Full wwPDB EM Validation 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 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 ⓘ 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:

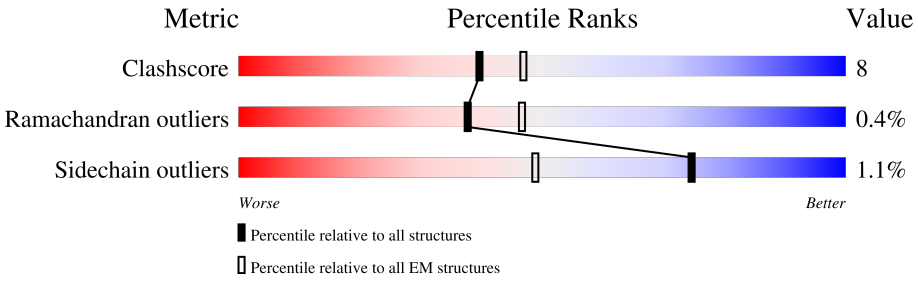
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

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	C	N	O	S	0	0
			701	461	121	116	3		

- Molecule 16 is a protein called ATP synthase subunit.

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

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	C	N	O	S	0	0
			577	364	106	106	1		

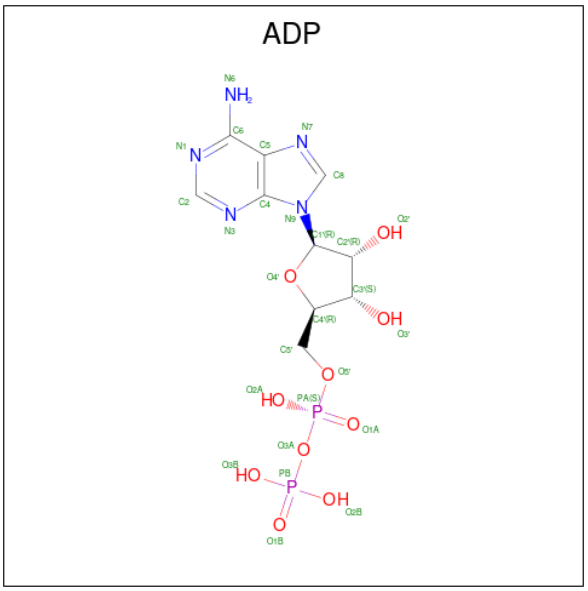
There are 3 discrepancies between the modelled and reference sequences:

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).

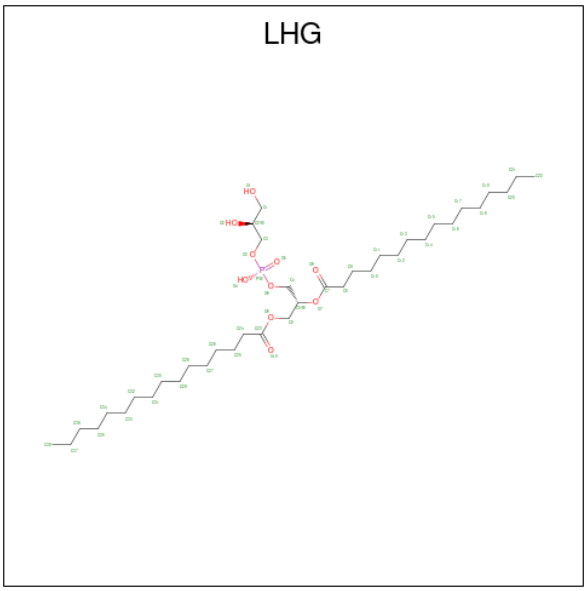
Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	Mg	0
			1	1	
18	C	1	Total	Mg	0
			1	1	
18	A	1	Total	Mg	0
			1	1	

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



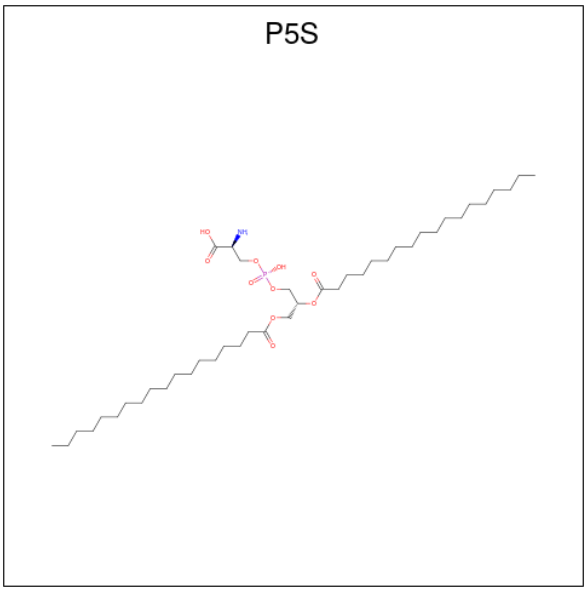
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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



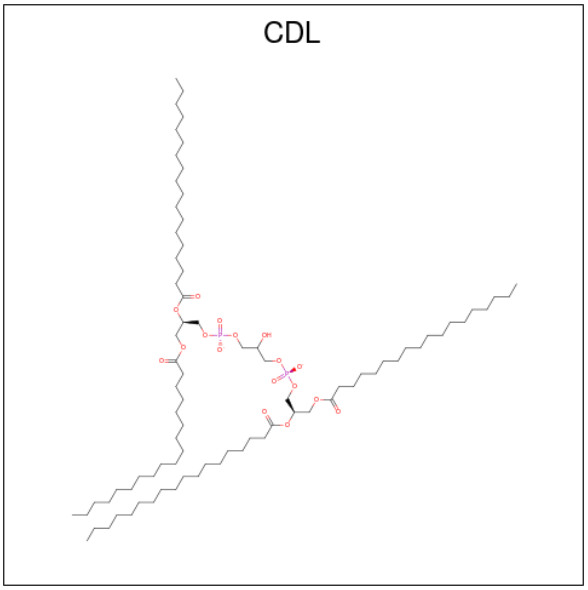
Mol	Chain	Residues	Atoms				AltConf
20	K	1	Total	C	O	P	0
			92	70	20	2	
20	K	1	Total	C	O	P	0
			92	70	20	2	
20	2	1	Total	C	O	P	0
			45	34	10	1	
20	R	1	Total	C	O	P	0
			49	38	10	1	
20	S	1	Total	C	O	P	0
			98	76	20	2	
20	S	1	Total	C	O	P	0
			98	76	20	2	

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



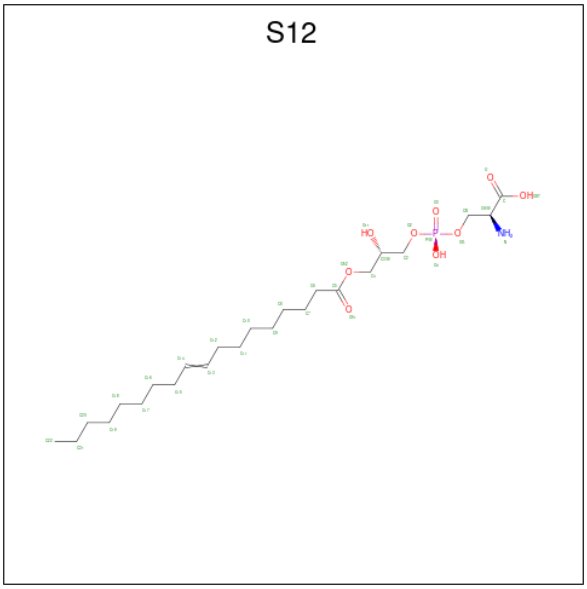
Mol	Chain	Residues	Atoms					AltConf
21	2	1	Total	C	N	O	P	0
			54	42	1	10	1	

- 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: $C_{24}H_{46}NO_9P$).



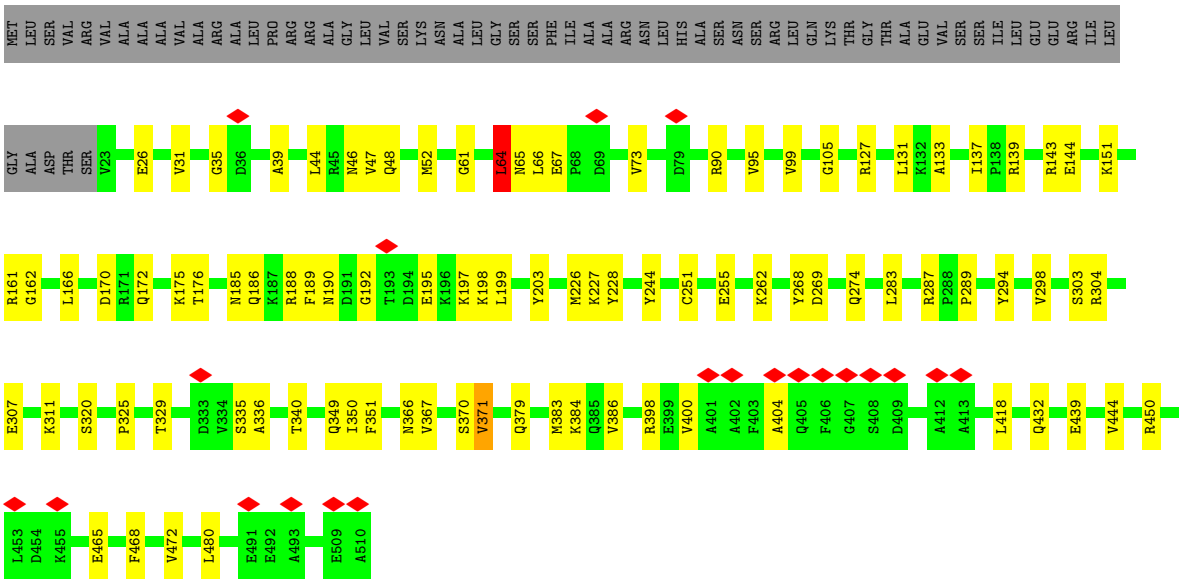
Mol	Chain	Residues	Atoms					AltConf
23	T	1	Total	C	N	O	P	0
			35	24	1	9	1	

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.

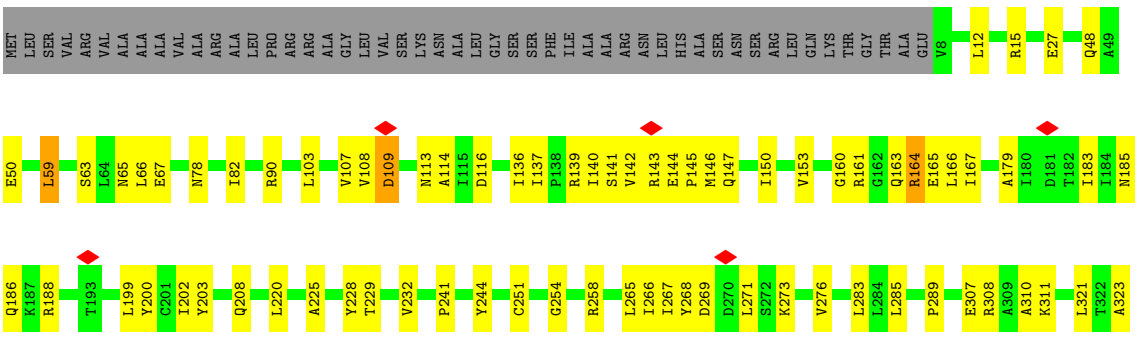
• Molecule 1: ATP synthase subunit alpha

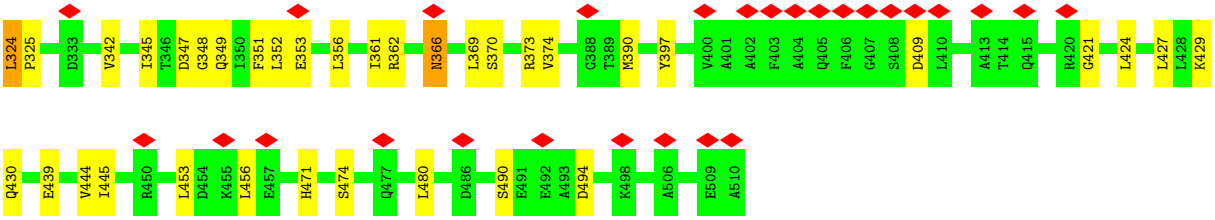
Chain B:



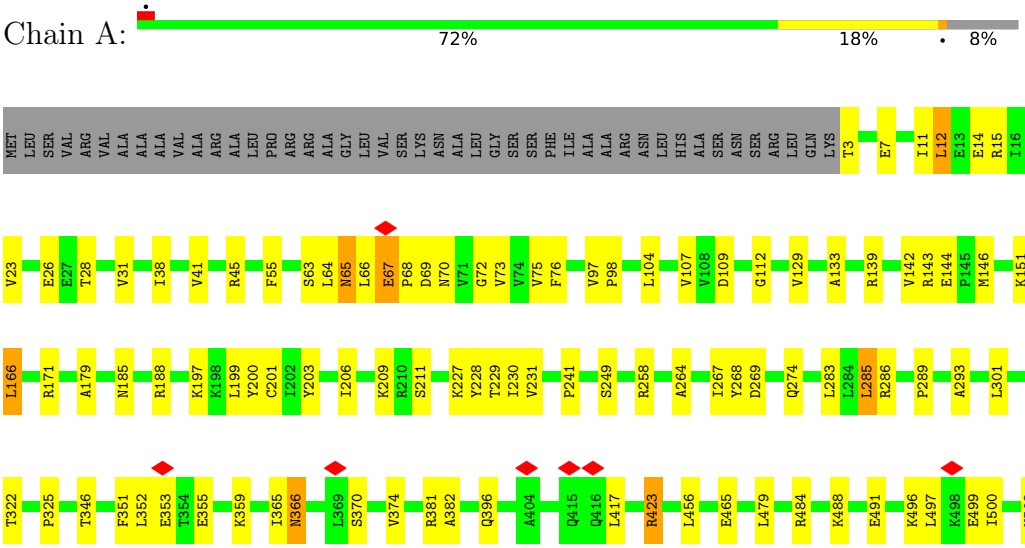
• Molecule 1: ATP synthase subunit alpha

Chain C:

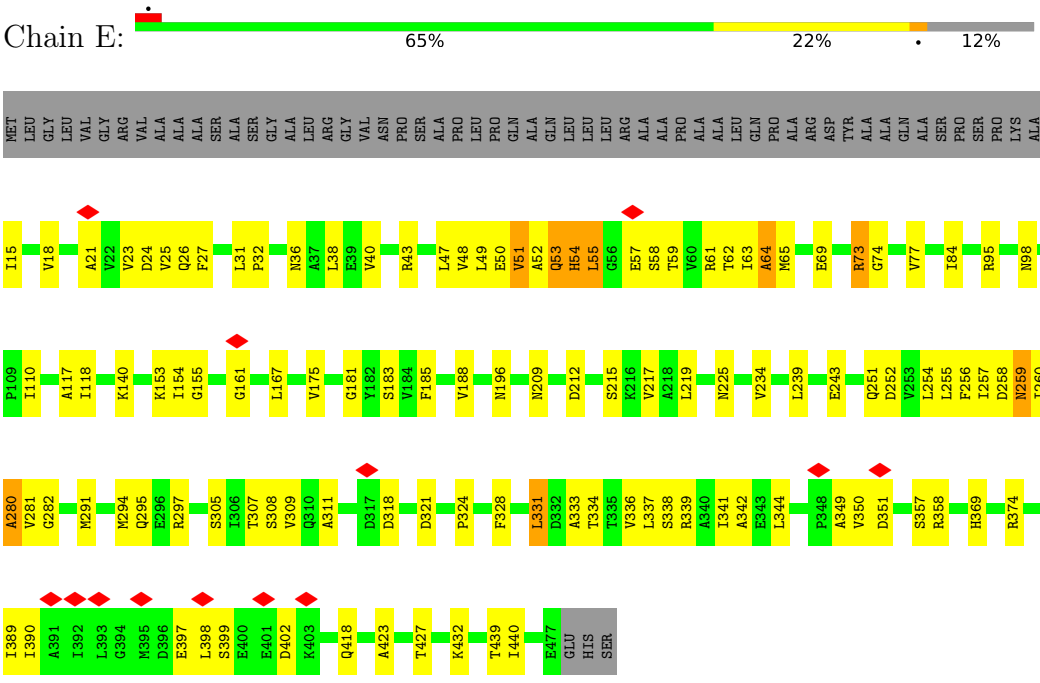




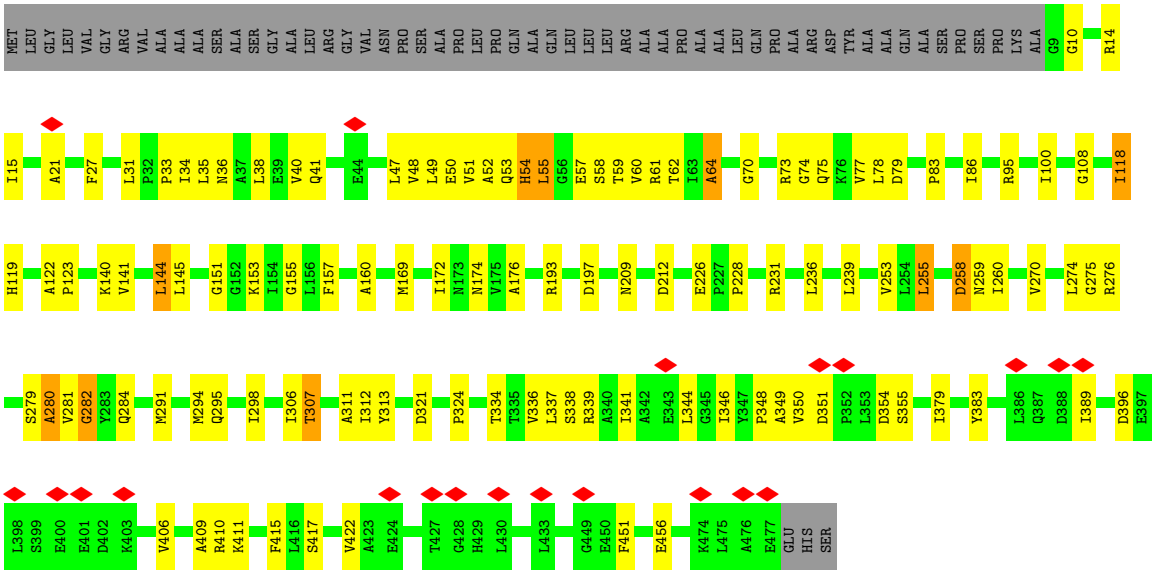
• Molecule 1: ATP synthase subunit alpha



• Molecule 2: ATP synthase subunit beta

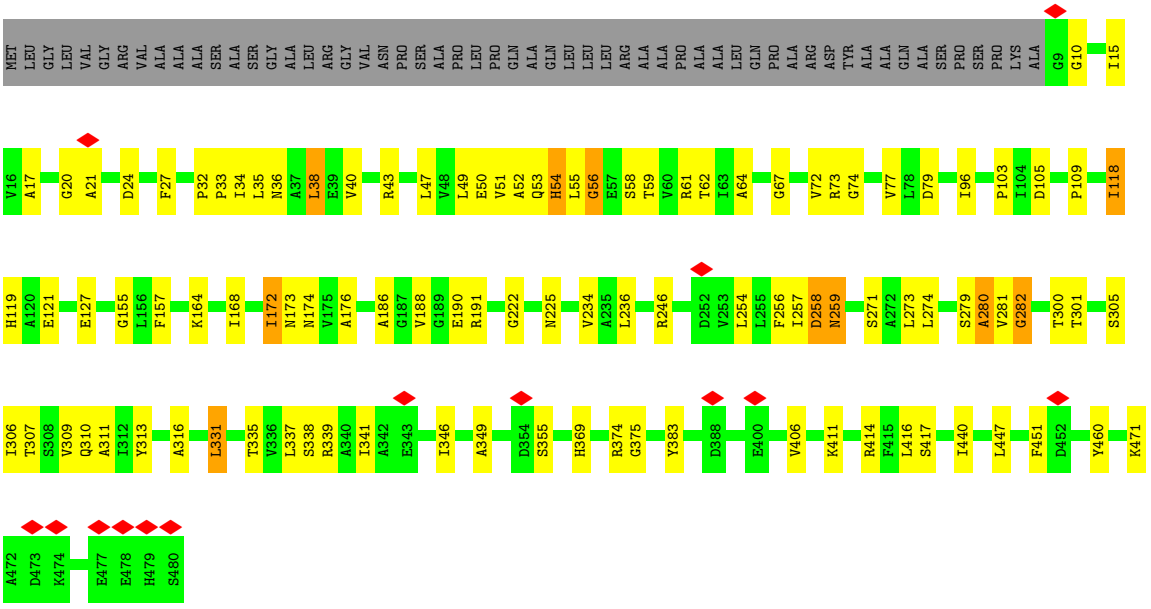


• Molecule 2: ATP synthase subunit beta



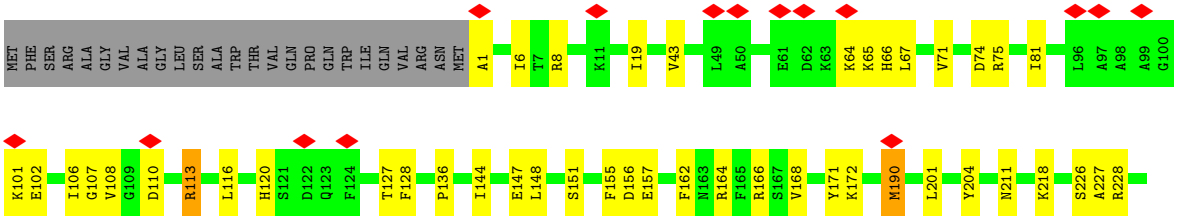
• Molecule 2: ATP synthase subunit beta

Chain F:



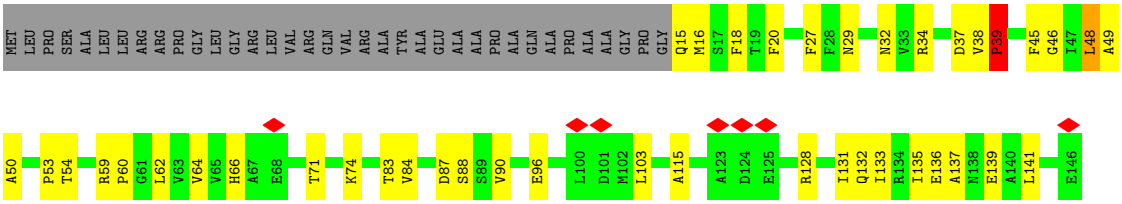
• Molecule 3: ATP synthase subunit gamma

Chain G:



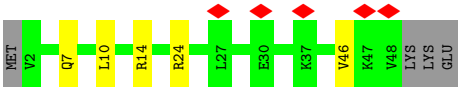
• Molecule 4: ATP synthase F1 subunit delta

Chain H:



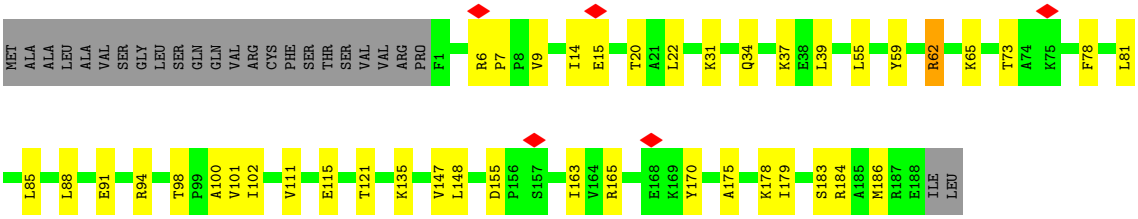
• Molecule 5: ATP synthase F1 subunit epsilon

Chain I:



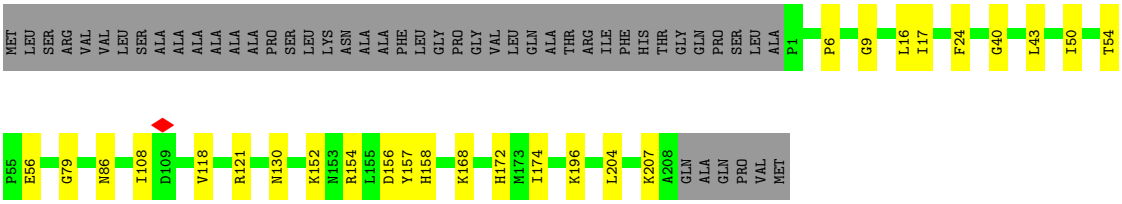
• Molecule 6: ATP synthase peripheral stalk subunit OSCP

Chain J:



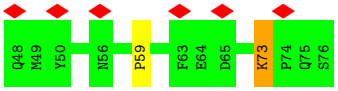
• Molecule 7: ATP synthase subunit b

Chain K:

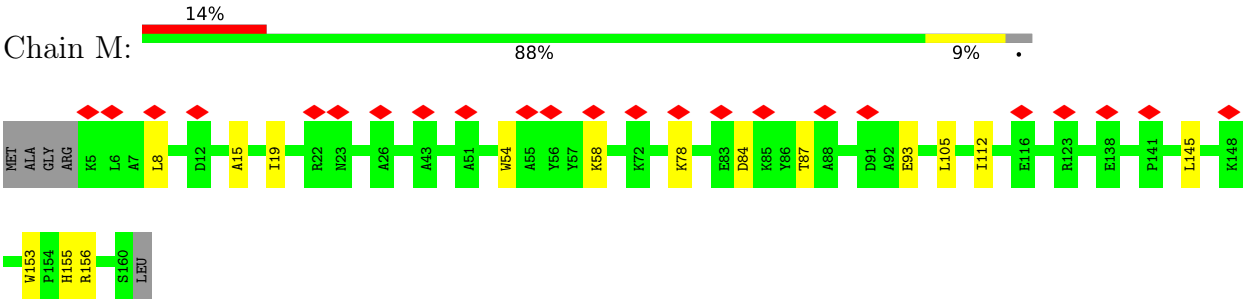


• Molecule 8: ATP synthase-coupling factor 6, mitochondrial

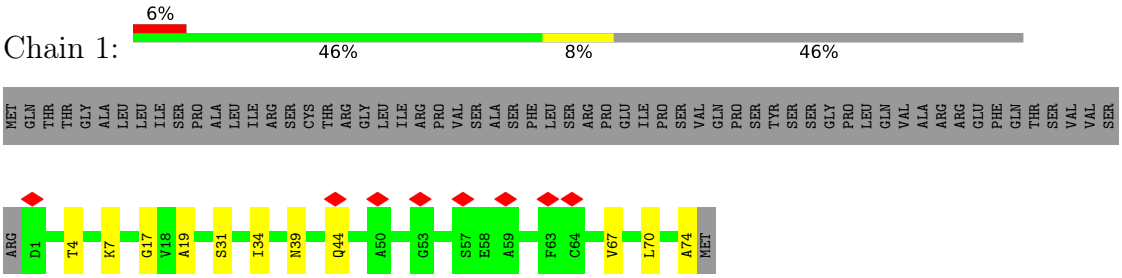
Chain L:



• Molecule 9: ATP synthase subunit d, mitochondrial



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



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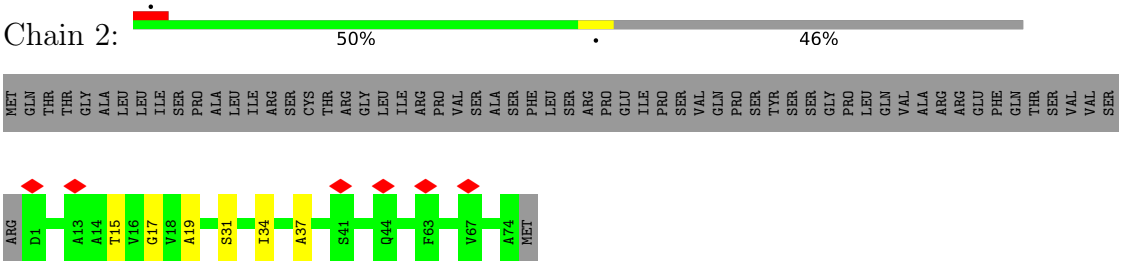

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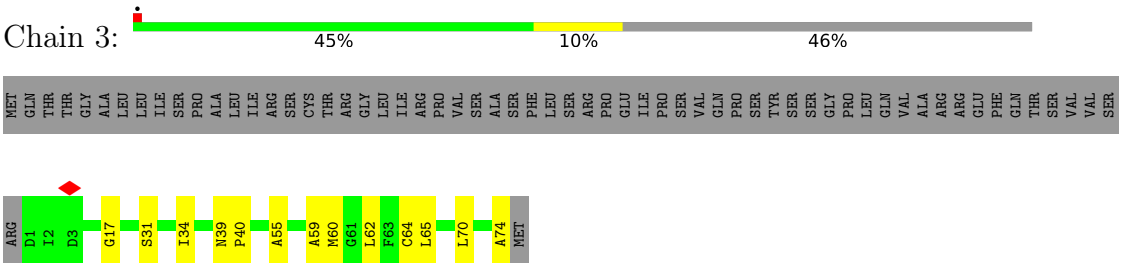

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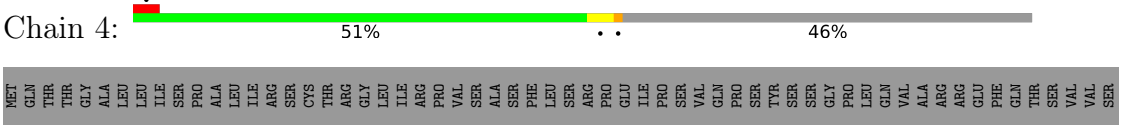
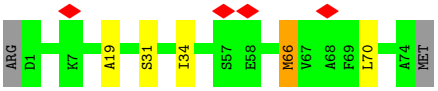
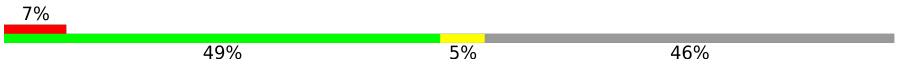
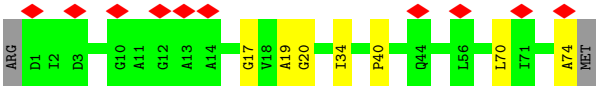




• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

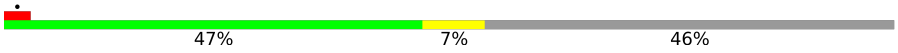
Chain 5:

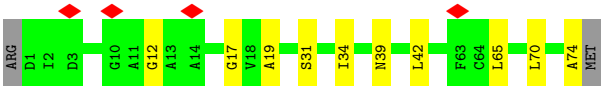




• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

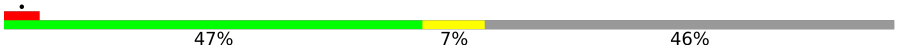
Chain 6:

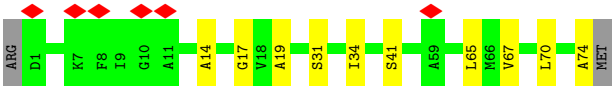




• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

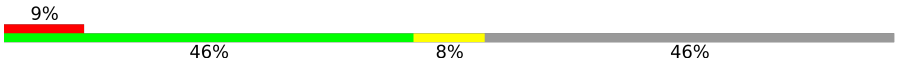
Chain 7:

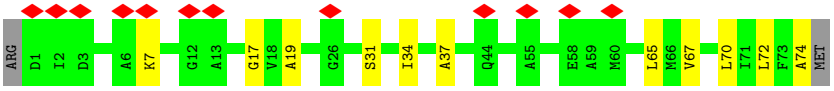




• Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

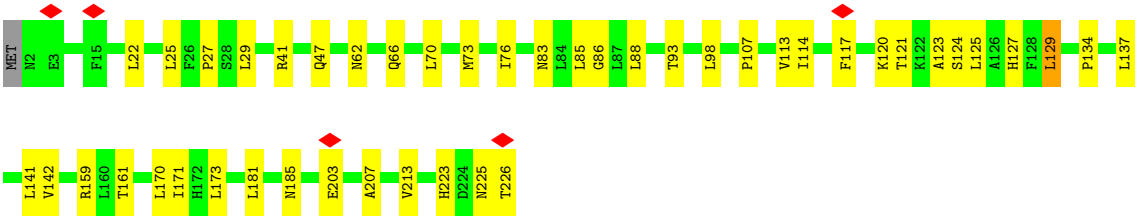
Chain 8:



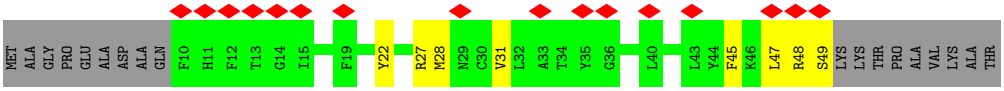


• Molecule 11: ATP synthase subunit a

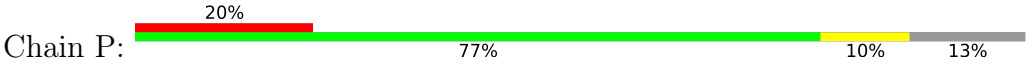
Chain N:

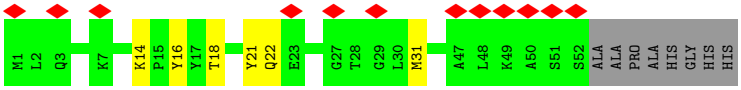


• Molecule 12: Subunit DAPIT

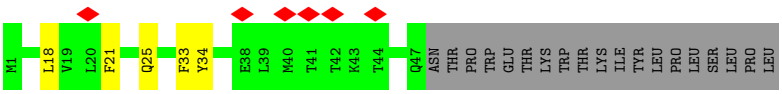


• Molecule 13: ATP synthase membrane subunit 6.8PL

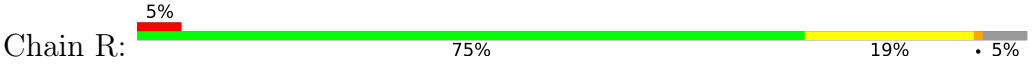


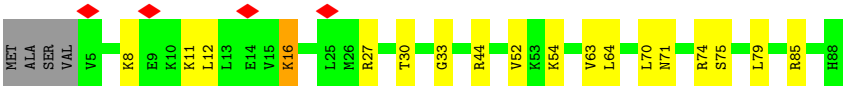


• Molecule 14: ATP synthase protein 8

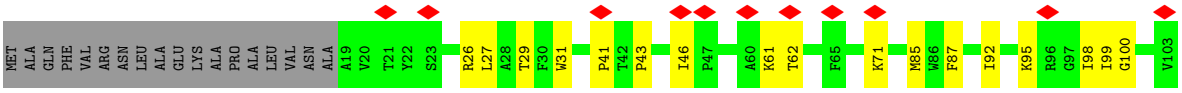


• Molecule 15: ATP synthase membrane subunit f

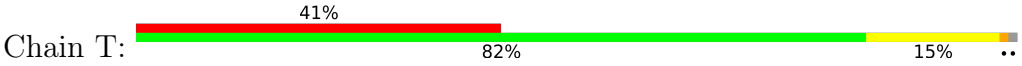


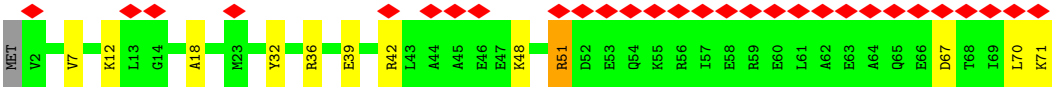


• Molecule 16: ATP synthase subunit



• 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

5.1 Standard geometry

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

All (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
1	C	324	LEU	CA-CB-CG	6.60	130.48	115.30
2	F	259	ASN	N-CA-C	-6.11	94.50	111.00
17	T	70	LEU	CA-CB-CG	6.00	129.11	115.30
1	C	103	LEU	CA-CB-CG	5.96	129.00	115.30
2	E	331	LEU	CB-CG-CD1	-5.90	100.96	111.00
2	F	258	ASP	C-N-CA	5.90	136.45	121.70
2	F	416	LEU	CA-CB-CG	5.83	128.70	115.30
1	B	64	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	166	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	143	ARG	C-N-CA	-5.72	107.40	121.70
1	C	12	LEU	CA-CB-CG	5.47	127.88	115.30
2	F	331	LEU	CB-CG-CD2	-5.44	101.75	111.00
11	N	129	LEU	CA-CB-CG	5.43	127.80	115.30
8	L	30	ASP	CB-CG-OD1	5.40	123.16	118.30
2	D	258	ASP	C-N-CA	5.39	135.17	121.70
2	D	64	ALA	C-N-CA	5.30	134.95	121.70
1	A	12	LEU	CB-CG-CD2	-5.28	102.02	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	255	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	B	418	LEU	CA-CB-CG	5.11	127.05	115.30
2	F	38	LEU	CA-CB-CG	5.08	126.99	115.30
1	C	59	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	LYS	Peptide
1	A	64	LEU	Mainchain,Peptide
1	A	65	ASN	Peptide
1	A	67	GLU	Peptide
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
1	C	352	LEU	Peptide
1	C	366	ASN	Peptide
2	D	118	ILE	Peptide
2	D	122	ALA	Peptide
2	D	258	ASP	Peptide
2	D	280	ALA	Peptide
2	D	54	HIS	Peptide
2	D	57	GLU	Peptide
2	D	83	PRO	Peptide
2	E	258	ASP	Peptide
2	E	397	GLU	Peptide
2	E	51	VAL	Peptide
2	E	52	ALA	Peptide
2	E	54	HIS	Peptide
2	E	64	ALA	Peptide
2	F	118	ILE	Peptide
2	F	20	GLY	Peptide
2	F	258	ASP	Peptide
2	F	280	ALA	Peptide
2	F	54	HIS	Peptide
2	F	56	GLY	Peptide
4	H	39	PRO	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
2:D:10:GLY:HA2	2:D:79:ASP:O	1.64	0.97
2:E:27:PHE:O	2:E:58:SER:HB2	1.65	0.97
2:E:338:SER:O	2:E:349:ALA:HB3	1.66	0.95
4:H:16:MET:HA	4:H:88:SER:O	1.70	0.91
1:A:199:LEU:O	1:A:228:TYR:HB3	1.75	0.85
6:J:115:GLU:HA	6:J:147:VAL:O	1.74	0.85
1:C:199:LEU:O	1:C:228:TYR:HB3	1.76	0.85
2:F:21:ALA:HA	2:F:64:ALA:H	1.42	0.83
2:F:27:PHE:O	2:F:58:SER:HA	1.81	0.81
2:E:21:ALA:O	2:E:63:ILE:HA	1.82	0.78
2:D:54:HIS:HA	2:D:59:THR:O	1.83	0.78
4:H:15:GLN:O	4:H:88:SER:HB2	1.85	0.76
2:E:259:ASN:HA	2:E:311:ALA:O	1.86	0.76
3:G:66:HIS:HA	3:G:157:GLU:O	1.87	0.74
2:D:27:PHE:O	2:D:58:SER:HB2	1.87	0.74
2:E:336:VAL:O	2:E:350:VAL:HA	1.89	0.73
10:5:70:LEU:O	10:5:74:ALA:HB3	1.88	0.73
2:F:54:HIS:HA	2:F:59:THR:O	1.88	0.72
10:3:70:LEU:O	10:3:74:ALA:HB3	1.88	0.72
1:C:362:ARG:HH22	2:F:374:ARG:HD2	1.57	0.70
2:D:21:ALA:HA	2:D:64:ALA:H	1.56	0.69
2:E:21:ALA:HA	2:E:64:ALA:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ARG:HA	1:C:323:ALA:O	1.93	0.68
2:D:259:ASN:CA	2:D:311:ALA:O	2.30	0.68
2:E:36:ASN:O	2:E:50:GLU:HA	1.92	0.68
2:E:50:GLU:O	2:E:62:THR:HA	1.93	0.68
2:F:259:ASN:CA	2:F:311:ALA:O	2.36	0.67
2:E:40:VAL:HB	2:E:47:LEU:HB3	1.75	0.67
2:D:40:VAL:HB	2:D:47:LEU:HB3	1.77	0.67
2:F:346:ILE:HG23	2:F:417:SER:HB3	1.77	0.67
1:C:347:ASP:OD2	2:D:193:ARG:NH1	2.29	0.66
1:B:268:TYR:HB2	1:B:325:PRO:HA	1.77	0.66
2:F:40:VAL:HB	2:F:47:LEU:HB3	1.77	0.66
10:6:19:ALA:HB2	10:7:17:GLY:HA2	1.77	0.66
1:B:144:GLU:HB2	1:B:161:ARG:HB2	1.76	0.66
2:D:141:VAL:HG11	2:D:350:VAL:HG11	1.78	0.66
2:D:54:HIS:CA	2:D:59:THR:O	2.44	0.65
2:F:27:PHE:O	2:F:58:SER:CA	2.45	0.64
2:E:31:LEU:HD13	2:E:58:SER:HB3	1.78	0.64
2:F:300:THR:HG23	2:F:305:SER:HA	1.78	0.64
7:K:6:PRO:HG2	15:R:52:VAL:HG12	1.78	0.64
2:F:15:ILE:O	2:F:74:GLY:N	2.30	0.64
1:B:251:CYS:SG	1:B:268:TYR:OH	2.56	0.64
2:F:369:HIS:HD2	2:F:440:ILE:HD11	1.63	0.64
2:F:54:HIS:CA	2:F:59:THR:O	2.45	0.64
1:B:137:ILE:HG13	2:F:105:ASP:HA	1.80	0.63
1:A:144:GLU:HB2	1:A:161:ARG:HB2	1.80	0.63
2:F:21:ALA:CA	2:F:64:ALA:H	2.11	0.63
2:F:54:HIS:C	2:F:59:THR:O	2.37	0.63
2:F:96:ILE:HD12	2:F:105:ASP:HB3	1.81	0.63
1:A:423:ARG:NH2	1:A:456:LEU:O	2.32	0.63
1:C:59:LEU:HD11	1:C:82:ILE:HD11	1.81	0.62
1:C:351:PHE:H	1:C:370:SER:HB3	1.63	0.62
4:H:136:GLU:HA	4:H:139:GLU:HG2	1.81	0.62
2:F:10:GLY:HA2	2:F:79:ASP:O	2.00	0.62
2:F:36:ASN:O	2:F:50:GLU:HA	2.00	0.62
4:H:39:PRO:HB2	4:H:62:LEU:H	1.63	0.62
1:C:144:GLU:HB2	1:C:161:ARG:HB2	1.82	0.62
1:B:133:ALA:HB3	2:F:225:ASN:HD22	1.65	0.62
1:C:66:LEU:HD23	2:D:73:ARG:HG3	1.83	0.61
2:D:14:ARG:HA	2:D:75:GLN:O	2.00	0.61
1:C:349:GLN:NE2	1:C:369:LEU:O	2.33	0.61
2:E:54:HIS:HA	2:E:59:THR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:172:HIS:NE2	8:L:29:VAL:O	2.31	0.61
1:C:251:CYS:SG	1:C:268:TYR:OH	2.58	0.61
4:H:48:LEU:HD23	4:H:49:ALA:H	1.64	0.61
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.34	0.60
7:K:79:GLY:O	11:N:41:ARG:NH2	2.34	0.60
1:A:161:ARG:HH12	1:A:197:LYS:HA	1.67	0.60
10:4:66:MET:HG2	11:N:170:LEU:HD13	1.84	0.60
2:E:15:ILE:O	2:E:74:GLY:N	2.34	0.60
20:S:201:LHG:H172	20:S:201:LHG:H371	1.84	0.60
2:D:34:ILE:HG23	2:D:52:ALA:HA	1.84	0.60
1:B:349:GLN:HG3	1:B:371:VAL:HG12	1.83	0.60
2:D:54:HIS:C	2:D:59:THR:O	2.40	0.60
7:K:54:THR:HG22	7:K:56:GLU:H	1.67	0.60
22:R:301:CDL:H851	22:R:301:CDL:H381	1.84	0.60
1:C:179:ALA:HB1	1:C:267:ILE:HD13	1.84	0.60
10:7:19:ALA:HB2	10:8:17:GLY:HA2	1.84	0.60
2:E:95:ARG:NH2	2:E:108:GLY:O	2.35	0.60
10:6:31:SER:HA	10:6:34:ILE:HG22	1.84	0.59
11:N:29:LEU:HD21	22:R:302:CDL:H162	1.84	0.59
1:B:251:CYS:O	1:B:255:GLU:HB2	2.02	0.59
1:B:350:ILE:HA	1:B:371:VAL:O	2.02	0.59
1:C:185:ASN:OD1	1:C:188:ARG:NH2	2.36	0.59
22:R:303:CDL:H351	22:R:303:CDL:H211	1.83	0.59
2:D:226:GLU:O	2:D:231:ARG:NH1	2.36	0.59
2:D:31:LEU:HD13	2:D:58:SER:HB3	1.84	0.59
9:M:15:ALA:O	9:M:19:ILE:HB	2.02	0.59
1:A:63:SER:HA	1:A:73:VAL:HA	1.85	0.59
2:F:27:PHE:O	2:F:58:SER:CB	2.51	0.59
3:G:166:ARG:HE	3:G:172:LYS:HB2	1.68	0.59
16:S:41:PRO:HG3	17:T:12:LYS:HE2	1.84	0.59
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.35	0.59
2:D:379:ILE:HG12	2:D:409:ALA:HB2	1.84	0.59
1:A:65:ASN:O	1:A:72:GLY:N	2.36	0.58
2:D:172:ILE:O	2:D:176:ALA:HB3	2.04	0.58
16:S:87:PHE:HB2	17:T:18:ALA:HB1	1.85	0.58
2:E:31:LEU:HD12	2:E:32:PRO:HD2	1.83	0.58
2:E:336:VAL:HB	2:E:351:ASP:HB2	1.85	0.58
4:H:66:HIS:ND1	4:H:71:THR:O	2.37	0.58
11:N:25:LEU:HB3	22:R:302:CDL:H341	1.86	0.58
1:A:151:LYS:NZ	1:A:465:GLU:OE2	2.34	0.58
10:7:31:SER:HA	10:7:34:ILE:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:ARG:NH2	2:F:67:GLY:O	2.37	0.58
23:T:201:S12:H27	23:T:201:S12:H7	1.86	0.58
2:E:140:LYS:HG2	2:E:439:THR:HG22	1.85	0.57
2:F:280:ALA:O	2:F:282:GLY:N	2.34	0.57
2:E:84:ILE:O	2:E:117:ALA:HA	2.04	0.57
2:D:155:GLY:O	2:D:334:THR:HA	2.04	0.57
10:7:70:LEU:O	10:7:74:ALA:HB3	2.04	0.57
1:C:140:ILE:O	1:C:311:LYS:HB3	2.04	0.57
2:D:253:VAL:O	2:D:306:ILE:HA	2.04	0.57
10:8:7:LYS:NZ	10:8:72:LEU:O	2.38	0.57
2:F:341:ILE:HG22	2:F:346:ILE:HB	1.87	0.57
1:B:64:LEU:HD23	1:B:65:ASN:H	1.70	0.57
1:C:145:PRO:HB2	1:C:147:GLN:HE21	1.69	0.57
1:A:107:VAL:HG22	1:A:231:VAL:HB	1.87	0.57
3:G:75:ARG:O	3:G:228:ARG:NH2	2.38	0.57
10:1:44:GLN:NE2	12:O:22:TYR:OH	2.37	0.57
1:C:67:GLU:O	2:D:73:ARG:NH1	2.37	0.57
1:C:307:GLU:HG3	1:C:345:ILE:HD11	1.85	0.57
4:H:53:PRO:HA	4:H:84:VAL:HG23	1.86	0.57
1:B:383:MET:HA	1:B:386:VAL:HG12	1.87	0.57
1:A:286:ARG:NH2	2:D:275:GLY:O	2.38	0.57
2:D:15:ILE:O	2:D:74:GLY:N	2.31	0.57
11:N:25:LEU:HD21	14:Q:18:LEU:HD12	1.87	0.57
1:A:3:THR:HG23	6:J:14:ILE:HD11	1.87	0.56
1:A:67:GLU:O	1:A:69:ASP:N	2.38	0.56
1:A:479:LEU:HD13	1:A:496:LYS:HD3	1.87	0.56
2:F:38:LEU:HD22	2:F:51:VAL:HG23	1.87	0.56
4:H:96:GLU:OE2	5:I:24:ARG:NH2	2.38	0.56
15:R:75:SER:O	15:R:79:LEU:N	2.38	0.56
15:R:30:THR:HG23	15:R:33:GLY:H	1.68	0.56
1:C:50:GLU:HA	1:C:63:SER:O	2.05	0.56
1:C:439:GLU:HG3	1:C:480:LEU:HB3	1.87	0.56
2:E:399:SER:H	2:E:402:ASP:HB3	1.71	0.56
1:C:183:ILE:HG23	1:C:228:TYR:HE2	1.70	0.56
1:A:355:GLU:O	1:A:359:LYS:HB2	2.05	0.56
2:F:34:ILE:HG23	2:F:52:ALA:HA	1.87	0.56
10:3:31:SER:HA	10:3:34:ILE:HG22	1.87	0.56
14:Q:21:PHE:O	14:Q:25:GLN:CB	2.54	0.56
20:S:201:LHG:H111	20:S:201:LHG:H282	1.87	0.56
2:D:209:ASN:ND2	2:D:212:ASP:OD1	2.39	0.56
6:J:31:LYS:HD2	6:J:81:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:8:31:SER:HA	10:8:34:ILE:HG22	1.88	0.56
1:A:133:ALA:HB3	2:E:225:ASN:HD22	1.71	0.56
7:K:16:LEU:HD12	7:K:17:ILE:HG23	1.88	0.56
1:C:147:GLN:O	1:C:186:GLN:NE2	2.39	0.56
10:2:31:SER:HA	10:2:34:ILE:HG22	1.86	0.56
16:S:61:LYS:HG3	16:S:62:THR:HG23	1.87	0.56
2:D:396:ASP:HB3	3:G:75:ARG:HD2	1.87	0.55
1:B:294:TYR:HB3	1:B:298:VAL:HG21	1.88	0.55
21:2:201:P5S:H33A	21:2:201:P5S:H52A	1.88	0.55
2:E:53:GLN:OE1	2:E:61:ARG:NH1	2.39	0.55
2:F:335:THR:HA	2:F:355:SER:HB2	1.88	0.55
17:T:48:LYS:HD2	17:T:51:ARG:HD2	1.88	0.55
1:B:170:ASP:O	1:B:175:LYS:NZ	2.32	0.55
1:C:390:MET:HG3	1:C:424:LEU:HD13	1.89	0.55
2:D:36:ASN:O	2:D:50:GLU:HA	2.05	0.55
2:D:95:ARG:NH2	2:D:108:GLY:O	2.39	0.55
3:G:164:ARG:HH21	3:G:166:ARG:HD3	1.71	0.55
10:6:70:LEU:O	10:6:74:ALA:HB3	2.06	0.55
1:B:379:GLN:HB2	1:B:384:LYS:HE3	1.89	0.55
11:N:86:GLY:HA3	11:N:93:THR:HG22	1.89	0.55
16:S:27:LEU:O	16:S:31:TRP:N	2.37	0.55
1:C:220:LEU:HD13	1:C:229:THR:HG21	1.89	0.55
15:R:85:ARG:NH2	16:S:99:ILE:O	2.39	0.55
2:E:95:ARG:HE	2:E:110:ILE:HG12	1.72	0.55
1:B:31:VAL:O	6:J:59:TYR:OH	2.25	0.55
2:E:418:GLN:NE2	2:E:432:LYS:O	2.40	0.55
16:S:92:ILE:HD12	16:S:95:LYS:HD3	1.88	0.55
2:D:280:ALA:O	2:D:282:GLY:N	2.39	0.55
6:J:98:THR:HA	6:J:101:VAL:HG12	1.88	0.55
2:E:155:GLY:O	2:E:334:THR:HA	2.07	0.55
10:1:31:SER:HA	10:1:34:ILE:HG22	1.88	0.55
11:N:41:ARG:NE	15:R:54:LYS:O	2.38	0.55
1:B:67:GLU:O	2:F:73:ARG:NH1	2.40	0.54
2:E:38:LEU:HB2	2:E:49:LEU:HB2	1.89	0.54
2:E:53:GLN:O	2:E:59:THR:O	2.24	0.54
2:F:341:ILE:HB	2:F:349:ALA:HB1	1.88	0.54
7:K:204:LEU:HA	7:K:207:LYS:HG2	1.89	0.54
9:M:145:LEU:HB3	9:M:155:HIS:HB2	1.89	0.54
1:A:258:ARG:HD3	1:A:321:LEU:HB2	1.90	0.54
2:D:38:LEU:HB2	2:D:49:LEU:HB2	1.89	0.54
2:E:374:ARG:NH2	2:E:377:GLN:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:VAL:O	2:D:274:LEU:N	2.40	0.54
1:A:499:GLU:OE2	1:A:503:ASN:ND2	2.40	0.54
9:M:84:ASP:OD2	9:M:87:THR:OG1	2.23	0.54
1:A:201:CYS:HB2	1:A:229:THR:HG22	1.90	0.54
8:L:73:LYS:NZ	9:M:93:GLU:OE2	2.41	0.54
2:F:17:ALA:HB3	2:F:24:ASP:HB2	1.89	0.54
10:6:65:LEU:HD11	10:7:67:VAL:HG21	1.89	0.54
17:T:32:TYR:OH	17:T:36:ARG:NH2	2.41	0.54
2:E:54:HIS:CA	2:E:59:THR:O	2.56	0.54
2:D:21:ALA:CA	2:D:64:ALA:H	2.19	0.54
15:R:63:VAL:HG22	22:R:303:CDL:H591	1.89	0.54
1:B:439:GLU:HG3	1:B:480:LEU:HB3	1.90	0.54
1:A:163:GLN:O	1:A:322:THR:HA	2.08	0.54
1:C:136:ILE:HD12	1:C:137:ILE:HG12	1.90	0.54
1:A:14:GLU:HA	1:A:17:LEU:HD22	1.89	0.54
2:E:54:HIS:C	2:E:59:THR:O	2.47	0.53
4:H:59:ARG:HH11	4:H:60:PRO:HD2	1.72	0.53
1:C:166:LEU:HD23	1:C:325:PRO:HG2	1.90	0.53
14:Q:21:PHE:O	14:Q:25:GLN:HB2	2.07	0.53
1:C:139:ARG:NH2	1:C:307:GLU:O	2.36	0.53
1:A:15:ARG:NH1	6:J:91:GLU:OE1	2.39	0.53
2:D:169:MET:HB3	2:D:422:VAL:HG21	1.90	0.53
4:H:50:ALA:HB3	10:7:41:SER:HB2	1.89	0.53
1:C:166:LEU:HD21	1:C:342:VAL:HG12	1.90	0.53
1:C:203:TYR:OH	1:C:269:ASP:OD2	2.26	0.53
6:J:22:LEU:HG	6:J:85:LEU:HD22	1.89	0.53
6:J:55:LEU:O	6:J:65:LYS:NZ	2.42	0.53
2:E:84:ILE:HB	2:E:118:ILE:HG12	1.91	0.53
2:F:257:ILE:O	2:F:310:GLN:HA	2.09	0.53
21:2:201:P5S:H24	21:2:201:P5S:H43A	1.90	0.53
2:E:280:ALA:O	2:E:282:GLY:N	2.42	0.53
2:F:21:ALA:HA	2:F:64:ALA:N	2.17	0.53
2:F:32:PRO:HG2	2:F:51:VAL:HG21	1.91	0.53
10:1:19:ALA:HB2	10:2:17:GLY:HA2	1.90	0.53
2:D:51:VAL:HA	2:D:62:THR:HG22	1.90	0.53
2:D:346:ILE:HG23	2:D:417:SER:HB2	1.91	0.53
2:F:460:TYR:O	2:F:471:LYS:NZ	2.41	0.53
15:R:85:ARG:HD2	16:S:100:GLY:HA3	1.90	0.53
1:C:199:LEU:O	1:C:228:TYR:CB	2.51	0.53
2:E:95:ARG:HH12	2:E:107:ARG:HB2	1.73	0.53
2:F:279:SER:OG	2:F:280:ALA:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:37:ASP:HB2	4:H:64:VAL:HB	1.90	0.53
1:C:65:ASN:HD22	1:C:285:LEU:HG	1.74	0.53
1:A:12:LEU:HG	6:J:88:LEU:HD21	1.91	0.53
1:A:203:TYR:OH	1:A:269:ASP:OD2	2.27	0.53
2:D:341:ILE:HG22	2:D:346:ILE:HB	1.90	0.53
6:J:183:SER:HA	6:J:186:MET:HG2	1.91	0.53
11:N:181:LEU:O	11:N:185:ASN:N	2.40	0.53
1:C:139:ARG:HD3	1:C:310:ALA:HB3	1.91	0.52
2:D:239:LEU:HD22	2:D:298:ILE:HB	1.91	0.52
2:D:294:MET:SD	2:D:295:GLN:NE2	2.77	0.52
10:4:31:SER:HA	10:4:34:ILE:HG22	1.90	0.52
9:M:153:TRP:HB3	11:N:70:LEU:HB2	1.91	0.52
2:F:50:GLU:O	2:F:62:THR:HA	2.09	0.52
2:D:41:GLN:HE22	2:D:78:LEU:HB2	1.74	0.52
3:G:65:LYS:HB2	3:G:155:PHE:HA	1.90	0.52
2:E:38:LEU:O	2:E:48:VAL:HA	2.10	0.52
2:D:260:ILE:HG13	2:D:312:ILE:HG12	1.92	0.52
4:H:46:GLY:H	10:6:39:ASN:HA	1.75	0.52
20:K:302:LHG:H321	20:K:302:LHG:H122	1.91	0.52
10:1:70:LEU:O	10:1:74:ALA:HB3	2.09	0.52
2:F:33:PRO:O	2:F:36:ASN:ND2	2.42	0.52
2:E:256:PHE:HA	2:E:309:VAL:O	2.10	0.52
11:N:98:LEU:HA	11:N:161:THR:HG21	1.91	0.52
1:B:303:SER:O	1:B:307:GLU:HB2	2.09	0.52
2:F:164:LYS:NZ	19:F:600:ADP:O1B	2.38	0.52
2:D:351:ASP:O	2:D:355:SER:OG	2.26	0.52
22:R:302:CDL:H181	22:R:303:CDL:H601	1.90	0.52
2:F:10:GLY:CA	2:F:79:ASP:O	2.57	0.52
7:K:9:GLY:HA3	15:R:52:VAL:HG11	1.91	0.52
17:T:7:VAL:HG23	17:T:12:LYS:HD2	1.91	0.52
1:C:241:PRO:HA	1:C:244:TYR:HB3	1.92	0.51
1:A:353:GLU:HG2	1:A:366:ASN:HB3	1.92	0.51
1:A:497:LEU:HA	1:A:500:ILE:HG22	1.92	0.51
3:G:64:LYS:O	3:G:66:HIS:ND1	2.40	0.51
1:C:27:GLU:OE1	1:C:90:ARG:NH2	2.42	0.51
2:D:151:GLY:H	2:D:307:THR:HB	1.74	0.51
11:N:107:PRO:HD3	13:P:31:MET:HG3	1.92	0.51
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.92	0.51
2:F:40:VAL:HG22	2:F:77:VAL:HG22	1.92	0.51
1:B:340:THR:HG21	2:F:316:ALA:HA	1.91	0.51
1:C:220:LEU:HB3	1:C:225:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:LEU:HA	1:C:456:LEU:HD13	1.92	0.51
2:E:40:VAL:HG22	2:E:77:VAL:HG22	1.92	0.51
10:8:70:LEU:O	10:8:74:ALA:HB3	2.11	0.51
2:E:48:VAL:HG13	2:E:65:MET:HG3	1.93	0.51
6:J:62:ARG:HA	6:J:65:LYS:HD3	1.92	0.51
1:B:176:THR:N	19:B:602:ADP:O2A	2.41	0.51
1:A:109:ASP:O	1:A:112:GLY:N	2.40	0.51
2:D:153:LYS:HZ3	2:D:298:ILE:HG23	1.76	0.51
1:B:366:ASN:O	1:B:370:SER:N	2.34	0.50
3:G:204:TYR:HH	4:H:83:THR:HG1	1.58	0.50
10:2:19:ALA:HB2	10:3:17:GLY:HA2	1.92	0.50
16:S:98:ILE:HG21	20:S:201:LHG:H132	1.93	0.50
17:T:39:GLU:OE1	17:T:42:ARG:NH2	2.44	0.50
1:C:108:VAL:HA	1:C:114:ALA:HA	1.93	0.50
6:J:135:LYS:HE2	6:J:148:LEU:HD21	1.92	0.50
1:B:186:GLN:O	1:B:190:ASN:ND2	2.39	0.50
1:B:170:ASP:OD1	1:B:329:THR:OG1	2.27	0.50
1:C:167:ILE:HD11	1:C:324:LEU:HD12	1.94	0.50
1:C:186:GLN:HG3	1:C:199:LEU:HD22	1.94	0.50
1:A:382:ALA:HB2	1:A:488:LYS:HA	1.93	0.50
2:F:103:PRO:HG3	2:F:109:PRO:HA	1.93	0.50
3:G:64:LYS:HG2	3:G:101:LYS:HE2	1.92	0.50
3:G:166:ARG:NH2	3:G:171:TYR:O	2.38	0.50
6:J:34:GLN:HA	6:J:37:LYS:HE2	1.93	0.50
7:K:43:LEU:HD21	20:S:201:LHG:H212	1.93	0.50
1:A:199:LEU:O	1:A:228:TYR:CB	2.54	0.50
2:E:209:ASN:ND2	2:E:212:ASP:OD1	2.45	0.50
2:E:181:GLY:HA2	2:E:251:GLN:HG2	1.93	0.49
2:F:56:GLY:H	2:F:59:THR:HB	1.77	0.49
4:H:20:PHE:HB3	4:H:27:PHE:HB2	1.94	0.49
9:M:54:TRP:O	9:M:58:LYS:HB2	2.11	0.49
2:D:336:VAL:HB	2:D:351:ASP:HB3	1.93	0.49
2:F:259:ASN:OD1	2:F:313:TYR:N	2.45	0.49
11:N:137:LEU:O	11:N:141:LEU:HB2	2.11	0.49
1:B:44:LEU:HG	1:B:47:VAL:HB	1.94	0.49
2:D:33:PRO:O	2:D:36:ASN:ND2	2.46	0.49
6:J:7:PRO:HG3	6:J:20:THR:HG22	1.93	0.49
2:E:243:GLU:OE1	2:E:297:ARG:NH2	2.39	0.49
2:E:341:ILE:HG13	2:E:344:LEU:HD12	1.93	0.49
2:D:276:ARG:HH12	2:D:284:GLN:HB2	1.76	0.49
3:G:246:LEU:HA	3:G:249:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:GLY:HA3	1:C:266:ILE:HD11	1.94	0.49
1:C:361:ILE:HA	1:C:429:LYS:HG2	1.93	0.49
7:K:118:VAL:HG11	9:M:105:LEU:HD13	1.94	0.49
7:K:152:LYS:NZ	7:K:156:ASP:OD2	2.35	0.49
1:C:78:ASN:ND2	2:F:121:GLU:OE2	2.46	0.49
2:D:157:PHE:O	2:D:337:LEU:HB2	2.13	0.49
1:A:396:GLN:HB3	1:A:417:LEU:HD21	1.94	0.49
2:F:38:LEU:HB2	2:F:79:ASP:HA	1.95	0.49
5:I:10:LEU:HD11	5:I:14:ARG:HG2	1.95	0.49
13:P:18:THR:O	13:P:22:GLN:NE2	2.43	0.49
15:R:70:LEU:HB3	22:R:302:CDL:H442	1.95	0.49
1:C:273:LYS:HA	1:C:276:VAL:HG12	1.95	0.49
2:F:118:ILE:O	2:F:119:HIS:ND1	2.46	0.49
4:H:45:PHE:HA	10:6:39:ASN:HB3	1.95	0.49
10:3:55:ALA:HB3	11:N:213:VAL:HG21	1.95	0.49
10:5:19:ALA:HB2	10:6:17:GLY:HA2	1.95	0.49
1:C:165:GLU:HA	1:C:348:GLY:O	2.12	0.49
2:D:410:ARG:NE	2:D:456:GLU:OE1	2.42	0.49
2:F:338:SER:O	2:F:349:ALA:CB	2.45	0.48
2:D:279:SER:OG	2:D:280:ALA:N	2.46	0.48
2:D:411:LYS:NZ	2:D:451:PHE:O	2.34	0.48
2:F:172:ILE:O	2:F:176:ALA:HB3	2.12	0.48
1:A:66:LEU:C	1:A:70:ASN:O	2.51	0.48
2:D:118:ILE:O	2:D:119:HIS:ND1	2.45	0.48
2:F:346:ILE:HD11	2:F:414:ARG:HD3	1.95	0.48
1:A:66:LEU:HD13	2:E:18:VAL:HB	1.94	0.48
1:B:311:LYS:HD2	1:B:320:SER:HB3	1.95	0.48
8:L:12:VAL:HA	8:L:15:ILE:HD12	1.94	0.48
1:B:127:ARG:HH22	1:B:131:LEU:HD12	1.78	0.48
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.95	0.48
2:E:255:LEU:O	2:E:308:SER:HA	2.14	0.48
2:E:279:SER:OG	2:E:280:ALA:N	2.40	0.48
2:E:185:PHE:HB3	2:E:219:LEU:HD23	1.95	0.48
2:F:254:LEU:HD23	2:F:307:THR:HB	1.96	0.48
10:1:17:GLY:HA2	10:8:19:ALA:HB2	1.96	0.48
3:G:74:ASP:OD1	3:G:110:ASP:N	2.46	0.48
22:R:301:CDL:H552	22:R:301:CDL:H422	1.96	0.48
10:8:70:LEU:O	10:8:74:ALA:CB	2.62	0.47
11:N:134:PRO:HG2	11:N:137:LEU:HD13	1.96	0.47
15:R:44:ARG:NH1	20:R:304:LHG:O5	2.46	0.47
1:C:353:GLU:H	1:C:366:ASN:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:136:PRO:HG2	3:G:218:LYS:HG2	1.95	0.47
1:B:367:VAL:HB	1:B:398:ARG:HH21	1.79	0.47
1:C:258:ARG:HD3	1:C:321:LEU:HB2	1.95	0.47
3:G:81:ILE:HD11	3:G:227:ALA:HB3	1.97	0.47
4:H:133:ILE:HA	4:H:136:GLU:HG2	1.96	0.47
7:K:154:ARG:HH21	8:L:59:PRO:HD2	1.79	0.47
11:N:124:SER:HA	11:N:127:HIS:HD1	1.79	0.47
2:E:175:VAL:HG21	2:E:254:LEU:HD11	1.96	0.47
10:4:19:ALA:HB2	10:5:17:GLY:HA2	1.95	0.47
1:B:203:TYR:OH	1:B:269:ASP:OD2	2.29	0.47
2:D:389:ILE:HA	3:G:19:ILE:HD13	1.95	0.47
22:R:303:CDL:H531	22:R:303:CDL:H322	1.97	0.47
2:E:51:VAL:HA	2:E:62:THR:HG22	1.97	0.47
11:N:83:ASN:HB3	11:N:207:ALA:HB1	1.96	0.47
2:E:209:ASN:H	2:E:215:SER:HB3	1.80	0.47
2:F:55:LEU:HD13	2:F:61:ARG:HH21	1.80	0.47
4:H:87:ASP:OD1	4:H:87:ASP:N	2.47	0.47
11:N:113:VAL:HA	11:N:225:ASN:HD21	1.80	0.47
1:B:283:LEU:HD21	1:B:289:PRO:HB3	1.97	0.47
1:C:141:SER:OG	2:D:197:ASP:OD1	2.26	0.47
1:A:7:GLU:OE2	6:J:94:ARG:NH1	2.47	0.47
1:A:206:ILE:HG21	1:A:274:GLN:HB2	1.96	0.47
2:F:168:ILE:HD11	2:F:311:ALA:HB2	1.96	0.47
2:F:246:ARG:HD3	2:F:306:ILE:HG13	1.98	0.47
4:H:54:THR:HG22	4:H:84:VAL:HG22	1.96	0.47
6:J:186:MET:HG3	7:K:174:ILE:HD11	1.97	0.47
1:C:136:ILE:H	1:C:136:ILE:HG13	1.60	0.46
1:C:424:LEU:HD23	1:C:427:LEU:HD13	1.96	0.46
2:E:24:ASP:OD1	2:E:24:ASP:N	2.47	0.46
2:F:222:GLY:HA3	2:F:234:VAL:HG21	1.98	0.46
3:G:71:VAL:HA	3:G:108:VAL:HG22	1.97	0.46
16:S:26:ARG:NH2	16:S:29:THR:OG1	2.49	0.46
1:B:26:GLU:HG3	1:B:46:ASN:HB2	1.98	0.46
4:H:115:ALA:HA	4:H:131:ILE:HD11	1.97	0.46
6:J:121:THR:HB	6:J:163:ILE:HG13	1.98	0.46
1:C:48:GLN:HB2	2:D:70:GLY:HA2	1.97	0.46
1:A:20:ASP:OD1	1:A:20:ASP:N	2.48	0.46
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.96	0.46
1:A:209:LYS:HE2	1:A:211:SER:HB3	1.97	0.46
3:G:113:ARG:HG2	3:G:127:THR:HG21	1.97	0.46
7:K:130:ASN:HB2	9:M:8:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:NH2	1:B:307:GLU:O	2.33	0.46
3:G:147:GLU:O	3:G:151:SER:OG	2.27	0.46
2:D:21:ALA:HA	2:D:64:ALA:N	2.29	0.46
2:D:55:LEU:HD11	2:D:61:ARG:HE	1.80	0.46
1:B:195:GLU:OE2	1:B:262:LYS:NZ	2.43	0.46
1:C:347:ASP:HB2	1:C:373:ARG:HD3	1.98	0.46
3:G:64:LYS:HE2	3:G:102:GLU:HG2	1.97	0.46
1:A:23:VAL:O	1:A:28:THR:OG1	2.34	0.46
1:A:26:GLU:HG2	1:A:45:ARG:HB2	1.97	0.46
2:D:49:LEU:HB3	2:D:62:THR:HB	1.97	0.46
15:R:8:LYS:O	15:R:27:ARG:NH2	2.49	0.46
1:B:105:GLY:HA2	1:B:226:MET:HG3	1.98	0.46
1:B:351:PHE:HB3	1:B:370:SER:HA	1.98	0.46
1:C:362:ARG:O	1:C:430:GLN:N	2.44	0.46
1:A:55:PHE:HE2	1:A:75:VAL:HG22	1.81	0.46
11:N:47:GLN:HG3	14:Q:33:PHE:HE1	1.81	0.46
2:D:291:MET:HA	2:D:294:MET:HG3	1.98	0.45
10:1:39:ASN:ND2	10:8:37:ALA:O	2.49	0.45
11:N:27:PRO:HG3	11:N:85:LEU:HD22	1.97	0.45
1:C:199:LEU:HD11	1:C:265:LEU:HD23	1.99	0.45
2:E:341:ILE:HB	2:E:349:ALA:HB1	1.98	0.45
2:E:21:ALA:CA	2:E:64:ALA:O	2.64	0.45
2:D:35:LEU:N	2:D:51:VAL:O	2.48	0.45
2:D:160:ALA:O	2:D:339:ARG:NH2	2.49	0.45
3:G:127:THR:HB	5:I:46:VAL:HB	1.98	0.45
9:M:54:TRP:O	9:M:58:LYS:CB	2.64	0.45
10:7:65:LEU:HD11	10:8:67:VAL:HG21	1.98	0.45
1:C:444:VAL:HG13	1:C:445:ILE:HD12	1.99	0.45
1:A:274:GLN:HE22	1:A:301:LEU:HD21	1.81	0.45
1:A:65:ASN:HA	1:A:66:LEU:HD12	1.99	0.45
6:J:165:ARG:HB2	6:J:170:TYR:HD1	1.82	0.45
11:N:22:LEU:HD12	22:R:302:CDL:H372	1.98	0.45
11:N:73:MET:HA	11:N:76:ILE:HG22	1.99	0.45
1:A:166:LEU:HB2	1:A:346:THR:HG21	1.99	0.45
2:D:40:VAL:HG22	2:D:77:VAL:HG12	1.98	0.45
6:J:155:ASP:N	6:J:155:ASP:OD1	2.50	0.45
2:D:321:ASP:HB3	2:D:324:PRO:HD2	1.99	0.45
3:G:168:VAL:O	3:G:226:SER:OG	2.35	0.45
11:N:120:LYS:HB3	11:N:123:ALA:HB3	1.99	0.45
13:P:14:LYS:O	13:P:18:THR:CB	2.64	0.45
1:B:39:ALA:HB3	1:B:73:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ARG:NH2	1:C:308:ARG:O	2.50	0.45
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.99	0.45
1:C:471:HIS:O	1:C:474:SER:OG	2.34	0.45
1:A:31:VAL:HA	1:A:41:VAL:HG12	1.99	0.45
1:A:381:ARG:HB2	1:A:488:LYS:HB3	1.99	0.45
2:E:43:ARG:NH1	2:E:69:GLU:O	2.42	0.45
2:F:186:ALA:HB3	2:F:257:ILE:HG12	1.99	0.45
7:K:50:ILE:HD13	20:K:302:LHG:HC91	1.99	0.45
2:F:155:GLY:HA3	2:F:331:LEU:HD21	1.99	0.44
7:K:121:ARG:HH11	9:M:19:ILE:HG13	1.81	0.44
12:O:45:PHE:O	12:O:49:SER:OG	2.29	0.44
2:E:333:ALA:HA	2:E:357:SER:HA	1.98	0.44
3:G:106:ILE:HD13	3:G:148:LEU:HD13	1.99	0.44
11:N:129:LEU:HD11	12:O:27:ARG:HG2	1.99	0.44
2:E:154:ILE:HB	2:E:333:ALA:HB3	1.99	0.44
7:K:154:ARG:O	7:K:158:HIS:ND1	2.38	0.44
2:D:348:PRO:O	2:D:350:VAL:N	2.51	0.44
1:A:139:ARG:O	2:E:196:ASN:ND2	2.51	0.44
2:E:49:LEU:HB3	2:E:62:THR:HB	1.99	0.44
6:J:179:ILE:O	6:J:183:SER:OG	2.27	0.44
7:K:168:LYS:HD3	8:L:39:LEU:HD22	2.00	0.44
1:A:98:PRO:HD2	1:A:112:GLY:HA3	2.00	0.44
2:F:188:VAL:HG22	2:F:234:VAL:HB	1.99	0.44
2:F:411:LYS:NZ	2:F:451:PHE:O	2.43	0.44
4:H:38:VAL:HA	4:H:39:PRO:HD3	1.79	0.44
1:C:142:VAL:HG21	1:C:374:VAL:HB	2.00	0.44
2:E:18:VAL:HA	2:E:23:VAL:HG12	2.00	0.44
6:J:175:ALA:HB1	8:L:10:LEU:HD21	2.00	0.44
8:L:13:ASP:OD1	8:L:16:ARG:NH2	2.47	0.44
1:C:15:ARG:HG2	6:J:186:MET:HA	1.99	0.43
1:C:199:LEU:O	1:C:228:TYR:HA	2.18	0.43
2:D:236:LEU:HD13	2:D:239:LEU:HD12	1.99	0.43
2:F:375:GLY:HA3	2:F:447:LEU:HD11	2.00	0.43
1:B:35:GLY:HA2	2:E:53:GLN:HG2	1.99	0.43
2:E:239:LEU:HD21	2:E:297:ARG:HB2	1.99	0.43
2:D:259:ASN:OD1	2:D:313:TYR:N	2.51	0.43
12:O:47:LEU:HG	12:O:48:ARG:HE	1.81	0.43
3:G:107:GLY:O	3:G:127:THR:HA	2.17	0.43
5:I:7:GLN:HE22	10:3:40:PRO:HB2	1.82	0.43
6:J:15:GLU:HG2	6:J:100:ALA:HB3	2.01	0.43
2:E:369:HIS:CD2	2:E:440:ILE:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2:37:ALA:O	10:3:39:ASN:ND2	2.51	0.43
1:B:351:PHE:H	1:B:370:SER:HB2	1.83	0.43
2:E:38:LEU:HD13	2:E:77:VAL:HG11	2.01	0.43
2:F:118:ILE:HG23	2:F:236:LEU:HB3	1.99	0.43
2:F:338:SER:OG	2:F:339:ARG:N	2.51	0.43
3:G:71:VAL:HG13	3:G:162:PHE:HA	1.99	0.43
1:B:189:PHE:HB3	1:B:197:LYS:HG3	2.01	0.43
2:E:341:ILE:HA	2:E:344:LEU:HB2	2.01	0.43
1:C:200:TYR:HA	1:C:228:TYR:HA	2.01	0.43
1:C:342:VAL:HA	1:C:345:ILE:HG22	2.01	0.43
2:E:387:GLN:HA	2:E:390:ILE:HG22	2.00	0.43
2:F:157:PHE:O	2:F:337:LEU:HB2	2.18	0.43
6:J:73:THR:HG23	6:J:78:PHE:HB2	2.01	0.43
1:C:108:VAL:HG13	1:C:232:VAL:HG22	2.00	0.43
3:G:1:ALA:HB3	3:G:6:ILE:HD11	2.01	0.43
10:3:62:LEU:HD13	10:3:65:LEU:HB3	1.99	0.43
3:G:190:MET:HG2	3:G:201:LEU:HD11	2.00	0.43
6:J:178:LYS:HB2	8:L:10:LEU:HD22	2.01	0.43
7:K:157:TYR:HE1	8:L:46:LEU:HB3	1.84	0.43
11:N:88:LEU:HD11	15:R:64:LEU:HD22	2.00	0.43
15:R:71:ASN:HA	15:R:74:ARG:HG2	2.00	0.43
16:S:43:PRO:HA	16:S:46:ILE:HG12	2.00	0.43
1:A:11:ILE:HA	1:A:14:GLU:HG3	2.01	0.43
1:A:268:TYR:HB2	1:A:325:PRO:HA	2.01	0.43
2:D:140:LYS:NZ	2:D:415:PHE:O	2.46	0.43
2:F:190:GLU:HG3	2:F:191:ARG:H	1.84	0.43
3:G:164:ARG:HB3	3:G:172:LYS:HB3	2.01	0.43
1:B:251:CYS:O	1:B:255:GLU:CB	2.65	0.42
1:C:362:ARG:HB3	19:C:602:ADP:C6	2.53	0.42
2:F:27:PHE:O	2:F:58:SER:OG	2.37	0.42
4:H:37:ASP:HA	4:H:46:GLY:HA2	2.01	0.42
10:4:70:LEU:HD12	11:N:173:LEU:HD11	2.01	0.42
11:N:142:VAL:HG21	12:O:31:VAL:HG22	2.01	0.42
11:N:171:ILE:HD11	11:N:203:GLU:HG3	2.01	0.42
2:D:341:ILE:HB	2:D:349:ALA:HB1	2.00	0.42
2:F:383:TYR:HE1	2:F:406:VAL:HG13	1.83	0.42
4:H:128:ARG:HA	4:H:131:ILE:HG22	2.01	0.42
10:4:34:ILE:HD12	10:5:34:ILE:HG23	2.00	0.42
1:C:356:LEU:HB3	1:C:361:ILE:HG22	2.01	0.42
1:C:397:TYR:CG	1:C:421:GLY:HA3	2.54	0.42
1:A:66:LEU:HB3	2:E:73:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:HD23	1:A:365:ILE:HA	2.01	0.42
2:E:26:GLN:NE2	2:E:57:GLU:OE1	2.51	0.42
11:N:125:LEU:HD23	12:O:28:MET:HG3	2.00	0.42
15:R:12:LEU:H	20:R:304:LHG:HC11	1.84	0.42
1:B:151:LYS:NZ	1:B:465:GLU:OE2	2.49	0.42
2:E:98:ASN:O	2:E:101:GLY:N	2.41	0.42
2:D:341:ILE:HG23	2:D:344:LEU:HD12	2.01	0.42
10:5:40:PRO:HG3	10:6:42:LEU:HD21	2.02	0.42
17:T:67:ASP:HA	17:T:71:LYS:HE2	2.00	0.42
1:B:52:MET:HA	1:B:61:GLY:O	2.18	0.42
1:B:432:GLN:HG3	19:B:602:ADP:C6	2.54	0.42
1:C:160:GLY:N	1:C:163:GLN:OE1	2.45	0.42
1:C:490:SER:O	1:C:494:ASP:N	2.50	0.42
2:D:21:ALA:HA	2:D:64:ALA:O	2.20	0.42
4:H:84:VAL:HG12	4:H:90:VAL:HA	2.00	0.42
10:1:4:THR:HA	10:1:7:LYS:HG2	2.01	0.42
1:A:104:LEU:HD13	1:A:230:ILE:HG13	2.01	0.42
2:E:15:ILE:HD13	2:E:25:VAL:HG22	2.02	0.42
2:E:423:ALA:O	2:E:427:THR:OG1	2.32	0.42
2:D:228:PRO:HB2	2:D:270:VAL:HG13	2.00	0.42
7:K:196:LYS:HZ2	8:L:8:GLN:N	2.18	0.42
10:1:67:VAL:HG21	10:8:65:LEU:HD11	2.00	0.42
1:A:166:LEU:HD23	1:A:325:PRO:HG2	2.00	0.42
2:E:252:ASP:OD1	2:E:305:SER:OG	2.33	0.42
2:D:144:LEU:HG	2:D:145:LEU:HG	2.00	0.42
13:P:21:TYR:HE2	14:Q:25:GLN:HE22	1.66	0.42
1:B:472:VAL:HG12	1:B:480:LEU:HD11	2.01	0.42
2:E:257:ILE:HG22	2:E:259:ASN:H	1.84	0.42
2:E:260:ILE:HD12	2:E:260:ILE:HA	1.90	0.42
9:M:153:TRP:N	13:P:16:TYR:OH	2.53	0.42
1:A:264:ALA:O	1:A:321:LEU:HA	2.20	0.42
3:G:249:THR:HA	3:G:252:ARG:HG2	2.00	0.42
4:H:18:PHE:HA	4:H:90:VAL:HB	2.02	0.42
15:R:16:LYS:HD2	15:R:16:LYS:HA	1.75	0.42
1:A:311:LYS:NZ	1:A:318:GLY:O	2.53	0.42
2:E:188:VAL:HG22	2:E:234:VAL:HB	2.01	0.42
10:4:19:ALA:HB1	10:5:20:GLY:HA3	2.02	0.42
1:A:66:LEU:CA	1:A:70:ASN:O	2.68	0.41
2:E:328:PHE:HA	2:E:331:LEU:HB2	2.01	0.41
2:D:86:ILE:HD13	2:D:118:ILE:HD11	2.01	0.41
1:C:202:ILE:HB	1:C:266:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HG12	1:A:285:LEU:HD22	2.01	0.41
1:A:76:PHE:HE1	1:A:241:PRO:HB2	1.85	0.41
1:A:200:TYR:HA	1:A:228:TYR:HA	2.02	0.41
2:D:383:TYR:HE1	2:D:406:VAL:HG13	1.85	0.41
6:J:6:ARG:HD3	6:J:7:PRO:HD2	2.02	0.41
7:K:40:GLY:HA3	16:S:85:MET:HB3	2.01	0.41
7:K:108:ILE:HG23	9:M:112:ILE:HD11	2.02	0.41
20:K:302:LHG:H222	22:R:303:CDL:H392	2.02	0.41
2:E:321:ASP:HB3	2:E:324:PRO:HD2	2.01	0.41
10:3:59:ALA:HB1	11:N:159:ARG:HB2	2.01	0.41
1:B:335:SER:HA	1:B:340:THR:HG23	2.02	0.41
2:E:23:VAL:HG22	2:E:64:ALA:HB2	2.02	0.41
22:R:302:CDL:H181	22:R:303:CDL:H741	2.01	0.41
1:A:97:VAL:HG21	1:A:249:SER:HA	2.03	0.41
2:F:35:LEU:N	2:F:51:VAL:O	2.51	0.41
4:H:137:ALA:O	4:H:141:LEU:HB2	2.20	0.41
1:C:321:LEU:HA	1:C:321:LEU:HD12	1.83	0.41
1:A:479:LEU:HD21	1:A:497:LEU:HG	2.02	0.41
2:E:23:VAL:O	2:E:62:THR:OG1	2.34	0.41
2:E:55:LEU:H	2:E:55:LEU:HG	1.60	0.41
2:E:342:ALA:N	2:E:349:ALA:HB2	2.34	0.41
11:N:22:LEU:HB3	22:R:302:CDL:H402	2.02	0.41
11:N:62:ASN:O	11:N:66:GLN:N	2.54	0.41
11:N:117:PHE:O	11:N:121:THR:OG1	2.30	0.41
1:B:44:LEU:HD11	1:B:90:ARG:HG3	2.03	0.41
1:B:172:GLN:OE1	2:E:358:ARG:NH2	2.54	0.41
13:P:14:LYS:O	13:P:18:THR:OG1	2.33	0.41
1:A:171:ARG:NH2	2:D:354:ASP:OD1	2.53	0.41
7:K:24:PHE:HE1	16:S:71:LYS:HG3	1.86	0.41
1:B:244:TYR:OH	1:B:304:ARG:NH2	2.54	0.41
1:C:150:ILE:HG22	1:C:153:VAL:H	1.85	0.41
1:C:268:TYR:HE2	1:C:323:ALA:HB1	1.85	0.41
2:E:161:GLY:H	2:E:339:ARG:HH11	1.68	0.41
2:E:291:MET:O	2:E:295:GLN:HB2	2.21	0.41
3:G:43:VAL:HG11	4:H:29:ASN:HD22	1.86	0.41
3:G:116:LEU:HD12	3:G:120:HIS:HB2	2.03	0.41
6:J:9:VAL:HG23	6:J:111:VAL:HG11	2.02	0.41
6:J:39:LEU:HD12	6:J:102:ILE:HG12	2.03	0.41
10:2:15:THR:HG22	10:3:64:CYS:HB2	2.03	0.41
10:6:12:GLY:HA2	10:7:14:ALA:HB2	2.03	0.41
16:S:92:ILE:HD11	16:S:98:ILE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:VAL:HB	1:C:116:ASP:HB3	2.03	0.41
1:C:208:GLN:NE2	1:C:269:ASP:OD2	2.54	0.41
1:A:142:VAL:HG21	1:A:374:VAL:HG11	2.02	0.41
2:E:386:LEU:HD23	2:E:389:ILE:HD12	2.03	0.41
2:D:54:HIS:CD2	2:D:60:VAL:HG12	2.56	0.41
11:N:223:HIS:HA	11:N:226:THR:HB	2.02	0.41
1:B:287:ARG:HH12	2:F:273:LEU:HD21	1.86	0.40
1:B:400:VAL:O	1:B:404:ALA:N	2.54	0.40
1:C:109:ASP:HB3	1:C:113:ASN:O	2.21	0.40
1:C:409:ASP:OD1	1:C:409:ASP:N	2.54	0.40
1:A:66:LEU:HA	1:A:70:ASN:O	2.20	0.40
2:E:183:SER:O	2:E:217:VAL:HA	2.21	0.40
2:D:259:ASN:HD21	2:D:313:TYR:HB2	1.85	0.40
2:F:256:PHE:HA	2:F:309:VAL:O	2.21	0.40
3:G:67:LEU:HD11	3:G:106:ILE:HG23	2.03	0.40
9:M:156:ARG:NH1	14:Q:34:TYR:O	2.54	0.40
10:3:70:LEU:O	10:3:74:ALA:CB	2.64	0.40
20:S:202:LHG:H142	20:S:202:LHG:H112	1.91	0.40
1:B:99:VAL:HG11	1:B:127:ARG:HB2	2.04	0.40
2:F:271:SER:HA	2:F:274:LEU:HB2	2.04	0.40
3:G:108:VAL:HA	3:G:128:PHE:HB2	2.03	0.40
1:B:444:VAL:HA	1:B:468:PHE:HZ	1.86	0.40
1:A:351:PHE:H	1:A:370:SER:HB2	1.85	0.40
4:H:132:GLN:HA	4:H:135:ILE:HG22	2.04	0.40
2:E:167:LEU:HD13	2:E:337:LEU:HD21	2.03	0.40
2:E:277:ILE:HG23	3:G:266:ILE:HG21	2.03	0.40
2:D:48:VAL:HG11	2:D:100:ILE:HG12	2.02	0.40
1:B:48:GLN:HB3	2:F:72:VAL:HG22	2.03	0.40
1:B:66:LEU:HB3	2:F:73:ARG:HD3	2.02	0.40
1:B:192:GLY:O	1:B:198:LYS:NZ	2.53	0.40
1:C:356:LEU:HD13	1:C:361:ILE:HG21	2.03	0.40
2:E:254:LEU:HA	2:E:307:THR:O	2.21	0.40
2:E:318:ASP:OD2	2:E:321:ASP:N	2.55	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	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

All (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
2	F	281	VAL
2	D	55	LEU
4	H	39	PRO
2	E	279	SER
2	D	53	GLN
6	J	62	ARG
1	A	491	GLU
2	E	398	LEU
2	F	53	GLN
1	B	336	ALA
1	A	68	PRO
2	E	55	LEU
2	F	282	GLY
2	D	123	PRO
2	D	282	GLY

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	95	VAL

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Mol	Chain	Res	Type
1	B	166	LEU
1	B	274	GLN
1	B	450	ARG
1	C	146	MET
1	C	164	ARG
1	A	17	LEU
1	A	129	VAL
1	A	146	MET
1	A	285	LEU
1	A	366	ASN
1	A	423	ARG
1	A	484	ARG
2	E	73	ARG
2	E	153	LYS
2	E	294	MET
2	D	144	LEU
2	D	174	ASN
2	D	255	LEU
2	D	307	THR
2	F	127	GLU
2	F	172	ILE
2	F	173	ASN
2	F	174	ASN
2	F	301	THR
3	G	8	ARG
3	G	113	ARG
3	G	144	ILE
3	G	190	MET
3	G	211	ASN
4	H	32	ASN
4	H	34	ARG
4	H	48	LEU
4	H	74	LYS
4	H	103	LEU
6	J	184	ARG
7	K	86	ASN
8	L	19	ARG
8	L	21	LYS
8	L	73	LYS
9	M	78	LYS
10	3	60	MET
10	4	66	MET

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Mol	Chain	Res	Type
11	N	114	ILE
15	R	11	LYS
15	R	16	LYS
17	T	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	366	ASN
1	C	147	GLN
1	C	366	ASN
1	C	405	GLN
1	A	366	ASN
1	A	405	GLN
2	E	54	HIS
2	D	26	GLN
2	F	132	GLN
2	F	173	ASN
2	F	174	ASN
2	F	179	HIS
2	F	223	GLN
3	G	163	ASN
4	H	15	GLN
4	H	32	ASN
5	I	7	GLN
7	K	86	ASN
7	K	145	HIS
10	1	44	GLN
14	Q	31	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (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
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	-

All (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
22	R	301	CDL	C22-C21	-3.47	1.32	1.51
22	R	302	CDL	C22-C21	-3.47	1.32	1.51
22	R	303	CDL	C19-C18	-3.46	1.32	1.51
22	R	302	CDL	C19-C18	-3.45	1.32	1.51
22	R	303	CDL	C62-C61	-3.45	1.32	1.51
22	R	303	CDL	C59-C58	-3.44	1.32	1.51
22	R	301	CDL	C39-C38	-3.44	1.32	1.51
22	R	301	CDL	C79-C78	-3.44	1.32	1.51
22	R	301	CDL	C62-C61	-3.44	1.32	1.51
22	R	301	CDL	C59-C58	-3.44	1.32	1.51
22	R	303	CDL	C22-C21	-3.44	1.32	1.51
22	R	301	CDL	C82-C81	-3.43	1.32	1.51
22	R	302	CDL	C59-C58	-3.43	1.32	1.51
22	R	302	CDL	C62-C61	-3.41	1.32	1.51
22	R	303	CDL	C42-C41	-3.41	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	303	CDL	C39-C38	-3.36	1.32	1.51
20	R	304	LHG	O7-C5	-2.48	1.40	1.46
20	2	202	LHG	O7-C5	-2.48	1.40	1.46
20	K	302	LHG	O7-C5	-2.45	1.40	1.46
19	D	600	ADP	C5-C4	2.32	1.47	1.40
19	C	602	ADP	C5-C4	2.30	1.47	1.40
19	A	602	ADP	C5-C4	2.29	1.47	1.40
20	S	202	LHG	O7-C5	-2.28	1.40	1.46
19	B	602	ADP	C5-C4	2.25	1.46	1.40
19	F	600	ADP	C5-C4	2.18	1.46	1.40
22	R	302	CDL	C79-C78	-2.16	1.32	1.49
20	S	201	LHG	P-O6	2.15	1.68	1.59
19	A	602	ADP	O4'-C1'	2.14	1.44	1.41

All (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
20	R	304	LHG	O4-P-O5	4.11	132.57	112.24
19	F	600	ADP	PA-O3A-PB	-3.95	119.28	132.83
19	F	600	ADP	C3'-C2'-C1'	3.76	106.64	100.98
19	D	600	ADP	PA-O3A-PB	-3.64	120.34	132.83
19	C	602	ADP	PA-O3A-PB	-3.54	120.67	132.83
19	A	602	ADP	PA-O3A-PB	-3.42	121.08	132.83
19	C	602	ADP	N3-C2-N1	-3.36	123.42	128.68
19	F	600	ADP	N3-C2-N1	-3.33	123.48	128.68
20	K	302	LHG	O8-C23-C24	3.22	122.03	111.91
19	D	600	ADP	N3-C2-N1	-3.18	123.70	128.68
19	A	602	ADP	C4-C5-N7	-3.11	106.15	109.40
19	A	602	ADP	N3-C2-N1	-3.10	123.83	128.68
19	B	602	ADP	N3-C2-N1	-3.06	123.90	128.68
19	B	602	ADP	PA-O3A-PB	-2.96	122.66	132.83
19	C	602	ADP	C3'-C2'-C1'	2.90	105.34	100.98
19	B	602	ADP	C4-C5-N7	-2.84	106.44	109.40
19	D	600	ADP	C3'-C2'-C1'	2.82	105.22	100.98
20	2	202	LHG	O8-C23-C24	2.76	120.56	111.91
22	R	303	CDL	C40-C39-C38	2.61	127.67	114.42
20	R	304	LHG	C11-C10-C9	-2.58	101.32	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	K	302	LHG	C11-C10-C9	-2.58	101.32	114.42
22	R	301	CDL	C62-C61-C60	2.56	127.42	114.42
22	R	303	CDL	C62-C61-C60	2.55	127.38	114.42
22	R	303	CDL	C22-C21-C20	2.52	127.24	114.42
20	K	301	LHG	O8-C23-C24	2.52	119.83	111.91
22	R	301	CDL	C40-C39-C38	2.52	127.23	114.42
20	S	202	LHG	O8-C23-C24	2.51	119.80	111.91
20	S	202	LHG	C11-C10-C9	-2.51	101.69	114.42
20	S	201	LHG	C11-C10-C9	-2.51	101.69	114.42
22	R	302	CDL	C60-C59-C58	2.50	127.14	114.42
22	R	302	CDL	C40-C39-C38	2.50	127.11	114.42
22	R	301	CDL	C80-C79-C78	2.50	127.09	114.42
22	R	302	CDL	C19-C18-C17	2.49	127.08	114.42
22	R	302	CDL	C62-C61-C60	2.49	127.07	114.42
22	R	301	CDL	C22-C21-C20	2.49	127.05	114.42
22	R	303	CDL	C60-C59-C58	2.48	127.03	114.42
22	R	301	CDL	C20-C19-C18	2.48	127.02	114.42
22	R	302	CDL	C42-C41-C40	2.47	126.96	114.42
22	R	302	CDL	C22-C21-C20	2.46	126.91	114.42
20	K	302	LHG	C20-C19-C18	-2.44	102.02	114.42
22	R	303	CDL	C19-C18-C17	2.44	126.81	114.42
22	R	303	CDL	C42-C41-C40	2.44	126.80	114.42
22	R	301	CDL	C60-C59-C58	2.43	126.74	114.42
22	R	301	CDL	C42-C41-C40	2.42	126.71	114.42
22	R	303	CDL	C20-C19-C18	2.41	126.66	114.42
20	2	202	LHG	C11-C10-C9	-2.41	102.20	114.42
20	S	201	LHG	O8-C23-C24	2.40	119.43	111.91
22	R	302	CDL	C20-C19-C18	2.39	126.58	114.42
22	R	301	CDL	C82-C81-C80	2.39	126.57	114.42
22	R	301	CDL	C59-C58-C57	2.39	126.57	114.42
19	D	600	ADP	C4-C5-N7	-2.38	106.92	109.40
20	R	304	LHG	O8-C23-C24	2.38	119.37	111.91
22	R	303	CDL	C63-C62-C61	2.38	126.49	114.42
22	R	303	CDL	C43-C42-C41	2.38	126.49	114.42
22	R	302	CDL	C23-C22-C21	2.37	126.45	114.42
22	R	302	CDL	C59-C58-C57	2.37	126.45	114.42
20	K	301	LHG	C11-C10-C9	-2.37	102.41	114.42
19	C	602	ADP	C4-C5-N7	-2.36	106.94	109.40
20	2	202	LHG	C20-C19-C18	-2.36	102.44	114.42
22	R	302	CDL	C39-C38-C37	2.36	126.40	114.42
22	R	301	CDL	C23-C22-C21	2.35	126.38	114.42
22	R	302	CDL	C63-C62-C61	2.35	126.37	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	202	LHG	C5-O7-C7	-2.35	112.00	117.79
22	R	302	CDL	C43-C42-C41	2.34	126.30	114.42
22	R	301	CDL	C79-C78-C77	2.34	126.29	114.42
22	R	301	CDL	C19-C18-C17	2.32	126.20	114.42
20	S	202	LHG	C20-C19-C18	-2.32	102.67	114.42
20	S	201	LHG	C20-C19-C18	-2.31	102.71	114.42
20	R	304	LHG	C20-C19-C18	-2.30	102.72	114.42
20	2	202	LHG	C18-C17-C16	-2.29	102.80	114.42
22	R	301	CDL	C39-C38-C37	2.29	126.03	114.42
20	K	302	LHG	C18-C17-C16	-2.27	102.91	114.42
22	R	303	CDL	C23-C22-C21	2.26	125.89	114.42
20	S	202	LHG	C18-C17-C16	-2.26	102.96	114.42
22	R	303	CDL	C59-C58-C57	2.26	125.89	114.42
22	R	301	CDL	C43-C42-C41	2.26	125.88	114.42
20	R	304	LHG	C18-C17-C16	-2.25	103.02	114.42
19	A	602	ADP	C3'-C2'-C1'	2.22	104.32	100.98
22	R	301	CDL	C63-C62-C61	2.20	125.57	114.42
20	S	201	LHG	C18-C17-C16	-2.19	103.31	114.42
22	R	303	CDL	C39-C38-C37	2.18	125.48	114.42
20	S	202	LHG	C27-C26-C25	-2.16	103.47	114.42
20	K	301	LHG	C27-C26-C25	-2.12	103.68	114.42
22	R	301	CDL	C83-C82-C81	2.11	125.11	114.42
20	S	201	LHG	C27-C26-C25	-2.10	103.75	114.42
20	R	304	LHG	C27-C26-C25	-2.10	103.75	114.42
19	B	602	ADP	O3B-PB-O2B	2.07	115.55	107.64
22	R	303	CDL	CB4-OB6-CB5	2.06	122.87	117.79
19	F	600	ADP	C4-C5-N7	-2.05	107.26	109.40
22	R	303	CDL	CA4-OA6-CA5	2.03	122.79	117.79
20	K	302	LHG	C27-C26-C25	-2.02	104.16	114.42
20	K	302	LHG	C5-O7-C7	-2.02	112.82	117.79

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

All (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
19	D	600	ADP	C5'-O5'-PA-O1A
19	F	600	ADP	C5'-O5'-PA-O3A
20	K	301	LHG	C1-C2-C3-O3
20	K	301	LHG	C3-O3-P-O5
20	K	301	LHG	C3-O3-P-O6
20	K	301	LHG	C4-O6-P-O3
20	K	301	LHG	C4-O6-P-O5
20	K	302	LHG	C3-O3-P-O5
20	K	302	LHG	C8-C7-O7-C5
20	K	302	LHG	O10-C23-O8-C6
20	K	302	LHG	C24-C23-O8-C6
20	2	202	LHG	O1-C1-C2-C3
20	2	202	LHG	C1-C2-C3-O3
20	2	202	LHG	C4-O6-P-O5
20	2	202	LHG	C8-C7-O7-C5
20	R	304	LHG	O1-C1-C2-C3
20	R	304	LHG	C3-O3-P-O4
20	R	304	LHG	C3-O3-P-O5
20	R	304	LHG	C3-O3-P-O6
20	R	304	LHG	C4-O6-P-O5
20	S	201	LHG	O1-C1-C2-C3
20	S	201	LHG	C4-O6-P-O5
20	S	201	LHG	O6-C4-C5-O7
20	S	201	LHG	O9-C7-O7-C5
20	S	201	LHG	C8-C7-O7-C5
20	S	202	LHG	O1-C1-C2-C3
20	S	202	LHG	C1-C2-C3-O3
20	S	202	LHG	C4-O6-P-O5
21	2	201	P5S	CA-CB-OG-P12
21	2	201	P5S	CB-OG-P12-O15
21	2	201	P5S	C3-O16-P12-O13
22	R	301	CDL	CB2-C1-CA2-OA2
22	R	301	CDL	CA2-OA2-PA1-OA3
22	R	301	CDL	CA3-OA5-PA1-OA2
22	R	301	CDL	CA3-OA5-PA1-OA4
22	R	301	CDL	CB3-OB5-PB2-OB3
22	R	302	CDL	CA3-OA5-PA1-OA2
22	R	302	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
22	R	302	CDL	CA3-OA5-PA1-OA4
22	R	303	CDL	O1-C1-CA2-OA2
22	R	303	CDL	CA3-OA5-PA1-OA2
22	R	303	CDL	CA3-OA5-PA1-OA3
22	R	303	CDL	CA3-OA5-PA1-OA4
22	R	303	CDL	CB2-OB2-PB2-OB5
23	T	201	S12	CB-OG-P-O4
23	T	201	S12	C2-O2-P-OG
23	T	201	S12	C2-O2-P-O3
23	T	201	S12	C2-O2-P-O4
20	S	202	LHG	C24-C23-O8-C6
20	2	202	LHG	O10-C23-O8-C6
20	S	201	LHG	O10-C23-O8-C6
20	K	301	LHG	O9-C7-O7-C5
20	2	202	LHG	O9-C7-O7-C5
20	S	201	LHG	C24-C23-O8-C6
22	R	301	CDL	C20-C21-C22-C23
22	R	301	CDL	C37-C38-C39-C40
22	R	301	CDL	C40-C41-C42-C43
22	R	301	CDL	C80-C81-C82-C83
22	R	302	CDL	C20-C21-C22-C23
22	R	302	CDL	C37-C38-C39-C40
22	R	302	CDL	C40-C41-C42-C43
22	R	302	CDL	C57-C58-C59-C60
22	R	303	CDL	C57-C58-C59-C60
22	R	303	CDL	C61-C62-C63-C64
20	K	302	LHG	O9-C7-O7-C5
20	S	202	LHG	O10-C23-O8-C6
20	K	301	LHG	O2-C2-C3-O3
20	2	202	LHG	O2-C2-C3-O3
20	S	202	LHG	O2-C2-C3-O3
22	R	301	CDL	O1-C1-CA2-OA2
22	R	302	CDL	O1-C1-CB2-OB2
20	2	202	LHG	C24-C23-O8-C6
19	B	602	ADP	O4'-C4'-C5'-O5'
20	K	301	LHG	C24-C23-O8-C6
20	R	304	LHG	C1-C2-C3-O3
22	R	302	CDL	CA2-C1-CB2-OB2
22	R	303	CDL	CB2-C1-CA2-OA2
22	R	301	CDL	C61-C62-C63-C64
20	R	304	LHG	O2-C2-C3-O3
22	R	301	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
22	R	302	CDL	O1-C1-CA2-OA2
22	R	301	CDL	CA7-C31-C32-C33
20	S	201	LHG	C7-C8-C9-C10
21	2	201	P5S	C38-C39-C40-C41
22	R	302	CDL	CA5-C11-C12-C13
20	R	304	LHG	C7-C8-C9-C10
20	K	301	LHG	O10-C23-O8-C6
20	2	202	LHG	C3-O3-P-O6
20	R	304	LHG	C4-O6-P-O3
20	S	201	LHG	C3-O3-P-O6
20	S	202	LHG	C4-O6-P-O3
21	2	201	P5S	CB-OG-P12-O16
22	R	301	CDL	CB3-OB5-PB2-OB2
22	R	303	CDL	CA2-OA2-PA1-OA5
20	S	202	LHG	C23-C24-C25-C26
20	K	302	LHG	C32-C33-C34-C35
20	S	201	LHG	C24-C25-C26-C27
22	R	301	CDL	C19-C20-C21-C22
22	R	301	CDL	C36-C37-C38-C39
22	R	302	CDL	C18-C19-C20-C21
22	R	302	CDL	C39-C40-C41-C42
23	T	201	S12	C11-C10-C9-C8
19	B	602	ADP	C4'-C5'-O5'-PA
22	R	301	CDL	C39-C40-C41-C42
20	K	302	LHG	O2-C2-C3-O3
20	K	302	LHG	C30-C31-C32-C33
20	2	202	LHG	C27-C28-C29-C30
22	R	301	CDL	C21-C22-C23-C24
22	R	302	CDL	C36-C37-C38-C39
20	K	301	LHG	C28-C29-C30-C31
20	K	301	LHG	C31-C32-C33-C34
20	K	302	LHG	C28-C29-C30-C31
20	S	202	LHG	C30-C31-C32-C33
22	R	302	CDL	C16-C17-C18-C19
20	K	302	LHG	O1-C1-C2-C3
20	R	304	LHG	C24-C25-C26-C27
20	S	201	LHG	C27-C28-C29-C30
21	2	201	P5S	C22-C23-C24-C25
22	R	303	CDL	C38-C39-C40-C41
20	K	301	LHG	C7-C8-C9-C10
22	R	302	CDL	C61-C62-C63-C64
22	R	303	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	R	303	CDL	CB7-C71-C72-C73
20	S	202	LHG	C27-C28-C29-C30
20	K	302	LHG	C9-C10-C11-C12
20	S	202	LHG	C32-C33-C34-C35
22	R	303	CDL	C18-C19-C20-C21
22	R	303	CDL	C52-C53-C54-C55
20	S	202	LHG	C4-C5-C6-O8
20	R	304	LHG	C29-C30-C31-C32
20	K	301	LHG	C8-C7-O7-C5
20	S	201	LHG	O1-C1-C2-O2
20	S	202	LHG	O1-C1-C2-O2
20	S	202	LHG	C28-C29-C30-C31
21	2	201	P5S	OXT-C-CA-N
22	R	301	CDL	C78-C79-C80-C81
22	R	301	CDL	C41-C42-C43-C44
22	R	302	CDL	C59-C60-C61-C62
20	S	202	LHG	C12-C13-C14-C15
20	S	202	LHG	C24-C25-C26-C27
20	K	302	LHG	C7-C8-C9-C10
20	2	202	LHG	C11-C12-C13-C14
20	S	202	LHG	C29-C30-C31-C32
22	R	302	CDL	C62-C63-C64-C65
20	K	301	LHG	C23-C24-C25-C26
20	2	202	LHG	C23-C24-C25-C26
20	S	201	LHG	C12-C13-C14-C15
20	R	304	LHG	C27-C28-C29-C30
22	R	302	CDL	C19-C20-C21-C22
22	R	302	CDL	C51-CB5-OB6-CB4
22	R	302	CDL	OB7-CB5-OB6-CB4
22	R	301	CDL	OA6-CA4-CA6-OA8
22	R	302	CDL	OA6-CA4-CA6-OA8
20	K	301	LHG	C24-C25-C26-C27
20	S	201	LHG	C4-O6-P-O3
20	R	304	LHG	C12-C13-C14-C15
22	R	303	CDL	C1-CB2-OB2-PB2
20	K	301	LHG	O6-C4-C5-C6
22	R	301	CDL	CA2-C1-CB2-OB2
20	S	202	LHG	C7-C8-C9-C10
22	R	301	CDL	CA3-CA4-CA6-OA8
20	K	302	LHG	C19-C20-C21-C22
20	K	301	LHG	C30-C31-C32-C33
20	K	302	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
20	2	202	LHG	O1-C1-C2-O2
20	R	304	LHG	O1-C1-C2-O2
20	K	301	LHG	C9-C10-C11-C12
20	R	304	LHG	C19-C20-C21-C22
20	K	302	LHG	C18-C19-C20-C21
20	K	301	LHG	C4-C5-O7-C7
20	K	302	LHG	C15-C16-C17-C18
20	S	201	LHG	C32-C33-C34-C35
22	R	302	CDL	CA4-CA3-OA5-PA1
22	R	301	CDL	C58-C59-C60-C61
22	R	302	CDL	CB5-C51-C52-C53
22	R	302	CDL	C56-C57-C58-C59
20	R	304	LHG	C15-C16-C17-C18
20	S	202	LHG	C15-C16-C17-C18
20	2	202	LHG	C19-C20-C21-C22
20	K	302	LHG	O6-C4-C5-C6
20	R	304	LHG	C30-C31-C32-C33
23	T	201	S12	C7-C8-C9-C10
20	2	202	LHG	C7-C8-C9-C10
20	K	302	LHG	C33-C34-C35-C36
20	S	202	LHG	O9-C7-O7-C5
20	R	304	LHG	C9-C10-C11-C12
20	2	202	LHG	C2-C3-O3-P
20	2	202	LHG	C13-C14-C15-C16
20	S	202	LHG	C9-C10-C11-C12
22	R	303	CDL	C58-C59-C60-C61
20	2	202	LHG	C29-C30-C31-C32
20	K	302	LHG	O6-C4-C5-O7
20	R	304	LHG	O6-C4-C5-O7
22	R	301	CDL	C81-C82-C83-C84
20	K	302	LHG	O7-C5-C6-O8
22	R	302	CDL	C76-C77-C78-C79
21	2	201	P5S	O-C-CA-N
22	R	302	CDL	CB2-C1-CA2-OA2
20	R	304	LHG	C28-C29-C30-C31
20	R	304	LHG	C33-C34-C35-C36
20	K	301	LHG	C26-C27-C28-C29
20	K	301	LHG	C35-C36-C37-C38
20	R	304	LHG	C11-C10-C9-C8
19	A	602	ADP	C4'-C5'-O5'-PA
20	K	301	LHG	C2-C3-O3-P
20	R	304	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
22	R	301	CDL	C1-CA2-OA2-PA1
20	S	201	LHG	C9-C10-C11-C12
20	S	202	LHG	C8-C7-O7-C5
20	R	304	LHG	O6-C4-C5-C6
20	S	201	LHG	O6-C4-C5-C6
22	R	302	CDL	OB5-CB3-CB4-CB6
20	S	202	LHG	C11-C10-C9-C8
22	R	303	CDL	C16-C17-C18-C19
20	K	302	LHG	C31-C32-C33-C34
22	R	301	CDL	C1-CB2-OB2-PB2
22	R	302	CDL	CA3-CA4-CA6-OA8
20	K	301	LHG	O6-C4-C5-O7
22	R	302	CDL	OB5-CB3-CB4-OB6
23	T	201	S12	C9-C10-C11-C12
20	K	301	LHG	O7-C5-C6-O8
22	R	302	CDL	OB6-CB4-CB6-OB8
19	B	602	ADP	C3'-C4'-C5'-O5'
22	R	301	CDL	C84-C85-C86-C87
22	R	301	CDL	C62-C63-C64-C65
21	2	201	P5S	N-CA-CB-OG
22	R	301	CDL	CB4-CB3-OB5-PB2
19	B	602	ADP	C5'-O5'-PA-O1A
19	A	602	ADP	C5'-O5'-PA-O2A
19	F	600	ADP	C5'-O5'-PA-O1A
20	K	301	LHG	C3-O3-P-O4
20	2	202	LHG	C3-O3-P-O5
20	R	304	LHG	C4-O6-P-O4
20	S	201	LHG	C3-O3-P-O5
22	R	301	CDL	CA3-OA5-PA1-OA3
22	R	303	CDL	CA2-OA2-PA1-OA3
22	R	303	CDL	CA2-OA2-PA1-OA4
22	R	303	CDL	CB2-OB2-PB2-OB4
23	T	201	S12	CB-OG-P-O3
22	R	303	CDL	CB5-C51-C52-C53
20	2	202	LHG	O6-C4-C5-C6
20	S	201	LHG	C15-C16-C17-C18
20	S	202	LHG	C16-C17-C18-C19
22	R	301	CDL	C52-C51-CB5-OB6
23	T	201	S12	C13-C14-C15-C16
22	R	302	CDL	C12-C11-CA5-OA6
20	S	201	LHG	C26-C27-C28-C29
20	S	201	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
20	R	304	LHG	O7-C5-C6-O8
20	S	202	LHG	O7-C5-C6-O8
20	R	304	LHG	C25-C26-C27-C28
22	R	303	CDL	C1-CA2-OA2-PA1
22	R	303	CDL	C59-C60-C61-C62
20	S	201	LHG	C31-C32-C33-C34
20	K	302	LHG	C16-C17-C18-C19
22	R	303	CDL	C12-C13-C14-C15
20	2	202	LHG	C12-C13-C14-C15
22	R	301	CDL	C79-C80-C81-C82
21	2	201	P5S	C1-C2-O37-C38
20	R	304	LHG	C13-C14-C15-C16
20	2	202	LHG	O6-C4-C5-O7
21	2	201	P5S	C45-C46-C48-C49
20	R	304	LHG	C10-C11-C12-C13
22	R	302	CDL	C58-C59-C60-C61
20	K	302	LHG	C27-C28-C29-C30
20	K	302	LHG	C3-O3-P-O6
20	2	202	LHG	C4-O6-P-O3
22	R	301	CDL	CA2-OA2-PA1-OA5
22	R	301	CDL	CB2-OB2-PB2-OB5
20	2	202	LHG	C18-C19-C20-C21
23	T	201	S12	C11-C12-C13-C14
20	S	202	LHG	C25-C26-C27-C28
22	R	302	CDL	C1-CB2-OB2-PB2
22	R	303	CDL	C51-C52-C53-C54
20	K	302	LHG	O1-C1-C2-O2
19	D	600	ADP	C3'-C4'-C5'-O5'
20	S	202	LHG	C14-C15-C16-C17
20	S	201	LHG	C10-C11-C12-C13
20	S	201	LHG	C28-C29-C30-C31
20	R	304	LHG	C14-C15-C16-C17
19	B	602	ADP	PA-O3A-PB-O1B
22	R	301	CDL	C11-C12-C13-C14
20	2	202	LHG	C9-C10-C11-C12
20	K	301	LHG	C27-C28-C29-C30
21	2	201	P5S	C46-C48-C49-C50
19	A	602	ADP	O4'-C4'-C5'-O5'
22	R	302	CDL	C74-C75-C76-C77
21	2	201	P5S	C23-C24-C25-C26
22	R	301	CDL	C14-C15-C16-C17
22	R	302	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
20	S	201	LHG	C34-C35-C36-C37
20	R	304	LHG	C31-C32-C33-C34
22	R	303	CDL	C22-C23-C24-C25
20	S	202	LHG	O8-C23-C24-C25
22	R	303	CDL	C14-C15-C16-C17
23	T	201	S12	OXT-C-CA-N
20	S	202	LHG	O7-C7-C8-C9
23	T	201	S12	O52-C5-C6-C7
20	K	302	LHG	C4-C5-C6-O8
22	R	302	CDL	CB3-CB4-CB6-OB8
20	K	302	LHG	C24-C25-C26-C27
20	2	202	LHG	C24-C25-C26-C27
22	R	302	CDL	C32-C33-C34-C35
19	B	602	ADP	PA-O3A-PB-O2B
19	B	602	ADP	PA-O3A-PB-O3B
20	S	201	LHG	C29-C30-C31-C32
19	C	602	ADP	C5'-O5'-PA-O3A
23	T	201	S12	CA-CB-OG-P
23	T	201	S12	O51-C5-C6-C7
22	R	302	CDL	C52-C53-C54-C55
20	S	202	LHG	O9-C7-C8-C9
22	R	301	CDL	C82-C83-C84-C85
20	R	304	LHG	O9-C7-C8-C9
20	K	301	LHG	O9-C7-C8-C9
20	K	301	LHG	C4-O6-P-O4
21	2	201	P5S	CB-OG-P12-O13
22	R	301	CDL	CB2-OB2-PB2-OB3
22	R	303	CDL	CA6-CA4-OA6-CA5
22	R	303	CDL	CB6-CB4-OB6-CB5
20	2	202	LHG	C28-C29-C30-C31
21	2	201	P5S	C29-C30-C31-C32
20	S	201	LHG	C33-C34-C35-C36
22	R	301	CDL	C35-C36-C37-C38

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

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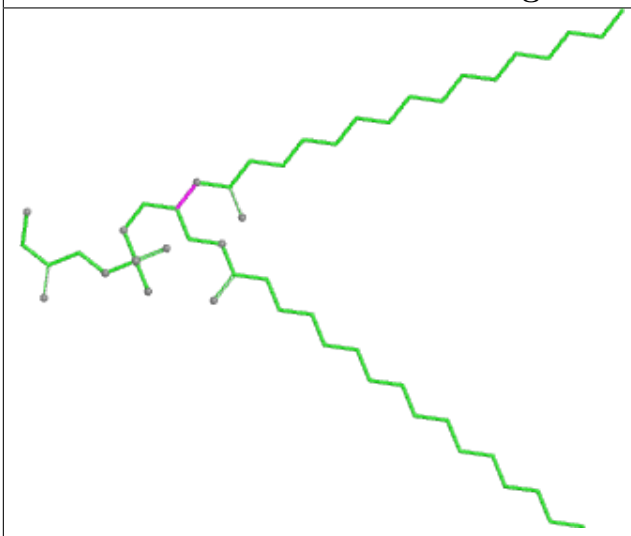
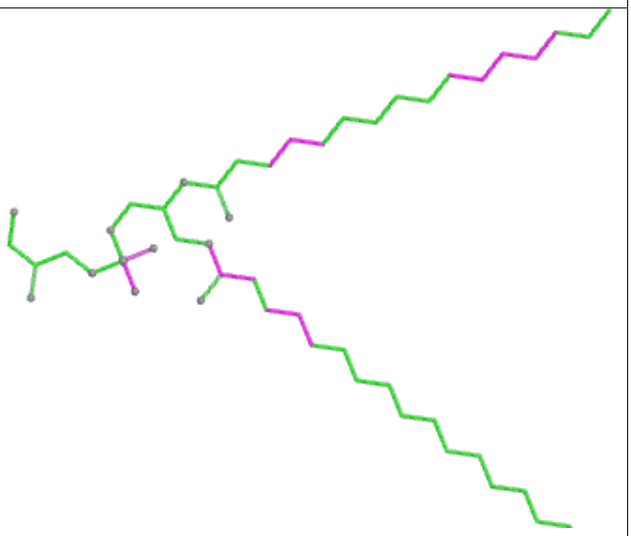
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	R	302	CDL	7	0
19	F	600	ADP	1	0
20	K	302	LHG	3	0
21	2	201	P5S	2	0
22	R	301	CDL	2	0
22	R	303	CDL	6	0
19	B	602	ADP	2	0
23	T	201	S12	1	0

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.

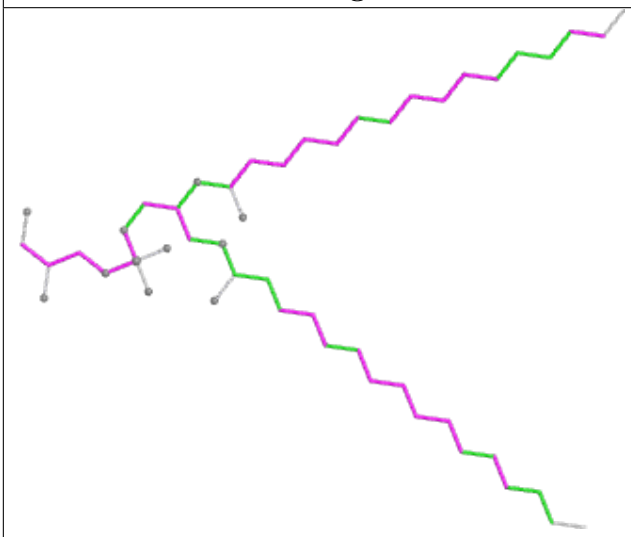
Ligand LHG R 304



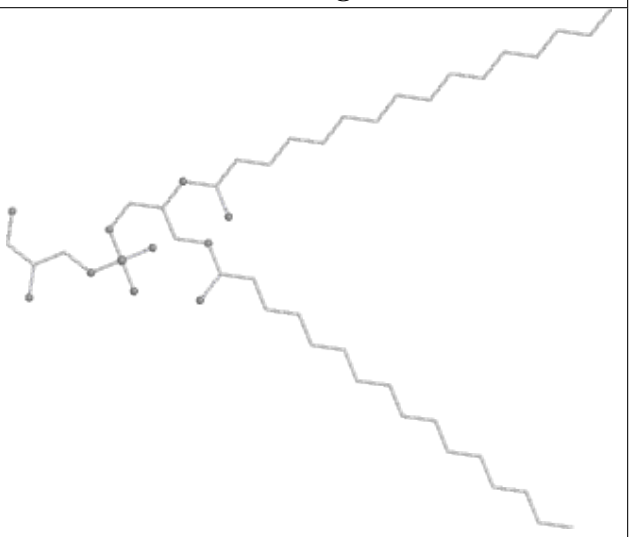
Bond lengths



Bond angles

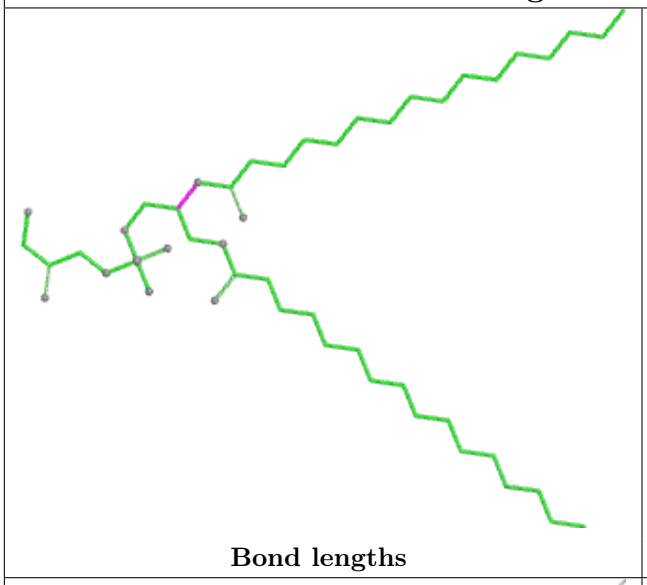


Torsions

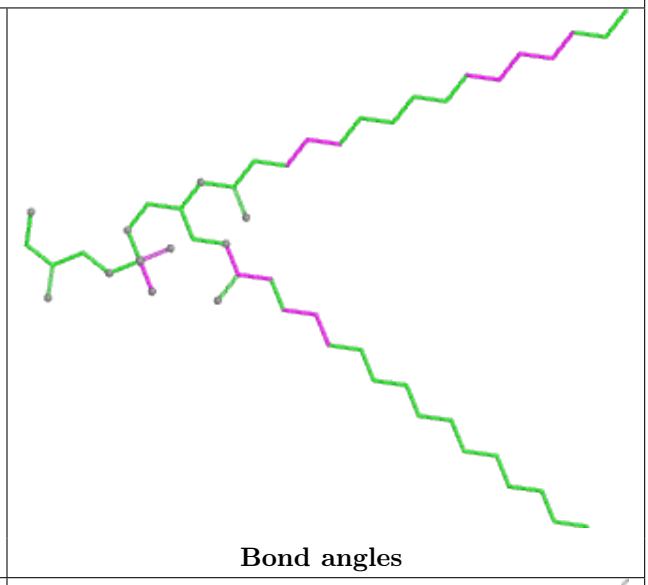


Rings

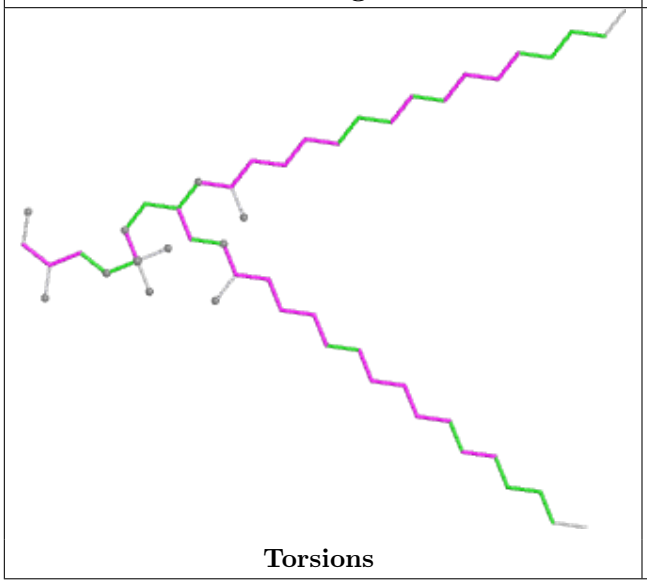
Ligand LHG S 202



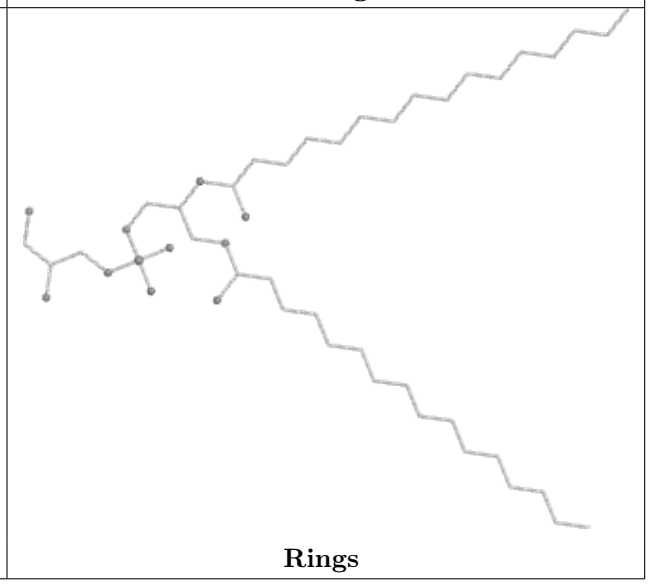
Bond lengths



Bond angles

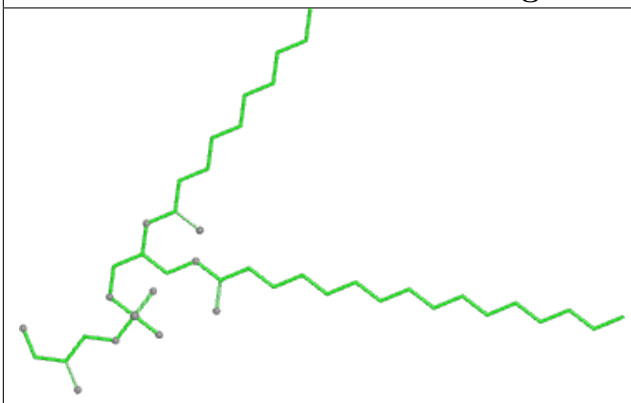


Torsions

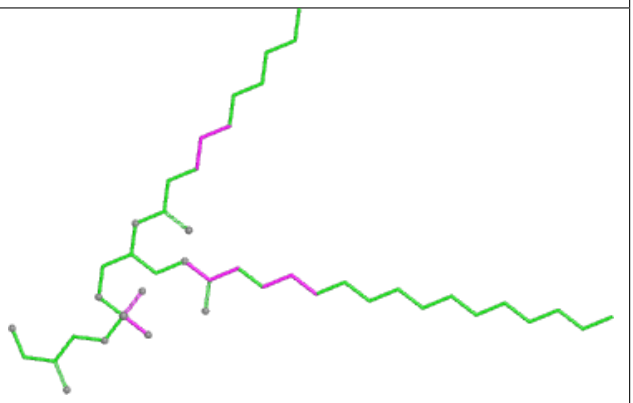


Rings

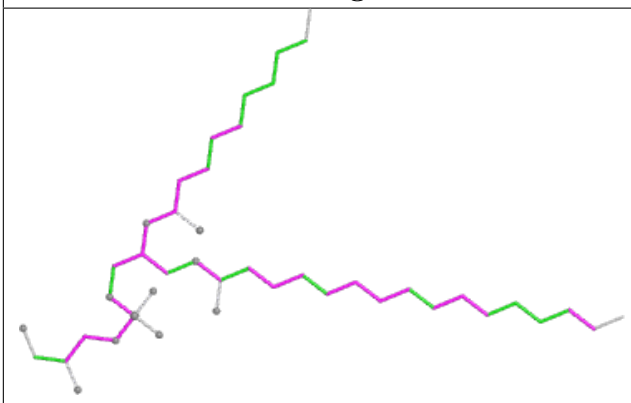
Ligand LHG K 301



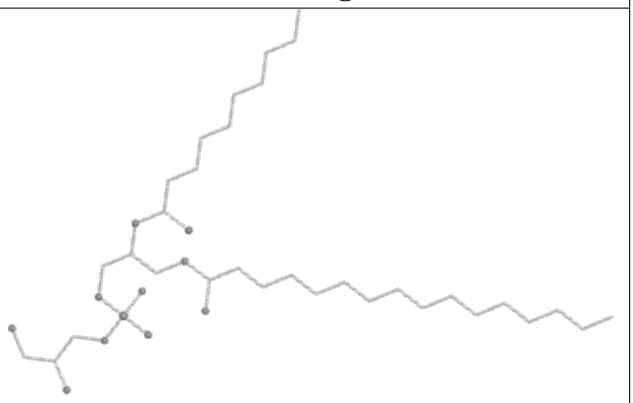
Bond lengths



Bond angles

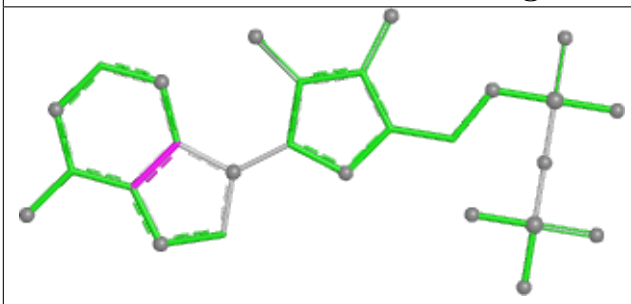


Torsions

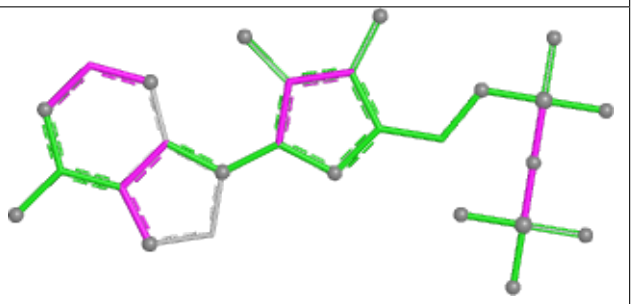


Rings

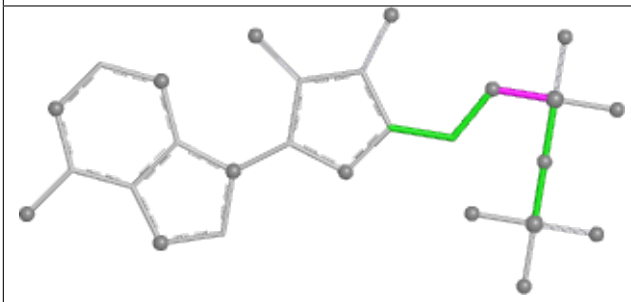
Ligand ADP C 602



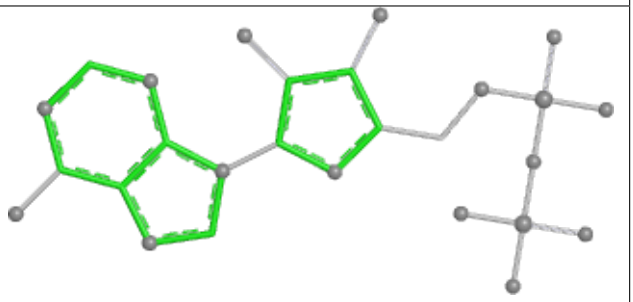
Bond lengths



Bond angles

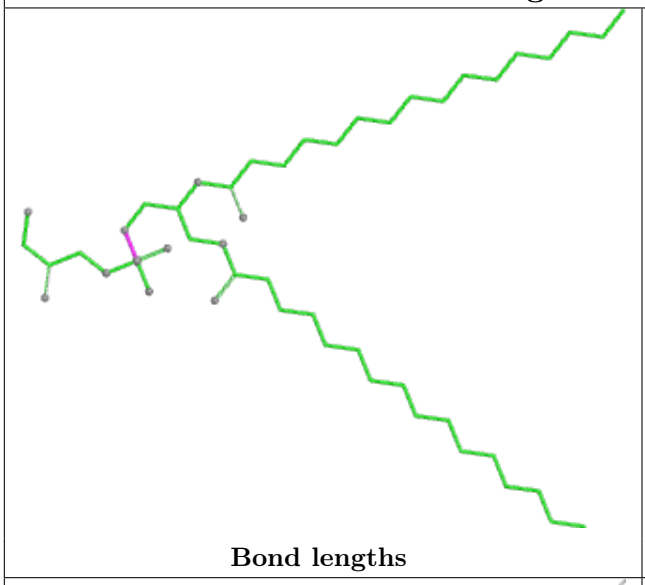


Torsions

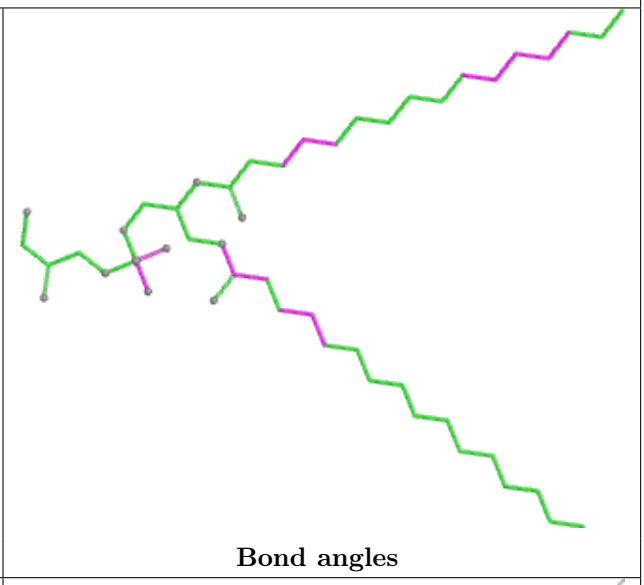


Rings

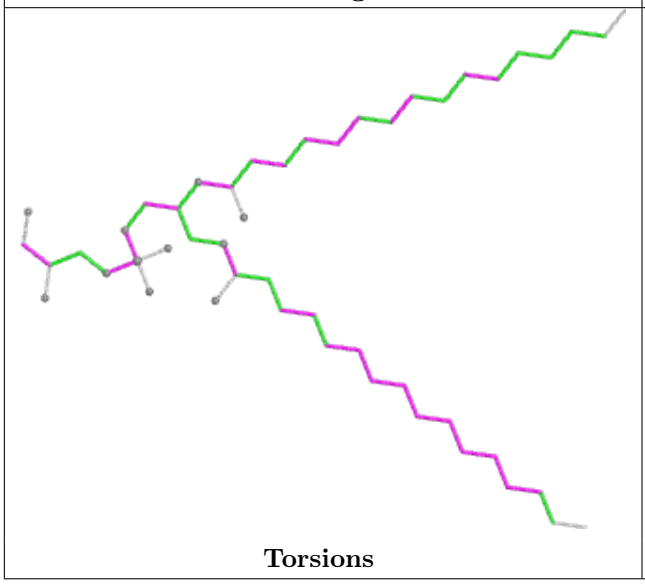
Ligand LHG S 201



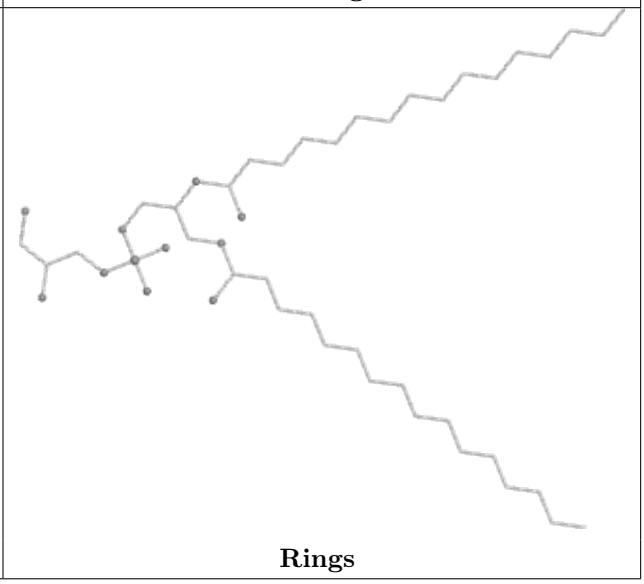
Bond lengths



Bond angles

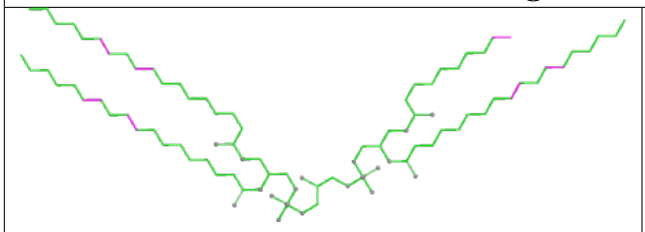


Torsions

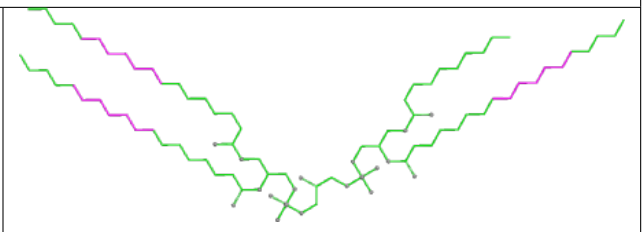


Rings

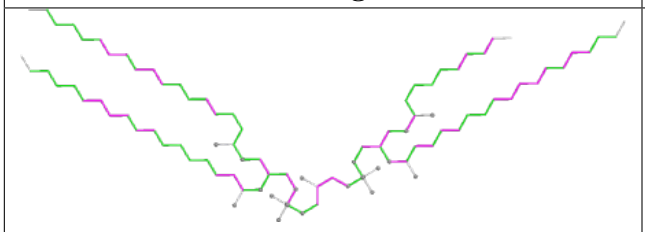
Ligand CDL R 302



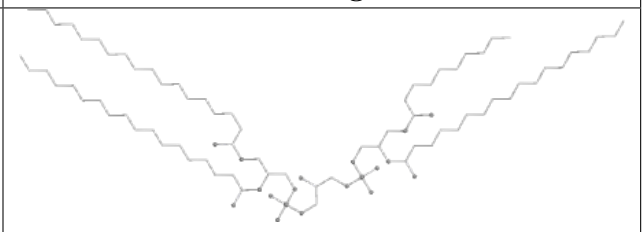
Bond lengths



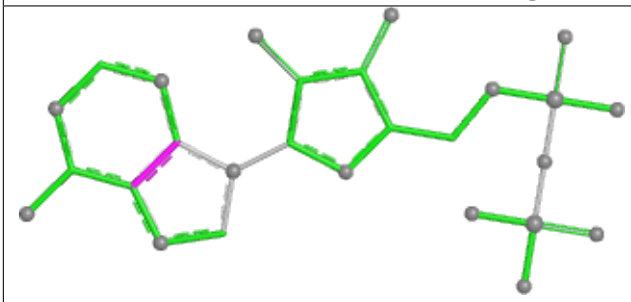
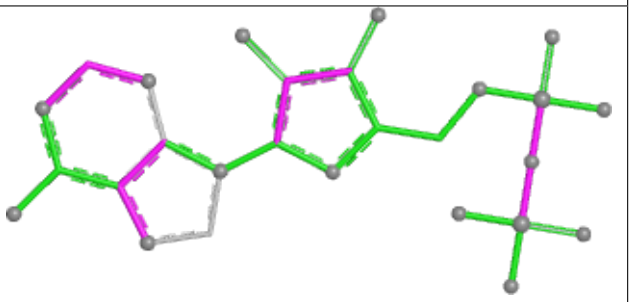
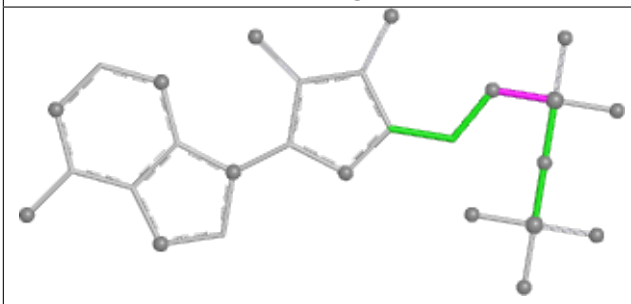
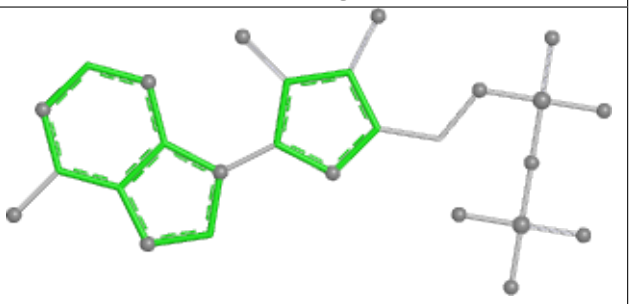
Bond angles



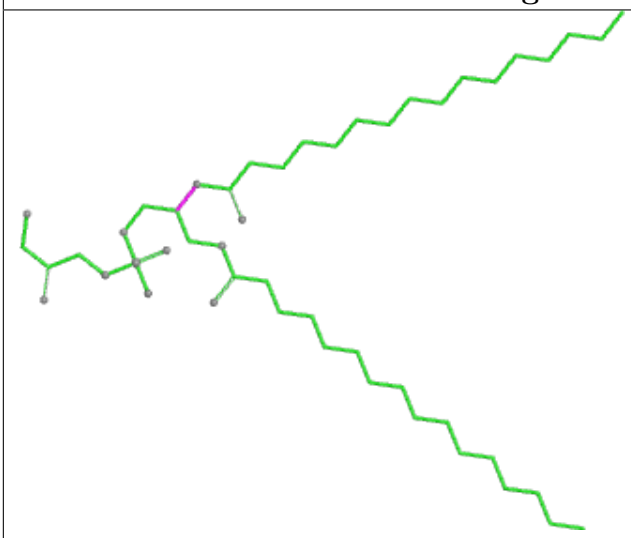
Torsions



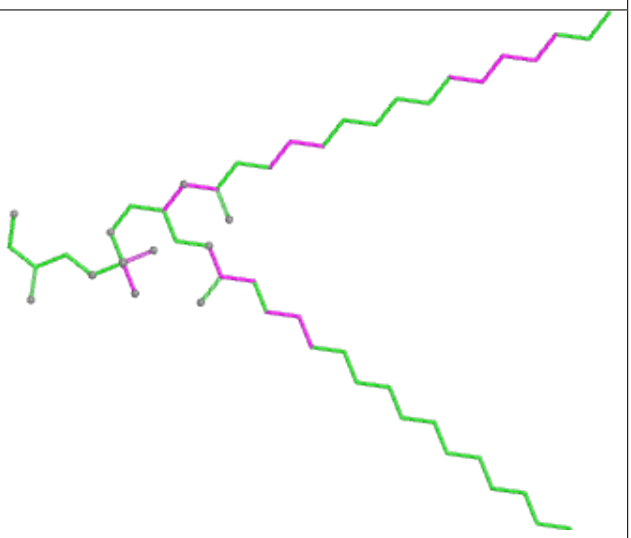
Rings

Ligand ADP F 600	
 Bond lengths	 Bond angles
 Torsions	 Rings

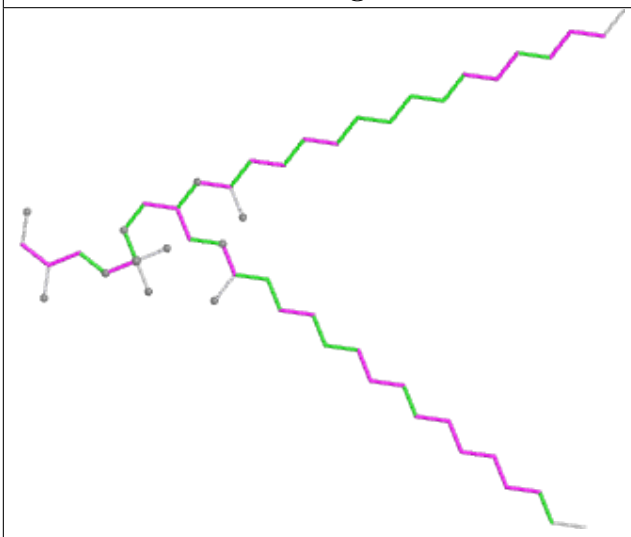
Ligand LHG K 302



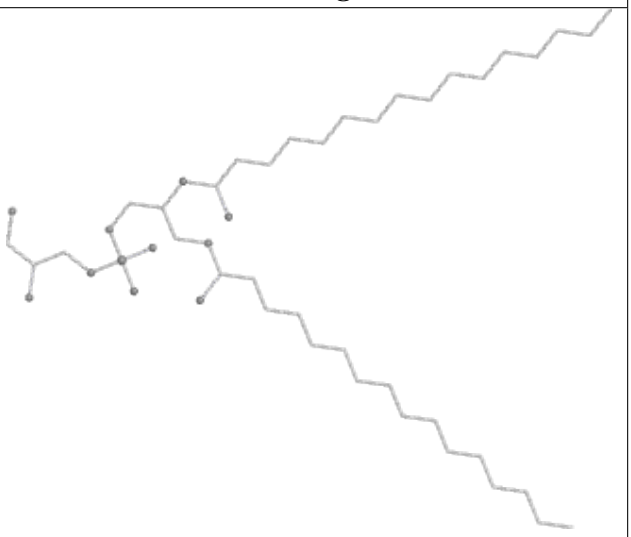
Bond lengths



Bond angles

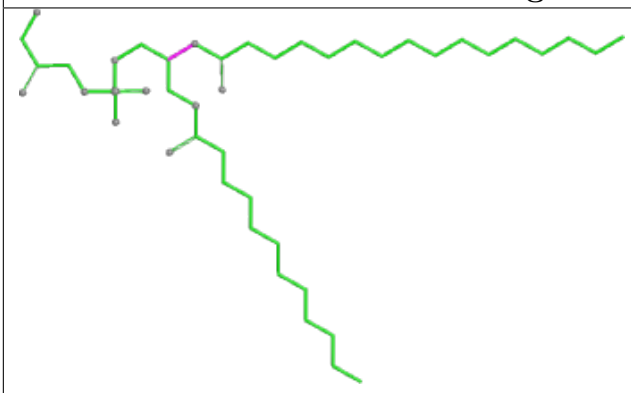


Torsions

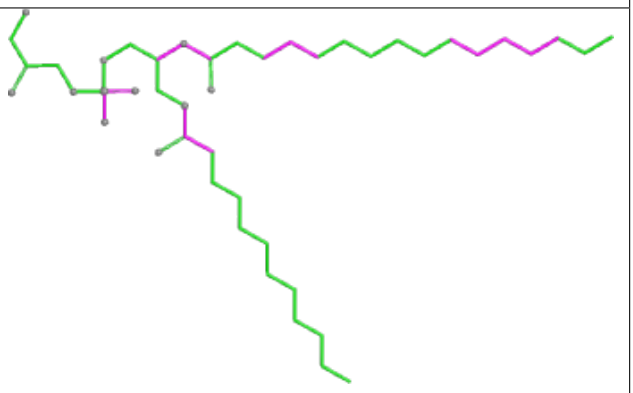


Rings

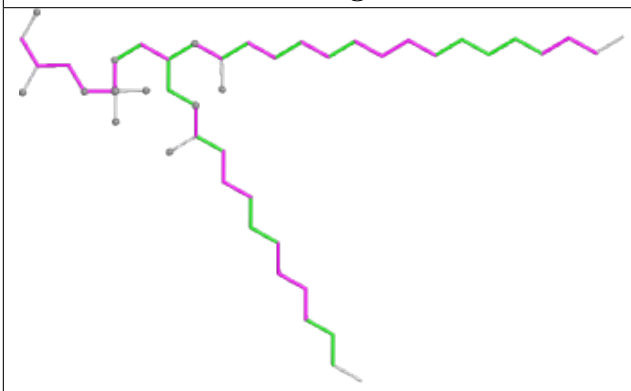
Ligand LHG 2 202



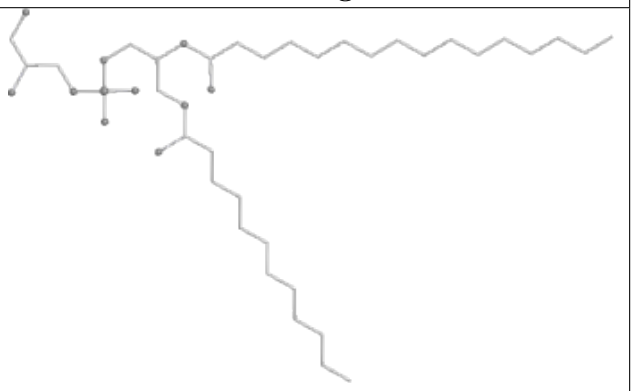
Bond lengths



Bond angles



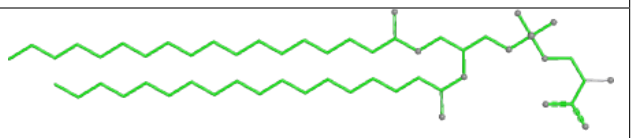
Torsions



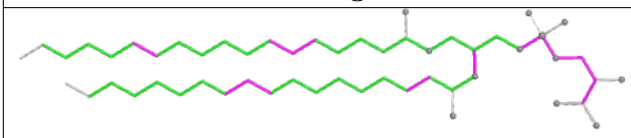
Rings

Ligand P5S 2 201

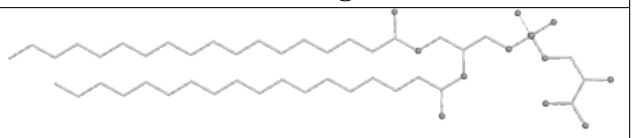
Bond lengths



Bond angles

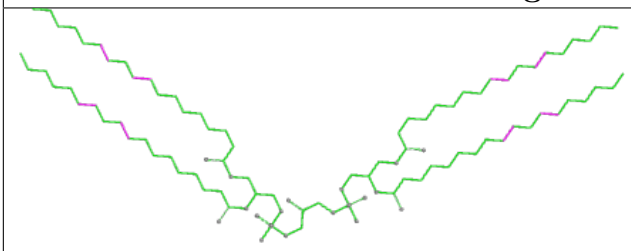


Torsions

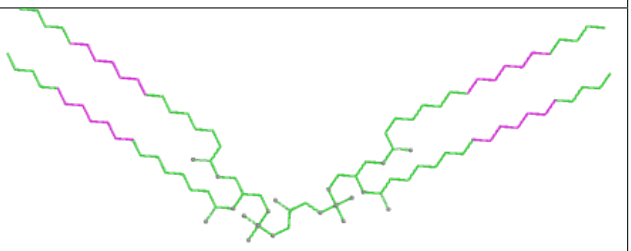


Rings

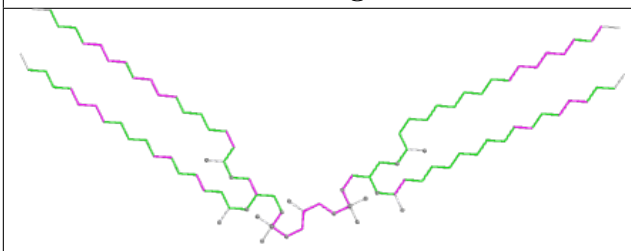
Ligand CDL R 301



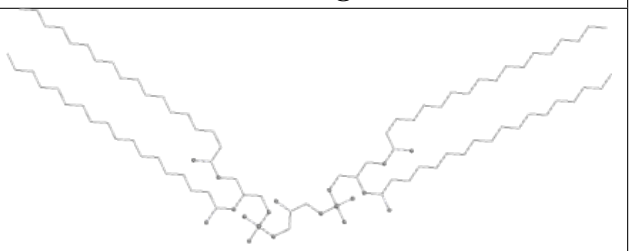
Bond lengths



Bond angles

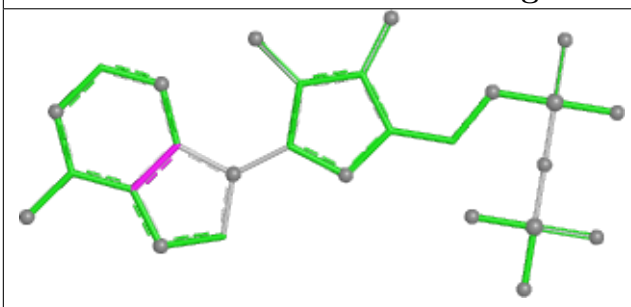


Torsions

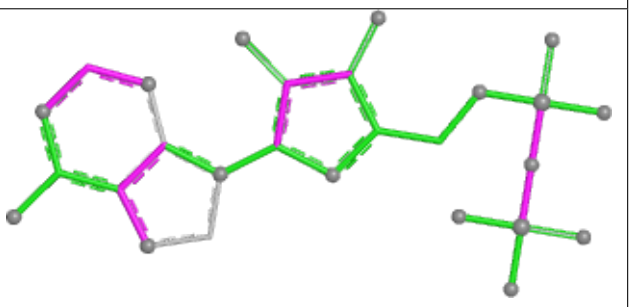


Rings

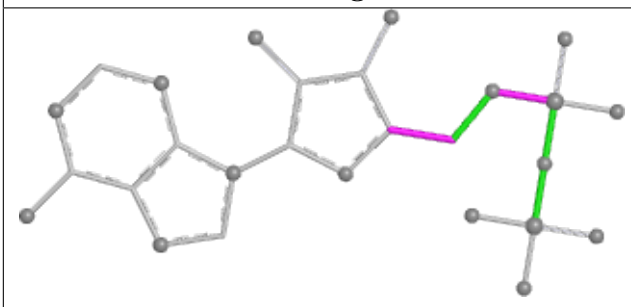
Ligand ADP D 600



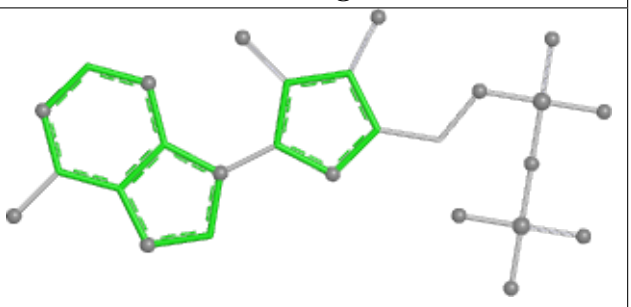
Bond lengths



Bond angles

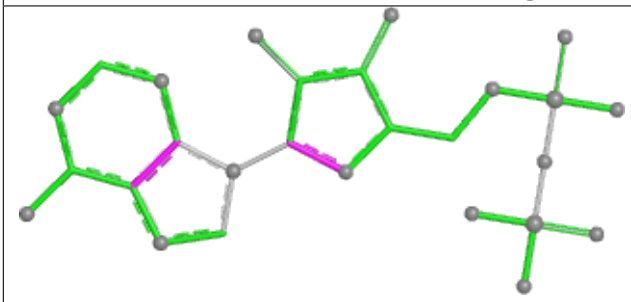


Torsions

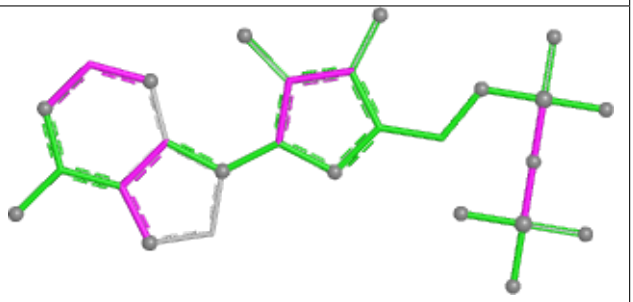


Rings

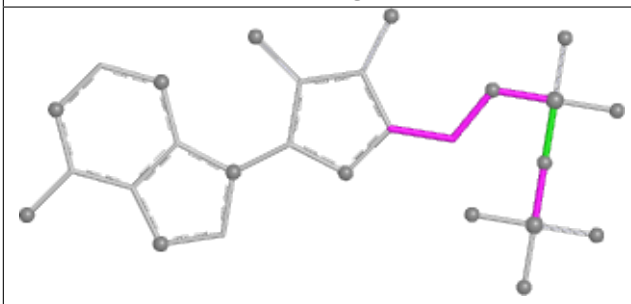
Ligand ADP A 602



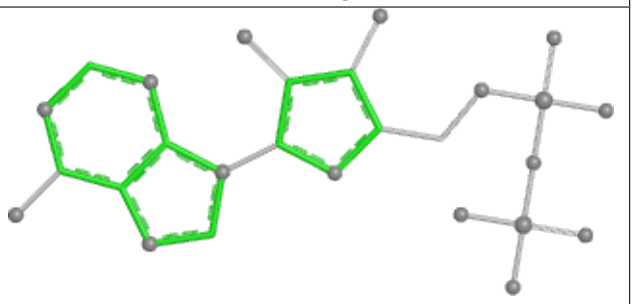
Bond lengths



Bond angles

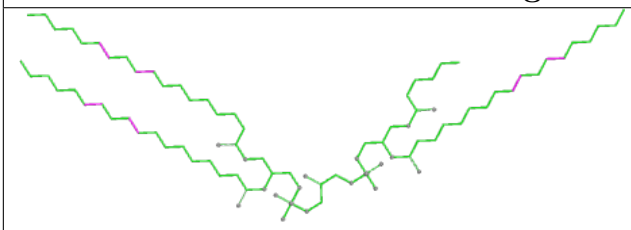


Torsions

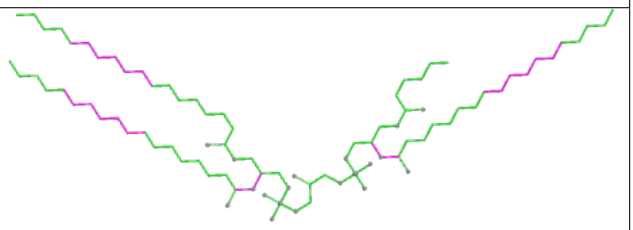


Rings

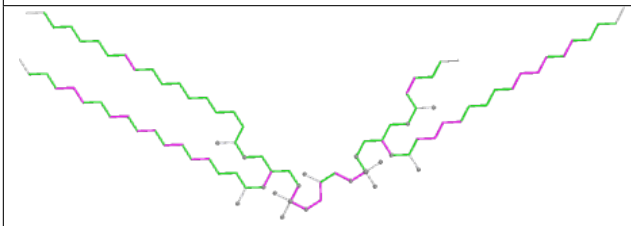
Ligand CDL R 303



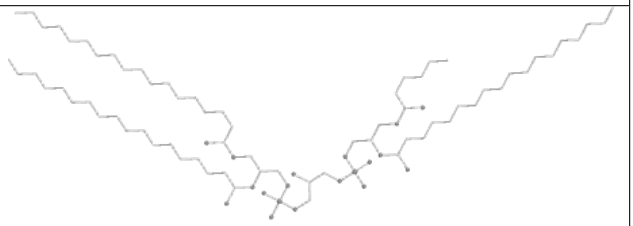
Bond lengths



Bond angles

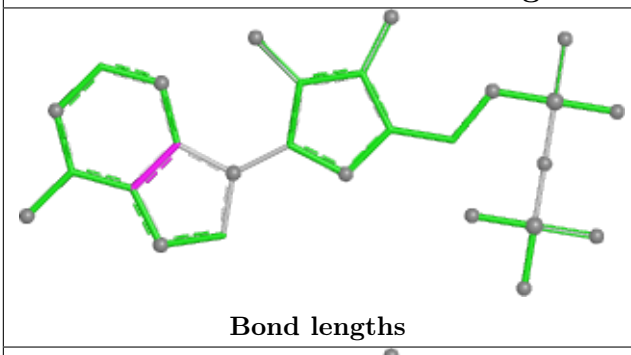


Torsions

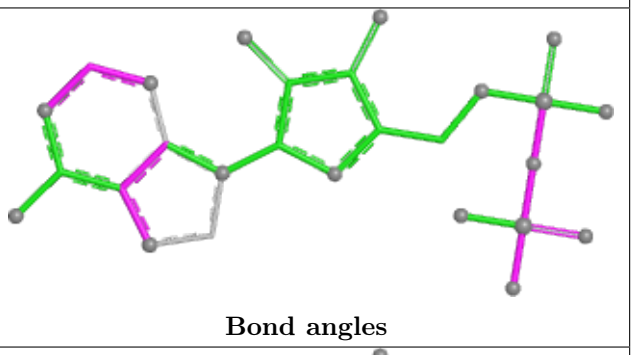


Rings

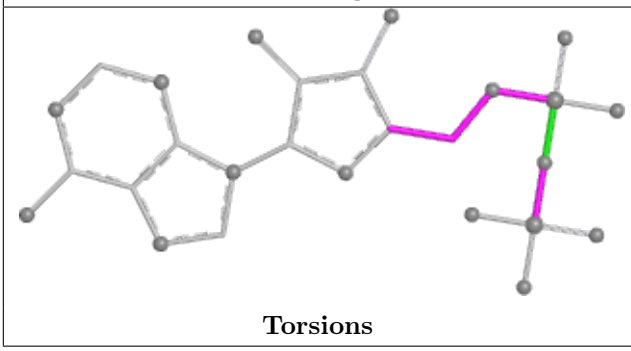
Ligand ADP B 602



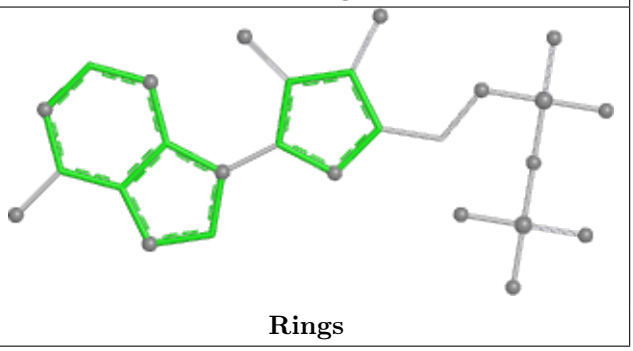
Bond lengths



Bond angles

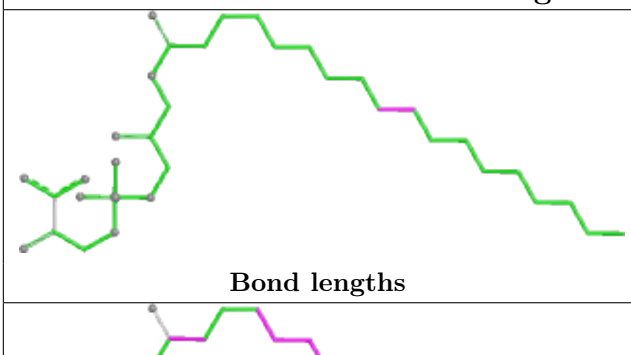


Torsions

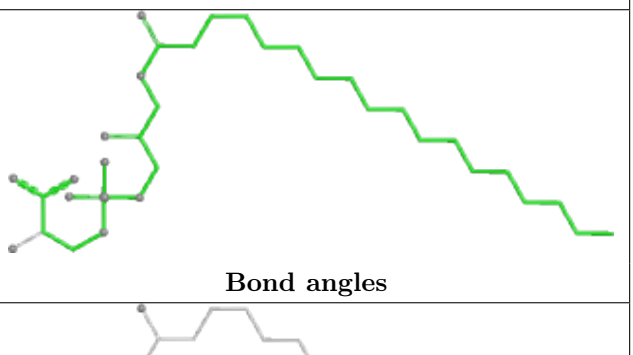


Rings

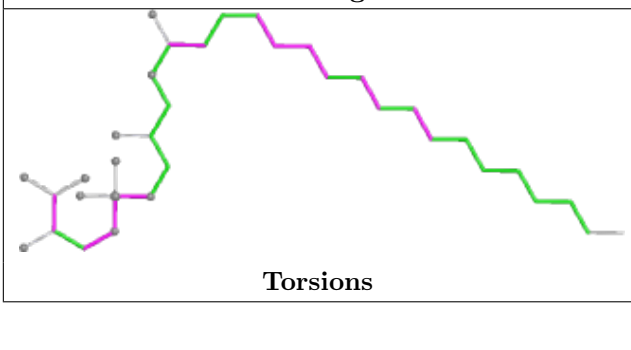
Ligand S12 T 201



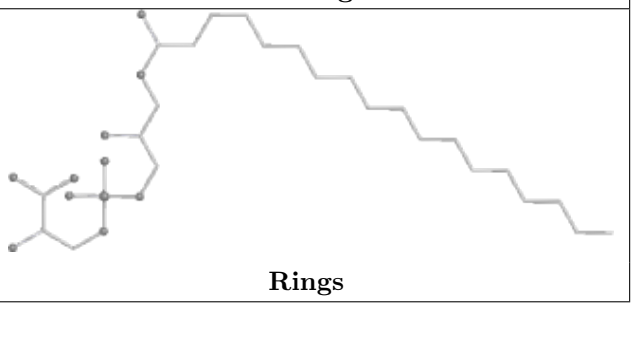
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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

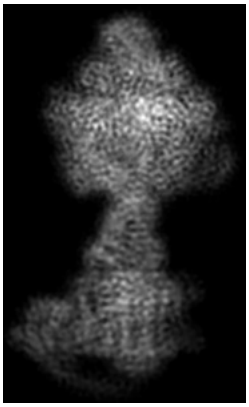
6 Map visualisation

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.

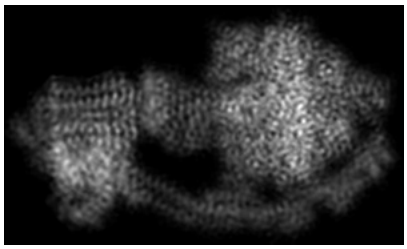
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

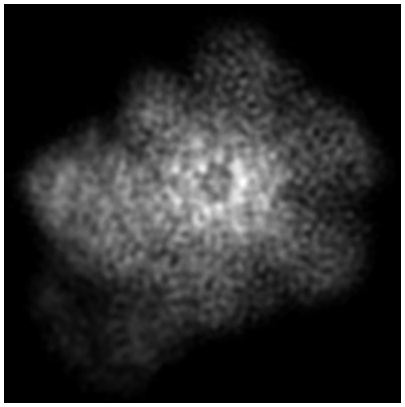
6.1.1 Primary map



X



Y



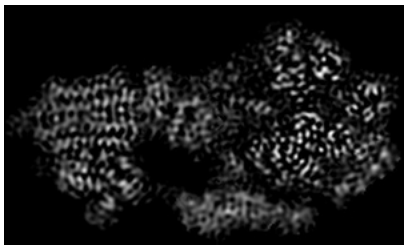
Z

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

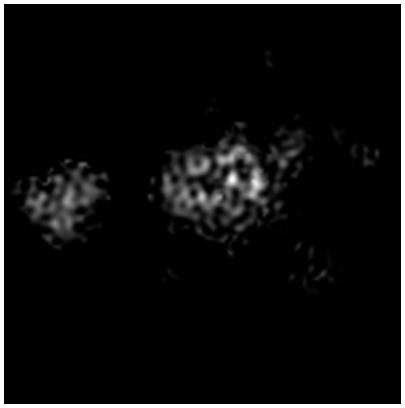
6.2 Central slices

6.2.1 Primary map

X Index: 69



Y Index: 69



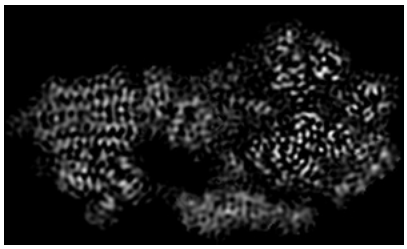
Z Index: 115

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

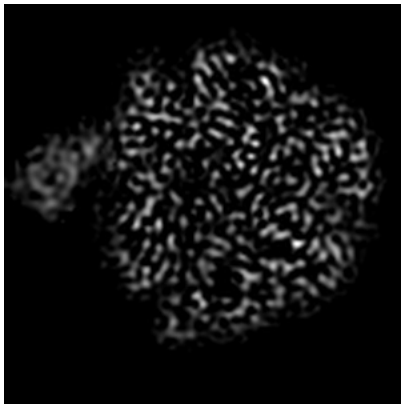
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 81



Y Index: 69



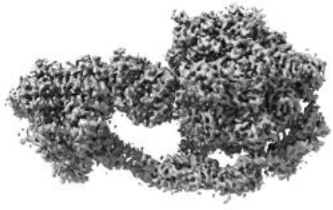
Z Index: 167

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.

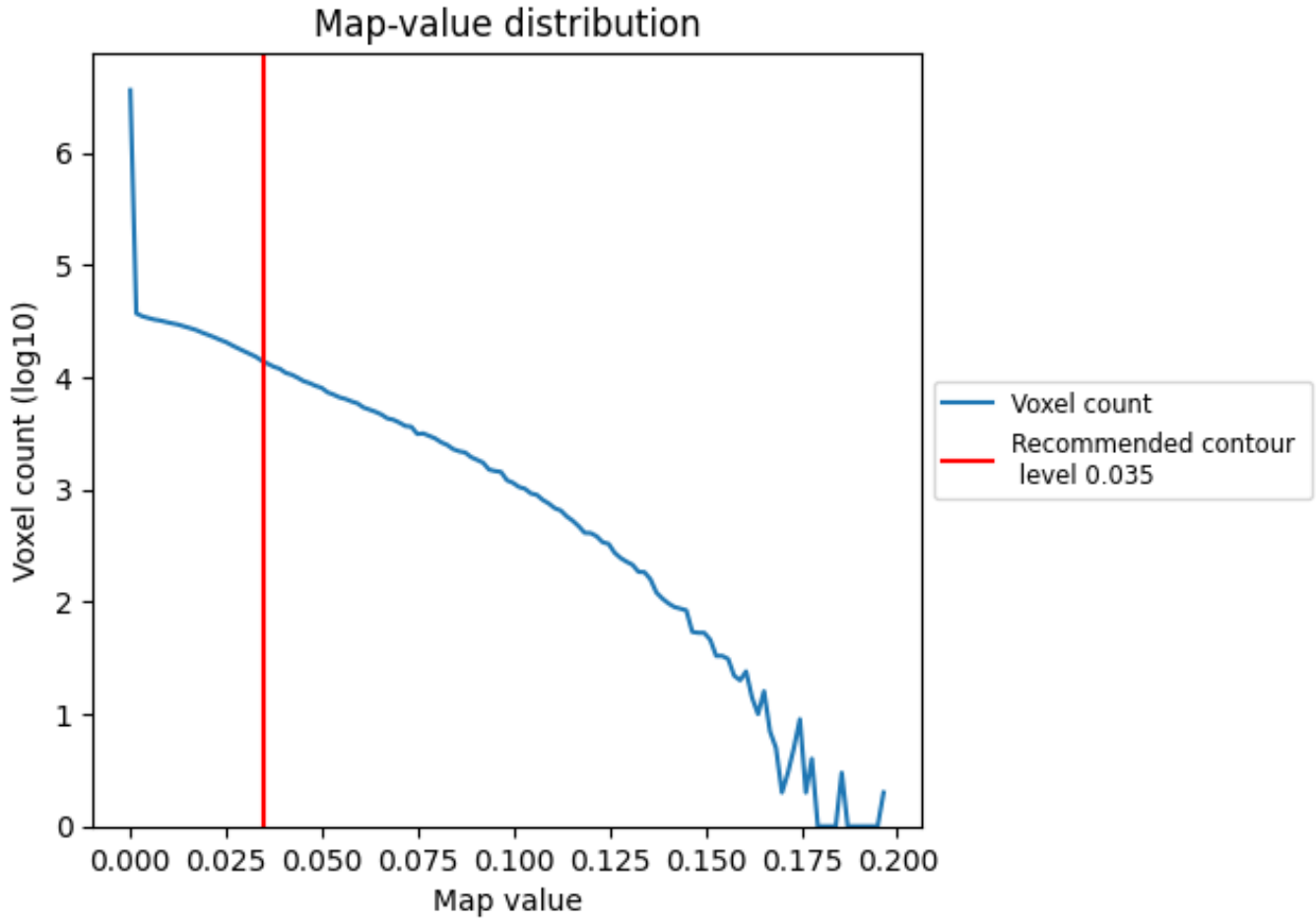
6.5 Mask visualisation (i)

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

7 Map analysis

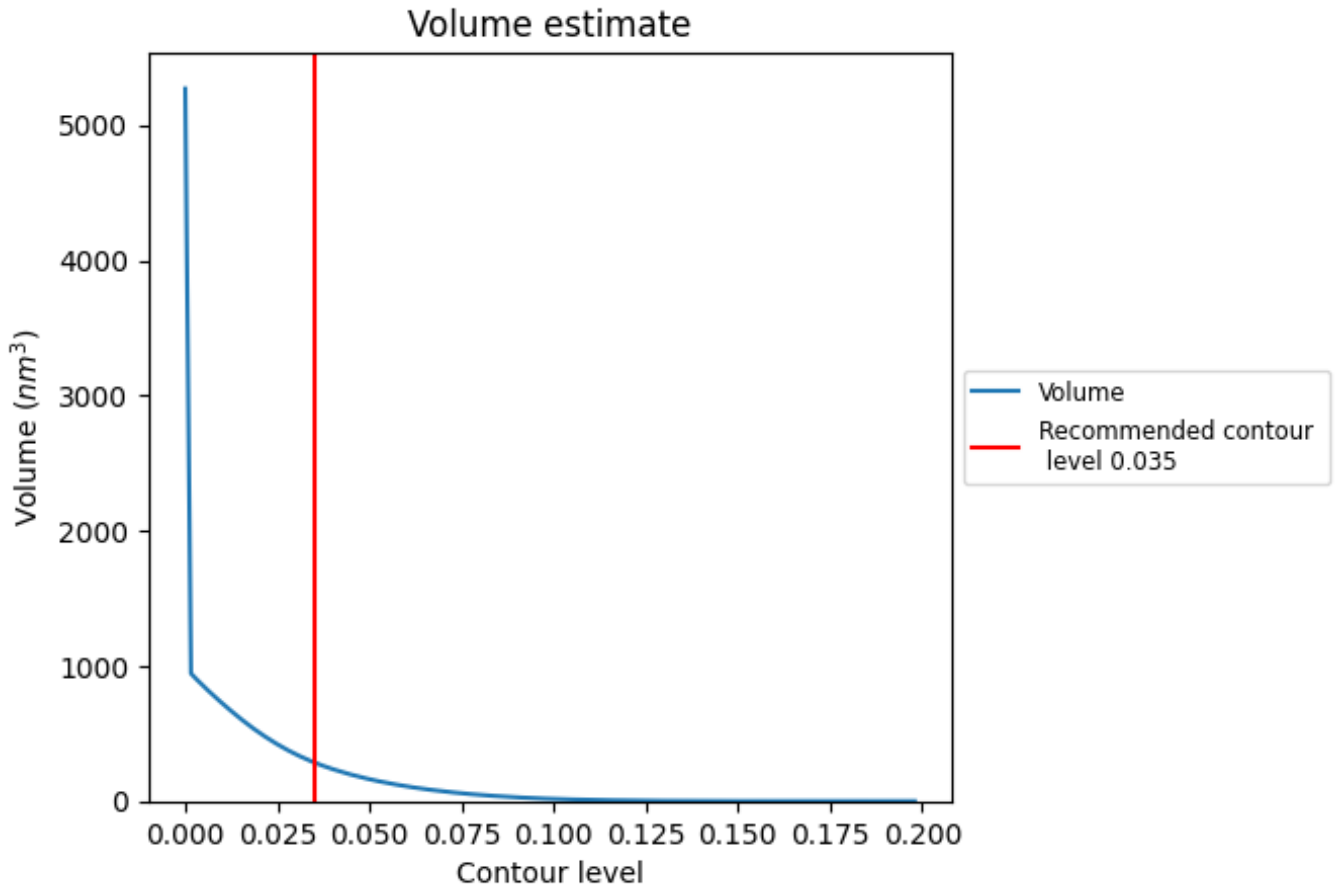
This section contains the results of statistical analysis of the map.

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.

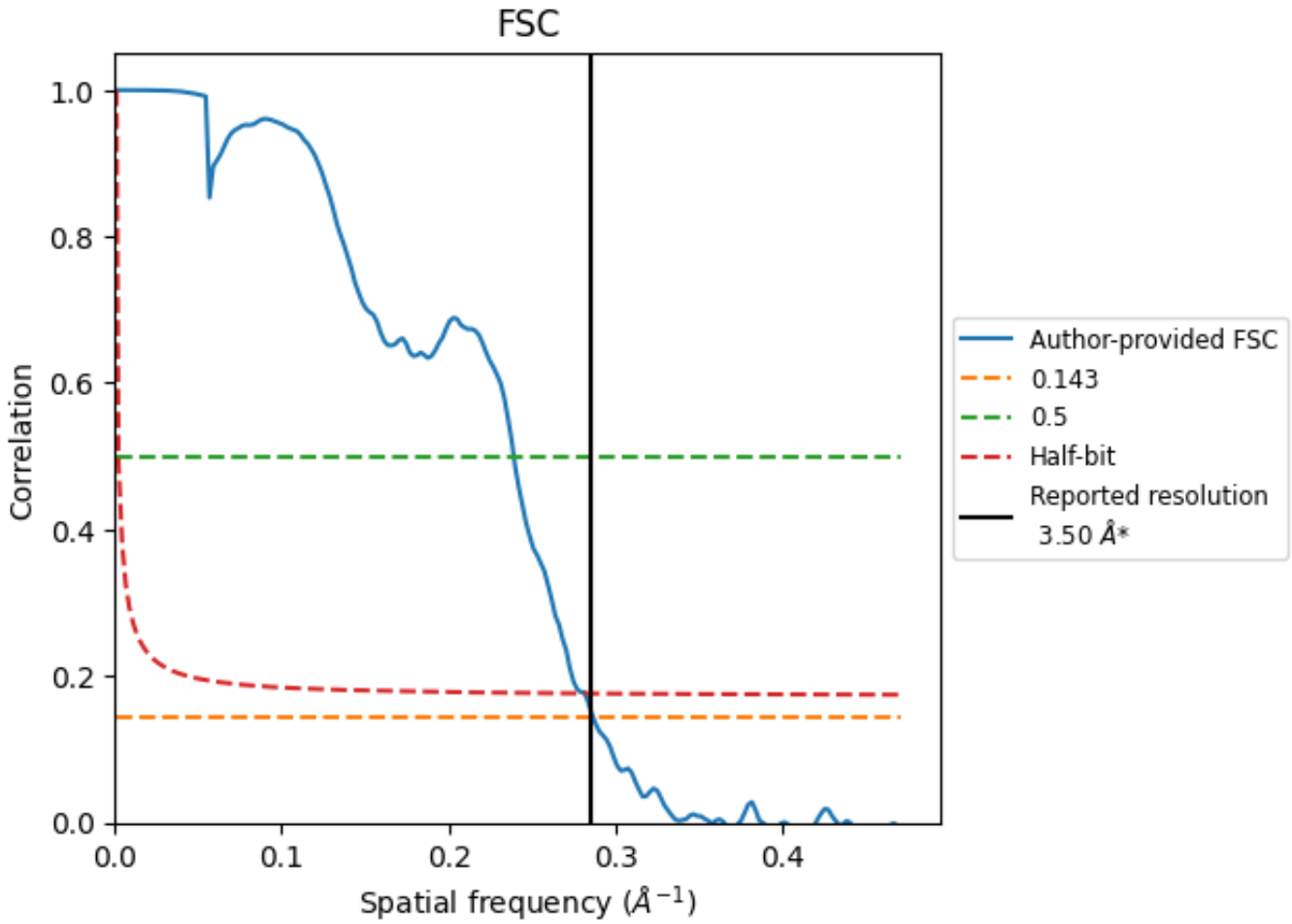
7.3 Rotationally averaged power spectrum (i)

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)

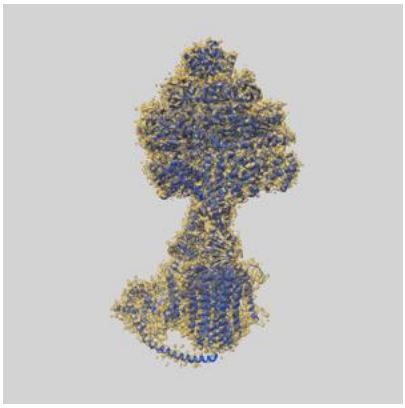
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.18	3.55
Unmasked-calculated*	-	-	-

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

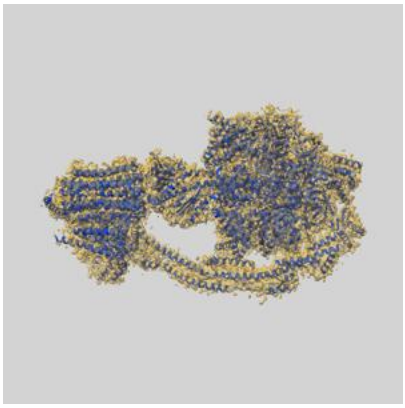
9 Map-model fit

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.

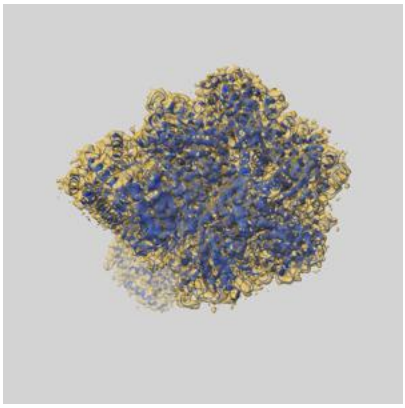
9.1 Map-model overlay



X



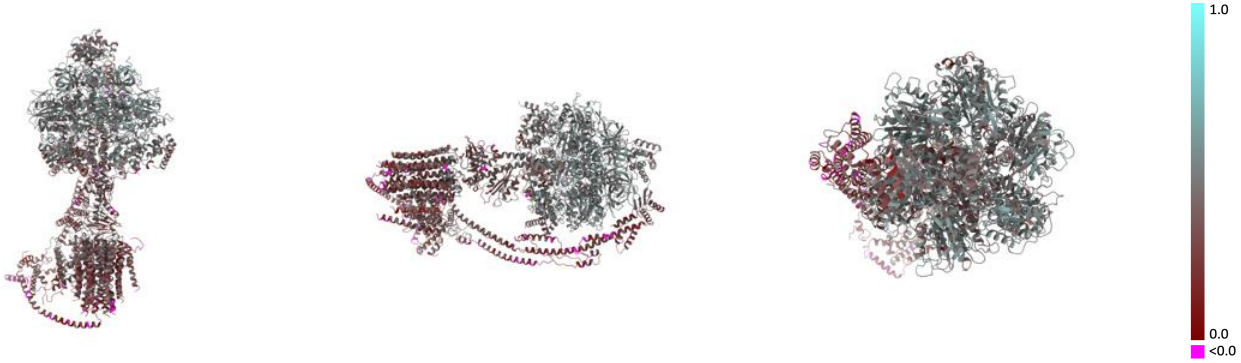
Y



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.

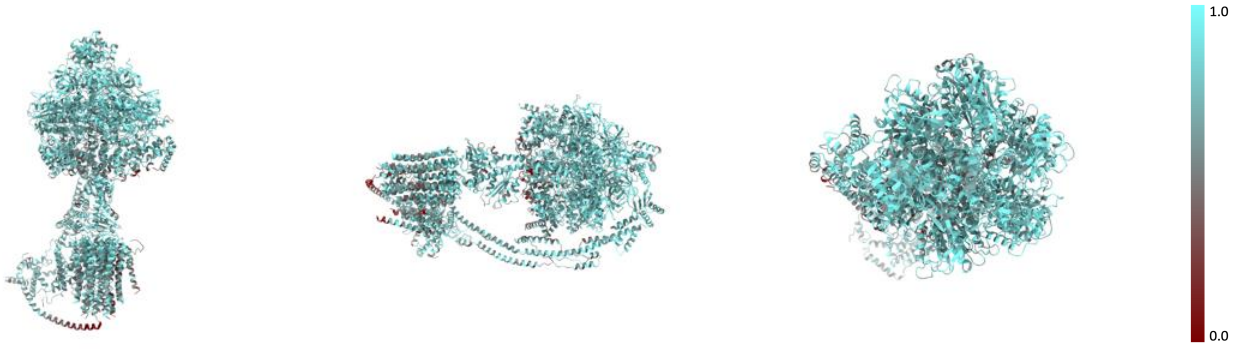
9.2 Q-score mapped to coordinate model (i)



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.

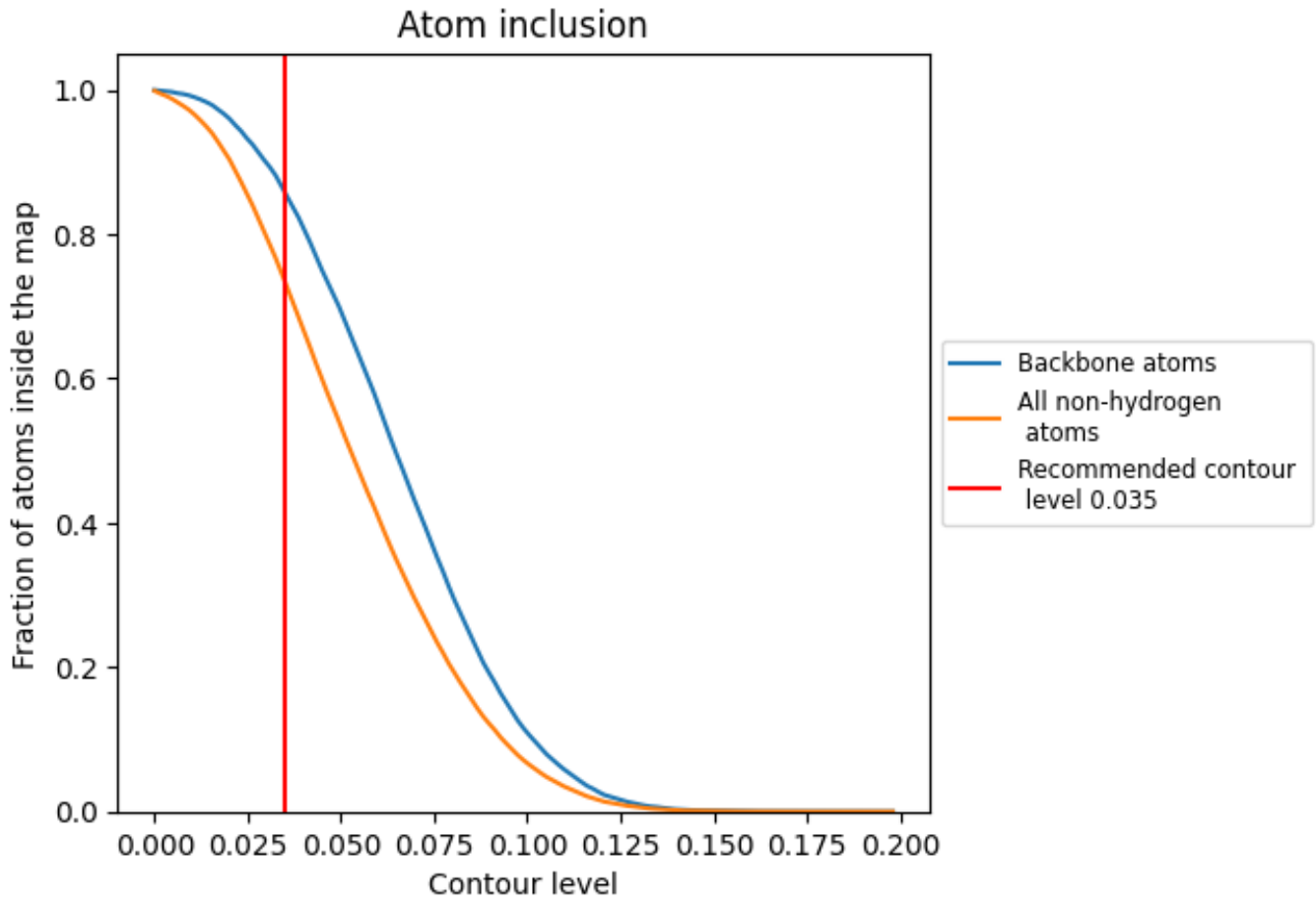
9.3 Atom inclusion mapped to coordinate model (i)



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