	2.34	0.57
3:G:365:THR:O	3:G:786:ARG:NH2	2.38	0.57
7:H:79:ASP:OD2	13:J:27:HIS:NE2	2.33	0.57
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.87	0.57
10:M:123:ILE:HG13	10:M:149:PRO:HB2	1.87	0.57
1:F:288:LYS:HD2	1:F:331:HIS:HA	1.87	0.56
9:L:318:TYR:OH	9:L:418:GLY:O	2.22	0.56
11:N:134:LEU:HD11	13:J:143:LEU:HB3	1.86	0.56
11:N:4:THR:HG23	11:N:7:ASN:H	1.71	0.56
2:E:23:GLU:HA	2:E:26:MET:HE2	1.88	0.56
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.87	0.56
9:L:75:ILE:HG21	9:L:137:LEU:HD23	1.87	0.56
1:F:85:ARG:HB2	1:F:125:ALA:HA	1.87	0.56
10:M:306:PHE:O	10:M:442:ARG:NH2	2.39	0.56
7:H:211:PRO:HG3	7:H:289:LEU:HD12	1.89	0.55
10:M:463:ARG:NH1	10:M:464:GLU:OE2	2.36	0.55
7:H:263:PRO:HG2	7:H:264:LEU:HD12	1.87	0.55
1:F:85:ARG:HG2	1:F:213:PRO:HG2	1.89	0.55
11:N:248:ILE:HD11	11:N:334:LEU:HB2	1.89	0.55
11:N:311:VAL:HA	11:N:314:ILE:HD12	1.89	0.55
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.87	0.55
5:B:94:ASP:OD1	5:B:94:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:356:PRO:HB2	1:F:396:THR:HG22	1.89	0.55
3:G:55:TYR:HB3	3:G:60:ASP:HB3	1.89	0.55
10:M:224:MET:HE2	10:M:282:ALA:HB1	1.89	0.55
5:B:101:THR:HA	5:B:129:CYS:HB3	1.89	0.55
7:H:118:PHE:HA	7:H:121:MET:HG3	1.89	0.54
3:G:283:GLN:NE2	3:G:644:LYS:O	2.40	0.54
3:G:165:ASP:OD1	3:G:165:ASP:N	2.39	0.54
5:B:47:ASN:ND2	5:B:179:GLU:O	2.36	0.54
11:N:412:GLY:HA3	19:N:601:LFA:H81	1.89	0.54
3:G:814:ILE:HD11	3:G:902:LEU:HD13	1.88	0.54
10:M:332:THR:HB	10:M:417:VAL:HG21	1.90	0.54
4:C:462:ASP:OD1	4:C:462:ASP:N	2.33	0.54
3:G:626:GLU:OE1	3:G:786:ARG:NH1	2.40	0.53
10:M:3:LEU:HB3	10:M:132:LEU:HD13	1.89	0.53
8:A:94:GLU:OE1	8:A:94:GLU:N	2.38	0.53
4:C:192:LEU:HD12	5:B:108:PRO:HB2	1.90	0.53
4:C:77:LEU:HB3	4:C:137:TYR:HB3	1.90	0.53
4:C:143:ASP:OD1	4:C:157:ARG:NH1	2.39	0.53
7:H:146:ALA:HB2	7:H:225:TYR:HB3	1.91	0.53
9:L:344:LEU:HB2	9:L:460:LEU:HB3	1.89	0.53
4:C:123:HIS:HA	4:C:148:THR:O	2.08	0.53
4:C:501:THR:HG23	4:C:521:GLN:HB3	1.91	0.53
6:I:51:THR:HG22	6:I:139:ILE:HD11	1.91	0.53
12:K:16:VAL:HG21	13:J:104:LEU:HB2	1.90	0.53
12:K:96:SER:O	12:K:96:SER:OG	2.26	0.52
10:M:338:TYR:HB3	10:M:493:ILE:HD12	1.90	0.52
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.91	0.52
9:L:599:SER:HB3	12:K:19:LEU:HD21	1.92	0.52
10:M:405:VAL:O	10:M:409:MET:HG3	2.09	0.52
11:N:42:VAL:O	11:N:46:ASN:ND2	2.43	0.52
5:B:68:MET:HB3	5:B:126:MET:HE1	1.92	0.52
1:F:182:GLU:O	1:F:186:LEU:N	2.37	0.52
3:G:138:ARG:NH1	6:I:162:ASP:OD2	2.39	0.52
11:N:66:LEU:HA	11:N:124:HIS:HB2	1.92	0.52
3:G:397:GLN:O	3:G:404:ARG:NH2	2.42	0.51
7:H:149:ALA:HB1	7:H:208:HIS:HE1	1.74	0.51
12:K:96:SER:OG	12:K:99:ARG:NH2	2.44	0.51
5:B:101:THR:OG1	5:B:129:CYS:SG	2.64	0.51
9:L:378:CYS:HA	9:L:461:LEU:HD21	1.92	0.51
10:M:141:PHE:O	10:M:145:MET:HB2	2.11	0.51
8:A:66:ALA:HB3	13:J:161:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:624:ASN:HB2	3:G:628:ARG:H	1.75	0.50
10:M:252:PRO:HD2	10:M:257:VAL:HG11	1.92	0.50
1:F:431:HIS:O	4:C:510:GLN:NE2	2.37	0.50
4:C:276:GLU:O	4:C:283:ASN:ND2	2.40	0.50
9:L:82:ASP:N	9:L:82:ASP:OD1	2.43	0.50
9:L:134:ASP:OD2	9:L:196:ASN:ND2	2.44	0.50
12:K:28:LEU:HA	12:K:31:MET:HG3	1.92	0.50
3:G:118:ASP:OD1	3:G:762:ASN:ND2	2.42	0.50
3:G:482:GLN:NE2	3:G:486:ASP:OD2	2.44	0.50
2:E:87:HIS:ND1	2:E:146:ASP:OD2	2.45	0.50
4:C:312:GLU:OE2	4:C:447:TYR:OH	2.27	0.50
3:G:727:ARG:HD3	4:C:179:GLU:HB2	1.93	0.50
6:I:161:LYS:HD2	6:I:166:ALA:HB2	1.94	0.49
3:G:243:GLU:HG2	3:G:636:TYR:HB3	1.95	0.49
3:G:267:ARG:HB2	3:G:820:LEU:HG	1.95	0.49
4:C:339:ALA:N	4:C:394:TYR:HH	2.11	0.49
4:C:461:SER:OG	4:C:466:ARG:NH1	2.45	0.49
5:B:53:SER:OG	7:H:66:LYS:NZ	2.32	0.49
1:F:83:ASN:OD1	1:F:83:ASN:N	2.46	0.49
11:N:485:MET:SD	11:N:485:MET:N	2.86	0.49
3:G:472:PRO:HG3	3:G:799:THR:HA	1.94	0.49
9:L:240:ALA:O	9:L:306:ARG:NH1	2.45	0.49
11:N:16:ILE:HD12	11:N:51:SER:HB3	1.95	0.49
11:N:125:LEU:HD13	11:N:174:MET:HB3	1.94	0.49
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.78	0.48
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.94	0.48
3:G:212:THR:HG22	3:G:832:VAL:HG21	1.95	0.48
2:E:138:ASP:OD1	2:E:138:ASP:N	2.47	0.48
3:G:320:PRO:HB2	3:G:537:SER:HB2	1.95	0.48
10:M:248:HIS:ND1	10:M:258:ASP:OD2	2.33	0.48
3:G:97:LEU:HD22	3:G:154:ILE:HB	1.95	0.48
4:C:254:ARG:HG3	5:B:103:PHE:HE1	1.76	0.48
9:L:103:ALA:HA	9:L:106:TYR:HB3	1.95	0.48
9:L:179:VAL:HG22	10:M:426:THR:HG22	1.94	0.48
2:E:141:PRO:HG2	2:E:153:LEU:HB2	1.96	0.48
4:C:569:LEU:HD22	4:C:598:VAL:HG21	1.96	0.48
5:B:61:LEU:HB3	5:B:100:GLY:HA3	1.95	0.48
7:H:88:MET:O	7:H:92:THR:OG1	2.31	0.48
3:G:454:GLU:OE1	3:G:813:ARG:NH1	2.44	0.47
5:B:215:ARG:HB2	6:I:42:PRO:HB3	1.96	0.47
8:A:80:VAL:HA	8:A:83:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:802:3PE:H2B1	20:L:802:3PE:H3A2	1.96	0.47
3:G:843:LYS:HB2	3:G:885:GLY:HA3	1.97	0.47
9:L:263:VAL:HG13	9:L:323:LEU:HD11	1.95	0.47
10:M:404:PHE:O	10:M:408:PHE:HB2	2.14	0.47
3:G:226:ALA:HB3	3:G:635:VAL:HG22	1.96	0.47
10:M:263:LEU:HD21	10:M:352:ALA:HB3	1.96	0.47
11:N:367:TRP:NE1	11:N:434:LEU:O	2.36	0.47
13:J:20:ILE:HG13	13:J:21:THR:HG23	1.97	0.47
8:A:20:LEU:HD12	20:J:301:3PE:H382	1.96	0.47
8:A:94:GLU:OE2	13:J:127:LYS:NZ	2.47	0.47
1:F:348:ARG:HD2	6:I:180:PRO:HB2	1.96	0.47
4:C:429:LEU:O	4:C:432:THR:OG1	2.32	0.47
6:I:44:TYR:HD2	6:I:118:PRO:HA	1.79	0.47
11:N:291:GLN:O	11:N:427:ARG:NH2	2.47	0.47
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.96	0.47
7:H:113:ASN:N	7:H:113:ASN:OD1	2.48	0.47
9:L:542:ASP:OD1	9:L:542:ASP:N	2.47	0.47
10:M:422:THR:O	10:M:426:THR:OG1	2.33	0.47
11:N:386:ILE:O	11:N:389:THR:OG1	2.27	0.47
11:N:360:PHE:CE2	11:N:362:TYR:HB3	2.50	0.47
4:C:455:PRO:HB2	4:C:469:LEU:HD22	1.97	0.47
7:H:293:ARG:NH2	7:H:296:GLN:OE1	2.47	0.47
9:L:260:THR:HB	9:L:335:LEU:HD11	1.97	0.47
3:G:364:TYR:OH	3:G:370:GLU:OE1	2.26	0.47
4:C:85:ARG:HB3	4:C:88:ARG:HD2	1.97	0.47
7:H:204:VAL:HG22	7:H:209:ARG:HB2	1.98	0.46
9:L:430:PHE:CD2	9:L:505:ILE:HD12	2.49	0.46
10:M:151:TYR:HB2	10:M:175:PHE:HD2	1.80	0.46
4:C:401:ASN:HB3	4:C:404:LEU:HB3	1.98	0.46
9:L:385:ALA:HA	9:L:393:THR:HB	1.97	0.46
10:M:264:LEU:HA	10:M:264:LEU:HD12	1.83	0.46
11:N:176:LEU:HD22	11:N:202:LEU:HD11	1.95	0.46
1:F:320:ARG:NH1	16:F:503:NAI:O2D	2.47	0.46
9:L:173:VAL:HG22	20:M:1001:3PE:H391	1.96	0.46
1:F:62:ARG:O	1:F:100:LYS:NZ	2.49	0.46
2:E:117:PRO:HB3	2:E:130:PRO:HD3	1.97	0.46
1:F:241:LYS:HE2	1:F:241:LYS:HB2	1.75	0.46
3:G:443:ASP:OD1	3:G:443:ASP:N	2.46	0.46
4:C:215:PHE:HA	4:C:237:LEU:O	2.15	0.46
20:A:202:3PE:H321	20:J:301:3PE:H341	1.98	0.46
11:N:288:ALA:HB2	11:N:300:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:LYS:HA	1:F:286:LYS:HD3	1.80	0.46
2:E:116:LYS:HA	2:E:116:LYS:HD3	1.79	0.46
3:G:679:VAL:HG11	3:G:689:LYS:HB2	1.98	0.46
12:K:80:LEU:HD11	12:K:90:LEU:HD13	1.98	0.46
3:G:224:GLN:O	3:G:242:GLY:HA2	2.16	0.46
5:B:60:GLY:HA2	5:B:65:TYR:CG	2.51	0.46
6:I:154:ALA:O	6:I:161:LYS:NZ	2.37	0.46
8:A:67:LYS:NZ	8:A:125:TRP:O	2.47	0.46
10:M:84:ASP:N	10:M:84:ASP:OD1	2.48	0.46
20:J:301:3PE:H3D1	20:J:301:3PE:H2A1	1.98	0.46
12:K:96:SER:HG	12:K:99:ARG:NH2	2.14	0.45
7:H:183:GLN:NE2	7:H:258:GLY:H	2.13	0.45
10:M:314:LEU:O	10:M:318:THR:HG23	2.16	0.45
11:N:285:ASN:HB3	11:N:420:ILE:HB	1.97	0.45
3:G:307:ILE:HG21	3:G:591:LEU:HD13	1.98	0.45
12:K:85:ARG:HE	12:K:85:ARG:HB2	1.47	0.45
3:G:611:SER:OG	3:G:646:VAL:O	2.31	0.45
9:L:431:ARG:HG3	9:L:512:TRP:CE2	2.50	0.45
11:N:81:LEU:HD21	11:N:117:ILE:HD11	1.98	0.45
11:N:119:LEU:HD22	11:N:253:VAL:HG11	1.99	0.45
8:A:75:PHE:O	8:A:79:ASP:HB2	2.17	0.45
10:M:315:ILE:HD13	10:M:355:LEU:HB3	1.98	0.45
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.99	0.45
1:F:434:ASN:HB3	6:I:146:PRO:HD2	1.99	0.45
5:B:39:MET:N	5:B:41:LYS:HZ2	2.13	0.45
6:I:45:ARG:HG2	6:I:116:LEU:HD22	1.98	0.45
9:L:222:LEU:HD22	9:L:265:LEU:HD11	1.98	0.45
11:N:214:LEU:HD13	11:N:254:VAL:HG22	1.99	0.45
1:F:308:PRO:O	1:F:313:SER:OG	2.30	0.45
5:B:217:PRO:HG3	6:I:144:LYS:HD2	1.98	0.45
6:I:109:CYS:HB2	6:I:114:ILE:HG22	1.99	0.45
9:L:179:VAL:HG21	10:M:430:VAL:HG23	1.97	0.45
13:J:86:GLN:HA	13:J:89:LYS:NZ	2.32	0.45
3:G:812:TRP:HB2	3:G:902:LEU:HB3	1.99	0.45
9:L:389:LEU:O	9:L:393:THR:OG1	2.28	0.45
11:N:14:LEU:HD21	11:N:118:LEU:HD23	1.99	0.45
13:J:37:LEU:HD22	20:J:301:3PE:H2A2	1.97	0.45
5:B:117:MET:HB2	5:B:121:LYS:HE2	1.97	0.45
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.99	0.45
11:N:311:VAL:HG22	11:N:410:LEU:HD13	1.99	0.45
8:A:83:LEU:HB2	13:J:54:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:499:VAL:HA	9:L:502:VAL:HG22	1.98	0.44
10:M:82:ALA:HB3	10:M:134:ILE:HG21	1.98	0.44
10:M:119:ASN:HB3	10:M:149:PRO:HB3	2.00	0.44
1:F:61:GLY:N	1:F:67:PHE:O	2.48	0.44
4:C:576:ILE:HG12	4:C:584:LEU:HD23	1.99	0.44
20:L:801:3PE:H262	20:L:801:3PE:H322	1.99	0.44
13:J:65:VAL:O	13:J:69:PHE:HB2	2.17	0.44
10:M:246:ASP:OD1	10:M:246:ASP:N	2.50	0.44
1:F:239:ILE:HD11	1:F:246:GLY:HA2	2.00	0.44
3:G:288:ARG:HH21	3:G:293:ILE:HD11	1.82	0.44
3:G:295:LEU:HB3	3:G:299:GLN:HG3	1.98	0.44
11:N:416:VAL:O	11:N:420:ILE:HG13	2.18	0.44
12:K:87:ARG:HE	12:K:95:VAL:HG21	1.82	0.44
9:L:501:ALA:O	9:L:505:ILE:HG12	2.18	0.44
3:G:106:PRO:HD3	4:C:515:LEU:HD21	2.00	0.44
3:G:431:LEU:O	3:G:446:ALA:N	2.51	0.44
4:C:464:TYR:O	4:C:468:MET:HG2	2.18	0.44
11:N:265:ASP:HA	11:N:270:ARG:HH22	1.82	0.44
4:C:62:ASP:OD1	4:C:66:LYS:NZ	2.49	0.44
11:N:206:GLY:O	11:N:210:MET:HG3	2.18	0.44
3:G:807:PRO:HB3	3:G:882:GLY:HA3	2.00	0.43
7:H:6:PRO:HD2	7:H:7:GLU:H	1.82	0.43
9:L:135:ASN:OD1	9:L:135:ASN:N	2.51	0.43
10:M:115:PHE:O	10:M:119:ASN:ND2	2.48	0.43
10:M:299:PHE:HE2	10:M:424:ILE:HG22	1.83	0.43
3:G:624:ASN:HD22	3:G:626:GLU:HG2	1.82	0.43
9:L:273:PHE:HB3	9:L:280:LEU:HD13	2.00	0.43
10:M:65:SER:HB3	10:M:83:ILE:HG22	1.99	0.43
3:G:613:ALA:HB1	3:G:617:GLU:HB2	2.01	0.43
4:C:233:ILE:HA	4:C:247:PRO:HA	2.00	0.43
4:C:277:TYR:CG	5:B:63:CYS:HB3	2.53	0.43
7:H:295:ASP:N	7:H:295:ASP:OD1	2.51	0.43
12:K:4:LEU:N	13:J:116:ASP:OD2	2.51	0.43
1:F:93:GLU:OE1	1:F:136:TYR:OH	2.29	0.43
2:E:81:ARG:HD2	2:E:81:ARG:HA	1.78	0.43
3:G:250:ARG:HE	3:G:252:GLU:HG2	1.84	0.43
10:M:2:LEU:HG	10:M:42:LEU:HD11	2.00	0.43
13:J:12:ALA:O	13:J:16:THR:HG22	2.18	0.43
3:G:854:VAL:HG13	3:G:858:THR:HG23	2.01	0.43
1:F:291:GLN:O	1:F:326:ALA:HA	2.18	0.43
11:N:52:LEU:HD23	11:N:52:LEU:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:185:ARG:NH1	3:G:187:GLU:O	2.52	0.43
5:B:39:MET:N	5:B:39:MET:SD	2.92	0.43
12:K:89:ASN:ND2	12:K:91:ASN:HB2	2.34	0.43
4:C:389:LYS:HE3	4:C:389:LYS:HB3	1.87	0.43
1:F:96:PRO:HB3	2:E:94:SER:HB3	2.01	0.43
3:G:227:PRO:HG2	3:G:633:PHE:CD1	2.54	0.43
3:G:232:GLN:HB2	14:G:1003:SF4:S3	2.59	0.43
7:H:6:PRO:HD2	7:H:7:GLU:N	2.34	0.43
20:L:801:3PE:H2I3	20:L:802:3PE:H391	1.99	0.43
3:G:117:GLN:HB3	4:C:520:LEU:HD11	2.01	0.43
4:C:254:ARG:NH2	5:B:62:SER:OG	2.52	0.43
10:M:117:HIS:O	10:M:121:MET:HG2	2.18	0.43
10:M:159:HIS:HD2	10:M:253:THR:HB	1.84	0.43
10:M:442:ARG:NH1	20:M:1001:3PE:O12	2.52	0.43
2:E:98:HIS:HA	2:E:102:TYR:HD1	1.82	0.42
7:H:21:ILE:HG12	19:H:601:LFA:H62	2.01	0.42
9:L:178:ASP:OD1	9:L:178:ASP:N	2.48	0.42
3:G:669:THR:OG1	3:G:670:GLN:N	2.52	0.42
6:I:74:CYS:HB2	6:I:95:ASN:HB3	2.00	0.42
9:L:421:GLY:O	9:L:425:THR:OG1	2.26	0.42
10:M:236:PRO:HG2	10:M:320:VAL:HG22	2.01	0.42
3:G:624:ASN:HB2	3:G:628:ARG:HB3	2.01	0.42
2:E:90:ARG:HA	2:E:129:LEU:O	2.18	0.42
4:C:281:CYS:HA	4:C:284:GLU:HB2	2.01	0.42
5:B:91:ARG:HB3	7:H:230:SER:HB3	2.02	0.42
3:G:740:MET:SD	3:G:740:MET:N	2.85	0.42
7:H:188:ASN:HA	7:H:191:PRO:HD2	2.02	0.42
11:N:12:LEU:HD12	11:N:12:LEU:HA	1.88	0.42
3:G:369:ARG:NH2	3:G:775:GLY:O	2.50	0.42
3:G:505:ASN:HA	3:G:536:ARG:HH21	1.85	0.42
6:I:80:ALA:HB2	6:I:90:GLU:HB2	2.01	0.42
7:H:280:MET:SD	7:H:280:MET:N	2.92	0.42
13:J:57:ILE:HG22	13:J:58:VAL:HG23	2.01	0.42
1:F:63:GLY:O	16:F:503:NAI:H2N	2.20	0.42
9:L:342:LYS:HD3	9:L:342:LYS:HA	1.83	0.42
9:L:506:LEU:HD13	9:L:506:LEU:HA	1.92	0.42
4:C:547:TYR:HB3	4:C:560:ARG:HB3	2.02	0.42
4:C:569:LEU:HA	4:C:569:LEU:HD12	1.81	0.42
5:B:58:ASN:HB3	5:B:65:TYR:HE1	1.85	0.42
8:A:83:LEU:HD11	12:K:63:ILE:HG23	2.01	0.42
20:L:804:3PE:H252	11:N:423:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:258:ASP:HA	10:M:262:ILE:HG13	2.01	0.42
11:N:150:LYS:HA	12:K:87:ARG:HH22	1.85	0.42
1:F:72:LYS:NZ	1:F:216:VAL:O	2.36	0.41
1:F:397:PHE:HB3	14:F:501:SF4:S2	2.60	0.41
3:G:102:PRO:HG3	3:G:151:ASN:HB3	2.02	0.41
4:C:377:ASP:OD1	4:C:377:ASP:N	2.47	0.41
10:M:144:GLU:HB2	11:N:387:PRO:HG2	2.02	0.41
10:M:220:GLU:HG2	10:M:279:PHE:HB3	2.02	0.41
11:N:305:HIS:ND1	11:N:329:TYR:OH	2.37	0.41
1:F:240:SER:HG	1:F:242:SER:HG	1.65	0.41
1:F:396:THR:HG21	1:F:401:ALA:HB3	2.02	0.41
11:N:171:LEU:HD23	12:K:42:SER:HB2	2.02	0.41
12:K:43:ALA:HB1	12:K:62:TYR:CD2	2.55	0.41
7:H:210:HIS:CD2	7:H:211:PRO:HA	2.56	0.41
4:C:277:TYR:CE1	5:B:66:VAL:HG21	2.56	0.41
9:L:233:LEU:HA	9:L:234:PRO:HA	1.78	0.41
11:N:101:ASN:OD1	11:N:101:ASN:N	2.51	0.41
4:C:85:ARG:NH2	4:C:532:GLU:OE2	2.47	0.41
4:C:156:ARG:NH1	4:C:203:GLU:O	2.53	0.41
5:B:218:ASP:OD1	5:B:218:ASP:N	2.47	0.41
10:M:107:LYS:HD2	10:M:107:LYS:HA	1.87	0.41
12:K:9:ILE:HG12	13:J:108:VAL:HG22	2.03	0.41
13:J:129:VAL:O	13:J:133:LEU:HB2	2.20	0.41
3:G:830:ALA:HA	3:G:831:PRO:HD3	1.95	0.41
4:C:342:ASP:OD1	4:C:342:ASP:N	2.53	0.41
5:B:100:GLY:HA2	14:B:301:SF4:S4	2.61	0.41
7:H:314:LEU:HD23	7:H:314:LEU:HA	1.92	0.41
9:L:563:ASP:OD1	10:M:300:TYR:OH	2.25	0.41
10:M:339:GLN:OE1	10:M:489:SER:OG	2.31	0.41
20:M:1001:3PE:H331	20:M:1001:3PE:H231	2.03	0.41
11:N:70:ASP:OD1	11:N:70:ASP:N	2.52	0.41
11:N:352:ARG:HA	11:N:352:ARG:HD3	1.84	0.41
9:L:230:SER:HB3	9:L:316:ILE:HG21	2.01	0.41
9:L:495:ILE:O	9:L:499:VAL:HG13	2.20	0.41
10:M:368:THR:HG21	10:M:373:MET:SD	2.61	0.41
11:N:119:LEU:HD23	11:N:119:LEU:HA	1.84	0.41
11:N:399:LEU:HD23	11:N:399:LEU:HA	1.92	0.41
1:F:381:ILE:HG12	1:F:423:ILE:HD11	2.03	0.41
3:G:628:ARG:HG2	3:G:630:GLN:HG3	2.03	0.41
13:J:15:ALA:HB3	13:J:35:SER:HB3	2.03	0.41
1:F:20:ASP:N	1:F:20:ASP:OD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:114:CYS:HB3	3:G:117:GLN:HB2	2.03	0.41
3:G:466:ALA:HB3	3:G:489:VAL:HG21	2.03	0.41
3:G:745:GLN:O	3:G:750:ARG:NH2	2.54	0.41
4:C:52:ILE:HD12	4:C:60:VAL:HG21	2.02	0.41
7:H:265:LEU:HB2	7:H:270:TRP:CD1	2.56	0.41
8:A:83:LEU:HD13	13:J:54:LEU:HD13	2.03	0.41
1:F:269:THR:HA	1:F:308:PRO:HA	2.03	0.41
3:G:592:VAL:HB	3:G:606:ALA:HA	2.03	0.41
7:H:96:LEU:HD13	8:A:20:LEU:HD22	2.03	0.41
13:J:1:MET:HB2	13:J:1:MET:HE2	1.85	0.41
4:C:300:PRO:HG3	4:C:492:PRO:HG2	2.02	0.40
7:H:6:PRO:HA	7:H:9:ILE:HB	2.03	0.40
8:A:106:PHE:CE2	13:J:145:SER:HB3	2.57	0.40
9:L:12:LEU:HD23	9:L:12:LEU:HA	1.89	0.40
9:L:139:MET:HE2	9:L:139:MET:HB3	1.97	0.40
11:N:421:GLY:HA2	11:N:424:TYR:CE2	2.56	0.40
1:F:103:LEU:HD22	1:F:261:LEU:HD23	2.04	0.40
4:C:67:LEU:HD23	4:C:67:LEU:HA	1.92	0.40
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.55	0.40
4:C:594:VAL:HG23	4:C:597:ASP:HB2	2.03	0.40
1:F:384:LEU:HD22	1:F:408:LEU:HD21	2.04	0.40
7:H:60:LEU:HA	7:H:60:LEU:HD22	1.83	0.40
10:M:115:PHE:CD2	19:M:1002:LFA:H82	2.56	0.40
13:J:37:LEU:HA	13:J:56:ILE:HD11	2.02	0.40
1:F:274:LEU:HD23	1:F:305:LEU:HD21	2.02	0.40
3:G:451:ALA:HB1	3:G:455:ASP:HB2	2.03	0.40
3:G:694:ASP:OD1	3:G:694:ASP:N	2.42	0.40
4:C:136:TRP:CZ2	4:C:247:PRO:HG2	2.57	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%)	872 (97%)	31 (3%)	0	100	100
4	C	563/600 (94%)	548 (97%)	15 (3%)	0	100	100
5	B	163/220 (74%)	153 (94%)	10 (6%)	0	100	100
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%)	576 (96%)	21 (4%)	0	100	100
10	M	502/509 (99%)	493 (98%)	9 (2%)	0	100	100
11	N	476/485 (98%)	463 (97%)	12 (2%)	1 (0%)	47	82
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	160/184 (87%)	153 (96%)	7 (4%)	0	100	100
All	All	4601/4882 (94%)	4464 (97%)	136 (3%)	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	356/359 (99%)	343 (96%)	13 (4%)	34	70
2	E	129/139 (93%)	128 (99%)	1 (1%)	81	93
3	G	732/735 (100%)	708 (97%)	24 (3%)	38	73
4	C	486/519 (94%)	470 (97%)	16 (3%)	38	73
5	B	146/192 (76%)	139 (95%)	7 (5%)	25	62
6	I	124/154 (80%)	123 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	H	255/269 (95%)	238 (93%)	17 (7%)	16 49
8	A	79/119 (66%)	75 (95%)	4 (5%)	24 60
9	L	477/486 (98%)	458 (96%)	19 (4%)	31 68
10	M	413/418 (99%)	395 (96%)	18 (4%)	28 65
11	N	381/385 (99%)	368 (97%)	13 (3%)	37 72
12	K	79/79 (100%)	73 (92%)	6 (8%)	13 43
13	J	128/146 (88%)	122 (95%)	6 (5%)	26 63
All	All	3785/4000 (95%)	3640 (96%)	145 (4%)	36 69

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	22	GLN
1	F	78	LYS
1	F	94	MET
1	F	119	SER
1	F	126	TYR
1	F	221	THR
1	F	240	SER
1	F	255	ARG
1	F	286	LYS
1	F	298	ASP
1	F	386	GLN
1	F	398	CYS
1	F	430	THR
2	E	111	LYS
3	G	31	ASP
3	G	59	GLU
3	G	61	THR
3	G	62	ARG
3	G	67	MET
3	G	135	ARG
3	G	165	ASP
3	G	187	GLU
3	G	291	ASP
3	G	310	GLN
3	G	385	THR
3	G	411	LYS
3	G	459	LEU
3	G	665	GLU

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Mol	Chain	Res	Type
3	G	681	LYS
3	G	714	ARG
3	G	740	MET
3	G	750	ARG
3	G	791	SER
3	G	804	ARG
3	G	806	GLN
3	G	841	TYR
3	G	858	THR
3	G	868	THR
4	C	22	ASP
4	C	30	ARG
4	C	65	LYS
4	C	78	HIS
4	C	183	PHE
4	C	228	HIS
4	C	273	ASP
4	C	356	PHE
4	C	389	LYS
4	C	417	LYS
4	C	469	LEU
4	C	488	MET
4	C	531	ASN
4	C	537	ILE
4	C	584	LEU
4	C	600	ARG
5	B	39	MET
5	B	41	LYS
5	B	91	ARG
5	B	94	ASP
5	B	170	MET
5	B	194	ARG
5	B	207	GLU
6	I	77	LEU
7	H	60	LEU
7	H	67	MET
7	H	68	PHE
7	H	80	ARG
7	H	88	MET
7	H	92	THR
7	H	113	ASN
7	H	136	SER

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Mol	Chain	Res	Type
7	H	164	LEU
7	H	170	GLN
7	H	176	MET
7	H	204	VAL
7	H	212	PHE
7	H	238	PHE
7	H	288	SER
7	H	298	MET
7	H	323	GLN
8	A	12	HIS
8	A	14	TRP
8	A	83	LEU
8	A	119	ARG
9	L	1	MET
9	L	3	MET
9	L	77	PHE
9	L	111	GLU
9	L	123	PHE
9	L	139	MET
9	L	275	MET
9	L	311	SER
9	L	342	LYS
9	L	359	GLU
9	L	364	LYS
9	L	374	LEU
9	L	379	PHE
9	L	415	MET
9	L	424	MET
9	L	431	ARG
9	L	483	THR
9	L	542	ASP
9	L	562	ARG
10	M	1	MET
10	M	74	ARG
10	M	106	TRP
10	M	174	PHE
10	M	202	VAL
10	M	215	MET
10	M	246	ASP
10	M	253	THR
10	M	259	LEU
10	M	262	ILE

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Mol	Chain	Res	Type
10	M	279	PHE
10	M	303	TRP
10	M	365	ARG
10	M	373	MET
10	M	408	PHE
10	M	418	VAL
10	M	426	THR
10	M	435	TYR
11	N	36	LEU
11	N	61	MET
11	N	63	VAL
11	N	70	ASP
11	N	127	SER
11	N	150	LYS
11	N	200	GLU
11	N	227	THR
11	N	292	THR
11	N	323	MET
11	N	324	GLU
11	N	362	TYR
11	N	485	MET
12	K	1	MET
12	K	25	ARG
12	K	46	PHE
12	K	72	GLU
12	K	96	SER
12	K	98	MET
13	J	18	ARG
13	J	23	THR
13	J	59	TYR
13	J	86	GLN
13	J	100	SER
13	J	146	MET

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

Mol	Chain	Res	Type
2	E	106	GLN
3	G	283	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	LFA	M	1002	-	19,19,19	0.17	0	18,18,18	0.15	0
19	LFA	N	601	-	19,19,19	0.12	0	18,18,18	0.14	0
14	SF4	I	201	6	0,12,12	-	-	-		
19	LFA	H	601	-	19,19,19	0.15	0	18,18,18	0.14	0
14	SF4	B	301	5	0,12,12	-	-	-		
14	SF4	F	501	1	0,12,12	-	-	-		
20	3PE	M	1001	-	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	0.27	0
19	LFA	L	803	-	19,19,19	0.15	0	18,18,18	0.11	0
16	NAI	F	503	-	42,48,48	0.52	0	47,73,73	0.53	1 (2%)
20	3PE	L	804	-	50,50,50	0.30	0	53,55,55	0.30	0
20	3PE	J	301	-	50,50,50	0.31	0	53,55,55	0.33	0
20	3PE	L	802	-	50,50,50	0.30	0	53,55,55	0.30	0
14	SF4	I	202	6	0,12,12	-	-	-		
17	FES	E	201	2	0,4,4	-	-	-		
14	SF4	G	1003	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LFA	A	201	-	19,19,19	0.15	0	18,18,18	0.20	0
14	SF4	G	1001	3	0,12,12	-	-	-		
20	3PE	A	202	-	50,50,50	0.29	0	53,55,55	0.28	0
15	FMN	F	502	-	33,33,33	1.12	3 (9%)	48,50,50	1.32	6 (12%)
17	FES	G	1004	3	0,4,4	-	-	-		

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	LFA	M	1002	-	-	3/17/17/17	-
19	LFA	N	601	-	-	0/17/17/17	-
14	SF4	I	201	6	-	-	0/6/5/5
19	LFA	H	601	-	-	1/17/17/17	-
14	SF4	B	301	5	-	-	0/6/5/5
14	SF4	F	501	1	-	-	0/6/5/5
20	3PE	M	1001	-	-	8/54/54/54	-
14	SF4	G	1002	3	-	-	0/6/5/5
20	3PE	L	801	-	-	8/54/54/54	-
19	LFA	L	803	-	-	1/17/17/17	-
16	NAI	F	503	-	-	8/25/72/72	0/5/5/5
20	3PE	L	804	-	-	13/54/54/54	-
20	3PE	J	301	-	-	12/54/54/54	-
20	3PE	L	802	-	-	15/54/54/54	-
14	SF4	I	202	6	-	-	0/6/5/5
17	FES	E	201	2	-	-	0/1/1/1
14	SF4	G	1003	3	-	-	0/6/5/5
19	LFA	A	201	-	-	1/17/17/17	-
14	SF4	G	1001	3	-	-	0/6/5/5
20	3PE	A	202	-	-	9/54/54/54	-
15	FMN	F	502	-	-	9/18/18/18	0/3/3/3
17	FES	G	1004	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.29	1.37	1.30
15	F	502	FMN	C4A-C10	-2.04	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C10-N1	2.02	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	-3.36	119.44	125.64
15	F	502	FMN	C4A-C10-N10	2.95	120.80	116.48
15	F	502	FMN	C4A-C4-N3	2.72	120.09	113.19
15	F	502	FMN	O4-C4-C4A	-2.59	119.73	126.60
16	F	503	NAI	C5A-C6A-N6A	2.33	123.89	120.35
15	F	502	FMN	C4A-C10-N1	-2.33	119.32	124.73
15	F	502	FMN	C10-C4A-N5	-2.26	120.05	124.86

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	502	FMN	N10-C1'-C2'-O2'
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	A	202	3PE	C1-O11-P-O12
20	A	202	3PE	C1-O11-P-O13
20	A	202	3PE	C1-O11-P-O14
20	A	202	3PE	O13-C11-C12-N
20	L	801	3PE	O13-C11-C12-N
20	L	802	3PE	C11-O13-P-O11
20	L	802	3PE	C11-O13-P-O12
20	L	802	3PE	C11-O13-P-O14
20	L	802	3PE	O13-C11-C12-N
20	L	804	3PE	C1-O11-P-O14
20	L	804	3PE	C11-O13-P-O11
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	M	1001	3PE	O13-C11-C12-N
20	J	301	3PE	C1-O11-P-O14
20	J	301	3PE	C11-O13-P-O14
20	J	301	3PE	O13-C11-C12-N
20	L	804	3PE	C1-O11-P-O13
20	M	1001	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
20	M	1001	3PE	C11-O13-P-O11
20	L	802	3PE	C3C-C3D-C3E-C3F
19	L	803	LFA	C6-C7-C8-C9
19	H	601	LFA	C14-C15-C16-C17
20	L	801	3PE	C2C-C2D-C2E-C2F
20	L	801	3PE	C3E-C3F-C3G-C3H
20	J	301	3PE	C1-O11-P-O13
20	J	301	3PE	C11-O13-P-O11
20	L	802	3PE	O11-C1-C2-C3
20	L	804	3PE	C1-C2-C3-O31
20	L	802	3PE	C31-C32-C33-C34
15	F	502	FMN	C5'-O5'-P-O1P
19	M	1002	LFA	C15-C16-C17-C18
20	L	801	3PE	C37-C38-C39-C3A
19	M	1002	LFA	C11-C12-C13-C14
20	L	802	3PE	C3D-C3E-C3F-C3G
20	A	202	3PE	C11-O13-P-O11
20	A	202	3PE	C21-C22-C23-C24
20	L	802	3PE	C39-C3A-C3B-C3C
20	L	804	3PE	O21-C2-C3-O31
20	A	202	3PE	C2-C1-O11-P
20	L	802	3PE	C2-C1-O11-P
20	J	301	3PE	C21-C22-C23-C24
16	F	503	NAI	C5B-O5B-PA-O2A
20	A	202	3PE	C11-O13-P-O12
20	L	804	3PE	C1-O11-P-O12
20	M	1001	3PE	C1-O11-P-O12
20	M	1001	3PE	C1-O11-P-O14
20	M	1001	3PE	C11-O13-P-O14
20	J	301	3PE	C1-O11-P-O12
20	J	301	3PE	C11-O13-P-O12
15	F	502	FMN	N10-C1'-C2'-C3'
20	L	802	3PE	O11-C1-C2-O21
15	F	502	FMN	C2'-C3'-C4'-O4'
20	L	801	3PE	C25-C26-C27-C28
20	J	301	3PE	C3B-C3C-C3D-C3E
15	F	502	FMN	O3'-C3'-C4'-C5'
20	L	801	3PE	C23-C24-C25-C26
15	F	502	FMN	O3'-C3'-C4'-O4'
16	F	503	NAI	O4D-C1D-N1N-C2N
16	F	503	NAI	PN-O3-PA-O2A
15	F	502	FMN	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
20	J	301	3PE	C22-C23-C24-C25
16	F	503	NAI	C2D-C1D-N1N-C2N
19	M	1002	LFA	C13-C14-C15-C16
20	J	301	3PE	C2F-C2G-C2H-C2I
20	L	804	3PE	C25-C26-C27-C28
20	L	804	3PE	C23-C24-C25-C26
20	L	802	3PE	C32-C33-C34-C35
19	A	201	LFA	C12-C13-C14-C15
20	M	1001	3PE	O21-C2-C3-O31
20	A	202	3PE	O21-C21-C22-C23
20	L	802	3PE	C37-C38-C39-C3A
20	L	804	3PE	C28-C29-C2A-C2B
20	L	801	3PE	C34-C35-C36-C37
16	F	503	NAI	C2D-C1D-N1N-C6N
20	J	301	3PE	C39-C3A-C3B-C3C
20	L	802	3PE	C1-O11-P-O14
20	L	802	3PE	C3F-C3G-C3H-C3I
16	F	503	NAI	O4D-C1D-N1N-C6N
20	L	801	3PE	C2F-C2G-C2H-C2I
20	M	1001	3PE	O31-C31-C32-C33
20	L	804	3PE	C2D-C2E-C2F-C2G

There are no ring outliers.

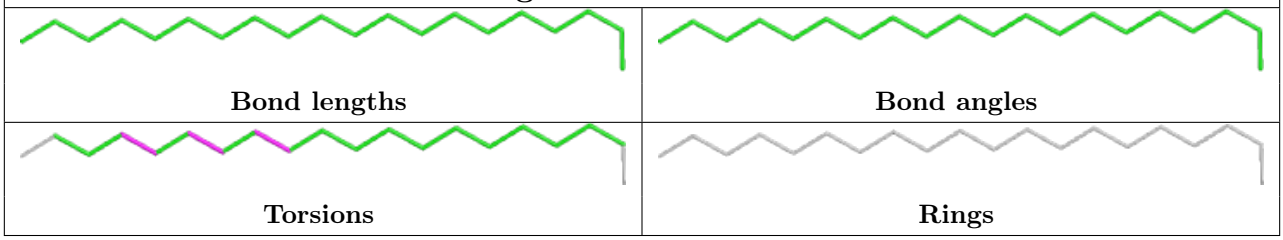
13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	M	1002	LFA	1	0
19	N	601	LFA	1	0
19	H	601	LFA	1	0
14	B	301	SF4	1	0
14	F	501	SF4	1	0
20	M	1001	3PE	3	0
20	L	801	3PE	2	0
16	F	503	NAI	3	0
20	L	804	3PE	1	0
20	J	301	3PE	4	0
20	L	802	3PE	3	0
14	G	1003	SF4	1	0
20	A	202	3PE	1	0

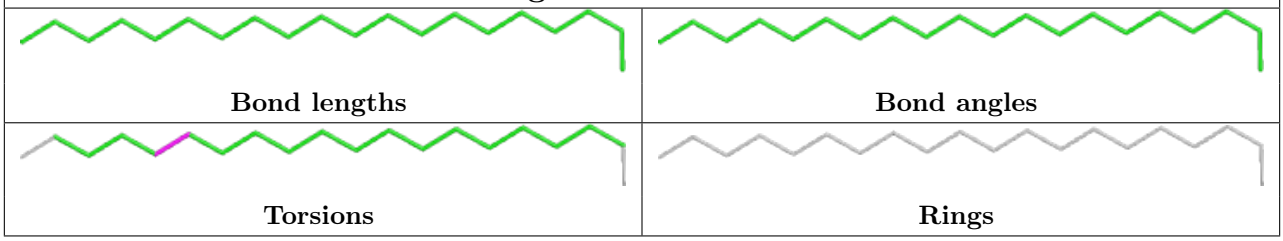
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

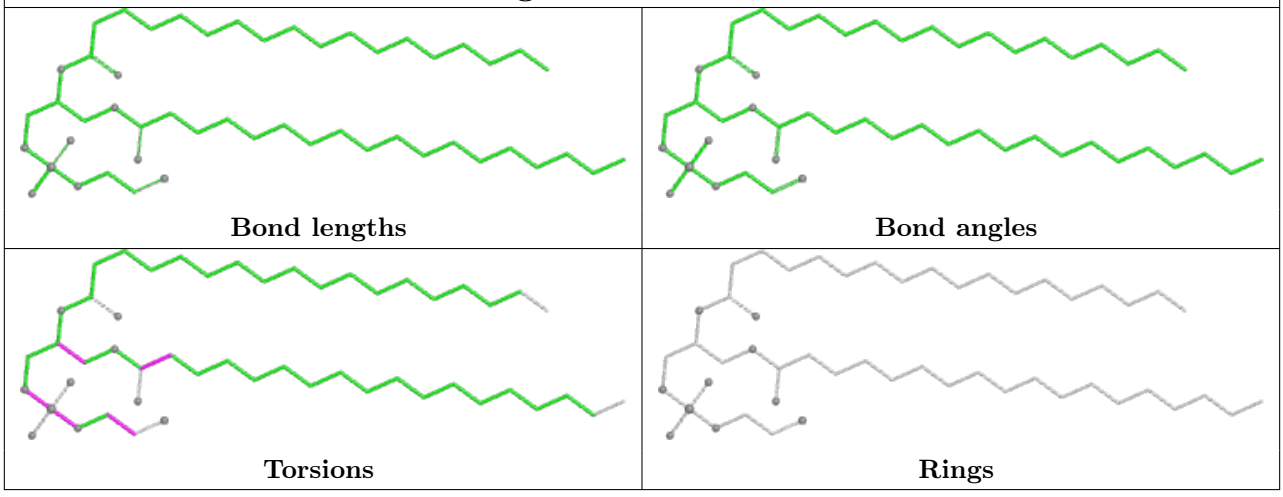
Ligand LFA M 1002



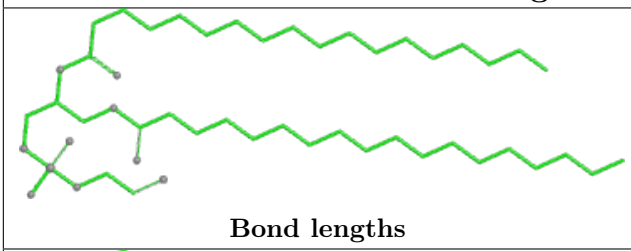
Ligand LFA H 601



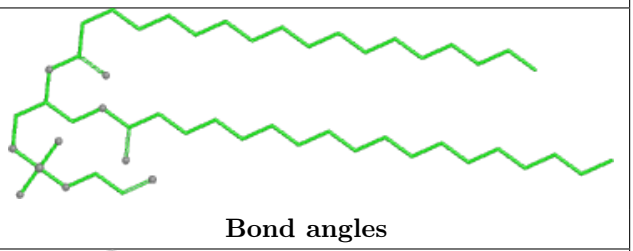
Ligand 3PE M 1001



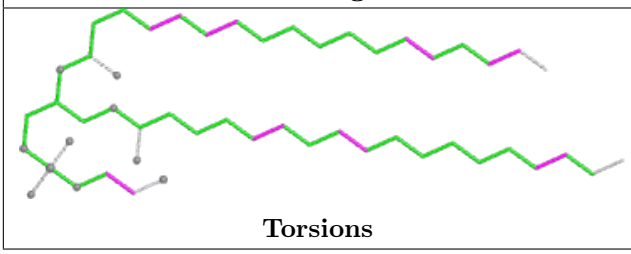
Ligand 3PE L 801



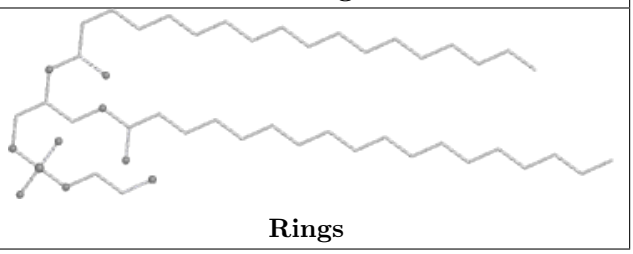
Bond lengths



Bond angles

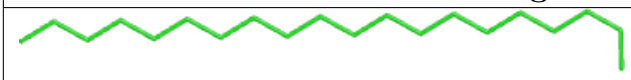


Torsions

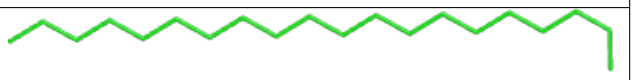


Rings

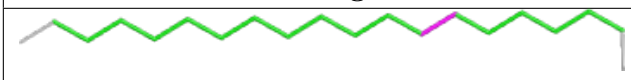
Ligand LFA L 803



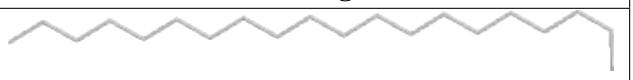
Bond lengths



Bond angles

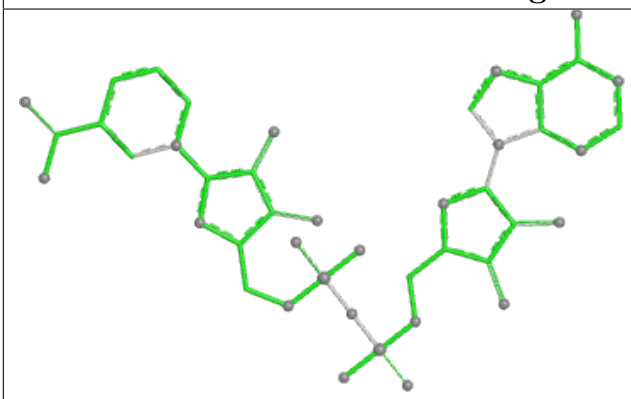


Torsions

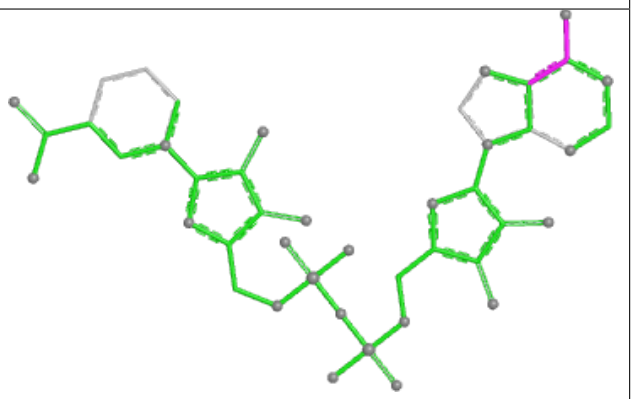


Rings

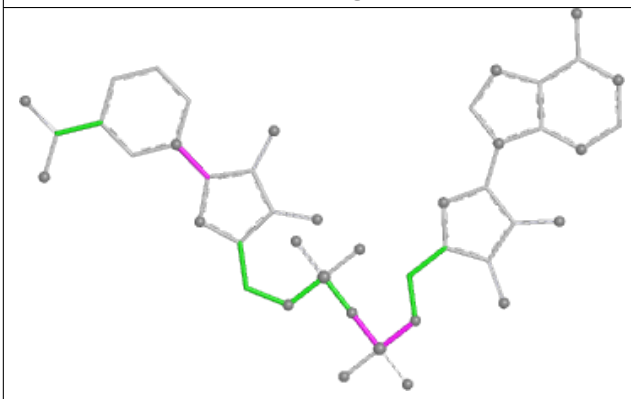
Ligand NAI F 503



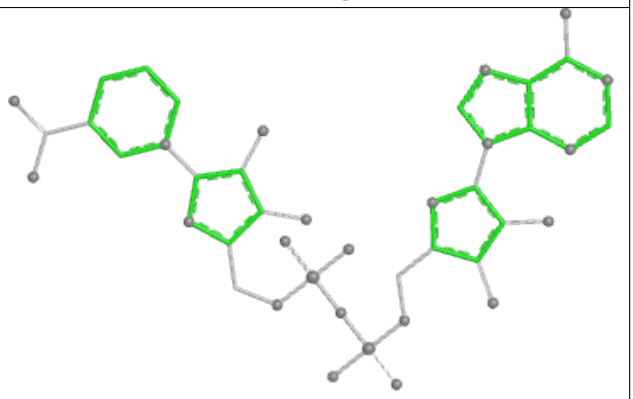
Bond lengths



Bond angles

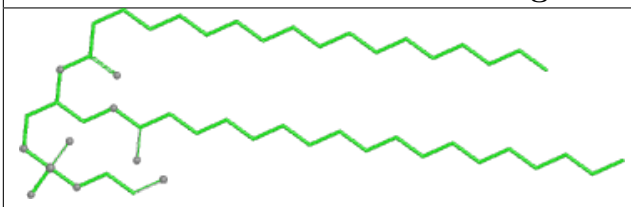


Torsions

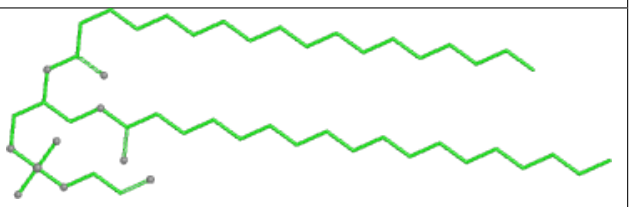


Rings

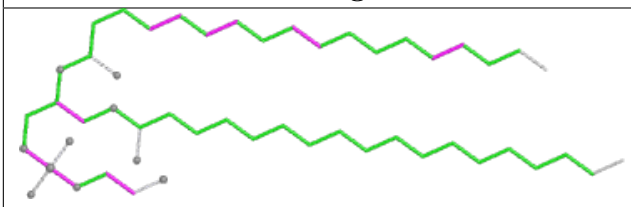
Ligand 3PE L 804



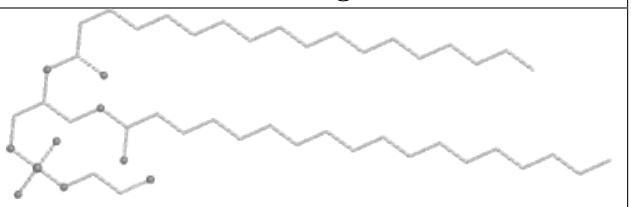
Bond lengths



Bond angles

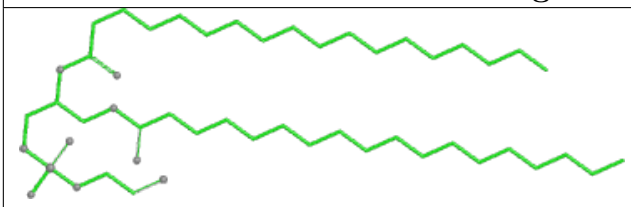


Torsions

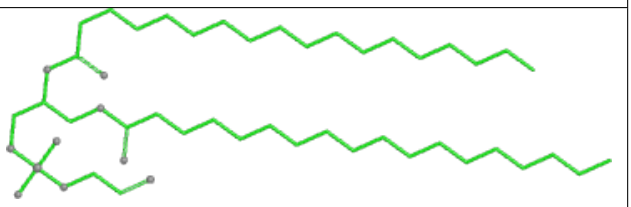


Rings

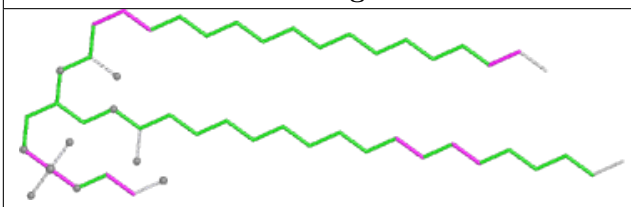
Ligand 3PE J 301



Bond lengths



Bond angles



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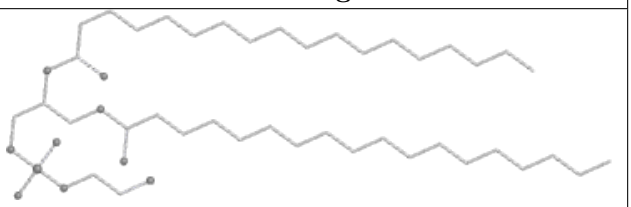
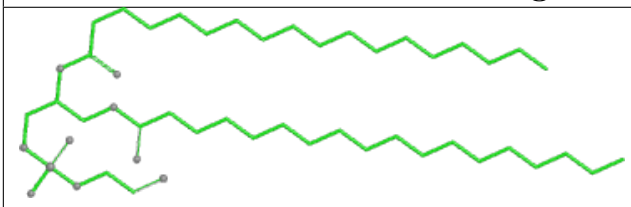
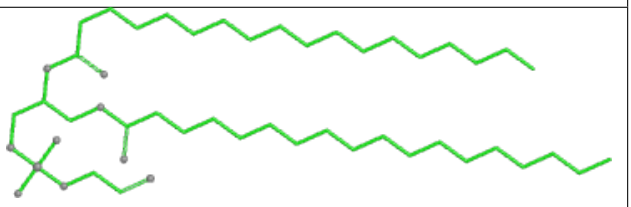


Rings

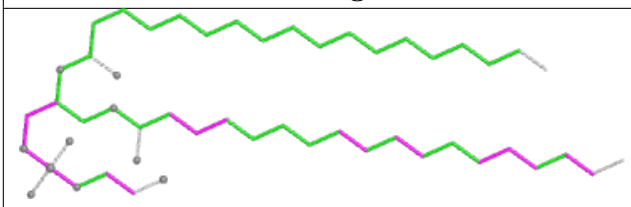
Ligand 3PE L 802



Bond lengths



Bond angles



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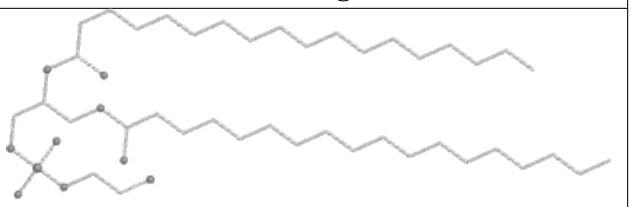
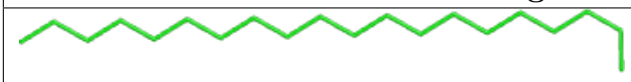
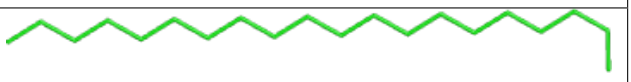
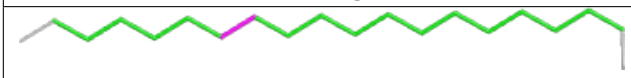
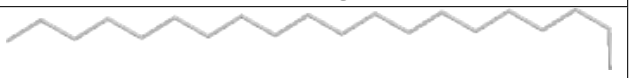
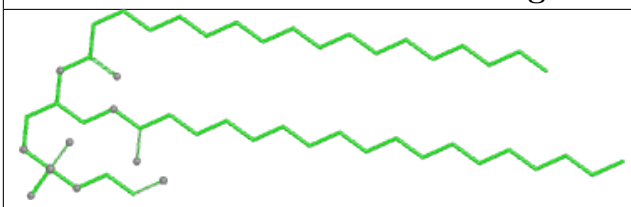
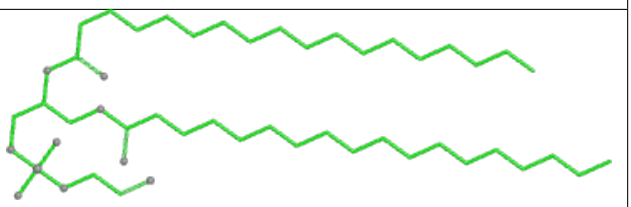
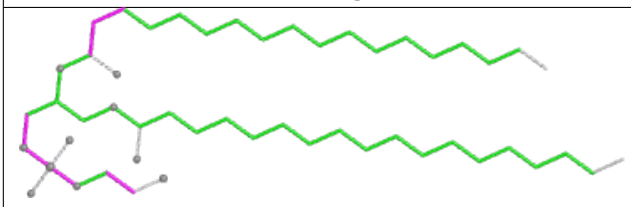
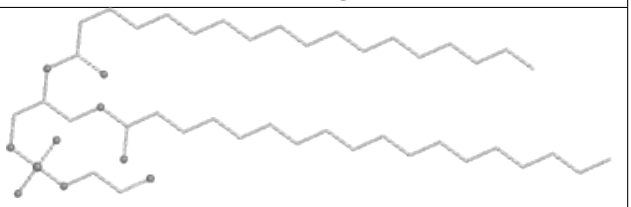
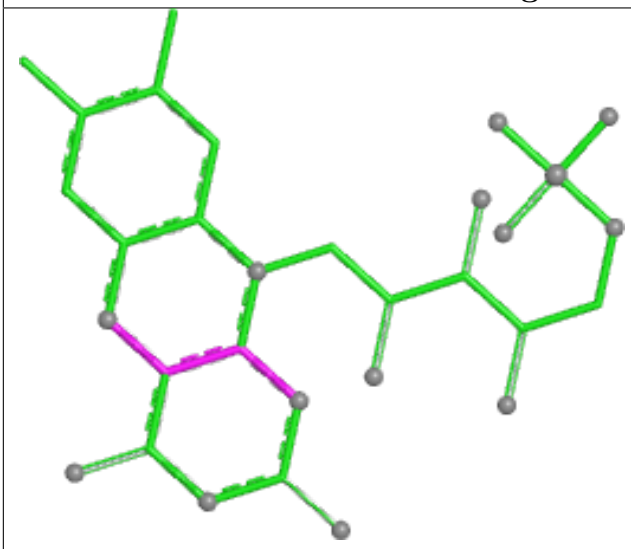
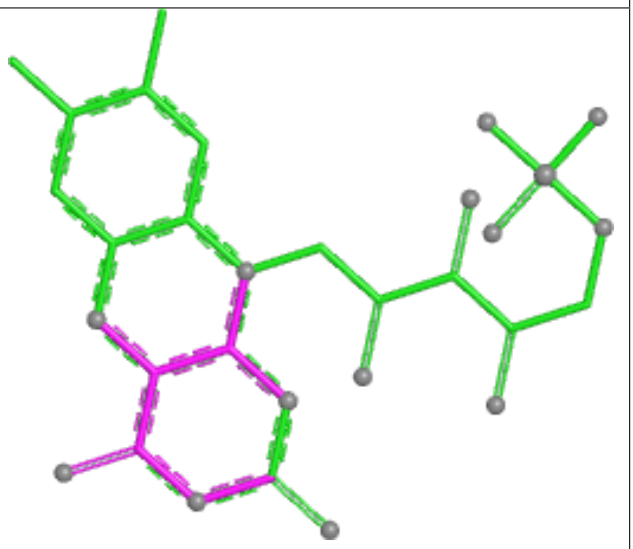
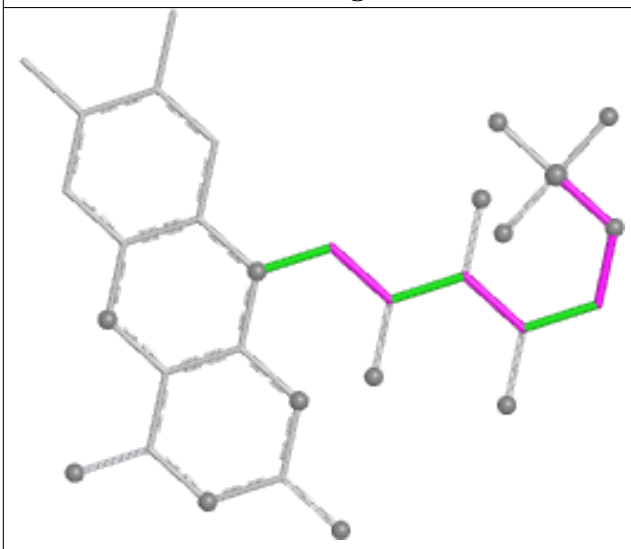
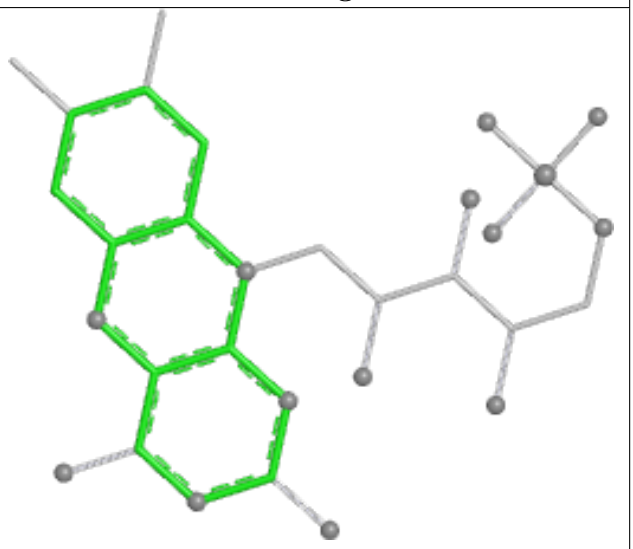


Rings

Ligand LFA A 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE A 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FMN F 502	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

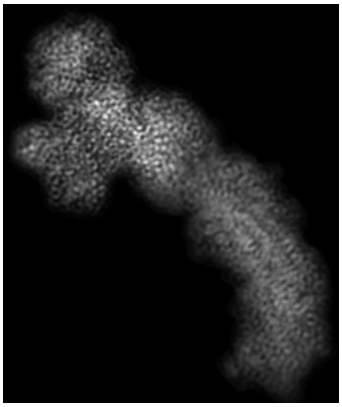
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14620. These allow visual inspection of the internal detail of the map and identification of artifacts.

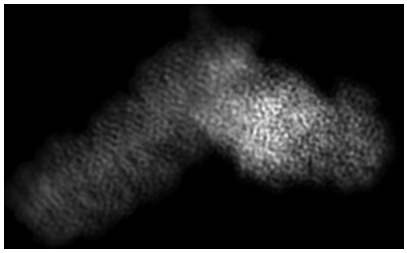
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

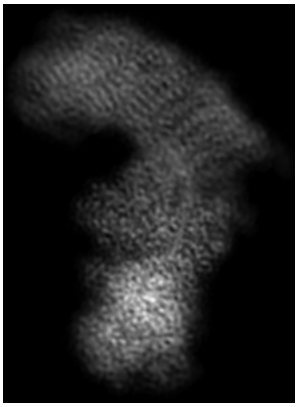
6.1.1 Primary map



X



Y

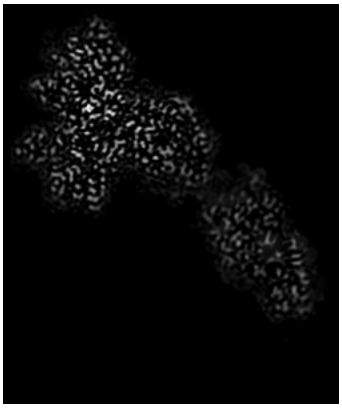


Z

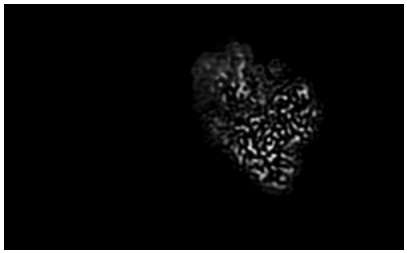
The images above show the map projected in three orthogonal directions.

6.2 Central slices

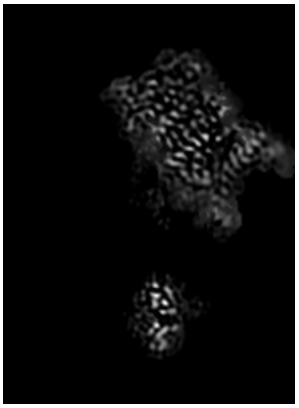
6.2.1 Primary map



X Index: 71



Y Index: 98

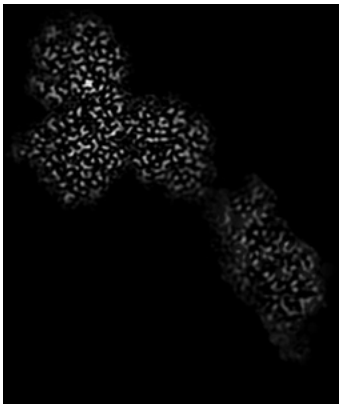


Z Index: 117

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

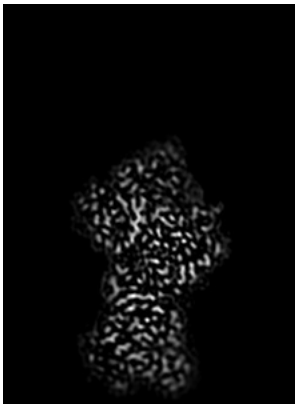
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 65

Y Index: 50



Z Index: 154

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

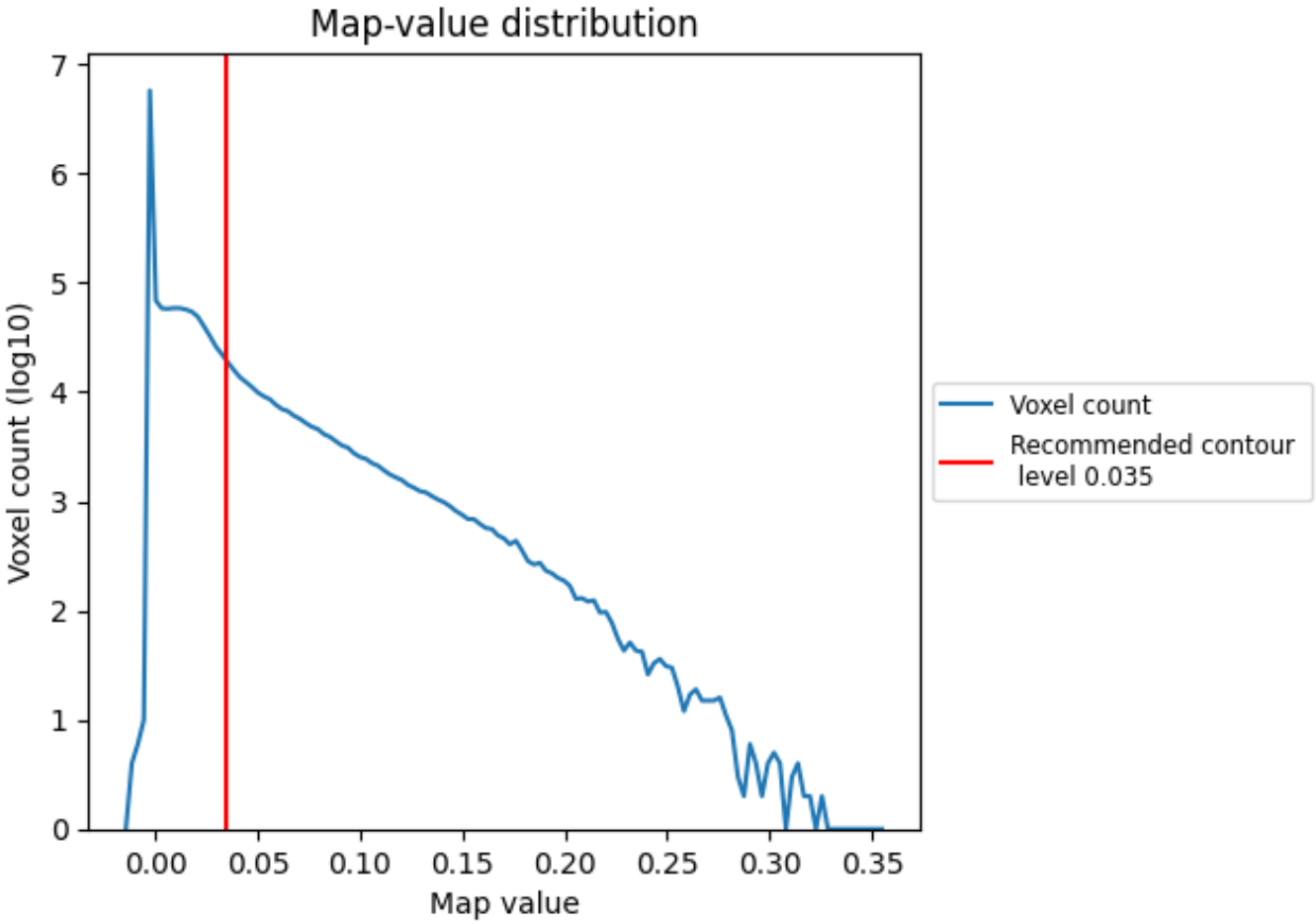
6.5 Mask visualisation (i)

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

7 Map analysis

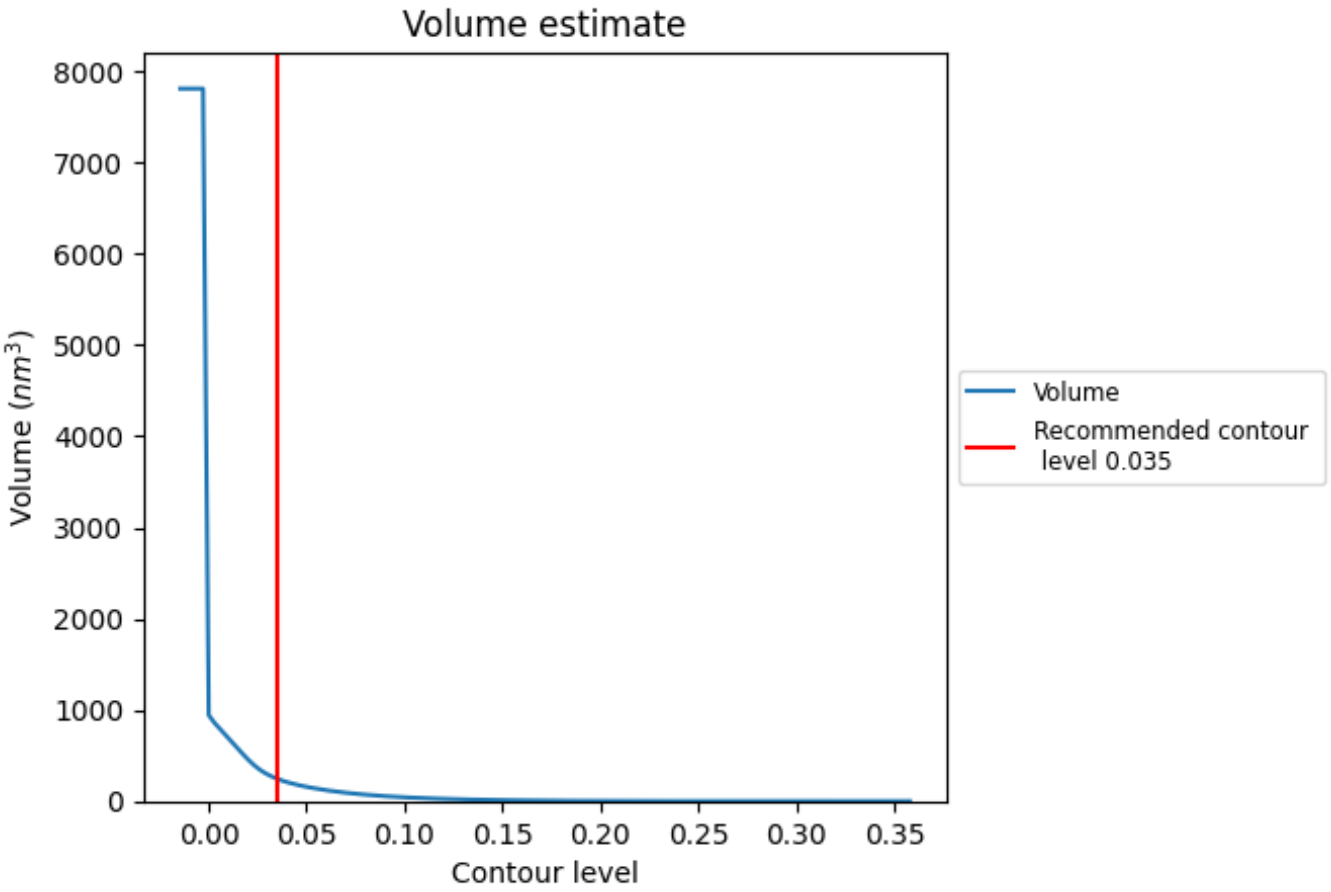
This section contains the results of statistical analysis of the map.

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 246 nm^3; this corresponds to an approximate mass of 222 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.

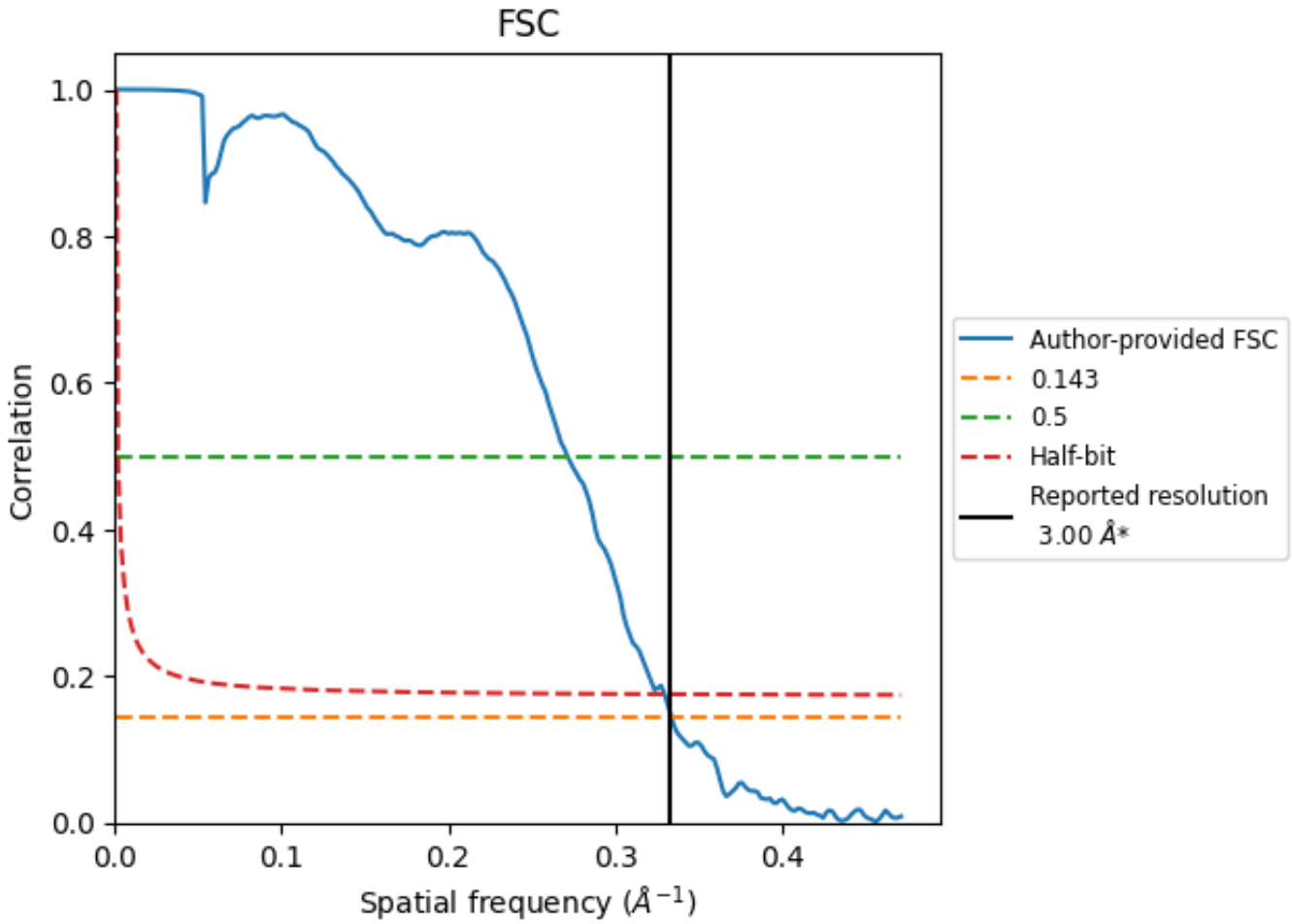
7.3 Rotationally averaged power spectrum

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

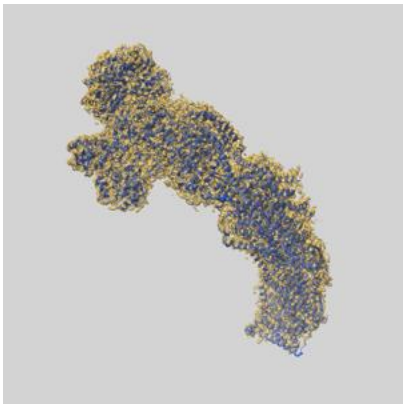
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.68	3.03
Unmasked-calculated*	-	-	-

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

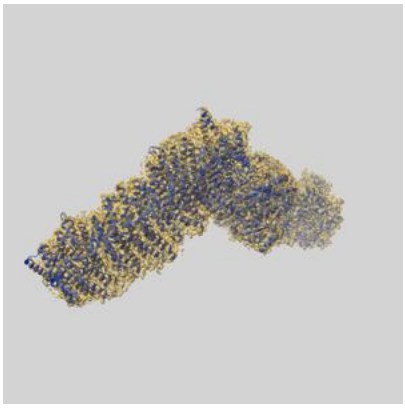
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14620 and PDB model 7ZC5. Per-residue inclusion information can be found in section 3 on page 10.

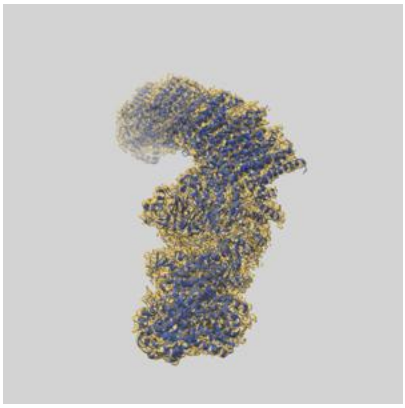
9.1 Map-model overlay



X



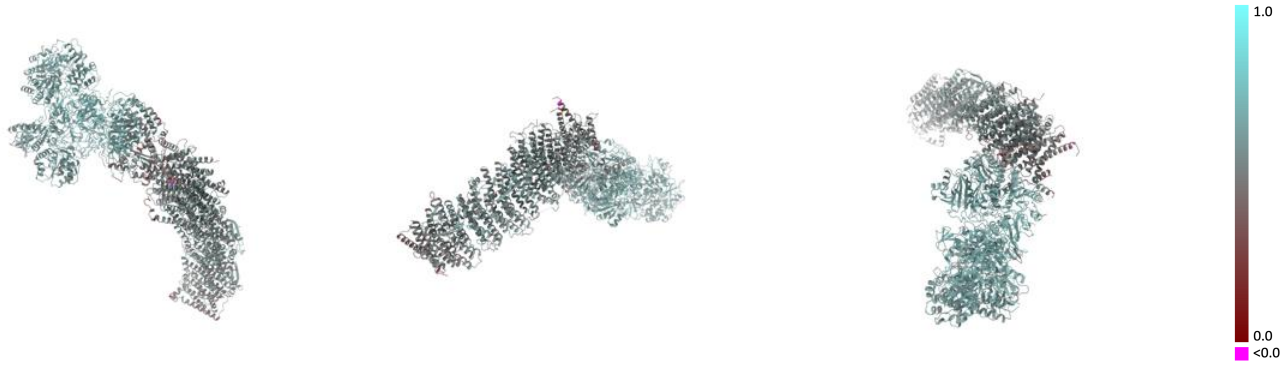
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

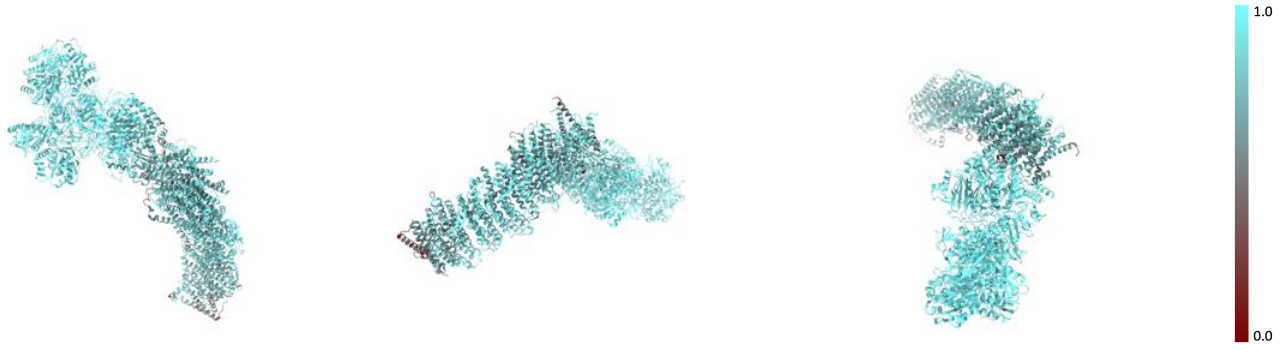
9.2 Q-score mapped to coordinate model (i)



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.

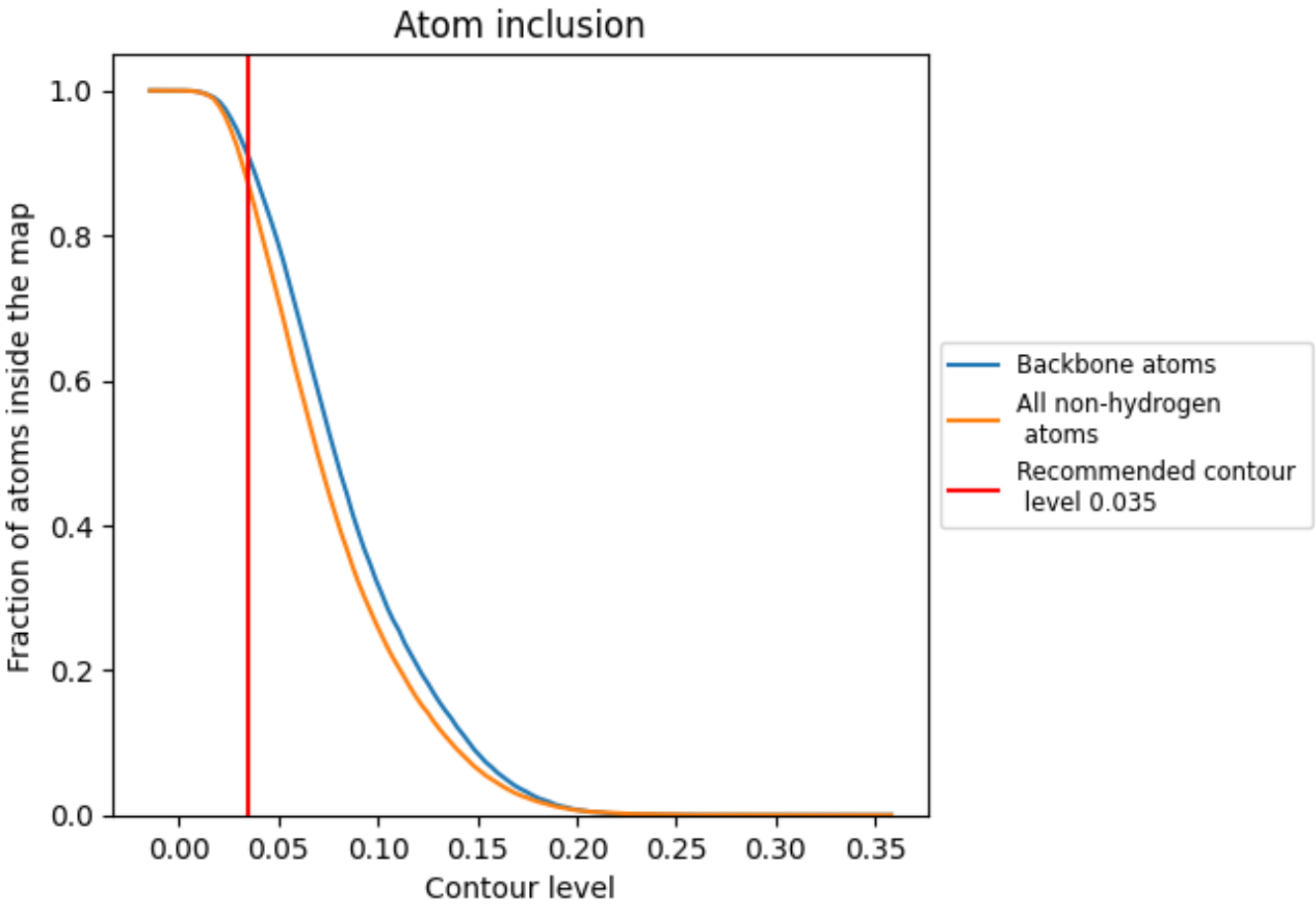
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 91% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8708	0.5710
A	0.7474	0.4900
B	0.9557	0.6010
C	0.9359	0.6150
E	0.9509	0.6160
F	0.9433	0.6150
G	0.9590	0.6360
H	0.7444	0.4720
I	0.9762	0.6630
J	0.7676	0.4880
K	0.8497	0.5290
L	0.7118	0.4980
M	0.8525	0.5420
N	0.8425	0.5390