Full wwPDB EM Validation Report

Aug 26, 2026 – 11:41 am BST

PDB ID	:	7P69 / pdb_00007p69
EMDB ID	:	EMD-13222
Title	:	Complex I from E. coli, DDM/LMNG-purified, under Turnover at pH 6, Resting state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2021-07-15
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 (i) 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 (1)) were used in the production of this report:

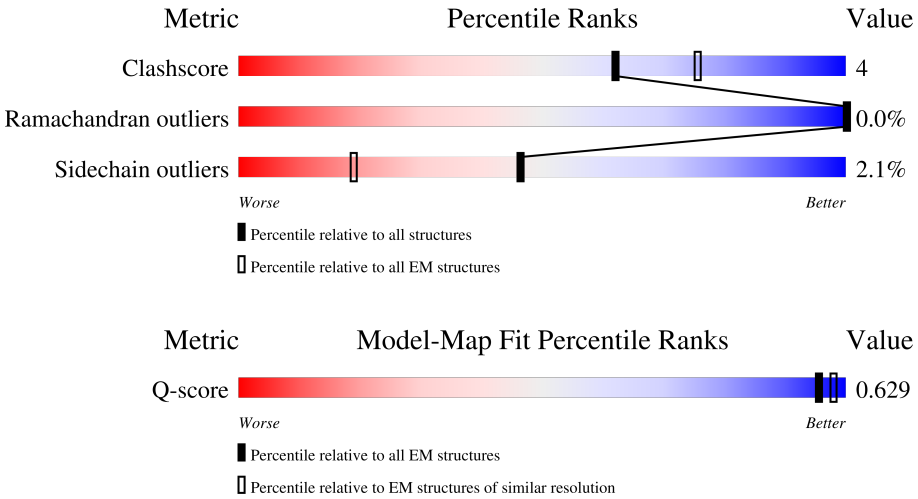
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	F	442	90% 10%
2	E	156	90% 10%
3	G	905	89% 10%
4	C	600	83% 12% 5%

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Mol	Chain	Length	Quality of chain
5	B	220	
6	I	145	
7	H	325	
8	A	147	
9	L	613	
10	M	504	
11	N	485	
12	K	100	
13	J	162	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 37577 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	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 Proton-translocating NADH-quinone oxidoreductase, chain 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		

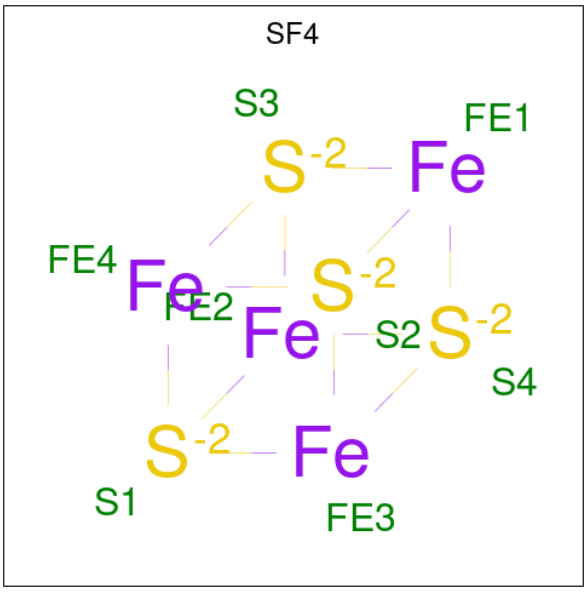
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

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.

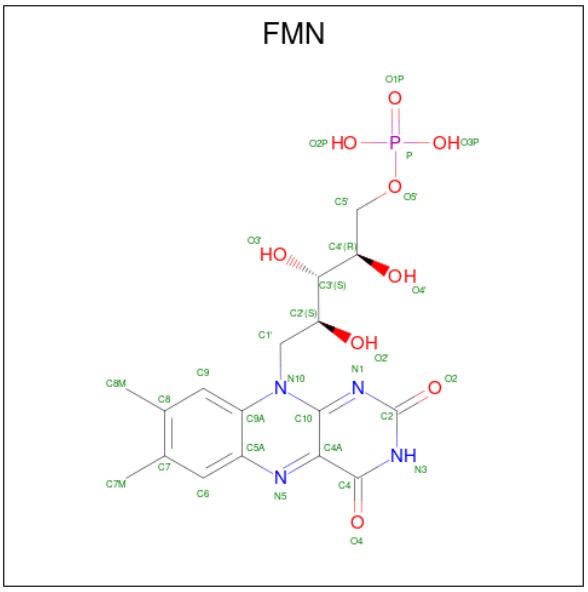
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	162	Total	C	N	O	S	0	0
			1226	824	188	207	7		

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



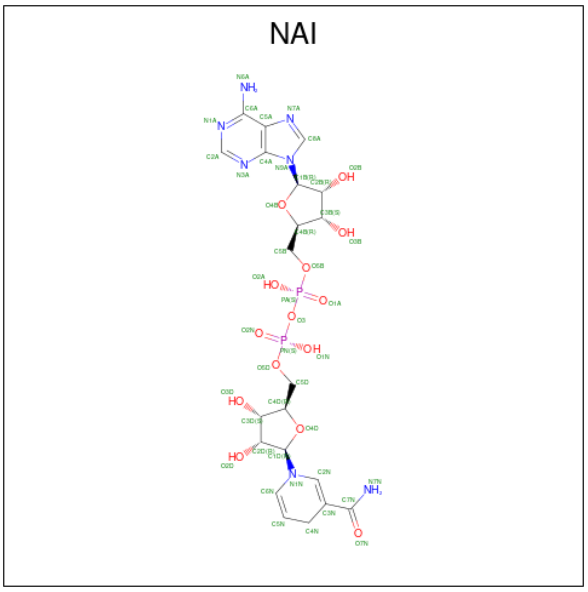
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 8 4 4	0
14	B	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 8 4 4	0

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



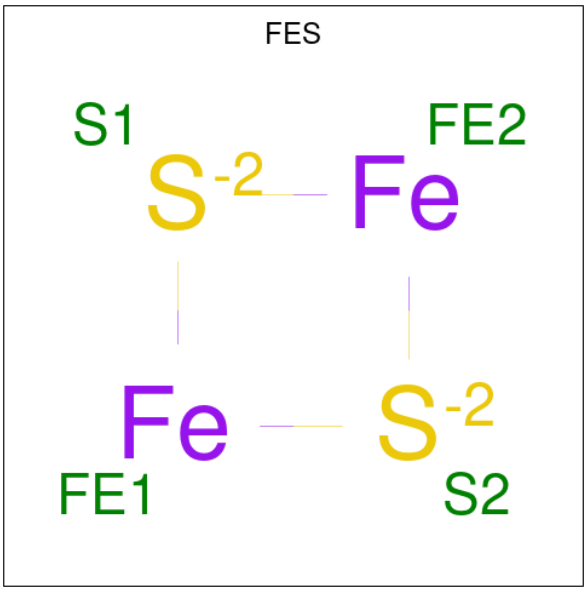
Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 16 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: 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 (CCD ID: FES) (formula: Fe_2S_2).

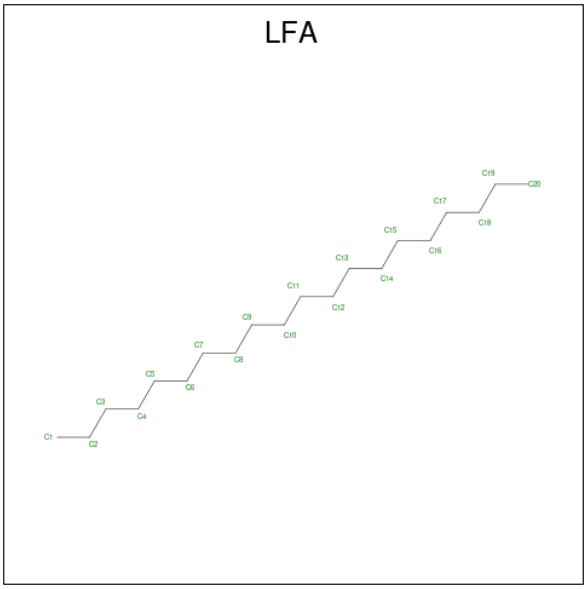


Mol	Chain	Residues	Atoms	AltConf
17	E	1	Total Fe S 4 2 2	0
17	G	1	Total Fe S 4 2 2	0

- Molecule 18 is CALCIUM ION (CCD ID: CA) (formula: Ca).

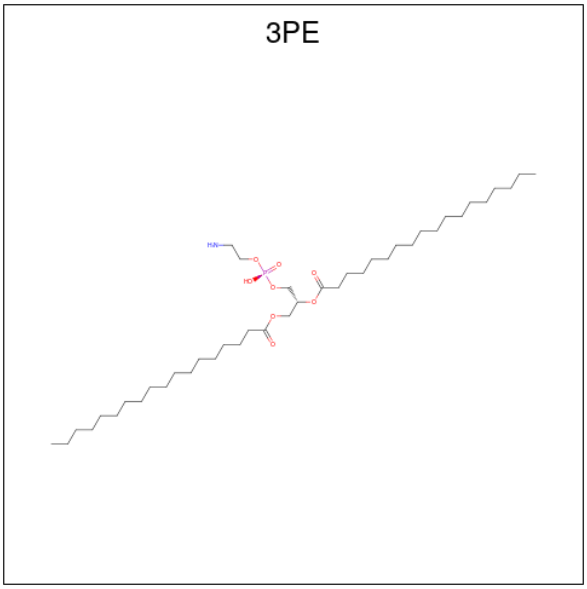
Mol	Chain	Residues	Atoms	AltConf
18	G	1	Total Ca 1 1	0

- Molecule 19 is EICOSANE (CCD ID: 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 15 15	0
19	L	1	Total C 20 20	0
19	N	1	Total C 20 20	0
19	N	1	Total C 20 20	0

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



Mol	Chain	Residues	Atoms	AltConf
20	H	1	Total C N O P 51 41 1 8 1	0
20	A	1	Total C N O P 34 24 1 8 1	0
20	A	1	Total C N O P 51 41 1 8 1	0
20	L	1	Total C N O P 51 41 1 8 1	0
20	L	1	Total C N O P 51 41 1 8 1	0

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Mol	Chain	Residues	Atoms					AltConf
20	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
20	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
20	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
20	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
20	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
20	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
20	N	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	F	27	Total	O	0
			27	27	
21	E	8	Total	O	0
			8	8	
21	G	231	Total	O	0
			231	231	
21	C	97	Total	O	0
			97	97	
21	B	12	Total	O	0
			12	12	
21	I	46	Total	O	0
			46	46	
21	H	10	Total	O	0
			10	10	
21	A	5	Total	O	0
			5	5	
21	L	32	Total	O	0
			32	32	
21	M	54	Total	O	0
			54	54	
21	N	32	Total	O	0
			32	32	
21	K	15	Total	O	0
			15	15	

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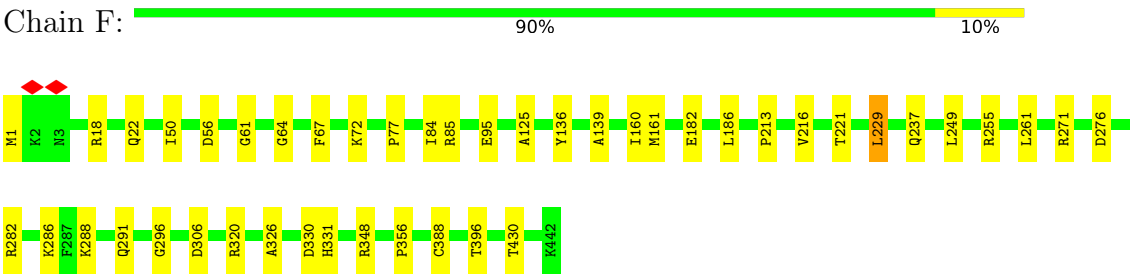
Mol	Chain	Residues	Atoms		AltConf
21	J	12	Total	O	0
			12	12	

3 Residue-property plots (i)

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

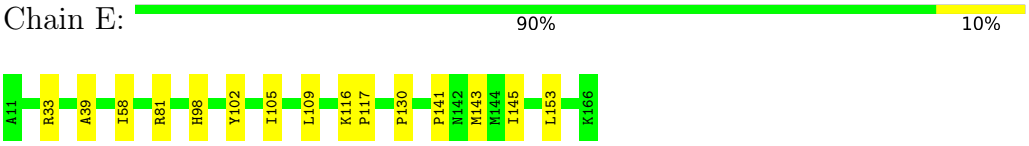
• Molecule 1: NADH-quinone oxidoreductase subunit F

Chain F:



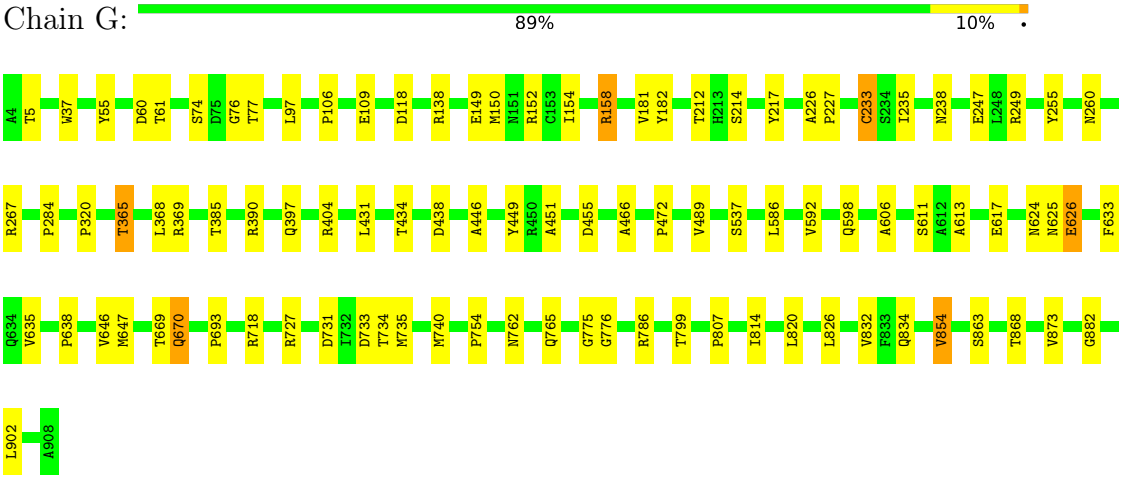
• Molecule 2: NADH dehydrogenase I subunit E

Chain E:



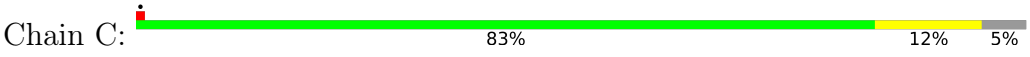
• Molecule 3: NADH-quinone oxidoreductase

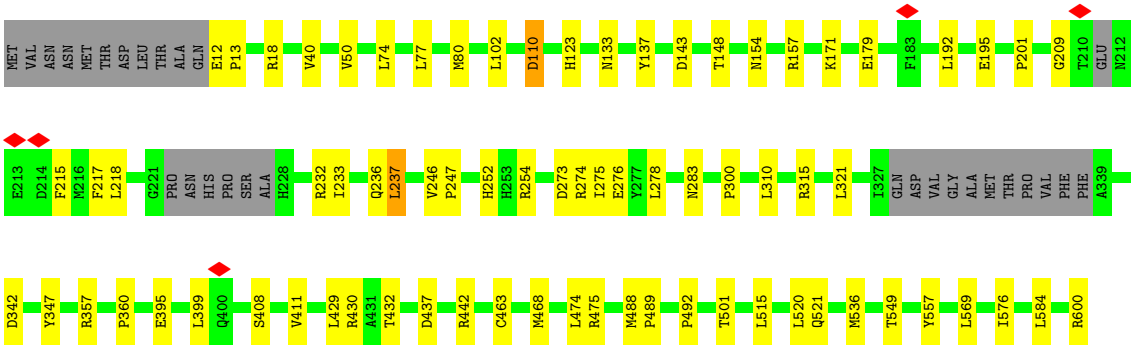
Chain G:



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

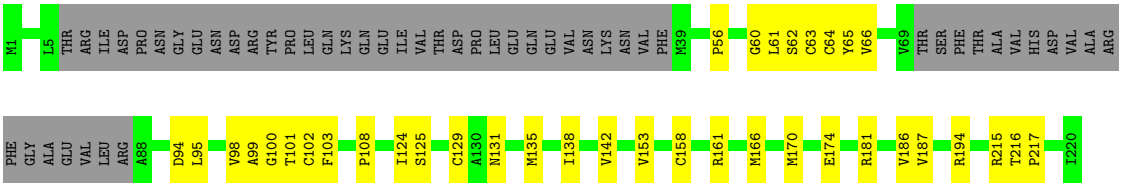
Chain C:



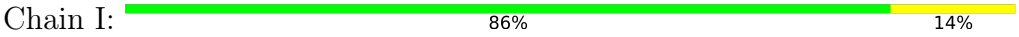


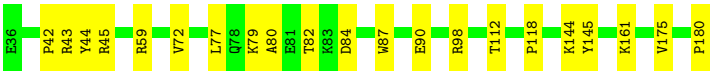
• Molecule 5: NADH-quinone oxidoreductase subunit B



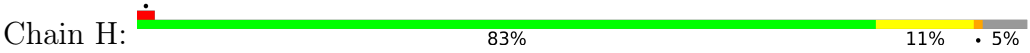


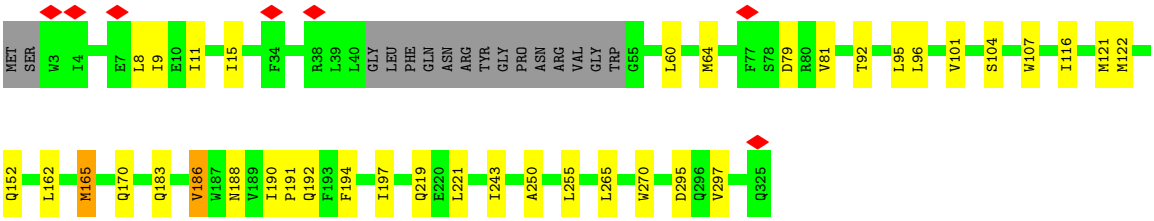
• Molecule 6: NADH-quinone oxidoreductase subunit I





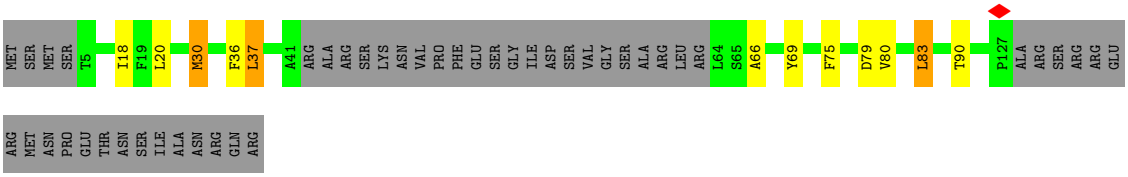
• Molecule 7: NADH-quinone oxidoreductase subunit H





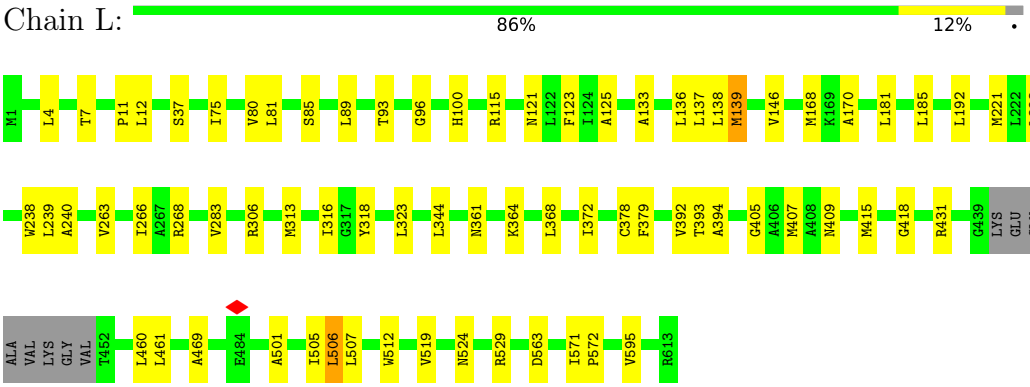
• Molecule 8: NADH-quinone oxidoreductase subunit A





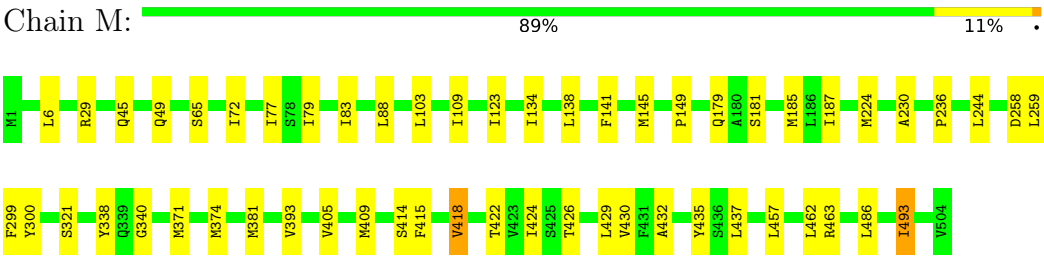
• Molecule 9: Proton-translocating NADH-quinone oxidoreductase, chain L

Chain L:



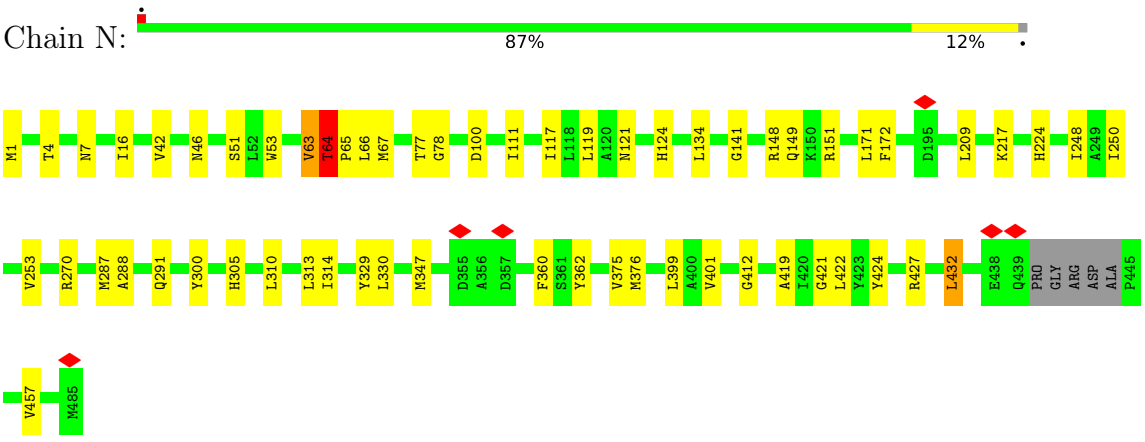
• Molecule 10: NADH dehydrogenase I subunit M

Chain M:



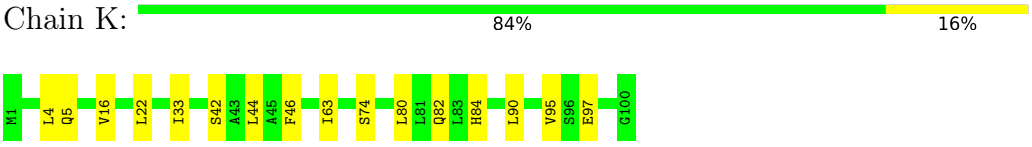
• Molecule 11: NADH-quinone oxidoreductase subunit N

Chain N:



• Molecule 12: NADH-quinone oxidoreductase subunit K

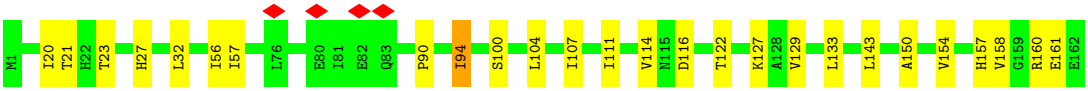
Chain K:



• Molecule 13: NADH-quinone oxidoreductase subunit J

Chain J:




M1
I20
T21
H22
T23
H27
L32
I56
I57
L76
E80
I81
E82
Q83
P90
I94
S100
L104
I107
I111
V114
N115
D116
T122
K127
A128
V129
L133
L143
A150
V154
H157
V158
G159
R160
E161
E162

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	92922	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	0.532	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	154.5, 205.0, 247.5	wwPDB
Map dimensions	495, 410, 309	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.21	0/3511	0.37	0/4745
2	E	0.21	0/1248	0.38	0/1691
3	G	0.27	0/7173	0.39	0/9726
4	C	0.25	0/4719	0.39	0/6400
5	B	0.22	0/1367	0.36	0/1847
6	I	0.28	0/1176	0.41	0/1590
7	H	0.24	0/2492	0.38	0/3391
8	A	0.22	0/821	0.38	0/1119
9	L	0.21	0/4713	0.39	0/6423
10	M	0.26	0/4074	0.42	0/5546
11	N	0.26	0/3724	0.45	1/5081 (0.0%)
12	K	0.22	0/769	0.35	0/1040
13	J	0.22	0/1252	0.41	0/1708
All	All	0.24	0/37039	0.40	1/50307 (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
3	G	0	1
11	N	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	64	THR	N-CA-C	-5.75	97.10	109.81

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	260	ASN	Peptide
11	N	63	VAL	Peptide
11	N	64	THR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3432	0	3405	28	0
2	E	1220	0	1187	10	0
3	G	7022	0	6824	50	0
4	C	4597	0	4506	45	0
5	B	1339	0	1330	25	0
6	I	1149	0	1114	16	0
7	H	2422	0	2469	25	0
8	A	796	0	804	10	0
9	L	4595	0	4736	41	0
10	M	3953	0	4053	29	0
11	N	3635	0	3802	39	0
12	K	760	0	817	13	0
13	J	1226	0	1297	20	0
14	B	8	0	0	1	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	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	0	0
19	L	35	0	71	0	0
19	N	40	0	84	2	0
20	A	85	0	124	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	H	51	0	82	4	0
20	L	306	0	492	9	0
20	M	102	0	164	4	0
20	N	51	0	82	2	0
21	A	5	0	0	0	0
21	B	12	0	0	0	0
21	C	97	0	0	1	0
21	E	8	0	0	1	0
21	F	27	0	0	0	0
21	G	231	0	0	1	0
21	H	10	0	0	0	0
21	I	46	0	0	2	0
21	J	12	0	0	0	0
21	K	15	0	0	0	0
21	L	32	0	0	1	0
21	M	54	0	0	0	0
21	N	32	0	0	0	0
All	All	37577	0	37573	321	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (321) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:64:THR:HB	11:N:66:LEU:H	1.46	0.80
11:N:63:VAL:O	11:N:67:MET:HB2	1.90	0.72
7:H:170:GLN:HE22	7:H:191:PRO:HB2	1.58	0.69
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.75	0.69
10:M:181:SER:HB2	10:M:230:ALA:HA	1.76	0.68
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.76	0.68
1:F:85:ARG:HG2	1:F:213:PRO:HG2	1.79	0.65
7:H:152:GLN:HE21	7:H:297:VAL:HG11	1.62	0.65
3:G:434:THR:HG23	3:G:449:TYR:HB3	1.77	0.65
7:H:64:MET:HE1	8:A:30:MET:HE3	1.81	0.63
7:H:121:MET:HE3	13:J:56:ILE:HD12	1.79	0.63
11:N:134:LEU:HD11	13:J:143:LEU:HB3	1.79	0.63
1:F:95:GLU:HB2	16:F:503:NAI:H42N	1.81	0.62
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.79	0.62
20:M:702:3PE:H3C1	20:M:702:3PE:H2C2	1.81	0.62
3:G:150:MET:HE2	3:G:182:TYR:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:MET:HB2	2:E:153:LEU:HD11	1.82	0.62
20:L:701:3PE:H2G2	20:M:701:3PE:H3D2	1.81	0.61
7:H:121:MET:HG2	13:J:56:ILE:HB	1.82	0.61
12:K:16:VAL:HG13	13:J:100:SER:HB3	1.82	0.61
2:E:141:PRO:HG2	2:E:153:LEU:HB2	1.82	0.60
1:F:56:ASP:O	1:F:237:GLN:NE2	2.35	0.60
4:C:360:PRO:O	6:I:45:ARG:NH1	2.33	0.60
4:C:408:SER:HB2	4:C:463:CYS:HB2	1.84	0.60
1:F:348:ARG:HD2	6:I:180:PRO:HB2	1.84	0.59
11:N:117:ILE:O	11:N:121:ASN:ND2	2.35	0.59
11:N:100:ASP:OD2	11:N:148:ARG:NH1	2.35	0.59
3:G:118:ASP:OD1	3:G:762:ASN:ND2	2.36	0.59
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.85	0.59
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.72	0.59
9:L:85:SER:OG	9:L:268:ARG:NH2	2.36	0.58
1:F:85:ARG:HB2	1:F:125:ALA:HA	1.85	0.58
5:B:124:ILE:HG12	5:B:153:VAL:HB	1.85	0.58
11:N:305:HIS:ND1	11:N:329:TYR:OH	2.35	0.58
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.84	0.58
11:N:42:VAL:O	11:N:46:ASN:ND2	2.38	0.57
4:C:110:ASP:OD2	4:C:442:ARG:NH1	2.37	0.57
4:C:488:MET:HE3	4:C:489:PRO:HD2	1.87	0.57
7:H:96:LEU:HD22	8:A:20:LEU:HD23	1.86	0.57
7:H:219:GLN:HG2	7:H:221:LEU:H	1.70	0.57
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.86	0.57
10:M:45:GLN:NE2	10:M:49:GLN:OE1	2.38	0.57
3:G:765:GLN:NE2	21:G:1116:HOH:O	2.37	0.57
4:C:576:ILE:HD13	4:C:584:LEU:HD13	1.87	0.57
11:N:151:ARG:NH1	12:K:97:GLU:OE2	2.38	0.57
10:M:187:ILE:HD11	11:N:399:LEU:HD22	1.87	0.56
13:J:20:ILE:HG13	13:J:21:THR:HG23	1.88	0.56
3:G:472:PRO:HG3	3:G:799:THR:HA	1.87	0.56
1:F:288:LYS:HD2	1:F:331:HIS:HA	1.88	0.55
9:L:240:ALA:O	9:L:306:ARG:NH1	2.40	0.55
11:N:78:GLY:HA3	20:N:902:3PE:H392	1.88	0.55
5:B:101:THR:HA	5:B:129:CYS:HB3	1.89	0.55
9:L:263:VAL:HG13	9:L:323:LEU:HD11	1.89	0.55
4:C:80:MET:HE1	4:C:549:THR:HG21	1.89	0.55
5:B:186:VAL:HG23	5:B:187:VAL:HG23	1.89	0.55
1:F:320:ARG:NH1	16:F:503:NAI:O2D	2.38	0.55
4:C:254:ARG:HG3	5:B:103:PHE:HE1	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:706:3PE:H2B1	20:L:706:3PE:H3A2	1.89	0.55
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.88	0.55
3:G:669:THR:OG1	3:G:670:GLN:N	2.39	0.55
3:G:365:THR:O	3:G:786:ARG:NH2	2.39	0.55
9:L:239:LEU:HD23	9:L:313:MET:HG3	1.89	0.55
10:M:103:LEU:O	10:M:463:ARG:NH1	2.40	0.55
20:H:602:3PE:H341	20:A:203:3PE:H321	1.88	0.54
4:C:195:GLU:OE1	4:C:232:ARG:NH1	2.39	0.54
7:H:121:MET:HG3	13:J:57:ILE:HG13	1.89	0.54
10:M:258:ASP:HA	10:M:262:ILE:HG13	1.89	0.54
4:C:254:ARG:NH2	5:B:62:SER:OG	2.41	0.54
9:L:136:LEU:HD12	9:L:139:MET:HE2	1.90	0.54
9:L:139:MET:HE1	9:L:181:LEU:HD21	1.89	0.54
4:C:218:LEU:HD23	4:C:237:LEU:HD13	1.91	0.53
7:H:170:GLN:OE1	7:H:188:ASN:ND2	2.41	0.53
4:C:399:LEU:HD22	4:C:468:MET:HG2	1.89	0.53
10:M:141:PHE:O	10:M:145:MET:HB2	2.08	0.53
4:C:276:GLU:O	4:C:283:ASN:ND2	2.36	0.53
6:I:161:LYS:NZ	21:I:303:HOH:O	2.42	0.53
20:L:702:3PE:H322	20:L:702:3PE:H262	1.89	0.53
3:G:613:ALA:HB1	3:G:617:GLU:HB2	1.89	0.53
9:L:524:ASN:O	9:L:529:ARG:NH1	2.42	0.53
9:L:378:CYS:HA	9:L:461:LEU:HD21	1.89	0.53
4:C:13:PRO:O	4:C:18:ARG:NH2	2.40	0.53
6:I:80:ALA:HB2	6:I:90:GLU:HB2	1.90	0.53
4:C:278:LEU:HD21	4:C:321:LEU:HD23	1.90	0.52
6:I:59:ARG:NH1	6:I:112:THR:OG1	2.43	0.52
11:N:1:MET:HG2	11:N:65:PRO:HD3	1.91	0.52
11:N:291:GLN:O	11:N:427:ARG:NH2	2.41	0.52
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.92	0.52
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.90	0.52
4:C:110:ASP:OD1	4:C:110:ASP:N	2.42	0.52
11:N:412:GLY:HA3	19:N:903:LFA:H81	1.91	0.52
7:H:95:LEU:HD12	7:H:243:ILE:HG21	1.91	0.52
4:C:77:LEU:HB3	4:C:137:TYR:HB3	1.92	0.52
3:G:138:ARG:NH2	21:I:301:HOH:O	2.44	0.51
8:A:90:THR:O	13:J:127:LYS:NZ	2.38	0.51
4:C:143:ASP:OD1	4:C:157:ARG:NH1	2.42	0.51
6:I:59:ARG:NH2	6:I:145:TYR:O	2.40	0.51
8:A:69:TYR:OH	12:K:74:SER:O	2.28	0.51
11:N:347:MET:HB2	11:N:360:PHE:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:338:TYR:HB3	10:M:493:ILE:HD12	1.93	0.51
12:K:84:HIS:HB2	12:K:90:LEU:HD21	1.93	0.51
4:C:201:PRO:HG2	4:C:209:GLY:HA3	1.93	0.51
7:H:79:ASP:OD2	13:J:27:HIS:NE2	2.43	0.51
7:H:162:LEU:HA	7:H:165:MET:HB2	1.93	0.51
10:M:236:PRO:HG3	10:M:244:LEU:HD22	1.92	0.51
4:C:395:GLU:OE2	4:C:475:ARG:NH1	2.39	0.51
12:K:5:GLN:NE2	13:J:114:VAL:O	2.44	0.51
3:G:727:ARG:HD3	4:C:179:GLU:HB2	1.93	0.51
9:L:571:ILE:HG13	9:L:572:PRO:HD3	1.92	0.51
3:G:369:ARG:NH2	3:G:775:GLY:O	2.38	0.50
4:C:357:ARG:HH21	5:B:161:ARG:HH22	1.57	0.50
11:N:4:THR:HG23	11:N:7:ASN:H	1.76	0.50
3:G:397:GLN:O	3:G:404:ARG:NH2	2.41	0.50
10:M:29:ARG:HD3	10:M:109:ILE:HD11	1.92	0.50
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.93	0.50
11:N:419:ALA:HA	11:N:422:LEU:HD12	1.93	0.50
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.94	0.49
3:G:814:ILE:HD11	3:G:902:LEU:HD13	1.94	0.49
5:B:61:LEU:HB3	5:B:100:GLY:HA3	1.93	0.49
13:J:157:HIS:O	13:J:160:ARG:NH1	2.45	0.49
3:G:807:PRO:HB3	3:G:882:GLY:HA3	1.93	0.49
6:I:82:THR:OG1	6:I:84:ASP:OD1	2.26	0.49
8:A:80:VAL:HA	8:A:83:LEU:HD23	1.94	0.49
1:F:50:ILE:HG23	1:F:229:LEU:HD21	1.94	0.49
10:M:185:MET:HB2	10:M:230:ALA:HB2	1.94	0.49
13:J:90:PRO:O	13:J:94:ILE:HB	2.13	0.49
5:B:64:CYS:HB3	5:B:99:ALA:HB1	1.95	0.49
10:M:65:SER:HB3	10:M:83:ILE:HG22	1.95	0.49
10:M:414:SER:O	10:M:418:VAL:N	2.38	0.49
11:N:171:LEU:HD23	12:K:42:SER:HB2	1.94	0.49
3:G:74:SER:O	3:G:77:THR:OG1	2.28	0.49
7:H:95:LEU:HD12	7:H:243:ILE:HD13	1.95	0.49
20:H:602:3PE:N	20:A:203:3PE:O14	2.43	0.49
20:L:706:3PE:H3A2	20:L:706:3PE:H2E2	1.95	0.49
11:N:310:LEU:HD12	11:N:313:LEU:HD23	1.95	0.48
3:G:320:PRO:HB2	3:G:537:SER:HB3	1.94	0.48
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.95	0.48
7:H:295:ASP:OD1	7:H:295:ASP:N	2.46	0.48
3:G:247:GLU:HG3	3:G:249:ARG:HE	1.78	0.48
3:G:598:GLN:HG3	3:G:826:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:217:PRO:HG3	6:I:144:LYS:HD2	1.96	0.48
5:B:166:MET:HE3	5:B:170:MET:HE2	1.96	0.48
20:H:602:3PE:H3B1	20:A:203:3PE:H3B2	1.95	0.48
9:L:405:GLY:O	9:L:409:ASN:ND2	2.40	0.48
1:F:77:PRO:O	1:F:85:ARG:NH2	2.44	0.48
12:K:33:ILE:HG23	13:J:32:LEU:HD22	1.96	0.48
2:E:109:LEU:HD11	2:E:143:MET:HE2	1.96	0.47
3:G:670:GLN:HE21	3:G:733:ASP:HA	1.78	0.47
20:M:702:3PE:H351	19:N:903:LFA:H171	1.96	0.47
11:N:376:MET:HB3	11:N:432:LEU:HD21	1.96	0.47
2:E:117:PRO:HB3	2:E:130:PRO:HD3	1.96	0.47
1:F:1:MET:N	1:F:276:ASP:O	2.43	0.47
3:G:611:SER:OG	3:G:646:VAL:O	2.31	0.47
9:L:318:TYR:OH	9:L:418:GLY:O	2.27	0.47
9:L:392:VAL:HG23	9:L:393:THR:HG23	1.97	0.47
1:F:72:LYS:NZ	1:F:216:VAL:O	2.42	0.47
9:L:168:MET:HG3	10:M:437:LEU:HD23	1.97	0.47
9:L:563:ASP:OD1	10:M:300:TYR:OH	2.22	0.47
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.49	0.47
12:K:80:LEU:HD11	12:K:90:LEU:HD13	1.96	0.47
3:G:731:ASP:OD2	3:G:734:THR:OG1	2.26	0.47
10:M:371:MET:HA	10:M:374:MET:HG2	1.96	0.47
11:N:53:TRP:HA	20:N:902:3PE:H242	1.97	0.47
4:C:12:GLU:HG2	4:C:18:ARG:HH12	1.80	0.47
4:C:133:ASN:OD1	4:C:133:ASN:N	2.46	0.47
4:C:429:LEU:O	4:C:432:THR:OG1	2.30	0.47
3:G:267:ARG:HB2	3:G:820:LEU:HG	1.96	0.46
4:C:217:PHE:HE1	4:C:236:GLN:HE21	1.63	0.46
9:L:37:SER:OG	9:L:121:ASN:OD1	2.28	0.46
10:M:123:ILE:HG13	10:M:149:PRO:HB2	1.96	0.46
10:M:409:MET:HE1	10:M:486:LEU:HD21	1.96	0.46
11:N:421:GLY:HA2	11:N:424:TYR:CE2	2.50	0.46
5:B:215:ARG:HB2	6:I:42:PRO:HB3	1.97	0.46
3:G:37:TRP:O	3:G:158:ARG:NH1	2.49	0.46
9:L:75:ILE:HG21	9:L:137:LEU:HD23	1.97	0.46
10:M:72:ILE:HB	10:M:77:ILE:HB	1.98	0.46
11:N:64:THR:HG22	11:N:65:PRO:HD2	1.97	0.46
4:C:315:ARG:NH2	21:C:713:HOH:O	2.49	0.46
5:B:125:SER:OG	5:B:131:ASN:OD1	2.33	0.46
3:G:431:LEU:O	3:G:446:ALA:N	2.49	0.46
8:A:75:PHE:O	8:A:79:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:375:VAL:HG11	11:N:457:VAL:HB	1.98	0.46
10:M:224:MET:HE3	10:M:224:MET:HB3	1.81	0.46
2:E:116:LYS:HA	2:E:116:LYS:HD3	1.81	0.45
3:G:255:TYR:OH	3:G:776:GLY:O	2.32	0.45
3:G:212:THR:HG22	3:G:832:VAL:HG21	1.99	0.45
12:K:16:VAL:HG21	13:J:104:LEU:HB2	1.99	0.45
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.98	0.45
4:C:123:HIS:HA	4:C:148:THR:O	2.16	0.45
8:A:66:ALA:HB3	13:J:161:GLU:HB2	1.98	0.45
1:F:61:GLY:N	1:F:67:PHE:O	2.50	0.45
9:L:4:LEU:O	9:L:7:THR:OG1	2.30	0.45
20:L:704:3PE:H2G2	20:L:708:3PE:H2C1	1.99	0.45
6:I:44:TYR:HD2	6:I:118:PRO:HA	1.80	0.45
9:L:96:GLY:O	9:L:100:HIS:ND1	2.45	0.45
9:L:230:SER:HB3	9:L:316:ILE:HG21	1.99	0.45
10:M:405:VAL:HG12	10:M:409:MET:HE2	1.98	0.45
12:K:82:GLN:NE2	13:J:158:VAL:O	2.49	0.45
1:F:249:LEU:HD13	1:F:261:LEU:HD21	1.99	0.45
9:L:115:ARG:NH1	21:L:807:HOH:O	2.49	0.45
11:N:360:PHE:CE2	11:N:362:TYR:HB3	2.52	0.44
5:B:135:MET:HA	6:I:72:VAL:HG13	1.99	0.44
1:F:64:GLY:HA3	16:F:503:NAI:H1D	1.98	0.44
3:G:55:TYR:HB3	3:G:60:ASP:HB3	1.99	0.44
5:B:94:ASP:OD1	5:B:94:ASP:N	2.50	0.44
1:F:160:ILE:HG22	1:F:161:MET:HG3	1.99	0.44
20:L:701:3PE:H262	20:L:701:3PE:H321	1.99	0.44
20:M:701:3PE:H322	20:M:702:3PE:H392	2.00	0.44
1:F:291:GLN:O	1:F:326:ALA:HA	2.17	0.44
4:C:192:LEU:HD12	5:B:108:PRO:HB2	1.99	0.44
3:G:97:LEU:HD22	3:G:154:ILE:HB	2.00	0.44
3:G:624:ASN:OD1	3:G:625:ASN:N	2.51	0.44
4:C:357:ARG:HE	5:B:161:ARG:HH12	1.66	0.44
12:K:4:LEU:N	13:J:116:ASP:OD2	2.49	0.44
5:B:56:PRO:HB3	5:B:95:LEU:HD23	2.00	0.44
4:C:501:THR:HG23	4:C:521:GLN:HB3	1.99	0.44
4:C:233:ILE:HA	4:C:247:PRO:HA	1.99	0.43
8:A:36:PHE:HD2	8:A:37:LEU:HD22	1.82	0.43
9:L:221:MET:HE1	20:L:708:3PE:H3B1	1.99	0.43
9:L:361:ASN:HB3	9:L:364:LYS:HG2	2.00	0.43
2:E:98:HIS:HA	2:E:102:TYR:HD1	1.83	0.43
3:G:466:ALA:HB3	3:G:489:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:863:SER:HB3	3:G:868:THR:HG22	2.01	0.43
1:F:271:ARG:NE	1:F:306:ASP:OD1	2.43	0.43
2:E:81:ARG:HD2	2:E:81:ARG:HA	1.81	0.43
3:G:149:GLU:HG2	3:G:152:ARG:CZ	2.49	0.43
3:G:227:PRO:HD3	3:G:754:PRO:HB3	2.00	0.43
3:G:854:VAL:HG11	3:G:873:VAL:HG21	2.00	0.43
3:G:106:PRO:HD3	4:C:515:LEU:HD21	2.01	0.43
3:G:284:PRO:HD3	3:G:646:VAL:HB	2.01	0.43
5:B:217:PRO:HD3	6:I:144:LYS:HB3	2.00	0.43
4:C:40:VAL:HG22	4:C:50:VAL:HG12	1.99	0.43
9:L:170:ALA:HA	9:L:238:TRP:HB2	2.00	0.43
4:C:252:HIS:NE2	5:B:61:LEU:O	2.51	0.43
13:J:107:ILE:O	13:J:111:ILE:HG12	2.19	0.43
4:C:215:PHE:HA	4:C:237:LEU:O	2.19	0.43
7:H:183:GLN:NE2	7:H:255:LEU:O	2.52	0.43
8:A:83:LEU:HD11	12:K:63:ILE:HG23	2.00	0.43
9:L:431:ARG:HG3	9:L:512:TRP:CE2	2.54	0.43
11:N:149:GLN:HE21	11:N:151:ARG:HB2	1.84	0.43
1:F:356:PRO:HB2	1:F:396:THR:HG22	2.01	0.43
9:L:12:LEU:HD23	9:L:12:LEU:HA	1.88	0.43
9:L:595:VAL:HG11	12:K:22:LEU:HG	2.00	0.43
3:G:438:ASP:OD1	3:G:438:ASP:N	2.50	0.42
7:H:116:ILE:HD12	7:H:116:ILE:HA	1.94	0.42
3:G:451:ALA:HB1	3:G:455:ASP:HB2	2.01	0.42
9:L:89:LEU:O	9:L:93:THR:OG1	2.30	0.42
11:N:16:ILE:HD12	11:N:51:SER:HB3	1.99	0.42
4:C:310:LEU:HD23	4:C:310:LEU:HA	1.89	0.42
11:N:270:ARG:HG3	11:N:314:ILE:HG23	2.01	0.42
1:F:296:GLY:O	1:F:320:ARG:NH2	2.52	0.42
3:G:626:GLU:OE1	3:G:786:ARG:NH1	2.52	0.42
7:H:15:ILE:HG23	8:A:18:ILE:HG21	2.01	0.42
11:N:119:LEU:HD22	11:N:253:VAL:HG11	2.01	0.42
11:N:172:PHE:HD2	11:N:209:LEU:HD13	1.84	0.42
11:N:288:ALA:HB2	11:N:300:TYR:HB2	2.02	0.42
7:H:8:LEU:HD12	7:H:11:ILE:HD11	2.01	0.42
7:H:170:GLN:NE2	7:H:192:GLN:HE21	2.18	0.42
9:L:123:PHE:HE1	9:L:146:VAL:HB	1.84	0.42
3:G:740:MET:HE2	3:G:740:MET:HB2	1.89	0.42
10:M:179:GLN:HG2	11:N:422:LEU:HD21	2.01	0.42
2:E:39:ALA:HB1	2:E:58:ILE:HD12	2.02	0.42
3:G:592:VAL:HB	3:G:606:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:520:LEU:HD23	4:C:520:LEU:HA	1.87	0.42
7:H:186:VAL:HG23	7:H:190:ILE:HD12	2.02	0.42
9:L:394:ALA:HA	9:L:469:ALA:HB2	2.02	0.42
10:M:381:MET:HG2	10:M:457:LEU:HD12	2.01	0.42
11:N:224:HIS:CD2	11:N:287:MET:HE1	2.54	0.42
2:E:105:ILE:HG21	2:E:153:LEU:HD13	2.02	0.42
3:G:227:PRO:HG2	3:G:633:PHE:CD1	2.54	0.42
5:B:100:GLY:HA2	14:B:301:SF4:S4	2.60	0.42
9:L:266:ILE:HB	9:L:323:LEU:HD13	2.02	0.42
9:L:415:MET:HE2	9:L:415:MET:HB3	1.93	0.42
20:L:706:3PE:H3D1	20:L:706:3PE:H292	2.01	0.42
1:F:18:ARG:HH11	1:F:22:GLN:HB2	1.85	0.41
2:E:33:ARG:NH1	21:E:302:HOH:O	2.45	0.41
6:I:59:ARG:HH12	6:I:145:TYR:HB2	1.84	0.41
1:F:286:LYS:HE3	1:F:331:HIS:HB3	2.03	0.41
4:C:74:LEU:HA	4:C:102:LEU:HD23	2.02	0.41
10:M:493:ILE:HD13	10:M:493:ILE:HA	1.85	0.41
11:N:66:LEU:HA	11:N:124:HIS:HB2	2.01	0.41
4:C:171:LYS:HE3	4:C:557:TYR:CZ	2.55	0.41
4:C:347:TYR:HB3	4:C:357:ARG:HH11	1.85	0.41
10:M:299:PHE:CE1	10:M:424:ILE:HG22	2.55	0.41
1:F:255:ARG:HD3	1:F:282:ARG:HH21	1.85	0.41
9:L:313:MET:HE2	9:L:313:MET:HB3	1.91	0.41
9:L:344:LEU:HB2	9:L:460:LEU:HB3	2.03	0.41
11:N:217:LYS:HA	11:N:217:LYS:HD3	1.85	0.41
13:J:129:VAL:O	13:J:133:LEU:HB2	2.19	0.41
1:F:182:GLU:O	1:F:186:LEU:N	2.48	0.41
3:G:5:THR:O	3:G:76:GLY:N	2.52	0.41
3:G:233:CYS:SG	3:G:235:ILE:HG12	2.60	0.41
4:C:430:ARG:NH1	4:C:437:ASP:OD1	2.54	0.41
7:H:265:LEU:HB2	7:H:270:TRP:CD1	2.55	0.41
9:L:368:LEU:HD12	9:L:368:LEU:HA	1.94	0.41
11:N:141:GLY:HA3	13:J:154:VAL:HG22	2.01	0.41
5:B:181:ARG:HH12	5:B:194:ARG:HH12	1.68	0.41
7:H:101:VAL:HG11	7:H:250:ALA:HB1	2.03	0.41
9:L:501:ALA:O	9:L:505:ILE:HG12	2.21	0.41
1:F:286:LYS:HE3	1:F:286:LYS:HB3	1.88	0.41
3:G:226:ALA:HB3	3:G:635:VAL:HG22	2.02	0.41
3:G:693:PRO:HG2	3:G:735:MET:SD	2.61	0.41
4:C:569:LEU:HD23	4:C:569:LEU:HA	1.93	0.41
9:L:235:LEU:HD21	20:L:704:3PE:H3D2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:133:ALA:HB1	9:L:138:LEU:HB3	2.02	0.41
10:M:340:GLY:HA2	10:M:409:MET:HE3	2.03	0.41
1:F:1:MET:HE3	1:F:276:ASP:HB3	2.03	0.40
4:C:275:ILE:O	4:C:283:ASN:ND2	2.54	0.40
4:C:300:PRO:HG3	4:C:492:PRO:HG2	2.03	0.40
5:B:102:CYS:HB3	5:B:142:VAL:HB	2.02	0.40
6:I:84:ASP:OD1	6:I:84:ASP:N	2.51	0.40
5:B:216:THR:HA	5:B:217:PRO:HD3	1.95	0.40
6:I:79:LYS:HE3	6:I:87:TRP:CE2	2.56	0.40
3:G:217:TYR:HB3	6:I:79:LYS:HD2	2.03	0.40
9:L:407:MET:HE2	9:L:407:MET:HB3	2.01	0.40
5:B:60:GLY:HA2	5:B:65:TYR:CG	2.56	0.40
7:H:122:MET:HE1	20:H:602:3PE:H2B1	2.04	0.40
10:M:6:LEU:HD23	10:M:6:LEU:HA	1.98	0.40
1:F:255:ARG:NH1	1:F:330:ASP:OD2	2.55	0.40
3:G:109:GLU:OE2	3:G:214:SER:OG	2.35	0.40
7:H:194:PHE:HA	7:H:197:ILE:HG12	2.04	0.40
9:L:506:LEU:HD13	9:L:506:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	440/442 (100%)	429 (98%)	11 (2%)	0	100	100
2	E	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
3	G	903/905 (100%)	880 (98%)	23 (2%)	0	100	100
4	C	563/600 (94%)	550 (98%)	13 (2%)	0	100	100
5	B	163/220 (74%)	157 (96%)	6 (4%)	0	100	100
6	I	143/145 (99%)	140 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	305/325 (94%)	291 (95%)	14 (5%)	0	100	100
8	A	97/147 (66%)	97 (100%)	0	0	100	100
9	L	597/613 (97%)	580 (97%)	17 (3%)	0	100	100
10	M	502/504 (100%)	495 (99%)	7 (1%)	0	100	100
11	N	476/485 (98%)	462 (97%)	13 (3%)	1 (0%)	43	76
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
All	All	4601/4804 (96%)	4482 (97%)	118 (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	356/356 (100%)	351 (99%)	5 (1%)	59	80
2	E	129/129 (100%)	128 (99%)	1 (1%)	73	86
3	G	732/732 (100%)	718 (98%)	14 (2%)	50	76
4	C	486/519 (94%)	476 (98%)	10 (2%)	47	75
5	B	146/192 (76%)	141 (97%)	5 (3%)	32	66
6	I	124/124 (100%)	120 (97%)	4 (3%)	34	67
7	H	255/269 (95%)	249 (98%)	6 (2%)	43	73
8	A	79/119 (66%)	76 (96%)	3 (4%)	29	63
9	L	477/486 (98%)	467 (98%)	10 (2%)	47	75
10	M	413/413 (100%)	400 (97%)	13 (3%)	35	68
11	N	381/385 (99%)	378 (99%)	3 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	K	79/79 (100%)	76 (96%)	3 (4%)	29 63
13	J	128/128 (100%)	125 (98%)	3 (2%)	44 74
All	All	3785/3931 (96%)	3705 (98%)	80 (2%)	46 75

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	84	ILE
1	F	221	THR
1	F	229	LEU
1	F	388	CYS
1	F	430	THR
2	E	145	ILE
3	G	61	THR
3	G	158	ARG
3	G	181	VAL
3	G	233	CYS
3	G	238	ASN
3	G	365	THR
3	G	385	THR
3	G	586	LEU
3	G	626	GLU
3	G	647	MET
3	G	670	GLN
3	G	718	ARG
3	G	834	GLN
3	G	854	VAL
4	C	110	ASP
4	C	154	ASN
4	C	237	LEU
4	C	246	VAL
4	C	273	ASP
4	C	342	ASP
4	C	411	VAL
4	C	474	LEU
4	C	536	MET
4	C	600	ARG
5	B	63	CYS
5	B	66	VAL
5	B	98	VAL
5	B	138	ILE

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Mol	Chain	Res	Type
5	B	174	GLU
6	I	43	ARG
6	I	77	LEU
6	I	98	ARG
6	I	175	VAL
7	H	9	ILE
7	H	60	LEU
7	H	81	VAL
7	H	92	THR
7	H	165	MET
7	H	186	VAL
8	A	30	MET
8	A	37	LEU
8	A	83	LEU
9	L	80	VAL
9	L	81	LEU
9	L	139	MET
9	L	185	LEU
9	L	192	LEU
9	L	372	ILE
9	L	379	PHE
9	L	506	LEU
9	L	507	LEU
9	L	519	VAL
10	M	88	LEU
10	M	134	ILE
10	M	259	LEU
10	M	262	ILE
10	M	263	LEU
10	M	321	SER
10	M	393	VAL
10	M	418	VAL
10	M	426	THR
10	M	429	LEU
10	M	430	VAL
10	M	462	LEU
10	M	493	ILE
11	N	64	THR
11	N	401	VAL
11	N	432	LEU
12	K	44	LEU
12	K	46	PHE

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Mol	Chain	Res	Type
12	K	95	VAL
13	J	23	THR
13	J	94	ILE
13	J	122	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	22	GLN
1	F	224	ASN
1	F	434	ASN
2	E	78	GLN
2	E	150	HIS
3	G	218	ASN
3	G	224	GLN
3	G	238	ASN
3	G	256	ASN
3	G	465	HIS
3	G	655	HIS
3	G	673	HIS
3	G	768	ASN
3	G	806	GLN
3	G	867	ASN
4	C	135	ASN
4	C	219	ASN
6	I	64	ASN
7	H	152	GLN
7	H	192	GLN
7	H	312	ASN
8	A	12	HIS
9	L	55	ASN
9	L	78	ASN
9	L	163	ASN
10	M	198	ASN
10	M	308	GLN
11	N	149	GLN
11	N	180	GLN
11	N	472	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	SF4	G	1002	3	0,12,12	-	-	-		
17	FES	G	1004	3	0,4,4	-	-	-		
16	NAI	F	503	-	45,48,48	0.26	0	60,73,73	0.29	0
14	SF4	B	301	5	0,12,12	-	-	-		
20	3PE	A	202	-	33,33,50	0.36	0	36,38,55	0.34	0
19	LFA	N	903	-	19,19,19	0.09	0	18,18,18	0.16	0
20	3PE	H	602	-	50,50,50	0.31	0	53,55,55	0.34	0
20	3PE	M	702	-	50,50,50	0.29	0	53,55,55	0.28	0
19	LFA	A	201	-	19,19,19	0.13	0	18,18,18	0.18	0
19	LFA	N	901	-	19,19,19	0.12	0	18,18,18	0.17	0
20	3PE	L	706	-	50,50,50	0.30	0	53,55,55	0.35	0
19	LFA	L	703	-	14,14,19	0.16	0	13,13,18	0.13	0
14	SF4	F	501	1	0,12,12	-	-	-		
20	3PE	L	705	-	50,50,50	0.31	0	53,55,55	0.30	0
17	FES	E	201	2	0,4,4	-	-	-		
14	SF4	G	1001	3	0,12,12	-	-	-		
15	FMN	F	502	-	33,33,33	1.06	2 (6%)	48,50,50	1.30	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LFA	H	601	-	19,19,19	0.14	0	18,18,18	0.11	0
20	3PE	L	704	-	50,50,50	0.30	0	53,55,55	0.33	0
19	LFA	L	707	-	19,19,19	0.15	0	18,18,18	0.11	0
14	SF4	I	202	6	0,12,12	-	-	-		
20	3PE	L	702	-	50,50,50	0.30	0	53,55,55	0.30	0
14	SF4	G	1003	3	0,12,12	-	-	-		
20	3PE	M	701	-	50,50,50	0.30	0	53,55,55	0.28	0
20	3PE	A	203	-	50,50,50	0.30	0	53,55,55	0.26	0
20	3PE	L	701	-	50,50,50	0.30	0	53,55,55	0.31	0
20	3PE	N	902	-	50,50,50	0.30	0	53,55,55	0.28	0
20	3PE	L	708	-	50,50,50	0.30	0	53,55,55	0.31	0
14	SF4	I	201	6	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	G	1002	3	-	-	0/6/5/5
17	FES	G	1004	3	-	-	0/1/1/1
16	NAI	F	503	-	-	6/29/72/72	0/5/5/5
20	3PE	A	202	-	-	6/37/37/54	-
14	SF4	B	301	5	-	-	0/6/5/5
19	LFA	N	903	-	-	0/17/17/17	-
20	3PE	H	602	-	-	9/54/54/54	-
20	3PE	M	702	-	-	6/54/54/54	-
19	LFA	A	201	-	-	1/17/17/17	-
19	LFA	N	901	-	-	3/17/17/17	-
20	3PE	L	706	-	-	17/54/54/54	-
19	LFA	L	703	-	-	0/12/12/17	-
14	SF4	F	501	1	-	-	0/6/5/5
20	3PE	L	705	-	-	10/54/54/54	-
17	FES	E	201	2	-	-	0/1/1/1
14	SF4	G	1001	3	-	-	0/6/5/5
15	FMN	F	502	-	-	5/18/18/18	0/3/3/3
19	LFA	H	601	-	-	1/17/17/17	-
20	3PE	L	704	-	-	8/54/54/54	-
19	LFA	L	707	-	-	1/17/17/17	-
20	3PE	L	702	-	-	8/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	I	202	6	-	-	0/6/5/5
14	SF4	G	1003	3	-	-	0/6/5/5
20	3PE	M	701	-	-	9/54/54/54	-
20	3PE	A	203	-	-	13/54/54/54	-
20	3PE	L	701	-	-	11/54/54/54	-
20	3PE	N	902	-	-	10/54/54/54	-
20	3PE	L	708	-	-	12/54/54/54	-
14	SF4	I	201	6	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.51	1.37	1.30
15	F	502	FMN	C10-N1	2.14	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	119.37	125.64
15	F	502	FMN	C4A-C10-N10	2.98	120.83	116.48
15	F	502	FMN	C4A-C4-N3	2.77	120.22	113.19
15	F	502	FMN	O4-C4-C4A	-2.53	119.90	126.60
15	F	502	FMN	C4A-C10-N1	-2.45	119.05	124.73
15	F	502	FMN	C10-C4A-N5	-2.30	119.97	124.86
15	F	502	FMN	C4-C4A-C10	2.01	120.17	116.79

There are no chirality outliers.

All (136) 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
20	H	602	3PE	C1-O11-P-O14
20	H	602	3PE	O13-C11-C12-N
20	A	202	3PE	O13-C11-C12-N
20	A	203	3PE	O13-C11-C12-N
20	L	701	3PE	C11-O13-P-O11
20	L	701	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
20	L	701	3PE	C11-O13-P-O14
20	L	704	3PE	C1-O11-P-O14
20	L	704	3PE	O13-C11-C12-N
20	L	705	3PE	C1-O11-P-O12
20	L	705	3PE	C11-O13-P-O14
20	L	706	3PE	C11-O13-P-O11
20	L	706	3PE	C11-O13-P-O12
20	L	706	3PE	C11-O13-P-O14
20	L	706	3PE	O13-C11-C12-N
20	L	708	3PE	C11-O13-P-O11
20	L	708	3PE	C11-O13-P-O14
20	M	701	3PE	C1-O11-P-O14
20	M	701	3PE	O13-C11-C12-N
20	M	702	3PE	C11-O13-P-O12
20	M	702	3PE	C11-O13-P-O14
20	N	902	3PE	C1-O11-P-O12
20	N	902	3PE	C1-O11-P-O13
20	N	902	3PE	C1-O11-P-O14
20	N	902	3PE	O13-C11-C12-N
20	L	701	3PE	O21-C2-C3-O31
20	L	708	3PE	C25-C26-C27-C28
20	A	203	3PE	C1-O11-P-O13
20	L	705	3PE	C1-O11-P-O13
20	M	702	3PE	C11-O13-P-O11
20	L	708	3PE	C21-C22-C23-C24
19	L	707	LFA	C6-C7-C8-C9
20	L	706	3PE	C3C-C3D-C3E-C3F
20	L	708	3PE	C35-C36-C37-C38
20	L	705	3PE	C35-C36-C37-C38
19	H	601	LFA	C14-C15-C16-C17
20	A	202	3PE	C21-C22-C23-C24
20	L	708	3PE	C37-C38-C39-C3A
20	L	702	3PE	C23-C24-C25-C26
20	L	702	3PE	C2C-C2D-C2E-C2F
20	L	702	3PE	C3E-C3F-C3G-C3H
20	L	704	3PE	C1-O11-P-O13
20	L	705	3PE	C11-O13-P-O11
20	L	706	3PE	O11-C1-C2-C3
20	M	701	3PE	C24-C25-C26-C27
20	L	701	3PE	C1-C2-C3-O31
20	L	706	3PE	C31-C32-C33-C34
15	F	502	FMN	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
20	M	701	3PE	C25-C26-C27-C28
20	H	602	3PE	C3C-C3D-C3E-C3F
20	M	701	3PE	C2-C1-O11-P
19	A	201	LFA	C12-C13-C14-C15
20	L	706	3PE	C2-C1-O11-P
20	L	706	3PE	C3D-C3E-C3F-C3G
20	H	602	3PE	C21-C22-C23-C24
16	F	503	NAI	C2D-C1D-N1N-C2N
20	L	706	3PE	C39-C3A-C3B-C3C
20	M	702	3PE	C29-C2A-C2B-C2C
20	A	203	3PE	C23-C24-C25-C26
20	A	203	3PE	C2-C1-O11-P
20	L	706	3PE	C3F-C3G-C3H-C3I
20	A	202	3PE	C11-O13-P-O11
20	M	701	3PE	C1-O11-P-O13
20	L	701	3PE	C2-C1-O11-P
20	M	702	3PE	C2-C1-O11-P
20	A	203	3PE	C1-O11-P-O12
20	A	203	3PE	C1-O11-P-O14
20	L	704	3PE	C1-O11-P-O12
20	L	705	3PE	C1-O11-P-O14
20	L	705	3PE	C11-O13-P-O12
20	A	203	3PE	O11-C1-C2-C3
20	L	708	3PE	O13-C11-C12-N
19	N	901	LFA	C11-C12-C13-C14
20	L	706	3PE	O11-C1-C2-O21
20	N	902	3PE	C38-C39-C3A-C3B
16	F	503	NAI	O4D-C1D-N1N-C2N
20	L	701	3PE	C25-C26-C27-C28
20	N	902	3PE	O31-C31-C32-C33
19	N	901	LFA	C15-C16-C17-C18
20	H	602	3PE	C2F-C2G-C2H-C2I
20	L	701	3PE	C29-C2A-C2B-C2C
20	A	203	3PE	O11-C1-C2-O21
20	A	203	3PE	O21-C21-C22-C23
20	H	602	3PE	C1-O11-P-O13
20	A	203	3PE	C11-O13-P-O11
20	L	704	3PE	C11-O13-P-O11
20	L	708	3PE	C1-O11-P-O13
20	M	701	3PE	C11-O13-P-O11
20	N	902	3PE	C11-O13-P-O11
20	N	902	3PE	C2-C1-O11-P

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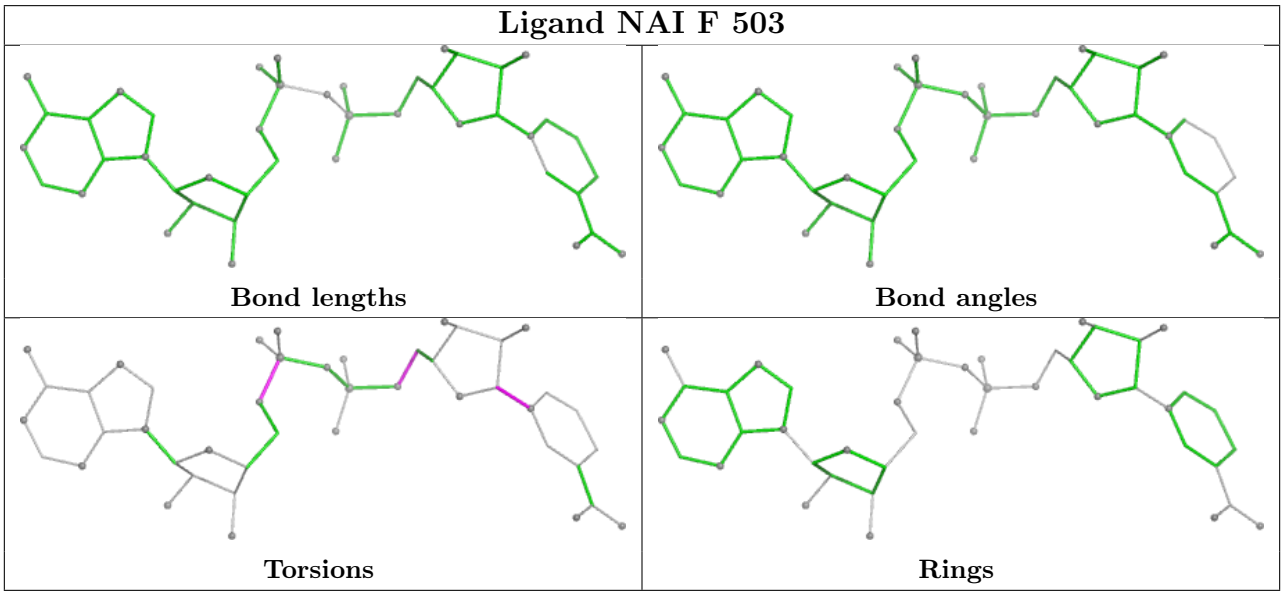
Mol	Chain	Res	Type	Atoms
20	L	702	3PE	C37-C38-C39-C3A
20	L	704	3PE	C37-C38-C39-C3A
16	F	503	NAI	O4D-C1D-N1N-C6N
16	F	503	NAI	C2D-C1D-N1N-C6N
20	H	602	3PE	C22-C23-C24-C25
20	A	203	3PE	C21-C22-C23-C24
20	L	708	3PE	C2F-C2G-C2H-C2I
20	L	706	3PE	C37-C38-C39-C3A
16	F	503	NAI	C4D-C5D-O5D-PN
20	L	706	3PE	C32-C33-C34-C35
20	L	705	3PE	O31-C31-C32-C33
20	L	706	3PE	C3E-C3F-C3G-C3H
20	A	202	3PE	O21-C21-C22-C23
20	L	704	3PE	O31-C31-C32-C33
20	A	202	3PE	C23-C24-C25-C26
20	L	702	3PE	C29-C2A-C2B-C2C
20	A	203	3PE	O21-C2-C3-O31
20	L	705	3PE	O21-C21-C22-C23
20	L	702	3PE	C25-C26-C27-C28
20	L	705	3PE	O32-C31-C32-C33
20	L	704	3PE	O32-C31-C32-C33
16	F	503	NAI	C5B-O5B-PA-O1A
20	H	602	3PE	C1-O11-P-O12
20	A	203	3PE	C11-O13-P-O14
20	L	701	3PE	C1-O11-P-O14
20	L	702	3PE	C1-O11-P-O14
20	M	701	3PE	C11-O13-P-O14
20	N	902	3PE	C11-O13-P-O14
20	M	702	3PE	C3C-C3D-C3E-C3F
20	L	701	3PE	C2D-C2E-C2F-C2G
20	M	701	3PE	C35-C36-C37-C38
20	L	708	3PE	C12-C11-O13-P
20	A	202	3PE	O22-C21-C22-C23
20	L	708	3PE	O21-C21-C22-C23
19	N	901	LFA	C13-C14-C15-C16
20	L	706	3PE	O31-C31-C32-C33
20	N	902	3PE	C2F-C2G-C2H-C2I
20	L	706	3PE	O32-C31-C32-C33
20	H	602	3PE	C3B-C3C-C3D-C3E
20	L	701	3PE	O21-C21-C22-C23
20	L	708	3PE	O22-C21-C22-C23
20	L	702	3PE	C34-C35-C36-C37

There are no ring outliers.

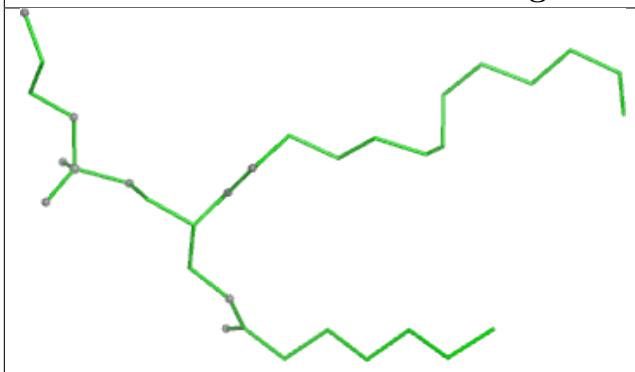
13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	F	503	NAI	3	0
14	B	301	SF4	1	0
19	N	903	LFA	2	0
20	H	602	3PE	4	0
20	M	702	3PE	3	0
20	L	706	3PE	3	0
20	L	704	3PE	2	0
20	L	702	3PE	1	0
20	M	701	3PE	2	0
20	A	203	3PE	3	0
20	L	701	3PE	2	0
20	N	902	3PE	2	0
20	L	708	3PE	2	0

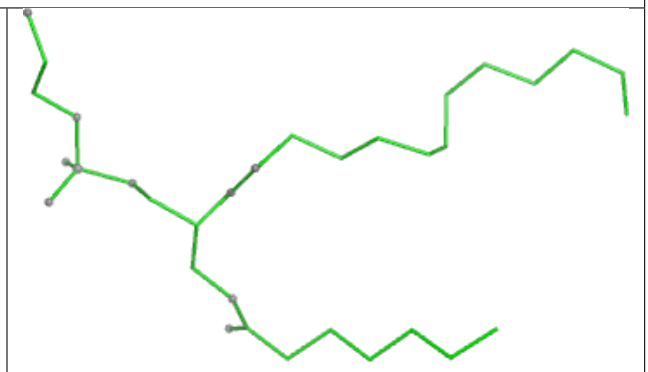
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



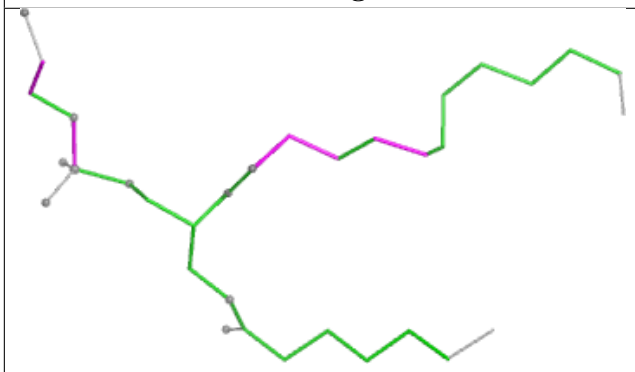
Ligand 3PE A 202



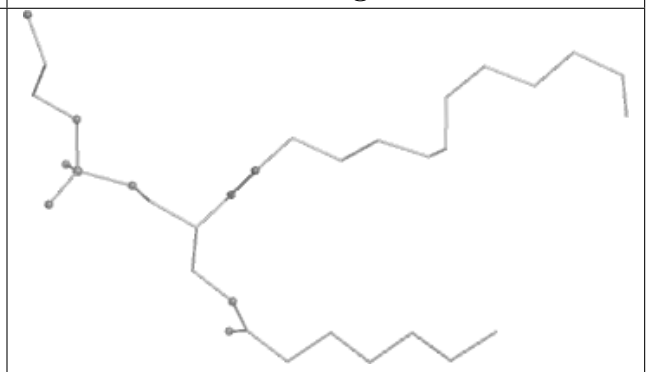
Bond lengths



Bond angles

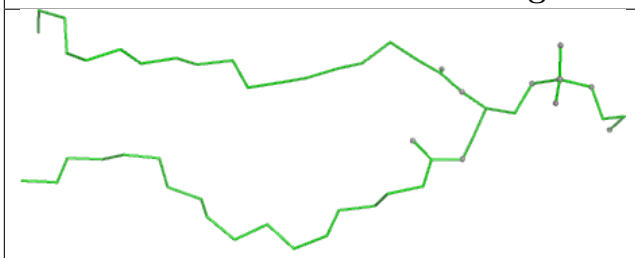


Torsions

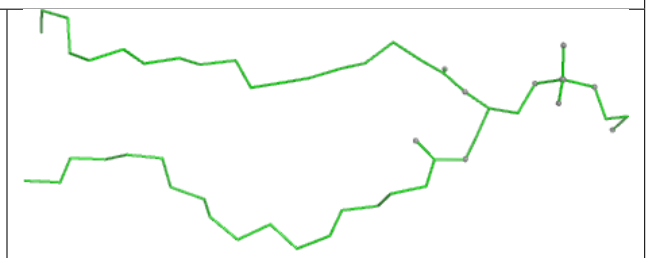


Rings

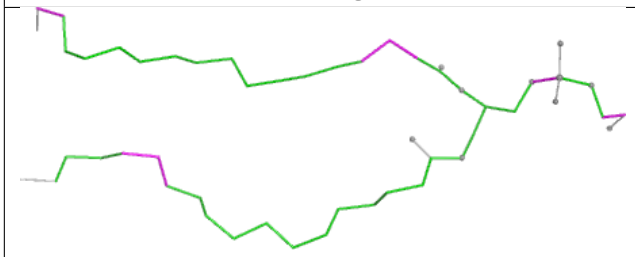
Ligand 3PE H 602



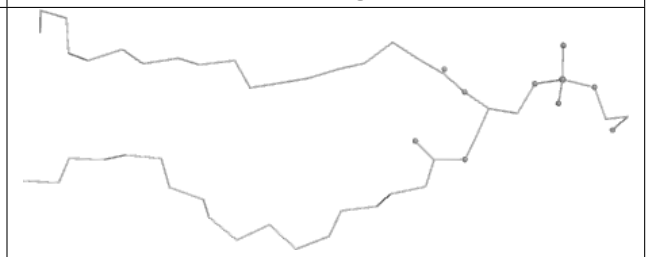
Bond lengths



Bond angles

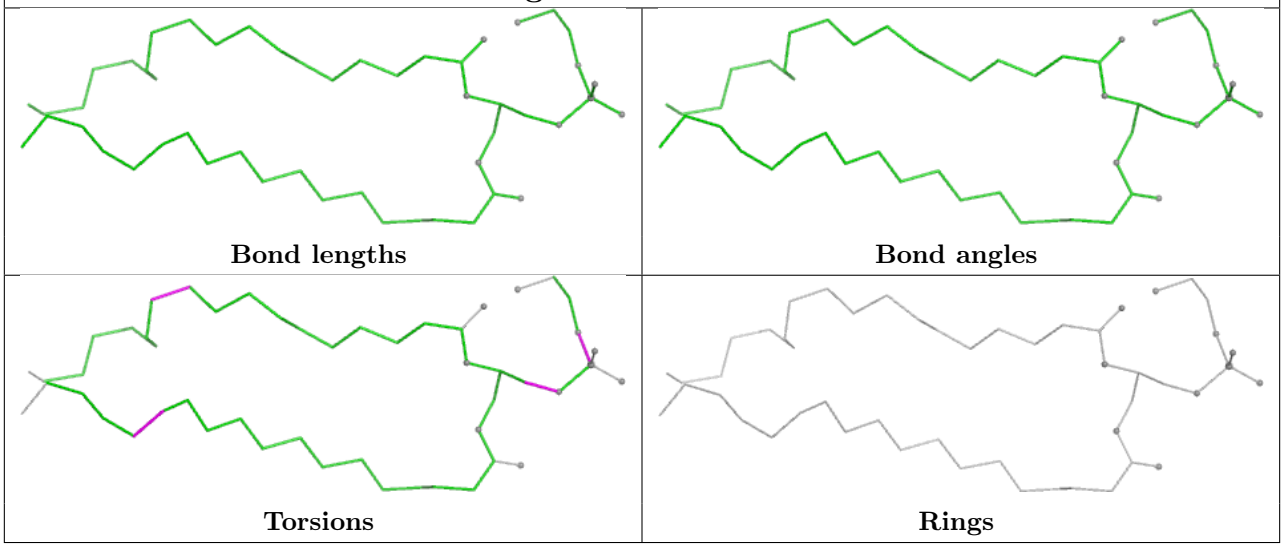


Torsions

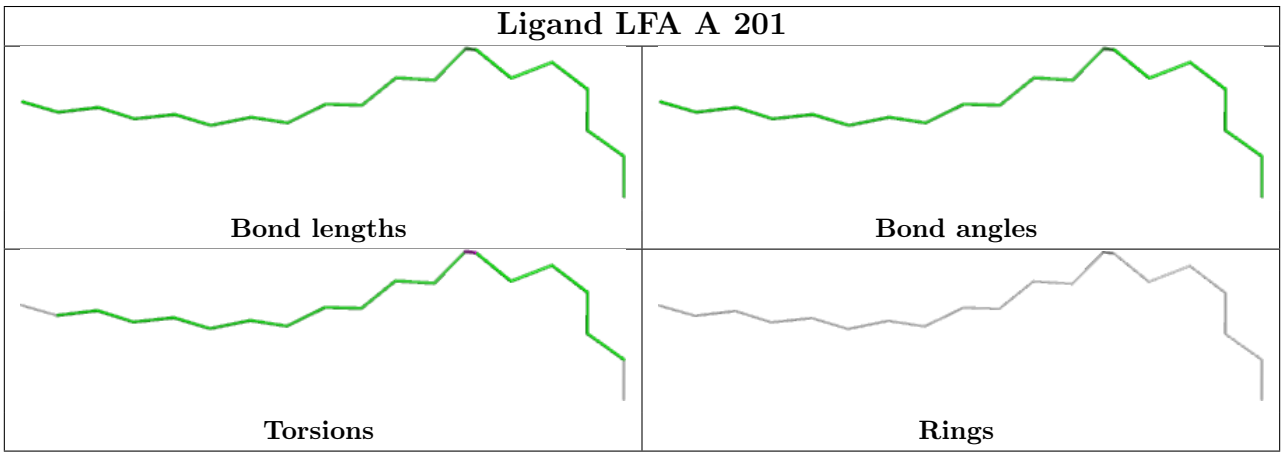


Rings

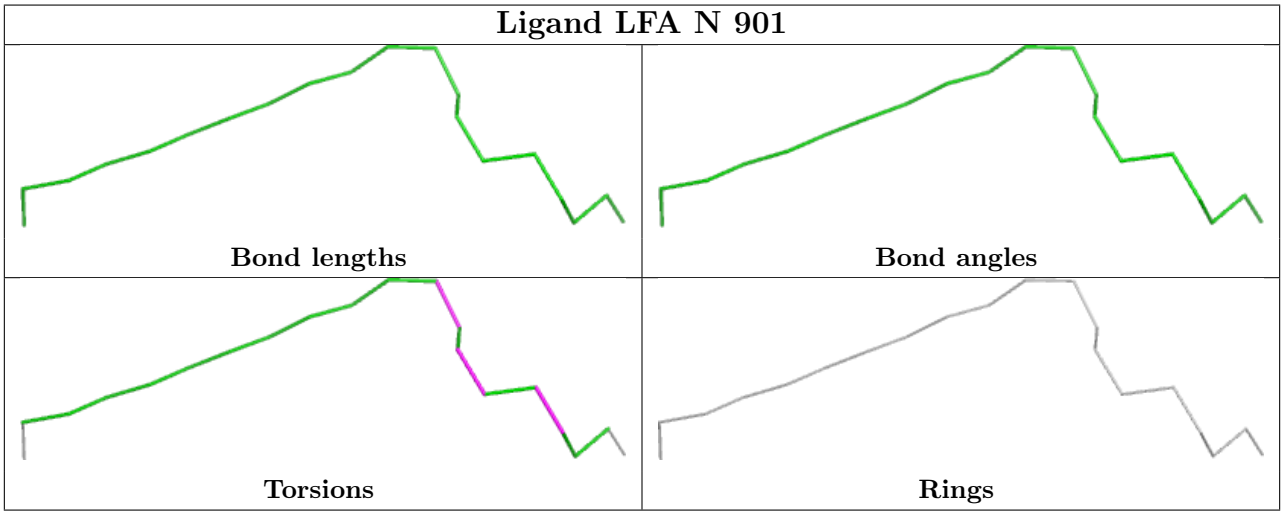
Ligand 3PE M 702



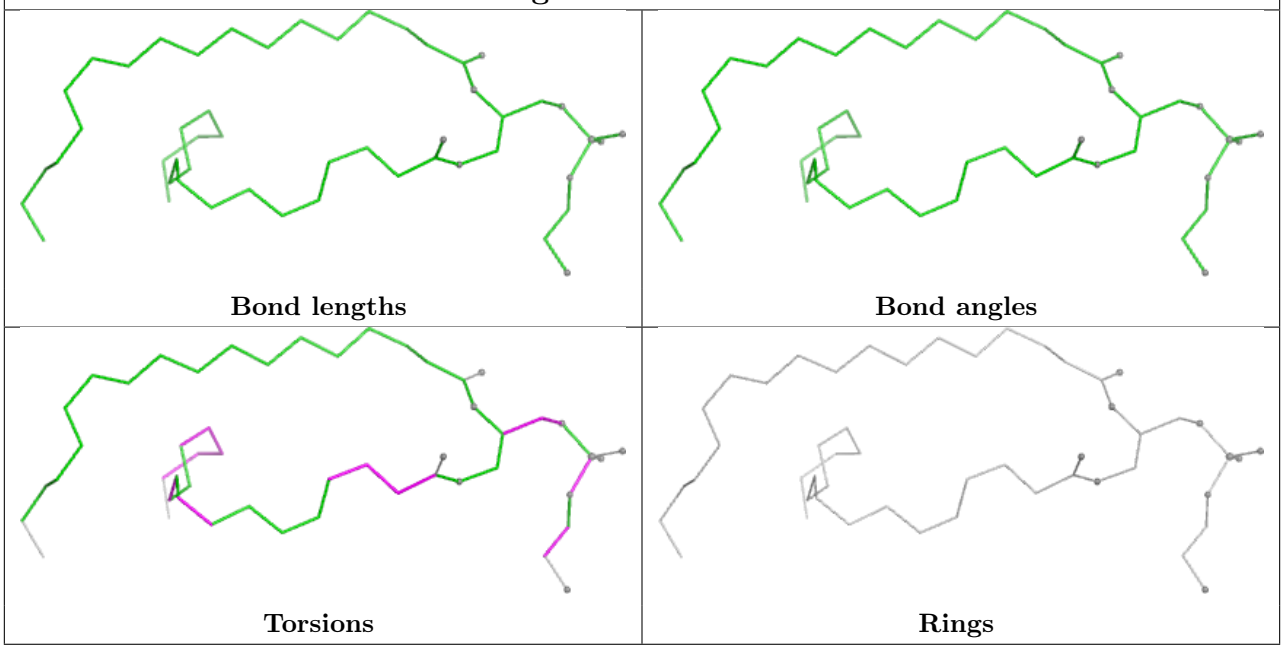
Ligand LFA A 201



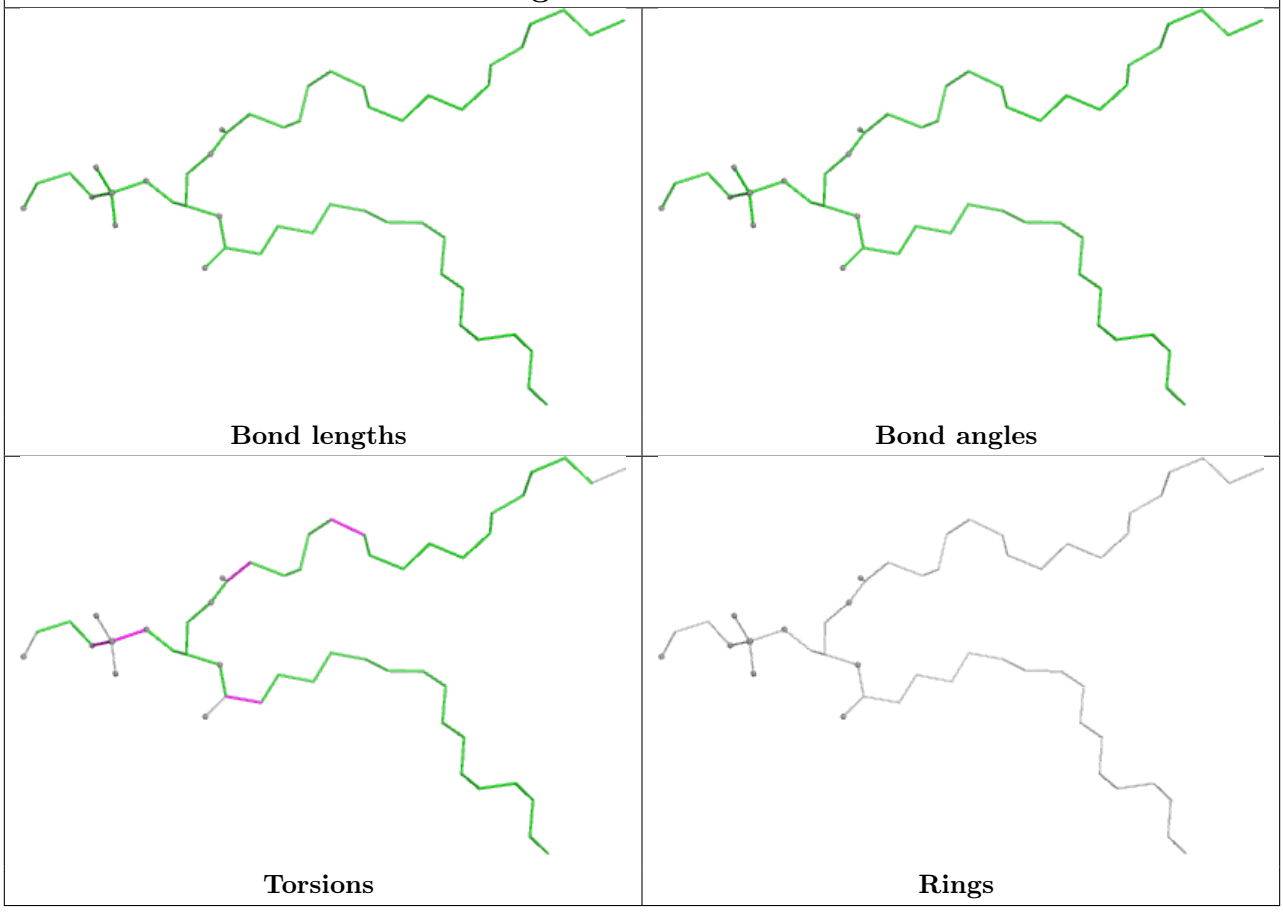
Ligand LFA N 901



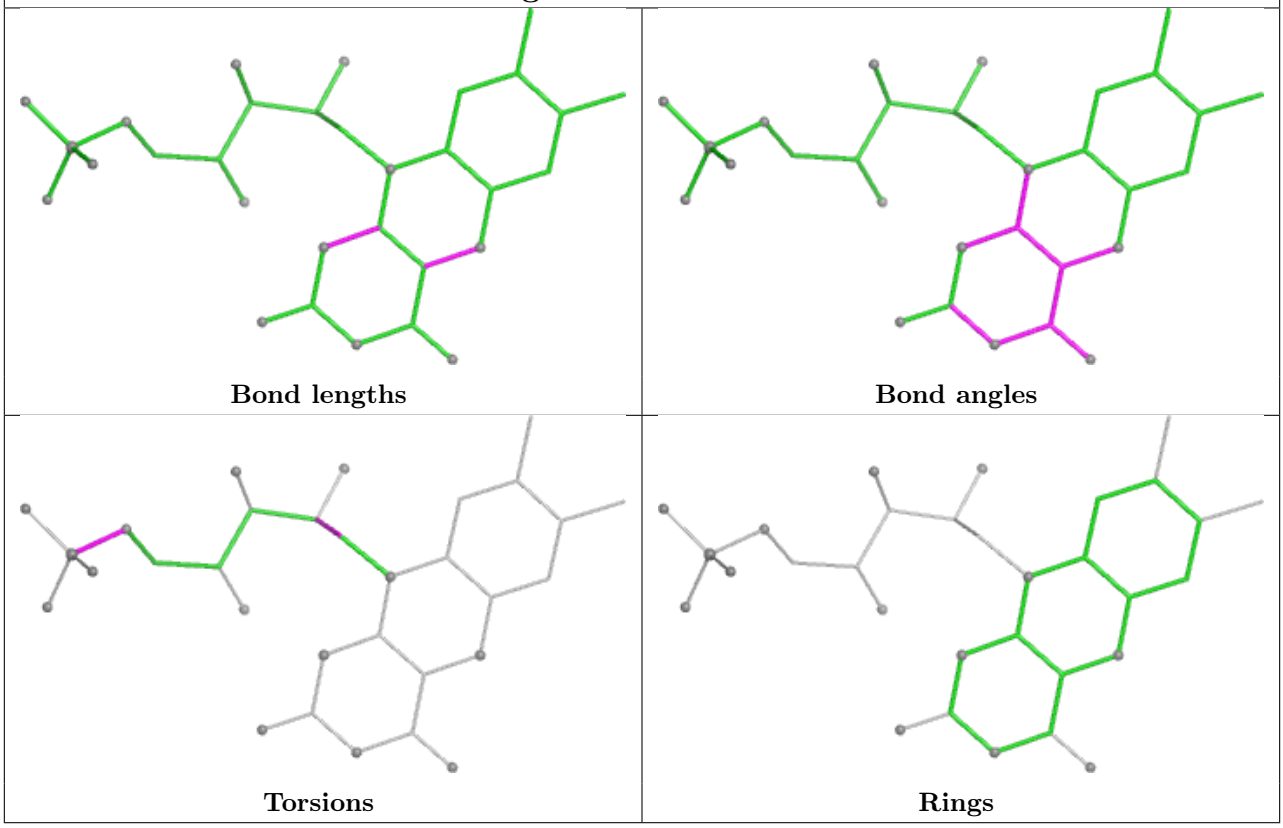
Ligand 3PE L 706



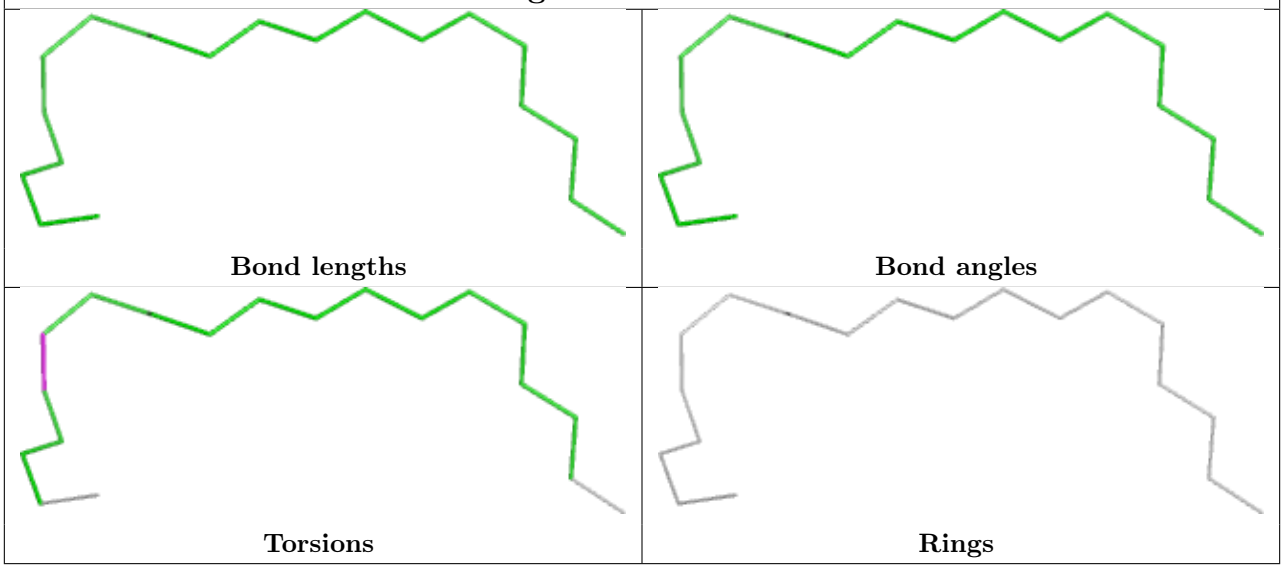
Ligand 3PE L 705



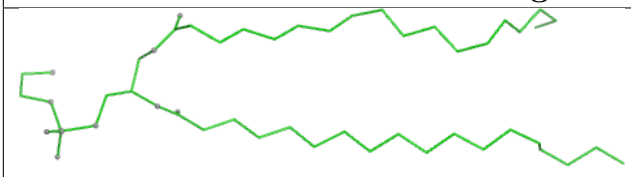
Ligand FMN F 502



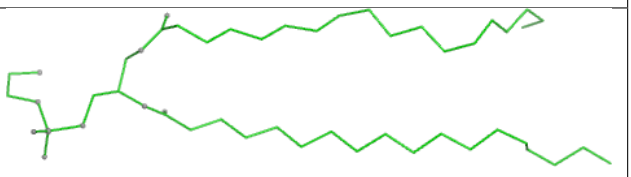
Ligand LFA H 601



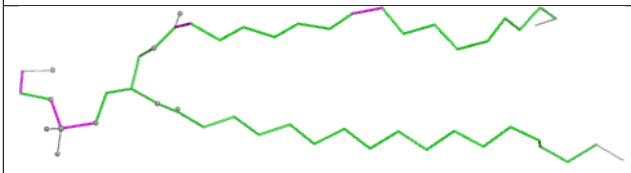
Ligand 3PE L 704



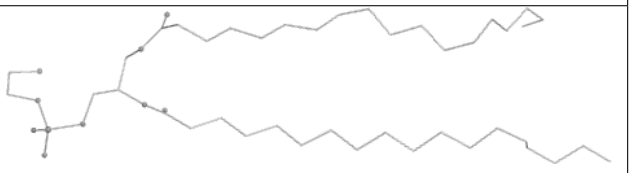
Bond lengths



Bond angles



Torsions



Rings

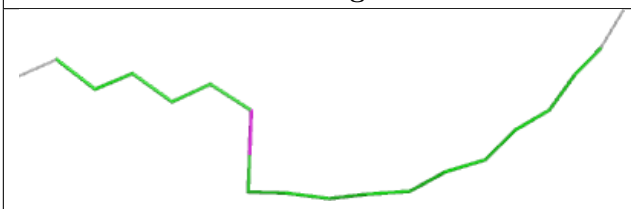
Ligand LFA L 707



Bond lengths



Bond angles



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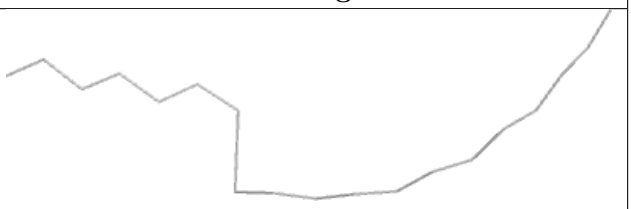

Rings

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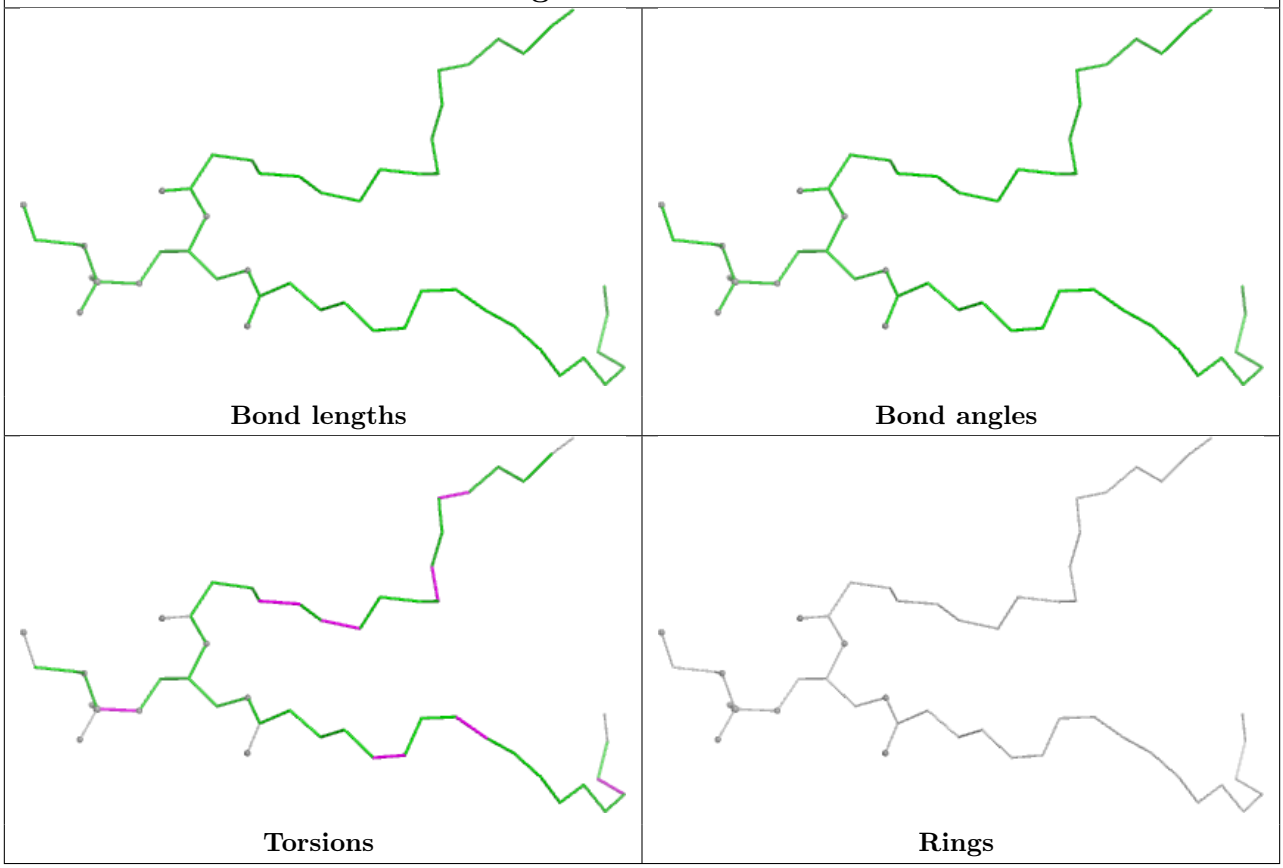
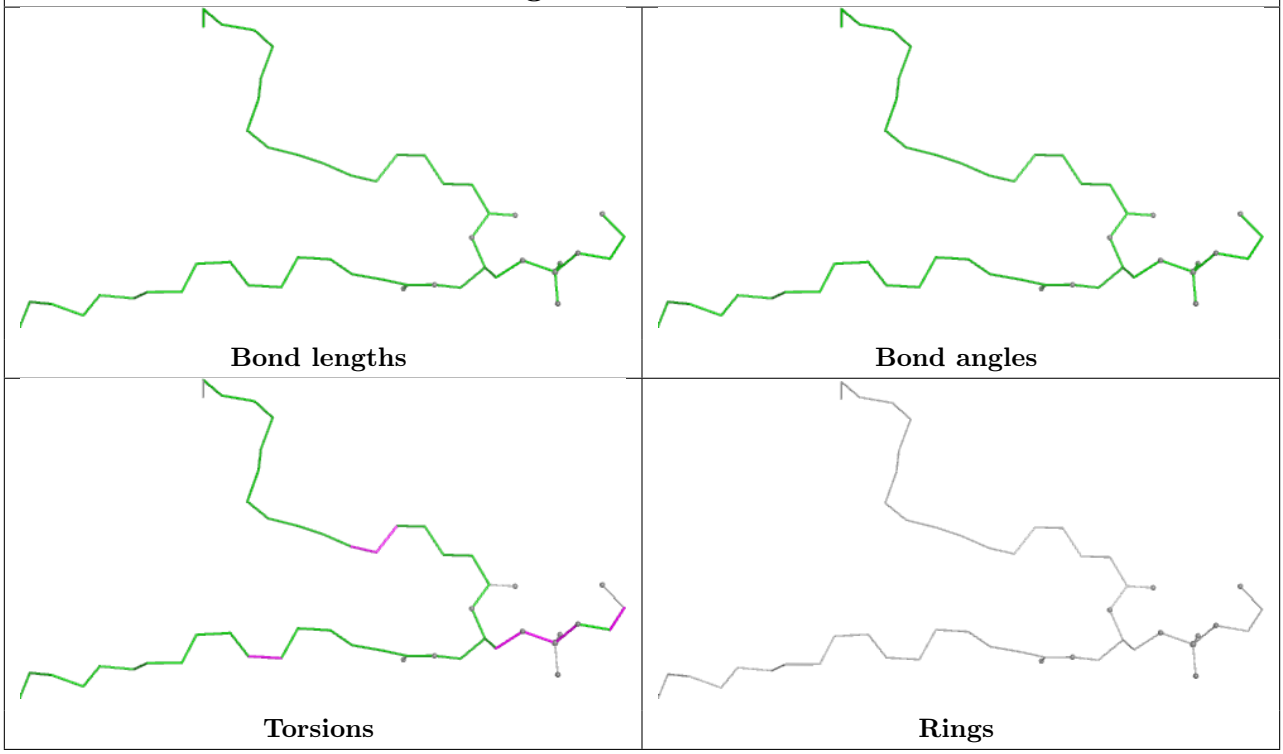
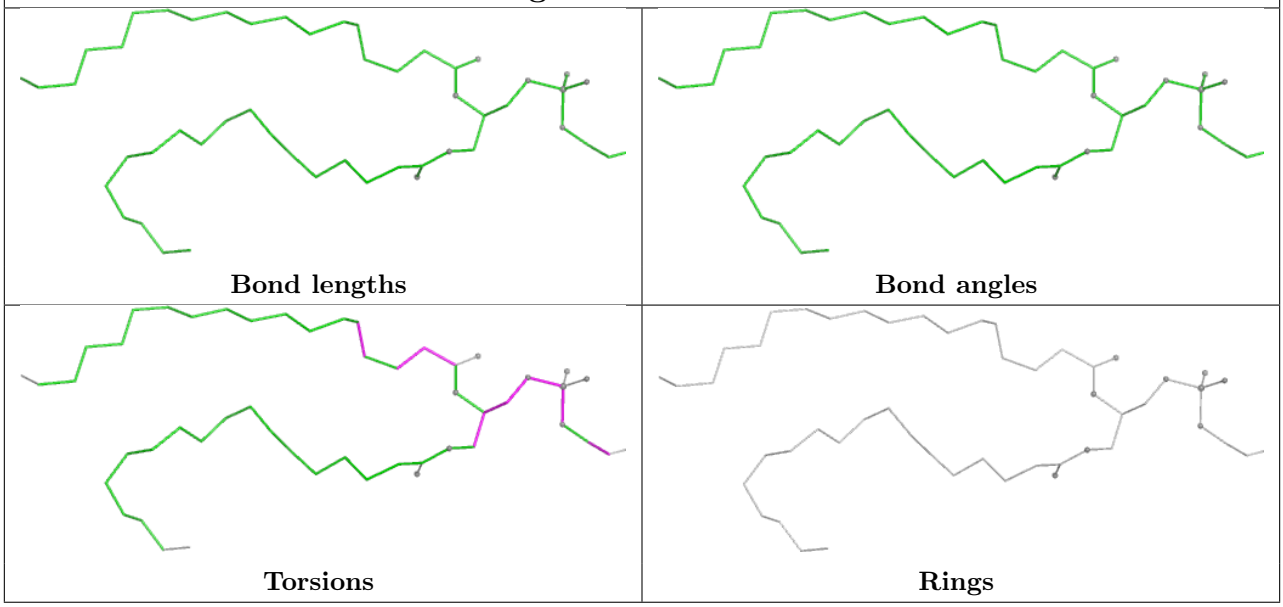


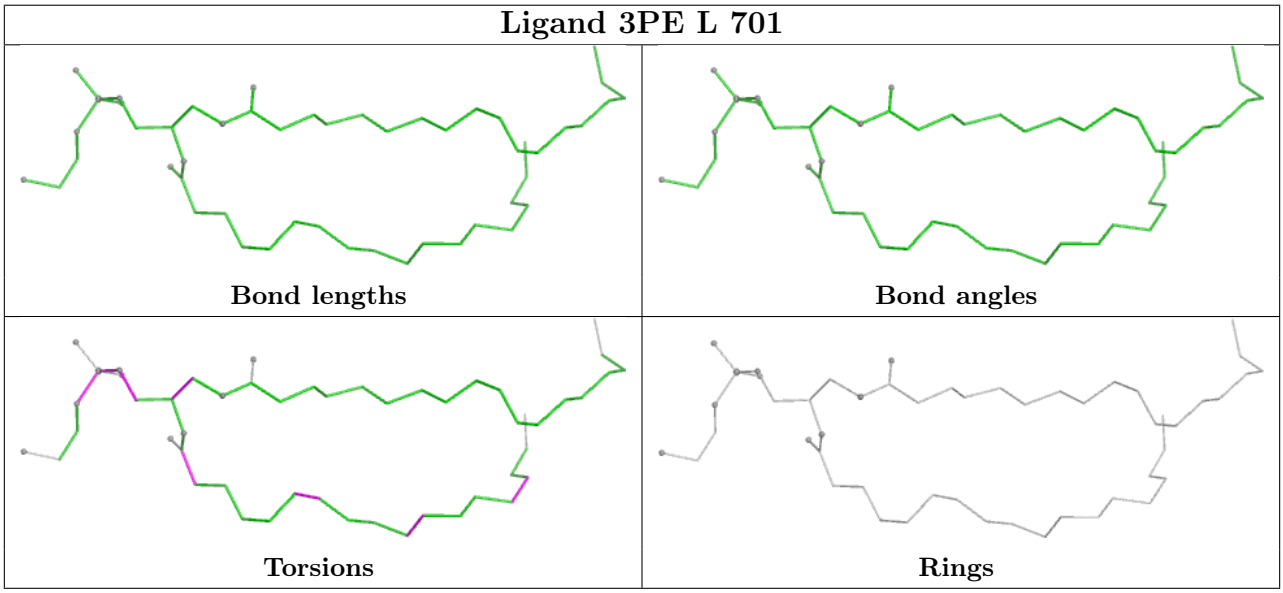
Ligand 3PE M 701



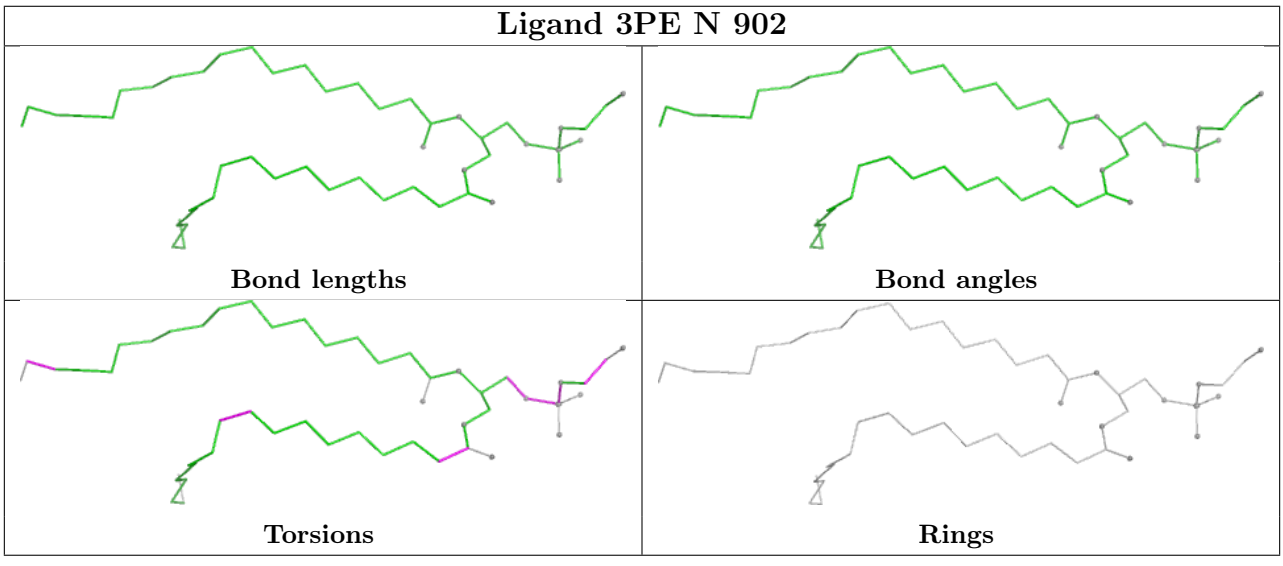
Ligand 3PE A 203

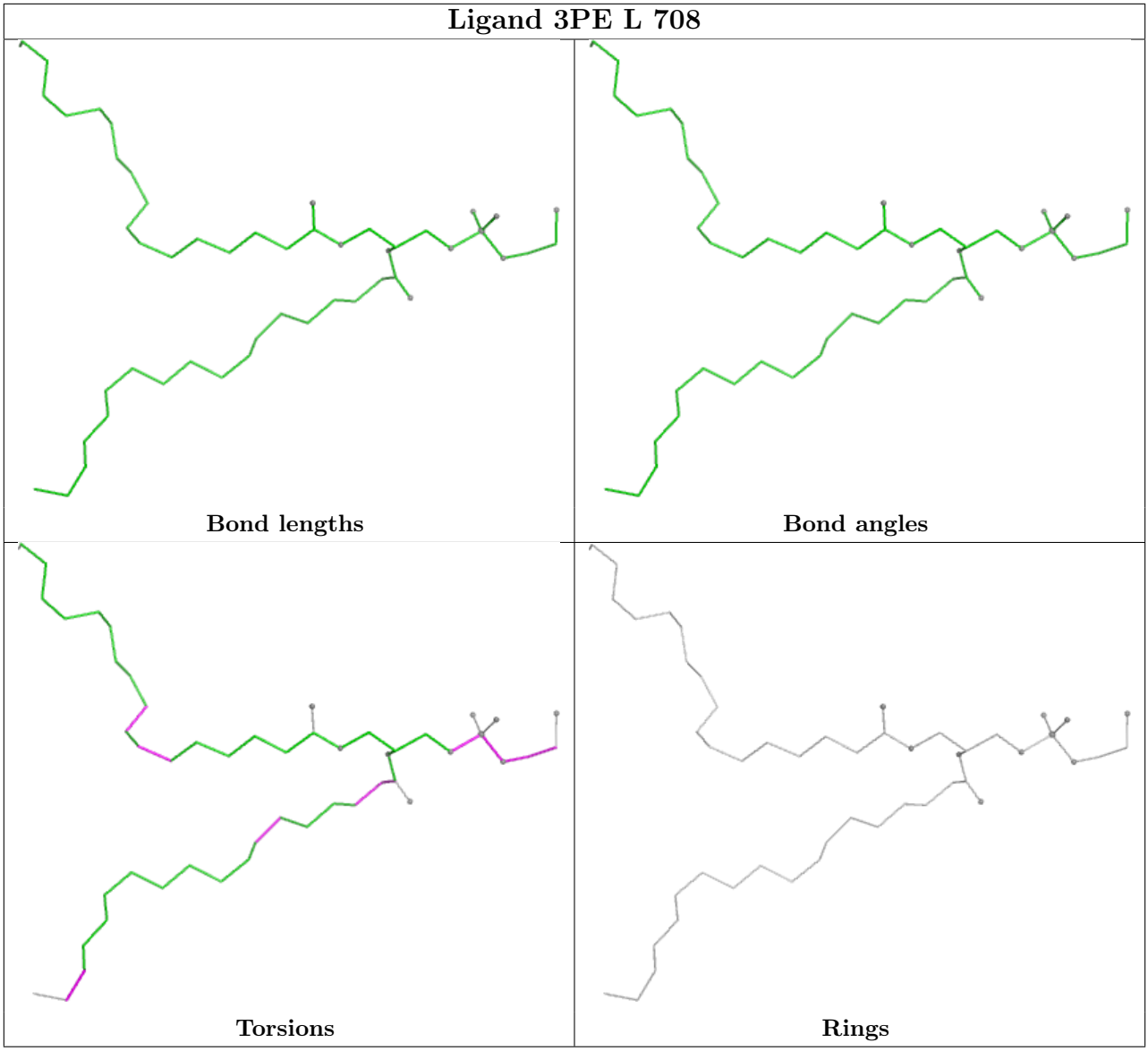


Ligand 3PE L 701



Ligand 3PE N 902





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.

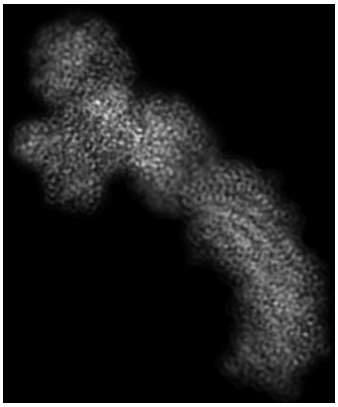
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13222. These allow visual inspection of the internal detail of the map and identification of artifacts.

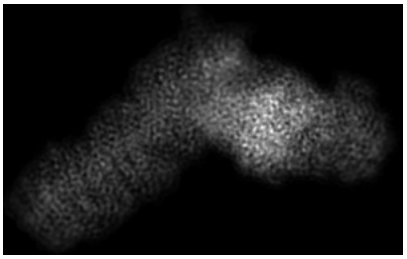
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

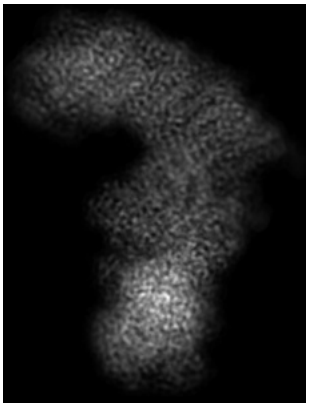
6.1.1 Primary map



X



Y

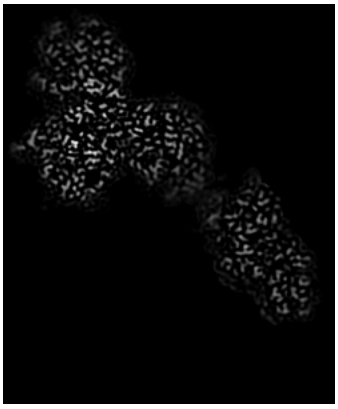


Z

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

6.2 Central slices

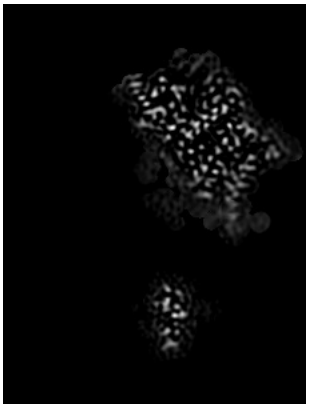
6.2.1 Primary map



X Index: 154



Y Index: 205



Z Index: 247

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: 176



Y Index: 110

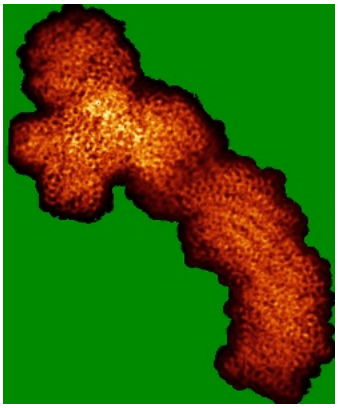


Z Index: 331

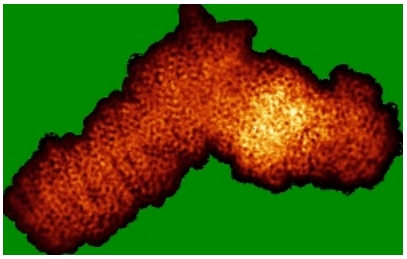
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

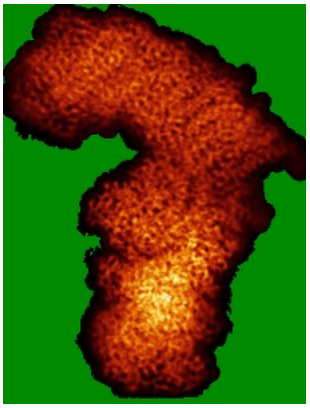
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 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.

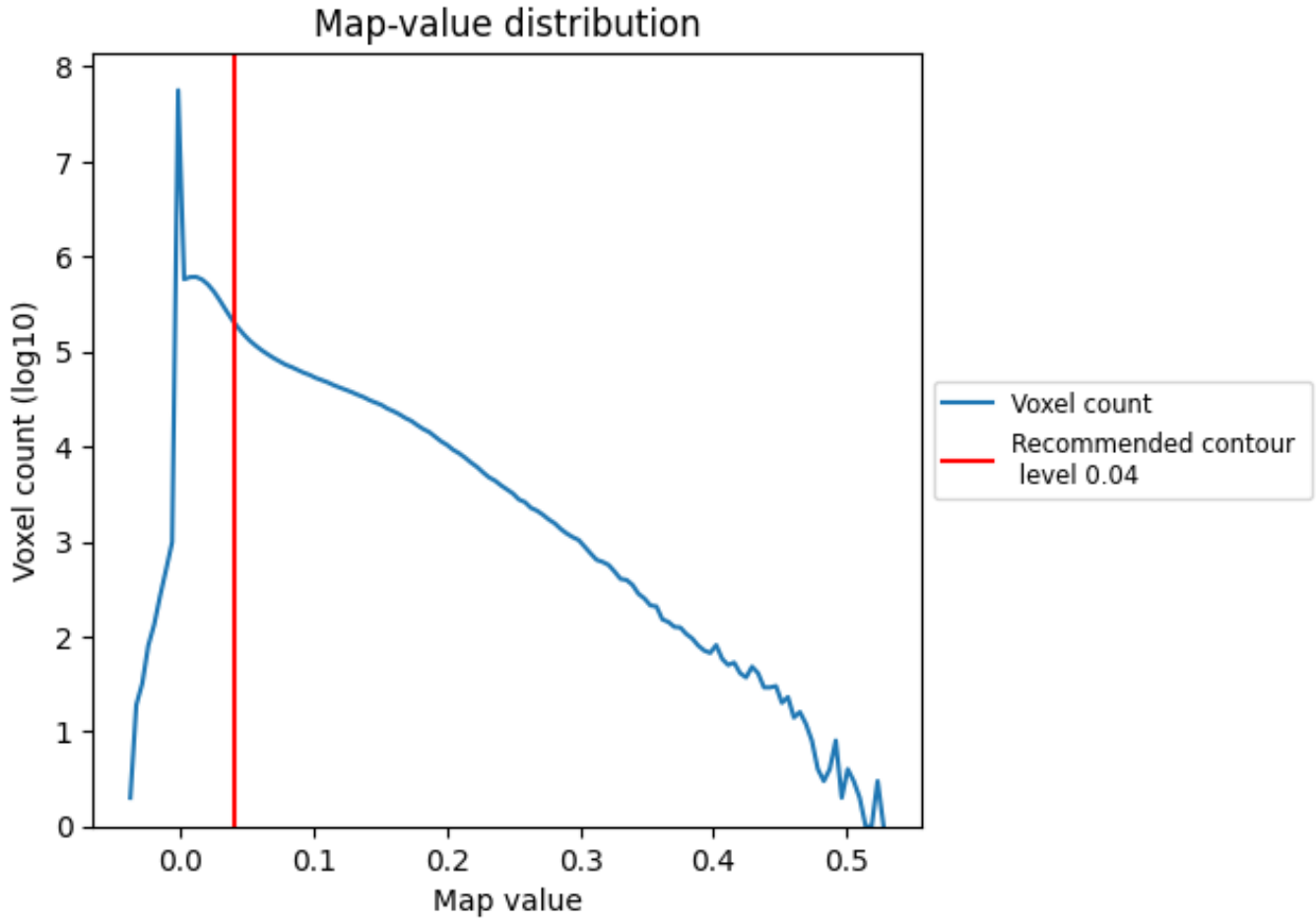
6.6 Mask visualisation (i)

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

7 Map analysis

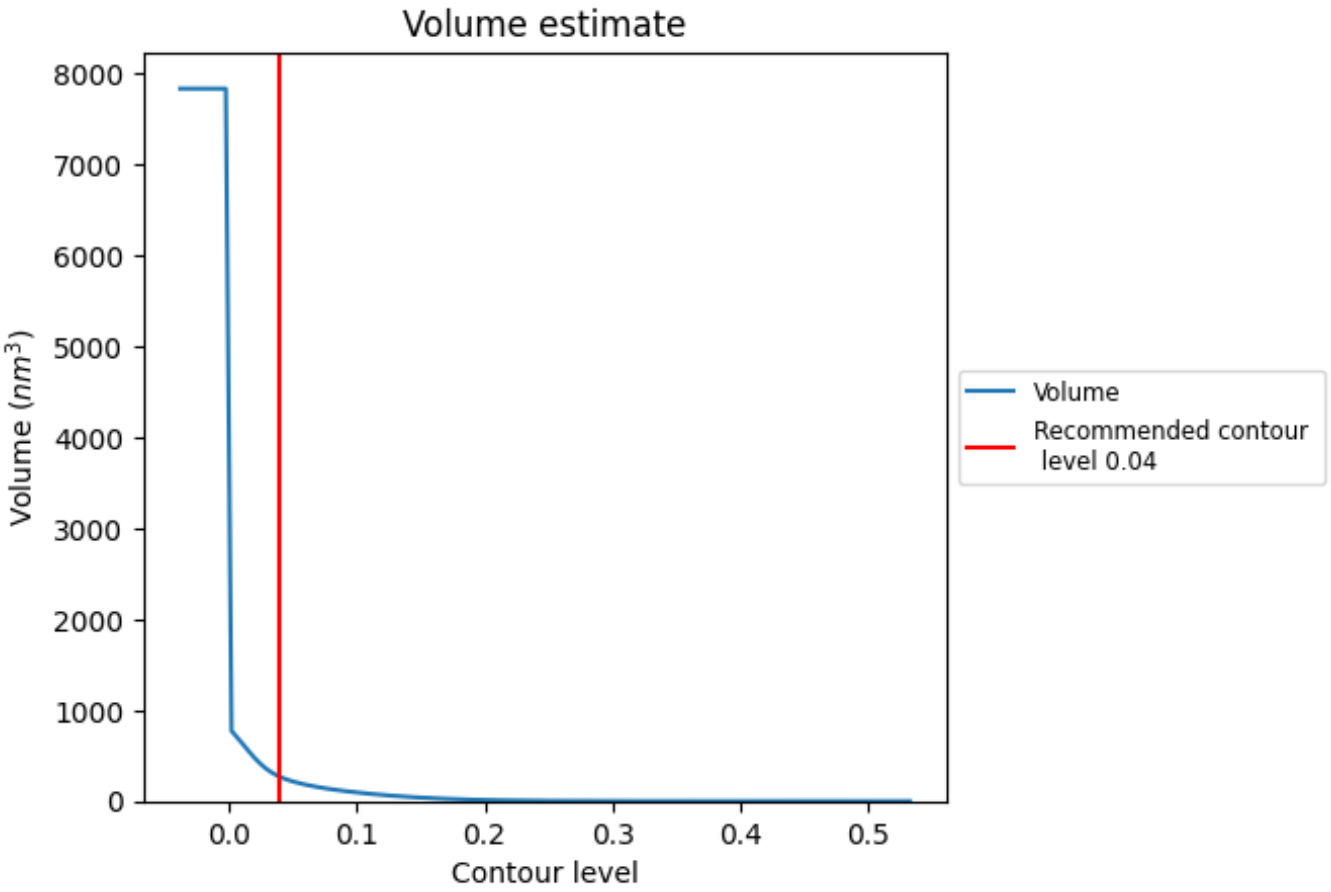
This section contains the results of statistical analysis of the map.

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 269 nm^3; this corresponds to an approximate mass of 243 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.

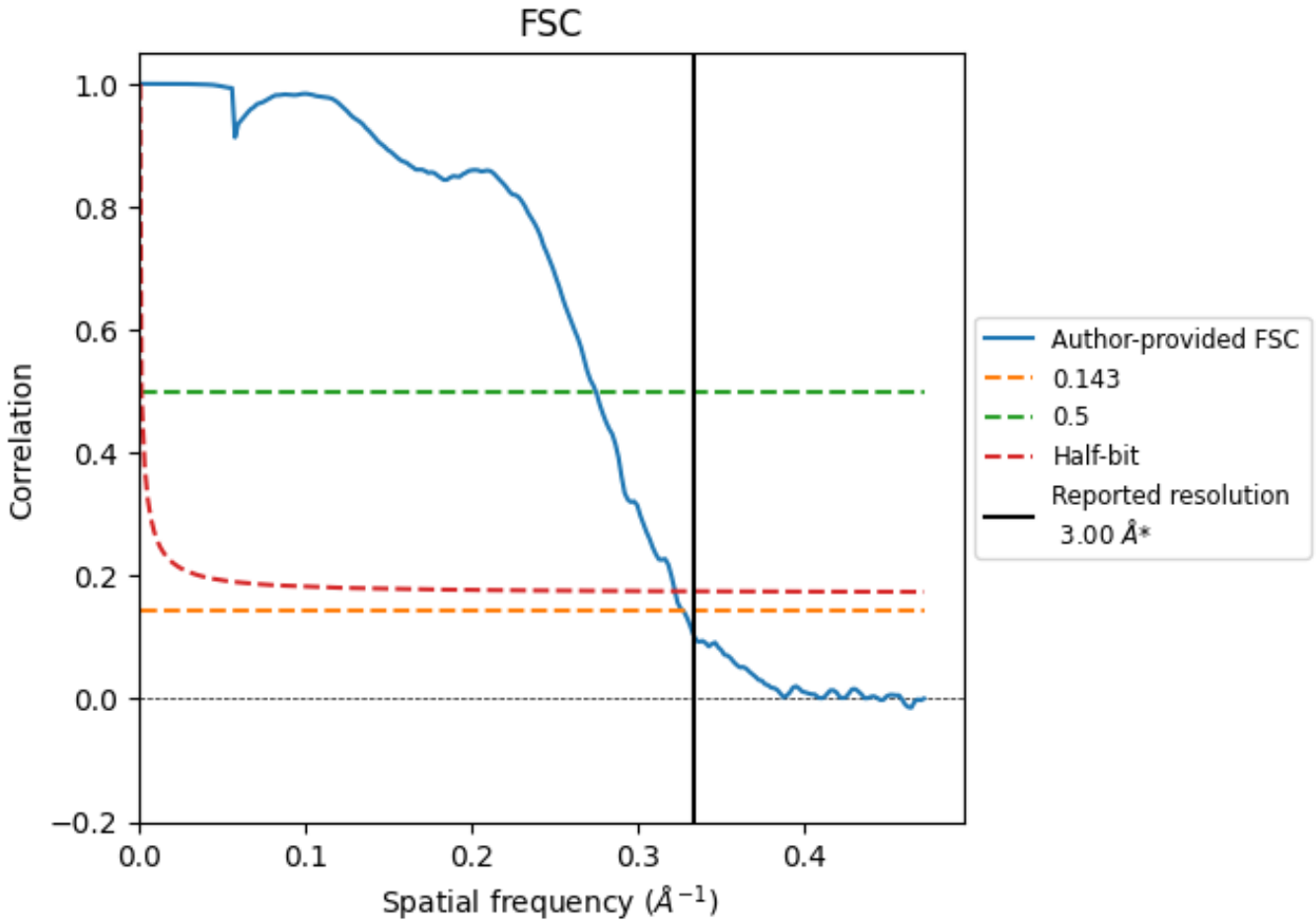
7.3 Rotationally averaged power spectrum

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)

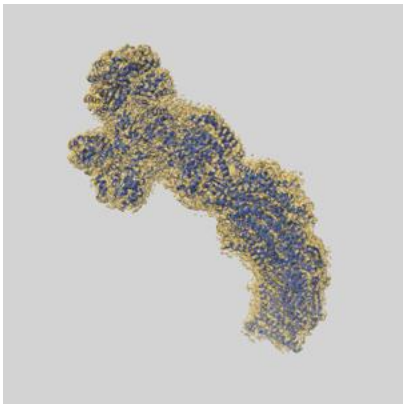
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.06	3.64	3.10
Unmasked-calculated*	-	-	-

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

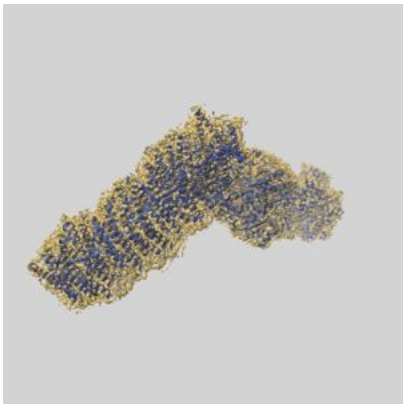
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13222 and PDB model 7P69. Per-residue inclusion information can be found in section 3 on page 12.

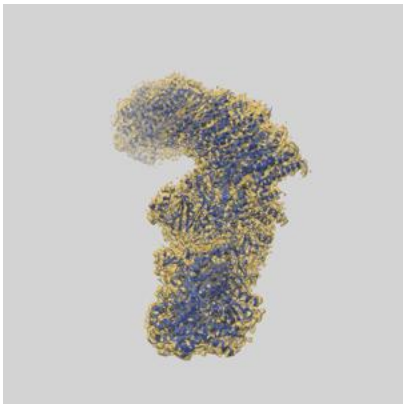
9.1 Map-model overlay



X



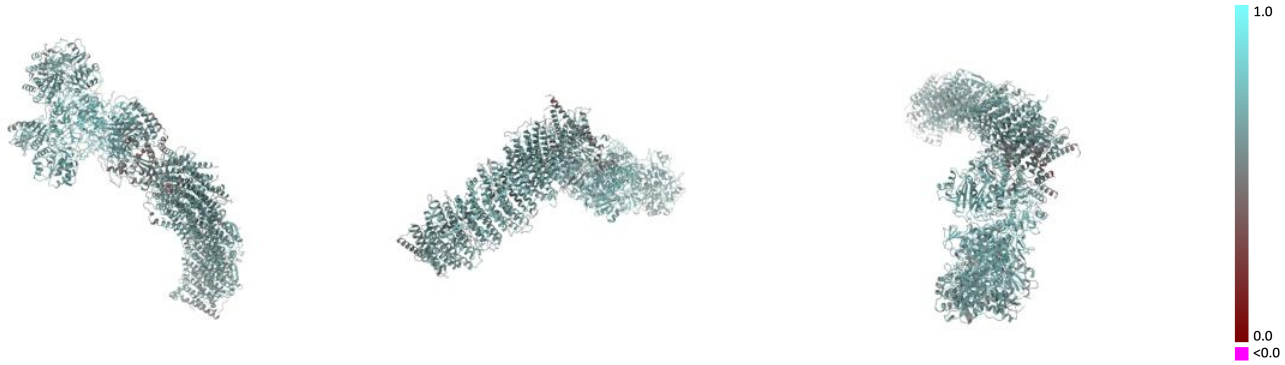
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

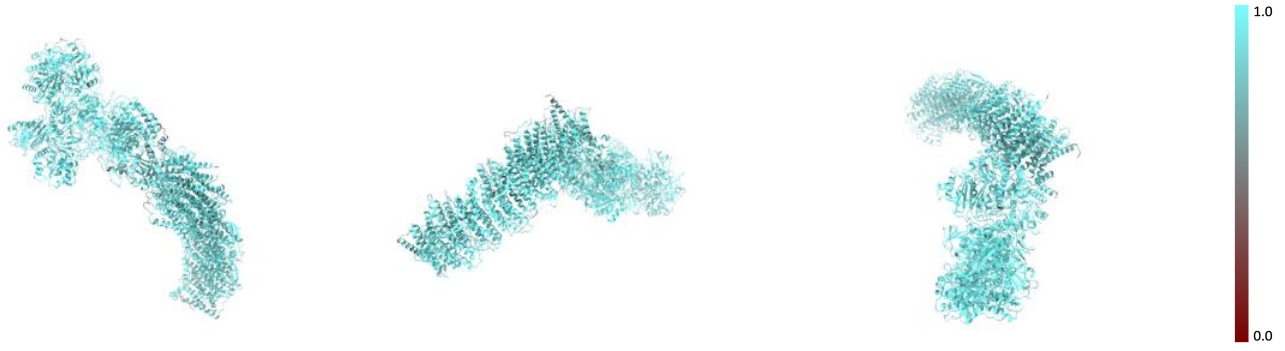
9.2 Q-score mapped to coordinate model (i)



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.

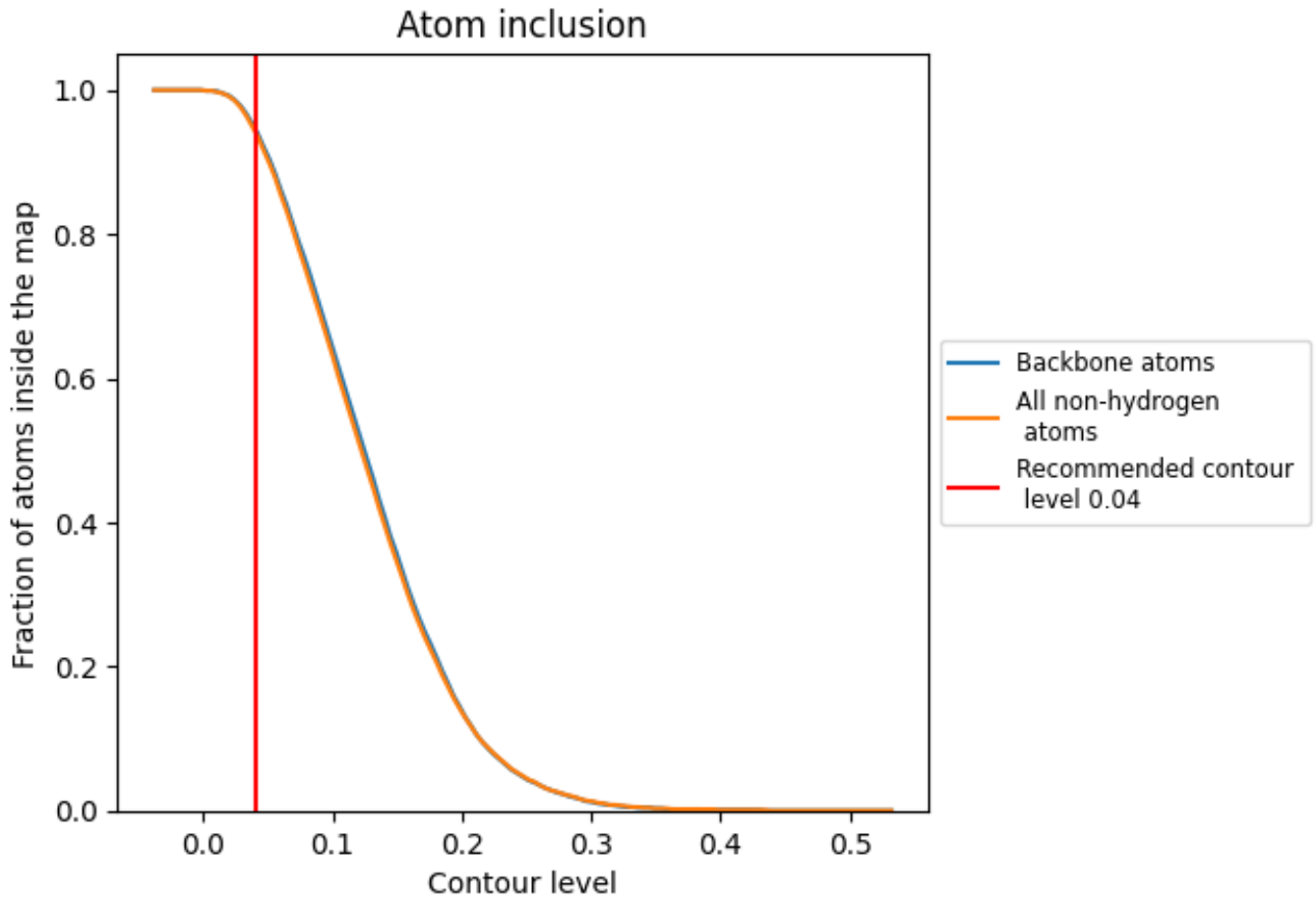
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% 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	0.9430	0.6290
A	0.9210	0.5950
B	0.9340	0.5950
C	0.9430	0.6430
E	0.9440	0.6200
F	0.9400	0.6120
G	0.9740	0.6780
H	0.8730	0.5580
I	0.9760	0.6900
J	0.9340	0.6060
K	0.9830	0.6460
L	0.9210	0.5980
M	0.9600	0.6300
N	0.9580	0.6350

