Full wwPDB EM Validation Report (i)

Jul 14, 2024 – 09:57 pm BST

PDB ID	:	7Z7V
EMDB ID	:	EMD-14538
Title	:	Complex I from E. coli, LMNG-purified, under Turnover at pH 6, Open-ready state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2022-03-16
Resolution	:	2.29 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:

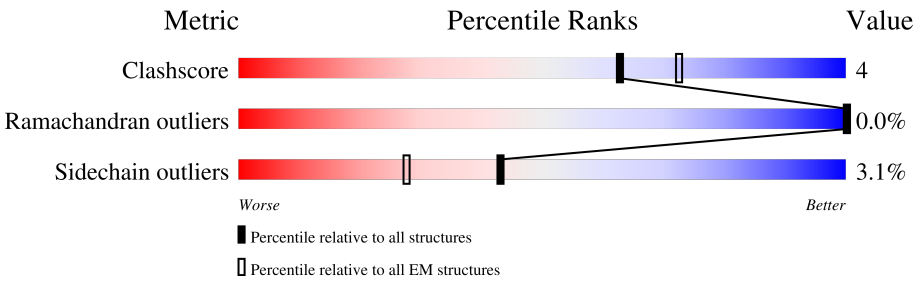
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.29 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	87% 11% •
2	E	166	• 80% 13% • 6%
3	G	908	88% 11%
4	C	596	• 87% 12% •
5	B	220	74% 16% 10%
6	I	180	88% 12%
7	H	325	• 82% 15% • •
8	A	147	• 59% 15% • 25%

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Mol	Chain	Length	Quality of chain
9	L	613	84% 14%
10	M	509	84% 14%
11	N	485	87% 11%
12	K	100	81% 18%
13	J	184	75% 11% 12%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 39106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	905	7027	4392	1269	1329	37	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	588	4739	3038	824	853	24	0	0

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	198	1568	994	272	286	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	180	1436	915	242	264	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	323	2544	1707	400	419	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	110	875	596	140	135	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	605	4627	3076	740	779	32	0	0

- Molecule 10 is a protein called NADH dehydrogenase I subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	504	3953	2661	617	646	29	0	0

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	478	3620	2418	571	611	20	0	0

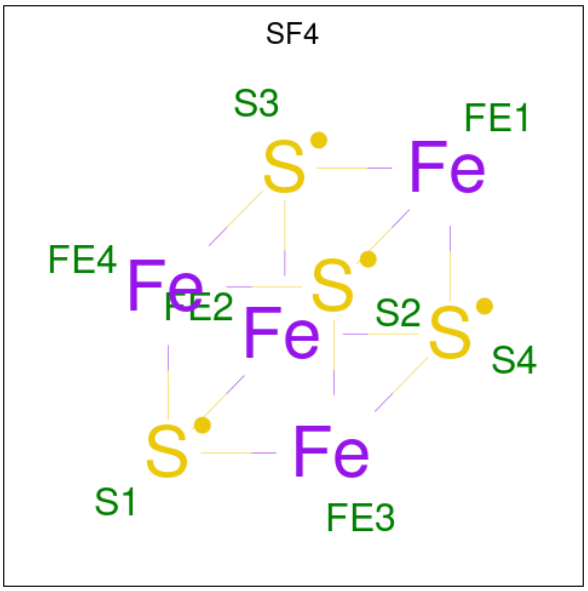
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	100	760	494	132	129	5	0	0

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit J.

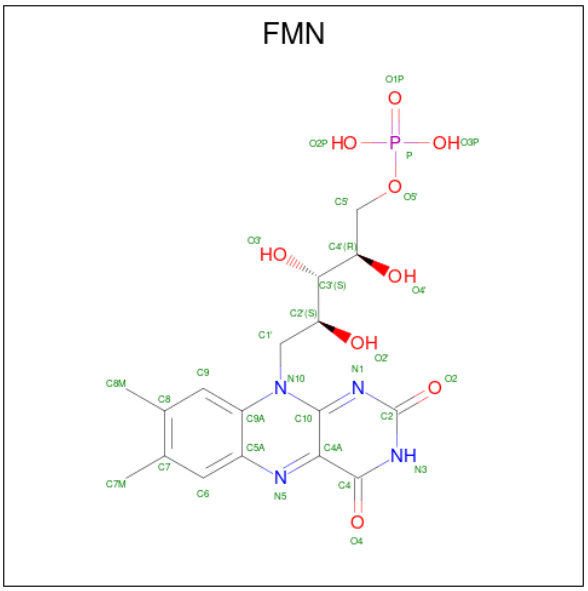
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	162	1226	824	188	207	7	0	0

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



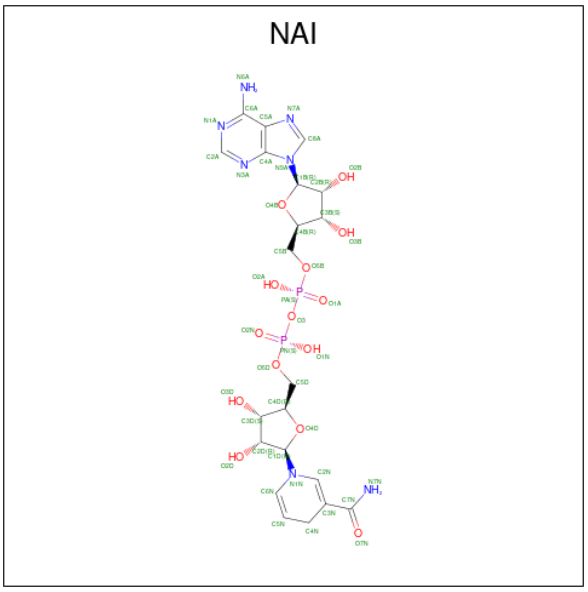
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
14	F	1	8	4	4	0
14	G	1	8	4	4	0
14	G	1	8	4	4	0
14	G	1	8	4	4	0
14	B	1	8	4	4	0
14	I	1	8	4	4	0
14	I	1	8	4	4	0

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



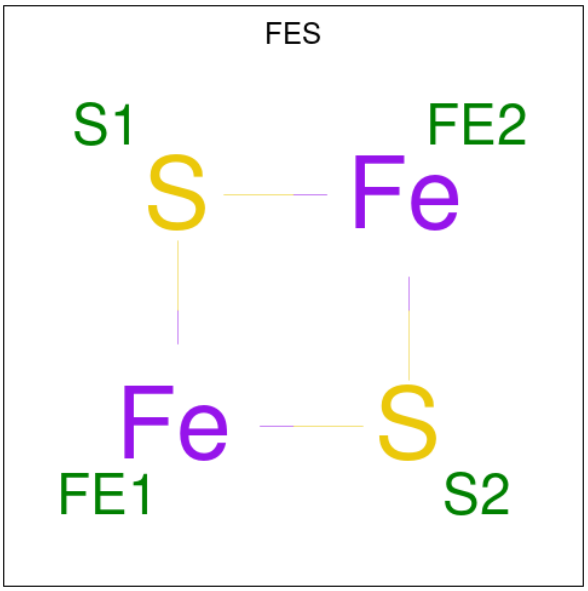
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
15	F	1	31	17	4	9	1	0

- 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
			Total	C	N	O	P	
16	F	1	44	21	7	14	2	0

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

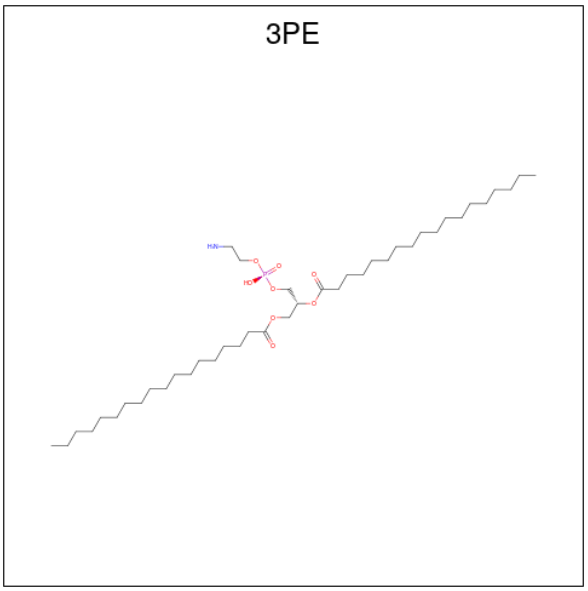


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	E	1	4	2	2	0
17	G	1	4	2	2	0

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

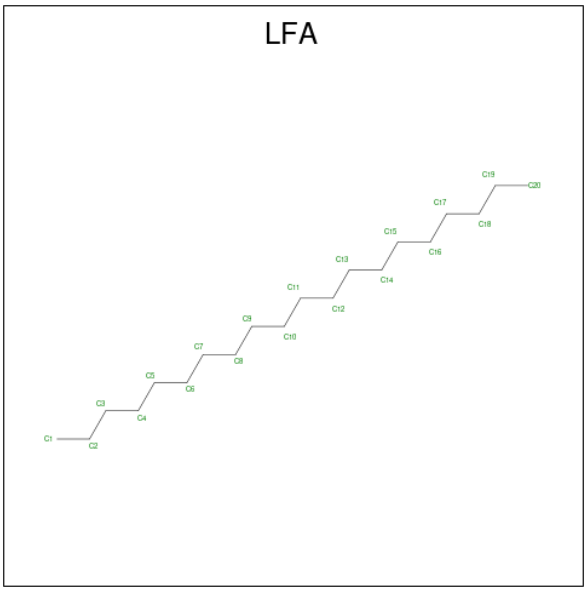
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
18	G	1	1	1	0

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



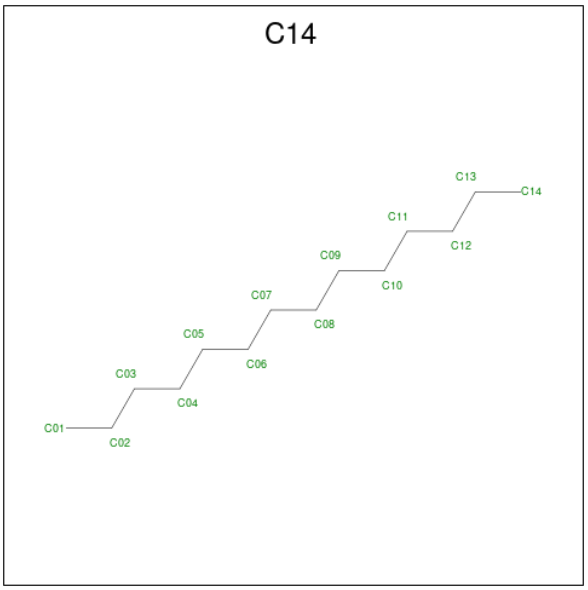
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	I	1	51	41	1	8	1	0
19	H	1	51	41	1	8	1	0
19	H	1	51	41	1	8	1	0
19	A	1	34	24	1	8	1	0
19	L	1	51	41	1	8	1	0
19	L	1	49	39	1	8	1	0
19	L	1	51	41	1	8	1	0
19	M	1	51	41	1	8	1	0
19	M	1	51	41	1	8	1	0
19	M	1	51	41	1	8	1	0
19	N	1	51	41	1	8	1	0
19	J	1	51	41	1	8	1	0

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



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
20	H	1	20	20	0
			Total	C	
20	L	1	20	20	0
			Total	C	
20	M	1	20	20	0

- Molecule 21 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
21	N	1	14	14	0

- Molecule 22 is water.

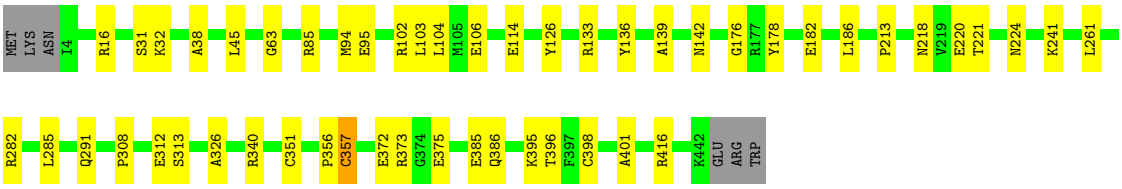
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
22	F	122	122	122	0
22	E	30	30	30	0
22	G	374	374	374	0
22	C	194	194	194	0
22	B	67	67	67	0
22	I	96	96	96	0
22	H	49	49	49	0
22	A	14	14	14	0
22	L	95	95	95	0
22	M	115	115	115	0
22	N	93	93	93	0
22	K	21	21	21	0
22	J	27	27	27	0

3 Residue-property plots (i)

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

• Molecule 1: NADH-quinone oxidoreductase subunit F

Chain F:

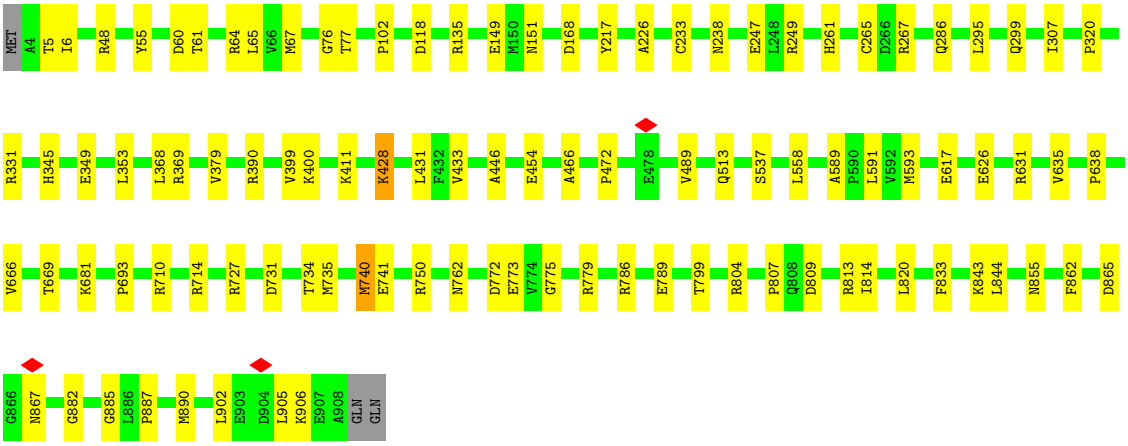


• Molecule 2: NADH dehydrogenase I subunit E

Chain E:

• Molecule 3: NADH-quinone oxidoreductase

Chain G:



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

Chain C: 87% 12%

MET THR ASP LEU THR ALA GLN E12 P13 I52 V60 K69 L74 L77 H78 G79 M80 L102 D106 R107 D110 N120 D121 L122 F127 N133 Y137 E140 P168 Y173 R176 E179 L192 E193 M194 L197 T198 M206 K207 R208

G209 T210 GLU N212 E213 D214 F215 M216 F217 L218 H224 R232 I233 V234 D248 H252 H253 R254 S264 E276 N283 I297 P300 E312 H319 S324 I327 M333 T334 P335 V336 F337 L349 M358 R374 D377 R378 L379 L391 R407

R442 Y447 Y464 M468 L474 P492 H497 T501 L520 Q521 N544 R562 L569 S582 I585 V598 D599 R600

- Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B: 74% 16% 10%

MET D2 R7 ILE ASP PRO ASN GLY GLU ASN ASP ARG TYR PRO LEU GLN LYS GLN E23 T26 D27 P28 L29 GLU GLN GLU VAL ASN LYS N36 V37 Y57 C63 E67 S71 A74 V78 V85 L86 R87 R91 G100 T101 C102 F103 V109 L113

I124 S125 M126 C129 F148 I149 V153 Y154 I155 P156 P159 R180 V186 V187 Y193 S199 P217 D218 E219 I220

- Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I: 88% 12%

M1 R15 I20 A24 R28 R43 I48 R59 L77 G78 K79 A80 E90 F96 L116 M122 P142 A154 G155 M156 D159 G160 K161 D162 K163 A166 P180

- Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H: 82% 15%

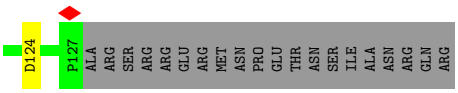
MET SER W3 I4 S5 P6 E7 C28 M32 E36 G41 L42 F43 R46 M64 I65 K66 E71 P75 K76 F77 S78 D79 I89 T92 L96 V103 S104 W107 I114 L117 F118 M121 A129 S137 Y141 S142 L143 R148

Q152 Q170 A171 G172 I179 N188 I201 R209 D213 E218 L221 A222 D223 E228 F238 Y242 I245 L255 G262 W270 M280 M281 F282 I283 L284 I285 R286 A287 R293 M298 S299 I311 Q325

- Molecule 8: NADH-quinone oxidoreductase subunit A

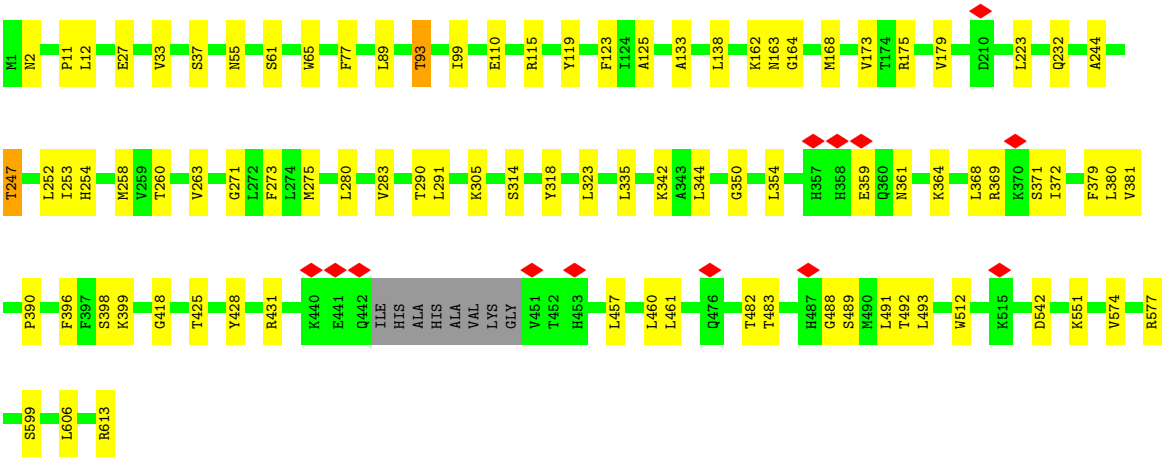
Chain A: 59% 15% 25%

MET SER MET SER THR S6 T7 I10 L20 L26 M30 L31 A41 R42 A43 R44 S45 K46 N47 V48 P49 F50 GLU SER GLY ILE ASP SER VAL GLY SER ALA ARG LEU R63 L64 K67 F68 Y69 L70 V71 F75 D79 V80 L83 L110 V115 R119



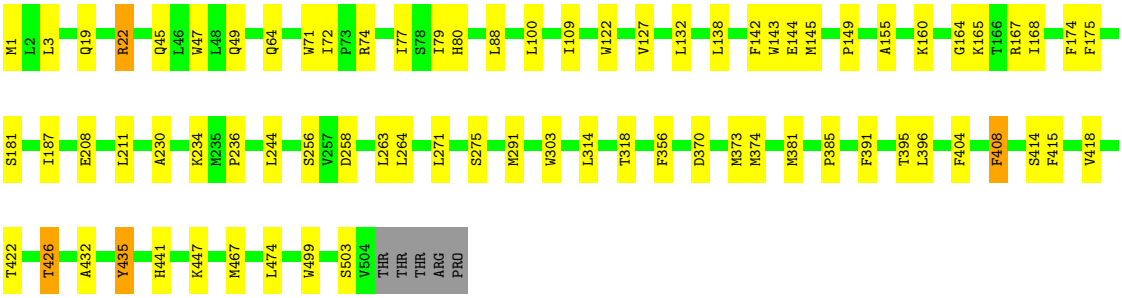
• Molecule 9: NADH dehydrogenase subunit L

Chain L:



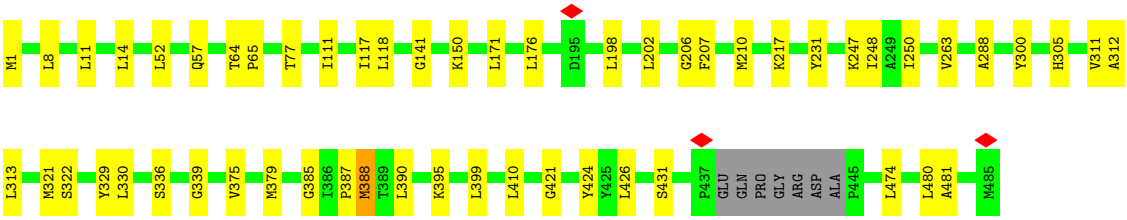
• Molecule 10: NADH dehydrogenase I subunit M

Chain M:



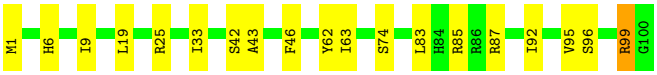
• Molecule 11: NADH-quinone oxidoreductase subunit N

Chain N:



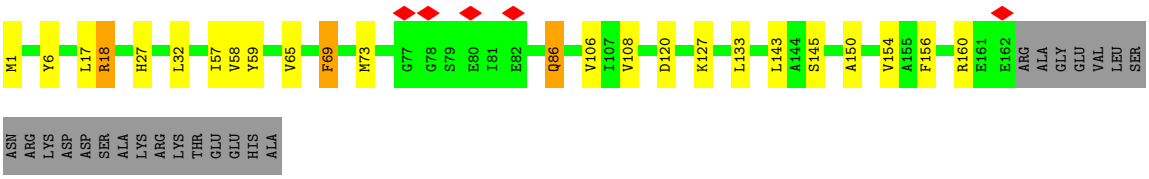
• Molecule 12: NADH-quinone oxidoreductase subunit K

Chain K:



• Molecule 13: NADH-quinone oxidoreductase subunit J

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	317174	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	0.748	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	153.0, 210.5, 237.5	wwPDB
Map dimensions	306, 421, 475	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FMN, C14, SF4, 3PE, LFA, NAI, CA

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	0.31	0/3486	0.52	0/4713
2	E	0.30	0/1248	0.53	0/1691
3	G	0.31	0/7178	0.55	0/9733
4	C	0.31	0/4869	0.55	1/6607 (0.0%)
5	B	0.32	0/1601	0.54	0/2168
6	I	0.32	0/1470	0.56	0/1985
7	H	0.33	0/2620	0.53	1/3565 (0.0%)
8	A	0.32	0/902	0.53	2/1226 (0.2%)
9	L	0.29	0/4745	0.49	0/6465
10	M	0.31	0/4074	0.53	1/5546 (0.0%)
11	N	0.31	0/3709	0.52	1/5061 (0.0%)
12	K	0.29	0/769	0.57	1/1040 (0.1%)
13	J	0.31	0/1252	0.49	0/1708
All	All	0.31	0/37923	0.53	7/51508 (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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	109	ILE	CG1-CB-CG2	-6.76	96.52	111.40
11	N	313	LEU	CA-CB-CG	6.52	130.29	115.30
8	A	83	LEU	CA-CB-CG	6.11	129.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	79	ASP	CB-CG-OD2	6.03	123.73	118.30
4	C	218	LEU	CA-CB-CG	5.62	128.23	115.30
12	K	95	VAL	CG1-CB-CG2	-5.44	102.20	110.90
8	A	110	LEU	CB-CG-CD1	-5.30	101.99	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	145	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3407	0	3374	29	0
2	E	1220	0	1187	14	0
3	G	7027	0	6829	48	0
4	C	4739	0	4650	40	0
5	B	1568	0	1553	19	0
6	I	1436	0	1415	15	0
7	H	2544	0	2591	35	0
8	A	875	0	890	20	0
9	L	4627	0	4770	42	0
10	M	3953	0	4053	41	0
11	N	3620	0	3790	33	0
12	K	760	0	817	14	0
13	J	1226	0	1297	23	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	1	0
16	F	44	0	27	3	0
17	E	4	0	0	0	0
17	G	4	0	0	0	0
18	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	34	0	42	3	0
19	H	102	0	164	7	0
19	I	51	0	82	1	0
19	J	51	0	82	5	0
19	L	151	0	239	6	0
19	M	153	0	246	3	0
19	N	51	0	82	2	0
20	H	20	0	42	2	0
20	L	20	0	42	0	0
20	M	20	0	42	1	0
21	N	14	0	30	1	0
22	A	14	0	0	0	0
22	B	67	0	0	0	0
22	C	194	0	0	2	0
22	E	30	0	0	2	0
22	F	122	0	0	1	0
22	G	374	0	0	1	0
22	H	49	0	0	0	0
22	I	96	0	0	0	0
22	J	27	0	0	0	0
22	K	21	0	0	2	0
22	L	95	0	0	1	0
22	M	115	0	0	0	0
22	N	93	0	0	0	0
All	All	39106	0	38355	333	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 (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:GLU:HB2	16:F:503:NAI:H42N	1.62	0.78
12:K:6:HIS:HD1	13:J:6:TYR:HH	1.35	0.73
10:M:181:SER:HB2	10:M:230:ALA:HA	1.74	0.67
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.77	0.67
1:F:357:CYS:HB2	1:F:401:ALA:HB2	1.78	0.65
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.79	0.64
7:H:36:GLU:HG2	7:H:283:ILE:HD12	1.78	0.64
3:G:862:PHE:HB3	3:G:905:LEU:HD23	1.79	0.63
11:N:385:GLY:HA3	11:N:395:LYS:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:276:GLU:HB3	4:C:283:ASN:HD21	1.64	0.62
12:K:85:ARG:NH1	22:K:201:HOH:O	2.33	0.61
12:K:9:ILE:HG12	13:J:108:VAL:HG22	1.82	0.61
9:L:179:VAL:HG22	10:M:426:THR:HG22	1.81	0.61
2:E:84:VAL:HB	2:E:127:THR:HG21	1.83	0.60
8:A:64:LEU:HD12	13:J:73:MET:HA	1.84	0.60
7:H:218:GLU:HB3	7:H:221:LEU:HD13	1.82	0.60
7:H:96:LEU:HD22	8:A:20:LEU:HD23	1.84	0.59
3:G:626:GLU:OE1	3:G:786:ARG:NH1	2.36	0.59
6:I:24:ALA:HB2	7:H:43:PHE:HD1	1.68	0.58
2:E:90:ARG:NH1	22:E:302:HOH:O	2.35	0.58
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.86	0.58
10:M:187:ILE:HD11	11:N:399:LEU:HD22	1.85	0.58
5:B:126:MET:HG3	5:B:155:ILE:HD12	1.86	0.58
10:M:19:GLN:OE1	10:M:22:ARG:NH1	2.35	0.57
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.86	0.57
4:C:77:LEU:HB3	4:C:137:TYR:HB3	1.86	0.56
1:F:373:ARG:NH1	1:F:375:GLU:OE1	2.37	0.56
4:C:283:ASN:ND2	22:C:714:HOH:O	2.36	0.56
19:H:403:3PE:H341	19:J:201:3PE:H321	1.87	0.56
4:C:232:ARG:HB2	4:C:248:ASP:HB3	1.87	0.56
11:N:118:LEU:HD22	13:J:143:LEU:HD13	1.86	0.56
19:H:401:3PE:H2H2	19:H:401:3PE:H3E2	1.87	0.56
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.87	0.56
9:L:247:THR:HG21	9:L:350:GLY:HA3	1.86	0.56
6:I:15:ARG:HH22	19:I:203:3PE:H112	1.69	0.55
8:A:68:PHE:HB3	13:J:69:PHE:HE2	1.70	0.55
8:A:119:ARG:NH1	19:A:201:3PE:O12	2.37	0.55
5:B:180:ARG:HB2	5:B:193:TYR:HB2	1.89	0.55
3:G:472:PRO:HG3	3:G:799:THR:HA	1.88	0.55
4:C:69:LYS:HB3	4:C:107:ARG:HG3	1.89	0.55
7:H:179:ILE:HG21	7:H:255:LEU:HD23	1.89	0.55
6:I:156:MET:O	6:I:161:LYS:NZ	2.40	0.54
3:G:727:ARG:HD3	4:C:179:GLU:HB2	1.90	0.54
9:L:164:GLY:CA	10:M:441:HIS:HE1	2.20	0.54
9:L:577:ARG:NH1	19:L:804:3PE:O22	2.33	0.54
10:M:122:TRP:CD2	10:M:149:PRO:HG3	2.42	0.54
3:G:814:ILE:HD11	3:G:902:LEU:HD13	1.91	0.53
1:F:16:ARG:HG2	1:F:32:LYS:HD2	1.91	0.53
1:F:218:ASN:ND2	15:F:502:FMN:O2	2.36	0.53
6:I:154:ALA:O	6:I:161:LYS:NZ	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:ILE:HG22	3:G:77:THR:HB	1.91	0.53
9:L:115:ARG:NH1	22:L:910:HOH:O	2.42	0.53
5:B:7:ARG:NH2	5:B:23:GLU:OE1	2.42	0.53
4:C:569:LEU:HD22	4:C:598:VAL:HG21	1.91	0.52
11:N:312:ALA:O	11:N:322:SER:OG	2.26	0.52
11:N:57:GLN:NE2	19:N:602:3PE:O32	2.43	0.52
3:G:5:THR:O	3:G:76:GLY:N	2.40	0.52
10:M:414:SER:O	10:M:418:VAL:N	2.34	0.52
9:L:368:LEU:HD23	9:L:372:ILE:HD11	1.91	0.52
2:E:90:ARG:NH1	22:E:305:HOH:O	2.42	0.51
2:E:123:ASP:OD1	2:E:123:ASP:N	2.39	0.51
7:H:148:ARG:NH1	7:H:218:GLU:OE2	2.43	0.51
12:K:99:ARG:NH1	22:K:203:HOH:O	2.43	0.51
4:C:254:ARG:HG3	5:B:103:PHE:HE1	1.74	0.51
7:H:76:LYS:HE2	8:A:47:ASN:HD21	1.75	0.51
6:I:59:ARG:NH2	6:I:142:PRO:O	2.43	0.51
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.92	0.51
5:B:91:ARG:NH2	8:A:46:LYS:O	2.44	0.51
19:L:801:3PE:H2A2	19:L:803:3PE:H2I2	1.92	0.50
1:F:282:ARG:HB2	1:F:285:LEU:HD12	1.93	0.50
8:A:41:ALA:O	8:A:46:LYS:NZ	2.40	0.50
5:B:101:THR:HA	5:B:129:CYS:HB3	1.92	0.50
7:H:213:ASP:OD1	7:H:213:ASP:N	2.41	0.50
7:H:242:TYR:HA	7:H:245:ILE:HD12	1.94	0.50
10:M:3:LEU:HB3	10:M:132:LEU:HD13	1.93	0.50
4:C:69:LYS:HG2	4:C:106:ASP:HB3	1.94	0.50
6:I:48:ILE:HG12	6:I:116:LEU:HG	1.94	0.50
11:N:8:LEU:HD23	11:N:11:LEU:HD12	1.94	0.50
8:A:80:VAL:O	8:A:83:LEU:HG	2.12	0.50
4:C:334:THR:OG1	7:H:287:ALA:O	2.24	0.49
11:N:171:LEU:HD23	12:K:42:SER:HB2	1.93	0.49
4:C:110:ASP:OD2	4:C:442:ARG:NH1	2.46	0.49
5:B:217:PRO:HB3	6:I:43:ARG:HB3	1.92	0.49
10:M:404:PHE:O	10:M:408:PHE:HB2	2.12	0.49
9:L:344:LEU:HB2	9:L:460:LEU:HB3	1.94	0.49
10:M:142:PHE:HA	10:M:145:MET:HG2	1.95	0.49
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.95	0.49
2:E:87:HIS:NE2	2:E:166:LYS:OXT	2.46	0.49
3:G:261:HIS:CD2	3:G:369:ARG:HD2	2.48	0.49
3:G:295:LEU:HA	3:G:299:GLN:HE21	1.78	0.49
4:C:407:ARG:NH2	22:C:729:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:401:3PE:H3B2	19:H:401:3PE:H2A1	1.95	0.49
3:G:168:ASP:OD1	3:G:400:LYS:NZ	2.46	0.49
3:G:865:ASP:OD2	3:G:867:ASN:ND2	2.45	0.49
8:A:83:LEU:HD23	13:J:58:VAL:HG21	1.95	0.49
3:G:887:PRO:HB2	3:G:890:MET:HG3	1.95	0.48
1:F:220:GLU:O	1:F:224:ASN:ND2	2.40	0.48
9:L:163:ASN:HD22	9:L:244:ALA:HB1	1.79	0.48
10:M:499:TRP:O	10:M:503:SER:OG	2.29	0.48
4:C:337:PHE:HB3	5:B:74:ALA:HB2	1.95	0.48
5:B:186:VAL:HG23	5:B:187:VAL:HG23	1.95	0.48
7:H:137:SER:HB2	7:H:228:GLU:HG3	1.96	0.48
7:H:209:ARG:HD3	7:H:245:ILE:HD11	1.96	0.48
9:L:431:ARG:HG3	9:L:512:TRP:CE2	2.49	0.48
1:F:63:GLY:O	16:F:503:NAI:H2N	2.13	0.48
1:F:308:PRO:O	1:F:313:SER:OG	2.28	0.48
4:C:52:ILE:HD12	4:C:60:VAL:HG21	1.95	0.47
1:F:176:GLY:O	2:E:77:SER:OG	2.32	0.47
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.95	0.47
4:C:544:ASN:ND2	4:C:562:ARG:O	2.45	0.47
11:N:1:MET:H3	11:N:65:PRO:HD3	1.79	0.47
11:N:305:HIS:ND1	11:N:329:TYR:OH	2.38	0.47
3:G:431:LEU:O	3:G:446:ALA:N	2.47	0.47
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.96	0.47
8:A:67:LYS:HD3	8:A:70:LEU:HD12	1.96	0.47
10:M:127:VAL:HG11	10:M:264:LEU:HD13	1.96	0.47
3:G:307:ILE:HG21	3:G:591:LEU:HD13	1.97	0.47
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.96	0.47
11:N:421:GLY:HA2	11:N:424:TYR:CE2	2.50	0.47
5:B:26:THR:OG1	5:B:27:ASP:N	2.47	0.47
9:L:89:LEU:O	9:L:93:THR:OG1	2.27	0.47
9:L:260:THR:HB	9:L:335:LEU:HD11	1.96	0.47
10:M:314:LEU:O	10:M:318:THR:HG23	2.14	0.47
1:F:176:GLY:HA3	2:E:78:GLN:HG2	1.97	0.47
2:E:86:ARG:NH1	2:E:166:LYS:O	2.48	0.47
10:M:381:MET:HB2	10:M:385:PRO:HD3	1.96	0.47
19:H:403:3PE:H3B1	19:J:201:3PE:H3B2	1.97	0.47
7:H:71:GLU:OE2	8:A:46:LYS:NZ	2.41	0.47
9:L:273:PHE:HB3	9:L:280:LEU:HD13	1.97	0.47
10:M:391:PHE:O	10:M:395:THR:HG23	2.15	0.47
1:F:356:PRO:HB2	1:F:396:THR:HG22	1.97	0.46
3:G:741:GLU:OE2	4:C:176:ARG:NH1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:115:VAL:HG21	19:A:201:3PE:H252	1.96	0.46
11:N:231:TYR:OH	11:N:247:LYS:NZ	2.48	0.46
7:H:103:VAL:HG21	20:H:402:LFA:H81	1.97	0.46
3:G:149:GLU:OE2	6:I:163:LYS:NZ	2.42	0.46
4:C:391:LEU:HD22	4:C:474:LEU:HD22	1.97	0.46
7:H:28:CYS:O	7:H:32:MET:HB2	2.15	0.46
10:M:236:PRO:HG3	10:M:244:LEU:HD22	1.96	0.46
13:J:120:ASP:OD1	13:J:120:ASP:N	2.42	0.46
3:G:320:PRO:HB2	3:G:537:SER:HB2	1.98	0.46
10:M:474:LEU:HD22	20:M:1002:LFA:H41	1.97	0.46
2:E:112:LYS:HD2	2:E:162:LEU:HD12	1.98	0.46
3:G:286:GLN:HB2	3:G:295:LEU:HD11	1.98	0.46
1:F:38:ALA:HB2	1:F:114:GLU:HG3	1.97	0.46
3:G:428:LYS:HE3	3:G:428:LYS:HB3	1.76	0.46
3:G:731:ASP:OD2	3:G:734:THR:OG1	2.31	0.46
11:N:141:GLY:HA3	13:J:154:VAL:HG22	1.97	0.46
3:G:399:VAL:HG13	3:G:428:LYS:HB2	1.97	0.46
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.97	0.46
10:M:45:GLN:HE22	10:M:49:GLN:HE21	1.63	0.46
4:C:133:ASN:OD1	4:C:133:ASN:N	2.43	0.45
3:G:843:LYS:HB2	3:G:885:GLY:HA3	1.98	0.45
4:C:374:ARG:NH2	5:B:218:ASP:OD2	2.49	0.45
19:H:403:3PE:N	19:J:201:3PE:O14	2.46	0.45
10:M:370:ASP:HB3	10:M:373:MET:HG2	1.98	0.45
1:F:386:GLN:NE2	22:F:618:HOH:O	2.49	0.45
3:G:247:GLU:HG3	3:G:249:ARG:HE	1.81	0.45
3:G:267:ARG:HA	3:G:833:PHE:HZ	1.82	0.45
7:H:75:PRO:HB2	7:H:78:SER:HB3	1.98	0.45
4:C:78:HIS:HE2	4:C:140:GLU:HG2	1.81	0.45
9:L:33:VAL:O	9:L:37:SER:OG	2.30	0.45
2:E:116:LYS:HD3	2:E:116:LYS:HA	1.73	0.45
10:M:72:ILE:HB	10:M:77:ILE:HB	1.97	0.45
10:M:175:PHE:CD1	11:N:426:LEU:HD21	2.51	0.45
1:F:85:ARG:HG2	1:F:213:PRO:HB2	1.98	0.45
11:N:330:LEU:HD23	11:N:330:LEU:HA	1.81	0.45
11:N:336:SER:HA	11:N:379:MET:SD	2.56	0.45
11:N:481:ALA:HB2	19:N:602:3PE:H241	1.99	0.45
4:C:297:ILE:HG12	4:C:497:HIS:CG	2.51	0.45
7:H:311:ILE:HD11	19:A:201:3PE:H371	1.98	0.45
9:L:457:LEU:O	9:L:461:LEU:HB2	2.17	0.45
9:L:488:GLY:O	9:L:492:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:170:GLN:NE2	7:H:188:ASN:OD1	2.49	0.45
8:A:31:LEU:HD23	8:A:31:LEU:HA	1.83	0.45
2:E:106:GLN:O	2:E:110:GLU:HG2	2.16	0.45
7:H:201:ILE:HG12	19:H:401:3PE:H381	1.98	0.45
13:J:1:MET:HB2	19:J:201:3PE:H112	1.98	0.45
5:B:67:GLU:HG3	5:B:159:PRO:HB2	1.98	0.44
7:H:41:GLY:HA2	7:H:46:ARG:HG3	2.00	0.44
5:B:156:PRO:HG2	6:I:122:MET:HB3	1.99	0.44
7:H:79:ASP:OD1	13:J:27:HIS:NE2	2.42	0.44
10:M:208:GLU:HA	10:M:211:LEU:HD12	2.00	0.44
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.52	0.44
11:N:339:GLY:HA3	11:N:379:MET:HE3	1.99	0.44
11:N:387:PRO:O	11:N:388:MET:HG2	2.16	0.44
9:L:606:LEU:HB3	13:J:106:VAL:HG11	1.98	0.44
3:G:102:PRO:HG3	3:G:151:ASN:HB3	1.98	0.44
10:M:71:TRP:HB2	10:M:79:ILE:HG13	1.98	0.44
7:H:172:GLY:O	13:J:127:LYS:NZ	2.51	0.44
7:H:262:GLY:HA3	7:H:270:TRP:CD1	2.52	0.44
13:J:18:ARG:HE	13:J:18:ARG:HB3	1.62	0.44
1:F:178:TYR:OH	16:F:503:NAI:H5N	2.18	0.44
1:F:340:ARG:NE	1:F:372:GLU:OE1	2.46	0.44
4:C:224:HIS:CE1	4:C:585:ILE:HD11	2.53	0.44
5:B:57:TYR:HE2	5:B:113:LEU:HD13	1.82	0.44
5:B:148:PHE:CD2	5:B:149:ILE:HG23	2.52	0.44
8:A:7:THR:HA	8:A:10:ILE:HG12	1.99	0.44
13:J:57:ILE:HG22	13:J:58:VAL:HG23	2.00	0.44
2:E:138:ASP:OD1	2:E:138:ASP:N	2.48	0.44
7:H:89:ILE:HB	7:H:129:ALA:HB2	1.99	0.44
19:M:1004:3PE:H351	21:N:601:C14:H122	2.00	0.44
4:C:324:SER:HB2	4:C:336:VAL:HA	2.00	0.44
3:G:267:ARG:HB2	3:G:820:LEU:HG	1.99	0.43
7:H:36:GLU:OE2	7:H:286:ARG:NH1	2.49	0.43
7:H:114:ILE:HB	7:H:117:LEU:HB2	2.00	0.43
6:I:24:ALA:HB2	7:H:43:PHE:CD1	2.51	0.43
12:K:33:ILE:HG23	13:J:32:LEU:HD22	1.99	0.43
1:F:182:GLU:O	1:F:186:LEU:N	2.44	0.43
3:G:379:VAL:HB	3:G:433:VAL:HG12	2.00	0.43
9:L:173:VAL:HG22	19:M:1001:3PE:H391	1.99	0.43
3:G:118:ASP:OD1	3:G:762:ASN:ND2	2.47	0.43
9:L:551:LYS:HA	9:L:551:LYS:HD3	1.67	0.43
7:H:103:VAL:HG11	20:H:402:LFA:H61	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:361:ASN:HB3	9:L:364:LYS:HG2	1.99	0.43
1:F:103:LEU:HD22	1:F:261:LEU:HD23	2.01	0.43
4:C:74:LEU:HA	4:C:102:LEU:HD23	2.00	0.43
4:C:276:GLU:HB3	4:C:283:ASN:ND2	2.33	0.43
6:I:161:LYS:HE3	6:I:166:ALA:HB2	2.00	0.43
9:L:168:MET:HG3	10:M:441:HIS:CE1	2.53	0.43
3:G:710:ARG:NH1	22:G:1136:HOH:O	2.43	0.43
5:B:85:VAL:HG12	5:B:87:ARG:HH11	1.83	0.43
9:L:425:THR:HA	9:L:428:TYR:CE2	2.54	0.43
10:M:155:ALA:O	10:M:167:ARG:NH1	2.52	0.43
12:K:43:ALA:HB1	12:K:62:TYR:HD1	1.84	0.43
3:G:226:ALA:HB3	3:G:635:VAL:HG22	2.00	0.43
9:L:164:GLY:CA	10:M:441:HIS:CE1	3.01	0.43
9:L:164:GLY:O	10:M:441:HIS:HE1	2.02	0.43
9:L:318:TYR:OH	9:L:418:GLY:O	2.25	0.43
19:L:804:3PE:H2F1	19:M:1003:3PE:H3D2	2.00	0.43
1:F:106:GLU:O	1:F:142:ASN:ND2	2.49	0.42
3:G:772:ASP:OD1	3:G:773:GLU:N	2.50	0.42
8:A:64:LEU:HB2	13:J:73:MET:HG3	2.01	0.42
7:H:141:TYR:HB3	7:H:223:ASP:HA	2.01	0.42
9:L:263:VAL:HG13	9:L:323:LEU:HD11	2.01	0.42
9:L:354:LEU:HD23	9:L:354:LEU:HA	1.91	0.42
11:N:176:LEU:HD22	11:N:202:LEU:HD11	2.01	0.42
11:N:198:LEU:HD21	11:N:263:VAL:HA	2.00	0.42
7:H:298:MET:HE1	8:A:71:VAL:HG21	2.01	0.42
9:L:133:ALA:HB1	9:L:138:LEU:HB3	2.01	0.42
1:F:395:LYS:HE3	3:G:65:LEU:HD12	2.02	0.42
11:N:52:LEU:HD23	11:N:52:LEU:HA	1.91	0.42
11:N:390:LEU:HD21	11:N:474:LEU:HD22	2.01	0.42
12:K:92:ILE:HD12	12:K:92:ILE:HA	1.91	0.42
1:F:16:ARG:NH1	1:F:32:LYS:O	2.49	0.42
4:C:120:ASN:OD1	4:C:120:ASN:N	2.52	0.42
4:C:464:TYR:O	4:C:468:MET:HG2	2.20	0.42
8:A:75:PHE:O	8:A:79:ASP:HB2	2.19	0.42
10:M:263:LEU:HD11	10:M:356:PHE:HD2	1.83	0.42
11:N:311:VAL:HG22	11:N:410:LEU:HD13	2.01	0.42
3:G:558:LEU:HD22	3:G:589:ALA:HB2	2.02	0.42
2:E:141:PRO:HG2	2:E:153:LEU:HB2	2.01	0.42
3:G:353:LEU:HD21	3:G:513:GLN:HG3	2.01	0.42
8:A:69:TYR:HB2	13:J:73:MET:HE1	2.02	0.42
3:G:454:GLU:OE1	3:G:813:ARG:NH1	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:285:ILE:HD13	7:H:285:ILE:HA	1.86	0.42
9:L:390:PRO:HA	9:L:396:PHE:CG	2.54	0.42
3:G:368:LEU:HD21	3:G:390:ARG:HB3	2.02	0.42
9:L:99:ILE:HG21	9:L:252:LEU:HG	2.01	0.42
9:L:271:GLY:O	9:L:275:MET:HG3	2.20	0.42
2:E:98:HIS:HA	2:E:102:TYR:HD1	1.84	0.42
3:G:345:HIS:NE2	3:G:349:GLU:OE1	2.52	0.42
3:G:772:ASP:HB3	3:G:779:ARG:HA	2.01	0.42
9:L:65:TRP:HB2	19:L:803:3PE:H122	2.01	0.42
9:L:175:ARG:NH2	10:M:396:LEU:O	2.52	0.42
11:N:206:GLY:O	11:N:210:MET:HG3	2.20	0.41
11:N:288:ALA:HB2	11:N:300:TYR:HB2	2.01	0.41
13:J:86:GLN:H	13:J:86:GLN:HG3	1.64	0.41
5:B:124:ILE:HG12	5:B:153:VAL:HB	2.01	0.41
1:F:102:ARG:O	1:F:106:GLU:HB2	2.21	0.41
4:C:327:ILE:HG21	4:C:335:PRO:HG2	2.01	0.41
9:L:380:LEU:HD23	9:L:380:LEU:HA	1.89	0.41
13:J:65:VAL:O	13:J:69:PHE:HB2	2.21	0.41
3:G:466:ALA:HB3	3:G:489:VAL:HG21	2.02	0.41
3:G:693:PRO:HG2	3:G:735:MET:SD	2.61	0.41
4:C:12:GLU:HA	4:C:13:PRO:HD3	1.90	0.41
6:I:80:ALA:HB2	6:I:90:GLU:HB2	2.01	0.41
7:H:66:LYS:HB3	7:H:66:LYS:HE3	1.85	0.41
10:M:143:TRP:CZ2	10:M:234:LYS:HE2	2.55	0.41
10:M:164:GLY:O	10:M:168:ILE:HG12	2.21	0.41
10:M:271:LEU:HA	10:M:275:SER:HB2	2.03	0.41
13:J:156:PHE:CZ	13:J:160:ARG:HD3	2.56	0.41
3:G:369:ARG:NH2	3:G:775:GLY:O	2.48	0.41
3:G:714:ARG:NH1	3:G:740:MET:SD	2.93	0.41
4:C:334:THR:HG21	6:I:20:ILE:HD12	2.02	0.41
8:A:26:LEU:O	8:A:30:MET:HG3	2.20	0.41
11:N:375:VAL:O	11:N:379:MET:HG2	2.21	0.41
12:K:43:ALA:HB1	12:K:62:TYR:CD1	2.56	0.41
3:G:844:LEU:HD23	3:G:844:LEU:HA	1.95	0.41
12:K:83:LEU:O	12:K:87:ARG:HB2	2.20	0.41
3:G:217:TYR:HB3	6:I:79:LYS:HD2	2.03	0.41
4:C:168:PRO:HA	4:C:173:TYR:CG	2.56	0.41
7:H:118:PHE:HA	7:H:121:MET:SD	2.60	0.41
9:L:232:GLN:HA	9:L:290:THR:HG21	2.03	0.41
10:M:144:GLU:HB2	11:N:387:PRO:HG2	2.02	0.41
10:M:258:ASP:O	10:M:263:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:501:THR:HG23	4:C:521:GLN:HB3	2.02	0.41
7:H:92:THR:O	7:H:96:LEU:HG	2.21	0.41
9:L:253:ILE:HG23	9:L:258:MET:HB3	2.03	0.41
11:N:14:LEU:HD21	13:J:143:LEU:HD11	2.03	0.41
12:K:63:ILE:HD13	13:J:133:LEU:HD11	2.03	0.41
3:G:48:ARG:HA	3:G:67:MET:SD	2.61	0.41
3:G:55:TYR:HB3	3:G:60:ASP:HB3	2.02	0.41
3:G:807:PRO:HB3	3:G:882:GLY:HA3	2.03	0.41
4:C:300:PRO:HG3	4:C:492:PRO:HG2	2.03	0.41
9:L:119:TYR:OH	19:L:801:3PE:O32	2.30	0.41
19:L:804:3PE:H232	19:L:804:3PE:H262	1.93	0.41
10:M:160:LYS:HD3	10:M:160:LYS:HA	1.90	0.41
1:F:385:GLU:OE2	1:F:416:ARG:NH1	2.45	0.40
4:C:192:LEU:HD21	5:B:109:VAL:HG22	2.04	0.40
4:C:520:LEU:HD23	4:C:520:LEU:HA	1.91	0.40
5:B:100:GLY:HA2	14:B:301:SF4:S4	2.62	0.40
9:L:253:ILE:HG22	9:L:254:HIS:HD2	1.86	0.40
12:K:25:ARG:HD2	12:K:25:ARG:HA	1.82	0.40
1:F:104:LEU:HD23	1:F:104:LEU:HA	1.94	0.40
1:F:291:GLN:O	1:F:326:ALA:HA	2.21	0.40
4:C:122:LEU:HD23	4:C:122:LEU:HA	1.92	0.40
4:C:252:HIS:O	4:C:252:HIS:ND1	2.51	0.40
4:C:349:LEU:HD13	4:C:379:LEU:HB2	2.03	0.40
6:I:48:ILE:HB	6:I:96:PHE:HZ	1.87	0.40
10:M:100:LEU:HD22	10:M:467:MET:HB2	2.03	0.40
4:C:333:MET:H	4:C:333:MET:HG3	1.64	0.40
9:L:291:LEU:HA	9:L:314:SER:HA	2.04	0.40
9:L:599:SER:HB3	12:K:19:LEU:HD21	2.04	0.40
1:F:45:LEU:HD23	1:F:45:LEU:HA	1.94	0.40
1:F:133:ARG:HD3	1:F:136:TYR:CE1	2.56	0.40
10:M:47:TRP:CG	10:M:88:LEU:HD11	2.56	0.40
10:M:291:MET:SD	10:M:418:VAL:HG21	2.62	0.40
11:N:480:LEU:HD23	11:N:480:LEU:HA	1.87	0.40
4:C:312:GLU:OE2	4:C:447:TYR:OH	2.31	0.40
19:H:403:3PE:H261	19:J:201:3PE:H271	2.03	0.40
8:A:69:TYR:OH	12:K:74:SER:O	2.36	0.40
9:L:12:LEU:HD23	9:L:12:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	437/445 (98%)	429 (98%)	8 (2%)	0	100	100
2	E	154/166 (93%)	150 (97%)	4 (3%)	0	100	100
3	G	903/908 (99%)	884 (98%)	18 (2%)	1 (0%)	51	64
4	C	584/596 (98%)	570 (98%)	14 (2%)	0	100	100
5	B	192/220 (87%)	182 (95%)	10 (5%)	0	100	100
6	I	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
7	H	321/325 (99%)	313 (98%)	8 (2%)	0	100	100
8	A	106/147 (72%)	106 (100%)	0	0	100	100
9	L	601/613 (98%)	588 (98%)	13 (2%)	0	100	100
10	M	502/509 (99%)	493 (98%)	9 (2%)	0	100	100
11	N	474/485 (98%)	465 (98%)	8 (2%)	1 (0%)	47	58
12	K	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
13	J	160/184 (87%)	159 (99%)	1 (1%)	0	100	100
All	All	4710/4878 (97%)	4609 (98%)	99 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	669	THR
11	N	64	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	353/359 (98%)	344 (98%)	9 (2%)	47	65
2	E	129/139 (93%)	125 (97%)	4 (3%)	40	55
3	G	733/736 (100%)	713 (97%)	20 (3%)	44	61
4	C	505/515 (98%)	494 (98%)	11 (2%)	52	69
5	B	171/192 (89%)	166 (97%)	5 (3%)	42	58
6	I	154/154 (100%)	151 (98%)	3 (2%)	57	73
7	H	267/269 (99%)	254 (95%)	13 (5%)	25	35
8	A	87/119 (73%)	86 (99%)	1 (1%)	73	86
9	L	480/485 (99%)	453 (94%)	27 (6%)	21	29
10	M	413/418 (99%)	399 (97%)	14 (3%)	37	51
11	N	380/385 (99%)	375 (99%)	5 (1%)	69	82
12	K	79/79 (100%)	75 (95%)	4 (5%)	24	33
13	J	128/146 (88%)	122 (95%)	6 (5%)	26	37
All	All	3879/3996 (97%)	3757 (97%)	122 (3%)	43	55

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	31	SER
1	F	94	MET
1	F	126	TYR
1	F	221	THR
1	F	241	LYS
1	F	312	GLU
1	F	351	CYS
1	F	357	CYS
1	F	398	CYS
2	E	47	ARG
2	E	127	THR
2	E	147	GLU
2	E	149	THR
3	G	61	THR
3	G	64	ARG
3	G	135	ARG
3	G	233	CYS
3	G	238	ASN
3	G	265	CYS
3	G	331	ARG

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Mol	Chain	Res	Type
3	G	411	LYS
3	G	428	LYS
3	G	593	MET
3	G	631	ARG
3	G	666	VAL
3	G	681	LYS
3	G	740	MET
3	G	750	ARG
3	G	789	GLU
3	G	804	ARG
3	G	809	ASP
3	G	855	ASN
3	G	906	LYS
4	C	80	MET
4	C	110	ASP
4	C	127	PHE
4	C	206	MET
4	C	216	MET
4	C	234	VAL
4	C	264	SER
4	C	319	HIS
4	C	358	MET
4	C	377	ASP
4	C	582	SER
5	B	37	VAL
5	B	63	CYS
5	B	71	SER
5	B	78	VAL
5	B	199	SER
6	I	28	ARG
6	I	77	LEU
6	I	159	ASP
7	H	64	MET
7	H	66	LYS
7	H	76	LYS
7	H	78	SER
7	H	92	THR
7	H	143	LEU
7	H	152	GLN
7	H	238	PHE
7	H	280	MET
7	H	282	PHE

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Mol	Chain	Res	Type
7	H	286	ARG
7	H	293	ARG
7	H	299	SER
8	A	124	ASP
9	L	2	ASN
9	L	27	GLU
9	L	55	ASN
9	L	61	SER
9	L	77	PHE
9	L	93	THR
9	L	110	GLU
9	L	123	PHE
9	L	162	LYS
9	L	247	THR
9	L	305	LYS
9	L	342	LYS
9	L	359	GLU
9	L	369	ARG
9	L	371	SER
9	L	379	PHE
9	L	381	VAL
9	L	398	SER
9	L	399	LYS
9	L	482	THR
9	L	483	THR
9	L	489	SER
9	L	491	LEU
9	L	493	LEU
9	L	542	ASP
9	L	574	VAL
9	L	613	ARG
10	M	1	MET
10	M	22	ARG
10	M	64	GLN
10	M	74	ARG
10	M	80	HIS
10	M	165	LYS
10	M	174	PHE
10	M	256	SER
10	M	303	TRP
10	M	374	MET
10	M	408	PHE

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Mol	Chain	Res	Type
10	M	426	THR
10	M	435	TYR
10	M	447	LYS
11	N	150	LYS
11	N	207	PHE
11	N	321	MET
11	N	388	MET
11	N	431	SER
12	K	1	MET
12	K	46	PHE
12	K	96	SER
12	K	99	ARG
13	J	17	LEU
13	J	18	ARG
13	J	59	TYR
13	J	69	PHE
13	J	86	GLN
13	J	145	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
9	L	163	ASN
10	M	45	GLN
10	M	441	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	C14	N	601	-	13,13,13	0.14	0	12,12,12	0.11	0
19	3PE	H	403	-	50,50,50	0.31	0	53,55,55	0.34	0
14	SF4	F	501	1	0,12,12	-	-	-		
14	SF4	G	1001	3	0,12,12	-	-	-		
19	3PE	M	1003	-	50,50,50	0.31	0	53,55,55	0.28	0
17	FES	E	201	2	0,4,4	-	-	-		
14	SF4	B	301	5	0,12,12	-	-	-		
19	3PE	M	1004	-	50,50,50	0.29	0	53,55,55	0.27	0
20	LFA	L	802	-	19,19,19	0.15	0	18,18,18	0.11	0
15	FMN	F	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.28	7 (14%)
14	SF4	G	1003	3	0,12,12	-	-	-		
19	3PE	L	803	-	48,48,50	0.30	0	51,53,55	0.35	0
19	3PE	L	804	-	50,50,50	0.30	0	53,55,55	0.29	0
20	LFA	H	402	-	19,19,19	0.14	0	18,18,18	0.12	0
19	3PE	A	201	-	33,33,50	0.36	0	36,38,55	0.32	0
16	NAI	F	503	-	42,48,48	0.52	0	47,73,73	0.56	1 (2%)
19	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.28	0
20	LFA	M	1002	-	19,19,19	0.13	0	18,18,18	0.12	0
14	SF4	G	1002	3	0,12,12	-	-	-		
19	3PE	J	201	-	50,50,50	0.30	0	53,55,55	0.27	0
14	SF4	I	201	6	0,12,12	-	-	-		
17	FES	G	1004	3	0,4,4	-	-	-		
19	3PE	H	401	-	50,50,50	0.30	0	53,55,55	0.29	0
19	3PE	N	602	-	50,50,50	0.30	0	53,55,55	0.32	0
19	3PE	I	203	-	50,50,50	0.30	0	53,55,55	0.29	0
14	SF4	I	202	6	0,12,12	-	-	-		
19	3PE	M	1001	-	50,50,50	0.30	0	53,55,55	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	C14	N	601	-	-	0/11/11/11	-
19	3PE	H	403	-	-	10/54/54/54	-
14	SF4	F	501	1	-	-	0/6/5/5
14	SF4	G	1001	3	-	-	0/6/5/5
19	3PE	M	1003	-	-	11/54/54/54	-
19	3PE	M	1004	-	-	14/54/54/54	-
14	SF4	B	301	5	-	-	0/6/5/5
20	LFA	L	802	-	-	0/17/17/17	-
17	FES	E	201	2	-	-	0/1/1/1
15	FMN	F	502	-	-	10/18/18/18	0/3/3/3
14	SF4	G	1003	3	-	-	0/6/5/5
19	3PE	L	804	-	-	14/54/54/54	-
19	3PE	L	803	-	-	14/52/52/54	-
20	LFA	H	402	-	-	1/17/17/17	-
19	3PE	A	201	-	-	9/37/37/54	-
16	NAI	F	503	-	-	5/25/72/72	0/5/5/5
19	3PE	L	801	-	-	11/54/54/54	-
20	LFA	M	1002	-	-	0/17/17/17	-
14	SF4	G	1002	3	-	-	0/6/5/5
19	3PE	J	201	-	-	12/54/54/54	-
14	SF4	I	201	6	-	-	0/6/5/5
17	FES	G	1004	3	-	-	0/1/1/1
19	3PE	H	401	-	-	11/54/54/54	-
19	3PE	N	602	-	-	11/54/54/54	-
19	3PE	I	203	-	-	13/54/54/54	-
14	SF4	I	202	6	-	-	0/6/5/5
19	3PE	M	1001	-	-	6/54/54/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.60	1.37	1.30
15	F	502	FMN	C10-N1	2.24	1.37	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4-N3-C2	-3.25	119.64	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4A-C10-N10	2.80	120.57	116.48
15	F	502	FMN	C4A-C4-N3	2.75	120.16	113.19
15	F	502	FMN	O4-C4-C4A	-2.41	120.21	126.60
15	F	502	FMN	C4A-C10-N1	-2.40	119.16	124.73
15	F	502	FMN	C10-C4A-N5	-2.38	119.80	124.86
16	F	503	NAI	C5A-C6A-N6A	2.30	123.84	120.35
15	F	502	FMN	O3P-P-O5'	2.04	112.16	106.73

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	502	FMN	C5'-O5'-P-O1P
15	F	502	FMN	C5'-O5'-P-O2P
16	F	503	NAI	C5B-O5B-PA-O1A
19	I	203	3PE	C11-O13-P-O12
19	I	203	3PE	C11-O13-P-O14
19	H	401	3PE	C11-O13-P-O11
19	H	401	3PE	C11-O13-P-O14
19	H	401	3PE	O13-C11-C12-N
19	H	403	3PE	C11-O13-P-O12
19	H	403	3PE	O13-C11-C12-N
19	A	201	3PE	C1-O11-P-O12
19	A	201	3PE	O13-C11-C12-N
19	L	801	3PE	C1-O11-P-O14
19	L	801	3PE	O13-C11-C12-N
19	L	803	3PE	C1-O11-P-O14
19	L	803	3PE	C11-O13-P-O14
19	L	804	3PE	C11-O13-P-O12
19	M	1001	3PE	C11-O13-P-O12
19	M	1001	3PE	C11-O13-P-O14
19	M	1003	3PE	C1-O11-P-O14
19	M	1003	3PE	C11-O13-P-O14
19	M	1003	3PE	O13-C11-C12-N
19	M	1004	3PE	C1-O11-P-O12
19	M	1004	3PE	C11-O13-P-O11
19	M	1004	3PE	C11-O13-P-O14
19	M	1004	3PE	O13-C11-C12-N
19	N	602	3PE	O13-C11-C12-N
19	J	201	3PE	C1-O11-P-O12
19	J	201	3PE	C1-O11-P-O13
19	J	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
19	J	201	3PE	C11-O13-P-O12
19	J	201	3PE	C11-O13-P-O14
19	A	201	3PE	C31-C32-C33-C34
19	M	1004	3PE	C2-C1-O11-P
19	I	203	3PE	C11-O13-P-O11
19	A	201	3PE	C1-O11-P-O13
19	A	201	3PE	C11-O13-P-O11
19	L	803	3PE	C1-O11-P-O13
19	L	804	3PE	C1-O11-P-O13
19	L	804	3PE	C11-O13-P-O11
19	M	1001	3PE	C11-O13-P-O11
19	N	602	3PE	C1-O11-P-O13
19	J	201	3PE	C11-O13-P-O11
19	H	401	3PE	C3D-C3E-C3F-C3G
19	M	1004	3PE	C3E-C3F-C3G-C3H
19	L	801	3PE	C2C-C2D-C2E-C2F
19	L	804	3PE	C24-C25-C26-C27
19	L	804	3PE	C2A-C2B-C2C-C2D
19	I	203	3PE	C31-C32-C33-C34
19	I	203	3PE	C2A-C2B-C2C-C2D
19	N	602	3PE	C25-C26-C27-C28
19	M	1004	3PE	C26-C27-C28-C29
19	L	801	3PE	C37-C38-C39-C3A
19	L	804	3PE	C3B-C3C-C3D-C3E
20	H	402	LFA	C14-C15-C16-C17
19	L	801	3PE	C23-C24-C25-C26
19	H	403	3PE	C11-O13-P-O11
19	I	203	3PE	C3A-C3B-C3C-C3D
19	J	201	3PE	C23-C24-C25-C26
19	L	803	3PE	C3A-C3B-C3C-C3D
19	L	803	3PE	C37-C38-C39-C3A
19	L	804	3PE	O21-C2-C3-O31
19	N	602	3PE	C2-C1-O11-P
19	M	1004	3PE	C2E-C2F-C2G-C2H
19	L	804	3PE	C1-C2-C3-O31
19	H	401	3PE	C29-C2A-C2B-C2C
19	M	1003	3PE	C23-C24-C25-C26
19	H	401	3PE	C36-C37-C38-C39
19	L	803	3PE	C35-C36-C37-C38
15	F	502	FMN	C5'-O5'-P-O3P
19	J	201	3PE	C21-C22-C23-C24
19	L	804	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
19	M	1003	3PE	C2-C1-O11-P
19	I	203	3PE	C3B-C3C-C3D-C3E
16	F	503	NAI	C5B-O5B-PA-O3
19	M	1003	3PE	C1-O11-P-O13
15	F	502	FMN	C4'-C5'-O5'-P
19	L	803	3PE	C2-C1-O11-P
19	J	201	3PE	C2-C1-O11-P
19	H	403	3PE	C11-O13-P-O14
19	A	201	3PE	C11-O13-P-O14
19	L	803	3PE	C1-O11-P-O12
19	L	804	3PE	C1-O11-P-O12
19	L	804	3PE	C1-O11-P-O14
19	L	804	3PE	C11-O13-P-O14
19	N	602	3PE	C1-O11-P-O12
19	N	602	3PE	C1-O11-P-O14
19	M	1003	3PE	C24-C25-C26-C27
15	F	502	FMN	N10-C1'-C2'-O2'
15	F	502	FMN	N10-C1'-C2'-C3'
19	L	803	3PE	O11-C1-C2-O21
19	N	602	3PE	O11-C1-C2-O21
15	F	502	FMN	C2'-C3'-C4'-O4'
19	N	602	3PE	O21-C21-C22-C23
19	L	803	3PE	O11-C1-C2-C3
19	J	201	3PE	O21-C21-C22-C23
19	L	803	3PE	C11-O13-P-O11
19	M	1003	3PE	C11-O13-P-O11
19	N	602	3PE	C11-O13-P-O11
16	F	503	NAI	O4D-C1D-N1N-C2N
19	L	801	3PE	C31-C32-C33-C34
19	A	201	3PE	C34-C35-C36-C37
19	H	403	3PE	C3C-C3D-C3E-C3F
15	F	502	FMN	C2'-C3'-C4'-C5'
19	L	803	3PE	O21-C2-C3-O31
19	H	403	3PE	C2F-C2G-C2H-C2I
16	F	503	NAI	C2D-C1D-N1N-C2N
15	F	502	FMN	O3'-C3'-C4'-C5'
19	N	602	3PE	C3B-C3C-C3D-C3E
19	I	203	3PE	C32-C33-C34-C35
19	J	201	3PE	O11-C1-C2-C3
19	H	401	3PE	C1-C2-C3-O31
19	J	201	3PE	O11-C1-C2-O21
19	L	801	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
15	F	502	FMN	O3'-C3'-C4'-O4'
19	H	401	3PE	O21-C2-C3-O31
19	M	1004	3PE	O31-C31-C32-C33
19	M	1003	3PE	C35-C36-C37-C38
19	L	801	3PE	C1-O11-P-O13
19	H	403	3PE	C34-C35-C36-C37
19	M	1004	3PE	C2F-C2G-C2H-C2I
19	A	201	3PE	O31-C31-C32-C33
19	N	602	3PE	O31-C31-C32-C33
19	I	203	3PE	C2C-C2D-C2E-C2F
19	I	203	3PE	O31-C31-C32-C33
19	M	1001	3PE	O31-C31-C32-C33
19	I	203	3PE	C38-C39-C3A-C3B
19	L	801	3PE	O21-C2-C3-O31
19	L	801	3PE	C25-C26-C27-C28
19	M	1004	3PE	O32-C31-C32-C33
19	L	804	3PE	C23-C24-C25-C26
19	M	1004	3PE	C29-C2A-C2B-C2C
19	A	201	3PE	O32-C31-C32-C33
19	L	803	3PE	O21-C21-C22-C23
19	I	203	3PE	C26-C27-C28-C29
16	F	503	NAI	C5B-O5B-PA-O2A
19	M	1001	3PE	C1-O11-P-O14
19	M	1004	3PE	C1-O11-P-O14
19	M	1001	3PE	O32-C31-C32-C33
19	I	203	3PE	O32-C31-C32-C33
19	H	403	3PE	C23-C24-C25-C26
19	L	801	3PE	C12-C11-O13-P
19	M	1003	3PE	C12-C11-O13-P
19	H	401	3PE	C38-C39-C3A-C3B
19	H	403	3PE	C3B-C3C-C3D-C3E
19	H	401	3PE	O31-C31-C32-C33
19	L	803	3PE	O22-C21-C22-C23
19	H	401	3PE	C25-C26-C27-C28
19	L	804	3PE	C2F-C2G-C2H-C2I
19	M	1004	3PE	O21-C21-C22-C23
19	H	403	3PE	C26-C27-C28-C29
19	M	1003	3PE	C2C-C2D-C2E-C2F

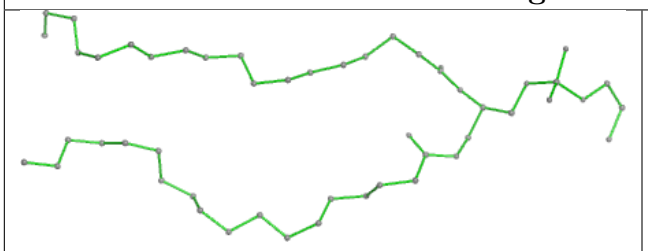
There are no ring outliers.

18 monomers are involved in 30 short contacts:

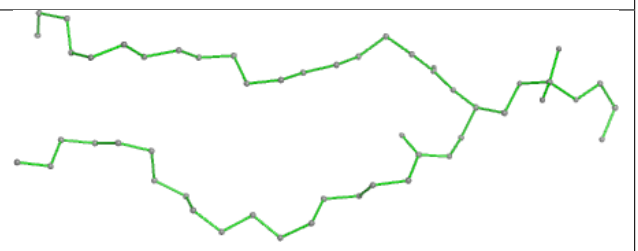
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	601	C14	1	0
19	H	403	3PE	4	0
19	M	1003	3PE	1	0
14	B	301	SF4	1	0
19	M	1004	3PE	1	0
15	F	502	FMN	1	0
19	L	803	3PE	2	0
19	L	804	3PE	3	0
20	H	402	LFA	2	0
19	A	201	3PE	3	0
16	F	503	NAI	3	0
19	L	801	3PE	2	0
20	M	1002	LFA	1	0
19	J	201	3PE	5	0
19	H	401	3PE	3	0
19	N	602	3PE	2	0
19	I	203	3PE	1	0
19	M	1001	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.

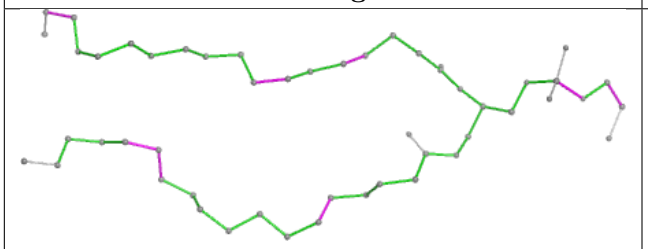
Ligand 3PE H 403



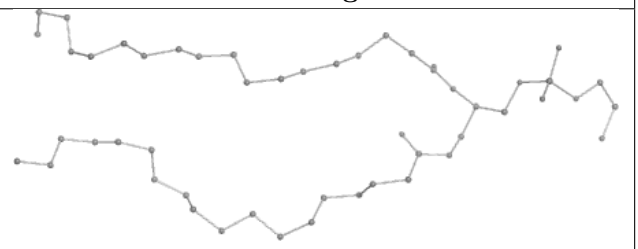
Bond lengths



Bond angles

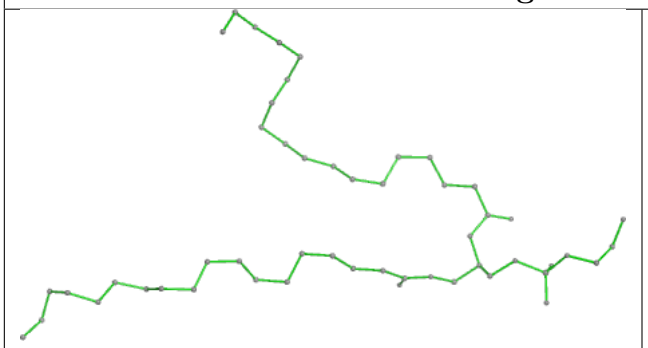


Torsions

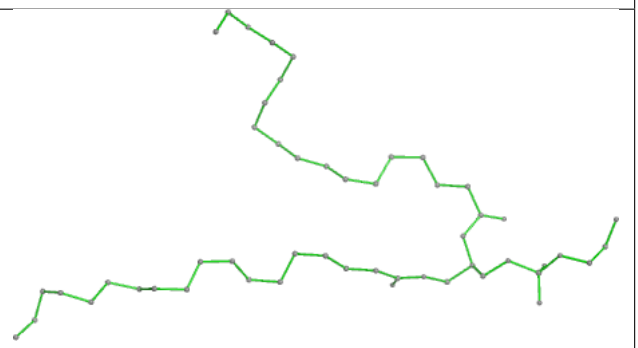


Rings

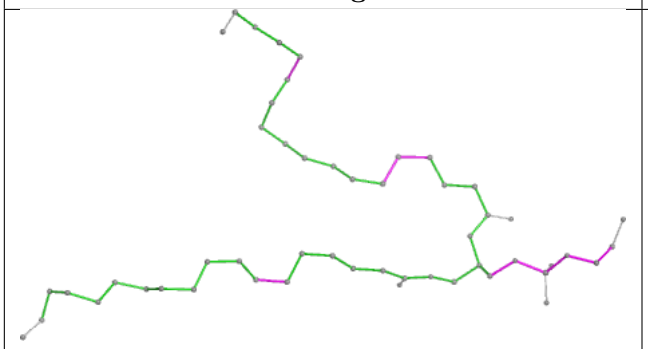
Ligand 3PE M 1003



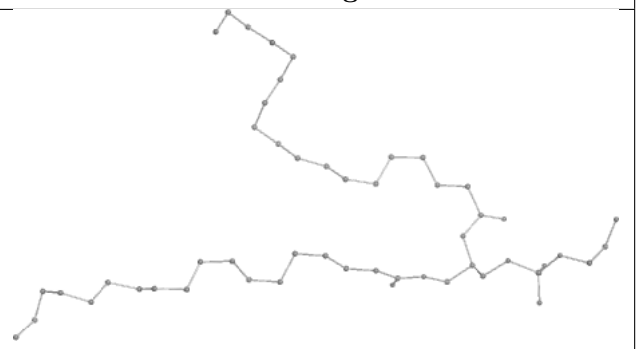
Bond lengths



Bond angles

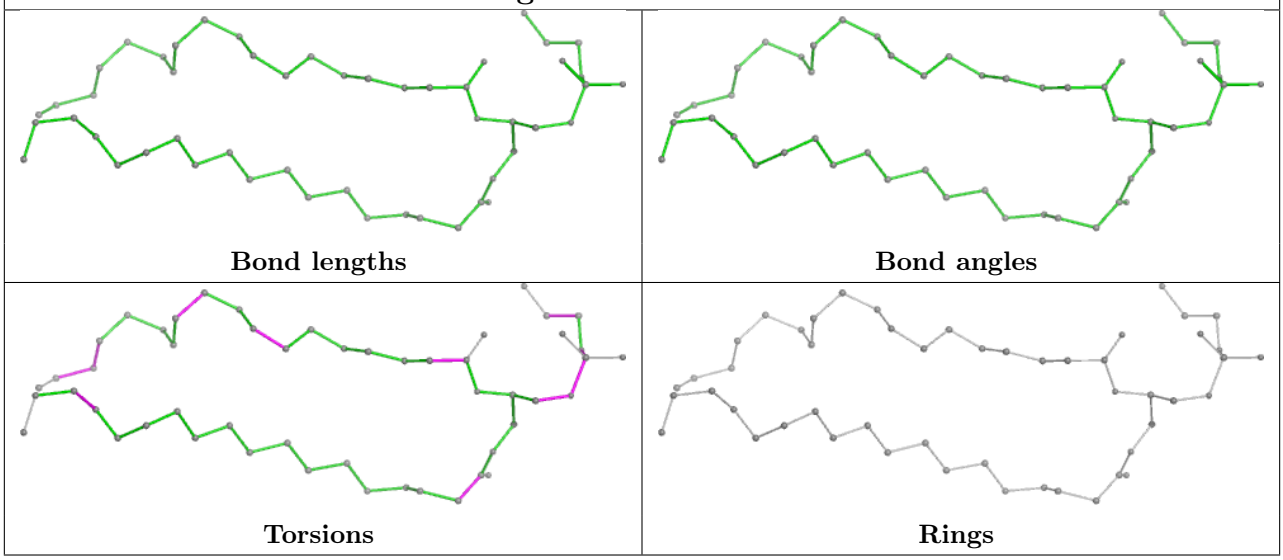


Torsions

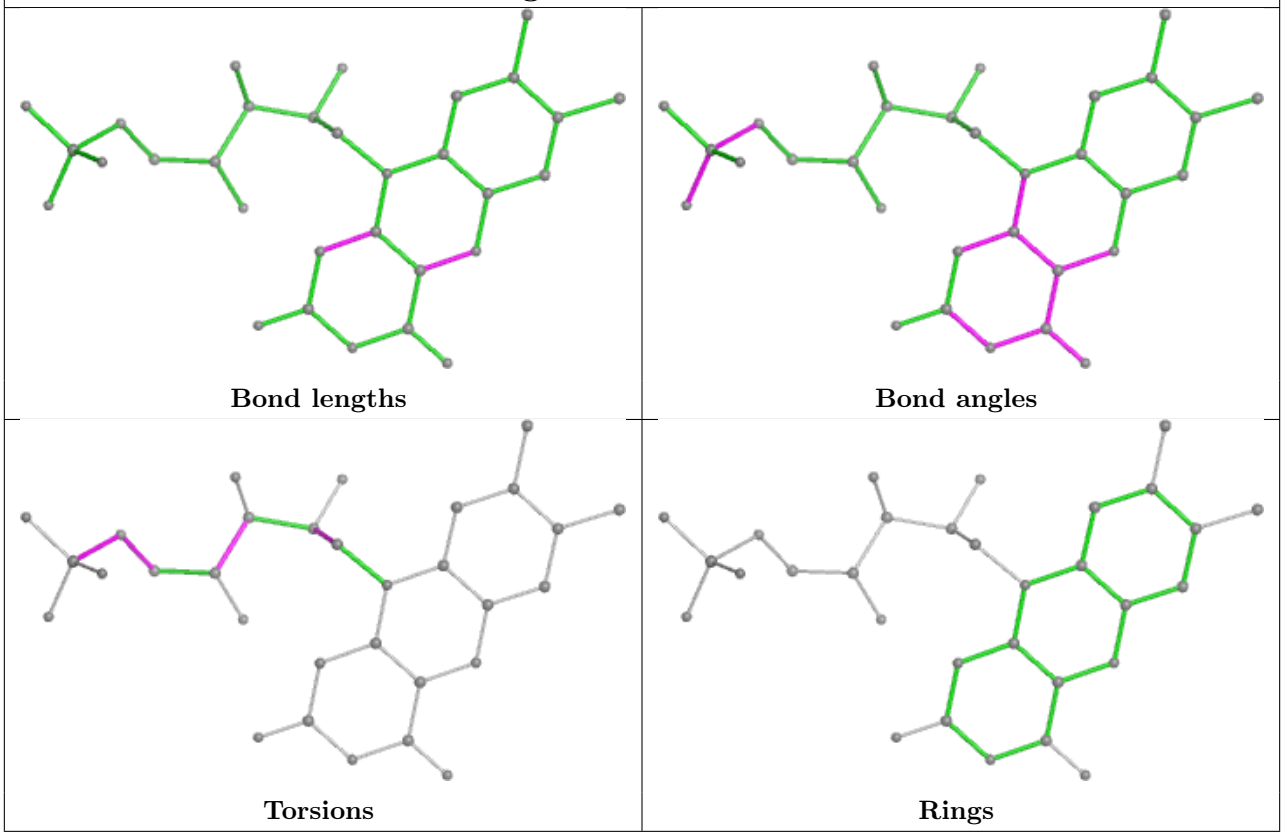


Rings

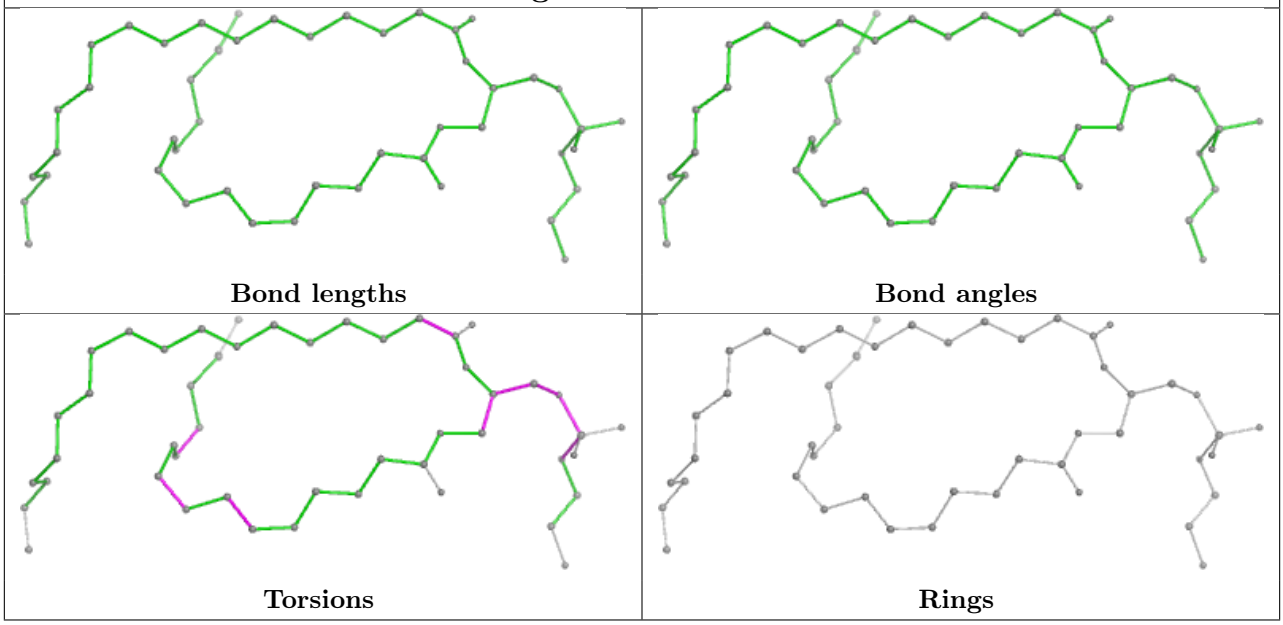
Ligand 3PE M 1004



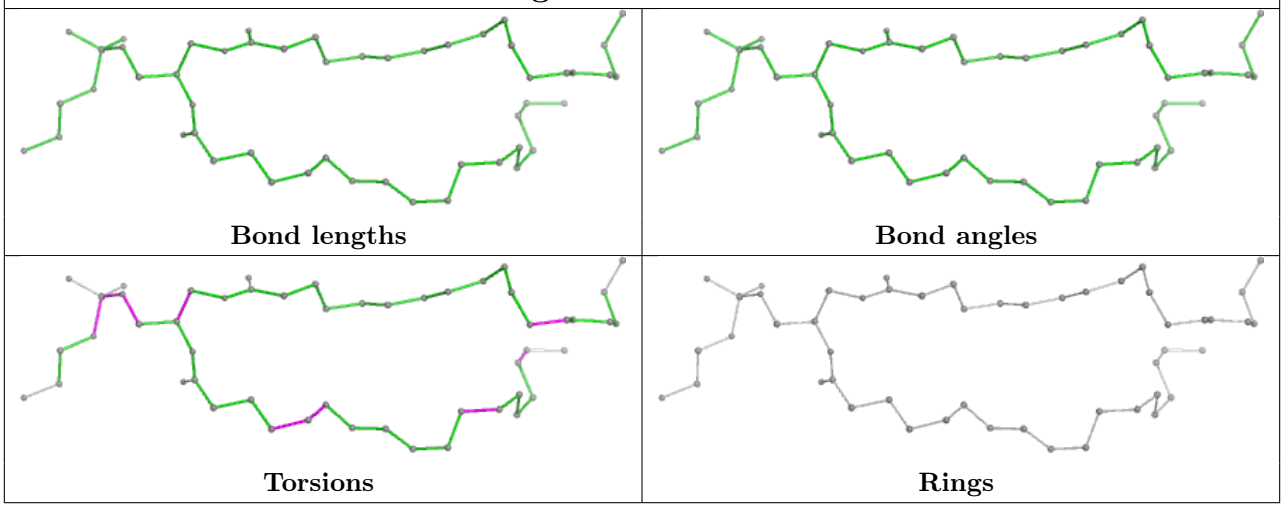
Ligand FMN F 502



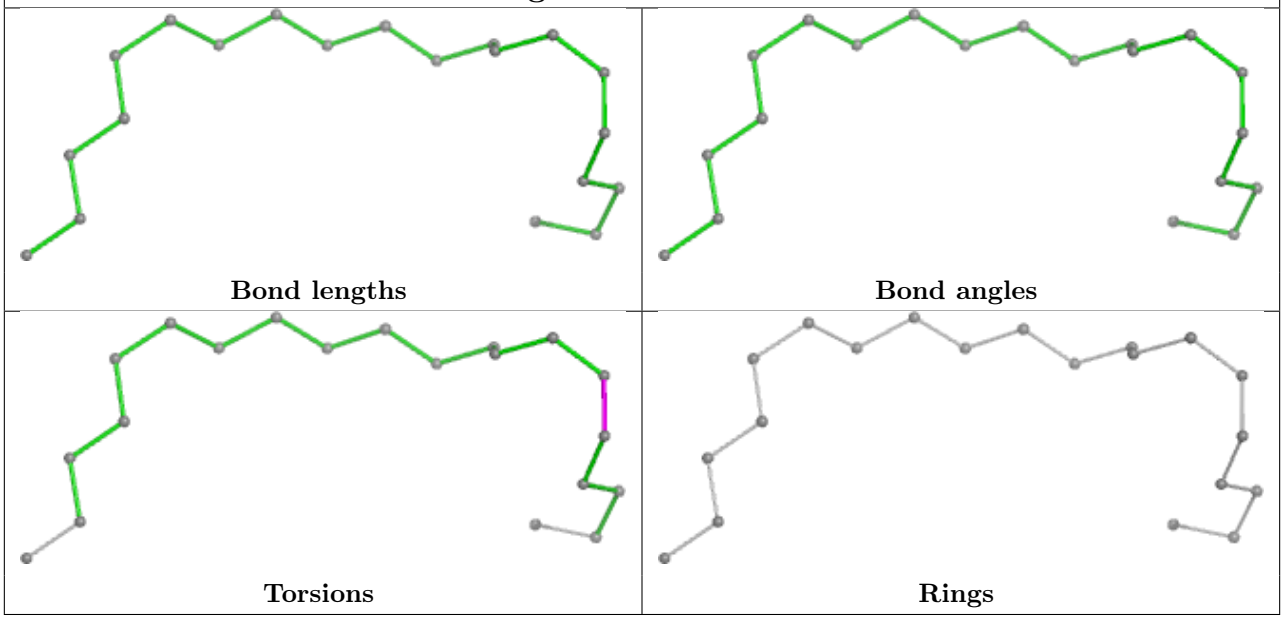
Ligand 3PE L 803



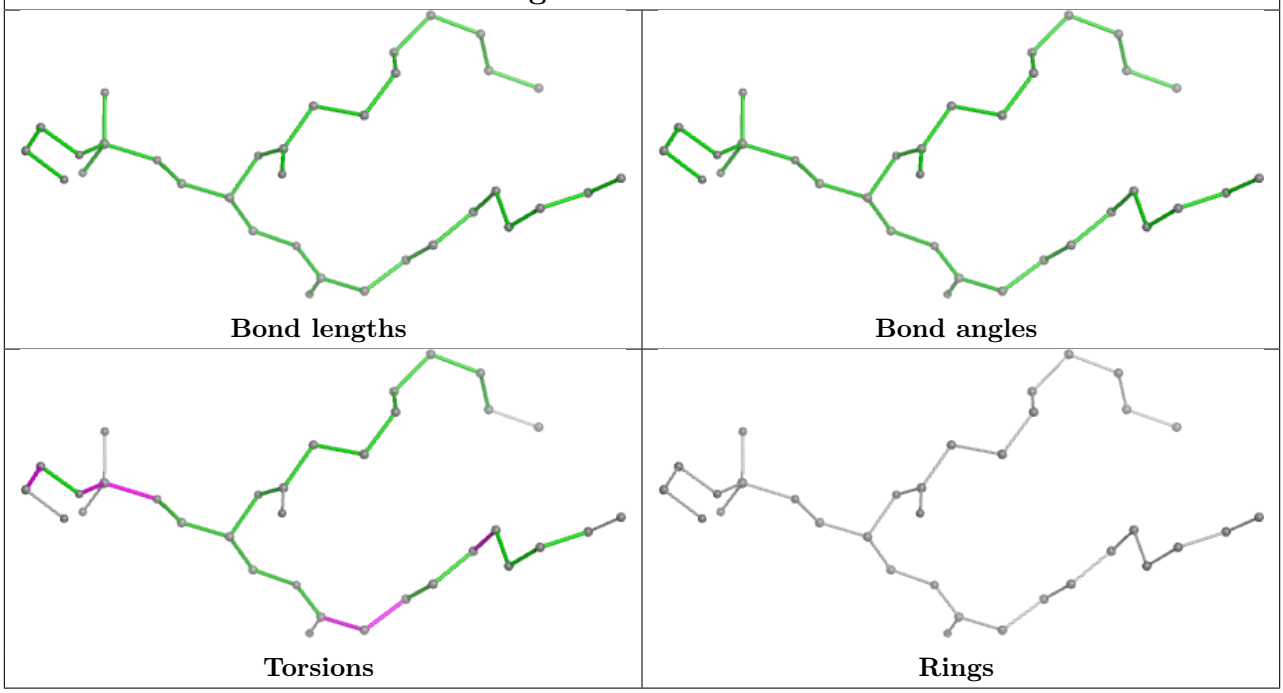
Ligand 3PE L 804



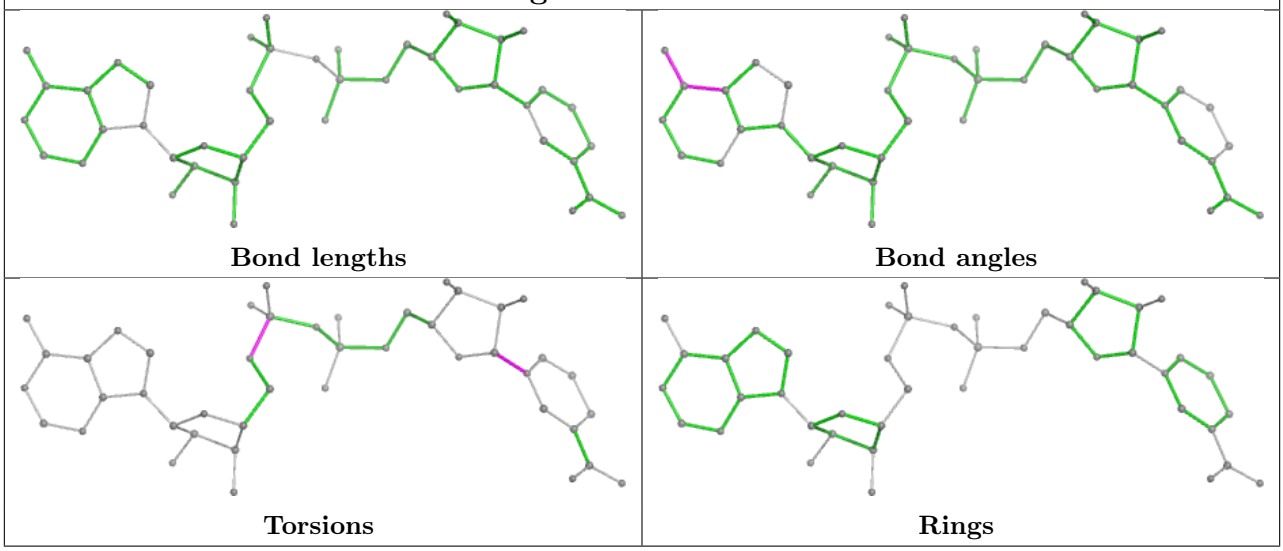
Ligand LFA H 402



Ligand 3PE A 201



Ligand NAI F 503



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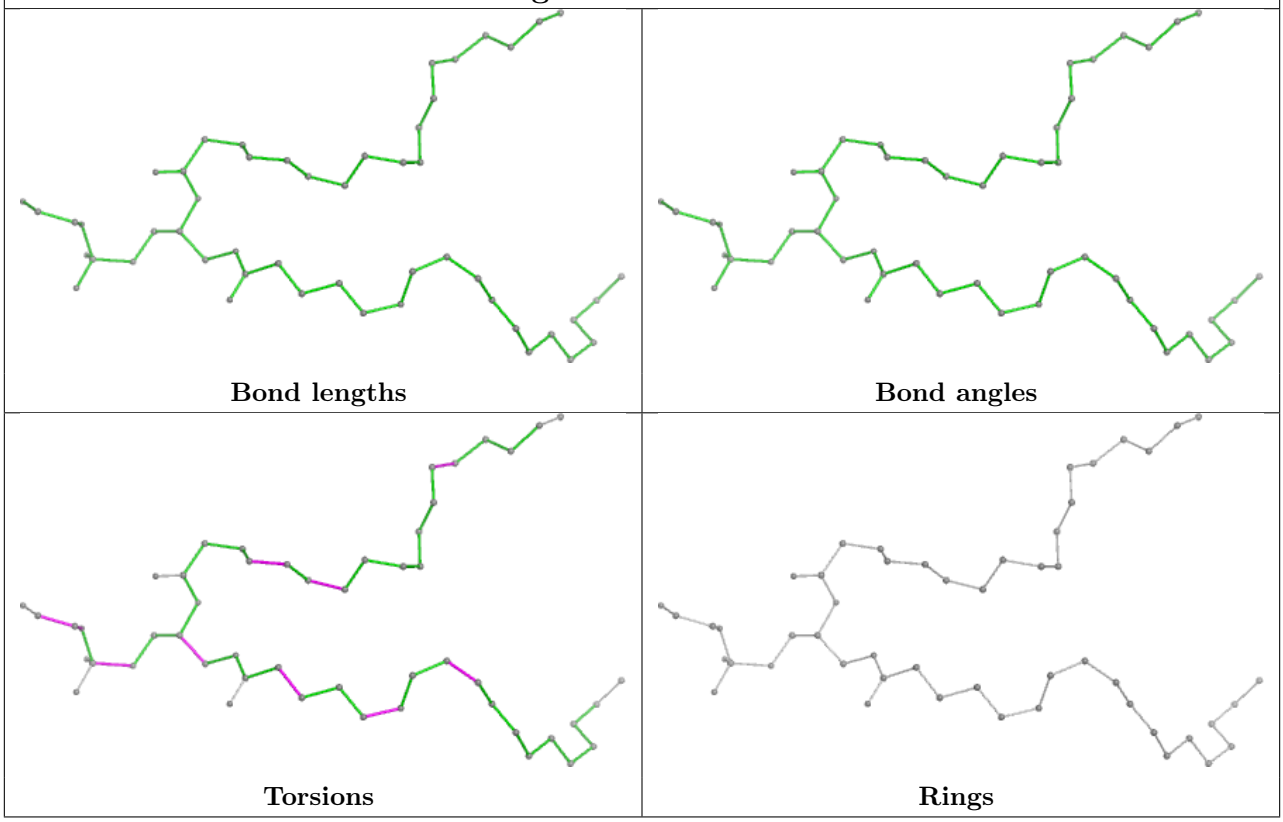
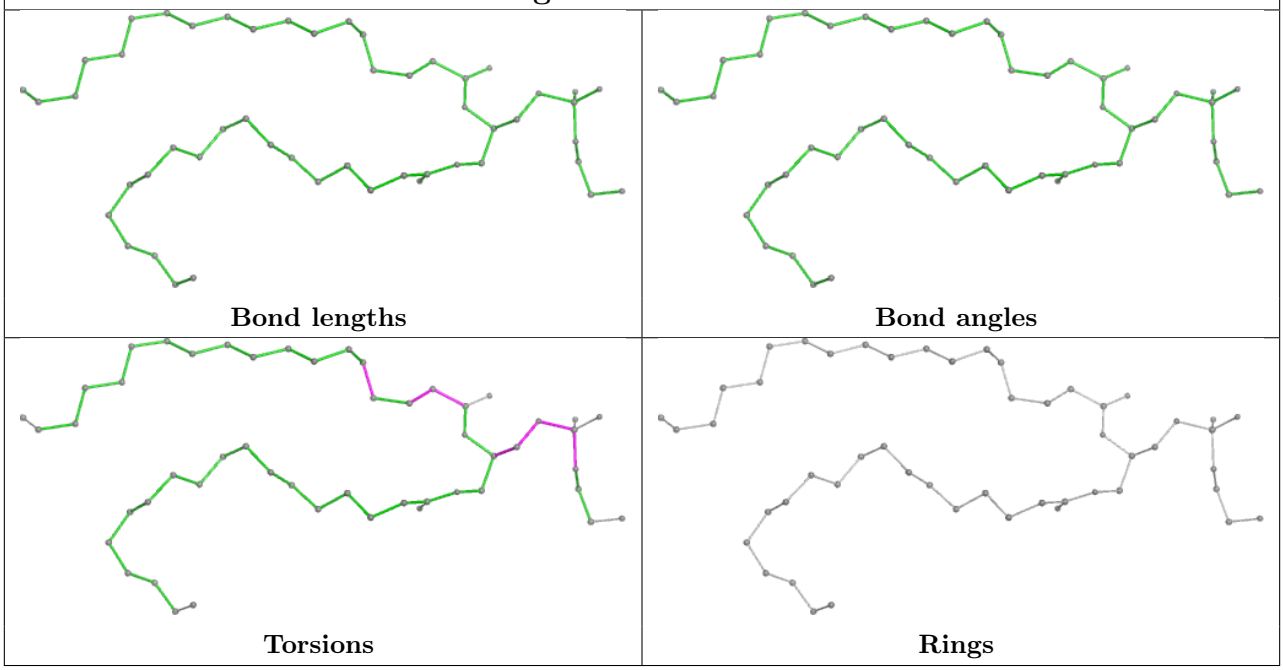


Ligand 3PE J 201



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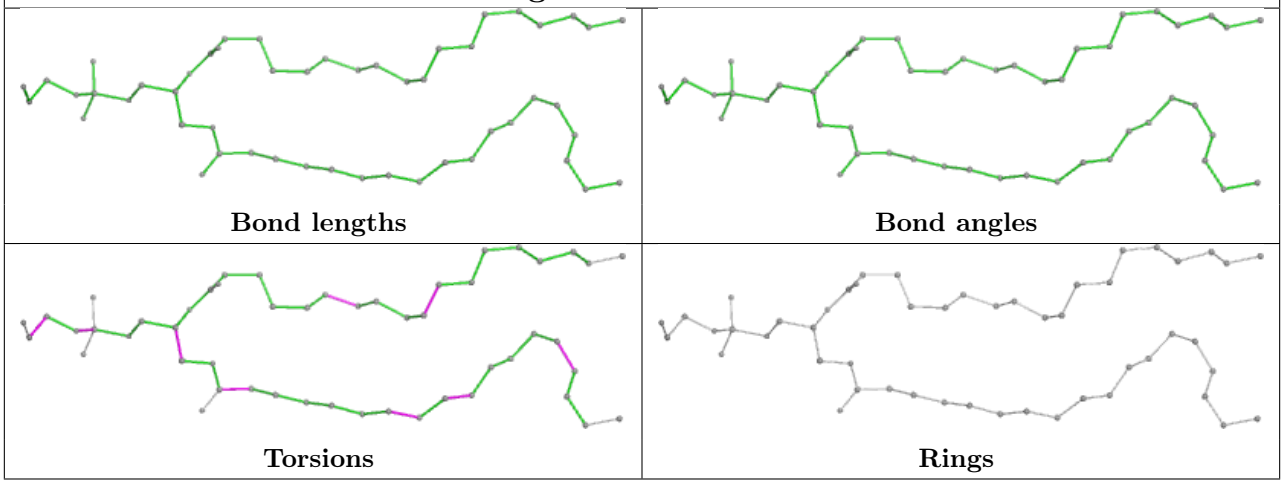
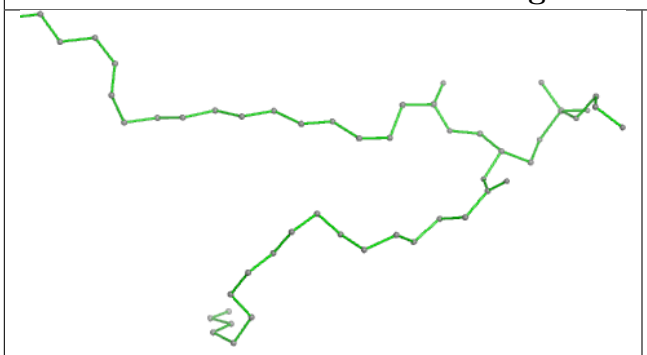
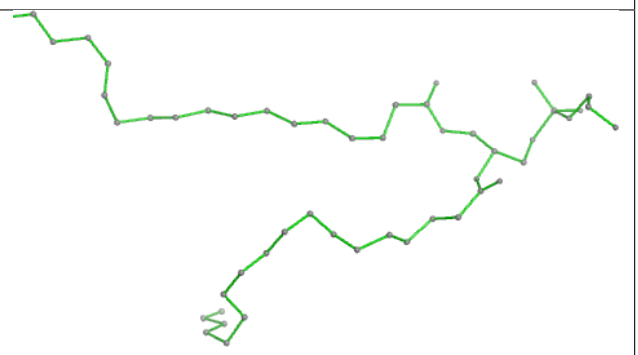


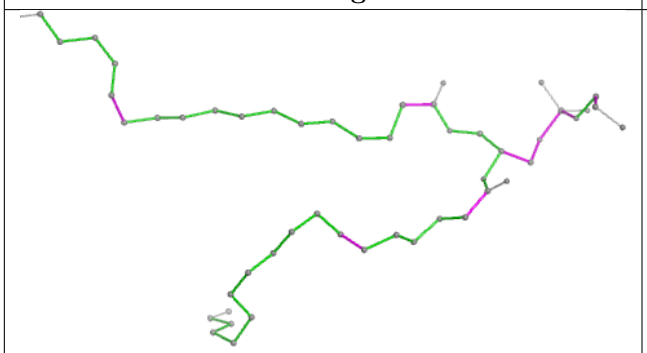
Ligand 3PE N 602



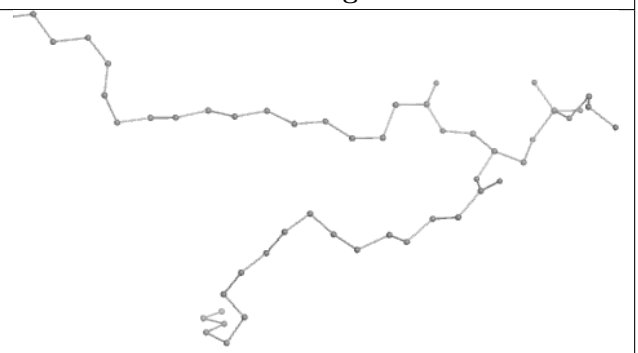
Bond lengths



Bond angles

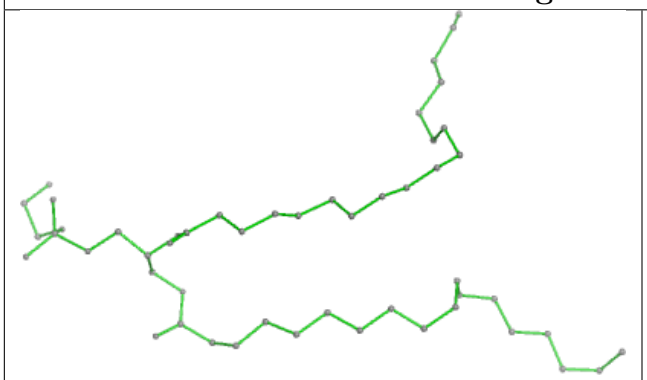


Torsions

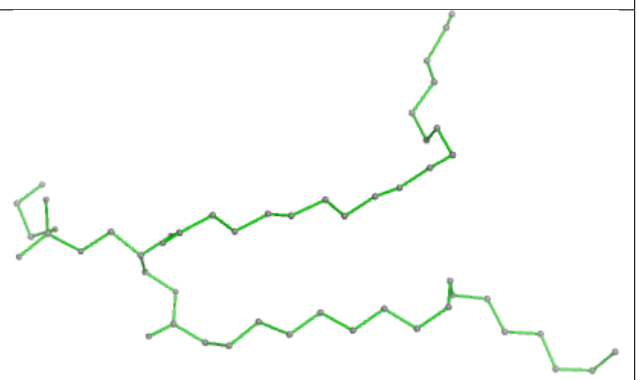


Rings

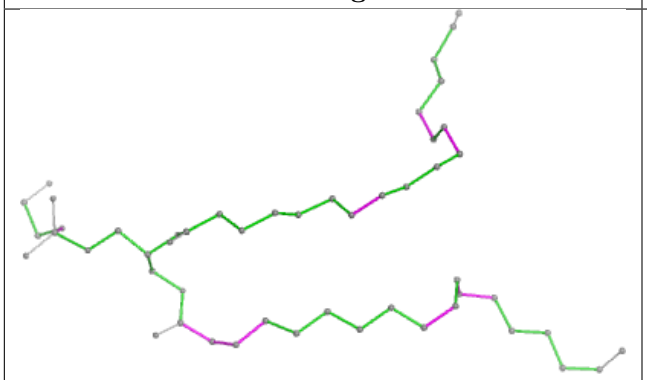
Ligand 3PE I 203



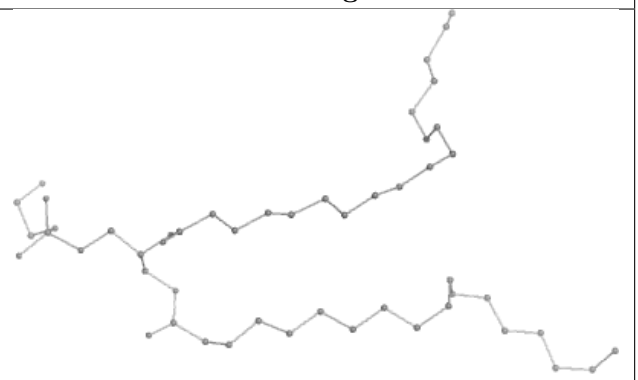
Bond lengths



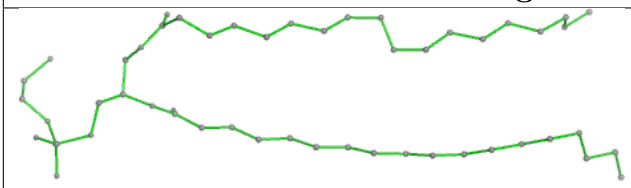
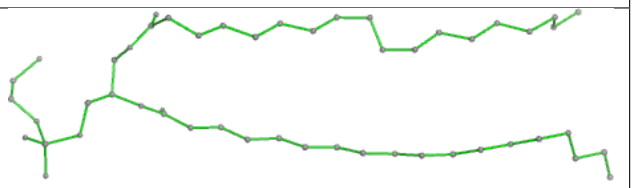
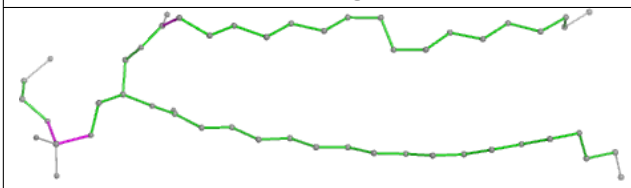
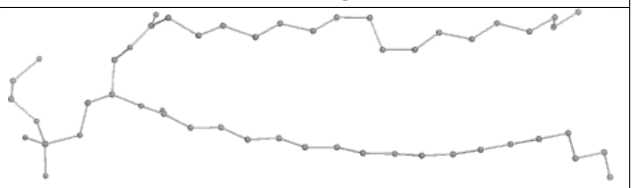
Bond angles



Torsions



Rings

Ligand 3PE M 1001	
 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.

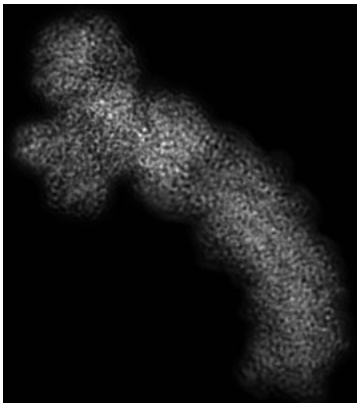
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14538. These allow visual inspection of the internal detail of the map and identification of artifacts.

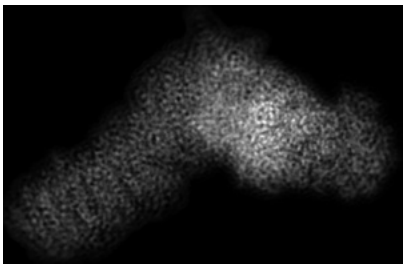
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

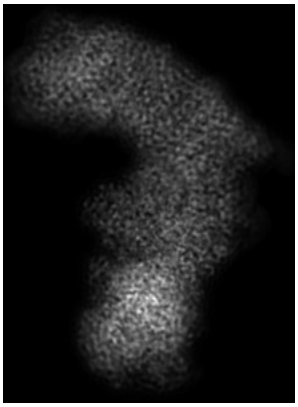
6.1.1 Primary map



X



Y



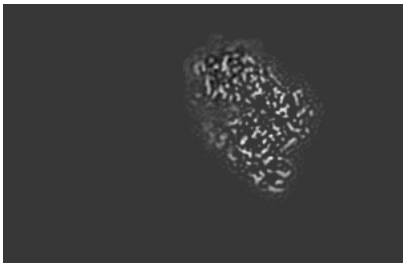
Z

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

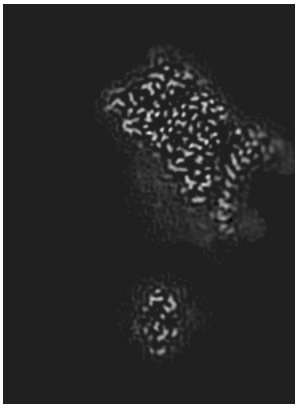
6.2 Central slices (i)

6.2.1 Primary map

X Index: 153



Y Index: 210

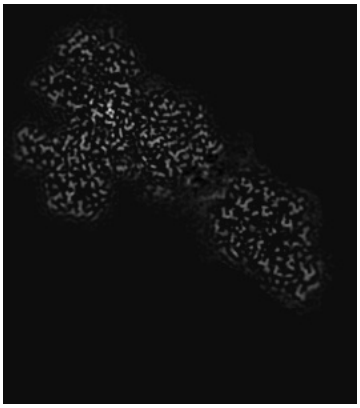


Z Index: 237

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

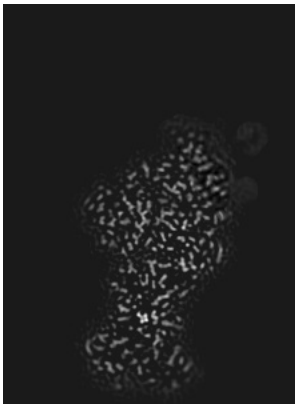
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 167

Y Index: 110

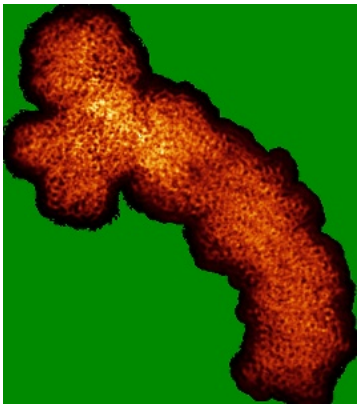


Z Index: 309

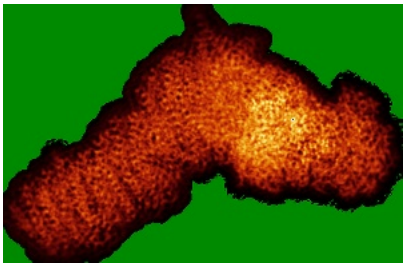
The images above show the largest variance slices of the map in three orthogonal directions.

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

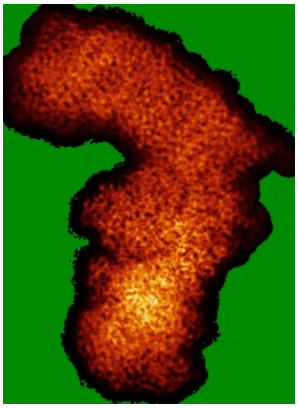
6.4.1 Primary map



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

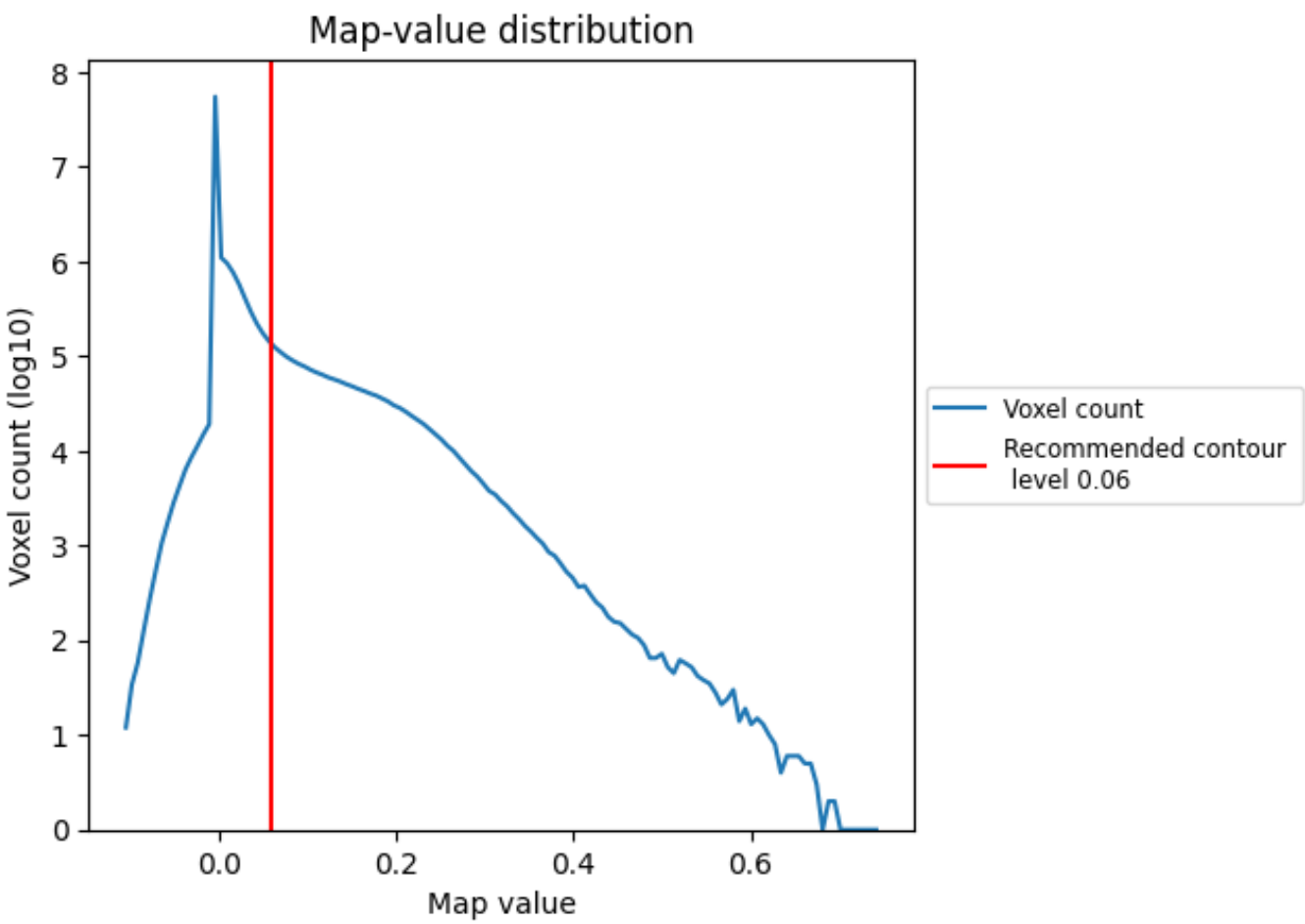
6.6 Mask visualisation (i)

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

7 Map analysis (i)

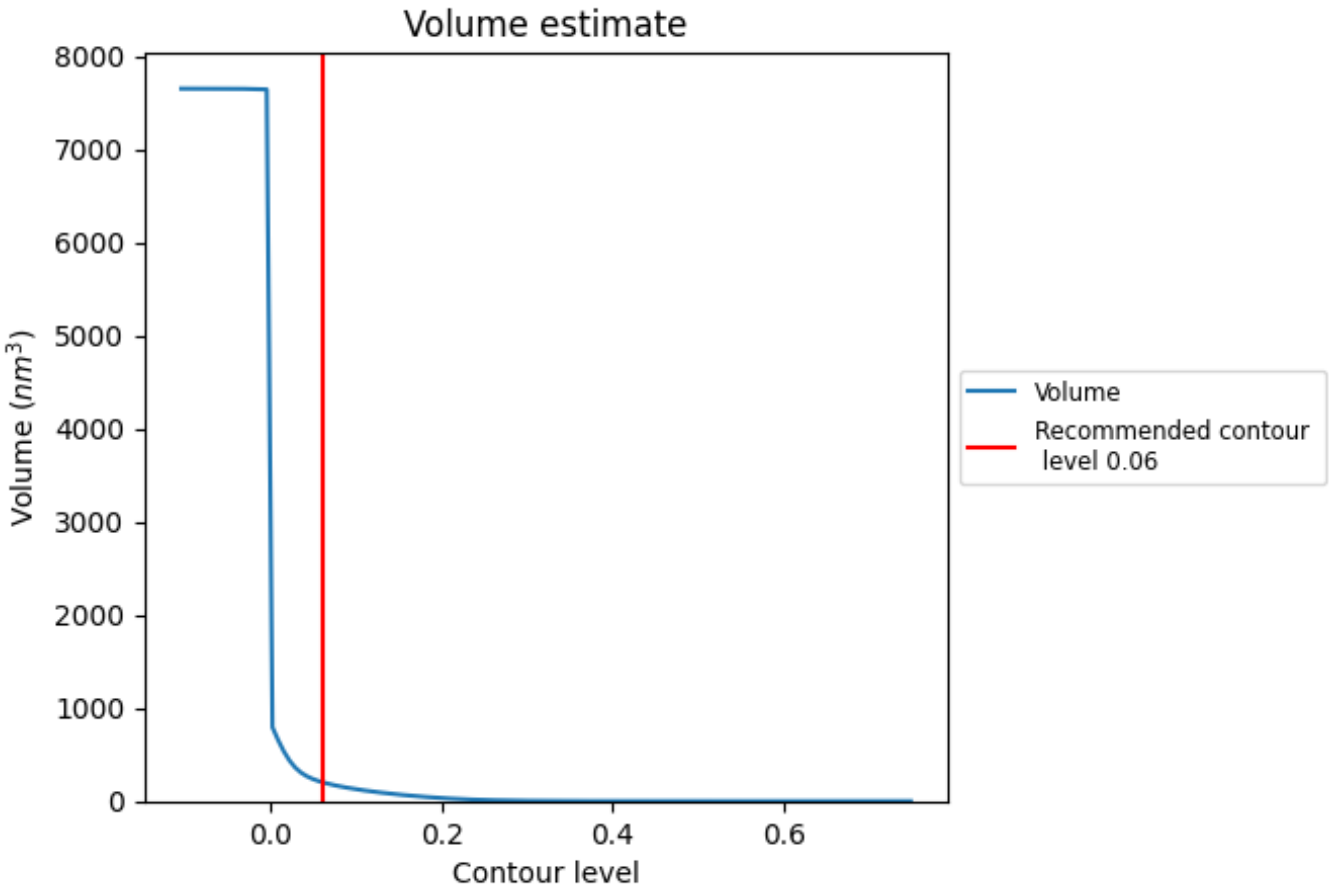
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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 (i)



The volume at the recommended contour level is 205 nm^3; this corresponds to an approximate mass of 185 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.

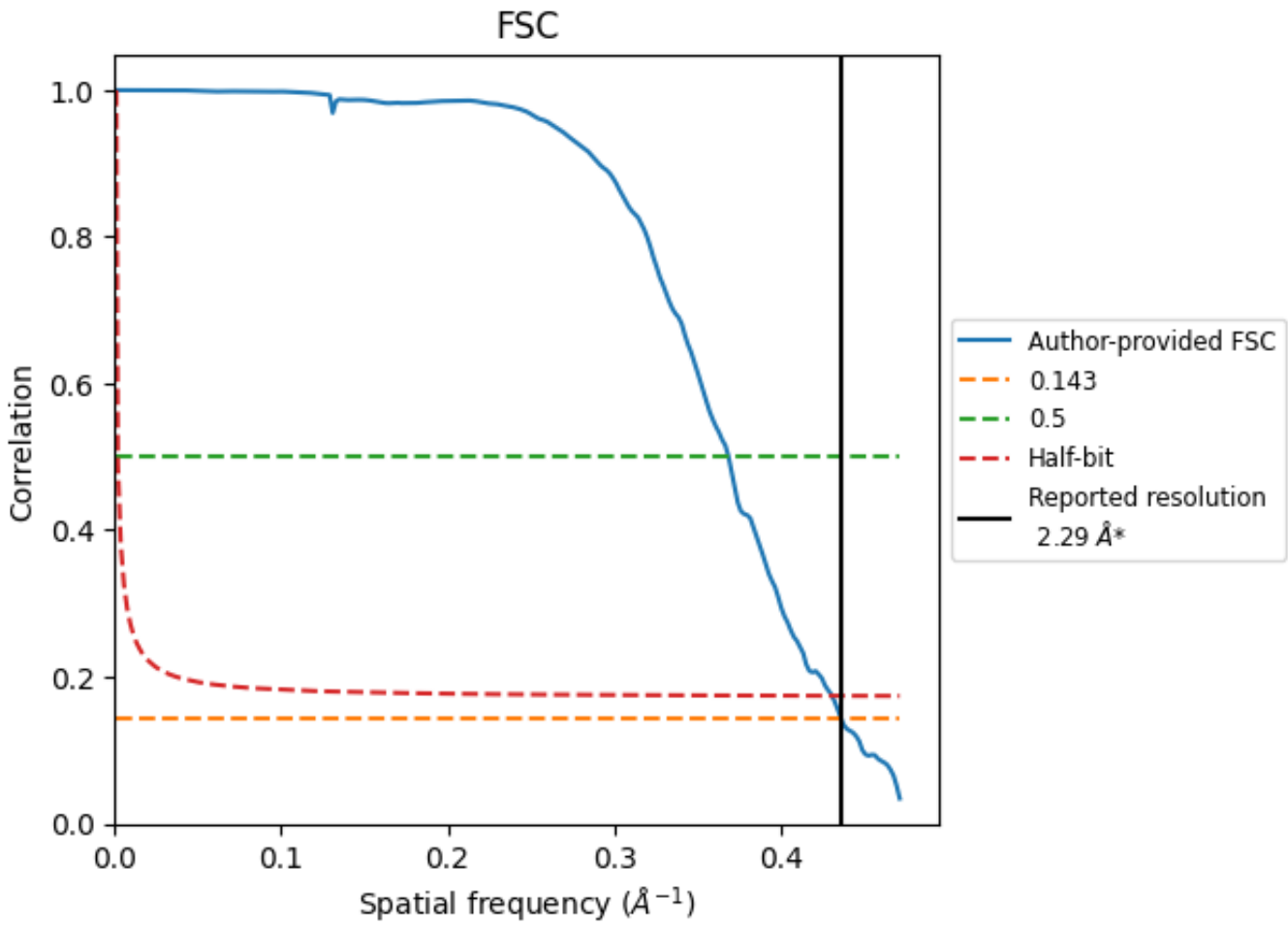
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.437 Å^{-1}

8.2 Resolution estimates (i)

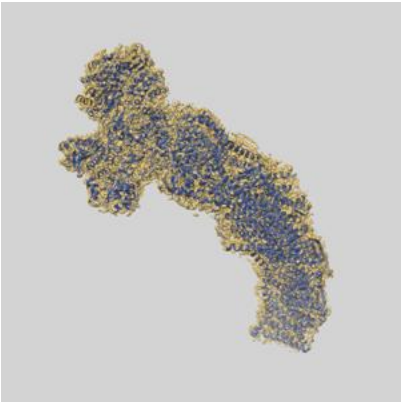
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	2.29	2.71	2.32
Unmasked-calculated*	-	-	-

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

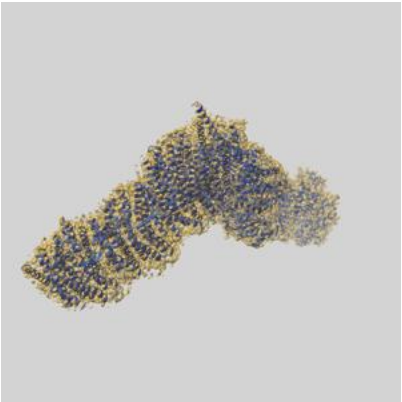
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14538 and PDB model 7Z7V. Per-residue inclusion information can be found in section 3 on page 12.

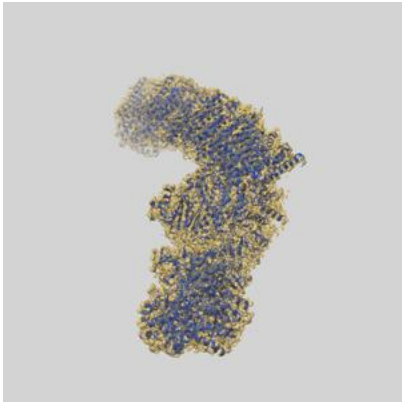
9.1 Map-model overlay (i)



X



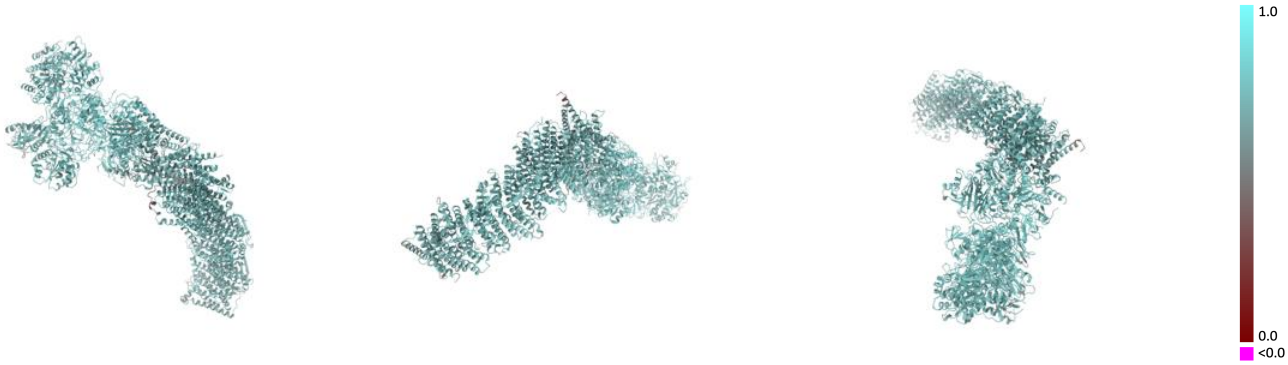
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

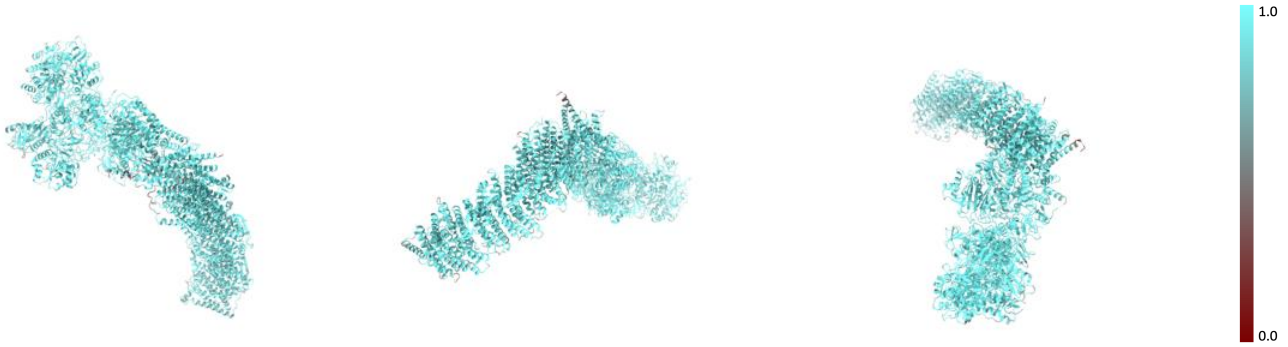
9.2 Q-score mapped to coordinate model (i)



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.

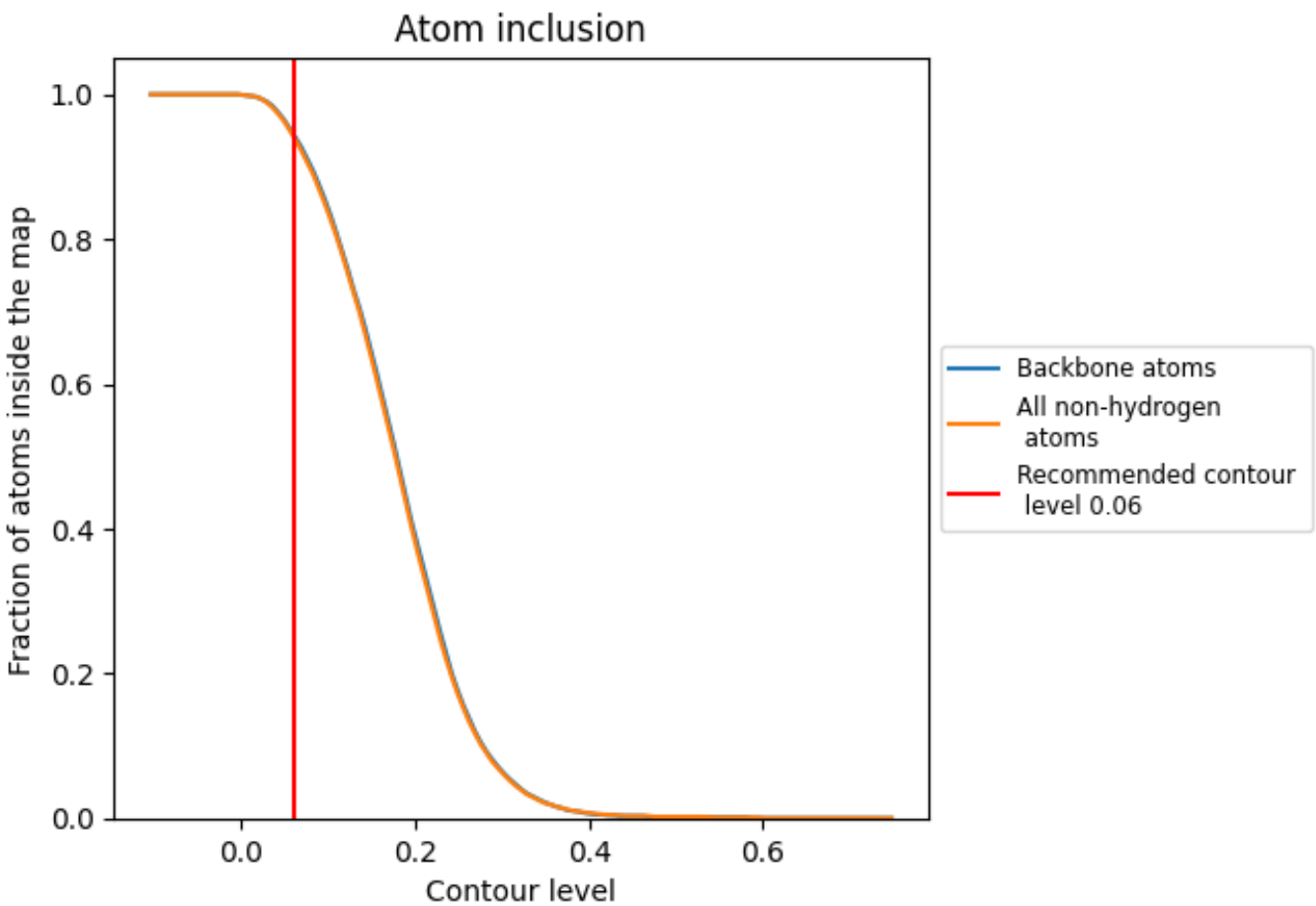
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9410	0.7090
A	0.8830	0.6660
B	0.9590	0.7270
C	0.9520	0.7310
E	0.9420	0.7050
F	0.9610	0.7170
G	0.9610	0.7370
H	0.9160	0.6610
I	0.9510	0.7430
J	0.9100	0.6830
K	0.9760	0.7290
L	0.9110	0.6710
M	0.9410	0.6990
N	0.9550	0.7120