Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 04:03 AM EST

PDB ID	:	6WM2
EMDB ID	:	EMD-21847
Title	:	Human V-ATPase in state 1 with SidK and ADP
Authors	:	Wang, L.; Wu, H.; Fu, T.M.
Deposited on	:	2020-04-20
Resolution	:	3.10 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:

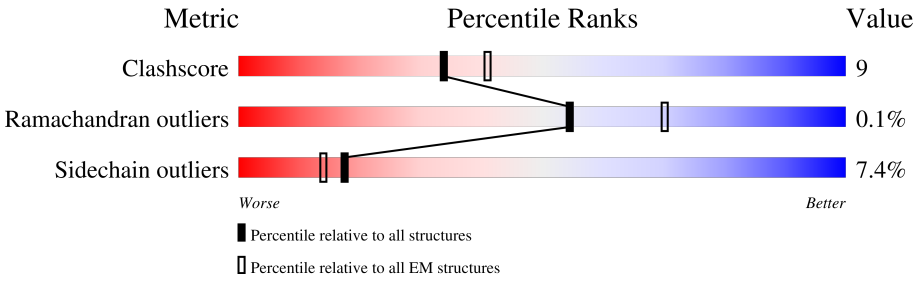
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	H	226	5% 71% 26%
1	I	226	7% 73% 27%
1	J	226	14% 76% 22%
2	K	118	13% 56% 37%
2	L	118	19% 59% 35%
2	M	118	37% 56% 31% 9%
3	O	382	37% 49% 8% 6%
4	P	483	39% 41% 9% 12%

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Mol	Chain	Length	Quality of chain
5	R	837	63% 25% 10%
6	A	617	81% 14%
6	B	617	79% 17%
6	C	617	82% 15%
7	D	511	79% 10% 10%
7	E	511	76% 14% 10%
7	F	511	78% 11% 10%
8	X	573	8% 28% 16% 54%
8	Y	573	5% 33% 12% 53%
8	Z	573	14% 30% 14% 54%
9	G	247	70% 15% 14%
10	N	119	68% 22% 8%
11	0	205	84% 14%
12	1	155	87% 8%
12	2	155	88% 9%
12	3	155	86% 10%
12	4	155	82% 14%
12	5	155	85% 12%
12	6	155	85% 12%
12	7	155	89% 7%
12	8	155	83% 12%
12	9	155	87% 8%
13	Q	351	83% 16%
14	S	81	77% 19% 5%
15	T	137	55% 5% 38%

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Mol	Chain	Length	Quality of chain
16	U	470	31% 12% 56%
17	V	350	13% 86%
18	W	5	60% 40%
19	a	4	100%
20	b	2	100%
20	c	2	50% 50%
20	d	2	100%
20	s	2	50% 50%
20	u	2	100%
21	r	11	36% 64%

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
19	NGA	a	2	X	-	-	-
21	NAG	r	1	X	-	-	-
21	MAN	r	11	X	-	-	-
24	PTY	0	307	X	-	-	-
24	PTY	R	904	X	-	-	-
24	PTY	U	503	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 73243 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 subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	225	Total	C	N	O	S	0	0
			1822	1143	322	347	10		
1	I	225	Total	C	N	O	S	0	0
			1822	1143	322	347	10		
1	J	225	Total	C	N	O	S	0	0
			1822	1143	322	347	10		

- Molecule 2 is a protein called V-type proton ATPase subunit G 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
2	L	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
2	M	114	Total	C	N	O	S	0	0
			938	573	179	183	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	359	Total	C	N	O	S	0	0
			2916	1869	493	545	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	427	Total	C	N	O	S	0	0
			3508	2228	605	648	27		

- Molecule 5 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	753	Total	C	N	O	S	0	0
			6141	4013	1020	1068	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	600	Total	C	N	O	S	0	0
			4652	2949	785	890	28		
6	B	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
6	C	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		

- Molecule 7 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	460	Total	C	N	O	S	0	0
			3600	2284	616	680	20		
7	E	460	Total	C	N	O	S	0	0
			3589	2278	616	676	19		
7	F	460	Total	C	N	O	S	0	0
			3596	2282	616	678	20		

- Molecule 8 is a protein called SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	262	Total	C	N	O	S	0	0
			2111	1339	354	408	10		
8	Y	267	Total	C	N	O	S	0	0
			2136	1355	359	411	11		
8	Z	262	Total	C	N	O	S	0	0
			2105	1333	354	408	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	213	Total	C	N	O	S	0	0
			1713	1087	309	312	5		

- Molecule 10 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	110	Total	C	N	O	S	0	0
			875	552	157	164	2		

- Molecule 11 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	0	204	Total	C	N	O	S	0	0
			1495	988	238	259	10		

- Molecule 12 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	7	150	Total	C	N	O	S	0	0
			1059	695	166	191	7		
12	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

- Molecule 13 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	350	Total	C	N	O	S	0	0
			2829	1825	461	530	13		

- Molecule 14 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	77	Total	C	N	O	S	0	0
			631	436	97	93	5		

- Molecule 15 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	85	Total	C	N	O	S	0	0
			654	431	101	115	7		

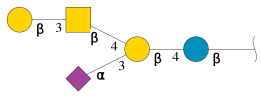
- Molecule 16 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	205	Total	C	N	O	S	0	0
			1664	1089	265	300	10		

- Molecule 17 is a protein called Renin receptor.

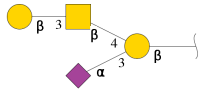
Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	50	Total	C	N	O	S	0	0
			417	283	58	73	3		

- Molecule 18 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
18	W	5	Total	C	N	O	0	0
			68	37	2	29		

- Molecule 19 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose.



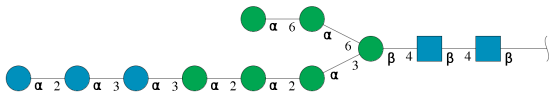
Mol	Chain	Residues	Atoms				AltConf	Trace
19	a	4	Total	C	N	O	0	0
			56	31	2	23		

- Molecule 20 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-

acetamido-2-deoxy-beta-D-glucopyranose.

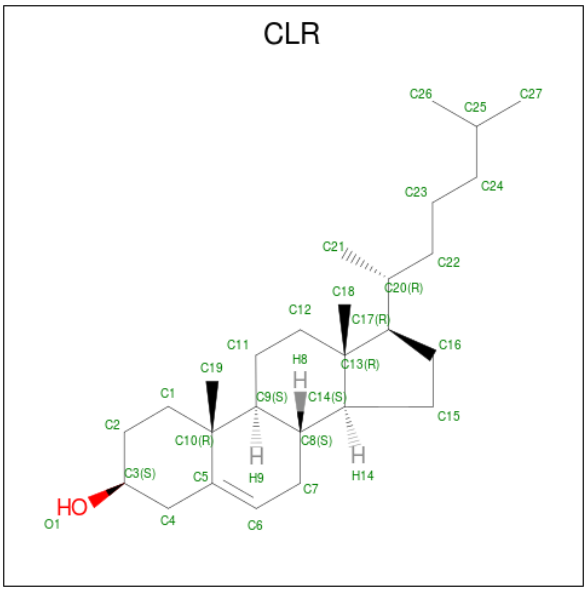
Mol	Chain	Residues	Atoms				AltConf	Trace
20	u	2	Total	C	N	O	0	0
			28	16	2	10		
20	b	2	Total	C	N	O	0	0
			28	16	2	10		
20	c	2	Total	C	N	O	0	0
			28	16	2	10		
20	d	2	Total	C	N	O	0	0
			28	16	2	10		
20	s	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 21 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)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



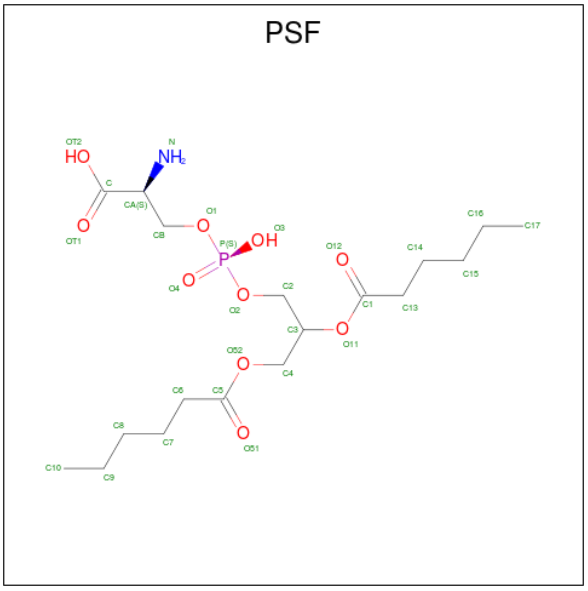
Mol	Chain	Residues	Atoms				AltConf	Trace
21	r	11	Total	C	N	O	0	0
			127	70	2	55		

- Molecule 22 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



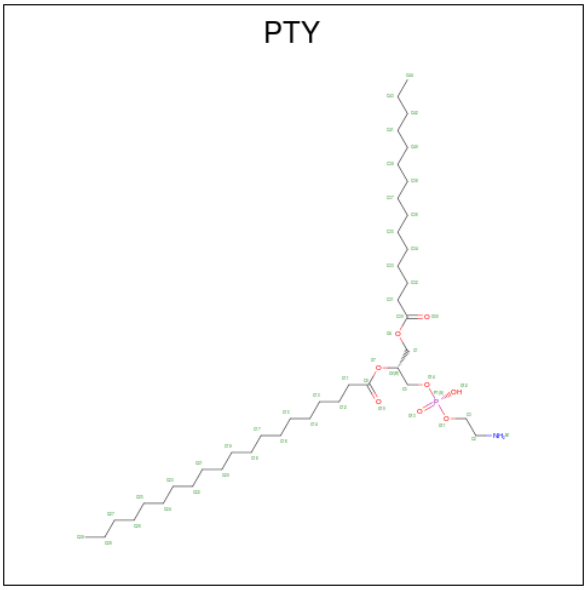
Mol	Chain	Residues	Atoms	AltConf
22	R	1	Total C O 28 27 1	0
22	0	1	Total C O 28 27 1	0
22	5	1	Total C O 28 27 1	0
22	V	1	Total C O 28 27 1	0

- Molecule 23 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (three-letter code: PSF) (formula: $C_{18}H_{34}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
23	R	1	Total	C	N	O	P	0
			30	18	1	10	1	

- Molecule 24 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total	C	N	O	P	0
			61	47	1	12	1	
24	R	1	Total	C	N	O	P	0
			61	47	1	12	1	
24	0	1	Total	C	N	O	P	0
			65	47	1	15	2	
24	0	1	Total	C	N	O	P	0
			65	47	1	15	2	
24	2	1	Total	C	N	O	P	0
			29	20	1	7	1	
24	5	1	Total	C	N	O	P	0
			35	25	1	8	1	
24	6	1	Total	C	O	P		0
			21	13	7	1		
24	7	1	Total	C	N	O	P	0
			42	32	1	8	1	
24	8	1	Total	C	N	O	P	0
			83	68	1	13	1	
24	8	1	Total	C	N	O	P	0
			83	68	1	13	1	

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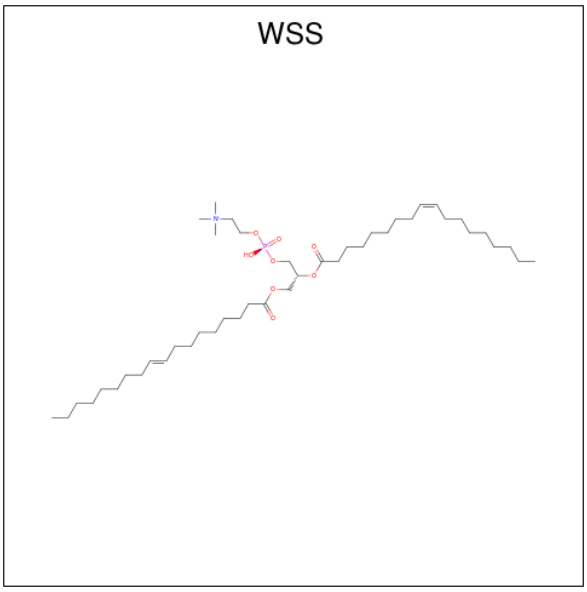
Mol	Chain	Residues	Atoms	AltConf
24	Q	1	Total C N O P 30 20 1 8 1	0
24	U	1	Total C O 26 21 5	0
24	V	1	Total C N O P 29 20 1 7 1	0

- Molecule 25 is tri(methyl)-[2-[[(2 {R})-2-[({Z})-octadec-9-enoyl]oxy-3-[({E})-1-oxidanylideneoctadec-9-enoxy]propoxy]-oxidanyl-phosphoryl]oxyethyl]azanium (three-letter code: WSS) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
25	R	1	Total C N O P 40 30 1 8 1	0
25	0	1	Total C N O P 142 103 3 32 4	0
25	0	1	Total C N O P 142 103 3 32 4	0
25	0	1	Total C N O P 142 103 3 32 4	0
25	0	1	Total C N O P 142 103 3 32 4	0
25	1	1	Total C N O P 34 24 1 8 1	0
25	3	1	Total C O P 41 32 8 1	0

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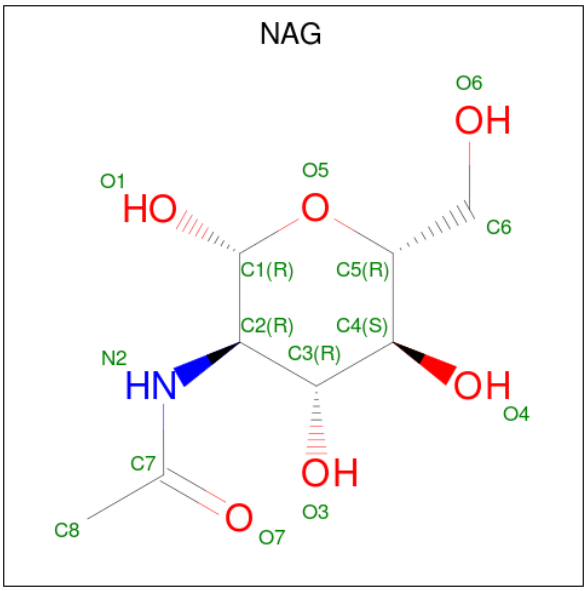
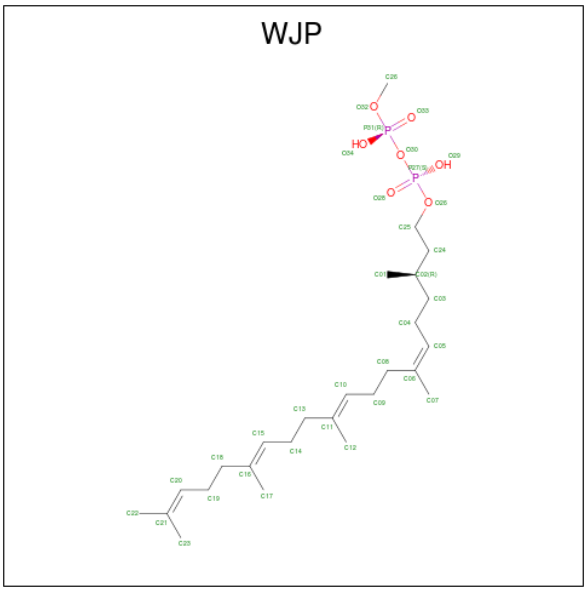
Mol	Chain	Residues	Atoms					AltConf
25	U	1	Total	C	N	O	P	0
			76	56	2	16	2	
25	U	1	Total	C	N	O	P	0
			76	56	2	16	2	
25	V	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 26 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



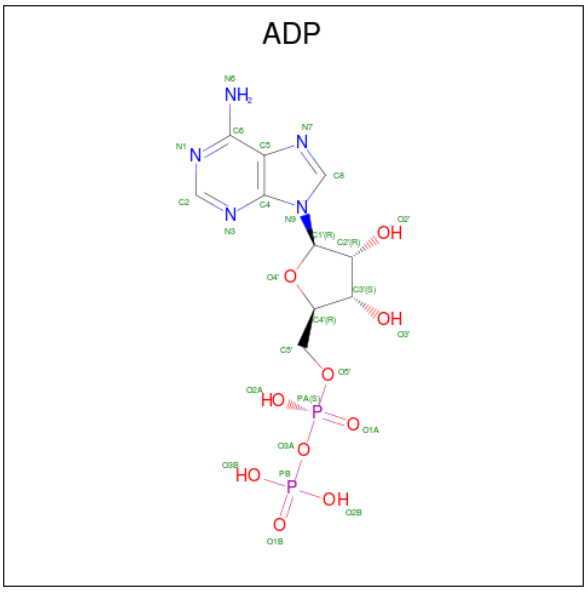
Mol	Chain	Residues	Atoms				AltConf
26	R	1	Total	C	N	O	0
			14	8	1	5	
26	U	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 27 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: $C_{26}H_{48}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
27	R	1	Total	C	O	P	0
			34	25	7	2	

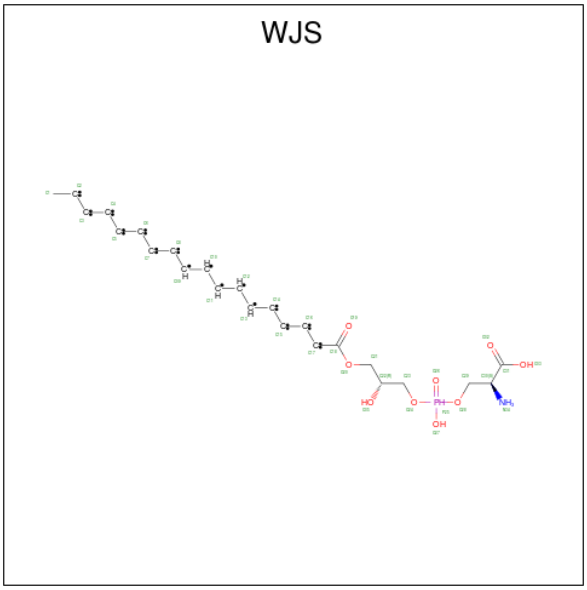
- Molecule 28 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 29 is (2 {S})-2-$l^{4}-azanyl-3-[[(2 {R})-3-octadecanoyloxy-2-oxidanyl-propoxy]-oxidanyl-oxidanylidene-$l^{6}-phosphanyl]oxy-propanoic acid (three-letter code: WJS)

(formula: $C_{24}H_{20}NO_9P$).



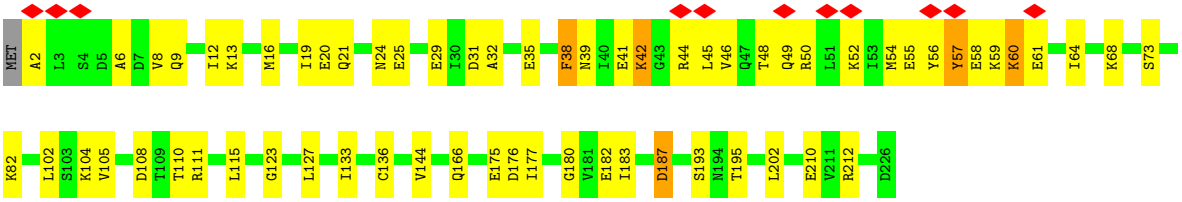
Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	N	O	P	0
			27	16	1	9	1	

3 Residue-property plots (i)

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

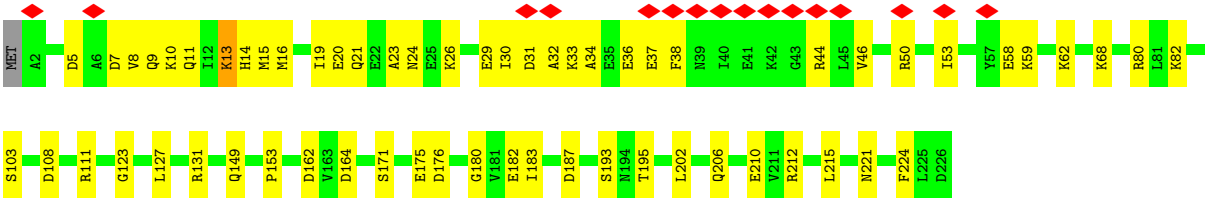
• Molecule 1: V-type proton ATPase subunit E 1

Chain H:



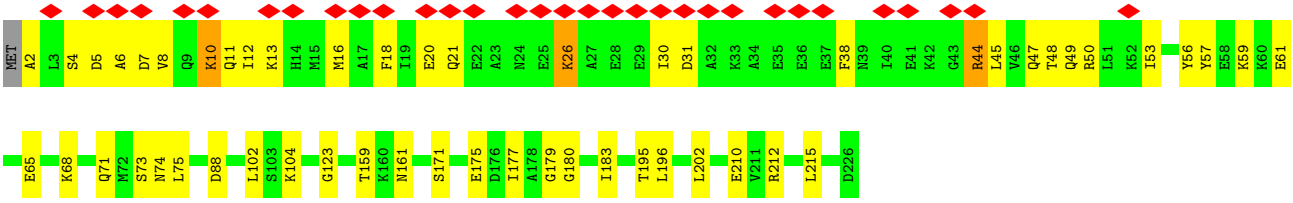
• Molecule 1: V-type proton ATPase subunit E 1

Chain I:



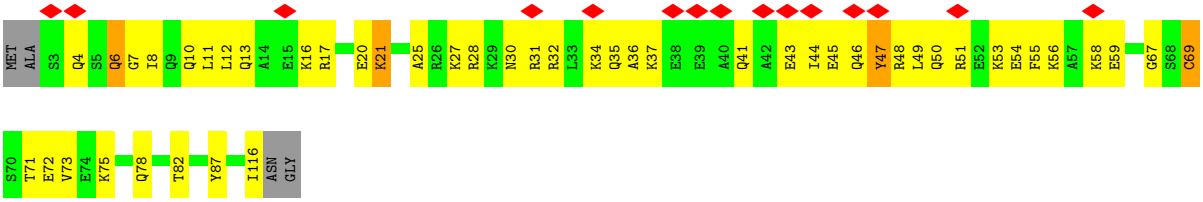
• Molecule 1: V-type proton ATPase subunit E 1

Chain J:



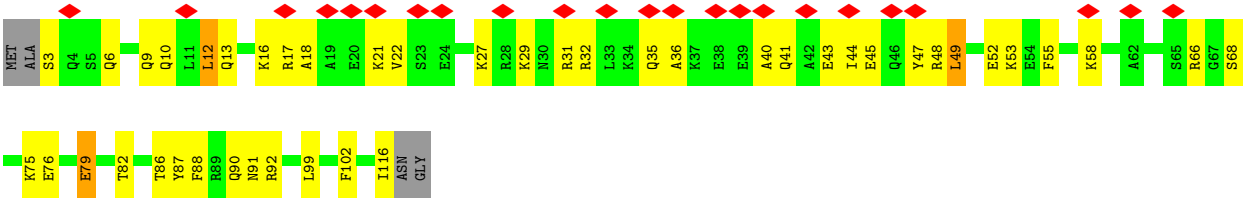
• Molecule 2: V-type proton ATPase subunit G 1

Chain K:



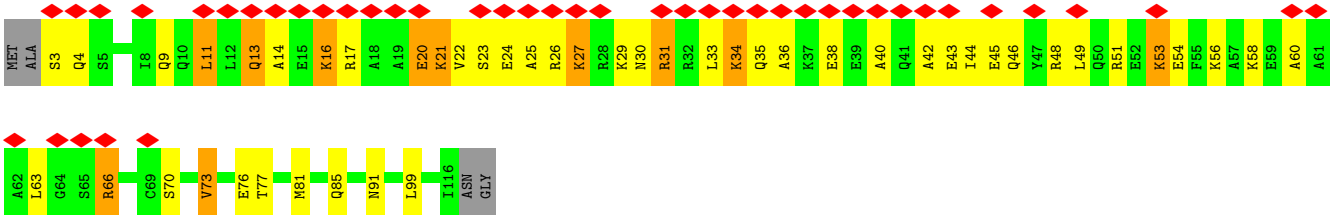
• Molecule 2: V-type proton ATPase subunit G 1

Chain L:



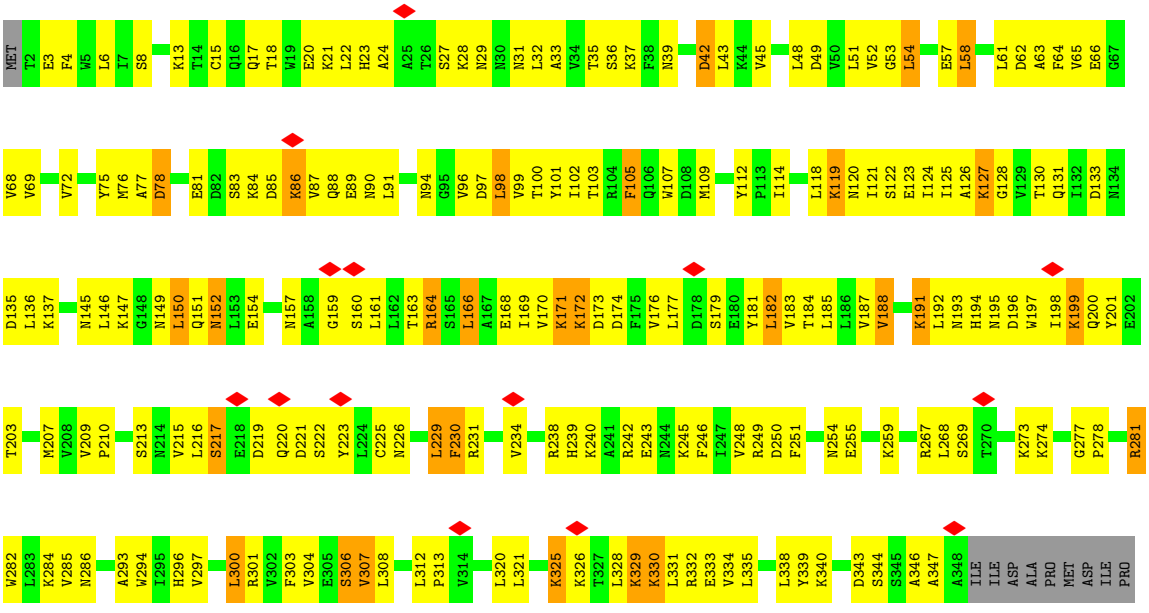
• Molecule 2: V-type proton ATPase subunit G 1

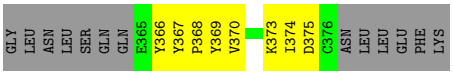
Chain M:



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

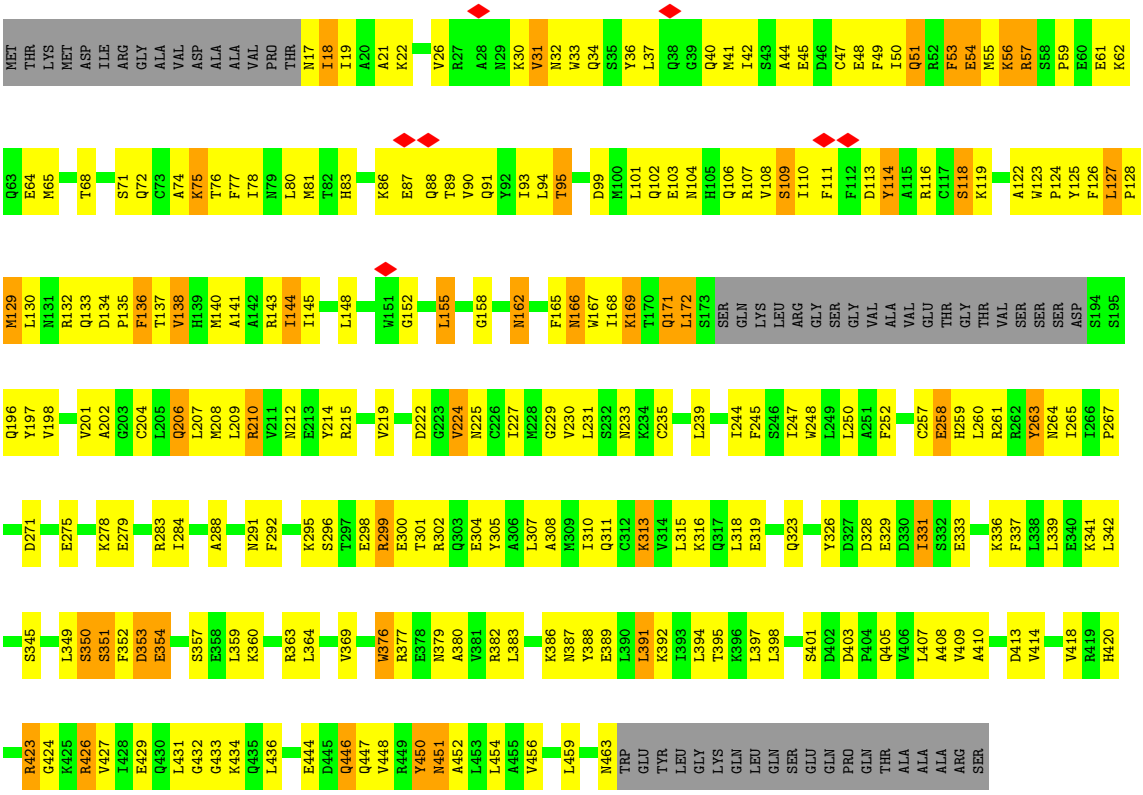
Chain O:





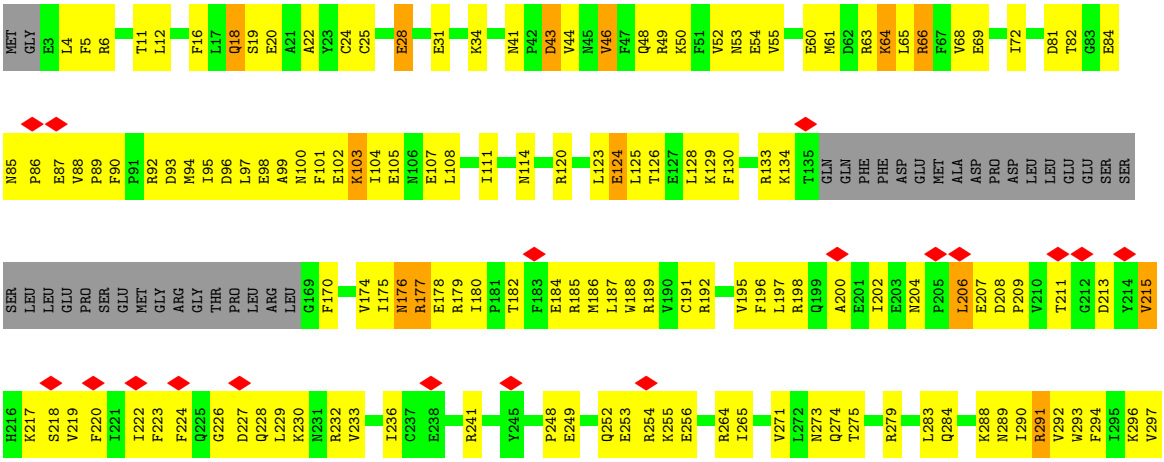
• Molecule 4: V-type proton ATPase subunit H

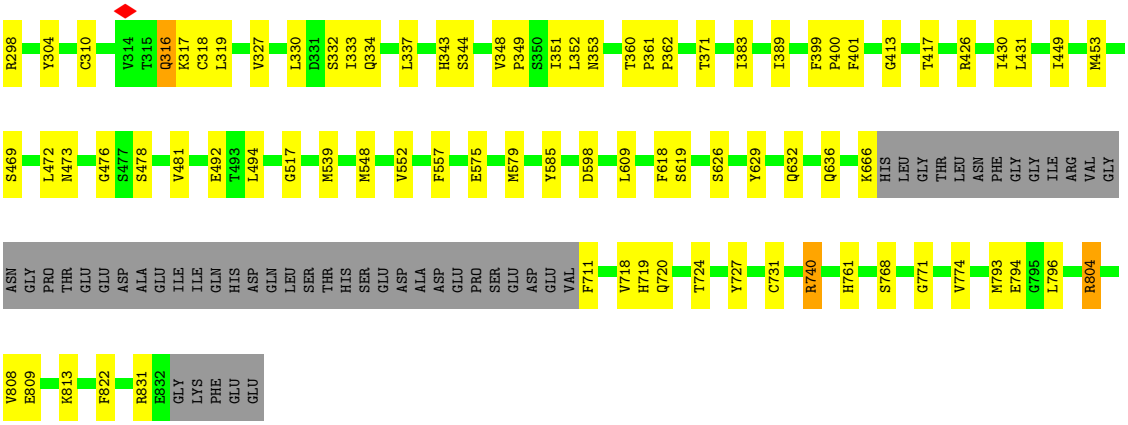
Chain P:



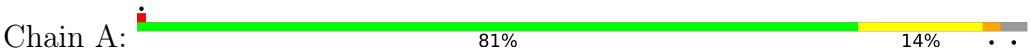
• Molecule 5: V-type proton ATPase 116 kDa subunit a isoform 1

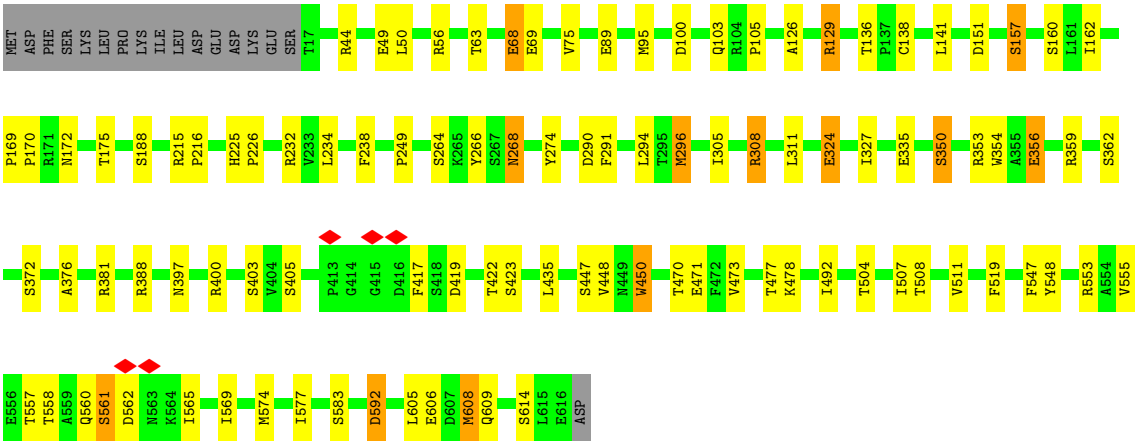
Chain R:



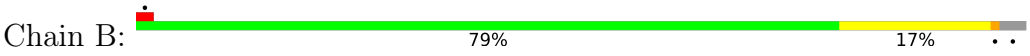


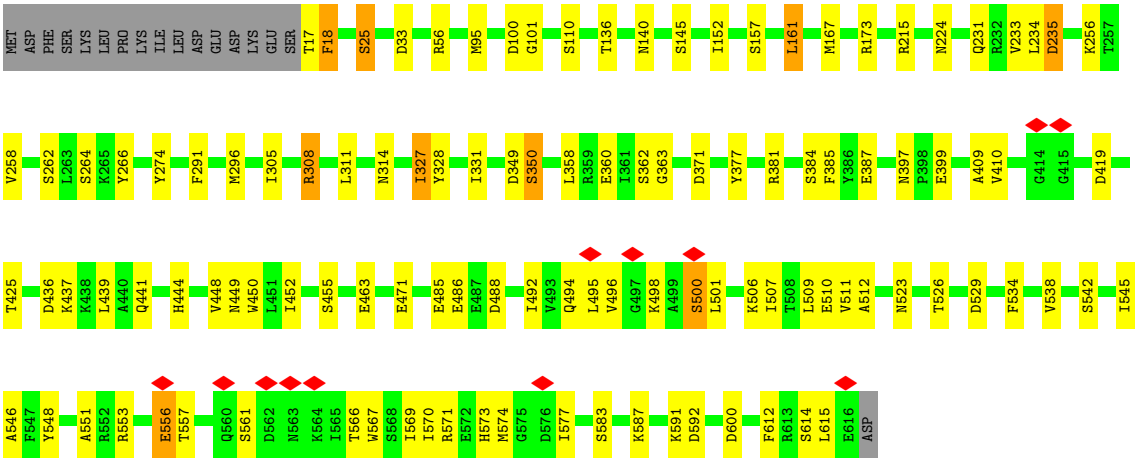
• Molecule 6: V-type proton ATPase catalytic subunit A





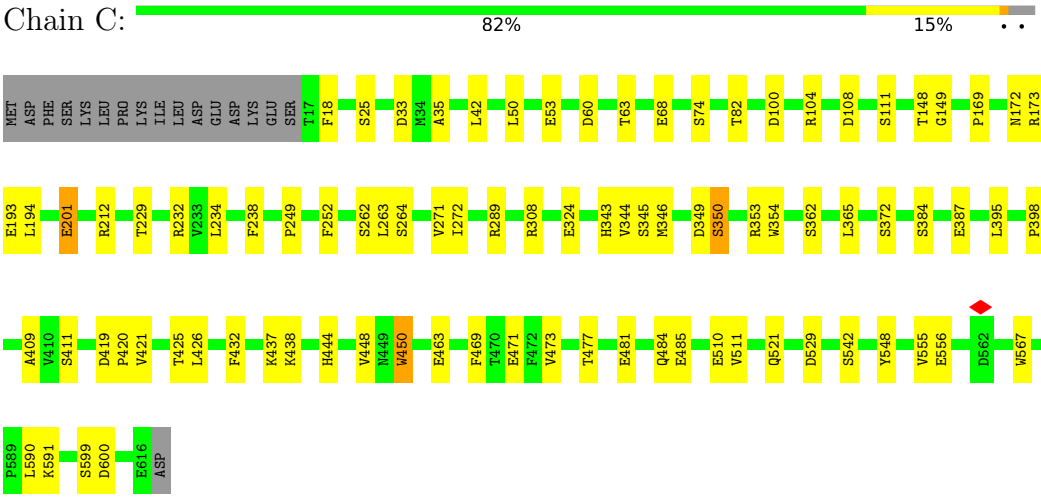
• Molecule 6: V-type proton ATPase catalytic subunit A





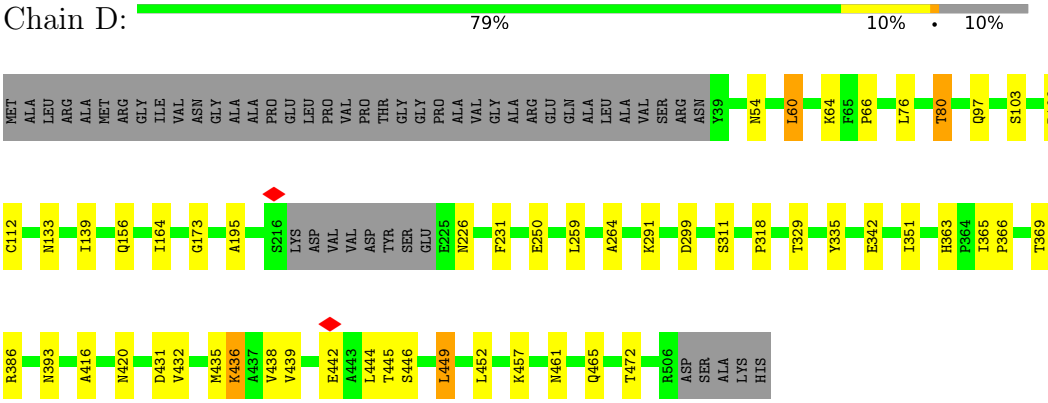
• Molecule 6: V-type proton ATPase catalytic subunit A

Chain C:



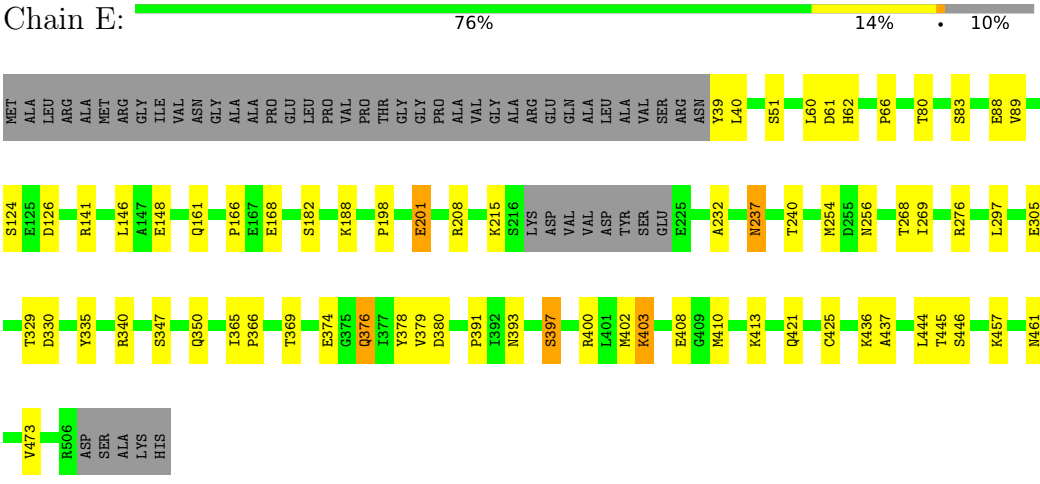
• Molecule 7: V-type proton ATPase subunit B, brain isoform

Chain D:



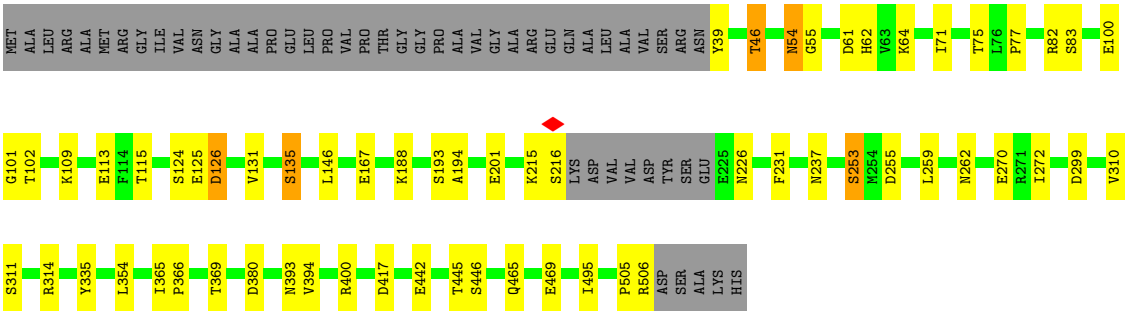
• Molecule 7: V-type proton ATPase subunit B, brain isoform

Chain E:



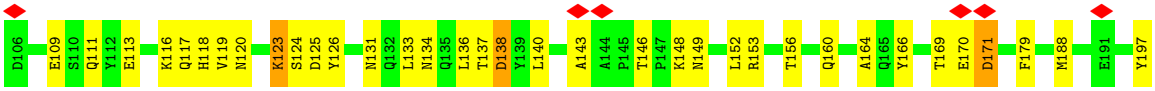
• Molecule 7: V-type proton ATPase subunit B, brain isoform

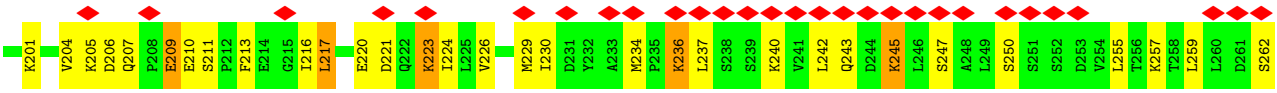
Chain F:

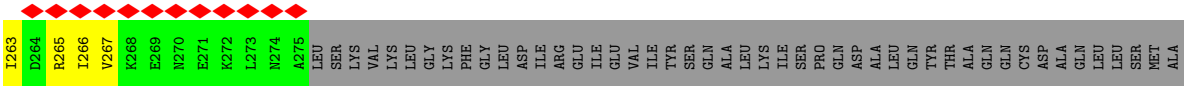


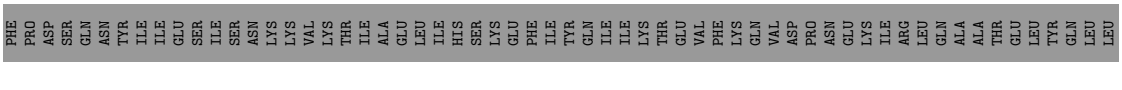
• Molecule 8: SidK

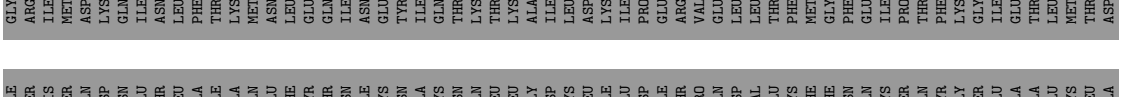
Chain X:

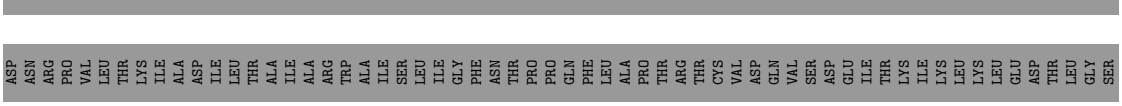


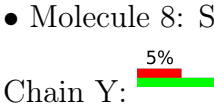






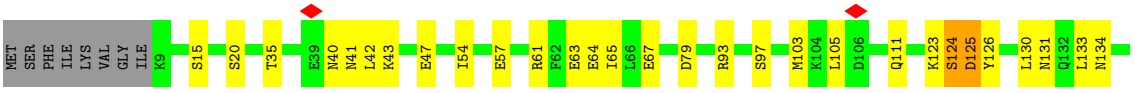


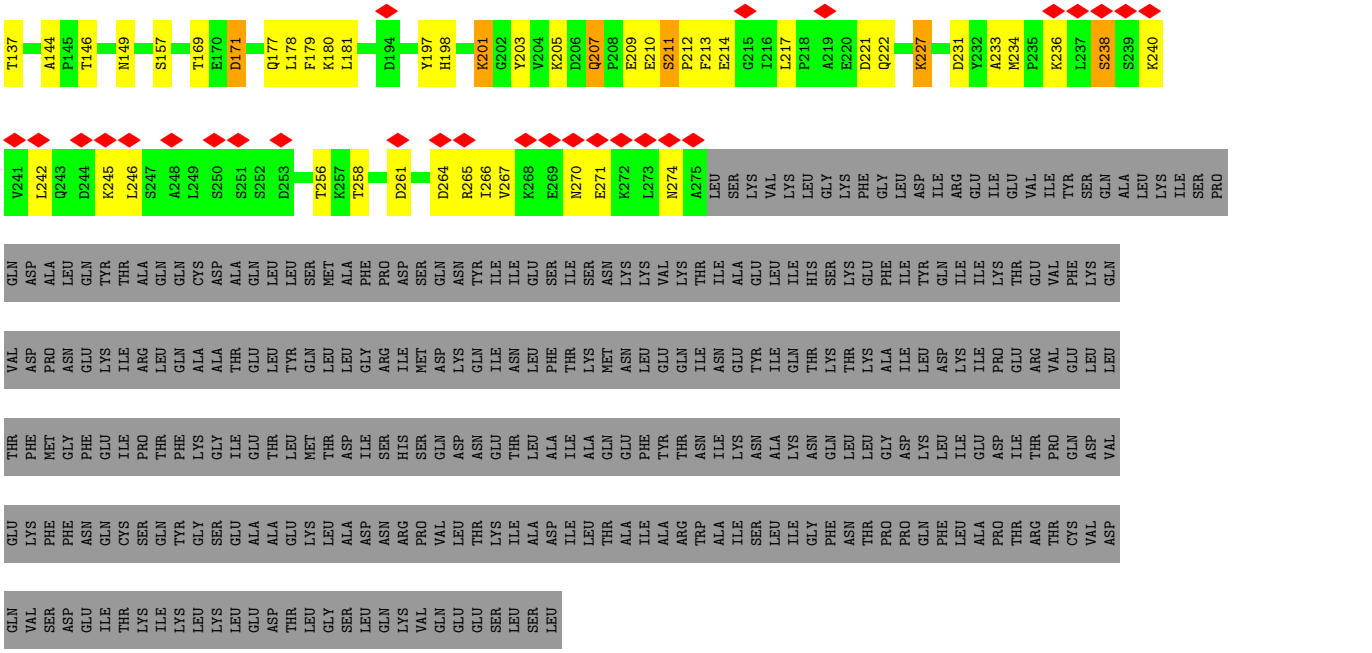




• Molecule 8: SidK

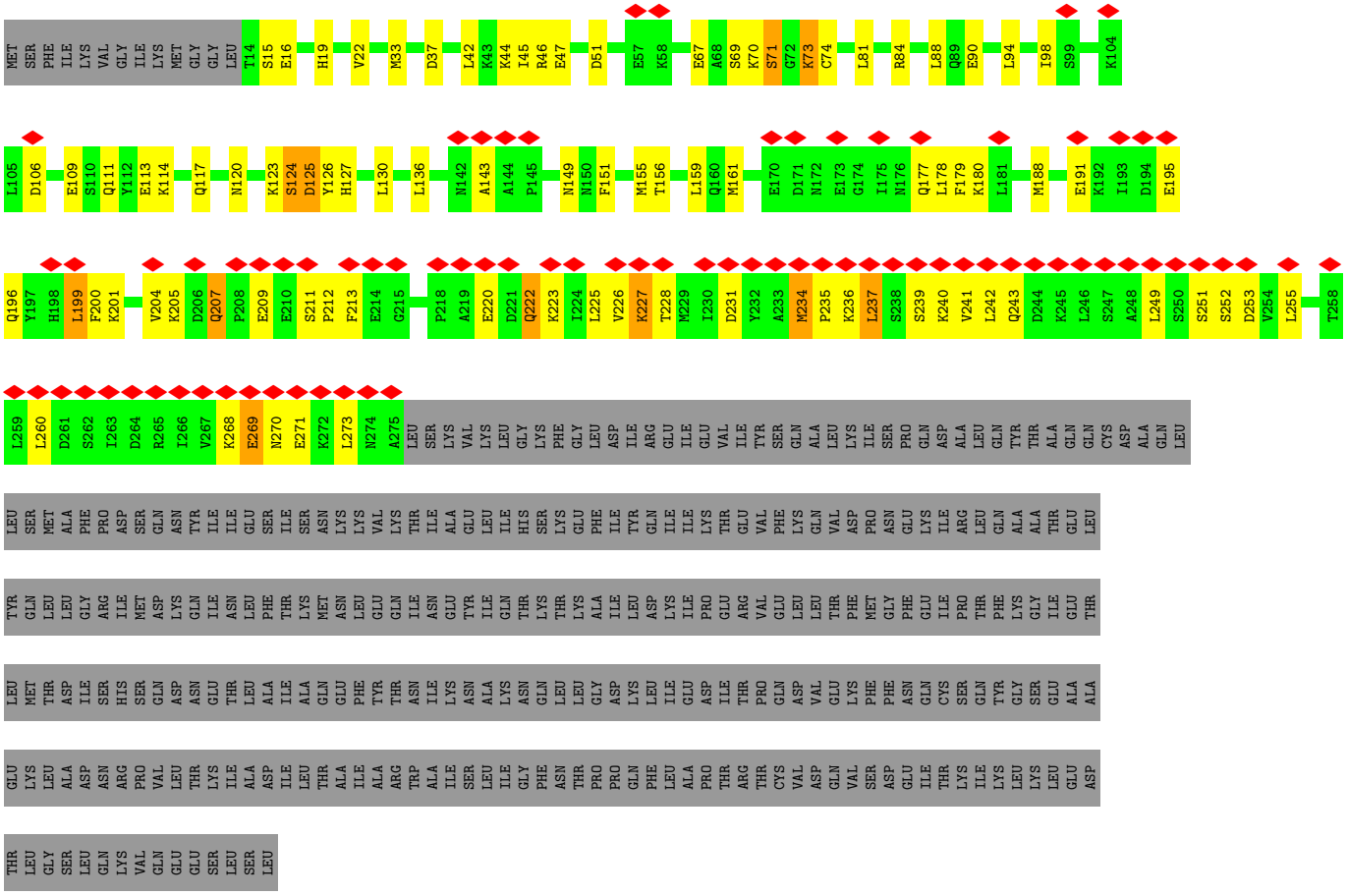
Chain Y:





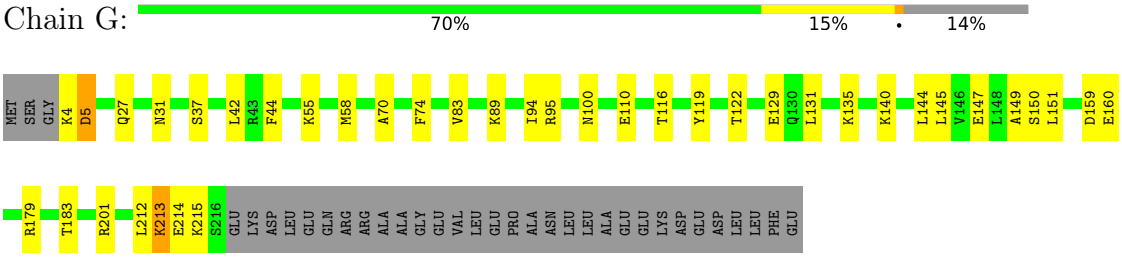
• Molecule 8: SidK

Chain Z:



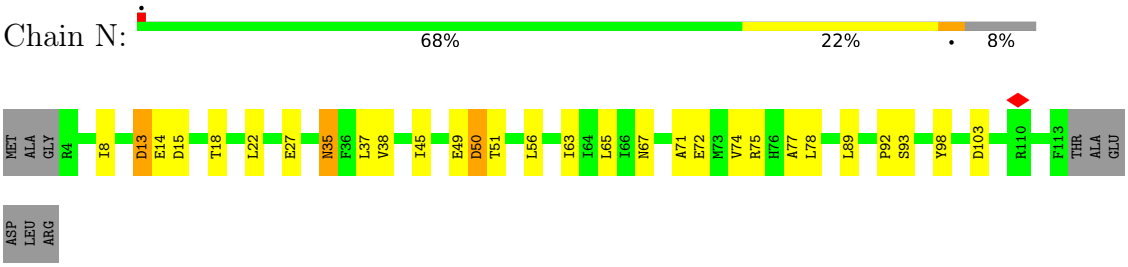
• Molecule 9: V-type proton ATPase subunit D

Chain G:



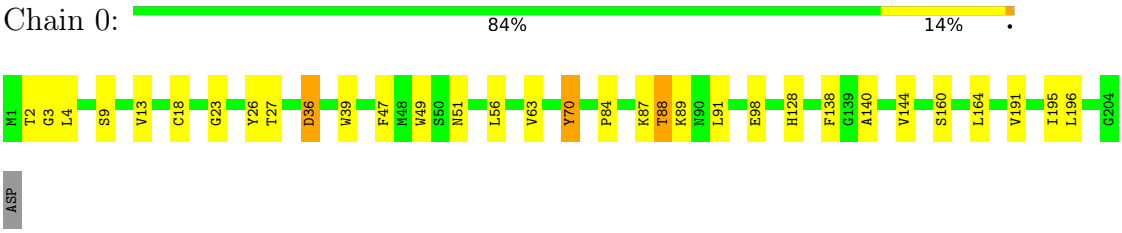
• Molecule 10: V-type proton ATPase subunit F

Chain N:



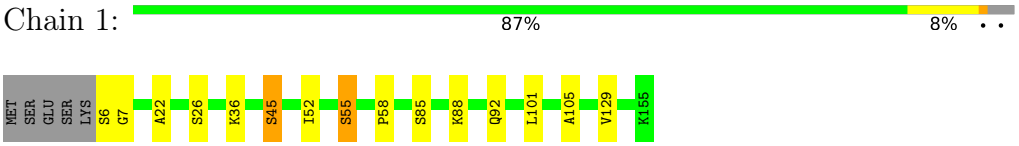
• Molecule 11: V-type proton ATPase 21 kDa proteolipid subunit

Chain 0:



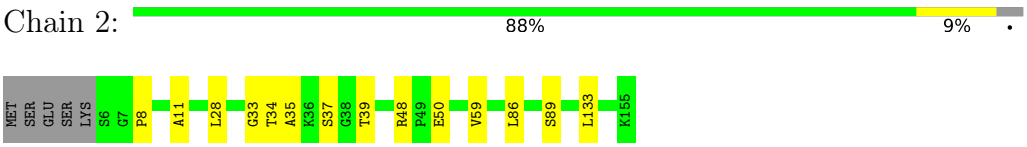
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 1:



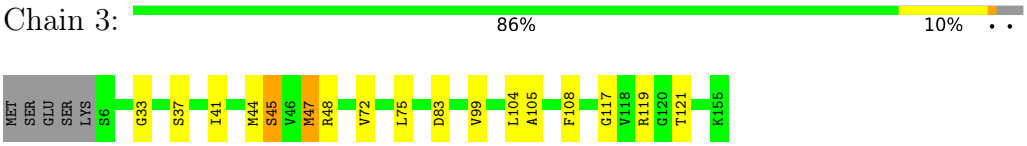
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 2:



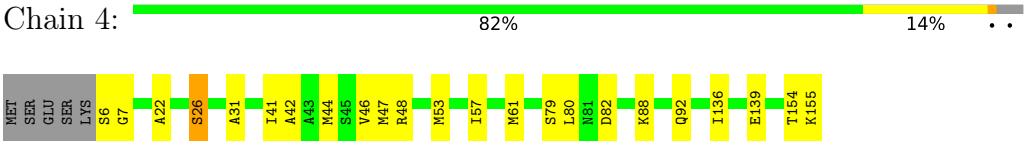
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 3:



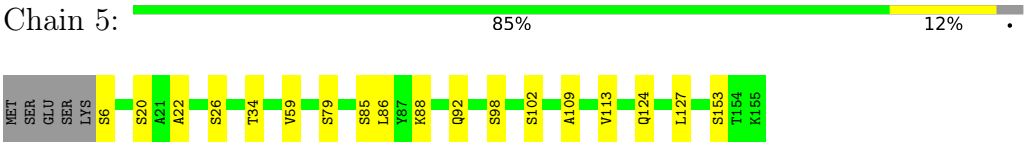
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 4:



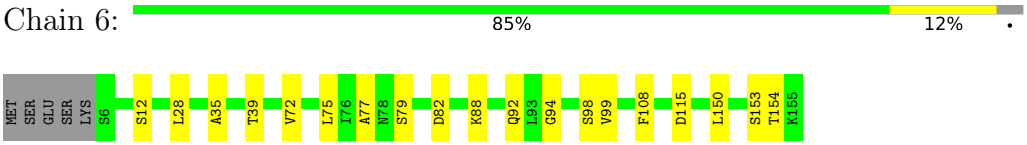
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 5:



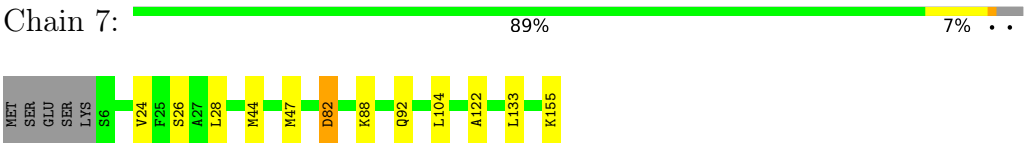
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 6:



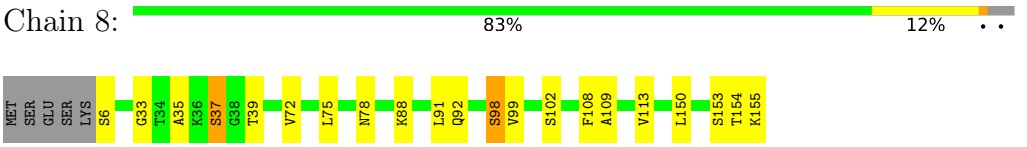
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 7:



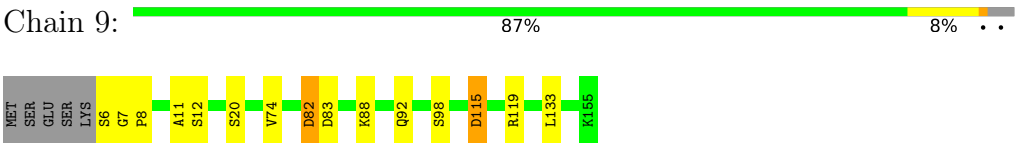
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 8:



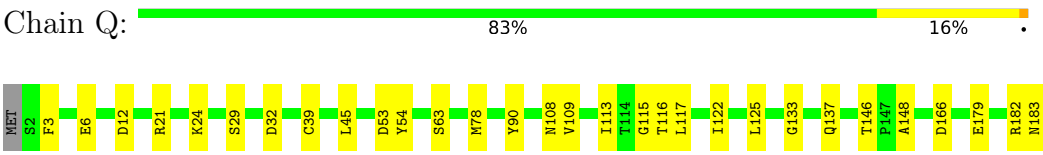
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

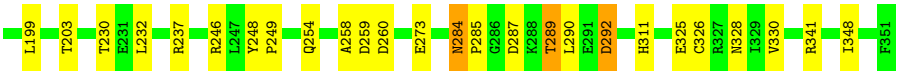
Chain 9:



• Molecule 13: V-type proton ATPase subunit d 1

Chain Q:





• Molecule 14: V-type proton ATPase subunit e 1

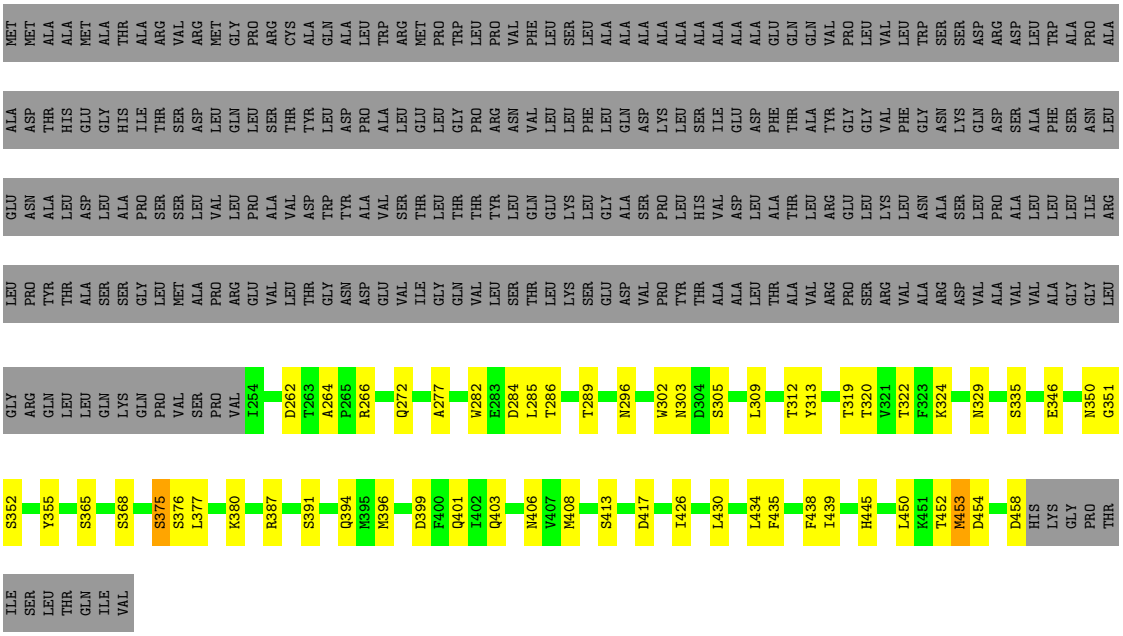
Chain S:

• Molecule 15: Ribonuclease kappa

Chain T:

• Molecule 16: V-type proton ATPase subunit S1

Chain U:

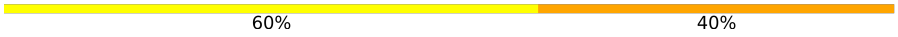


• Molecule 17: Renin receptor

Chain V:

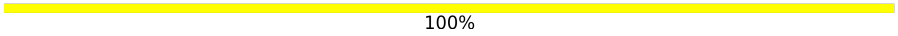
• Molecule 18: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain W:



• Molecule 19: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose

Chain a:



• Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:

• Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

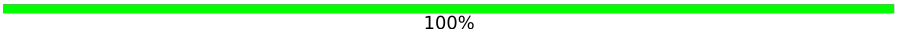
Chain b:

• Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

• Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

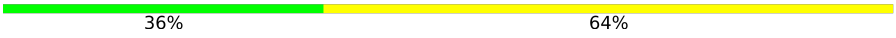


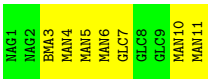
• Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

• Molecule 21: 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)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1000000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.1	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	30.271	Depositor
Minimum map value	-15.824	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.986	Depositor
Recommended contour level	2.8	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, PSF, NGA, BGC, MAN, NAG, SIA, WJP, WSS, GLC, WJS, PTY, CLR, BMA, ADP

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	H	0.32	0/1839	0.47	0/2462
1	I	0.33	0/1839	0.46	0/2462
1	J	0.32	0/1839	0.45	0/2462
2	K	0.31	0/945	0.49	0/1258
2	L	0.33	0/945	0.49	1/1258 (0.1%)
2	M	0.34	0/945	0.50	0/1258
3	O	0.29	0/2970	0.56	1/4013 (0.0%)
4	P	0.31	0/3576	0.51	0/4819
5	R	0.40	0/6299	0.48	0/8523
6	A	0.41	0/4748	0.46	0/6431
6	B	0.39	0/4752	0.47	0/6435
6	C	0.43	0/4752	0.47	0/6435
7	D	0.43	0/3671	0.47	0/4973
7	E	0.43	0/3660	0.47	0/4960
7	F	0.42	0/3667	0.47	0/4968
8	X	0.29	0/2145	0.47	0/2893
8	Y	0.28	0/2170	0.43	0/2926
8	Z	0.28	0/2138	0.46	0/2884
9	G	0.37	0/1731	0.50	0/2316
10	N	0.34	0/889	0.51	0/1200
11	0	0.47	0/1529	0.48	0/2079
12	1	0.47	0/1080	0.48	0/1461
12	2	0.46	0/1080	0.48	0/1461
12	3	0.46	0/1080	0.46	0/1461
12	4	0.48	0/1080	0.47	0/1461
12	5	0.46	0/1080	0.47	0/1461
12	6	0.43	0/1080	0.48	0/1461
12	7	0.43	0/1074	0.46	0/1454
12	8	0.45	0/1080	0.48	0/1461
12	9	0.47	0/1080	0.48	0/1461
13	Q	0.49	0/2895	0.46	0/3922
14	S	0.42	0/657	0.45	0/902

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
15	T	0.38	0/670	0.44	0/911
16	U	0.41	0/1718	0.48	0/2337
17	V	0.50	0/431	0.43	0/591
All	All	0.39	0/73134	0.48	2/98820 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	O	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	300	LEU	CA-CB-CG	5.27	127.41	115.30
2	L	12	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	O	312	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1822	0	1886	42	0
1	I	1822	0	1886	44	0
1	J	1822	0	1886	32	0
2	K	938	0	947	31	0
2	L	938	0	947	36	0
2	M	938	0	947	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	2916	0	2955	162	0
4	P	3508	0	3483	196	0
5	R	6141	0	6161	145	0
6	A	4652	0	4631	45	0
6	B	4656	0	4642	56	0
6	C	4656	0	4642	46	0
7	D	3600	0	3605	26	0
7	E	3589	0	3590	39	0
7	F	3596	0	3601	32	0
8	X	2111	0	2134	52	0
8	Y	2136	0	2158	40	0
8	Z	2105	0	2127	51	0
9	G	1713	0	1818	21	0
10	N	875	0	878	23	0
11	0	1495	0	1537	22	0
12	1	1065	0	1131	8	0
12	2	1065	0	1131	8	0
12	3	1065	0	1131	14	0
12	4	1065	0	1131	13	0
12	5	1065	0	1131	9	0
12	6	1065	0	1131	8	0
12	7	1059	0	1120	9	0
12	8	1065	0	1131	12	0
12	9	1065	0	1131	8	0
13	Q	2829	0	2757	30	0
14	S	631	0	646	10	0
15	T	654	0	641	4	0
16	U	1664	0	1584	45	0
17	V	417	0	405	4	0
18	W	68	0	58	3	0
19	a	56	0	47	0	0
20	b	28	0	25	0	0
20	c	28	0	25	0	0
20	d	28	0	25	0	0
20	s	28	0	25	0	0
20	u	28	0	25	0	0
21	r	127	0	106	0	0
22	0	28	0	46	1	0
22	5	28	0	46	16	0
22	R	28	0	46	1	0
22	V	28	0	46	11	0
23	R	30	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	0	65	0	85	4	0
24	2	29	0	40	1	0
24	5	35	0	46	6	0
24	6	21	0	19	7	0
24	7	42	0	60	7	0
24	8	83	0	129	10	0
24	Q	30	0	33	6	0
24	R	61	0	85	2	0
24	U	26	0	33	21	0
24	V	29	0	40	9	0
25	0	142	0	0	1	0
25	1	34	0	0	0	0
25	3	41	0	0	0	0
25	R	40	0	0	5	0
25	U	76	0	0	0	0
25	V	37	0	0	0	0
26	R	14	0	13	0	0
26	U	14	0	13	0	0
27	R	34	0	0	0	0
28	C	27	0	12	1	0
29	3	27	0	0	5	0
All	All	73243	0	73822	1307	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 9.

All (1307) 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)
5:R:473:ASN:ND2	25:R:905:WSS:C4	1.82	1.39
5:R:473:ASN:HD22	25:R:905:WSS:C4	1.38	1.33
16:U:438:PHE:CE2	24:U:503:PTY:H181	1.71	1.25
16:U:438:PHE:HE2	24:U:503:PTY:C18	1.56	1.17
24:6:201:PTY:O13	24:7:201:PTY:C2	1.95	1.14
22:5:201:CLR:C2	24:V:403:PTY:HC51	1.83	1.08
22:5:201:CLR:C1	24:V:403:PTY:HC51	1.83	1.08
24:6:201:PTY:O13	24:7:201:PTY:HC22	1.56	1.04
24:Q:401:PTY:H322	24:U:503:PTY:H321	1.37	1.02
4:P:37:LEU:HD11	4:P:48:GLU:HG2	1.43	1.00
22:5:201:CLR:H21	24:V:403:PTY:C5	1.90	1.00
24:6:201:PTY:O13	24:7:201:PTY:HC21	1.61	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5:202:PTY:O13	24:6:201:PTY:C3	2.11	0.98
16:U:438:PHE:CE2	24:U:503:PTY:C18	2.39	0.98
24:5:202:PTY:H121	22:V:402:CLR:H193	1.45	0.95
16:U:438:PHE:HE2	24:U:503:PTY:H181	1.13	0.95
24:Q:401:PTY:H112	24:U:503:PTY:O10	1.65	0.94
22:5:201:CLR:H21	24:V:403:PTY:HC51	1.41	0.94
12:8:108:PHE:HB3	24:8:201:PTY:O13	1.71	0.91
12:3:108:PHE:CE2	29:3:202:WJS:O27	2.23	0.90
24:Q:401:PTY:C32	24:U:503:PTY:H321	2.00	0.90
12:8:108:PHE:HZ	24:8:202:PTY:H341	1.38	0.88
5:R:97:LEU:O	5:R:100:ASN:HB3	1.73	0.88
22:5:201:CLR:H11	24:V:403:PTY:HC51	1.55	0.88
12:3:108:PHE:CD2	29:3:202:WJS:O27	2.26	0.88
5:R:618:PHE:O	18:W:5:SIA:O1A	1.91	0.87
2:K:50:GLN:HA	2:K:53:LYS:HE2	1.57	0.85
16:U:438:PHE:HE2	24:U:503:PTY:H182	1.39	0.85
4:P:37:LEU:HD12	4:P:44:ALA:HA	1.58	0.84
4:P:26:VAL:HG21	4:P:95:THR:HB	1.60	0.83
4:P:51:GLN:HA	4:P:54:GLU:HB2	1.59	0.83
5:R:473:ASN:HD21	25:R:905:WSS:C4	1.89	0.82
4:P:267:PRO:HG3	4:P:311:GLN:HB3	1.61	0.82
4:P:158:GLY:O	4:P:162:ASN:HB2	1.81	0.81
24:5:202:PTY:H121	22:V:402:CLR:C19	2.11	0.80
4:P:165:PHE:HB3	4:P:169:LYS:H	1.45	0.80
16:U:438:PHE:CD2	24:U:503:PTY:H181	2.17	0.79
2:M:4:GLN:NE2	3:O:210:PRO:O	2.16	0.79
4:P:307:LEU:O	4:P:311:GLN:N	2.17	0.78
4:P:86:LYS:O	4:P:90:VAL:N	2.15	0.78
12:6:108:PHE:HE2	24:6:201:PTY:HC6	1.47	0.78
5:R:24:CYS:HG	5:R:344:SER:HG	1.23	0.77
4:P:141:ALA:HA	4:P:144:ILE:HG22	1.66	0.77
11:0:13:VAL:HG11	24:0:306:PTY:H312	1.66	0.77
2:K:13:GLN:HA	2:K:16:LYS:HE2	1.66	0.76
1:H:61:GLU:OE1	2:K:58:LYS:NZ	2.16	0.76
8:Z:207:GLN:HE22	8:Z:212:PRO:HG3	1.51	0.76
1:H:19:ILE:HD12	5:R:316:GLN:HG2	1.68	0.76
4:P:31:VAL:HG21	4:P:33:TRP:CE2	2.21	0.75
5:R:473:ASN:ND2	25:R:905:WSS:C5	2.49	0.75
8:Y:264:ASP:HA	8:Y:267:VAL:HG12	1.66	0.75
3:O:183:VAL:HB	3:O:231:ARG:HE	1.51	0.75
2:L:27:LYS:HE3	2:L:31:ARG:HH22	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:208:ARG:NH2	7:E:467:PRO:O	2.19	0.75
4:P:140:MET:SD	4:P:141:ALA:N	2.60	0.74
6:B:410:VAL:HG11	6:B:425:THR:HG21	1.70	0.74
8:Z:37:ASP:HB3	8:Z:46:ARG:HH21	1.49	0.74
3:O:20:GLU:OE1	3:O:28:LYS:NZ	2.19	0.74
13:Q:230:THR:HG22	13:Q:232:LEU:H	1.53	0.74
1:H:49:GLN:HG3	2:K:44:ILE:HD13	1.70	0.74
4:P:395:THR:HA	4:P:398:LEU:HD12	1.69	0.74
12:8:108:PHE:CZ	24:8:202:PTY:H341	2.23	0.74
6:C:229:THR:HG22	6:C:263:LEU:HG	1.69	0.73
8:X:242:LEU:HD12	8:X:245:LYS:HE2	1.71	0.73
3:O:170:VAL:HA	3:O:216:LEU:HD11	1.70	0.73
1:I:34:ALA:HB2	2:L:29:LYS:HE2	1.69	0.73
5:R:294:PHE:HE2	5:R:298:ARG:HH11	1.33	0.73
5:R:66:ARG:HH12	5:R:294:PHE:HB2	1.54	0.72
4:P:451:ASN:OD1	4:P:451:ASN:N	2.20	0.72
3:O:161:LEU:HD13	3:O:219:ASP:HB3	1.71	0.71
22:5:201:CLR:C2	24:V:403:PTY:C5	2.57	0.71
5:R:125:LEU:HD23	5:R:265:ILE:HG13	1.72	0.71
8:X:48:ASP:OD2	8:X:116:LYS:NZ	2.22	0.71
10:N:37:LEU:HG	10:N:51:THR:HG21	1.73	0.71
8:Z:177:GLN:HE22	8:Z:180:LYS:HE3	1.55	0.71
4:P:166:ASN:OD1	4:P:166:ASN:N	2.24	0.71
5:R:316:GLN:OE1	5:R:317:LYS:N	2.23	0.71
3:O:163:THR:O	3:O:249:ARG:NH1	2.24	0.70
5:R:174:VAL:HA	5:R:219:VAL:HG21	1.72	0.70
4:P:446:GLN:NE2	4:P:447:GLN:OE1	2.24	0.70
4:P:74:ALA:HA	4:P:77:PHE:HD2	1.56	0.70
2:K:48:ARG:HE	2:K:49:LEU:HD22	1.56	0.70
4:P:74:ALA:HA	4:P:77:PHE:CD2	2.27	0.70
12:1:36:LYS:HG3	16:U:450:LEU:HD21	1.72	0.70
2:L:3:SER:O	2:L:6:GLN:NE2	2.25	0.70
6:A:138:CYS:HB2	6:A:141:LEU:HD12	1.72	0.69
12:3:108:PHE:HE2	29:3:202:WJS:O27	1.72	0.69
4:P:130:LEU:H	4:P:138:VAL:HB	1.58	0.69
8:Z:223:LYS:NZ	8:Z:253:ASP:OD2	2.22	0.69
5:R:249:GLU:H	5:R:254:ARG:HG2	1.56	0.68
5:R:100:ASN:O	5:R:103:LYS:HG3	1.94	0.68
3:O:33:ALA:HB1	3:O:321:LEU:HD11	1.75	0.68
10:N:35:ASN:N	10:N:35:ASN:OD1	2.27	0.68
6:A:565:ILE:HA	6:A:569:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:289:ARG:NH1	7:F:167:GLU:OE2	2.26	0.68
3:O:3:GLU:OE2	3:O:373:LYS:NZ	2.25	0.68
7:D:133:ASN:HB3	7:D:139:ILE:HD12	1.76	0.67
1:J:210:GLU:OE2	7:F:39:TYR:OH	2.12	0.67
4:P:202:ALA:O	4:P:206:GLN:NE2	2.28	0.67
5:R:473:ASN:HD22	25:R:905:WSS:C5	2.06	0.67
7:F:445:THR:HG22	7:F:446:SER:H	1.59	0.67
1:H:24:ASN:OD1	2:K:21:LYS:NZ	2.26	0.67
6:B:264:SER:O	6:B:308:ARG:NH2	2.28	0.67
2:M:51:ARG:NH2	2:M:54:GLU:OE1	2.22	0.67
4:P:353:ASP:N	4:P:353:ASP:OD1	2.27	0.67
1:H:180:GLY:HA3	1:H:195:THR:HA	1.76	0.67
3:O:335:LEU:HD22	3:O:369:TYR:CZ	2.30	0.67
6:A:419:ASP:HB3	6:A:422:THR:HG22	1.75	0.67
3:O:277:GLY:O	3:O:281:ARG:NH2	2.28	0.67
6:B:486:GLU:HG2	6:B:509:LEU:HD22	1.78	0.66
4:P:296:SER:HB2	4:P:302:ARG:HD3	1.75	0.66
1:J:180:GLY:HA3	1:J:195:THR:HA	1.77	0.66
3:O:45:VAL:HG23	3:O:51:LEU:HD11	1.78	0.66
4:P:102:GLN:HE21	4:P:140:MET:HA	1.61	0.66
6:A:264:SER:O	6:A:308:ARG:NH2	2.29	0.66
24:5:202:PTY:H312	24:5:202:PTY:H122	1.76	0.66
3:O:255:GLU:HG3	3:O:259:LYS:HD2	1.77	0.66
8:X:220:GLU:HA	8:X:223:LYS:HE3	1.78	0.66
4:P:350:SER:HA	4:P:369:VAL:HG12	1.77	0.66
6:B:17:THR:OG1	6:B:18:PHE:N	2.29	0.66
4:P:37:LEU:HD13	4:P:47:CYS:HB3	1.78	0.66
6:C:232:ARG:NH2	6:C:529:ASP:OD1	2.29	0.66
9:G:27:GLN:O	9:G:31:ASN:ND2	2.29	0.66
3:O:240:LYS:O	3:O:243:GLU:HB3	1.96	0.66
6:B:101:GLY:H	6:B:314:ASN:HD21	1.43	0.65
13:Q:39:CYS:O	13:Q:341:ARG:NH2	2.29	0.65
6:B:567:TRP:HA	6:B:570:ILE:HD12	1.78	0.65
3:O:160:SER:HB2	3:O:220:GLN:HE22	1.61	0.65
8:Y:111:GLN:NE2	8:Y:169:THR:OG1	2.28	0.65
16:U:435:PHE:HE1	24:U:503:PTY:C20	2.10	0.65
16:U:319:THR:HG22	16:U:320:THR:H	1.61	0.65
2:M:31:ARG:O	2:M:35:GLN:HG3	1.97	0.65
4:P:55:MET:HB2	4:P:61:GLU:HG3	1.78	0.65
5:R:123:LEU:HD22	5:R:206:LEU:HD13	1.78	0.65
13:Q:179:GLU:OE1	13:Q:182:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:193:ASN:O	3:O:196:ASP:HB3	1.97	0.65
3:O:145:ASN:O	3:O:149:ASN:ND2	2.30	0.64
12:3:108:PHE:HD2	29:3:202:WJS:O27	1.80	0.64
3:O:332:ARG:HA	3:O:335:LEU:HD12	1.79	0.64
6:B:140:ASN:ND2	8:Y:35:THR:OG1	2.30	0.64
8:X:93:ARG:NH2	8:X:131:ASN:OD1	2.25	0.64
6:B:56:ARG:HD3	7:F:54:ASN:HD22	1.63	0.64
12:2:33:GLY:O	12:2:37:SER:OG	2.16	0.64
6:A:151:ASP:OD2	6:A:397:ASN:ND2	2.30	0.64
24:2:201:PTY:O12	29:3:202:WJS:C29	2.45	0.64
12:7:82:ASP:OD1	12:7:82:ASP:N	2.30	0.64
3:O:23:HIS:N	3:O:27:SER:OG	2.30	0.64
8:X:171:ASP:OD1	8:X:171:ASP:N	2.29	0.64
13:Q:108:ASN:ND2	13:Q:133:GLY:O	2.30	0.64
4:P:102:GLN:O	4:P:143:ARG:NH1	2.31	0.64
5:R:176:ASN:HD21	5:R:215:VAL:HG23	1.62	0.64
3:O:29:ASN:HB3	3:O:32:LEU:HB2	1.78	0.63
1:H:6:ALA:O	1:H:9:GLN:NE2	2.31	0.63
4:P:116:ARG:HH12	4:P:119:LYS:HD3	1.62	0.63
1:I:53:ILE:HD11	2:L:47:TYR:HD1	1.64	0.63
5:R:126:THR:O	5:R:129:LYS:HB2	1.98	0.63
3:O:185:LEU:HD11	3:O:248:VAL:HB	1.80	0.63
8:Z:111:GLN:HA	8:Z:114:LYS:HZ1	1.63	0.63
4:P:271:ASP:O	4:P:275:GLU:HB2	1.98	0.63
3:O:209:VAL:HG23	3:O:229:LEU:HA	1.79	0.63
4:P:328:ASP:HB3	4:P:331:ILE:HB	1.80	0.63
8:X:226:VAL:HG12	8:X:255:LEU:HD23	1.80	0.63
8:X:240:LYS:HG3	8:X:243:GLN:HG3	1.81	0.63
3:O:35:THR:HB	3:O:321:LEU:HD13	1.80	0.63
3:O:157:ASN:ND2	3:O:168:GLU:OE2	2.31	0.63
4:P:389:GLU:HA	4:P:392:LYS:HB3	1.81	0.63
1:H:41:GLU:HG2	1:H:44:ARG:HH11	1.63	0.62
4:P:224:VAL:HG21	4:P:260:LEU:HD21	1.81	0.62
22:5:201:CLR:H193	22:V:402:CLR:C19	2.29	0.62
2:L:55:PHE:HA	2:L:58:LYS:HZ1	1.63	0.62
1:H:123:GLY:HA3	1:H:183:ILE:HD13	1.80	0.62
12:7:47:MET:SD	13:Q:254:GLN:NE2	2.72	0.62
5:R:95:ILE:HA	5:R:98:GLU:HG2	1.80	0.62
8:X:236:LYS:NZ	8:X:236:LYS:HA	2.14	0.62
8:Y:93:ARG:NH2	8:Y:131:ASN:OD1	2.32	0.62
8:Y:213:PHE:O	8:Y:222:GLN:NE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:1:BGC:O4	18:W:1:BGC:O2	2.10	0.62
13:Q:29:SER:OG	13:Q:32:ASP:OD1	2.16	0.62
10:N:67:ASN:ND2	10:N:93:SER:OG	2.33	0.62
5:R:81:ASP:HA	5:R:291:ARG:HB3	1.82	0.62
5:R:93:ASP:OD1	5:R:94:MET:N	2.32	0.62
8:Y:144:ALA:O	8:Y:149:ASN:ND2	2.31	0.62
8:Y:209:GLU:OE2	8:Y:210:GLU:N	2.33	0.62
13:Q:246:ARG:NH2	13:Q:273:GLU:OE2	2.32	0.62
5:R:108:LEU:HD21	5:R:283:LEU:HD13	1.81	0.62
1:H:2:ALA:HB2	5:R:337:LEU:HB3	1.82	0.62
3:O:150:LEU:HB2	3:O:268:LEU:HD13	1.81	0.62
3:O:125:ILE:HD11	3:O:293:ALA:HB1	1.81	0.61
5:R:96:ASP:OD2	5:R:97:LEU:N	2.33	0.61
5:R:134:LYS:HE3	5:R:200:ALA:HA	1.81	0.61
16:U:355:TYR:HB2	16:U:387:ARG:HG3	1.81	0.61
13:Q:146:THR:HG22	13:Q:148:ALA:H	1.64	0.61
5:R:413:GLY:O	5:R:417:THR:HG23	2.00	0.61
1:I:53:ILE:HD11	2:L:47:TYR:CD1	2.36	0.61
4:P:72:GLN:HA	4:P:76:THR:HG23	1.82	0.61
4:P:101:LEU:O	4:P:104:ASN:ND2	2.33	0.61
16:U:272:GLN:NE2	16:U:399:ASP:OD2	2.33	0.61
5:R:585:TYR:OH	5:R:629:TYR:OH	2.13	0.61
5:R:720:GLN:O	5:R:724:THR:HG23	2.00	0.61
22:5:201:CLR:H193	22:V:402:CLR:H191	1.83	0.61
4:P:307:LEU:HD13	4:P:311:GLN:HE21	1.66	0.61
5:R:94:MET:O	5:R:98:GLU:N	2.34	0.61
2:M:30:ASN:O	2:M:34:LYS:HD2	2.00	0.61
1:J:8:VAL:HB	3:O:210:PRO:HG2	1.82	0.61
8:X:25:LYS:HE3	8:X:82:SER:HB2	1.82	0.61
4:P:215:ARG:O	4:P:219:VAL:HG23	2.01	0.61
6:A:504:THR:O	6:A:508:THR:HG23	2.00	0.61
7:F:82:ARG:NH1	7:F:101:GLY:O	2.34	0.61
8:Z:201:LYS:HB3	8:Z:205:LYS:HE3	1.83	0.61
5:R:49:ARG:NH2	5:R:310:CYS:O	2.34	0.60
24:5:202:PTY:H111	22:V:402:CLR:H22	1.82	0.60
4:P:279:GLU:OE2	4:P:326:TYR:OH	2.18	0.60
5:R:349:PRO:HB2	5:R:351:ILE:HG23	1.82	0.60
6:C:324:GLU:HG3	6:C:354:TRP:HE1	1.65	0.60
7:D:195:ALA:O	7:D:381:ARG:NH2	2.31	0.60
7:D:173:GLY:O	7:D:465:GLN:NE2	2.28	0.60
12:8:88:LYS:O	12:8:92:GLN:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:65:LEU:HG	5:R:290:ILE:HD11	1.84	0.60
6:B:161:LEU:HD11	6:B:296:MET:HE1	1.83	0.60
2:M:26:ARG:HH11	2:M:29:LYS:HD3	1.67	0.60
4:P:395:THR:HG21	4:P:431:LEU:HD22	1.84	0.60
16:U:458:ASP:N	16:U:458:ASP:OD1	2.35	0.60
3:O:62:ASP:OD2	3:O:63:ALA:N	2.33	0.60
3:O:321:LEU:HD21	3:O:331:LEU:HD11	1.82	0.60
5:R:177:ARG:HD2	5:R:218:SER:HB2	1.84	0.60
12:6:108:PHE:CE2	24:6:201:PTY:HC6	2.34	0.60
5:R:64:LYS:HE2	5:R:102:GLU:HG2	1.82	0.59
8:X:209:GLU:OE2	8:X:211:SER:N	2.35	0.59
12:2:8:PRO:HD2	12:2:11:ALA:HB2	1.84	0.59
3:O:194:HIS:O	3:O:198:ILE:HG13	2.02	0.59
7:D:318:PRO:HG3	9:G:201:ARG:HD2	1.85	0.59
12:4:22:ALA:O	12:4:26:SER:OG	2.18	0.59
4:P:104:ASN:O	4:P:109:SER:OG	2.21	0.59
4:P:283:ARG:HA	4:P:331:ILE:HD11	1.84	0.59
6:B:296:MET:HG3	6:B:305:ILE:HG22	1.85	0.59
8:X:213:PHE:HB3	8:X:217:LEU:HD11	1.83	0.59
1:J:7:ASP:HA	1:J:10:LYS:HE3	1.84	0.59
3:O:328:LEU:HD23	3:O:328:LEU:H	1.68	0.59
4:P:423:ARG:HG2	4:P:426:ARG:HG2	1.85	0.59
8:Z:205:LYS:HE2	8:Z:260:LEU:HB3	1.84	0.59
4:P:108:VAL:O	4:P:110:ILE:HG12	2.03	0.59
4:P:224:VAL:HG11	4:P:260:LEU:HD11	1.84	0.59
5:R:362:PRO:HB2	5:R:822:PHE:HB2	1.84	0.59
8:X:14:THR:HG22	8:X:15:SER:H	1.68	0.59
8:Y:256:THR:HG22	8:Y:258:THR:H	1.67	0.59
1:H:8:VAL:O	1:H:12:ILE:HG13	2.03	0.59
7:D:106:ASP:OD2	7:D:109:LYS:NZ	2.33	0.59
9:G:95:ARG:NH1	9:G:110:GLU:OE2	2.36	0.59
14:S:79:HIS:NE2	15:T:75:HIS:O	2.35	0.59
16:U:445:HIS:CE1	24:U:503:PTY:H311	2.38	0.59
3:O:20:GLU:HA	3:O:27:SER:HA	1.84	0.59
3:O:150:LEU:HD12	3:O:268:LEU:HD13	1.85	0.59
6:A:473:VAL:O	6:A:477:THR:HG23	2.03	0.59
1:J:71:GLN:HE22	2:M:66:ARG:HD2	1.68	0.59
4:P:77:PHE:HD1	4:P:80:LEU:HD13	1.67	0.59
8:Y:238:SER:O	8:Y:238:SER:OG	2.21	0.59
1:I:180:GLY:HA3	1:I:195:THR:HA	1.84	0.58
5:R:120:ARG:HG2	5:R:124:GLU:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:8:ILE:O	2:K:12:LEU:HD12	2.03	0.58
6:B:274:TYR:HB3	6:B:311:LEU:HD23	1.84	0.58
4:P:424:GLY:HA2	4:P:427:VAL:HG12	1.85	0.58
8:Z:51:ASP:OD2	8:Z:84:ARG:NH1	2.30	0.58
1:I:108:ASP:OD2	1:I:111:ARG:NH2	2.36	0.58
2:M:40:ALA:O	2:M:44:ILE:HG13	2.02	0.58
3:O:118:LEU:HD21	3:O:303:PHE:HE1	1.68	0.58
7:E:403:LYS:H	7:E:403:LYS:HD2	1.69	0.58
9:G:149:ALA:HB2	10:N:89:LEU:HD11	1.84	0.58
16:U:303:ASN:HB3	16:U:305:SER:H	1.68	0.58
2:K:28:ARG:HA	2:K:31:ARG:HG2	1.85	0.58
1:I:5:ASP:HA	1:I:8:VAL:HG22	1.86	0.58
1:J:61:GLU:O	1:J:65:GLU:HG2	2.03	0.58
8:X:51:ASP:OD1	8:X:51:ASP:N	2.37	0.58
9:G:83:VAL:HG21	10:N:18:THR:HG23	1.86	0.58
9:G:119:TYR:O	9:G:135:LYS:NZ	2.37	0.58
1:I:16:MET:HG2	2:L:10:GLN:HG3	1.84	0.58
3:O:29:ASN:HD22	3:O:33:ALA:HB2	1.69	0.58
4:P:263:TYR:HB2	4:P:265:ILE:HD11	1.86	0.58
5:R:64:LYS:HE2	5:R:102:GLU:HA	1.85	0.58
8:Z:195:GLU:O	8:Z:199:LEU:HD23	2.04	0.58
8:Z:227:LYS:NZ	8:Z:231:ASP:OD1	2.35	0.58
5:R:632:GLN:HE21	5:R:636:GLN:NE2	2.02	0.58
6:A:169:PRO:HB2	6:A:172:ASN:HD22	1.69	0.58
6:B:233:VAL:HG13	6:B:234:LEU:HG	1.86	0.58
16:U:435:PHE:CE1	24:U:503:PTY:C20	2.87	0.57
2:K:28:ARG:HA	2:K:31:ARG:HE	1.69	0.57
4:P:22:LYS:O	4:P:26:VAL:HG22	2.04	0.57
5:R:125:LEU:O	5:R:128:LEU:HB2	2.04	0.57
8:X:230:ILE:HG21	8:X:250:SER:HB3	1.85	0.57
10:N:98:TYR:OH	10:N:103:ASP:OD2	2.22	0.57
13:Q:203:THR:HB	13:Q:311:HIS:HB3	1.86	0.57
8:Z:42:LEU:HD23	8:Z:45:ILE:HD12	1.85	0.57
24:Q:401:PTY:C32	24:U:503:PTY:C32	2.79	0.57
1:H:16:MET:HA	1:H:19:ILE:HG22	1.86	0.57
6:A:89:GLU:OE1	6:A:129:ARG:NH2	2.37	0.57
5:R:20:GLU:OE2	5:R:20:GLU:N	2.37	0.57
8:Y:181:LEU:HD23	8:Y:203:TYR:HB2	1.86	0.57
3:O:98:LEU:H	3:O:98:LEU:HD12	1.70	0.57
3:O:367:TYR:HB3	3:O:369:TYR:CZ	2.40	0.57
5:R:11:THR:HG23	5:R:327:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:598:ASP:HA	14:S:61:ASN:HB3	1.87	0.57
8:Y:242:LEU:HA	8:Y:245:LYS:HB2	1.86	0.57
12:5:98:SER:O	12:5:102:SER:OG	2.21	0.57
16:U:329:ASN:ND2	16:U:365:SER:OG	2.37	0.57
6:C:421:VAL:O	6:C:425:THR:HG23	2.04	0.57
7:F:55:GLY:O	7:F:102:THR:OG1	2.22	0.56
12:7:104:LEU:HD21	24:7:201:PTY:H322	1.86	0.56
12:9:12:SER:O	12:9:12:SER:OG	2.23	0.56
7:D:380:ASP:HB2	7:D:393:ASN:HB2	1.87	0.56
4:P:56:LYS:HZ2	4:P:57:ARG:HH21	1.52	0.56
5:R:28:GLU:O	5:R:31:GLU:HG3	2.06	0.56
6:C:100:ASP:OD1	6:C:100:ASP:N	2.36	0.56
16:U:368:SER:HB3	16:U:403:GLN:HB2	1.85	0.56
4:P:391:LEU:O	4:P:394:LEU:CB	2.54	0.56
5:R:87:GLU:HG3	5:R:89:PRO:HD3	1.86	0.56
5:R:99:ALA:O	5:R:102:GLU:HB2	2.06	0.56
4:P:387:ASN:HB3	4:P:389:GLU:HB2	1.87	0.56
5:R:18:GLN:NE2	5:R:20:GLU:OE2	2.34	0.56
5:R:100:ASN:HD22	5:R:101:PHE:HD1	1.54	0.56
2:K:78:GLN:O	2:K:82:THR:HG23	2.05	0.56
4:P:145:ILE:HD11	4:P:204:CYS:HB2	1.88	0.56
4:P:168:ILE:HA	4:P:171:GLN:OE1	2.06	0.56
8:Y:124:SER:OG	8:Y:125:ASP:N	2.39	0.56
4:P:17:ASN:O	4:P:21:ALA:N	2.37	0.56
12:1:88:LYS:O	12:1:92:GLN:HG2	2.06	0.56
6:B:360:GLU:OE2	7:E:329:THR:OG1	2.15	0.56
9:G:131:LEU:O	9:G:135:LYS:HG2	2.06	0.56
24:Q:401:PTY:H321	24:U:503:PTY:H312	1.88	0.56
3:O:54:LEU:O	3:O:58:LEU:HB2	2.06	0.55
5:R:101:PHE:O	5:R:104:ILE:HB	2.06	0.55
6:C:463:GLU:N	6:C:463:GLU:OE1	2.39	0.55
13:Q:12:ASP:OD1	13:Q:12:ASP:N	2.38	0.55
6:A:50:LEU:HB3	6:A:68:GLU:HG3	1.88	0.55
7:F:82:ARG:HD3	7:F:100:GLU:HB2	1.89	0.55
11:0:56:LEU:HD21	16:U:435:PHE:CZ	2.41	0.55
12:1:22:ALA:O	12:1:26:SER:OG	2.23	0.55
3:O:126:ALA:O	3:O:130:THR:HG23	2.05	0.55
4:P:316:LYS:HE2	4:P:316:LYS:H	1.71	0.55
4:P:359:LEU:HA	4:P:364:LEU:HD11	1.88	0.55
5:R:44:VAL:HG13	5:R:48:GLN:HB2	1.89	0.55
8:X:105:LEU:HD22	8:X:105:LEU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:GLN:N	1:H:49:GLN:OE1	2.39	0.55
16:U:296:ASN:O	16:U:312:THR:OG1	2.24	0.55
3:O:29:ASN:O	3:O:32:LEU:HB2	2.07	0.55
3:O:306:SER:HB2	3:O:370:VAL:HG21	1.89	0.55
4:P:56:LYS:HZ3	4:P:57:ARG:HE	1.54	0.55
6:A:507:ILE:HD11	6:A:555:VAL:HG21	1.88	0.55
6:B:231:GLN:O	6:B:235:ASP:HB2	2.06	0.55
8:X:201:LYS:HA	8:X:204:VAL:HG12	1.87	0.55
13:Q:179:GLU:O	13:Q:183:ASN:ND2	2.40	0.55
4:P:408:ALA:HB2	4:P:448:VAL:HG12	1.89	0.55
6:A:561:SER:OG	6:A:562:ASP:N	2.39	0.55
8:Z:151:PHE:O	8:Z:155:MET:HG2	2.06	0.55
22:5:201:CLR:H121	22:V:402:CLR:H181	1.89	0.55
8:Z:237:LEU:HD13	8:Z:243:GLN:HA	1.89	0.55
24:8:201:PTY:H122	24:8:201:PTY:HC12	1.88	0.55
16:U:401:GLN:HE22	17:V:296:ALA:H	1.53	0.55
7:F:124:SER:OG	7:F:125:GLU:N	2.39	0.55
12:4:42:ALA:HA	12:5:127:LEU:HD21	1.89	0.55
3:O:49:ASP:OD2	5:R:228:GLN:HB2	2.06	0.55
6:B:511:VAL:HG11	6:B:548:TYR:CD1	2.42	0.55
9:G:4:LYS:HG2	9:G:5:ASP:H	1.71	0.55
1:I:8:VAL:HB	5:R:196:PHE:CE1	2.41	0.54
2:K:7:GLY:O	2:K:11:LEU:HG	2.07	0.54
3:O:4:PHE:HZ	3:O:99:VAL:HG12	1.72	0.54
4:P:405:GLN:O	4:P:409:VAL:HG23	2.08	0.54
8:Z:114:LYS:NZ	8:Z:114:LYS:HB3	2.22	0.54
1:H:55:GLU:O	1:H:59:LYS:HG2	2.08	0.54
2:M:11:LEU:HD22	3:O:182:LEU:HD11	1.89	0.54
8:X:207:GLN:NE2	8:X:209:GLU:O	2.40	0.54
2:K:41:GLN:HA	2:K:44:ILE:HG12	1.89	0.54
5:R:87:GLU:OE2	5:R:296:LYS:HE3	2.08	0.54
7:D:416:ALA:O	7:D:420:ASN:ND2	2.38	0.54
10:N:74:VAL:HG12	10:N:77:ALA:HB3	1.90	0.54
12:5:88:LYS:O	12:5:92:GLN:HG2	2.07	0.54
12:8:109:ALA:O	12:8:113:VAL:HG12	2.08	0.54
1:I:187:ASP:OD1	1:I:187:ASP:N	2.35	0.54
1:J:16:MET:HG3	2:M:14:ALA:HB2	1.89	0.54
4:P:145:ILE:HD13	4:P:208:MET:HG3	1.90	0.54
5:R:330:LEU:O	5:R:334:GLN:HG3	2.08	0.54
8:Z:237:LEU:HD13	8:Z:243:GLN:HG3	1.90	0.54
22:5:201:CLR:H212	22:V:402:CLR:H181	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:553:ARG:O	6:A:557:THR:HG23	2.06	0.54
8:X:152:LEU:O	8:X:156:THR:HG23	2.07	0.54
3:O:28:LYS:HE3	3:O:335:LEU:HD23	1.88	0.54
6:A:296:MET:HG2	6:A:305:ILE:HG22	1.90	0.54
6:C:484:GLN:O	6:C:484:GLN:NE2	2.41	0.54
8:X:148:LYS:NZ	8:X:188:MET:O	2.41	0.54
8:Z:227:LYS:HZ1	8:Z:228:THR:HA	1.72	0.54
6:A:350:SER:HB3	6:A:353:ARG:HG3	1.89	0.54
6:C:178:TYR:HB3	6:C:193:GLU:HB3	1.90	0.54
8:Y:207:GLN:NE2	8:Y:212:PRO:HB3	2.23	0.54
12:8:72:VAL:HG11	12:8:99:VAL:HG11	1.89	0.54
4:P:127:LEU:HG	4:P:128:PRO:HD3	1.90	0.54
6:B:25:SER:O	6:B:25:SER:OG	2.26	0.54
6:B:397:ASN:O	6:B:399:GLU:N	2.41	0.54
4:P:99:ASP:HA	4:P:102:GLN:HB2	1.89	0.53
3:O:24:ALA:HA	3:O:31:ASN:HB2	1.89	0.53
4:P:108:VAL:O	4:P:110:ILE:N	2.42	0.53
4:P:244:ILE:HG22	4:P:284:ILE:HG22	1.89	0.53
4:P:299:ARG:O	4:P:299:ARG:NH1	2.42	0.53
6:A:372:SER:O	6:A:372:SER:OG	2.25	0.53
16:U:377:LEU:HB2	16:U:380:LYS:HB2	1.91	0.53
3:O:300:LEU:HA	3:O:303:PHE:HB3	1.90	0.53
6:C:372:SER:O	6:C:372:SER:OG	2.25	0.53
2:M:23:SER:O	2:M:27:LYS:HE2	2.09	0.53
5:R:288:LYS:HG3	5:R:289:ASN:HD22	1.73	0.53
6:C:387:GLU:HG3	7:D:264:ALA:HB3	1.90	0.53
7:F:262:ASN:ND2	7:F:270:GLU:OE1	2.41	0.53
8:X:216:ILE:HB	8:X:217:LEU:HD23	1.91	0.53
3:O:216:LEU:HD23	3:O:217:SER:HB3	1.90	0.53
4:P:155:LEU:HD11	4:P:158:GLY:HA2	1.91	0.53
8:Y:63:GLU:OE2	8:Y:63:GLU:N	2.38	0.53
8:Z:143:ALA:HB1	8:Z:149:ASN:ND2	2.23	0.53
11:0:36:ASP:HB3	11:0:39:TRP:HB3	1.91	0.53
12:5:34:THR:HG23	12:5:59:VAL:HG13	1.90	0.53
2:L:41:GLN:HA	2:L:44:ILE:HD12	1.90	0.53
4:P:278:LYS:HA	5:R:20:GLU:OE1	2.09	0.53
9:G:70:ALA:O	9:G:74:PHE:HD2	1.92	0.53
4:P:71:SER:O	4:P:75:LYS:HE3	2.08	0.53
4:P:257:CYS:O	4:P:261:ARG:NH1	2.41	0.53
5:R:273:ASN:OD1	5:R:274:GLN:N	2.42	0.53
6:A:232:ARG:NH1	6:A:519:PHE:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:13:GLN:HA	2:M:16:LYS:HE3	1.91	0.53
2:M:60:ALA:HA	2:M:63:LEU:HD12	1.90	0.53
4:P:206:GLN:HG2	4:P:245:PHE:HD2	1.73	0.53
5:R:18:GLN:O	5:R:22:ALA:N	2.41	0.53
7:F:365:ILE:HB	7:F:366:PRO:HD3	1.91	0.53
3:O:147:LYS:HA	3:O:150:LEU:HD22	1.91	0.52
4:P:261:ARG:NH2	4:P:301:THR:O	2.40	0.52
5:R:54:GLU:HG2	5:R:304:TYR:CZ	2.44	0.52
7:D:438:VAL:HG22	7:D:439:VAL:HG23	1.91	0.52
3:O:96:VAL:HG23	3:O:101:TYR:HB2	1.91	0.52
3:O:188:VAL:HG22	3:O:222:SER:OG	2.08	0.52
4:P:75:LYS:HA	4:P:78:ILE:HG13	1.90	0.52
7:F:193:SER:OG	7:F:194:ALA:N	2.43	0.52
9:G:94:ILE:HD13	10:N:63:ILE:HD12	1.92	0.52
9:G:179:ARG:O	9:G:183:THR:HG22	2.09	0.52
2:L:18:ALA:O	2:L:22:VAL:HG23	2.09	0.52
4:P:64:GLU:O	4:P:68:THR:HG23	2.09	0.52
4:P:108:VAL:HG13	4:P:113:ASP:H	1.74	0.52
4:P:145:ILE:O	4:P:148:LEU:HB2	2.09	0.52
5:R:808:VAL:HG21	12:4:136:ILE:HD11	1.91	0.52
8:Y:61:ARG:NH1	8:Y:64:GLU:OE2	2.42	0.52
12:5:109:ALA:O	12:5:113:VAL:HG12	2.08	0.52
3:O:66:GLU:HA	3:O:69:VAL:HG12	1.91	0.52
5:R:43:ASP:N	5:R:43:ASP:OD2	2.43	0.52
5:R:481:VAL:HG11	14:S:73:ILE:HG23	1.91	0.52
16:U:375:SER:HB2	16:U:396:MET:HA	1.90	0.52
3:O:234:VAL:O	3:O:238:ARG:N	2.34	0.52
6:A:324:GLU:HA	6:A:354:TRP:CD1	2.44	0.52
6:C:53:GLU:OE2	6:C:212:ARG:NH2	2.42	0.52
1:J:16:MET:O	1:J:20:GLU:HG2	2.09	0.52
6:B:350:SER:H	6:B:409:ALA:HB3	1.74	0.52
8:Y:238:SER:N	8:Y:270:ASN:HD21	2.08	0.52
8:Z:159:LEU:HB2	8:Z:178:LEU:HD22	1.91	0.52
16:U:438:PHE:CE2	24:U:503:PTY:H182	2.31	0.52
1:I:16:MET:CG	2:L:10:GLN:HG3	2.40	0.52
4:P:351:SER:OG	4:P:354:GLU:OE2	2.28	0.52
7:D:365:ILE:HB	7:D:366:PRO:HD3	1.92	0.52
8:X:259:LEU:O	8:X:263:ILE:HD12	2.10	0.52
1:I:9:GLN:O	1:I:13:LYS:HD3	2.09	0.52
1:J:57:TYR:O	1:J:61:GLU:HG2	2.09	0.52
4:P:148:LEU:HD11	4:P:155:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:553:ARG:O	6:B:557:THR:HG23	2.10	0.52
7:F:465:GLN:NE2	7:F:469:GLU:O	2.43	0.52
10:N:50:ASP:OD2	10:N:51:THR:N	2.43	0.52
11:0:18:CYS:SG	22:0:304:CLR:H273	2.50	0.52
12:4:6:SER:OG	12:4:7:GLY:N	2.41	0.52
4:P:108:VAL:C	4:P:110:ILE:H	2.13	0.51
4:P:111:PHE:CG	4:P:152:GLY:HA3	2.45	0.51
5:R:399:PHE:HB3	5:R:400:PRO:HD3	1.90	0.51
6:B:500:SER:O	6:B:500:SER:OG	2.28	0.51
7:F:253:SER:OG	7:F:255:ASP:OD1	2.22	0.51
17:V:329:TRP:CE3	24:V:403:PTY:O30	2.62	0.51
2:K:27:LYS:HD2	2:K:27:LYS:N	2.26	0.51
3:O:83:SER:HA	3:O:88:GLN:O	2.10	0.51
4:P:376:TRP:HA	4:P:376:TRP:CE3	2.44	0.51
12:3:72:VAL:HG11	12:3:99:VAL:HG11	1.91	0.51
4:P:162:ASN:HA	4:P:167:TRP:CH2	2.46	0.51
16:U:445:HIS:CE1	24:U:503:PTY:C30	2.94	0.51
4:P:210:ARG:O	4:P:215:ARG:NH2	2.43	0.51
5:R:228:GLN:HB3	5:R:232:ARG:NH2	2.26	0.51
1:I:215:LEU:HD23	2:L:91:ASN:HB2	1.92	0.51
3:O:76:MET:HG2	3:O:91:LEU:HD11	1.93	0.51
4:P:257:CYS:O	4:P:261:ARG:HG2	2.10	0.51
4:P:307:LEU:O	4:P:310:ILE:N	2.44	0.51
4:P:450:TYR:OH	5:R:107:GLU:OE2	2.28	0.51
12:7:88:LYS:O	12:7:92:GLN:HG2	2.11	0.51
16:U:445:HIS:ND1	24:U:503:PTY:C30	2.74	0.51
3:O:187:VAL:HG11	3:O:197:TRP:CZ2	2.46	0.51
8:Y:54:ILE:HA	8:Y:57:GLU:HG2	1.92	0.51
8:Z:200:PHE:O	8:Z:204:VAL:HG12	2.11	0.51
2:M:22:VAL:O	2:M:26:ARG:HG2	2.11	0.51
3:O:102:ILE:HD12	3:O:103:THR:N	2.26	0.51
4:P:247:ILE:HA	4:P:250:LEU:HD12	1.92	0.51
8:X:83:ARG:NH1	8:X:119:VAL:O	2.33	0.51
2:K:6:GLN:O	2:K:10:GLN:HG2	2.11	0.51
4:P:47:CYS:HA	4:P:50:ILE:HD12	1.93	0.51
28:C:701:ADP:O1B	7:F:400:ARG:NH2	2.42	0.51
7:E:376:GLN:HG3	7:E:378:TYR:CE2	2.45	0.51
11:0:2:THR:HG22	11:0:3:GLY:H	1.75	0.51
13:Q:284:ASN:HD22	13:Q:285:PRO:HD2	1.76	0.51
1:I:20:GLU:O	1:I:24:ASN:ND2	2.43	0.51
1:J:2:ALA:HB2	3:O:203:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:176:VAL:H	3:O:184:THR:HG1	1.59	0.51
6:A:75:VAL:HB	7:D:66:PRO:HD2	1.93	0.51
9:G:144:LEU:O	9:G:147:GLU:HG3	2.11	0.51
12:8:33:GLY:O	12:8:37:SER:OG	2.29	0.51
2:L:18:ALA:O	2:L:21:LYS:HG2	2.11	0.50
3:O:29:ASN:ND2	3:O:33:ALA:HB2	2.26	0.50
3:O:42:ASP:N	3:O:42:ASP:OD1	2.44	0.50
3:O:220:GLN:HE21	3:O:221:ASP:CG	2.13	0.50
4:P:337:PHE:CZ	4:P:341:LYS:HD2	2.47	0.50
6:B:173:ARG:HD3	8:Y:20:SER:OG	2.11	0.50
6:C:398:PRO:O	6:C:400:ARG:HD3	2.11	0.50
1:I:149:GLN:O	1:I:153:PRO:HD2	2.12	0.50
4:P:162:ASN:HA	4:P:167:TRP:HH2	1.76	0.50
3:O:149:ASN:HA	3:O:152:ASN:OD1	2.12	0.50
4:P:329:GLU:H	4:P:329:GLU:CD	2.15	0.50
6:B:511:VAL:HG11	6:B:548:TYR:HD1	1.74	0.50
6:B:566:THR:H	6:B:569:ILE:HD12	1.75	0.50
1:I:38:PHE:CD2	2:L:36:ALA:HB2	2.47	0.50
1:J:38:PHE:CD1	2:M:36:ALA:HB2	2.47	0.50
2:K:25:ALA:HA	2:K:28:ARG:NE	2.27	0.50
3:O:86:LYS:HE2	3:O:87:VAL:HG22	1.93	0.50
4:P:56:LYS:HB2	4:P:107:ARG:NH2	2.25	0.50
7:D:226:ASN:N	7:D:226:ASN:OD1	2.44	0.50
22:5:201:CLR:H261	22:V:402:CLR:H261	1.92	0.50
24:8:202:PTY:H332	24:8:202:PTY:C17	2.41	0.50
16:U:289:THR:HG1	16:U:313:TYR:HH	1.40	0.50
1:J:212:ARG:NH1	7:F:126:ASP:OD2	2.44	0.50
2:K:67:GLY:O	2:K:71:THR:HG23	2.12	0.50
9:G:145:LEU:HD23	10:N:65:LEU:HD23	1.93	0.50
6:C:511:VAL:HG11	6:C:548:TYR:CD1	2.46	0.50
3:O:231:ARG:O	3:O:234:VAL:HG22	2.11	0.50
3:O:238:ARG:HG2	3:O:248:VAL:HG21	1.93	0.50
3:O:329:LYS:HG3	3:O:330:LYS:H	1.77	0.50
4:P:145:ILE:O	4:P:148:LEU:N	2.45	0.50
4:P:388:TYR:O	4:P:392:LYS:N	2.44	0.50
5:R:41:ASN:OD1	5:R:49:ARG:NH2	2.45	0.50
24:R:904:PTY:H181	14:S:40:MET:HB3	1.94	0.50
6:B:492:ILE:O	6:B:496:VAL:HG22	2.12	0.50
6:B:534:PHE:O	6:B:538:VAL:HG22	2.12	0.50
6:C:42:LEU:O	6:C:82:THR:OG1	2.30	0.50
12:6:88:LYS:O	12:6:92:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:48:THR:OG1	1:J:49:GLN:OE1	2.24	0.50
3:O:17:GLN:HE22	3:O:37:LYS:HG2	1.77	0.50
3:O:68:VAL:HB	3:O:133:ASP:OD2	2.12	0.50
4:P:37:LEU:H	4:P:37:LEU:HD23	1.76	0.50
4:P:72:GLN:N	4:P:72:GLN:OE1	2.45	0.50
5:R:46:VAL:HA	5:R:49:ARG:HB2	1.93	0.50
8:X:97:SER:O	8:X:160:GLN:NE2	2.45	0.50
12:9:88:LYS:O	12:9:92:GLN:HG2	2.11	0.50
1:I:162:ASP:N	1:I:162:ASP:OD1	2.45	0.50
4:P:65:MET:HA	4:P:68:THR:OG1	2.12	0.50
2:L:13:GLN:O	2:L:17:ARG:HG2	2.11	0.49
3:O:4:PHE:HB2	3:O:374:ILE:HG23	1.94	0.49
3:O:334:VAL:O	3:O:338:LEU:HB2	2.12	0.49
8:X:111:GLN:HG2	8:X:169:THR:HG23	1.93	0.49
2:M:13:GLN:HB3	2:M:17:ARG:HH11	1.77	0.49
3:O:278:PRO:HA	3:O:281:ARG:HH21	1.77	0.49
4:P:391:LEU:O	4:P:394:LEU:HB3	2.12	0.49
5:R:170:PHE:CD2	5:R:223:PHE:HB3	2.47	0.49
1:H:57:TYR:CE2	1:H:58:GLU:HG2	2.47	0.49
1:I:131:ARG:NH1	1:I:164:ASP:OD1	2.45	0.49
3:O:58:LEU:HB3	3:O:301:ARG:HG2	1.94	0.49
3:O:166:LEU:HD21	3:O:249:ARG:HG2	1.94	0.49
3:O:346:ALA:HB2	5:R:192:ARG:HD3	1.94	0.49
4:P:463:ASN:OD1	5:R:264:ARG:NH2	2.44	0.49
6:B:553:ARG:HA	6:B:556:GLU:OE2	2.12	0.49
8:Z:236:LYS:O	8:Z:236:LYS:HD3	2.12	0.49
8:Z:268:LYS:HA	8:Z:271:GLU:HB3	1.93	0.49
6:B:327:ILE:HG23	6:B:385:PHE:CE1	2.47	0.49
8:Y:214:GLU:O	8:Y:214:GLU:HG2	2.12	0.49
10:N:14:GLU:HG3	10:N:38:VAL:HG11	1.94	0.49
16:U:350:ASN:OD1	16:U:351:GLY:N	2.45	0.49
3:O:28:LYS:HE3	3:O:335:LEU:CD2	2.42	0.49
3:O:173:ASP:OD1	3:O:173:ASP:N	2.45	0.49
4:P:104:ASN:HB2	4:P:107:ARG:HB2	1.93	0.49
4:P:118:SER:O	4:P:122:ALA:N	2.45	0.49
4:P:315:LEU:O	4:P:319:GLU:HG2	2.13	0.49
5:R:771:GLY:HA2	5:R:774:VAL:HG12	1.94	0.49
7:E:421:GLN:NE2	7:E:425:CYS:SG	2.84	0.49
12:1:6:SER:OG	12:1:7:GLY:N	2.44	0.49
4:P:316:LYS:HA	4:P:319:GLU:HG2	1.95	0.49
1:H:20:GLU:HG2	2:K:17:ARG:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:5:201:CLR:H11	24:V:403:PTY:HC12	1.93	0.49
4:P:394:LEU:HD12	4:P:397:LEU:HD11	1.95	0.49
5:R:575:GLU:O	5:R:727:TYR:OH	2.27	0.49
6:A:583:SER:O	6:A:583:SER:OG	2.25	0.49
7:D:436:LYS:HB2	7:D:444:LEU:HD11	1.93	0.49
8:Z:239:SER:O	8:Z:243:GLN:N	2.46	0.49
11:0:47:PHE:O	11:0:51:ASN:ND2	2.42	0.49
11:0:164:LEU:HD13	13:Q:21:ARG:HD2	1.95	0.49
1:H:136:CYS:SG	1:H:144:VAL:HG11	2.53	0.49
4:P:129:MET:HG2	4:P:137:THR:O	2.12	0.49
4:P:206:GLN:HG2	4:P:245:PHE:CD2	2.47	0.49
12:4:88:LYS:O	12:4:92:GLN:HG2	2.13	0.49
1:I:212:ARG:NH1	7:E:126:ASP:OD2	2.46	0.49
3:O:347:ALA:HA	3:O:366:TYR:HB3	1.95	0.49
6:A:574:MET:HE2	6:A:577:ILE:HG21	1.94	0.49
1:H:29:GLU:OE2	4:P:283:ARG:NH1	2.46	0.48
1:H:39:ASN:O	1:H:42:LYS:HG3	2.13	0.48
4:P:56:LYS:HD3	4:P:57:ARG:HE	1.78	0.48
4:P:90:VAL:O	4:P:94:LEU:HB2	2.13	0.48
8:Z:33:MET:HE2	8:Z:88:LEU:HD21	1.94	0.48
8:Z:143:ALA:HB1	8:Z:149:ASN:HD22	1.78	0.48
1:H:12:ILE:O	1:H:16:MET:HG2	2.13	0.48
1:H:127:LEU:HD12	1:H:183:ILE:HG22	1.95	0.48
12:2:28:LEU:HD23	12:3:105:ALA:HB2	1.94	0.48
12:3:47:MET:HG2	12:3:48:ARG:HG3	1.94	0.48
15:T:100:LEU:O	15:T:104:VAL:HG22	2.12	0.48
5:R:197:LEU:HD13	5:R:220:PHE:HB3	1.94	0.48
5:R:224:PHE:CD2	5:R:233:VAL:HB	2.47	0.48
7:D:231:PHE:HB3	7:D:259:LEU:HD23	1.94	0.48
12:8:35:ALA:O	12:8:39:THR:HG23	2.13	0.48
1:H:46:VAL:O	1:H:50:ARG:HB2	2.13	0.48
4:P:380:ALA:HA	4:P:383:LEU:HD23	1.96	0.48
1:I:32:ALA:O	1:I:36:GLU:HG2	2.13	0.48
4:P:135:PRO:HB2	4:P:137:THR:HG23	1.96	0.48
5:R:334:GLN:HG2	5:R:352:LEU:HD21	1.95	0.48
5:R:494:LEU:O	14:S:70:ASN:ND2	2.41	0.48
8:X:98:ILE:HD12	8:X:164:ALA:HB2	1.94	0.48
1:I:127:LEU:HD12	1:I:183:ILE:HG22	1.96	0.48
1:I:206:GLN:NE2	7:E:40:LEU:O	2.43	0.48
2:M:34:LYS:O	2:M:38:GLU:HG2	2.14	0.48
8:Z:22:VAL:HG21	8:Z:69:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:242:LEU:HD22	8:Z:269:GLU:HG3	1.96	0.48
12:8:150:LEU:O	12:8:154:THR:OG1	2.29	0.48
1:I:33:LYS:HA	1:I:36:GLU:HG2	1.95	0.48
4:P:45:GLU:O	4:P:49:PHE:HB2	2.13	0.48
4:P:323:GLN:CD	5:R:53:ASN:HB2	2.33	0.48
6:C:587:LYS:HE3	6:C:600:ASP:HB3	1.96	0.48
7:E:365:ILE:HB	7:E:366:PRO:HD3	1.96	0.48
8:X:54:ILE:HA	8:X:57:GLU:HG2	1.96	0.48
22:5:201:CLR:H11	24:V:403:PTY:C1	2.44	0.48
3:O:151:GLN:O	3:O:154:GLU:HG2	2.13	0.48
13:Q:237:ARG:NH2	13:Q:258:ALA:O	2.46	0.48
1:H:187:ASP:OD2	1:H:187:ASP:N	2.47	0.48
3:O:131:GLN:NE2	3:O:135:ASP:OD1	2.47	0.48
6:B:349:ASP:HA	6:B:409:ALA:HB3	1.95	0.48
10:N:13:ASP:OD1	10:N:13:ASP:N	2.38	0.48
12:2:35:ALA:O	12:2:39:THR:HG23	2.14	0.48
1:H:61:GLU:O	1:H:64:ILE:HG13	2.14	0.47
3:O:17:GLN:HG3	3:O:21:LYS:HZ3	1.78	0.47
9:G:119:TYR:HB3	9:G:122:THR:HG21	1.95	0.47
12:9:115:ASP:OD2	12:9:119:ARG:NH2	2.47	0.47
1:H:102:LEU:O	1:H:105:VAL:HG12	2.14	0.47
2:K:25:ALA:HA	2:K:28:ARG:HE	1.79	0.47
3:O:48:LEU:O	3:O:52:VAL:HG23	2.14	0.47
4:P:296:SER:O	4:P:296:SER:OG	2.29	0.47
4:P:452:ALA:O	4:P:456:VAL:HG13	2.14	0.47
5:R:310:CYS:SG	5:R:319:LEU:HB3	2.54	0.47
5:R:831:ARG:HA	5:R:831:ARG:HH11	1.78	0.47
6:C:350:SER:HB3	6:C:353:ARG:HG2	1.95	0.47
8:Y:197:TYR:O	8:Y:201:LYS:HG3	2.14	0.47
8:Z:237:LEU:CD1	8:Z:243:GLN:HG3	2.44	0.47
16:U:266:ARG:HD2	16:U:302:TRP:CE3	2.49	0.47
1:J:159:THR:OG1	1:J:161:ASN:OD1	2.21	0.47
3:O:120:ASN:O	3:O:124:ILE:HG23	2.14	0.47
4:P:75:LYS:C	4:P:75:LYS:HZ2	2.18	0.47
8:Y:134:ASN:HA	8:Y:137:THR:HG22	1.96	0.47
1:I:182:GLU:HG2	1:I:193:SER:HA	1.96	0.47
4:P:31:VAL:HG21	4:P:33:TRP:CD2	2.49	0.47
5:R:19:SER:HA	5:R:22:ALA:HB3	1.95	0.47
6:C:444:HIS:ND1	6:C:521:GLN:OE1	2.48	0.47
1:I:26:LYS:HA	1:I:29:GLU:HG2	1.96	0.47
3:O:193:ASN:HD22	3:O:245:LYS:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:170:PHE:HA	5:R:223:PHE:CD2	2.49	0.47
6:B:377:TYR:O	6:B:381:ARG:HG2	2.14	0.47
7:E:61:ASP:OD1	7:E:62:HIS:N	2.45	0.47
8:X:209:GLU:OE2	8:X:210:GLU:N	2.48	0.47
8:Z:225:LEU:HD12	8:Z:226:VAL:HG23	1.96	0.47
4:P:101:LEU:HA	4:P:104:ASN:HB3	1.96	0.47
4:P:198:VAL:HA	4:P:201:VAL:HG22	1.96	0.47
17:V:319:LEU:HD23	17:V:319:LEU:HA	1.74	0.47
1:J:177:ILE:HG22	1:J:179:GLY:H	1.79	0.47
4:P:230:VAL:O	4:P:233:ASN:HB2	2.14	0.47
4:P:333:GLU:OE2	4:P:333:GLU:HA	2.15	0.47
4:P:389:GLU:HA	4:P:392:LYS:CB	2.44	0.47
4:P:405:GLN:CD	4:P:405:GLN:H	2.18	0.47
6:A:56:ARG:HB3	6:A:63:THR:HB	1.95	0.47
6:A:100:ASP:N	6:A:100:ASP:OD1	2.44	0.47
6:C:238:PHE:CZ	6:C:450:TRP:HA	2.50	0.47
8:Y:233:ALA:HA	8:Y:236:LYS:HD3	1.96	0.47
12:8:75:LEU:HD23	12:8:75:LEU:HA	1.79	0.47
16:U:324:LYS:HB2	16:U:346:GLU:HG3	1.97	0.47
2:K:50:GLN:O	2:K:54:GLU:HG2	2.14	0.47
2:L:12:LEU:O	2:L:16:LYS:HB2	2.15	0.47
5:R:232:ARG:O	5:R:236:ILE:HG12	2.15	0.47
14:S:28:ILE:O	14:S:34:ARG:NH1	2.47	0.47
1:H:182:GLU:HG2	1:H:193:SER:HA	1.96	0.47
1:I:46:VAL:O	1:I:50:ARG:HB2	2.15	0.47
1:J:44:ARG:HD2	1:J:45:LEU:HD22	1.97	0.47
3:O:332:ARG:NH2	3:O:333:GLU:OE1	2.48	0.47
4:P:426:ARG:O	4:P:429:GLU:HG2	2.14	0.47
6:A:592:ASP:N	6:A:592:ASP:OD1	2.47	0.47
7:D:442:GLU:CD	7:D:442:GLU:H	2.18	0.47
7:E:457:LYS:O	7:E:461:ASN:HB2	2.15	0.47
3:O:90:ASN:HB3	3:O:98:LEU:HD11	1.97	0.47
3:O:282:TRP:CE2	3:O:286:ASN:ND2	2.83	0.47
4:P:209:LEU:HD22	4:P:215:ARG:HA	1.97	0.47
4:P:377:ARG:CZ	4:P:420:HIS:HE1	2.28	0.47
5:R:182:THR:O	5:R:186:MET:HG2	2.14	0.47
6:B:362:SER:OG	6:B:363:GLY:N	2.48	0.47
7:D:435:MET:HA	7:D:438:VAL:HG12	1.96	0.47
7:F:505:PRO:O	7:F:506:ARG:HG3	2.14	0.47
16:U:319:THR:HG21	16:U:350:ASN:HA	1.96	0.47
2:L:49:LEU:O	2:L:53:LYS:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:343:ASP:OD2	3:O:344:SER:N	2.47	0.46
4:P:33:TRP:HB2	4:P:47:CYS:SG	2.55	0.46
4:P:116:ARG:O	4:P:116:ARG:NH1	2.48	0.46
6:A:492:ILE:HG21	7:E:437:ALA:HB1	1.96	0.46
8:Y:246:LEU:HD12	8:Y:266:ILE:HD12	1.96	0.46
10:N:71:ALA:HB1	10:N:78:LEU:HD21	1.97	0.46
12:7:24:VAL:HG11	24:8:201:PTY:H392	1.97	0.46
1:J:6:ALA:O	1:J:10:LYS:HG3	2.15	0.46
2:K:10:GLN:O	2:K:13:GLN:HB2	2.15	0.46
2:L:12:LEU:HD12	2:L:13:GLN:N	2.30	0.46
2:L:79:GLU:O	2:L:82:THR:HG22	2.16	0.46
3:O:6:LEU:HB3	3:O:320:LEU:HD13	1.97	0.46
3:O:75:TYR:HA	3:O:78:ASP:OD1	2.14	0.46
3:O:249:ARG:O	3:O:251:PHE:N	2.48	0.46
1:H:50:ARG:O	1:H:54:MET:HG2	2.15	0.46
3:O:197:TRP:HB2	3:O:246:PHE:CE1	2.50	0.46
3:O:254:ASN:N	3:O:254:ASN:OD1	2.49	0.46
3:O:343:ASP:HB2	5:R:192:ARG:HH21	1.80	0.46
7:F:380:ASP:HB2	7:F:393:ASN:HB2	1.96	0.46
12:3:117:GLY:O	12:3:121:THR:HG22	2.15	0.46
12:9:6:SER:OG	12:9:7:GLY:N	2.47	0.46
3:O:77:ALA:HA	3:O:83:SER:O	2.16	0.46
6:B:152:ILE:HG12	6:B:167:MET:HG2	1.97	0.46
6:C:481:GLU:O	6:C:485:GLU:HG3	2.16	0.46
7:F:237:ASN:H	7:F:237:ASN:ND2	2.13	0.46
12:6:35:ALA:O	12:6:39:THR:HG23	2.16	0.46
13:Q:260:ASP:N	13:Q:260:ASP:OD1	2.46	0.46
2:M:54:GLU:O	2:M:58:LYS:HE2	2.15	0.46
3:O:84:LYS:O	3:O:89:GLU:HA	2.15	0.46
5:R:175:ILE:HG22	5:R:219:VAL:HG13	1.97	0.46
5:R:188:TRP:HB3	5:R:192:ARG:HD2	1.96	0.46
7:E:436:LYS:HG3	7:E:444:LEU:HD11	1.97	0.46
7:F:226:ASN:N	7:F:226:ASN:OD1	2.49	0.46
12:7:28:LEU:HD22	24:8:201:PTY:HC11	1.98	0.46
3:O:183:VAL:HB	3:O:231:ARG:NE	2.27	0.46
5:R:111:ILE:HA	5:R:114:ASN:HB2	1.98	0.46
5:R:170:PHE:O	5:R:198:ARG:NH2	2.49	0.46
5:R:761:HIS:HD2	15:T:82:ASP:OD1	1.99	0.46
7:F:71:ILE:O	7:F:115:THR:OG1	2.31	0.46
8:Y:227:LYS:HB2	8:Y:227:LYS:HE2	1.48	0.46
3:O:36:SER:OG	3:O:37:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:62:ASP:HA	3:O:65:VAL:HG22	1.98	0.46
4:P:77:PHE:CD1	4:P:80:LEU:HD13	2.48	0.46
22:R:901:CLR:H213	24:R:904:PTY:H191	1.97	0.46
6:A:547:PHE:HB2	6:A:608:MET:SD	2.56	0.46
7:E:379:VAL:HG13	7:E:391:PRO:HG2	1.96	0.46
11:0:128:HIS:HB3	12:9:82:ASP:HB2	1.97	0.46
1:I:31:ASP:HA	2:L:32:ARG:NH1	2.30	0.46
2:L:32:ARG:O	2:L:35:GLN:HG2	2.15	0.46
4:P:87:GLU:HA	4:P:90:VAL:HG12	1.97	0.46
4:P:144:ILE:HD12	4:P:144:ILE:HA	1.74	0.46
4:P:376:TRP:HA	4:P:376:TRP:HE3	1.80	0.46
6:A:157:SER:O	6:A:157:SER:OG	2.32	0.46
6:B:463:GLU:OE2	6:B:463:GLU:N	2.46	0.46
6:B:523:ASN:O	6:B:526:THR:OG1	2.33	0.46
7:D:432:VAL:HG12	7:D:452:LEU:HD21	1.97	0.46
8:Y:207:GLN:HE21	8:Y:209:GLU:HB3	1.79	0.46
8:Z:19:HIS:CG	8:Z:70:LYS:HG3	2.51	0.46
5:R:90:PHE:HE2	5:R:343:HIS:CD2	2.34	0.46
5:R:740:ARG:NH2	12:4:139:GLU:OE1	2.49	0.46
8:X:17:GLN:O	8:X:21:GLN:HG2	2.15	0.46
8:X:72:GLY:HA2	8:X:76:ASN:ND2	2.30	0.46
8:X:220:GLU:O	8:X:224:ILE:HG13	2.16	0.46
3:O:176:VAL:HG12	3:O:184:THR:OG1	2.16	0.46
4:P:315:LEU:HA	4:P:318:LEU:HD12	1.97	0.46
6:B:224:ASN:OD1	8:Y:123:LYS:NZ	2.49	0.46
8:X:250:SER:O	8:X:250:SER:OG	2.29	0.46
10:N:75:ARG:HA	10:N:75:ARG:HD2	1.72	0.46
11:0:191:VAL:O	11:0:195:ILE:HG13	2.16	0.46
4:P:18:ILE:HG13	4:P:19:ILE:N	2.31	0.45
4:P:313:LYS:HB2	4:P:313:LYS:HE2	1.76	0.45
4:P:351:SER:OG	4:P:353:ASP:OD1	2.32	0.45
4:P:379:ASN:HD21	4:P:382:ARG:HH11	1.64	0.45
6:C:234:LEU:HD21	6:C:448:VAL:HG21	1.97	0.45
2:L:10:GLN:O	2:L:13:GLN:HG3	2.16	0.45
2:M:81:MET:O	2:M:85:GLN:HG2	2.16	0.45
3:O:166:LEU:O	3:O:170:VAL:HG12	2.16	0.45
5:R:476:GLY:O	14:S:4:HIS:NE2	2.45	0.45
8:Z:270:ASN:O	8:Z:273:LEU:HB2	2.16	0.45
1:I:80:ARG:NH2	7:E:254:MET:O	2.49	0.45
3:O:304:VAL:HA	3:O:307:VAL:HG12	1.98	0.45
4:P:212:ASN:O	4:P:215:ARG:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:113:GLU:O	8:X:117:GLN:HG2	2.16	0.45
11:0:88:THR:OG1	11:0:89:LYS:N	2.50	0.45
24:5:202:PTY:O10	24:6:201:PTY:HC12	2.16	0.45
4:P:17:ASN:OD1	4:P:196:GLN:NE2	2.50	0.45
5:R:389:ILE:HD11	5:R:557:PHE:HB2	1.99	0.45
11:0:56:LEU:HD21	16:U:435:PHE:HZ	1.81	0.45
24:7:201:PTY:O10	24:7:201:PTY:HC12	2.16	0.45
1:I:68:LYS:HB3	1:I:68:LYS:HE3	1.77	0.45
3:O:171:LYS:HG3	3:O:172:LYS:H	1.82	0.45
4:P:59:PRO:O	4:P:62:LYS:HB2	2.17	0.45
5:R:84:GLU:HG3	5:R:292:VAL:HB	1.98	0.45
6:B:545:ILE:HD12	6:B:546:ALA:N	2.32	0.45
6:C:42:LEU:HD23	6:C:53:GLU:HG3	1.99	0.45
6:C:169:PRO:HB2	6:C:172:ASN:HD22	1.82	0.45
7:D:363:HIS:HB3	7:D:366:PRO:HD2	1.99	0.45
7:F:131:VAL:HG22	7:F:259:LEU:HD12	1.99	0.45
8:Y:261:ASP:HA	8:Y:264:ASP:OD2	2.17	0.45
11:0:49:TRP:HB3	11:0:138:PHE:HB2	1.98	0.45
12:3:121:THR:O	12:3:121:THR:OG1	2.35	0.45
13:Q:115:GLY:HA3	13:Q:125:LEU:HD11	1.99	0.45
13:Q:289:THR:OG1	13:Q:290:LEU:N	2.50	0.45
1:I:210:GLU:OE1	7:E:39:TYR:OH	2.30	0.45
2:K:32:ARG:HA	2:K:35:GLN:NE2	2.31	0.45
4:P:71:SER:O	4:P:75:LYS:HB3	2.17	0.45
7:E:380:ASP:HB2	7:E:393:ASN:HB2	1.98	0.45
7:F:417:ASP:HB3	7:F:495:ILE:HG23	1.99	0.45
9:G:55:LYS:NZ	10:N:103:ASP:OD2	2.42	0.45
12:7:133:LEU:HD23	12:7:133:LEU:HA	1.71	0.45
3:O:98:LEU:O	3:O:102:ILE:HG13	2.17	0.45
4:P:133:GLN:NE2	4:P:166:ASN:HA	2.32	0.45
4:P:363:ARG:HA	4:P:363:ARG:NH1	2.32	0.45
5:R:129:LYS:HD3	5:R:133:ARG:HH11	1.82	0.45
6:B:439:LEU:HD23	6:B:444:HIS:CD2	2.51	0.45
6:C:148:THR:OG1	6:C:149:GLY:N	2.49	0.45
6:C:249:PRO:HG2	6:C:432:PHE:HE1	1.82	0.45
1:H:48:THR:HG23	1:H:49:GLN:H	1.82	0.45
3:O:107:TRP:HA	3:O:296:HIS:HE1	1.82	0.45
3:O:121:ILE:O	3:O:124:ILE:HG13	2.16	0.45
4:P:165:PHE:HD1	4:P:168:ILE:HB	1.82	0.45
6:A:376:ALA:HB1	7:E:309:GLU:HA	1.98	0.45
6:B:100:ASP:OD1	6:B:100:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:350:GLN:HE21	7:E:350:GLN:HB3	1.51	0.45
7:E:393:ASN:O	7:E:397:SER:OG	2.28	0.45
8:Z:213:PHE:CE2	8:Z:255:LEU:HD22	2.52	0.45
12:6:150:LEU:O	12:6:154:THR:OG1	2.35	0.45
3:O:284:LYS:HA	3:O:284:LYS:HD2	1.85	0.45
4:P:47:CYS:O	4:P:50:ILE:HB	2.17	0.45
4:P:114:TYR:CD1	4:P:114:TYR:N	2.85	0.45
4:P:197:TYR:O	4:P:201:VAL:HG13	2.17	0.45
6:A:234:LEU:HD21	6:A:448:VAL:HG21	1.98	0.45
6:C:238:PHE:HZ	6:C:450:TRP:HA	1.81	0.45
7:D:445:THR:HG22	7:D:446:SER:N	2.32	0.45
7:F:231:PHE:HB3	7:F:259:LEU:HD23	1.99	0.45
8:Z:240:LYS:HA	8:Z:243:GLN:HB2	1.99	0.45
16:U:284:ASP:OD2	16:U:286:THR:HG22	2.16	0.45
3:O:4:PHE:CZ	3:O:99:VAL:HG12	2.51	0.45
3:O:66:GLU:HB3	3:O:294:TRP:NE1	2.32	0.45
3:O:195:ASN:HA	3:O:198:ILE:HD12	1.99	0.45
4:P:379:ASN:ND2	4:P:382:ARG:HG3	2.32	0.45
8:X:49:TYR:O	8:X:53:LEU:HB2	2.17	0.45
8:X:170:GLU:CD	8:X:170:GLU:H	2.20	0.45
12:2:133:LEU:HA	12:2:133:LEU:HD23	1.74	0.45
1:H:38:PHE:CE1	2:K:36:ALA:HA	2.52	0.44
1:I:13:LYS:HG3	2:L:10:GLN:NE2	2.32	0.44
1:I:221:ASN:OD1	1:I:221:ASN:N	2.43	0.44
1:J:47:GLN:HE22	1:J:50:ARG:HH11	1.63	0.44
5:R:473:ASN:ND2	5:R:473:ASN:O	2.50	0.44
6:A:238:PHE:CZ	6:A:450:TRP:HA	2.52	0.44
6:A:356:GLU:OE2	6:A:359:ARG:NH2	2.41	0.44
6:C:63:THR:HG21	6:C:365:LEU:HD21	1.99	0.44
8:Z:44:LYS:O	8:Z:47:GLU:HG3	2.17	0.44
9:G:44:PHE:HE1	9:G:159:ASP:HB2	1.81	0.44
1:I:123:GLY:HA3	1:I:183:ILE:HD13	1.98	0.44
2:M:42:ALA:O	2:M:45:GLU:HB3	2.18	0.44
3:O:267:ARG:HB3	3:O:267:ARG:HH21	1.81	0.44
5:R:50:LYS:HB3	5:R:50:LYS:HE3	1.62	0.44
5:R:65:LEU:HA	5:R:68:VAL:HG12	2.00	0.44
7:F:335:TYR:CE2	7:F:369:THR:HG23	2.52	0.44
8:X:223:LYS:HA	8:X:226:VAL:HG22	1.98	0.44
8:Z:88:LEU:HD12	8:Z:88:LEU:HA	1.83	0.44
8:Z:114:LYS:HB3	8:Z:114:LYS:HZ2	1.82	0.44
1:J:30:ILE:HG21	2:M:25:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:105:PHE:HE1	3:O:296:HIS:CE1	2.35	0.44
4:P:434:LYS:HE2	4:P:459:LEU:HD11	2.00	0.44
5:R:271:VAL:O	5:R:275:THR:HG22	2.18	0.44
5:R:793:MET:HE3	5:R:794:GLU:HG2	1.99	0.44
7:E:201:GLU:H	7:E:201:GLU:HG2	1.41	0.44
7:E:376:GLN:HG3	7:E:378:TYR:HE2	1.82	0.44
13:Q:292:ASP:OD1	13:Q:292:ASP:N	2.50	0.44
2:M:51:ARG:HD3	2:M:51:ARG:HA	1.74	0.44
2:M:73:VAL:O	2:M:77:THR:HG22	2.17	0.44
3:O:72:VAL:HG12	3:O:136:LEU:HG	1.99	0.44
3:O:166:LEU:HD12	3:O:169:ILE:HD12	1.98	0.44
3:O:335:LEU:HD13	3:O:369:TYR:OH	2.18	0.44
4:P:401:SER:HB3	4:P:407:LEU:HD12	1.99	0.44
8:Y:93:ARG:O	8:Y:97:SER:OG	2.33	0.44
2:L:86:THR:O	2:L:90:GLN:NE2	2.51	0.44
3:O:43:LEU:HB2	3:O:303:PHE:CZ	2.53	0.44
3:O:112:TYR:HE2	3:O:296:HIS:CD2	2.36	0.44
3:O:197:TRP:O	3:O:201:TYR:HD2	2.01	0.44
4:P:291:ASN:O	4:P:295:LYS:HG2	2.18	0.44
5:R:69:GLU:HA	5:R:72:ILE:HG22	1.98	0.44
5:R:81:ASP:HA	5:R:291:ARG:CB	2.46	0.44
5:R:449:ILE:O	5:R:453:MET:HG3	2.18	0.44
5:R:517:GLY:O	14:S:59:GLN:NE2	2.51	0.44
6:C:469:PHE:O	6:C:471:GLU:N	2.50	0.44
8:Z:234:MET:HG3	8:Z:235:PRO:HD3	1.99	0.44
1:I:58:GLU:O	1:I:62:LYS:HG2	2.18	0.44
2:L:10:GLN:NE2	2:L:13:GLN:HE21	2.15	0.44
2:M:73:VAL:HA	2:M:76:GLU:CD	2.38	0.44
3:O:18:THR:O	3:O:23:HIS:HB2	2.18	0.44
4:P:37:LEU:HB3	4:P:42:ILE:HB	1.99	0.44
9:G:89:LYS:HA	10:N:27:GLU:OE1	2.17	0.44
11:0:140:ALA:O	11:0:144:VAL:HG12	2.17	0.44
13:Q:284:ASN:HB3	13:Q:287:ASP:OD2	2.16	0.44
1:I:23:ALA:O	1:I:26:LYS:HG2	2.18	0.44
1:J:75:LEU:HD21	2:M:70:SER:HA	2.00	0.44
2:M:31:ARG:HD3	2:M:34:LYS:HB2	1.98	0.44
3:O:28:LYS:HB3	3:O:331:LEU:HG	1.99	0.44
4:P:134:ASP:HB3	4:P:135:PRO:HD3	1.99	0.44
6:A:605:LEU:O	6:A:609:GLN:HG3	2.17	0.44
8:X:143:ALA:HB1	8:X:149:ASN:OD1	2.18	0.44
8:Y:177:GLN:HG3	8:Y:178:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:4:41:ILE:O	12:4:44:MET:HG3	2.17	0.44
16:U:426:ILE:HG22	16:U:430:LEU:HD13	1.99	0.44
3:O:64:PHE:O	3:O:68:VAL:HG13	2.17	0.44
3:O:99:VAL:HG23	3:O:100:THR:H	1.83	0.44
3:O:112:TYR:HB3	3:O:121:ILE:HD12	1.99	0.44
5:R:60:GLU:O	5:R:63:ARG:HG3	2.18	0.44
5:R:176:ASN:ND2	5:R:215:VAL:HG23	2.29	0.44
5:R:224:PHE:CD2	5:R:229:LEU:HB3	2.53	0.44
6:A:249:PRO:HG2	6:A:435:LEU:HB2	1.99	0.44
8:X:140:LEU:HD13	8:X:153:ARG:HA	2.00	0.44
8:Z:94:LEU:HB2	8:Z:130:LEU:HD21	1.99	0.44
13:Q:113:ILE:O	13:Q:117:LEU:HG	2.16	0.44
16:U:365:SER:O	16:U:406:ASN:ND2	2.39	0.44
1:J:123:GLY:HA3	1:J:183:ILE:HD13	1.99	0.44
3:O:179:SER:OG	3:O:182:LEU:N	2.47	0.44
3:O:191:LYS:HB3	3:O:223:TYR:CD1	2.52	0.44
12:1:45:SER:HB2	12:1:52:ILE:HG12	2.00	0.44
2:L:6:GLN:O	2:L:10:GLN:HB2	2.18	0.43
2:L:75:LYS:NZ	2:L:79:GLU:HB3	2.33	0.43
4:P:212:ASN:HA	4:P:215:ARG:NE	2.33	0.43
4:P:342:LEU:HD23	4:P:342:LEU:HA	1.77	0.43
6:B:485:GLU:HA	6:B:488:ASP:OD2	2.18	0.43
6:C:438:LYS:HA	6:C:438:LYS:HD3	1.81	0.43
8:X:133:LEU:O	8:X:137:THR:HG22	2.18	0.43
12:2:86:LEU:HD12	12:2:86:LEU:HA	1.87	0.43
12:6:77:ALA:O	12:7:155:LYS:HE2	2.18	0.43
3:O:151:GLN:HA	3:O:154:GLU:OE2	2.18	0.43
4:P:165:PHE:HB3	4:P:169:LYS:N	2.22	0.43
4:P:235:CYS:HB3	4:P:239:LEU:HD23	2.00	0.43
5:R:185:ARG:O	5:R:189:ARG:HG3	2.18	0.43
6:C:473:VAL:O	6:C:477:THR:HG23	2.18	0.43
7:E:168:GLU:OE2	7:E:410:MET:HG2	2.19	0.43
8:Z:124:SER:OG	8:Z:125:ASP:N	2.52	0.43
1:J:65:GLU:HA	1:J:68:LYS:HG2	2.00	0.43
2:L:44:ILE:HA	2:L:47:TYR:CZ	2.53	0.43
3:O:61:LEU:O	3:O:65:VAL:HG13	2.18	0.43
3:O:213:SER:HA	3:O:226:ASN:O	2.17	0.43
4:P:357:SER:HA	4:P:360:LYS:HZ2	1.84	0.43
8:Z:209:GLU:HG2	8:Z:211:SER:H	1.83	0.43
16:U:277:ALA:HB2	16:U:282:TRP:CD2	2.53	0.43
3:O:339:TYR:O	3:O:368:PRO:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:263:TYR:HB2	4:P:265:ILE:CD1	2.48	0.43
6:C:511:VAL:HG11	6:C:548:TYR:HD1	1.83	0.43
7:E:335:TYR:CE2	7:E:369:THR:HG23	2.52	0.43
9:G:83:VAL:HG11	10:N:22:LEU:HD21	2.01	0.43
12:5:22:ALA:O	12:5:26:SER:OG	2.27	0.43
22:5:201:CLR:H121	22:V:402:CLR:C18	2.47	0.43
1:I:13:LYS:NZ	2:L:10:GLN:OE1	2.36	0.43
2:K:17:ARG:O	2:K:20:GLU:HG3	2.18	0.43
2:M:21:LYS:HE3	2:M:21:LYS:HB3	1.81	0.43
4:P:56:LYS:NZ	4:P:57:ARG:HH21	2.16	0.43
6:C:350:SER:H	6:C:409:ALA:HB3	1.84	0.43
7:E:269:ILE:HD12	7:E:269:ILE:H	1.83	0.43
8:Y:43:LYS:O	8:Y:47:GLU:HG2	2.19	0.43
8:Z:106:ASP:OD2	8:Z:106:ASP:N	2.51	0.43
9:G:145:LEU:HD23	10:N:65:LEU:CD2	2.49	0.43
12:6:72:VAL:HG11	12:6:99:VAL:HG11	2.00	0.43
12:9:8:PRO:HD2	12:9:11:ALA:HB2	2.00	0.43
1:H:60:LYS:HA	1:H:60:LYS:HD3	1.69	0.43
5:R:224:PHE:HD2	5:R:229:LEU:O	2.01	0.43
6:B:234:LEU:HD21	6:B:448:VAL:HG21	1.99	0.43
7:E:66:PRO:HB2	7:E:89:VAL:HG22	2.01	0.43
8:Y:270:ASN:O	8:Y:274:ASN:ND2	2.52	0.43
8:Z:220:GLU:CD	8:Z:220:GLU:H	2.22	0.43
10:N:8:ILE:HG23	10:N:63:ILE:HB	2.00	0.43
12:4:47:MET:HG3	12:4:48:ARG:HG3	2.01	0.43
13:Q:190:LEU:HD12	13:Q:190:LEU:HA	1.82	0.43
2:M:11:LEU:HD22	3:O:182:LEU:CD1	2.49	0.43
5:R:188:TRP:CD1	5:R:222:ILE:HD11	2.54	0.43
24:0:307:PTY:H412	24:0:307:PTY:H161	2.00	0.43
24:8:202:PTY:HC6	24:8:202:PTY:H111	1.70	0.43
1:H:108:ASP:OD2	1:H:111:ARG:HD3	2.19	0.43
1:I:26:LYS:O	1:I:30:ILE:HG12	2.19	0.43
1:J:26:LYS:HB3	2:M:21:LYS:HD3	2.00	0.43
2:M:29:LYS:HB3	2:M:29:LYS:HE2	1.72	0.43
4:P:426:ARG:HG3	4:P:427:VAL:N	2.34	0.43
6:C:252:PHE:O	6:C:437:LYS:NZ	2.51	0.43
11:0:9:SER:O	11:0:13:VAL:HG12	2.19	0.43
24:0:307:PTY:H112	24:0:307:PTY:C30	2.48	0.43
12:4:46:VAL:HA	12:5:124:GLN:HB2	2.01	0.43
1:H:82:LYS:HE2	1:H:82:LYS:HB3	1.82	0.43
2:K:43:GLU:O	2:K:46:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:53:LYS:HB3	2:M:53:LYS:HE3	1.69	0.43
3:O:196:ASP:O	3:O:199:LYS:HD3	2.19	0.43
3:O:215:VAL:HA	3:O:225:CYS:HB3	2.00	0.43
4:P:248:TRP:HD1	4:P:288:ALA:HA	1.84	0.43
6:A:511:VAL:HG11	6:A:548:TYR:HB2	2.01	0.43
6:B:511:VAL:HG21	6:B:548:TYR:HB2	2.01	0.43
8:X:136:LEU:HD13	8:X:156:THR:HG22	2.00	0.43
8:X:197:TYR:CE2	8:X:201:LYS:HD3	2.53	0.43
9:G:213:LYS:HB3	9:G:213:LYS:HE3	1.72	0.43
10:N:92:PRO:HB3	10:N:98:TYR:HB2	2.00	0.43
13:Q:326:CYS:O	13:Q:330:VAL:HG23	2.19	0.43
1:H:115:LEU:HD12	1:H:115:LEU:HA	1.91	0.43
1:I:11:GLN:NE2	1:I:14:HIS:HD1	2.17	0.43
1:I:15:MET:O	1:I:19:ILE:HG12	2.19	0.43
3:O:118:LEU:HD21	3:O:303:PHE:CE1	2.51	0.43
3:O:179:SER:HG	3:O:182:LEU:N	2.17	0.43
4:P:40:GLN:O	4:P:83:HIS:NE2	2.45	0.43
4:P:129:MET:HA	4:P:132:ARG:HH21	1.83	0.43
4:P:264:ASN:ND2	4:P:267:PRO:HG2	2.34	0.43
5:R:52:VAL:O	5:R:55:VAL:HG22	2.19	0.43
5:R:207:GLU:HB2	5:R:213:ASP:N	2.33	0.43
7:E:188:LYS:HE2	7:E:188:LYS:HB2	1.75	0.43
8:Y:181:LEU:CD2	8:Y:203:TYR:HB2	2.48	0.43
2:L:48:ARG:O	2:L:52:GLU:HG2	2.17	0.42
2:M:29:LYS:O	2:M:33:LEU:HG	2.19	0.42
4:P:264:ASN:HD21	4:P:267:PRO:HG2	1.83	0.42
5:R:180:ILE:O	5:R:184:GLU:HG2	2.19	0.42
6:B:574:MET:HB3	6:B:577:ILE:HB	1.99	0.42
6:C:510:GLU:HG3	6:C:567:TRP:CE2	2.54	0.42
8:X:134:ASN:O	8:X:138:ASP:HB2	2.18	0.42
8:Y:217:LEU:HB3	8:Y:221:ASP:OD1	2.19	0.42
13:Q:116:THR:HG22	13:Q:122:ILE:HD11	2.01	0.42
13:Q:248:TYR:HB3	13:Q:249:PRO:HD3	2.00	0.42
16:U:309:LEU:O	16:U:324:LYS:HA	2.20	0.42
3:O:76:MET:SD	3:O:81:GLU:HB3	2.59	0.42
3:O:304:VAL:O	3:O:308:LEU:HG	2.19	0.42
4:P:90:VAL:HA	4:P:93:ILE:HG13	2.01	0.42
5:R:84:GLU:HG2	5:R:87:GLU:HG2	2.00	0.42
6:A:105:PRO:HG3	6:A:126:ALA:HA	2.01	0.42
7:D:457:LYS:O	7:D:461:ASN:HB2	2.19	0.42
7:F:215:LYS:HE2	7:F:215:LYS:HB2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:0:23:GLY:O	11:0:27:THR:HG22	2.19	0.42
13:Q:54:TYR:OH	13:Q:325:GLU:OE1	2.37	0.42
24:Q:401:PTY:H361	24:Q:401:PTY:H332	1.72	0.42
1:H:41:GLU:O	1:H:45:LEU:HG	2.18	0.42
3:O:114:ILE:HD12	3:O:114:ILE:HA	1.82	0.42
3:O:176:VAL:HG21	3:O:182:LEU:HD22	2.02	0.42
6:B:95:MET:HE3	6:B:308:ARG:HA	2.01	0.42
16:U:439:ILE:HG12	24:U:503:PTY:H192	2.01	0.42
1:J:4:SER:H	1:J:7:ASP:HB2	1.85	0.42
3:O:29:ASN:HB2	3:O:33:ALA:H	1.84	0.42
3:O:102:ILE:HD13	3:O:320:LEU:HD21	2.02	0.42
3:O:196:ASP:O	3:O:200:GLN:HB2	2.18	0.42
5:R:16:PHE:CZ	5:R:318:CYS:HB2	2.54	0.42
5:R:248:PRO:HA	5:R:254:ARG:HE	1.84	0.42
7:D:335:TYR:CE2	7:D:369:THR:HG23	2.54	0.42
12:3:104:LEU:HD11	17:V:324:THR:HG21	2.02	0.42
12:4:57:ILE:O	12:4:61:MET:HG3	2.20	0.42
1:H:68:LYS:HA	1:H:68:LYS:HD3	1.73	0.42
1:I:33:LYS:O	1:I:37:GLU:HG2	2.19	0.42
1:J:104:LYS:HE2	1:J:104:LYS:HB2	1.78	0.42
3:O:177:LEU:HD12	3:O:177:LEU:HA	1.75	0.42
3:O:338:LEU:HD23	3:O:338:LEU:HA	1.91	0.42
3:O:347:ALA:HB1	3:O:367:TYR:N	2.33	0.42
4:P:37:LEU:CB	4:P:42:ILE:HB	2.49	0.42
5:R:187:LEU:HB3	5:R:222:ILE:HD12	2.00	0.42
6:A:290:ASP:O	6:A:294:LEU:HD13	2.19	0.42
6:B:498:LYS:HG2	6:B:501:LEU:HD22	2.01	0.42
8:X:263:ILE:O	8:X:266:ILE:HG13	2.19	0.42
12:8:98:SER:O	12:8:102:SER:OG	2.35	0.42
16:U:438:PHE:CE1	24:U:503:PTY:C36	3.03	0.42
1:H:32:ALA:HA	1:H:35:GLU:OE1	2.20	0.42
1:H:177:ILE:HD13	1:H:177:ILE:HA	1.89	0.42
3:O:159:GLY:C	3:O:164:ARG:HG2	2.39	0.42
4:P:126:PHE:O	4:P:129:MET:HB2	2.20	0.42
5:R:293:TRP:O	5:R:297:VAL:HG23	2.20	0.42
5:R:579:MET:HE2	5:R:579:MET:HB2	1.66	0.42
5:R:796:LEU:HD12	5:R:796:LEU:HA	1.83	0.42
7:E:408:GLU:HG2	7:E:413:LYS:HB3	2.01	0.42
7:F:272:ILE:HD11	7:F:310:VAL:HG11	2.01	0.42
8:X:61:ARG:H	8:X:64:GLU:HG3	1.85	0.42
8:X:205:LYS:HA	8:X:257:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:222:GLN:O	8:Z:226:VAL:HG23	2.19	0.42
3:O:238:ARG:HB3	3:O:242:ARG:HH22	1.85	0.42
4:P:299:ARG:NH1	4:P:302:ARG:O	2.53	0.42
5:R:279:ARG:O	5:R:283:LEU:HB2	2.20	0.42
7:E:198:PRO:HB2	7:E:201:GLU:HG3	2.02	0.42
7:F:188:LYS:HD3	7:F:335:TYR:O	2.19	0.42
8:Y:40:ASN:O	8:Y:41:ASN:ND2	2.51	0.42
8:Y:211:SER:O	8:Y:211:SER:OG	2.33	0.42
12:2:48:ARG:NH2	12:2:50:GLU:OE2	2.53	0.42
12:4:31:ALA:HB1	12:5:109:ALA:HB2	2.02	0.42
16:U:376:SER:O	16:U:376:SER:OG	2.32	0.42
1:J:102:LEU:HG	1:J:196:LEU:HD13	2.01	0.42
2:K:4:GLN:H	5:R:353:ASN:ND2	2.18	0.42
3:O:297:VAL:O	3:O:300:LEU:HD23	2.19	0.42
4:P:108:VAL:HG22	4:P:113:ASP:OD1	2.20	0.42
4:P:410:ALA:O	4:P:414:VAL:HG12	2.19	0.42
6:B:486:GLU:HG3	6:B:512:ALA:HB3	2.00	0.42
6:B:507:ILE:O	6:B:511:VAL:HG12	2.20	0.42
6:B:566:THR:OG1	6:B:567:TRP:N	2.52	0.42
6:C:350:SER:OG	6:C:411:SER:OG	2.37	0.42
7:E:60:LEU:HD21	7:E:112:CYS:SG	2.60	0.42
12:6:94:GLY:O	12:6:98:SER:OG	2.33	0.42
16:U:277:ALA:HB3	16:U:394:GLN:HB2	2.02	0.42
3:O:119:LYS:HG3	3:O:123:GLU:OE2	2.20	0.42
3:O:191:LYS:HA	3:O:194:HIS:HB2	2.02	0.42
4:P:31:VAL:HG22	4:P:32:ASN:N	2.35	0.42
4:P:313:LYS:HE2	4:P:313:LYS:H	1.84	0.42
4:P:426:ARG:HA	4:P:429:GLU:CD	2.40	0.42
6:B:256:LYS:HB3	6:B:256:LYS:HE2	1.79	0.42
6:B:258:VAL:O	6:B:262:SER:OG	2.30	0.42
8:X:52:VAL:HG12	8:X:75:PRO:HG2	2.02	0.42
22:5:201:CLR:H261	22:V:402:CLR:C26	2.49	0.42
24:7:201:PTY:H432	24:8:201:PTY:H261	2.01	0.42
15:T:123:PHE:O	15:T:126:VAL:HG12	2.20	0.42
1:H:102:LEU:HD12	1:H:102:LEU:HA	1.83	0.42
3:O:54:LEU:HA	3:O:57:GLU:HG3	2.02	0.42
3:O:127:LYS:HD2	3:O:128:GLY:N	2.34	0.42
4:P:231:LEU:O	4:P:231:LEU:HD23	2.20	0.42
4:P:395:THR:CA	4:P:398:LEU:HD12	2.45	0.42
4:P:432:GLY:O	4:P:436:LEU:HG	2.20	0.42
5:R:609:LEU:HD12	5:R:609:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:169:PRO:HA	6:A:170:PRO:HD3	1.93	0.42
6:A:274:TYR:HB3	6:A:311:LEU:HD23	2.02	0.42
6:C:372:SER:HB3	6:C:420:PRO:HG2	2.01	0.42
7:E:146:LEU:HD12	7:E:146:LEU:HA	1.90	0.42
8:X:120:ASN:HD21	8:X:123:LYS:HB2	1.85	0.42
1:I:11:GLN:HE22	1:I:14:HIS:HD1	1.68	0.41
4:P:53:PHE:H	4:P:61:GLU:CD	2.23	0.41
4:P:204:CYS:O	4:P:207:LEU:HG	2.20	0.41
4:P:394:LEU:O	4:P:398:LEU:N	2.53	0.41
5:R:64:LYS:HD3	5:R:105:GLU:HB2	2.02	0.41
6:A:225:HIS:HA	6:A:226:PRO:HD3	1.96	0.41
6:B:328:TYR:HA	6:B:331:ILE:HG22	2.02	0.41
6:C:108:ASP:OD1	6:C:108:ASP:N	2.52	0.41
7:F:77:PRO:HB3	7:F:109:LYS:HE2	2.02	0.41
8:Y:42:LEU:HD21	8:Y:105:LEU:HD12	2.02	0.41
24:0:307:PTY:HC11	24:U:503:PTY:H141	2.01	0.41
12:3:33:GLY:O	12:3:37:SER:OG	2.36	0.41
24:7:201:PTY:H392	24:8:201:PTY:H252	2.02	0.41
5:R:86:PRO:O	5:R:88:VAL:HG23	2.20	0.41
6:A:44:ARG:HD2	6:A:49:GLU:HB3	2.02	0.41
6:A:350:SER:HB3	6:A:353:ARG:CG	2.49	0.41
6:B:449:ASN:HD22	6:B:452:ILE:HG12	1.84	0.41
6:C:264:SER:HB2	6:C:272:ILE:HG21	2.02	0.41
8:Z:188:MET:HE1	8:Z:196:GLN:HA	2.02	0.41
1:J:5:ASP:HA	1:J:8:VAL:HG22	2.01	0.41
1:J:49:GLN:O	1:J:53:ILE:HG12	2.20	0.41
2:L:116:ILE:H	2:L:116:ILE:HG12	1.64	0.41
4:P:94:LEU:HD12	4:P:136:PHE:HB3	2.02	0.41
5:R:333:ILE:HG13	5:R:334:GLN:N	2.35	0.41
5:R:431:LEU:HD12	5:R:431:LEU:HA	1.86	0.41
6:A:268:ASN:OD1	6:A:268:ASN:N	2.46	0.41
6:B:501:LEU:HB3	6:B:506:LYS:HE2	2.02	0.41
7:E:445:THR:HG22	7:E:446:SER:H	1.85	0.41
7:F:146:LEU:HD12	7:F:146:LEU:HA	1.85	0.41
8:X:72:GLY:HA2	8:X:76:ASN:HD21	1.85	0.41
8:Z:90:GLU:OE1	8:Z:127:HIS:ND1	2.53	0.41
10:N:72:GLU:HA	10:N:75:ARG:HG2	2.02	0.41
13:Q:24:LYS:O	13:Q:24:LYS:HG2	2.20	0.41
1:J:10:LYS:HA	1:J:13:LYS:HB2	2.03	0.41
2:K:30:ASN:O	2:K:34:LYS:HE3	2.19	0.41
2:K:45:GLU:O	2:K:49:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:88:PHE:CZ	2:L:92:ARG:HD3	2.55	0.41
3:O:53:GLY:O	3:O:57:GLU:HG3	2.20	0.41
4:P:259:HIS:CG	4:P:260:LEU:N	2.87	0.41
5:R:18:GLN:NE2	5:R:20:GLU:HB2	2.35	0.41
5:R:430:ILE:H	5:R:430:ILE:HG13	1.68	0.41
6:C:50:LEU:HB3	6:C:68:GLU:HG3	2.02	0.41
7:D:60:LEU:HD21	7:D:112:CYS:SG	2.59	0.41
7:D:291:LYS:HE2	7:D:291:LYS:HB3	1.78	0.41
8:X:58:LYS:HE2	8:X:58:LYS:HB2	1.72	0.41
8:X:118:HIS:CE1	8:X:124:SER:HB3	2.56	0.41
8:Y:133:LEU:O	8:Y:137:THR:HG22	2.19	0.41
13:Q:284:ASN:HD22	13:Q:285:PRO:CD	2.33	0.41
1:J:12:ILE:HG22	1:J:16:MET:CE	2.49	0.41
2:K:72:GLU:HG3	2:K:73:VAL:N	2.34	0.41
3:O:150:LEU:HD23	3:O:151:GLN:N	2.36	0.41
4:P:45:GLU:HG2	4:P:49:PHE:HD2	1.86	0.41
4:P:162:ASN:O	4:P:168:ILE:HG13	2.21	0.41
4:P:172:LEU:O	4:P:172:LEU:HD13	2.20	0.41
5:R:252:GLN:HE22	5:R:255:LYS:HD2	1.86	0.41
8:Z:120:ASN:ND2	8:Z:123:LYS:HB2	2.36	0.41
8:Z:222:GLN:HA	8:Z:225:LEU:HG	2.01	0.41
22:5:201:CLR:C26	22:V:402:CLR:C26	2.98	0.41
12:9:83:ASP:OD1	12:9:83:ASP:N	2.49	0.41
3:O:65:VAL:HA	3:O:68:VAL:HG22	2.02	0.41
5:R:24:CYS:SG	5:R:344:SER:OG	2.53	0.41
5:R:360:THR:HB	5:R:361:PRO:N	2.36	0.41
6:A:95:MET:HE2	6:A:162:ILE:HG13	2.02	0.41
6:B:587:LYS:NZ	6:B:600:ASP:OD1	2.52	0.41
6:C:173:ARG:NH1	8:Z:16:GLU:OE1	2.42	0.41
7:F:46:THR:HG23	7:F:113:GLU:HB2	2.03	0.41
8:X:36:ILE:HG13	8:X:95:VAL:HG21	2.02	0.41
8:Y:61:ARG:O	8:Y:65:ILE:HG13	2.21	0.41
8:Y:130:LEU:HD23	8:Y:130:LEU:HA	1.85	0.41
10:N:56:LEU:HD23	10:N:56:LEU:HA	1.87	0.41
11:0:4:LEU:HD23	11:0:4:LEU:HA	1.84	0.41
13:Q:12:ASP:HB2	13:Q:90:TYR:CD2	2.56	0.41
13:Q:328:ASN:ND2	13:Q:348:ILE:O	2.48	0.41
1:I:21:GLN:NE2	3:O:45:VAL:HG13	2.35	0.41
3:O:325:LYS:HD2	3:O:325:LYS:HA	1.61	0.41
4:P:123:TRP:HB2	4:P:124:PRO:HD3	2.03	0.41
4:P:298:GLU:O	4:P:301:THR:OG1	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:335:GLU:OE1	6:A:388:ARG:NH1	2.48	0.41
6:B:573:HIS:CG	6:B:615:LEU:HD13	2.55	0.41
7:E:374:GLU:HA	7:E:400:ARG:HD2	2.02	0.41
7:F:135:SER:O	7:F:135:SER:OG	2.38	0.41
14:S:72:THR:O	14:S:76:LEU:HG	2.21	0.41
4:P:414:VAL:O	4:P:418:VAL:HG22	2.21	0.41
5:R:208:ASP:OD1	5:R:209:PRO:HD2	2.21	0.41
6:C:194:LEU:HD23	6:C:201:GLU:HB3	2.03	0.41
8:Z:113:GLU:O	8:Z:117:GLN:HG2	2.21	0.41
10:N:45:ILE:O	10:N:49:GLU:HG2	2.20	0.41
11:0:63:VAL:HG22	12:1:105:ALA:HB2	2.02	0.41
11:0:91:LEU:HD12	11:0:91:LEU:HA	1.83	0.41
12:3:41:ILE:O	12:3:45:SER:HB3	2.21	0.41
16:U:312:THR:HG22	16:U:322:THR:OG1	2.21	0.41
18:W:5:SIA:O7	18:W:5:SIA:H113	2.21	0.41
1:H:127:LEU:HD23	1:H:127:LEU:HA	1.92	0.41
2:L:40:ALA:O	2:L:43:GLU:HG2	2.21	0.41
3:O:163:THR:HA	3:O:249:ARG:NH2	2.34	0.41
3:O:281:ARG:O	3:O:285:VAL:HG22	2.21	0.41
4:P:132:ARG:C	4:P:135:PRO:HD2	2.41	0.41
4:P:258:GLU:H	4:P:258:GLU:HG3	1.38	0.41
4:P:433:GLY:HA2	4:P:436:LEU:HD12	2.02	0.41
5:R:61:MET:SD	5:R:64:LYS:HE3	2.61	0.41
6:B:437:LYS:O	6:B:441:GLN:HG3	2.20	0.41
6:C:426:LEU:HD23	6:C:426:LEU:HA	1.90	0.41
6:C:511:VAL:HG21	6:C:548:TYR:HB2	2.03	0.41
7:D:164:ILE:HD11	7:D:342:GLU:HA	2.02	0.41
8:Z:241:VAL:HG13	8:Z:242:LEU:HG	2.03	0.41
11:0:3:GLY:HA3	25:0:305:WSS:C1	2.50	0.41
11:0:84:PRO:O	11:0:87:LYS:HG2	2.21	0.41
12:1:55:SER:O	12:1:58:PRO:HD2	2.21	0.41
12:3:44:MET:HG2	12:3:119:ARG:HA	2.03	0.41
12:4:154:THR:O	12:4:154:THR:OG1	2.36	0.41
13:Q:179:GLU:H	13:Q:179:GLU:HG2	1.72	0.41
16:U:284:ASP:O	16:U:285:LEU:HD23	2.21	0.41
1:H:21:GLN:O	1:H:25:GLU:HG2	2.20	0.41
1:H:31:ASP:OD2	1:H:32:ALA:N	2.54	0.41
3:O:63:ALA:O	3:O:66:GLU:HG2	2.20	0.41
4:P:229:GLY:O	4:P:233:ASN:ND2	2.47	0.41
4:P:336:LYS:O	4:P:339:LEU:HG	2.21	0.41
8:X:242:LEU:HD23	8:X:242:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:101:LEU:HD23	12:1:101:LEU:HA	1.89	0.41
12:2:34:THR:HG23	12:2:59:VAL:HG13	2.03	0.41
1:H:133:ILE:HA	1:H:166:GLN:O	2.22	0.40
1:I:82:LYS:HB3	1:I:82:LYS:HE3	1.76	0.40
2:K:47:TYR:HA	2:K:50:GLN:HG2	2.04	0.40
2:L:76:GLU:O	2:L:79:GLU:HG3	2.20	0.40
2:M:20:GLU:OE1	2:M:21:LYS:N	2.53	0.40
3:O:181:TYR:HD2	3:O:230:PHE:CE1	2.39	0.40
4:P:304:GLU:O	4:P:308:ALA:HB3	2.21	0.40
5:R:130:PHE:HB3	5:R:202:ILE:HG12	2.03	0.40
6:C:104:ARG:HE	6:C:104:ARG:HB2	1.66	0.40
6:C:271:VAL:HB	6:C:344:VAL:HG22	2.03	0.40
7:D:444:LEU:HD23	7:D:449:LEU:HG	2.03	0.40
16:U:445:HIS:CE1	24:U:503:PTY:C31	3.03	0.40
16:U:453:MET:SD	16:U:453:MET:N	2.92	0.40
1:I:202:LEU:O	1:I:206:GLN:HG2	2.21	0.40
1:J:215:LEU:HD23	2:M:91:ASN:HB2	2.04	0.40
3:O:13:LYS:HB2	3:O:13:LYS:HE2	1.77	0.40
5:R:22:ALA:HA	5:R:25:CYS:SG	2.61	0.40
5:R:188:TRP:HB3	5:R:192:ARG:HE	1.87	0.40
5:R:226:GLY:O	5:R:230:LYS:N	2.46	0.40
5:R:253:GLU:HA	5:R:256:GLU:OE1	2.21	0.40
5:R:401:PHE:HZ	14:S:51:PHE:HB2	1.86	0.40
6:B:551:ALA:HB2	6:B:612:PHE:HZ	1.86	0.40
7:E:232:ALA:HB3	7:E:297:LEU:HD23	2.02	0.40
7:E:237:ASN:ND2	7:E:240:THR:H	2.19	0.40
8:X:263:ILE:O	8:X:267:VAL:HG13	2.21	0.40
8:Z:71:SER:OG	8:Z:73:LYS:HD2	2.22	0.40
12:7:44:MET:HB2	12:7:122:ALA:HB2	2.03	0.40
2:M:43:GLU:O	2:M:46:GLN:HB2	2.22	0.40
7:D:76:LEU:HB2	7:D:80:THR:HG23	2.04	0.40
7:F:61:ASP:OD1	7:F:62:HIS:N	2.50	0.40
8:Z:98:ILE:H	8:Z:98:ILE:HG12	1.79	0.40
12:4:80:LEU:HD23	12:4:80:LEU:HA	1.88	0.40
16:U:262:ASP:C	16:U:264:ALA:H	2.24	0.40
2:L:18:ALA:HA	2:L:21:LYS:HD3	2.03	0.40
2:L:45:GLU:O	2:L:49:LEU:HD22	2.22	0.40
3:O:21:LYS:HG3	3:O:22:LEU:H	1.86	0.40
3:O:150:LEU:HB2	3:O:268:LEU:HD22	2.02	0.40
4:P:130:LEU:O	4:P:133:GLN:NE2	2.49	0.40
5:R:202:ILE:HB	5:R:217:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:215:ARG:HA	6:A:216:PRO:HD3	1.94	0.40
7:E:166:PRO:HA	7:E:340:ARG:HD3	2.02	0.40
7:E:182:SER:HB2	7:E:402:MET:HG3	2.03	0.40
7:E:445:THR:HG22	7:E:446:SER:N	2.37	0.40
8:Y:171:ASP:OD2	8:Y:171:ASP:N	2.54	0.40
9:G:131:LEU:HD23	9:G:131:LEU:HA	1.86	0.40
11:0:70:TYR:CD1	11:0:70:TYR:C	2.95	0.40
11:0:196:LEU:HD12	12:9:74:VAL:HG22	2.02	0.40
12:8:91:LEU:HD13	12:8:155:LYS:HB3	2.03	0.40
1:H:57:TYR:CE1	2:K:51:ARG:HD2	2.57	0.40
1:I:8:VAL:HB	5:R:196:PHE:HE1	1.87	0.40
1:J:18:PHE:O	1:J:21:GLN:HB2	2.22	0.40
2:K:69:CYS:O	2:K:73:VAL:HG23	2.22	0.40
2:L:9:GLN:HA	2:L:12:LEU:HG	2.02	0.40
4:P:103:GLU:O	4:P:104:ASN:ND2	2.54	0.40
4:P:394:LEU:HD12	4:P:394:LEU:HA	1.89	0.40
5:R:12:LEU:HD12	5:R:12:LEU:HA	1.87	0.40
5:R:548:MET:HG2	5:R:813:LYS:HE2	2.04	0.40
5:R:804:ARG:NH1	5:R:809:GLU:OE2	2.52	0.40
6:B:25:SER:HB2	7:E:88:GLU:HG3	2.04	0.40
6:C:343:HIS:ND1	6:C:403:SER:HB3	2.36	0.40
7:E:124:SER:HA	7:E:148:GLU:HB2	2.04	0.40
12:3:83:ASP:OD2	12:3:83:ASP:N	2.55	0.40
12:5:86:LEU:HD12	12:5:86:LEU:HA	1.87	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	H	223/226 (99%)	213 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	223/226 (99%)	218 (98%)	5 (2%)	0	100	100
1	J	223/226 (99%)	221 (99%)	2 (1%)	0	100	100
2	K	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
2	L	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
2	M	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
3	O	355/382 (93%)	325 (92%)	29 (8%)	1 (0%)	41	73
4	P	423/483 (88%)	379 (90%)	41 (10%)	3 (1%)	22	57
5	R	745/837 (89%)	698 (94%)	47 (6%)	0	100	100
6	A	598/617 (97%)	572 (96%)	26 (4%)	0	100	100
6	B	598/617 (97%)	562 (94%)	36 (6%)	0	100	100
6	C	598/617 (97%)	567 (95%)	30 (5%)	1 (0%)	47	79
7	D	456/511 (89%)	432 (95%)	24 (5%)	0	100	100
7	E	456/511 (89%)	434 (95%)	22 (5%)	0	100	100
7	F	456/511 (89%)	440 (96%)	16 (4%)	0	100	100
8	X	260/573 (45%)	248 (95%)	12 (5%)	0	100	100
8	Y	265/573 (46%)	250 (94%)	15 (6%)	0	100	100
8	Z	260/573 (45%)	238 (92%)	22 (8%)	0	100	100
9	G	211/247 (85%)	201 (95%)	10 (5%)	0	100	100
10	N	108/119 (91%)	97 (90%)	11 (10%)	0	100	100
11	0	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
12	1	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
12	2	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
12	3	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
12	4	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
12	5	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
12	6	148/155 (96%)	139 (94%)	9 (6%)	0	100	100
12	7	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
12	8	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	9	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
13	Q	348/351 (99%)	333 (96%)	15 (4%)	0	100	100
14	S	75/81 (93%)	70 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	T	83/137 (61%)	76 (92%)	7 (8%)	0	100 100
16	U	203/470 (43%)	187 (92%)	16 (8%)	0	100 100
17	V	48/350 (14%)	44 (92%)	4 (8%)	0	100 100
All	All	9085/11192 (81%)	8610 (95%)	470 (5%)	5 (0%)	54 83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	P	109	SER
4	P	30	LYS
6	C	35	ALA
3	O	313	PRO
4	P	31	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	198/199 (100%)	182 (92%)	16 (8%)	11 39
1	I	198/199 (100%)	188 (95%)	10 (5%)	24 56
1	J	198/199 (100%)	185 (93%)	13 (7%)	16 47
2	K	99/101 (98%)	88 (89%)	11 (11%)	6 24
2	L	99/101 (98%)	92 (93%)	7 (7%)	14 44
2	M	99/101 (98%)	81 (82%)	18 (18%)	1 7
3	O	323/344 (94%)	274 (85%)	49 (15%)	3 12
4	P	385/429 (90%)	320 (83%)	65 (17%)	2 9
5	R	673/746 (90%)	622 (92%)	51 (8%)	13 41
6	A	507/525 (97%)	470 (93%)	37 (7%)	14 43
6	B	508/525 (97%)	471 (93%)	37 (7%)	14 43
6	C	508/525 (97%)	479 (94%)	29 (6%)	20 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	393/430 (91%)	376 (96%)	17 (4%)	29	62
7	E	390/430 (91%)	369 (95%)	21 (5%)	22	53
7	F	392/430 (91%)	376 (96%)	16 (4%)	30	64
8	X	238/519 (46%)	210 (88%)	28 (12%)	5	21
8	Y	239/519 (46%)	215 (90%)	24 (10%)	7	28
8	Z	237/519 (46%)	212 (90%)	25 (10%)	7	26
9	G	183/212 (86%)	168 (92%)	15 (8%)	11	38
10	N	94/100 (94%)	90 (96%)	4 (4%)	29	62
11	0	153/155 (99%)	147 (96%)	6 (4%)	32	65
12	1	107/112 (96%)	103 (96%)	4 (4%)	34	66
12	2	107/112 (96%)	106 (99%)	1 (1%)	78	91
12	3	107/112 (96%)	104 (97%)	3 (3%)	43	73
12	4	107/112 (96%)	102 (95%)	5 (5%)	26	59
12	5	107/112 (96%)	102 (95%)	5 (5%)	26	59
12	6	107/112 (96%)	100 (94%)	7 (6%)	17	47
12	7	106/112 (95%)	104 (98%)	2 (2%)	57	81
12	8	107/112 (96%)	102 (95%)	5 (5%)	26	59
12	9	107/112 (96%)	102 (95%)	5 (5%)	26	59
13	Q	303/306 (99%)	288 (95%)	15 (5%)	24	57
14	S	69/72 (96%)	66 (96%)	3 (4%)	29	62
15	T	70/116 (60%)	65 (93%)	5 (7%)	14	44
16	U	182/397 (46%)	171 (94%)	11 (6%)	19	49
17	V	45/308 (15%)	44 (98%)	1 (2%)	52	78
All	All	7745/9515 (81%)	7174 (93%)	571 (7%)	17	42

All (571) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	13	LYS
1	H	38	PHE
1	H	42	LYS
1	H	52	LYS
1	H	56	TYR
1	H	57	TYR

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Mol	Chain	Res	Type
1	H	60	LYS
1	H	73	SER
1	H	104	LYS
1	H	110	THR
1	H	175	GLU
1	H	176	ASP
1	H	187	ASP
1	H	202	LEU
1	H	210	GLU
1	H	212	ARG
1	I	7	ASP
1	I	10	LYS
1	I	13	LYS
1	I	44	ARG
1	I	59	LYS
1	I	103	SER
1	I	171	SER
1	I	175	GLU
1	I	176	ASP
1	I	224	PHE
1	J	10	LYS
1	J	11	GLN
1	J	26	LYS
1	J	31	ASP
1	J	44	ARG
1	J	56	TYR
1	J	59	LYS
1	J	73	SER
1	J	74	ASN
1	J	88	ASP
1	J	171	SER
1	J	175	GLU
1	J	202	LEU
2	K	6	GLN
2	K	21	LYS
2	K	37	LYS
2	K	47	TYR
2	K	55	PHE
2	K	56	LYS
2	K	59	GLU
2	K	69	CYS
2	K	75	LYS

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Mol	Chain	Res	Type
2	K	87	TYR
2	K	116	ILE
2	L	49	LEU
2	L	66	ARG
2	L	68	SER
2	L	79	GLU
2	L	87	TYR
2	L	99	LEU
2	L	102	PHE
2	M	3	SER
2	M	9	GLN
2	M	11	LEU
2	M	13	GLN
2	M	16	LYS
2	M	20	GLU
2	M	21	LYS
2	M	24	GLU
2	M	27	LYS
2	M	31	ARG
2	M	34	LYS
2	M	48	ARG
2	M	49	LEU
2	M	53	LYS
2	M	56	LYS
2	M	66	ARG
2	M	73	VAL
2	M	99	LEU
3	O	8	SER
3	O	15	CYS
3	O	39	ASN
3	O	42	ASP
3	O	54	LEU
3	O	58	LEU
3	O	78	ASP
3	O	85	ASP
3	O	86	LYS
3	O	94	ASN
3	O	97	ASP
3	O	98	LEU
3	O	105	PHE
3	O	109	MET
3	O	119	LYS

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Mol	Chain	Res	Type
3	O	122	SER
3	O	127	LYS
3	O	137	LYS
3	O	146	LEU
3	O	150	LEU
3	O	152	ASN
3	O	164	ARG
3	O	166	LEU
3	O	171	LYS
3	O	172	LYS
3	O	174	ASP
3	O	182	LEU
3	O	188	VAL
3	O	191	LYS
3	O	192	LEU
3	O	199	LYS
3	O	207	MET
3	O	217	SER
3	O	229	LEU
3	O	230	PHE
3	O	239	HIS
3	O	250	ASP
3	O	269	SER
3	O	273	LYS
3	O	274	LYS
3	O	281	ARG
3	O	306	SER
3	O	307	VAL
3	O	325	LYS
3	O	326	LYS
3	O	329	LYS
3	O	330	LYS
3	O	340	LYS
3	O	375	ASP
4	P	18	ILE
4	P	34	GLN
4	P	36	TYR
4	P	41	MET
4	P	51	GLN
4	P	53	PHE
4	P	54	GLU
4	P	56	LYS

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Mol	Chain	Res	Type
4	P	57	ARG
4	P	75	LYS
4	P	81	MET
4	P	88	GLN
4	P	89	THR
4	P	91	GLN
4	P	95	THR
4	P	106	GLN
4	P	114	TYR
4	P	118	SER
4	P	125	TYR
4	P	127	LEU
4	P	129	MET
4	P	136	PHE
4	P	138	VAL
4	P	144	ILE
4	P	155	LEU
4	P	162	ASN
4	P	166	ASN
4	P	169	LYS
4	P	171	GLN
4	P	172	LEU
4	P	206	GLN
4	P	210	ARG
4	P	214	TYR
4	P	222	ASP
4	P	224	VAL
4	P	225	ASN
4	P	227	ILE
4	P	252	PHE
4	P	258	GLU
4	P	263	TYR
4	P	292	PHE
4	P	299	ARG
4	P	300	GLU
4	P	305	TYR
4	P	313	LYS
4	P	331	ILE
4	P	345	SER
4	P	349	LEU
4	P	350	SER
4	P	351	SER

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Mol	Chain	Res	Type
4	P	352	PHE
4	P	353	ASP
4	P	354	GLU
4	P	376	TRP
4	P	386	LYS
4	P	391	LEU
4	P	403	ASP
4	P	413	ASP
4	P	423	ARG
4	P	426	ARG
4	P	444	GLU
4	P	446	GLN
4	P	450	TYR
4	P	451	ASN
4	P	454	LEU
5	R	4	LEU
5	R	5	PHE
5	R	6	ARG
5	R	18	GLN
5	R	28	GLU
5	R	34	LYS
5	R	43	ASP
5	R	46	VAL
5	R	64	LYS
5	R	66	ARG
5	R	82	THR
5	R	85	ASN
5	R	92	ARG
5	R	103	LYS
5	R	124	GLU
5	R	176	ASN
5	R	177	ARG
5	R	178	GLU
5	R	179	ARG
5	R	191	CYS
5	R	195	VAL
5	R	204	ASN
5	R	206	LEU
5	R	211	THR
5	R	215	VAL
5	R	227	ASP
5	R	241	ARG

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Mol	Chain	Res	Type
5	R	284	GLN
5	R	291	ARG
5	R	316	GLN
5	R	332	SER
5	R	348	VAL
5	R	371	THR
5	R	383	ILE
5	R	426	ARG
5	R	469	SER
5	R	472	LEU
5	R	478	SER
5	R	492	GLU
5	R	539	MET
5	R	552	VAL
5	R	619	SER
5	R	626	SER
5	R	666	LYS
5	R	711	PHE
5	R	718	VAL
5	R	719	HIS
5	R	731	CYS
5	R	740	ARG
5	R	768	SER
5	R	804	ARG
6	A	68	GLU
6	A	69	GLU
6	A	103	GLN
6	A	129	ARG
6	A	136	THR
6	A	157	SER
6	A	160	SER
6	A	175	THR
6	A	188	SER
6	A	266	TYR
6	A	268	ASN
6	A	291	PHE
6	A	296	MET
6	A	308	ARG
6	A	324	GLU
6	A	327	ILE
6	A	350	SER
6	A	356	GLU

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Mol	Chain	Res	Type
6	A	362	SER
6	A	381	ARG
6	A	400	ARG
6	A	403	SER
6	A	405	SER
6	A	417	PHE
6	A	423	SER
6	A	447	SER
6	A	450	TRP
6	A	470	THR
6	A	471	GLU
6	A	478	LYS
6	A	558	THR
6	A	560	GLN
6	A	561	SER
6	A	592	ASP
6	A	606	GLU
6	A	608	MET
6	A	614	SER
6	B	18	PHE
6	B	25	SER
6	B	33	ASP
6	B	110	SER
6	B	136	THR
6	B	145	SER
6	B	157	SER
6	B	161	LEU
6	B	215	ARG
6	B	235	ASP
6	B	266	TYR
6	B	291	PHE
6	B	308	ARG
6	B	327	ILE
6	B	350	SER
6	B	358	LEU
6	B	371	ASP
6	B	384	SER
6	B	387	GLU
6	B	419	ASP
6	B	436	ASP
6	B	450	TRP
6	B	455	SER

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Mol	Chain	Res	Type
6	B	471	GLU
6	B	494	GLN
6	B	495	LEU
6	B	500	SER
6	B	510	GLU
6	B	529	ASP
6	B	542	SER
6	B	556	GLU
6	B	561	SER
6	B	571	ARG
6	B	583	SER
6	B	591	LYS
6	B	592	ASP
6	B	614	SER
6	C	18	PHE
6	C	25	SER
6	C	33	ASP
6	C	60	ASP
6	C	74	SER
6	C	111	SER
6	C	177	THR
6	C	201	GLU
6	C	262	SER
6	C	308	ARG
6	C	345	SER
6	C	346	MET
6	C	349	ASP
6	C	350	SER
6	C	362	SER
6	C	384	SER
6	C	395	LEU
6	C	400	ARG
6	C	403	SER
6	C	419	ASP
6	C	450	TRP
6	C	542	SER
6	C	555	VAL
6	C	556	GLU
6	C	571	ARG
6	C	588	ASP
6	C	590	LEU
6	C	591	LYS

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Mol	Chain	Res	Type
6	C	599	SER
7	D	54	ASN
7	D	60	LEU
7	D	64	LYS
7	D	80	THR
7	D	97	GLN
7	D	103	SER
7	D	156	GLN
7	D	250	GLU
7	D	299	ASP
7	D	311	SER
7	D	329	THR
7	D	351	ILE
7	D	386	ARG
7	D	431	ASP
7	D	436	LYS
7	D	449	LEU
7	D	472	THR
7	E	51	SER
7	E	80	THR
7	E	83	SER
7	E	103	SER
7	E	141	ARG
7	E	161	GLN
7	E	201	GLU
7	E	215	LYS
7	E	237	ASN
7	E	256	ASN
7	E	268	THR
7	E	276	ARG
7	E	305	GLU
7	E	311	SER
7	E	330	ASP
7	E	347	SER
7	E	376	GLN
7	E	397	SER
7	E	403	LYS
7	E	470	ASN
7	E	473	VAL
7	F	46	THR
7	F	54	ASN
7	F	64	LYS

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Mol	Chain	Res	Type
7	F	75	THR
7	F	83	SER
7	F	126	ASP
7	F	135	SER
7	F	201	GLU
7	F	216	SER
7	F	253	SER
7	F	299	ASP
7	F	311	SER
7	F	314	ARG
7	F	354	LEU
7	F	394	VAL
7	F	442	GLU
8	X	32	CYS
8	X	48	ASP
8	X	71	SER
8	X	99	SER
8	X	104	LYS
8	X	105	LEU
8	X	109	GLU
8	X	123	LYS
8	X	125	ASP
8	X	126	TYR
8	X	138	ASP
8	X	146	THR
8	X	166	TYR
8	X	171	ASP
8	X	179	PHE
8	X	206	ASP
8	X	209	GLU
8	X	217	LEU
8	X	221	ASP
8	X	223	LYS
8	X	229	MET
8	X	234	MET
8	X	236	LYS
8	X	237	LEU
8	X	245	LYS
8	X	247	SER
8	X	262	SER
8	X	265	ARG
8	Y	15	SER

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Mol	Chain	Res	Type
8	Y	67	GLU
8	Y	79	ASP
8	Y	103	MET
8	Y	124	SER
8	Y	125	ASP
8	Y	126	TYR
8	Y	146	THR
8	Y	157	SER
8	Y	171	ASP
8	Y	179	PHE
8	Y	180	LYS
8	Y	198	HIS
8	Y	201	LYS
8	Y	205	LYS
8	Y	207	GLN
8	Y	211	SER
8	Y	227	LYS
8	Y	231	ASP
8	Y	234	MET
8	Y	238	SER
8	Y	240	LYS
8	Y	265	ARG
8	Y	271	GLU
8	Z	15	SER
8	Z	67	GLU
8	Z	71	SER
8	Z	73	LYS
8	Z	74	CYS
8	Z	81	LEU
8	Z	109	GLU
8	Z	124	SER
8	Z	125	ASP
8	Z	126	TYR
8	Z	136	LEU
8	Z	156	THR
8	Z	161	MET
8	Z	179	PHE
8	Z	191	GLU
8	Z	199	LEU
8	Z	207	GLN
8	Z	222	GLN
8	Z	227	LYS

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Mol	Chain	Res	Type
8	Z	234	MET
8	Z	237	LEU
8	Z	249	LEU
8	Z	251	SER
8	Z	252	SER
8	Z	269	GLU
9	G	5	ASP
9	G	37	SER
9	G	42	LEU
9	G	58	MET
9	G	100	ASN
9	G	116	THR
9	G	129	GLU
9	G	140	LYS
9	G	150	SER
9	G	151	LEU
9	G	160	GLU
9	G	212	LEU
9	G	213	LYS
9	G	214	GLU
9	G	215	LYS
10	N	13	ASP
10	N	15	ASP
10	N	35	ASN
10	N	50	ASP
11	0	26	TYR
11	0	36	ASP
11	0	70	TYR
11	0	88	THR
11	0	98	GLU
11	0	160	SER
12	1	45	SER
12	1	55	SER
12	1	85	SER
12	1	129	VAL
12	2	89	SER
12	3	45	SER
12	3	47	MET
12	3	75	LEU
12	4	26	SER
12	4	53	MET
12	4	79	SER

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Mol	Chain	Res	Type
12	4	82	ASP
12	4	155	LYS
12	5	6	SER
12	5	20	SER
12	5	79	SER
12	5	85	SER
12	5	153	SER
12	6	12	SER
12	6	28	LEU
12	6	75	LEU
12	6	79	SER
12	6	82	ASP
12	6	115	ASP
12	6	153	SER
12	7	26	SER
12	7	82	ASP
12	8	6	SER
12	8	37	SER
12	8	78	ASN
12	8	98	SER
12	8	153	SER
12	9	20	SER
12	9	82	ASP
12	9	98	SER
12	9	115	ASP
12	9	133	LEU
13	Q	3	PHE
13	Q	6	GLU
13	Q	45	LEU
13	Q	53	ASP
13	Q	63	SER
13	Q	78	MET
13	Q	109	VAL
13	Q	137	GLN
13	Q	166	ASP
13	Q	193	PHE
13	Q	199	LEU
13	Q	259	ASP
13	Q	284	ASN
13	Q	289	THR
13	Q	292	ASP
14	S	24	VAL

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Mol	Chain	Res	Type
14	S	26	TRP
14	S	30	LYS
15	T	53	CYS
15	T	88	LYS
15	T	97	ILE
15	T	104	VAL
15	T	126	VAL
16	U	335	SER
16	U	352	SER
16	U	375	SER
16	U	391	SER
16	U	408	MET
16	U	413	SER
16	U	417	ASP
16	U	434	LEU
16	U	452	THR
16	U	453	MET
16	U	454	ASP
17	V	304	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	100	GLN
1	H	149	GLN
1	H	166	GLN
1	H	219	ASN
1	I	11	GLN
1	I	24	ASN
1	I	47	GLN
1	I	66	GLN
1	I	149	GLN
1	J	21	GLN
1	J	24	ASN
1	J	47	GLN
1	J	63	GLN
1	J	67	GLN
1	J	74	ASN
1	J	77	ASN
1	J	100	GLN
1	J	149	GLN
1	J	219	ASN

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Mol	Chain	Res	Type
2	K	6	GLN
2	K	13	GLN
2	K	46	GLN
2	K	50	GLN
2	K	85	GLN
2	L	13	GLN
2	M	10	GLN
3	O	29	ASN
3	O	94	ASN
3	O	134	ASN
3	O	157	ASN
3	O	193	ASN
3	O	220	GLN
3	O	244	ASN
3	O	252	GLN
3	O	296	HIS
3	O	315	ASN
3	O	322	GLN
4	P	17	ASN
4	P	40	GLN
4	P	51	GLN
4	P	102	GLN
4	P	196	GLN
4	P	264	ASN
4	P	291	ASN
4	P	379	ASN
4	P	420	HIS
4	P	430	GLN
4	P	439	ASN
4	P	457	GLN
5	R	100	ASN
5	R	176	ASN
5	R	289	ASN
5	R	308	ASN
5	R	353	ASN
5	R	433	GLN
5	R	473	ASN
5	R	503	ASN
5	R	547	HIS
5	R	604	ASN
5	R	636	GLN
5	R	734	ASN

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Mol	Chain	Res	Type
5	R	761	HIS
6	A	172	ASN
6	A	213	GLN
6	A	430	GLN
6	A	441	GLN
6	A	444	HIS
6	A	603	GLN
6	B	65	GLN
6	B	140	ASN
6	B	172	ASN
6	B	261	GLN
6	B	314	ASN
6	B	521	GLN
6	B	560	GLN
6	C	140	ASN
6	C	172	ASN
6	C	261	GLN
6	C	441	GLN
6	C	449	ASN
7	D	85	GLN
7	D	97	GLN
7	D	156	GLN
7	D	350	GLN
7	E	156	GLN
7	E	237	ASN
7	E	256	ASN
7	E	350	GLN
7	E	363	HIS
7	E	382	GLN
7	E	470	ASN
7	F	54	ASN
7	F	85	GLN
7	F	97	GLN
7	F	237	ASN
7	F	350	GLN
8	X	59	ASN
8	X	134	ASN
8	X	198	HIS
8	X	243	GLN
8	Y	41	ASN
8	Y	160	GLN
8	Y	176	ASN

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Mol	Chain	Res	Type
8	Y	190	ASN
8	Y	196	GLN
8	Y	207	GLN
8	Y	270	ASN
8	Y	274	ASN
8	Z	149	ASN
8	Z	150	ASN
8	Z	177	GLN
8	Z	207	GLN
8	Z	274	ASN
9	G	31	ASN
9	G	85	GLN
9	G	88	ASN
9	G	91	GLN
9	G	100	ASN
9	G	152	GLN
9	G	206	GLN
10	N	67	ASN
10	N	83	GLN
11	0	90	ASN
12	5	51	GLN
12	5	78	ASN
12	5	123	GLN
13	Q	50	GLN
13	Q	137	GLN
13	Q	284	ASN
13	Q	338	GLN
14	S	67	GLN
15	T	107	ASN
16	U	272	GLN
16	U	329	ASN
16	U	348	HIS
16	U	398	GLN
16	U	401	GLN
16	U	411	GLN
16	U	445	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

30 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	BGC	W	1	18	12,12,12	0.55	0	17,17,17	1.39	4 (23%)
18	GAL	W	2	18	11,11,12	0.77	0	15,15,17	1.44	2 (13%)
18	NGA	W	3	18	14,14,15	0.43	0	17,19,21	1.94	6 (35%)
18	GAL	W	4	18	11,11,12	0.33	0	15,15,17	0.86	1 (6%)
18	SIA	W	5	18	20,20,21	0.60	0	24,28,31	1.37	2 (8%)
19	GAL	a	1	19	11,11,12	0.59	0	15,15,17	1.41	2 (13%)
19	NGA	a	2	19	14,14,15	0.70	0	17,19,21	1.85	4 (23%)
19	GAL	a	3	19	11,11,12	0.58	0	15,15,17	1.79	2 (13%)
19	SIA	a	4	19	20,20,21	0.73	1 (5%)	24,28,31	1.13	2 (8%)
20	NAG	b	1	16,20	14,14,15	0.23	0	17,19,21	0.51	0
20	NAG	b	2	20	14,14,15	0.27	0	17,19,21	0.47	0
20	NAG	c	1	16,20	14,14,15	0.53	0	17,19,21	0.74	0
20	NAG	c	2	20	14,14,15	0.24	0	17,19,21	0.85	1 (5%)
20	NAG	d	1	20	14,14,15	0.44	0	17,19,21	0.34	0
20	NAG	d	2	20	14,14,15	0.18	0	17,19,21	0.45	0
21	NAG	r	1	21,27	14,14,15	0.37	0	17,19,21	0.49	0
21	MAN	r	10	21	11,11,12	0.57	0	15,15,17	1.10	1 (6%)
21	MAN	r	11	21	11,11,12	0.37	0	15,15,17	0.82	1 (6%)
21	NAG	r	2	21	14,14,15	0.43	0	17,19,21	0.49	0
21	BMA	r	3	21	11,11,12	0.86	0	15,15,17	1.03	1 (6%)
21	MAN	r	4	21	11,11,12	0.91	1 (9%)	15,15,17	1.06	1 (6%)
21	MAN	r	5	21	11,11,12	0.95	1 (9%)	15,15,17	1.23	2 (13%)
21	MAN	r	6	21	11,11,12	0.86	1 (9%)	15,15,17	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	GLC	r	7	21	11,11,12	0.78	0	15,15,17	0.90	1 (6%)
21	GLC	r	8	21	11,11,12	0.64	0	15,15,17	0.90	0
21	GLC	r	9	21	11,11,12	0.66	0	15,15,17	0.75	0
20	NAG	s	1	14,20	14,14,15	0.25	0	17,19,21	0.66	1 (5%)
20	NAG	s	2	20	14,14,15	0.21	0	17,19,21	0.50	0
20	NAG	u	1	16,20	14,14,15	0.22	0	17,19,21	0.53	0
20	NAG	u	2	20	14,14,15	0.29	0	17,19,21	0.46	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	BGC	W	1	18	-	1/2/22/22	0/1/1/1
18	GAL	W	2	18	-	0/2/19/22	0/1/1/1
18	NGA	W	3	18	-	2/6/23/26	0/1/1/1
18	GAL	W	4	18	-	1/2/19/22	0/1/1/1
18	SIA	W	5	18	-	2/18/34/38	0/1/1/1
19	GAL	a	1	19	-	0/2/19/22	0/1/1/1
19	NGA	a	2	19	1/1/5/7	3/6/23/26	0/1/1/1
19	GAL	a	3	19	-	1/2/19/22	0/1/1/1
19	SIA	a	4	19	-	13/18/34/38	0/1/1/1
20	NAG	b	1	16,20	-	1/6/23/26	0/1/1/1
20	NAG	b	2	20	-	4/6/23/26	0/1/1/1
20	NAG	c	1	16,20	-	3/6/23/26	0/1/1/1
20	NAG	c	2	20	-	2/6/23/26	0/1/1/1
20	NAG	d	1	20	-	3/6/23/26	0/1/1/1
20	NAG	d	2	20	-	2/6/23/26	0/1/1/1
21	NAG	r	1	21,27	1/1/5/7	2/6/23/26	0/1/1/1
21	MAN	r	10	21	-	2/2/19/22	0/1/1/1
21	MAN	r	11	21	1/1/4/5	0/2/19/22	0/1/1/1
21	NAG	r	2	21	-	2/6/23/26	0/1/1/1
21	BMA	r	3	21	-	0/2/19/22	0/1/1/1
21	MAN	r	4	21	-	2/2/19/22	0/1/1/1
21	MAN	r	5	21	-	2/2/19/22	0/1/1/1
21	MAN	r	6	21	-	2/2/19/22	0/1/1/1
21	GLC	r	7	21	-	1/2/19/22	0/1/1/1
21	GLC	r	8	21	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	GLC	r	9	21	-	0/2/19/22	0/1/1/1
20	NAG	s	1	14,20	-	2/6/23/26	0/1/1/1
20	NAG	s	2	20	-	3/6/23/26	0/1/1/1
20	NAG	u	1	16,20	-	2/6/23/26	0/1/1/1
20	NAG	u	2	20	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	4	SIA	O1B-C1	-2.83	1.21	1.30
21	r	6	MAN	O5-C1	-2.62	1.39	1.43
21	r	4	MAN	O5-C1	-2.55	1.39	1.43
21	r	5	MAN	O5-C1	-2.02	1.40	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	2	NGA	C1-O5-C5	4.82	118.72	112.19
19	a	3	GAL	C1-C2-C3	4.51	115.20	109.67
19	a	3	GAL	C1-O5-C5	4.03	117.66	112.19
19	a	2	NGA	C2-N2-C7	-3.71	117.62	122.90
18	W	3	NGA	C1-C2-N2	3.71	116.82	110.49
18	W	5	SIA	C11-C10-N5	3.70	122.37	116.10
18	W	3	NGA	O5-C1-C2	-3.66	105.51	111.29
18	W	3	NGA	C4-C3-C2	-3.32	106.15	111.02
20	c	2	NAG	C1-O5-C5	3.15	116.46	112.19
19	a	4	SIA	O6-C2-C3	-3.12	106.17	110.46
21	r	5	MAN	O2-C2-C3	-3.09	103.94	110.14
18	W	3	NGA	C1-O5-C5	2.94	116.18	112.19
19	a	1	GAL	C1-C2-C3	2.79	113.10	109.67
21	r	4	MAN	O2-C2-C3	-2.72	104.69	110.14
21	r	3	BMA	O2-C2-C3	-2.70	104.72	110.14
18	W	2	GAL	O4-C4-C3	2.61	116.37	110.35
18	W	4	GAL	C1-C2-C3	2.58	112.83	109.67
18	W	1	BGC	C4-C3-C2	-2.50	106.46	110.82
18	W	1	BGC	O5-C5-C6	2.49	112.63	106.44
19	a	1	GAL	C1-O5-C5	-2.48	108.83	112.19
18	W	5	SIA	O9-C9-C8	-2.48	105.67	111.07
21	r	10	MAN	O2-C2-C3	-2.44	105.25	110.14
19	a	2	NGA	C1-C2-N2	2.42	114.62	110.49
21	r	6	MAN	O2-C2-C3	-2.40	105.33	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	2	NGA	O3-C3-C2	-2.38	104.54	109.47
18	W	3	NGA	O3-C3-C2	2.33	114.30	109.47
21	r	11	MAN	C1-O5-C5	-2.32	109.05	112.19
20	s	1	NAG	C1-O5-C5	2.26	115.25	112.19
18	W	1	BGC	O2-C2-C1	-2.24	103.96	109.16
18	W	2	GAL	C1-C2-C3	2.24	112.41	109.67
19	a	4	SIA	O1B-C1-C2	2.20	119.31	113.03
21	r	7	GLC	C1-C2-C3	2.16	112.32	109.67
21	r	5	MAN	C1-O5-C5	2.15	115.11	112.19
18	W	3	NGA	O3-C3-C4	-2.04	105.63	110.35
18	W	1	BGC	O2-C2-C3	-2.01	105.71	110.35

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	a	2	NGA	C1
21	r	1	NAG	C1
21	r	11	MAN	C1

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	W	3	NGA	C8-C7-N2-C2
18	W	3	NGA	O7-C7-N2-C2
19	a	4	SIA	C5-C6-C7-C8
19	a	4	SIA	C5-C6-C7-O7
19	a	4	SIA	O6-C6-C7-C8
19	a	4	SIA	O6-C6-C7-O7
19	a	4	SIA	C6-C7-C8-C9
19	a	4	SIA	C7-C8-C9-O9
21	r	10	MAN	O5-C5-C6-O6
20	s	2	NAG	C4-C5-C6-O6
19	a	4	SIA	O8-C8-C9-O9
20	b	2	NAG	O5-C5-C6-O6
20	d	1	NAG	O5-C5-C6-O6
21	r	4	MAN	O5-C5-C6-O6
20	c	2	NAG	O5-C5-C6-O6
21	r	4	MAN	C4-C5-C6-O6
20	d	1	NAG	C4-C5-C6-O6
21	r	10	MAN	C4-C5-C6-O6
20	s	1	NAG	O5-C5-C6-O6
20	s	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
20	b	2	NAG	C4-C5-C6-O6
19	a	4	SIA	O7-C7-C8-O8
21	r	1	NAG	O5-C5-C6-O6
21	r	6	MAN	O5-C5-C6-O6
19	a	4	SIA	C6-C7-C8-O8
19	a	4	SIA	C11-C10-N5-C5
19	a	4	SIA	O10-C10-N5-C5
19	a	4	SIA	O7-C7-C8-C9
20	u	1	NAG	C4-C5-C6-O6
21	r	1	NAG	C4-C5-C6-O6
21	r	6	MAN	C4-C5-C6-O6
20	s	1	NAG	C4-C5-C6-O6
18	W	5	SIA	C11-C10-N5-C5
18	W	5	SIA	O10-C10-N5-C5
19	a	2	NGA	C8-C7-N2-C2
20	b	2	NAG	C8-C7-N2-C2
20	b	2	NAG	O7-C7-N2-C2
20	d	2	NAG	C8-C7-N2-C2
20	d	2	NAG	O7-C7-N2-C2
20	c	2	NAG	C4-C5-C6-O6
20	c	1	NAG	O5-C5-C6-O6
20	u	1	NAG	O5-C5-C6-O6
21	r	5	MAN	O5-C5-C6-O6
19	a	2	NGA	O7-C7-N2-C2
21	r	5	MAN	C4-C5-C6-O6
18	W	4	GAL	O5-C5-C6-O6
20	u	2	NAG	O5-C5-C6-O6
20	b	1	NAG	O5-C5-C6-O6
20	c	1	NAG	C4-C5-C6-O6
21	r	7	GLC	O5-C5-C6-O6
20	c	1	NAG	C3-C2-N2-C7
19	a	2	NGA	C4-C5-C6-O6
21	r	2	NAG	C4-C5-C6-O6
19	a	3	GAL	O5-C5-C6-O6
19	a	4	SIA	O1A-C1-C2-O6
20	s	2	NAG	C3-C2-N2-C7
18	W	1	BGC	O5-C5-C6-O6
21	r	2	NAG	O5-C5-C6-O6
20	u	2	NAG	C3-C2-N2-C7
20	d	1	NAG	C3-C2-N2-C7

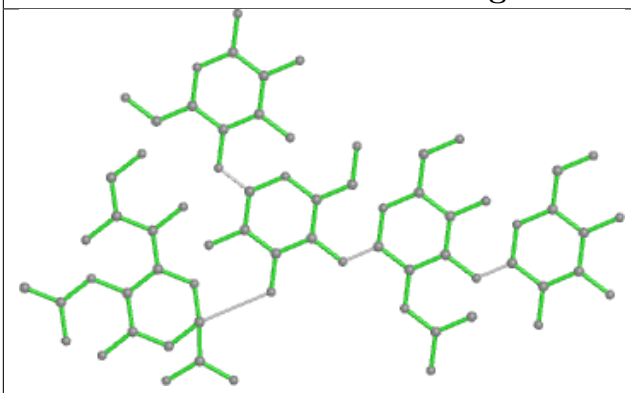
There are no ring outliers.

2 monomers are involved in 3 short contacts:

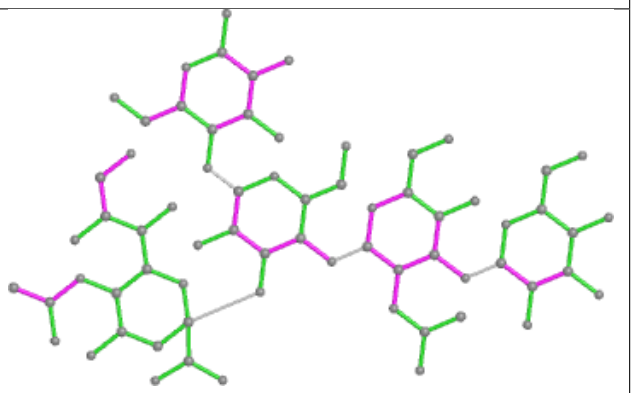
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	W	5	SIA	2	0
18	W	1	BGC	1	0

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

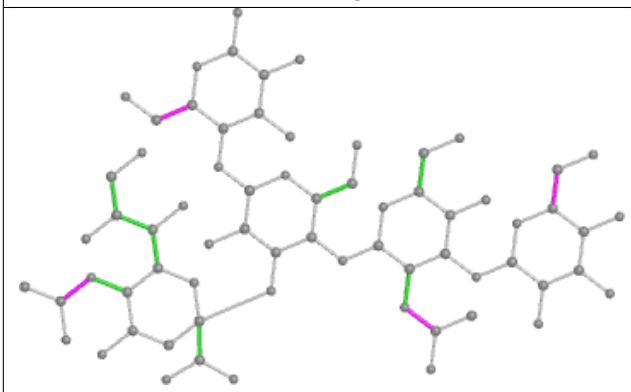
Oligosaccharide Chain W



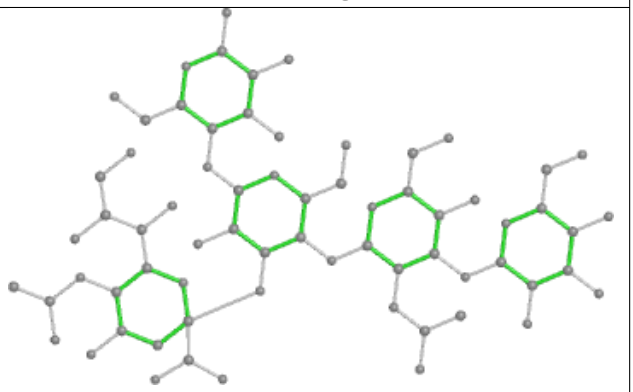
Bond lengths



Bond angles

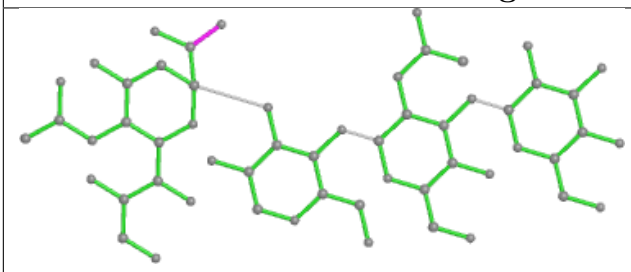


Torsions

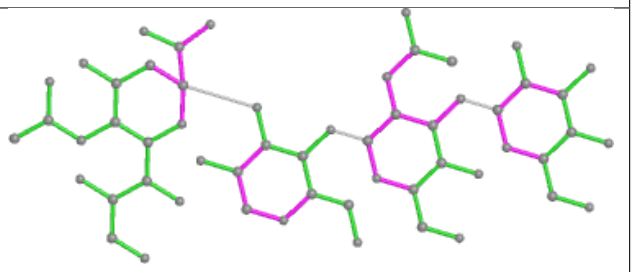


Rings

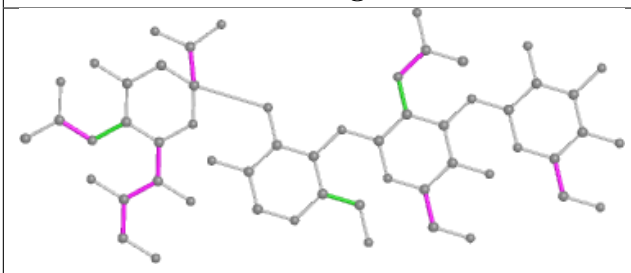
Oligosaccharide Chain a



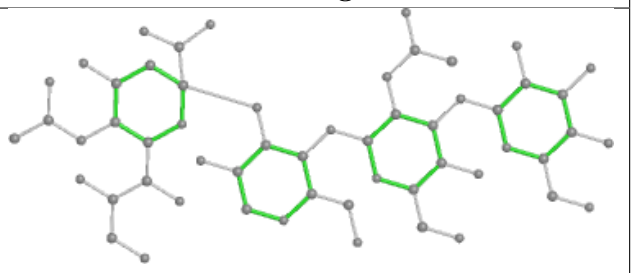
Bond lengths



Bond angles

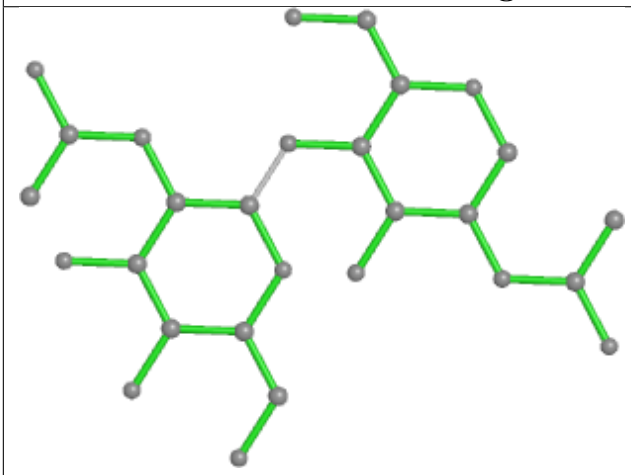


Torsions

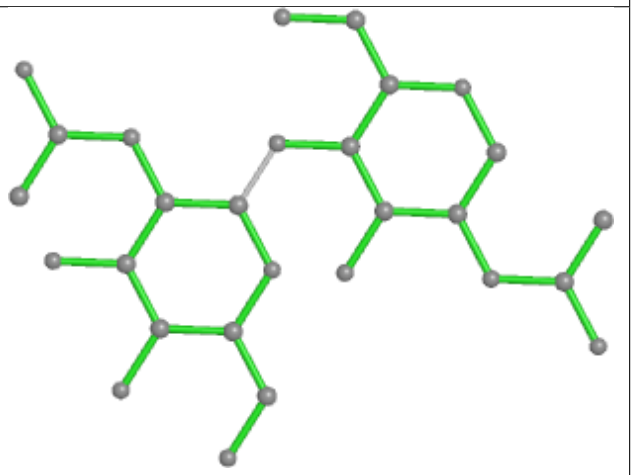


Rings

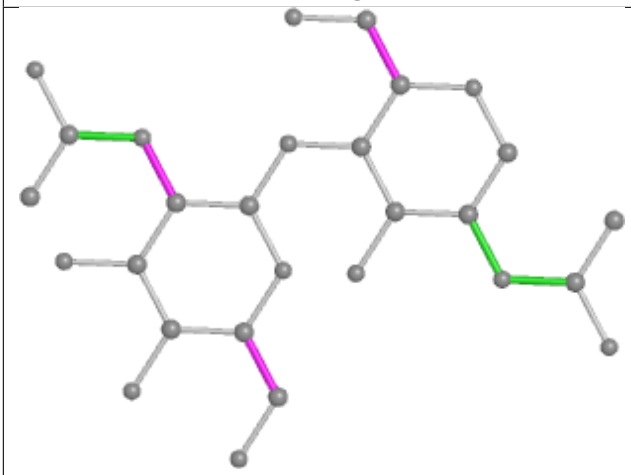
Oligosaccharide Chain u



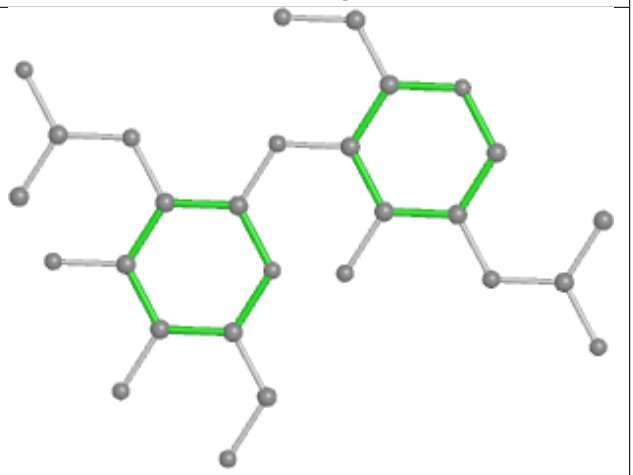
Bond lengths



Bond angles

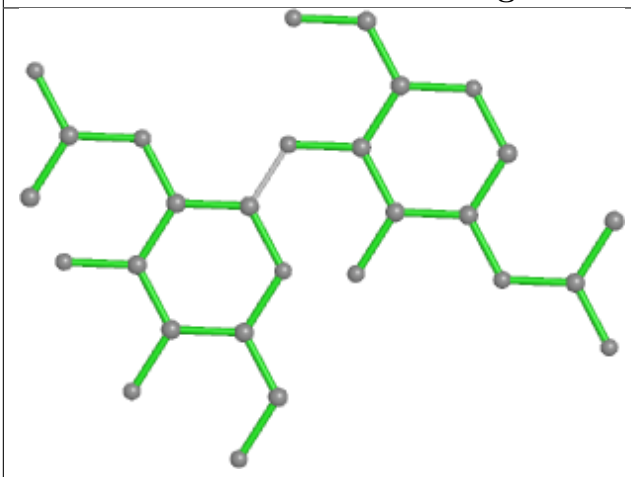


Torsions

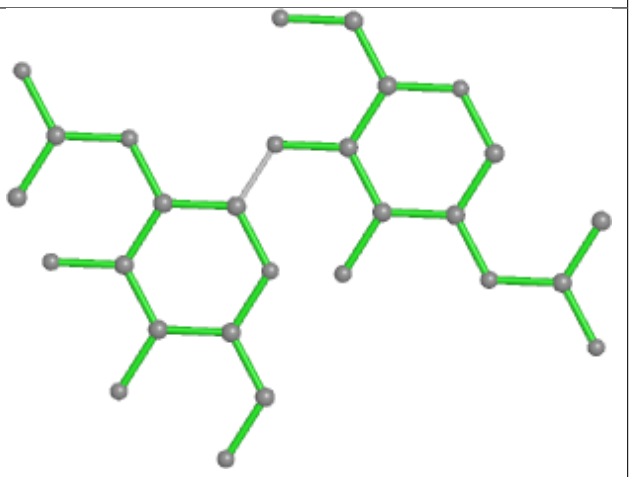


Rings

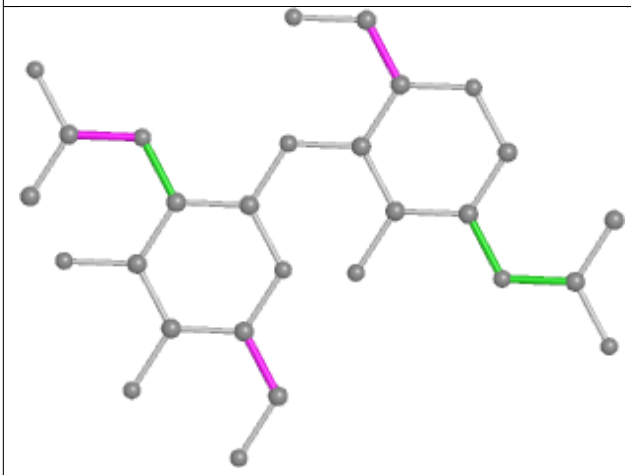
Oligosaccharide Chain b



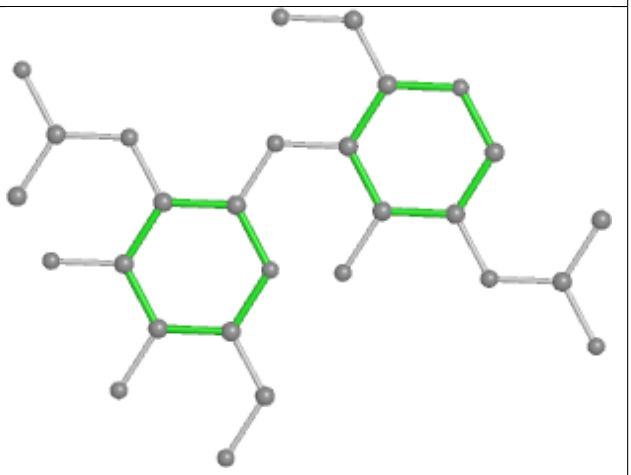
Bond lengths



Bond angles

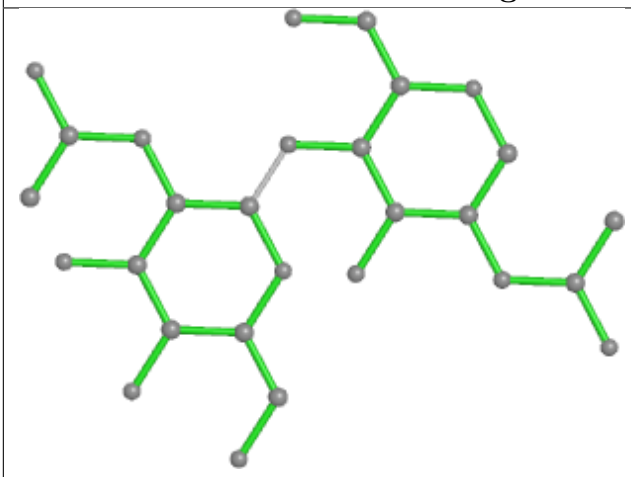


Torsions

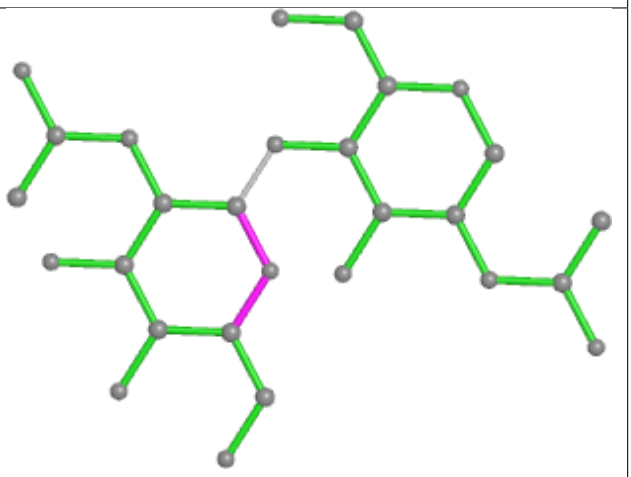


Rings

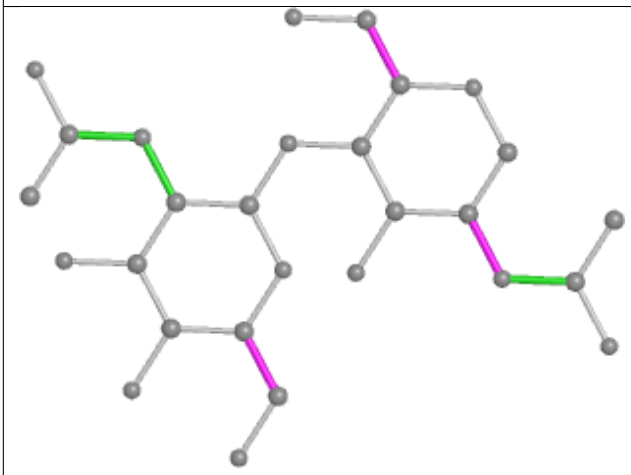
Oligosaccharide Chain c



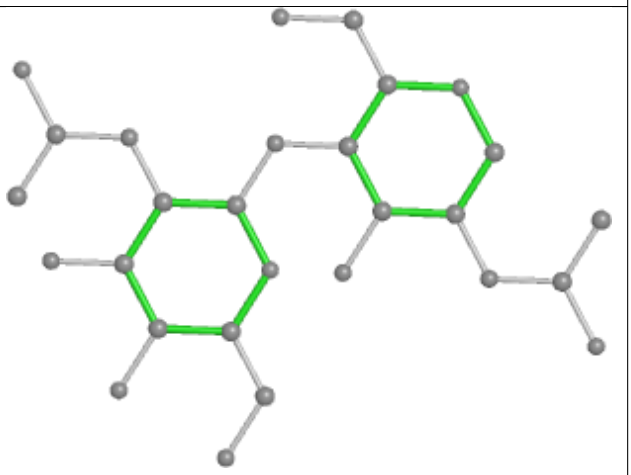
Bond lengths



Bond angles

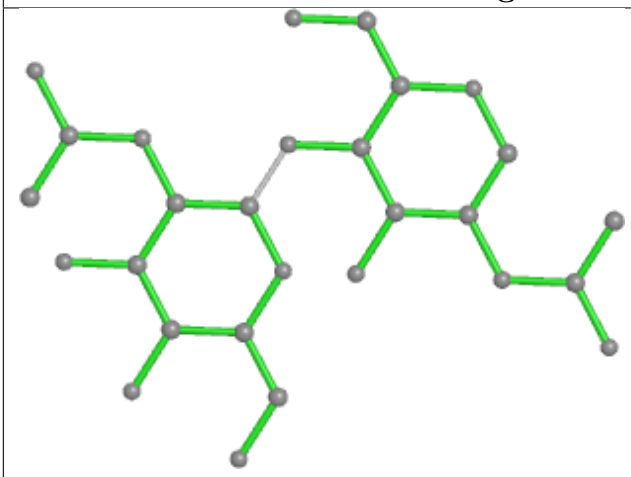


Torsions

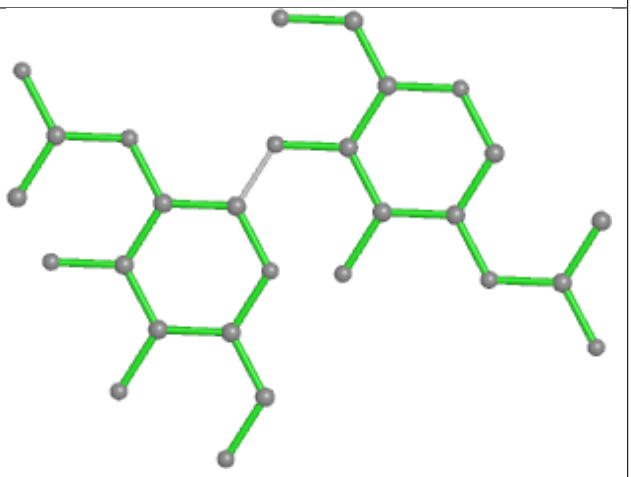


Rings

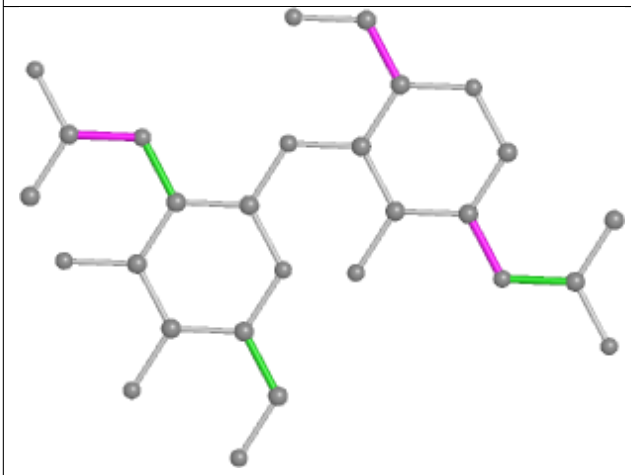
Oligosaccharide Chain d



Bond lengths



Bond angles



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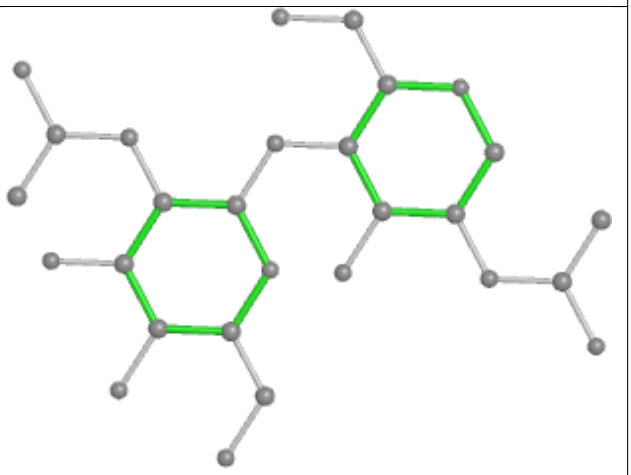
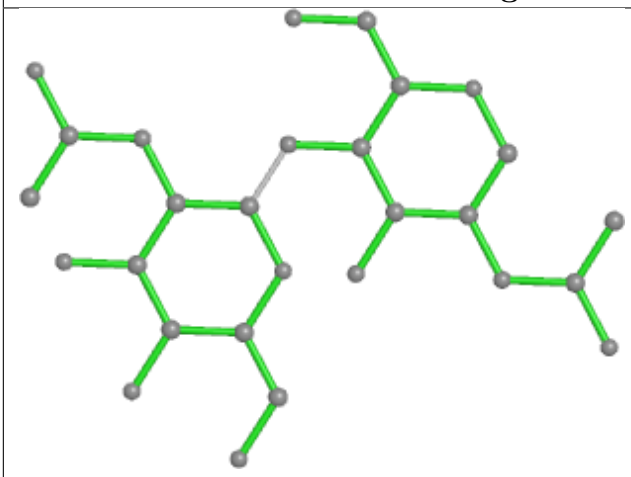
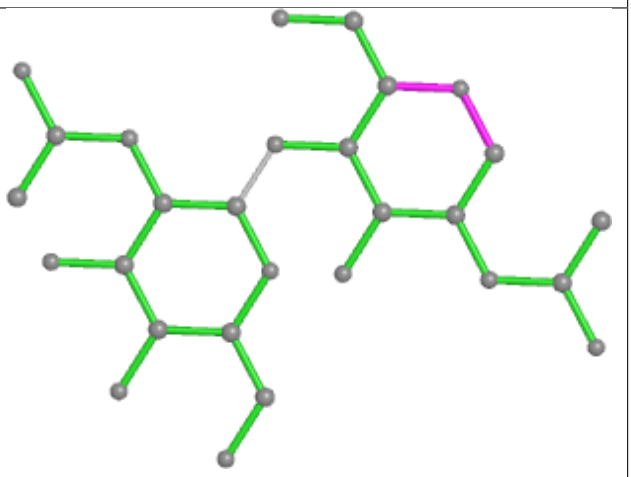


Rings

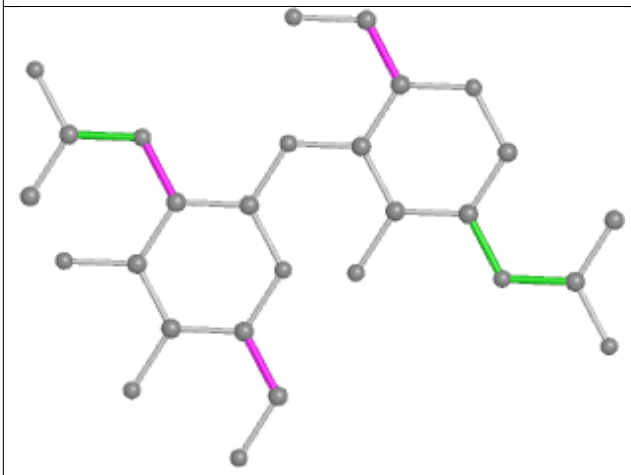
Oligosaccharide Chain s



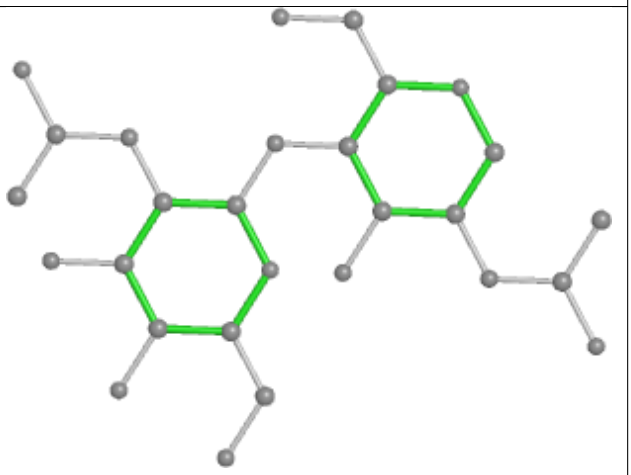
Bond lengths



Bond angles

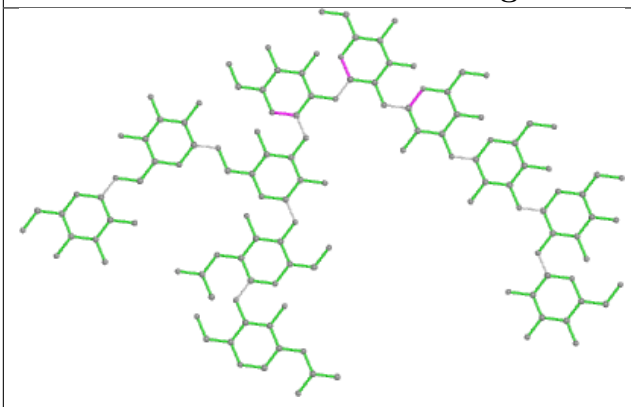


Torsions

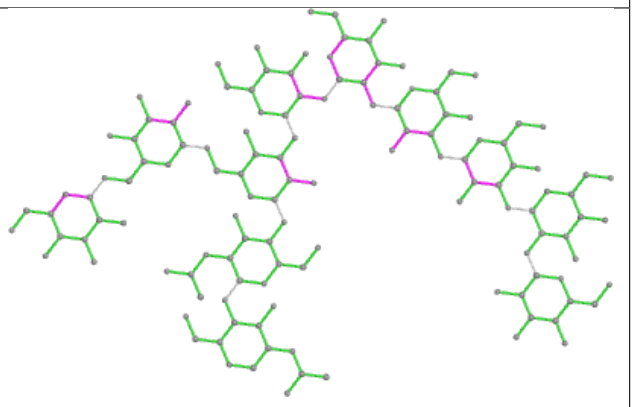


Rings

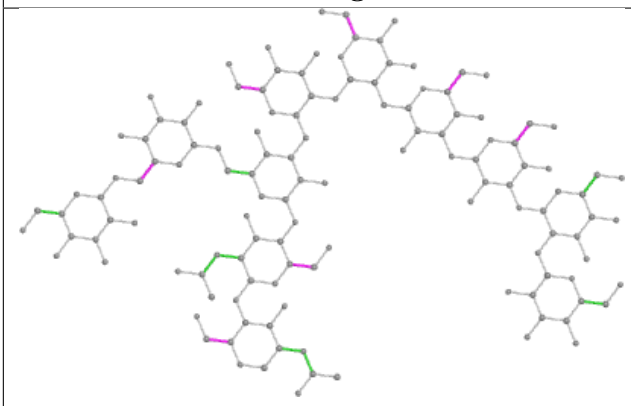
Oligosaccharide Chain r



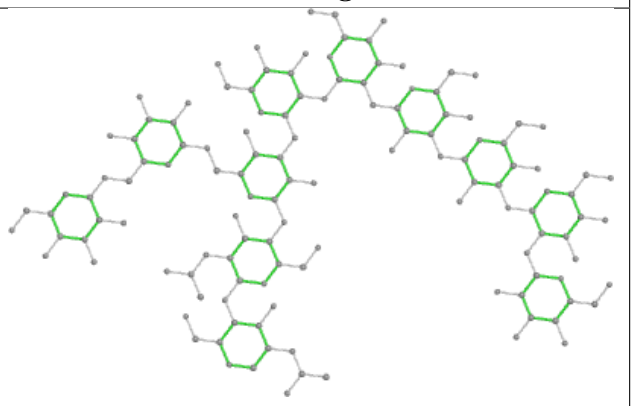
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

33 ligands 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	$\#\|Z\| > 2$
23	PSF	R	902	-	28,29,29	0.51	0	32,36,36	0.57	0
25	WSS	0	302	-	40,40,53	0.34	0	45,48,61	0.41	0
24	PTY	8	201	-	49,49,49	0.29	0	52,54,54	0.31	0
22	CLR	V	402	-	31,31,31	0.52	0	48,48,48	0.61	0
24	PTY	0	306	-	16,16,49	0.58	0	19,20,54	0.72	1 (5%)
25	WSS	3	201	-	40,40,53	0.46	0	43,45,61	0.69	1 (2%)
25	WSS	V	401	-	36,36,53	0.35	0	42,44,61	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	NAG	U	504	16	14,14,15	0.20	0	17,19,21	0.42	0
24	PTY	0	307	-	47,47,49	0.28	0	50,52,54	0.34	0
24	PTY	2	201	-	28,28,49	0.34	0	30,32,54	0.48	0
22	CLR	R	901	-	31,31,31	0.27	0	48,48,48	0.49	0
25	WSS	R	905	-	39,39,53	0.35	0	45,47,61	0.39	0
24	PTY	5	202	-	34,34,49	0.36	0	37,39,54	0.43	0
22	CLR	5	201	-	31,31,31	0.30	0	48,48,48	0.64	1 (2%)
24	PTY	R	904	-	28,28,49	0.32	0	30,32,54	0.45	0
29	WJS	3	202	-	25,26,34	1.40	2 (8%)	28,32,40	1.54	2 (7%)
24	PTY	V	403	-	28,28,49	0.35	0	30,32,54	0.40	0
25	WSS	0	301	-	43,43,53	0.36	0	48,51,61	0.81	1 (2%)
22	CLR	0	304	-	31,31,31	0.32	0	48,48,48	0.41	0
25	WSS	U	501	-	38,38,53	0.38	0	43,46,61	0.34	0
25	WSS	0	303	-	25,25,53	0.39	0	31,33,61	0.81	1 (3%)
24	PTY	U	503	-	25,25,49	0.34	0	27,27,54	0.32	0
25	WSS	1	201	-	33,33,53	0.37	0	39,41,61	0.66	1 (2%)
24	PTY	7	201	-	41,41,49	0.30	0	44,46,54	0.38	0
25	WSS	U	502	-	36,36,53	0.39	0	42,44,61	0.54	0
25	WSS	0	305	-	30,30,53	0.47	0	33,35,61	0.63	1 (3%)
28	ADP	C	701	-	24,29,29	0.96	1 (4%)	29,45,45	1.43	4 (13%)
26	NAG	R	906	5	14,14,15	0.42	0	17,19,21	0.47	0
24	PTY	Q	401	-	29,29,49	0.36	0	32,34,54	0.46	0
24	PTY	8	202	-	32,32,49	0.28	0	34,34,54	0.44	0
27	WJP	R	907	21	31,33,34	1.53	5 (16%)	39,43,44	1.97	11 (28%)
24	PTY	R	903	-	31,31,49	0.31	0	33,33,54	0.32	0
24	PTY	6	201	-	20,20,49	0.42	0	22,24,54	0.43	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
23	PSF	R	902	-	-	18/35/35/35	-
25	WSS	0	302	-	-	12/44/44/57	-
24	PTY	8	201	-	-	29/53/53/53	-
22	CLR	V	402	-	-	0/10/68/68	0/4/4/4
24	PTY	0	306	-	-	6/16/16/53	-
25	WSS	3	201	-	-	10/44/44/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	WSS	V	401	-	-	6/40/40/57	-
26	NAG	U	504	16	-	2/6/23/26	0/1/1/1
24	PTY	0	307	-	1/1/4/4	35/51/51/53	-
24	PTY	2	201	-	-	11/30/30/53	-
22	CLR	R	901	-	-	6/10/68/68	0/4/4/4
25	WSS	R	905	-	-	18/43/43/57	-
24	PTY	5	202	-	-	23/38/38/53	-
22	CLR	5	201	-	-	0/10/68/68	0/4/4/4
24	PTY	R	904	-	1/1/3/4	20/31/31/53	-
29	WJS	3	202	-	-	13/30/30/38	-
24	PTY	V	403	-	-	18/30/30/53	-
25	WSS	0	301	-	-	15/47/47/57	-
22	CLR	0	304	-	-	0/10/68/68	0/4/4/4
25	WSS	U	501	-	-	4/42/42/57	-
25	WSS	0	303	-	-	7/29/29/57	-
24	PTY	U	503	-	-	10/27/27/53	-
25	WSS	1	201	-	-	5/37/37/57	-
24	PTY	7	201	-	-	22/45/45/53	-
25	WSS	U	502	-	-	4/40/40/57	-
25	WSS	0	305	-	-	9/32/32/57	-
28	ADP	C	701	-	-	1/12/32/32	0/3/3/3
26	NAG	R	906	5	-	4/6/23/26	0/1/1/1
24	PTY	Q	401	-	-	15/33/33/53	-
24	PTY	8	202	-	-	18/34/34/53	-
27	WJP	R	907	21	-	10/37/37/40	-
24	PTY	R	903	-	-	20/33/33/53	-
24	PTY	6	201	-	-	11/22/22/53	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	907	WJP	P31-O34	4.69	1.72	1.54
29	3	202	WJS	P25-O24	4.29	1.76	1.59
27	R	907	WJP	P27-O26	3.00	1.71	1.59
27	R	907	WJP	C15-C16	2.98	1.40	1.33
27	R	907	WJP	C10-C11	2.87	1.39	1.33
27	R	907	WJP	C12-C11	-2.29	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	701	ADP	C5-C4	2.19	1.46	1.40
29	3	202	WJS	C29-C30	2.07	1.58	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	3	202	WJS	O28-C29-C30	6.21	113.47	108.06
27	R	907	WJP	C12-C11-C13	5.49	124.50	115.27
27	R	907	WJP	C04-C05-C06	-4.97	115.68	127.66
27	R	907	WJP	C17-C16-C18	4.39	122.65	115.27
25	0	301	WSS	O2-C31-C32	4.05	120.22	111.50
25	0	303	WSS	O2-C31-C32	3.34	118.70	111.50
28	C	701	ADP	C3'-C2'-C1'	3.30	105.95	100.98
25	3	201	WSS	O2-C31-C32	3.09	118.15	111.50
28	C	701	ADP	N3-C2-N1	-2.99	124.00	128.68
27	R	907	WJP	C03-C04-C05	2.83	119.70	112.23
25	1	201	WSS	O2-C31-C32	2.73	117.39	111.50
28	C	701	ADP	C4-C5-N7	-2.62	106.67	109.40
28	C	701	ADP	PA-O3A-PB	-2.61	123.89	132.83
27	R	907	WJP	C17-C16-C15	-2.56	117.10	123.68
25	0	305	WSS	O2P-P-O1P	2.44	120.23	110.68
24	0	306	PTY	O12-P1-O13	2.43	120.18	110.68
29	3	202	WJS	O27-P25-O26	2.34	123.82	112.24
27	R	907	WJP	O26-P27-O28	-2.30	100.06	109.07
27	R	907	WJP	O34-P31-O30	2.30	112.36	104.64
22	5	201	CLR	C15-C14-C13	2.29	106.60	103.84
27	R	907	WJP	C08-C06-C05	-2.28	116.50	121.12
27	R	907	WJP	C07-C06-C05	2.17	129.25	123.68
27	R	907	WJP	C13-C14-C15	2.10	118.79	111.88
27	R	907	WJP	C12-C11-C10	-2.08	118.35	123.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	R	904	PTY	C6
24	0	307	PTY	C6

All (382) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	R	902	PSF	C2-O2-P-O4
23	R	902	PSF	C2-O2-P-O3

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Mol	Chain	Res	Type	Atoms
23	R	902	PSF	C13-C1-O11-C3
24	R	903	PTY	C11-C8-O7-C6
24	R	904	PTY	C11-C8-O7-C6
24	R	904	PTY	C5-O14-P1-O11
24	R	904	PTY	C5-O14-P1-O12
24	R	904	PTY	C5-O14-P1-O13
24	0	306	PTY	C5-O14-P1-O11
24	0	307	PTY	O4-C1-C6-O7
24	0	307	PTY	O10-C8-O7-C6
24	0	307	PTY	C11-C8-O7-C6
24	0	307	PTY	C3-O11-P1-O14
24	2	201	PTY	N1-C2-C3-O11
24	2	201	PTY	O14-C5-C6-C1
24	2	201	PTY	C5-O14-P1-O11
24	2	201	PTY	C5-O14-P1-O12
24	2	201	PTY	C5-O14-P1-O13
24	5	202	PTY	N1-C2-C3-O11
24	5	202	PTY	C3-O11-P1-O12
24	5	202	PTY	C3-O11-P1-O13
24	5	202	PTY	C5-O14-P1-O12
24	6	201	PTY	C5-O14-P1-O12
24	7	201	PTY	N1-C2-C3-O11
24	7	201	PTY	C3-O11-P1-O12
24	7	201	PTY	C5-O14-P1-O12
24	8	201	PTY	N1-C2-C3-O11
24	8	202	PTY	O10-C8-O7-C6
24	8	202	PTY	C11-C8-O7-C6
24	Q	401	PTY	O30-C30-O4-C1
24	U	503	PTY	O14-C5-C6-C1
24	U	503	PTY	O14-C5-C6-O7
24	V	403	PTY	O4-C1-C6-O7
24	V	403	PTY	C3-O11-P1-O12
24	V	403	PTY	C5-O14-P1-O13
25	0	301	WSS	C32-C31-O2-C2
25	0	301	WSS	O31-C31-O2-C2
25	0	301	WSS	C39-C40-C41-C42
25	0	301	WSS	C1-O3P-P-O1P
25	0	301	WSS	C4-O4P-P-O1P
25	0	301	WSS	C4-O4P-P-O3P
25	0	302	WSS	C5-C4-O4P-P
25	0	303	WSS	C32-C31-O2-C2
25	0	303	WSS	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
25	0	305	WSS	C39-C40-C41-C42
25	1	201	WSS	O31-C31-O2-C2
25	3	201	WSS	C32-C31-O2-C2
25	3	201	WSS	O31-C31-O2-C2
25	V	401	WSS	C1-O3P-P-O2P
27	R	907	WJP	C02-C03-C04-C05
29	3	202	WJS	C29-O28-P25-O24
29	3	202	WJS	C29-O28-P25-O26
29	3	202	WJS	C30-C29-O28-P25
29	3	202	WJS	O28-C29-C30-C31
29	3	202	WJS	O28-C29-C30-N34
24	8	201	PTY	O30-C30-O4-C1
26	R	906	NAG	O5-C5-C6-O6
23	R	902	PSF	O12-C1-O11-C3
24	R	903	PTY	O10-C8-O7-C6
24	R	904	PTY	O10-C8-O7-C6
24	8	201	PTY	C31-C30-O4-C1
24	Q	401	PTY	C31-C30-O4-C1
25	1	201	WSS	C32-C31-O2-C2
23	R	902	PSF	OT2-C-CA-N
24	8	202	PTY	O30-C30-O4-C1
24	R	903	PTY	O30-C30-O4-C1
29	3	202	WJS	O20-C21-C22-O35
25	R	905	WSS	C32-C31-O2-C2
24	0	307	PTY	C33-C34-C35-C36
29	3	202	WJS	C12-C13-C14-C15
24	0	307	PTY	C17-C18-C19-C20
22	R	901	CLR	C13-C17-C20-C22
24	R	903	PTY	C31-C30-O4-C1
24	8	202	PTY	C31-C30-O4-C1
26	R	906	NAG	C4-C5-C6-O6
26	R	906	NAG	C1-C2-N2-C7
24	0	307	PTY	C36-C37-C38-C39
24	V	403	PTY	O14-C5-C6-C1
24	8	202	PTY	C32-C33-C34-C35
24	6	201	PTY	C31-C30-O4-C1
29	3	202	WJS	C10-C11-C12-C13
26	U	504	NAG	C8-C7-N2-C2
26	U	504	NAG	O7-C7-N2-C2
24	0	306	PTY	C30-C31-C32-C33
24	V	403	PTY	C30-C31-C32-C33
27	R	907	WJP	C01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
22	R	901	CLR	C13-C17-C20-C21
24	0	307	PTY	C30-C31-C32-C33
24	8	201	PTY	C8-C11-C12-C13
24	8	202	PTY	C8-C11-C12-C13
24	8	202	PTY	C30-C31-C32-C33
25	R	905	WSS	O31-C31-O2-C2
22	R	901	CLR	C22-C23-C24-C25
24	7	201	PTY	C30-C31-C32-C33
24	6	201	PTY	O30-C30-O4-C1
27	R	907	WJP	C16-C18-C19-C20
24	2	201	PTY	O14-C5-C6-O7
24	V	403	PTY	O14-C5-C6-O7
24	U	503	PTY	C31-C30-O4-C1
23	R	902	PSF	C2-O2-P-O1
24	0	307	PTY	C5-O14-P1-O11
24	5	202	PTY	C3-O11-P1-O14
24	5	202	PTY	C5-O14-P1-O11
24	7	201	PTY	C3-O11-P1-O14
24	7	201	PTY	C5-O14-P1-O11
24	V	403	PTY	C3-O11-P1-O14
24	V	403	PTY	C5-O14-P1-O11
25	0	301	WSS	C1-O3P-P-O4P
25	0	302	WSS	C1-O3P-P-O4P
25	0	302	WSS	C4-O4P-P-O3P
25	U	501	WSS	C1-O3P-P-O4P
25	V	401	WSS	C1-O3P-P-O4P
25	V	401	WSS	C31-C32-C33-C34
24	8	201	PTY	C11-C8-O7-C6
24	0	307	PTY	C14-C15-C16-C17
24	7	201	PTY	C37-C38-C39-C40
24	8	201	PTY	C18-C19-C20-C21
25	0	305	WSS	C34-C35-C36-C37
24	0	307	PTY	C23-C24-C25-C26
25	R	905	WSS	C32-C33-C34-C35
24	8	201	PTY	O10-C8-O7-C6
24	2	201	PTY	C31-C32-C33-C34
24	7	201	PTY	C34-C35-C36-C37
24	8	201	PTY	C39-C40-C41-C42
24	Q	401	PTY	C35-C36-C37-C38
24	R	903	PTY	C36-C37-C38-C39
24	R	904	PTY	C20-C21-C22-C23
24	8	201	PTY	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	3	202	WJS	C13-C14-C15-C16
24	U	503	PTY	O30-C30-O4-C1
27	R	907	WJP	C17-C16-C18-C19
24	R	903	PTY	C14-C15-C16-C17
24	R	904	PTY	C19-C20-C21-C22
24	0	307	PTY	C35-C36-C37-C38
24	5	202	PTY	C39-C40-C41-C42
24	8	202	PTY	C40-C41-C42-C43
24	R	903	PTY	C12-C13-C14-C15
24	0	307	PTY	C31-C32-C33-C34
24	8	201	PTY	C12-C13-C14-C15
24	8	201	PTY	C32-C33-C34-C35
24	8	202	PTY	C34-C35-C36-C37
24	U	503	PTY	C32-C33-C34-C35
24	8	201	PTY	C30-C31-C32-C33
24	R	904	PTY	C18-C19-C20-C21
24	0	307	PTY	C12-C13-C14-C15
24	0	307	PTY	C16-C17-C18-C19
25	R	905	WSS	C42-C43-C44-C45
24	R	903	PTY	O4-C1-C6-C5
24	R	904	PTY	C11-C12-C13-C14
23	R	902	PSF	C6-C5-O52-C4
24	2	201	PTY	C31-C30-O4-C1
24	V	403	PTY	C31-C32-C33-C34
25	R	905	WSS	C43-C44-C45-C46
25	R	905	WSS	C11-C12-C13-C14
24	R	903	PTY	C32-C33-C34-C35
24	0	307	PTY	C21-C22-C23-C24
24	5	202	PTY	C32-C33-C34-C35
22	R	901	CLR	C16-C17-C20-C21
24	0	307	PTY	C19-C20-C21-C22
24	0	306	PTY	C31-C32-C33-C34
24	5	202	PTY	C11-C12-C13-C14
27	R	907	WJP	C15-C16-C18-C19
25	R	905	WSS	C38-C39-C40-C41
24	5	202	PTY	C31-C30-O4-C1
24	7	201	PTY	C31-C30-O4-C1
24	V	403	PTY	C39-C40-C41-C42
23	R	902	PSF	O51-C5-O52-C4
24	5	202	PTY	C40-C41-C42-C43
24	V	403	PTY	C31-C30-O4-C1
22	R	901	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
24	7	201	PTY	C36-C37-C38-C39
24	Q	401	PTY	C11-C8-O7-C6
24	R	903	PTY	C35-C36-C37-C38
24	7	201	PTY	C13-C14-C15-C16
24	R	904	PTY	C15-C16-C17-C18
24	Q	401	PTY	O10-C8-O7-C6
24	R	904	PTY	C13-C14-C15-C16
24	V	403	PTY	C36-C37-C38-C39
24	7	201	PTY	C12-C13-C14-C15
24	8	201	PTY	C23-C24-C25-C26
24	U	503	PTY	C11-C12-C13-C14
24	5	202	PTY	O30-C30-O4-C1
24	7	201	PTY	C39-C40-C41-C42
22	R	901	CLR	C20-C22-C23-C24
24	R	904	PTY	C3-O11-P1-O14
24	6	201	PTY	C5-O14-P1-O11
24	0	307	PTY	C20-C21-C22-C23
24	0	307	PTY	C6-C5-O14-P1
24	2	201	PTY	O30-C30-O4-C1
24	R	904	PTY	O14-C5-C6-C1
25	0	301	WSS	O3P-C1-C2-C3
24	0	307	PTY	C32-C33-C34-C35
24	0	307	PTY	C38-C39-C40-C41
24	8	201	PTY	C22-C23-C24-C25
24	0	307	PTY	O4-C1-C6-C5
25	0	305	WSS	C1-C2-C3-O3
24	R	903	PTY	C15-C16-C17-C18
24	0	307	PTY	C15-C16-C17-C18
24	Q	401	PTY	C11-C12-C13-C14
25	R	905	WSS	C35-C36-C37-C38
24	2	201	PTY	C30-C31-C32-C33
24	7	201	PTY	C41-C42-C43-C44
24	8	202	PTY	C36-C37-C38-C39
24	Q	401	PTY	C36-C37-C38-C39
23	R	902	PSF	C7-C8-C9-C10
24	8	202	PTY	C41-C42-C43-C44
24	7	201	PTY	O30-C30-O4-C1
24	0	306	PTY	C32-C33-C34-C35
24	8	202	PTY	C15-C16-C17-C18
25	0	301	WSS	C1-C2-O2-C31
24	0	306	PTY	C5-O14-P1-O13
24	6	201	PTY	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
24	R	903	PTY	C37-C38-C39-C40
24	V	403	PTY	O30-C30-O4-C1
24	R	904	PTY	C21-C22-C23-C24
25	R	905	WSS	C41-C42-C43-C44
24	5	202	PTY	O4-C1-C6-O7
25	0	303	WSS	O2-C2-C3-O3
23	R	902	PSF	C1-C13-C14-C15
24	8	201	PTY	C25-C26-C27-C28
24	0	307	PTY	O14-C5-C6-C1
24	5	202	PTY	C30-C31-C32-C33
24	8	202	PTY	C33-C34-C35-C36
24	8	201	PTY	C17-C18-C19-C20
24	6	201	PTY	C30-C31-C32-C33
25	0	302	WSS	C31-C32-C33-C34
24	8	201	PTY	C24-C25-C26-C27
24	8	202	PTY	C14-C15-C16-C17
24	7	201	PTY	C6-C5-O14-P1
24	Q	401	PTY	C33-C34-C35-C36
24	5	202	PTY	O4-C1-C6-C5
24	7	201	PTY	O4-C1-C6-C5
25	3	201	WSS	C1-C2-C3-O3
24	V	403	PTY	O4-C1-C6-C5
24	8	202	PTY	C11-C12-C13-C14
23	R	902	PSF	C13-C14-C15-C16
25	0	302	WSS	C33-C34-C35-C36
29	3	202	WJS	C23-O24-P25-O28
24	8	201	PTY	C26-C27-C28-C29
24	0	307	PTY	O14-C5-C6-O7
25	0	301	WSS	O3P-C1-C2-O2
25	0	303	WSS	O3P-C1-C2-O2
24	8	202	PTY	C37-C38-C39-C40
24	R	903	PTY	C41-C42-C43-C44
24	Q	401	PTY	C31-C32-C33-C34
23	R	902	PSF	OT1-C-CA-N
24	8	201	PTY	C6-C5-O14-P1
24	6	201	PTY	C32-C33-C34-C35
24	5	202	PTY	C37-C38-C39-C40
24	0	307	PTY	C18-C19-C20-C21
25	0	302	WSS	C19-C20-C21-C22
27	R	907	WJP	P31-O30-P27-O26
24	5	202	PTY	O14-C5-C6-C1
24	Q	401	PTY	O14-C5-C6-C1

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Mol	Chain	Res	Type	Atoms
27	R	907	WJP	C24-C02-C03-C04
25	0	305	WSS	C37-C38-C39-C40
24	8	201	PTY	C35-C36-C37-C38
24	5	202	PTY	C31-C32-C33-C34
24	5	202	PTY	C36-C37-C38-C39
25	3	201	WSS	C19-C20-C21-C22
24	Q	401	PTY	C1-C6-O7-C8
24	8	201	PTY	C33-C34-C35-C36
24	Q	401	PTY	O4-C1-C6-C5
25	0	301	WSS	C2-C1-O3P-P
25	U	501	WSS	C2-C1-O3P-P
24	R	904	PTY	O14-C5-C6-O7
24	Q	401	PTY	O14-C5-C6-O7
25	U	502	WSS	C17-C18-C19-C20
25	0	302	WSS	C11-C12-C13-C14
24	R	903	PTY	O4-C1-C6-O7
25	3	201	WSS	O2-C2-C3-O3
25	R	905	WSS	C4-C5-N1-C8
24	R	903	PTY	C11-C12-C13-C14
23	R	902	PSF	N-CA-CB-O1
24	0	307	PTY	C31-C30-O4-C1
24	5	202	PTY	C34-C35-C36-C37
25	0	303	WSS	C1-O3P-P-O4P
24	7	201	PTY	C40-C41-C42-C43
24	0	307	PTY	C3-O11-P1-O12
24	0	307	PTY	C5-O14-P1-O13
24	5	202	PTY	C5-O14-P1-O13
24	6	201	PTY	C5-O14-P1-O13
24	V	403	PTY	C5-O14-P1-O12
25	0	301	WSS	C1-O3P-P-O2P
25	0	302	WSS	C1-O3P-P-O2P
25	0	302	WSS	C4-O4P-P-O2P
25	U	502	WSS	C5-C4-O4P-P
23	R	902	PSF	C5-C6-C7-C8
24	6	201	PTY	O14-C5-C6-C1
29	3	202	WJS	C21-C22-C23-O24
25	3	201	WSS	C17-C18-C19-C20
25	0	302	WSS	O4P-C4-C5-N1
25	U	502	WSS	O4P-C4-C5-N1
24	0	307	PTY	O30-C30-O4-C1
25	0	305	WSS	O2-C2-C3-O3
24	V	403	PTY	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
25	3	201	WSS	C36-C37-C38-C39
25	R	905	WSS	C4-C5-N1-C7
24	7	201	PTY	C14-C15-C16-C17
25	0	301	WSS	C12-C13-C14-C15
25	0	301	WSS	C17-C18-C19-C20
24	R	903	PTY	C5-C6-O7-C8
24	7	201	PTY	C1-C6-O7-C8
24	5	202	PTY	O14-C5-C6-O7
24	7	201	PTY	C33-C34-C35-C36
24	6	201	PTY	C33-C34-C35-C36
24	Q	401	PTY	O4-C1-C6-O7
23	R	902	PSF	CB-O1-P-O2
24	8	201	PTY	C5-O14-P1-O11
25	1	201	WSS	C4-O4P-P-O3P
25	3	201	WSS	C4-O4P-P-O3P
24	6	201	PTY	C3-O11-P1-O13
24	7	201	PTY	C35-C36-C37-C38
24	8	201	PTY	C20-C21-C22-C23
24	V	403	PTY	C37-C38-C39-C40
25	0	303	WSS	C1-C2-C3-O3
25	0	301	WSS	C19-C20-C21-C22
24	0	307	PTY	C37-C38-C39-C40
24	U	503	PTY	C12-C13-C14-C15
25	R	905	WSS	C34-C35-C36-C37
25	V	401	WSS	C13-C14-C15-C16
25	U	501	WSS	C17-C18-C19-C20
24	U	503	PTY	C6-C1-O4-C30
24	8	201	PTY	O4-C1-C6-O7
24	0	306	PTY	C6-C5-O14-P1
24	5	202	PTY	C35-C36-C37-C38
24	U	503	PTY	C13-C14-C15-C16
24	8	201	PTY	C34-C35-C36-C37
23	R	902	PSF	OT1-C-CA-CB
23	R	902	PSF	OT2-C-CA-CB
29	3	202	WJS	C29-C30-C31-O32
29	3	202	WJS	C29-C30-C31-O33
28	C	701	ADP	O4'-C4'-C5'-O5'
24	0	307	PTY	C40-C41-C42-C43
25	R	905	WSS	C4-C5-N1-C9
24	Q	401	PTY	C34-C35-C36-C37
25	0	303	WSS	O3P-C1-C2-C3
24	R	904	PTY	O4-C1-C6-C5

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Mol	Chain	Res	Type	Atoms
24	R	903	PTY	C39-C40-C41-C42
25	R	905	WSS	O11-C11-O3-C3
25	0	302	WSS	C37-C38-C39-C40
25	3	201	WSS	C39-C40-C41-C42
24	0	307	PTY	C13-C14-C15-C16
25	R	905	WSS	C12-C11-O3-C3
24	R	904	PTY	C12-C13-C14-C15
24	R	904	PTY	O4-C1-C6-O7
25	0	302	WSS	C17-C18-C19-C20
27	R	907	WJP	C12-C11-C13-C14
24	2	201	PTY	C33-C34-C35-C36
24	8	201	PTY	O4-C1-C6-C5
25	U	502	WSS	C2-C1-O3P-P
24	0	307	PTY	C41-C42-C43-C44
25	0	305	WSS	O3-C11-C12-C13
25	R	905	WSS	C37-C38-C39-C40
25	3	201	WSS	C37-C38-C39-C40
27	R	907	WJP	C25-O26-P27-O30
24	R	903	PTY	C38-C39-C40-C41
24	R	903	PTY	C13-C14-C15-C16
25	V	401	WSS	C14-C15-C16-C17
25	R	905	WSS	C31-C32-C33-C34
27	R	907	WJP	P31-O30-P27-O28
26	R	906	NAG	C3-C2-N2-C7
24	V	403	PTY	C33-C34-C35-C36
23	R	902	PSF	CB-O1-P-O4
24	R	904	PTY	C3-O11-P1-O13
25	R	905	WSS	C1-O3P-P-O1P
25	1	201	WSS	C4-O4P-P-O1P
25	U	501	WSS	C1-O3P-P-O1P
24	0	307	PTY	N1-C2-C3-O11
24	8	202	PTY	C12-C11-C8-O7
24	8	201	PTY	C38-C39-C40-C41
25	0	305	WSS	O11-C11-C12-C13
24	8	201	PTY	C41-C42-C43-C44
24	R	904	PTY	C17-C18-C19-C20
24	R	903	PTY	C12-C11-C8-O7
25	1	201	WSS	O2-C31-C32-C33
25	V	401	WSS	O3P-C1-C2-O2
24	8	201	PTY	C12-C11-C8-O7
25	0	305	WSS	O2-C31-C32-C33
24	U	503	PTY	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	0	305	WSS	O31-C31-C32-C33
24	8	202	PTY	C12-C11-C8-O10

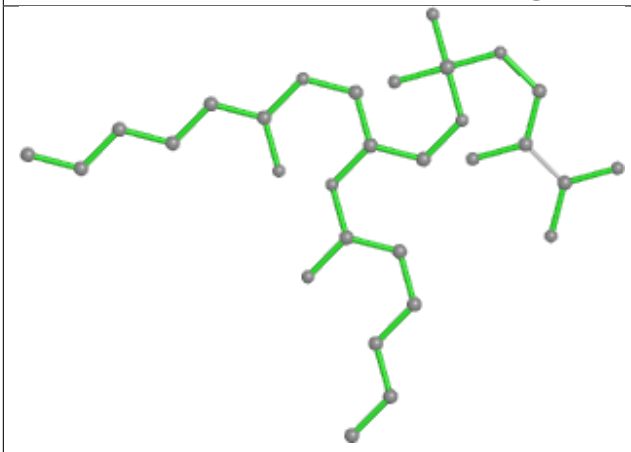
There are no ring outliers.

20 monomers are involved in 80 short contacts:

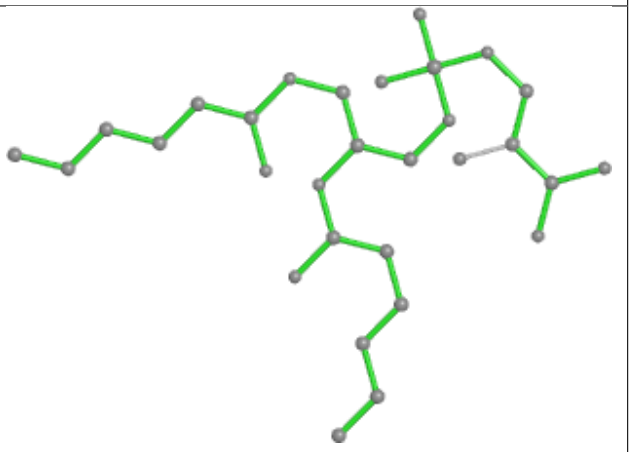
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	8	201	PTY	6	0
22	V	402	CLR	11	0
24	0	306	PTY	1	0
24	0	307	PTY	3	0
24	2	201	PTY	1	0
22	R	901	CLR	1	0
25	R	905	WSS	5	0
24	5	202	PTY	6	0
22	5	201	CLR	16	0
24	R	904	PTY	2	0
29	3	202	WJS	5	0
24	V	403	PTY	9	0
22	0	304	CLR	1	0
24	U	503	PTY	21	0
24	7	201	PTY	7	0
25	0	305	WSS	1	0
28	C	701	ADP	1	0
24	Q	401	PTY	6	0
24	8	202	PTY	4	0
24	6	201	PTY	7	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.

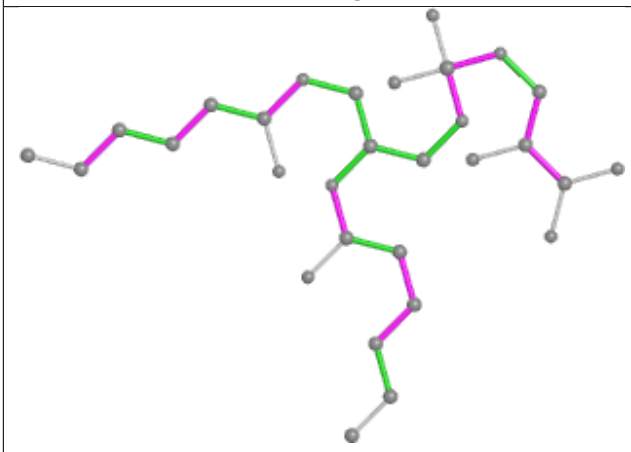
Ligand PSF R 902



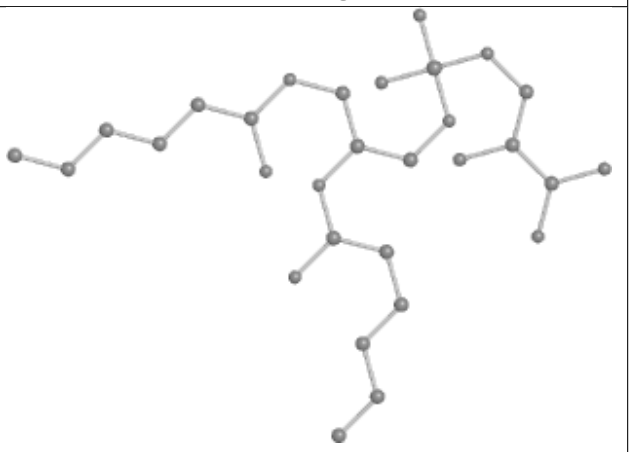
Bond lengths



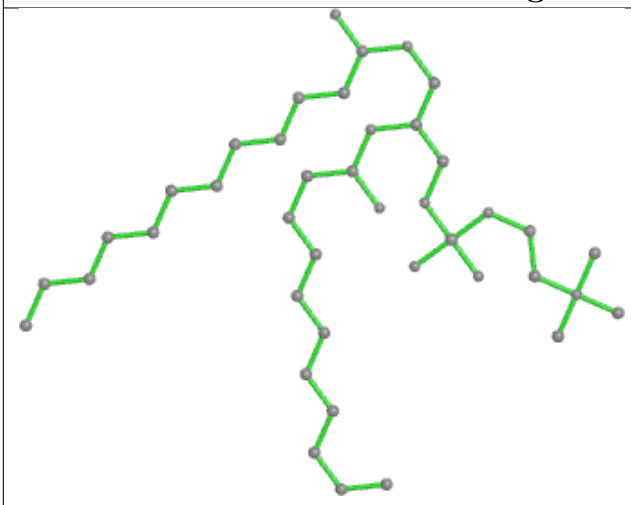
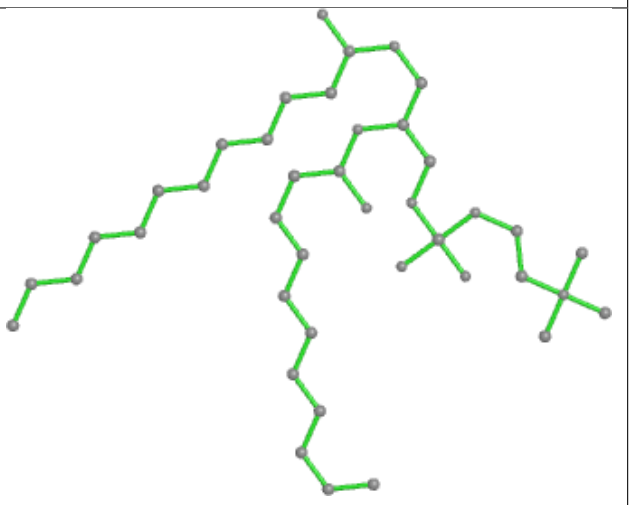
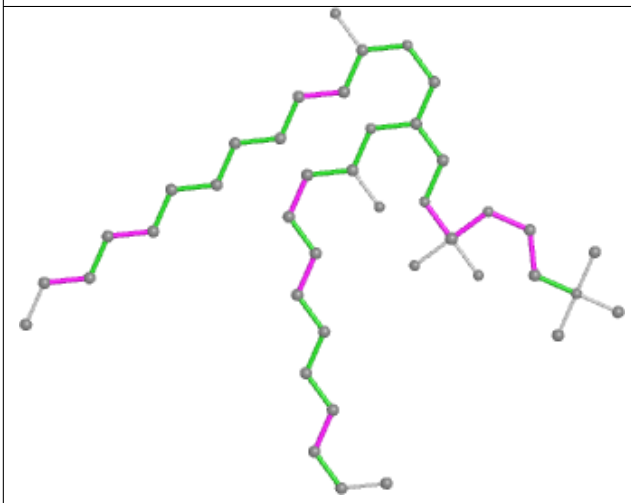
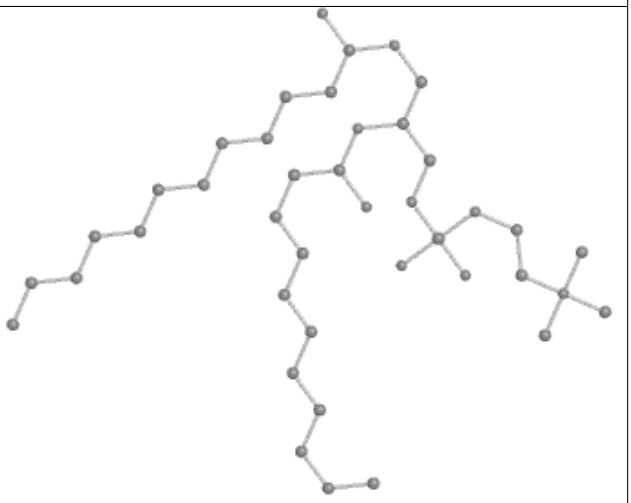
Bond angles

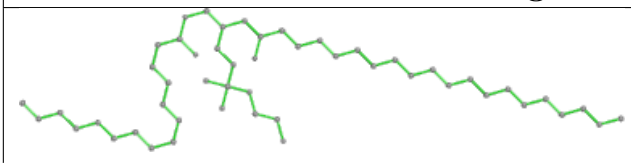
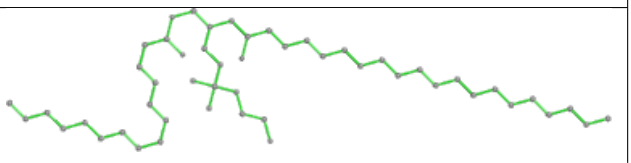
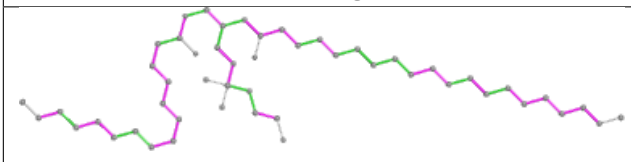
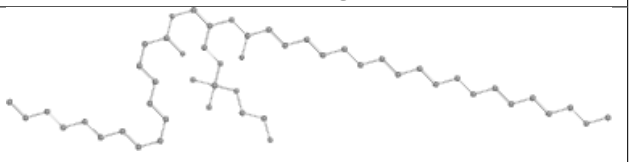


Torsions

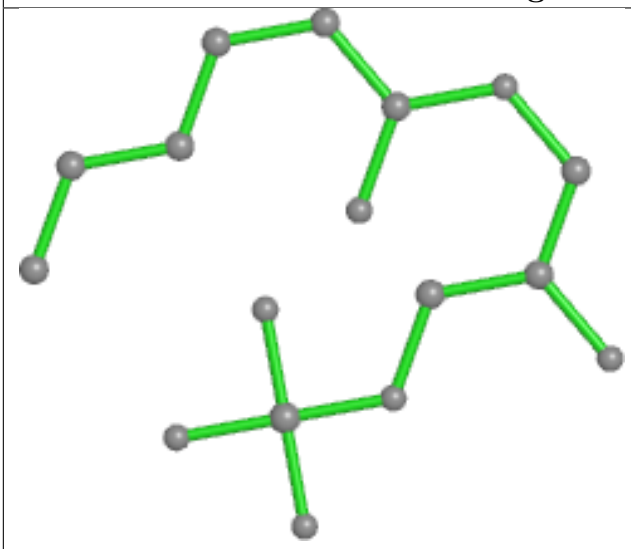


Rings

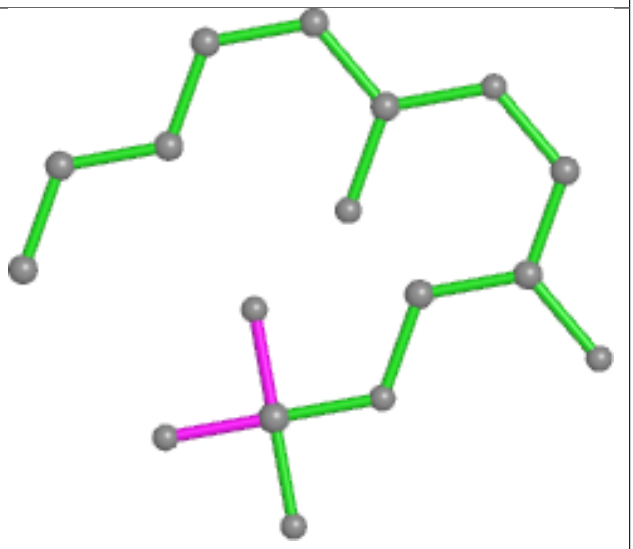
Ligand WSS 0 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY 8 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

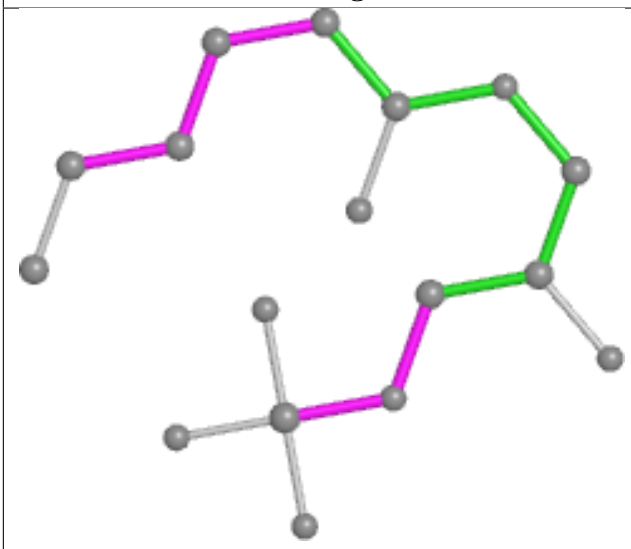
Ligand PTY 0 306



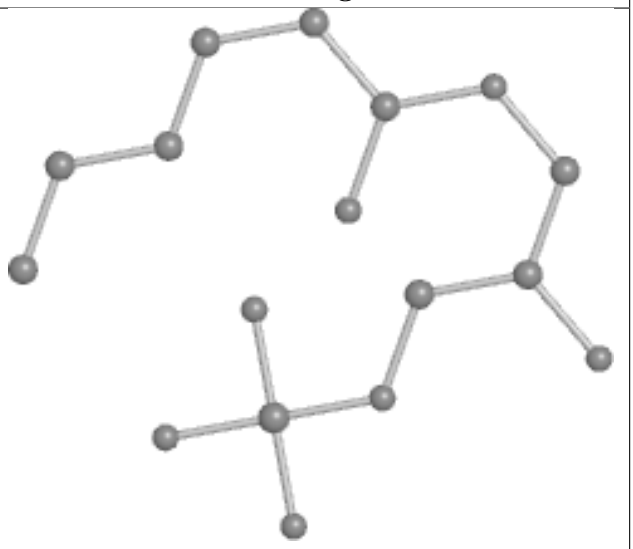
Bond lengths



Bond angles

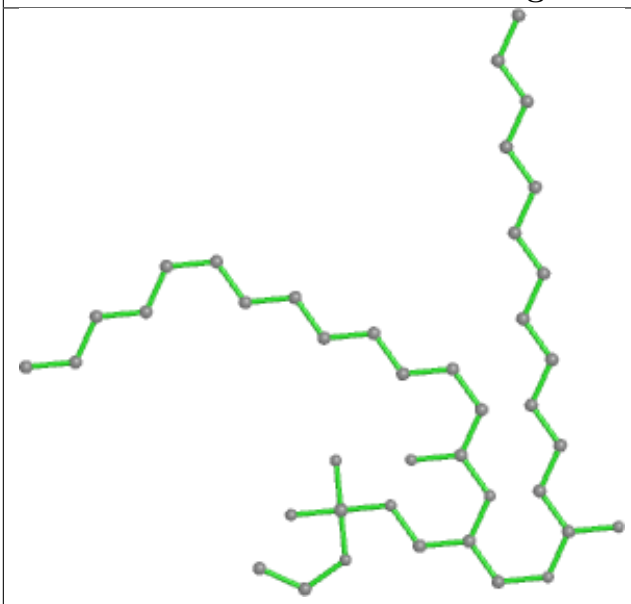


Torsions

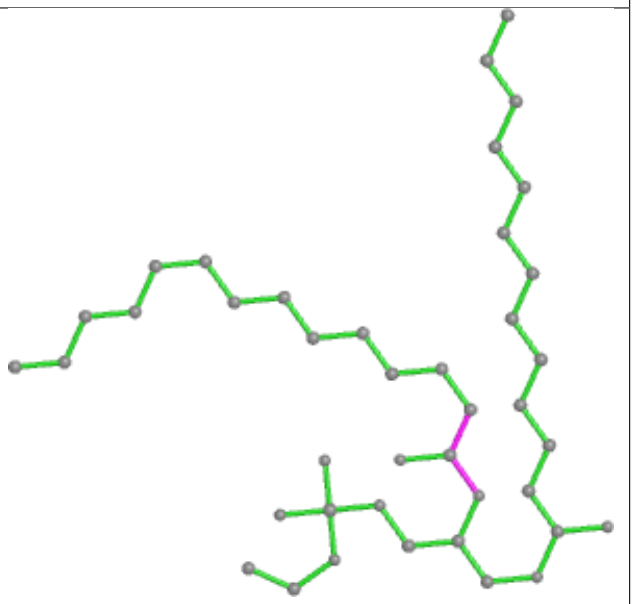


Rings

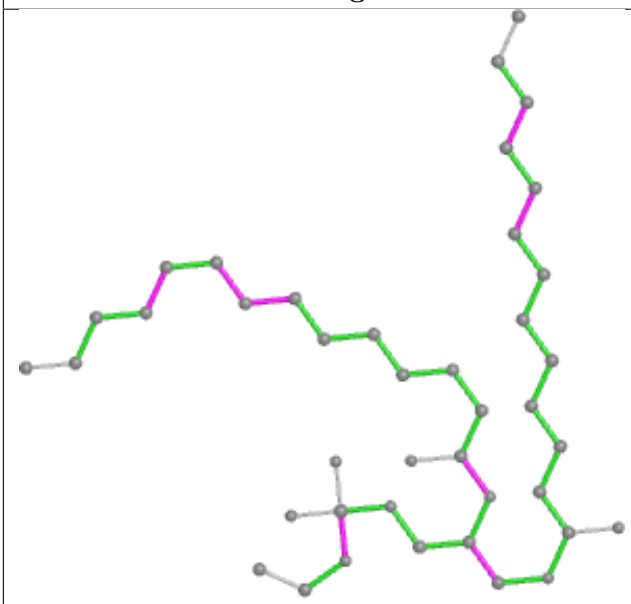
Ligand WSS 3 201



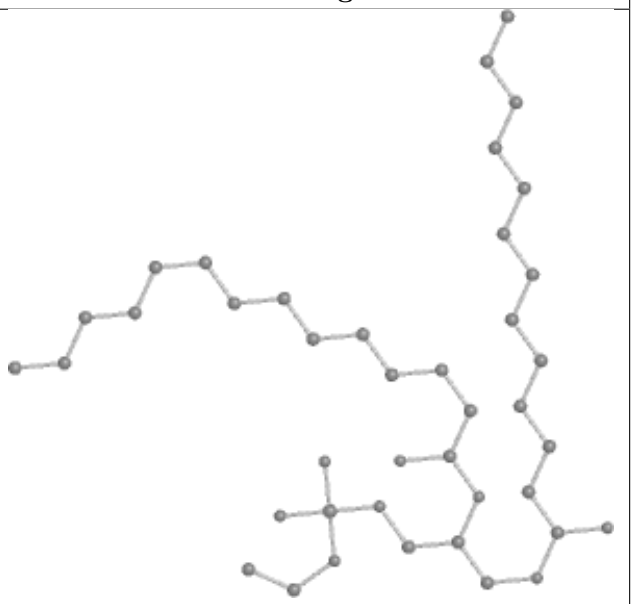
Bond lengths



Bond angles

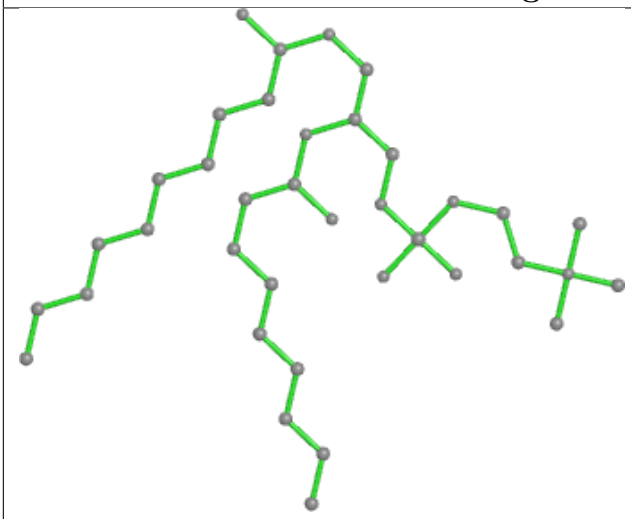


Torsions

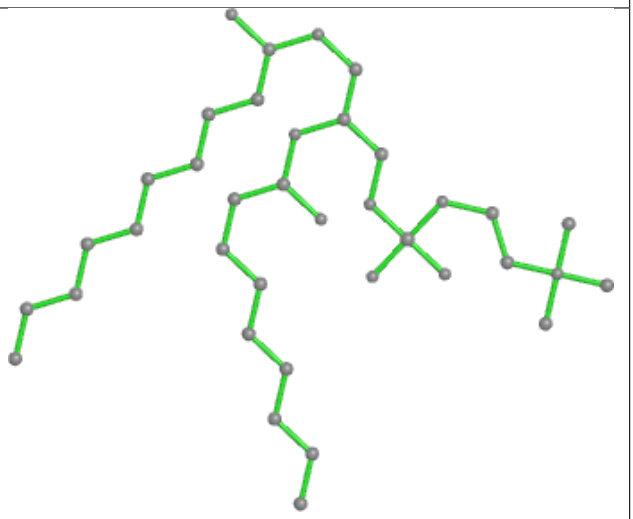


Rings

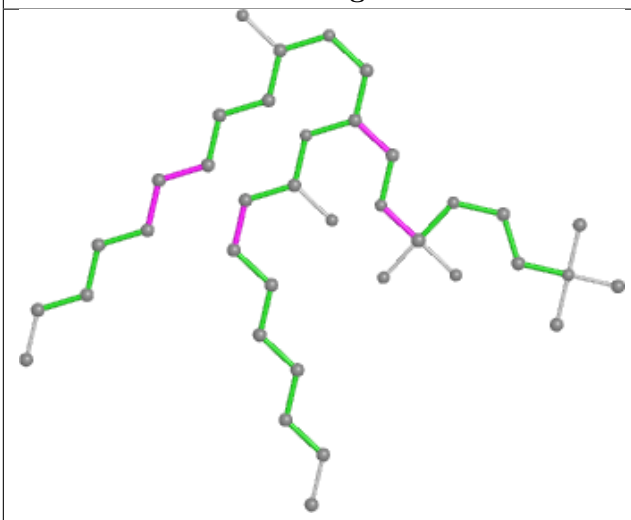
Ligand WSS V 401



Bond lengths



Bond angles



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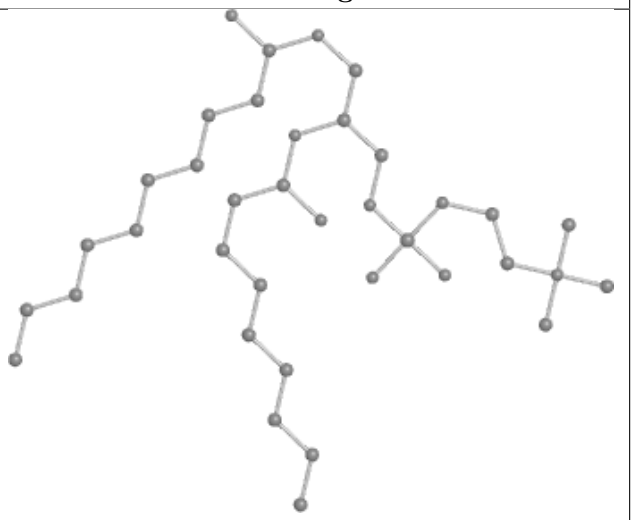
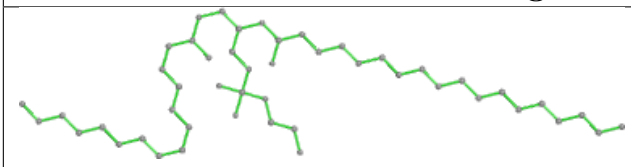
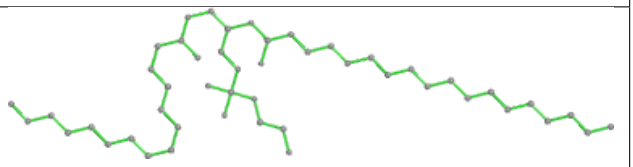


Rings

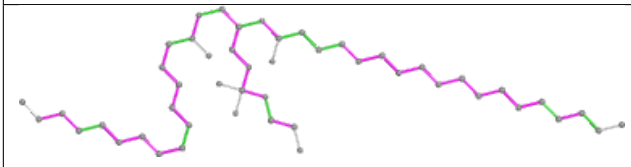
Ligand PTY 0 307



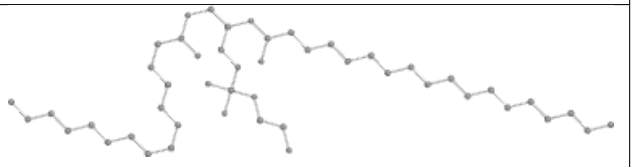
Bond lengths



Bond angles

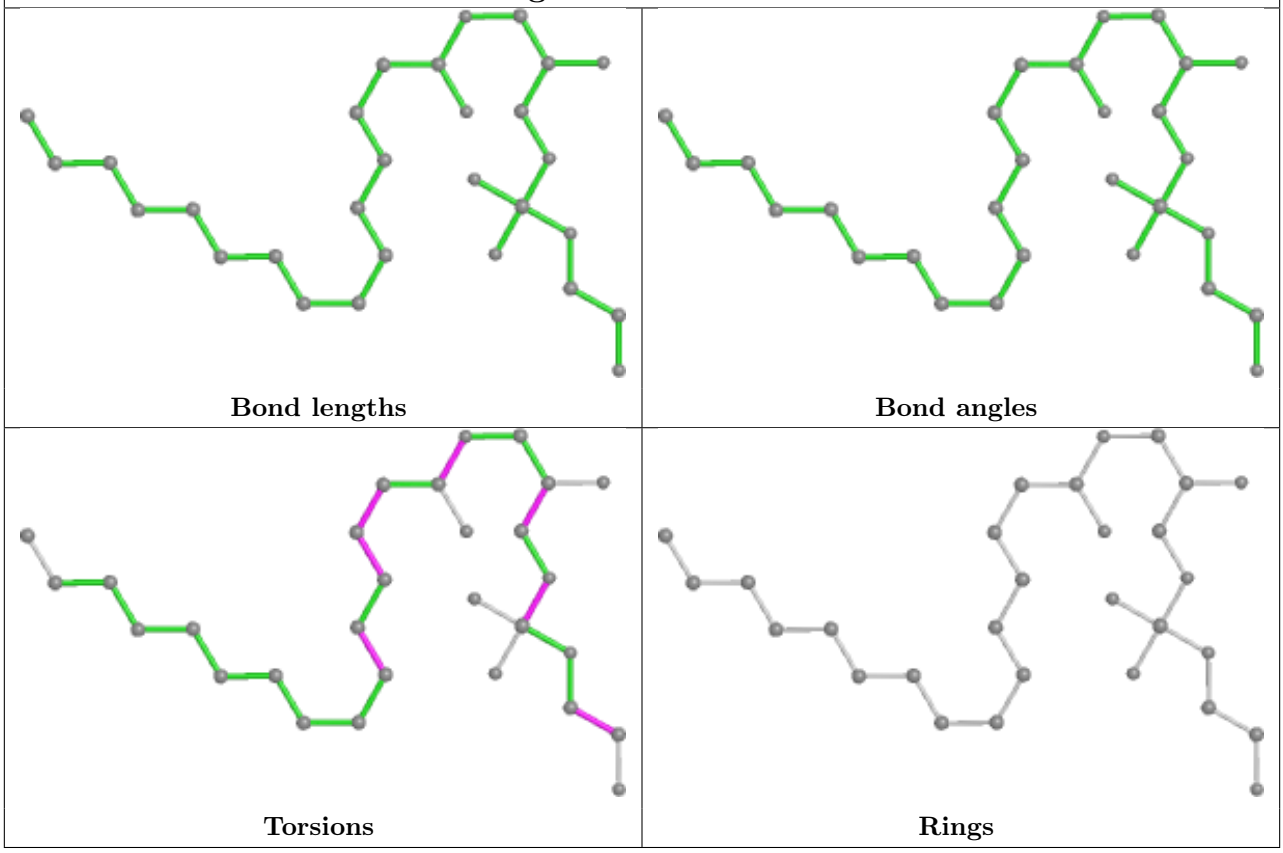


Torsions

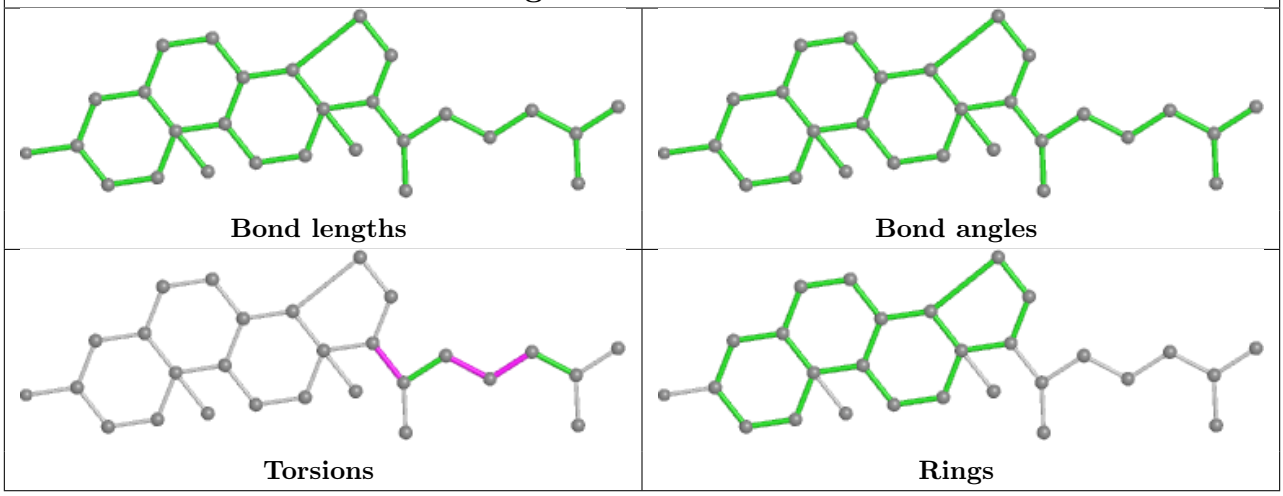


Rings

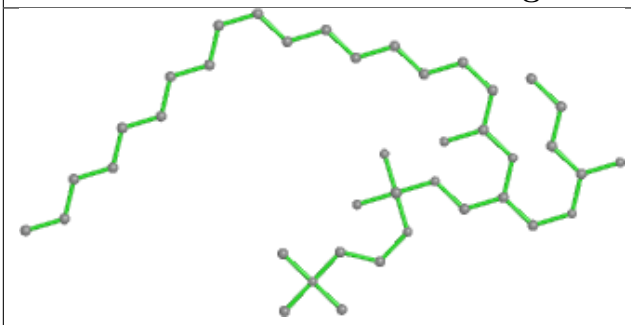
Ligand PTY 2 201



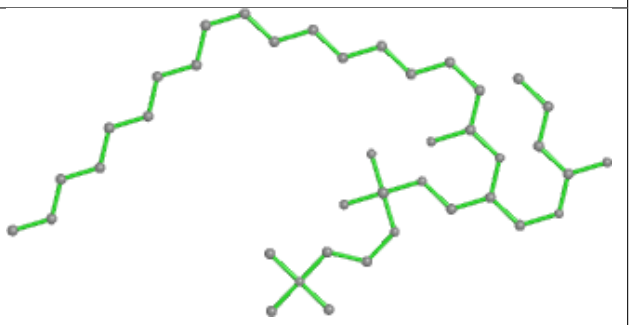
Ligand CLR R 901



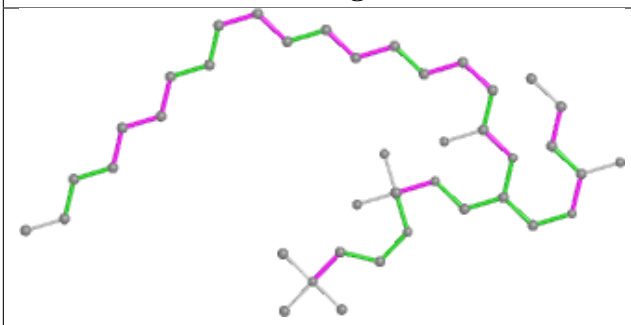
Ligand WSS R 905



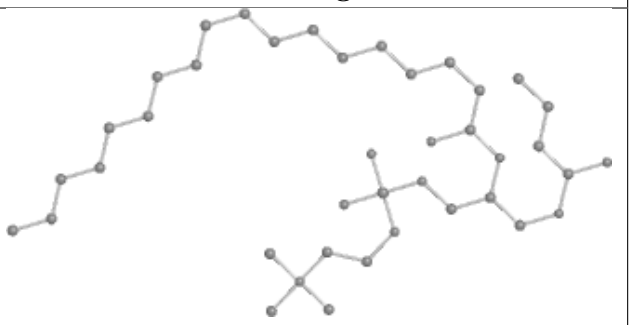
Bond lengths



Bond angles

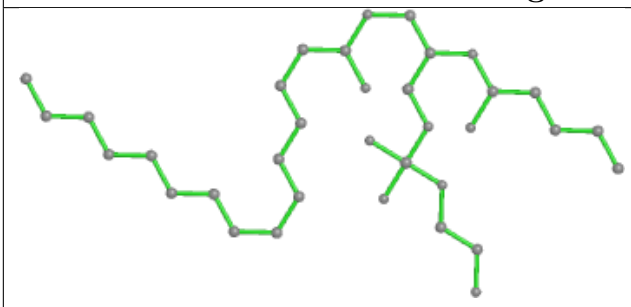


Torsions

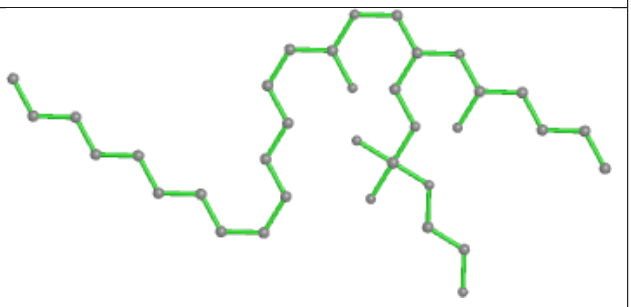


Rings

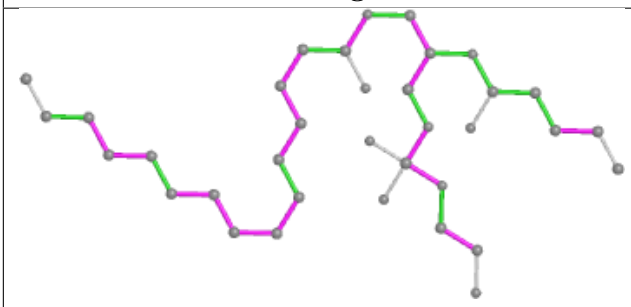
Ligand PTY 5 202



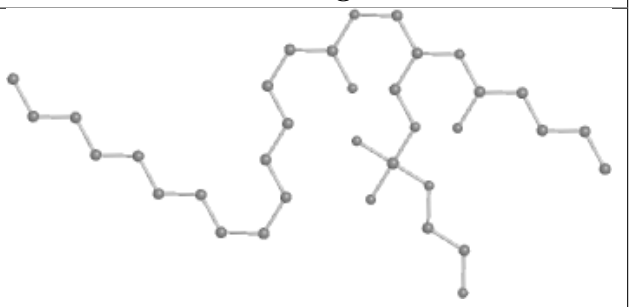
Bond lengths



Bond angles

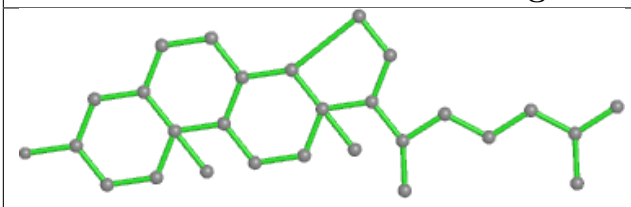


Torsions

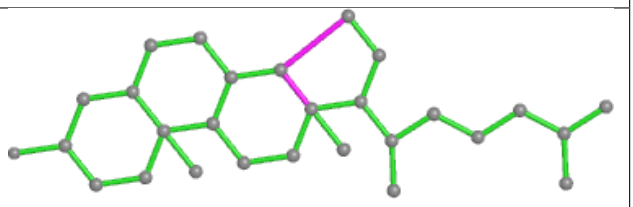


Rings

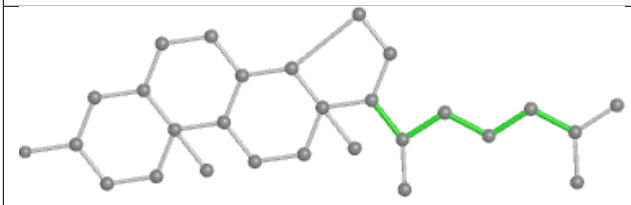
Ligand CLR 5 201



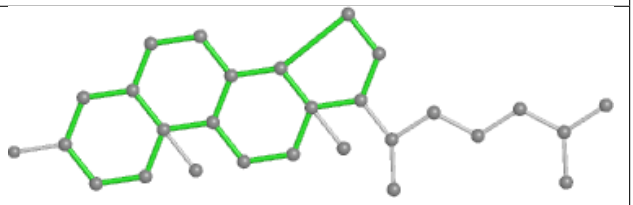
Bond lengths



Bond angles

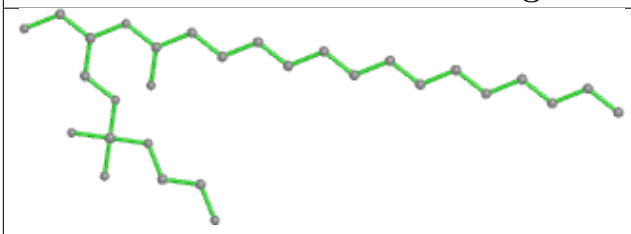


Torsions

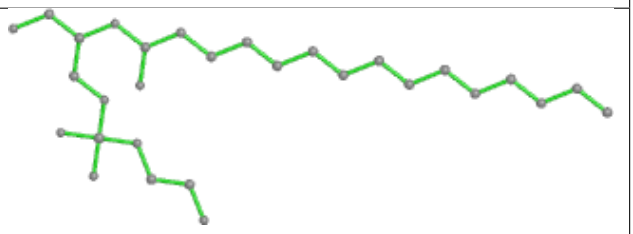


Rings

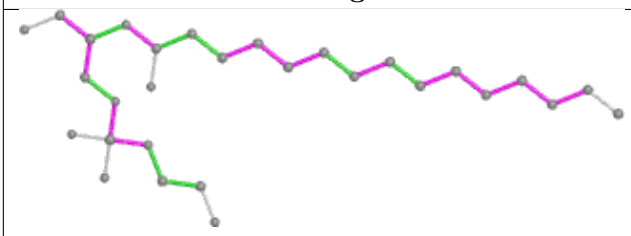
Ligand PTY R 904



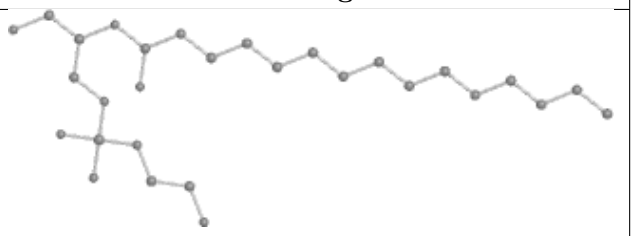
Bond lengths



Bond angles

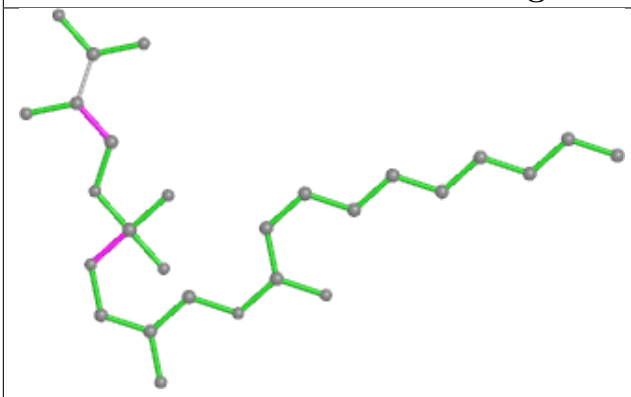


Torsions



Rings

Ligand WJS 3 202



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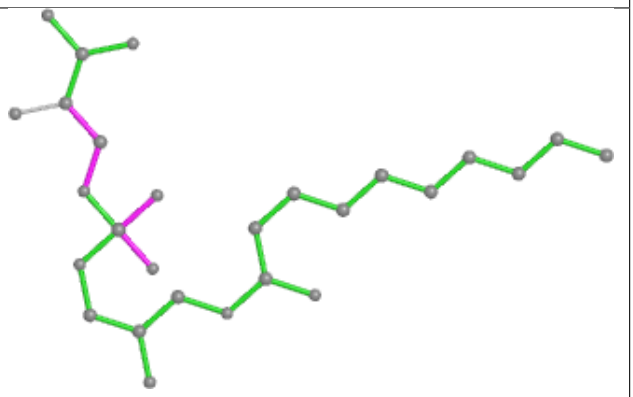
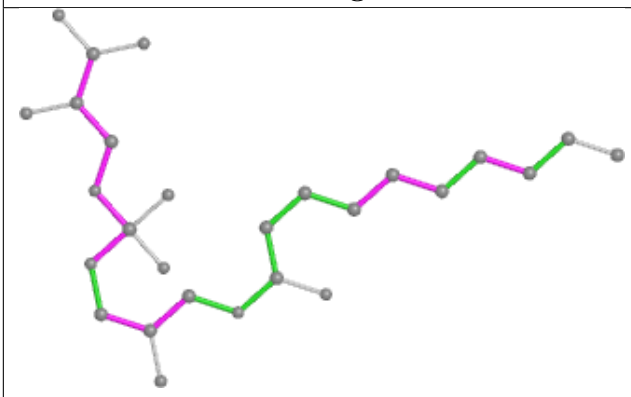


Bond angles



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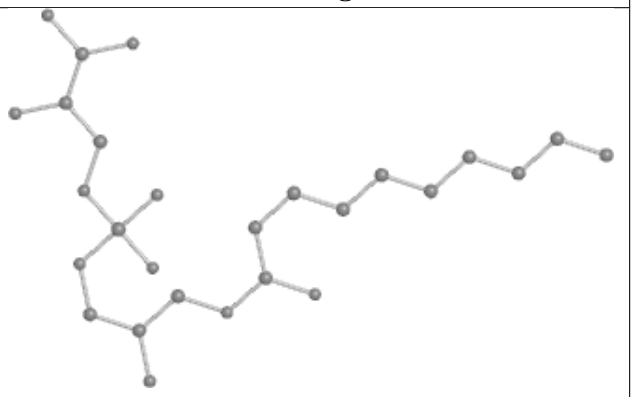
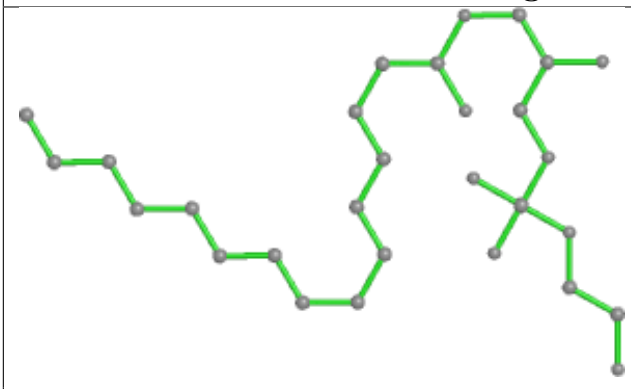
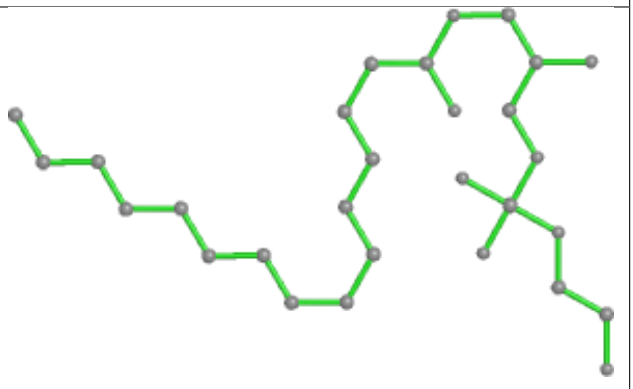


Rings

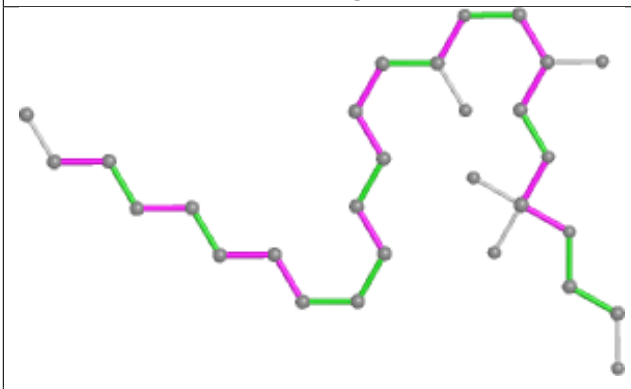
Ligand PTY V 403



Bond lengths



Bond angles



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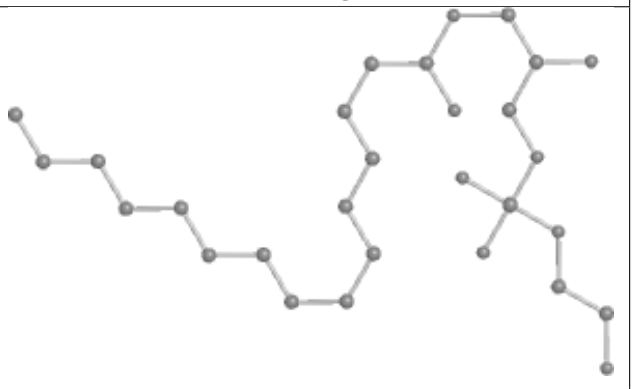
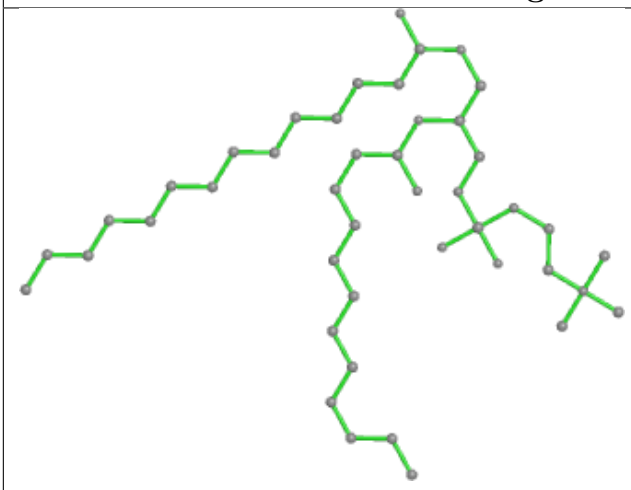


Rings

Ligand WSS 0 301



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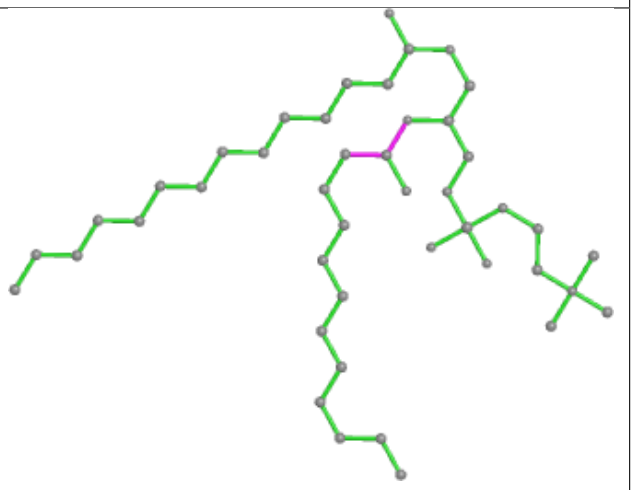
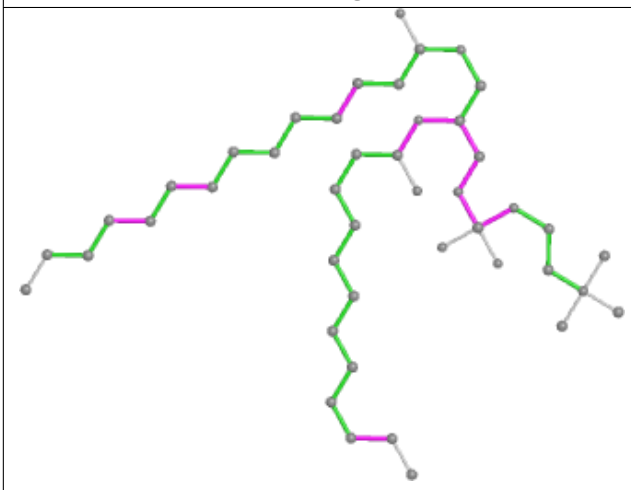


Bond angles



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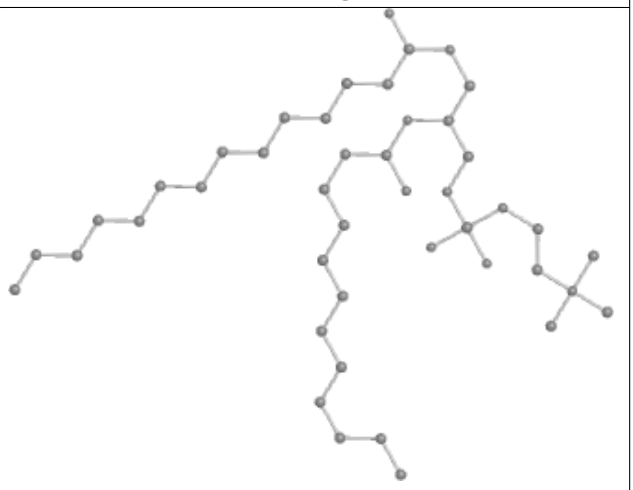
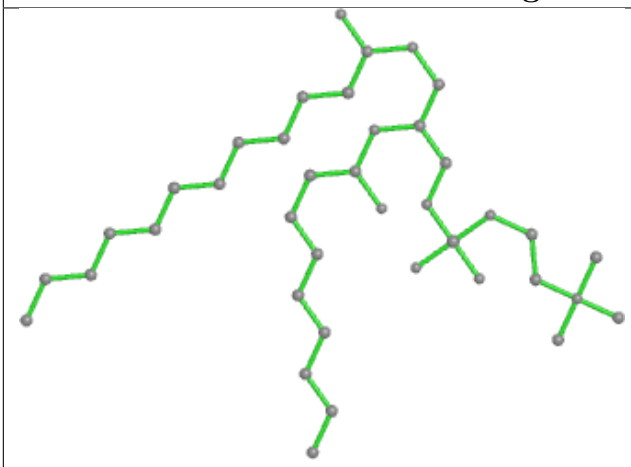
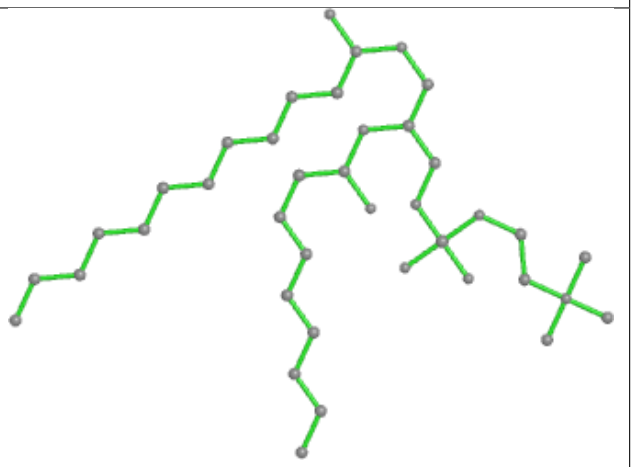


Rings

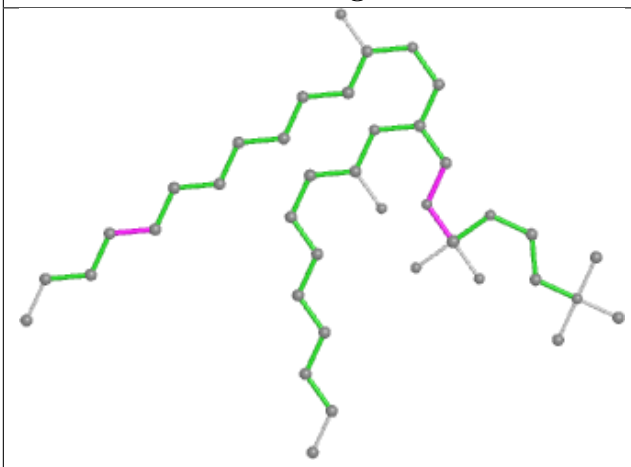
Ligand WSS U 501



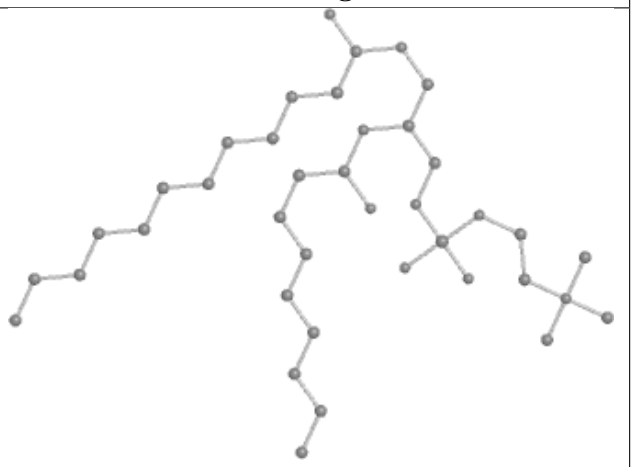
Bond lengths



Bond angles

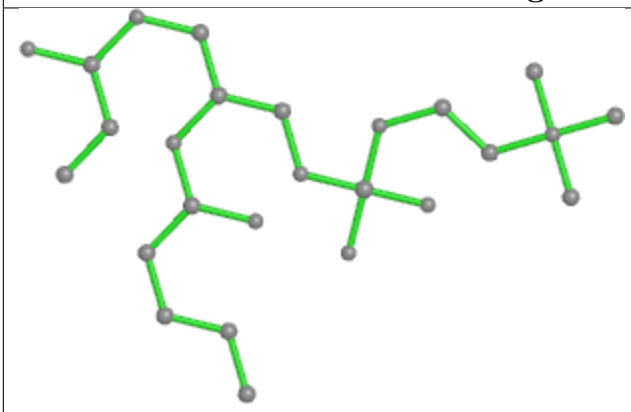


Torsions

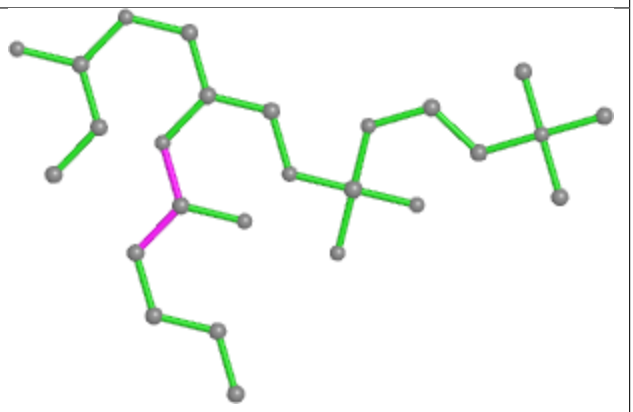


Rings

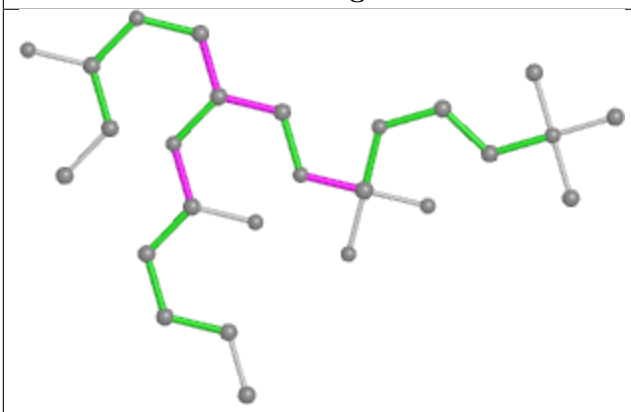
Ligand WSS 0 303



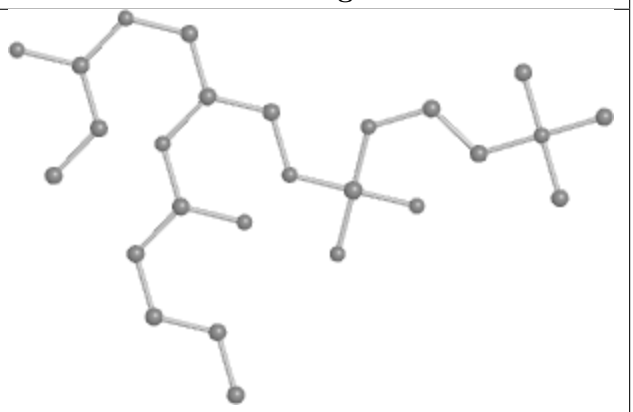
Bond lengths



Bond angles

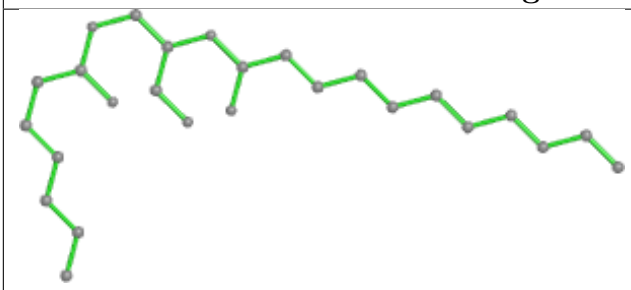


Torsions

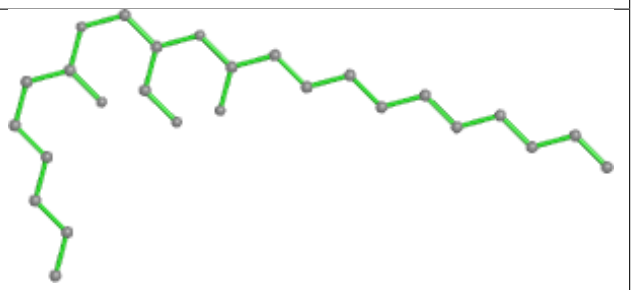


Rings

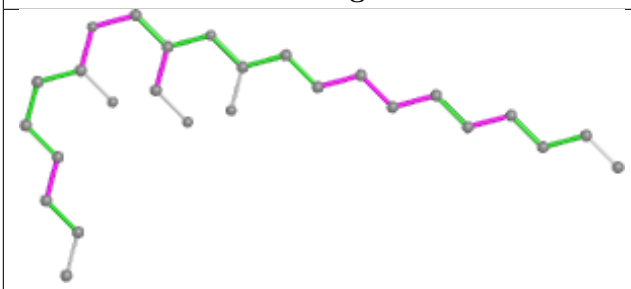
Ligand PTY U 503



Bond lengths



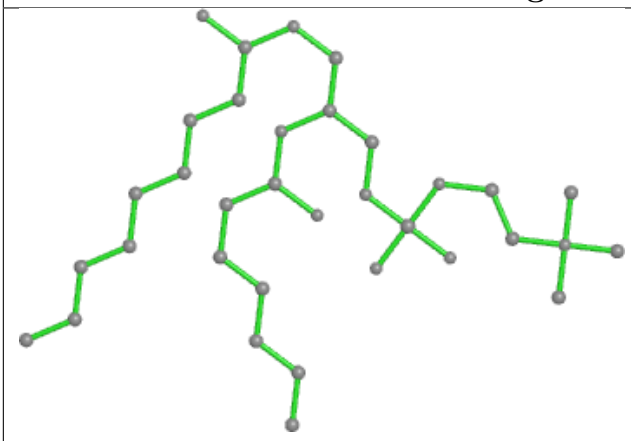
Bond angles



Torsions

Rings

Ligand WSS 1 201



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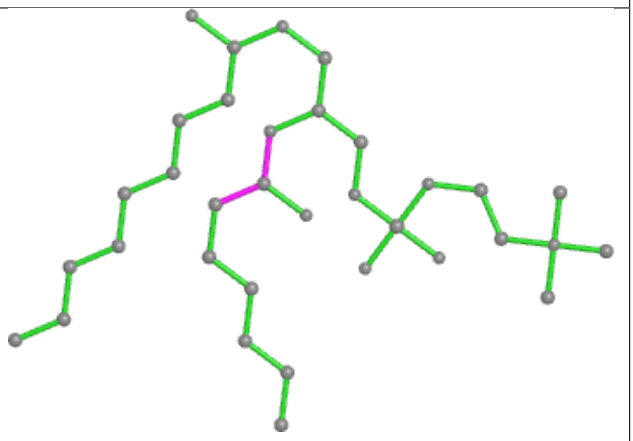
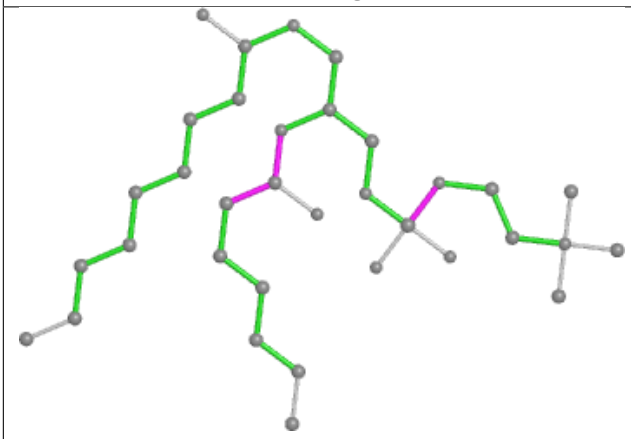
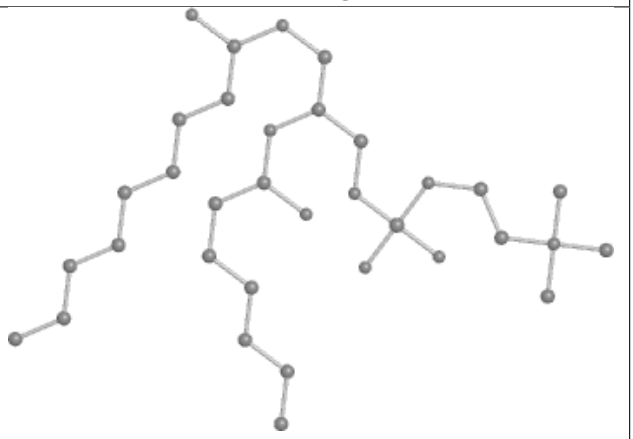


Bond angles

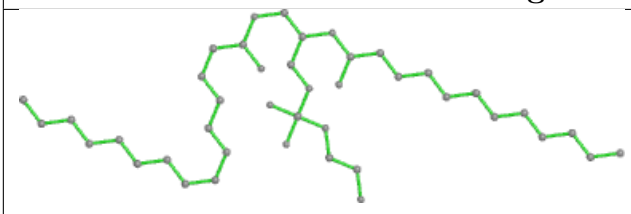


Torsions



Rings

Ligand PTY 7 201



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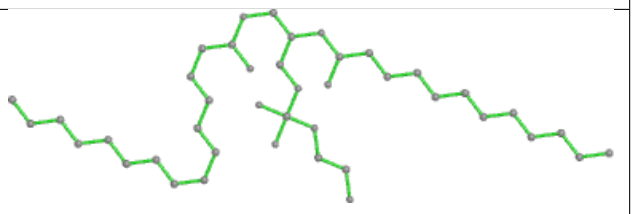
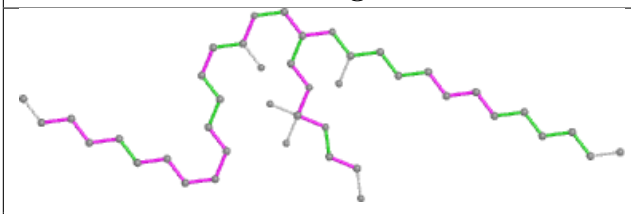
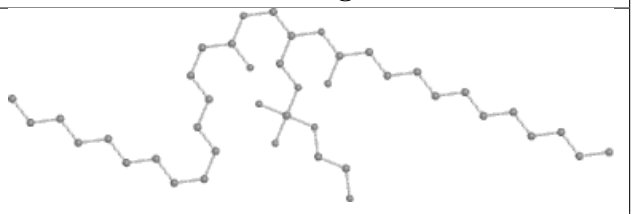


Bond angles

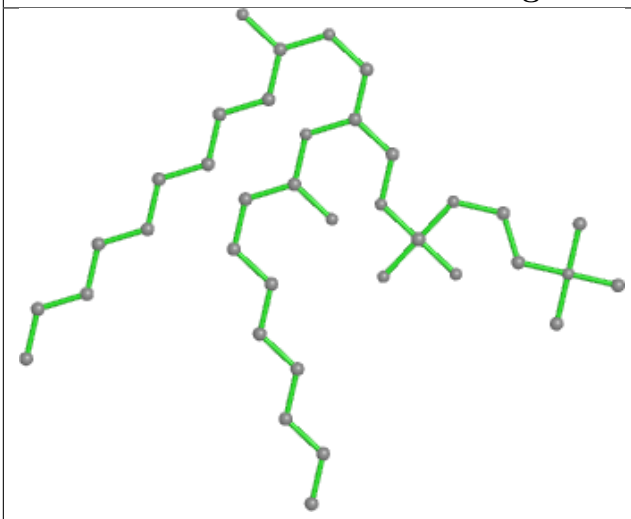


Torsions

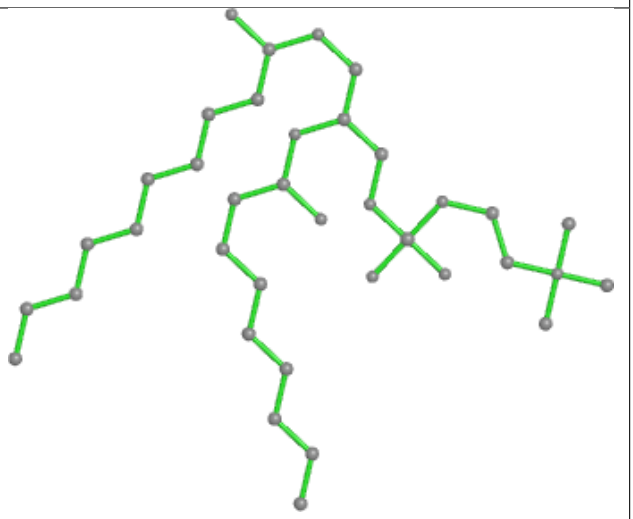


Rings

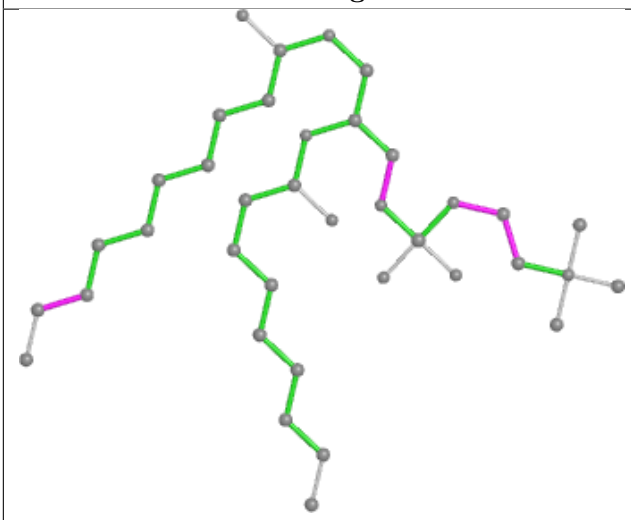
Ligand WSS U 502



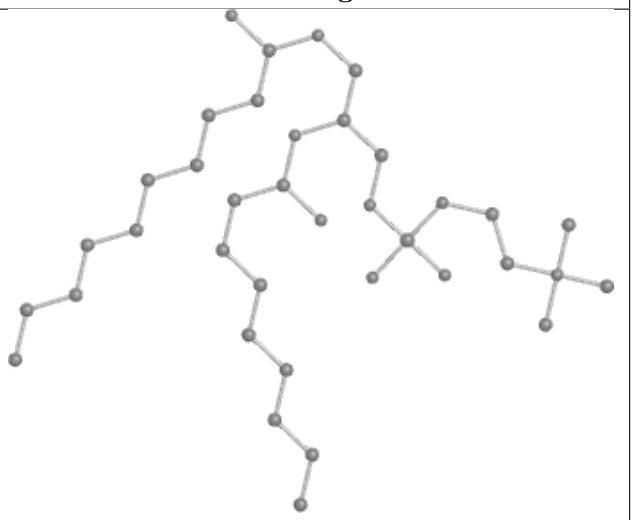
Bond lengths



Bond angles

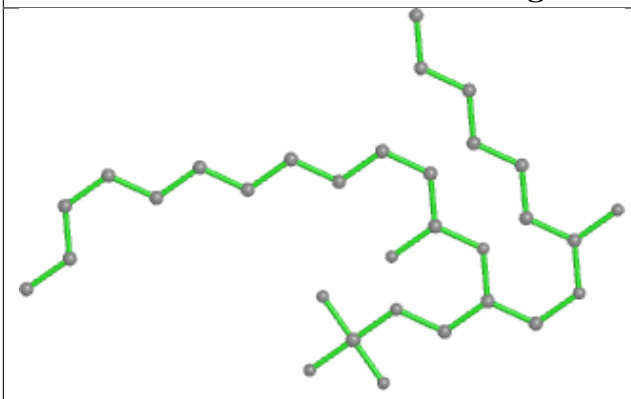


Torsions

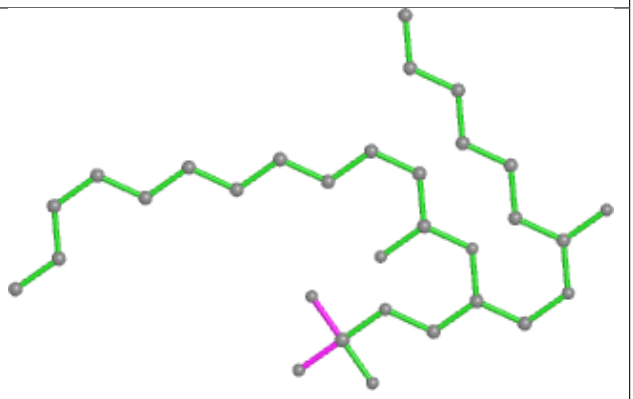


Rings

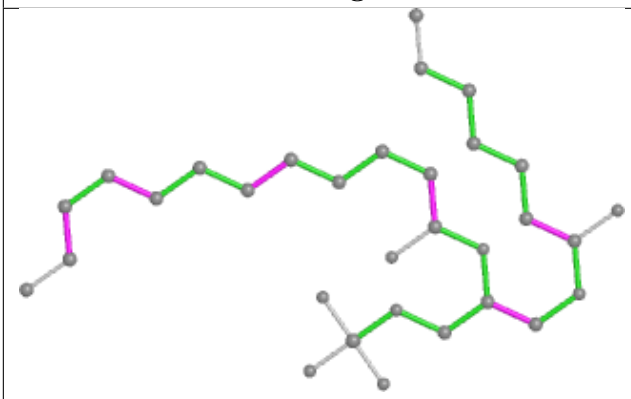
Ligand WSS 0 305



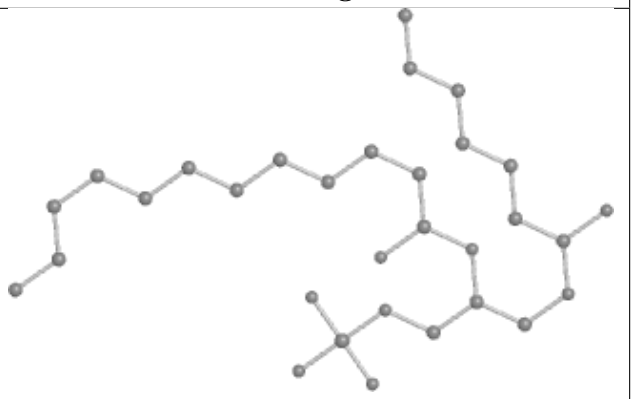
Bond lengths



Bond angles

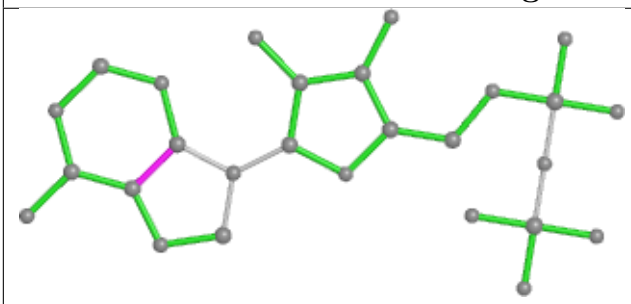


Torsions

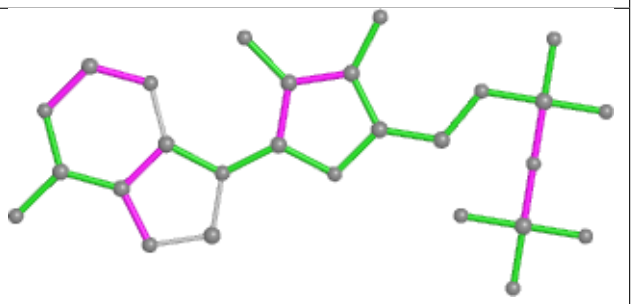


Rings

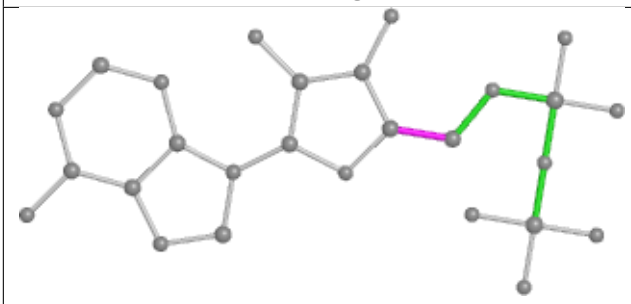
Ligand ADP C 701



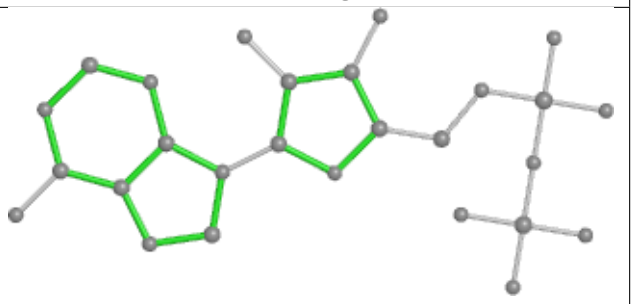
Bond lengths



Bond angles

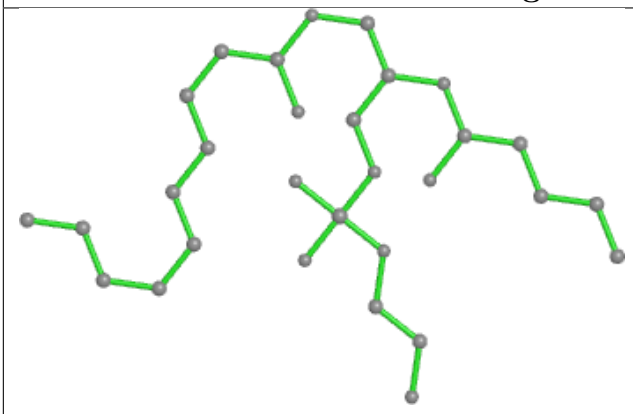


Torsions

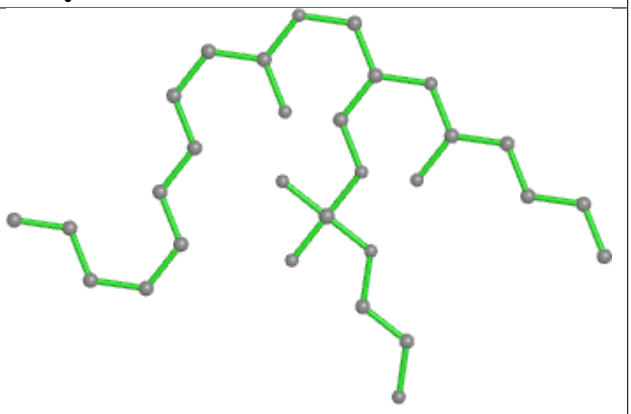


Rings

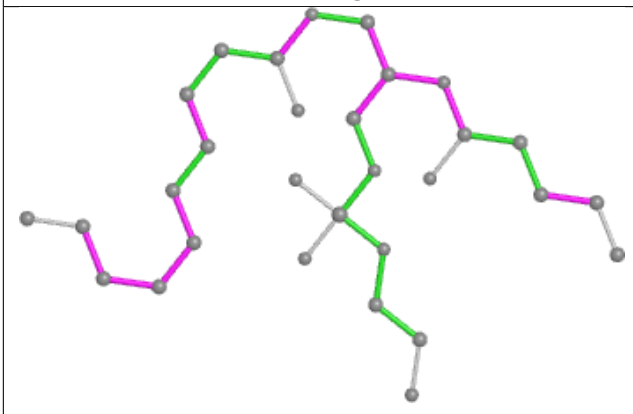
Ligand PTY Q 401



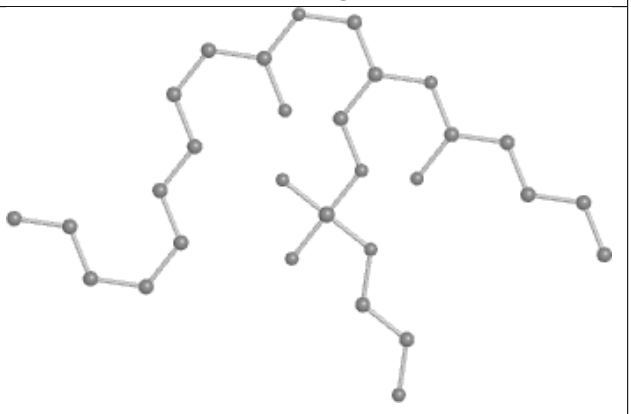
Bond lengths



Bond angles

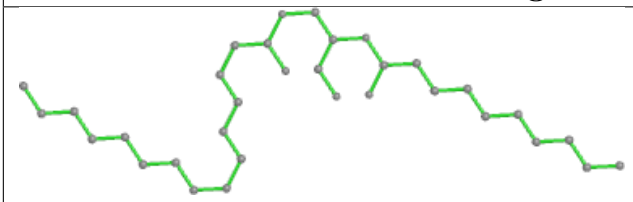


Torsions

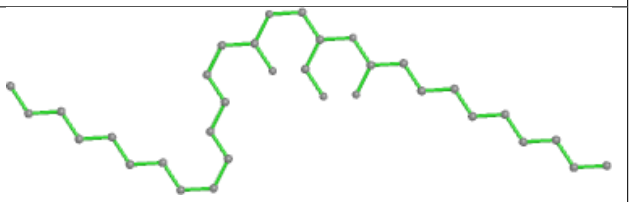


Rings

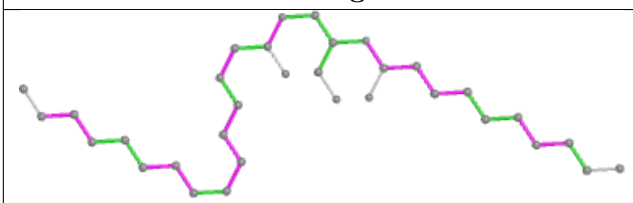
Ligand PTY 8 202



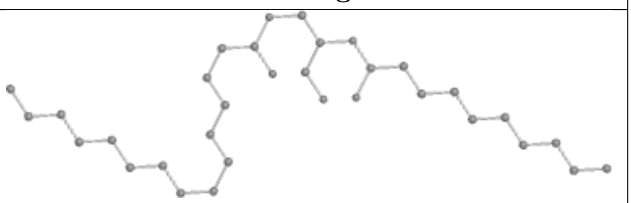
Bond lengths



Bond angles

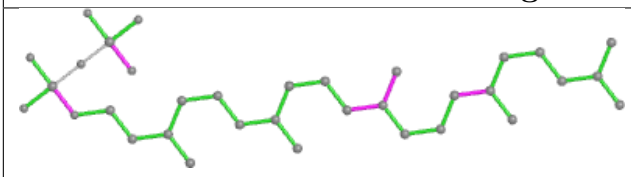


Torsions

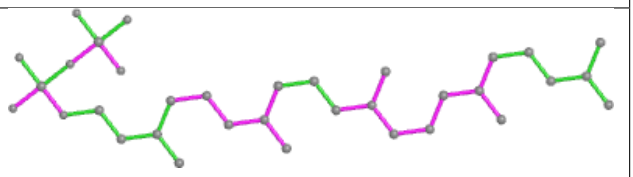


Rings

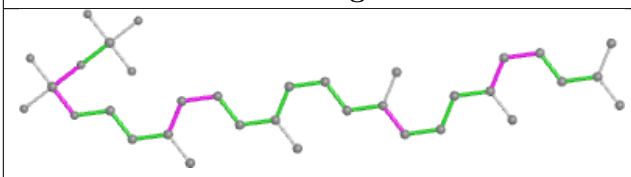
Ligand WJP R 907



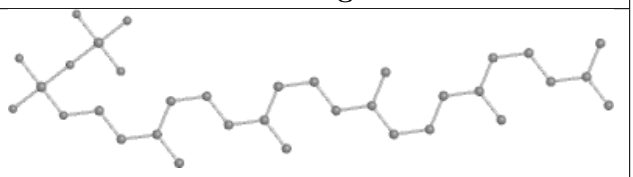
Bond lengths



Bond angles

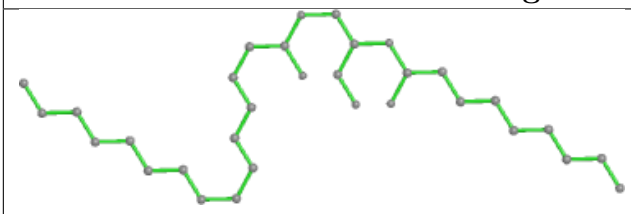


Torsions

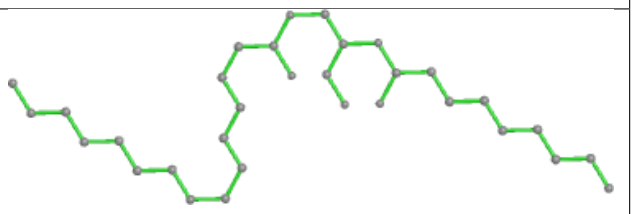


Rings

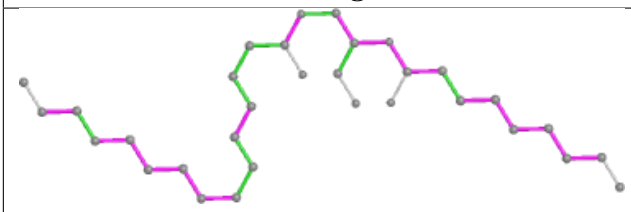
Ligand PTY R 903



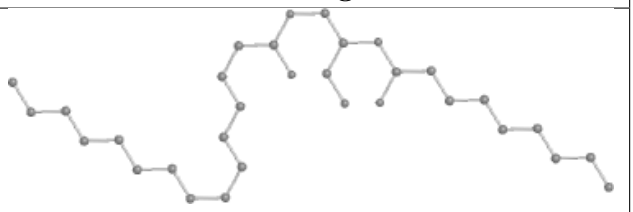
Bond lengths



Bond angles

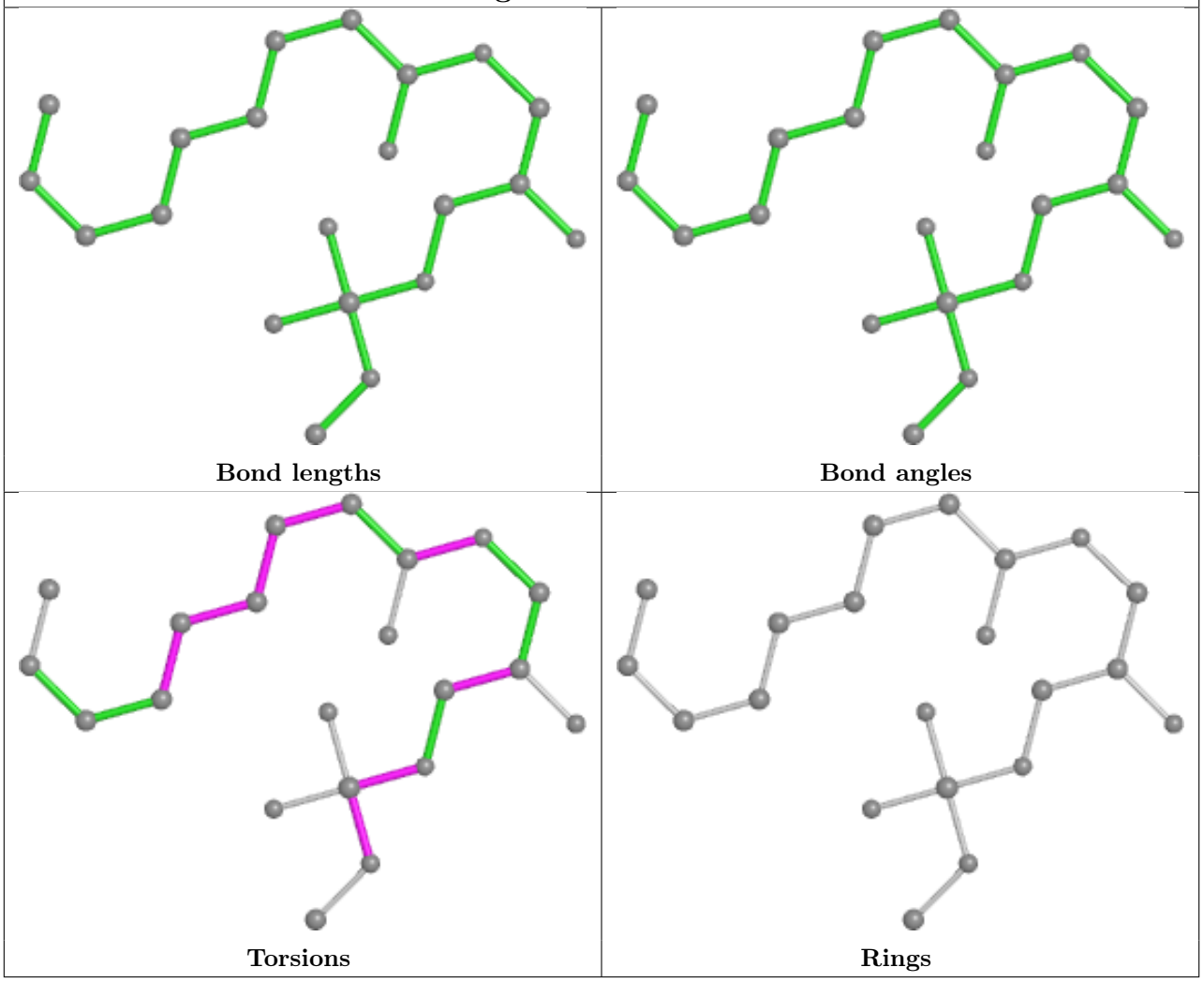


Torsions



Rings

Ligand PTY 6 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	360:THR	C	361:PRO	N	5.02

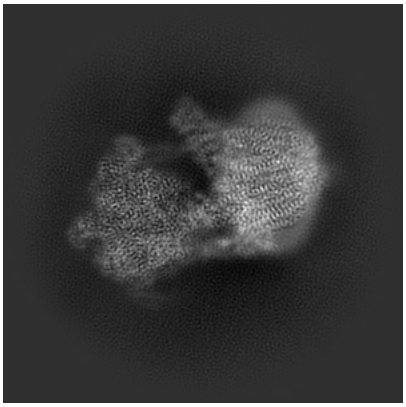
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21847. These allow visual inspection of the internal detail of the map and identification of artifacts.

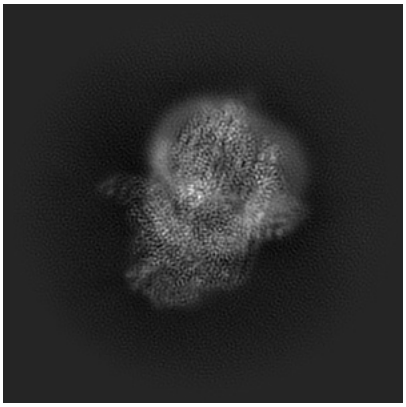
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

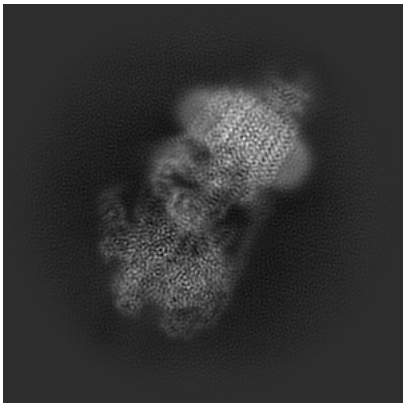
6.1.1 Primary map



X



Y

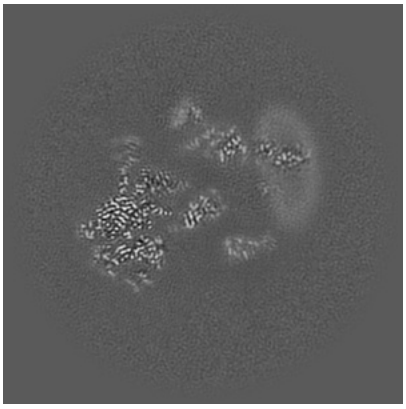


Z

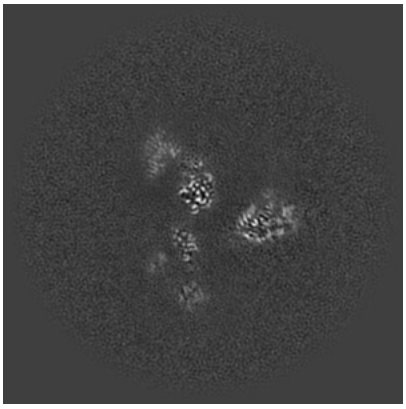
The images above show the map projected in three orthogonal directions.

6.2 Central slices

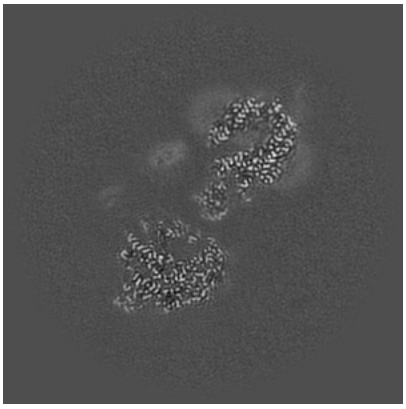
6.2.1 Primary map



X Index: 180



Y Index: 180

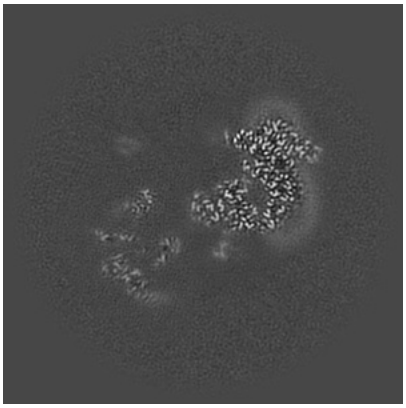


Z Index: 180

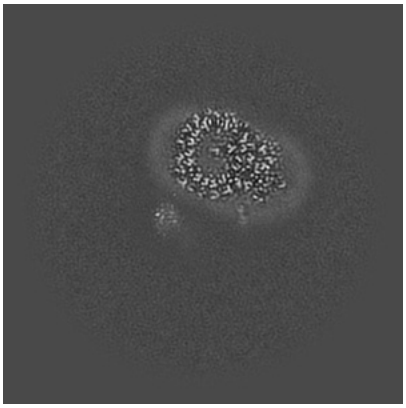
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

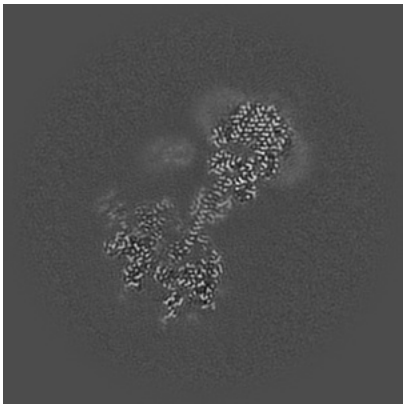
6.3.1 Primary map



X Index: 199



Y Index: 242



Z Index: 170

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

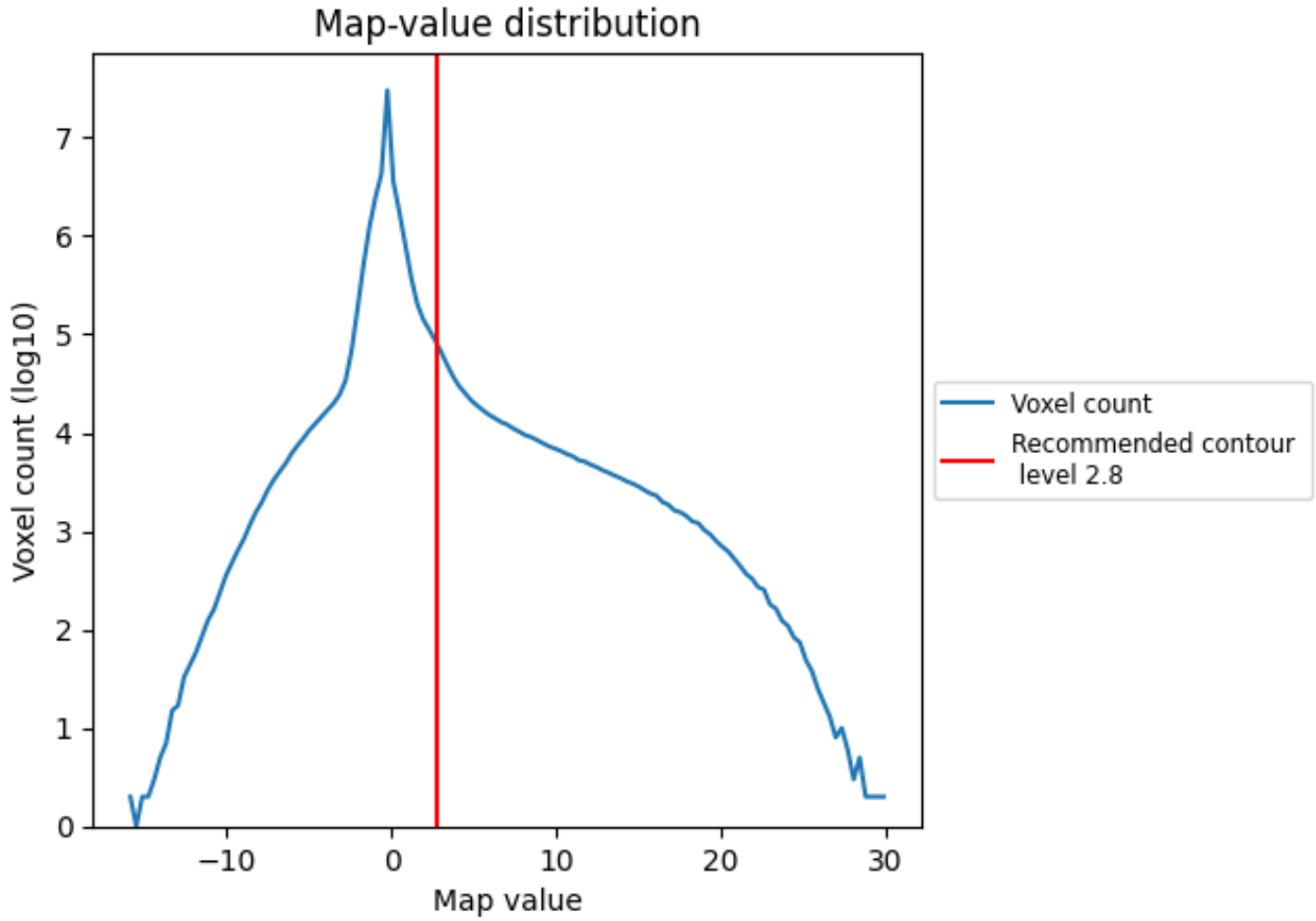
6.5 Mask visualisation (i)

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

7 Map analysis

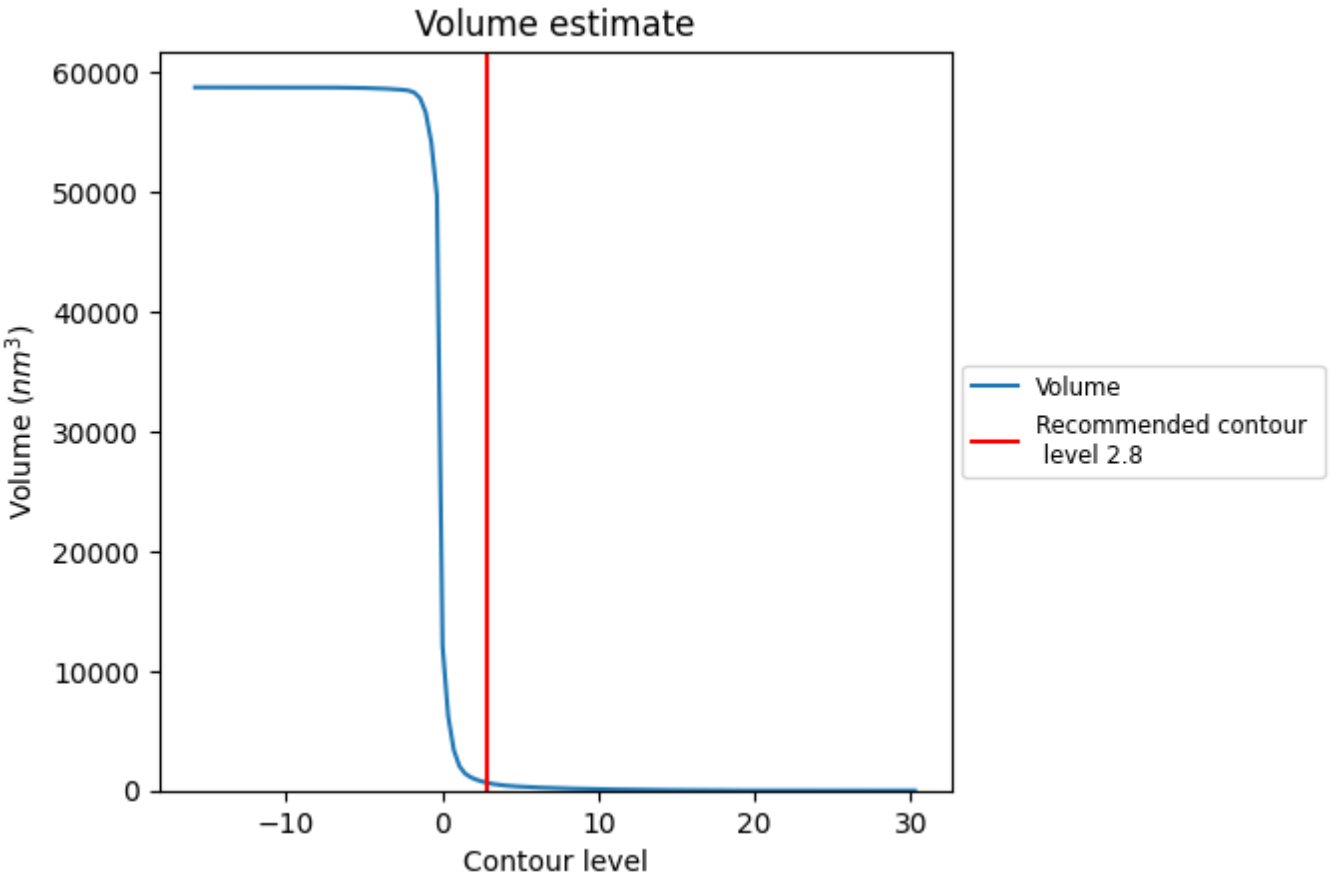
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

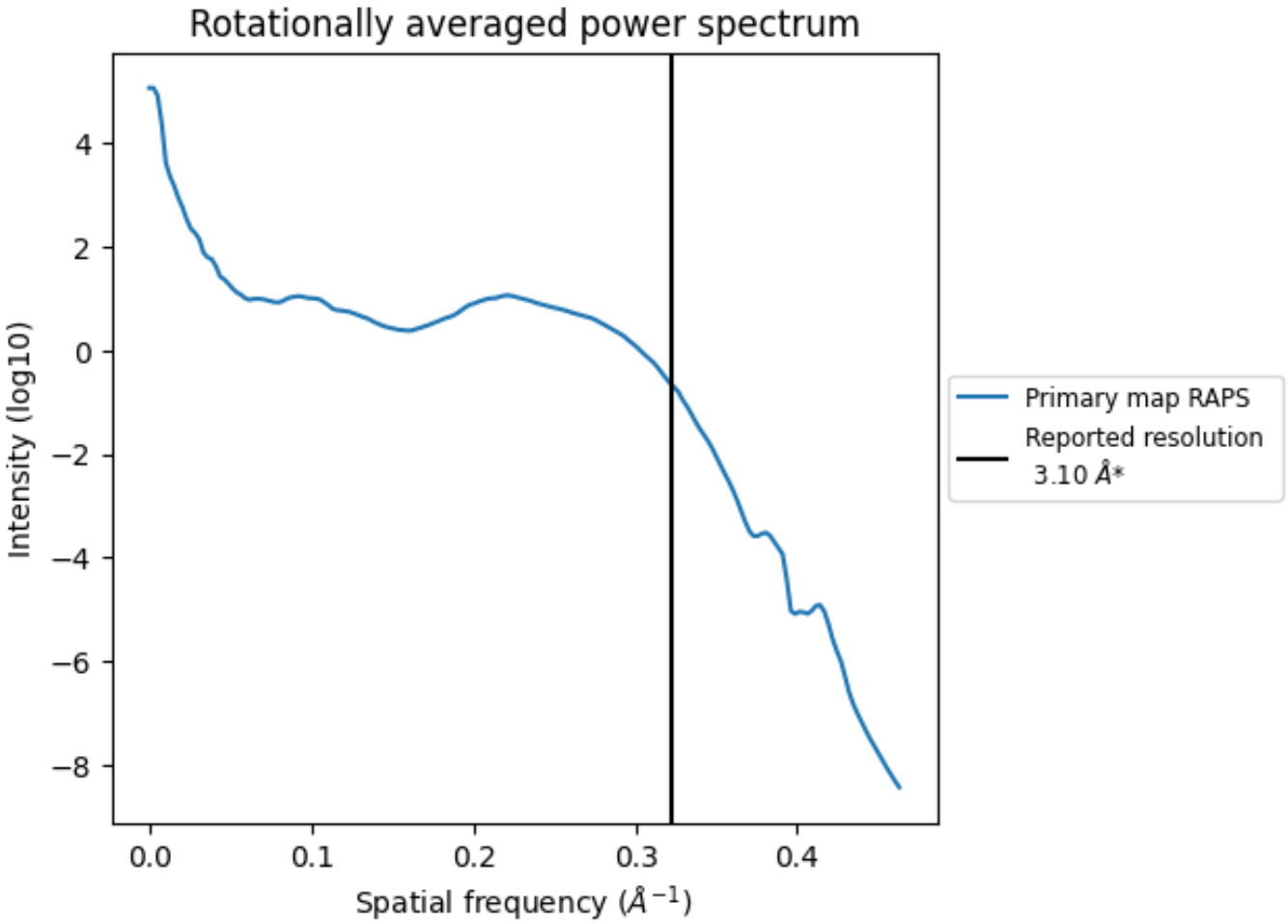
7.2 Volume estimate



The volume at the recommended contour level is 675 nm^3; this corresponds to an approximate mass of 610 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 0.323 Å^{-1}

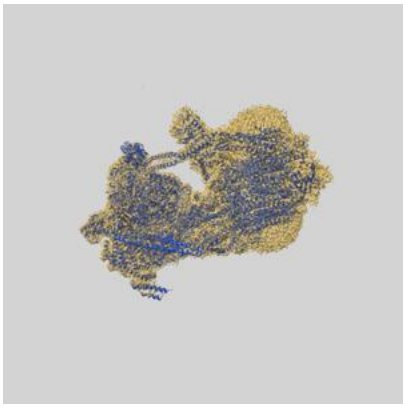
8 Fourier-Shell correlation

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

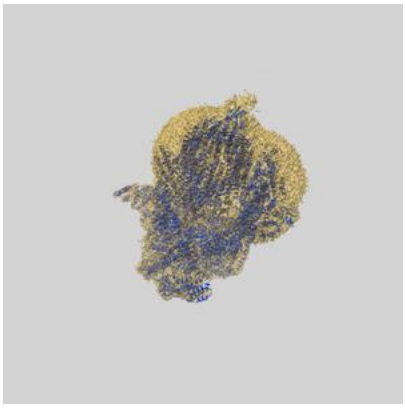
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21847 and PDB model 6WM2. Per-residue inclusion information can be found in section 3 on page 16.

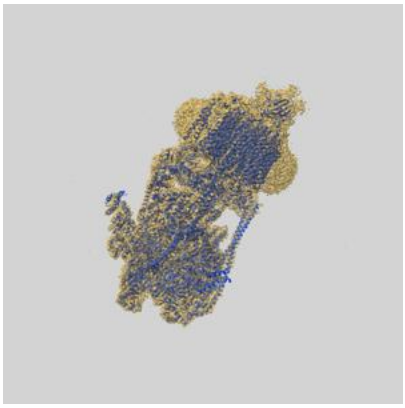
9.1 Map-model overlay



X



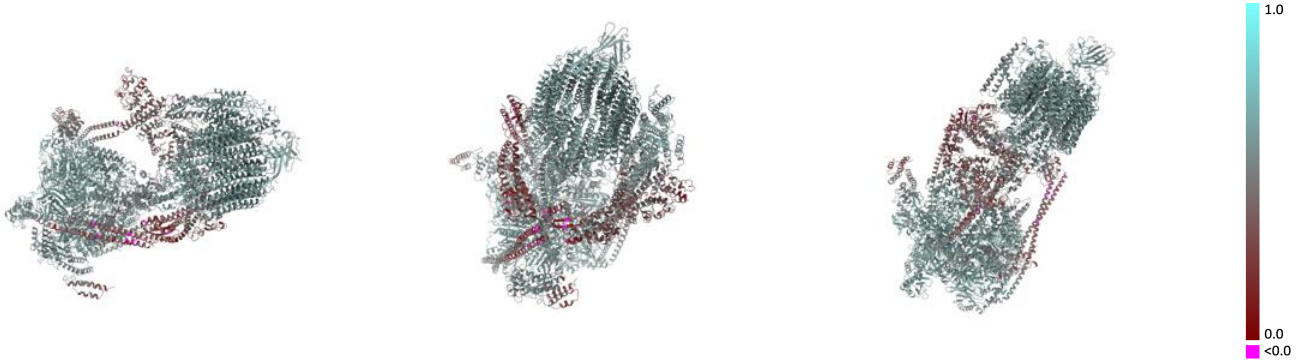
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.8 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.

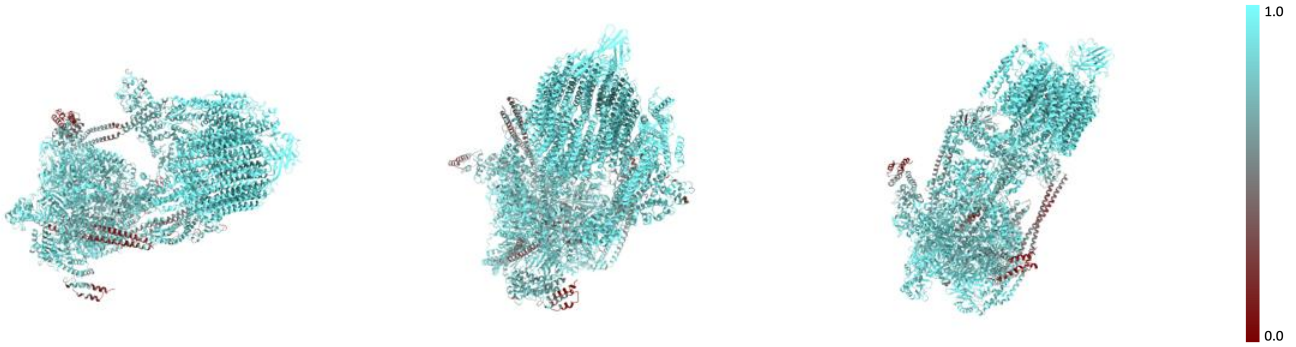
9.2 Q-score mapped to coordinate model (i)



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.

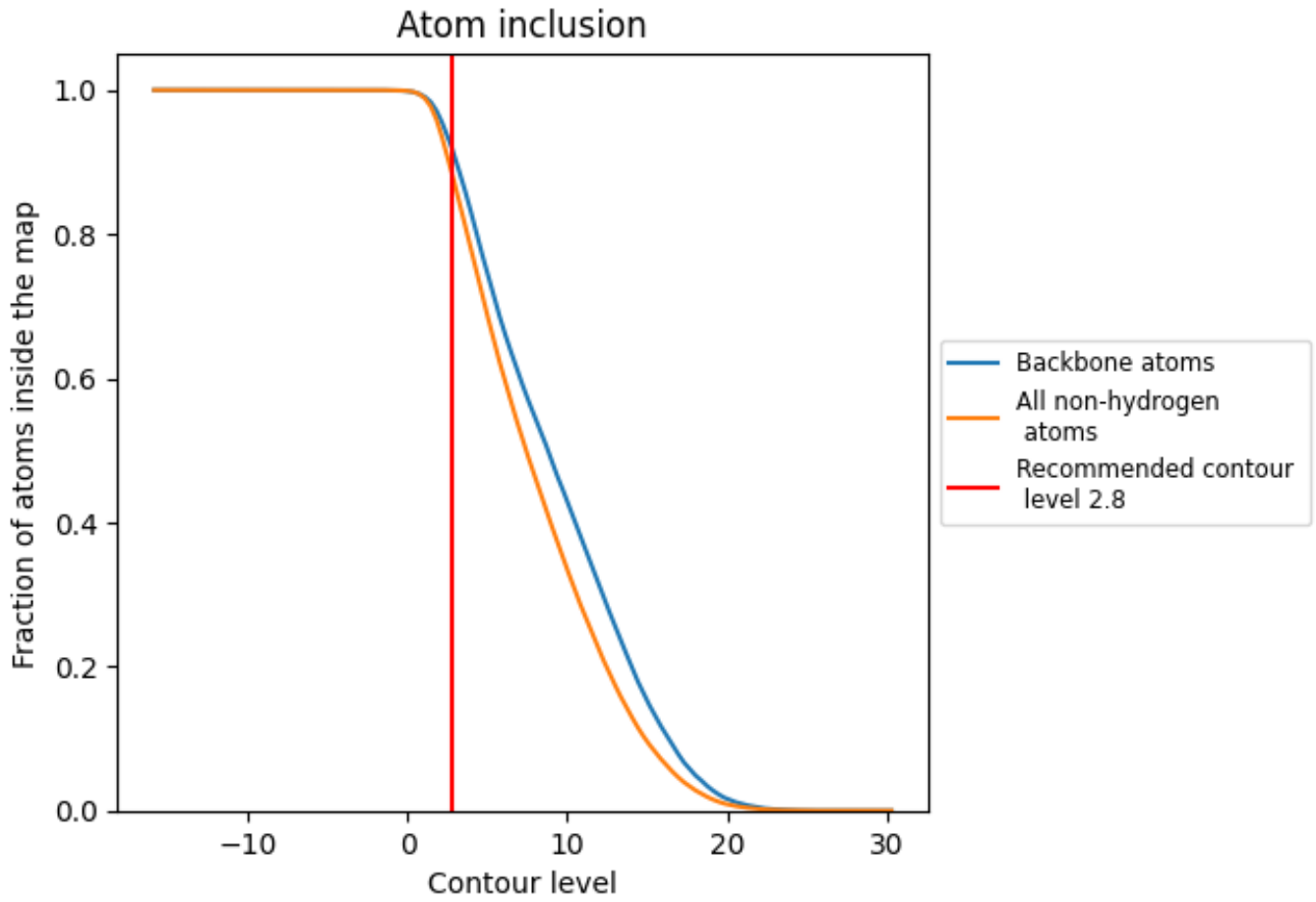
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.8).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8841	0.5350
0	0.9819	0.5860
1	0.9881	0.5870
2	0.9778	0.5800
3	0.9786	0.5880
4	0.9801	0.5790
5	0.9722	0.5780
6	0.9674	0.5770
7	0.9753	0.5750
8	0.9719	0.5750
9	0.9820	0.5840
A	0.9164	0.5980
B	0.9005	0.5860
C	0.9372	0.6080
D	0.9441	0.6150
E	0.9539	0.6120
F	0.9486	0.6160
G	0.8913	0.5490
H	0.8265	0.5230
I	0.8097	0.4800
J	0.7493	0.4990
K	0.6959	0.4500
L	0.6740	0.3890
M	0.5587	0.3840
N	0.9078	0.5140
O	0.7844	0.2890
P	0.8723	0.3600
Q	0.9637	0.5850
R	0.8992	0.4760
S	0.9646	0.5650
T	0.9567	0.5230
U	0.9869	0.5750
V	0.9741	0.5780
W	0.8088	0.3900
X	0.6599	0.4920

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	0.7309	0.5200
Z	0.5665	0.4900
a	0.8571	0.4310
b	0.8929	0.4270
c	0.9286	0.4260
d	0.8571	0.4170
r	0.9843	0.5560
s	1.0000	0.5130
u	0.9286	0.4320