Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 01:42 AM EDT

PDB ID	:	7KHR
EMDB ID	:	EMD-22880
Title	:	Cryo-EM structure of bafilomycin A1-bound intact V-ATPase from bovine brain
Authors	:	Wang, R.; Li, X.
Deposited on	:	2020-10-21
Resolution	:	3.62 Å(reported)

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:

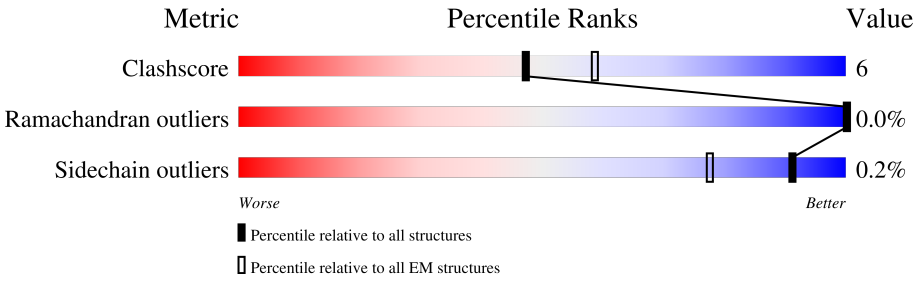
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.62 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	617	84% 11% 5%
1	B	617	82% 13% •
1	C	617	86% 11% •
2	D	511	79% 12% 10%
2	E	511	79% 11% 10%
2	F	511	80% 9% 10%
3	G	382	30% 91% 9%
4	H	247	77% 9% 14%

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Mol	Chain	Length	Quality of chain
5	I	226	15% 89% 8%
5	J	226	7% 88% 9%
5	K	226	92% 6%
6	L	119	75% 12% 13%
7	M	118	19% 92% 8%
7	N	118	14% 90% 8%
7	O	118	19% 89% 8%
8	P	465	8% 70% 9% 21%
9	a	838	89% 11%
10	b	205	98%
11	d	351	99%
12	e	81	90% 10%
13	s	468	43% 56%
14	r	351	13% 87%
15	c	155	97%
15	g	155	97%
15	k	155	97%
15	l	155	97%
15	m	155	97%
15	n	155	97%
15	o	155	97%
15	p	155	97%
15	q	155	97%
16	f	98	66% 34%
17	t	9	44% 56%

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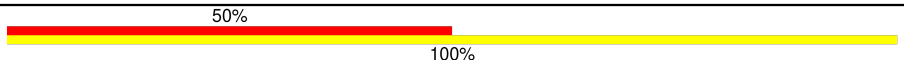
Mol	Chain	Length	Quality of chain
18	Q	2	

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
25	WEV	g	202	-	X	-	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 61913 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 V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	589	Total	C	N	O	S	0	0
			4568	2900	770	870	28		
1	B	591	Total	C	N	O	S	0	0
			4591	2911	774	879	27		
1	C	600	Total	C	N	O	S	0	0
			4654	2950	785	891	28		

- Molecule 2 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	461	Total	C	N	O	S	0	0
			3609	2288	618	683	20		
2	E	458	Total	C	N	O	S	0	0
			3585	2273	613	679	20		
2	F	458	Total	C	N	O	S	0	0
			3585	2273	613	679	20		

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	346	Total	C	N	O	0	0
			1720	1028	346	346		

- Molecule 4 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	212	Total	C	N	O	S	0	0
			1708	1084	308	311	5		

- Molecule 5 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	218	Total	C	N	O	S	0	0
			1543	960	288	289	6		
5	J	218	Total	C	N	O	S	0	0
			1636	1024	301	304	7		
5	K	220	Total	C	N	O	S	0	0
			1568	977	293	292	6		

- Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	103	Total	C	N	O	S	0	0
			816	516	143	156	1		

- Molecule 7 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	109	Total	C	N	O	S	0	0
			663	396	138	126	3		
7	N	109	Total	C	N	O	S	0	0
			684	408	140	133	3		
7	O	109	Total	C	N	O	S	0	0
			677	404	139	131	3		

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	368	Total	C	N	O	S	0	0
			2499	1558	460	473	8		

- Molecule 9 is a protein called V-type proton ATPase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	750	Total	C	N	O	S	0	0
			5827	3788	972	1031	36		

- Molecule 10 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	204	Total	C	N	O	S	0	0
			1503	996	238	259	10		

- Molecule 11 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	348	Total	C	N	O	S	0	0
			2819	1817	460	528	14		

- Molecule 12 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	e	73	Total	C	N	O	S	0	0
			590	409	91	87	3		

- Molecule 13 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	204	Total	C	N	O	S	0	0
			1660	1078	263	311	8		

- Molecule 14 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	r	46	Total	C	N	O	S	0	0
			385	261	54	67	3		

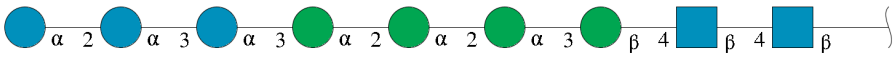
- Molecule 15 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	g	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	k	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	l	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	m	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	n	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
15	o	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		
15	p	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		
15	q	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		

- Molecule 16 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	f	65	501	336	75	86	4	0	0

- Molecule 17 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	t	9	105	58	2	45	0	0

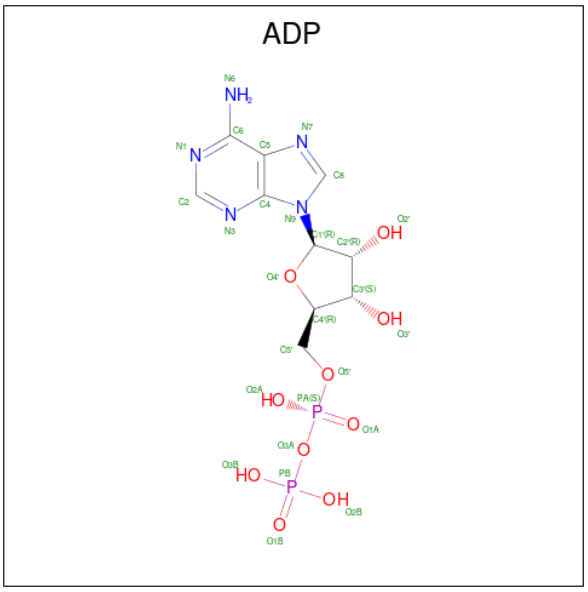
- Molecule 18 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
18	Q	2	22	12	10	0	0

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

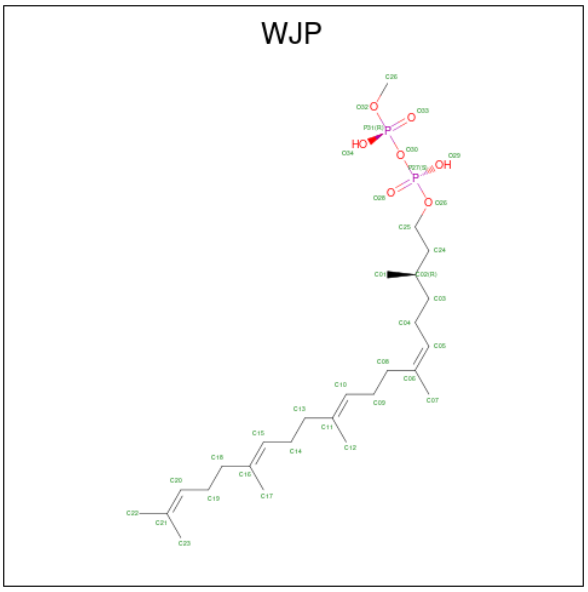
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
19	C	1	1	1	0

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



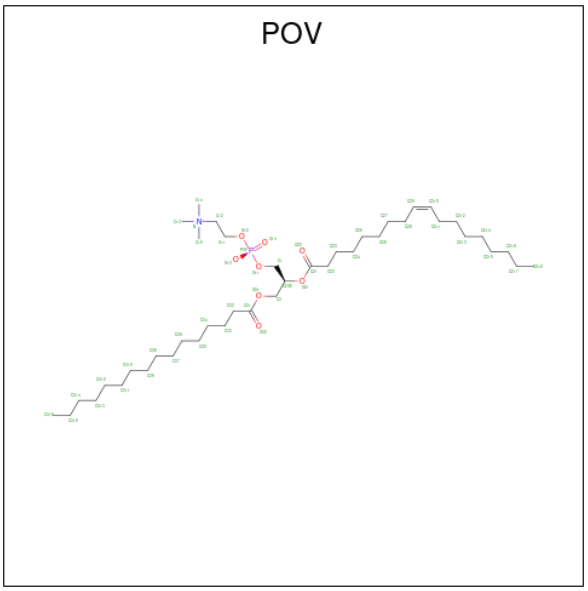
Mol	Chain	Residues	Atoms					AltConf
20	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 21 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylicosa-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (three-letter code: WJP) (formula: $C_{26}H_{48}O_7P_2$).



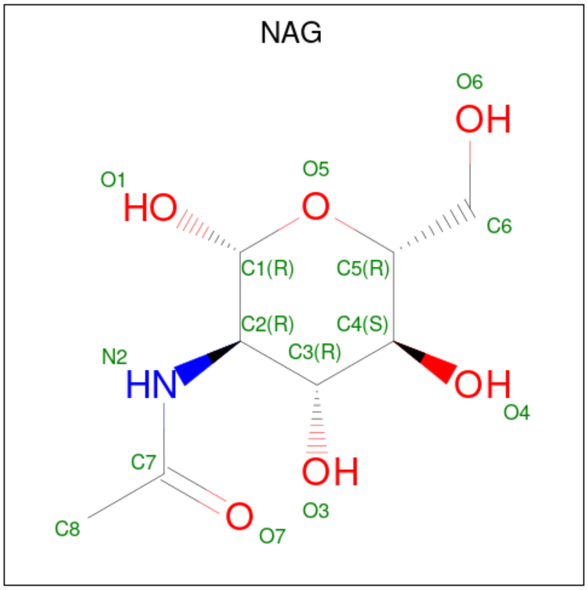
Mol	Chain	Residues	Atoms				AltConf
21	a	1	Total	C	O	P	0
			34	25	7	2	

- Molecule 22 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



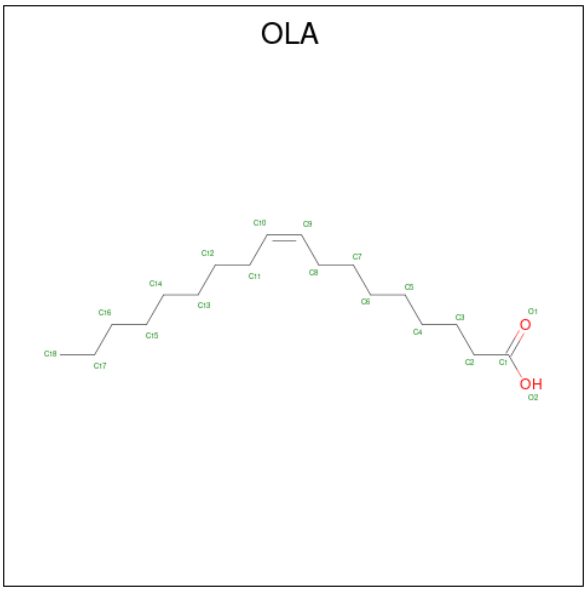
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
22	b	1	Total	C	N	O	P	0
			43	33	1	8	1	
22	s	1	Total	C	N	O	P	0
			40	30	1	8	1	
22	s	1	Total	C	N	O	P	0
			39	29	1	8	1	
22	r	1	Total	C	N	O	P	0
			47	37	1	8	1	
22	r	1	Total	C	N	O	P	0
			45	35	1	8	1	
22	r	1	Total	C	N	O	P	0
			47	37	1	8	1	
22	l	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 23 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



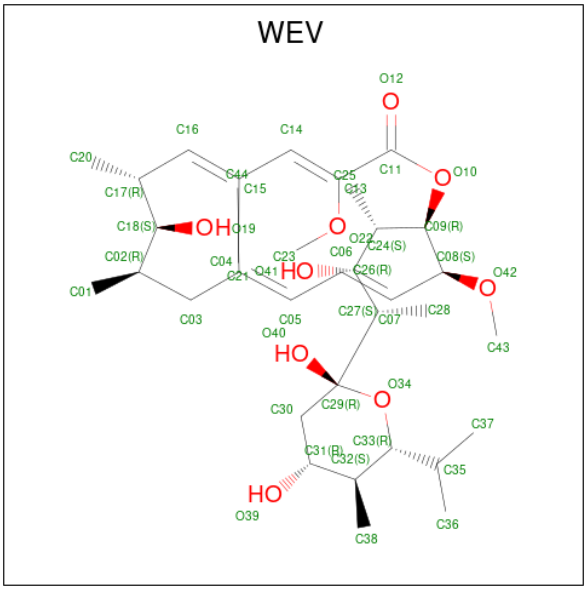
Mol	Chain	Residues	Atoms	AltConf
23	s	1	Total C N O 14 8 1 5	0
23	s	1	Total C N O 14 8 1 5	0
23	s	1	Total C N O 14 8 1 5	0
23	s	1	Total C N O 14 8 1 5	0
23	s	1	Total C N O 14 8 1 5	0
23	s	1	Total C N O 14 8 1 5	0
23	s	1	Total C N O 14 8 1 5	0

- Molecule 24 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			AltConf
24	r	1	Total	C	O	0
			20	18	2	

- Molecule 25 is (5R)-2,4-dideoxy-1-C-{(2S,3R,4S)-3-hydroxy-4-[(2R,3S,4E,6E,9R,10S,11R,12E,14Z)-10-hydroxy-3,15-dimethoxy-7,9,11,13-tetramethyl-16-oxo-1-oxacyclohexadeca-4,6,12,14-tetraen-2-yl]pentan-2-yl}-4-methyl-5-propan-2-yl-alpha-D-threo-pentopyranose (three-letter code: WEV) (formula: $C_{35}H_{58}O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	g	1	Total	C	O	0
			44	35	9	

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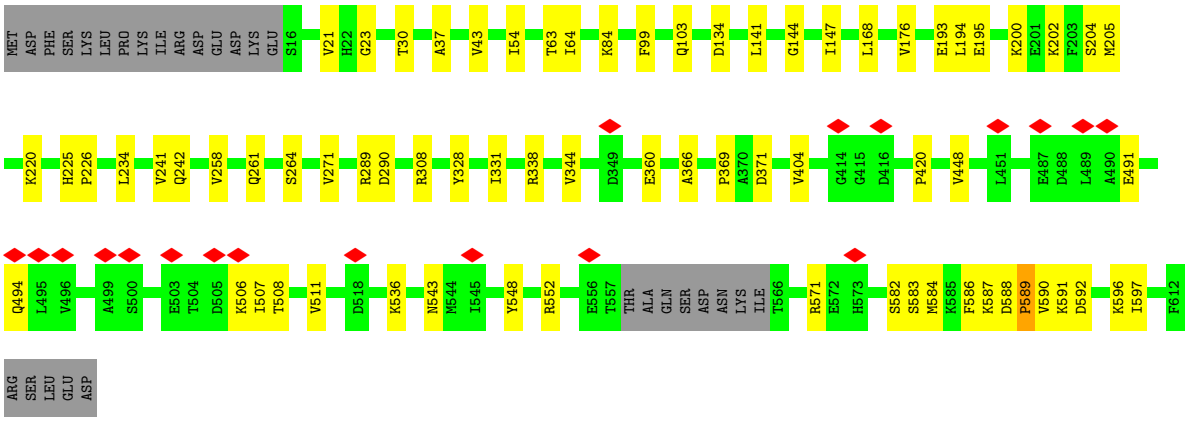
Mol	Chain	Residues	Atoms	AltConf
25	g	1	Total C O 44 35 9	0
25	l	1	Total C O 44 35 9	0
25	m	1	Total C O 44 35 9	0
25	o	1	Total C O 44 35 9	0
25	p	1	Total C O 44 35 9	0

3 Residue-property plots (i)

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

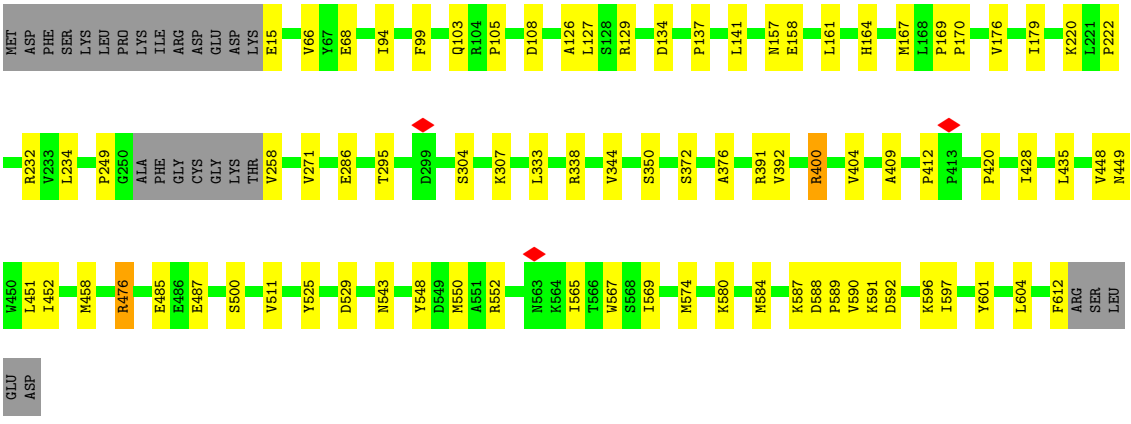
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain A:



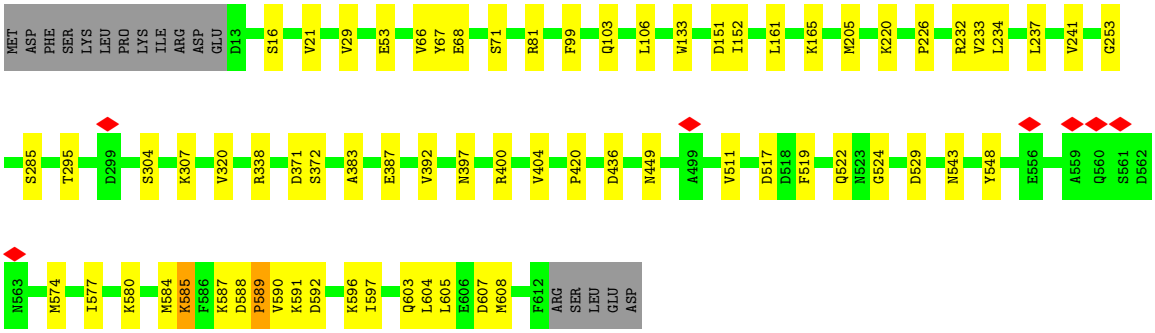
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain B:



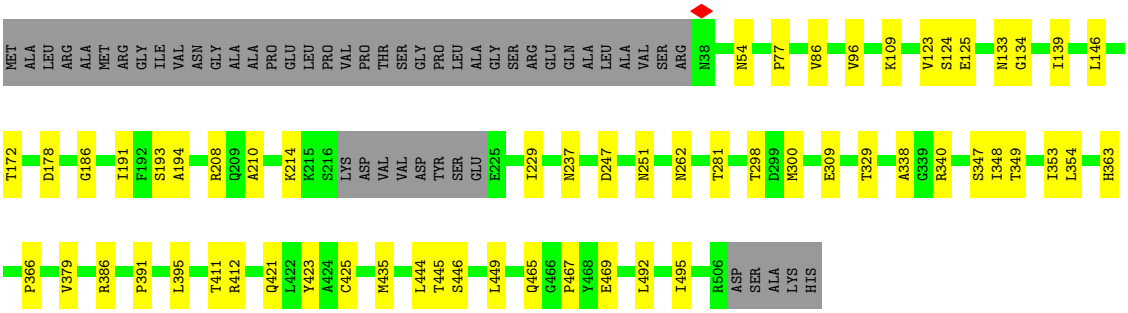
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain C:



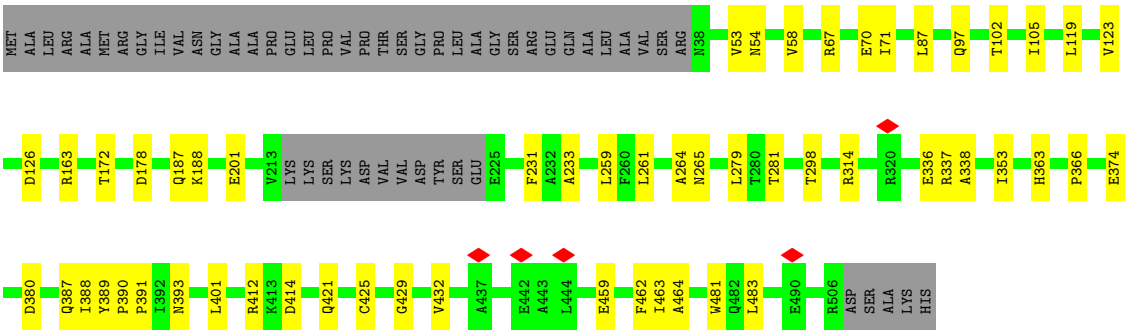
• Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain D:



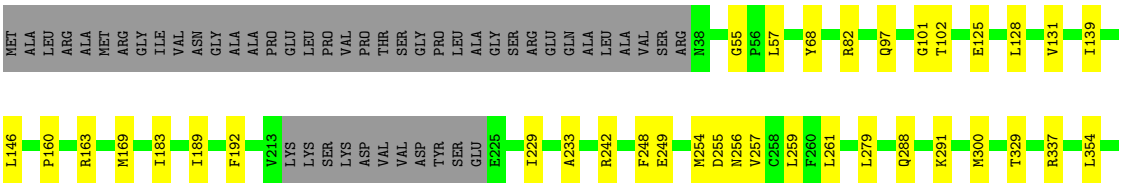
• Molecule 2: V-type proton ATPase subunit B, brain isoform

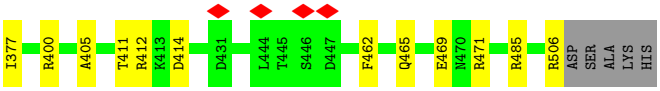
Chain E:



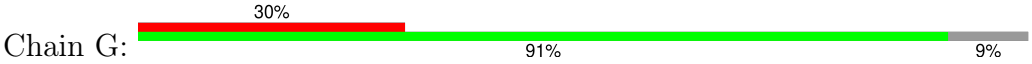
• Molecule 2: V-type proton ATPase subunit B, brain isoform

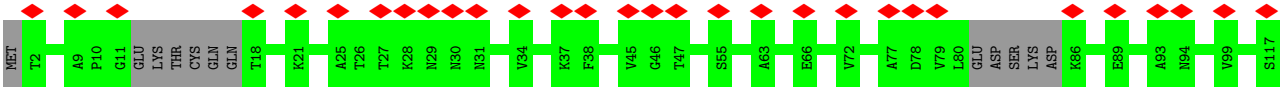
Chain F:

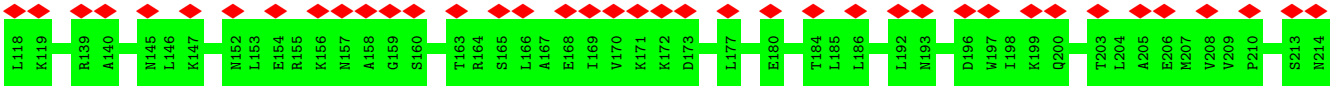


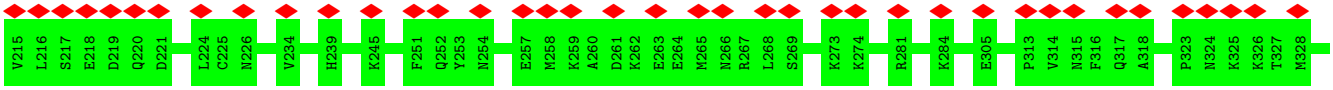


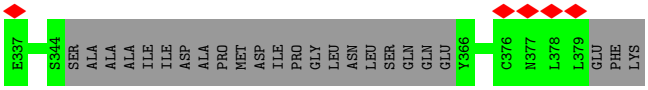
• Molecule 3: V-type proton ATPase subunit C 1



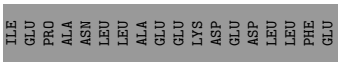




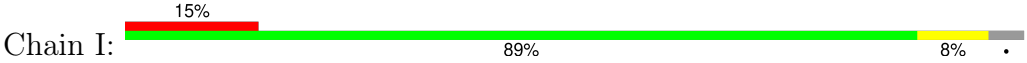


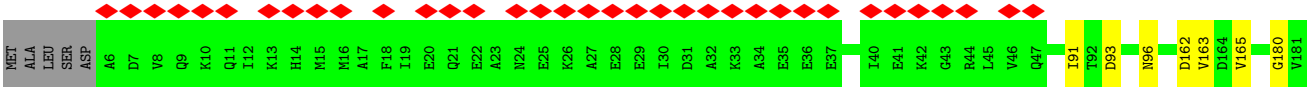


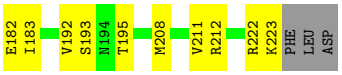
• Molecule 4: V-type proton ATPase subunit D



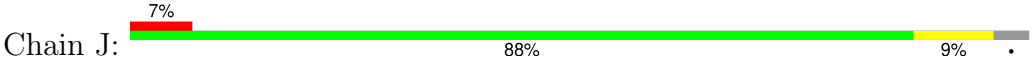
• Molecule 5: V-type proton ATPase subunit E 1

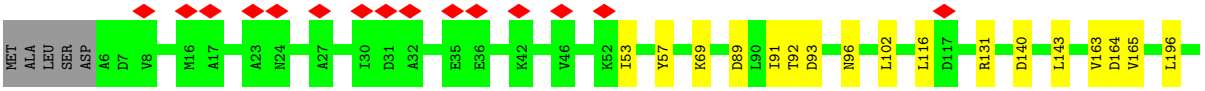


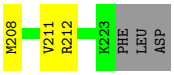




• Molecule 5: V-type proton ATPase subunit E 1

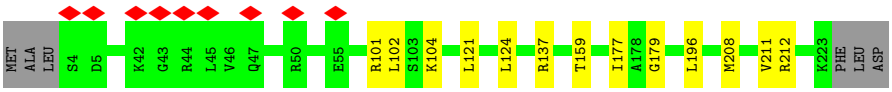






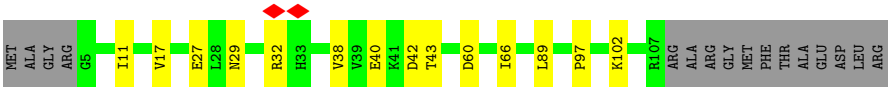
• Molecule 5: V-type proton ATPase subunit E 1

Chain K:



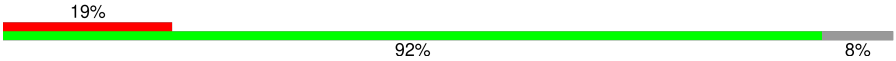
• Molecule 6: V-type proton ATPase subunit F

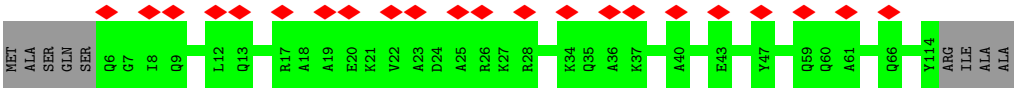
Chain L:



• Molecule 7: V-type proton ATPase subunit G

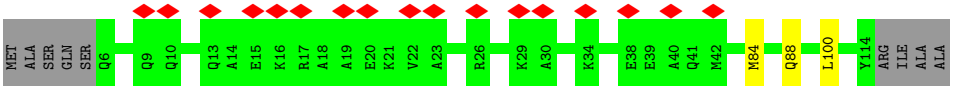
Chain M:





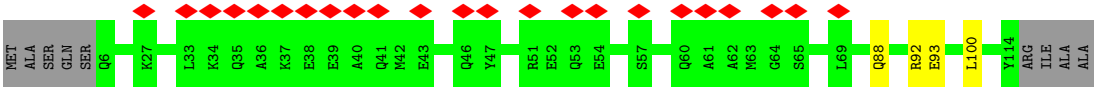
• Molecule 7: V-type proton ATPase subunit G

Chain N:



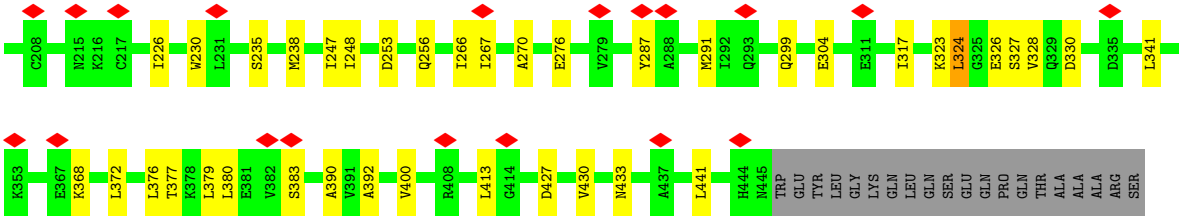
• Molecule 7: V-type proton ATPase subunit G

Chain O:

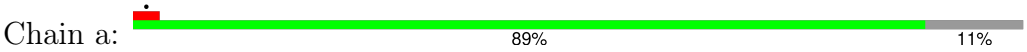


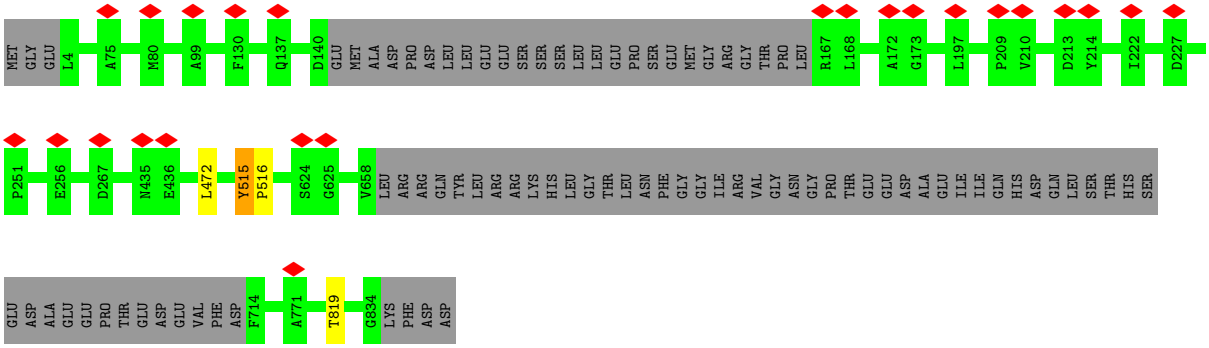
• Molecule 8: V-type proton ATPase subunit H

Chain P:

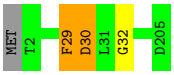


• Molecule 9: V-type proton ATPase subunit a

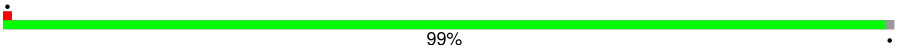


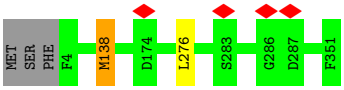


• Molecule 10: V-type proton ATPase 21 kDa proteolipid subunit

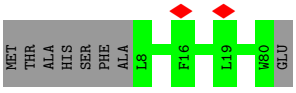


• Molecule 11: V-type proton ATPase subunit d 1

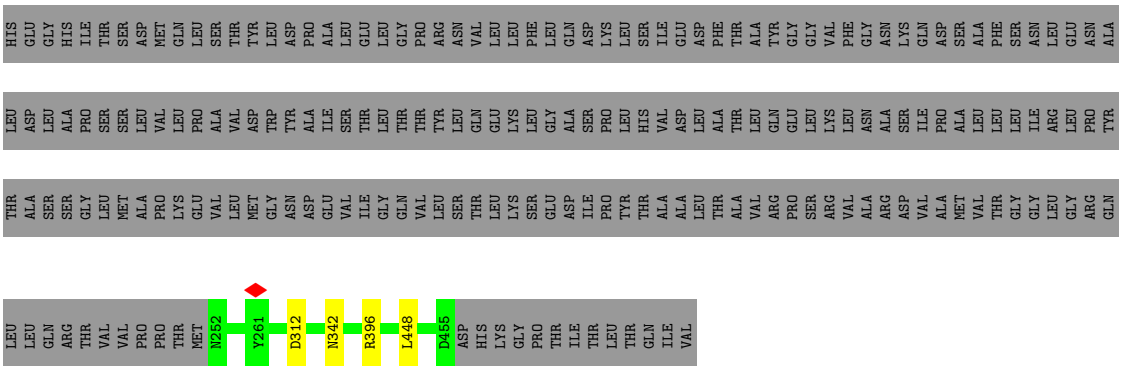




• Molecule 12: V-type proton ATPase subunit e 2

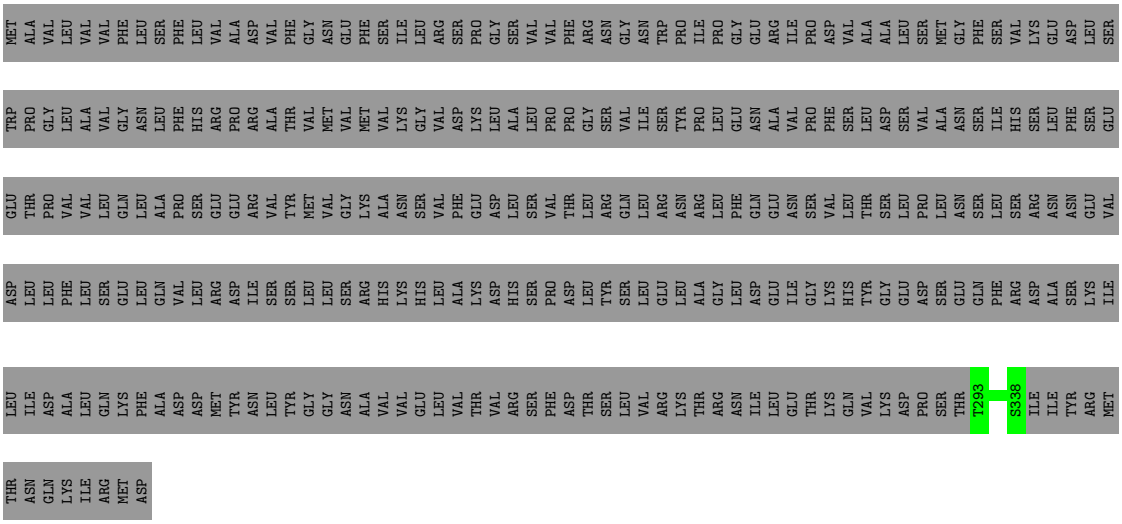


• Molecule 13: V-type proton ATPase subunit S1



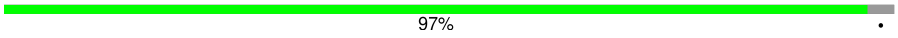
• Molecule 14: Renin receptor

Chain r:



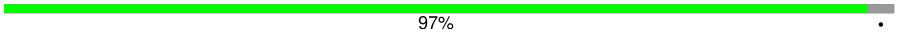
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain c:



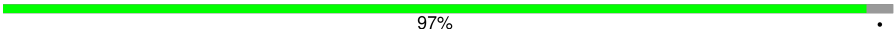
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain g:



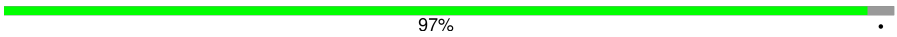
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain k:



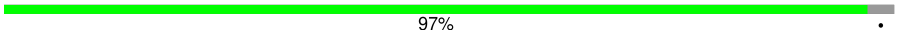
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain l:



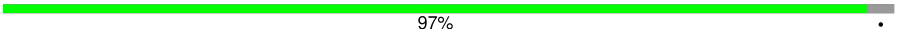
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain m:



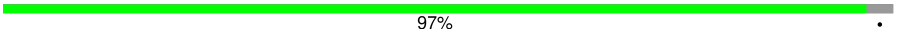
• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

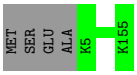
Chain n:



• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

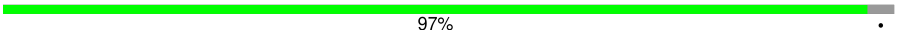
Chain o:

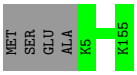




• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

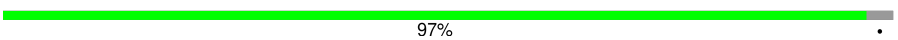
Chain p:

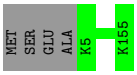




• Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

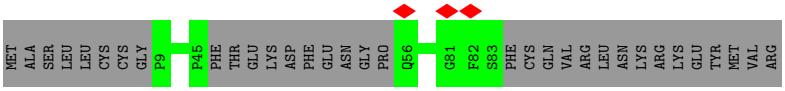
Chain q:





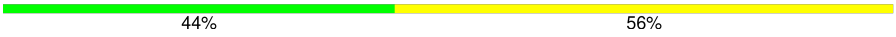
• Molecule 16: Ribonuclease kappa

Chain f:



• Molecule 17: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:



• Molecule 18: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose

Chain Q:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26530	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	28.118	Depositor
Minimum map value	-14.814	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.046	Depositor
Recommended contour level	3.4	Depositor
Map size (Å)	413.168, 413.168, 413.168	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, WJP, OLA, GLC, MAN, MG, NAG, POV, WEV, BMA

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	0.38	2/4663 (0.0%)	0.52	0/6314
1	B	0.38	1/4685 (0.0%)	0.53	1/6345 (0.0%)
1	C	0.40	1/4750 (0.0%)	0.55	1/6432 (0.0%)
2	D	0.31	0/3680	0.53	0/4986
2	E	0.33	1/3656 (0.0%)	0.54	2/4956 (0.0%)
2	F	0.30	0/3656	0.50	0/4956
3	G	0.23	0/1716	0.43	0/2390
4	H	0.25	0/1726	0.49	1/2309 (0.0%)
5	I	0.27	0/1554	0.46	0/2108
5	J	0.25	0/1649	0.46	0/2223
5	K	0.26	0/1579	0.46	0/2139
6	L	0.26	0/829	0.50	0/1122
7	M	0.23	0/666	0.39	0/912
7	N	0.24	0/687	0.41	0/939
7	O	0.23	0/680	0.40	0/930
8	P	0.31	0/2526	0.56	1/3439 (0.0%)
9	a	0.33	1/5965 (0.0%)	0.55	2/8090 (0.0%)
10	b	0.47	1/1537 (0.1%)	0.60	3/2090 (0.1%)
11	d	0.29	0/2884	0.54	2/3906 (0.1%)
12	e	0.27	0/613	0.45	0/844
13	s	0.42	0/1712	0.66	3/2331 (0.1%)
14	r	0.28	0/398	0.52	0/547
15	c	0.30	0/1079	0.49	0/1459
15	g	0.29	0/1079	0.49	0/1459
15	k	0.29	0/1079	0.48	0/1459
15	l	0.29	0/1079	0.48	0/1459
15	m	0.29	0/1079	0.46	0/1459
15	n	0.29	0/1079	0.49	0/1459
15	o	0.30	0/1088	0.48	0/1470
15	p	0.30	0/1088	0.50	0/1470
15	q	0.29	0/1088	0.51	0/1470
16	f	0.27	0/512	0.52	0/695

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.33	7/62061 (0.0%)	0.52	16/84167 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	589	PRO	N-CD	-14.12	1.28	1.47
1	B	589	PRO	N-CD	-14.07	1.28	1.47
1	A	589	PRO	N-CD	-14.06	1.28	1.47
2	E	387	GLN	C-N	7.05	1.50	1.34
1	A	582	SER	C-N	5.63	1.47	1.34
9	a	515	TYR	CE1-CZ	-5.46	1.31	1.38
10	b	32	GLY	C-O	-5.28	1.15	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	s	448	LEU	CA-CB-CG	8.88	135.73	115.30
9	a	515	TYR	C-N-CD	-8.69	101.48	120.60
9	a	515	TYR	N-CA-C	7.95	132.46	111.00
2	E	391	PRO	O-C-N	-7.91	110.05	122.70
10	b	29	PHE	N-CA-C	-7.56	90.59	111.00
1	B	525	TYR	C-N-CA	6.38	137.66	121.70
8	P	324	LEU	CA-CB-CG	-5.91	101.71	115.30
10	b	30	ASP	N-CA-C	5.86	126.82	111.00
11	d	276	LEU	CA-CB-CG	5.80	128.64	115.30
13	s	342	ASN	CB-CA-C	-5.64	99.12	110.40
11	d	138	MET	CA-CB-CG	5.63	122.88	113.30
1	C	585	LYS	O-C-N	5.58	131.63	122.70
13	s	312	ASP	CB-CG-OD2	5.35	123.12	118.30
10	b	30	ASP	CB-CG-OD1	5.32	123.09	118.30
2	E	387	GLN	O-C-N	-5.28	114.25	122.70
4	H	217	ASP	CB-CG-OD2	5.19	122.97	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4568	0	4551	61	0
1	B	4591	0	4571	70	0
1	C	4654	0	4630	59	0
2	D	3609	0	3611	38	0
2	E	3585	0	3579	31	0
2	F	3585	0	3580	34	0
3	G	1720	0	758	0	0
4	H	1708	0	1816	15	0
5	I	1543	0	1435	11	0
5	J	1636	0	1614	13	0
5	K	1568	0	1476	9	0
6	L	816	0	818	10	0
7	M	663	0	495	0	0
7	N	684	0	532	2	0
7	O	677	0	516	3	0
8	P	2499	0	2069	33	0
9	a	5827	0	5639	0	0
10	b	1503	0	1550	0	0
11	d	2819	0	2756	0	0
12	e	590	0	613	0	0
13	s	1660	0	1542	0	0
14	r	385	0	373	0	0
15	c	1064	0	1132	0	0
15	g	1064	0	1132	0	0
15	k	1064	0	1132	0	0
15	l	1064	0	1132	0	0
15	m	1064	0	1132	0	0
15	n	1064	0	1132	0	0
15	o	1073	0	1145	0	0
15	p	1073	0	1145	0	0
15	q	1073	0	1145	0	0
16	f	501	0	510	0	0
17	t	105	0	87	0	0
18	Q	22	0	19	0	0
19	C	1	0	0	0	0
20	C	27	0	12	2	0
21	a	34	0	0	0	0
22	b	90	0	125	0	0
22	l	40	0	52	0	0
22	r	139	0	194	0	0
22	s	79	0	103	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	s	98	0	91	0	0
24	r	20	0	33	0	0
25	g	88	0	0	0	0
25	l	44	0	0	0	0
25	m	44	0	0	0	0
25	o	44	0	0	0	0
25	p	44	0	0	0	0
All	All	61913	0	59977	358	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 6.

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LYS:NZ	1:A:597:ILE:HD13	1.44	1.32
1:C:587:LYS:O	1:C:597:ILE:HD11	1.07	1.24
1:C:587:LYS:O	1:C:597:ILE:CD1	1.86	1.23
8:P:291:MET:CE	8:P:324:LEU:HD21	1.75	1.15
8:P:291:MET:SD	8:P:324:LEU:HD21	1.89	1.13
1:A:536:LYS:HE3	1:A:589:PRO:HD3	1.31	1.11
8:P:291:MET:SD	8:P:324:LEU:CD2	2.42	1.07
1:B:574:MET:HE1	1:B:612:PHE:CD1	1.93	1.03
1:B:15:GLU:OE2	2:D:109:LYS:HE2	1.57	1.03
1:A:536:LYS:NZ	1:A:597:ILE:CD1	2.22	1.01
8:P:291:MET:HE3	8:P:324:LEU:HD21	1.44	0.99
1:A:536:LYS:HZ3	1:A:597:ILE:HD13	1.28	0.99
1:A:588:ASP:O	1:A:592:ASP:HB2	1.67	0.95
1:C:588:ASP:O	1:C:592:ASP:HB2	1.67	0.94
1:A:536:LYS:HZ1	1:A:597:ILE:HD13	1.20	0.94
1:B:588:ASP:O	1:B:592:ASP:HB2	1.67	0.94
1:A:588:ASP:O	1:A:592:ASP:CB	2.18	0.92
1:B:588:ASP:O	1:B:592:ASP:CB	2.18	0.92
1:C:588:ASP:O	1:C:592:ASP:CB	2.18	0.90
1:A:536:LYS:HZ1	1:A:597:ILE:CD1	1.83	0.87
1:A:590:VAL:HG13	1:A:591:LYS:HG3	1.60	0.84
1:C:590:VAL:HG13	1:C:591:LYS:HG3	1.60	0.83
8:P:341:LEU:CB	8:P:376:LEU:HD23	2.09	0.83
1:B:574:MET:CE	1:B:612:PHE:CE1	2.62	0.82
1:B:590:VAL:HG13	1:B:591:LYS:HG3	1.60	0.81
8:P:291:MET:SD	8:P:324:LEU:HD22	2.19	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:341:LEU:CB	8:P:376:LEU:CD2	2.59	0.80
1:A:536:LYS:HZ3	1:A:597:ILE:CD1	1.89	0.80
1:A:536:LYS:HE3	1:A:589:PRO:CD	2.10	0.80
1:B:543:ASN:HD22	1:B:584:MET:CE	1.97	0.78
1:B:574:MET:CE	1:B:612:PHE:CD1	2.66	0.76
1:B:574:MET:HE3	1:B:612:PHE:CE1	2.19	0.76
1:B:574:MET:HE3	1:B:612:PHE:HE1	1.53	0.73
1:B:588:ASP:O	1:B:592:ASP:HB3	1.90	0.72
8:P:276:GLU:OE1	8:P:323:LYS:HE2	1.90	0.72
1:C:588:ASP:O	1:C:592:ASP:HB3	1.89	0.72
1:B:580:LYS:HB3	1:B:604:LEU:HD21	1.72	0.71
1:C:580:LYS:HB3	1:C:604:LEU:HD21	1.72	0.70
1:A:588:ASP:OD1	1:A:590:VAL:HG12	1.92	0.70
8:P:256:GLN:HA	8:P:299:GLN:HE22	1.57	0.70
1:B:588:ASP:OD1	1:B:590:VAL:HG12	1.92	0.70
8:P:291:MET:HE3	8:P:324:LEU:CD2	2.19	0.69
1:A:588:ASP:O	1:A:592:ASP:HB3	1.90	0.69
1:C:588:ASP:OD1	1:C:590:VAL:HG12	1.92	0.69
8:P:291:MET:CE	8:P:324:LEU:CD2	2.65	0.67
1:B:587:LYS:O	1:B:597:ILE:HD11	1.94	0.67
1:C:580:LYS:HB3	1:C:604:LEU:CD2	2.24	0.67
1:A:587:LYS:O	1:A:597:ILE:HD11	1.94	0.66
1:C:71:SER:HA	2:F:68:TYR:HD2	1.61	0.66
1:B:15:GLU:OE2	2:D:109:LYS:CE	2.40	0.66
1:A:371:ASP:OD2	1:A:420:PRO:HB3	1.98	0.64
1:B:350:SER:H	1:B:409:ALA:HB3	1.63	0.63
1:B:550:MET:SD	1:B:612:PHE:HD2	2.22	0.62
1:B:574:MET:HE1	1:B:612:PHE:HD1	1.62	0.62
1:C:592:ASP:OD1	1:C:596:LYS:HG2	1.99	0.61
2:E:163:ARG:NH2	2:E:338:ALA:O	2.33	0.61
1:A:587:LYS:O	1:A:597:ILE:CD1	2.49	0.60
1:B:574:MET:HE1	1:B:612:PHE:CE1	2.26	0.60
1:B:550:MET:HB2	1:B:612:PHE:CE2	2.36	0.60
2:D:134:GLY:HA3	2:D:262:ASN:HD22	1.66	0.60
8:P:390:ALA:HB1	8:P:433:ASN:HD22	1.67	0.60
2:F:146:LEU:HD23	5:I:212:ARG:HD2	1.83	0.60
1:B:66:VAL:HG12	1:B:68:GLU:H	1.66	0.59
1:B:587:LYS:O	1:B:597:ILE:CD1	2.49	0.59
2:F:249:GLU:HG2	2:F:254:MET:HG3	1.84	0.59
8:P:247:ILE:HG23	8:P:248:ILE:HD12	1.84	0.59
1:B:543:ASN:HD22	1:B:584:MET:HE3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:388:ILE:HG23	2:E:464:ALA:HB2	1.84	0.59
6:L:40:GLU:HG2	6:L:43:THR:HG23	1.85	0.59
1:B:550:MET:SD	1:B:612:PHE:CD2	2.95	0.59
1:B:550:MET:HB3	1:B:612:PHE:CD2	2.37	0.58
5:K:102:LEU:HD13	7:O:100:LEU:HD22	1.85	0.58
1:A:43:VAL:HG21	1:A:64:ILE:HD13	1.85	0.58
1:C:220:LYS:HA	1:C:392:VAL:HG23	1.84	0.58
1:A:226:PRO:HA	1:A:241:VAL:HA	1.87	0.57
2:E:87:LEU:HD13	2:E:314:ARG:HD2	1.86	0.57
8:P:276:GLU:CD	8:P:323:LYS:HE2	2.25	0.57
1:B:249:PRO:HG2	1:B:435:LEU:HB2	1.86	0.57
2:D:86:VAL:HG22	2:D:96:VAL:HG12	1.86	0.57
2:E:126:ASP:OD1	5:K:212:ARG:NH2	2.38	0.57
1:A:234:LEU:HD21	1:A:448:VAL:HG21	1.86	0.56
2:D:421:GLN:NE2	2:D:425:CYS:SG	2.77	0.56
1:A:289:ARG:NH1	1:A:290:ASP:OD1	2.39	0.56
1:B:234:LEU:HD21	1:B:448:VAL:HG21	1.86	0.56
4:H:149:ALA:HB2	6:L:89:LEU:HD11	1.88	0.56
1:C:233:VAL:HG23	1:C:237:LEU:HD12	1.88	0.56
1:A:204:SER:OG	1:A:205:MET:N	2.39	0.56
1:A:264:SER:O	1:A:308:ARG:NH2	2.35	0.55
2:D:77:PRO:HB3	2:D:109:LYS:HB2	1.88	0.55
1:B:222:PRO:O	1:B:391:ARG:NH1	2.39	0.55
2:E:188:LYS:NZ	2:E:374:GLU:OE2	2.40	0.55
8:P:400:VAL:HG21	8:P:441:LEU:HD23	1.88	0.55
1:A:220:LYS:O	2:F:242:ARG:NH2	2.39	0.55
1:B:428:ILE:O	2:D:237:ASN:ND2	2.39	0.55
1:C:511:VAL:HG21	1:C:548:TYR:HB2	1.89	0.55
1:A:543:ASN:HD22	1:A:584:MET:HE3	1.71	0.55
1:C:580:LYS:HB3	1:C:604:LEU:CD1	2.37	0.55
2:E:188:LYS:HE2	2:E:336:GLU:HA	1.88	0.54
1:B:543:ASN:HB2	1:B:584:MET:HE1	1.89	0.54
20:C:702:ADP:O3A	2:F:400:ARG:NH1	2.39	0.54
1:B:548:TYR:OH	1:B:552:ARG:NH2	2.40	0.54
1:C:517:ASP:O	1:C:585:LYS:NZ	2.40	0.54
1:C:603:GLN:NE2	1:C:607:ASP:OD1	2.41	0.54
5:I:162:ASP:N	5:I:162:ASP:OD1	2.41	0.54
8:P:377:THR:HA	8:P:380:LEU:HD12	1.90	0.54
2:F:125:GLU:OE2	2:F:291:LYS:NZ	2.40	0.54
1:A:99:PHE:HB3	1:A:103:GLN:HA	1.90	0.54
1:A:590:VAL:HG13	1:A:591:LYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:VAL:HG13	1:B:591:LYS:N	2.23	0.54
1:C:590:VAL:HG13	1:C:591:LYS:N	2.23	0.53
2:F:279:LEU:HB3	2:F:337:ARG:HD2	1.89	0.53
1:A:271:VAL:HG23	1:A:344:VAL:HG13	1.90	0.53
2:E:380:ASP:HB2	2:E:393:ASN:HB2	1.90	0.53
1:A:536:LYS:HE2	1:A:589:PRO:HB3	1.91	0.53
1:B:592:ASP:OD1	1:B:596:LYS:HG2	2.09	0.53
1:C:580:LYS:CB	1:C:604:LEU:HD11	2.38	0.53
4:H:193:GLU:HG2	4:H:196:ARG:HH21	1.72	0.53
4:H:204:LYS:HG3	4:H:208:LYS:HE2	1.91	0.53
8:P:235:SER:HB3	8:P:238:MET:HG3	1.91	0.53
1:C:151:ASP:HB3	1:C:397:ASN:H	1.74	0.53
1:C:226:PRO:HA	1:C:241:VAL:HA	1.90	0.53
6:L:40:GLU:HG3	6:L:42:ASP:H	1.74	0.53
2:D:193:SER:OG	2:D:194:ALA:N	2.42	0.53
1:A:592:ASP:OD1	1:A:596:LYS:HG2	2.09	0.52
1:C:580:LYS:HB3	1:C:604:LEU:HD11	1.90	0.52
4:H:30:ARG:O	4:H:34:LYS:N	2.43	0.52
1:A:491:GLU:O	1:A:494:GLN:NE2	2.43	0.52
2:D:123:VAL:HG12	2:D:281:THR:HG22	1.92	0.52
4:H:30:ARG:HD2	4:H:173:GLU:HG2	1.92	0.52
2:D:395:LEU:HA	2:D:423:TYR:HE1	1.75	0.52
5:I:180:GLY:HA3	5:I:195:THR:HA	1.92	0.51
5:I:182:GLU:HG2	5:I:193:SER:HA	1.91	0.51
2:E:279:LEU:HB3	2:E:337:ARG:HD2	1.92	0.51
2:F:465:GLN:NE2	2:F:469:GLU:O	2.43	0.51
1:A:168:LEU:HD11	1:A:194:LEU:HD11	1.91	0.51
1:A:371:ASP:OD1	1:A:371:ASP:O	2.27	0.51
1:A:583:SER:HA	1:A:586:PHE:CD1	2.46	0.51
1:C:320:VAL:HG22	2:F:329:THR:HG21	1.93	0.51
1:C:574:MET:HB3	1:C:577:ILE:HB	1.93	0.51
2:F:82:ARG:NH1	2:F:101:GLY:O	2.44	0.51
1:A:141:LEU:HD21	1:A:147:ILE:HD12	1.92	0.51
8:P:253:ASP:O	8:P:256:GLN:NE2	2.39	0.51
2:F:183:ILE:HG22	2:F:189:ILE:HD13	1.93	0.51
1:B:550:MET:CB	1:B:612:PHE:CE2	2.94	0.50
8:P:390:ALA:HB2	8:P:430:VAL:HA	1.93	0.50
1:C:371:ASP:OD1	1:C:371:ASP:N	2.42	0.50
2:F:229:ILE:HB	2:F:257:VAL:HG22	1.93	0.50
5:J:93:ASP:HA	5:J:96:ASN:HB2	1.94	0.50
8:P:230:TRP:HD1	8:P:270:ALA:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:VAL:N	1:B:286:GLU:OE2	2.45	0.50
5:I:208:MET:HA	5:I:211:VAL:HG22	1.94	0.50
2:D:379:VAL:HG13	2:D:391:PRO:HG2	1.94	0.49
1:A:369:PRO:HG2	4:H:196:ARG:HG2	1.94	0.49
5:K:101:ARG:NH1	7:O:93:GLU:OE1	2.44	0.49
5:I:163:VAL:HB	5:I:165:VAL:HG23	1.94	0.49
8:P:379:LEU:O	8:P:383:SER:OG	2.30	0.49
1:C:161:LEU:HD12	1:C:307:LYS:HB2	1.95	0.49
5:I:93:ASP:HA	5:I:96:ASN:HB2	1.94	0.49
1:C:524:GLY:H	20:C:702:ADP:HN62	1.61	0.49
2:E:390:PRO:HD2	2:E:463:ILE:O	2.13	0.49
8:P:266:ILE:O	8:P:270:ALA:N	2.41	0.49
2:F:169:MET:HB2	2:F:405:ALA:HB1	1.94	0.48
1:B:451:LEU:HD11	1:B:487:GLU:HG3	1.95	0.48
1:A:338:ARG:HG3	1:A:404:VAL:HG23	1.93	0.48
1:B:137:PRO:HB3	1:B:179:ILE:HD11	1.95	0.48
8:P:168:ILE:O	8:P:172:LEU:N	2.47	0.48
8:P:380:LEU:HD21	8:P:392:ALA:HB3	1.96	0.48
1:C:71:SER:HA	2:F:68:TYR:CD2	2.47	0.48
1:C:580:LYS:C	1:C:604:LEU:HD21	2.34	0.48
2:E:201:GLU:HB3	2:E:389:TYR:OH	2.14	0.48
4:H:178:PRO:HA	4:H:181:GLU:HG2	1.96	0.48
2:E:414:ASP:OD2	2:E:481:TRP:NE1	2.37	0.48
2:F:131:VAL:HG12	2:F:259:LEU:HB2	1.96	0.48
2:E:412:ARG:NE	2:E:414:ASP:OD1	2.45	0.47
5:J:131:ARG:HG3	5:J:164:ASP:HB3	1.97	0.47
1:B:565:ILE:HG22	1:B:567:TRP:H	1.79	0.47
2:F:412:ARG:NE	2:F:414:ASP:OD1	2.44	0.47
1:A:30:THR:HG22	1:A:63:THR:HG23	1.96	0.47
2:D:133:ASN:HB3	2:D:139:ILE:HD11	1.97	0.47
8:P:368:LYS:HB3	8:P:372:LEU:HB2	1.97	0.47
1:A:507:ILE:HD13	1:A:571:ARG:HH21	1.79	0.47
1:C:16:SER:O	1:C:81:ARG:NH2	2.47	0.47
5:J:53:ILE:O	5:J:57:TYR:N	2.47	0.47
5:K:121:LEU:HA	5:K:124:LEU:HD12	1.96	0.47
8:P:304:GLU:HA	8:P:317:ILE:HD12	1.95	0.47
2:F:131:VAL:HG23	2:F:139:ILE:HB	1.97	0.47
1:A:508:THR:HA	1:A:511:VAL:HG12	1.97	0.47
1:B:376:ALA:HB1	2:D:309:GLU:HA	1.97	0.47
1:B:550:MET:CB	1:B:612:PHE:CD2	2.97	0.47
4:H:145:LEU:HD12	6:L:89:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:465:GLN:NE2	2:D:469:GLU:O	2.48	0.47
2:D:210:ALA:HB3	2:D:229:ILE:HD11	1.97	0.46
2:E:123:VAL:HG12	2:E:281:THR:HG22	1.95	0.46
2:D:445:THR:OG1	2:D:446:SER:N	2.49	0.46
2:E:87:LEU:HG	2:E:97:GLN:HG2	1.96	0.46
2:E:187:GLN:HB2	2:E:401:LEU:HD12	1.97	0.46
1:A:195:GLU:HG3	1:A:200:LYS:HD3	1.97	0.46
1:C:522:GLN:HG3	1:C:529:ASP:HB3	1.97	0.46
2:F:128:LEU:HG	2:F:256:ASN:HA	1.96	0.46
1:B:157:ASN:OD1	1:B:157:ASN:N	2.47	0.46
1:B:458:MET:SD	1:B:476:ARG:NH2	2.89	0.46
1:C:99:PHE:HB3	1:C:103:GLN:HA	1.97	0.46
2:F:192:PHE:N	2:F:377:ILE:O	2.44	0.46
8:P:377:THR:HG21	8:P:413:LEU:HD11	1.98	0.46
1:B:584:MET:O	1:B:601:TYR:OH	2.32	0.46
1:B:338:ARG:HG3	1:B:404:VAL:HG23	1.98	0.45
1:B:565:ILE:HG23	1:B:569:ILE:HB	1.97	0.45
2:E:231:PHE:HB3	2:E:259:LEU:HD23	1.98	0.45
1:C:232:ARG:NH1	1:C:519:PHE:O	2.47	0.45
5:I:222:ARG:HD2	5:I:222:ARG:HA	1.70	0.45
2:D:435:MET:HG2	4:H:35:LYS:HD3	1.99	0.45
2:E:102:THR:HG22	2:E:105:ILE:HD12	1.99	0.45
2:E:233:ALA:HB3	2:E:261:LEU:HA	1.99	0.45
1:A:258:VAL:HA	1:A:261:GLN:HG2	1.99	0.45
2:D:247:ASP:O	2:D:251:ASN:ND2	2.49	0.45
2:D:298:THR:HA	2:D:353:ILE:HB	1.99	0.45
2:E:388:ILE:HD13	2:E:459:GLU:HB3	1.99	0.45
5:J:163:VAL:HB	5:J:165:VAL:HG23	1.98	0.45
1:B:158:GLU:OE2	1:B:164:HIS:ND1	2.46	0.45
1:C:436:ASP:HB2	1:C:449:ASN:HB2	1.99	0.45
1:C:592:ASP:OD1	1:C:596:LYS:CG	2.64	0.45
5:K:208:MET:HA	5:K:211:VAL:HG22	1.99	0.45
1:A:193:GLU:HG3	1:A:202:LYS:HB3	1.99	0.45
1:B:141:LEU:HD21	1:B:176:VAL:HG21	1.98	0.45
2:E:71:ILE:HD12	2:E:119:LEU:HD13	1.99	0.45
1:B:587:LYS:HA	1:B:587:LYS:HD3	1.80	0.44
2:D:124:SER:OG	2:D:125:GLU:N	2.50	0.44
6:L:29:ASN:HB3	6:L:32:ARG:HH21	1.82	0.44
1:A:583:SER:O	1:A:583:SER:OG	2.30	0.44
1:A:590:VAL:CG1	1:A:591:LYS:N	2.80	0.44
1:B:161:LEU:HD12	1:B:307:LYS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:ASN:OD1	2:E:54:ASN:N	2.49	0.44
2:F:233:ALA:HB3	2:F:261:LEU:HA	1.99	0.44
5:J:102:LEU:HD13	7:N:100:LEU:HD22	1.99	0.44
1:B:590:VAL:CG1	1:B:591:LYS:N	2.80	0.44
2:F:146:LEU:HD11	5:I:91:ILE:HG13	1.99	0.44
6:L:17:VAL:HG21	6:L:38:VAL:HG22	1.97	0.44
1:B:372:SER:HB3	1:B:420:PRO:HG2	2.00	0.44
5:I:183:ILE:HG23	5:I:192:VAL:HB	1.99	0.44
2:D:54:ASN:N	2:D:54:ASN:OD1	2.50	0.44
1:B:99:PHE:HB3	1:B:103:GLN:HA	1.99	0.44
1:C:133:TRP:HB2	1:C:205:MET:HE1	1.99	0.44
2:D:146:LEU:HD11	5:J:91:ILE:HG13	1.99	0.44
1:C:66:VAL:HG12	1:C:68:GLU:H	1.83	0.44
1:A:366:ALA:O	4:H:203:LYS:NZ	2.43	0.44
1:B:105:PRO:HD3	1:B:126:ALA:HA	2.00	0.44
2:D:340:ARG:HG2	2:D:347:SER:HB2	1.99	0.44
2:E:53:VAL:HG22	2:E:58:VAL:HG22	2.00	0.44
2:F:462:PHE:O	2:F:471:ARG:NH1	2.50	0.44
1:B:232:ARG:NH2	1:B:529:ASP:OD1	2.50	0.44
1:B:249:PRO:HB2	1:B:412:PRO:HA	2.00	0.44
2:F:255:ASP:N	2:F:255:ASP:OD1	2.42	0.44
1:C:253:GLY:HA2	2:F:400:ARG:HH12	1.82	0.43
1:C:543:ASN:ND2	1:C:584:MET:HE1	2.33	0.43
1:C:587:LYS:C	1:C:597:ILE:HD11	2.12	0.43
8:P:226:ILE:HG21	8:P:267:ILE:HG12	2.00	0.43
1:A:37:ALA:HB1	1:A:54:ILE:HD13	1.98	0.43
1:C:372:SER:HB3	1:C:420:PRO:HG3	2.00	0.43
2:D:492:LEU:HD23	2:D:495:ILE:HD12	1.99	0.43
1:A:536:LYS:HE3	1:A:589:PRO:CG	2.49	0.43
1:C:53:GLU:OE1	1:C:67:TYR:OH	2.32	0.43
2:D:172:THR:OG1	2:D:178:ASP:OD1	2.35	0.43
1:C:543:ASN:HD22	1:C:584:MET:CE	2.30	0.43
2:F:411:THR:OG1	2:F:412:ARG:N	2.51	0.43
5:K:177:ILE:HG22	5:K:179:GLY:H	1.83	0.43
1:C:587:LYS:HB3	1:C:597:ILE:HG12	2.01	0.43
1:C:590:VAL:CG1	1:C:591:LYS:N	2.80	0.43
2:E:462:PHE:HB2	2:E:483:LEU:HD11	2.00	0.43
6:L:60:ASP:OD1	6:L:60:ASP:N	2.46	0.43
1:B:500:SER:O	1:B:500:SER:OG	2.31	0.43
1:C:285:SER:OG	2:F:163:ARG:O	2.29	0.43
2:D:146:LEU:HD23	5:J:212:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:GLY:H	2:D:349:THR:HB	1.84	0.43
2:D:300:MET:HB2	2:D:354:LEU:HB3	2.00	0.43
2:D:363:HIS:HB3	2:D:366:PRO:HD2	2.00	0.43
2:F:55:GLY:O	2:F:102:THR:OG1	2.31	0.43
1:A:328:TYR:HA	1:A:331:ILE:HG22	2.00	0.43
2:D:208:ARG:NH2	2:D:467:PRO:O	2.52	0.43
2:E:429:GLY:HA2	2:E:432:VAL:HG22	1.99	0.43
8:P:276:GLU:OE1	8:P:323:LYS:CE	2.63	0.43
1:C:233:VAL:HG13	1:C:234:LEU:HD12	2.01	0.43
1:C:580:LYS:O	1:C:604:LEU:HD21	2.19	0.43
4:H:30:ARG:HD3	4:H:177:ILE:HD12	2.01	0.43
8:P:122:ALA:O	8:P:126:PHE:N	2.52	0.43
1:A:21:VAL:HG12	1:A:23:GLY:H	1.84	0.42
1:B:220:LYS:HD3	1:B:392:VAL:HG12	1.99	0.42
1:B:271:VAL:HG23	1:B:344:VAL:HG13	2.01	0.42
2:E:172:THR:OG1	2:E:178:ASP:OD1	2.37	0.42
2:F:248:PHE:HB3	2:F:254:MET:HG2	2.01	0.42
5:J:140:ASP:HA	5:J:143:LEU:HD12	2.01	0.42
1:C:584:MET:H	1:C:584:MET:HG3	1.67	0.42
2:F:288:GLN:O	5:I:223:LYS:N	2.52	0.42
4:H:84:ILE:HD13	6:L:38:VAL:HG21	2.00	0.42
1:A:506:LYS:O	1:A:571:ARG:NH2	2.53	0.42
1:B:580:LYS:HB3	1:B:604:LEU:CD2	2.48	0.42
1:C:152:ILE:HD13	1:C:165:LYS:HD3	2.01	0.42
8:P:427:ASP:HB2	8:P:430:VAL:HG22	2.00	0.42
1:A:360:GLU:OE2	2:D:329:THR:OG1	2.32	0.42
1:B:94:ILE:HD11	1:B:333:LEU:HD22	2.01	0.42
1:B:295:THR:HA	1:B:304:SER:HA	2.01	0.42
2:D:214:LYS:HD2	2:D:214:LYS:HA	1.79	0.42
2:E:298:THR:HA	2:E:353:ILE:HB	2.00	0.42
2:E:67:ARG:HB2	2:E:70:GLU:HB2	2.02	0.42
4:H:19:MET:HG3	4:H:180:ILE:HG23	2.01	0.42
7:N:84:MET:O	7:N:88:GLN:N	2.52	0.42
1:A:134:ASP:OD1	1:A:134:ASP:N	2.41	0.42
1:C:588:ASP:HA	1:C:589:PRO:HD2	1.89	0.42
2:D:444:LEU:HD11	2:D:449:LEU:HD13	2.01	0.42
1:C:338:ARG:HG3	1:C:404:VAL:HG23	2.02	0.42
1:C:383:ALA:HB1	2:E:264:ALA:HB1	2.00	0.42
2:F:300:MET:HB2	2:F:354:LEU:HB3	2.02	0.42
6:L:11:ILE:HD12	6:L:66:ILE:HD12	2.00	0.42
1:C:21:VAL:HG13	1:C:29:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:287:TYR:CZ	8:P:327:SER:OG	2.69	0.41
1:B:449:ASN:HD21	1:B:452:ILE:HG12	1.85	0.41
1:C:295:THR:HA	1:C:304:SER:HA	2.02	0.41
2:E:363:HIS:HB3	2:E:366:PRO:HD2	2.01	0.41
5:J:89:ASP:HA	5:J:92:THR:HG22	2.02	0.41
2:F:291:LYS:HE3	2:F:291:LYS:HB2	1.98	0.41
7:O:88:GLN:HE22	7:O:92:ARG:HH21	1.67	0.41
2:D:411:THR:OG1	2:D:412:ARG:N	2.53	0.41
1:B:167:MET:SD	1:B:400:ARG:NH2	2.94	0.41
2:D:191:ILE:HB	2:D:353:ILE:HG12	2.01	0.41
1:A:144:GLY:N	1:A:176:VAL:O	2.52	0.41
1:B:127:LEU:O	1:B:129:ARG:NH1	2.53	0.41
1:C:387:GLU:HG2	2:E:265:ASN:HB3	2.01	0.41
2:F:485:ARG:NH2	2:F:506:ARG:O	2.54	0.41
5:J:208:MET:HA	5:J:211:VAL:HG22	2.01	0.41
8:P:256:GLN:H	8:P:256:GLN:HG3	1.70	0.41
1:A:543:ASN:HB2	1:A:584:MET:HE1	2.03	0.41
1:B:134:ASP:OD1	1:B:134:ASP:N	2.43	0.41
1:A:494:GLN:H	1:A:494:GLN:HG3	1.75	0.41
1:B:511:VAL:HG11	1:B:548:TYR:HB2	2.03	0.41
1:B:588:ASP:CG	1:B:590:VAL:HG12	2.41	0.41
2:D:338:ALA:HA	2:D:348:ILE:HG23	2.03	0.41
4:H:90:ALA:HB2	6:L:27:GLU:HB2	2.02	0.41
1:B:169:PRO:HA	1:B:170:PRO:HD3	1.91	0.41
1:C:588:ASP:CG	1:C:590:VAL:HG12	2.41	0.41
5:K:137:ARG:HD2	5:K:179:GLY:HA2	2.03	0.41
1:A:225:HIS:HB3	1:A:242:GLN:HE21	1.85	0.40
1:B:105:PRO:HG2	1:B:108:ASP:HB2	2.03	0.40
1:B:485:GLU:OE2	2:D:386:ARG:NH1	2.55	0.40
5:J:69:LYS:HB3	5:J:69:LYS:HE2	1.77	0.40
5:J:116:LEU:HD12	5:J:116:LEU:HA	1.94	0.40
5:J:196:LEU:HD23	5:J:196:LEU:HA	1.95	0.40
1:A:84:LYS:HD3	1:A:84:LYS:HA	1.91	0.40
1:C:605:LEU:HA	1:C:608:MET:HE2	2.03	0.40
1:C:106:LEU:HD13	2:F:160:PRO:HD2	2.03	0.40
4:H:97:LYS:HB2	4:H:108:VAL:HG23	2.04	0.40
2:D:208:ARG:HE	2:D:208:ARG:HB2	1.79	0.40
2:E:421:GLN:NE2	2:E:425:CYS:SG	2.81	0.40
2:F:57:LEU:HD23	2:F:97:GLN:HB3	2.04	0.40
5:K:102:LEU:HD21	5:K:196:LEU:HD12	2.03	0.40
1:A:141:LEU:HD23	1:A:176:VAL:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ASN:ND2	1:A:584:MET:HE3	2.37	0.40
1:A:548:TYR:OH	1:A:552:ARG:NH1	2.52	0.40
1:A:587:LYS:HD3	1:A:587:LYS:HA	1.80	0.40
5:K:101:ARG:HA	5:K:104:LYS:HE2	2.04	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	585/617 (95%)	554 (95%)	31 (5%)	0	100	100
1	B	587/617 (95%)	552 (94%)	35 (6%)	0	100	100
1	C	598/617 (97%)	575 (96%)	23 (4%)	0	100	100
2	D	457/511 (89%)	421 (92%)	36 (8%)	0	100	100
2	E	454/511 (89%)	430 (95%)	24 (5%)	0	100	100
2	F	454/511 (89%)	429 (94%)	25 (6%)	0	100	100
3	G	338/382 (88%)	326 (96%)	12 (4%)	0	100	100
4	H	210/247 (85%)	203 (97%)	7 (3%)	0	100	100
5	I	216/226 (96%)	214 (99%)	2 (1%)	0	100	100
5	J	216/226 (96%)	213 (99%)	3 (1%)	0	100	100
5	K	218/226 (96%)	215 (99%)	3 (1%)	0	100	100
6	L	101/119 (85%)	93 (92%)	7 (7%)	1 (1%)	13	46
7	M	107/118 (91%)	106 (99%)	1 (1%)	0	100	100
7	N	107/118 (91%)	107 (100%)	0	0	100	100
7	O	107/118 (91%)	103 (96%)	4 (4%)	0	100	100
8	P	364/465 (78%)	342 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	a	744/838 (89%)	678 (91%)	65 (9%)	1 (0%)	48 79
10	b	202/205 (98%)	196 (97%)	5 (2%)	1 (0%)	25 59
11	d	346/351 (99%)	320 (92%)	26 (8%)	0	100 100
12	e	71/81 (88%)	69 (97%)	2 (3%)	0	100 100
13	s	202/468 (43%)	175 (87%)	27 (13%)	0	100 100
14	r	44/351 (12%)	40 (91%)	4 (9%)	0	100 100
15	c	148/155 (96%)	145 (98%)	3 (2%)	0	100 100
15	g	148/155 (96%)	148 (100%)	0	0	100 100
15	k	148/155 (96%)	146 (99%)	2 (1%)	0	100 100
15	l	148/155 (96%)	146 (99%)	2 (1%)	0	100 100
15	m	148/155 (96%)	148 (100%)	0	0	100 100
15	n	148/155 (96%)	146 (99%)	2 (1%)	0	100 100
15	o	149/155 (96%)	148 (99%)	1 (1%)	0	100 100
15	p	149/155 (96%)	149 (100%)	0	0	100 100
15	q	149/155 (96%)	149 (100%)	0	0	100 100
16	f	61/98 (62%)	58 (95%)	3 (5%)	0	100 100
All	All	8124/9416 (86%)	7744 (95%)	377 (5%)	3 (0%)	100 100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	a	516	PRO
10	b	30	ASP
6	L	97	PRO

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	497/524 (95%)	497 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	501/524 (96%)	499 (100%)	2 (0%)	89 94
1	C	507/524 (97%)	506 (100%)	1 (0%)	92 96
2	D	394/432 (91%)	394 (100%)	0	100 100
2	E	391/432 (90%)	391 (100%)	0	100 100
2	F	391/432 (90%)	391 (100%)	0	100 100
4	H	183/212 (86%)	183 (100%)	0	100 100
5	I	133/198 (67%)	133 (100%)	0	100 100
5	J	156/198 (79%)	156 (100%)	0	100 100
5	K	137/198 (69%)	136 (99%)	1 (1%)	81 89
6	L	89/100 (89%)	88 (99%)	1 (1%)	70 83
7	M	35/97 (36%)	35 (100%)	0	100 100
7	N	42/97 (43%)	42 (100%)	0	100 100
7	O	39/97 (40%)	39 (100%)	0	100 100
8	P	185/415 (45%)	182 (98%)	3 (2%)	58 76
9	a	597/744 (80%)	594 (100%)	3 (0%)	86 92
10	b	156/158 (99%)	155 (99%)	1 (1%)	84 91
11	d	303/306 (99%)	302 (100%)	1 (0%)	91 96
12	e	62/68 (91%)	62 (100%)	0	100 100
13	s	183/398 (46%)	182 (100%)	1 (0%)	86 92
14	r	42/315 (13%)	42 (100%)	0	100 100
15	c	106/110 (96%)	106 (100%)	0	100 100
15	g	106/110 (96%)	106 (100%)	0	100 100
15	k	106/110 (96%)	106 (100%)	0	100 100
15	l	106/110 (96%)	106 (100%)	0	100 100
15	m	106/110 (96%)	106 (100%)	0	100 100
15	n	106/110 (96%)	106 (100%)	0	100 100
15	o	107/110 (97%)	107 (100%)	0	100 100
15	p	107/110 (97%)	107 (100%)	0	100 100
15	q	107/110 (97%)	107 (100%)	0	100 100
16	f	54/84 (64%)	54 (100%)	0	100 100
All	All	6034/7543 (80%)	6020 (100%)	14 (0%)	91 96

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	400	ARG
1	B	476	ARG
1	C	400	ARG
5	K	159	THR
6	L	102	LYS
8	P	326	GLU
8	P	328	VAL
8	P	330	ASP
9	a	472	LEU
9	a	515	TYR
9	a	819	THR
10	b	29	PHE
11	d	138	MET
13	s	396	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	159	ASN
1	A	444	HIS
1	A	523	ASN
1	A	543	ASN
1	B	314	ASN
1	B	430	GLN
1	B	521	GLN
1	B	543	ASN
1	C	114	GLN
1	C	282	ASN
1	C	468	HIS
1	C	522	GLN
1	C	543	ASN
1	C	603	GLN
2	D	38	ASN
2	D	205	GLN
2	D	237	ASN
2	D	262	ASN
2	D	382	GLN
2	D	421	GLN
2	D	482	GLN
2	E	171	GLN

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Mol	Chain	Res	Type
2	E	251	ASN
2	E	358	ASN
2	E	385	ASN
2	E	482	GLN
2	F	482	GLN
4	H	113	HIS
4	H	174	HIS
5	J	74	ASN
5	J	100	GLN
5	J	194	ASN
5	J	206	GLN
5	K	71	GLN
5	K	100	GLN
5	K	122	GLN
6	L	31	ASN
7	M	85	GLN
7	N	111	HIS
7	N	113	ASN
7	O	89	GLN
7	O	111	HIS
8	P	222	GLN
8	P	241	HIS
8	P	299	GLN
8	P	305	GLN
8	P	402	HIS
8	P	417	GLN
8	P	421	ASN
8	P	433	ASN
8	P	445	ASN
9	a	53	ASN
9	a	106	ASN
9	a	121	ASN
9	a	375	GLN
9	a	412	HIS
9	a	433	GLN
9	a	465	ASN
9	a	524	ASN
9	a	534	ASN
9	a	548	HIS
9	a	735	ASN
10	b	168	GLN
11	d	152	ASN

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Mol	Chain	Res	Type
11	d	171	GLN
11	d	183	ASN
11	d	254	GLN
11	d	266	ASN
11	d	297	HIS
12	e	59	GLN
12	e	67	GLN
13	s	342	ASN
13	s	380	ASN
13	s	404	ASN
15	c	78	ASN
15	g	78	ASN
15	k	78	ASN
15	l	78	ASN
15	l	92	GLN
15	m	78	ASN
15	p	78	ASN
15	p	92	GLN
15	q	78	ASN
15	q	92	GLN
15	q	123	GLN
16	f	68	ASN

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

11 monosaccharides are modelled in this entry.

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	$\#\|Z\|>2$
18	MAN	Q	1	18	11,11,12	0.93	1 (9%)	15,15,17	1.10	2 (13%)
18	MAN	Q	2	18	11,11,12	0.85	0	15,15,17	1.29	2 (13%)
17	NAG	t	1	17	14,14,15	0.29	0	17,19,21	0.53	0
17	NAG	t	2	17	14,14,15	0.32	0	17,19,21	1.06	2 (11%)
17	BMA	t	3	17	11,11,12	0.82	0	15,15,17	0.98	1 (6%)
17	MAN	t	4	17	11,11,12	0.87	1 (9%)	15,15,17	1.03	1 (6%)
17	MAN	t	5	17	11,11,12	0.90	0	15,15,17	1.19	2 (13%)
17	MAN	t	6	17	11,11,12	0.82	1 (9%)	15,15,17	0.88	1 (6%)
17	GLC	t	7	17	11,11,12	0.76	0	15,15,17	0.74	0
17	GLC	t	8	17	11,11,12	0.61	0	15,15,17	0.76	0
17	GLC	t	9	17	11,11,12	0.64	0	15,15,17	0.62	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
18	MAN	Q	1	18	-	2/2/19/22	0/1/1/1
18	MAN	Q	2	18	-	1/2/19/22	1/1/1/1
17	NAG	t	1	17	-	4/6/23/26	0/1/1/1
17	NAG	t	2	17	-	2/6/23/26	0/1/1/1
17	BMA	t	3	17	-	0/2/19/22	0/1/1/1
17	MAN	t	4	17	-	2/2/19/22	0/1/1/1
17	MAN	t	5	17	-	2/2/19/22	0/1/1/1
17	MAN	t	6	17	-	2/2/19/22	0/1/1/1
17	GLC	t	7	17	-	1/2/19/22	0/1/1/1
17	GLC	t	8	17	-	0/2/19/22	0/1/1/1
17	GLC	t	9	17	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	t	6	MAN	O5-C1	-2.50	1.39	1.43
17	t	4	MAN	O5-C1	-2.42	1.39	1.43
18	Q	1	MAN	C1-C2	2.15	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Q	2	MAN	C1-O5-C5	4.11	117.70	112.19
17	t	5	MAN	O2-C2-C3	-2.99	103.96	110.15
17	t	4	MAN	O2-C2-C3	-2.65	104.66	110.15
17	t	3	BMA	O2-C2-C3	-2.60	104.77	110.15
18	Q	1	MAN	C1-O5-C5	2.58	115.64	112.19
17	t	2	NAG	O5-C1-C2	-2.46	107.48	111.29
17	t	6	MAN	O2-C2-C3	-2.34	105.31	110.15
17	t	2	NAG	C3-C4-C5	2.16	114.16	110.23
17	t	5	MAN	C1-O5-C5	2.16	115.08	112.19
18	Q	2	MAN	O2-C2-C3	-2.09	105.82	110.15
18	Q	1	MAN	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	t	1	NAG	C8-C7-N2-C2
17	t	1	NAG	O7-C7-N2-C2
18	Q	1	MAN	O5-C5-C6-O6
17	t	4	MAN	O5-C5-C6-O6
17	t	4	MAN	C4-C5-C6-O6
17	t	6	MAN	O5-C5-C6-O6
18	Q	1	MAN	C4-C5-C6-O6
17	t	6	MAN	C4-C5-C6-O6
17	t	5	MAN	O5-C5-C6-O6
17	t	1	NAG	C4-C5-C6-O6
17	t	2	NAG	C8-C7-N2-C2
17	t	5	MAN	C4-C5-C6-O6
17	t	1	NAG	O5-C5-C6-O6
17	t	2	NAG	O7-C7-N2-C2
17	t	7	GLC	O5-C5-C6-O6
18	Q	2	MAN	O5-C5-C6-O6

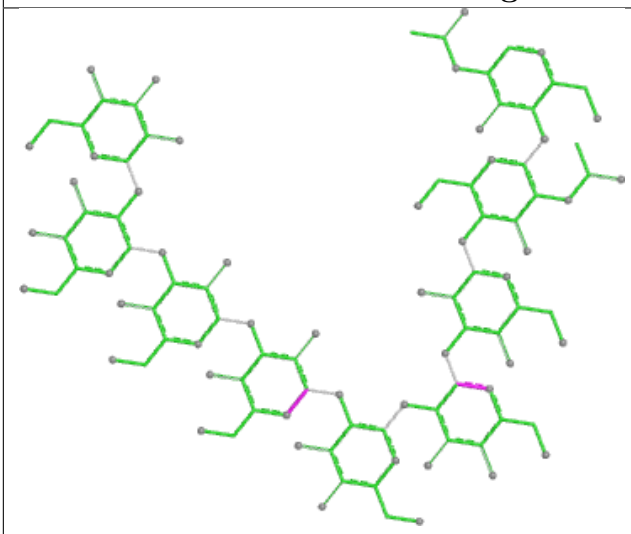
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	Q	2	MAN	C1-C2-C3-C4-C5-O5

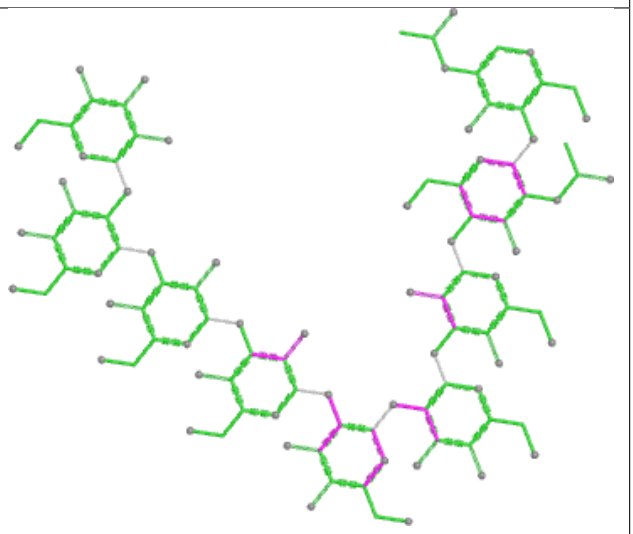
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

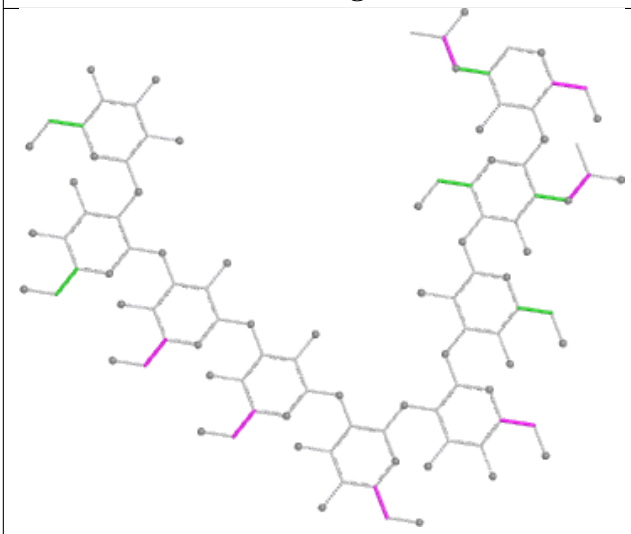
Oligosaccharide Chain t



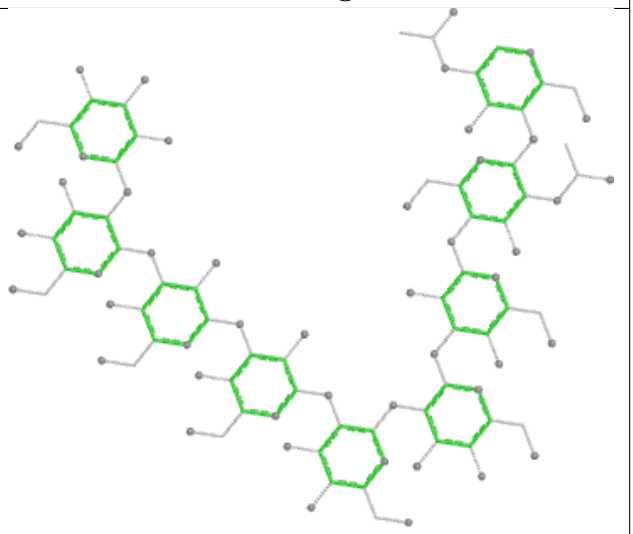
Bond lengths



Bond angles

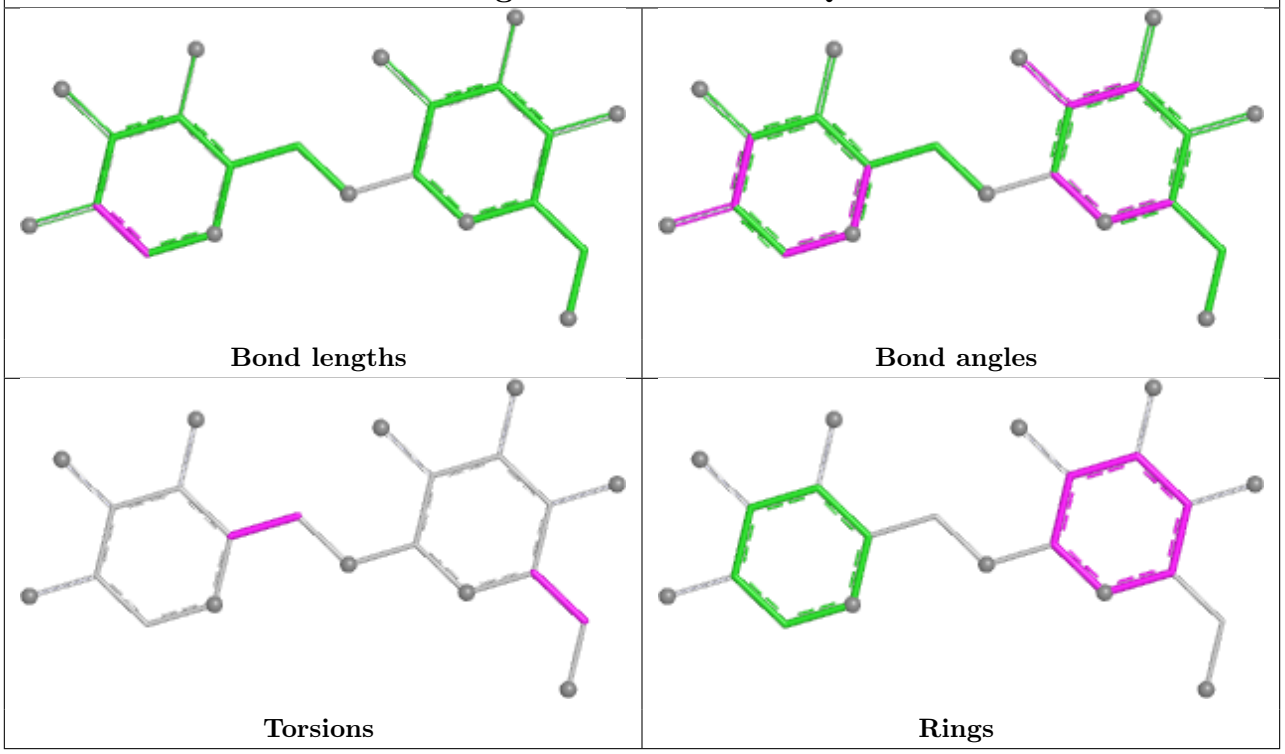


Torsions



Rings

Oligosaccharide Chain Q



5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 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	$\#\|Z\| > 2$
23	NAG	s	504	-	14,14,15	0.55	0	17,19,21	0.55	0
20	ADP	C	702	19	24,29,29	1.23	2 (8%)	29,45,45	1.28	3 (10%)
25	WEV	g	202	-	43,45,45	2.06	18 (41%)	47,65,65	4.30	28 (59%)
22	POV	s	502	-	38,38,51	1.14	3 (7%)	44,46,59	1.02	3 (6%)
25	WEV	m	201	-	43,45,45	2.01	15 (34%)	47,65,65	3.22	24 (51%)
23	NAG	s	505	13	14,14,15	0.39	0	17,19,21	0.61	1 (5%)
25	WEV	o	201	-	43,45,45	2.29	18 (41%)	47,65,65	3.85	24 (51%)
23	NAG	s	506	13	14,14,15	0.65	0	17,19,21	0.48	0
25	WEV	l	202	-	43,45,45	2.22	20 (46%)	47,65,65	4.32	26 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	NAG	s	508	-	14,14,15	0.30	0	19,19,21	0.41	0
23	NAG	s	507	13	14,14,15	0.43	0	17,19,21	0.50	0
25	WEV	p	201	-	43,45,45	2.29	16 (37%)	47,65,65	3.93	29 (61%)
22	POV	b	301	-	46,46,51	1.05	4 (8%)	52,54,59	0.96	2 (3%)
25	WEV	g	201	-	43,45,45	2.25	17 (39%)	47,65,65	4.55	26 (55%)
22	POV	r	403	-	46,46,51	1.04	4 (8%)	52,54,59	0.88	3 (5%)
24	OLA	r	404	-	19,19,19	0.47	0	19,19,19	0.78	0
22	POV	b	302	-	42,42,51	1.09	4 (9%)	48,50,59	0.91	2 (4%)
22	POV	l	201	-	39,39,51	1.12	4 (10%)	45,47,59	0.87	2 (4%)
22	POV	r	402	-	44,44,51	1.04	4 (9%)	50,52,59	1.02	2 (4%)
21	WJP	a	901	-	32,33,34	1.02	2 (6%)	39,43,44	1.36	7 (17%)
23	NAG	s	509	13	14,14,15	0.47	0	17,19,21	0.60	0
23	NAG	s	503	13	14,14,15	0.40	0	17,19,21	0.53	0
22	POV	r	401	-	46,46,51	1.01	4 (8%)	52,54,59	0.85	2 (3%)
22	POV	s	501	-	39,39,51	1.12	4 (10%)	45,47,59	0.96	2 (4%)

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
23	NAG	s	504	-	-	1/6/23/26	0/1/1/1
20	ADP	C	702	19	-	3/12/32/32	0/3/3/3
25	WEV	g	202	-	-	39/64/82/82	0/1/2/2
22	POV	s	502	-	-	25/42/42/55	-
25	WEV	m	201	-	-	30/64/82/82	0/1/2/2
23	NAG	s	505	13	-	0/6/23/26	0/1/1/1
25	WEV	o	201	-	-	26/64/82/82	0/1/2/2
23	NAG	s	506	13	-	2/6/23/26	0/1/1/1
25	WEV	l	202	-	-	30/64/82/82	0/1/2/2
23	NAG	s	508	-	-	2/6/22/26	0/1/1/1
23	NAG	s	507	13	-	2/6/23/26	0/1/1/1
25	WEV	p	201	-	-	32/64/82/82	0/1/2/2
22	POV	b	301	-	-	22/50/50/55	-
25	WEV	g	201	-	-	22/64/82/82	0/1/2/2
22	POV	r	403	-	-	25/50/50/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	OLA	r	404	-	-	9/17/17/17	-
22	POV	b	302	-	-	24/46/46/55	-
22	POV	l	201	-	-	21/43/43/55	-
22	POV	r	402	-	-	24/48/48/55	-
21	WJP	a	901	-	-	10/37/37/40	-
23	NAG	s	509	13	-	0/6/23/26	0/1/1/1
23	NAG	s	503	13	-	2/6/23/26	0/1/1/1
22	POV	r	401	-	-	26/50/50/55	-
22	POV	s	501	-	-	19/43/43/55	-

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	o	201	WEV	C14-C15	6.73	1.58	1.45
25	p	201	WEV	C09-C08	6.24	1.60	1.52
25	l	202	WEV	C14-C15	5.57	1.56	1.45
25	g	201	WEV	C14-C15	5.55	1.56	1.45
25	g	202	WEV	C14-C15	4.85	1.55	1.45
25	o	201	WEV	C30-C31	-4.80	1.46	1.53
25	p	201	WEV	C14-C15	4.58	1.54	1.45
25	l	202	WEV	O40-C29	-4.54	1.32	1.40
25	p	201	WEV	O40-C29	-4.54	1.32	1.40
25	m	201	WEV	O40-C29	-4.35	1.33	1.40
25	g	201	WEV	C30-C31	-4.25	1.46	1.53
25	g	201	WEV	O40-C29	-4.09	1.33	1.40
25	p	201	WEV	O41-C26	-3.93	1.33	1.43
25	p	201	WEV	O12-C11	-3.90	1.13	1.21
25	m	201	WEV	C06-C05	3.85	1.55	1.43
25	g	201	WEV	O41-C26	-3.84	1.33	1.43
25	l	202	WEV	C32-C31	-3.82	1.42	1.53
25	m	201	WEV	C14-C15	3.80	1.53	1.45
25	o	201	WEV	C32-C31	-3.76	1.42	1.53
25	o	201	WEV	O12-C11	-3.75	1.14	1.21
25	g	202	WEV	C32-C31	-3.73	1.42	1.53
25	g	202	WEV	O12-C11	-3.71	1.14	1.21
25	o	201	WEV	O34-C33	3.71	1.49	1.44
25	o	201	WEV	O34-C29	3.69	1.49	1.43
25	m	201	WEV	O41-C26	-3.67	1.33	1.43
25	g	202	WEV	C30-C31	-3.64	1.47	1.53
25	l	202	WEV	C16-C15	-3.64	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	o	201	WEV	O41-C26	-3.64	1.33	1.43
25	m	201	WEV	O34-C33	3.62	1.49	1.44
20	C	702	ADP	O4'-C1'	3.52	1.45	1.40
25	g	202	WEV	O40-C29	-3.51	1.34	1.40
21	a	901	WJP	P31-O33	3.45	1.61	1.50
25	l	202	WEV	O41-C26	-3.43	1.34	1.43
25	g	201	WEV	C32-C31	-3.41	1.43	1.53
25	p	201	WEV	C17-C18	-3.28	1.42	1.54
25	g	201	WEV	O19-C18	-3.24	1.34	1.43
22	s	502	POV	O21-C2	-3.16	1.39	1.46
25	m	201	WEV	O10-C09	-3.15	1.40	1.44
25	g	201	WEV	O12-C11	-3.15	1.15	1.21
25	g	201	WEV	C16-C15	-3.12	1.26	1.34
25	m	201	WEV	O12-C11	-3.10	1.15	1.21
25	l	202	WEV	O12-C11	-3.08	1.15	1.21
25	g	201	WEV	C28-C27	-3.02	1.46	1.53
25	l	202	WEV	O42-C08	-3.01	1.36	1.43
25	p	201	WEV	O42-C08	-2.99	1.36	1.43
25	o	201	WEV	O42-C08	-2.97	1.36	1.43
25	g	201	WEV	C25-C24	-2.97	1.47	1.53
25	g	201	WEV	C32-C33	-2.97	1.47	1.53
25	g	202	WEV	O34-C33	2.96	1.48	1.44
25	o	201	WEV	O40-C29	-2.94	1.35	1.40
21	a	901	WJP	P27-O28	2.93	1.61	1.50
25	l	202	WEV	C30-C31	-2.92	1.48	1.53
25	g	202	WEV	C06-C05	2.90	1.52	1.43
22	b	302	POV	O21-C2	-2.89	1.39	1.46
25	g	202	WEV	C32-C33	-2.89	1.47	1.53
22	r	403	POV	O21-C2	-2.87	1.39	1.46
25	g	201	WEV	O10-C11	2.84	1.40	1.34
25	p	201	WEV	O19-C18	-2.82	1.36	1.43
25	p	201	WEV	C06-C05	2.81	1.51	1.43
22	b	301	POV	O21-C2	-2.76	1.40	1.46
22	l	201	POV	O21-C2	-2.76	1.40	1.46
25	m	201	WEV	C38-C32	2.75	1.59	1.53
25	m	201	WEV	C30-C31	-2.75	1.49	1.53
25	l	202	WEV	C32-C33	-2.72	1.47	1.53
25	m	201	WEV	C32-C31	-2.71	1.45	1.53
22	s	501	POV	O21-C2	-2.70	1.40	1.46
25	g	201	WEV	O42-C08	-2.68	1.36	1.43
22	r	402	POV	O21-C2	-2.68	1.40	1.46
25	l	202	WEV	O19-C18	-2.68	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	202	WEV	O10-C09	-2.65	1.40	1.44
25	g	202	WEV	O22-C23	-2.65	1.39	1.45
25	l	202	WEV	O10-C11	2.63	1.40	1.34
25	l	202	WEV	C09-C08	2.62	1.55	1.52
25	g	202	WEV	C25-C24	-2.60	1.48	1.53
25	o	201	WEV	C03-C02	-2.59	1.49	1.53
25	m	201	WEV	C02-C18	-2.59	1.49	1.53
25	g	202	WEV	O42-C08	-2.58	1.37	1.43
25	p	201	WEV	C30-C31	-2.57	1.49	1.53
25	p	201	WEV	C02-C18	-2.51	1.49	1.53
25	l	202	WEV	C28-C27	-2.49	1.47	1.53
25	p	201	WEV	C32-C33	-2.49	1.48	1.53
25	p	201	WEV	C16-C15	-2.47	1.27	1.34
25	g	202	WEV	C13-C11	2.44	1.54	1.48
22	l	201	POV	O31-C31	2.43	1.40	1.33
22	b	302	POV	O31-C31	2.43	1.40	1.33
22	r	403	POV	O31-C31	2.42	1.40	1.33
22	s	501	POV	O31-C31	2.40	1.40	1.33
22	r	401	POV	O21-C21	2.39	1.41	1.34
25	l	202	WEV	C17-C16	-2.39	1.46	1.51
25	p	201	WEV	O22-C23	-2.38	1.40	1.45
22	r	401	POV	O31-C31	2.38	1.40	1.33
20	C	702	ADP	C8-N7	-2.38	1.30	1.34
25	o	201	WEV	C32-C33	-2.38	1.48	1.53
25	m	201	WEV	O19-C18	-2.36	1.37	1.43
22	s	502	POV	O31-C3	-2.35	1.39	1.45
25	o	201	WEV	O10-C11	2.34	1.39	1.34
22	r	402	POV	O31-C31	2.34	1.40	1.33
22	b	301	POV	O31-C3	-2.31	1.40	1.45
22	b	301	POV	O31-C31	2.28	1.40	1.33
25	g	202	WEV	C03-C02	-2.28	1.49	1.53
25	p	201	WEV	C32-C31	-2.27	1.46	1.53
25	g	201	WEV	C06-C05	2.26	1.50	1.43
25	g	202	WEV	C28-C27	-2.25	1.48	1.53
25	l	202	WEV	C06-C05	2.24	1.50	1.43
22	r	401	POV	O21-C2	-2.24	1.41	1.46
22	r	402	POV	O31-C3	-2.24	1.40	1.45
22	l	201	POV	O31-C3	-2.23	1.40	1.45
22	b	302	POV	O31-C3	-2.23	1.40	1.45
25	o	201	WEV	O22-C23	-2.22	1.40	1.45
22	r	401	POV	O31-C3	-2.22	1.40	1.45
22	s	502	POV	O31-C31	2.21	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	o	201	WEV	C25-C24	-2.21	1.48	1.53
25	l	202	WEV	C35-C33	-2.20	1.43	1.52
25	m	201	WEV	C16-C15	-2.19	1.28	1.34
25	g	202	WEV	O19-C18	-2.19	1.37	1.43
22	r	403	POV	O31-C3	-2.18	1.40	1.45
25	l	202	WEV	C25-C24	-2.18	1.49	1.53
22	s	501	POV	O31-C3	-2.17	1.40	1.45
22	s	501	POV	O21-C21	2.15	1.40	1.34
25	l	202	WEV	O22-C23	-2.13	1.40	1.45
22	r	402	POV	O21-C21	2.12	1.40	1.34
25	m	201	WEV	O22-C13	2.12	1.40	1.36
25	m	201	WEV	O10-C11	2.11	1.39	1.34
22	l	201	POV	O21-C21	2.11	1.40	1.34
25	p	201	WEV	C28-C27	-2.10	1.48	1.53
22	b	301	POV	O21-C21	2.10	1.40	1.34
25	l	202	WEV	C06-C07	-2.10	1.25	1.33
25	g	202	WEV	C24-C09	-2.10	1.48	1.54
25	o	201	WEV	O19-C18	-2.10	1.37	1.43
25	g	201	WEV	C05-C04	-2.10	1.28	1.35
22	b	302	POV	O21-C21	2.09	1.40	1.34
25	g	201	WEV	C24-C26	-2.05	1.48	1.54
25	o	201	WEV	C05-C04	-2.04	1.28	1.35
25	o	201	WEV	C28-C27	-2.03	1.48	1.53
25	o	201	WEV	C13-C11	-2.02	1.44	1.48
25	l	202	WEV	C13-C11	2.02	1.53	1.48
25	g	201	WEV	C01-C02	-2.01	1.47	1.53
25	g	202	WEV	C16-C15	-2.01	1.29	1.34
22	r	403	POV	O21-C21	2.01	1.39	1.34

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	201	WEV	C01-C02-C03	-13.80	90.69	109.92
25	l	202	WEV	O10-C11-C13	12.69	132.39	110.99
25	l	202	WEV	C06-C05-C04	-12.16	110.58	127.69
25	g	202	WEV	C05-C06-C07	-11.36	98.09	124.43
25	p	201	WEV	O10-C11-C13	11.06	129.64	110.99
25	l	202	WEV	C25-C24-C26	-10.47	90.83	111.43
25	l	202	WEV	O42-C08-C07	-10.45	80.69	111.05
25	g	202	WEV	O34-C33-C35	9.99	123.48	106.19
25	o	201	WEV	C31-C32-C33	-9.60	99.04	108.83
25	g	201	WEV	C31-C32-C33	-9.50	99.14	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	201	WEV	C17-C18-C02	9.37	133.95	114.88
25	g	201	WEV	C05-C06-C07	-9.19	103.12	124.43
25	g	201	WEV	O19-C18-C02	-8.78	93.06	109.79
25	g	202	WEV	O10-C11-C13	8.75	125.74	110.99
25	o	201	WEV	C01-C02-C03	-8.45	98.15	109.92
25	m	201	WEV	C08-C07-C06	8.23	142.56	125.88
25	g	202	WEV	O19-C18-C02	-8.21	94.14	109.79
25	m	201	WEV	O40-C29-O34	-8.07	94.33	110.00
25	p	201	WEV	C20-C17-C16	7.84	123.39	110.08
25	p	201	WEV	C05-C06-C07	-7.83	106.29	124.43
25	g	201	WEV	O10-C11-C13	7.72	124.00	110.99
25	o	201	WEV	O10-C11-C13	7.61	123.82	110.99
25	o	201	WEV	C09-O10-C11	7.57	132.16	117.72
25	l	202	WEV	C09-O10-C11	7.54	132.10	117.72
25	g	202	WEV	C31-C32-C33	-7.48	101.20	108.83
25	p	201	WEV	O42-C08-C07	-7.42	89.49	111.05
25	o	201	WEV	C05-C06-C07	-7.25	107.62	124.43
25	g	201	WEV	C06-C05-C04	-7.14	117.65	127.69
25	g	201	WEV	C03-C02-C18	7.06	126.38	111.09
25	m	201	WEV	C26-C24-C09	7.02	123.98	110.58
25	o	201	WEV	O40-C29-O34	-6.96	96.49	110.00
25	g	202	WEV	C29-O34-C33	-6.96	105.27	115.11
25	p	201	WEV	C21-C15-C16	-6.75	104.09	123.21
25	p	201	WEV	C29-O34-C33	-6.51	105.90	115.11
25	g	201	WEV	C25-C24-C26	-6.48	98.69	111.43
25	g	202	WEV	C01-C02-C03	-6.42	100.97	109.92
25	m	201	WEV	O34-C33-C35	6.42	117.30	106.19
25	p	201	WEV	C18-C17-C16	-6.30	95.27	109.55
25	g	202	WEV	C44-C04-C03	6.25	129.16	115.28
25	o	201	WEV	O22-C13-C11	-6.23	102.09	115.57
25	o	201	WEV	C44-C04-C03	6.01	128.64	115.28
25	g	202	WEV	O19-C18-C17	-5.95	90.67	108.46
25	m	201	WEV	C29-O34-C33	-5.92	106.74	115.11
25	g	201	WEV	O19-C18-C17	-5.64	91.60	108.46
25	p	201	WEV	O19-C18-C17	-5.52	91.97	108.46
25	l	202	WEV	O10-C11-O12	-5.49	113.17	123.40
25	l	202	WEV	C17-C18-C02	5.46	125.99	114.88
25	g	201	WEV	C21-C15-C14	5.30	130.74	119.05
25	o	201	WEV	C38-C32-C33	-5.30	101.98	112.22
25	o	201	WEV	O41-C26-C24	-5.06	98.33	109.56
25	p	201	WEV	C01-C02-C18	-5.04	102.31	111.45
20	C	702	ADP	N3-C2-N1	-4.98	121.91	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	p	201	WEV	C31-C32-C33	-4.98	103.75	108.83
25	g	202	WEV	C18-C17-C16	4.93	120.73	109.55
25	g	202	WEV	C17-C16-C15	4.93	142.06	126.72
25	m	201	WEV	O10-C09-C24	4.84	118.67	107.52
25	o	201	WEV	C23-O22-C13	-4.84	107.56	116.96
25	g	202	WEV	C03-C04-C05	-4.75	108.20	121.88
25	g	202	WEV	C21-C15-C16	-4.74	109.80	123.21
22	r	402	POV	O21-C21-C22	4.59	121.41	111.48
25	o	201	WEV	C25-C24-C26	-4.54	102.51	111.43
25	o	201	WEV	C21-C15-C16	-4.45	110.61	123.21
25	g	202	WEV	O40-C29-C30	-4.40	95.62	109.80
25	g	201	WEV	C20-C17-C18	4.39	120.85	111.45
25	m	201	WEV	C23-O22-C13	-4.38	108.46	116.96
25	p	201	WEV	C24-C26-C27	4.36	120.65	114.51
25	g	201	WEV	C09-O10-C11	4.35	126.02	117.72
25	g	201	WEV	C38-C32-C33	-4.30	103.91	112.22
25	o	201	WEV	C03-C04-C05	-4.26	109.62	121.88
25	p	201	WEV	O10-C11-O12	-4.22	115.53	123.40
25	g	202	WEV	O42-C08-C07	-4.21	98.82	111.05
22	b	301	POV	O21-C21-C22	4.19	120.55	111.48
25	p	201	WEV	C06-C05-C04	-4.13	121.88	127.69
25	p	201	WEV	C17-C16-C15	4.13	139.55	126.72
25	g	201	WEV	C24-C26-C27	-4.12	108.71	114.51
25	p	201	WEV	C38-C32-C31	-4.03	106.63	111.35
25	l	202	WEV	C08-C07-C06	-4.01	117.75	125.88
25	l	202	WEV	O10-C09-C24	-3.94	98.45	107.52
22	s	501	POV	O21-C21-C22	3.90	119.92	111.48
25	o	201	WEV	O34-C33-C35	3.90	112.94	106.19
22	s	502	POV	O21-C21-C22	3.89	119.90	111.48
25	p	201	WEV	C37-C35-C36	-3.89	99.89	110.58
25	l	202	WEV	C38-C32-C33	-3.88	104.72	112.22
22	b	302	POV	O21-C21-C22	3.81	119.73	111.48
22	r	403	POV	O21-C21-C22	3.81	119.73	111.48
25	o	201	WEV	C30-C31-C32	-3.75	104.01	111.16
25	m	201	WEV	C09-O10-C11	3.74	124.86	117.72
25	l	202	WEV	O40-C29-O34	-3.72	102.77	110.00
25	g	202	WEV	C23-O22-C13	-3.72	109.73	116.96
25	l	202	WEV	C26-C24-C09	3.69	117.63	110.58
25	g	202	WEV	O10-C09-C24	-3.66	99.07	107.52
25	g	202	WEV	C38-C32-C31	-3.64	107.08	111.35
25	m	201	WEV	O42-C08-C07	-3.63	100.50	111.05
25	m	201	WEV	C31-C32-C33	3.63	112.53	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	m	201	WEV	C24-C26-C27	3.60	119.58	114.51
22	l	201	POV	O21-C21-C22	3.56	119.18	111.48
22	r	401	POV	O21-C21-C22	3.51	119.07	111.48
25	p	201	WEV	C03-C04-C05	-3.50	111.79	121.88
25	g	201	WEV	C38-C32-C31	3.49	115.44	111.35
25	o	201	WEV	O42-C08-C07	-3.46	101.01	111.05
25	m	201	WEV	C14-C13-C11	-3.45	113.18	123.33
25	g	202	WEV	O10-C11-O12	-3.45	116.98	123.40
25	l	202	WEV	O19-C18-C02	-3.44	103.23	109.79
25	l	202	WEV	C21-C15-C14	3.41	126.57	119.05
25	m	201	WEV	O22-C13-C11	3.36	122.83	115.57
25	m	201	WEV	C05-C06-C07	3.35	132.21	124.43
25	p	201	WEV	C23-O22-C13	-3.34	110.47	116.96
25	l	202	WEV	C43-O42-C08	3.34	120.64	112.99
25	l	202	WEV	C18-C17-C16	-3.29	102.08	109.55
25	m	201	WEV	C36-C35-C33	3.28	121.86	111.78
25	m	201	WEV	C25-C24-C26	-3.28	104.98	111.43
25	m	201	WEV	O39-C31-C32	-3.27	103.91	110.62
25	g	201	WEV	C21-C15-C16	-3.27	113.96	123.21
25	g	201	WEV	O40-C29-O34	-3.25	103.68	110.00
25	g	201	WEV	O10-C09-C24	-3.16	100.24	107.52
25	g	202	WEV	O34-C33-C32	-3.13	103.99	109.59
25	p	201	WEV	C25-C24-C09	-3.09	105.96	111.40
25	o	201	WEV	O12-C11-C13	-3.09	112.19	121.76
25	o	201	WEV	C29-O34-C33	3.08	119.47	115.11
25	g	202	WEV	C25-C24-C26	-3.07	105.38	111.43
25	l	202	WEV	C03-C02-C18	3.07	117.74	111.09
25	p	201	WEV	C44-C04-C03	3.07	122.09	115.28
25	l	202	WEV	C01-C02-C18	-3.06	105.91	111.45
21	a	901	WJP	C07-C06-C08	3.05	120.53	115.23
25	p	201	WEV	O40-C29-C30	-3.00	100.13	109.80
25	m	201	WEV	C37-C35-C36	3.00	118.83	110.58
25	m	201	WEV	C03-C02-C18	2.97	117.52	111.09
25	l	202	WEV	C01-C02-C03	2.96	114.05	109.92
25	g	201	WEV	C44-C04-C03	2.94	121.81	115.28
25	g	202	WEV	C17-C18-C02	2.94	120.86	114.88
25	l	202	WEV	C05-C06-C07	-2.93	117.63	124.43
25	l	202	WEV	C30-C31-C32	-2.92	105.58	111.16
21	a	901	WJP	C12-C11-C13	2.88	120.22	115.23
22	b	301	POV	O31-C31-C32	2.84	120.50	111.83
25	g	202	WEV	C25-C24-C09	-2.78	106.51	111.40
25	g	202	WEV	C37-C35-C33	2.76	120.25	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	l	202	WEV	O39-C31-C32	-2.75	104.98	110.62
22	r	402	POV	O31-C31-C32	2.72	120.14	111.83
25	l	202	WEV	C17-C16-C15	-2.72	118.26	126.72
25	g	202	WEV	O41-C26-C24	-2.72	103.53	109.56
22	b	302	POV	O31-C31-C32	2.71	120.11	111.83
22	s	501	POV	O31-C31-C32	2.70	120.07	111.83
21	a	901	WJP	C17-C16-C18	2.68	119.88	115.23
25	l	202	WEV	C31-C32-C33	-2.67	106.10	108.83
22	r	401	POV	O31-C31-C32	2.66	119.95	111.83
25	g	201	WEV	O10-C11-O12	-2.60	118.55	123.40
22	s	502	POV	O31-C31-C32	2.59	119.72	111.83
25	o	201	WEV	C08-C07-C06	-2.58	120.64	125.88
25	p	201	WEV	C26-C24-C09	2.57	115.48	110.58
25	l	202	WEV	O12-C11-C13	-2.56	113.82	121.76
22	r	403	POV	O31-C31-C32	2.51	119.49	111.83
25	g	202	WEV	C01-C02-C18	2.50	115.99	111.45
22	s	502	POV	C2-O21-C21	-2.49	111.83	117.80
25	g	201	WEV	C26-C24-C09	2.49	115.34	110.58
22	l	201	POV	O31-C31-C32	2.46	119.34	111.83
25	g	201	WEV	O41-C26-C24	-2.45	104.11	109.56
25	l	202	WEV	C21-C15-C16	-2.42	116.35	123.21
25	m	201	WEV	C43-O42-C08	2.39	118.46	112.99
25	p	201	WEV	C36-C35-C33	-2.36	104.55	111.78
21	a	901	WJP	C14-C15-C16	-2.34	122.26	127.62
25	o	201	WEV	C14-C13-C11	2.34	130.23	123.33
25	m	201	WEV	O10-C11-C13	2.34	114.93	110.99
25	p	201	WEV	O34-C33-C35	2.34	110.24	106.19
25	o	201	WEV	C43-O42-C08	2.32	118.31	112.99
25	p	201	WEV	O12-C11-C13	-2.32	114.58	121.76
25	m	201	WEV	O19-C18-C02	-2.31	105.39	109.79
20	C	702	ADP	O3B-PB-O3A	2.30	112.35	104.64
25	g	202	WEV	C09-O10-C11	2.30	122.10	117.72
25	m	201	WEV	C06-C05-C04	-2.29	124.47	127.69
20	C	702	ADP	PA-O5'-C5'	-2.29	108.24	121.35
21	a	901	WJP	C04-C05-C06	-2.28	122.41	127.62
25	o	201	WEV	C03-C02-C18	2.27	116.00	111.09
25	p	201	WEV	C09-O10-C11	2.19	121.90	117.72
25	g	201	WEV	C23-O22-C13	-2.16	112.76	116.96
21	a	901	WJP	C07-C06-C05	-2.16	118.08	123.63
21	a	901	WJP	C23-C21-C22	2.15	119.55	114.59
25	p	201	WEV	C25-C24-C26	-2.12	107.26	111.43
22	r	403	POV	C2-O21-C21	-2.11	112.75	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	m	201	WEV	C17-C18-C02	-2.10	110.60	114.88
23	s	505	NAG	C1-O5-C5	2.10	115.00	112.19
25	g	201	WEV	C17-C16-C15	-2.08	120.24	126.72
25	g	201	WEV	C43-O42-C08	-2.06	108.27	112.99
25	g	202	WEV	C26-C24-C09	2.05	114.49	110.58
25	o	201	WEV	O10-C09-C24	-2.05	102.81	107.52
25	p	201	WEV	O41-C26-C24	-2.02	105.08	109.56
25	p	201	WEV	O22-C13-C11	-2.01	111.21	115.57

There are no chirality outliers.

All (396) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	C	702	ADP	C5'-O5'-PA-O1A
21	a	901	WJP	C02-C03-C04-C05
21	a	901	WJP	C02-C24-C25-O26
22	b	301	POV	C1-O11-P-O12
22	b	301	POV	C1-O11-P-O13
22	b	301	POV	C22-C21-O21-C2
22	b	302	POV	C1-O11-P-O12
22	b	302	POV	C11-O12-P-O11
22	b	302	POV	C11-O12-P-O13
22	b	302	POV	O12-C11-C12-N
22	b	302	POV	C22-C21-O21-C2
22	b	302	POV	O22-C21-O21-C2
22	s	501	POV	C1-O11-P-O12
22	s	501	POV	C1-O11-P-O13
22	s	501	POV	O12-C11-C12-N
22	s	501	POV	C22-C21-O21-C2
22	s	501	POV	C32-C31-O31-C3
22	s	501	POV	O32-C31-O31-C3
22	s	502	POV	C1-O11-P-O12
22	s	502	POV	C1-O11-P-O13
22	s	502	POV	C1-O11-P-O14
22	s	502	POV	C11-O12-P-O11
22	s	502	POV	C11-O12-P-O14
22	s	502	POV	O12-C11-C12-N
22	r	401	POV	C11-O12-P-O11
22	r	401	POV	C11-O12-P-O14
22	r	401	POV	O22-C21-O21-C2
22	r	402	POV	C1-O11-P-O12
22	r	402	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
22	r	402	POV	C1-O11-P-O14
22	r	402	POV	C11-O12-P-O11
22	r	402	POV	C11-O12-P-O14
22	r	403	POV	C11-O12-P-O11
22	r	403	POV	C11-O12-P-O13
22	r	403	POV	C11-O12-P-O14
22	r	403	POV	O12-C11-C12-N
22	r	403	POV	C22-C21-O21-C2
22	l	201	POV	C11-O12-P-O11
22	l	201	POV	C11-O12-P-O13
22	l	201	POV	C11-O12-P-O14
25	g	201	WEV	C01-C02-C18-O19
25	g	201	WEV	C03-C02-C18-O19
25	g	201	WEV	C07-C08-C09-C24
25	g	201	WEV	C07-C08-C09-O10
25	g	201	WEV	O42-C08-C09-C24
25	g	201	WEV	O42-C08-C09-O10
25	g	201	WEV	C09-C08-O42-C43
25	g	201	WEV	C08-C09-C24-C25
25	g	201	WEV	C08-C09-C24-C26
25	g	201	WEV	C13-C11-O10-C09
25	g	201	WEV	O12-C11-O10-C09
25	g	201	WEV	C24-C26-C27-C28
25	g	201	WEV	O41-C26-C27-C28
25	g	202	WEV	C03-C02-C18-C17
25	g	202	WEV	C02-C03-C04-C05
25	g	202	WEV	C02-C03-C04-C44
25	g	202	WEV	O42-C08-C09-C24
25	g	202	WEV	C09-C08-O42-C43
25	g	202	WEV	C15-C16-C17-C18
25	g	202	WEV	C16-C17-C18-C02
25	g	202	WEV	C16-C17-C18-O19
25	g	202	WEV	C20-C17-C18-C02
25	g	202	WEV	C09-C24-C26-O41
25	g	202	WEV	C24-C26-C27-C28
25	g	202	WEV	C24-C26-C27-C29
25	g	202	WEV	O41-C26-C27-C28
25	g	202	WEV	O41-C26-C27-C29
25	g	202	WEV	C26-C27-C29-C30
25	g	202	WEV	C26-C27-C29-O34
25	g	202	WEV	C26-C27-C29-O40
25	g	202	WEV	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
25	g	202	WEV	C28-C27-C29-O34
25	g	202	WEV	C28-C27-C29-O40
25	g	202	WEV	C32-C33-C35-C36
25	g	202	WEV	C32-C33-C35-C37
25	g	202	WEV	O34-C33-C35-C36
25	g	202	WEV	O34-C33-C35-C37
25	l	202	WEV	C01-C02-C03-C04
25	l	202	WEV	C18-C02-C03-C04
25	l	202	WEV	C03-C02-C18-C17
25	l	202	WEV	C03-C02-C18-O19
25	l	202	WEV	O42-C08-C09-C24
25	l	202	WEV	O42-C08-C09-O10
25	l	202	WEV	C08-C09-O10-C11
25	l	202	WEV	C13-C11-O10-C09
25	l	202	WEV	O12-C11-O10-C09
25	l	202	WEV	C20-C17-C18-O19
25	l	202	WEV	C09-C24-C26-C27
25	l	202	WEV	C09-C24-C26-O41
25	l	202	WEV	C25-C24-C26-C27
25	l	202	WEV	C24-C26-C27-C29
25	l	202	WEV	C26-C27-C29-C30
25	l	202	WEV	C26-C27-C29-O40
25	l	202	WEV	C28-C27-C29-O40
25	m	201	WEV	C07-C08-C09-C24
25	m	201	WEV	O42-C08-C09-C24
25	m	201	WEV	C09-C08-O42-C43
25	m	201	WEV	C24-C09-O10-C11
25	m	201	WEV	C15-C16-C17-C20
25	m	201	WEV	C20-C17-C18-C02
25	m	201	WEV	C20-C17-C18-O19
25	m	201	WEV	C24-C26-C27-C29
25	m	201	WEV	C26-C27-C29-C30
25	m	201	WEV	C26-C27-C29-O34
25	m	201	WEV	C28-C27-C29-O34
25	m	201	WEV	C28-C27-C29-O40
25	m	201	WEV	C32-C33-C35-C36
25	m	201	WEV	C32-C33-C35-C37
25	m	201	WEV	O34-C33-C35-C36
25	o	201	WEV	C01-C02-C18-O19
25	o	201	WEV	C06-C07-C08-O42
25	o	201	WEV	C09-C08-O42-C43
25	o	201	WEV	C08-C09-O10-C11

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Mol	Chain	Res	Type	Atoms
25	o	201	WEV	C13-C11-O10-C09
25	o	201	WEV	O12-C11-O10-C09
25	o	201	WEV	C15-C16-C17-C20
25	o	201	WEV	C26-C27-C29-C30
25	o	201	WEV	C26-C27-C29-O34
25	o	201	WEV	C26-C27-C29-O40
25	o	201	WEV	C28-C27-C29-C30
25	o	201	WEV	C28-C27-C29-O34
25	o	201	WEV	C28-C27-C29-O40
25	p	201	WEV	C01-C02-C03-C04
25	p	201	WEV	C18-C02-C03-C04
25	p	201	WEV	C07-C08-C09-C24
25	p	201	WEV	C07-C08-C09-O10
25	p	201	WEV	O42-C08-C09-C24
25	p	201	WEV	C09-C08-O42-C43
25	p	201	WEV	C08-C09-C24-C25
25	p	201	WEV	O10-C09-C24-C25
25	p	201	WEV	O10-C09-C24-C26
25	p	201	WEV	C08-C09-O10-C11
25	p	201	WEV	C13-C11-O10-C09
25	p	201	WEV	C14-C15-C16-C17
25	p	201	WEV	C15-C16-C17-C18
25	p	201	WEV	C24-C26-C27-C28
25	p	201	WEV	C24-C26-C27-C29
25	p	201	WEV	O41-C26-C27-C28
25	p	201	WEV	C26-C27-C29-C30
25	p	201	WEV	C32-C33-C35-C37
22	b	301	POV	O22-C21-O21-C2
22	s	501	POV	O22-C21-O21-C2
22	r	403	POV	O22-C21-O21-C2
22	r	401	POV	C22-C21-O21-C2
25	g	202	WEV	C08-C09-O10-C11
25	p	201	WEV	O12-C11-O10-C09
23	s	503	NAG	O5-C5-C6-O6
23	s	506	NAG	C4-C5-C6-O6
22	r	402	POV	C32-C31-O31-C3
22	s	502	POV	O32-C31-O31-C3
25	l	202	WEV	C25-C24-C26-O41
22	s	502	POV	C32-C31-O31-C3
21	a	901	WJP	C06-C08-C09-C10
21	a	901	WJP	C16-C18-C19-C20
23	s	507	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
22	r	402	POV	O32-C31-O31-C3
23	s	506	NAG	O5-C5-C6-O6
25	g	202	WEV	C04-C05-C06-C07
22	b	301	POV	C32-C31-O31-C3
23	s	503	NAG	C4-C5-C6-O6
23	s	507	NAG	C4-C5-C6-O6
22	r	403	POV	O21-C2-C3-O31
22	b	301	POV	C21-C22-C23-C24
25	g	202	WEV	C25-C24-C26-C27
20	C	702	ADP	O4'-C4'-C5'-O5'
22	s	501	POV	C21-C22-C23-C24
22	l	201	POV	C31-C32-C33-C34
22	b	302	POV	C31-C32-C33-C34
22	r	402	POV	C21-C22-C23-C24
22	r	403	POV	C21-C22-C23-C24
22	l	201	POV	C21-C22-C23-C24
22	b	301	POV	O32-C31-O31-C3
22	r	401	POV	C21-C22-C23-C24
22	r	401	POV	C31-C32-C33-C34
25	g	202	WEV	C25-C24-C26-O41
25	m	201	WEV	C25-C24-C26-O41
25	g	202	WEV	C20-C17-C18-O19
25	l	202	WEV	C16-C17-C18-O19
25	p	201	WEV	C20-C17-C18-O19
22	r	402	POV	C22-C21-O21-C2
22	r	402	POV	O22-C21-O21-C2
25	l	202	WEV	C01-C02-C18-O19
25	p	201	WEV	C25-C24-C26-O41
22	s	502	POV	C22-C21-O21-C2
25	g	201	WEV	C16-C17-C18-C02
25	l	202	WEV	C20-C17-C18-C02
25	m	201	WEV	C16-C17-C18-C02
22	r	401	POV	C32-C31-O31-C3
25	o	201	WEV	C03-C02-C18-O19
22	l	201	POV	C36-C37-C38-C39
22	s	501	POV	C32-C33-C34-C35
22	s	502	POV	C23-C24-C25-C26
22	s	501	POV	C31-C32-C33-C34
25	g	202	WEV	C24-C09-O10-C11
22	s	501	POV	C35-C36-C37-C38
22	r	402	POV	C23-C24-C25-C26
25	m	201	WEV	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
22	b	301	POV	C24-C25-C26-C27
22	b	302	POV	C24-C25-C26-C27
24	r	404	OLA	C4-C5-C6-C7
22	b	302	POV	C25-C26-C27-C28
22	r	401	POV	C24-C25-C26-C27
23	s	504	NAG	O5-C5-C6-O6
25	o	201	WEV	C01-C02-C18-C17
22	s	501	POV	C22-C23-C24-C25
22	s	502	POV	C31-C32-C33-C34
22	r	401	POV	O32-C31-O31-C3
22	s	502	POV	O22-C21-O21-C2
22	b	302	POV	C22-C23-C24-C25
22	r	403	POV	C37-C38-C39-C310
22	b	301	POV	C23-C24-C25-C26
22	r	401	POV	C36-C37-C38-C39
22	l	201	POV	C35-C36-C37-C38
22	r	402	POV	C29-C210-C211-C212
22	s	501	POV	C25-C26-C27-C28
25	g	201	WEV	O10-C09-C24-C25
22	r	402	POV	C36-C37-C38-C39
22	r	402	POV	C311-C310-C39-C38
25	m	201	WEV	C09-C24-C26-C27
25	g	201	WEV	O10-C09-C24-C26
22	r	403	POV	C26-C27-C28-C29
25	o	201	WEV	C03-C02-C18-C17
22	r	402	POV	C24-C25-C26-C27
22	l	201	POV	C33-C34-C35-C36
22	r	403	POV	C34-C35-C36-C37
25	o	201	WEV	C06-C07-C08-C09
25	m	201	WEV	C16-C17-C18-O19
25	p	201	WEV	C16-C17-C18-O19
25	p	201	WEV	C09-C24-C26-O41
22	r	401	POV	C26-C27-C28-C29
22	r	403	POV	C210-C211-C212-C213
22	l	201	POV	C26-C27-C28-C29
24	r	404	OLA	C6-C7-C8-C9
24	r	404	OLA	C2-C3-C4-C5
25	g	202	WEV	C09-C24-C26-C27
22	r	401	POV	C32-C33-C34-C35
22	l	201	POV	C32-C33-C34-C35
25	m	201	WEV	O34-C33-C35-C37
25	p	201	WEV	O34-C33-C35-C37

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Mol	Chain	Res	Type	Atoms
22	s	502	POV	C1-C2-C3-O31
22	r	401	POV	C1-C2-C3-O31
22	r	403	POV	C1-C2-C3-O31
22	b	301	POV	C210-C211-C212-C213
22	b	301	POV	C25-C26-C27-C28
22	r	403	POV	C32-C31-O31-C3
22	s	502	POV	C24-C25-C26-C27
22	r	403	POV	C35-C36-C37-C38
22	r	401	POV	C3-C2-O21-C21
25	g	202	WEV	C07-C08-O42-C43
25	o	201	WEV	C09-C24-C26-O41
22	r	401	POV	C210-C211-C212-C213
22	s	502	POV	O11-C1-C2-O21
25	p	201	WEV	C25-C24-C26-C27
25	o	201	WEV	C25-C24-C26-O41
22	b	301	POV	C22-C23-C24-C25
22	r	401	POV	C39-C310-C311-C312
25	p	201	WEV	C09-C24-C26-C27
25	l	202	WEV	C16-C17-C18-C02
25	p	201	WEV	C20-C17-C18-C02
22	r	401	POV	C311-C312-C313-C314
22	b	302	POV	C310-C311-C312-C313
25	l	202	WEV	C28-C27-C29-C30
25	m	201	WEV	C28-C27-C29-C30
23	s	508	NAG	C4-C5-C6-O6
24	r	404	OLA	C11-C12-C13-C14
22	r	403	POV	C22-C23-C24-C25
22	b	302	POV	O11-C1-C2-C3
22	s	502	POV	O11-C1-C2-C3
22	r	402	POV	C33-C34-C35-C36
20	C	702	ADP	C3'-C4'-C5'-O5'
22	r	403	POV	O32-C31-O31-C3
22	l	201	POV	C23-C24-C25-C26
25	g	201	WEV	C32-C33-C35-C36
22	r	401	POV	C22-C23-C24-C25
22	r	403	POV	C36-C37-C38-C39
25	g	201	WEV	C24-C09-O10-C11
22	s	502	POV	O21-C2-C3-O31
22	l	201	POV	O21-C2-C3-O31
25	g	202	WEV	O42-C08-C09-O10
24	r	404	OLA	C15-C16-C17-C18
22	r	401	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
22	s	502	POV	C33-C34-C35-C36
22	b	302	POV	C39-C310-C311-C312
22	r	402	POV	C39-C310-C311-C312
22	r	403	POV	O11-C1-C2-C3
22	b	302	POV	C21-C22-C23-C24
22	s	502	POV	C210-C211-C212-C213
22	l	201	POV	C25-C26-C27-C28
22	b	301	POV	C36-C37-C38-C39
24	r	404	OLA	C5-C6-C7-C8
22	s	501	POV	C27-C28-C29-C210
22	b	301	POV	O11-C1-C2-O21
22	b	302	POV	O11-C1-C2-O21
22	r	403	POV	O11-C1-C2-O21
22	l	201	POV	O11-C1-C2-O21
22	l	201	POV	C1-C2-C3-O31
22	b	302	POV	C312-C313-C314-C315
25	g	201	WEV	C13-C14-C15-C21
25	g	202	WEV	C13-C14-C15-C21
25	m	201	WEV	C14-C13-O22-C23
22	b	302	POV	C23-C24-C25-C26
22	r	402	POV	C34-C35-C36-C37
22	r	403	POV	C39-C310-C311-C312
22	r	401	POV	C37-C38-C39-C310
25	l	202	WEV	C06-C07-C08-C09
22	r	401	POV	O12-C11-C12-N
22	r	402	POV	O12-C11-C12-N
22	l	201	POV	O12-C11-C12-N
24	r	404	OLA	C3-C4-C5-C6
25	m	201	WEV	C09-C24-C26-O41
22	b	301	POV	O11-C1-C2-C3
22	l	201	POV	O11-C1-C2-C3
22	s	502	POV	C32-C33-C34-C35
21	a	901	WJP	C24-C02-C03-C04
22	l	201	POV	C22-C23-C24-C25
25	l	202	WEV	O41-C26-C27-C29
25	o	201	WEV	O10-C11-C13-C14
25	o	201	WEV	O10-C11-C13-O22
25	o	201	WEV	O12-C11-C13-C14
25	p	201	WEV	O41-C26-C27-C29
22	r	403	POV	C310-C311-C312-C313
21	a	901	WJP	C01-C02-C03-C04
22	b	302	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
25	p	201	WEV	C21-C15-C16-C17
22	r	401	POV	O21-C2-C3-O31
25	m	201	WEV	C06-C07-C08-O42
21	a	901	WJP	C25-O26-P27-O29
21	a	901	WJP	C25-O26-P27-O30
22	b	301	POV	C1-O11-P-O14
22	b	302	POV	C1-O11-P-O14
22	b	302	POV	C11-O12-P-O14
22	s	501	POV	C1-O11-P-O14
22	r	402	POV	C11-O12-P-O13
25	m	201	WEV	C11-C13-O22-C23
25	l	202	WEV	C01-C02-C18-C17
22	s	502	POV	C26-C27-C28-C29
22	b	301	POV	C310-C311-C312-C313
22	s	501	POV	C37-C38-C39-C310
23	s	508	NAG	O5-C5-C6-O6
22	s	502	POV	C25-C26-C27-C28
25	p	201	WEV	O42-C08-C09-O10
25	g	201	WEV	C08-C09-O10-C11
24	r	404	OLA	C13-C14-C15-C16
25	o	201	WEV	C04-C05-C06-C07
22	b	302	POV	C34-C35-C36-C37
22	b	301	POV	C26-C27-C28-C29
25	m	201	WEV	O42-C08-C09-O10
25	m	201	WEV	C06-C07-C08-C09
22	r	402	POV	C310-C311-C312-C313
25	l	202	WEV	C24-C26-C27-C28
25	o	201	WEV	C07-C08-O42-C43
25	g	202	WEV	C21-C15-C16-C17
25	o	201	WEV	C21-C15-C16-C17
24	r	404	OLA	C9-C10-C11-C12
25	m	201	WEV	C26-C27-C29-O40
25	p	201	WEV	C26-C27-C29-O40
21	a	901	WJP	C12-C11-C13-C14
22	b	301	POV	C311-C310-C39-C38
22	b	301	POV	C33-C34-C35-C36
22	r	401	POV	C35-C36-C37-C38
22	r	402	POV	C27-C28-C29-C210
21	a	901	WJP	C10-C11-C13-C14
22	s	502	POV	C27-C28-C29-C210
22	r	401	POV	C311-C310-C39-C38
25	m	201	WEV	C07-C08-C09-O10

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Mol	Chain	Res	Type	Atoms
22	s	501	POV	C1-C2-O21-C21
22	s	501	POV	C3-C2-O21-C21
22	r	403	POV	C27-C28-C29-C210
22	s	502	POV	C29-C210-C211-C212
22	r	401	POV	C29-C210-C211-C212
22	b	302	POV	C32-C33-C34-C35
25	p	201	WEV	C04-C05-C06-C07
25	g	201	WEV	C14-C13-O22-C23
25	l	202	WEV	C14-C13-O22-C23
22	r	403	POV	C29-C210-C211-C212
25	g	201	WEV	C13-C14-C15-C16
25	g	202	WEV	C13-C14-C15-C16
22	r	402	POV	C25-C26-C27-C28
25	g	202	WEV	C01-C02-C18-C17
22	l	201	POV	O22-C21-O21-C2
22	r	403	POV	C311-C310-C39-C38
22	s	501	POV	C39-C310-C311-C312
22	r	401	POV	C27-C28-C29-C210
22	l	201	POV	C22-C21-O21-C2
25	g	202	WEV	C08-C09-C24-C26
25	o	201	WEV	O12-C11-C13-O22
22	b	301	POV	C27-C28-C29-C210
22	s	502	POV	C2-C1-O11-P
25	g	202	WEV	O10-C09-C24-C26
22	b	302	POV	O31-C31-C32-C33
25	l	202	WEV	C24-C09-O10-C11
22	l	201	POV	C37-C38-C39-C310
22	b	302	POV	C26-C27-C28-C29
22	b	301	POV	C1-C2-C3-O31
25	l	202	WEV	O10-C09-C24-C26
22	r	402	POV	O31-C31-C32-C33

There are no ring outliers.

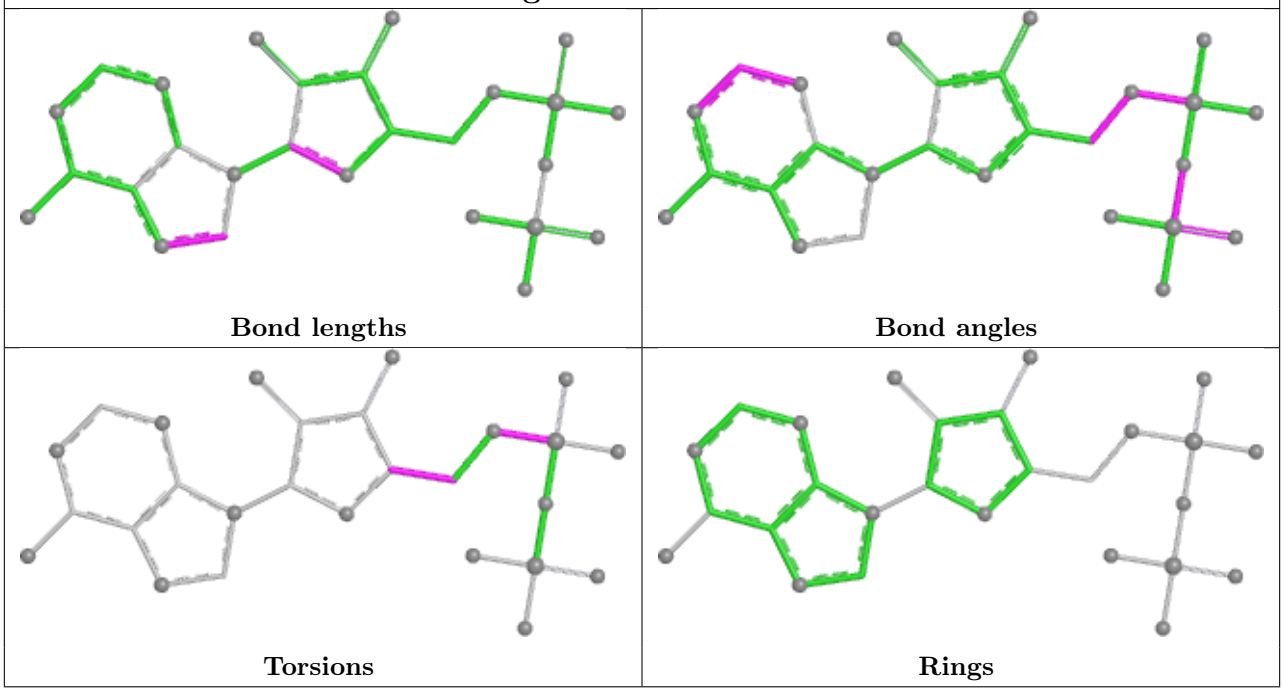
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	702	ADP	2	0

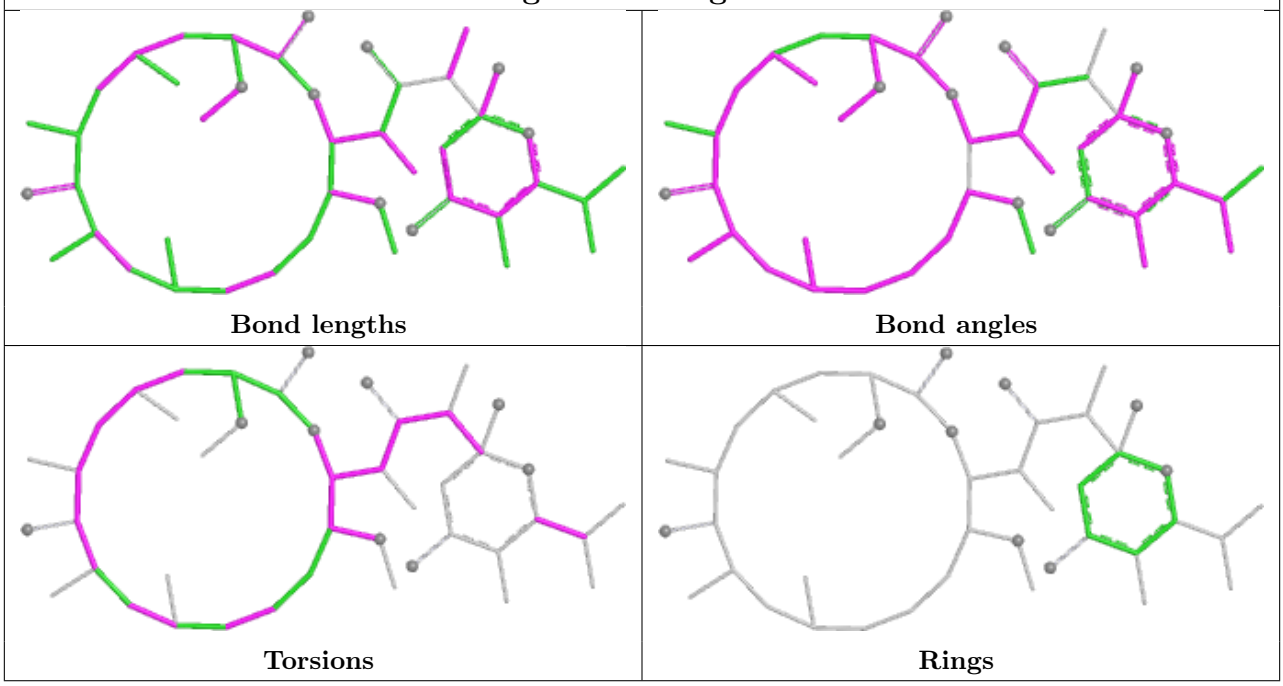
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

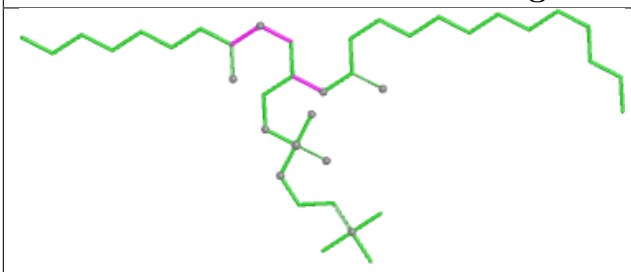
Ligand ADP C 702



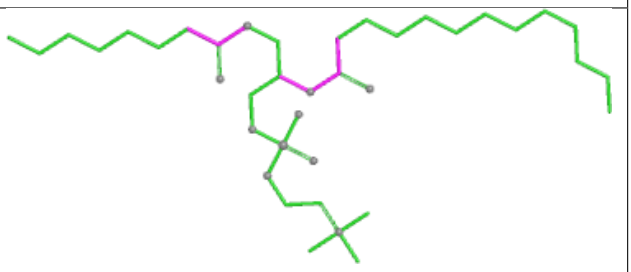
Ligand WEV g 202



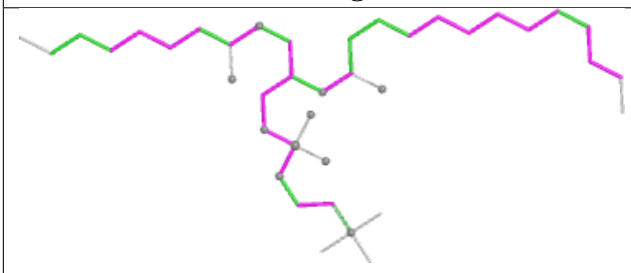
Ligand POV s 502



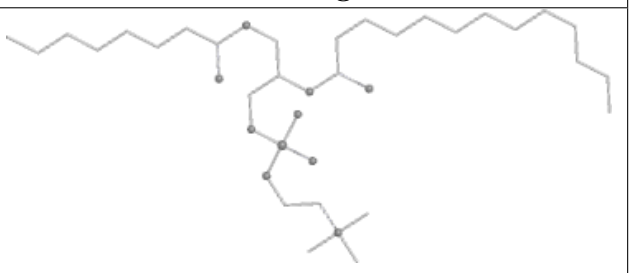
Bond lengths



Bond angles

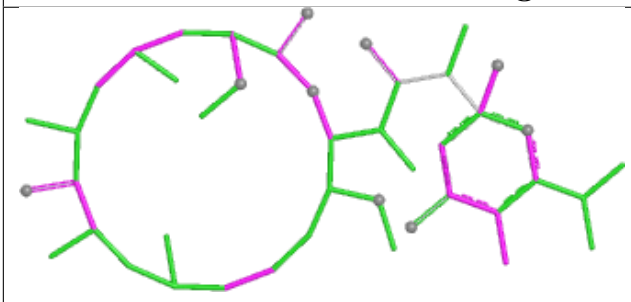


Torsions

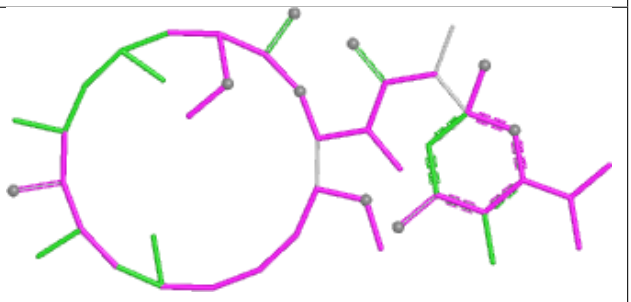


Rings

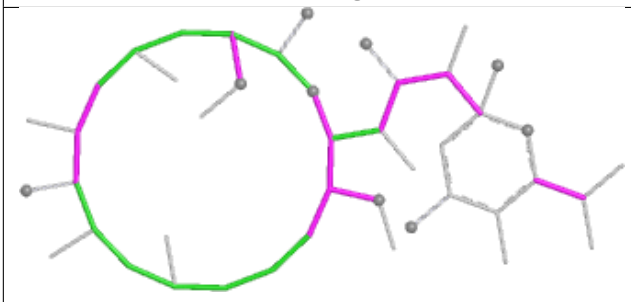
Ligand WEV m 201



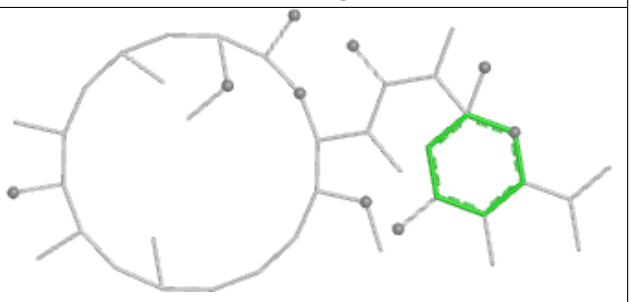
Bond lengths



Bond angles

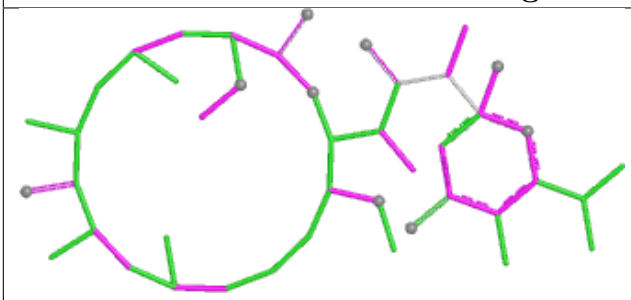


Torsions

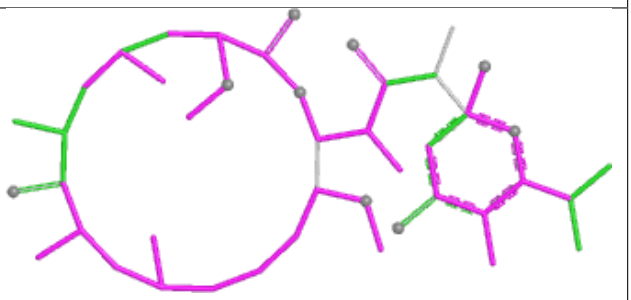


Rings

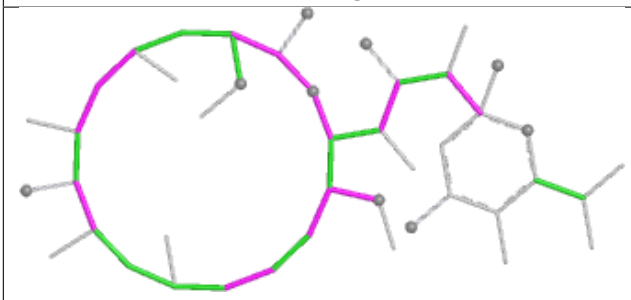
Ligand WEV o 201



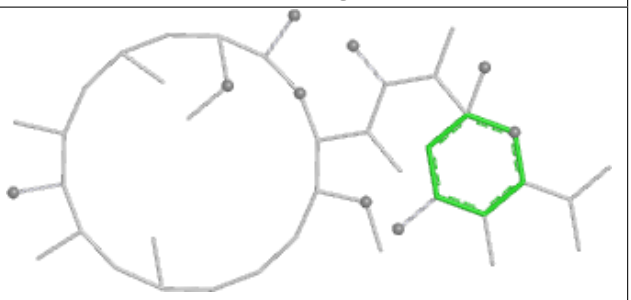
Bond lengths



Bond angles

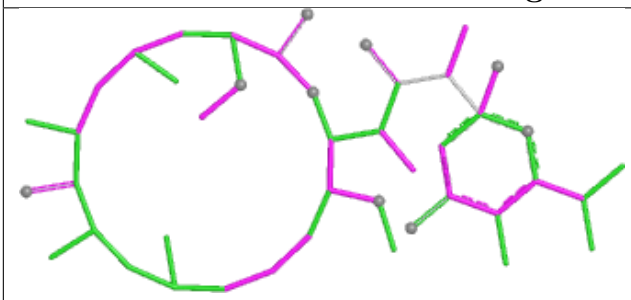


Torsions

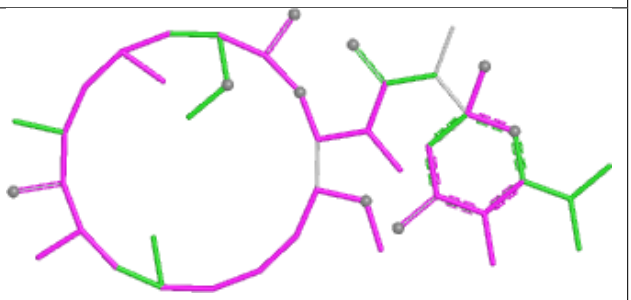


Rings

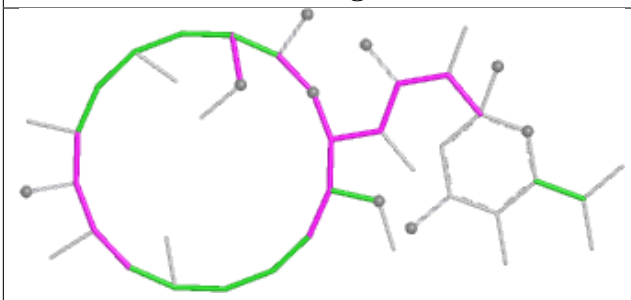
Ligand WEV l 202



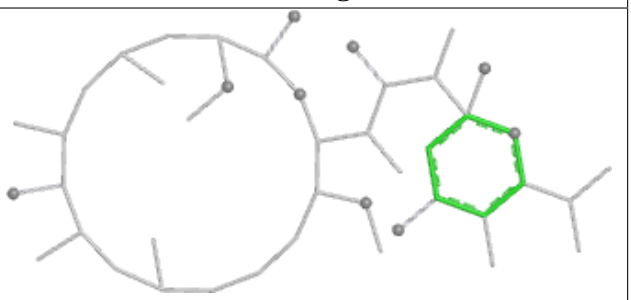
Bond lengths



Bond angles

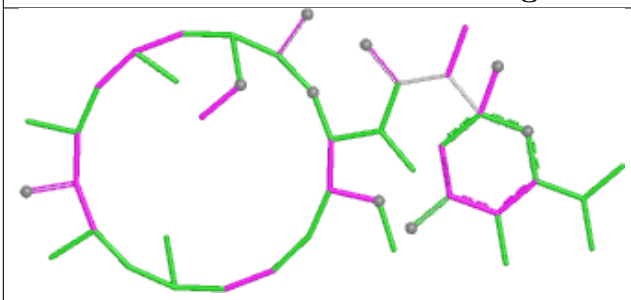


Torsions



Rings

Ligand WEV p 201



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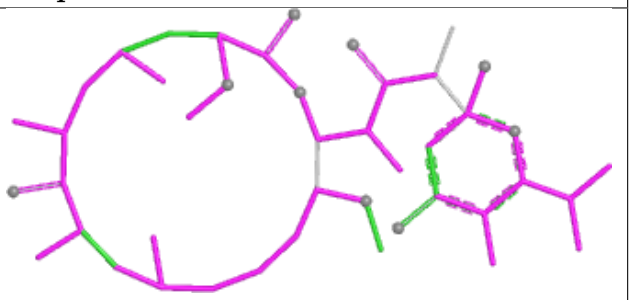
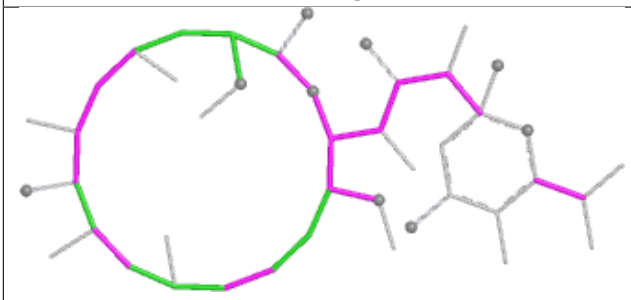


Bond angles



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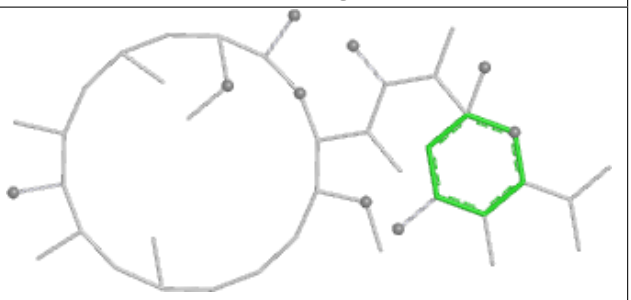
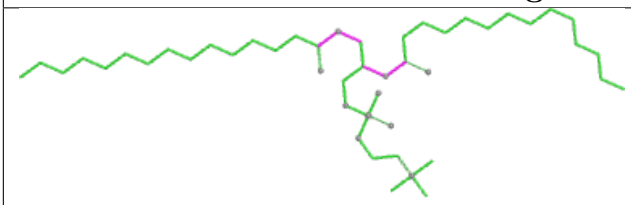
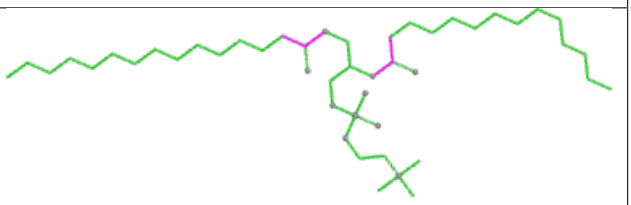


Rings

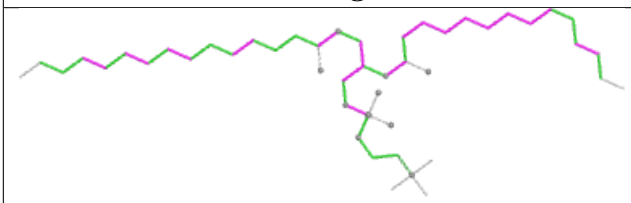
Ligand POV b 301



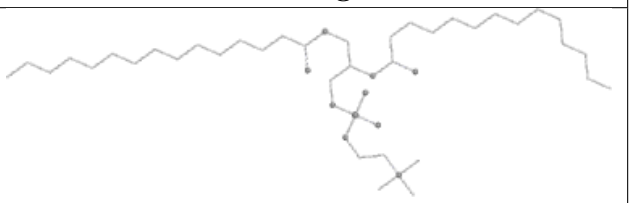
Bond lengths



Bond angles

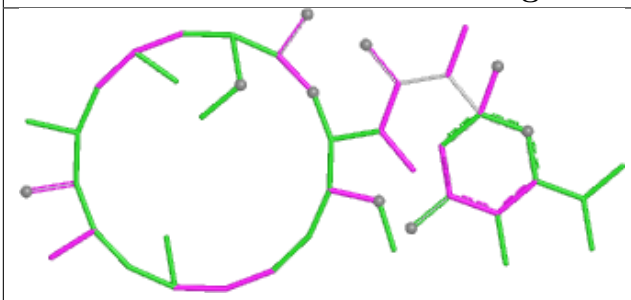


Torsions

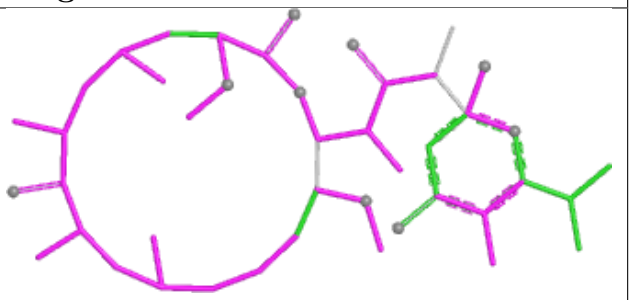


Rings

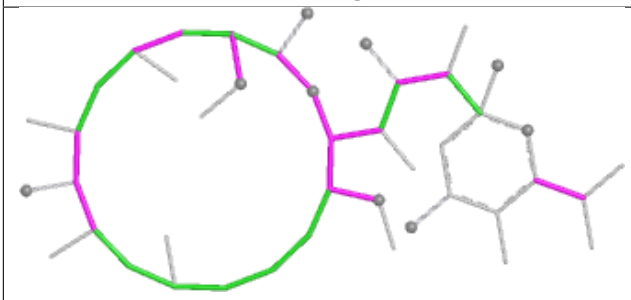
Ligand WEV g 201



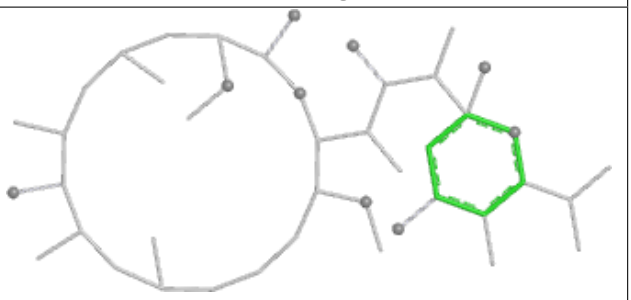
Bond lengths



Bond angles

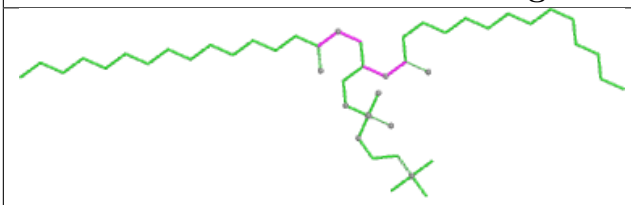


Torsions

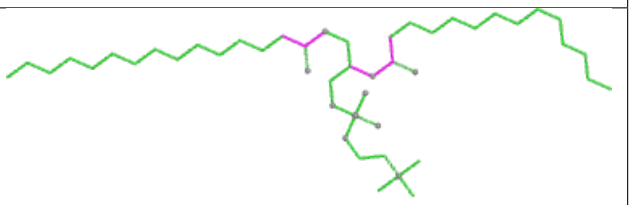


Rings

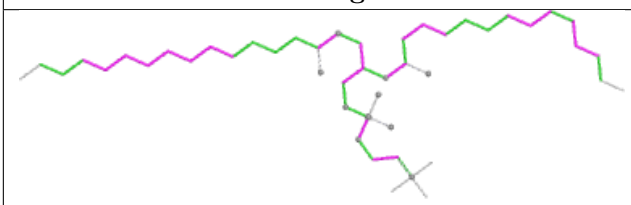
Ligand POV r 403



Bond lengths



Bond angles



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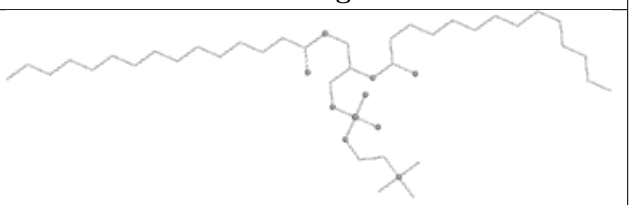
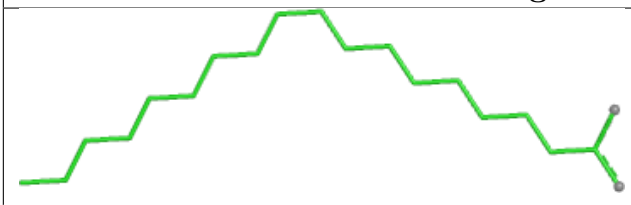
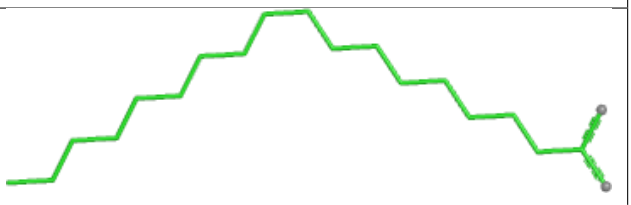


Rings

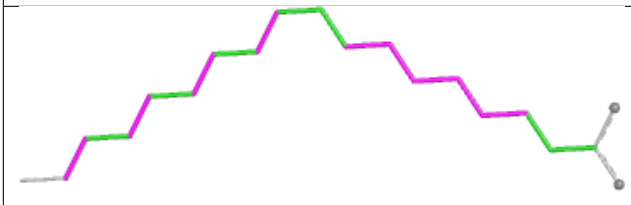
Ligand OLA r 404



Bond lengths



Bond angles



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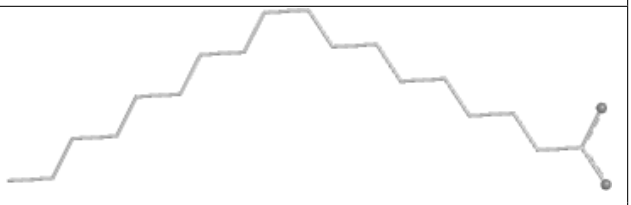
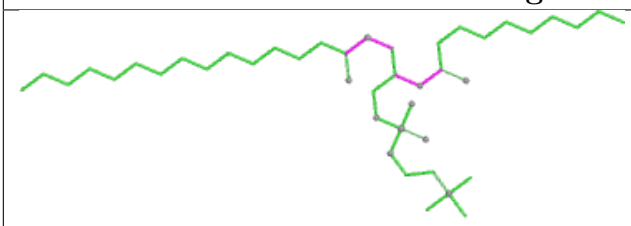
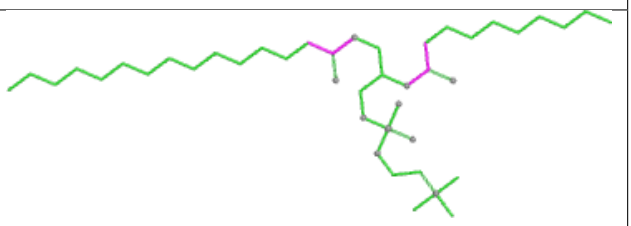
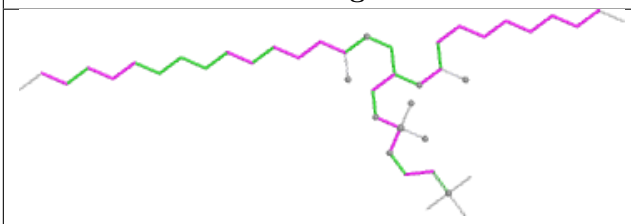


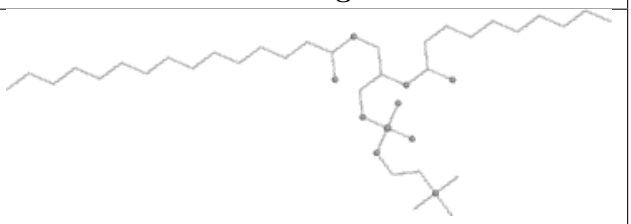
Rings

Ligand POV b 302

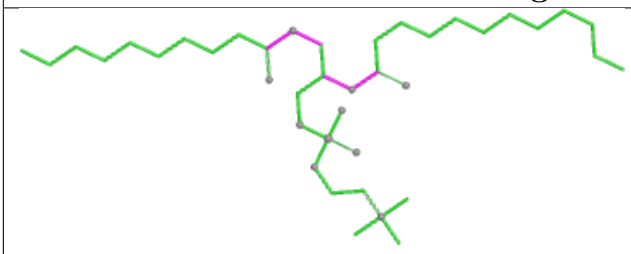

Bond lengths

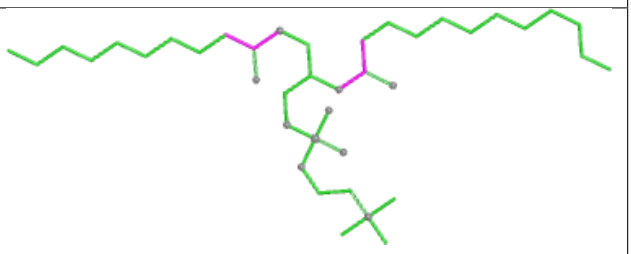

Bond angles

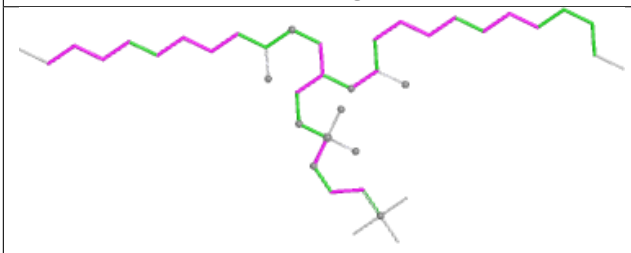

Torsions

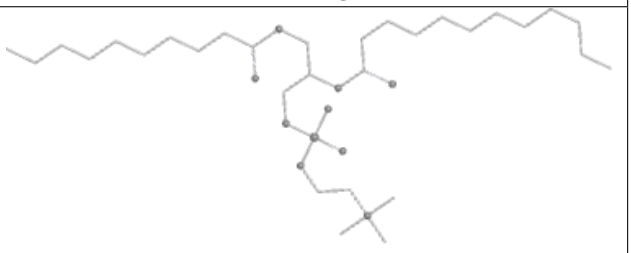

Rings

Ligand POV l 201

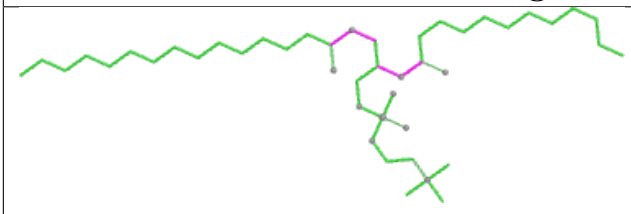

Bond lengths

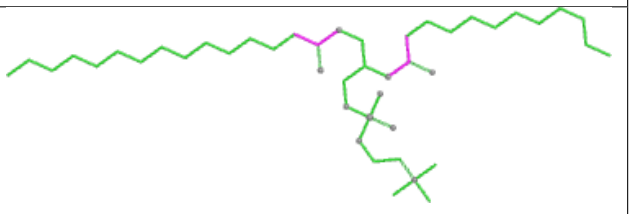

Bond angles

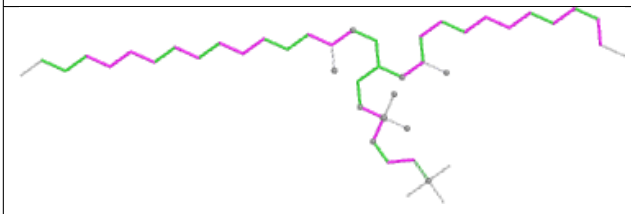

Torsions

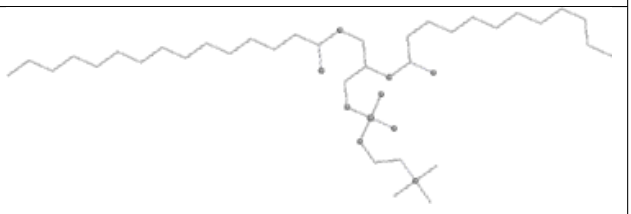

Rings

Ligand POV r 402

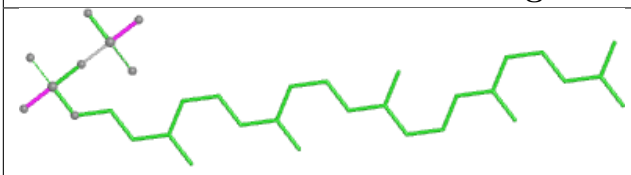

Bond lengths


Bond angles

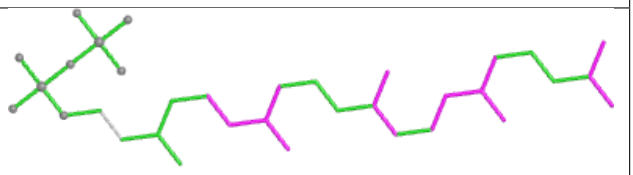

Torsions


Rings

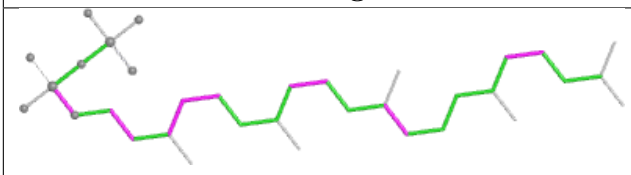
Ligand WJP a 901



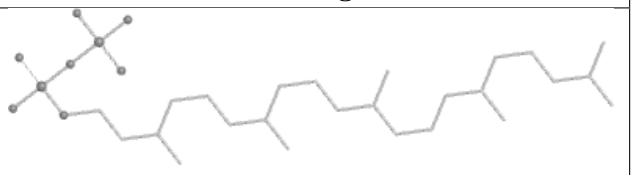
Bond lengths



Bond angles

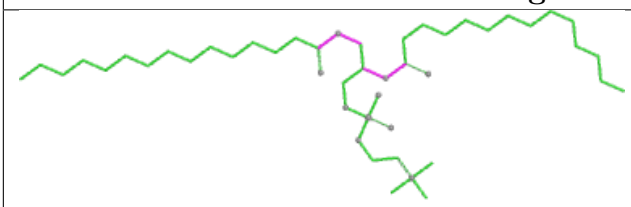


Torsions

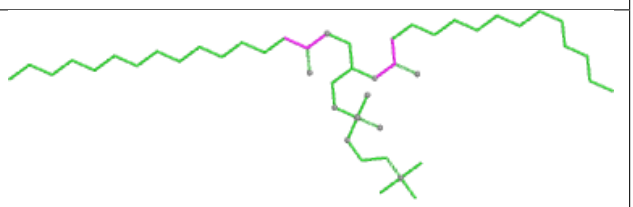


Rings

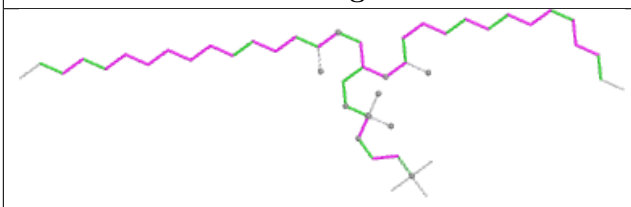
Ligand POV r 401



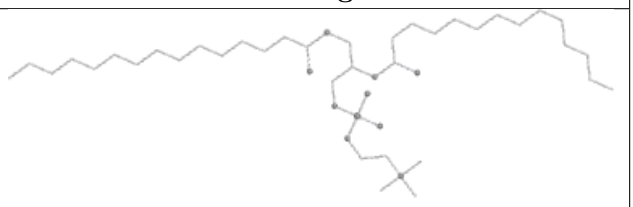
Bond lengths



Bond angles

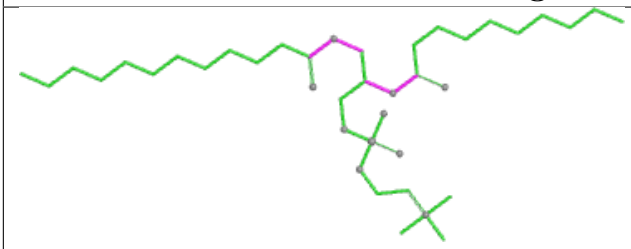


Torsions

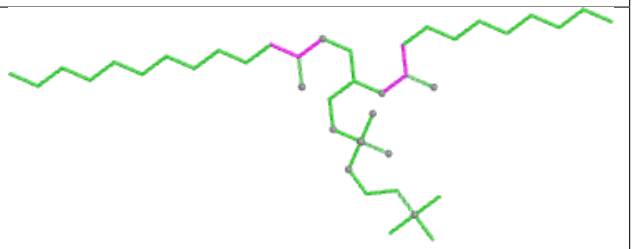


Rings

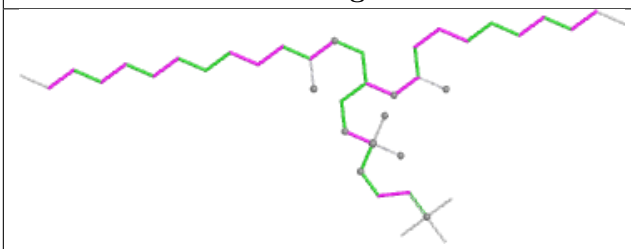
Ligand POV s 501



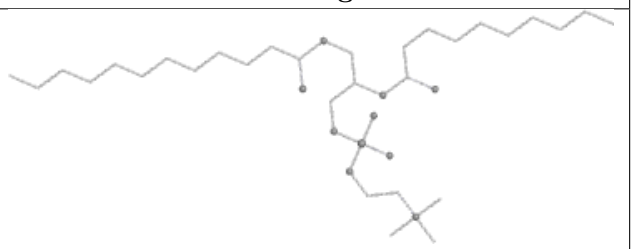
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

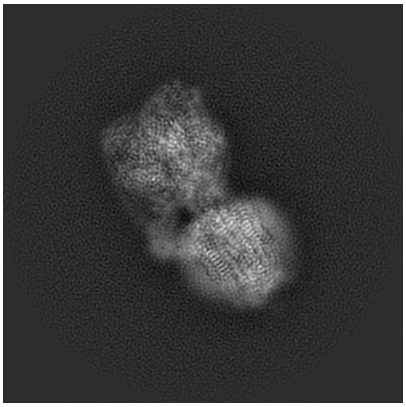
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22880. These allow visual inspection of the internal detail of the map and identification of artifacts.

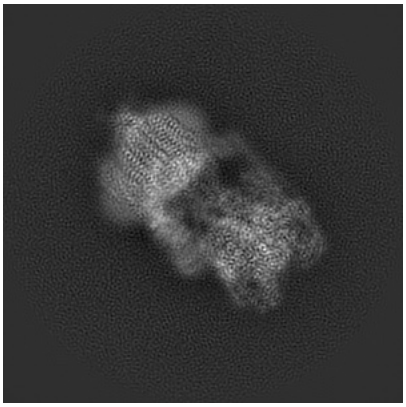
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

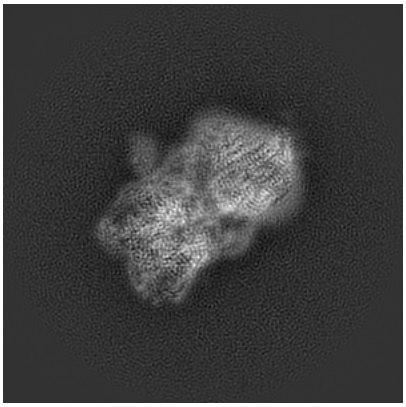
6.1.1 Primary map



X



Y

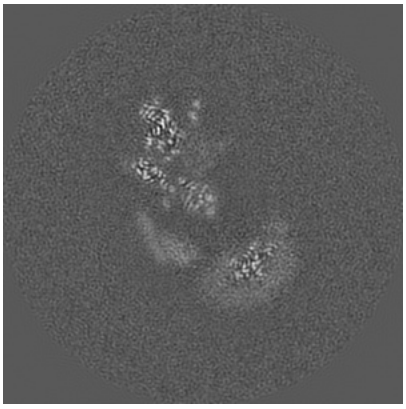


Z

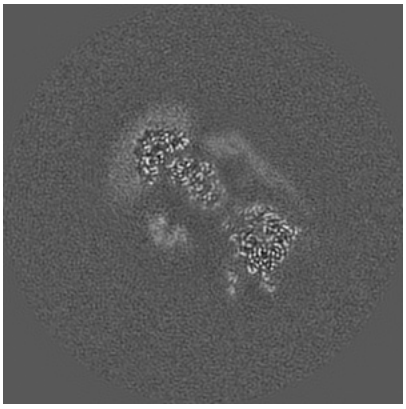
The images above show the map projected in three orthogonal directions.

6.2 Central slices

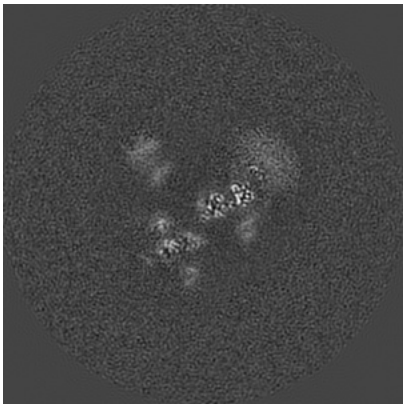
6.2.1 Primary map



X Index: 248



Y Index: 248

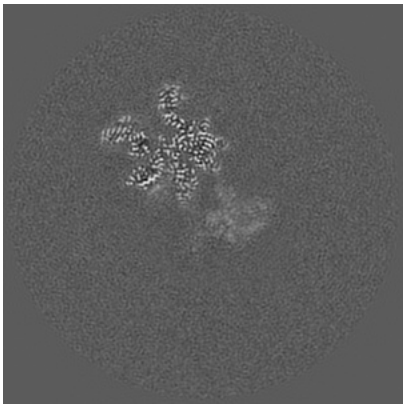


Z Index: 248

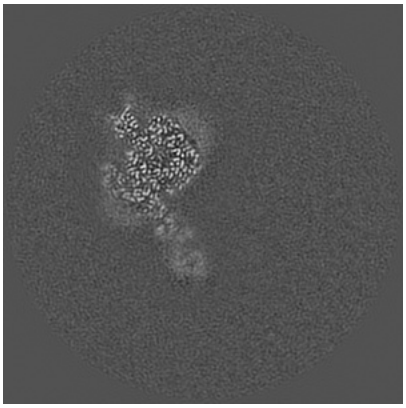
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

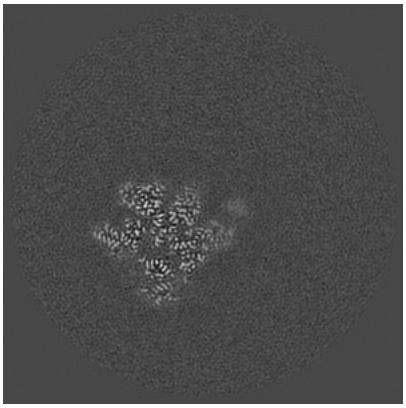
6.3.1 Primary map



X Index: 187



Y Index: 306

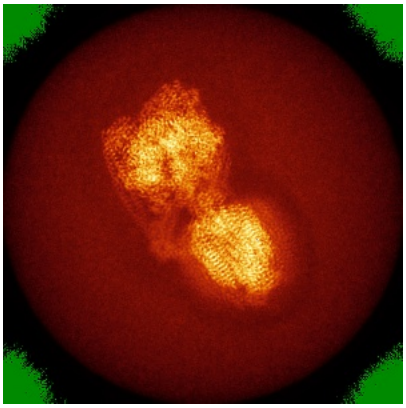


Z Index: 324

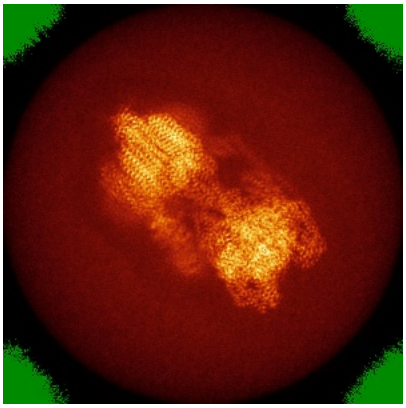
The images above show the largest variance slices of the map in three orthogonal directions.

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

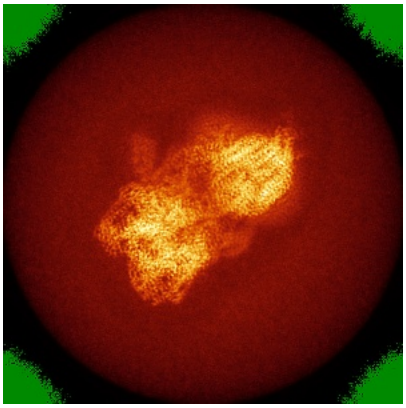
6.4.1 Primary map



X



Y

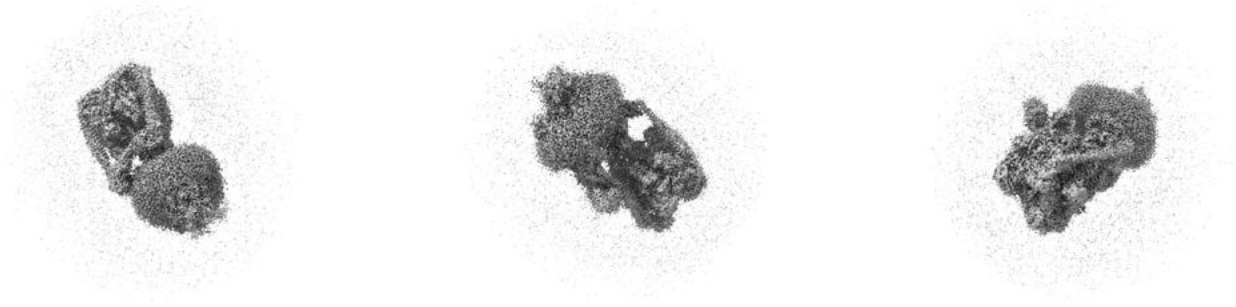


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

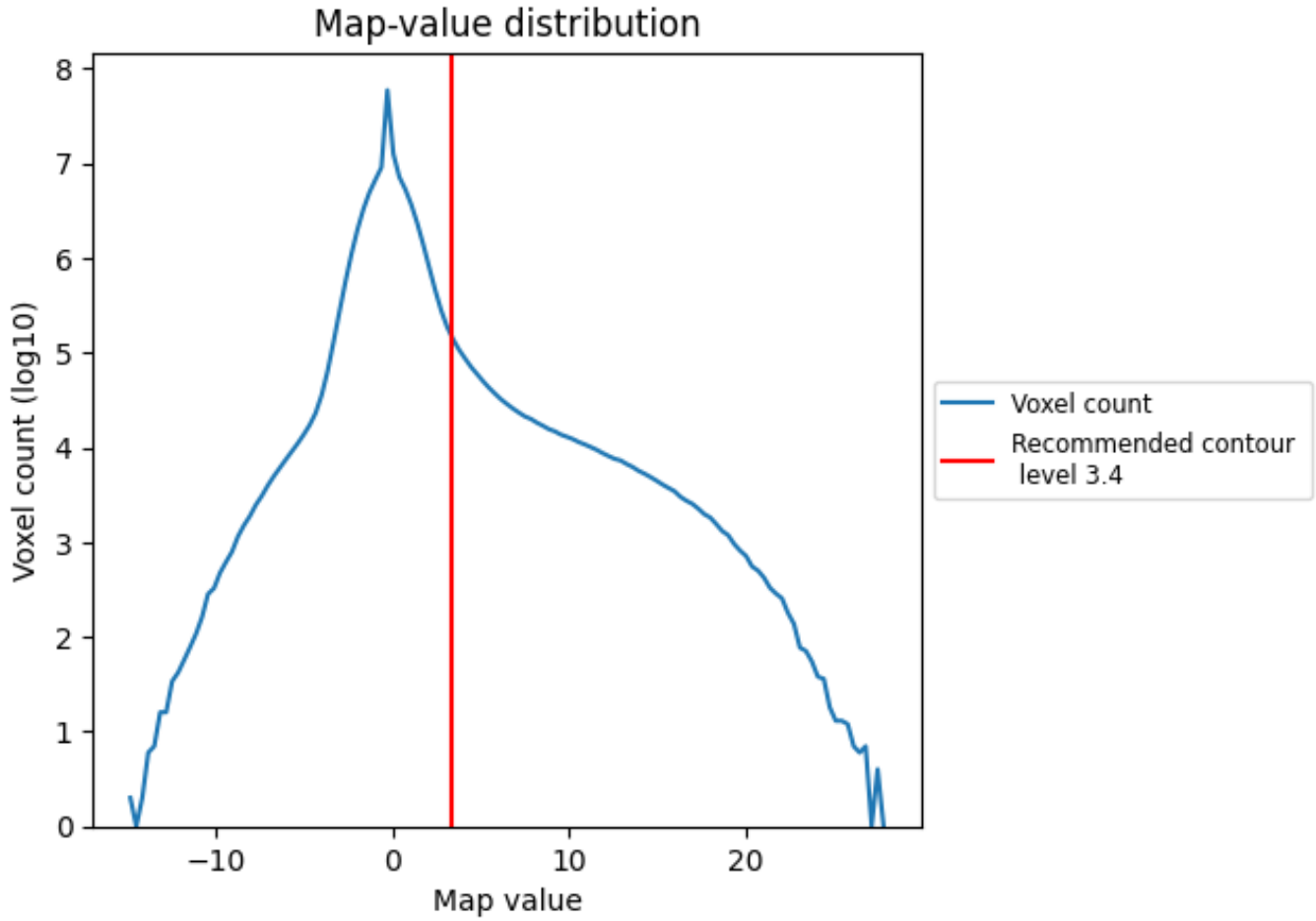
6.6 Mask visualisation (i)

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

7 Map analysis

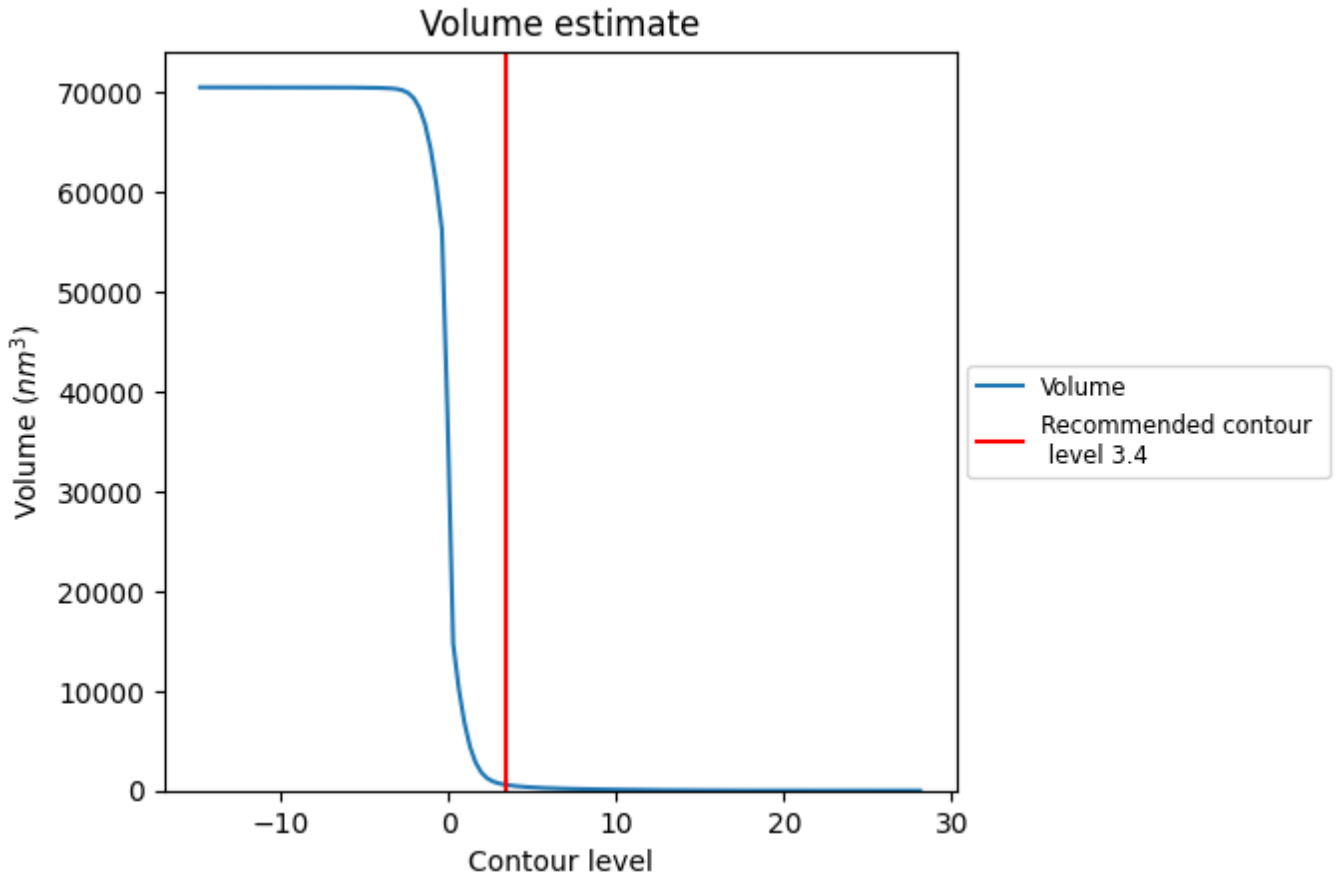
This section contains the results of statistical analysis of the map.

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.

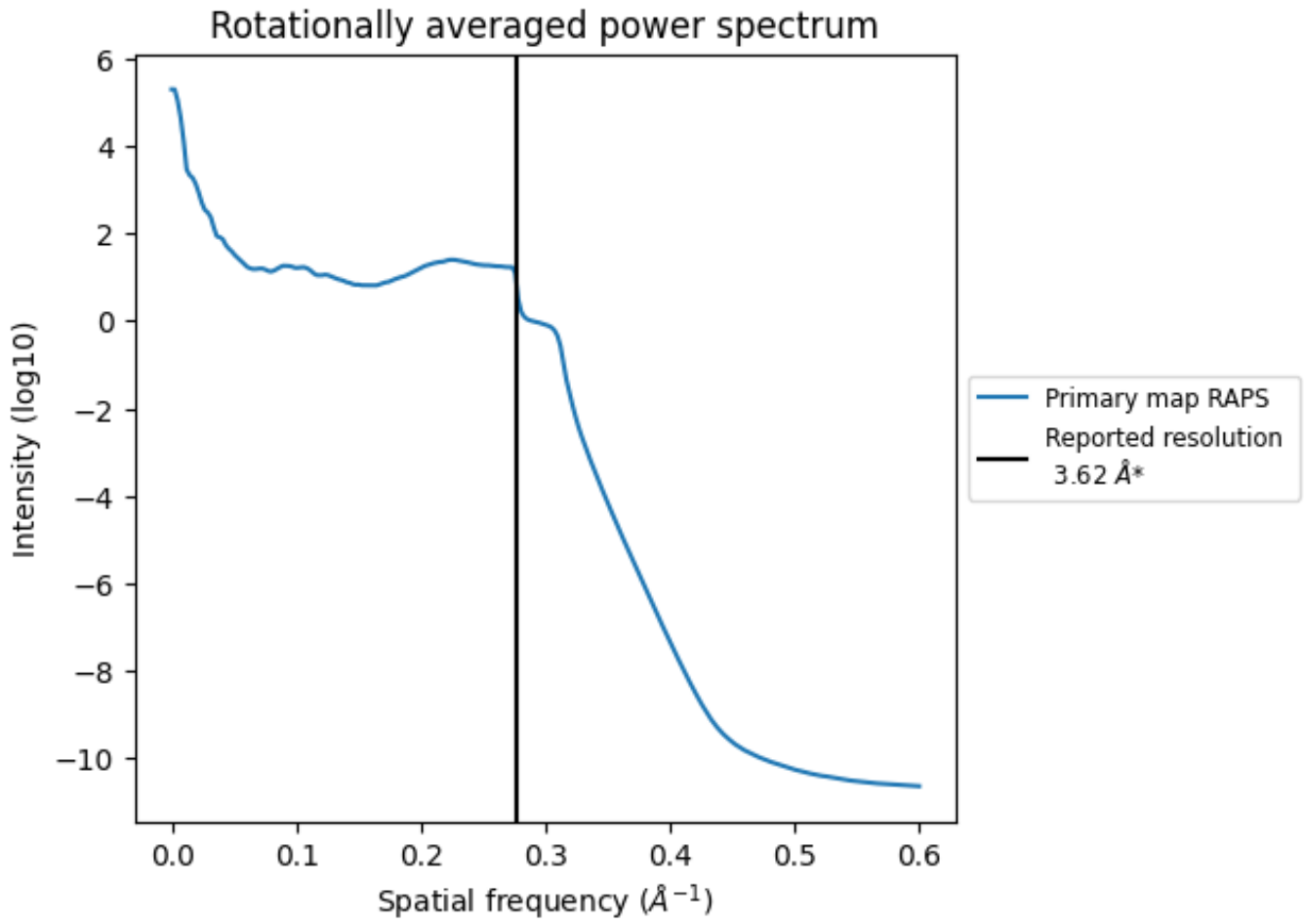
7.2 Volume estimate



The volume at the recommended contour level is 585 nm^3; this corresponds to an approximate mass of 528 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)



*Reported resolution corresponds to spatial frequency of 0.276 $Å^{-1}$

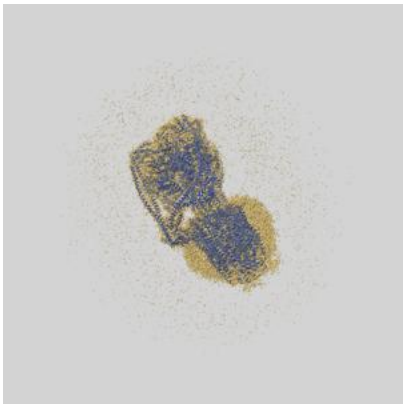
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

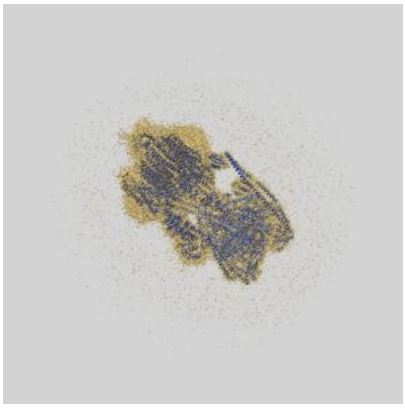
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22880 and PDB model 7KHR. Per-residue inclusion information can be found in section 3 on page 14.

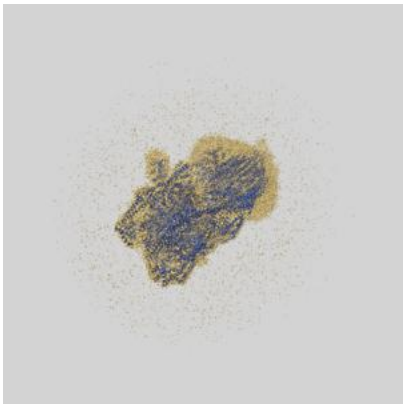
9.1 Map-model overlay



X



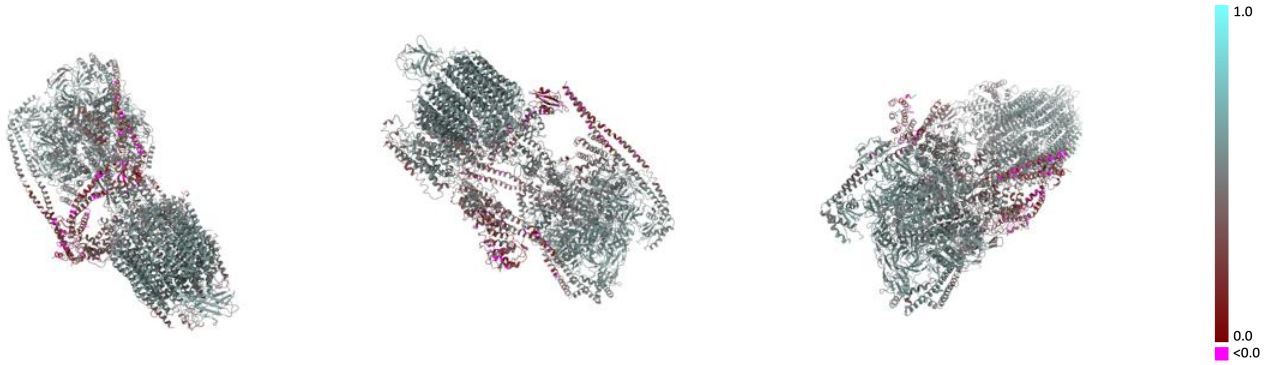
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.4 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.

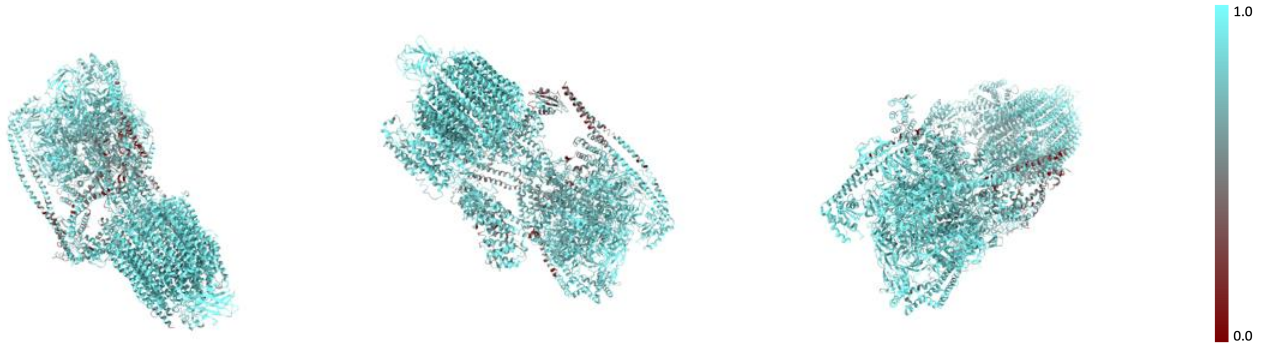
9.2 Q-score mapped to coordinate model (i)



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.

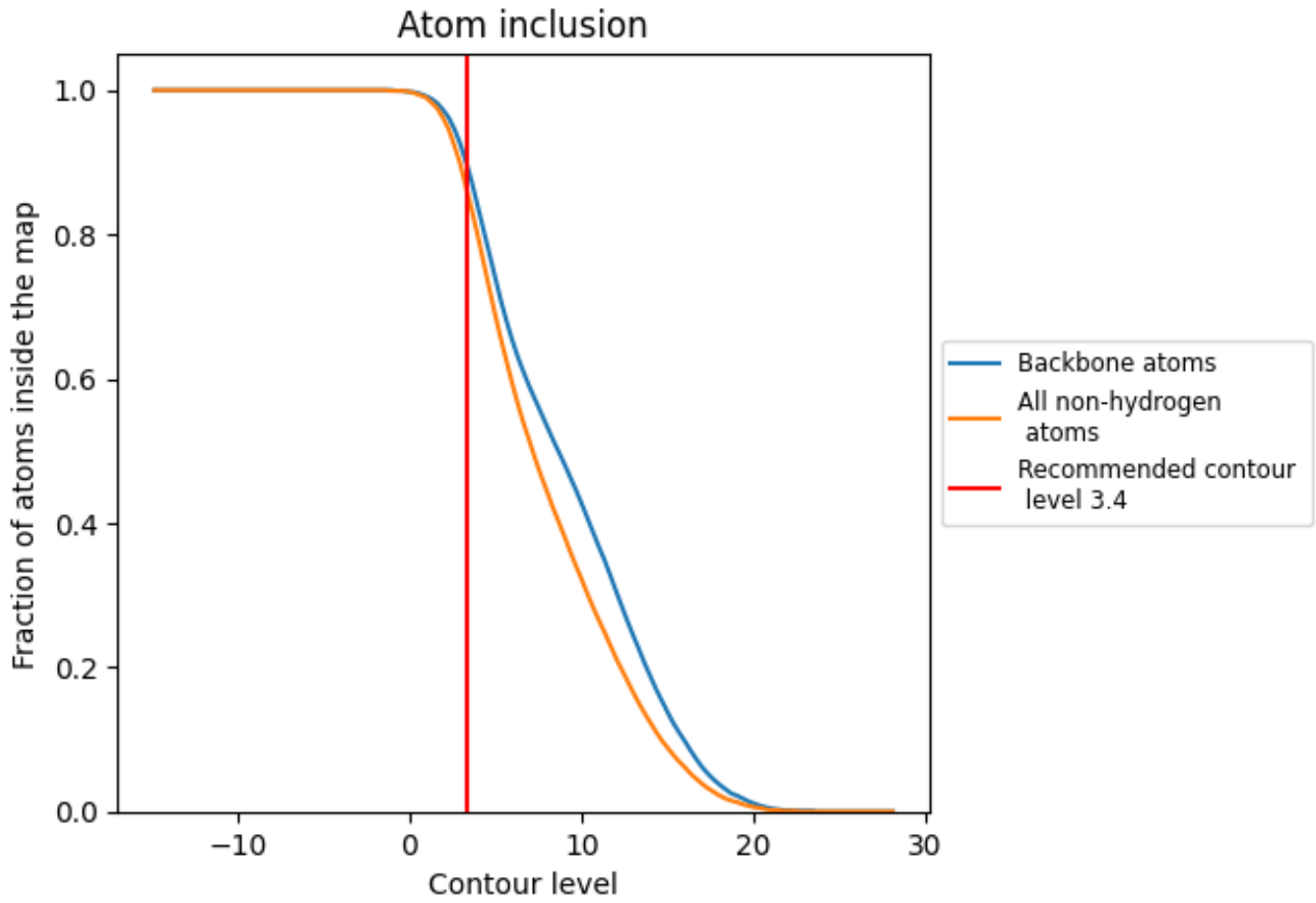
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.4).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (3.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8570	0.4930
A	0.8310	0.4920
B	0.8770	0.5260
C	0.8760	0.5350
D	0.9050	0.5510
E	0.8930	0.5470
F	0.8690	0.5360
G	0.6190	0.2050
H	0.8420	0.5030
I	0.8060	0.4680
J	0.8290	0.4860
K	0.8500	0.4780
L	0.8130	0.4630
M	0.7340	0.3860
N	0.7700	0.4100
O	0.7350	0.4000
P	0.7360	0.2810
Q	0.3640	0.2250
a	0.8260	0.4340
b	0.9300	0.5620
c	0.9290	0.5530
d	0.8750	0.5200
e	0.7930	0.4350
f	0.7640	0.4370
g	0.9400	0.5550
k	0.9320	0.5510
l	0.9280	0.5530
m	0.9230	0.5500
n	0.9170	0.5410
o	0.9290	0.5500
p	0.9190	0.5490
q	0.9320	0.5560
r	0.9230	0.5530
s	0.9150	0.5210
t	0.7810	0.4220