wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 02:32 am GMT

PDB ID	:	6TT7
EMDB ID	:	EMD-10573
Title	:	Ovine ATP synthase 1a state
Authors	:	Pinke, G.; Zhou, L.; Sazanov, L.A.
Deposited on	:	2019-12-23
Resolution	:	3.50 Å(reported)
Based on initial model	:	5ARA

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

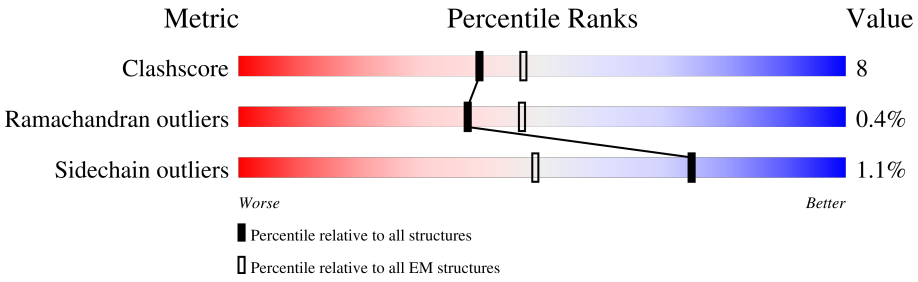
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 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)
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	A	553	72% 18% • 8%
1	B	553	71% 16% 12%
1	C	553	6% 71% 20% • 9%
2	D	528	66% 21% • 11%
2	E	528	65% 22% • 12%
2	F	528	70% 18% • 11%
3	G	298	5% 74% 16% • 9%
4	H	168	54% 24% •• 21%

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Mol	Chain	Length	Quality of chain
5	I	51	10% 82% 10% 8%
6	J	213	69% 19% 12%
7	K	256	71% 11% 19%
8	L	108	6% 51% 12% 36%
9	M	161	14% 88% 9%
10	1	136	6% 46% 8% 46%
10	2	136	50% 46%
10	3	136	45% 10% 46%
10	4	136	51% 46%
10	5	136	7% 49% 5% 46%
10	6	136	47% 7% 46%
10	7	136	47% 7% 46%
10	8	136	9% 46% 8% 46%
11	N	226	80% 19%
12	O	58	28% 55% 14% 31%
13	P	60	20% 77% 10% 13%
14	Q	66	9% 64% 8% 29%
15	R	88	5% 75% 19% 5%
16	S	103	11% 66% 17% 17%
17	T	71	41% 82% 15%

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
22	CDL	R	301	X	-	-	-
22	CDL	R	302	X	-	-	-
22	CDL	R	303	X	-	-	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 40337 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	488	Total	C	N	O	S	0	0
			3724	2347	657	708	12		
1	C	503	Total	C	N	O	S	0	0
			3834	2414	675	733	12		
1	A	507	Total	C	N	O	S	0	0
			3860	2429	679	740	12		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	467	Total	C	N	O	S	0	0
			3536	2242	601	682	11		
2	D	469	Total	C	N	O	S	0	0
			3544	2246	603	684	11		
2	F	472	Total	C	N	O	S	0	0
			3570	2260	608	691	11		

- Molecule 3 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	272	Total	C	N	O	S	0	0
			2115	1330	368	409	8		

- Molecule 4 is a protein called ATP synthase F1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	132	Total	C	N	O	S	0	0
			978	613	165	198	2		

- Molecule 5 is a protein called ATP synthase F1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	47	Total	C	N	O	S	0	0
			368	236	66	64	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	10	LEU	VAL	conflict	UNP W5Q3H8

- Molecule 6 is a protein called ATP synthase peripheral stalk subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	188	Total	C	N	O	S	0	0
			1452	922	251	269	10		

- Molecule 7 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	208	Total	C	N	O	S	0	0
			1689	1089	289	305	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	58	PHE	ALA	conflict	UNP W5QEA9

- Molecule 8 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	69	Total	C	N	O	S	0	0
			576	366	97	111	2		

- Molecule 9 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	156	Total	C	N	O	S	0	0
			1284	829	209	243	3		

- Molecule 10 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	74	Total	C	N	O	S	0	0
			526	348	82	93	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	2	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	3	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	4	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	5	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	6	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	7	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	8	74	Total	C	N	O	S	0	0
			526	348	82	93	3		

- Molecule 11 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	225	Total	C	N	O	S	0	0
			1734	1150	277	295	12		

- Molecule 12 is a protein called Subunit DAPIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	40	Total	C	N	O	S	0	0
			327	219	53	53	2		

- Molecule 13 is a protein called ATP synthase membrane subunit 6.8PL.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	52	Total	C	N	O	S	0	0
			425	281	70	71	3		

- Molecule 14 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	47	Total	C	N	O	S	0	0
			371	248	58	62	3		

- Molecule 15 is a protein called ATP synthase membrane subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	84	Total 701	C 461	N 121	O 116	S 3	0	0

- Molecule 16 is a protein called ATP synthase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	85	Total 673	C 448	N 106	O 118	S 1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	96	ARG	HIS	conflict	UNP W5Q5U7
S	99	ILE	THR	conflict	UNP W5Q5U7

- Molecule 17 is a protein called Subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	70	Total 577	C 364	N 106	O 106	S 1	0	0

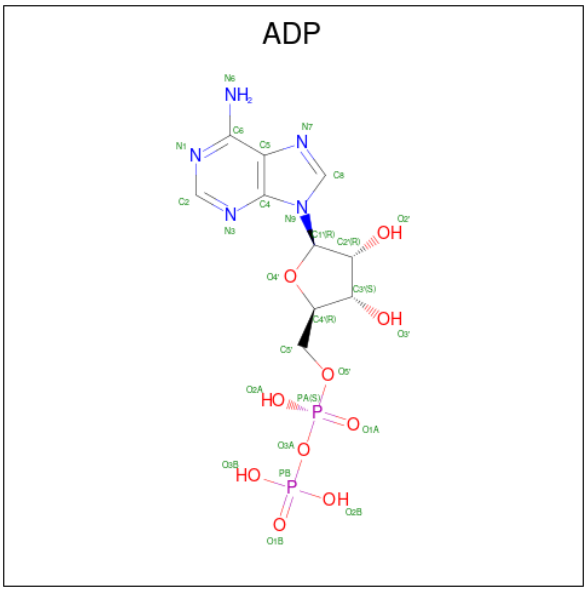
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	23	MET	VAL	conflict	UNP W5PF18
T	26	GLY	SER	conflict	UNP W5PF18
T	38	GLU	-	insertion	UNP W5PF18

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

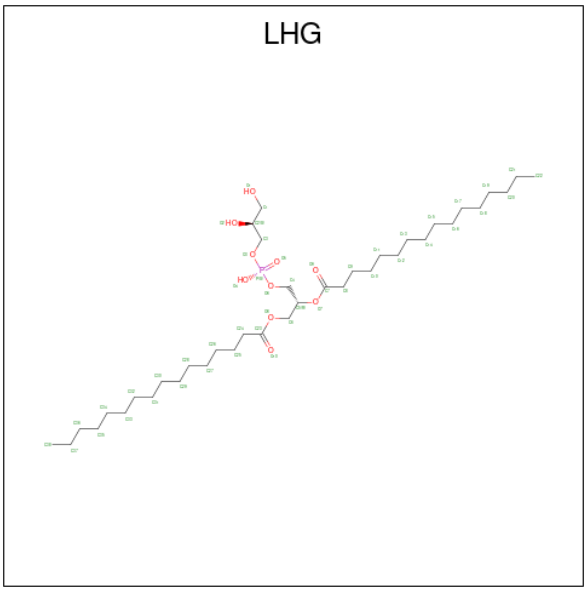
Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total 1	Mg 1	0
18	C	1	Total 1	Mg 1	0
18	A	1	Total 1	Mg 1	0

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



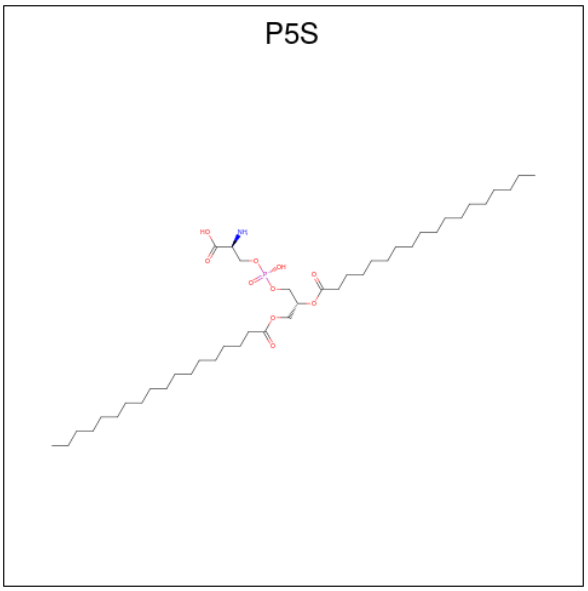
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



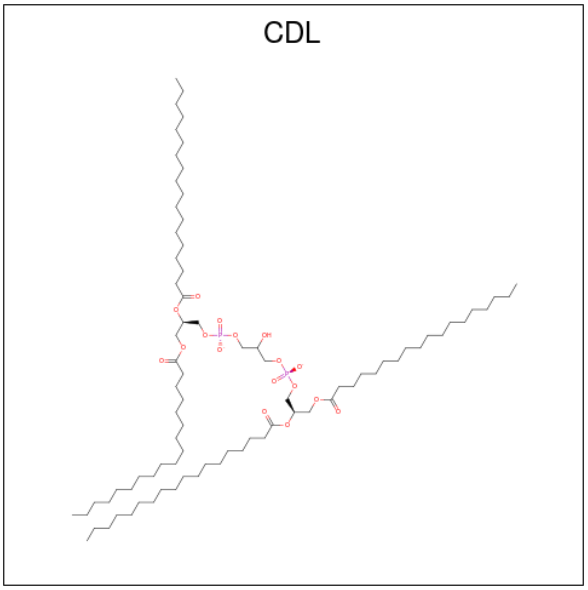
Mol	Chain	Residues	Atoms				AltConf
20	K	1	Total	C	O	P	0
			92	70	20	2	
20	K	1	Total	C	O	P	0
			92	70	20	2	
20	2	1	Total	C	O	P	0
			45	34	10	1	
20	R	1	Total	C	O	P	0
			49	38	10	1	
20	S	1	Total	C	O	P	0
			98	76	20	2	
20	S	1	Total	C	O	P	0
			98	76	20	2	

- Molecule 21 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



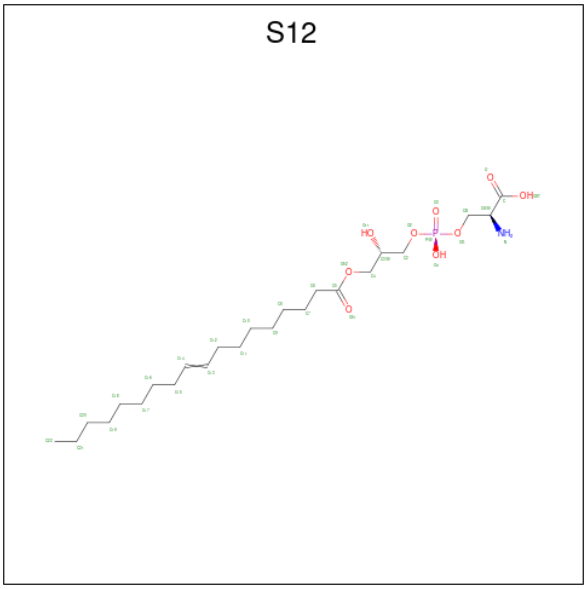
Mol	Chain	Residues	Atoms					AltConf
21	2	1	Total	C	N	O	P	0
			54	42	1	10	1	

- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
22	R	1	Total	C	O	P	0
			280	223	51	6	
22	R	1	Total	C	O	P	0
			280	223	51	6	
22	R	1	Total	C	O	P	0
			280	223	51	6	

- Molecule 23 is O-[(S)-hydroxy{[(2S)-2-hydroxy-3-(octadec-9-enoyloxy)propyl]oxy}phosphoryl]-L-serine (three-letter code: S12) (formula: $C_{24}H_{46}NO_9P$).



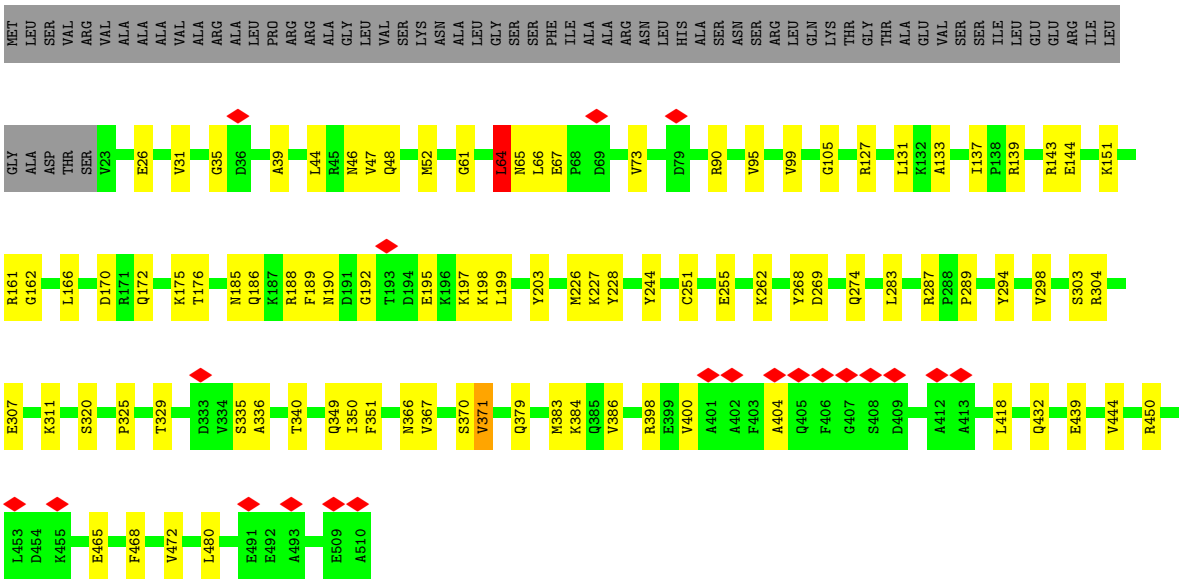
Mol	Chain	Residues	Atoms					AltConf
23	T	1	Total	C	N	O	P	0
			35	24	1	9	1	

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.

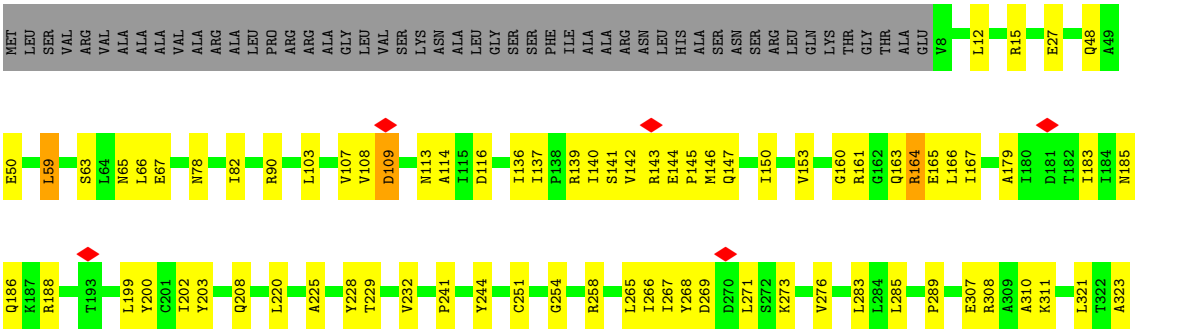
• Molecule 1: ATP synthase subunit alpha

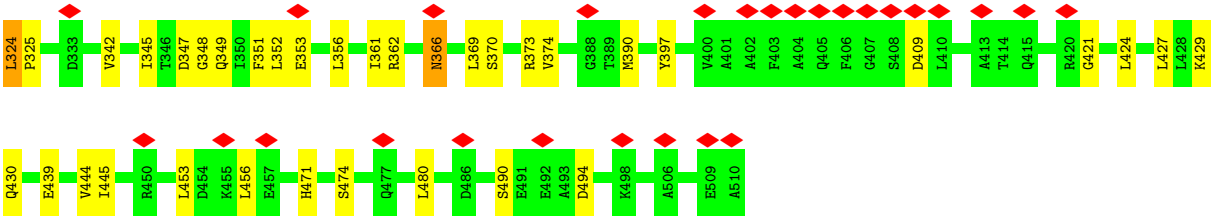
Chain B:



• Molecule 1: ATP synthase subunit alpha

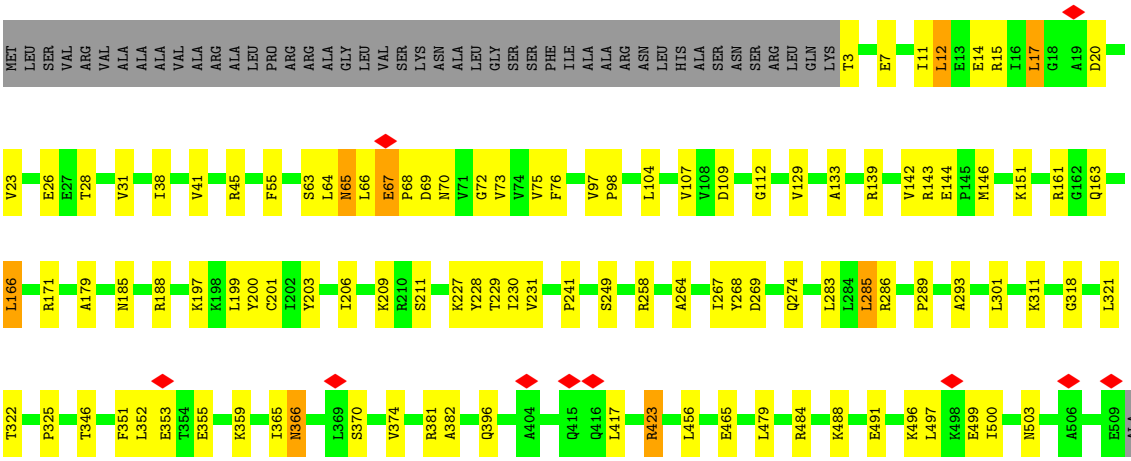
Chain C:





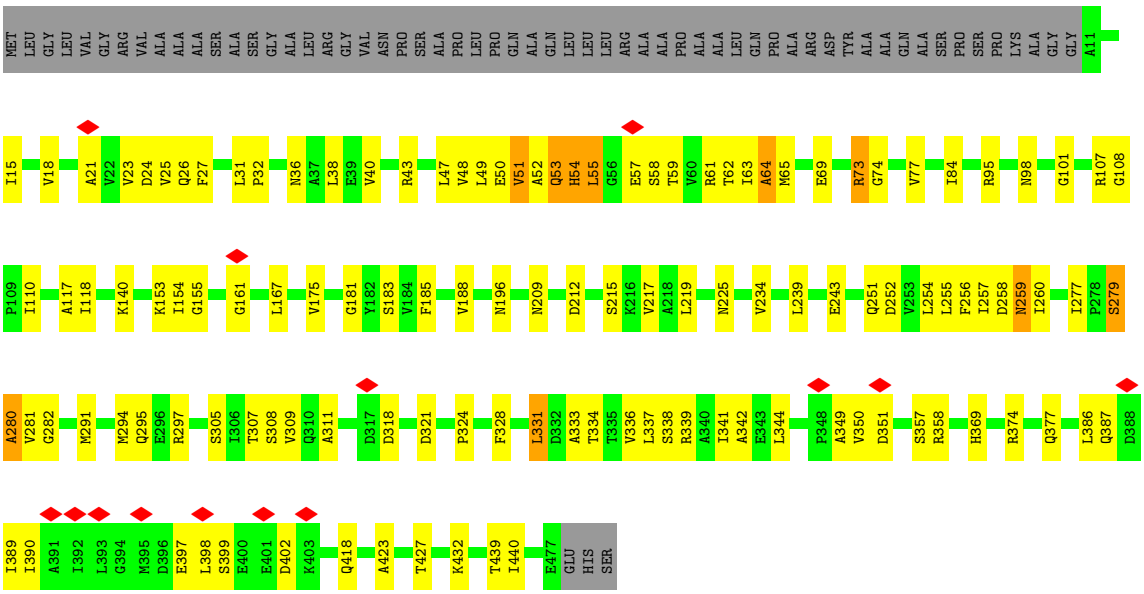
• Molecule 1: ATP synthase subunit alpha

Chain A:



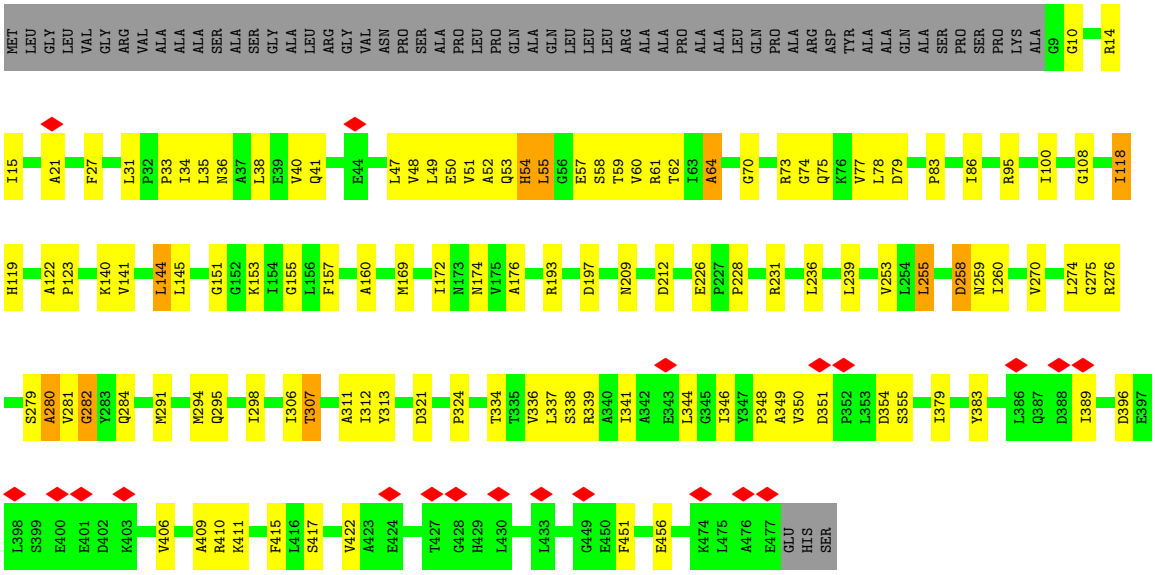
• Molecule 2: ATP synthase subunit beta

Chain E:



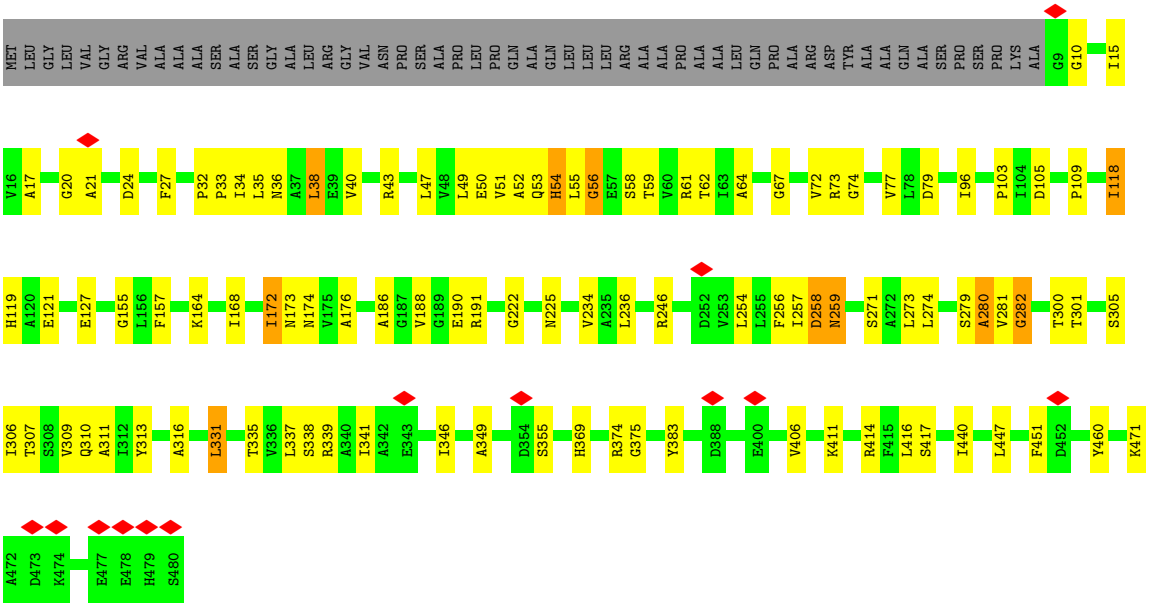
• Molecule 2: ATP synthase subunit beta

Chain D:



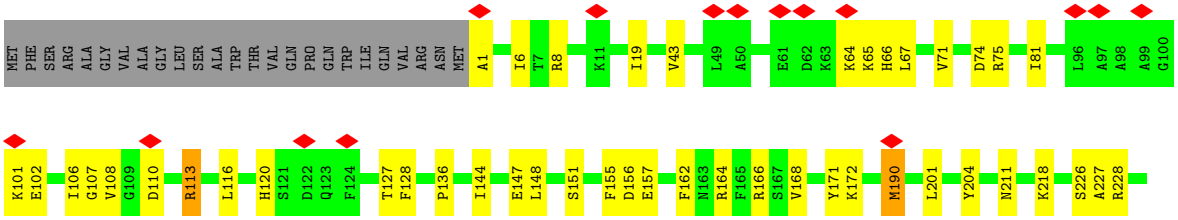
• Molecule 2: ATP synthase subunit beta

Chain F:



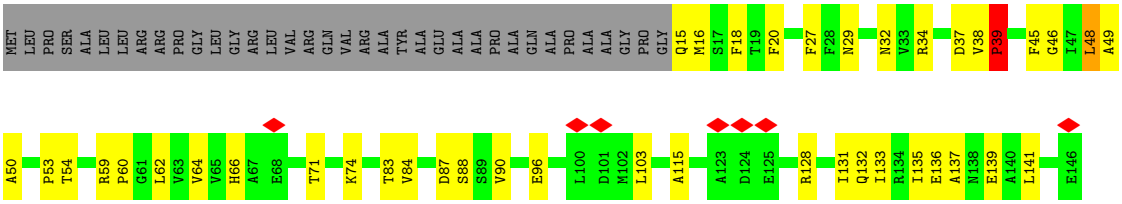
• Molecule 3: ATP synthase subunit gamma

Chain G:



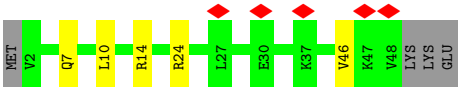
• Molecule 4: ATP synthase F1 subunit delta

Chain H:



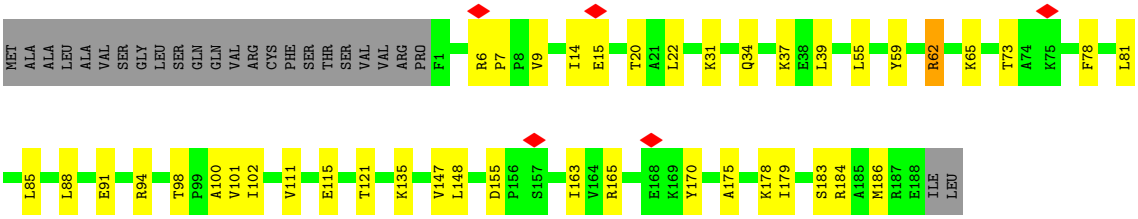
• Molecule 5: ATP synthase F1 subunit epsilon

Chain I:



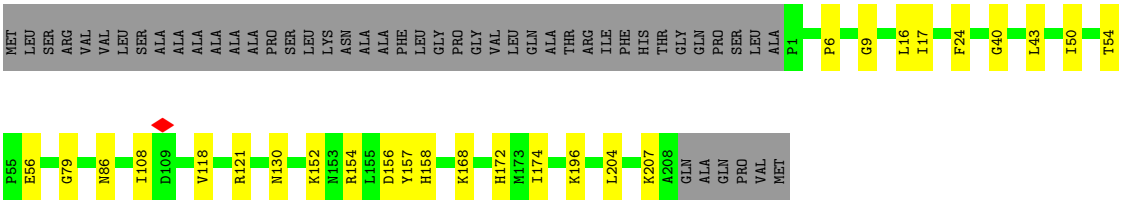
• Molecule 6: ATP synthase peripheral stalk subunit OSCP

Chain J:



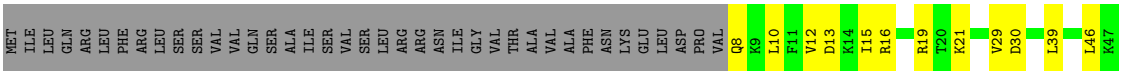
• Molecule 7: ATP synthase subunit b

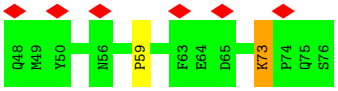
Chain K:



• Molecule 8: ATP synthase-coupling factor 6, mitochondrial

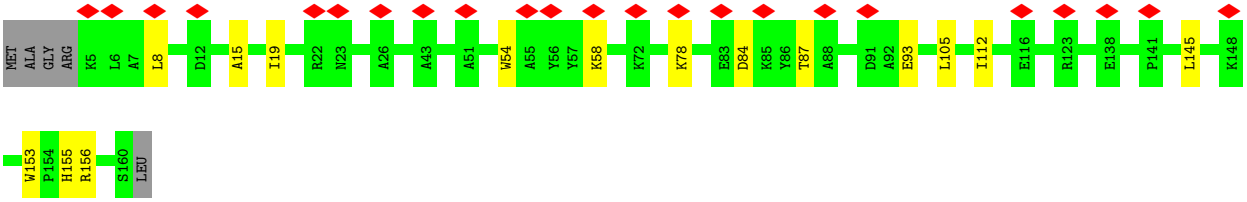
Chain L:





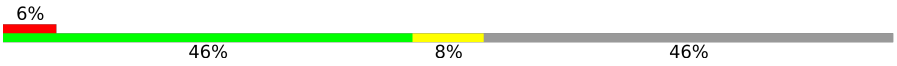
• Molecule 9: ATP synthase subunit d, mitochondrial

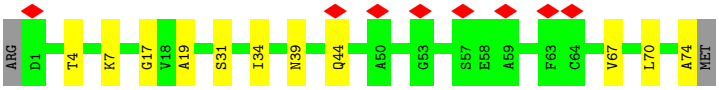
Chain M:



• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

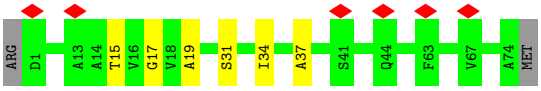
Chain 1:





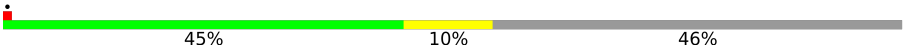
• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 2:



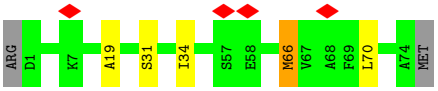
• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 3:



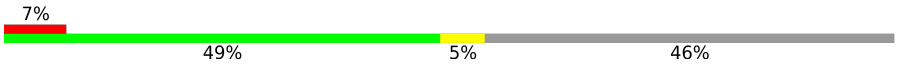
• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

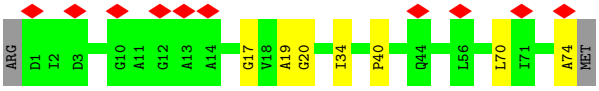
Chain 4:



• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

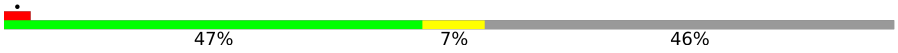
Chain 5:

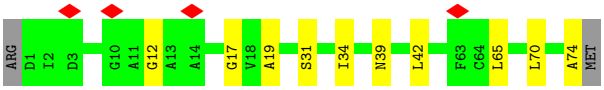




• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

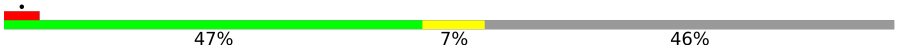
Chain 6:

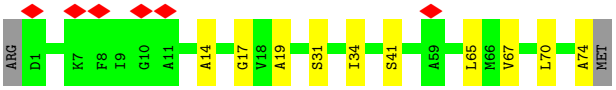




• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

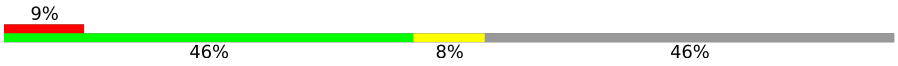
Chain 7:

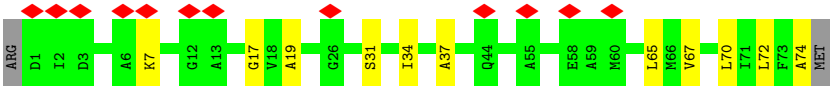




• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

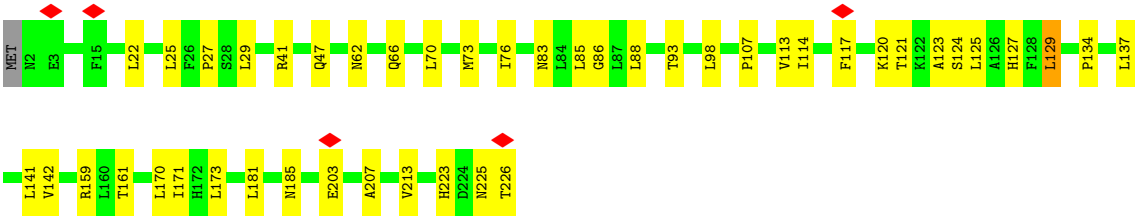
Chain 8:



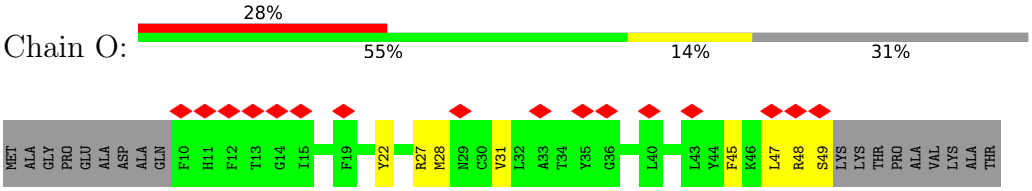


• Molecule 11: ATP synthase subunit a

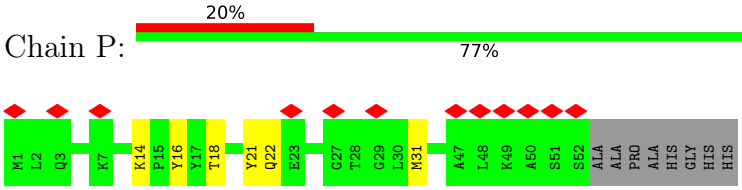
Chain N:



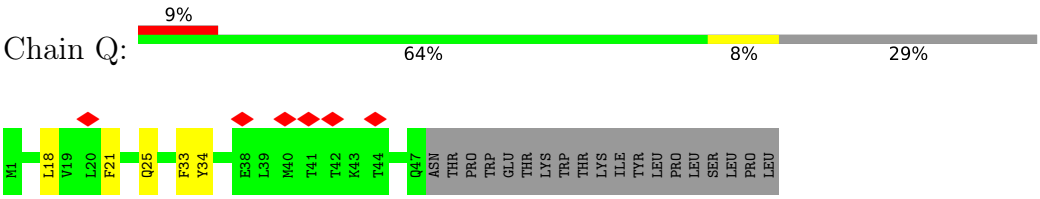
• Molecule 12: Subunit DAPIT



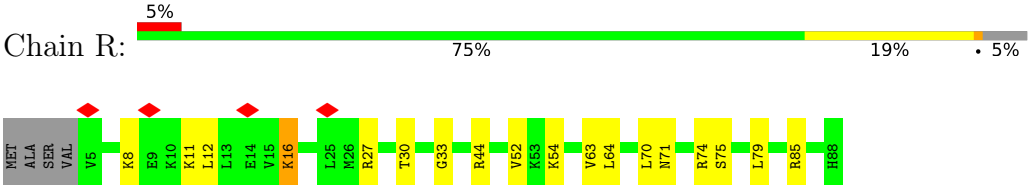
• Molecule 13: ATP synthase membrane subunit 6.8PL



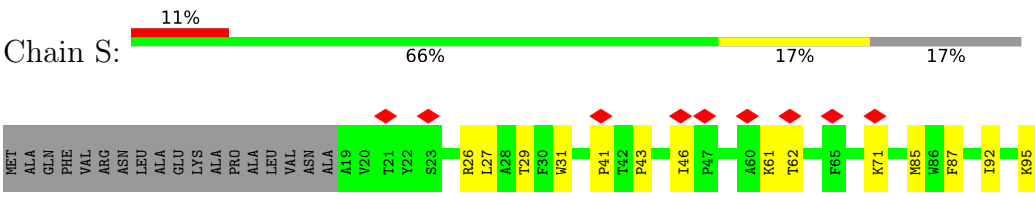
• Molecule 14: ATP synthase protein 8



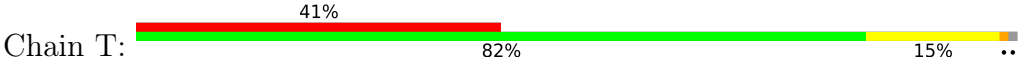
• Molecule 15: ATP synthase membrane subunit f

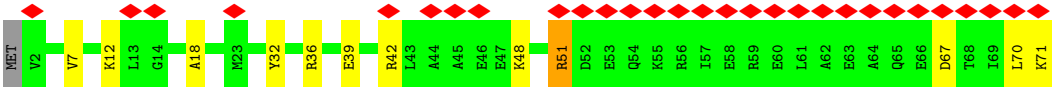


• Molecule 16: ATP synthase subunit



• Molecule 17: Subunit e




MET
V2
V7
K12
L13
G14
A18
M23
Y32
R36
E39
R42
L43
A44
A45
E46
E47
K48
R51
D52
E53
Q54
K55
R56
I57
E58
R59
E60
L61
A62
E63
A64
Q65
E66
D67
T68
I69
L70
K71

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35000	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 ($e^-/Å^2$)	106	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	131951	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	146.418, 147.479, 244.03	wwPDB
Map dimensions	230, 139, 138	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	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: CDL, ADP, LHG, P5S, MG, S12

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	A	0.40	0/3911	0.70	3/5278 (0.1%)
1	B	0.42	0/3775	0.68	3/5092 (0.1%)
1	C	0.46	1/3885 (0.0%)	0.73	6/5241 (0.1%)
2	D	0.40	0/3601	0.68	3/4884 (0.1%)
2	E	0.41	0/3593	0.68	1/4874 (0.0%)
2	F	0.42	0/3628	0.71	6/4919 (0.1%)
3	G	0.34	0/2141	0.62	1/2876 (0.0%)
4	H	0.36	0/990	0.70	0/1346
5	I	0.30	0/373	0.52	0/499
6	J	0.35	0/1470	0.63	0/1977
7	K	0.32	0/1722	0.56	0/2321
8	L	0.32	0/589	0.64	1/788 (0.1%)
9	M	0.29	0/1315	0.54	0/1781
10	1	0.35	0/535	0.58	0/722
10	2	0.37	0/535	0.60	0/722
10	3	0.38	0/535	0.63	0/722
10	4	0.36	0/535	0.60	0/722
10	5	0.36	0/535	0.56	0/722
10	6	0.36	0/535	0.58	0/722
10	7	0.34	0/535	0.58	0/722
10	8	0.36	0/535	0.58	0/722
11	N	0.33	0/1772	0.65	1/2421 (0.0%)
12	O	0.29	0/335	0.54	0/450
13	P	0.33	0/435	0.57	0/585
14	Q	0.33	0/381	0.62	0/518
15	R	0.35	0/719	0.56	0/963
16	S	0.30	0/691	0.55	0/940
17	T	0.30	0/585	0.66	1/780 (0.1%)
All	All	0.38	1/40191 (0.0%)	0.66	26/54309 (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
1	A	0	5
1	B	0	4
1	C	0	3
2	D	0	7
2	E	0	6
2	F	0	6
4	H	0	1
All	All	0	32

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	143	ARG	C-N	12.02	1.61	1.34

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	143	ARG	C-N-CA	-10.64	95.09	121.70
1	C	271	LEU	CA-CB-CG	7.36	132.23	115.30
1	B	143	ARG	C-N-CA	-7.26	103.56	121.70
3	G	156	ASP	CB-CG-OD1	7.19	124.78	118.30
2	F	49	LEU	CA-CB-CG	6.60	130.49	115.30

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162	GLY	Peptide
1	B	227	LYS	Peptide
1	B	371	VAL	Peptide
1	B	64	LEU	Peptide
1	C	109	ASP	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	A	3860	0	3961	66	0
1	B	3724	0	3825	55	0
1	C	3834	0	3937	75	0
2	D	3544	0	3597	77	0
2	E	3536	0	3591	85	0
2	F	3570	0	3615	73	0
3	G	2115	0	2185	33	0
4	H	978	0	976	27	0
5	I	368	0	390	4	0
6	J	1452	0	1557	28	0
7	K	1689	0	1739	22	0
8	L	576	0	560	10	0
9	M	1284	0	1292	13	0
10	1	526	0	544	8	0
10	2	526	0	544	5	0
10	3	526	0	544	10	0
10	4	526	0	544	6	0
10	5	526	0	544	6	0
10	6	526	0	544	9	0
10	7	526	0	544	8	0
10	8	526	0	544	9	0
11	N	1734	0	1856	33	0
12	O	327	0	337	6	0
13	P	425	0	455	6	0
14	Q	371	0	357	6	0
15	R	701	0	726	15	0
16	S	673	0	701	13	0
17	T	577	0	601	7	0
18	A	1	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
19	A	27	0	12	0	0
19	B	27	0	12	2	0
19	C	27	0	12	1	0
19	D	27	0	12	0	0
19	F	27	0	12	1	0
20	2	45	0	63	0	0
20	K	92	0	133	3	0
20	R	49	0	74	2	0
20	S	98	0	148	5	0
21	2	54	0	80	2	0
22	R	280	0	422	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	T	35	0	44	1	0
All	All	40337	0	41634	634	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 8.

The worst 5 of 634 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)
2:D:259:ASN:HA	2:D:311:ALA:O	1.38	1.22
2:F:259:ASN:HA	2:F:311:ALA:O	1.52	1.07
2:D:338:SER:O	2:D:349:ALA:HB3	1.54	1.05
2:F:338:SER:O	2:F:349:ALA:HB3	1.54	1.04
1:B:199:LEU:O	1:B:228:TYR:HB3	1.59	1.02

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	A	505/553 (91%)	457 (90%)	46 (9%)	2 (0%)	34 72
1	B	486/553 (88%)	448 (92%)	37 (8%)	1 (0%)	47 81
1	C	501/553 (91%)	456 (91%)	45 (9%)	0	100 100
2	D	467/528 (88%)	420 (90%)	42 (9%)	5 (1%)	14 52
2	E	465/528 (88%)	425 (91%)	33 (7%)	7 (2%)	10 45
2	F	470/528 (89%)	433 (92%)	34 (7%)	3 (1%)	25 64
3	G	270/298 (91%)	256 (95%)	14 (5%)	0	100 100
4	H	130/168 (77%)	119 (92%)	10 (8%)	1 (1%)	19 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	45/51 (88%)	43 (96%)	2 (4%)	0	100	100
6	J	186/213 (87%)	175 (94%)	10 (5%)	1 (0%)	29	68
7	K	206/256 (80%)	193 (94%)	13 (6%)	0	100	100
8	L	67/108 (62%)	60 (90%)	7 (10%)	0	100	100
9	M	154/161 (96%)	150 (97%)	4 (3%)	0	100	100
10	1	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	2	72/136 (53%)	72 (100%)	0	0	100	100
10	3	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	4	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
10	5	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
10	6	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	7	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	8	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
11	N	223/226 (99%)	212 (95%)	11 (5%)	0	100	100
12	O	38/58 (66%)	37 (97%)	1 (3%)	0	100	100
13	P	50/60 (83%)	49 (98%)	1 (2%)	0	100	100
14	Q	45/66 (68%)	42 (93%)	3 (7%)	0	100	100
15	R	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
16	S	83/103 (81%)	78 (94%)	5 (6%)	0	100	100
17	T	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	5117/6258 (82%)	4767 (93%)	330 (6%)	20 (0%)	38	72

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	53	GLN
2	E	259	ASN
2	E	280	ALA
2	E	281	VAL
2	D	281	VAL

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	A	410/443 (93%)	403 (98%)	7 (2%)	60	82
1	B	394/443 (89%)	390 (99%)	4 (1%)	76	88
1	C	407/443 (92%)	405 (100%)	2 (0%)	88	94
2	D	376/415 (91%)	372 (99%)	4 (1%)	73	88
2	E	376/415 (91%)	373 (99%)	3 (1%)	81	91
2	F	379/415 (91%)	374 (99%)	5 (1%)	69	86
3	G	230/251 (92%)	225 (98%)	5 (2%)	52	78
4	H	104/127 (82%)	99 (95%)	5 (5%)	25	60
5	I	38/42 (90%)	38 (100%)	0	100	100
6	J	164/185 (89%)	163 (99%)	1 (1%)	86	94
7	K	184/218 (84%)	183 (100%)	1 (0%)	88	94
8	L	63/98 (64%)	60 (95%)	3 (5%)	25	60
9	M	141/144 (98%)	140 (99%)	1 (1%)	84	93
10	1	50/105 (48%)	50 (100%)	0	100	100
10	2	50/105 (48%)	50 (100%)	0	100	100
10	3	50/105 (48%)	49 (98%)	1 (2%)	55	79
10	4	50/105 (48%)	49 (98%)	1 (2%)	55	79
10	5	50/105 (48%)	50 (100%)	0	100	100
10	6	50/105 (48%)	50 (100%)	0	100	100
10	7	50/105 (48%)	50 (100%)	0	100	100
10	8	50/105 (48%)	50 (100%)	0	100	100
11	N	197/198 (100%)	196 (100%)	1 (0%)	88	94
12	O	35/47 (74%)	35 (100%)	0	100	100
13	P	45/49 (92%)	45 (100%)	0	100	100
14	Q	39/66 (59%)	39 (100%)	0	100	100
15	R	73/76 (96%)	71 (97%)	2 (3%)	44	73
16	S	71/84 (84%)	71 (100%)	0	100	100
17	T	59/60 (98%)	58 (98%)	1 (2%)	60	82
All	All	4185/5059 (83%)	4138 (99%)	47 (1%)	74	88

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	190	MET
6	J	184	ARG
3	G	211	ASN
4	H	48	LEU
8	L	19	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	15	GLN
7	K	86	ASN
14	Q	31	HIS
7	K	145	HIS
5	I	7	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 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\#\|Z\|>2$
20	LHG	R	304	-	48,48,48	0.65	1 (2%)	51,54,54	1.24	6 (11%)
20	LHG	S	202	-	48,48,48	0.62	1 (2%)	51,54,54	1.23	6 (11%)
20	LHG	K	301	-	42,42,48	0.65	0	45,48,54	1.22	4 (8%)
19	ADP	C	602	18	24,29,29	0.94	1 (4%)	29,45,45	1.46	4 (13%)
20	LHG	S	201	-	48,48,48	0.66	1 (2%)	51,54,54	1.25	6 (11%)
22	CDL	R	302	-	91,91,99	0.95	7 (7%)	97,103,111	0.97	12 (12%)
19	ADP	F	600	-	24,29,29	0.92	1 (4%)	29,45,45	1.55	4 (13%)
20	LHG	K	302	-	48,48,48	0.68	1 (2%)	51,54,54	1.31	7 (13%)
20	LHG	2	202	-	44,44,48	0.68	1 (2%)	47,50,54	1.32	6 (12%)
21	P5S	2	201	-	52,53,53	0.33	0	56,60,60	0.54	0
22	CDL	R	301	-	99,99,99	1.01	8 (8%)	105,111,111	0.99	16 (15%)
19	ADP	D	600	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)
19	ADP	A	602	18	24,29,29	0.99	2 (8%)	29,45,45	1.38	4 (13%)
22	CDL	R	303	-	87,87,99	0.94	6 (6%)	93,99,111	1.02	14 (15%)
19	ADP	B	602	18	24,29,29	0.91	1 (4%)	29,45,45	1.31	4 (13%)
23	S12	T	201	-	33,34,34	0.67	1 (3%)	36,40,40	0.45	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
20	LHG	R	304	-	-	32/53/53/53	-
20	LHG	S	202	-	-	30/53/53/53	-
20	LHG	K	301	-	-	28/47/47/53	-
19	ADP	C	602	18	-	2/12/32/32	0/3/3/3
20	LHG	S	201	-	-	27/53/53/53	-
22	CDL	R	302	-	1/1/9/9	39/102/102/110	-
19	ADP	F	600	-	-	2/12/32/32	0/3/3/3
20	LHG	K	302	-	-	27/53/53/53	-
20	LHG	2	202	-	-	27/49/49/53	-
21	P5S	2	201	-	-	15/59/59/59	-
22	CDL	R	301	-	1/1/9/9	40/110/110/110	-
19	ADP	D	600	-	-	2/12/32/32	0/3/3/3
19	ADP	A	602	18	-	6/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CDL	R	303	-	2/2/9/9	29/98/98/110	-
19	ADP	B	602	18	-	8/12/32/32	0/3/3/3
23	S12	T	201	-	-	14/38/38/38	-

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	302	CDL	C42-C41	-3.49	1.32	1.51
23	T	201	S12	C14-C13	3.49	1.52	1.31
22	R	301	CDL	C42-C41	-3.49	1.32	1.51
22	R	302	CDL	C39-C38	-3.48	1.32	1.51
22	R	301	CDL	C19-C18	-3.47	1.32	1.51

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	202	LHG	O4-P-O5	4.26	133.29	112.24
20	K	302	LHG	O4-P-O5	4.20	133.02	112.24
20	K	301	LHG	O4-P-O5	4.18	132.92	112.24
20	S	202	LHG	O4-P-O5	4.16	132.82	112.24
20	S	201	LHG	O4-P-O5	4.16	132.80	112.24

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	R	301	CDL	CB4
22	R	302	CDL	CB4
22	R	303	CDL	CB4
22	R	303	CDL	CA4

5 of 328 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B	602	ADP	C5'-O5'-PA-O3A
19	C	602	ADP	C5'-O5'-PA-O1A
19	A	602	ADP	PA-O3A-PB-O2B
19	A	602	ADP	PA-O3A-PB-O3B
19	A	602	ADP	C5'-O5'-PA-O3A

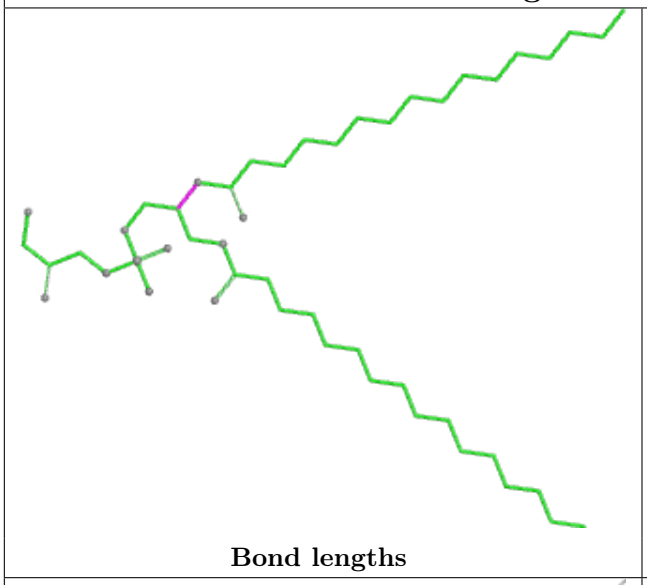
There are no ring outliers.

12 monomers are involved in 29 short contacts:

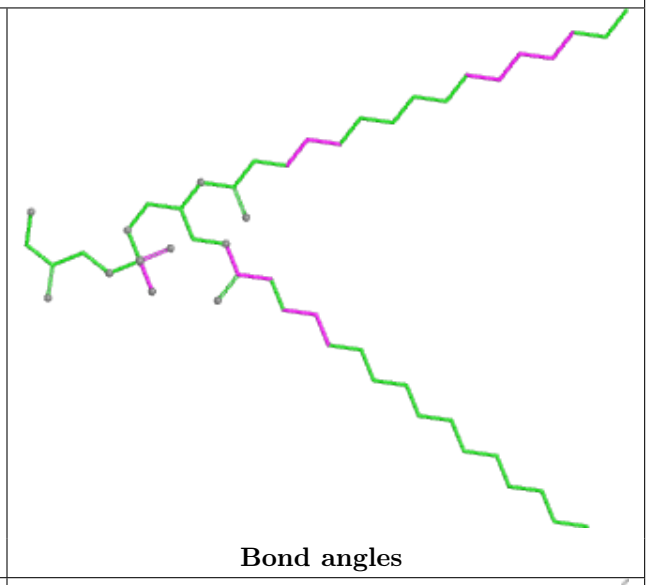
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	R	304	LHG	2	0
20	S	202	LHG	1	0
19	C	602	ADP	1	0
20	S	201	LHG	4	0
22	R	302	CDL	7	0
19	F	600	ADP	1	0
20	K	302	LHG	3	0
21	2	201	P5S	2	0
22	R	301	CDL	2	0
22	R	303	CDL	6	0
19	B	602	ADP	2	0
23	T	201	S12	1	0

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.

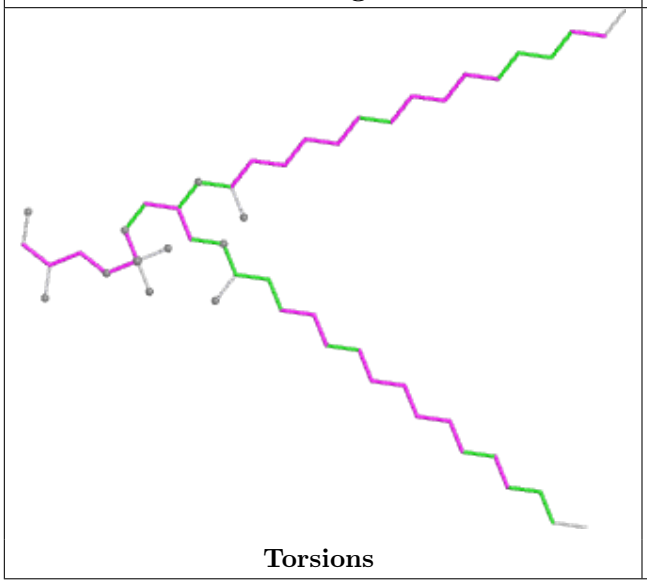
Ligand LHG R 304



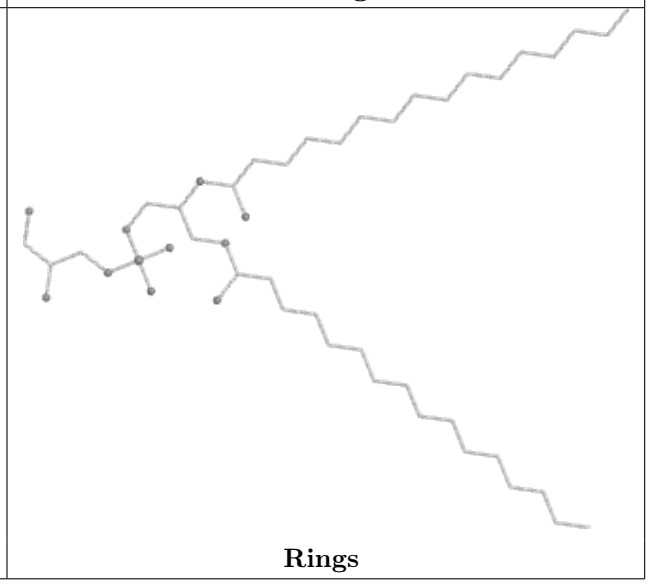
Bond lengths



Bond angles

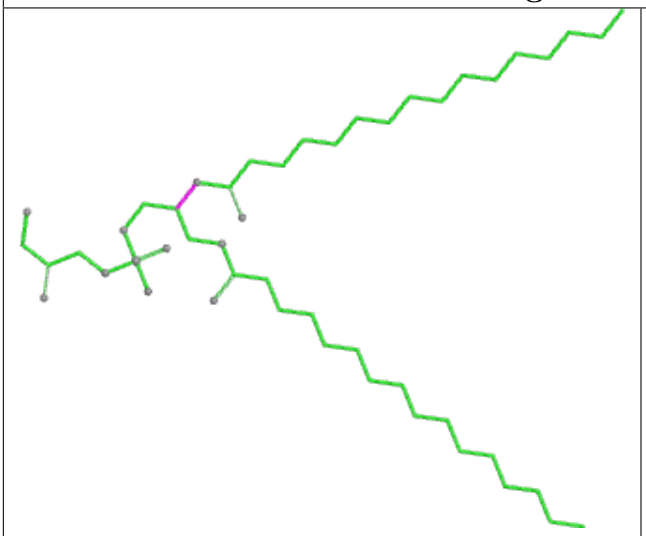


Torsions



Rings

Ligand LHG S 202



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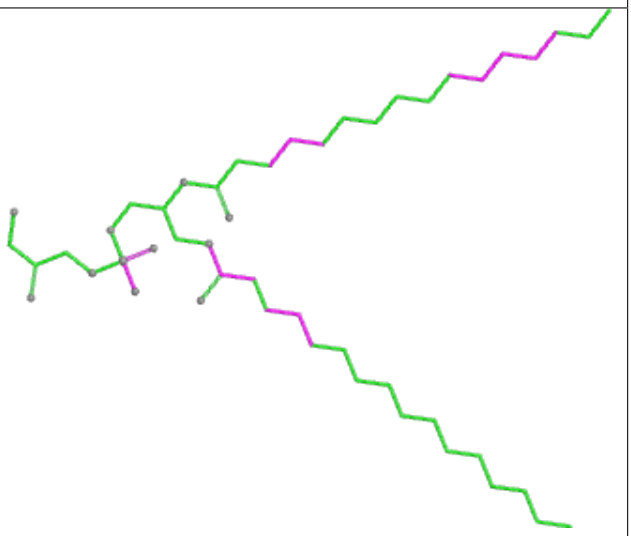
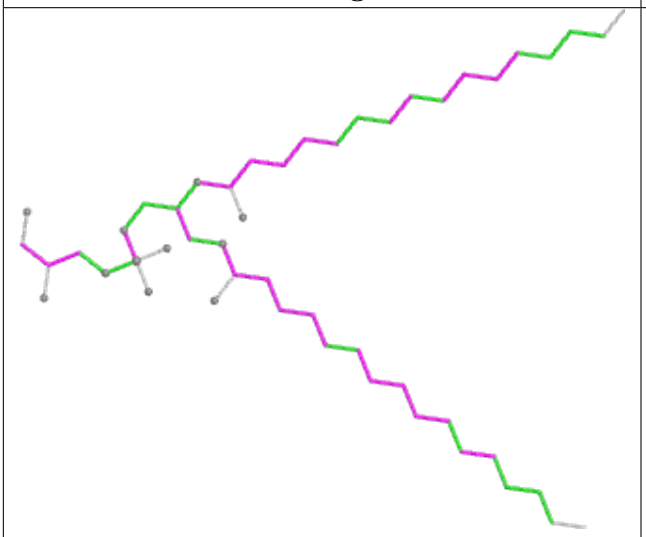


Bond angles



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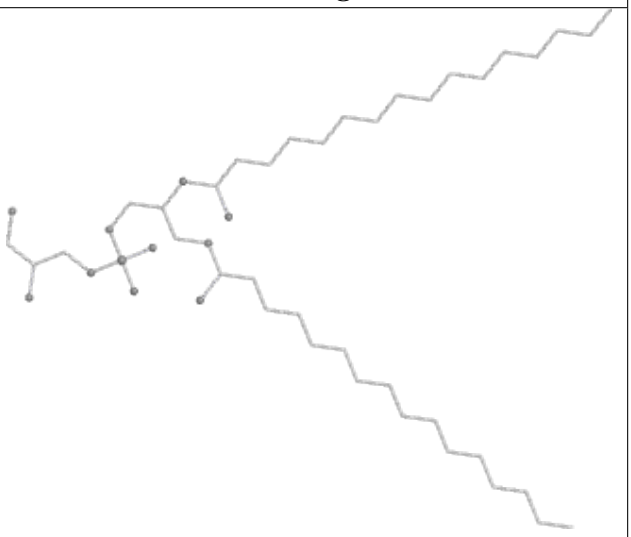
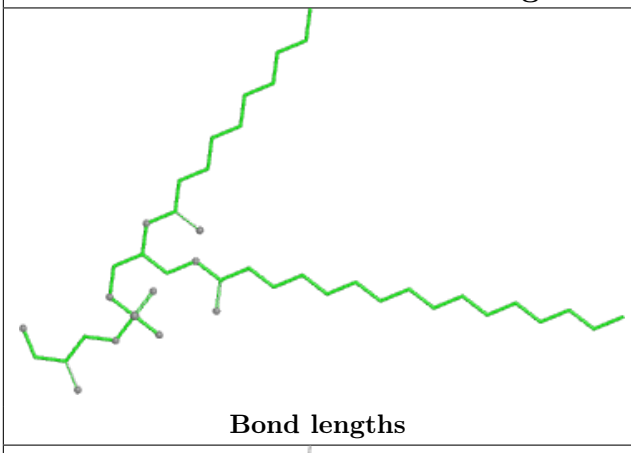


Rings

Ligand LHG K 301



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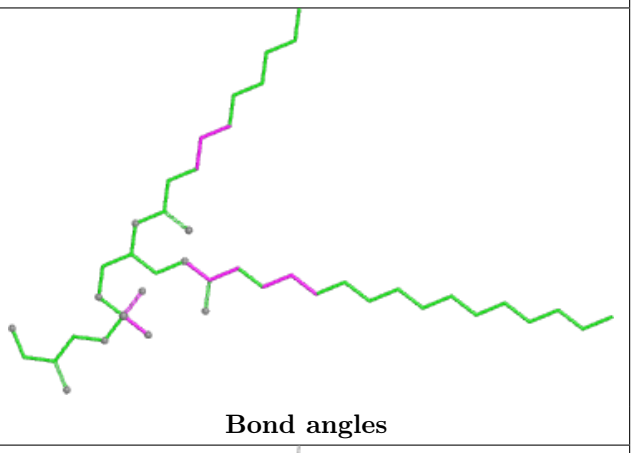
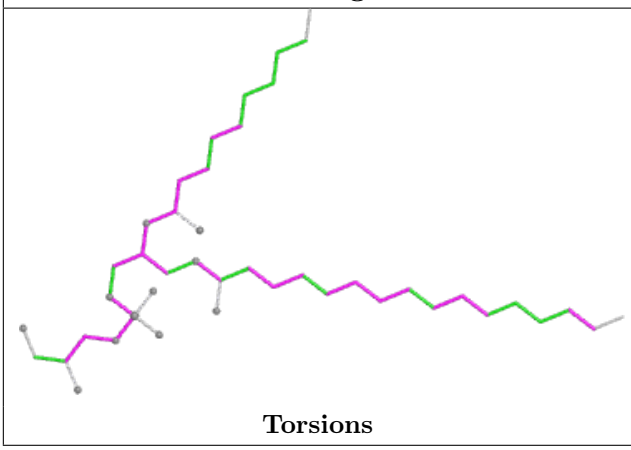


Bond angles



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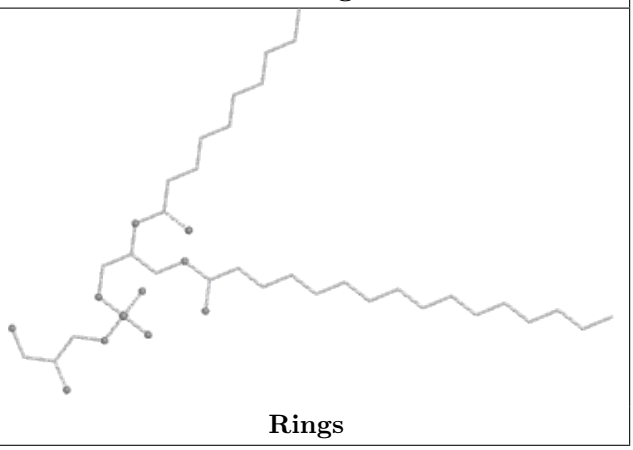
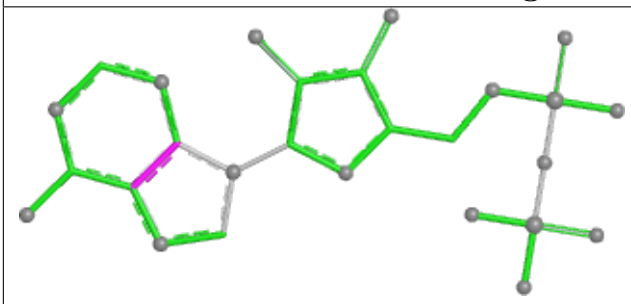


Rings

Ligand ADP C 602



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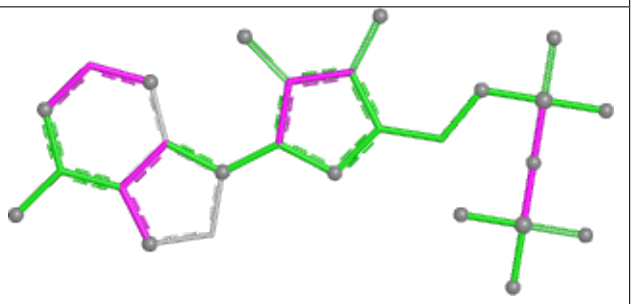
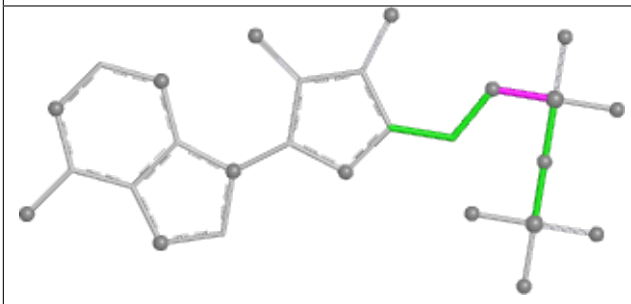


Bond angles



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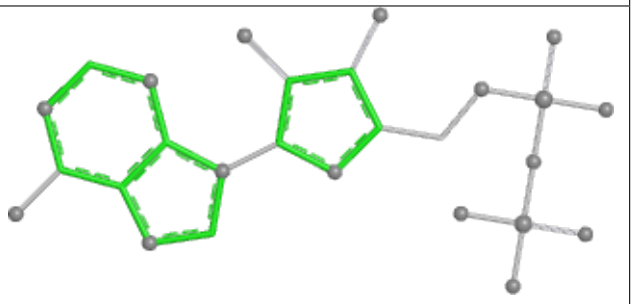
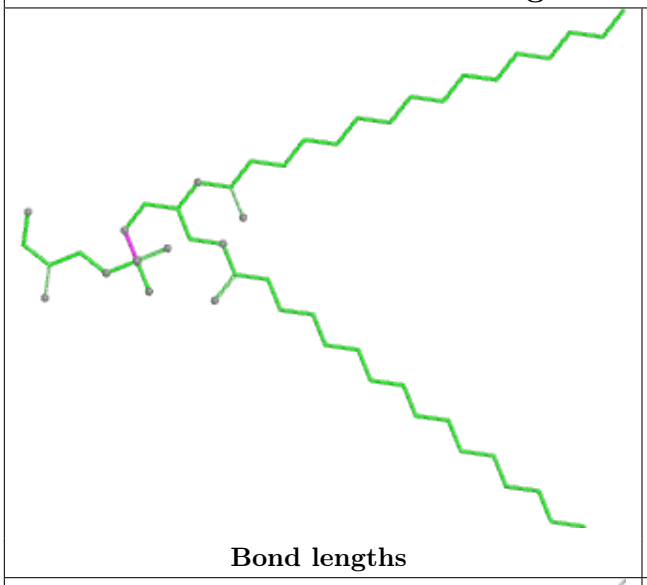


Rings

Ligand LHG S 201



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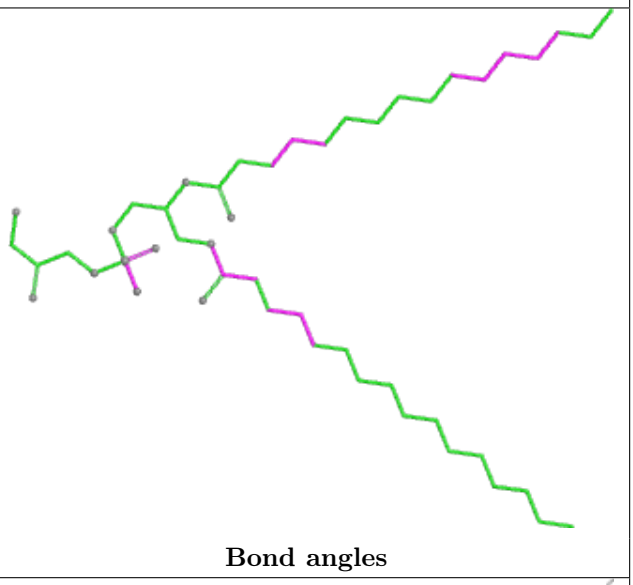

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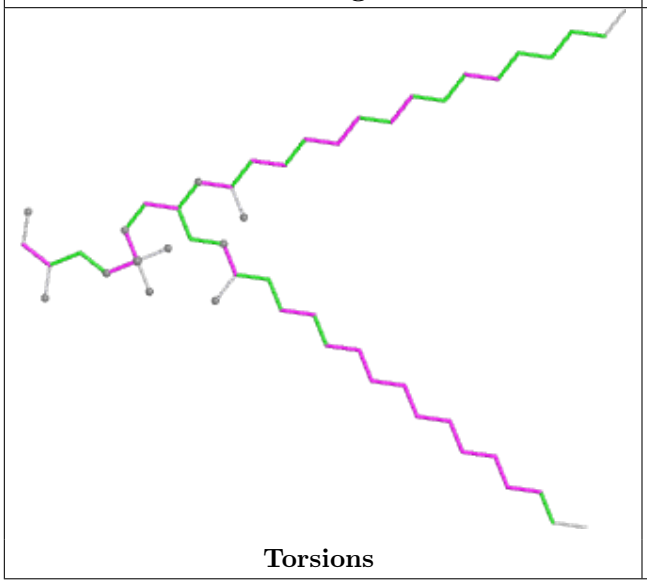

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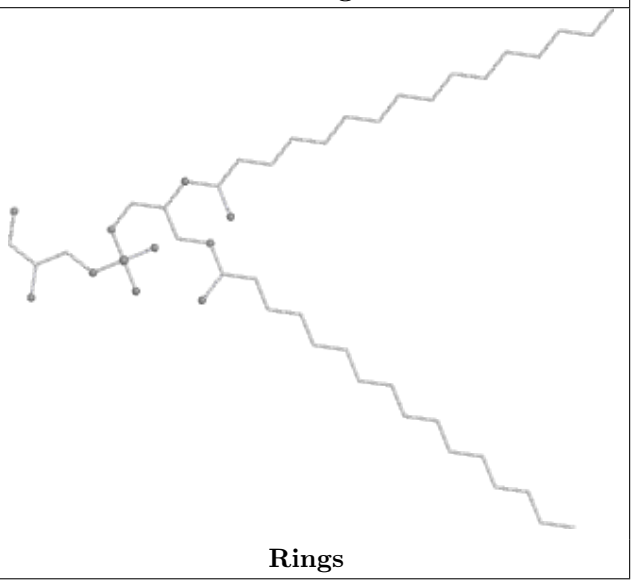
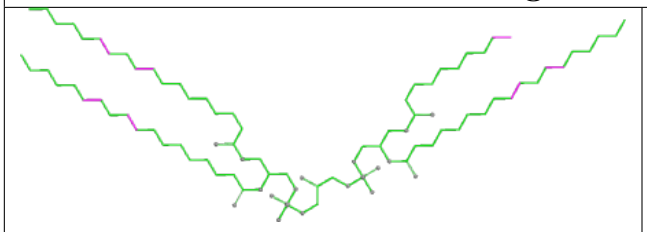


Rings

Ligand CDL R 302



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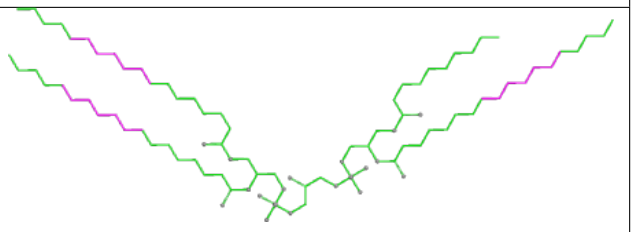
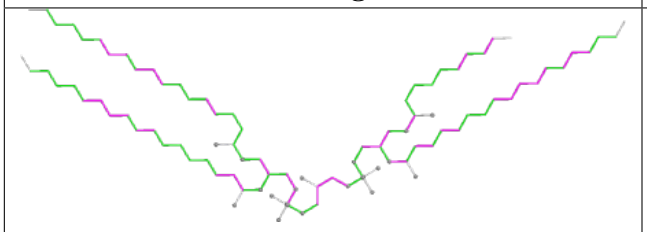


Bond angles



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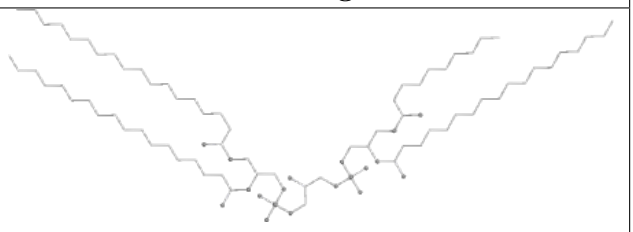
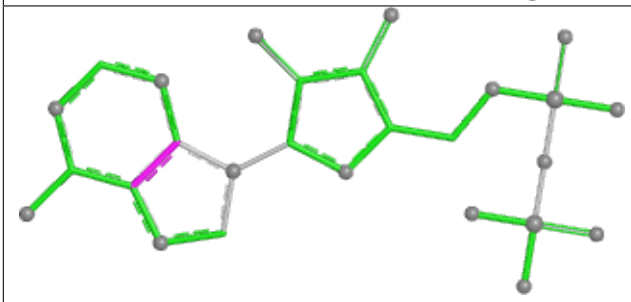
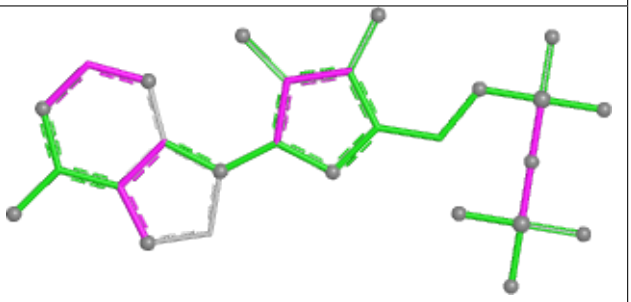


Rings

Ligand ADP F 600	
	
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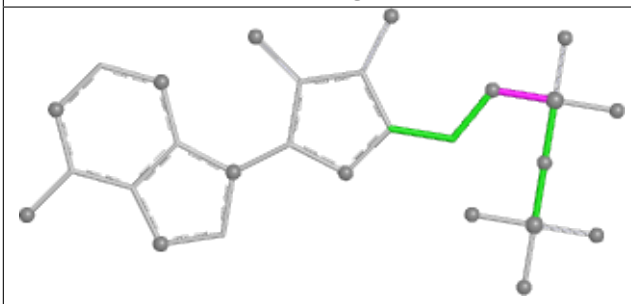
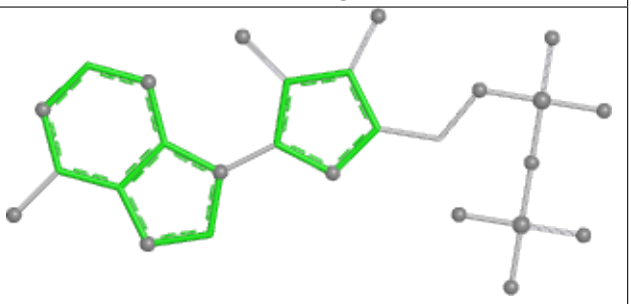
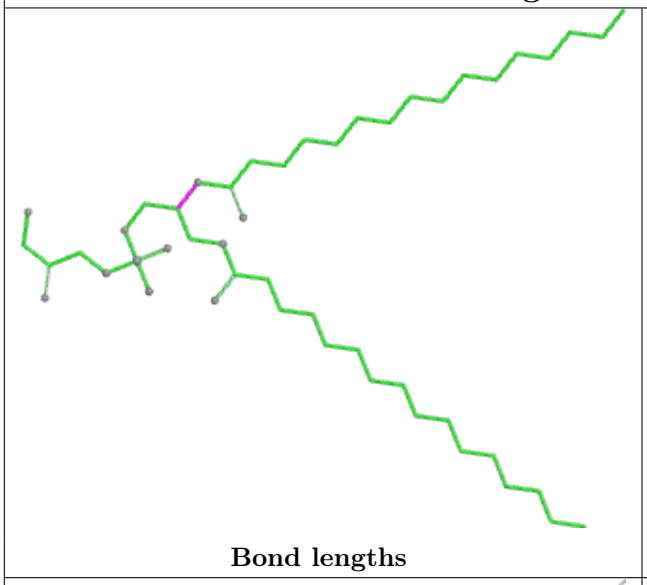
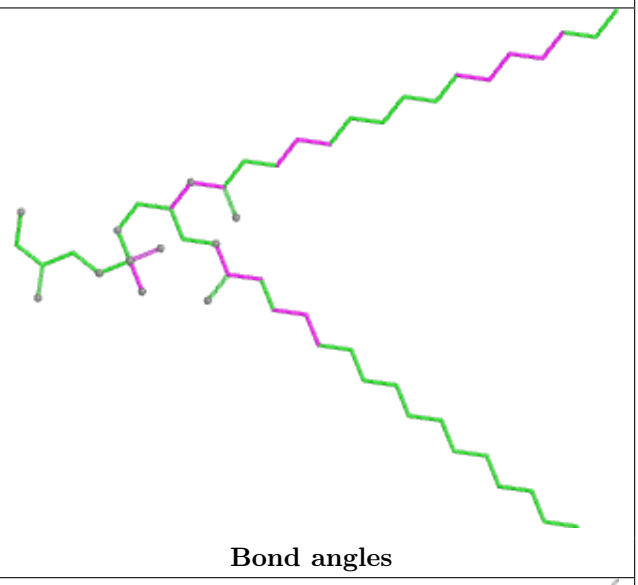
	
Torsions	**Rings**

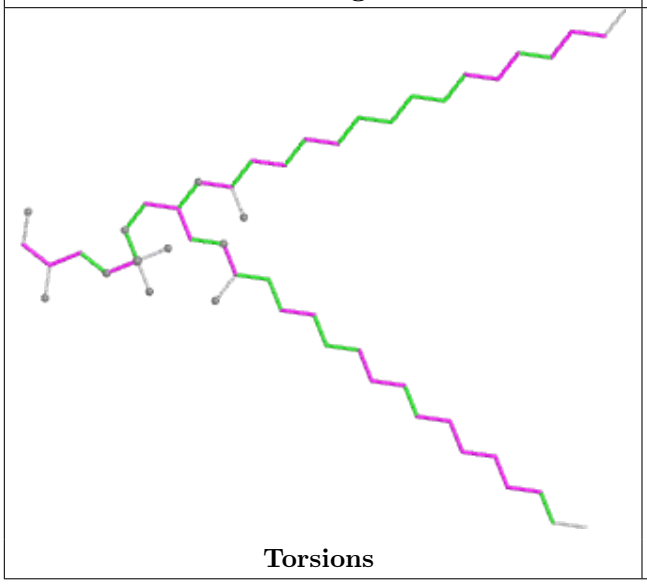
Ligand LHG K 302



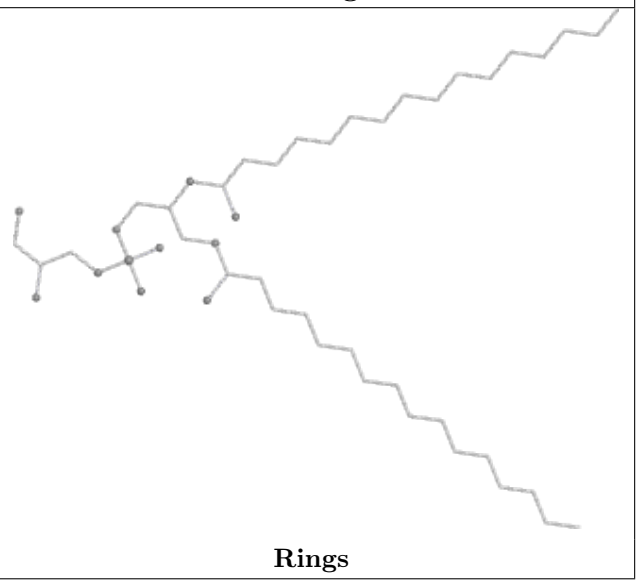
Bond lengths



Bond angles

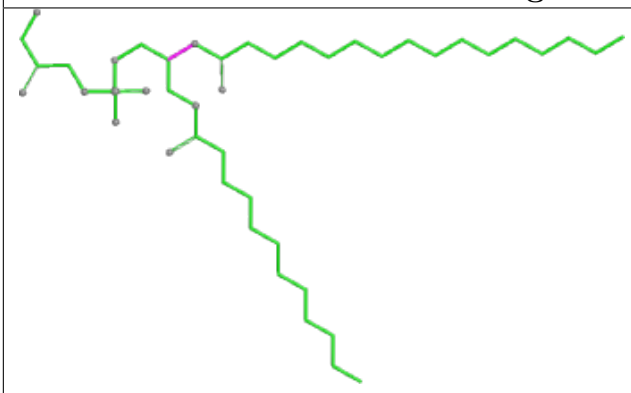


Torsions



Rings

Ligand LHG 2 202



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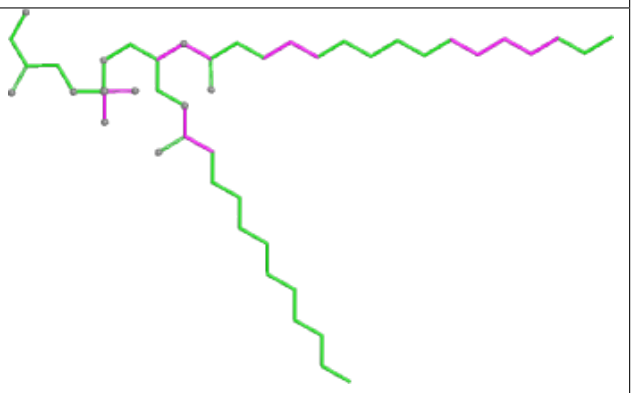

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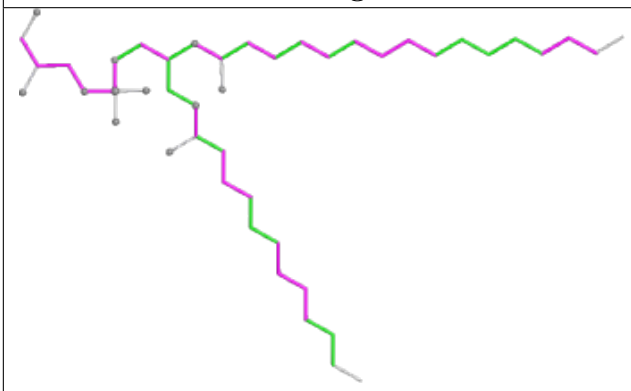

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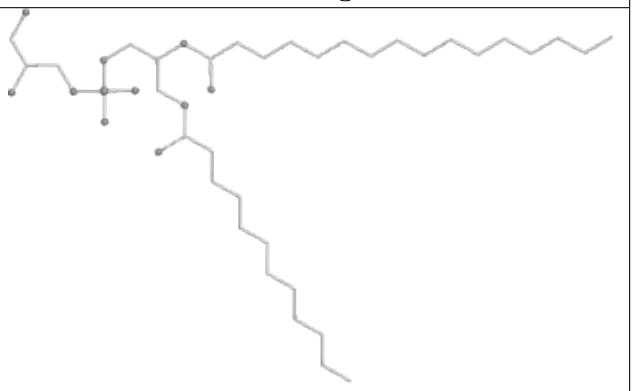
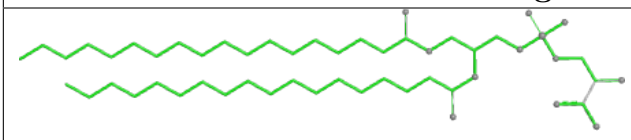


Rings

Ligand P5S 2 201



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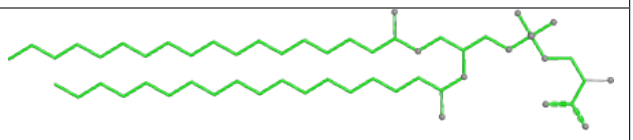

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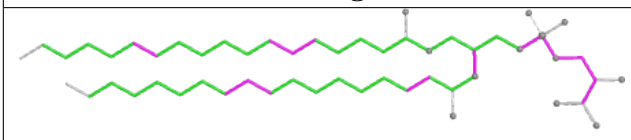

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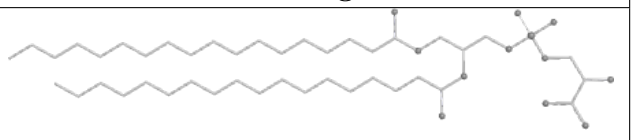
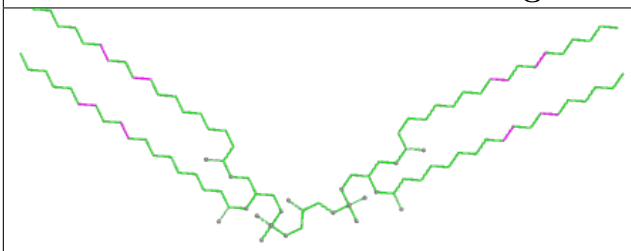
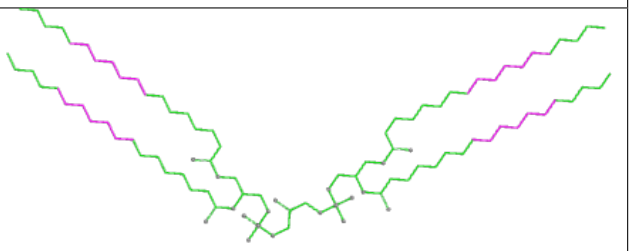


Rings

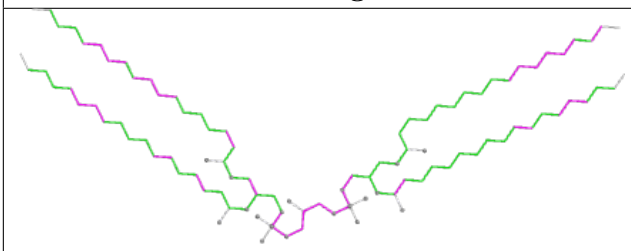
Ligand CDL R 301



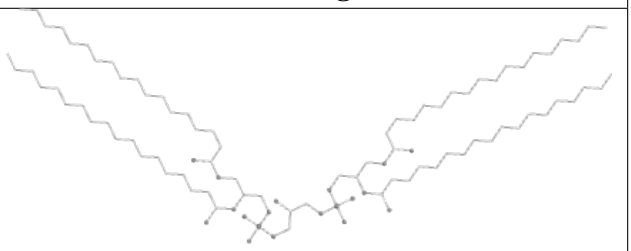
Bond lengths



Bond angles

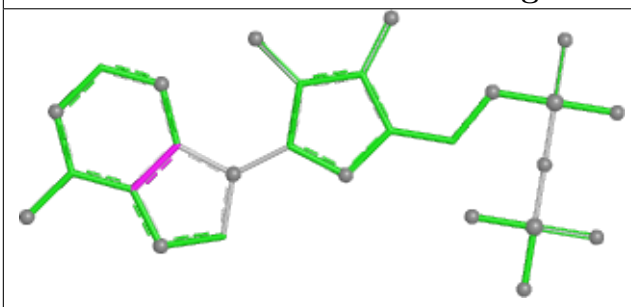


Torsions

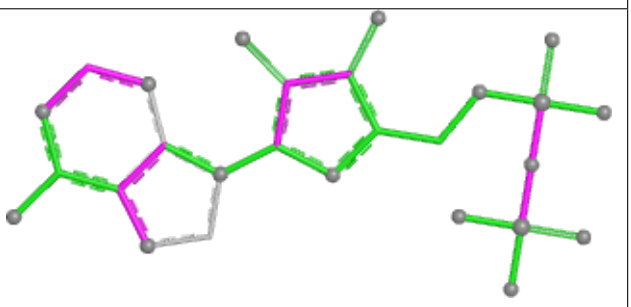


Rings

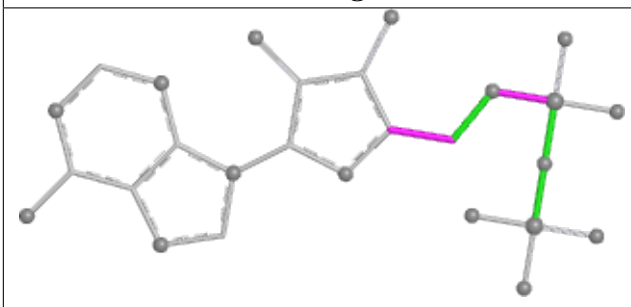
Ligand ADP D 600



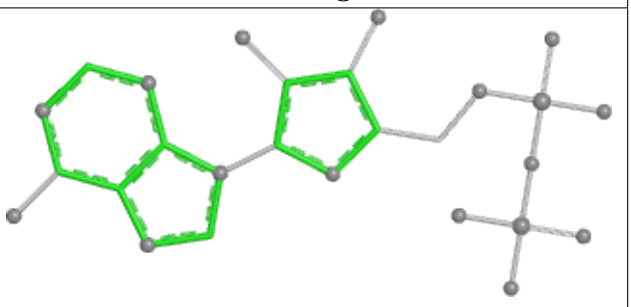
Bond lengths



Bond angles

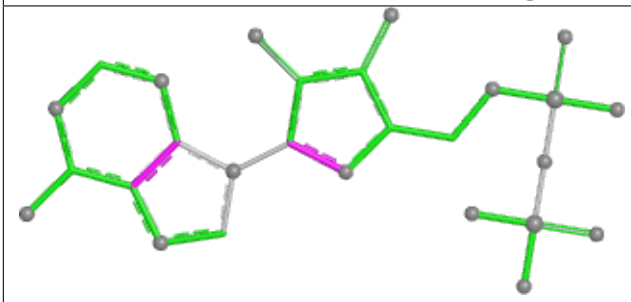


Torsions

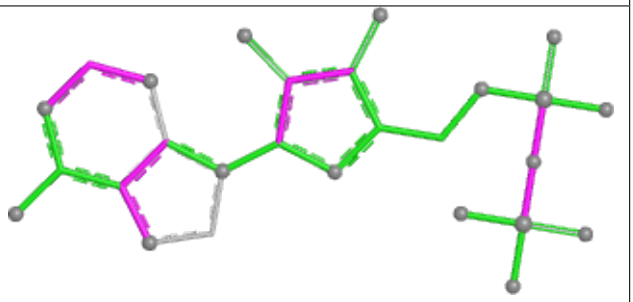


Rings

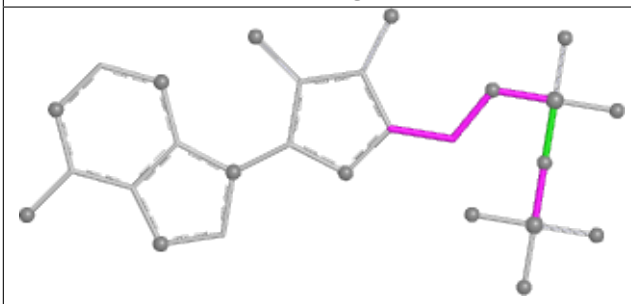
Ligand ADP A 602



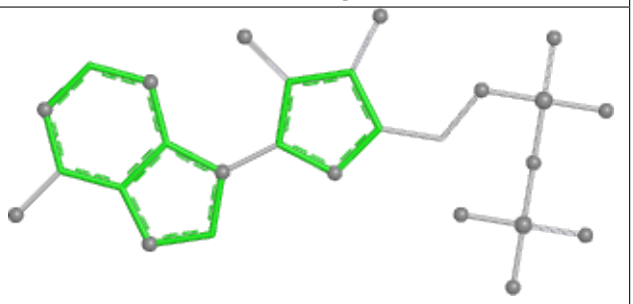
Bond lengths



Bond angles

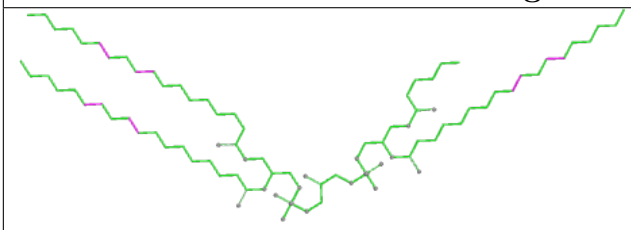


Torsions

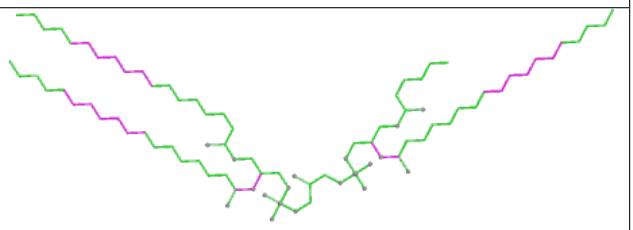


Rings

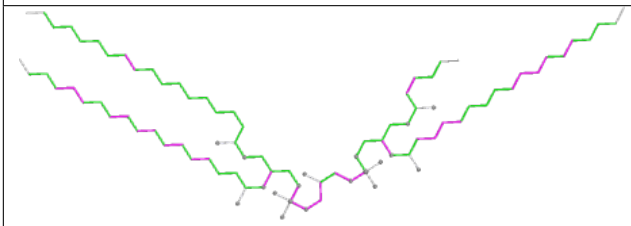
Ligand CDL R 303



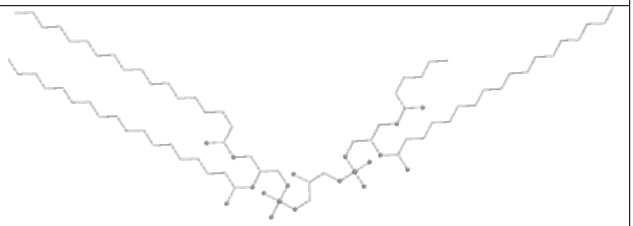
Bond lengths



Bond angles

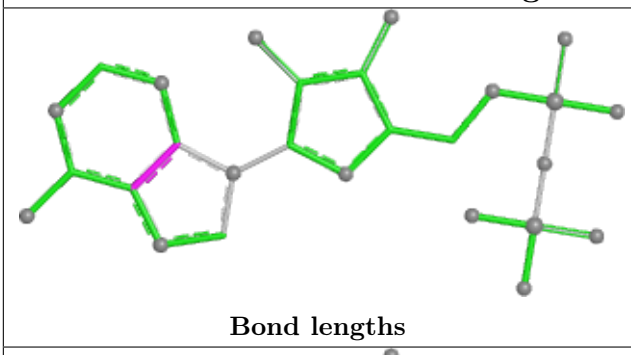


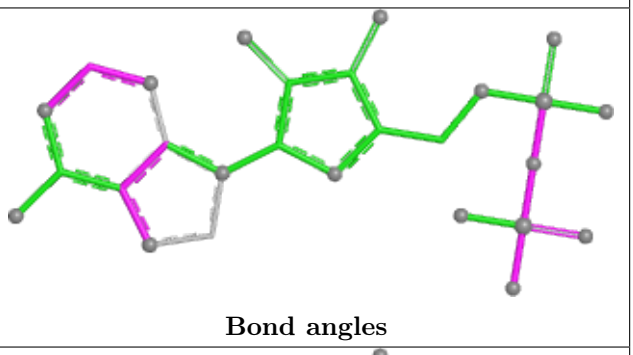
Torsions

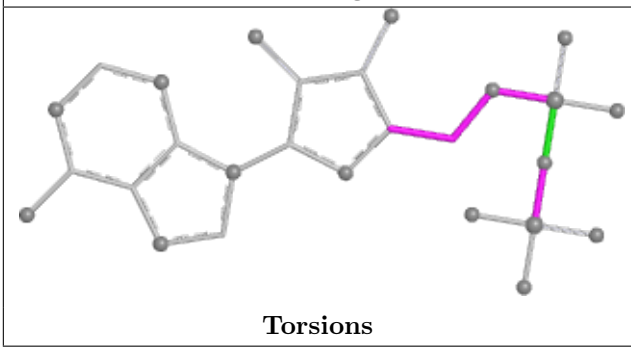


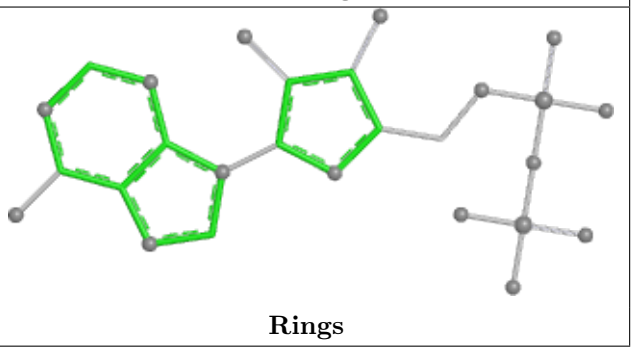
Rings

Ligand ADP B 602

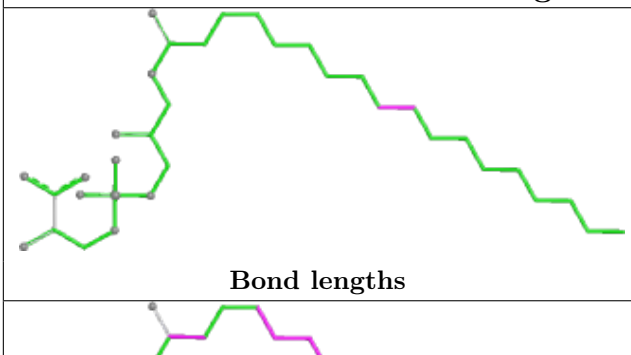

Bond lengths

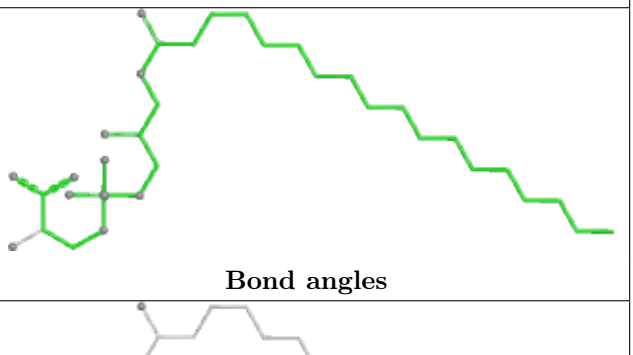

Bond angles

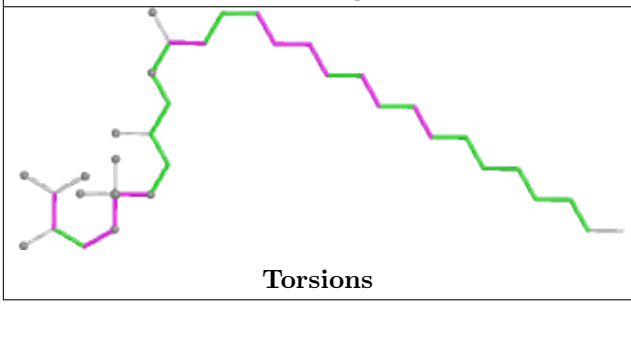

Torsions

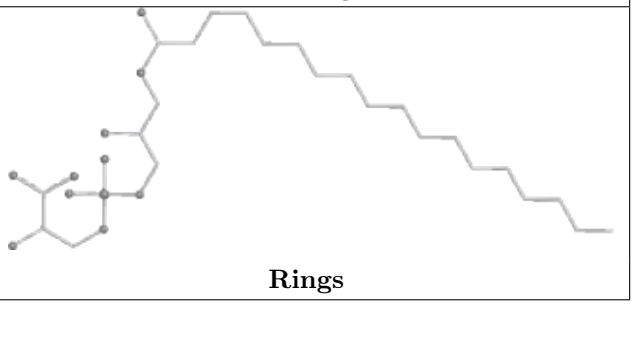

Rings

Ligand S12 T 201


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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	143:ARG	C	144:GLU	N	1.61

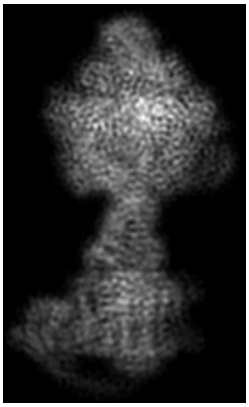
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10573. These allow visual inspection of the internal detail of the map and identification of artifacts.

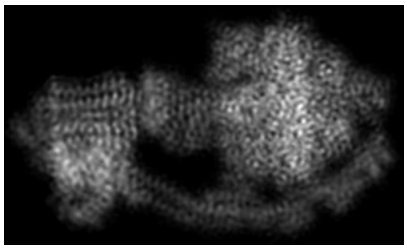
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

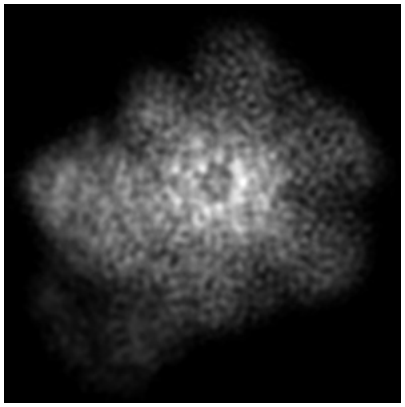
6.1.1 Primary map



X



Y



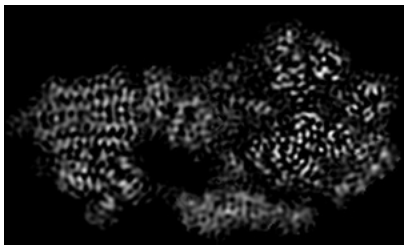
Z

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

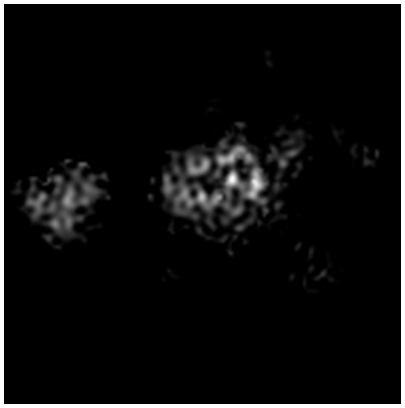
6.2 Central slices

6.2.1 Primary map

X Index: 69



Y Index: 69



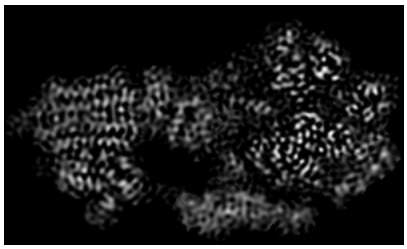
Z Index: 115

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

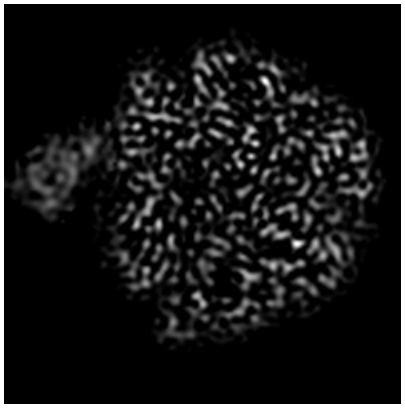
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 81



Y Index: 69



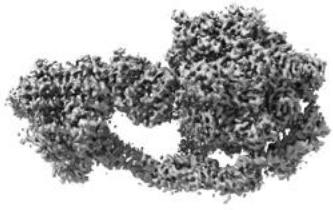
Z Index: 167

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

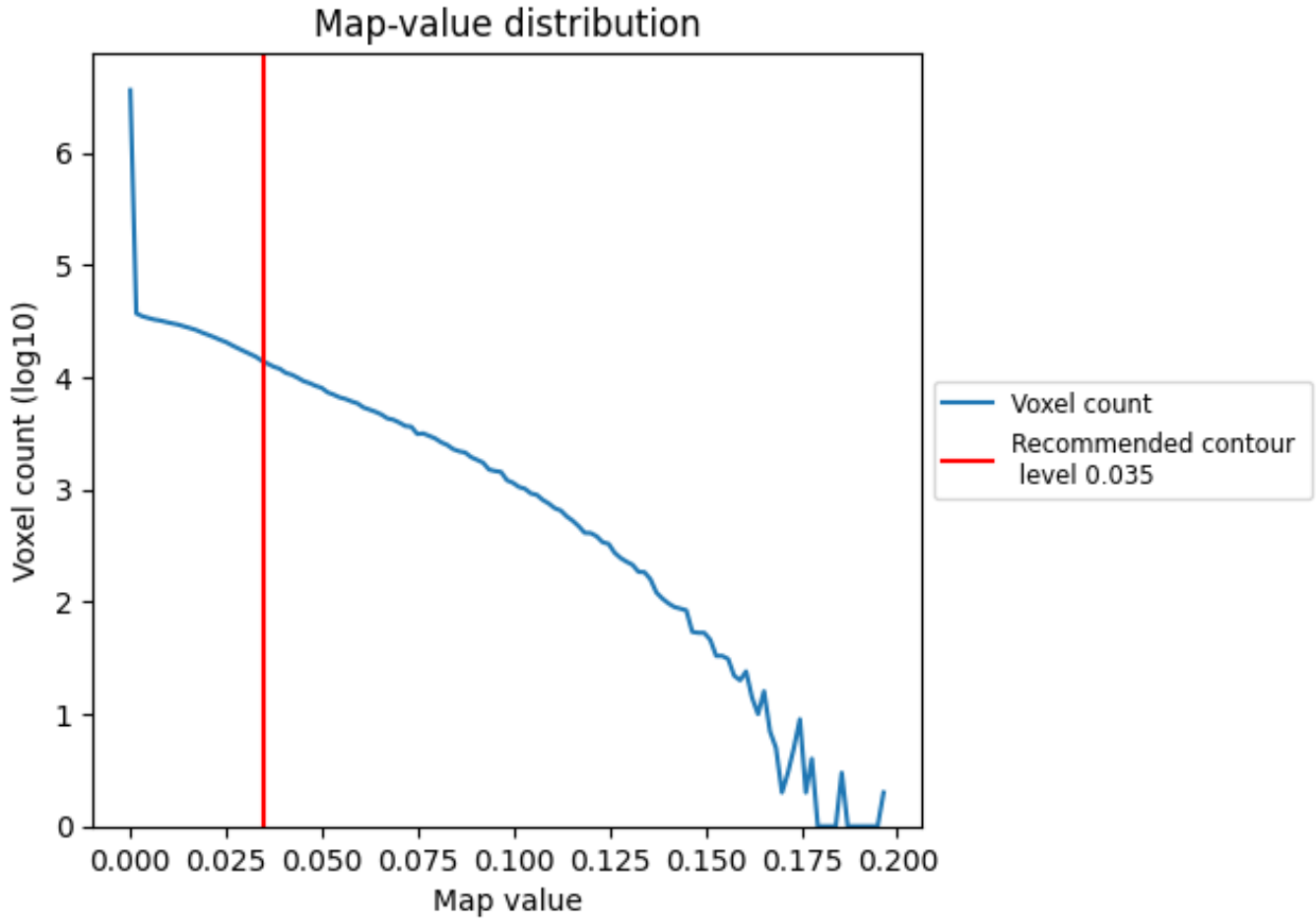
6.5 Mask visualisation (i)

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

7 Map analysis

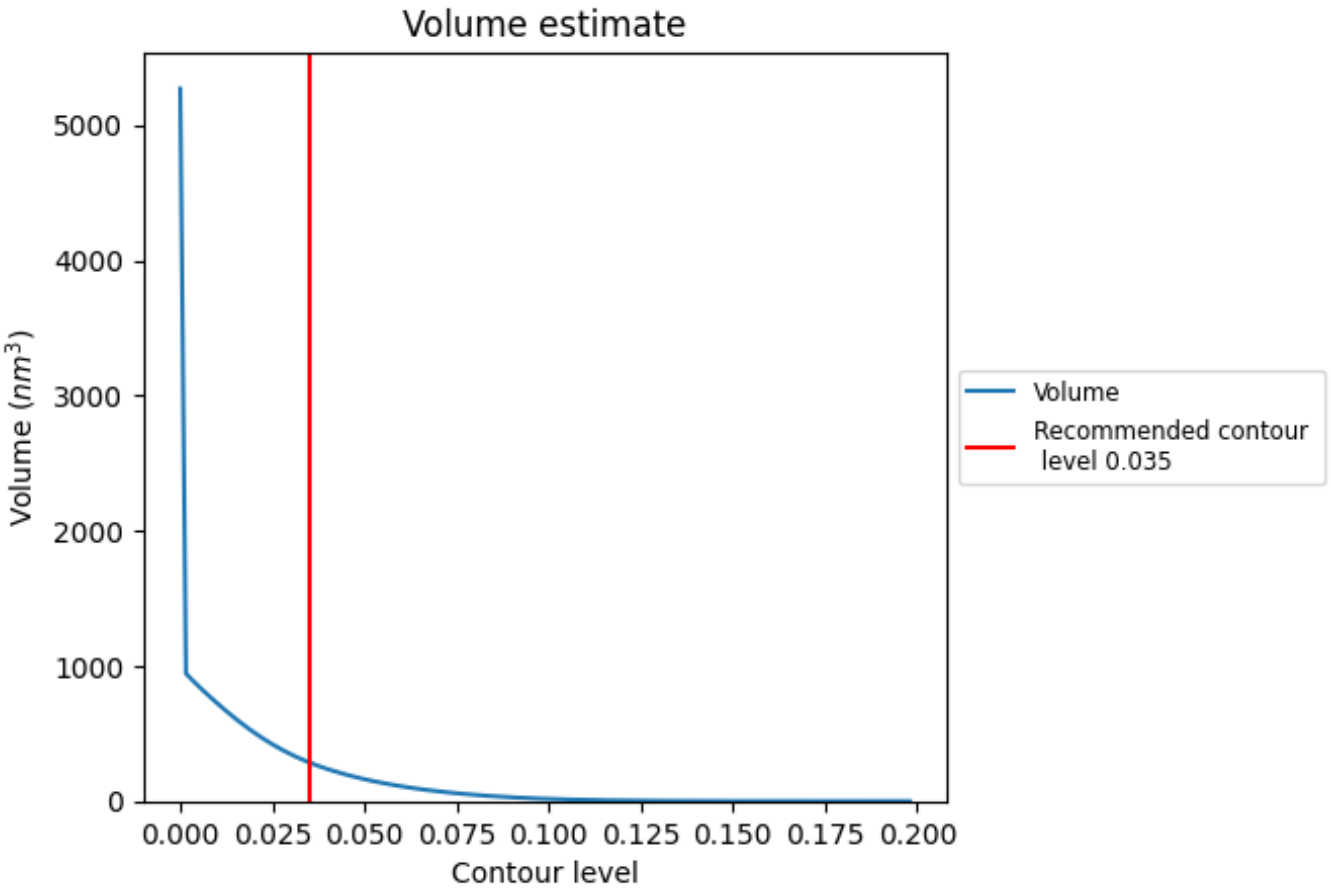
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 286 nm^3; this corresponds to an approximate mass of 259 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.

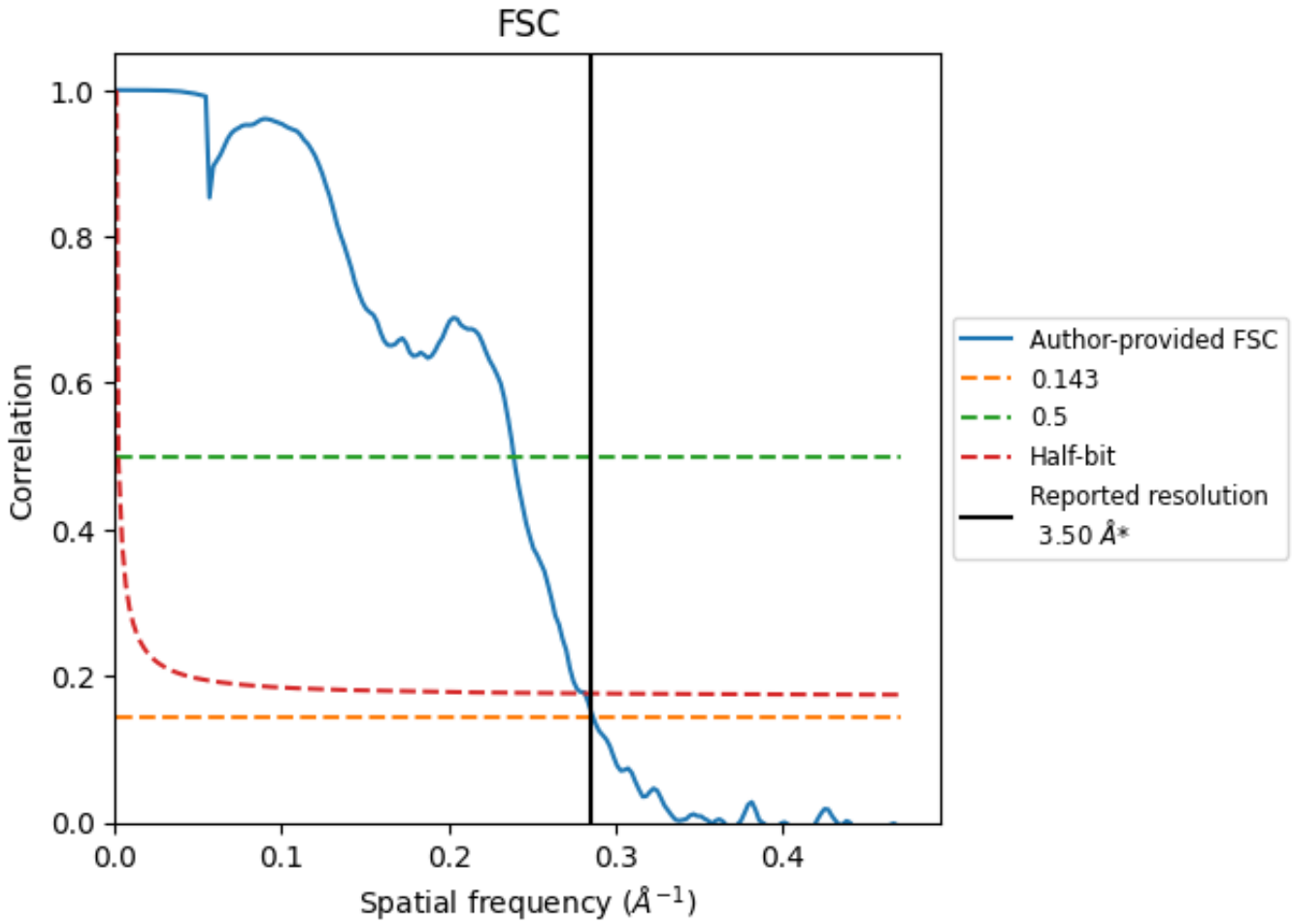
7.3 Rotationally averaged power spectrum (i)

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

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

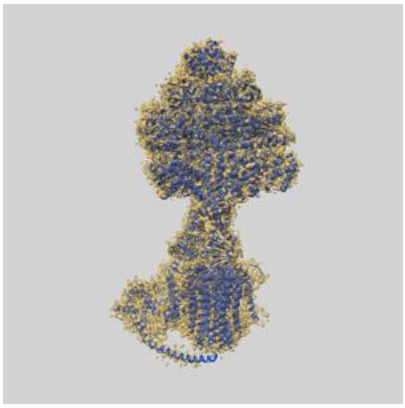
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.18	3.55
Unmasked-calculated*	-	-	-

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

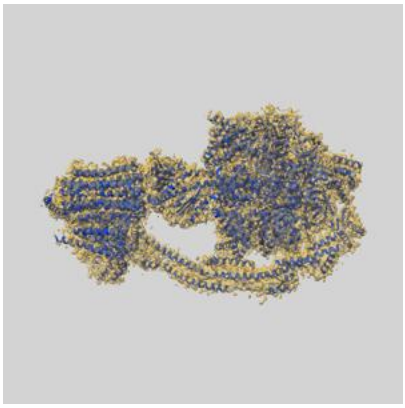
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10573 and PDB model 6TT7. Per-residue inclusion information can be found in section 3 on page 12.

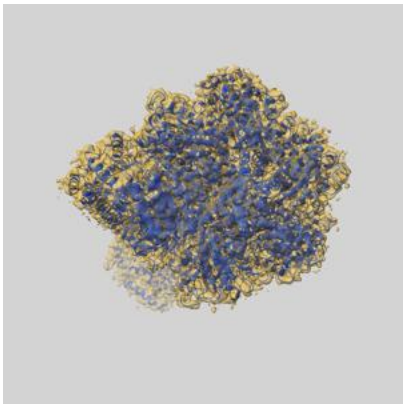
9.1 Map-model overlay



X



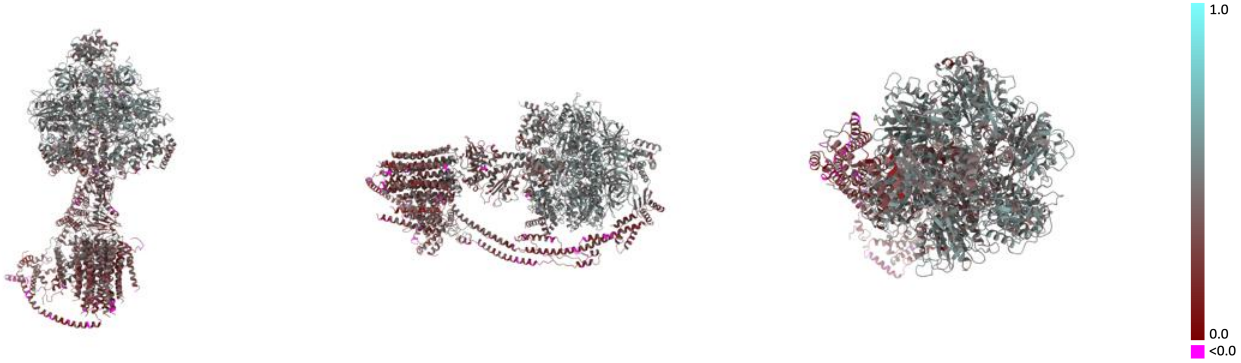
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

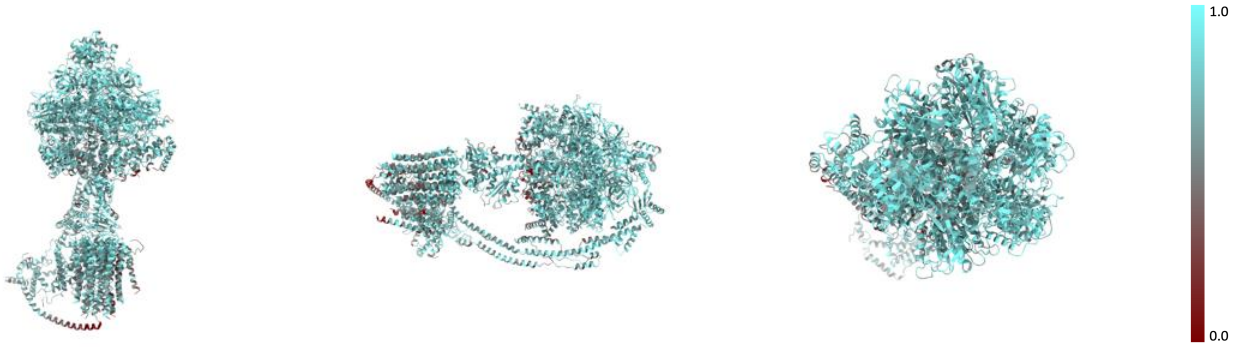
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

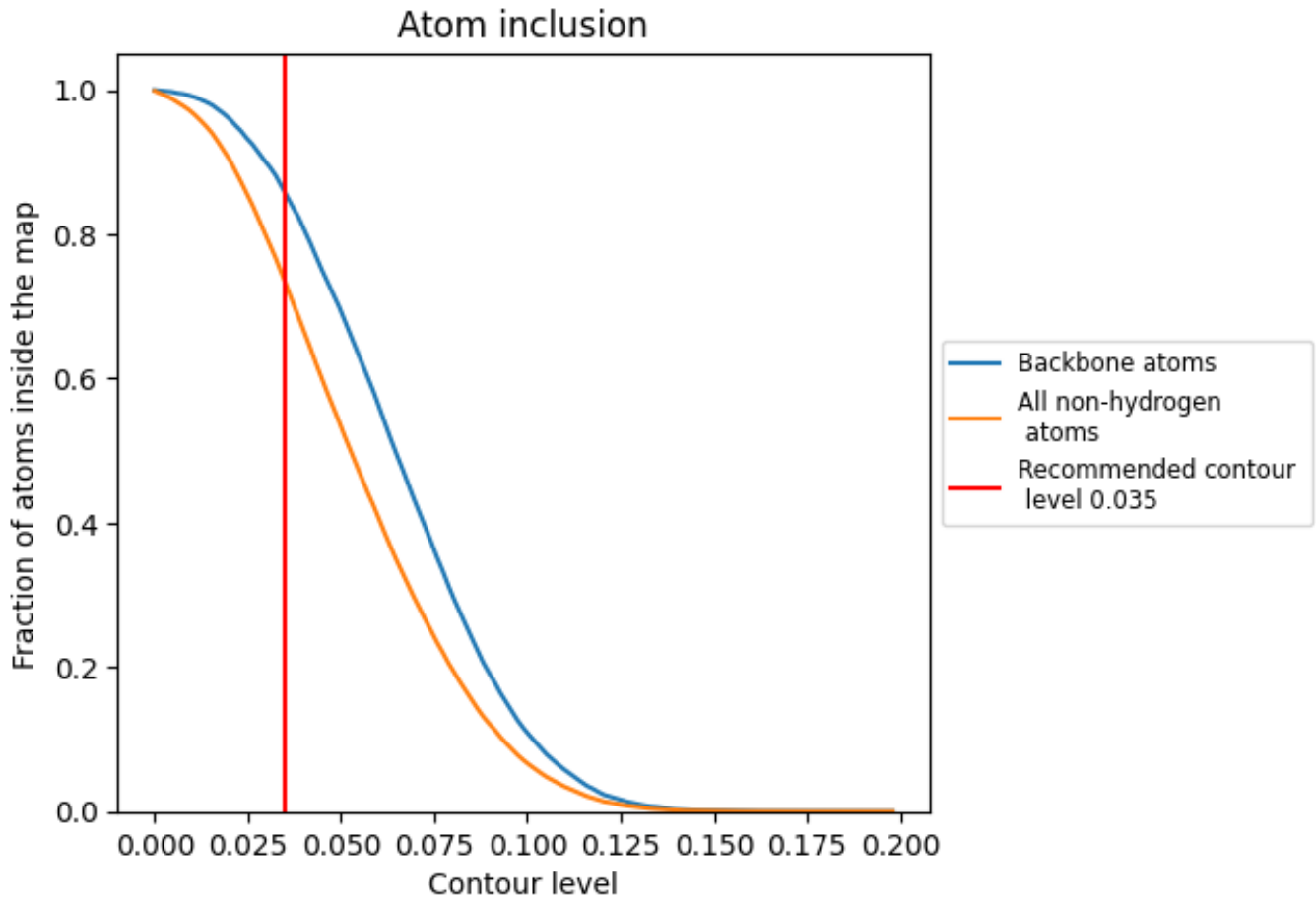
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7343	0.4010
1	0.6705	0.3020
2	0.6216	0.3180
3	0.7184	0.3370
4	0.6801	0.3380
5	0.6667	0.3030
6	0.7107	0.3270
7	0.7107	0.3430
8	0.6743	0.3060
A	0.7755	0.4720
B	0.7803	0.4810
C	0.7475	0.4500
D	0.7477	0.4660
E	0.7754	0.4770
F	0.7922	0.4940
G	0.7535	0.3780
H	0.7183	0.3100
I	0.7430	0.3210
J	0.7740	0.4110
K	0.7437	0.2870
L	0.7310	0.2230
M	0.6638	0.2340
N	0.7304	0.3570
O	0.4545	0.1830
P	0.6425	0.2780
Q	0.7182	0.3620
R	0.5794	0.2890
S	0.5797	0.2090
T	0.5068	0.2110