Full wwPDB EM Validation Report (i)

Aug 27, 2026 – 10:10 am BST

PDB ID	:	7P64 / pdb_00007p64
EMDB ID	:	EMD-13217
Title	:	Complex I from E. coli, DDM/LMNG-purified, under Turnover at pH 6, Open state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2021-07-15
Resolution	:	2.50 Å(reported)
Based on initial models	:	3RKO, 4HEA

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

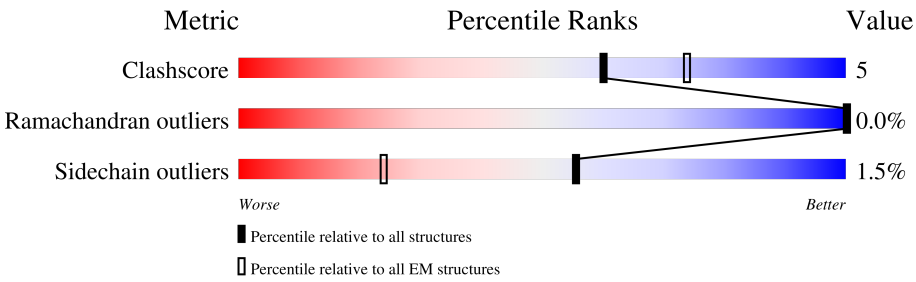
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

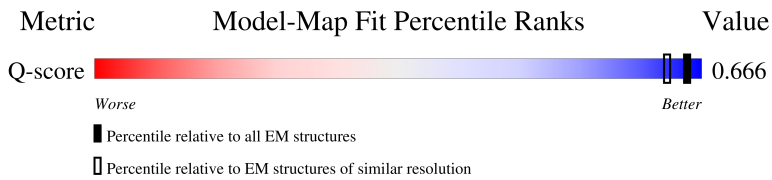
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	88% 11%
2	E	156	92% 8%
3	G	905	88% 12%
4	C	600	87% 10% • •

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Mol	Chain	Length	Quality of chain
5	B	220	79% 11% 10%
6	I	180	89% 10%
7	H	325	81% 15%
8	A	147	60% 10% 31%
9	L	613	87% 12%
10	M	504	88% 12%
11	N	485	86% 12%
12	K	100	84% 14%
13	J	162	81% 19%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 38981 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	588	4741	3039	824	854	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	314	2474	1665	389	402	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	606	4637	3083	741	781	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

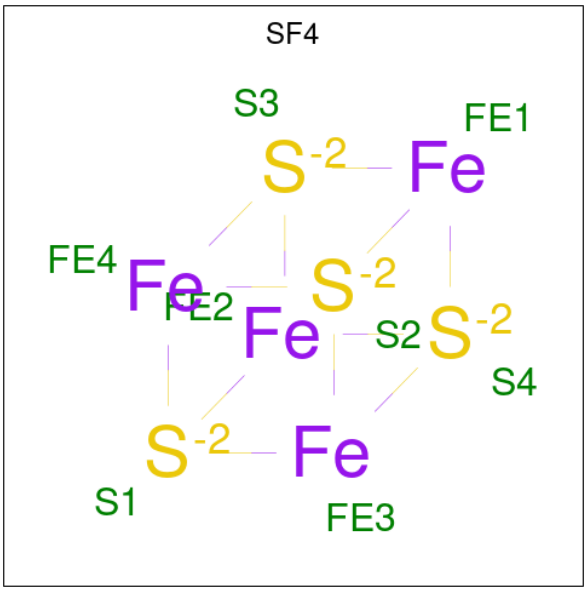
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

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.

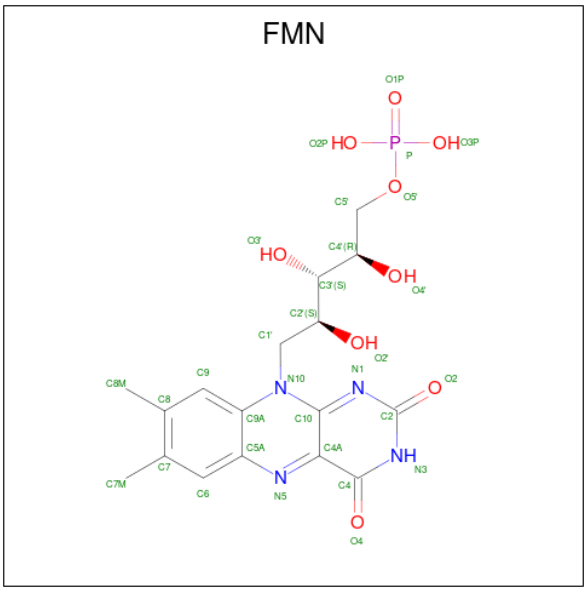
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	162	1226	824	188	207	7	0	0

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



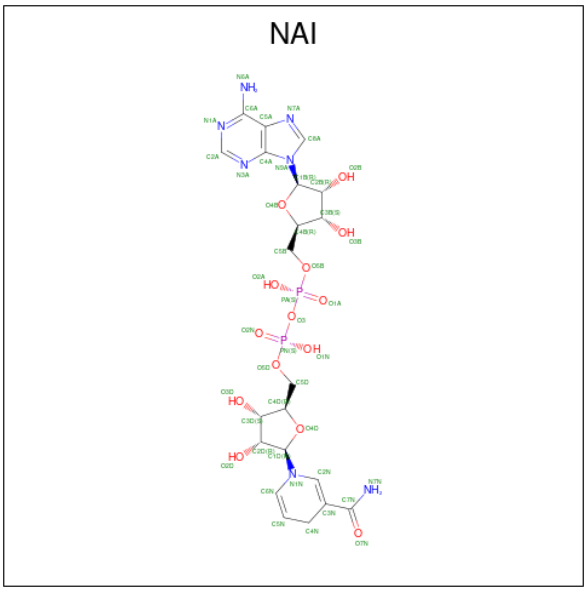
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
14	F	1	8	4	4	0
14	G	1	8	4	4	0
14	G	1	8	4	4	0
14	G	1	8	4	4	0
14	B	1	8	4	4	0
14	I	1	8	4	4	0
14	I	1	8	4	4	0

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



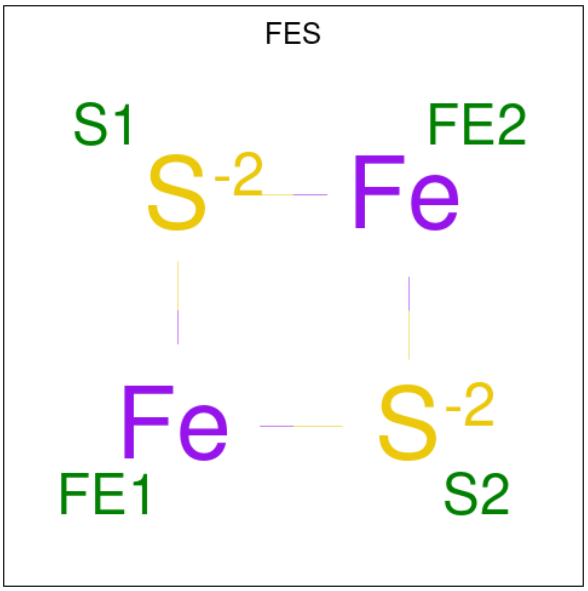
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
15	F	1	31	17	4	9	1	0

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

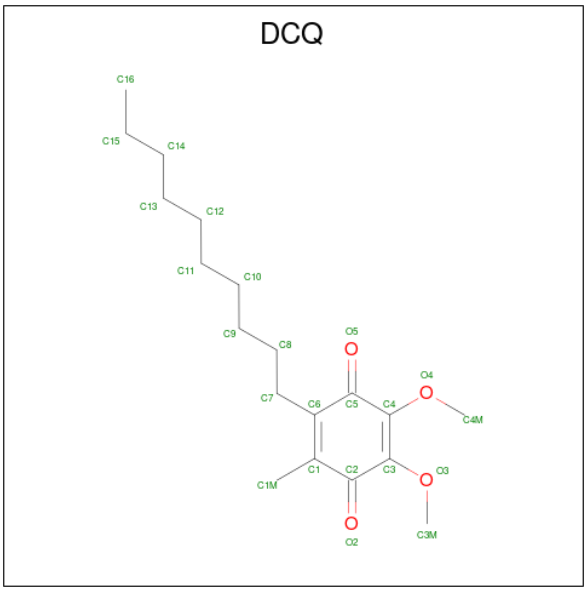


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	E	1	4	2	2	0
17	G	1	4	2	2	0

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

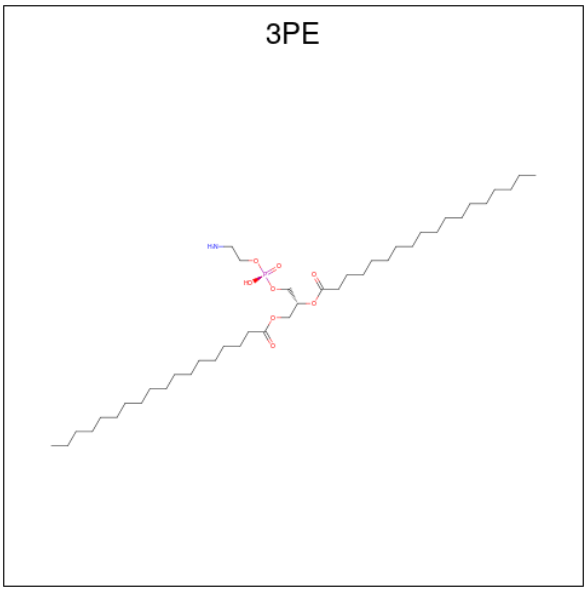
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
18	G	1	1	1	0

- Molecule 19 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: $C_{19}H_{30}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
19	B	1	23	19	4	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	I	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	I	1	28	20	1	6	1	0

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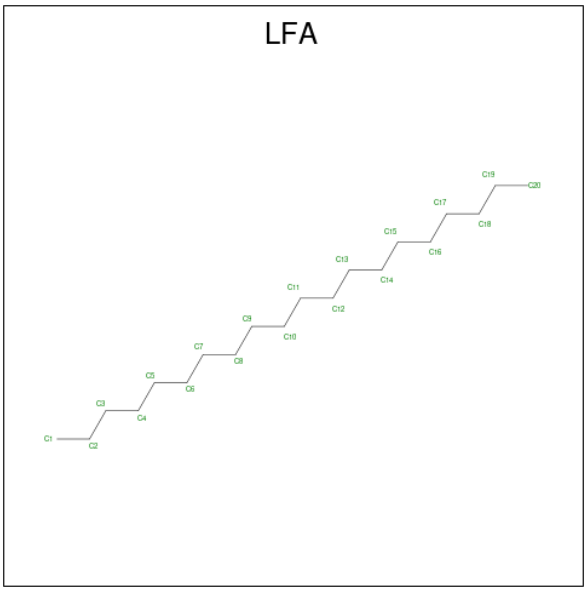
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	H	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	H	1	30	20	1	8	1	0
			Total	C	N	O	P	
20	H	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	H	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	A	1	42	32	1	8	1	0
			Total	C	N	O	P	
20	L	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	L	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	L	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	L	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	L	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	L	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	M	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	M	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	M	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	N	1	51	41	1	8	1	0
			Total	C	N	O	P	
20	J	1	51	41	1	8	1	0

- Molecule 21 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



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

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
22	F	34	34	34	0
			Total	O	
22	E	12	12	12	0
			Total	O	
22	G	308	308	308	0
			Total	O	
22	C	162	162	162	0
			Total	O	
22	B	57	57	57	0
			Total	O	
22	I	83	83	83	0
			Total	O	
22	H	47	47	47	0

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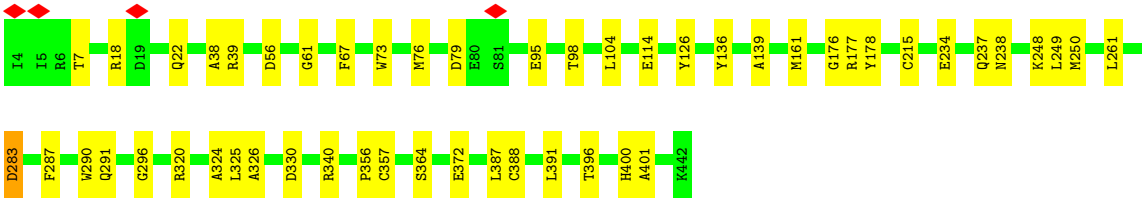
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
22	A	17	17	17	0
			Total	O	
22	L	62	62	62	0
			Total	O	
22	M	90	90	90	0
			Total	O	
22	N	73	73	73	0
			Total	O	
22	K	22	22	22	0
			Total	O	
22	J	20	20	20	0

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.

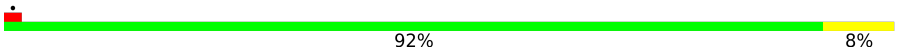
• Molecule 1: NADH-quinone oxidoreductase subunit F

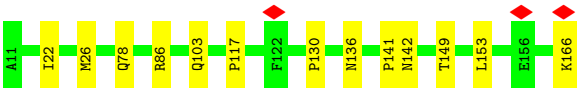
Chain F:



• Molecule 2: NADH dehydrogenase I subunit E

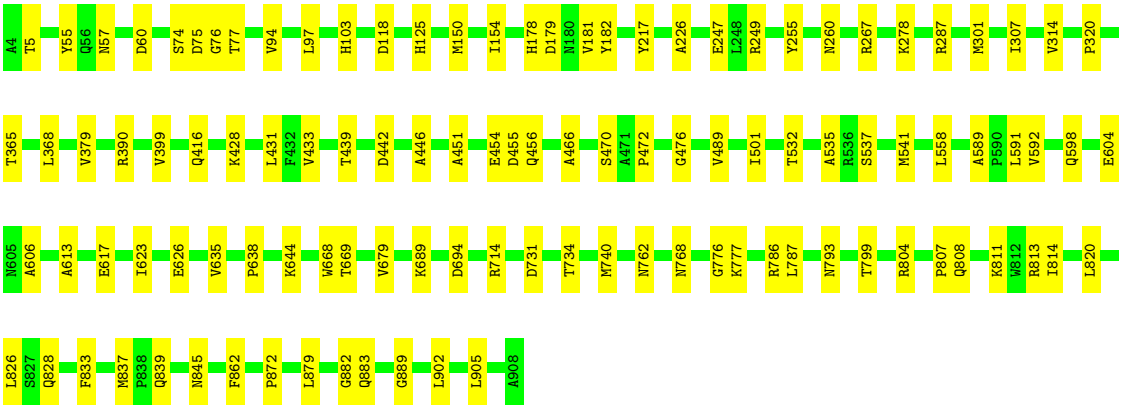
Chain E:





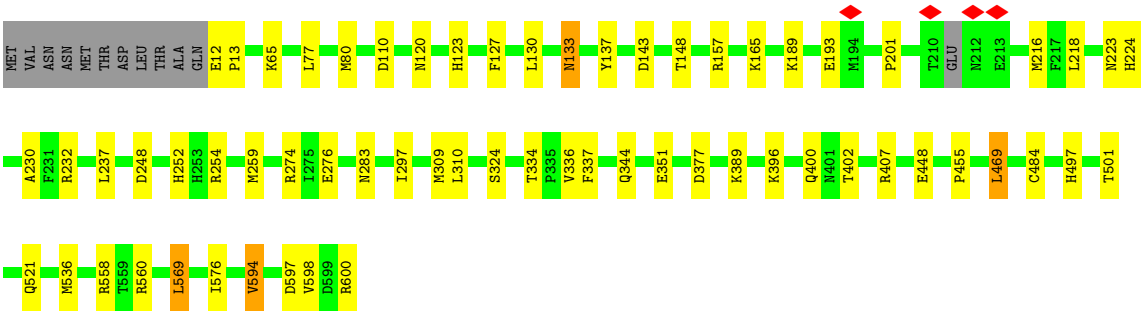
• Molecule 3: NADH-quinone oxidoreductase

Chain G:



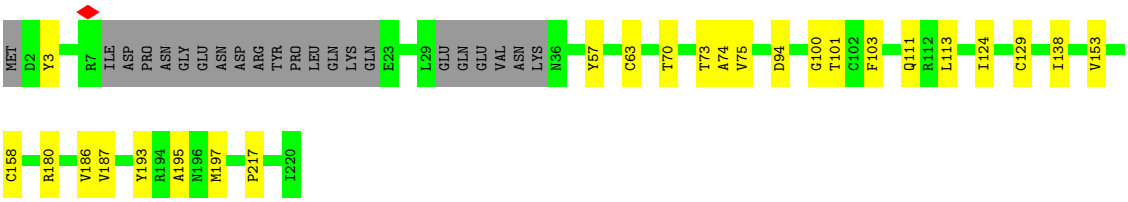
• Molecule 4: NADH-quinone oxidoreductase subunit C/D

Chain C:



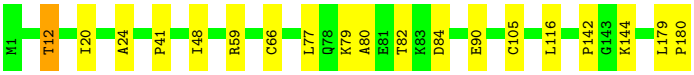
- Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:



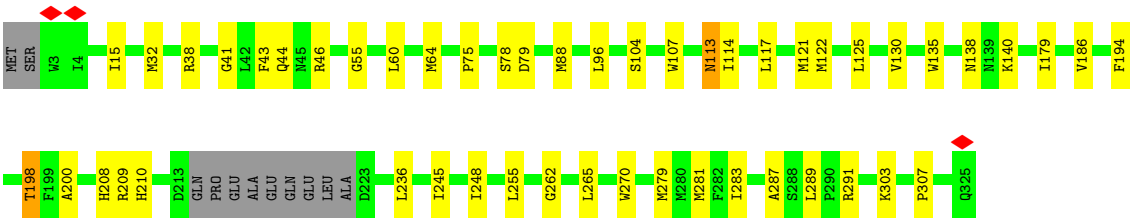
- Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:



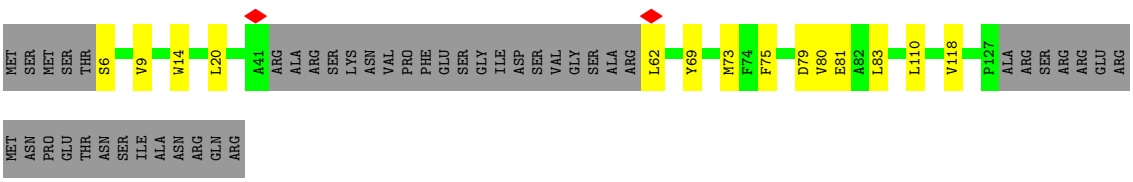
- Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:



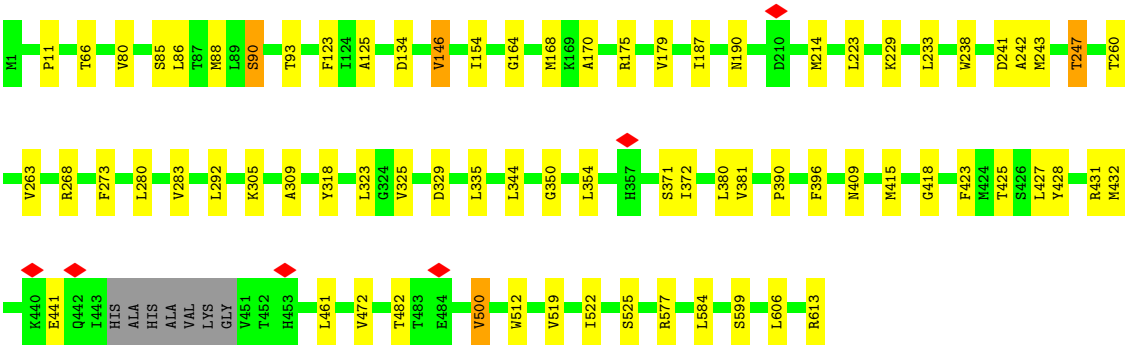
- Molecule 8: NADH-quinone oxidoreductase subunit A

Chain A:



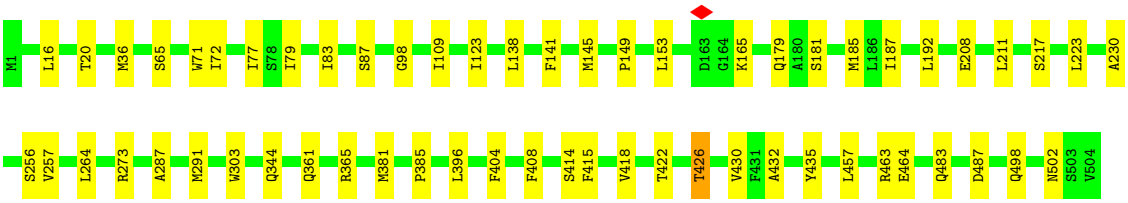
• Molecule 9: Proton-translocating NADH-quinone oxidoreductase, chain L

Chain L: 87% 12%



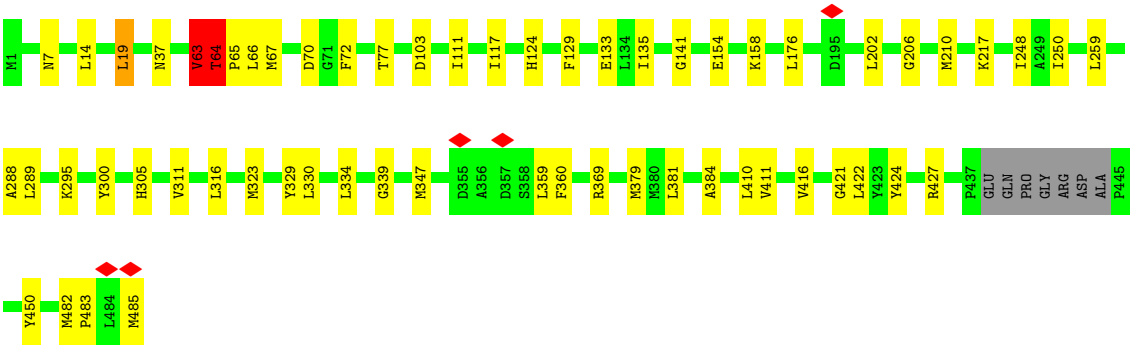
• Molecule 10: NADH dehydrogenase I subunit M

Chain M: 88% 12%



• Molecule 11: NADH-quinone oxidoreductase subunit N

Chain N: 86% 12%

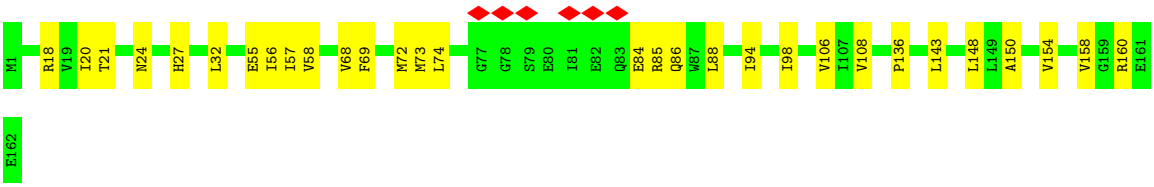


• Molecule 12: NADH-quinone oxidoreductase subunit K

Chain K: 84% 14%

• Molecule 13: NADH-quinone oxidoreductase subunit J

Chain J: 81% 19%


M1
R18
V19
I20
T21
N24
H27
L32
E55
I56
I57
V58
V68
F69
M72
M73
L74
G77
G78
S79
E80
I81
E82
Q83
E84
R85
Q86
W87
L88
I94
I98
V106
I107
V108
P136
L143
L148
L149
A150
V154
V158
G159
R160
E161
E162

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	97923	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	78	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.590	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	157.5, 210.5, 240.0	wwPDB
Map dimensions	480, 421, 315	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: DCQ, SF4, FMN, CA, LFA, NAI, FES, 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	0.17	0/3486	0.34	0/4713
2	E	0.17	0/1248	0.37	0/1691
3	G	0.21	0/7173	0.40	0/9726
4	C	0.23	0/4871	0.43	2/6610 (0.0%)
5	B	0.22	0/1601	0.39	0/2168
6	I	0.22	0/1470	0.40	0/1985
7	H	0.24	0/2548	0.42	0/3465
8	A	0.20	0/833	0.38	0/1134
9	L	0.19	0/4755	0.38	0/6479
10	M	0.23	0/4074	0.44	0/5546
11	N	0.23	0/3709	0.45	3/5061 (0.1%)
12	K	0.20	0/769	0.36	0/1040
13	J	0.20	0/1252	0.40	0/1708
All	All	0.21	0/37789	0.41	5/51326 (0.0%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	201	PRO	CA-N-CD	-12.00	95.20	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	64	THR	N-CA-C	-6.30	95.89	109.81
4	C	201	PRO	N-CD-CG	-5.89	94.36	103.20
11	N	63	VAL	CA-C-N	5.26	134.65	121.80
11	N	63	VAL	C-N-CA	5.26	134.65	121.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	260	ASN	Peptide
3	G	668	TRP	Peptide
11	N	63	VAL	Peptide
11	N	64	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3407	0	3374	28	0
2	E	1220	0	1187	6	0
3	G	7022	0	6824	64	0
4	C	4741	0	4652	40	0
5	B	1568	0	1553	16	0
6	I	1436	0	1415	13	0
7	H	2474	0	2528	39	0
8	A	808	0	821	13	0
9	L	4637	0	4783	50	0
10	M	3953	0	4053	35	0
11	N	3620	0	3790	39	0
12	K	760	0	817	12	0
13	J	1226	0	1297	27	0
14	B	8	0	0	1	0
14	F	8	0	0	0	0
14	G	24	0	0	0	0
14	I	16	0	0	0	0
15	F	31	0	19	0	0
16	F	44	0	27	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	E	4	0	0	0	0
17	G	4	0	0	0	0
18	G	1	0	0	0	0
19	B	23	0	30	0	0
20	A	42	0	61	2	0
20	H	183	0	280	11	0
20	I	79	0	119	2	0
20	J	51	0	82	3	0
20	L	306	0	492	11	0
20	M	153	0	246	5	0
20	N	51	0	82	1	0
21	H	20	0	42	0	0
21	L	20	0	42	0	0
21	M	20	0	42	0	0
21	N	34	0	69	1	0
22	A	17	0	0	0	0
22	B	57	0	0	0	0
22	C	162	0	0	1	0
22	E	12	0	0	0	0
22	F	34	0	0	0	0
22	G	308	0	0	7	0
22	H	47	0	0	1	0
22	I	83	0	0	0	0
22	J	20	0	0	0	0
22	K	22	0	0	0	0
22	L	62	0	0	3	0
22	M	90	0	0	1	0
22	N	73	0	0	0	0
All	All	38981	0	38727	346	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 (346) 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
4:C:560:ARG:HH12	4:C:600:ARG:HH21	1.37	0.72
11:N:64:THR:HB	11:N:66:LEU:H	1.53	0.71
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.73	0.70
11:N:482:MET:HE3	11:N:483:PRO:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:181:SER:HB2	10:M:230:ALA:HA	1.75	0.67
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.75	0.66
11:N:65:PRO:HG2	13:J:136:PRO:HB3	1.77	0.66
1:F:95:GLU:HB2	16:F:503:NAI:H42N	1.80	0.64
20:L:704:3PE:H331	20:L:704:3PE:H231	1.80	0.64
3:G:845:ASN:ND2	3:G:879:LEU:O	2.32	0.63
9:L:233:LEU:HD21	20:L:707:3PE:H3F2	1.80	0.63
4:C:389:LYS:H	4:C:389:LYS:HE2	1.63	0.62
4:C:309:MET:HE2	4:C:484:CYS:HB3	1.81	0.62
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.82	0.62
7:H:281:MET:HE2	20:H:401:3PE:H2G1	1.83	0.61
4:C:344:GLN:HG2	5:B:75:VAL:HG21	1.83	0.61
3:G:768:ASN:ND2	22:G:1108:HOH:O	2.34	0.60
10:M:36:MET:HE2	10:M:98:GLY:HA3	1.82	0.60
11:N:289:LEU:O	11:N:427:ARG:NH1	2.34	0.60
3:G:714:ARG:NH2	22:G:1113:HOH:O	2.35	0.59
7:H:32:MET:HE1	7:H:283:ILE:HD11	1.84	0.59
7:H:75:PRO:HB2	7:H:78:SER:HB3	1.85	0.59
4:C:254:ARG:HG3	5:B:103:PHE:HE1	1.68	0.59
4:C:402:THR:H	6:I:12:THR:HG21	1.67	0.59
9:L:187:ILE:HD11	20:M:703:3PE:H341	1.84	0.59
3:G:777:LYS:NZ	22:G:1120:HOH:O	2.37	0.58
9:L:519:VAL:HG13	20:L:705:3PE:H31	1.86	0.58
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.86	0.58
20:L:701:3PE:H2A2	11:N:416:VAL:HG13	1.86	0.57
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.86	0.57
3:G:862:PHE:HB3	3:G:905:LEU:HD23	1.86	0.57
8:A:83:LEU:HD23	13:J:58:VAL:HG21	1.87	0.57
20:H:405:3PE:H341	20:J:201:3PE:H321	1.85	0.57
3:G:118:ASP:OD1	3:G:762:ASN:ND2	2.38	0.56
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.87	0.56
9:L:243:MET:HE2	9:L:305:LYS:HB2	1.87	0.56
9:L:292:LEU:HB3	20:L:707:3PE:H2H1	1.87	0.56
12:K:9:ILE:HG12	13:J:108:VAL:HG22	1.87	0.56
3:G:828:GLN:NE2	3:G:889:GLY:O	2.39	0.56
7:H:179:ILE:HG21	7:H:255:LEU:HD23	1.87	0.56
9:L:66:THR:H	20:L:706:3PE:H112	1.69	0.56
3:G:476:GLY:O	3:G:804:ARG:NH2	2.39	0.56
3:G:808:GLN:HG3	3:G:811:LYS:HB2	1.88	0.56
7:H:291:ARG:NH1	22:H:508:HOH:O	2.39	0.55
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.88	0.55
12:K:80:LEU:HD21	13:J:74:LEU:HD11	1.89	0.55
5:B:186:VAL:HG23	5:B:187:VAL:HG23	1.89	0.55
1:F:56:ASP:O	1:F:237:GLN:NE2	2.38	0.54
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.90	0.54
7:H:79:ASP:OD2	13:J:27:HIS:NE2	2.38	0.54
6:I:59:ARG:NH2	6:I:142:PRO:O	2.40	0.54
4:C:65:LYS:NZ	4:C:130:LEU:O	2.40	0.54
6:I:24:ALA:HB2	7:H:43:PHE:HD1	1.73	0.54
11:N:37:ASN:ND2	11:N:103:ASP:OD2	2.38	0.54
11:N:305:HIS:ND1	11:N:329:TYR:OH	2.36	0.54
9:L:85:SER:OG	9:L:268:ARG:NH2	2.41	0.53
9:L:329:ASP:OD1	9:L:329:ASP:N	2.36	0.53
1:F:340:ARG:NE	1:F:372:GLU:OE1	2.42	0.53
3:G:883:GLN:NE2	22:G:1131:HOH:O	2.41	0.53
10:M:414:SER:O	10:M:418:VAL:N	2.36	0.53
13:J:68:VAL:O	13:J:72:MET:HG2	2.08	0.53
1:F:391:LEU:HD23	1:F:401:ALA:HB1	1.91	0.53
4:C:77:LEU:HB3	4:C:137:TYR:HB3	1.90	0.53
12:K:82:GLN:NE2	13:J:158:VAL:O	2.42	0.53
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.91	0.53
3:G:125:HIS:ND1	22:G:1104:HOH:O	2.33	0.53
9:L:371:SER:OG	9:L:441:GLU:OE2	2.25	0.53
2:E:86:ARG:NH2	2:E:166:LYS:O	2.42	0.52
12:K:85:ARG:NH1	13:J:160:ARG:O	2.42	0.52
3:G:626:GLU:OE1	3:G:786:ARG:NH1	2.42	0.52
4:C:80:MET:HE2	4:C:558:ARG:HG2	1.91	0.52
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.91	0.52
9:L:214:MET:HE1	20:M:703:3PE:H321	1.92	0.52
9:L:268:ARG:NH1	22:L:811:HOH:O	2.41	0.52
12:K:16:VAL:O	12:K:20:THR:OG1	2.28	0.52
9:L:179:VAL:HG22	10:M:426:THR:HG22	1.91	0.52
20:H:405:3PE:H3B1	20:J:201:3PE:H3B2	1.91	0.52
9:L:243:MET:HG3	9:L:309:ALA:HB2	1.92	0.52
5:B:180:ARG:HB2	5:B:193:TYR:HB2	1.91	0.52
11:N:176:LEU:HD22	11:N:202:LEU:HD11	1.92	0.52
5:B:101:THR:HA	5:B:129:CYS:HB3	1.90	0.52
10:M:344:GLN:NE2	22:M:817:HOH:O	2.39	0.51
4:C:189:LYS:HD2	5:B:111:GLN:HG2	1.90	0.51
4:C:230:ALA:O	4:C:252:HIS:NE2	2.40	0.51
11:N:369:ARG:HH22	11:N:450:TYR:HE2	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:GLU:O	1:F:238:ASN:ND2	2.44	0.51
1:F:357:CYS:HB2	1:F:401:ALA:HB2	1.92	0.51
4:C:133:ASN:OD1	4:C:133:ASN:N	2.40	0.51
7:H:121:MET:HE3	13:J:56:ILE:HD12	1.91	0.51
1:F:76:MET:HE2	1:F:215:CYS:HB2	1.91	0.51
1:F:98:THR:HA	1:F:325:LEU:HD12	1.93	0.51
3:G:454:GLU:OE1	3:G:813:ARG:NH1	2.38	0.51
3:G:74:SER:O	3:G:77:THR:OG1	2.29	0.50
20:H:405:3PE:H2C1	20:H:405:3PE:H3E1	1.92	0.50
4:C:110:ASP:OD1	4:C:110:ASP:N	2.41	0.50
9:L:318:TYR:OH	9:L:418:GLY:O	2.25	0.50
11:N:339:GLY:HA3	11:N:379:MET:HE3	1.94	0.50
7:H:209:ARG:HD3	7:H:245:ILE:HD11	1.92	0.50
20:L:704:3PE:H2E1	20:M:703:3PE:H2A1	1.93	0.50
4:C:276:GLU:O	4:C:283:ASN:ND2	2.33	0.50
7:H:38:ARG:NH1	7:H:55:GLY:O	2.44	0.50
10:M:208:GLU:HA	10:M:211:LEU:HD12	1.93	0.50
11:N:421:GLY:HA2	11:N:424:TYR:CE2	2.46	0.50
1:F:176:GLY:HA3	2:E:78:GLN:HG2	1.93	0.50
7:H:140:LYS:HD3	8:A:62:LEU:HB2	1.94	0.49
10:M:71:TRP:HB2	10:M:79:ILE:HG13	1.94	0.49
11:N:323:MET:HE1	11:N:485:MET:HE1	1.94	0.49
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.83	0.49
4:C:396:LYS:NZ	4:C:400:GLN:OE1	2.45	0.49
9:L:247:THR:HG21	9:L:350:GLY:HA3	1.92	0.49
4:C:224:HIS:HB2	4:C:230:ALA:HA	1.93	0.49
4:C:600:ARG:NH2	22:C:726:HOH:O	2.45	0.49
8:A:69:TYR:OH	12:K:74:SER:O	2.30	0.49
10:M:153:LEU:HD13	10:M:257:VAL:HG22	1.94	0.49
10:M:187:ILE:HD12	11:N:411:VAL:HG13	1.95	0.49
10:M:87:SER:OG	10:M:273:ARG:NH2	2.44	0.49
10:M:463:ARG:NH1	10:M:464:GLU:OE1	2.46	0.49
12:K:33:ILE:HG23	13:J:32:LEU:HD22	1.95	0.49
3:G:694:ASP:N	3:G:694:ASP:OD1	2.44	0.49
3:G:807:PRO:HB3	3:G:882:GLY:HA3	1.93	0.49
6:I:80:ALA:HB2	6:I:90:GLU:HB2	1.95	0.48
10:M:381:MET:HB2	10:M:385:PRO:HD3	1.95	0.48
4:C:324:SER:HB2	4:C:336:VAL:HA	1.95	0.48
7:H:113:ASN:OD1	7:H:113:ASN:N	2.46	0.48
9:L:606:LEU:HB3	13:J:106:VAL:HG11	1.96	0.48
3:G:399:VAL:HG13	3:G:428:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:5:THR:O	3:G:76:GLY:N	2.46	0.48
4:C:455:PRO:HB2	4:C:469:LEU:HD22	1.96	0.48
7:H:32:MET:HG2	7:H:279:MET:HE3	1.96	0.48
4:C:232:ARG:HB2	4:C:248:ASP:HB3	1.96	0.47
7:H:41:GLY:HA2	7:H:46:ARG:HG3	1.95	0.47
3:G:793:ASN:OD1	3:G:793:ASN:N	2.47	0.47
4:C:594:VAL:HG23	4:C:597:ASP:HB2	1.94	0.47
8:A:80:VAL:O	8:A:83:LEU:HG	2.14	0.47
9:L:170:ALA:HA	9:L:238:TRP:HB2	1.97	0.47
9:L:577:ARG:NH1	20:L:701:3PE:O22	2.42	0.47
11:N:311:VAL:HG22	11:N:410:LEU:HD13	1.97	0.47
9:L:154:ILE:HD13	9:L:242:ALA:HB1	1.97	0.47
3:G:451:ALA:O	3:G:456:GLN:NE2	2.47	0.47
4:C:143:ASP:OD1	4:C:157:ARG:NH1	2.45	0.47
1:F:39:ARG:HA	1:F:161:MET:HE1	1.95	0.47
1:F:73:TRP:CD1	1:F:215:CYS:HG	2.33	0.47
3:G:365:THR:O	3:G:786:ARG:NH2	2.46	0.47
3:G:679:VAL:HG11	3:G:689:LYS:HB2	1.97	0.47
20:I:203:3PE:H2I3	20:H:401:3PE:H2G2	1.96	0.47
10:M:65:SER:HB3	10:M:83:ILE:HG22	1.97	0.47
13:J:84:GLU:OE1	13:J:86:GLN:NE2	2.48	0.47
1:F:38:ALA:HB2	1:F:114:GLU:HG3	1.97	0.47
3:G:592:VAL:HB	3:G:606:ALA:HA	1.96	0.47
3:G:731:ASP:OD2	3:G:734:THR:OG1	2.30	0.47
7:H:303:LYS:HE3	8:A:118:VAL:HG13	1.96	0.47
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.95	0.47
4:C:569:LEU:HD12	4:C:598:VAL:HG11	1.97	0.47
9:L:80:VAL:HB	9:L:134:ASP:HB3	1.97	0.47
20:H:405:3PE:H382	8:A:20:LEU:HD12	1.96	0.46
11:N:129:PHE:O	11:N:133:GLU:HG2	2.15	0.46
11:N:66:LEU:HA	11:N:124:HIS:HB2	1.96	0.46
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.49	0.46
10:M:498:GLN:O	10:M:502:ASN:HB2	2.15	0.46
3:G:55:TYR:HB3	3:G:60:ASP:HB3	1.96	0.46
3:G:150:MET:HE2	3:G:182:TYR:HA	1.97	0.46
4:C:216:MET:HG3	4:C:237:LEU:HB2	1.98	0.46
11:N:14:LEU:HD21	13:J:143:LEU:HD11	1.97	0.46
3:G:598:GLN:HG3	3:G:826:LEU:HD22	1.98	0.46
7:H:121:MET:HG3	13:J:57:ILE:HG13	1.97	0.46
8:A:73:MET:HB3	8:A:73:MET:HE3	1.78	0.46
7:H:307:PRO:HB2	20:A:201:3PE:H2D2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:613:ALA:HB1	3:G:617:GLU:HB2	1.97	0.46
3:G:466:ALA:HB3	3:G:489:VAL:HG21	1.98	0.45
4:C:259:MET:HE2	5:B:138:ILE:HD13	1.98	0.45
9:L:179:VAL:HG21	10:M:430:VAL:HG23	1.98	0.45
9:L:263:VAL:HG13	9:L:323:LEU:HD11	1.97	0.45
9:L:273:PHE:HB3	9:L:280:LEU:HD13	1.98	0.45
11:N:70:ASP:N	11:N:70:ASP:OD1	2.47	0.45
10:M:404:PHE:O	10:M:408:PHE:HB2	2.16	0.45
3:G:267:ARG:HB2	3:G:820:LEU:HG	1.97	0.45
3:G:278:LYS:HA	3:G:278:LYS:HD3	1.71	0.45
9:L:381:VAL:HG21	9:L:461:LEU:HG	1.98	0.45
1:F:61:GLY:N	1:F:67:PHE:O	2.49	0.45
9:L:164:GLY:O	9:L:168:MET:HG3	2.16	0.45
1:F:296:GLY:O	1:F:320:ARG:NH2	2.48	0.45
9:L:415:MET:HE2	9:L:415:MET:HB3	1.83	0.45
10:M:483:GLN:NE2	10:M:487:ASP:OD1	2.44	0.45
3:G:740:MET:SD	22:G:1107:HOH:O	2.62	0.45
10:M:141:PHE:O	10:M:145:MET:HB2	2.17	0.45
1:F:178:TYR:HE2	1:F:400:HIS:HD2	1.64	0.45
2:E:136:ASN:O	2:E:142:ASN:ND2	2.43	0.45
3:G:178:HIS:HD1	3:G:179:ASP:H	1.64	0.45
3:G:839:GLN:NE2	3:G:872:PRO:HG3	2.32	0.45
8:A:118:VAL:HG11	20:A:201:3PE:H221	1.99	0.45
9:L:190:ASN:ND2	22:L:816:HOH:O	2.47	0.45
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.98	0.45
10:M:287:ALA:O	10:M:291:MET:HG3	2.15	0.45
11:N:288:ALA:HB2	11:N:300:TYR:HB2	1.98	0.45
3:G:255:TYR:OH	3:G:776:GLY:O	2.32	0.45
4:C:334:THR:HG21	6:I:20:ILE:HD12	1.99	0.45
7:H:114:ILE:HB	7:H:117:LEU:HB2	1.98	0.45
10:M:381:MET:HG2	10:M:457:LEU:HD12	1.99	0.45
4:C:123:HIS:HA	4:C:148:THR:O	2.17	0.44
9:L:243:MET:HE3	9:L:243:MET:HB3	1.76	0.44
10:M:109:ILE:HD12	10:M:109:ILE:HG23	1.80	0.44
10:M:361:GLN:O	10:M:365:ARG:HG2	2.17	0.44
3:G:247:GLU:HG3	3:G:249:ARG:HE	1.82	0.44
4:C:501:THR:HG23	4:C:521:GLN:HB3	2.00	0.44
6:I:82:THR:OG1	6:I:84:ASP:OD2	2.25	0.44
7:H:200:ALA:HB1	20:H:401:3PE:H3C2	1.99	0.44
10:M:185:MET:HB2	10:M:230:ALA:HB2	2.00	0.44
10:M:291:MET:HE1	10:M:418:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:330:ASP:OD1	1:F:330:ASP:N	2.41	0.44
1:F:364:SER:HB3	1:F:387:LEU:HD13	1.99	0.44
13:J:57:ILE:HG22	13:J:58:VAL:HG23	2.00	0.44
3:G:226:ALA:HB3	3:G:635:VAL:HG22	2.00	0.44
3:G:501:ILE:HG12	3:G:532:THR:HB	1.99	0.44
7:H:122:MET:HE1	20:H:405:3PE:H2B1	2.00	0.44
10:M:72:ILE:HB	10:M:77:ILE:HB	1.99	0.44
11:N:7:ASN:HB3	11:N:63:VAL:HG13	1.98	0.44
11:N:384:ALA:HB1	11:N:422:LEU:HD23	1.99	0.44
1:F:248:LYS:HB3	1:F:250:MET:HE3	2.00	0.44
3:G:97:LEU:HD22	3:G:154:ILE:HB	2.00	0.44
9:L:175:ARG:NH2	10:M:396:LEU:O	2.51	0.44
9:L:613:ARG:NH2	22:L:820:HOH:O	2.49	0.44
2:E:141:PRO:HG2	2:E:153:LEU:HB2	1.99	0.44
20:L:701:3PE:H2F1	20:M:701:3PE:H3B1	2.00	0.44
3:G:320:PRO:HB2	3:G:537:SER:HB2	2.00	0.44
7:H:130:VAL:HG21	7:H:208:HIS:CE1	2.53	0.44
9:L:241:ASP:OD2	9:L:241:ASP:N	2.51	0.44
2:E:22:ILE:O	2:E:26:MET:HG3	2.17	0.43
1:F:287:PHE:HZ	1:F:290:TRP:HB3	1.82	0.43
3:G:808:GLN:H	3:G:808:GLN:HG2	1.64	0.43
1:F:356:PRO:HB2	1:F:396:THR:HG22	2.01	0.43
3:G:307:ILE:HG22	3:G:591:LEU:HD22	2.00	0.43
4:C:334:THR:OG1	7:H:287:ALA:O	2.24	0.43
11:N:154:GLU:OE2	11:N:158:LYS:NZ	2.46	0.43
4:C:297:ILE:HG12	4:C:497:HIS:CG	2.53	0.43
9:L:431:ARG:HG3	9:L:512:TRP:CE2	2.54	0.43
20:I:203:3PE:H2F2	20:H:401:3PE:H2E1	1.99	0.43
8:A:81:GLU:HG2	13:J:148:LEU:HD13	2.00	0.43
10:M:123:ILE:HG13	10:M:149:PRO:HB2	1.99	0.43
13:J:20:ILE:HG13	13:J:21:THR:HG23	2.00	0.43
11:N:347:MET:HB2	11:N:360:PHE:HE1	1.83	0.43
3:G:439:THR:OG1	3:G:442:ASP:OD1	2.35	0.43
11:N:259:LEU:HB2	11:N:316:LEU:HD21	2.01	0.43
2:E:117:PRO:HB3	2:E:130:PRO:HD3	2.01	0.43
7:H:38:ARG:HA	7:H:38:ARG:HD2	1.81	0.43
9:L:599:SER:HB3	12:K:19:LEU:HD21	2.00	0.43
10:M:217:SER:O	20:M:701:3PE:N	2.40	0.43
11:N:330:LEU:HD23	11:N:330:LEU:HA	1.89	0.43
3:G:103:HIS:ND1	22:G:1105:HOH:O	2.34	0.43
4:C:407:ARG:NH1	7:H:291:ARG:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:217:PRO:HG3	6:I:144:LYS:HD2	2.01	0.43
7:H:15:ILE:HD11	8:A:14:TRP:HB3	2.00	0.43
11:N:206:GLY:O	11:N:210:MET:HG3	2.19	0.43
1:F:291:GLN:O	1:F:326:ALA:HA	2.19	0.43
3:G:431:LEU:O	3:G:446:ALA:N	2.52	0.43
5:B:100:GLY:HA2	14:B:301:SF4:S4	2.59	0.43
7:H:265:LEU:HB2	7:H:270:TRP:CD1	2.54	0.43
20:L:702:3PE:H2I3	20:L:706:3PE:H391	2.00	0.43
3:G:301:MET:HE2	3:G:301:MET:HA	2.00	0.42
9:L:325:VAL:O	9:L:409:ASN:ND2	2.52	0.42
10:M:192:LEU:HB2	10:M:223:LEU:HD13	2.01	0.42
1:F:18:ARG:HE	1:F:22:GLN:HB2	1.84	0.42
4:C:120:ASN:OD1	4:C:120:ASN:N	2.52	0.42
4:C:351:GLU:HB3	6:I:41:PRO:HG3	2.01	0.42
10:M:165:LYS:HD3	10:M:165:LYS:HA	1.66	0.42
6:I:24:ALA:HB2	7:H:43:PHE:CD1	2.53	0.42
6:I:48:ILE:HG12	6:I:116:LEU:HG	2.02	0.42
9:L:88:MET:HE3	9:L:88:MET:HB3	1.83	0.42
11:N:72:PHE:HB2	11:N:483:PRO:HB3	2.01	0.42
1:F:104:LEU:HD12	1:F:104:LEU:HA	1.90	0.42
5:B:70:THR:O	5:B:73:THR:OG1	2.36	0.42
7:H:96:LEU:HD13	8:A:20:LEU:HD22	2.00	0.42
7:H:262:GLY:HA3	7:H:270:TRP:CD1	2.55	0.42
11:N:67:MET:HE3	11:N:67:MET:HB3	1.89	0.42
1:F:283:ASP:OD1	1:F:283:ASP:N	2.50	0.42
9:L:423:PHE:HB2	9:L:500:VAL:HG13	2.00	0.42
9:L:390:PRO:HA	9:L:396:PHE:CG	2.55	0.42
5:B:197:MET:HE3	5:B:197:MET:HB3	1.92	0.42
7:H:210:HIS:NE2	7:H:289:LEU:O	2.43	0.42
10:M:179:GLN:HG2	11:N:422:LEU:HD11	2.00	0.42
11:N:19:LEU:HD11	20:N:503:3PE:H3F1	2.01	0.42
12:K:43:ALA:HB1	12:K:62:TYR:HD1	1.84	0.42
1:F:177:ARG:HA	1:F:177:ARG:HD3	1.79	0.42
8:A:6:SER:HB3	8:A:9:VAL:HG22	2.02	0.42
5:B:124:ILE:HG12	5:B:153:VAL:HB	2.00	0.42
9:L:522:ILE:O	9:L:525:SER:OG	2.34	0.42
4:C:12:GLU:HA	4:C:13:PRO:HD3	1.89	0.42
12:K:62:TYR:OH	13:J:55:GLU:OE1	2.31	0.42
13:J:69:PHE:O	13:J:73:MET:HG3	2.20	0.42
4:C:576:ILE:HD12	4:C:576:ILE:HA	1.91	0.41
7:H:88:MET:HE2	7:H:88:MET:HB3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:141:GLY:HA3	13:J:154:VAL:HG22	2.02	0.41
1:F:250:MET:HG2	1:F:324:ALA:HB1	2.03	0.41
3:G:379:VAL:HB	3:G:433:VAL:HG12	2.01	0.41
3:G:451:ALA:HB1	3:G:455:ASP:HB2	2.02	0.41
11:N:381:LEU:HD12	21:N:501:LFA:H181	2.00	0.41
13:J:18:ARG:HD2	13:J:18:ARG:HA	1.73	0.41
3:G:623:ILE:HD12	3:G:787:LEU:HD11	2.02	0.41
7:H:194:PHE:O	7:H:198:THR:OG1	2.31	0.41
9:L:260:THR:HB	9:L:335:LEU:HD11	2.01	0.41
3:G:287:ARG:NH2	3:G:604:GLU:O	2.53	0.41
4:C:310:LEU:HD23	4:C:310:LEU:HA	1.91	0.41
4:C:337:PHE:HB3	5:B:74:ALA:HB2	2.02	0.41
4:C:334:THR:HG23	7:H:44:GLN:HG2	2.02	0.41
13:J:94:ILE:HD12	13:J:94:ILE:HA	1.92	0.41
3:G:428:LYS:HE3	3:G:428:LYS:HB3	1.82	0.41
3:G:472:PRO:HG3	3:G:799:THR:HA	2.01	0.41
9:L:380:LEU:HD23	9:L:380:LEU:HA	1.91	0.41
3:G:833:PHE:O	3:G:837:MET:N	2.48	0.41
7:H:135:TRP:HB2	13:J:72:MET:HE1	2.02	0.41
20:H:405:3PE:H261	20:J:201:3PE:H271	2.01	0.41
9:L:123:PHE:HE1	9:L:146:VAL:HG13	1.85	0.41
3:G:535:ALA:HB2	3:G:541:MET:HE2	2.03	0.41
5:B:57:TYR:HE2	5:B:113:LEU:HD13	1.86	0.41
8:A:75:PHE:O	8:A:79:ASP:HB2	2.21	0.41
9:L:584:LEU:HD23	9:L:584:LEU:HA	1.94	0.41
11:N:248:ILE:HD11	11:N:334:LEU:HB2	2.02	0.41
3:G:390:ARG:HD2	3:G:390:ARG:HA	1.79	0.41
3:G:644:LYS:HB3	3:G:644:LYS:HE3	1.64	0.41
3:G:740:MET:HE2	3:G:740:MET:HB2	1.96	0.41
4:C:165:LYS:HA	4:C:165:LYS:HD3	1.84	0.41
9:L:432:MET:HE3	9:L:432:MET:HB3	1.90	0.41
10:M:16:LEU:O	10:M:20:THR:OG1	2.29	0.41
3:G:5:THR:H	3:G:75:ASP:HA	1.85	0.40
6:I:179:LEU:HA	6:I:180:PRO:HD3	1.91	0.40
9:L:86:LEU:O	9:L:90:SER:OG	2.32	0.40
9:L:425:THR:HA	9:L:428:TYR:CE2	2.56	0.40
12:K:93:ASP:O	12:K:96:SER:OG	2.31	0.40
13:J:85:ARG:HB3	13:J:88:LEU:HD12	2.03	0.40
3:G:558:LEU:HD22	3:G:589:ALA:HB2	2.03	0.40
7:H:125:LEU:HD13	20:H:405:3PE:H2G1	2.04	0.40
9:L:344:LEU:HD21	9:L:381:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:236:LEU:HD23	7:H:236:LEU:HA	1.95	0.40
7:H:248:ILE:HD13	7:H:248:ILE:HA	1.94	0.40
9:L:229:LYS:HA	9:L:229:LYS:HD3	1.85	0.40
9:L:427:LEU:HD21	20:L:705:3PE:H361	2.04	0.40
13:J:24:ASN:HB3	13:J:27:HIS:HB2	2.03	0.40
3:G:217:TYR:HB3	6:I:79:LYS:HD2	2.02	0.40
6:I:66:CYS:HB2	6:I:105:CYS:HB2	2.03	0.40
12:K:92:ILE:HD12	12:K:92:ILE:HA	1.92	0.40
3:G:814:ILE:HD11	3:G:902:LEU:HD13	2.03	0.40
3:G:837:MET:HE2	3:G:837:MET:HB2	1.96	0.40
5:B:3:TYR:CD1	5:B:195:ALA:HA	2.56	0.40
7:H:121:MET:HG2	13:J:56:ILE:HB	2.04	0.40
11:N:217:LYS:HA	11:N:217:LYS:HD3	1.83	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%)	150 (97%)	4 (3%)	0	100	100
3	G	903/905 (100%)	880 (98%)	22 (2%)	1 (0%)	48	68
4	C	584/600 (97%)	571 (98%)	13 (2%)	0	100	100
5	B	192/220 (87%)	183 (95%)	9 (5%)	0	100	100
6	I	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
7	H	310/325 (95%)	301 (97%)	9 (3%)	0	100	100
8	A	98/147 (67%)	98 (100%)	0	0	100	100
9	L	602/613 (98%)	591 (98%)	11 (2%)	0	100	100
10	M	502/504 (100%)	491 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	N	474/485 (98%)	464 (98%)	9 (2%)	1 (0%)	43	63
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	160/162 (99%)	160 (100%)	0	0	100	100
All	All	4692/4836 (97%)	4587 (98%)	103 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	N	64	THR
3	G	669	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%)	348 (99%)	5 (1%)	59	81
2	E	129/129 (100%)	127 (98%)	2 (2%)	55	79
3	G	732/732 (100%)	726 (99%)	6 (1%)	73	88
4	C	505/519 (97%)	494 (98%)	11 (2%)	45	73
5	B	171/192 (89%)	169 (99%)	2 (1%)	63	83
6	I	154/154 (100%)	152 (99%)	2 (1%)	61	82
7	H	260/269 (97%)	254 (98%)	6 (2%)	44	72
8	A	80/119 (67%)	79 (99%)	1 (1%)	61	82
9	L	482/486 (99%)	473 (98%)	9 (2%)	50	76
10	M	413/413 (100%)	409 (99%)	4 (1%)	68	86
11	N	380/385 (99%)	376 (99%)	4 (1%)	65	84
12	K	79/79 (100%)	75 (95%)	4 (5%)	21	43
13	J	128/128 (100%)	127 (99%)	1 (1%)	73	88
All	All	3866/3958 (98%)	3809 (98%)	57 (2%)	55	80

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	7	THR
1	F	79	ASP
1	F	126	TYR
1	F	283	ASP
1	F	388	CYS
2	E	103	GLN
2	E	149	THR
3	G	57	ASN
3	G	94	VAL
3	G	181	VAL
3	G	314	VAL
3	G	416	GLN
3	G	470	SER
4	C	127	PHE
4	C	133	ASN
4	C	193	GLU
4	C	218	LEU
4	C	223	ASN
4	C	377	ASP
4	C	448	GLU
4	C	469	LEU
4	C	536	MET
4	C	569	LEU
4	C	594	VAL
5	B	63	CYS
5	B	94	ASP
6	I	12	THR
6	I	77	LEU
7	H	60	LEU
7	H	64	MET
7	H	113	ASN
7	H	138	ASN
7	H	186	VAL
7	H	198	THR
8	A	110	LEU
9	L	90	SER
9	L	93	THR
9	L	146	VAL
9	L	247	THR
9	L	354	LEU
9	L	372	ILE
9	L	472	VAL

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Mol	Chain	Res	Type
9	L	482	THR
9	L	500	VAL
10	M	256	SER
10	M	264	LEU
10	M	303	TRP
10	M	426	THR
11	N	19	LEU
11	N	135	ILE
11	N	295	LYS
11	N	359	LEU
12	K	1	MET
12	K	20	THR
12	K	46	PHE
12	K	96	SER
13	J	98	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	400	HIS
1	F	431	HIS
1	F	437	GLN
2	E	100	ASN
3	G	7	HIS
3	G	232	GLN
3	G	238	ASN
3	G	256	ASN
3	G	416	GLN
3	G	422	ASN
3	G	490	GLN
3	G	730	GLN
3	G	845	ASN
4	C	135	ASN
4	C	223	ASN
4	C	328	GLN
4	C	487	ASN
5	B	52	ASN
5	B	213	ASN
7	H	312	ASN
9	L	74	ASN
9	L	409	ASN
10	M	117	HIS

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Mol	Chain	Res	Type
10	M	281	ASN
10	M	308	GLN
10	M	344	GLN
11	N	285	ASN
11	N	317	GLN
11	N	472	GLN
12	K	27	ASN
12	K	82	GLN
12	K	91	ASN
13	J	115	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 1 is monoatomic - leaving 35 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	LFA	M	704	-	19,19,19	0.14	0	18,18,18	0.11	0
14	SF4	I	201	6	0,12,12	-	-	-		
14	SF4	I	202	6	0,12,12	-	-	-		
14	SF4	B	301	5	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	LFA	N	502	-	13,13,19	0.14	0	12,12,18	0.12	0
14	SF4	G	1002	3	0,12,12	-	-	-		
21	LFA	N	501	-	19,19,19	0.14	0	18,18,18	0.17	0
17	FES	E	201	2	0,4,4	-	-	-		
20	3PE	L	706	-	50,50,50	0.30	0	53,55,55	0.31	0
20	3PE	L	702	-	50,50,50	0.30	0	53,55,55	0.28	0
21	LFA	L	703	-	19,19,19	0.14	0	18,18,18	0.16	0
20	3PE	H	405	-	50,50,50	0.31	0	53,55,55	0.30	0
20	3PE	L	701	-	50,50,50	0.30	0	53,55,55	0.29	0
21	LFA	H	402	-	19,19,19	0.14	0	18,18,18	0.11	0
20	3PE	H	403	-	29,29,50	0.39	0	32,34,55	0.37	0
20	3PE	H	404	-	50,50,50	0.30	0	53,55,55	0.35	0
20	3PE	A	201	-	41,41,50	0.33	0	44,46,55	0.29	0
20	3PE	M	701	-	50,50,50	0.31	0	53,55,55	0.30	0
17	FES	G	1004	3	0,4,4	-	-	-		
20	3PE	L	704	-	50,50,50	0.30	0	53,55,55	0.30	0
20	3PE	I	204	-	27,27,50	0.38	0	29,30,55	0.34	0
20	3PE	M	702	-	50,50,50	0.29	0	53,55,55	0.29	0
14	SF4	F	501	1	0,12,12	-	-	-		
14	SF4	G	1003	3	0,12,12	-	-	-		
20	3PE	L	707	-	50,50,50	0.32	0	53,55,55	0.57	1 (1%)
14	SF4	G	1001	3	0,12,12	-	-	-		
20	3PE	H	401	-	50,50,50	0.29	0	53,55,55	0.29	0
20	3PE	N	503	-	50,50,50	0.30	0	53,55,55	0.30	0
20	3PE	L	705	-	50,50,50	0.31	0	53,55,55	0.32	0
20	3PE	I	203	-	50,50,50	0.30	0	53,55,55	0.29	0
20	3PE	J	201	-	50,50,50	0.30	0	53,55,55	0.28	0
20	3PE	M	703	-	50,50,50	0.30	0	53,55,55	0.30	0
15	FMN	F	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.28	6 (12%)
16	NAI	F	503	-	45,48,48	0.27	0	60,73,73	0.35	0
19	DCQ	B	302	-	23,23,23	0.25	0	26,29,29	0.39	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	LFA	M	704	-	-	0/17/17/17	-
14	SF4	I	201	6	-	-	0/6/5/5
19	DCQ	B	302	-	-	1/14/38/38	0/1/1/1
14	SF4	I	202	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	B	301	5	-	-	0/6/5/5
21	LFA	N	502	-	-	0/11/11/17	-
14	SF4	G	1002	3	-	-	0/6/5/5
21	LFA	N	501	-	-	1/17/17/17	-
17	FES	E	201	2	-	-	0/1/1/1
20	3PE	L	706	-	-	16/54/54/54	-
20	3PE	L	702	-	-	14/54/54/54	-
21	LFA	L	703	-	-	0/17/17/17	-
20	3PE	H	405	-	-	8/54/54/54	-
20	3PE	L	701	-	-	15/54/54/54	-
21	LFA	H	402	-	-	1/17/17/17	-
20	3PE	H	403	-	-	10/33/33/54	-
20	3PE	H	404	-	-	9/54/54/54	-
20	3PE	A	201	-	-	14/45/45/54	-
20	3PE	M	701	-	-	10/54/54/54	-
17	FES	G	1004	3	-	-	0/1/1/1
20	3PE	L	704	-	-	13/54/54/54	-
20	3PE	M	702	-	-	12/54/54/54	-
20	3PE	I	204	-	-	4/28/28/54	-
14	SF4	F	501	1	-	-	0/6/5/5
14	SF4	G	1003	3	-	-	0/6/5/5
20	3PE	L	707	-	-	9/54/54/54	-
14	SF4	G	1001	3	-	-	0/6/5/5
20	3PE	H	401	-	-	13/54/54/54	-
20	3PE	N	503	-	-	13/54/54/54	-
20	3PE	L	705	-	-	9/54/54/54	-
20	3PE	I	203	-	-	8/54/54/54	-
20	3PE	J	201	-	-	14/54/54/54	-
15	FMN	F	502	-	-	5/18/18/18	0/3/3/3
16	NAI	F	503	-	-	5/29/72/72	0/5/5/5
20	3PE	M	703	-	-	12/54/54/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.65	1.37	1.30
15	F	502	FMN	C10-N1	2.21	1.37	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4-N3-C2	-3.33	119.49	125.64
15	F	502	FMN	C4A-C10-N10	2.96	120.81	116.48
15	F	502	FMN	C4A-C4-N3	2.75	120.17	113.19
15	F	502	FMN	O4-C4-C4A	-2.45	120.09	126.60
15	F	502	FMN	C10-C4A-N5	-2.42	119.73	124.86
15	F	502	FMN	C4A-C10-N1	-2.34	119.29	124.73
20	L	707	3PE	C2-O21-C21	2.33	123.52	117.79

There are no chirality outliers.

All (216) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	502	FMN	N10-C1'-C2'-O2'
15	F	502	FMN	N10-C1'-C2'-C3'
15	F	502	FMN	C5'-O5'-P-O2P
15	F	502	FMN	C5'-O5'-P-O3P
20	I	203	3PE	O13-C11-C12-N
20	I	204	3PE	C11-O13-P-O12
20	H	401	3PE	C11-O13-P-O12
20	H	401	3PE	C11-O13-P-O14
20	H	403	3PE	C11-O13-P-O11
20	H	403	3PE	C11-O13-P-O14
20	H	404	3PE	C11-O13-P-O11
20	H	404	3PE	C11-O13-P-O12
20	H	404	3PE	C11-O13-P-O14
20	H	404	3PE	O13-C11-C12-N
20	H	405	3PE	C1-O11-P-O12
20	H	405	3PE	C1-O11-P-O13
20	H	405	3PE	C1-O11-P-O14
20	A	201	3PE	C1-O11-P-O14
20	L	701	3PE	C1-O11-P-O14
20	L	701	3PE	O13-C11-C12-N
20	L	702	3PE	C1-O11-P-O14
20	L	702	3PE	C11-O13-P-O12
20	L	704	3PE	C1-O11-P-O14
20	L	704	3PE	C11-O13-P-O11
20	L	704	3PE	C11-O13-P-O12
20	L	704	3PE	C11-O13-P-O14
20	L	704	3PE	O13-C11-C12-N
20	L	705	3PE	C1-O11-P-O12
20	L	705	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
20	L	705	3PE	C11-O13-P-O11
20	L	705	3PE	C11-O13-P-O12
20	L	705	3PE	C11-O13-P-O14
20	L	706	3PE	C1-O11-P-O14
20	L	706	3PE	C2-C1-O11-P
20	L	706	3PE	O21-C2-C3-O31
20	L	707	3PE	C1-O11-P-O14
20	L	707	3PE	C11-O13-P-O14
20	L	707	3PE	O13-C11-C12-N
20	M	701	3PE	C11-O13-P-O11
20	M	701	3PE	C11-O13-P-O14
20	M	701	3PE	O13-C11-C12-N
20	M	702	3PE	C11-O13-P-O11
20	M	702	3PE	C11-O13-P-O12
20	M	702	3PE	C11-O13-P-O14
20	M	703	3PE	C1-O11-P-O12
20	M	703	3PE	C11-O13-P-O12
20	M	703	3PE	C11-O13-P-O14
20	M	703	3PE	O13-C11-C12-N
20	N	503	3PE	C1-O11-P-O12
20	N	503	3PE	C1-O11-P-O14
20	J	201	3PE	C1-O11-P-O12
20	J	201	3PE	C1-O11-P-O14
20	J	201	3PE	O13-C11-C12-N
20	L	706	3PE	C31-C32-C33-C34
20	I	204	3PE	C11-O13-P-O11
20	H	401	3PE	C11-O13-P-O11
20	L	701	3PE	C1-O11-P-O13
20	L	701	3PE	C11-O13-P-O11
20	L	702	3PE	C1-O11-P-O13
20	L	705	3PE	C1-O11-P-O13
20	L	706	3PE	C11-O13-P-O11
20	M	701	3PE	C1-O11-P-O13
20	M	703	3PE	C1-O11-P-O13
20	M	703	3PE	C11-O13-P-O11
20	N	503	3PE	C1-O11-P-O13
20	J	201	3PE	C1-O11-P-O13
20	L	702	3PE	C23-C24-C25-C26
20	L	707	3PE	C37-C38-C39-C3A
20	L	705	3PE	C35-C36-C37-C38
20	M	702	3PE	C3E-C3F-C3G-C3H
20	L	702	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
20	L	702	3PE	C2C-C2D-C2E-C2F
20	L	707	3PE	C24-C25-C26-C27
20	L	704	3PE	C3E-C3F-C3G-C3H
20	H	401	3PE	O13-C11-C12-N
20	H	403	3PE	O13-C11-C12-N
20	A	201	3PE	O13-C11-C12-N
21	H	402	LFA	C14-C15-C16-C17
20	L	701	3PE	C3B-C3C-C3D-C3E
20	L	701	3PE	C2B-C2C-C2D-C2E
20	M	701	3PE	C24-C25-C26-C27
20	M	702	3PE	C26-C27-C28-C29
20	L	702	3PE	C3E-C3F-C3G-C3H
20	I	203	3PE	C1-O11-P-O13
20	L	702	3PE	C11-O13-P-O11
20	L	704	3PE	C1-O11-P-O13
15	F	502	FMN	C5'-O5'-P-O1P
20	M	702	3PE	C2-C1-O11-P
20	L	701	3PE	O21-C2-C3-O31
20	H	401	3PE	C3D-C3E-C3F-C3G
20	H	405	3PE	C3B-C3C-C3D-C3E
20	M	703	3PE	C2D-C2E-C2F-C2G
20	L	706	3PE	C34-C35-C36-C37
20	M	703	3PE	C28-C29-C2A-C2B
20	J	201	3PE	O11-C1-C2-C3
20	L	706	3PE	C39-C3A-C3B-C3C
20	J	201	3PE	C21-C22-C23-C24
20	N	503	3PE	C2-C1-O11-P
20	J	201	3PE	C2-C1-O11-P
20	N	503	3PE	C2A-C2B-C2C-C2D
20	L	701	3PE	C1-C2-C3-O31
20	L	707	3PE	C11-O13-P-O11
20	I	203	3PE	C2-C1-O11-P
20	L	701	3PE	C2-C1-O11-P
20	M	701	3PE	C2-C1-O11-P
20	A	201	3PE	C28-C29-C2A-C2B
16	F	503	NAI	PN-O3-PA-O5B
20	H	403	3PE	O11-C1-C2-C3
20	J	201	3PE	C23-C24-C25-C26
20	J	201	3PE	O21-C21-C22-C23
20	H	401	3PE	C3C-C3D-C3E-C3F
20	L	702	3PE	C34-C35-C36-C37
20	H	403	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
20	H	404	3PE	C1-C2-C3-O31
20	L	706	3PE	C1-C2-C3-O31
20	J	201	3PE	O11-C1-C2-O21
20	L	706	3PE	C3C-C3D-C3E-C3F
20	M	703	3PE	C26-C27-C28-C29
20	H	404	3PE	O21-C2-C3-O31
20	L	704	3PE	O21-C2-C3-O31
16	F	503	NAI	C5B-O5B-PA-O3
20	H	401	3PE	C3F-C3G-C3H-C3I
19	B	302	DCQ	C11-C12-C13-C14
20	I	203	3PE	C1-O11-P-O12
20	I	204	3PE	C11-O13-P-O14
20	L	701	3PE	C1-O11-P-O12
20	L	701	3PE	C11-O13-P-O14
20	L	702	3PE	C1-O11-P-O12
20	L	702	3PE	C11-O13-P-O14
20	L	706	3PE	C11-O13-P-O14
20	M	701	3PE	C1-O11-P-O14
20	M	702	3PE	C2F-C2G-C2H-C2I
20	L	701	3PE	C24-C25-C26-C27
20	H	404	3PE	C12-C11-O13-P
20	M	702	3PE	C2E-C2F-C2G-C2H
20	L	706	3PE	C3E-C3F-C3G-C3H
20	H	403	3PE	O11-C1-C2-O21
20	A	201	3PE	O11-C1-C2-O21
20	H	405	3PE	C3C-C3D-C3E-C3F
20	A	201	3PE	C27-C28-C29-C2A
20	L	701	3PE	C28-C29-C2A-C2B
20	I	203	3PE	C32-C33-C34-C35
20	L	702	3PE	C25-C26-C27-C28
20	M	703	3PE	C37-C38-C39-C3A
20	H	404	3PE	C32-C33-C34-C35
20	I	203	3PE	C2D-C2E-C2F-C2G
20	H	405	3PE	C11-O13-P-O11
20	A	201	3PE	C1-O11-P-O13
20	L	706	3PE	C1-O11-P-O13
20	N	503	3PE	C11-O13-P-O11
20	J	201	3PE	C11-O13-P-O11
20	M	701	3PE	C35-C36-C37-C38
16	F	503	NAI	O4D-C1D-N1N-C2N
20	L	706	3PE	C37-C38-C39-C3A
20	H	405	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	L	701	3PE	C31-C32-C33-C34
20	H	404	3PE	C2-C1-O11-P
20	H	401	3PE	C1-C2-C3-O31
20	L	707	3PE	C1-C2-O21-C21
20	L	707	3PE	C1-O11-P-O13
20	A	201	3PE	O11-C1-C2-C3
20	I	203	3PE	C2A-C2B-C2C-C2D
20	H	405	3PE	C23-C24-C25-C26
20	H	401	3PE	O21-C2-C3-O31
16	F	503	NAI	C2D-C1D-N1N-C2N
20	M	703	3PE	O31-C31-C32-C33
20	L	706	3PE	O13-C11-C12-N
20	N	503	3PE	O13-C11-C12-N
20	L	707	3PE	C23-C24-C25-C26
20	A	201	3PE	C2-C1-O11-P
20	H	401	3PE	O31-C31-C32-C33
20	M	703	3PE	C2C-C2D-C2E-C2F
20	N	503	3PE	C2B-C2C-C2D-C2E
20	L	704	3PE	O21-C21-C22-C23
20	L	705	3PE	O31-C31-C32-C33
20	M	702	3PE	O31-C31-C32-C33
20	N	503	3PE	O21-C21-C22-C23
20	A	201	3PE	C2C-C2D-C2E-C2F
20	H	401	3PE	C29-C2A-C2B-C2C
20	N	503	3PE	O31-C31-C32-C33
20	H	403	3PE	C25-C26-C27-C28
20	L	702	3PE	O21-C2-C3-O31
20	L	702	3PE	C31-C32-C33-C34
20	M	702	3PE	C29-C2A-C2B-C2C
20	A	201	3PE	O21-C21-C22-C23
20	J	201	3PE	O22-C21-C22-C23
21	N	501	LFA	C11-C10-C9-C8
20	L	704	3PE	O22-C21-C22-C23
20	M	702	3PE	O32-C31-C32-C33
20	H	401	3PE	O32-C31-C32-C33
20	N	503	3PE	O32-C31-C32-C33
20	L	704	3PE	C1-C2-C3-O31
20	H	401	3PE	C25-C26-C27-C28
20	A	201	3PE	O22-C21-C22-C23
20	L	705	3PE	O32-C31-C32-C33
16	F	503	NAI	C5B-O5B-PA-O2A
20	L	704	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
20	L	706	3PE	C1-O11-P-O12
20	M	702	3PE	C1-O11-P-O14
20	N	503	3PE	C11-O13-P-O14
20	J	201	3PE	C11-O13-P-O14
20	N	503	3PE	O22-C21-C22-C23
20	H	403	3PE	O21-C21-C22-C23
20	L	701	3PE	C23-C24-C25-C26
20	L	706	3PE	C3D-C3E-C3F-C3G
20	I	203	3PE	C12-C11-O13-P
20	H	403	3PE	C12-C11-O13-P
20	M	701	3PE	C12-C11-O13-P
20	I	204	3PE	O31-C31-C32-C33
20	J	201	3PE	C24-C25-C26-C27
20	A	201	3PE	O31-C31-C32-C33
20	M	701	3PE	C2F-C2G-C2H-C2I
20	A	201	3PE	O32-C31-C32-C33
20	A	201	3PE	C26-C27-C28-C29
20	H	403	3PE	O22-C21-C22-C23
20	L	704	3PE	O31-C31-C32-C33

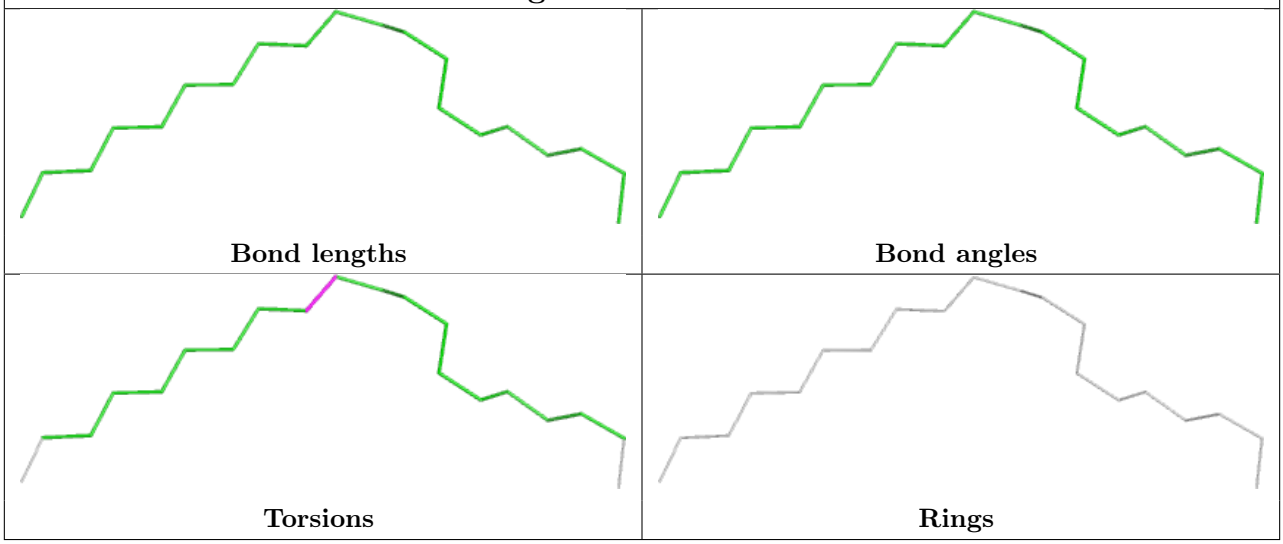
There are no ring outliers.

17 monomers are involved in 31 short contacts:

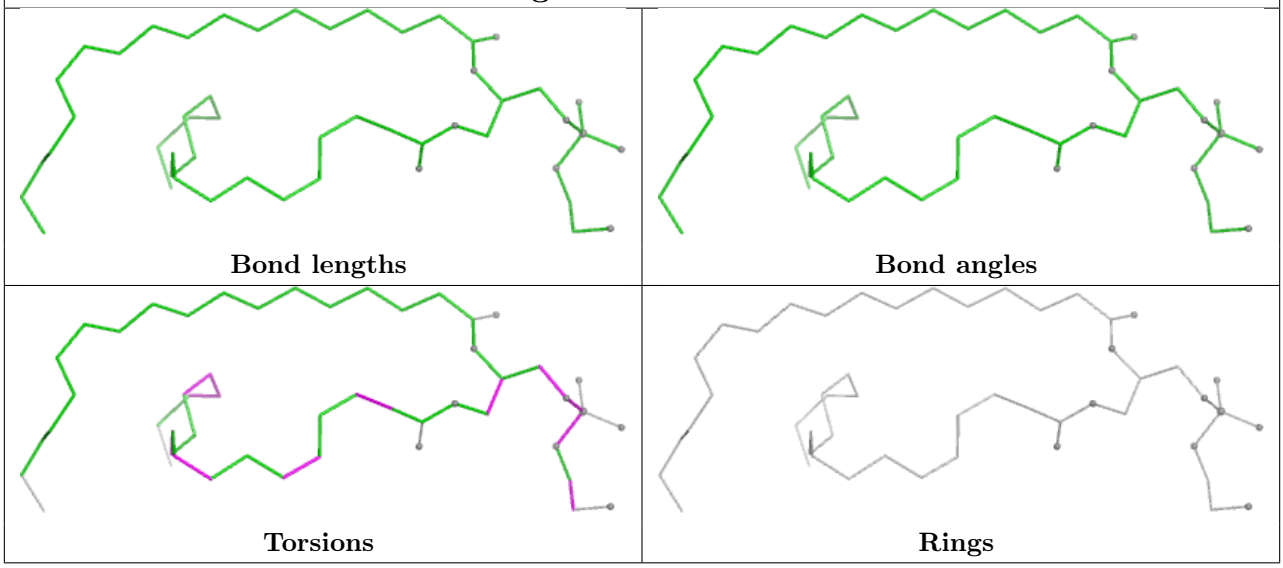
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	301	SF4	1	0
21	N	501	LFA	1	0
20	L	706	3PE	2	0
20	L	702	3PE	1	0
20	H	405	3PE	7	0
20	L	701	3PE	3	0
20	A	201	3PE	2	0
20	M	701	3PE	2	0
20	L	704	3PE	2	0
20	L	707	3PE	2	0
20	H	401	3PE	4	0
20	N	503	3PE	1	0
20	L	705	3PE	2	0
20	I	203	3PE	2	0
20	J	201	3PE	3	0
20	M	703	3PE	3	0
16	F	503	NAI	1	0

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

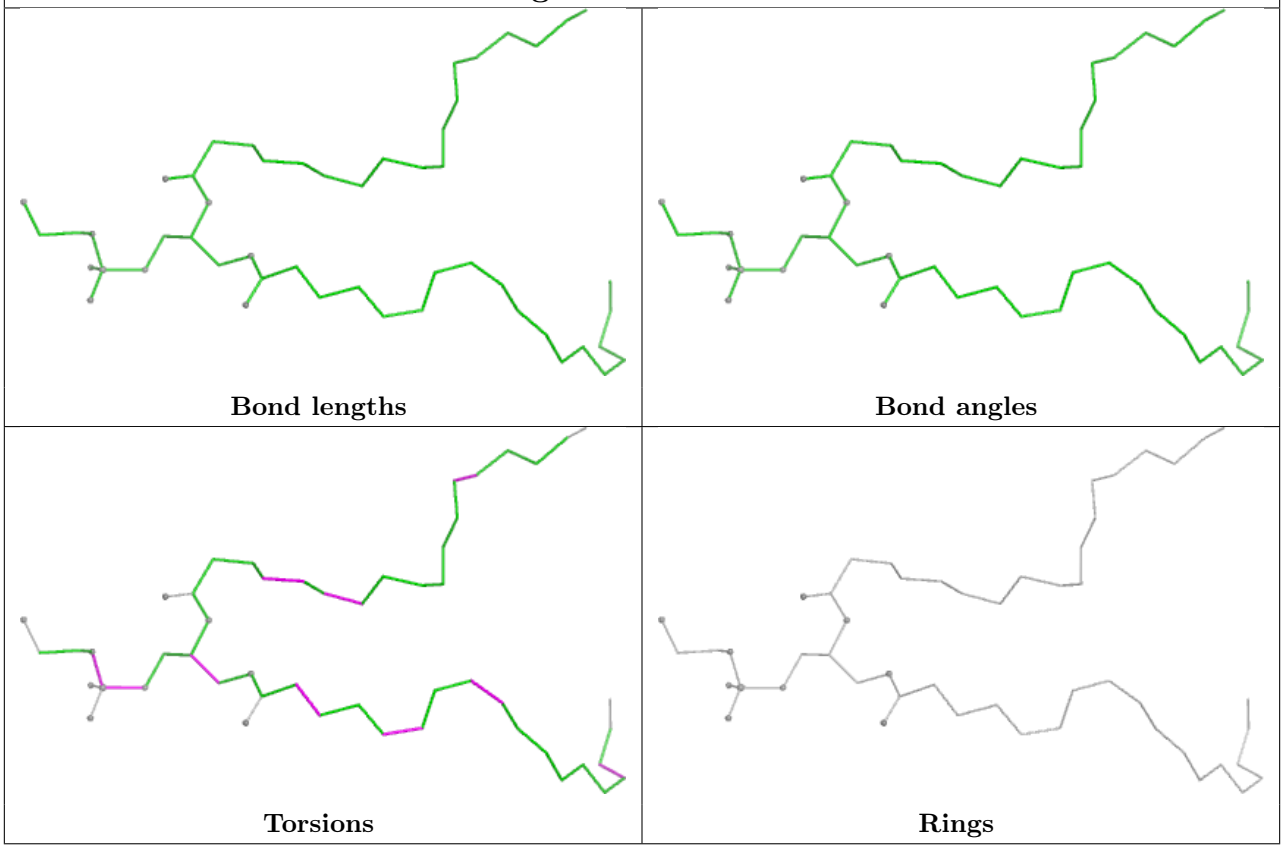
Ligand LFA N 501



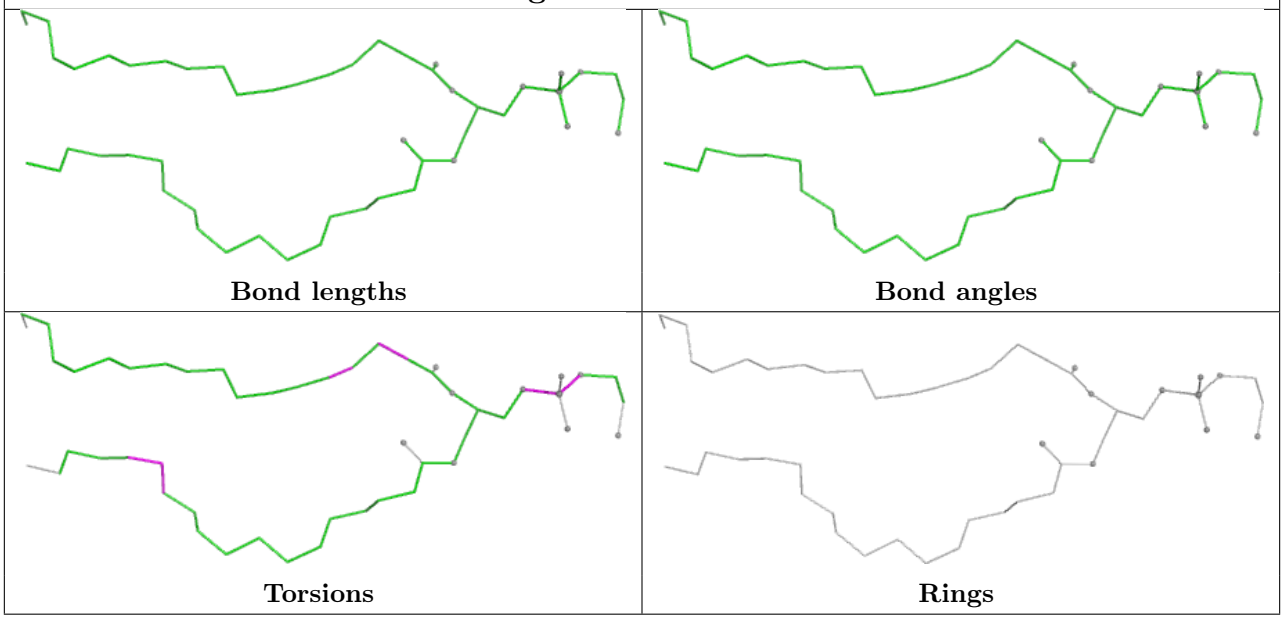
Ligand 3PE L 706

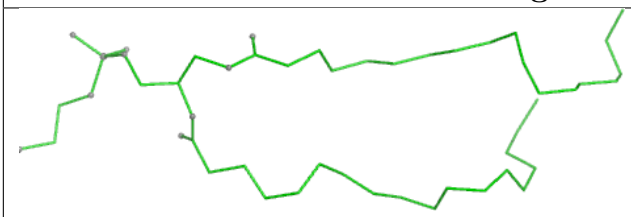
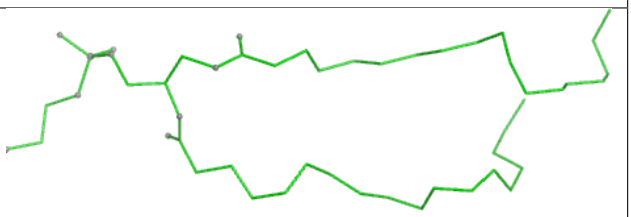
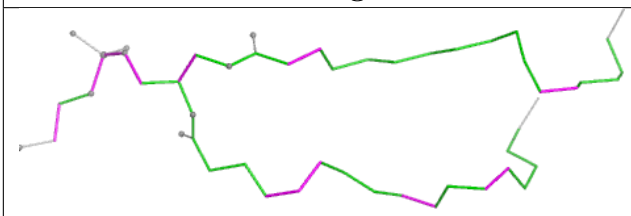
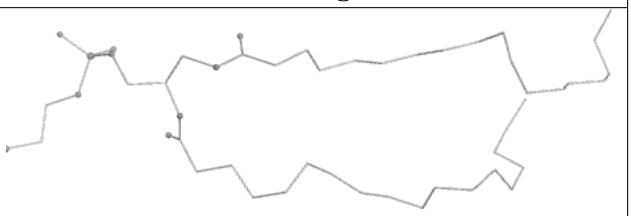


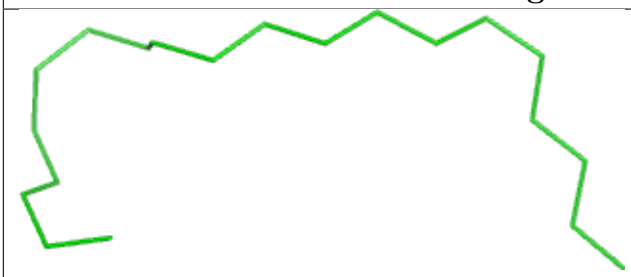
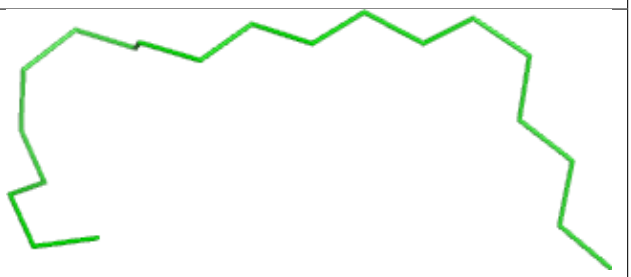
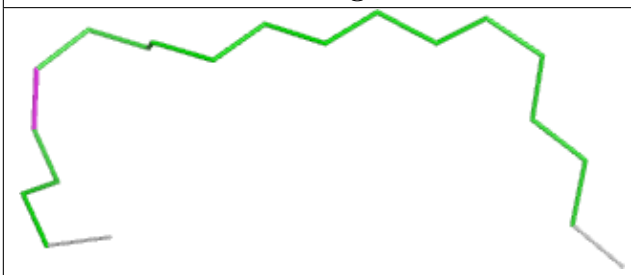
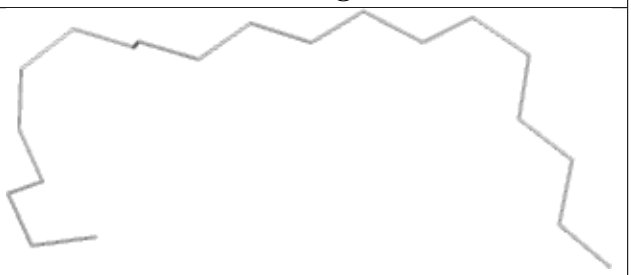
Ligand 3PE L 702



Ligand 3PE H 405



Ligand 3PE L 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LFA H 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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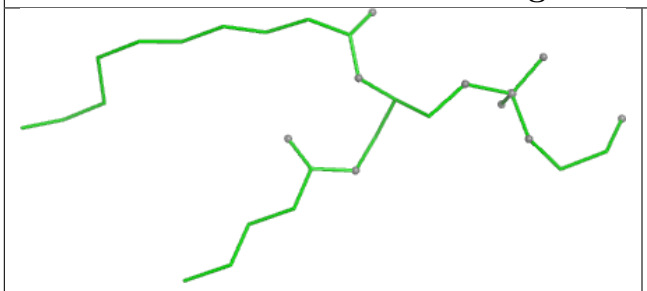

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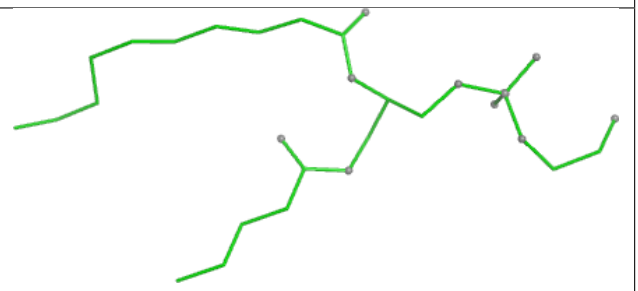

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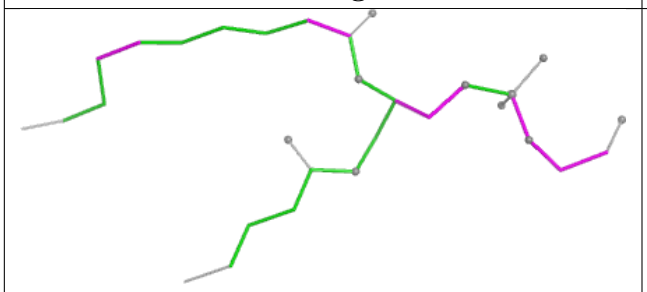

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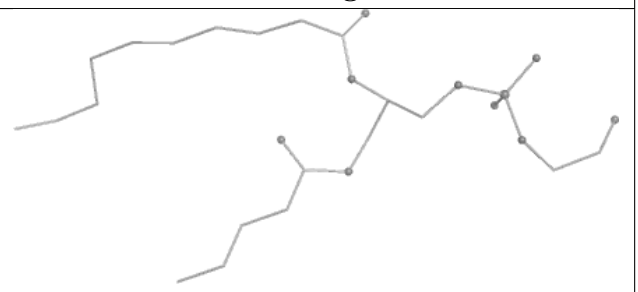
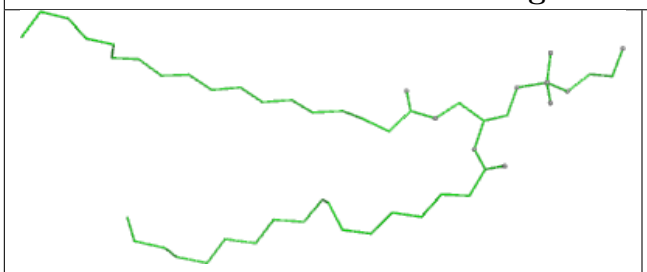


Rings

Ligand 3PE H 404



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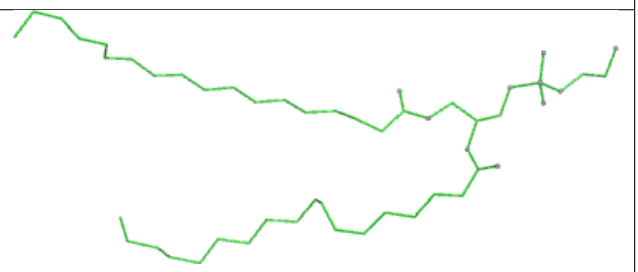

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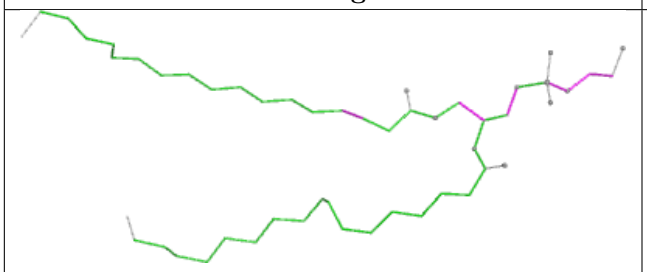

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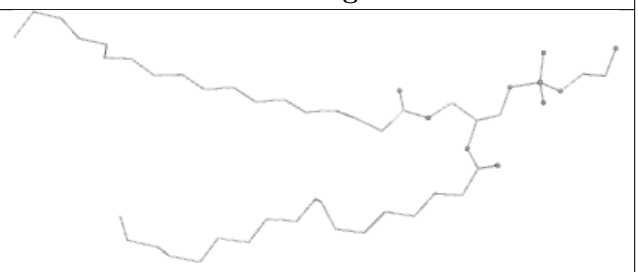
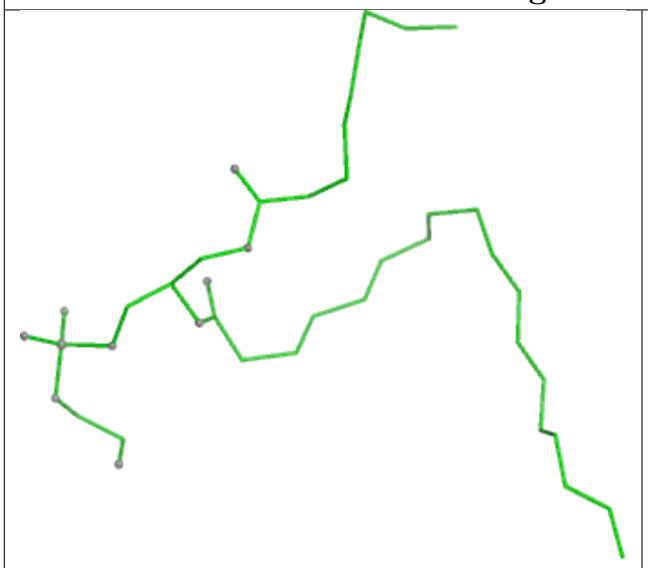


Rings

Ligand 3PE A 201



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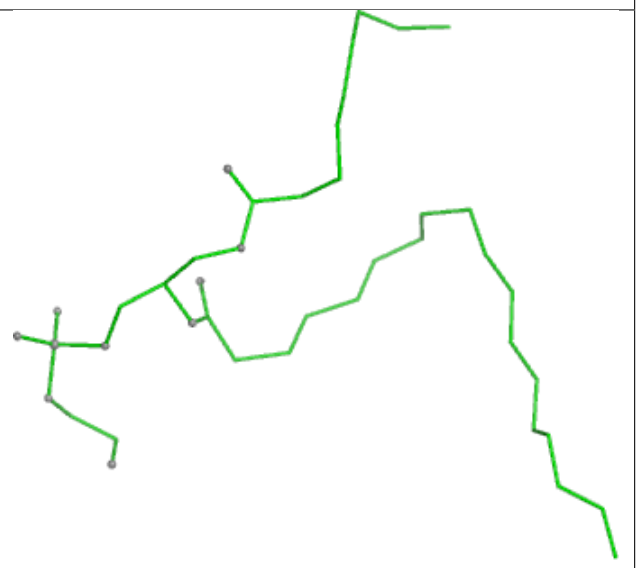
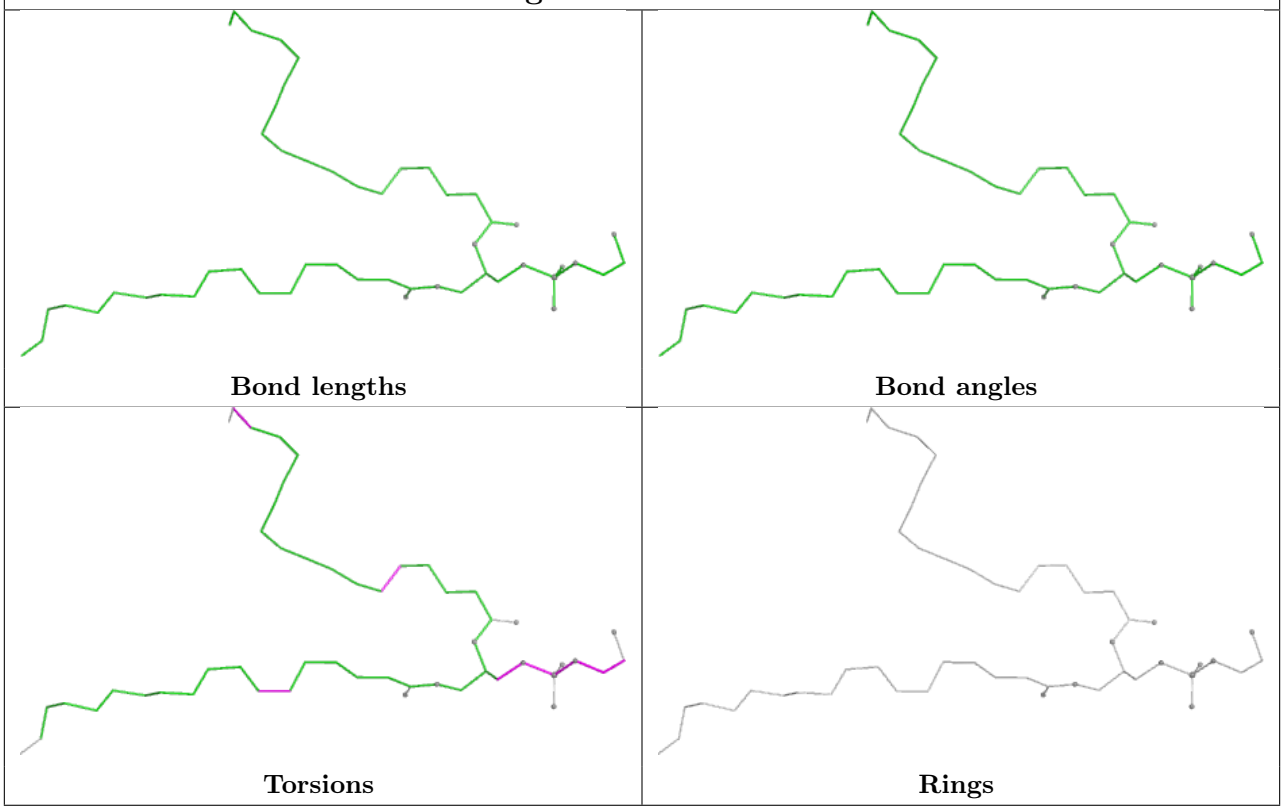


Bond angles

Torsions

Rings

Ligand 3PE M 701



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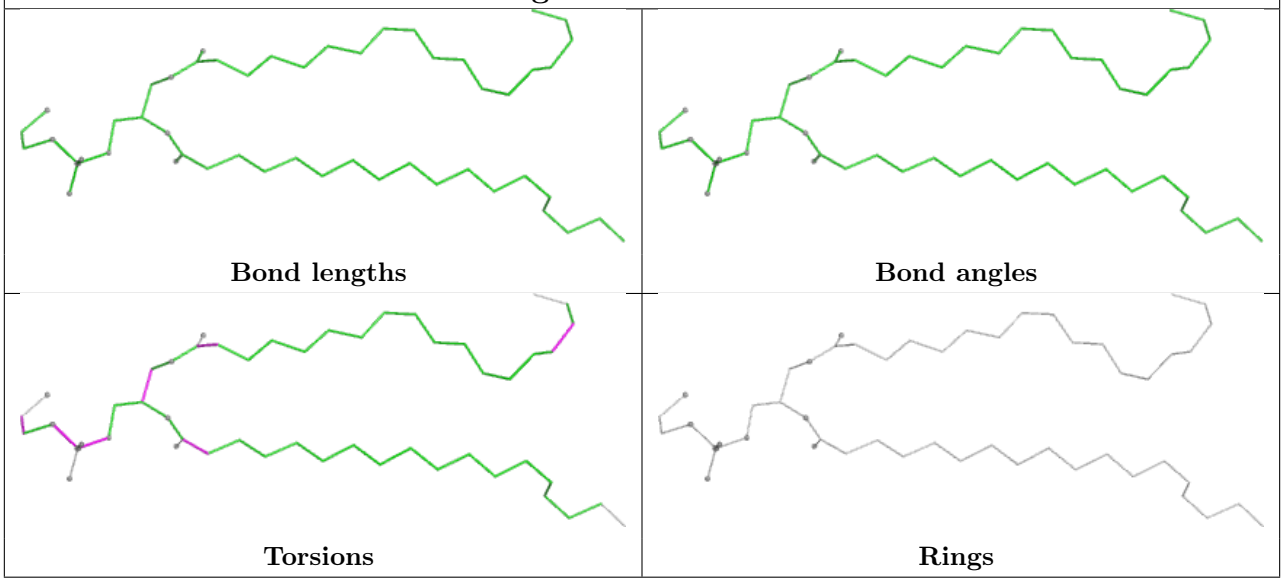

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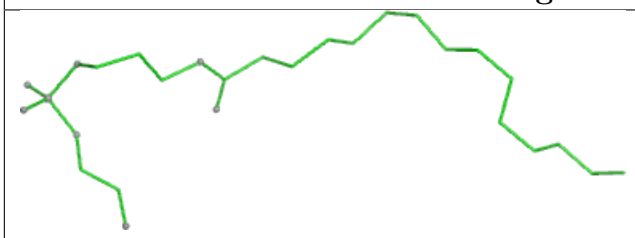
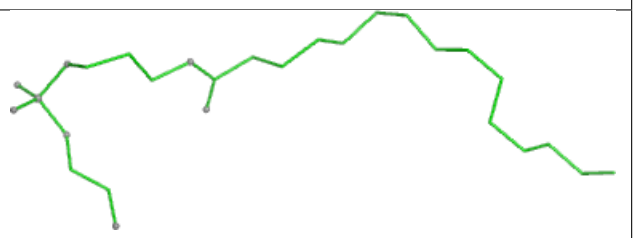
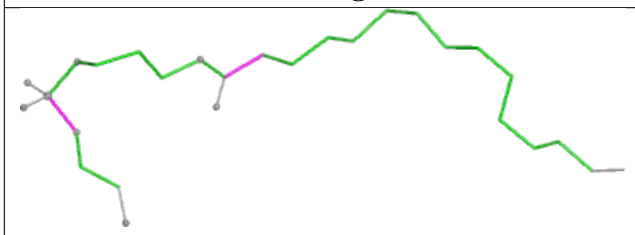
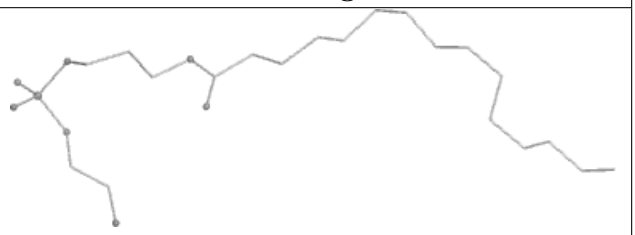
 Bond lengths	 Bond angles
 Torsions	 Rings

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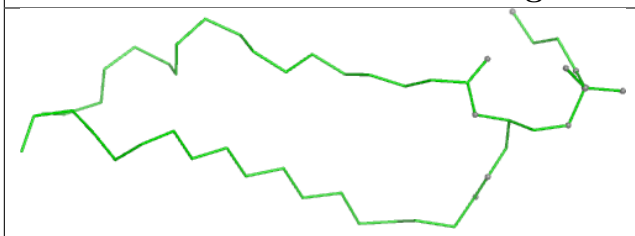
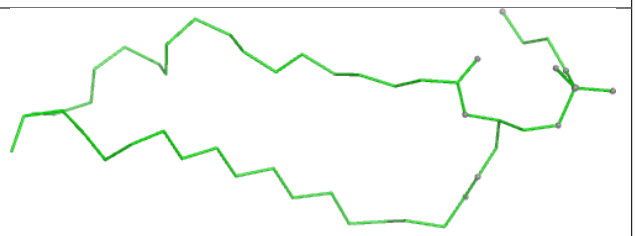
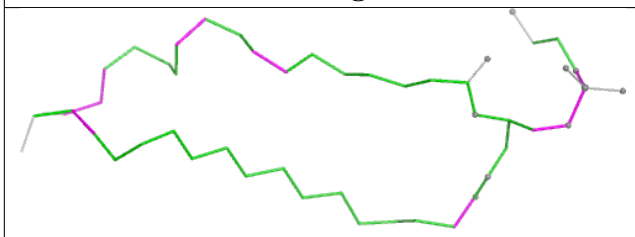
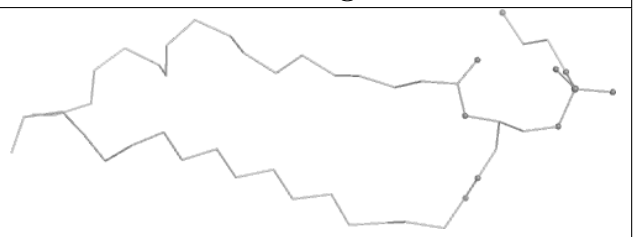
 Bond lengths	 Bond angles
 Torsions	 Rings

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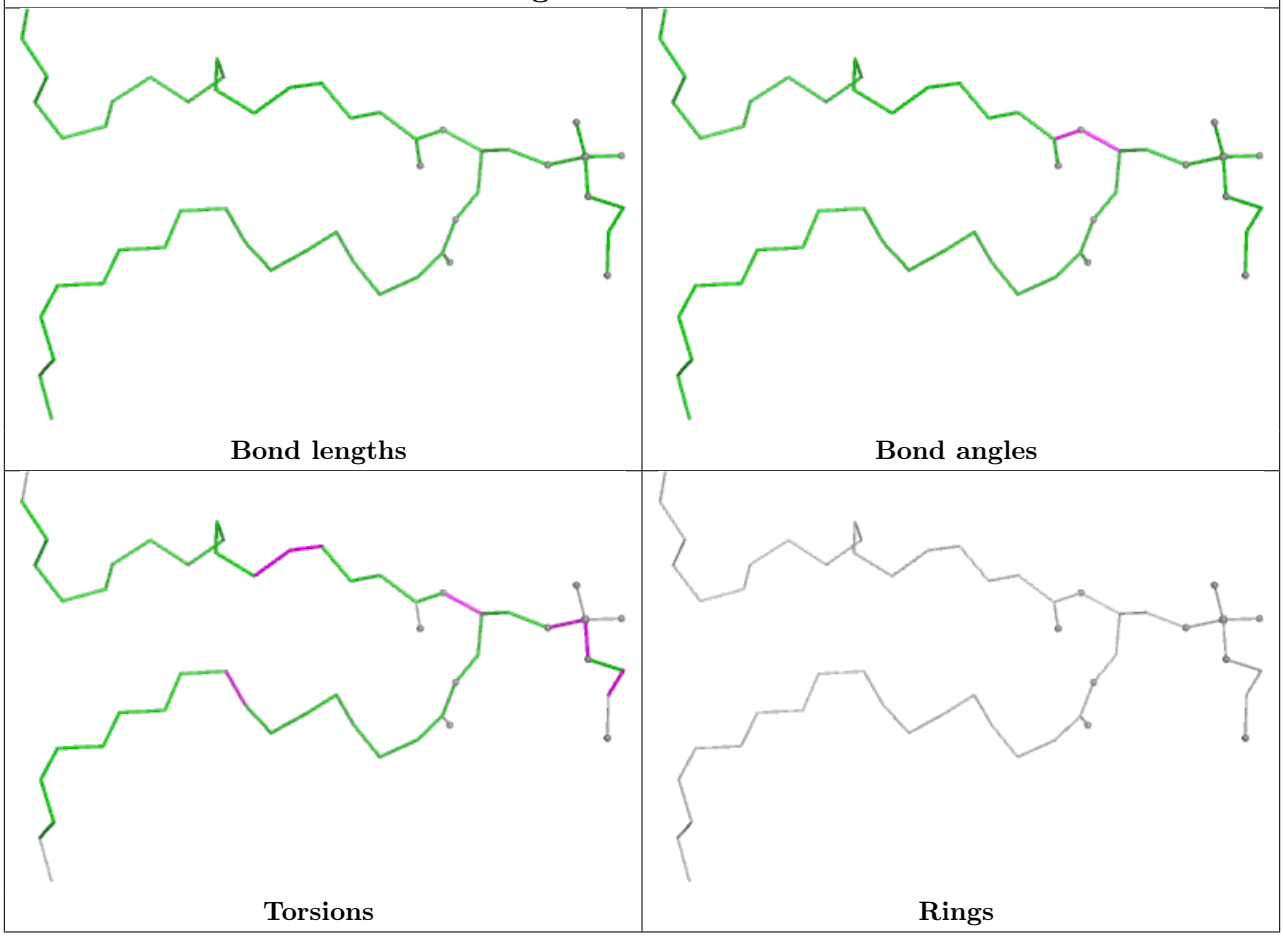

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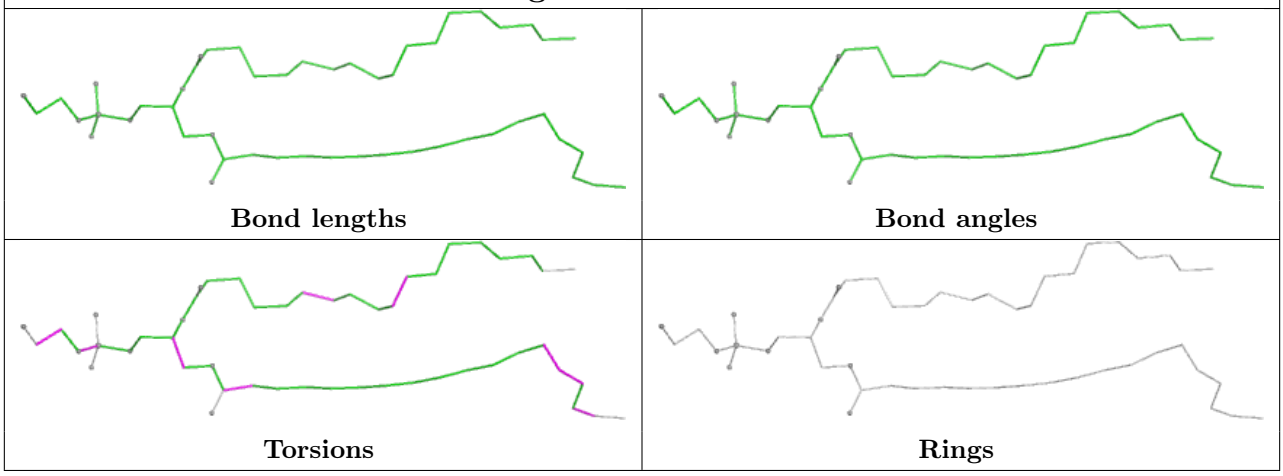
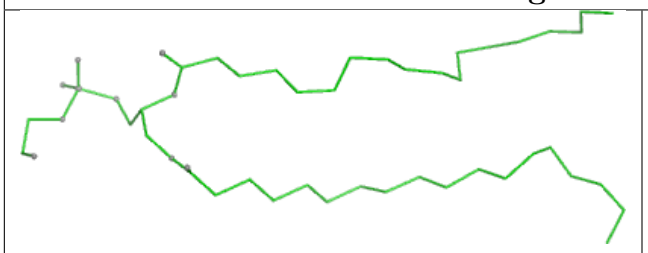
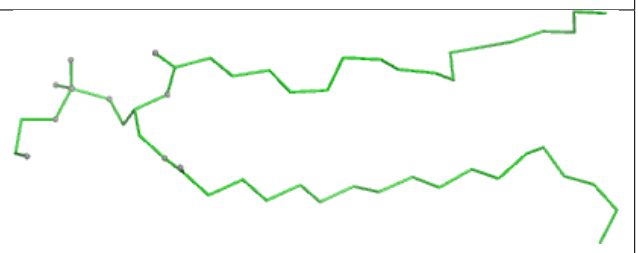


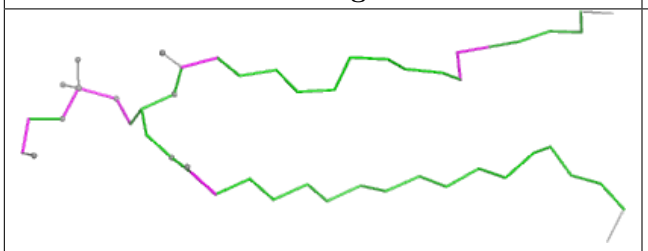
Ligand 3PE N 503



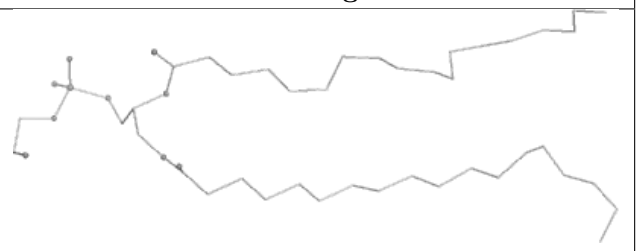
Bond lengths



Bond angles

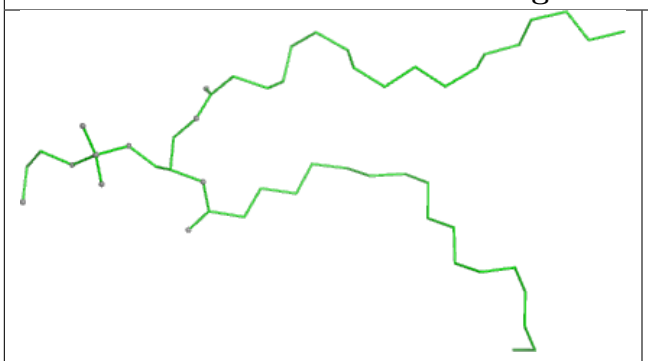


Torsions



Rings

Ligand 3PE L 705



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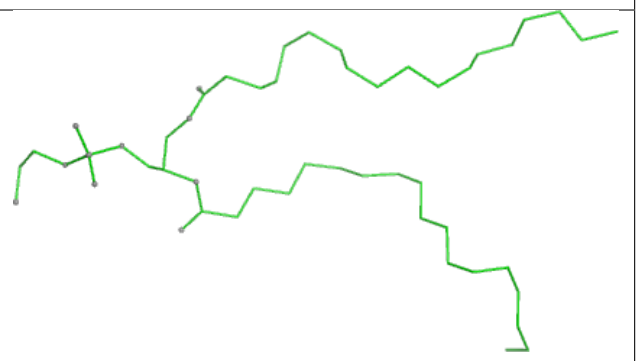

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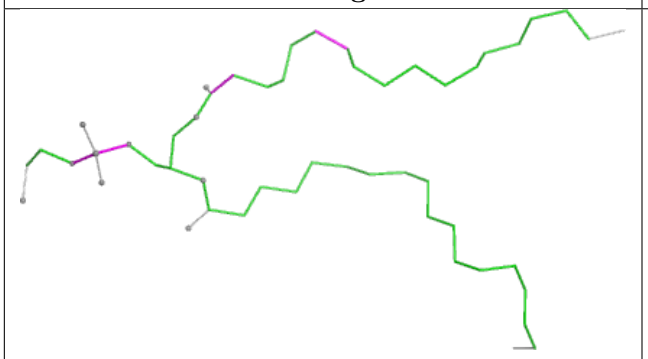

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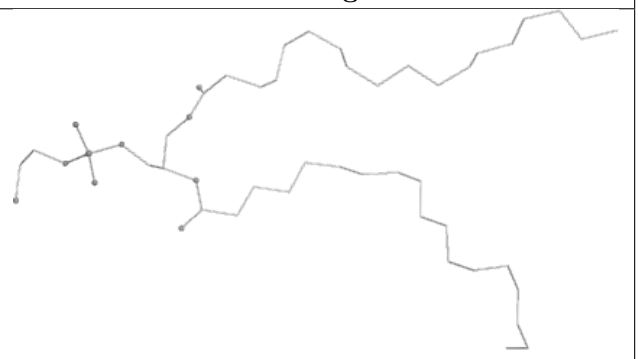
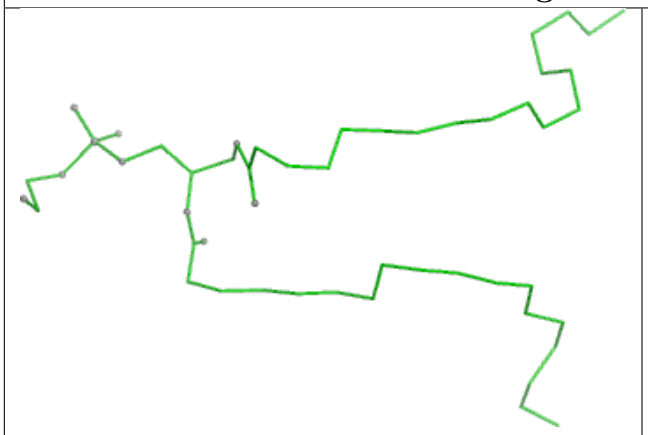


Rings

Ligand 3PE I 203



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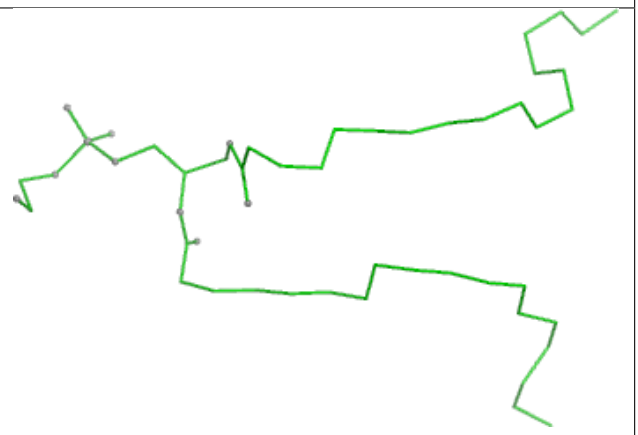

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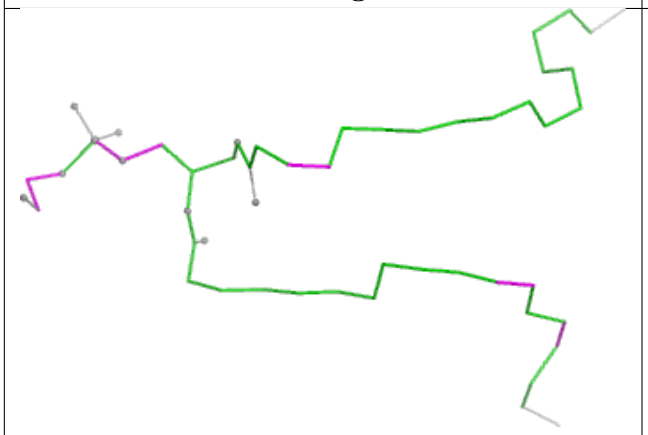

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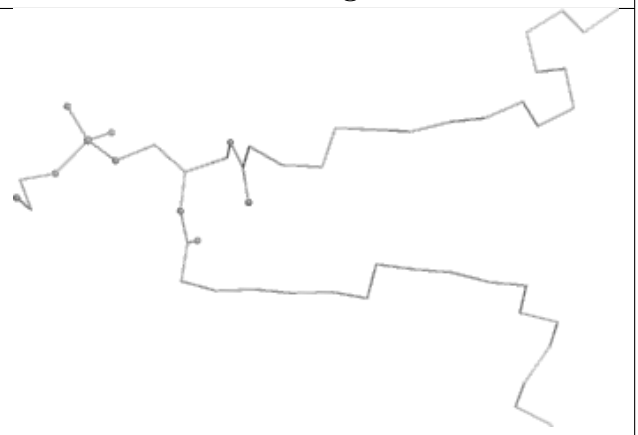

Rings

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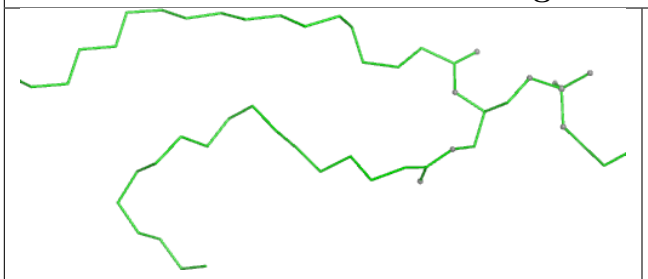

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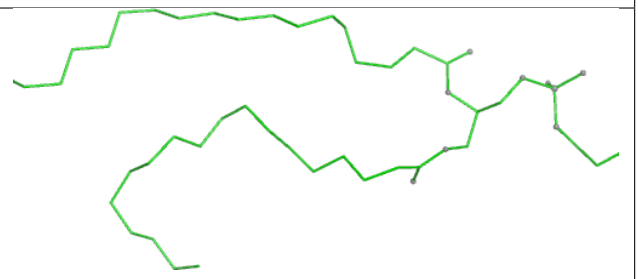

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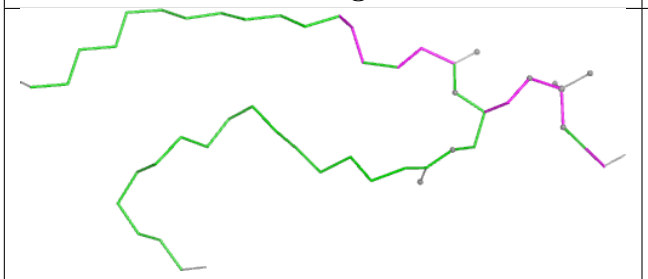

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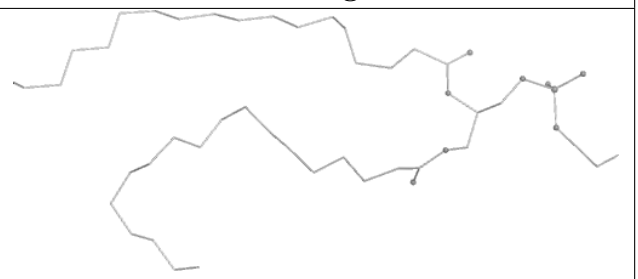
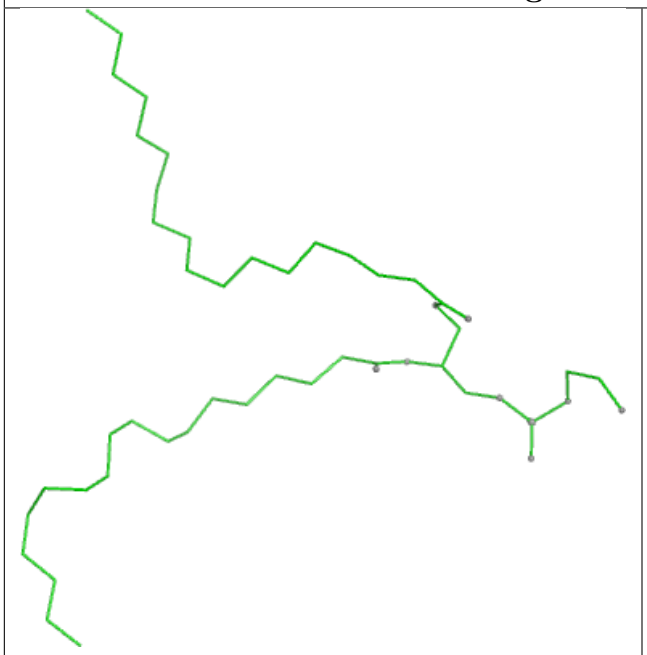


Rings

Ligand 3PE M 703



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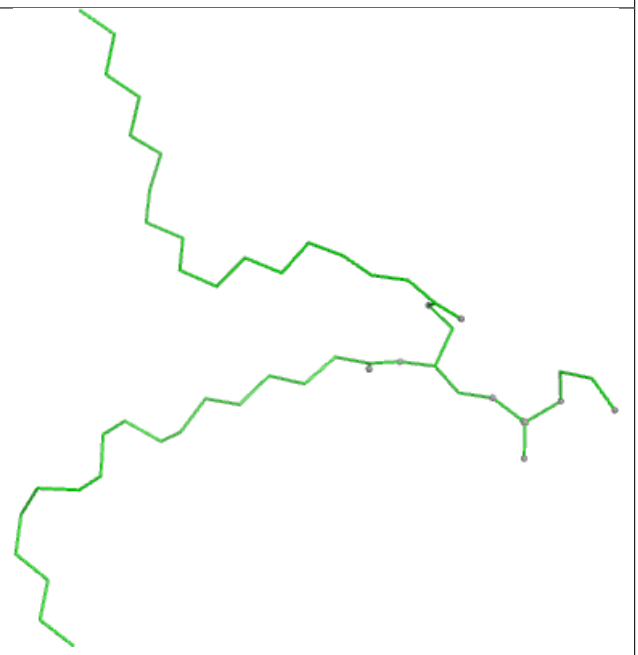

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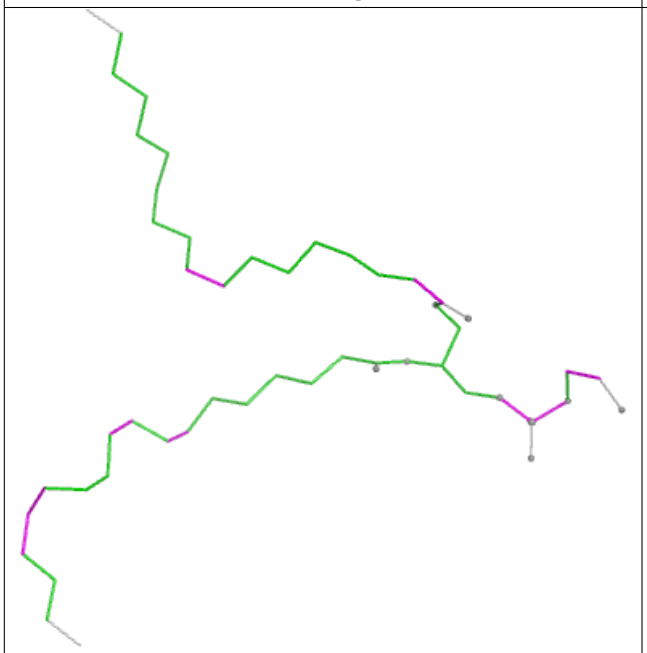

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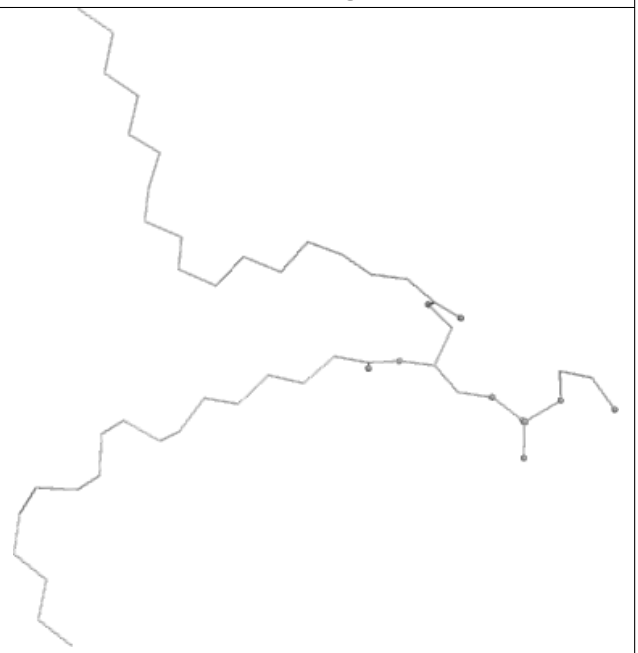
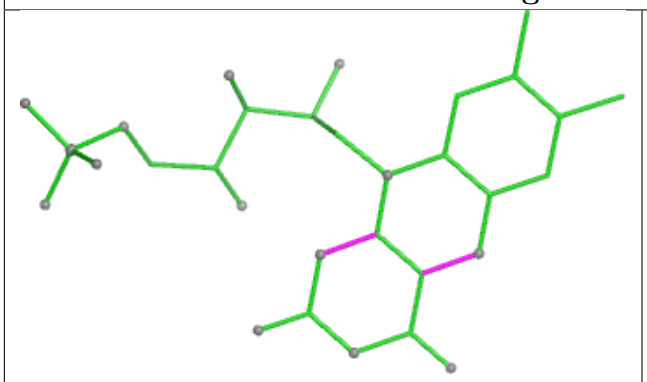
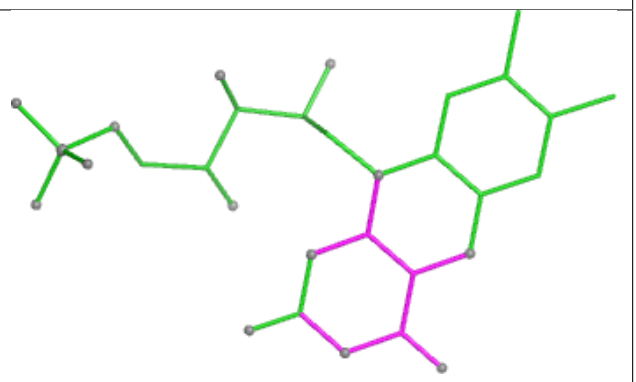


Rings

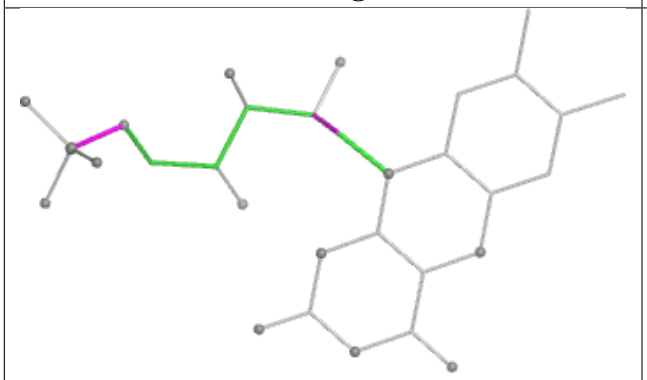
Ligand FMN F 502



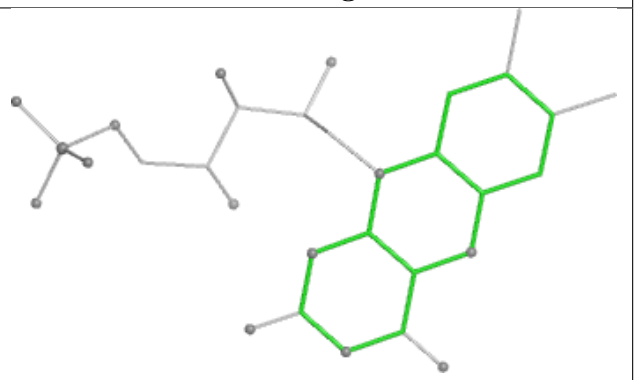
Bond lengths



Bond angles

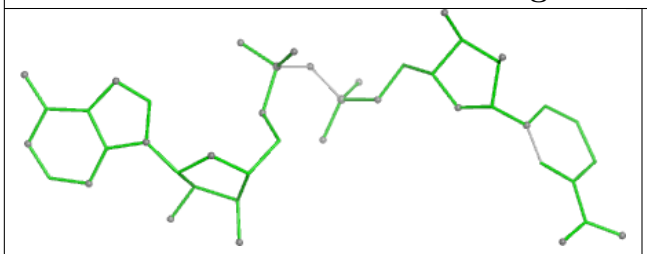


Torsions

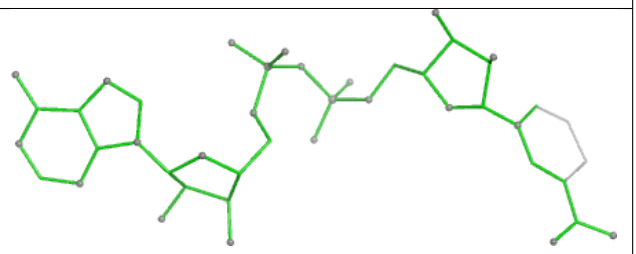


Rings

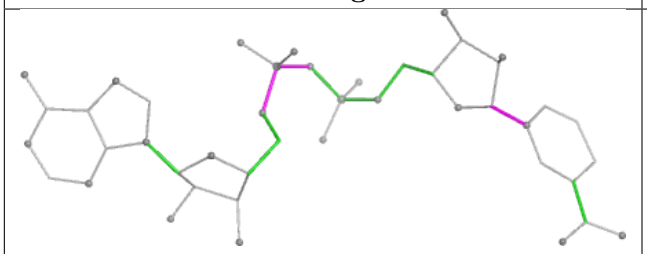
Ligand NAI F 503



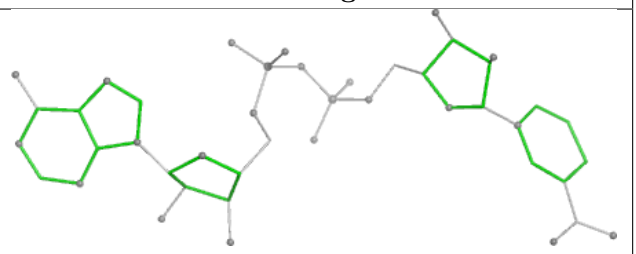
Bond lengths



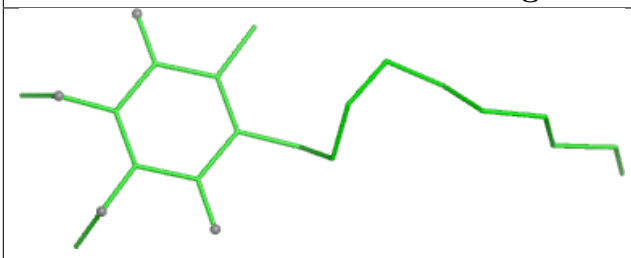
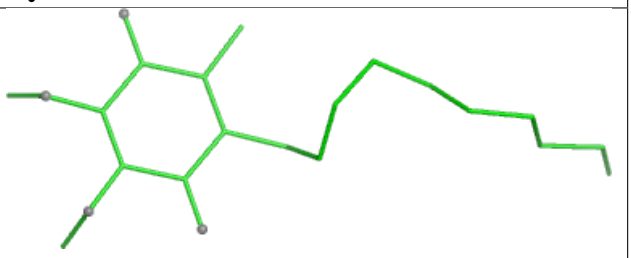
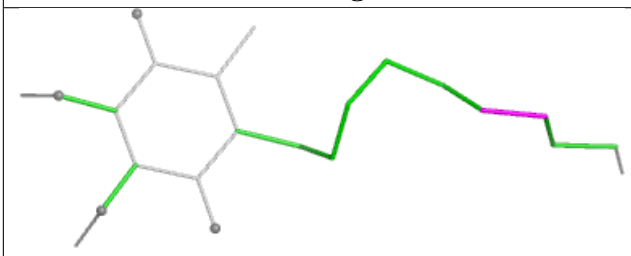
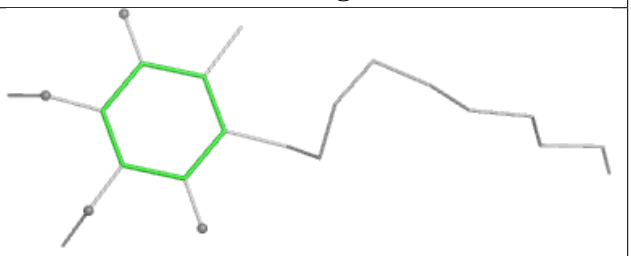
Bond angles



Torsions



Rings

Ligand DCQ B 302	
 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.

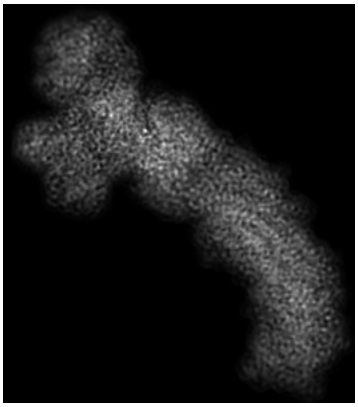
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13217. These allow visual inspection of the internal detail of the map and identification of artifacts.

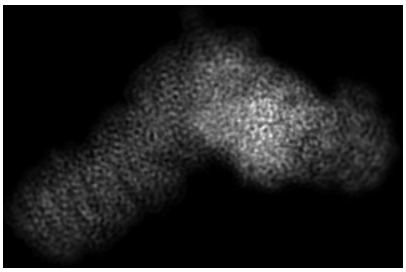
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

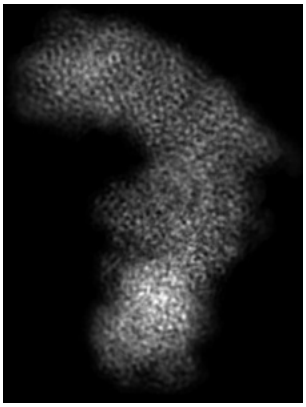
6.1.1 Primary map



X



Y



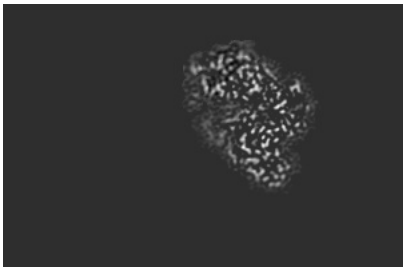
Z

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

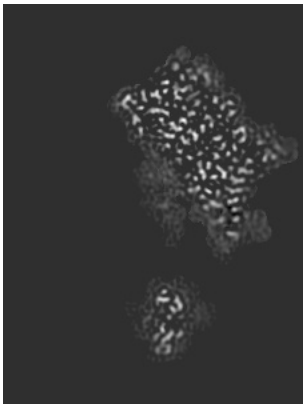
6.2 Central slices (i)

6.2.1 Primary map

X Index: 157



Y Index: 210



Z Index: 240

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: 168

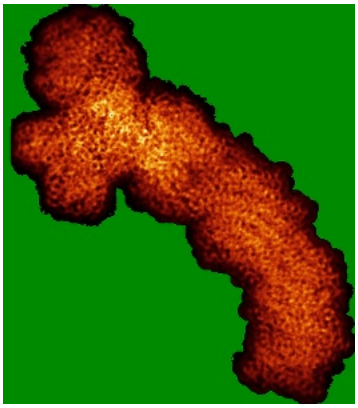
Y Index: 129

Z Index: 320

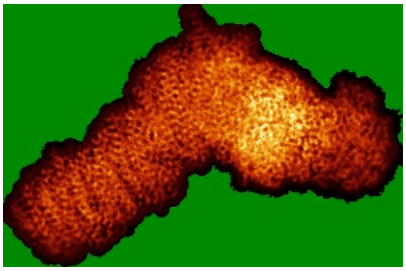
The images above show the largest variance slices of the map in three orthogonal directions.

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

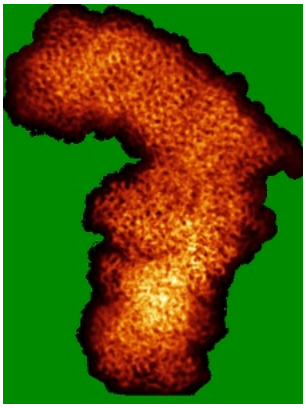
6.4.1 Primary map



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

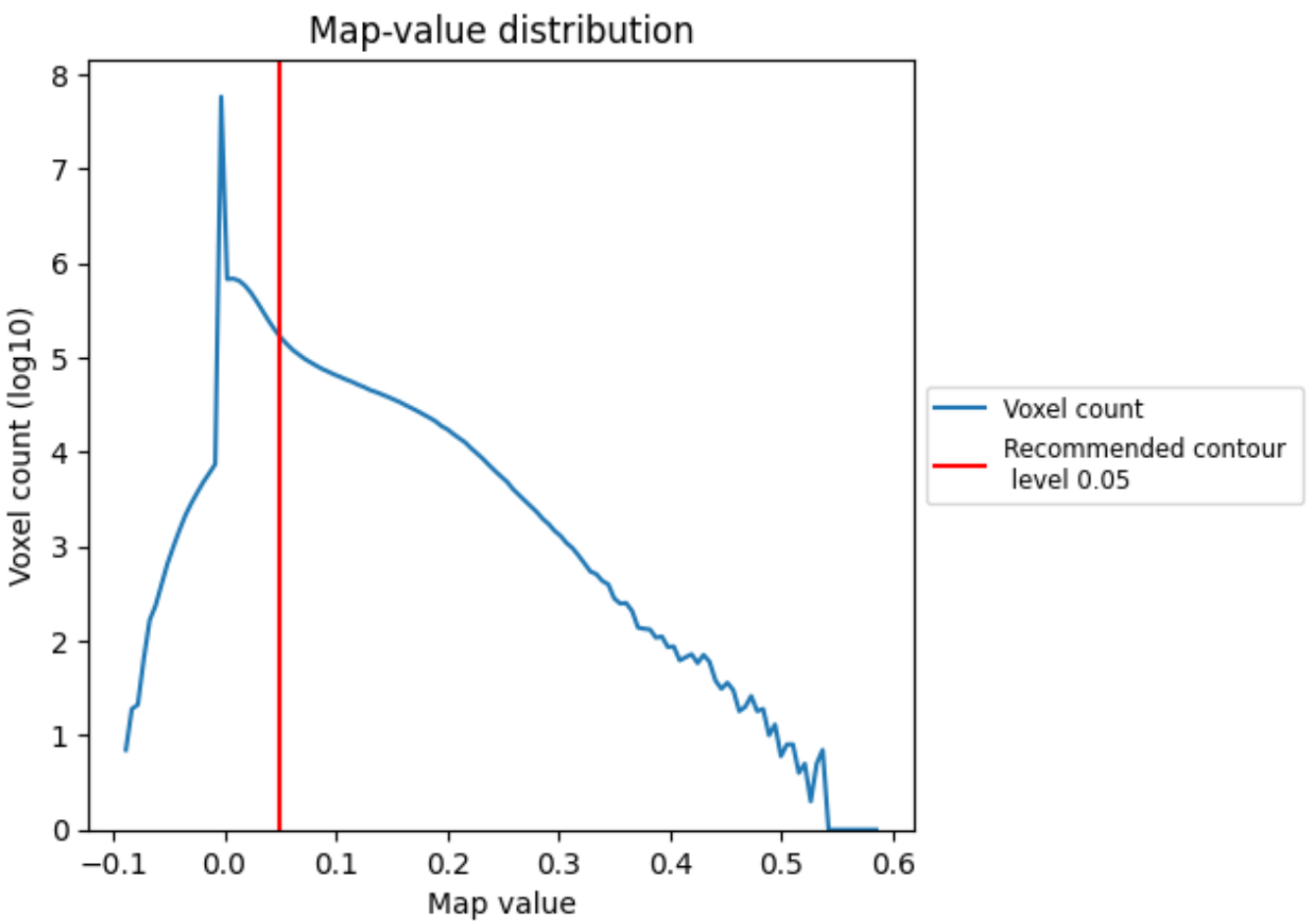
6.6 Mask visualisation (i)

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

7 Map analysis (i)

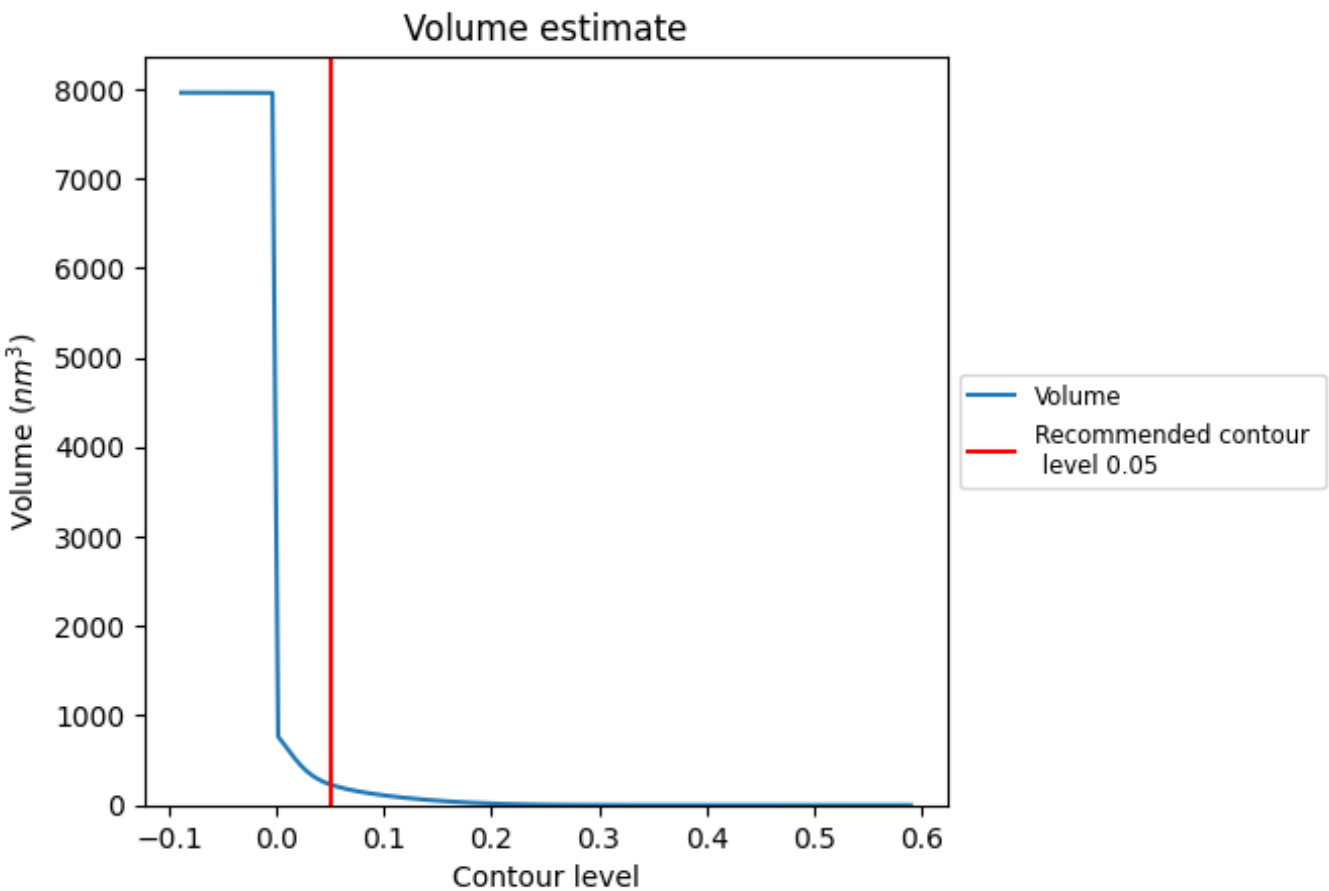
This section contains the results of statistical analysis of the map.

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 232 nm^3; this corresponds to an approximate mass of 210 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.

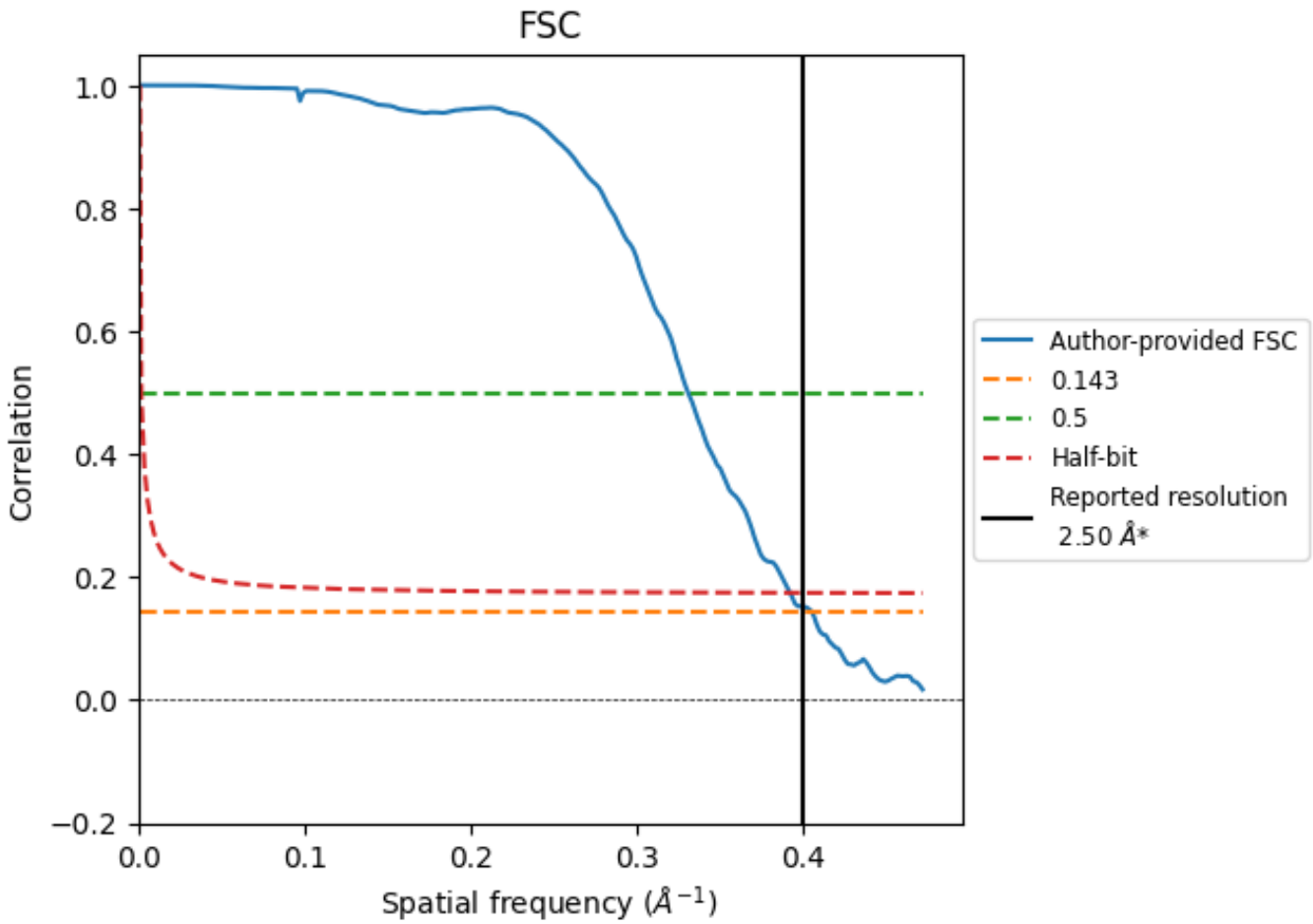
7.3 Rotationally averaged power spectrum (i)

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 0.400 Å^{-1}

8.2 Resolution estimates (i)

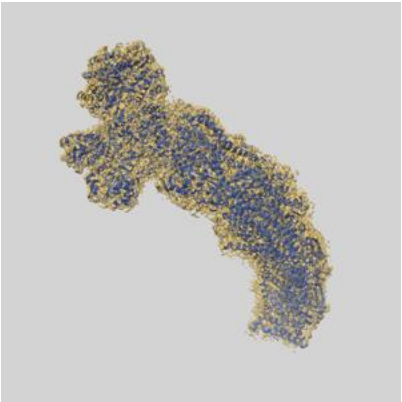
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.47	3.02	2.55
Unmasked-calculated*	-	-	-

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

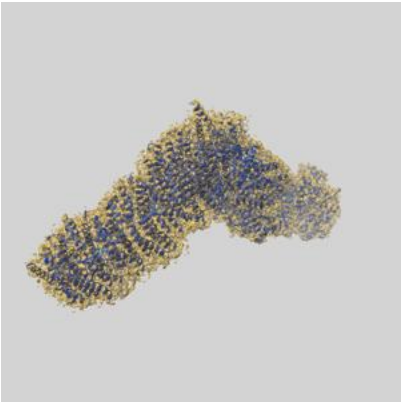
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13217 and PDB model 7P64. Per-residue inclusion information can be found in section 3 on page 13.

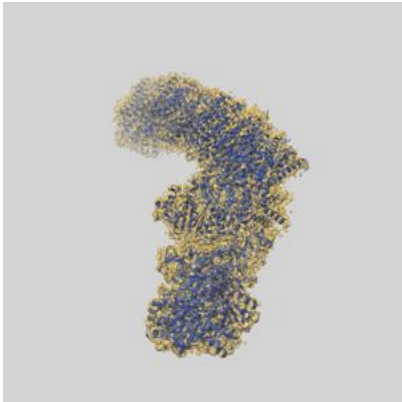
9.1 Map-model overlay (i)



X



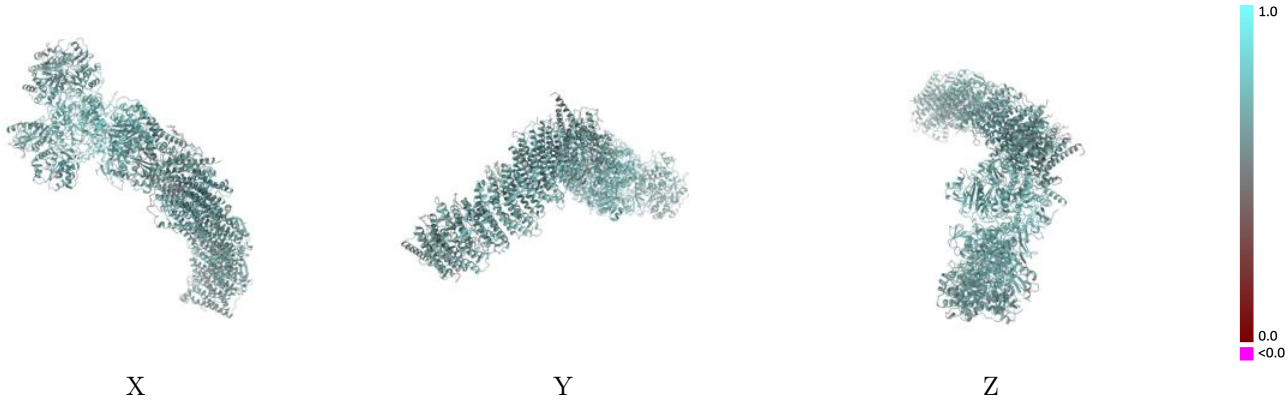
Y



Z

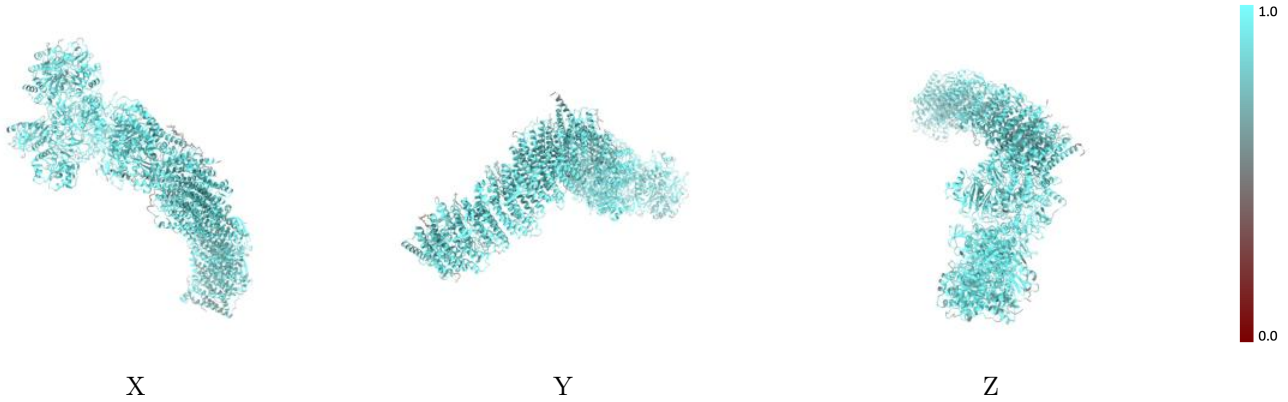
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



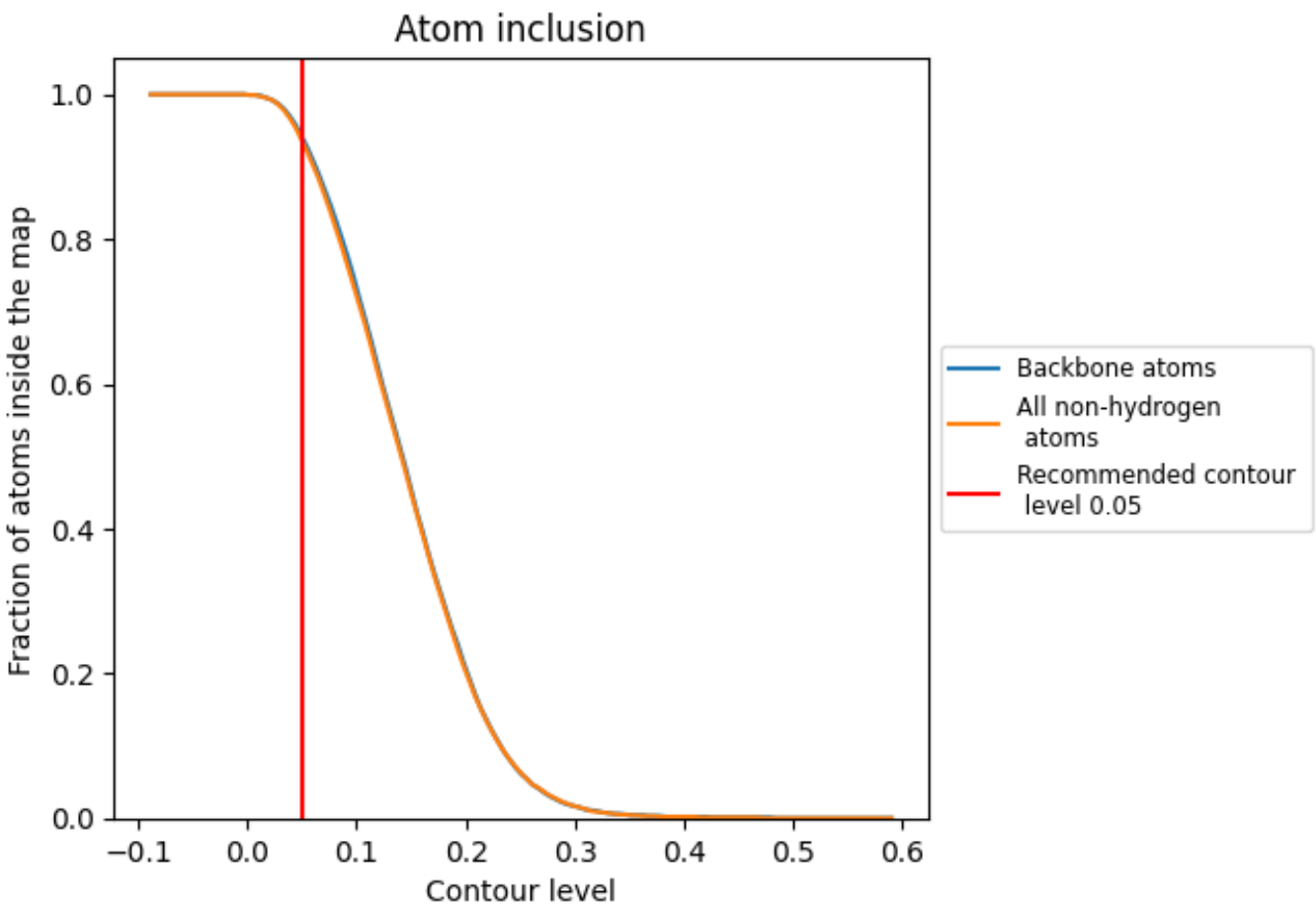
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9360	0.6660
A	0.9260	0.6410
B	0.9480	0.6920
C	0.9540	0.6970
E	0.9090	0.6350
F	0.9080	0.6330
G	0.9610	0.6980
H	0.9210	0.6300
I	0.9350	0.7000
J	0.9170	0.6460
K	0.9800	0.6950
L	0.9020	0.6240
M	0.9480	0.6590
N	0.9540	0.6740