Full wwPDB EM Validation Report (i)

Jul 8, 2024 – 12:47 am BST

PDB ID	:	7P7M
EMDB ID	:	EMD-13240
Title	:	Complex I from E. coli, DDM/LMNG-purified, inhibited by Piericidin A, Open state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2021-07-19
Resolution	:	3.20 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:

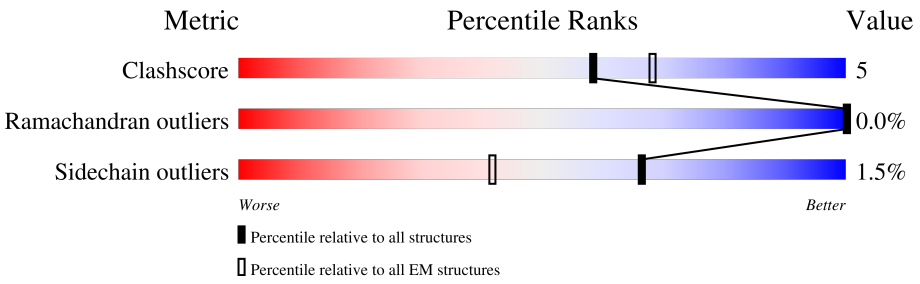
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	F	439	87% 13%
2	E	156	87% 13%
3	G	905	85% 15%
4	C	600	86% 11% •
5	B	220	80% 10% 10%
6	I	180	86% 14%
7	H	325	79% 16% • •
8	A	147	60% 8% • 31%

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Mol	Chain	Length	Quality of chain
9	L	613	85% 12%
10	M	504	88% 12%
11	N	485	84% 14%
12	K	100	83% 17%
13	J	184	66% 21% 13%

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

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

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 37390 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	589	4728	3032	822	850	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	311	2444	1644	385	397	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	102	808	555	124	125	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	596	4549	3029	721	767	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	480	3638	2428	574	616	20	0	0

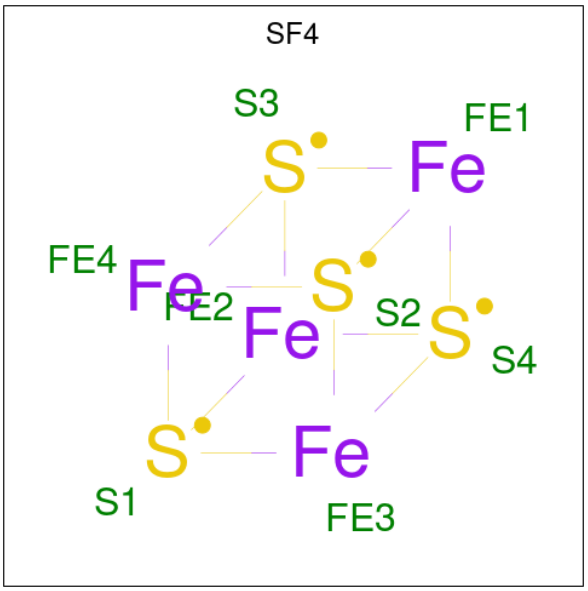
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

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.

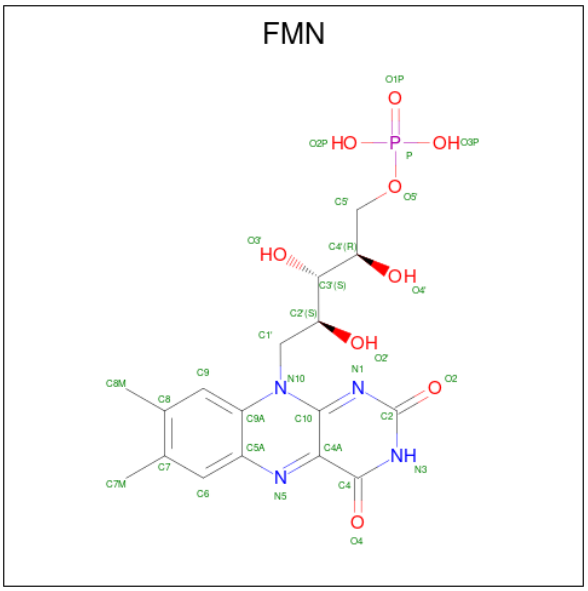
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	160	1218	820	186	205	7	0	0

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



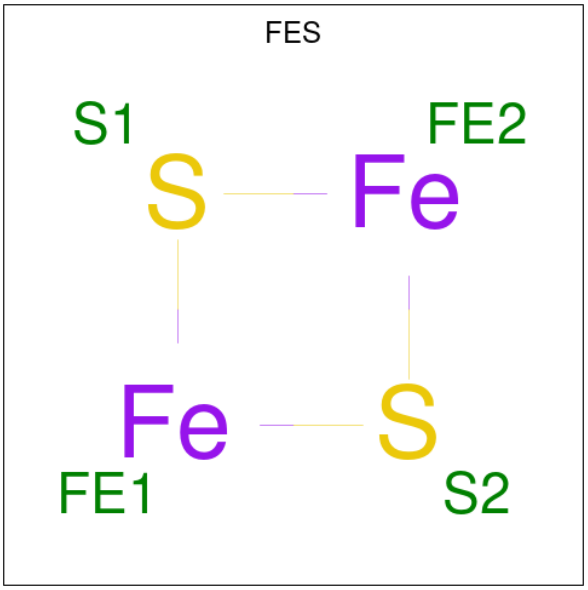
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
14	F	1	8	4	4	0
14	G	1	8	4	4	0
14	G	1	8	4	4	0
14	G	1	8	4	4	0
14	B	1	8	4	4	0
14	I	1	8	4	4	0
14	I	1	8	4	4	0

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

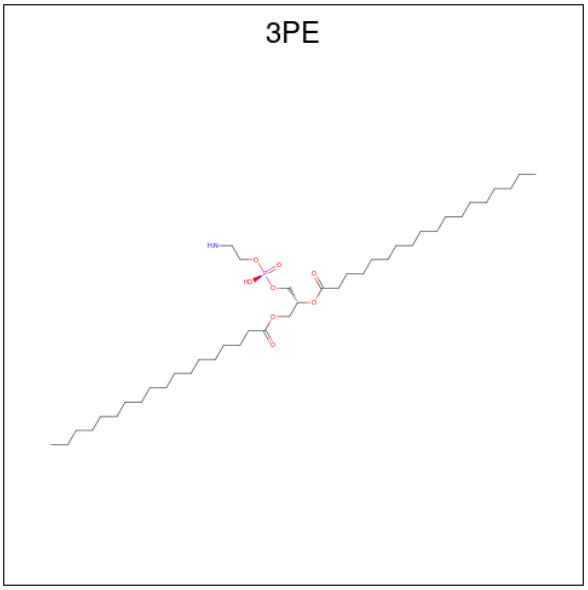


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
16	E	1	4	2	2	0
16	G	1	Total	Fe	S	
			4	2	2	0

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

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

- Molecule 18 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	
18	C	1	51	41	1	8	1	0
18	A	1	29	19	1	8	1	0
18	L	1	51	41	1	8	1	0
18	L	1	44	34	1	8	1	0
18	L	1	25	15	1	8	1	0
18	L	1	51	41	1	8	1	0
18	L	1	51	41	1	8	1	0
18	M	1	39	29	1	8	1	0
18	M	1	51	41	1	8	1	0
18	J	1	39	29	1	8	1	0

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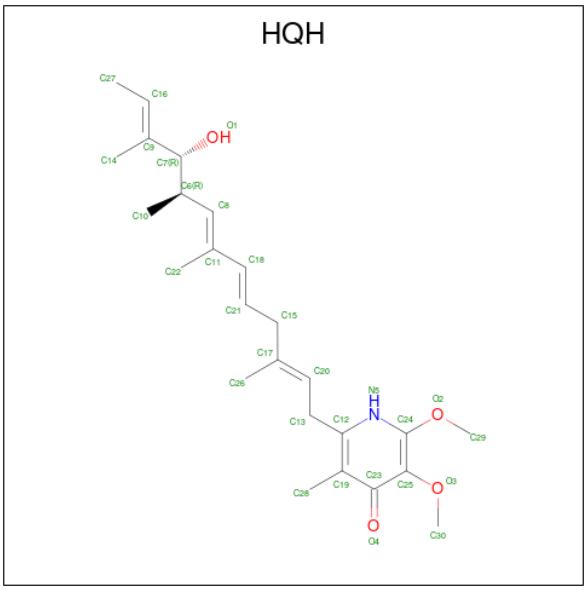
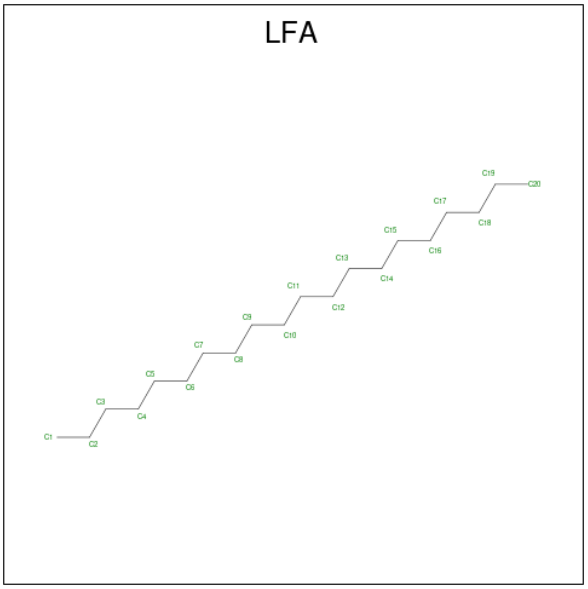
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	J	1	34	24	1	8	1	0

- Molecule 19 is Piericidin A (three-letter code: HQH) (formula: $C_{25}H_{37}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
19	H	1	30	25	1	4	0

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



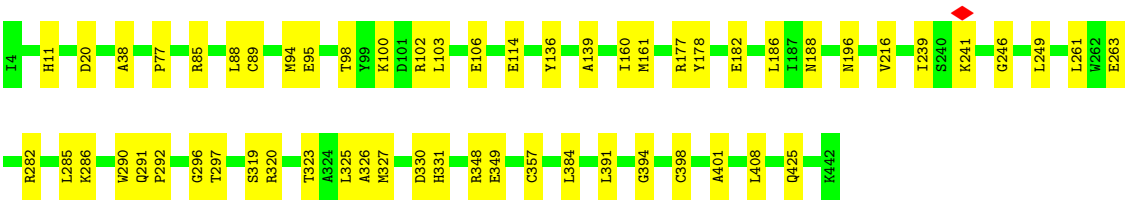
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
20	L	1	14	14	0
			Total	C	
20	N	1	20	20	0
			Total	C	
20	N	1	14	14	0

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.

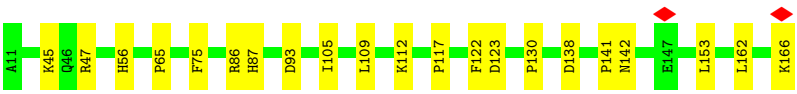
• Molecule 1: NADH-quinone oxidoreductase subunit F

Chain F: 87% 13%



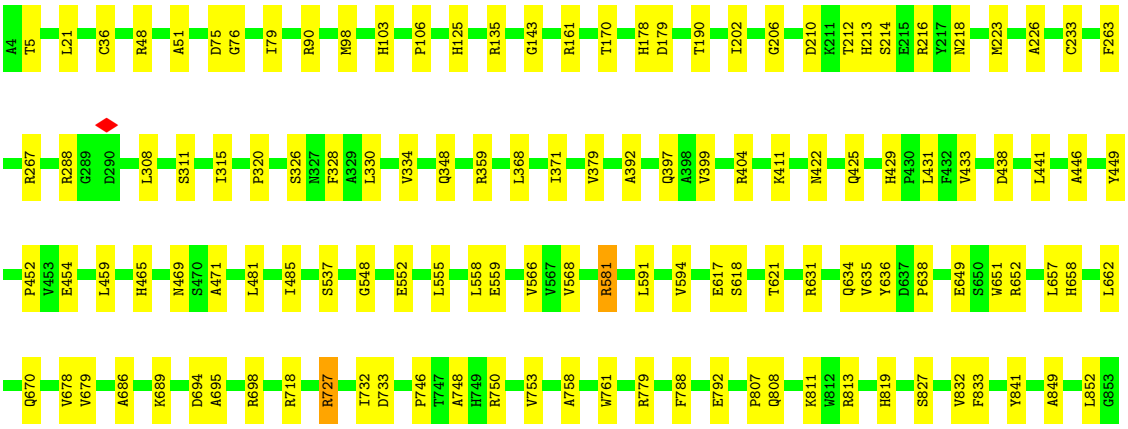
• Molecule 2: NADH dehydrogenase I subunit E

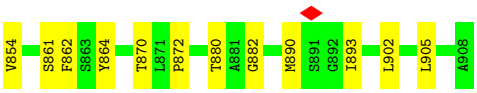
Chain E: 87% 13%



• Molecule 3: NADH-quinone oxidoreductase

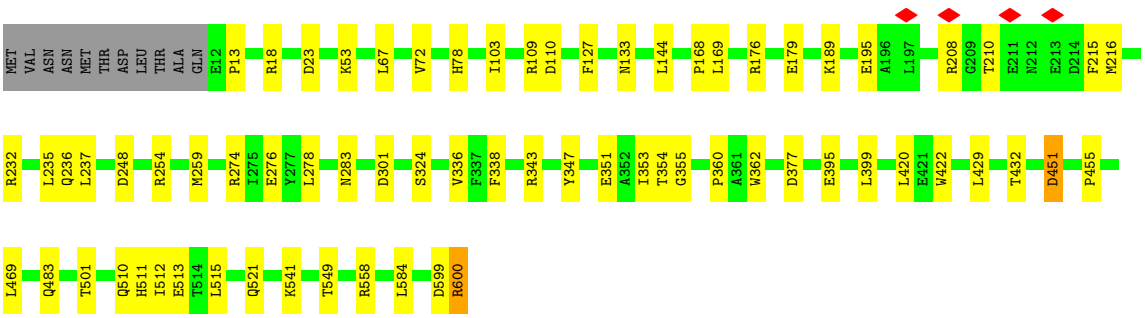
Chain G: 85% 15%





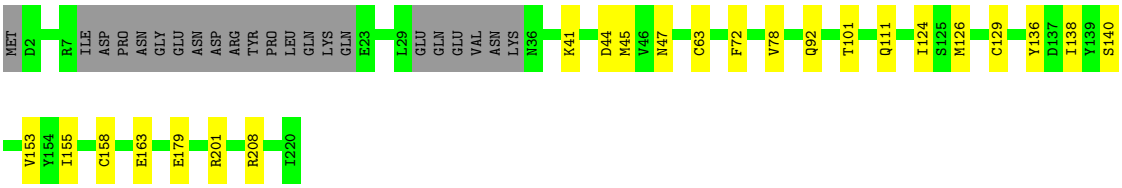
• Molecule 4: NADH-quinone oxidoreductase subunit C/D

Chain C:



• Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:

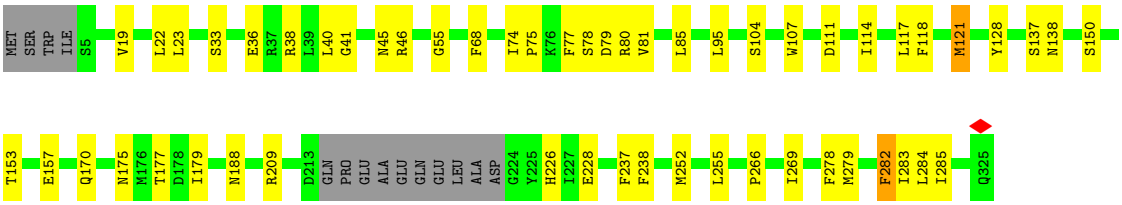


• Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:

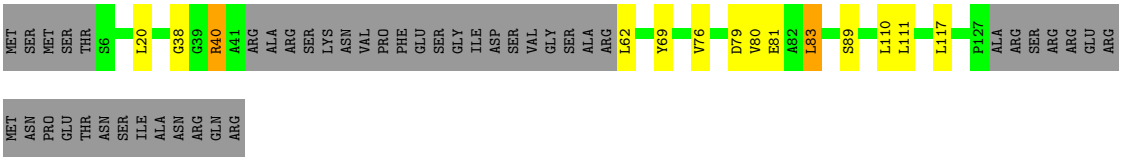
• Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:



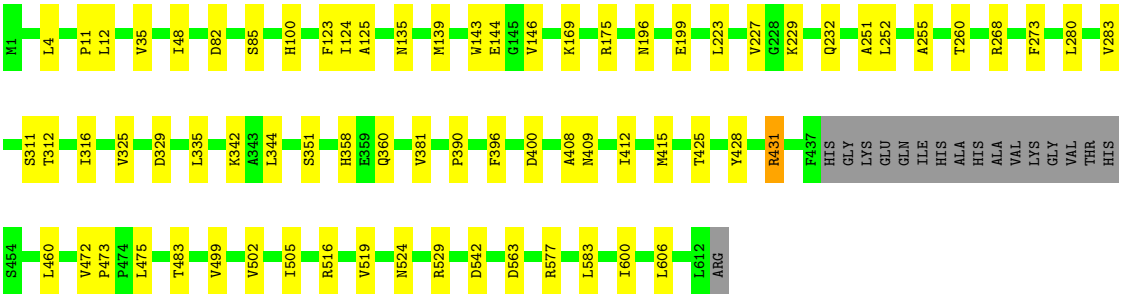
• Molecule 8: NADH-quinone oxidoreductase subunit A

Chain A:



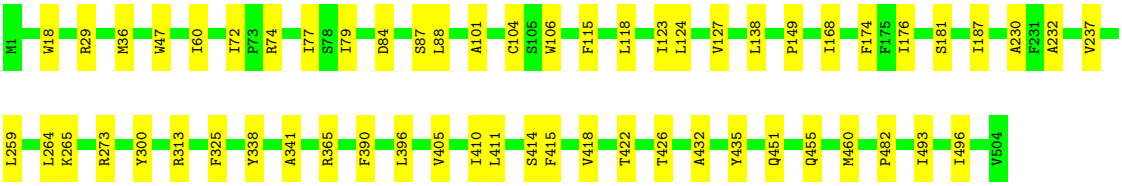
• Molecule 9: Proton-translocating NADH-quinone oxidoreductase, chain L

Chain L:



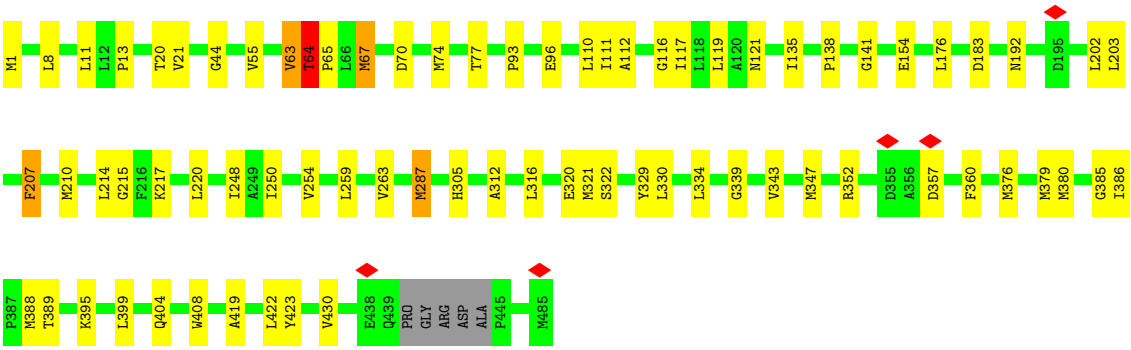
• Molecule 10: NADH dehydrogenase I subunit M

Chain M:



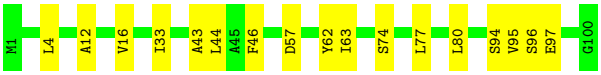
• Molecule 11: NADH-quinone oxidoreductase subunit N

Chain N:



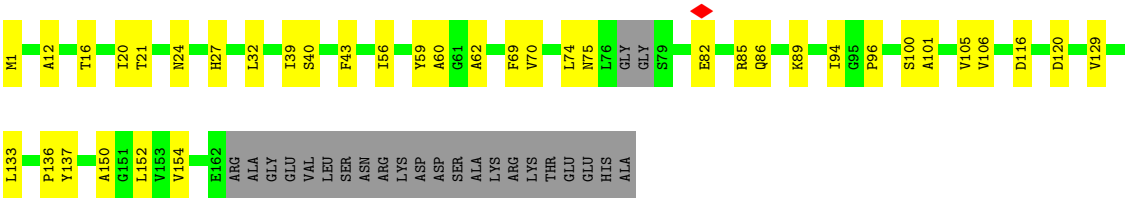
• Molecule 12: NADH-quinone oxidoreductase subunit K

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, C1	Depositor
Number of particles used	99940	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	90	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.395	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	156.09001, 216.59001, 238.37001	wwPDB
Map dimensions	197, 179, 129	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	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: CA, HQH, SF4, LFA, FES, FMN, 3PE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	F	0.26	0/3486	0.50	0/4713
2	E	0.26	0/1248	0.52	0/1691
3	G	0.28	0/7173	0.57	2/9726 (0.0%)
4	C	0.28	0/4859	0.53	0/6599
5	B	0.27	0/1601	0.55	0/2168
6	I	0.27	0/1470	0.53	0/1985
7	H	0.30	0/2516	0.52	0/3420
8	A	0.29	0/833	0.56	0/1134
9	L	0.27	0/4665	0.49	0/6360
10	M	0.28	0/4074	0.50	0/5546
11	N	0.29	0/3727	0.51	1/5085 (0.0%)
12	K	0.33	0/769	0.58	1/1040 (0.1%)
13	J	0.30	0/1243	0.57	0/1695
All	All	0.28	0/37664	0.53	4/51162 (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
11	N	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	872	PRO	CA-N-CD	-7.22	101.39	111.50
3	G	852	LEU	CA-CB-CG	6.19	129.54	115.30
11	N	183	ASP	CB-CG-OD1	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	K	95	VAL	CA-CB-CG1	5.08	118.53	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	N	63	VAL	Peptide
11	N	64	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3407	0	3374	37	0
2	E	1220	0	1187	15	0
3	G	7022	0	6824	76	0
4	C	4728	0	4623	47	0
5	B	1568	0	1553	15	0
6	I	1436	0	1415	17	0
7	H	2444	0	2503	30	0
8	A	808	0	821	10	0
9	L	4549	0	4688	48	0
10	M	3953	0	4053	32	0
11	N	3638	0	3804	46	0
12	K	760	0	817	13	0
13	J	1218	0	1290	27	0
14	B	8	0	0	2	0
14	F	8	0	0	0	0
14	G	24	0	0	1	0
14	I	16	0	0	0	0
15	F	31	0	19	0	0
16	E	4	0	0	1	0
16	G	4	0	0	0	0
17	G	1	0	0	0	0
18	A	29	0	32	1	0
18	C	51	0	82	3	0
18	J	73	0	94	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	222	0	335	9	0
18	M	90	0	134	2	0
19	H	30	0	0	0	0
20	L	14	0	27	1	0
20	N	34	0	69	0	0
All	All	37390	0	37744	370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (370) 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:63:VAL:O	11:N:67:MET:HB2	1.70	0.91
10:M:181:SER:HB2	10:M:230:ALA:HA	1.70	0.71
3:G:21:LEU:HD21	3:G:79:ILE:HG21	1.71	0.71
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.73	0.71
5:B:126:MET:HG3	5:B:155:ILE:HD12	1.76	0.67
13:J:96:PRO:O	13:J:100:SER:HB2	1.96	0.66
7:H:209:ARG:HG3	7:H:282:PHE:HE1	1.61	0.66
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.78	0.65
11:N:419:ALA:HA	11:N:422:LEU:HD12	1.78	0.64
4:C:276:GLU:O	4:C:283:ASN:ND2	2.30	0.64
11:N:65:PRO:HG2	13:J:136:PRO:HB3	1.79	0.64
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.81	0.63
18:J:201:3PE:H271	18:J:202:3PE:H261	1.81	0.62
11:N:305:HIS:HD1	11:N:329:TYR:HH	1.47	0.62
13:J:82:GLU:HG2	13:J:85:ARG:HH12	1.65	0.62
3:G:862:PHE:HB3	3:G:905:LEU:HD13	1.83	0.61
4:C:235:LEU:HD21	4:C:584:LEU:HD22	1.82	0.61
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.83	0.61
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.83	0.60
2:E:142:ASN:ND2	16:E:201:FES:S1	2.74	0.60
2:E:141:PRO:HG2	2:E:153:LEU:HB2	1.84	0.60
3:G:890:MET:HB2	3:G:893:ILE:HD12	1.84	0.60
18:C:701:3PE:H3E2	7:H:285:ILE:HG13	1.83	0.60
4:C:210:THR:HA	4:C:215:PHE:HB2	1.83	0.59
9:L:85:SER:OG	9:L:268:ARG:NH2	2.35	0.59
1:F:103:LEU:HD22	1:F:261:LEU:HD23	1.84	0.59
7:H:121:MET:HE2	13:J:56:ILE:HD12	1.83	0.59
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.83	0.59
3:G:103:HIS:HA	4:C:512:ILE:HD13	1.86	0.58
3:G:861:SER:HB2	3:G:870:THR:HG22	1.85	0.58
3:G:559:GLU:OE1	3:G:581:ARG:NH1	2.37	0.57
9:L:175:ARG:NH2	10:M:396:LEU:O	2.37	0.57
3:G:862:PHE:HB2	3:G:902:LEU:HD11	1.87	0.57
3:G:106:PRO:HD3	4:C:515:LEU:HD21	1.86	0.57
1:F:291:GLN:NE2	1:F:297:THR:O	2.36	0.57
1:F:348:ARG:NH2	2:E:93:ASP:OD1	2.37	0.57
9:L:144:GLU:OE1	9:L:175:ARG:NH1	2.37	0.57
8:A:62:LEU:O	13:J:75:ASN:ND2	2.38	0.57
9:L:325:VAL:O	9:L:409:ASN:ND2	2.36	0.57
3:G:5:THR:O	3:G:76:GLY:N	2.37	0.56
5:B:92:GLN:NE2	7:H:226:HIS:O	2.38	0.56
5:B:138:ILE:HG23	5:B:140:SER:H	1.68	0.56
3:G:454:GLU:OE2	3:G:813:ARG:NH1	2.38	0.56
4:C:215:PHE:HA	4:C:237:LEU:O	2.05	0.56
4:C:360:PRO:O	6:I:45:ARG:NH1	2.34	0.56
9:L:412:ILE:HA	9:L:415:MET:HE3	1.86	0.56
1:F:391:LEU:HD23	1:F:401:ALA:HB1	1.88	0.56
2:E:112:LYS:HD3	2:E:162:LEU:HD12	1.87	0.56
1:F:282:ARG:HB2	1:F:285:LEU:HD12	1.88	0.56
3:G:397:GLN:O	3:G:404:ARG:NH2	2.37	0.56
4:C:195:GLU:OE2	4:C:232:ARG:NH2	2.38	0.56
9:L:143:TRP:O	9:L:229:LYS:NZ	2.39	0.56
3:G:348:GLN:NE2	3:G:548:GLY:O	2.39	0.56
4:C:144:LEU:HA	4:C:168:PRO:HD2	1.87	0.56
4:C:208:ARG:O	4:C:236:GLN:NE2	2.35	0.56
10:M:451:GLN:O	10:M:455:GLN:NE2	2.39	0.56
8:A:69:TYR:OH	12:K:74:SER:O	2.24	0.55
4:C:189:LYS:HD2	5:B:111:GLN:HG2	1.88	0.55
4:C:451:ASP:O	4:C:483:GLN:NE2	2.40	0.55
9:L:499:VAL:HA	9:L:502:VAL:HG22	1.88	0.55
9:L:583:LEU:HB3	11:N:287:MET:HG2	1.87	0.55
10:M:365:ARG:HH21	10:M:460:MET:HA	1.71	0.55
10:M:123:ILE:HG13	10:M:149:PRO:HB2	1.90	0.54
10:M:168:ILE:HG12	11:N:430:VAL:HG11	1.90	0.54
9:L:577:ARG:NH1	18:L:806:3PE:O22	2.36	0.54
11:N:248:ILE:HD11	11:N:334:LEU:HB2	1.88	0.54
11:N:386:ILE:O	11:N:389:THR:OG1	2.21	0.54
12:K:44:LEU:HD13	13:J:39:ILE:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:552:GLU:HA	3:G:555:LEU:HD12	1.89	0.54
10:M:338:TYR:HB3	10:M:493:ILE:HD12	1.88	0.54
3:G:652:ARG:NH2	3:G:733:ASP:OD1	2.41	0.54
4:C:216:MET:HG2	4:C:237:LEU:HB2	1.89	0.54
8:A:81:GLU:HG3	8:A:110:LEU:HD13	1.90	0.53
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.90	0.53
18:M:702:3PE:H3B1	11:N:408:TRP:HB3	1.90	0.53
6:I:51:THR:HG22	6:I:139:ILE:HD11	1.89	0.53
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.89	0.53
1:F:357:CYS:HB2	1:F:401:ALA:HB2	1.90	0.53
7:H:77:PHE:O	7:H:138:ASN:ND2	2.42	0.53
9:L:519:VAL:HG13	18:L:804:3PE:H31	1.90	0.53
3:G:206:GLY:N	14:G:1001:SF4:S2	2.82	0.53
5:B:163:GLU:HG2	6:I:38:VAL:HG21	1.90	0.53
2:E:117:PRO:HB3	2:E:130:PRO:HD3	1.91	0.53
4:C:232:ARG:HB2	4:C:248:ASP:HB3	1.90	0.53
5:B:63:CYS:HB2	14:B:301:SF4:S1	2.48	0.53
3:G:438:ASP:OD1	3:G:438:ASP:N	2.40	0.52
6:I:17:ILE:HG23	7:H:284:LEU:HG	1.91	0.52
6:I:48:ILE:HG12	6:I:116:LEU:HG	1.90	0.52
9:L:408:ALA:HB1	9:L:483:THR:HG23	1.91	0.52
4:C:377:ASP:N	4:C:377:ASP:OD1	2.43	0.52
10:M:29:ARG:NH1	10:M:106:TRP:O	2.41	0.52
1:F:160:ILE:HG22	1:F:161:MET:HG2	1.91	0.52
4:C:13:PRO:O	4:C:18:ARG:NH2	2.42	0.52
3:G:267:ARG:NH2	3:G:819:HIS:O	2.43	0.52
3:G:368:LEU:HD12	3:G:371:ILE:HD12	1.92	0.52
9:L:273:PHE:HB3	9:L:280:LEU:HD13	1.92	0.52
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.81	0.52
4:C:395:GLU:HA	4:C:399:LEU:HB2	1.92	0.52
7:H:38:ARG:NH1	7:H:55:GLY:O	2.43	0.52
3:G:226:ALA:HB3	3:G:635:VAL:HG22	1.93	0.51
8:A:111:LEU:HD22	18:A:201:3PE:H271	1.93	0.51
9:L:431:ARG:NH2	18:L:804:3PE:O12	2.39	0.51
4:C:103:ILE:HG12	4:C:110:ASP:HB3	1.91	0.51
11:N:8:LEU:HD23	11:N:11:LEU:HD12	1.92	0.51
11:N:64:THR:HB	11:N:67:MET:H	1.75	0.51
4:C:144:LEU:HB3	4:C:169:LEU:HB2	1.93	0.51
11:N:215:GLY:HA2	11:N:220:LEU:HD12	1.93	0.51
8:A:20:LEU:HD21	18:J:202:3PE:H272	1.93	0.51
18:L:805:3PE:H2C2	18:L:805:3PE:H3A2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:80:LEU:HD21	13:J:74:LEU:HD11	1.93	0.51
3:G:670:GLN:NE2	3:G:732:ILE:O	2.43	0.50
10:M:127:VAL:HG11	10:M:264:LEU:HD23	1.91	0.50
9:L:143:TRP:NE1	9:L:229:LYS:HG3	2.26	0.50
12:K:57:ASP:OD2	13:J:137:TYR:OH	2.29	0.50
13:J:129:VAL:O	13:J:133:LEU:HB2	2.11	0.50
1:F:178:TYR:HB3	1:F:349:GLU:HB3	1.94	0.50
2:E:109:LEU:HD23	2:E:162:LEU:HD11	1.94	0.50
4:C:72:VAL:HG21	4:C:420:LEU:HD13	1.92	0.50
7:H:266:PRO:HD2	7:H:269:ILE:HD12	1.94	0.50
5:B:101:THR:HA	5:B:129:CYS:HB3	1.92	0.50
7:H:137:SER:HB2	7:H:228:GLU:HG3	1.93	0.50
11:N:385:GLY:HA3	11:N:395:LYS:HE2	1.94	0.50
1:F:98:THR:HA	1:F:325:LEU:HD12	1.94	0.50
3:G:308:LEU:HD23	3:G:591:LEU:HD21	1.94	0.50
4:C:23:ASP:OD1	4:C:109:ARG:NH1	2.45	0.50
10:M:414:SER:O	10:M:418:VAL:N	2.35	0.50
11:N:207:PHE:HA	11:N:210:MET:HG3	1.93	0.50
1:F:182:GLU:O	1:F:186:LEU:N	2.40	0.50
3:G:558:LEU:HD21	3:G:566:VAL:HB	1.94	0.50
7:H:75:PRO:HB2	7:H:78:SER:HB3	1.93	0.50
4:C:133:ASN:HB3	4:C:422:TRP:HA	1.94	0.50
9:L:606:LEU:HB3	13:J:106:VAL:HG11	1.93	0.50
9:L:502:VAL:HA	9:L:505:ILE:HG22	1.94	0.49
9:L:311:SER:OG	9:L:342:LYS:NZ	2.39	0.49
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.94	0.49
4:C:455:PRO:HB2	4:C:469:LEU:HD22	1.93	0.49
1:F:11:HIS:HD2	1:F:263:GLU:HB3	1.78	0.49
3:G:452:PRO:HD3	3:G:880:THR:HG21	1.94	0.49
3:G:558:LEU:HD11	3:G:566:VAL:HG21	1.94	0.49
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.94	0.49
3:G:481:LEU:O	3:G:485:ILE:HG12	2.13	0.49
7:H:79:ASP:OD2	13:J:27:HIS:NE2	2.45	0.48
9:L:516:ARG:HB2	9:L:519:VAL:HB	1.95	0.48
11:N:176:LEU:HD22	11:N:202:LEU:HD11	1.95	0.48
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.93	0.48
7:H:179:ILE:HG21	7:H:255:LEU:HD23	1.95	0.48
9:L:12:LEU:HD21	18:L:801:3PE:H3H1	1.95	0.48
11:N:1:MET:HG2	11:N:65:PRO:HD3	1.95	0.48
11:N:203:LEU:HD21	11:N:263:VAL:HG22	1.94	0.48
12:K:12:ALA:O	12:K:16:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:170:GLN:NE2	7:H:188:ASN:OD1	2.46	0.48
3:G:695:ALA:O	3:G:698:ARG:NH1	2.42	0.48
3:G:807:PRO:HB3	3:G:882:GLY:HA3	1.94	0.48
3:G:212:THR:HG22	3:G:832:VAL:HG21	1.96	0.48
3:G:51:ALA:O	3:G:90:ARG:NH1	2.47	0.48
9:L:123:PHE:HE1	9:L:146:VAL:HG13	1.79	0.48
11:N:117:ILE:O	11:N:121:ASN:ND2	2.47	0.48
10:M:422:THR:O	10:M:426:THR:OG1	2.25	0.48
1:F:331:HIS:H	1:F:331:HIS:CD2	2.31	0.48
4:C:429:LEU:O	4:C:432:THR:OG1	2.30	0.48
4:C:501:THR:HG23	4:C:521:GLN:HB3	1.95	0.48
8:A:76:VAL:HG22	13:J:62:ALA:HB1	1.96	0.48
11:N:352:ARG:NH2	11:N:357:ASP:O	2.47	0.48
1:F:102:ARG:O	1:F:106:GLU:HB2	2.14	0.47
6:I:154:ALA:O	6:I:161:LYS:NZ	2.36	0.47
10:M:36:MET:HE2	10:M:124:LEU:HD13	1.96	0.47
11:N:214:LEU:HD13	11:N:254:VAL:HG22	1.97	0.47
11:N:320:GLU:OE1	11:N:404:GLN:NE2	2.48	0.47
3:G:216:ARG:NH1	6:I:90:GLU:OE1	2.47	0.47
3:G:326:SER:HA	3:G:651:TRP:HB3	1.97	0.47
3:G:750:ARG:HH12	3:G:753:VAL:HA	1.80	0.47
7:H:279:MET:O	7:H:283:ILE:HG12	2.15	0.47
8:A:80:VAL:HA	8:A:83:LEU:HD23	1.95	0.47
18:C:701:3PE:H3I1	7:H:278:PHE:HB3	1.97	0.47
7:H:118:PHE:HA	7:H:121:MET:HG3	1.95	0.47
8:A:38:GLY:O	8:A:40:ARG:NH1	2.48	0.47
9:L:196:ASN:HB3	9:L:199:GLU:HB2	1.96	0.47
13:J:20:ILE:HG13	13:J:21:THR:HG23	1.96	0.47
3:G:143:GLY:HA3	3:G:190:THR:HG23	1.96	0.47
5:B:201:ARG:NH1	6:I:131:VAL:O	2.48	0.47
1:F:177:ARG:NH2	2:E:75:PHE:O	2.48	0.47
5:B:41:LYS:O	5:B:45:MET:HG3	2.15	0.47
10:M:187:ILE:HD11	11:N:399:LEU:HD22	1.97	0.47
4:C:324:SER:HB2	4:C:336:VAL:HA	1.96	0.46
5:B:72:PHE:HA	5:B:78:VAL:HG12	1.97	0.46
8:A:83:LEU:HD11	12:K:63:ILE:HG23	1.97	0.46
3:G:679:VAL:HG21	3:G:689:LYS:HB2	1.97	0.46
9:L:82:ASP:N	9:L:82:ASP:OD1	2.47	0.46
10:M:60:ILE:HD11	10:M:496:ILE:HA	1.97	0.46
1:F:95:GLU:OE2	1:F:296:GLY:N	2.48	0.46
1:F:394:GLY:O	3:G:48:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:600:ILE:HD11	20:L:802:LFA:H121	1.97	0.46
2:E:138:ASP:OD1	2:E:138:ASP:N	2.49	0.46
5:B:47:ASN:ND2	5:B:179:GLU:O	2.48	0.46
7:H:22:LEU:HD11	7:H:95:LEU:HD21	1.97	0.46
9:L:563:ASP:OD1	10:M:300:TYR:OH	2.30	0.46
12:K:77:LEU:HD22	13:J:70:VAL:HG11	1.97	0.46
3:G:36:CYS:O	3:G:161:ARG:NH1	2.37	0.46
3:G:315:ILE:HG13	3:G:566:VAL:HG23	1.98	0.46
3:G:392:ALA:HB1	3:G:441:LEU:HD21	1.97	0.46
9:L:344:LEU:HD21	9:L:381:VAL:HG23	1.97	0.46
4:C:53:LYS:HA	4:C:53:LYS:HD3	1.80	0.45
9:L:344:LEU:HB2	9:L:460:LEU:HB3	1.97	0.45
9:L:358:HIS:HB2	9:L:360:GLN:HE21	1.80	0.45
7:H:114:ILE:HB	7:H:117:LEU:HB2	1.98	0.45
9:L:542:ASP:OD1	9:L:542:ASP:N	2.48	0.45
3:G:214:SER:O	6:I:79:LYS:NZ	2.50	0.45
11:N:154:GLU:OE1	12:K:97:GLU:N	2.49	0.45
3:G:125:HIS:CD2	4:C:513:GLU:HG2	2.52	0.45
10:M:72:ILE:HB	10:M:77:ILE:HB	1.98	0.45
11:N:93:PRO:HA	11:N:96:GLU:HG3	1.99	0.45
1:F:88:LEU:HD12	1:F:216:VAL:HG22	1.99	0.45
3:G:808:GLN:HG3	3:G:811:LYS:HB2	1.98	0.45
5:B:208:ARG:NH1	6:I:132:TYR:OH	2.46	0.45
7:H:128:TYR:OH	13:J:60:ALA:O	2.22	0.45
1:F:348:ARG:NH1	2:E:93:ASP:OD2	2.49	0.45
4:C:110:ASP:OD1	4:C:110:ASP:N	2.49	0.45
10:M:176:ILE:HD11	11:N:423:TYR:HB2	1.99	0.45
11:N:20:THR:HG21	11:N:44:GLY:HA3	1.99	0.45
13:J:12:ALA:O	13:J:16:THR:OG1	2.29	0.45
3:G:330:LEU:O	3:G:334:VAL:HG22	2.16	0.45
4:C:549:THR:HB	4:C:558:ARG:HB3	1.98	0.45
10:M:87:SER:OG	10:M:273:ARG:NH2	2.48	0.45
3:G:618:SER:HB2	3:G:649:GLU:HG3	1.99	0.45
4:C:343:ARG:NH2	4:C:347:TYR:OH	2.50	0.45
9:L:329:ASP:HA	9:L:475:LEU:HD13	1.99	0.45
3:G:210:ASP:HB3	3:G:213:HIS:HB3	1.99	0.44
11:N:112:ALA:HB2	11:N:138:PRO:HB2	1.98	0.44
7:H:150:SER:HA	7:H:153:THR:HG22	2.00	0.44
11:N:343:VAL:HG11	11:N:376:MET:HB2	1.99	0.44
1:F:77:PRO:O	1:F:85:ARG:NH2	2.50	0.44
13:J:56:ILE:HA	13:J:60:ALA:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:727:ARG:HD2	4:C:179:GLU:HB2	2.00	0.44
7:H:81:VAL:O	7:H:85:LEU:HB2	2.17	0.44
8:A:117:LEU:HD11	13:J:152:LEU:HD21	1.98	0.44
9:L:524:ASN:HA	9:L:529:ARG:HH21	1.83	0.44
13:J:101:ALA:O	13:J:105:VAL:HG23	2.18	0.44
1:F:241:LYS:HA	1:F:241:LYS:HD3	1.79	0.44
3:G:694:ASP:OD1	3:G:694:ASP:N	2.47	0.44
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.52	0.44
18:L:801:3PE:H371	10:M:390:PHE:HD1	1.82	0.44
12:K:43:ALA:HB1	12:K:62:TYR:HD1	1.83	0.44
12:K:4:LEU:N	13:J:116:ASP:OD1	2.51	0.43
3:G:267:ARG:HA	3:G:833:PHE:HZ	1.82	0.43
6:I:82:THR:OG1	6:I:84:ASP:OD1	2.31	0.43
9:L:169:LYS:HG3	18:L:803:3PE:H341	2.00	0.43
1:F:286:LYS:HE3	1:F:286:LYS:HB3	1.81	0.43
3:G:328:PHE:CG	3:G:678:VAL:HG12	2.52	0.43
3:G:746:PRO:O	3:G:779:ARG:NH1	2.51	0.43
7:H:74:ILE:HG21	7:H:80:ARG:HG2	2.00	0.43
9:L:35:VAL:HG22	9:L:100:HIS:HB3	2.01	0.43
2:E:123:ASP:OD1	2:E:123:ASP:N	2.47	0.43
2:E:86:ARG:NH2	2:E:166:LYS:O	2.46	0.43
3:G:98:MET:HE3	4:C:512:ILE:HG23	2.00	0.43
3:G:320:PRO:HB2	3:G:537:SER:HB3	2.00	0.43
9:L:251:ALA:O	9:L:255:ALA:HB3	2.19	0.43
3:G:758:ALA:HB3	3:G:761:TRP:HB2	1.99	0.43
9:L:251:ALA:O	9:L:255:ALA:CB	2.67	0.43
18:L:801:3PE:H2I3	18:L:805:3PE:H391	2.00	0.43
10:M:411:LEU:HD13	10:M:426:THR:HG23	2.00	0.43
11:N:312:ALA:O	11:N:322:SER:OG	2.35	0.43
3:G:634:GLN:NE2	3:G:636:TYR:O	2.46	0.43
10:M:18:TRP:HB2	10:M:118:LEU:HD22	2.00	0.43
11:N:339:GLY:HA3	11:N:379:MET:HE3	2.01	0.43
3:G:288:ARG:NH1	3:G:288:ARG:HA	2.34	0.43
3:G:748:ALA:HB3	3:G:750:ARG:HE	1.82	0.43
10:M:405:VAL:HG11	10:M:482:PRO:HG3	1.99	0.43
18:J:201:3PE:H371	18:J:202:3PE:H351	2.00	0.43
4:C:301:ASP:OD1	4:C:301:ASP:N	2.52	0.43
4:C:353:ILE:O	6:I:43:ARG:NH1	2.44	0.43
12:K:33:ILE:HG23	13:J:32:LEU:HD22	2.00	0.43
2:E:45:LYS:HE2	2:E:45:LYS:HB2	1.85	0.42
3:G:568:VAL:O	3:G:594:VAL:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:4:LEU:HA	9:L:48:ILE:HD11	2.00	0.42
18:L:801:3PE:H3I3	18:L:805:3PE:H2H1	2.00	0.42
11:N:119:LEU:HD23	11:N:119:LEU:HA	1.89	0.42
13:J:24:ASN:HB3	13:J:27:HIS:HB2	2.01	0.42
11:N:259:LEU:HB2	11:N:316:LEU:HD21	2.01	0.42
1:F:297:THR:HG22	1:F:320:ARG:HB2	2.02	0.42
10:M:84:ASP:N	10:M:84:ASP:OD1	2.53	0.42
10:M:264:LEU:HD12	10:M:264:LEU:HA	1.81	0.42
11:N:347:MET:HB3	11:N:360:PHE:CE1	2.55	0.42
4:C:176:ARG:NH2	4:C:259:MET:SD	2.91	0.42
1:F:94:MET:HB3	1:F:94:MET:HE2	1.92	0.42
5:B:124:ILE:HG12	5:B:153:VAL:HB	2.00	0.42
9:L:12:LEU:HD23	9:L:12:LEU:HA	1.86	0.42
11:N:119:LEU:HD12	11:N:135:ILE:HD12	2.02	0.42
3:G:465:HIS:HA	3:G:471:ALA:HB3	2.02	0.42
18:M:701:3PE:H322	18:M:702:3PE:H392	2.01	0.42
3:G:422:ASN:O	3:G:425:GLN:NE2	2.44	0.42
3:G:689:LYS:HA	3:G:689:LYS:HD2	1.89	0.42
3:G:849:ALA:HB1	3:G:854:VAL:HB	2.01	0.42
4:C:278:LEU:HD12	4:C:541:LYS:HZ1	1.85	0.42
4:C:510:GLN:O	4:C:511:HIS:ND1	2.53	0.42
4:C:599:ASP:O	4:C:600:ARG:NH1	2.53	0.42
10:M:232:ALA:HB1	10:M:237:VAL:HB	2.02	0.42
11:N:21:VAL:HG22	11:N:110:LEU:HB3	2.00	0.42
2:E:105:ILE:HG21	2:E:153:LEU:HD13	2.02	0.42
3:G:218:ASN:ND2	3:G:223:MET:SD	2.85	0.42
6:I:171:LYS:HB3	6:I:171:LYS:HE3	1.75	0.42
9:L:280:LEU:HD12	9:L:280:LEU:HA	1.94	0.42
11:N:63:VAL:O	11:N:67:MET:CB	2.56	0.42
12:K:44:LEU:HD12	13:J:43:PHE:CE1	2.54	0.42
18:J:201:3PE:H342	18:J:202:3PE:H351	2.02	0.42
3:G:399:VAL:HA	3:G:429:HIS:HB2	2.01	0.41
4:C:254:ARG:HD3	5:B:136:TYR:CZ	2.55	0.41
4:C:351:GLU:HB3	6:I:41:PRO:HG3	2.00	0.41
9:L:390:PRO:HA	9:L:396:PHE:CG	2.54	0.41
1:F:20:ASP:OD1	1:F:20:ASP:N	2.45	0.41
1:F:290:TRP:HA	1:F:327:MET:O	2.20	0.41
10:M:101:ALA:HB2	10:M:259:LEU:HB2	2.02	0.41
11:N:13:PRO:HD3	11:N:55:VAL:HG21	2.01	0.41
11:N:70:ASP:O	11:N:74:MET:HG3	2.20	0.41
11:N:141:GLY:HA3	13:J:154:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:338:PHE:HE1	7:H:45:ASN:HB2	1.86	0.41
6:I:59:ARG:NH2	6:I:142:PRO:O	2.54	0.41
7:H:33:SER:O	7:H:36:GLU:HB3	2.21	0.41
12:K:43:ALA:HB1	12:K:62:TYR:CD1	2.55	0.41
1:F:330:ASP:OD1	1:F:330:ASP:N	2.40	0.41
3:G:679:VAL:HG22	3:G:686:ALA:HA	2.03	0.41
6:I:67:ALA:HA	6:I:75:ILE:HB	2.01	0.41
9:L:227:VAL:HB	9:L:232:GLN:HB2	2.01	0.41
10:M:265:LYS:HD3	10:M:265:LYS:HA	1.81	0.41
1:F:38:ALA:HB2	1:F:114:GLU:HG3	2.03	0.41
1:F:188:ASN:ND2	1:F:196:ASN:O	2.38	0.41
3:G:621:THR:OG1	3:G:631:ARG:NE	2.41	0.41
18:C:701:3PE:H232	6:I:6:LEU:HD12	2.03	0.41
1:F:291:GLN:HA	1:F:292:PRO:HD3	1.94	0.41
3:G:202:ILE:HD11	3:G:263:PHE:HE1	1.86	0.41
9:L:135:ASN:OD1	9:L:135:ASN:N	2.54	0.41
3:G:379:VAL:HB	3:G:433:VAL:HG12	2.03	0.41
3:G:657:LEU:HD12	3:G:657:LEU:HA	1.87	0.41
4:C:67:LEU:HD23	4:C:67:LEU:HA	1.92	0.41
1:F:100:LYS:HE3	1:F:323:THR:HB	2.03	0.41
1:F:384:LEU:HD22	1:F:408:LEU:HD21	2.02	0.41
2:E:87:HIS:NE2	2:E:166:LYS:OXT	2.45	0.41
3:G:178:HIS:CD2	3:G:178:HIS:H	2.39	0.41
3:G:431:LEU:O	3:G:446:ALA:N	2.54	0.41
7:H:19:VAL:O	7:H:23:LEU:HG	2.21	0.41
9:L:124:ILE:HD11	9:L:252:LEU:HD11	2.03	0.41
9:L:260:THR:HB	9:L:335:LEU:HD11	2.02	0.41
9:L:312:THR:O	9:L:316:ILE:HG12	2.21	0.41
13:J:94:ILE:HD12	13:J:94:ILE:HA	1.90	0.41
2:E:65:PRO:HB3	3:G:170:THR:HB	2.02	0.41
4:C:274:ARG:HG2	14:B:301:SF4:S2	2.61	0.41
1:F:291:GLN:O	1:F:326:ALA:HA	2.21	0.40
4:C:354:THR:OG1	4:C:355:GLY:N	2.54	0.40
7:H:153:THR:O	7:H:157:GLU:HB3	2.20	0.40
11:N:116:GLY:HA2	11:N:135:ILE:HD11	2.03	0.40
3:G:178:HIS:ND1	3:G:179:ASP:OD1	2.40	0.40
11:N:192:ASN:OD1	11:N:192:ASN:N	2.52	0.40
11:N:376:MET:O	11:N:380:MET:HG2	2.21	0.40
13:J:86:GLN:H	13:J:86:GLN:CD	2.25	0.40
10:M:47:TRP:CG	10:M:88:LEU:HD21	2.57	0.40
1:F:319:SER:OG	1:F:320:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:5:THR:H	3:G:75:ASP:HA	1.87	0.40
4:C:169:LEU:HD23	4:C:169:LEU:HA	1.89	0.40
7:H:40:LEU:HD23	7:H:40:LEU:HA	1.94	0.40
7:H:175:ASN:OD1	7:H:177:THR:OG1	2.38	0.40
10:M:341:ALA:HA	10:M:410:ILE:HD11	2.03	0.40
1:F:239:ILE:HD12	1:F:246:GLY:HA2	2.03	0.40
1:F:425:GLN:H	1:F:425:GLN:HG2	1.76	0.40
3:G:359:ARG:HB3	3:G:788:PHE:CG	2.56	0.40
3:G:449:TYR:CD2	3:G:459:LEU:HD22	2.56	0.40
3:G:658:HIS:CE1	3:G:662:LEU:HD11	2.57	0.40
7:H:41:GLY:HA2	7:H:46:ARG:HG3	2.03	0.40
9:L:396:PHE:O	9:L:400:ASP:HB2	2.21	0.40
9:L:425:THR:HA	9:L:428:TYR:CE2	2.56	0.40
9:L:472:VAL:HA	9:L:473:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	437/439 (100%)	428 (98%)	9 (2%)	0	100	100
2	E	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
3	G	903/905 (100%)	876 (97%)	27 (3%)	0	100	100
4	C	587/600 (98%)	574 (98%)	13 (2%)	0	100	100
5	B	192/220 (87%)	185 (96%)	7 (4%)	0	100	100
6	I	178/180 (99%)	176 (99%)	2 (1%)	0	100	100
7	H	307/325 (94%)	303 (99%)	4 (1%)	0	100	100
8	A	98/147 (67%)	98 (100%)	0	0	100	100
9	L	592/613 (97%)	578 (98%)	14 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	M	502/504 (100%)	489 (97%)	13 (3%)	0	100	100
11	N	476/485 (98%)	465 (98%)	10 (2%)	1 (0%)	47	79
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	156/184 (85%)	152 (97%)	4 (3%)	0	100	100
All	All	4680/4858 (96%)	4569 (98%)	110 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	N	64	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	353/353 (100%)	351 (99%)	2 (1%)	86	94
2	E	129/129 (100%)	126 (98%)	3 (2%)	50	78
3	G	732/732 (100%)	720 (98%)	12 (2%)	62	84
4	C	500/519 (96%)	495 (99%)	5 (1%)	76	90
5	B	171/192 (89%)	170 (99%)	1 (1%)	86	94
6	I	154/154 (100%)	152 (99%)	2 (1%)	69	87
7	H	257/269 (96%)	250 (97%)	7 (3%)	44	75
8	A	80/119 (67%)	76 (95%)	4 (5%)	24	60
9	L	472/486 (97%)	469 (99%)	3 (1%)	86	94
10	M	413/413 (100%)	407 (98%)	6 (2%)	65	85
11	N	382/385 (99%)	377 (99%)	5 (1%)	69	87
12	K	79/79 (100%)	76 (96%)	3 (4%)	33	67
13	J	128/146 (88%)	122 (95%)	6 (5%)	26	62
All	All	3850/3976 (97%)	3791 (98%)	59 (2%)	66	85

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	89	CYS
1	F	398	CYS
2	E	47	ARG
2	E	56	HIS
2	E	122	PHE
3	G	135	ARG
3	G	233	CYS
3	G	311	SER
3	G	411	LYS
3	G	469	ASN
3	G	581	ARG
3	G	718	ARG
3	G	727	ARG
3	G	792	GLU
3	G	827	SER
3	G	841	TYR
3	G	864	TYR
4	C	78	HIS
4	C	127	PHE
4	C	362	TRP
4	C	451	ASP
4	C	600	ARG
5	B	44	ASP
6	I	55	ASP
6	I	77	LEU
7	H	68	PHE
7	H	111	ASP
7	H	121	MET
7	H	237	PHE
7	H	238	PHE
7	H	252	MET
7	H	282	PHE
8	A	40	ARG
8	A	79	ASP
8	A	83	LEU
8	A	89	SER
9	L	139	MET
9	L	351	SER
9	L	431	ARG
10	M	74	ARG
10	M	104	CYS
10	M	115	PHE

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Mol	Chain	Res	Type
10	M	174	PHE
10	M	313	ARG
10	M	325	PHE
11	N	67	MET
11	N	207	PHE
11	N	287	MET
11	N	321	MET
11	N	388	MET
12	K	46	PHE
12	K	94	SER
12	K	96	SER
13	J	1	MET
13	J	40	SER
13	J	59	TYR
13	J	69	PHE
13	J	89	LYS
13	J	120	ASP

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

Mol	Chain	Res	Type
10	M	308	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	B	301	5	0,12,12	-	-	-		
18	3PE	L	804	-	24,24,50	0.42	0	27,29,55	0.36	0
18	3PE	J	202	-	33,33,50	0.36	0	36,38,55	0.33	0
19	HQH	H	701	-	29,30,30	0.33	0	28,40,40	1.02	2 (7%)
14	SF4	G	1002	3	0,12,12	-	-	-		
14	SF4	G	1003	3	0,12,12	-	-	-		
18	3PE	J	201	-	38,38,50	0.34	0	41,43,55	0.30	0
15	FMN	F	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.21	6 (12%)
20	LFA	N	502	-	13,13,19	0.16	0	12,12,18	0.12	0
18	3PE	A	201	-	28,28,50	0.39	0	31,33,55	0.33	0
16	FES	E	201	2	0,4,4	-	-	-		
18	3PE	L	805	-	50,50,50	0.30	0	53,55,55	0.30	0
14	SF4	I	201	6	0,12,12	-	-	-		
14	SF4	F	501	1	0,12,12	-	-	-		
20	LFA	N	501	-	19,19,19	0.13	0	18,18,18	0.16	0
20	LFA	L	802	-	13,13,19	0.15	0	12,12,18	0.11	0
16	FES	G	1004	3	0,4,4	-	-	-		
18	3PE	M	702	-	50,50,50	0.30	0	53,55,55	0.26	0
18	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.29	0
18	3PE	M	701	-	38,38,50	0.34	0	41,43,55	0.32	0
14	SF4	G	1001	3	0,12,12	-	-	-		
14	SF4	I	202	6	0,12,12	-	-	-		
18	3PE	C	701	-	50,50,50	0.30	0	53,55,55	0.32	0
18	3PE	L	806	-	50,50,50	0.30	0	53,55,55	0.28	0
18	3PE	L	803	-	43,43,50	0.32	0	46,48,55	0.31	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
14	SF4	B	301	5	-	-	0/6/5/5
18	3PE	L	804	-	-	8/28/28/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	3PE	J	202	-	-	4/37/37/54	-
19	HQH	H	701	-	-	9/27/29/29	0/1/1/1
14	SF4	G	1002	3	-	-	0/6/5/5
18	3PE	J	201	-	-	12/42/42/54	-
14	SF4	G	1003	3	-	-	0/6/5/5
15	FMN	F	502	-	-	7/18/18/18	0/3/3/3
20	LFA	N	502	-	-	0/11/11/17	-
18	3PE	A	201	-	-	12/32/32/54	-
16	FES	E	201	2	-	-	0/1/1/1
18	3PE	L	805	-	-	13/54/54/54	-
14	SF4	I	201	6	-	-	0/6/5/5
14	SF4	F	501	1	-	-	0/6/5/5
20	LFA	N	501	-	-	1/17/17/17	-
20	LFA	L	802	-	-	0/11/11/17	-
18	3PE	M	702	-	-	8/54/54/54	-
16	FES	G	1004	3	-	-	0/1/1/1
18	3PE	L	801	-	-	10/54/54/54	-
18	3PE	M	701	-	-	8/42/42/54	-
14	SF4	G	1001	3	-	-	0/6/5/5
14	SF4	I	202	6	-	-	0/6/5/5
18	3PE	C	701	-	-	12/54/54/54	-
18	3PE	L	806	-	-	13/54/54/54	-
18	3PE	L	803	-	-	10/47/47/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.76	1.38	1.30
15	F	502	FMN	C10-N1	2.40	1.38	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	-3.16	119.81	125.64
19	H	701	HQH	C6-C7-C9	3.08	123.23	112.68
19	H	701	HQH	C15-C21-C18	3.04	128.90	124.18
15	F	502	FMN	C4A-C10-N10	2.80	120.57	116.48
15	F	502	FMN	C4A-C4-N3	2.63	119.88	113.19
15	F	502	FMN	O4-C4-C4A	-2.46	120.06	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C10-C4A-N5	-2.32	119.93	124.86
15	F	502	FMN	C4A-C10-N1	-2.28	119.44	124.73

There are no chirality outliers.

All (127) 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
18	A	201	3PE	C11-O13-P-O12
18	A	201	3PE	O13-C11-C12-N
18	L	801	3PE	O13-C11-C12-N
18	L	803	3PE	C1-O11-P-O14
18	L	803	3PE	C11-O13-P-O12
18	L	804	3PE	C11-O13-P-O11
18	L	804	3PE	C11-O13-P-O12
18	L	804	3PE	C11-O13-P-O14
18	L	804	3PE	O13-C11-C12-N
18	L	805	3PE	O13-C11-C12-N
18	L	806	3PE	C1-O11-P-O12
18	L	806	3PE	C1-O11-P-O13
18	L	806	3PE	C1-O11-P-O14
18	L	806	3PE	C11-O13-P-O12
18	L	806	3PE	C11-O13-P-O14
18	L	806	3PE	O13-C11-C12-N
18	M	701	3PE	C1-O11-P-O13
18	M	701	3PE	C1-O11-P-O14
18	M	701	3PE	C11-O13-P-O14
18	M	701	3PE	O13-C11-C12-N
18	M	702	3PE	C1-O11-P-O12
18	J	201	3PE	C1-O11-P-O12
18	J	201	3PE	C1-O11-P-O13
18	J	201	3PE	C1-O11-P-O14
18	J	201	3PE	C11-O13-P-O12
18	J	201	3PE	C11-O13-P-O14
18	J	201	3PE	O13-C11-C12-N
18	J	202	3PE	C11-O13-P-O14
19	H	701	HQH	C8-C11-C18-C21
19	H	701	HQH	C10-C6-C7-C9
19	H	701	HQH	C10-C6-C7-O1

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Mol	Chain	Res	Type	Atoms
19	H	701	HQH	C22-C11-C18-C21
18	A	201	3PE	C11-O13-P-O11
18	L	805	3PE	C11-O13-P-O11
18	L	806	3PE	C11-O13-P-O11
18	M	702	3PE	C11-O13-P-O11
18	J	201	3PE	C11-O13-P-O11
18	J	202	3PE	C11-O13-P-O11
18	L	801	3PE	C37-C38-C39-C3A
18	L	801	3PE	C2C-C2D-C2E-C2F
18	M	702	3PE	C2-C1-O11-P
18	M	701	3PE	C24-C25-C26-C27
18	L	805	3PE	C39-C3A-C3B-C3C
18	L	803	3PE	C3E-C3F-C3G-C3H
18	M	702	3PE	C2E-C2F-C2G-C2H
18	A	201	3PE	O11-C1-C2-O21
18	J	201	3PE	C23-C24-C25-C26
19	H	701	HQH	C10-C6-C8-C11
18	L	803	3PE	C11-O13-P-O11
18	L	805	3PE	C3E-C3F-C3G-C3H
18	M	702	3PE	C26-C27-C28-C29
18	A	201	3PE	O11-C1-C2-C3
18	C	701	3PE	C1-C2-C3-O31
18	L	801	3PE	C3E-C3F-C3G-C3H
18	C	701	3PE	C3F-C3G-C3H-C3I
15	F	502	FMN	C5'-O5'-P-O1P
18	J	201	3PE	O11-C1-C2-C3
18	L	803	3PE	C1-O11-P-O13
20	N	501	LFA	C10-C11-C12-C13
18	C	701	3PE	O21-C2-C3-O31
18	M	701	3PE	C2-C1-O11-P
18	C	701	3PE	C3C-C3D-C3E-C3F
18	L	806	3PE	C23-C24-C25-C26
18	L	805	3PE	C2-C1-O11-P
18	J	201	3PE	C2-C1-O11-P
18	L	801	3PE	C23-C24-C25-C26
18	L	801	3PE	C25-C26-C27-C28
15	F	502	FMN	O2'-C2'-C3'-C4'
18	L	805	3PE	C1-O11-P-O13
18	M	701	3PE	C11-O13-P-O11
18	L	805	3PE	C3C-C3D-C3E-C3F
18	A	201	3PE	C11-O13-P-O14
18	L	803	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
18	L	805	3PE	C11-O13-P-O14
18	M	702	3PE	C11-O13-P-O14
18	J	202	3PE	C11-O13-P-O12
18	L	803	3PE	C12-C11-O13-P
18	J	201	3PE	O11-C1-C2-O21
18	J	202	3PE	C21-C22-C23-C24
18	C	701	3PE	C3B-C3C-C3D-C3E
18	C	701	3PE	C3E-C3F-C3G-C3H
18	C	701	3PE	C11-O13-P-O11
18	A	201	3PE	C1-O11-P-O13
18	L	804	3PE	C1-O11-P-O13
18	M	701	3PE	C35-C36-C37-C38
18	L	806	3PE	C25-C26-C27-C28
19	H	701	HQH	O1-C7-C9-C16
18	C	701	3PE	C28-C29-C2A-C2B
19	H	701	HQH	C7-C6-C8-C11
18	J	201	3PE	O21-C21-C22-C23
18	C	701	3PE	C25-C26-C27-C28
18	C	701	3PE	C29-C2A-C2B-C2C
18	C	701	3PE	O13-C11-C12-N
15	F	502	FMN	O2'-C2'-C3'-O3'
18	L	805	3PE	O21-C2-C3-O31
18	L	806	3PE	O21-C2-C3-O31
18	L	804	3PE	O31-C31-C32-C33
18	M	702	3PE	C1-O11-P-O13
18	L	806	3PE	C36-C37-C38-C39
18	A	201	3PE	O31-C31-C32-C33
18	A	201	3PE	O21-C21-C22-C23
18	L	805	3PE	O21-C21-C22-C23
18	L	804	3PE	O32-C31-C32-C33
18	L	801	3PE	C33-C34-C35-C36
18	A	201	3PE	O22-C21-C22-C23
18	L	806	3PE	C28-C29-C2A-C2B
19	H	701	HQH	C22-C11-C8-C6
19	H	701	HQH	O1-C7-C9-C14
18	A	201	3PE	C2-C1-O11-P
18	L	801	3PE	C1-O11-P-O14
18	L	804	3PE	C1-O11-P-O14
18	L	805	3PE	C1-O11-P-O12
18	M	702	3PE	C1-O11-P-O14
18	A	201	3PE	O32-C31-C32-C33
18	L	805	3PE	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
18	L	803	3PE	O21-C21-C22-C23
18	L	801	3PE	C12-C11-O13-P
18	C	701	3PE	O31-C31-C32-C33
18	L	805	3PE	O31-C31-C32-C33
18	L	801	3PE	C2F-C2G-C2H-C2I
18	L	803	3PE	O32-C31-C32-C33
18	L	806	3PE	C2D-C2E-C2F-C2G
18	L	803	3PE	O31-C31-C32-C33

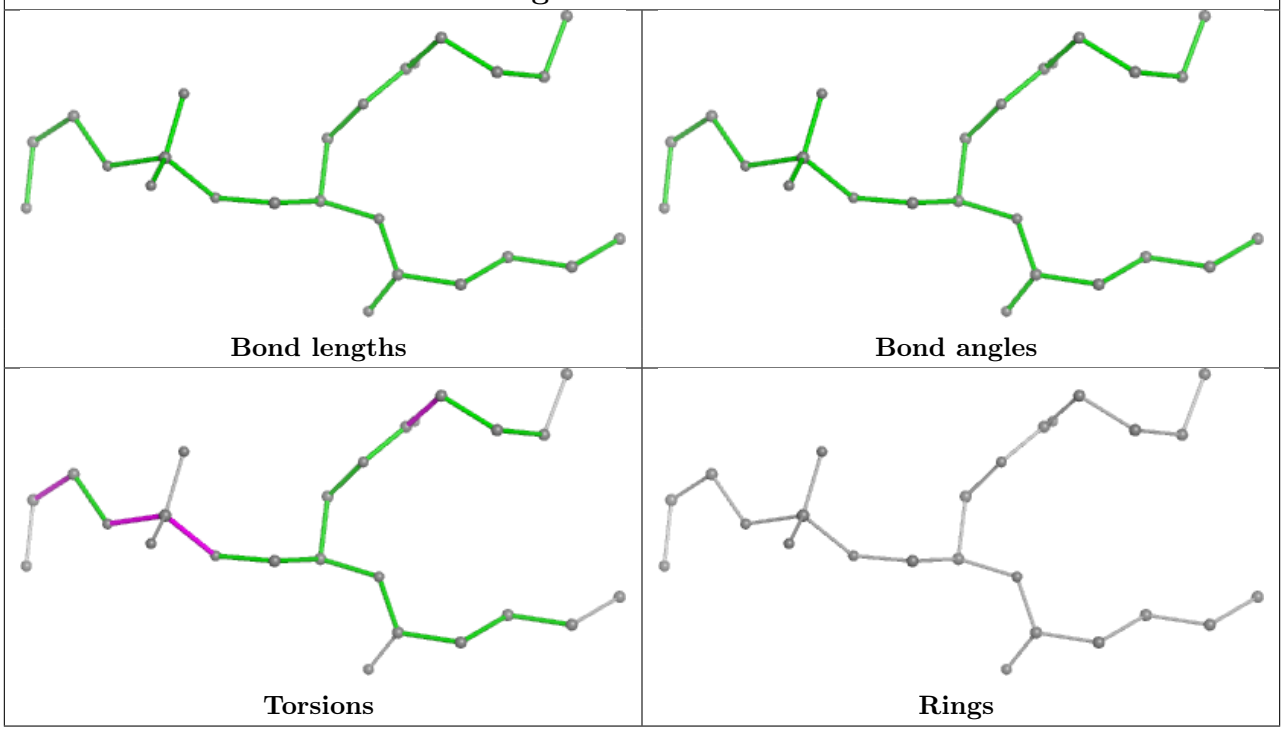
There are no ring outliers.

15 monomers are involved in 24 short contacts:

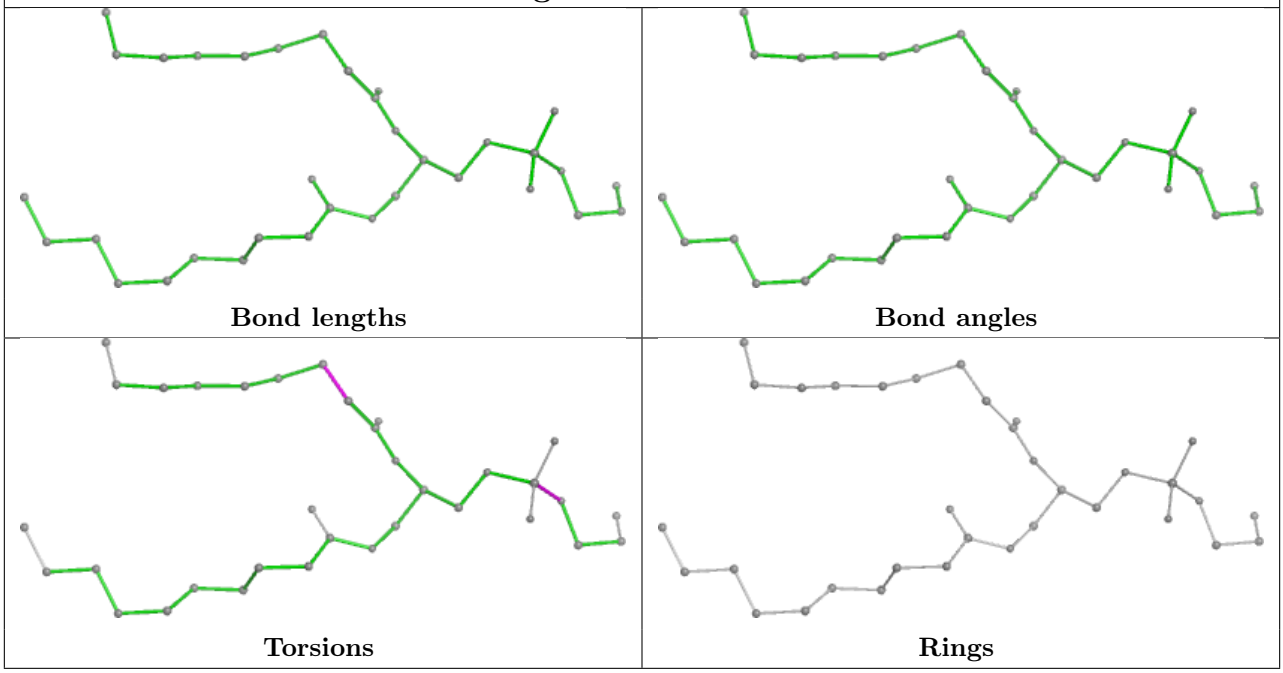
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	301	SF4	2	0
18	L	804	3PE	2	0
18	J	202	3PE	4	0
18	J	201	3PE	3	0
18	A	201	3PE	1	0
16	E	201	FES	1	0
18	L	805	3PE	3	0
20	L	802	LFA	1	0
18	M	702	3PE	2	0
18	L	801	3PE	4	0
18	M	701	3PE	1	0
14	G	1001	SF4	1	0
18	C	701	3PE	3	0
18	L	806	3PE	1	0
18	L	803	3PE	1	0

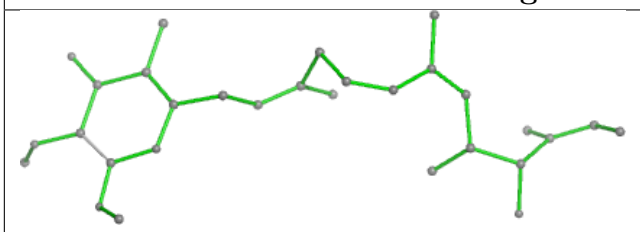
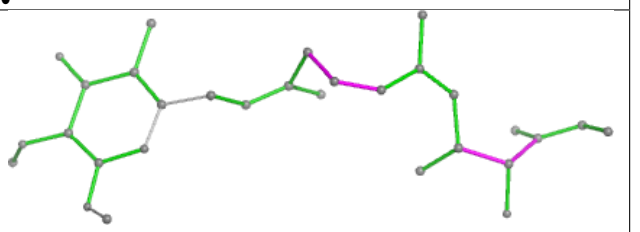
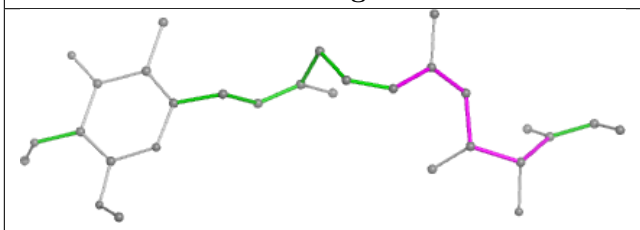
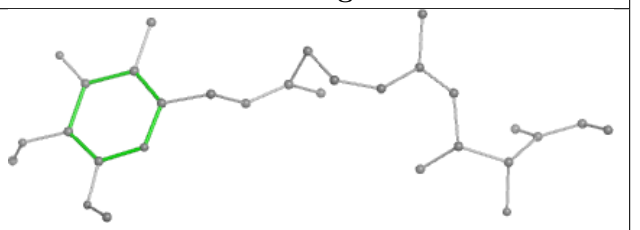
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

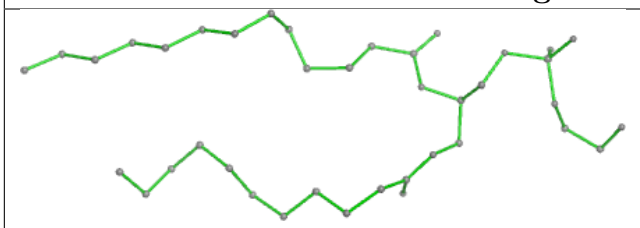
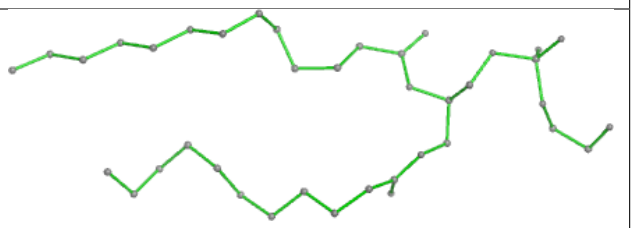
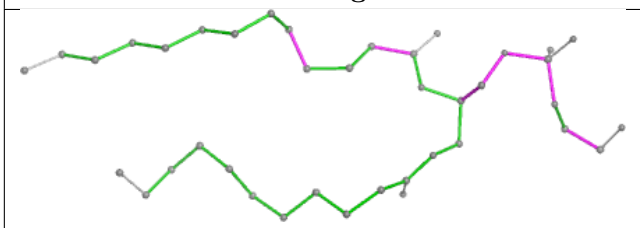
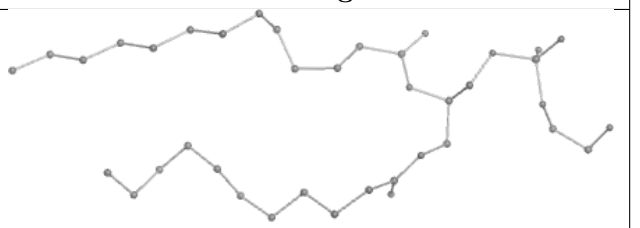
Ligand 3PE L 804



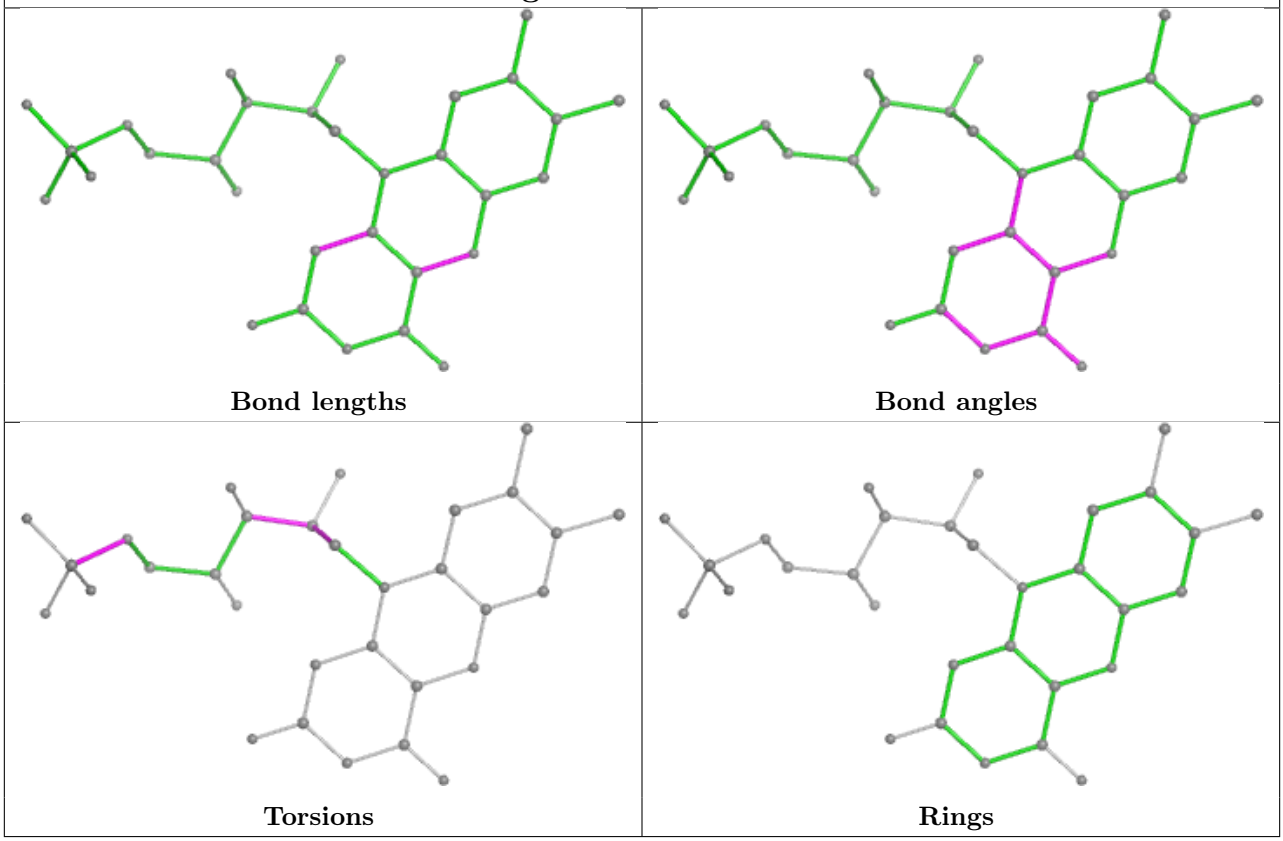
Ligand 3PE J 202



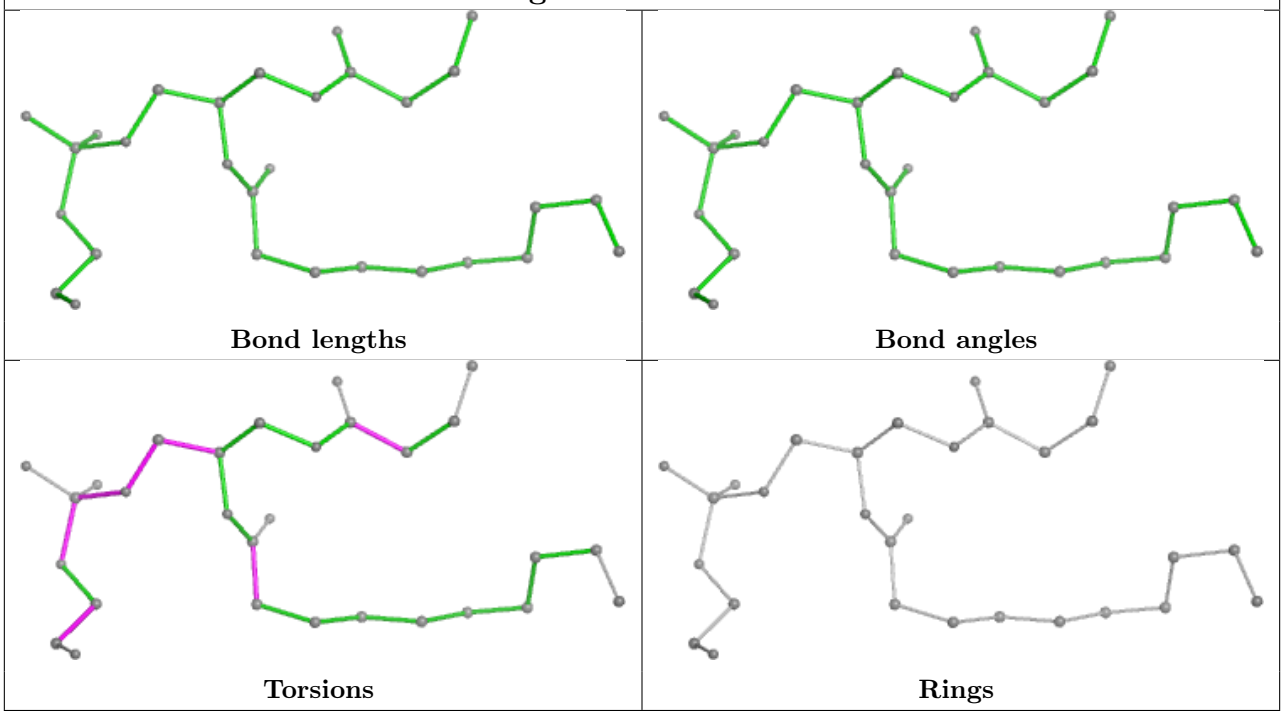
Ligand HQH H 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE J 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

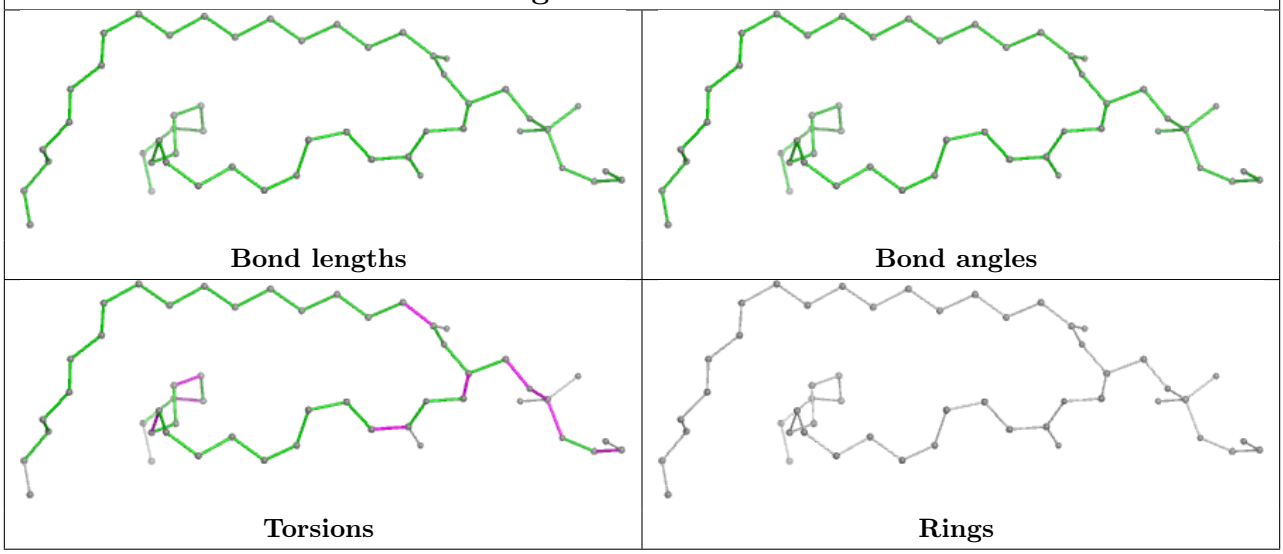
Ligand FMN F 502



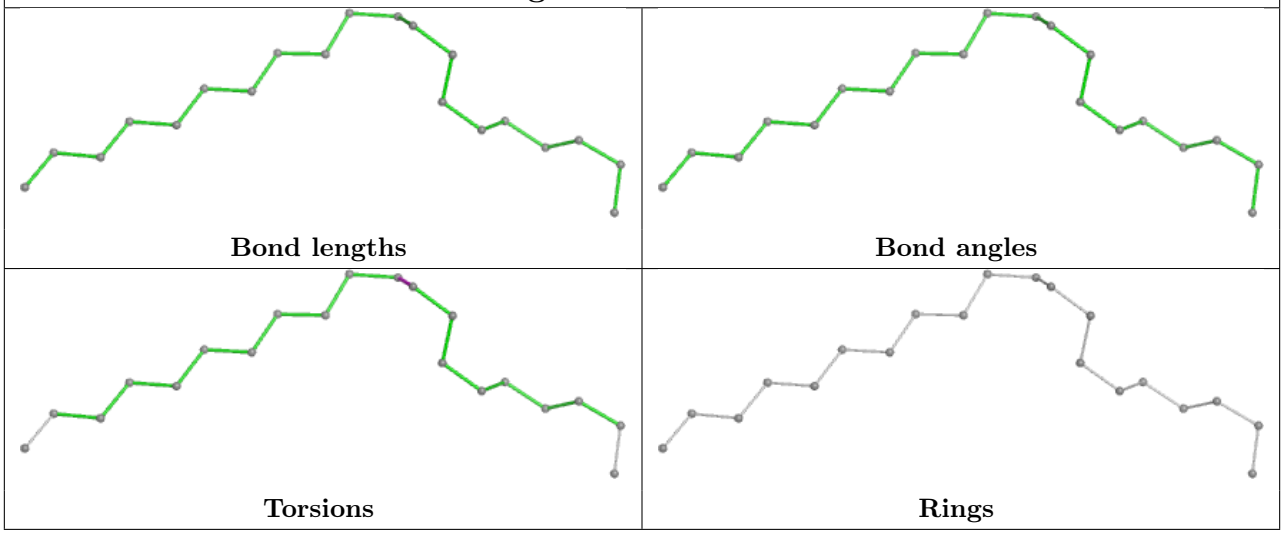
Ligand 3PE A 201



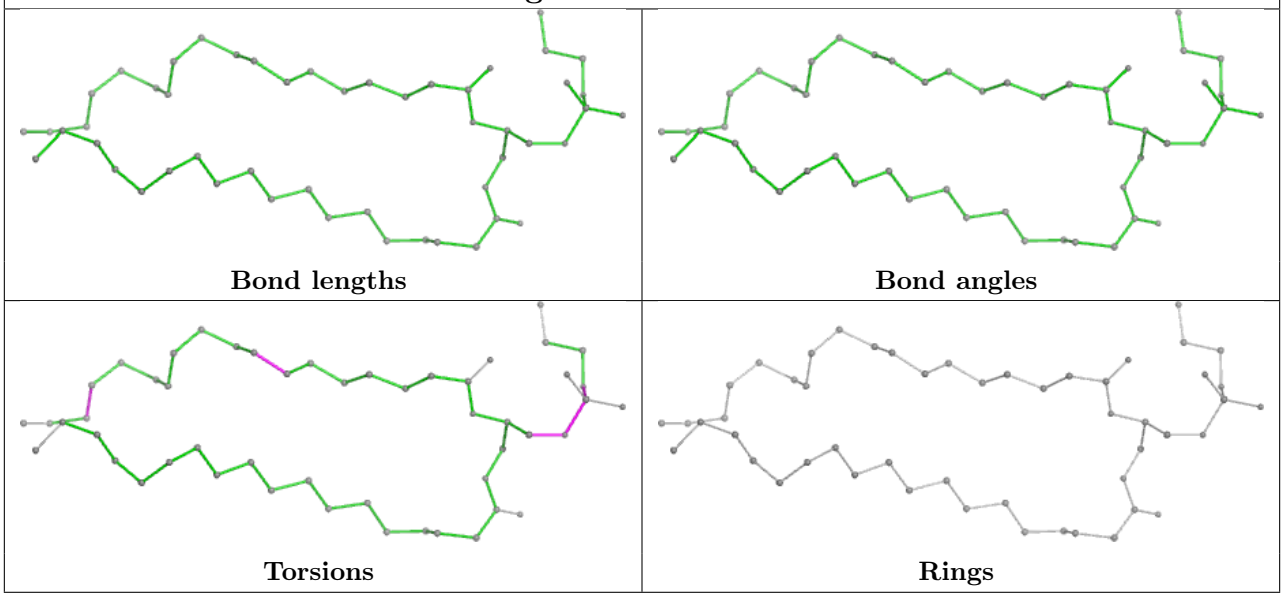
Ligand 3PE L 805



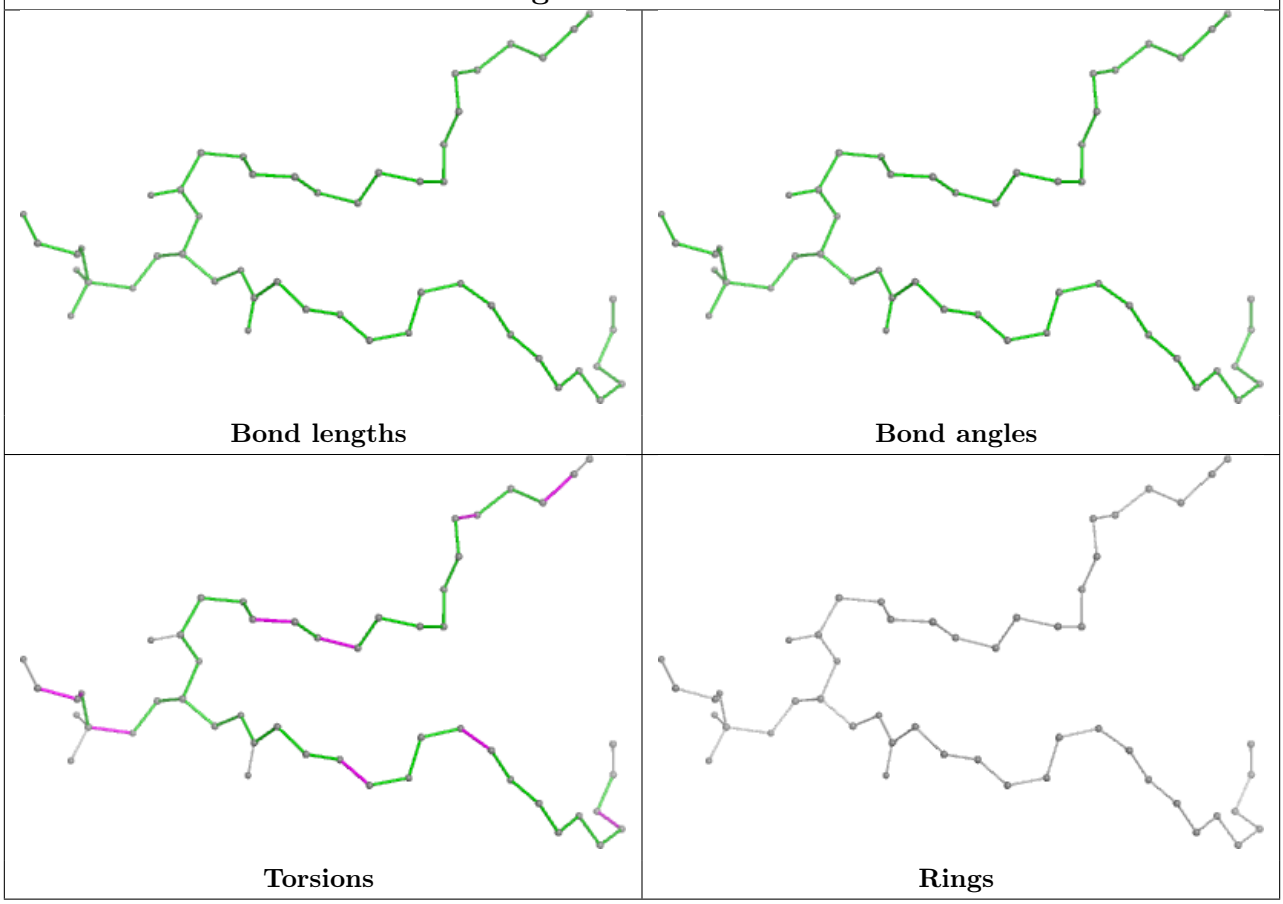
Ligand LFA N 501



Ligand 3PE M 702



Ligand 3PE L 801



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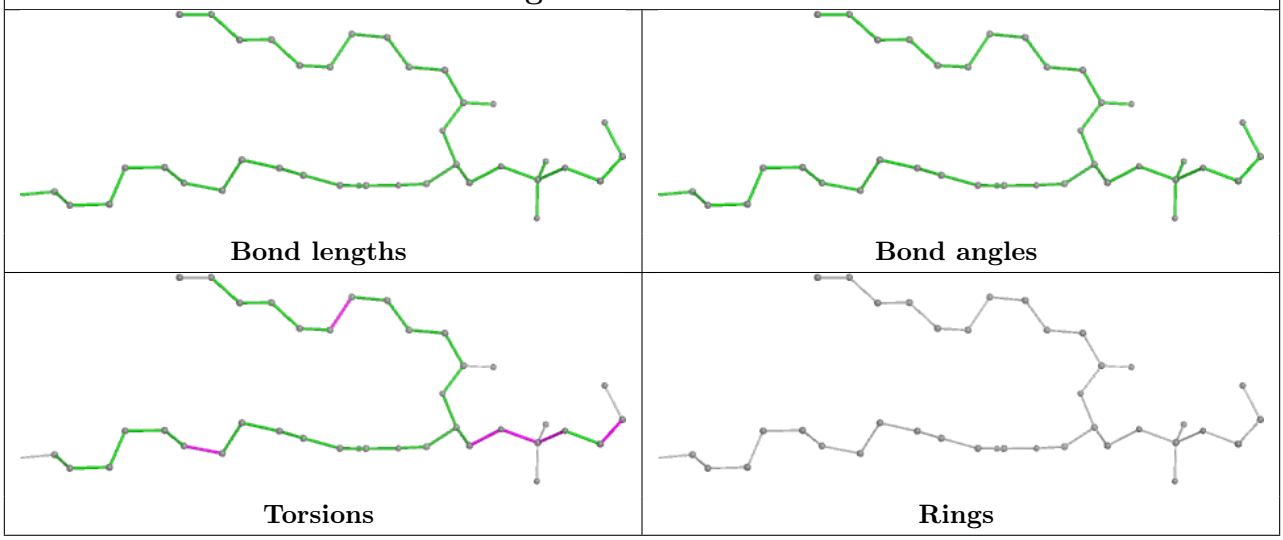

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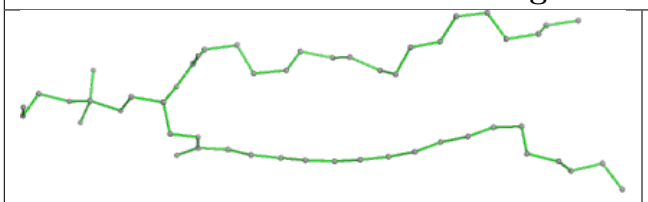
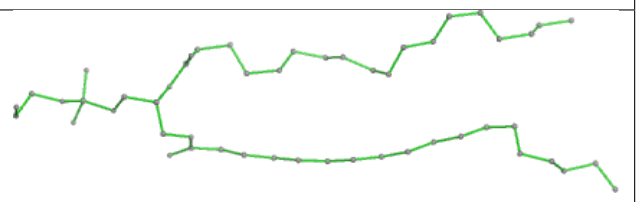
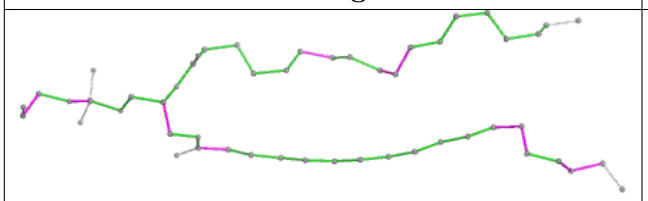


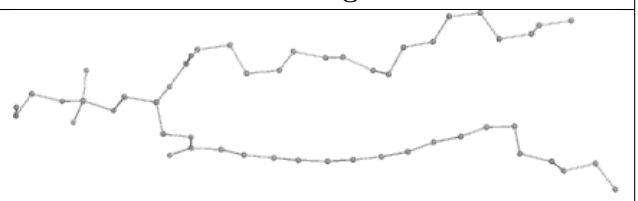
Bond lengths



Bond angles

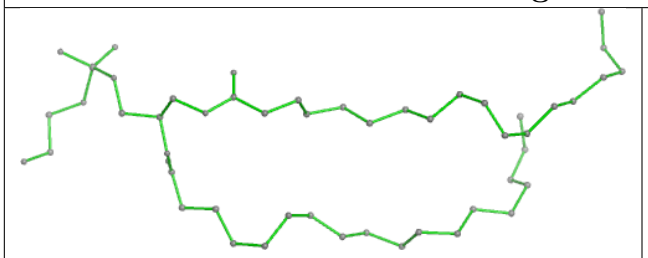


Torsions

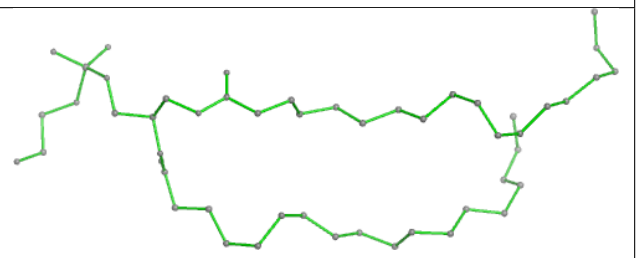


Rings

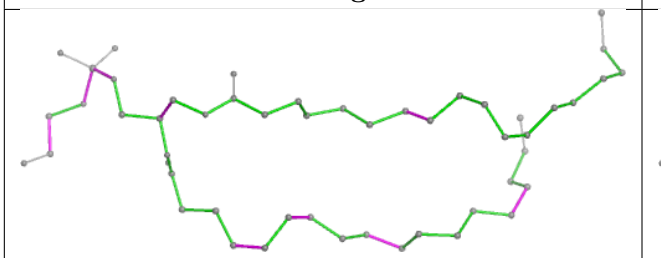
Ligand 3PE L 806



Bond lengths



Bond angles



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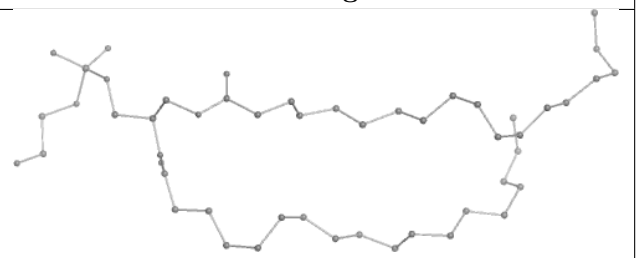
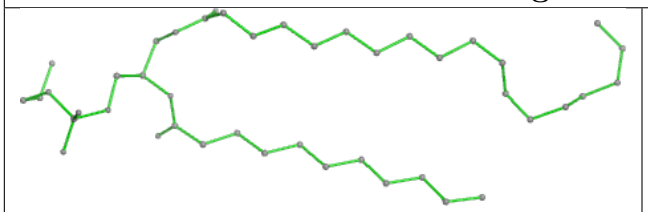
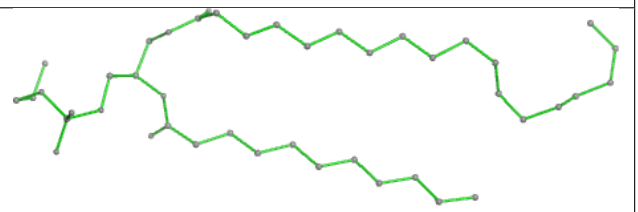


Rings

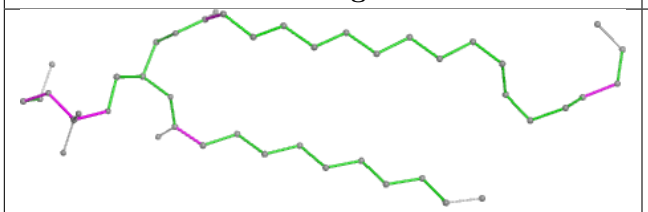
Ligand 3PE L 803



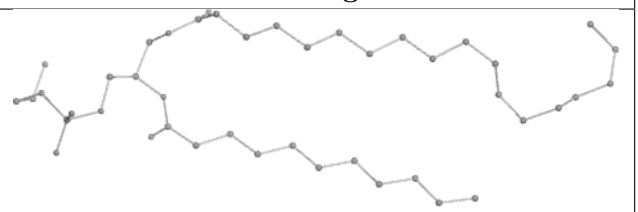
Bond lengths



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.

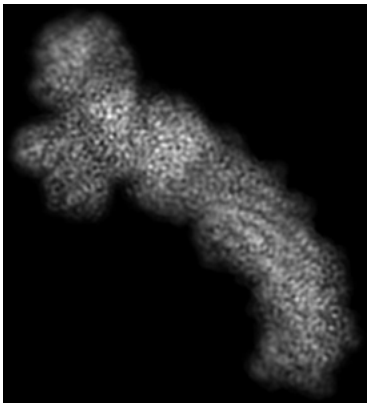
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13240. These allow visual inspection of the internal detail of the map and identification of artifacts.

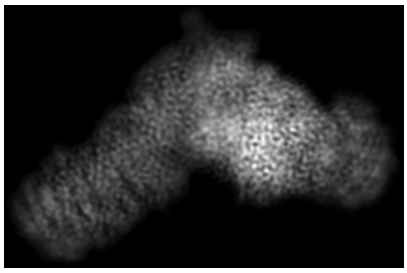
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

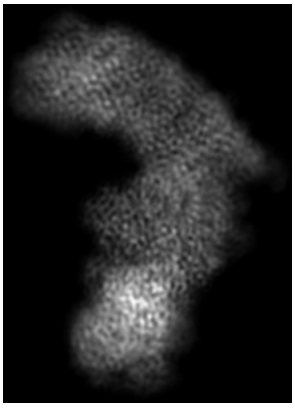
6.1.1 Primary map



X



Y

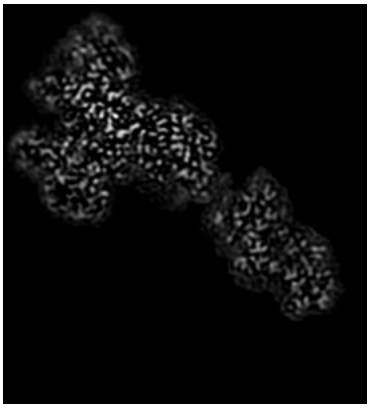


Z

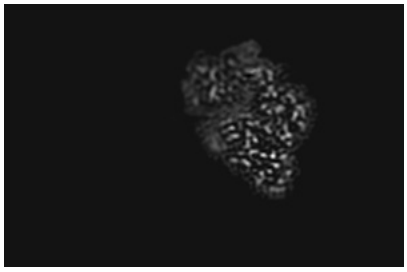
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

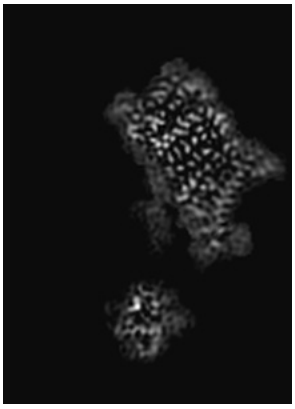
6.2.1 Primary map



X Index: 64



Y Index: 89



Z Index: 98

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: 62

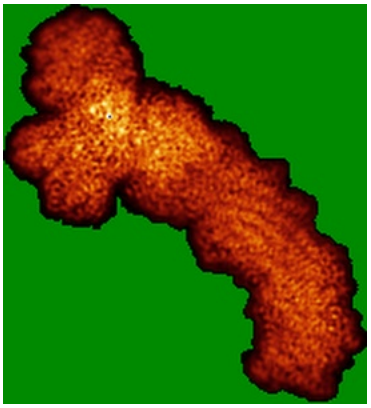
Y Index: 52

Z Index: 127

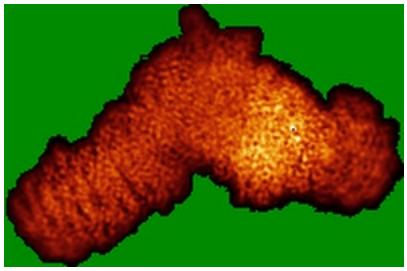
The images above show the largest variance slices of the map in three orthogonal directions.

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

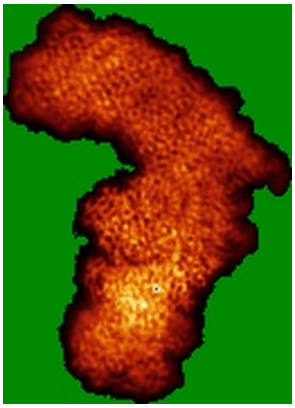
6.4.1 Primary map



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

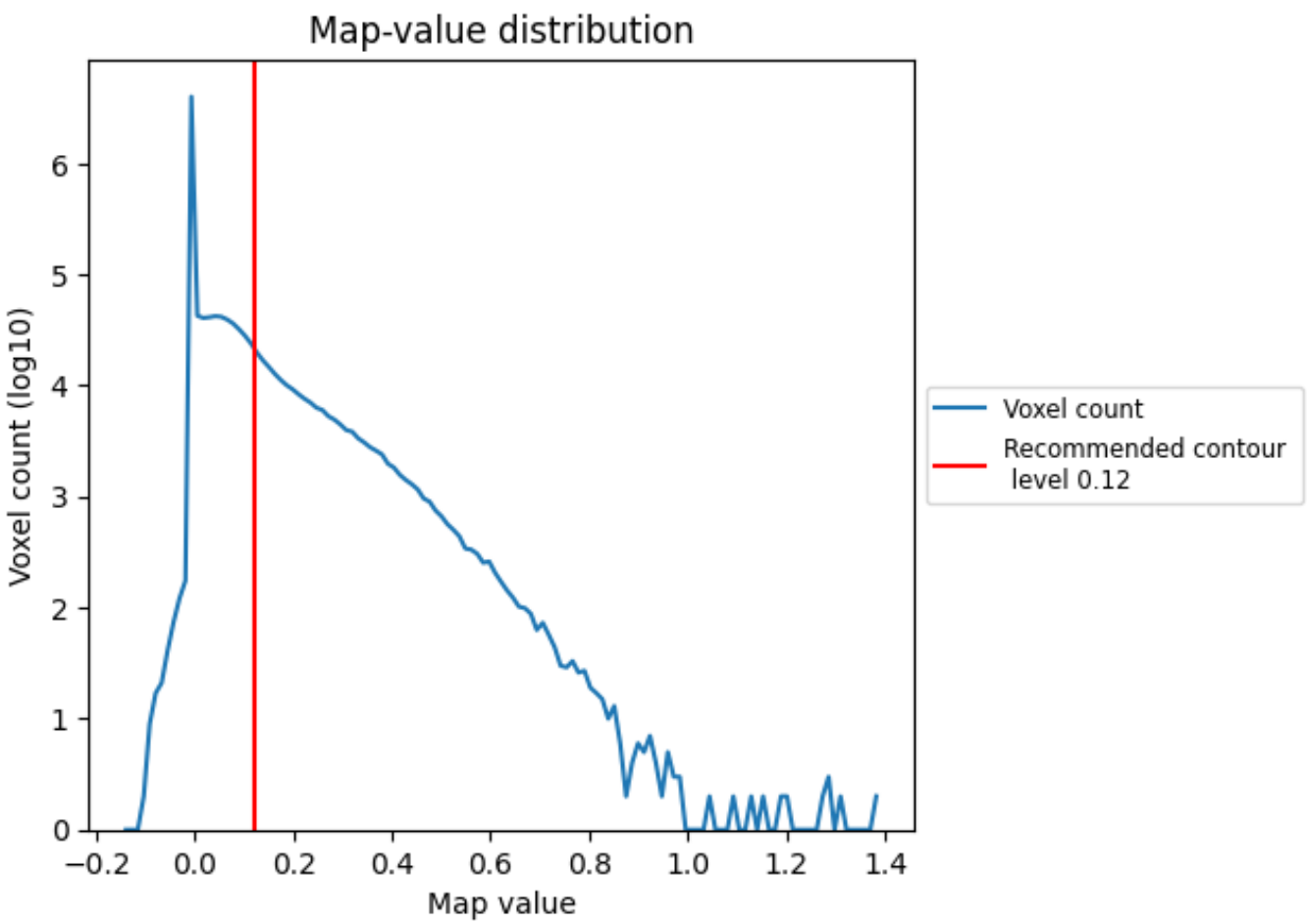
6.6 Mask visualisation (i)

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

7 Map analysis (i)

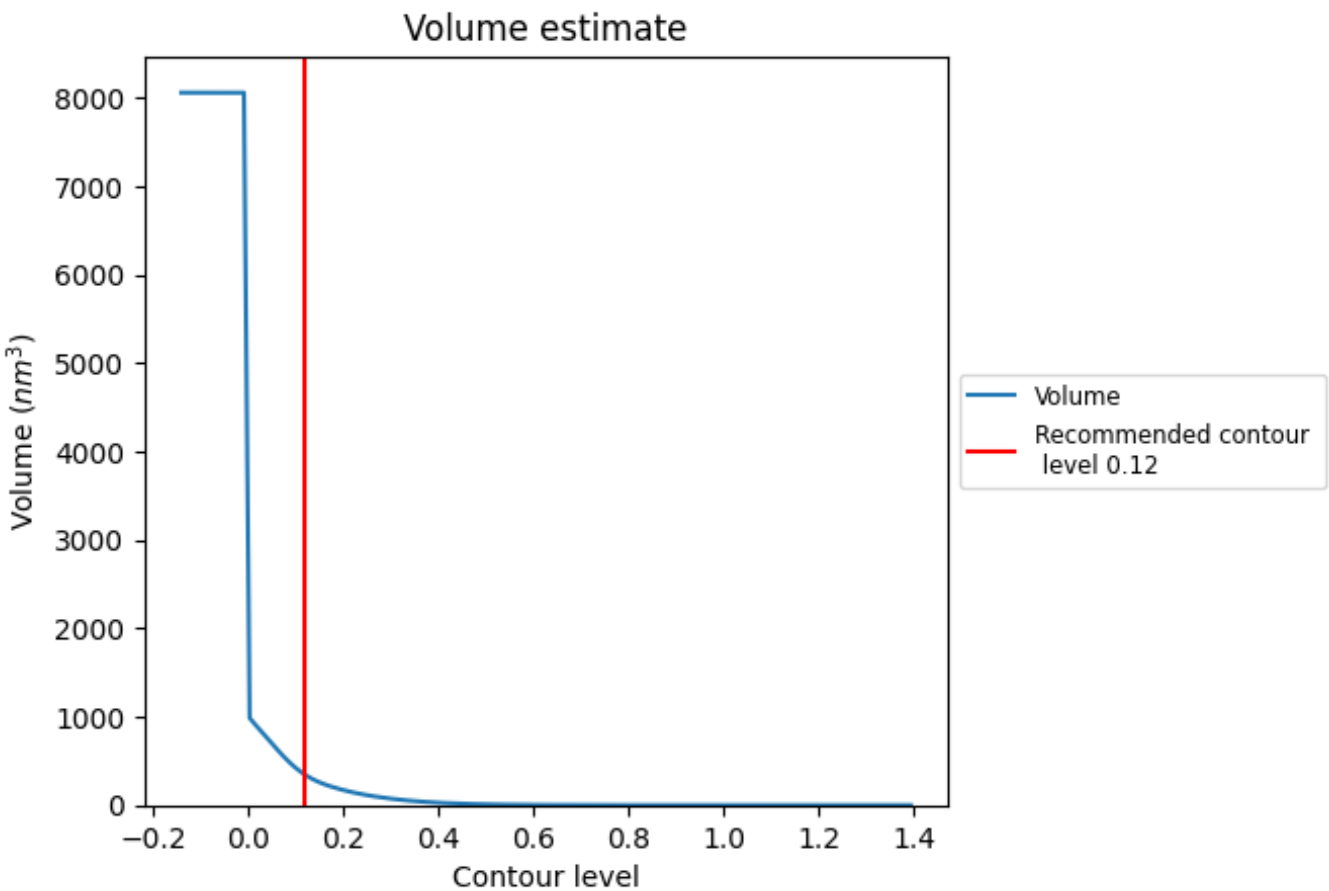
This section contains the results of statistical analysis of the map.

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 347 nm^3; this corresponds to an approximate mass of 313 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.

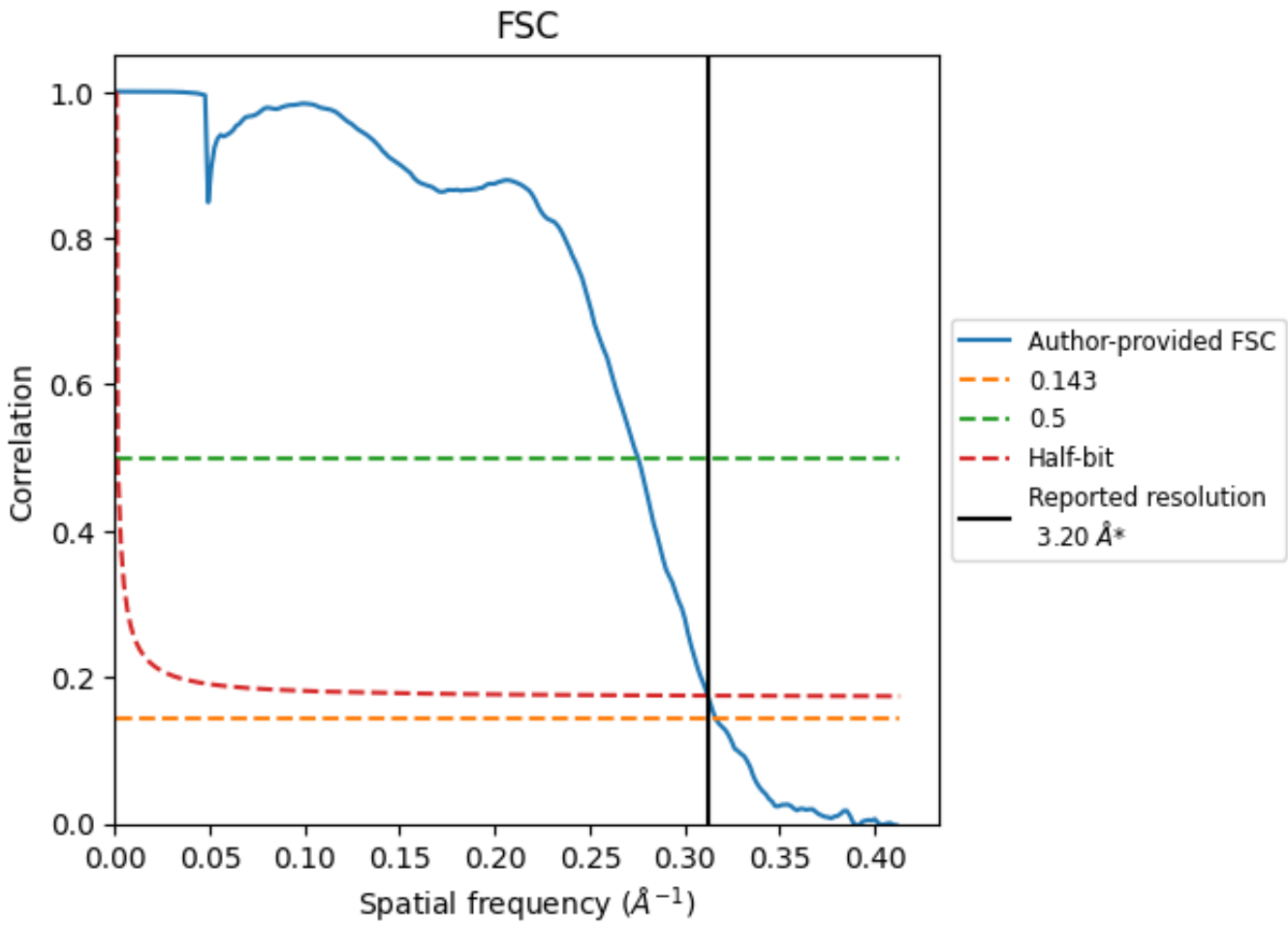
7.3 Rotationally averaged power spectrum (i)

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

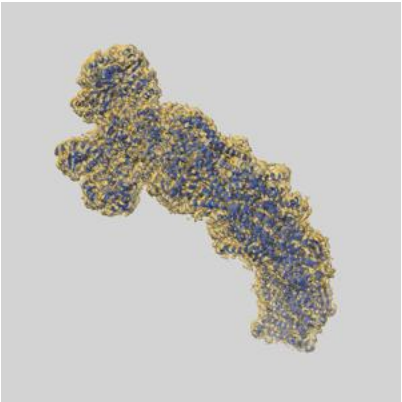
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.16	3.63	3.20
Unmasked-calculated*	-	-	-

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

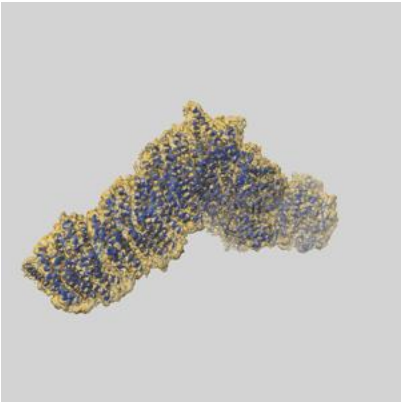
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13240 and PDB model 7P7M. Per-residue inclusion information can be found in section 3 on page 11.

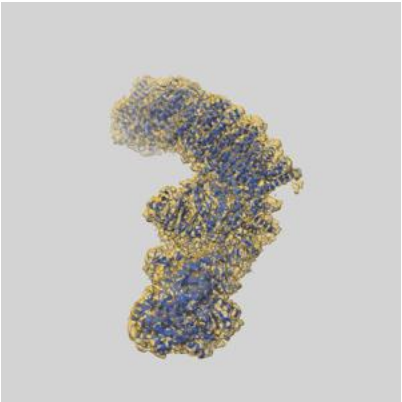
9.1 Map-model overlay (i)



X



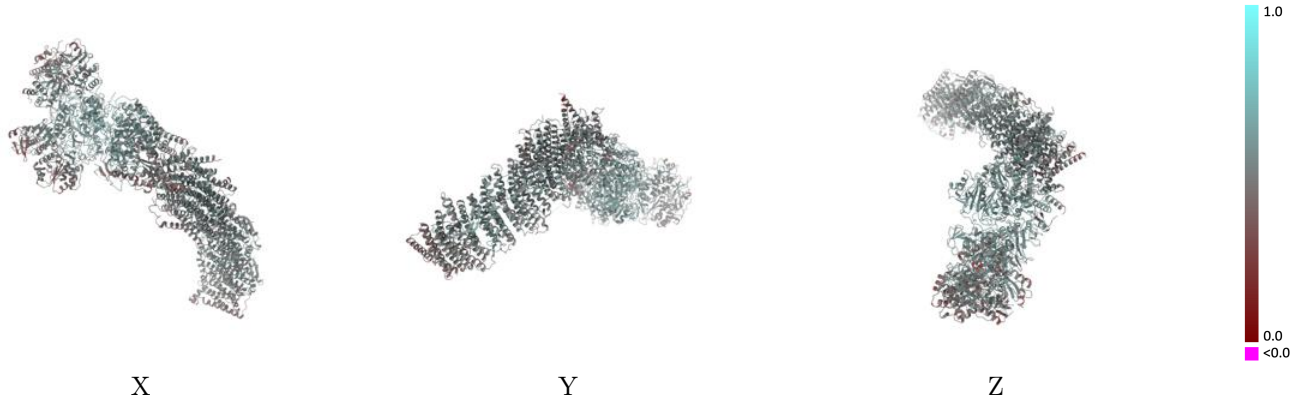
Y



Z

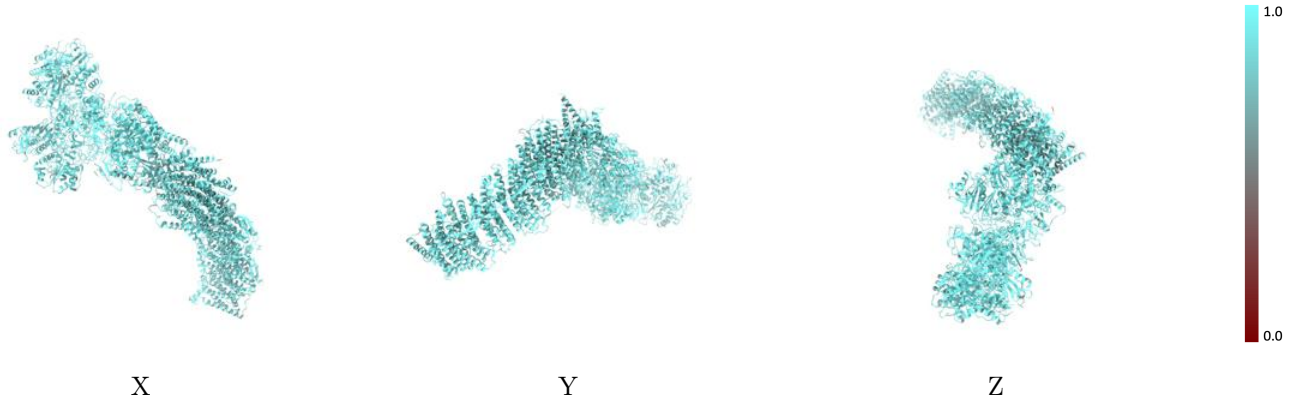
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



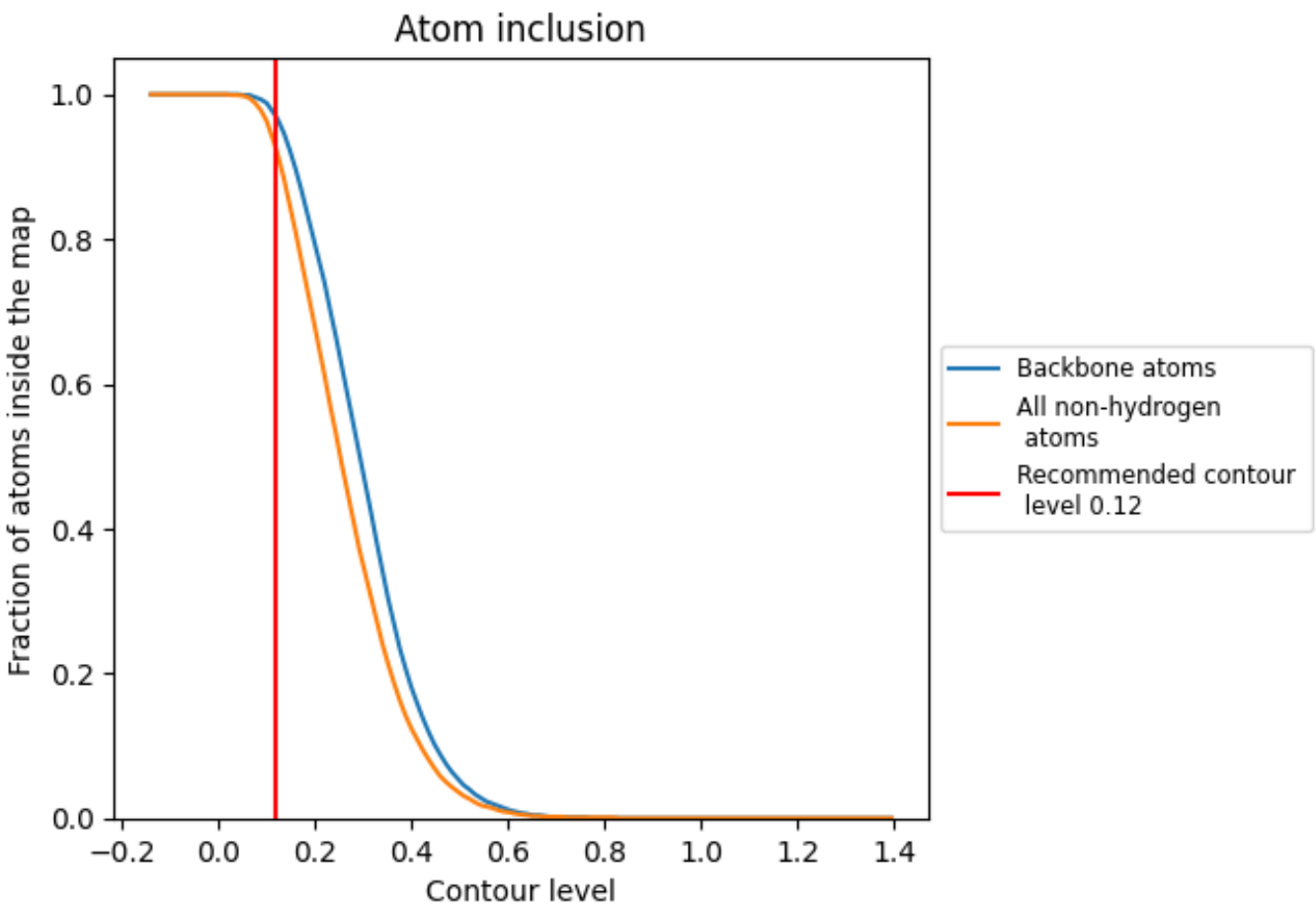
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9240	0.5190
A	0.8850	0.4990
B	0.9480	0.5400
C	0.9510	0.5680
E	0.9220	0.5000
F	0.9170	0.4810
G	0.9370	0.5270
H	0.9010	0.4910
I	0.9510	0.5660
J	0.8930	0.4920
K	0.9140	0.5130
L	0.8990	0.4870
M	0.9350	0.5260
N	0.9100	0.5230