Full wwPDB EM Validation Report (i)

May 19, 2024 – 09:26 PM JST

PDB ID	:	6L7O
EMDB ID	:	EMD-0849
Title	:	cryo-EM structure of cyanobacteria Fd-NDH-1L complex
Authors	:	Zhang, C.; Shuai, J.; Wu, J.; Lei, M.
Deposited on	:	2019-11-02
Resolution	:	3.20 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

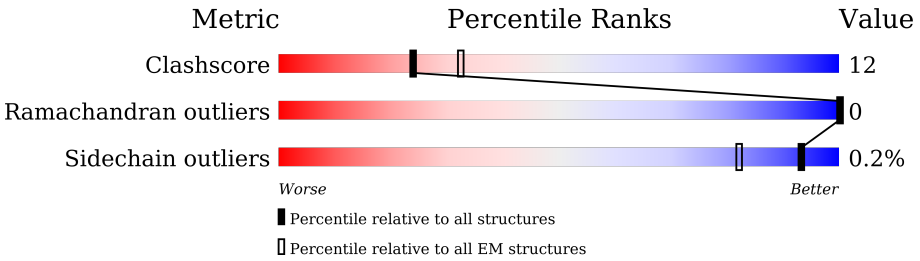
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	372	12% 81% 19%
2	B	515	• 80% 16% •
3	C	132	10% 70% 21% 8%
4	D	529	5% 74% 21% 5%
5	E	101	• 76% 24%
6	F	656	16% 79% 20% •
7	G	200	12% 78% 18% •
8	H	394	16% 81% 19%

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Mol	Chain	Length	Quality of chain
9	I	196	19% 77% 20%
10	J	168	12% 79% 14% 7%
11	K	237	6% 71% 16% 13%
12	L	76	16% 76% 20%
13	M	111	10% 89% 10%
14	N	150	11% 77% 22%
15	O	70	20% 84% 13%
16	P	44	11% 89% 5% 7%
17	Q	45	18% 78% 20%
18	R	98	77% 82% 17%
19	S	110	27% 45% 12% 44%
20	V	146	47% 51% 18% 29%

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
24	AJP	A	405	X	-	-	-
24	AJP	A	406	X	-	-	-
24	AJP	A	407	X	-	-	-
24	AJP	A	408	X	-	-	-
24	AJP	A	409	X	-	-	-
24	AJP	B	606	X	-	-	-
24	AJP	B	607	X	-	-	-
24	AJP	B	608	X	-	-	-
24	AJP	B	609	X	-	-	-
24	AJP	B	610	X	-	-	-
24	AJP	B	611	X	-	-	-
24	AJP	B	612	X	-	-	-
24	AJP	B	613	X	-	-	-
24	AJP	B	614	X	-	-	-
24	AJP	B	615	X	-	-	-
24	AJP	B	616	X	-	X	-
24	AJP	B	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	C	201	X	-	-	-
24	AJP	C	202	X	-	-	-
24	AJP	D	603	X	-	-	-
24	AJP	D	604	X	-	-	-
24	AJP	D	605	X	-	-	-
24	AJP	D	606	X	-	-	-
24	AJP	D	607	X	-	-	-
24	AJP	D	608	X	-	-	-
24	AJP	D	609	X	-	-	-
24	AJP	D	610	X	-	-	-
24	AJP	D	611	X	-	-	-
24	AJP	D	612	X	-	-	-
24	AJP	D	613	X	-	-	-
24	AJP	D	614	X	-	-	-
24	AJP	E	201	X	-	-	-
24	AJP	F	706	X	-	-	-
24	AJP	F	707	X	-	-	-
24	AJP	F	708	X	-	-	-
24	AJP	F	709	X	-	-	-
24	AJP	F	710	X	-	-	-
24	AJP	F	711	X	-	-	-
24	AJP	F	712	X	-	-	-
24	AJP	F	713	X	-	-	-
24	AJP	F	714	X	-	-	-
24	AJP	F	715	X	-	-	-
24	AJP	F	716	X	-	-	-
24	AJP	F	717	X	-	-	-
24	AJP	F	718	X	-	-	-
24	AJP	G	301	X	-	-	-
24	AJP	G	302	X	-	-	-
24	AJP	G	303	X	-	-	-
24	AJP	G	304	X	-	-	-
24	AJP	G	305	X	-	-	-
24	AJP	G	306	X	-	-	-
24	AJP	G	307	X	-	-	-
24	AJP	Q	101	X	-	-	-
24	AJP	Q	102	X	-	-	-
24	AJP	Q	103	X	-	-	-
24	AJP	Q	104	X	-	-	-
24	AJP	Q	105	X	-	-	-
24	AJP	Q	106	X	-	-	-
24	AJP	Q	107	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	Q	108	X	-	-	-
27	SF4	K	301	-	-	X	-
28	FES	R	101	-	-	X	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 35037 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 NAD(P)H-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	371	2859	1919	444	486	10	0	0

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	493	3732	2476	579	661	16	0	0

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	121	978	669	150	155	4	0	0

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase chain 4 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	504	3896	2613	606	656	21	0	0

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	101	783	517	128	134	4	0	0

- Molecule 6 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	647	5004	3318	796	852	38	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	192	1463	974	229	256	4	0	0

- Molecule 8 is a protein called NAD(P)H-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	393	3177	2048	545	565	19	0	0

- Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	190	1525	973	262	277	13	0	0

- Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	156	1278	817	218	238	5	0	0

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	206	1597	1024	276	284	13	0	0

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	73	590	406	90	93	1	0	0

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	110	879	548	160	169	2	0	0

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	148	1165	758	201	205	1	0	0

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	O	68	538	349	91	98	0	0

- Molecule 16 is a protein called NAD(P)H-quinone oxidoreductase subunit P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	41	321	212	52	55	2	0	0

- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	44	332	221	53	56	2	0	0

- Molecule 18 is a protein called Ferredoxin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	97	748	463	116	164	5	0	0

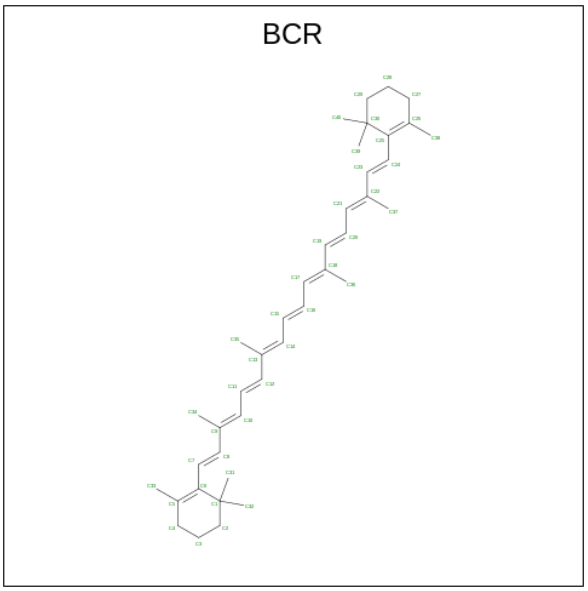
- Molecule 19 is a protein called Tlr0636 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	62	485	314	76	93	2	0	0

- Molecule 20 is a protein called Tlr0472 protein.

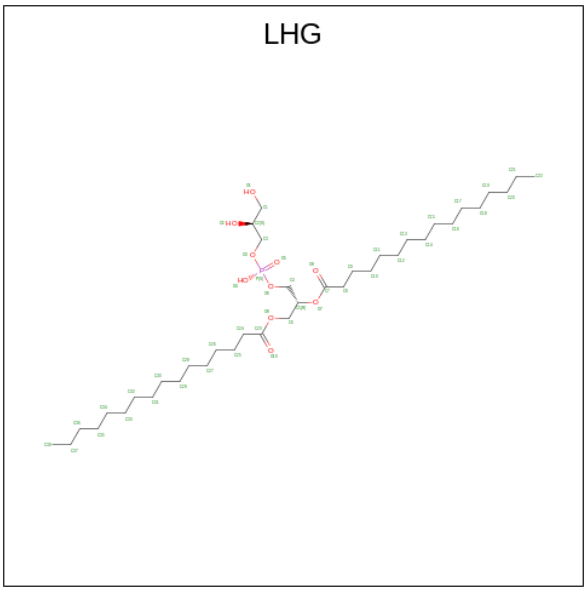
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	103	797	517	133	143	4	0	0

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



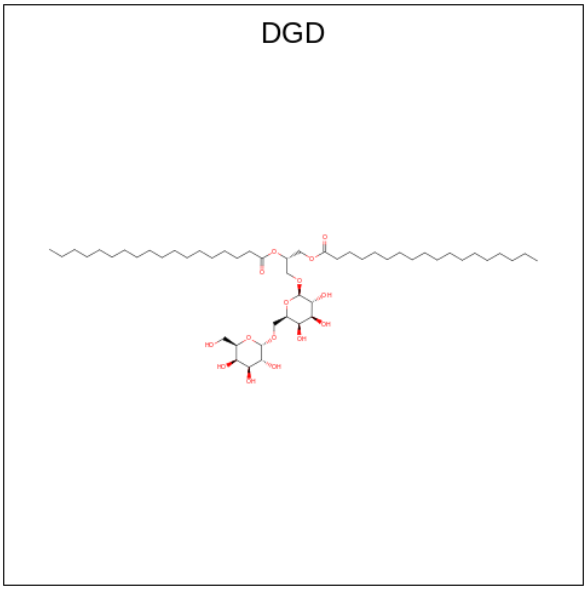
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
21	A	1	40	40	0
			Total	C	
21	F	1	40	40	0
			Total	C	
21	P	1	40	40	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



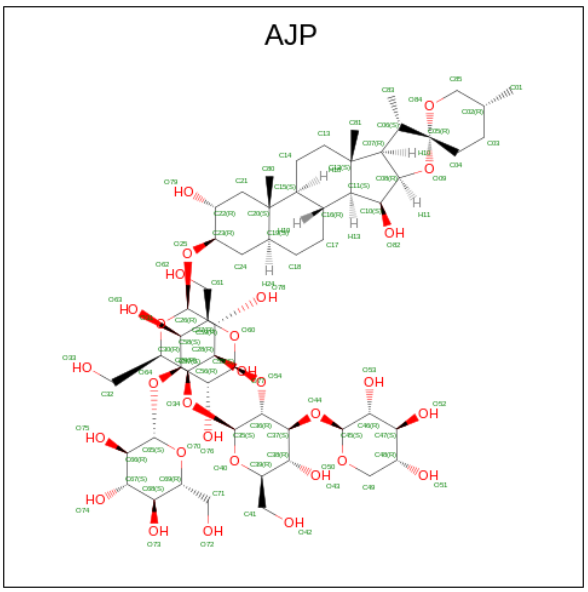
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
22	A	1	49	38	10	1	0
22	B	1	49	38	10	1	0
22	B	1	49	38	10	1	0
22	B	1	49	38	10	1	0
22	D	1	49	38	10	1	0
22	D	1	49	38	10	1	0
22	F	1	49	38	10	1	0
22	F	1	49	38	10	1	0
22	H	1	49	38	10	1	0

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	A	1	66	51	15	0
23	A	1	66	51	15	0

- Molecule 24 is Digitonin (three-letter code: AJP) (formula: $C_{56}H_{92}O_{29}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	A	1	32	27	5	0
24	A	1	32	27	5	0
24	A	1	32	27	5	0
24	A	1	32	27	5	0
24	A	1	32	27	5	0
24	B	1	32	27	5	0
24	B	1	32	27	5	0
24	B	1	32	27	5	0
24	B	1	32	27	5	0
24	B	1	32	27	5	0
24	B	1	32	27	5	0
24	B	1	32	27	5	0
24	B	1	32	27	5	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	B	1	32	27	5	0
24	B	1	32	27	5	0
24	B	1	32	27	5	0
24	B	1	32	27	5	0
24	C	1	32	27	5	0
24	C	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	D	1	32	27	5	0
24	E	1	32	27	5	0
24	F	1	32	27	5	0
24	F	1	32	27	5	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	F	1	32	27	5	0
24	F	1	32	27	5	0
24	F	1	32	27	5	0
24	F	1	32	27	5	0
24	F	1	32	27	5	0
24	F	1	32	27	5	0
24	F	1	32	27	5	0
24	F	1	32	27	5	0
24	F	1	32	27	5	0
24	F	1	32	27	5	0
24	F	1	32	27	5	0
24	G	1	32	27	5	0
24	G	1	32	27	5	0
24	G	1	32	27	5	0
24	G	1	32	27	5	0
24	G	1	32	27	5	0
24	G	1	32	27	5	0
24	G	1	32	27	5	0
24	G	1	32	27	5	0
24	Q	1	32	27	5	0
24	Q	1	32	27	5	0
24	Q	1	32	27	5	0

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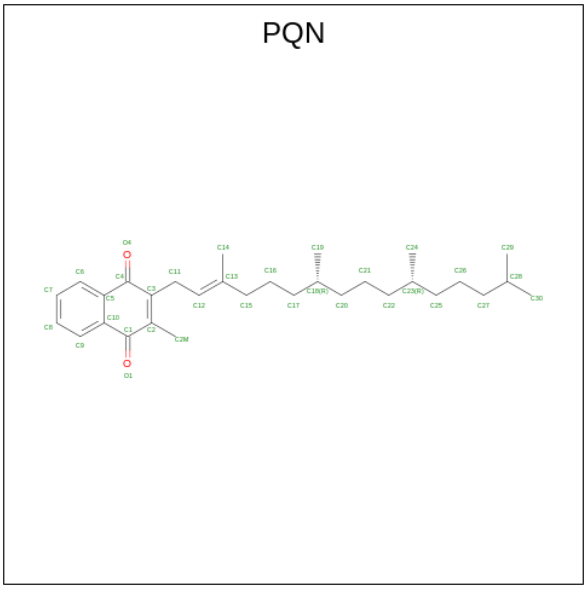
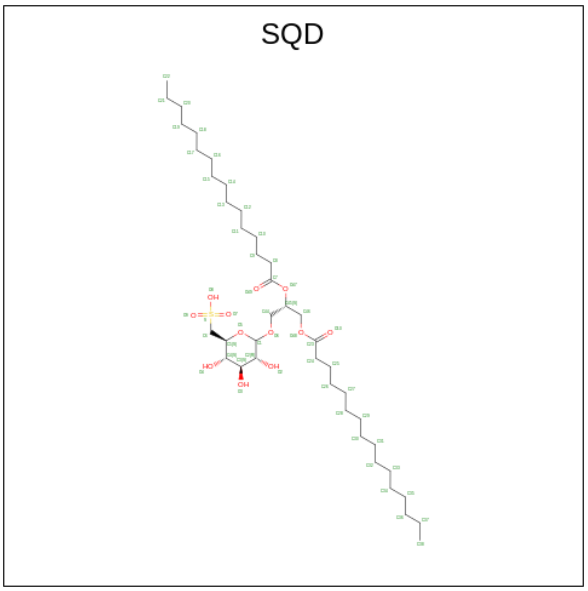
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	Q	1	32	27	5	0
24	Q	1	32	27	5	0
24	Q	1	32	27	5	0
24	Q	1	32	27	5	0
24	Q	1	32	27	5	0

- Molecule 25 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



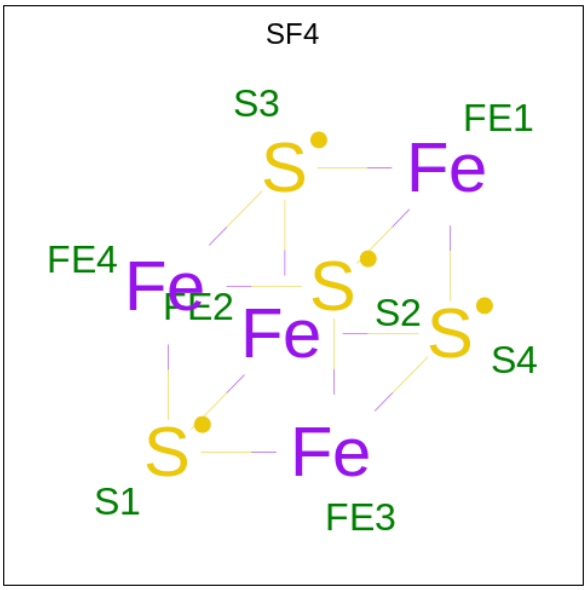
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	B	1	33	31	2	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



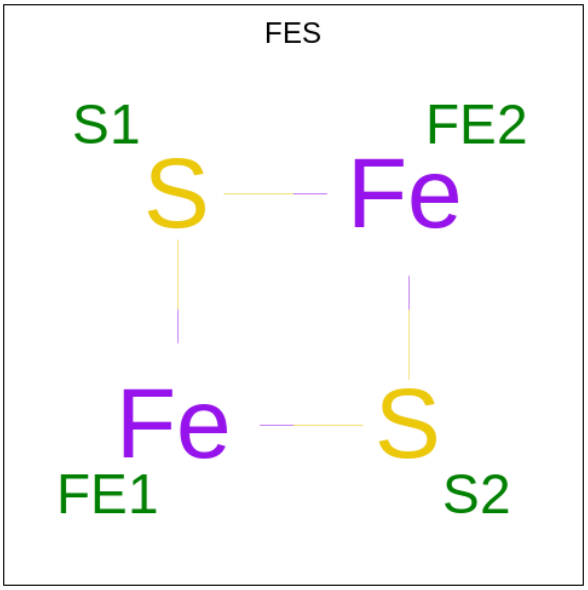
Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	S	0
			54	41	12	1	
26	F	1	Total	C	O	S	0
			54	41	12	1	
26	F	1	Total	C	O	S	0
			54	41	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
27	I	1	8	4	4	0
27	I	1	8	4	4	0
27	K	1	8	4	4	0

- Molecule 28 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



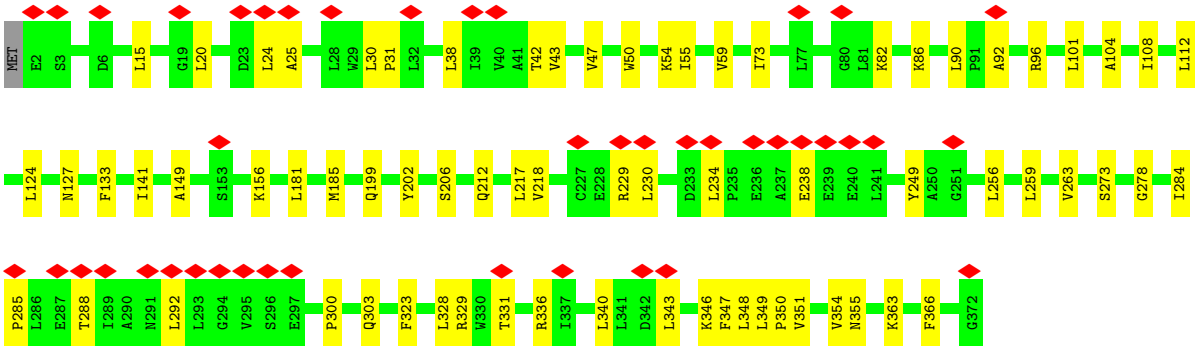
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
28	R	1	4	2	2	0

3 Residue-property plots (i)

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

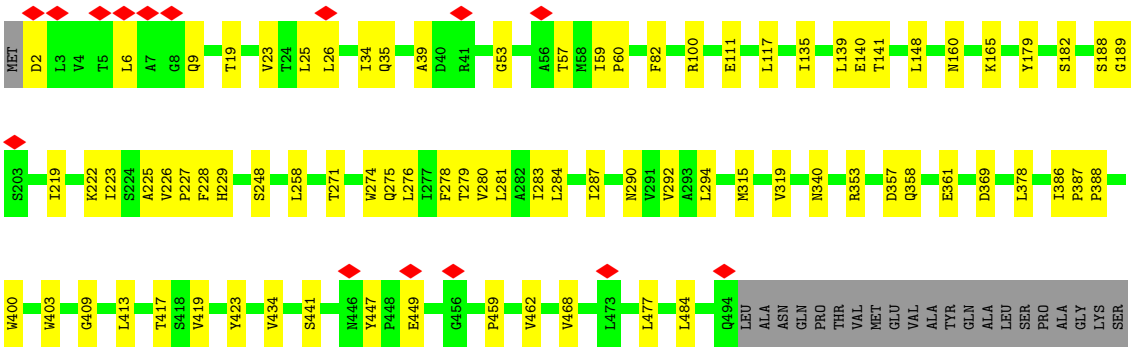
- Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1

Chain A:



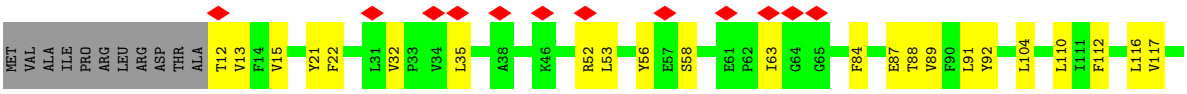
- Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2

Chain B:



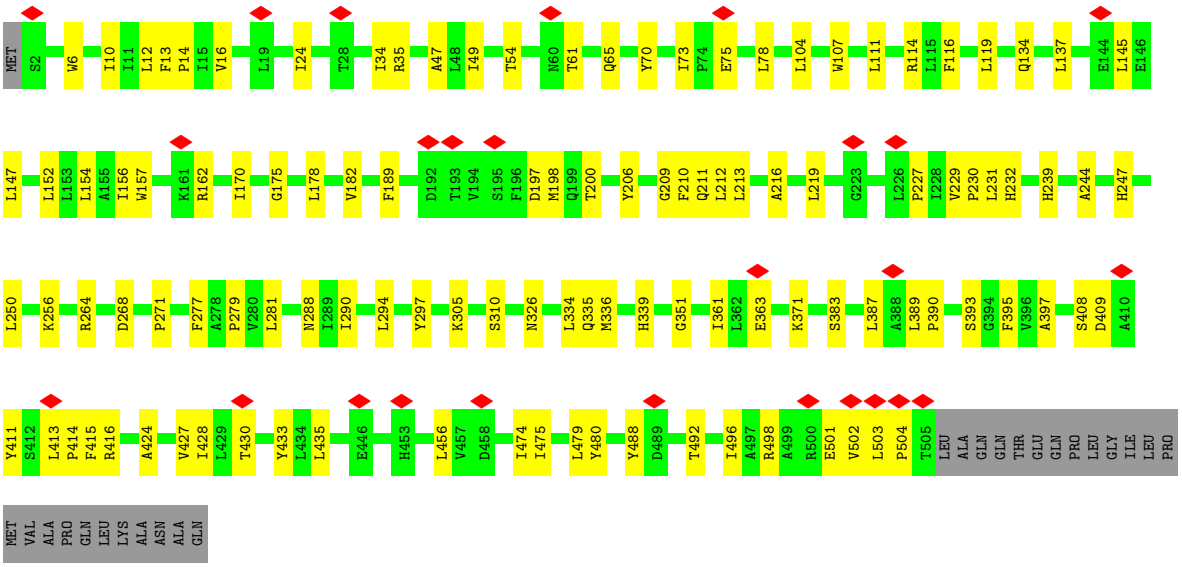
- Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3

Chain C:



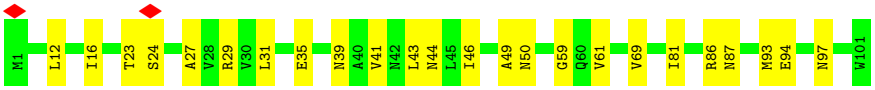
• Molecule 4: NAD(P)H-quinone oxidoreductase chain 4 1

Chain D:



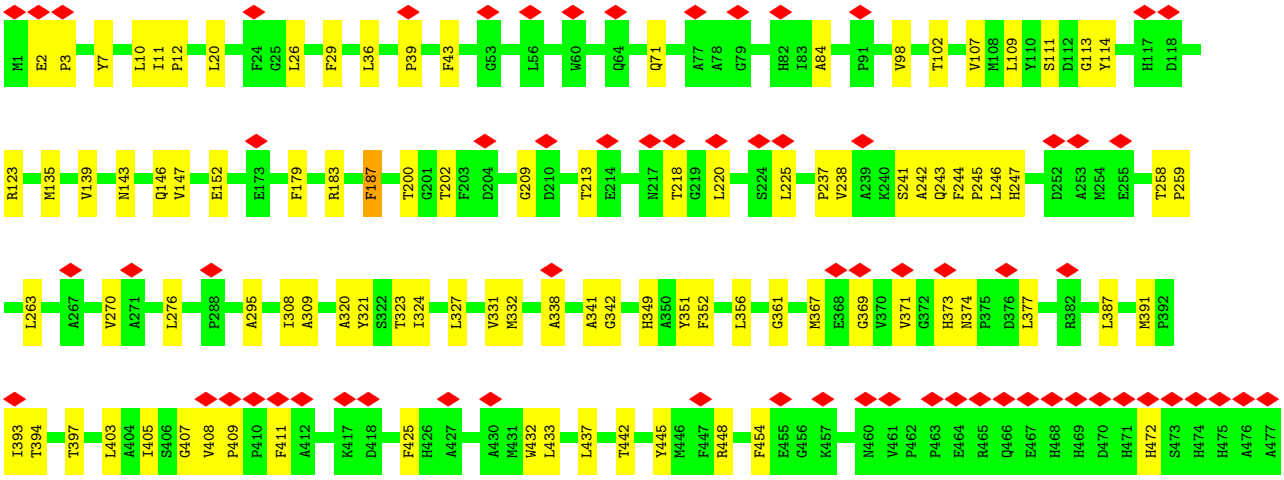
• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L

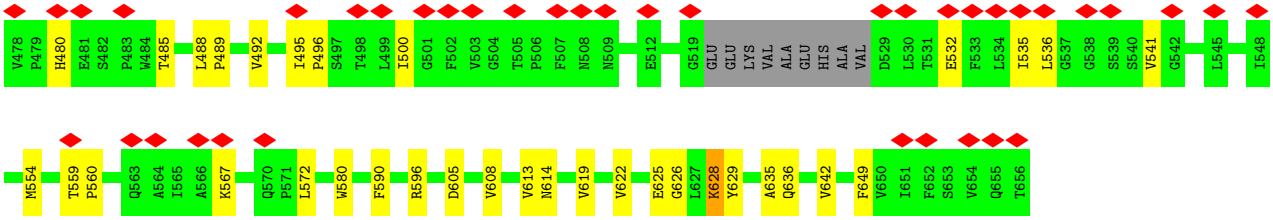
Chain E:



• Molecule 6: NADH dehydrogenase subunit 5

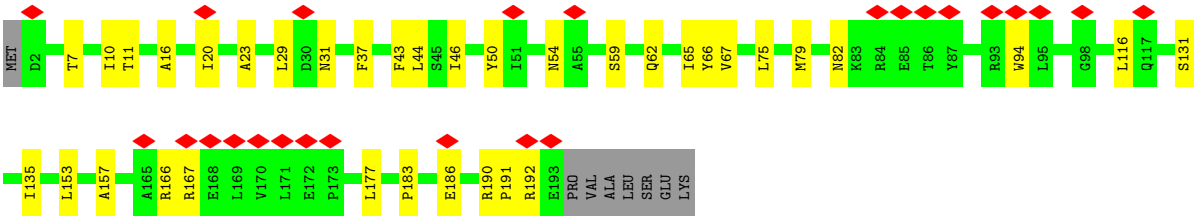
Chain F:





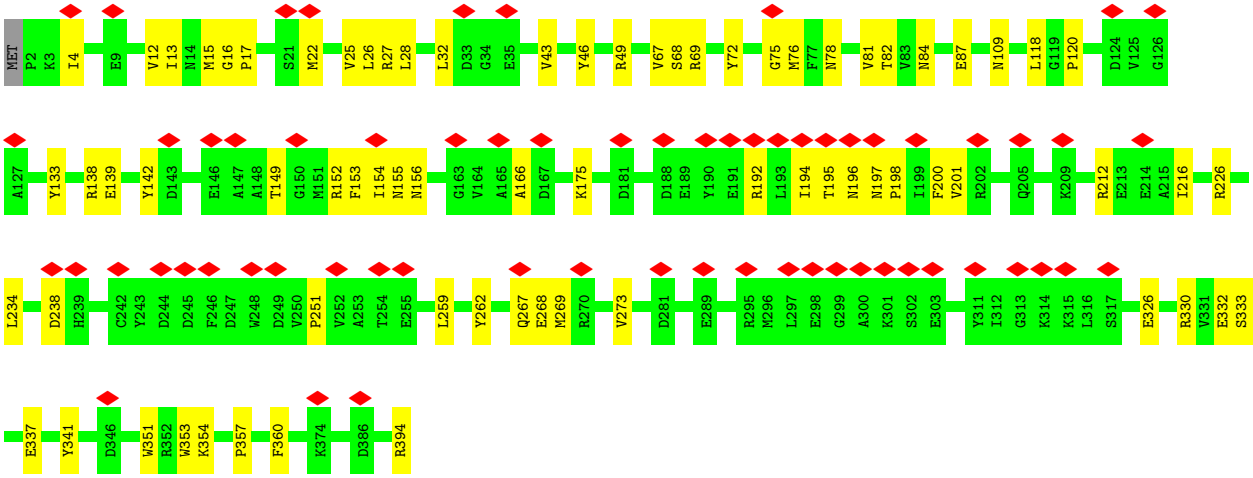
- Molecule 7: NADH-quinone oxidoreductase subunit J

Chain G:



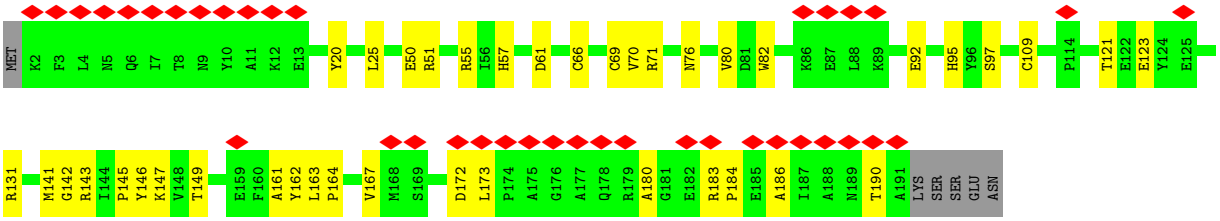
- Molecule 8: NAD(P)H-quinone oxidoreductase subunit H

Chain H:



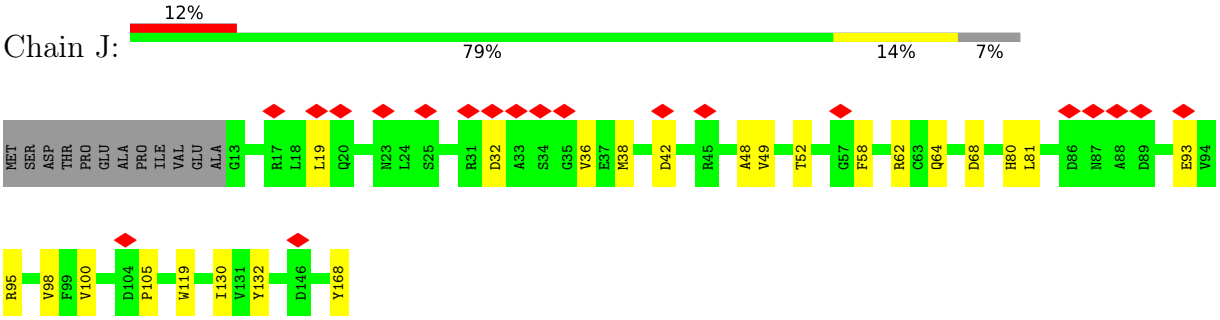
- Molecule 9: NAD(P)H-quinone oxidoreductase subunit I

Chain I:



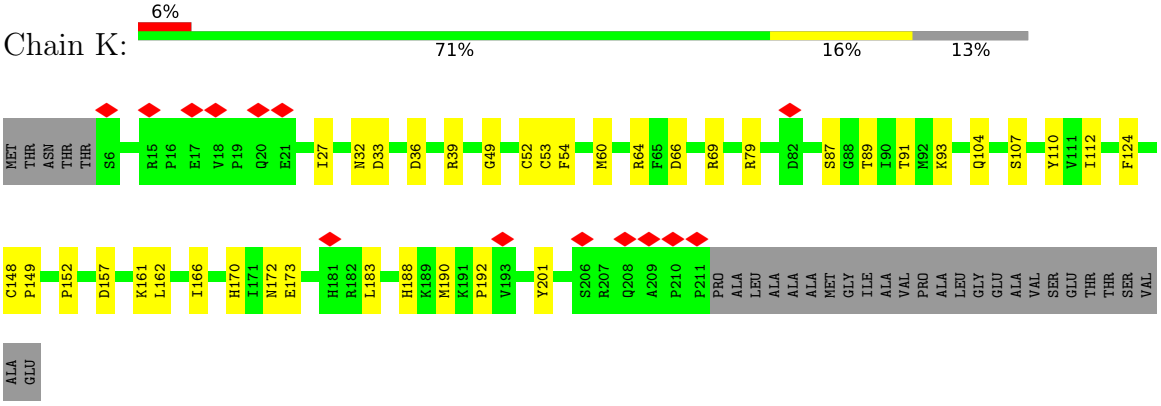
- Molecule 10: NAD(P)H-quinone oxidoreductase subunit J

Chain J:



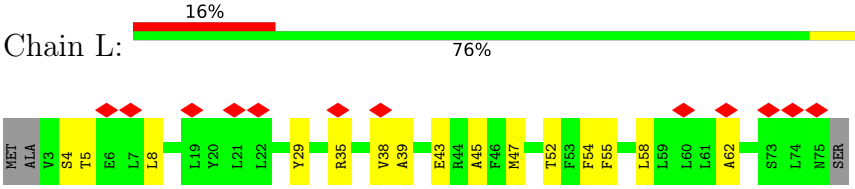
- Molecule 11: NAD(P)H-quinone oxidoreductase subunit K

Chain K:



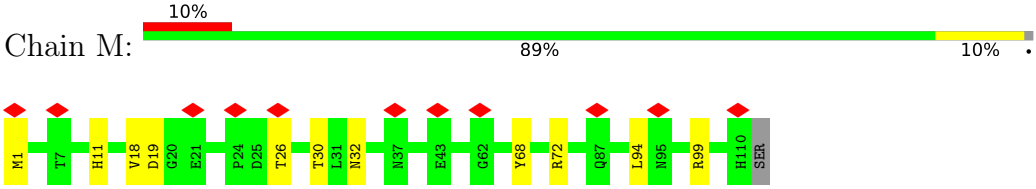
- Molecule 12: NAD(P)H-quinone oxidoreductase subunit L

Chain L:



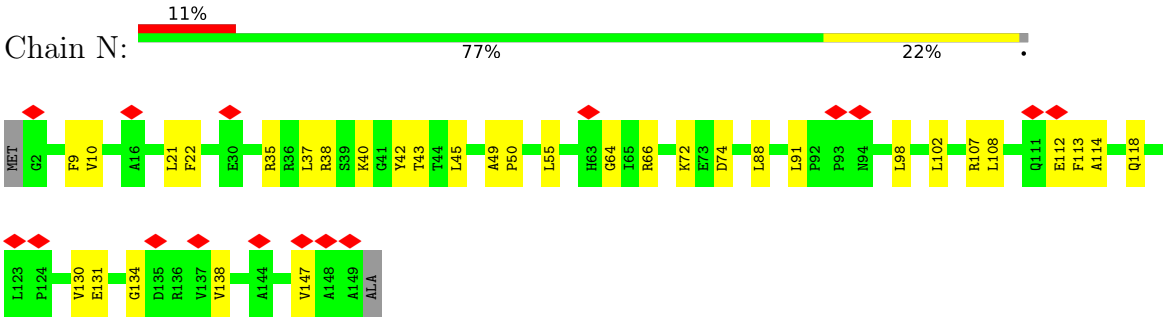
- Molecule 13: NAD(P)H-quinone oxidoreductase subunit M

Chain M:



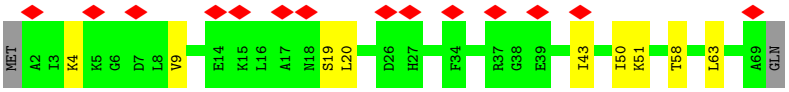
- Molecule 14: NAD(P)H-quinone oxidoreductase subunit N

Chain N:



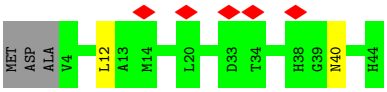
- Molecule 15: NAD(P)H-quinone oxidoreductase subunit O

Chain O: 20% 84% 13%



• Molecule 16: NAD(P)H-quinone oxidoreductase subunit P

Chain P: 11% 89% 5% 7%

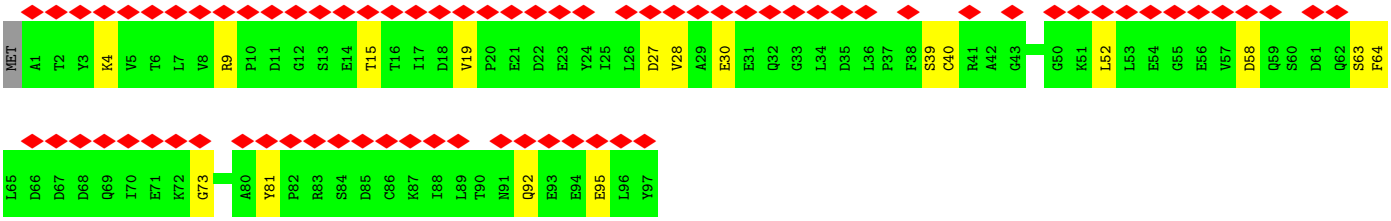


• Molecule 17: NAD(P)H-quinone oxidoreductase subunit Q

Chain Q: 18% 78% 20%

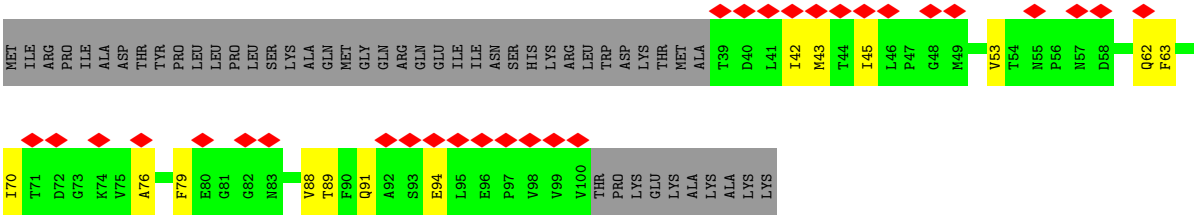
• Molecule 18: Ferredoxin-1

Chain R: 77% 82% 17%



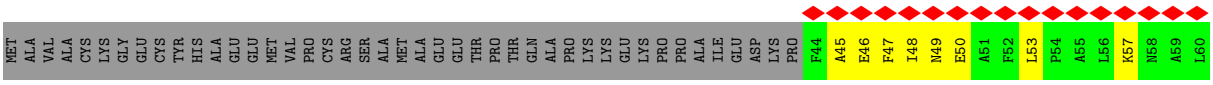
• Molecule 19: Tlr0636 protein

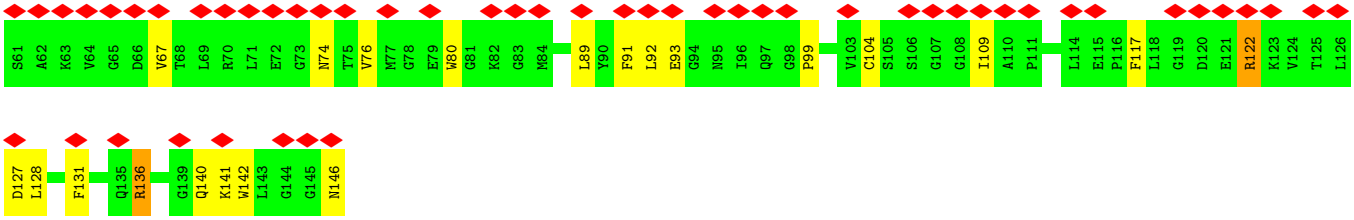
Chain S: 27% 45% 12% 44%



• Molecule 20: Tlr0472 protein

Chain V: 47% 51% 18% 29%




S61
A62
K63
V64
G65
D66
V67
T68
L69
R70
L71
E72
G73
N74
T75
V76
M77
G78
E79
W80
G81
K82
G83
M84
L89
Y90
F91
L92
E93
G94
N95
I96
Q97
G98
P99
V103
C104
S105
S106
G107
G108
I109
A110
P111
L114
E115
P116
F117
L118
G119
D120
E121
R122
K123
V124
T125
L126
D127
L128
F131
Q135
R136
G139
Q140
K141
W142
L143
G144
G145
N146

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	338822	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.401	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.038	Depositor
Map size (Å)	327.0, 327.0, 327.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AJP, SQD, BCR, FES, DGD, LHG, PQN, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.25	0/2932	0.41	0/4008
2	B	0.24	0/3818	0.39	0/5209
3	C	0.26	0/1008	0.40	0/1375
4	D	0.24	0/4003	0.40	0/5464
5	E	0.23	0/793	0.35	0/1077
6	F	0.24	0/5153	0.38	0/7020
7	G	0.24	0/1495	0.39	0/2050
8	H	0.24	0/3260	0.39	0/4417
9	I	0.24	0/1563	0.41	0/2119
10	J	0.23	0/1314	0.41	1/1789 (0.1%)
11	K	0.24	0/1638	0.40	0/2230
12	L	0.26	0/610	0.39	0/835
13	M	0.22	0/895	0.40	0/1214
14	N	0.24	0/1197	0.40	0/1628
15	O	0.23	0/550	0.40	0/748
16	P	0.26	0/330	0.39	0/448
17	Q	0.23	0/341	0.36	0/464
18	R	0.24	0/758	0.43	0/1029
19	S	0.23	0/494	0.44	0/674
20	V	0.25	0/814	0.45	0/1097
All	All	0.24	0/32966	0.40	1/44895 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	42	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2859	0	2983	70	0
2	B	3732	0	3864	107	0
3	C	978	0	1008	42	0
4	D	3896	0	4041	129	0
5	E	783	0	837	20	0
6	F	5004	0	5033	122	0
7	G	1463	0	1546	50	0
8	H	3177	0	3155	55	0
9	I	1525	0	1500	32	0
10	J	1278	0	1233	16	0
11	K	1597	0	1628	35	0
12	L	590	0	602	11	0
13	M	879	0	860	9	0
14	N	1165	0	1176	28	0
15	O	538	0	549	7	0
16	P	321	0	317	2	0
17	Q	332	0	331	12	0
18	R	748	0	709	11	0
19	S	485	0	488	9	0
20	V	797	0	800	22	0
21	A	40	0	55	4	0
21	F	40	0	54	3	0
21	P	40	0	54	5	0
22	A	49	0	73	3	0
22	B	147	0	222	4	0
22	D	98	0	148	1	0
22	F	98	0	145	8	0
22	H	49	0	73	3	0
23	A	132	0	191	3	0
24	A	160	0	0	26	0
24	B	384	0	0	84	0
24	C	64	0	0	17	0
24	D	384	0	0	99	0
24	E	32	0	0	1	0
24	F	416	0	0	65	0
24	G	224	0	0	43	0
24	Q	256	0	0	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	33	0	44	0	0
26	B	54	0	78	3	0
26	F	108	0	156	6	0
26	L	54	0	77	1	0
27	I	16	0	0	1	0
27	K	8	0	0	3	0
28	R	4	0	0	2	0
All	All	35037	0	34030	828	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 12.

All (828) 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)
4:D:413:LEU:HD21	24:D:608:AJP:C80	1.23	1.64
2:B:484:LEU:HD11	24:B:606:AJP:C13	1.27	1.60
2:B:287:ILE:CD1	24:B:616:AJP:C83	1.75	1.59
7:G:7:THR:HG22	24:G:302:AJP:C83	1.18	1.56
6:F:39:PRO:HB3	24:F:714:AJP:C83	1.23	1.55
7:G:7:THR:CG2	24:G:302:AJP:C83	1.84	1.54
4:D:413:LEU:CD1	24:D:608:AJP:C14	1.81	1.54
2:B:283:ILE:CD1	24:B:616:AJP:C80	1.88	1.51
2:B:484:LEU:CD1	24:B:606:AJP:C13	1.92	1.48
4:D:413:LEU:HD11	24:D:608:AJP:C14	1.04	1.47
3:C:121:VAL:HG22	24:C:202:AJP:C13	1.46	1.42
4:D:413:LEU:CD2	24:D:608:AJP:C80	2.02	1.36
6:F:29:PHE:CE2	24:F:707:AJP:O82	1.79	1.35
24:F:710:AJP:C03	24:Q:102:AJP:C13	2.04	1.35
4:D:70:TYR:OH	24:D:604:AJP:C24	1.73	1.34
6:F:39:PRO:CB	24:F:714:AJP:C83	2.05	1.33
3:C:117:VAL:HG11	24:C:202:AJP:C85	1.56	1.32
4:D:277:PHE:CZ	24:D:609:AJP:C80	2.15	1.29
4:D:212:LEU:HD12	24:D:613:AJP:C80	1.61	1.29
24:F:712:AJP:C14	24:F:718:AJP:C80	2.12	1.27
4:D:277:PHE:HE2	24:D:609:AJP:C81	1.49	1.26
1:A:101:LEU:CD2	24:G:301:AJP:C10	2.15	1.25
6:F:629:TYR:CD2	24:F:712:AJP:C11	2.15	1.20
1:A:366:PHE:CZ	24:A:409:AJP:C17	2.24	1.20
2:B:283:ILE:HD13	24:B:616:AJP:C80	1.60	1.19
2:B:59:ILE:CD1	24:B:606:AJP:O82	1.92	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ILE:HD12	24:B:616:AJP:C83	1.77	1.15
2:B:287:ILE:HD11	24:B:616:AJP:C83	1.48	1.14
7:G:94:TRP:HZ3	24:G:306:AJP:O25	1.31	1.13
24:A:408:AJP:O79	24:B:617:AJP:C18	1.99	1.11
3:C:121:VAL:CG2	24:C:202:AJP:C13	2.30	1.10
4:D:216:ALA:HB1	24:D:613:AJP:C03	1.79	1.10
4:D:277:PHE:CE2	24:D:609:AJP:C81	2.33	1.10
1:A:366:PHE:CE1	24:A:409:AJP:C17	2.37	1.08
4:D:47:ALA:HB1	24:D:607:AJP:C01	1.83	1.07
4:D:216:ALA:CB	24:D:613:AJP:C03	2.33	1.06
4:D:413:LEU:HD11	24:D:608:AJP:C15	1.89	1.03
7:G:7:THR:HG21	24:G:302:AJP:C83	1.88	1.03
1:A:101:LEU:HD21	24:G:301:AJP:C10	1.88	1.02
6:F:626:GLY:CA	24:F:718:AJP:O82	2.07	1.02
2:B:287:ILE:HD13	24:B:616:AJP:C83	1.85	1.01
2:B:59:ILE:HG23	24:B:606:AJP:C18	1.91	1.00
4:D:210:PHE:HE2	24:D:610:AJP:C21	1.73	0.99
1:A:366:PHE:CE1	24:A:409:AJP:C18	2.46	0.98
6:F:629:TYR:HD2	24:F:712:AJP:C11	1.69	0.98
2:B:283:ILE:HD11	24:B:616:AJP:C80	1.89	0.98
17:Q:18:PRO:HB3	24:Q:102:AJP:C18	1.94	0.97
2:B:484:LEU:HD12	24:B:606:AJP:C13	1.90	0.97
6:F:71:GLN:NE2	24:F:711:AJP:C80	2.28	0.97
2:B:283:ILE:HD12	24:B:616:AJP:C80	1.92	0.97
4:D:6:TRP:HH2	24:D:611:AJP:C13	1.78	0.97
4:D:277:PHE:CE2	24:D:609:AJP:C80	2.47	0.97
2:B:59:ILE:HD13	24:B:606:AJP:O82	1.66	0.96
4:D:70:TYR:CZ	24:D:604:AJP:C24	2.49	0.96
24:B:614:AJP:O79	24:D:610:AJP:C18	2.14	0.95
17:Q:20:MET:HE1	24:Q:106:AJP:C17	1.96	0.95
3:C:124:TRP:HH2	24:C:201:AJP:C13	1.79	0.95
1:A:366:PHE:HE1	24:A:409:AJP:C18	1.79	0.95
4:D:6:TRP:CH2	24:D:611:AJP:C13	2.50	0.95
6:F:29:PHE:CD2	24:F:707:AJP:O82	2.19	0.95
24:G:304:AJP:C21	24:G:307:AJP:C18	2.44	0.94
7:G:116:LEU:CD1	24:G:305:AJP:C14	2.46	0.94
6:F:626:GLY:HA3	24:F:718:AJP:O82	1.66	0.93
4:D:210:PHE:CE2	24:D:610:AJP:C21	2.52	0.93
7:G:94:TRP:CZ3	24:G:306:AJP:O25	2.21	0.93
2:B:477:LEU:HD22	24:B:609:AJP:C03	2.00	0.92
4:D:47:ALA:CB	24:D:607:AJP:C01	2.47	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:612:AJP:C13	22:F:703:LHG:H332	1.99	0.92
3:C:124:TRP:CH2	24:C:201:AJP:C13	2.54	0.90
17:Q:20:MET:CE	24:Q:106:AJP:C17	2.48	0.90
24:D:612:AJP:C13	22:F:703:LHG:C33	2.49	0.90
3:C:117:VAL:CG1	24:C:202:AJP:C85	2.47	0.90
2:B:280:VAL:HB	24:B:615:AJP:C81	2.03	0.89
1:A:285:PRO:HG2	24:A:407:AJP:C14	2.01	0.89
6:F:71:GLN:HE21	24:F:711:AJP:C21	1.85	0.88
2:B:59:ILE:HD12	24:B:606:AJP:C17	2.04	0.88
2:B:59:ILE:HD11	24:B:606:AJP:O82	1.72	0.87
4:D:16:VAL:HG11	24:D:605:AJP:C01	2.05	0.86
24:G:304:AJP:C13	24:G:307:AJP:O82	2.23	0.86
7:G:116:LEU:HD13	24:G:305:AJP:C14	2.05	0.85
24:B:617:AJP:C01	3:C:110:LEU:HD13	2.06	0.85
4:D:413:LEU:HD12	24:D:608:AJP:C14	2.02	0.84
7:G:37:PHE:O	24:G:301:AJP:C83	2.25	0.84
4:D:70:TYR:HH	24:D:604:AJP:C24	1.88	0.83
24:B:611:AJP:C10	3:C:121:VAL:HG11	2.09	0.82
2:B:2:ASP:N	24:B:617:AJP:C15	2.42	0.82
1:A:101:LEU:HD23	24:G:301:AJP:C10	2.09	0.82
2:B:283:ILE:CG2	24:B:616:AJP:C81	2.58	0.82
4:D:413:LEU:CD1	24:D:608:AJP:C21	2.58	0.80
4:D:212:LEU:CD1	24:D:613:AJP:C80	2.54	0.80
2:B:386:ILE:HG22	2:B:388:PRO:HD2	1.62	0.80
2:B:2:ASP:N	24:B:617:AJP:C19	2.46	0.79
17:Q:37:TRP:HH2	24:Q:107:AJP:C17	1.96	0.79
4:D:70:TYR:CE2	24:D:604:AJP:C24	2.65	0.78
4:D:182:VAL:CG1	24:D:610:AJP:C83	2.61	0.78
24:F:710:AJP:C03	24:Q:102:AJP:C14	2.61	0.78
4:D:213:LEU:CD2	24:D:613:AJP:O82	2.31	0.78
24:D:612:AJP:C14	22:F:703:LHG:H312	2.15	0.77
4:D:209:GLY:HA2	24:D:613:AJP:C80	2.15	0.76
4:D:413:LEU:CG	24:D:608:AJP:C14	2.62	0.76
7:G:116:LEU:CD1	24:G:305:AJP:C13	2.64	0.76
8:H:69:ARG:HG2	27:K:301:SF4:S2	2.25	0.76
8:H:139:GLU:HG2	11:K:64:ARG:HG2	1.67	0.76
2:B:283:ILE:HG23	24:B:616:AJP:C81	2.16	0.76
4:D:413:LEU:HD13	24:D:608:AJP:C21	2.16	0.76
2:B:276:LEU:HB2	24:B:615:AJP:C80	2.16	0.76
4:D:182:VAL:HG12	24:D:610:AJP:C83	2.16	0.75
1:A:366:PHE:HZ	24:A:409:AJP:C17	1.97	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:612:AJP:C13	22:F:703:LHG:H331	2.16	0.75
3:C:125:ARG:CD	24:C:202:AJP:O79	2.35	0.75
24:D:606:AJP:O82	24:D:611:AJP:C83	2.34	0.75
4:D:16:VAL:HG21	24:D:605:AJP:C03	2.16	0.74
24:G:303:AJP:C13	24:G:304:AJP:O82	2.35	0.74
6:F:11:ILE:HG23	6:F:12:PRO:HD3	1.69	0.74
4:D:6:TRP:HH2	24:D:611:AJP:C14	2.00	0.74
3:C:125:ARG:HD2	24:C:202:AJP:O79	1.87	0.74
4:D:413:LEU:HD11	24:D:608:AJP:C20	2.17	0.73
4:D:413:LEU:HD11	24:D:608:AJP:C21	2.18	0.73
2:B:82:PHE:CD2	24:B:606:AJP:C85	2.72	0.73
24:B:614:AJP:C23	24:D:614:AJP:C18	2.68	0.71
7:G:50:TYR:HB3	7:G:59:SER:HB2	1.70	0.71
6:F:270:VAL:HG13	6:F:327:LEU:HD21	1.70	0.71
24:F:710:AJP:C04	24:Q:102:AJP:C14	2.68	0.71
1:A:101:LEU:HD22	24:G:301:AJP:C10	2.17	0.71
2:B:287:ILE:HD11	24:B:616:AJP:C06	2.20	0.71
2:B:59:ILE:CD1	24:B:606:AJP:C17	2.68	0.70
24:A:408:AJP:O82	24:A:409:AJP:C07	2.39	0.70
4:D:6:TRP:CH2	24:D:611:AJP:C14	2.74	0.70
6:F:71:GLN:HE22	24:F:711:AJP:C80	2.02	0.70
7:G:10:ILE:HG12	24:G:304:AJP:C81	2.22	0.70
2:B:413:LEU:HD22	24:B:616:AJP:C13	2.21	0.69
4:D:413:LEU:HD22	24:D:608:AJP:C80	2.16	0.69
5:E:23:THR:HG22	5:E:24:SER:H	1.58	0.69
4:D:12:LEU:HD21	24:D:603:AJP:C04	2.22	0.69
4:D:411:TYR:HB3	4:D:415:PHE:HB3	1.74	0.69
2:B:283:ILE:HG21	24:B:616:AJP:C81	2.21	0.69
4:D:12:LEU:HD11	24:D:603:AJP:C83	2.22	0.69
6:F:29:PHE:CE2	24:F:707:AJP:C10	2.75	0.69
6:F:626:GLY:N	24:F:718:AJP:O82	2.26	0.69
24:B:614:AJP:C03	24:B:616:AJP:C13	2.72	0.68
8:H:69:ARG:NH2	11:K:148:CYS:SG	2.66	0.68
1:A:285:PRO:CG	24:A:407:AJP:C13	2.72	0.67
4:D:116:PHE:HB2	4:D:157:TRP:HH2	1.59	0.67
24:F:712:AJP:C13	24:F:718:AJP:C80	2.72	0.67
4:D:182:VAL:HG11	24:D:610:AJP:C83	2.24	0.67
2:B:283:ILE:HD11	24:B:616:AJP:C21	2.25	0.67
17:Q:20:MET:HE3	24:Q:106:AJP:C17	2.25	0.67
7:G:10:ILE:HD13	24:G:303:AJP:C83	2.24	0.67
6:F:338:ALA:HB1	6:F:341:ALA:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HG12	7:G:67:VAL:HG11	1.76	0.66
5:E:50:ASN:OD1	7:G:54:ASN:ND2	2.29	0.66
14:N:64:GLY:O	20:V:141:LYS:NZ	2.29	0.66
17:Q:37:TRP:CH2	24:Q:107:AJP:C17	2.77	0.66
2:B:34:ILE:HD11	24:B:611:AJP:C81	2.26	0.65
9:I:66:CYS:SG	27:I:202:SF4:FE4	1.88	0.65
8:H:27:ARG:HB3	8:H:43:VAL:HB	1.78	0.65
7:G:116:LEU:CD1	24:G:305:AJP:C15	2.74	0.65
1:A:366:PHE:CZ	24:A:409:AJP:C18	2.74	0.65
20:V:92:LEU:HD22	20:V:99:PRO:HB2	1.78	0.65
1:A:285:PRO:CD	24:A:407:AJP:C13	2.75	0.64
6:F:39:PRO:HB2	24:F:714:AJP:C83	2.24	0.64
7:G:7:THR:HG22	24:G:302:AJP:C06	2.19	0.64
3:C:124:TRP:CD2	24:C:202:AJP:C80	2.81	0.63
8:H:341:TYR:HB3	8:H:354:LYS:HB3	1.80	0.63
6:F:408:VAL:HG13	6:F:409:PRO:HD3	1.80	0.63
4:D:480:TYR:CE2	24:D:612:AJP:C80	2.82	0.63
7:G:7:THR:CB	24:G:302:AJP:C83	2.75	0.63
6:F:225:LEU:HD12	24:F:708:AJP:C81	2.29	0.62
24:D:603:AJP:C80	24:D:604:AJP:C81	2.77	0.62
4:D:16:VAL:CG1	24:D:605:AJP:C01	2.77	0.62
19:S:53:VAL:HG22	19:S:63:PHE:H	1.64	0.62
19:S:91:GLN:HB2	19:S:94:GLU:HG3	1.79	0.62
24:D:612:AJP:C14	22:F:703:LHG:H332	2.29	0.62
24:B:615:AJP:C13	24:B:616:AJP:C80	2.78	0.62
2:B:6:LEU:HB3	3:C:104:LEU:HD11	1.82	0.61
3:C:124:TRP:CE2	24:C:202:AJP:C80	2.83	0.61
4:D:219:LEU:HD11	4:D:281:LEU:HD21	1.82	0.61
24:Q:101:AJP:C04	24:Q:107:AJP:C83	2.78	0.61
2:B:140:GLU:HG3	5:E:69:VAL:HG11	1.82	0.61
13:M:68:TYR:OH	13:M:72:ARG:NH1	2.33	0.61
5:E:61:VAL:HG22	7:G:135:ILE:HG13	1.83	0.61
11:K:36:ASP:OD2	14:N:35:ARG:NH1	2.34	0.60
24:A:408:AJP:C14	24:B:617:AJP:O82	2.49	0.60
8:H:138:ARG:NH1	8:H:142:TYR:OH	2.35	0.60
4:D:24:ILE:HG21	4:D:34:ILE:HG12	1.82	0.60
4:D:70:TYR:CE2	24:D:604:AJP:C80	2.84	0.60
4:D:271:PRO:HG2	4:D:502:VAL:HG11	1.84	0.60
13:M:11:HIS:HB2	13:M:32:ASN:HB3	1.83	0.60
3:C:125:ARG:HD3	24:C:202:AJP:O79	2.01	0.60
4:D:268:ASP:O	4:D:498:ARG:NH2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:251:PRO:HG3	8:H:267:GLN:HB3	1.82	0.60
5:E:27:ALA:HB1	5:E:81:ILE:HD12	1.83	0.59
18:R:39:SER:N	28:R:101:FES:S1	2.71	0.59
9:I:70:VAL:O	9:I:76:ASN:ND2	2.35	0.59
10:J:36:VAL:HG22	10:J:93:GLU:HG3	1.85	0.59
4:D:229:VAL:HG23	4:D:230:PRO:HD3	1.84	0.59
18:R:40:CYS:N	28:R:101:FES:S1	2.75	0.59
1:A:47:VAL:HG11	12:L:52:THR:HG23	1.83	0.59
2:B:477:LEU:HD22	24:B:609:AJP:C04	2.33	0.59
2:B:484:LEU:HD12	24:B:606:AJP:C14	2.31	0.59
6:F:245:PRO:HB2	6:F:246:LEU:HD12	1.84	0.59
6:F:489:PRO:HA	6:F:492:VAL:HG22	1.84	0.59
7:G:116:LEU:HD12	24:G:305:AJP:C15	2.32	0.59
8:H:72:TYR:HB2	11:K:52:CYS:HB3	1.85	0.59
4:D:154:LEU:HD11	4:D:250:LEU:HD11	1.85	0.58
5:E:86:ARG:HH22	7:G:167:ARG:HG2	1.68	0.58
21:A:401:BCR:H393	9:I:25:LEU:HB3	1.85	0.58
8:H:15:MET:HB3	8:H:28:LEU:HB3	1.85	0.58
22:A:402:LHG:H211	7:G:44:LEU:HB3	1.85	0.58
24:A:408:AJP:O79	24:B:617:AJP:C17	2.51	0.58
7:G:116:LEU:HD11	24:G:305:AJP:C13	2.32	0.58
1:A:101:LEU:HD21	24:G:301:AJP:C08	2.33	0.58
2:B:409:GLY:HA2	24:B:614:AJP:C83	2.33	0.58
3:C:124:TRP:CH2	24:C:201:AJP:C14	2.86	0.57
6:F:152:GLU:OE1	6:F:183:ARG:NH1	2.36	0.57
14:N:10:VAL:HG21	14:N:40:LYS:HG3	1.86	0.57
2:B:275:GLN:O	2:B:279:THR:HG23	2.04	0.57
2:B:248:SER:OG	2:B:340:ASN:ND2	2.37	0.57
5:E:93:MET:HG2	6:F:636:GLN:HE22	1.68	0.57
9:I:143:ARG:NH1	14:N:50:PRO:O	2.37	0.57
13:M:18:VAL:HG23	13:M:19:ASP:H	1.69	0.57
6:F:84:ALA:O	6:F:143:ASN:ND2	2.38	0.57
10:J:62:ARG:HB3	10:J:80:HIS:HB3	1.86	0.57
1:A:285:PRO:CG	24:A:407:AJP:C14	2.78	0.57
6:F:369:GLY:HA3	6:F:480:HIS:HE1	1.69	0.57
6:F:590:PHE:HE1	26:F:705:SQD:H162	1.69	0.57
19:S:45:ILE:HG23	19:S:70:ILE:HG21	1.85	0.57
9:I:55:ARG:HH12	9:I:141:MET:HA	1.70	0.57
11:K:36:ASP:OD1	11:K:39:ARG:NH2	2.37	0.57
14:N:43:THR:HG21	14:N:91:LEU:HD11	1.86	0.57
6:F:225:LEU:CD1	24:F:708:AJP:C81	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:244:PHE:CZ	24:F:709:AJP:C01	2.88	0.57
1:A:285:PRO:HG2	24:A:407:AJP:C13	2.34	0.56
4:D:213:LEU:HD21	24:D:613:AJP:O82	2.04	0.56
2:B:280:VAL:CB	24:B:615:AJP:C81	2.78	0.56
1:A:346:LYS:HD2	3:C:124:TRP:CZ2	2.41	0.56
2:B:226:VAL:HG11	2:B:284:LEU:HB3	1.87	0.56
2:B:278:PHE:HB3	2:B:319:VAL:HG12	1.88	0.56
4:D:212:LEU:HB3	24:D:613:AJP:C81	2.35	0.56
6:F:608:VAL:HG22	24:Q:102:AJP:C83	2.35	0.56
4:D:479:LEU:O	24:D:612:AJP:C83	2.53	0.56
18:R:58:ASP:HB3	18:R:81:TYR:HB2	1.87	0.56
1:A:343:LEU:HD22	22:H:401:LHG:HC62	1.88	0.56
4:D:216:ALA:HB2	24:D:613:AJP:C03	2.30	0.56
24:D:606:AJP:O82	24:D:611:AJP:C81	2.54	0.56
6:F:572:LEU:HD11	22:F:702:LHG:H291	1.87	0.56
24:Q:101:AJP:C83	24:Q:107:AJP:C83	2.84	0.56
24:G:304:AJP:C81	24:G:304:AJP:C83	2.84	0.56
4:D:244:ALA:HB2	4:D:351:GLY:HA3	1.88	0.56
24:G:302:AJP:C83	24:G:302:AJP:C81	2.84	0.56
8:H:197:ASN:OD1	8:H:198:PRO:HD2	2.05	0.56
24:B:611:AJP:C81	24:B:611:AJP:C83	2.84	0.56
4:D:212:LEU:HD13	24:D:613:AJP:C81	2.36	0.56
24:D:612:AJP:C13	22:F:703:LHG:H312	2.35	0.56
14:N:66:ARG:HH22	20:V:146:ASN:HB3	1.71	0.56
24:A:407:AJP:C81	24:A:407:AJP:C83	2.84	0.55
24:B:606:AJP:C81	24:B:606:AJP:C83	2.85	0.55
24:B:607:AJP:C81	24:B:607:AJP:C83	2.85	0.55
14:N:114:ALA:HB3	20:V:109:ILE:HG21	1.88	0.55
4:D:213:LEU:HG	24:D:613:AJP:O82	2.05	0.55
10:J:119:TRP:HE1	11:K:201:TYR:HH	1.51	0.55
24:Q:103:AJP:C83	24:Q:103:AJP:C81	2.84	0.55
24:B:610:AJP:C83	24:B:610:AJP:C81	2.85	0.55
24:B:615:AJP:C81	24:B:615:AJP:C83	2.85	0.55
24:D:608:AJP:C81	24:D:608:AJP:C83	2.85	0.55
24:F:711:AJP:C81	24:F:711:AJP:C83	2.85	0.55
14:N:102:LEU:HD12	14:N:130:VAL:HG22	1.88	0.55
24:A:405:AJP:C81	24:A:405:AJP:C83	2.85	0.55
24:D:604:AJP:C81	24:D:604:AJP:C83	2.85	0.55
24:E:201:AJP:C81	24:E:201:AJP:C83	2.85	0.55
24:Q:101:AJP:C83	24:Q:101:AJP:C81	2.85	0.55
24:Q:106:AJP:C81	24:Q:106:AJP:C83	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:107:AJP:C83	24:Q:107:AJP:C81	2.85	0.55
1:A:230:LEU:HB2	1:A:329:ARG:HG3	1.88	0.55
24:C:201:AJP:C83	24:C:201:AJP:C81	2.85	0.55
24:C:202:AJP:C81	24:C:202:AJP:C83	2.84	0.55
4:D:277:PHE:CE1	24:D:609:AJP:C80	2.85	0.55
24:F:717:AJP:C81	24:F:717:AJP:C83	2.85	0.55
24:B:608:AJP:C81	24:B:608:AJP:C83	2.85	0.55
6:F:338:ALA:O	6:F:342:GLY:N	2.30	0.55
24:F:708:AJP:C81	24:F:708:AJP:C83	2.85	0.55
24:F:713:AJP:C81	24:F:713:AJP:C83	2.85	0.55
24:Q:104:AJP:C81	24:Q:104:AJP:C83	2.85	0.55
24:Q:105:AJP:C81	24:Q:105:AJP:C83	2.85	0.55
24:D:609:AJP:C81	24:D:609:AJP:C83	2.85	0.55
24:G:306:AJP:C81	24:G:306:AJP:C83	2.85	0.55
1:A:124:LEU:HD11	1:A:127:ASN:HB2	1.88	0.55
2:B:228:PHE:HD1	6:F:642:VAL:HG22	1.72	0.55
24:B:607:AJP:C14	24:B:608:AJP:O82	2.55	0.55
24:B:617:AJP:C83	24:B:617:AJP:C81	2.85	0.55
24:D:603:AJP:C83	24:D:603:AJP:C81	2.84	0.55
24:D:611:AJP:C83	24:D:611:AJP:C81	2.85	0.55
24:F:716:AJP:C83	24:F:716:AJP:C81	2.85	0.55
24:F:718:AJP:C81	24:F:718:AJP:C83	2.85	0.55
24:A:406:AJP:C81	24:A:406:AJP:C83	2.85	0.55
24:B:613:AJP:C81	24:B:613:AJP:C83	2.85	0.55
24:D:607:AJP:C83	24:D:607:AJP:C81	2.85	0.55
24:D:614:AJP:C81	24:D:614:AJP:C83	2.85	0.55
7:G:16:ALA:O	7:G:20:ILE:HG12	2.07	0.55
9:I:164:PRO:HA	9:I:180:ALA:HB2	1.89	0.55
24:F:712:AJP:C83	24:F:718:AJP:C83	2.85	0.55
24:F:715:AJP:C81	24:F:715:AJP:C83	2.85	0.55
24:Q:102:AJP:C83	24:Q:102:AJP:C81	2.84	0.55
24:B:614:AJP:C83	24:B:614:AJP:C81	2.84	0.54
4:D:197:ASP:HB3	4:D:200:THR:HG22	1.88	0.54
24:D:605:AJP:C83	24:D:605:AJP:C81	2.85	0.54
24:D:607:AJP:C83	24:D:607:AJP:C02	2.85	0.54
24:D:612:AJP:C83	24:D:612:AJP:C81	2.85	0.54
24:F:706:AJP:C81	24:F:706:AJP:C83	2.85	0.54
7:G:116:LEU:HD13	24:G:305:AJP:C15	2.35	0.54
24:A:409:AJP:C81	24:A:409:AJP:C83	2.85	0.54
24:B:616:AJP:C83	24:B:616:AJP:C81	2.85	0.54
4:D:305:LYS:HE2	4:D:433:TYR:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:707:AJP:C81	24:F:707:AJP:C83	2.85	0.54
24:G:301:AJP:C83	24:G:301:AJP:C81	2.85	0.54
11:K:170:HIS:HB3	11:K:173:GLU:HG2	1.90	0.54
15:O:9:VAL:HG11	15:O:50:ILE:HD12	1.88	0.54
24:B:612:AJP:C81	24:B:612:AJP:C83	2.85	0.54
3:C:89:VAL:HG21	7:G:65:ILE:HD11	1.88	0.54
4:D:498:ARG:HA	4:D:501:GLU:HG2	1.88	0.54
24:D:610:AJP:C83	24:D:610:AJP:C81	2.85	0.54
24:D:613:AJP:C81	24:D:613:AJP:C83	2.85	0.54
24:F:710:AJP:C81	24:F:710:AJP:C83	2.84	0.54
7:G:94:TRP:HZ3	24:G:306:AJP:C23	2.18	0.54
24:G:305:AJP:C83	24:G:305:AJP:C81	2.85	0.54
24:B:609:AJP:C81	24:B:609:AJP:C83	2.85	0.54
4:D:290:ILE:HG21	21:F:701:BCR:H323	1.89	0.54
24:D:606:AJP:C81	24:D:606:AJP:C83	2.85	0.54
6:F:209:GLY:O	6:F:213:THR:HG23	2.08	0.54
24:F:712:AJP:C83	24:F:712:AJP:C81	2.85	0.54
24:G:303:AJP:C83	24:G:303:AJP:C81	2.85	0.54
24:G:307:AJP:C83	24:G:307:AJP:C81	2.85	0.54
11:K:52:CYS:SG	27:K:301:SF4:S1	3.05	0.54
15:O:43:ILE:HD13	15:O:63:LEU:HD21	1.88	0.54
24:Q:108:AJP:C83	24:Q:108:AJP:C81	2.85	0.54
24:A:408:AJP:C81	24:A:408:AJP:C83	2.85	0.54
2:B:281:LEU:HD21	6:F:649:PHE:HZ	1.73	0.54
2:B:484:LEU:HD13	24:B:607:AJP:O82	2.08	0.54
4:D:209:GLY:HA3	24:D:613:AJP:C18	2.37	0.54
4:D:428:ILE:HD11	6:F:187:PHE:CG	2.42	0.54
24:F:711:AJP:C83	24:F:711:AJP:C02	2.85	0.54
8:H:22:MET:HG2	8:H:120:PRO:HG3	1.90	0.54
24:B:617:AJP:C01	3:C:110:LEU:CD1	2.83	0.54
24:F:714:AJP:C83	24:F:714:AJP:C81	2.85	0.54
11:K:188:HIS:HD2	11:K:190:MET:H	1.54	0.54
2:B:135:ILE:HG23	2:B:258:LEU:HD11	1.88	0.54
4:D:361:ILE:HG22	4:D:363:GLU:H	1.72	0.54
24:F:709:AJP:C81	24:F:709:AJP:C83	2.85	0.54
24:B:606:AJP:C83	24:B:606:AJP:C02	2.85	0.54
9:I:163:LEU:HD13	9:I:167:VAL:HB	1.88	0.54
9:I:131:ARG:NH1	10:J:168:TYR:O	2.41	0.53
7:G:82:ASN:ND2	8:H:4:ILE:O	2.40	0.53
8:H:72:TYR:HA	8:H:154:ILE:HD13	1.91	0.53
13:M:94:LEU:HD22	13:M:99:ARG:HH11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:67:VAL:HG21	8:H:82:THR:HG21	1.90	0.53
9:I:147:LYS:HG3	9:I:149:THR:H	1.74	0.53
20:V:127:ASP:OD1	20:V:128:LEU:N	2.40	0.53
3:C:124:TRP:CZ3	24:C:202:AJP:C81	2.92	0.53
4:D:35:ARG:NH1	4:D:107:TRP:O	2.41	0.53
5:E:16:ILE:HG21	7:G:23:ALA:HB1	1.90	0.53
9:I:80:VAL:HG12	9:I:82:TRP:HD1	1.73	0.53
11:K:39:ARG:NH1	11:K:110:TYR:OH	2.41	0.53
6:F:113:GLY:HA3	6:F:485:THR:HG21	1.91	0.53
7:G:116:LEU:HD12	24:G:305:AJP:C13	2.39	0.53
4:D:47:ALA:HB2	24:D:607:AJP:C01	2.38	0.53
24:F:706:AJP:O82	24:F:715:AJP:C83	2.57	0.53
8:H:269:MET:O	8:H:273:VAL:HG23	2.09	0.53
11:K:170:HIS:HD2	11:K:172:ASN:HB2	1.74	0.53
4:D:408:SER:O	4:D:416:ARG:NH2	2.42	0.52
6:F:387:LEU:HB2	6:F:454:PHE:HA	1.90	0.52
9:I:95:HIS:HE1	9:I:97:SER:HB2	1.74	0.52
9:I:123:GLU:OE1	9:I:146:TYR:N	2.40	0.52
2:B:35:GLN:HG2	2:B:39:ALA:HB2	1.89	0.52
4:D:206:TYR:HB2	4:D:211:GLN:HG3	1.90	0.52
11:K:49:GLY:HA3	11:K:54:PHE:HB2	1.91	0.52
2:B:283:ILE:HD13	24:B:616:AJP:C14	2.40	0.52
6:F:258:THR:HG21	6:F:361:GLY:HA3	1.90	0.52
1:A:285:PRO:HD3	24:A:407:AJP:C13	2.39	0.52
2:B:434:VAL:HA	4:D:156:ILE:HD13	1.92	0.52
4:D:104:LEU:O	4:D:107:TRP:NE1	2.42	0.52
6:F:238:VAL:HA	6:F:243:GLN:HG3	1.92	0.52
1:A:273:SER:O	1:A:278:GLY:N	2.39	0.52
10:J:64:GLN:NE2	10:J:132:TYR:OH	2.42	0.52
14:N:22:PHE:HB3	14:N:134:GLY:HA2	1.90	0.52
23:A:404:DGD:HA31	23:A:404:DGD:HB92	1.92	0.52
4:D:277:PHE:CD2	24:D:609:AJP:C81	2.91	0.52
20:V:122:ARG:H	20:V:122:ARG:HD3	1.75	0.52
6:F:532:GLU:O	6:F:536:LEU:HG	2.10	0.52
8:H:75:GLY:HA3	8:H:154:ILE:HG22	1.92	0.52
14:N:72:LYS:HD3	15:O:51:LYS:HE2	1.91	0.52
10:J:19:LEU:HD11	10:J:49:VAL:HG22	1.91	0.52
11:K:91:THR:HG22	11:K:93:LYS:H	1.75	0.52
2:B:6:LEU:HA	2:B:9:GLN:HG2	1.92	0.51
4:D:334:LEU:HD21	4:D:393:SER:HB2	1.91	0.51
6:F:532:GLU:HA	6:F:535:ILE:HG12	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:69:ARG:CG	27:K:301:SF4:S2	2.97	0.51
24:B:610:AJP:C06	24:B:610:AJP:C02	2.85	0.51
6:F:29:PHE:CZ	24:F:707:AJP:C17	2.93	0.51
8:H:153:PHE:CE2	11:K:149:PRO:HG3	2.45	0.51
17:Q:23:ILE:HA	17:Q:26:VAL:HG12	1.92	0.51
2:B:34:ILE:HD11	24:B:611:AJP:C16	2.40	0.51
4:D:73:ILE:HD12	4:D:75:GLU:HB2	1.92	0.51
6:F:237:PRO:HD3	6:F:276:LEU:HD23	1.92	0.51
4:D:310:SER:HA	4:D:339:HIS:CE1	2.46	0.51
24:D:606:AJP:C83	24:D:606:AJP:C02	2.88	0.51
6:F:619:VAL:HA	6:F:622:VAL:HG22	1.91	0.51
24:B:608:AJP:C06	24:B:608:AJP:C02	2.85	0.51
24:D:605:AJP:C02	24:D:605:AJP:C06	2.86	0.51
6:F:29:PHE:CZ	24:F:707:AJP:O82	2.55	0.51
4:D:383:SER:O	4:D:387:LEU:HG	2.11	0.51
12:L:39:ALA:HB1	12:L:43:GLU:HB3	1.92	0.51
24:B:608:AJP:C83	24:B:608:AJP:C02	2.88	0.51
6:F:442:THR:HA	6:F:445:TYR:CE2	2.46	0.51
14:N:88:LEU:HG	14:N:98:LEU:HD22	1.91	0.51
2:B:280:VAL:CG2	24:B:615:AJP:C81	2.88	0.51
8:H:238:ASP:N	8:H:238:ASP:OD2	2.44	0.51
1:A:43:VAL:HG13	12:L:55:PHE:HD2	1.76	0.51
24:B:606:AJP:C02	24:B:606:AJP:C06	2.87	0.51
4:D:213:LEU:CG	24:D:613:AJP:O82	2.59	0.51
24:D:606:AJP:C02	24:D:606:AJP:C06	2.85	0.51
9:I:70:VAL:HG12	9:I:76:ASN:HD22	1.76	0.51
20:V:80:TRP:HZ3	20:V:142:TRP:HB3	1.76	0.51
2:B:19:THR:O	2:B:23:VAL:HG23	2.11	0.50
4:D:54:THR:HG21	16:P:12:LEU:HD21	1.93	0.50
6:F:367:MET:O	6:F:371:VAL:N	2.38	0.50
18:R:52:LEU:N	18:R:73:GLY:O	2.34	0.50
6:F:393:ILE:O	6:F:397:THR:HG23	2.12	0.50
24:F:713:AJP:C06	24:F:713:AJP:C02	2.85	0.50
2:B:403:TRP:HD1	4:D:189:PHE:HD2	1.57	0.50
4:D:216:ALA:HB2	24:D:613:AJP:C04	2.42	0.50
6:F:135:MET:O	6:F:139:VAL:HG23	2.11	0.50
11:K:27:ILE:HD12	11:K:27:ILE:H	1.75	0.50
5:E:46:ILE:HG13	7:G:50:TYR:CE1	2.46	0.50
24:G:303:AJP:C02	24:G:303:AJP:C06	2.86	0.50
6:F:629:TYR:CD2	24:F:712:AJP:C10	2.92	0.50
7:G:183:PRO:HB2	7:G:186:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:192:ARG:HA	8:H:195:THR:HG22	1.94	0.50
4:D:61:THR:HB	4:D:65:GLN:HE22	1.77	0.50
7:G:190:ARG:HD3	7:G:191:PRO:HD2	1.93	0.50
1:A:284:ILE:HD13	24:A:407:AJP:C85	2.42	0.50
6:F:39:PRO:CG	24:F:714:AJP:C83	2.87	0.50
24:B:614:AJP:C06	24:B:614:AJP:C02	2.86	0.50
4:D:24:ILE:HB	4:D:114:ARG:HH22	1.76	0.50
6:F:36:LEU:CD1	24:F:707:AJP:C83	2.90	0.49
6:F:107:VAL:HG13	6:F:259:PRO:HB3	1.93	0.49
6:F:391:MET:HB3	6:F:394:THR:HB	1.93	0.49
6:F:629:TYR:HD2	24:F:712:AJP:C10	2.25	0.49
9:I:71:ARG:NH1	18:R:63:SER:O	2.45	0.49
20:V:104:CYS:SG	20:V:140:GLN:NE2	2.85	0.49
4:D:232:HIS:NE2	6:F:605:ASP:OD2	2.46	0.49
18:R:9:ARG:NH2	18:R:15:THR:HG23	2.27	0.49
3:C:84:PHE:O	3:C:88:THR:HG23	2.13	0.49
14:N:49:ALA:HB2	14:N:102:LEU:HB3	1.93	0.49
1:A:50:TRP:CE2	1:A:54:LYS:HG3	2.47	0.49
4:D:297:TYR:HA	4:D:433:TYR:HB3	1.92	0.49
1:A:351:VAL:HA	1:A:354:VAL:HG22	1.94	0.49
2:B:82:PHE:HD2	24:B:606:AJP:C85	2.25	0.49
2:B:139:LEU:HD11	2:B:222:LYS:HG3	1.95	0.49
2:B:59:ILE:HG23	24:B:606:AJP:C17	2.43	0.49
26:B:605:SQD:H152	6:F:613:VAL:HG13	1.95	0.49
24:B:614:AJP:C04	24:B:616:AJP:C11	2.91	0.49
6:F:629:TYR:CD2	24:F:712:AJP:C15	2.82	0.49
1:A:133:PHE:HE1	3:C:92:TYR:CE2	2.31	0.49
3:C:124:TRP:HD1	3:C:124:TRP:O	1.95	0.49
8:H:152:ARG:HG3	8:H:153:PHE:CD1	2.48	0.49
8:H:155:ASN:ND2	11:K:148:CYS:O	2.45	0.49
1:A:104:ALA:O	1:A:108:ILE:HG12	2.13	0.48
26:B:605:SQD:H302	26:B:605:SQD:H142	1.95	0.48
24:D:605:AJP:C83	24:D:605:AJP:C02	2.90	0.48
6:F:554:MET:HA	6:F:560:PRO:HG2	1.94	0.48
8:H:351:TRP:NE1	10:J:68:ASP:O	2.44	0.48
2:B:459:PRO:HA	2:B:462:VAL:HG12	1.93	0.48
3:C:58:SER:HB3	8:H:16:GLY:HA3	1.95	0.48
6:F:241:SER:OG	6:F:242:ALA:N	2.46	0.48
8:H:333:SER:OG	8:H:334:GLY:N	2.45	0.48
4:D:371:LYS:HB2	4:D:456:LEU:HD11	1.95	0.48
8:H:201:VAL:HA	8:H:259:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:SER:OG	5:E:44:ASN:ND2	2.46	0.48
2:B:387:PRO:HG2	2:B:388:PRO:HD3	1.95	0.48
24:Q:105:AJP:C13	24:Q:106:AJP:O82	2.61	0.48
2:B:179:TYR:HD1	5:E:41:VAL:HG12	1.77	0.48
3:C:88:THR:HA	3:C:91:LEU:HB2	1.96	0.48
10:J:119:TRP:NE1	11:K:201:TYR:OH	2.39	0.48
6:F:71:GLN:NE2	24:F:711:AJP:C21	2.67	0.48
9:I:71:ARG:HH12	18:R:64:PHE:HA	1.78	0.48
1:A:59:VAL:O	8:H:133:TYR:OH	2.31	0.48
1:A:288:THR:O	1:A:292:LEU:HG	2.12	0.48
5:E:29:ARG:NH1	7:G:29:LEU:O	2.47	0.48
11:K:157:ASP:O	11:K:161:LYS:HG2	2.14	0.48
12:L:4:SER:OG	12:L:5:THR:N	2.46	0.48
15:O:19:SER:OG	15:O:20:LEU:N	2.46	0.48
1:A:20:LEU:HD22	1:A:24:LEU:HD11	1.95	0.48
1:A:202:TYR:CE2	24:A:406:AJP:C80	2.97	0.48
2:B:271:THR:HA	2:B:274:TRP:CE2	2.49	0.47
6:F:218:THR:HG23	6:F:220:LEU:HD23	1.94	0.47
9:I:50:GLU:OE2	9:I:162:TYR:OH	2.32	0.47
11:K:170:HIS:CD2	11:K:172:ASN:H	2.32	0.47
1:A:185:MET:O	1:A:363:LYS:NZ	2.38	0.47
2:B:141:THR:HA	7:G:153:LEU:HD13	1.96	0.47
10:J:32:ASP:N	10:J:32:ASP:OD1	2.48	0.47
2:B:283:ILE:HD11	24:B:616:AJP:C20	2.44	0.47
4:D:408:SER:OG	4:D:409:ASP:N	2.46	0.47
4:D:413:LEU:HB3	4:D:414:PRO:HD3	1.95	0.47
6:F:143:ASN:H	6:F:146:GLN:HE21	1.62	0.47
9:I:121:THR:HG23	9:I:145:PRO:HB3	1.96	0.47
1:A:101:LEU:HD21	24:G:301:AJP:O09	2.14	0.47
1:A:156:LYS:NZ	8:H:12:VAL:O	2.48	0.47
6:F:20:LEU:HD11	21:P:101:BCR:H372	1.96	0.47
6:F:295:ALA:HA	6:F:332:MET:HA	1.97	0.47
20:V:45:ALA:O	20:V:49:ASN:ND2	2.47	0.47
4:D:227:PRO:O	4:D:288:ASN:ND2	2.44	0.47
6:F:71:GLN:HE21	24:F:711:AJP:C22	2.27	0.47
2:B:403:TRP:HD1	4:D:189:PHE:CD2	2.31	0.47
8:H:25:VAL:HG21	8:H:46:TYR:HB2	1.96	0.47
1:A:149:ALA:HB1	1:A:249:TYR:OH	2.15	0.47
2:B:160:ASN:HD21	5:E:87:ASN:HD22	1.62	0.47
22:F:703:LHG:H301	22:F:703:LHG:H271	1.66	0.47
1:A:284:ILE:CD1	24:A:407:AJP:C85	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:105:PRO:HB2	10:J:130:ILE:HA	1.96	0.47
2:B:226:VAL:O	2:B:229:HIS:ND1	2.46	0.47
26:B:605:SQD:H341	4:D:175:GLY:HA3	1.96	0.47
5:E:49:ALA:HB2	5:E:59:GLY:HA3	1.96	0.47
6:F:7:TYR:OH	24:F:716:AJP:C17	2.63	0.47
6:F:433:LEU:O	6:F:437:LEU:HG	2.15	0.47
6:F:622:VAL:O	24:F:718:AJP:C10	2.63	0.47
11:K:173:GLU:OE2	14:N:38:ARG:NH2	2.48	0.47
19:S:42:ILE:HG22	19:S:43:MET:H	1.79	0.47
6:F:425:PHE:HB2	6:F:432:TRP:CD1	2.50	0.46
18:R:92:GLN:HG3	18:R:95:GLU:HB2	1.96	0.46
1:A:331:THR:HG21	9:I:25:LEU:HG	1.96	0.46
2:B:315:MET:O	2:B:319:VAL:HG13	2.14	0.46
24:D:606:AJP:C13	24:D:607:AJP:C81	2.93	0.46
6:F:36:LEU:HD12	24:F:707:AJP:C83	2.44	0.46
8:H:84:ASN:HA	8:H:87:GLU:HG2	1.97	0.46
8:H:149:THR:HG21	8:H:156:ASN:HD22	1.79	0.46
8:H:194:ILE:HG21	8:H:262:TYR:HE2	1.79	0.46
2:B:59:ILE:HD12	24:B:606:AJP:C18	2.45	0.46
8:H:81:VAL:HA	8:H:84:ASN:ND2	2.30	0.46
6:F:308:ILE:HD11	6:F:580:TRP:HB2	1.96	0.46
2:B:148:LEU:HD11	7:G:157:ALA:HA	1.98	0.46
24:B:614:AJP:O79	24:D:610:AJP:C24	2.64	0.46
6:F:408:VAL:HG23	6:F:541:VAL:HB	1.96	0.46
6:F:614:ASN:HB3	24:F:710:AJP:C13	2.46	0.46
24:A:408:AJP:O82	24:A:409:AJP:C13	2.64	0.46
3:C:56:TYR:HD1	11:K:104:GLN:HE22	1.63	0.46
8:H:17:PRO:HA	8:H:26:LEU:H	1.81	0.46
14:N:49:ALA:HB1	14:N:108:LEU:HD11	1.98	0.46
4:D:70:TYR:HE2	24:D:604:AJP:C24	2.24	0.46
4:D:134:GLN:HE21	4:D:198:MET:HG2	1.80	0.46
8:H:49:ARG:HG2	11:K:89:THR:HG21	1.97	0.46
1:A:234:LEU:HD21	1:A:336:ARG:HA	1.97	0.46
4:D:70:TYR:HE2	24:D:604:AJP:C80	2.27	0.46
4:D:213:LEU:HD11	24:D:614:AJP:C81	2.46	0.46
2:B:357:ASP:N	2:B:357:ASP:OD1	2.49	0.46
2:B:358:GLN:HE22	7:G:192:ARG:HB3	1.81	0.46
4:D:10:ILE:HD13	4:D:49:ILE:HG12	1.97	0.46
7:G:62:GLN:HE22	7:G:66:TYR:HD2	1.64	0.46
1:A:199:GLN:O	1:A:206:SER:OG	2.32	0.46
1:A:202:TYR:HB2	1:A:206:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:GLY:CA	24:B:614:AJP:C83	2.94	0.46
6:F:7:TYR:CE2	24:F:716:AJP:C17	2.99	0.46
6:F:98:VAL:O	6:F:102:THR:HG23	2.14	0.46
6:F:323:THR:HG23	6:F:349:HIS:CE1	2.51	0.46
9:I:95:HIS:CE1	9:I:97:SER:HB2	2.50	0.46
1:A:92:ALA:HB2	3:C:53:LEU:HB3	1.98	0.45
21:A:401:BCR:H362	12:L:45:ALA:HB1	1.97	0.45
2:B:283:ILE:CD1	24:B:616:AJP:C14	2.93	0.45
6:F:409:PRO:HG2	6:F:411:PHE:CE2	2.51	0.45
17:Q:18:PRO:HA	17:Q:21:ILE:HG12	1.97	0.45
1:A:328:LEU:HD11	22:H:401:LHG:H291	1.97	0.45
4:D:24:ILE:HB	4:D:114:ARG:NH2	2.32	0.45
6:F:373:HIS:NE2	6:F:472:HIS:HB3	2.31	0.45
14:N:22:PHE:O	14:N:138:VAL:HA	2.16	0.45
1:A:202:TYR:CE1	24:A:407:AJP:C80	2.99	0.45
4:D:326:ASN:HA	4:D:496:ILE:HG13	1.98	0.45
8:H:118:LEU:HD23	8:H:118:LEU:H	1.80	0.45
9:I:55:ARG:HB3	9:I:121:THR:HB	1.98	0.45
9:I:92:GLU:HB3	20:V:131:PHE:CE1	2.52	0.45
6:F:26:LEU:HD23	26:F:704:SQD:H91	1.98	0.45
14:N:114:ALA:HB2	14:N:147:VAL:HG21	1.97	0.45
2:B:378:LEU:HD23	2:B:468:VAL:HG13	1.97	0.45
2:B:419:VAL:HG21	4:D:178:LEU:HD12	1.98	0.45
4:D:503:LEU:HD12	4:D:504:PRO:HD2	1.98	0.45
6:F:351:TYR:HD2	6:F:500:ILE:HD13	1.81	0.45
24:G:303:AJP:C83	24:G:303:AJP:C02	2.95	0.45
8:H:68:SER:OG	8:H:154:ILE:O	2.25	0.45
19:S:42:ILE:H	19:S:45:ILE:HG13	1.81	0.45
1:A:256:LEU:HD23	1:A:259:LEU:HD21	1.99	0.45
2:B:287:ILE:HD11	2:B:413:LEU:HD11	1.99	0.45
6:F:320:ALA:O	6:F:324:ILE:HG13	2.17	0.45
12:L:29:TYR:CZ	12:L:58:LEU:HD22	2.52	0.45
15:O:51:LYS:HG3	15:O:58:THR:HG22	1.98	0.45
5:E:43:LEU:HG	7:G:46:ILE:HD11	1.99	0.45
14:N:64:GLY:H	20:V:141:LYS:HZ2	1.64	0.45
17:Q:6:ASN:HB2	17:Q:11:LYS:HG3	1.97	0.45
1:A:38:LEU:O	1:A:42:THR:HG23	2.17	0.45
2:B:369:ASP:OD1	2:B:369:ASP:N	2.50	0.45
4:D:256:LYS:HD2	4:D:336:MET:HB3	1.99	0.45
8:H:337:GLU:OE2	10:J:62:ARG:NH2	2.50	0.45
1:A:82:LYS:HZ3	1:A:86:LYS:HE3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:596:ARG:HH12	17:Q:20:MET:HE1	1.82	0.44
13:M:99:ARG:HH22	14:N:45:LEU:HD12	1.82	0.44
2:B:25:LEU:HD12	2:B:117:LEU:HB2	1.99	0.44
3:C:87:GLU:HG3	3:C:116:LEU:HD13	1.99	0.44
4:D:335:GLN:HB2	4:D:397:ALA:HB1	1.99	0.44
9:I:183:ARG:HG2	9:I:184:PRO:HD2	1.98	0.44
20:V:46:GLU:HA	20:V:49:ASN:HD21	1.82	0.44
8:H:326:GLU:OE2	10:J:95:ARG:NH1	2.50	0.44
9:I:69:CYS:HB2	9:I:109:CYS:HB2	1.99	0.44
19:S:76:ALA:HA	19:S:89:THR:HG22	2.00	0.44
5:E:31:LEU:O	5:E:35:GLU:HG2	2.18	0.44
6:F:123:ARG:HD2	26:F:704:SQD:H242	1.98	0.44
6:F:243:GLN:HE22	6:F:331:VAL:HG21	1.81	0.44
9:I:163:LEU:HD22	9:I:173:LEU:HD21	1.99	0.44
1:A:20:LEU:HD13	1:A:25:ALA:HB2	1.99	0.44
22:D:601:LHG:H191	22:D:601:LHG:H383	1.99	0.44
7:G:116:LEU:HD13	24:G:305:AJP:C21	2.48	0.44
3:C:124:TRP:CE3	24:C:202:AJP:C81	3.01	0.44
5:E:12:LEU:CD1	24:G:306:AJP:C01	2.96	0.44
12:L:8:LEU:HD23	12:L:8:LEU:HA	1.89	0.44
2:B:35:GLN:OE1	24:B:612:AJP:C21	2.66	0.44
2:B:294:LEU:HD22	2:B:423:TYR:HD2	1.83	0.44
5:E:39:ASN:HD21	7:G:43:PHE:HE1	1.66	0.44
1:A:349:LEU:HB3	1:A:350:PRO:HD3	2.00	0.43
22:B:603:LHG:H212	22:B:603:LHG:H181	1.81	0.43
4:D:279:PRO:HG3	4:D:411:TYR:HE1	1.82	0.43
11:K:53:CYS:HB3	11:K:87:SER:HB2	1.99	0.43
1:A:31:PRO:HB3	22:A:402:LHG:H352	1.69	0.43
2:B:292:VAL:HG13	6:F:628:LYS:HB3	2.00	0.43
4:D:147:LEU:HD11	4:D:170:ILE:HG13	2.00	0.43
4:D:231:LEU:HD12	24:D:609:AJP:C01	2.48	0.43
8:H:13:ILE:HD12	8:H:32:LEU:HD21	2.00	0.43
14:N:38:ARG:HA	14:N:42:TYR:O	2.18	0.43
17:Q:18:PRO:CB	24:Q:102:AJP:C18	2.82	0.43
1:A:217:LEU:HD21	22:H:401:LHG:H162	1.99	0.43
2:B:387:PRO:HG2	4:D:145:LEU:HD23	2.00	0.43
9:I:186:ALA:O	9:I:190:THR:HG22	2.18	0.43
15:O:4:LYS:HB2	15:O:4:LYS:HE2	1.85	0.43
18:R:4:LYS:HA	18:R:4:LYS:HD3	1.89	0.43
3:C:56:TYR:HB2	11:K:79:ARG:HE	1.83	0.43
6:F:107:VAL:HG21	6:F:263:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:THR:HG21	5:E:50:ASN:HD21	1.83	0.43
6:F:243:GLN:O	6:F:247:HIS:HB3	2.18	0.43
6:F:323:THR:HG23	6:F:349:HIS:HE1	1.83	0.43
6:F:349:HIS:HA	6:F:352:PHE:CZ	2.53	0.43
6:F:495:ILE:HG13	6:F:496:PRO:HD3	2.00	0.43
24:F:712:AJP:C13	24:F:718:AJP:C81	2.96	0.43
9:I:172:ASP:N	9:I:172:ASP:OD2	2.51	0.43
14:N:10:VAL:HG22	14:N:37:LEU:HD23	2.00	0.43
3:C:124:TRP:CZ2	24:C:201:AJP:C14	3.01	0.43
4:D:427:VAL:HA	4:D:430:THR:HG22	2.01	0.43
4:D:475:ILE:HD12	21:P:101:BCR:H21C	1.99	0.43
8:H:175:LYS:HG3	9:I:161:ALA:HA	2.01	0.43
11:K:66:ASP:OD2	11:K:69:ARG:HB3	2.19	0.43
1:A:349:LEU:HD21	3:C:84:PHE:CE2	2.53	0.43
3:C:63:ILE:HD13	13:M:1:MET:HG2	2.01	0.43
6:F:488:LEU:HB3	6:F:489:PRO:HD3	2.01	0.43
26:F:704:SQD:H112	26:F:704:SQD:H142	1.86	0.43
4:D:239:HIS:O	4:D:247:HIS:NE2	2.46	0.43
8:H:67:VAL:HG22	8:H:78:ASN:HB3	2.01	0.43
11:K:32:ASN:HD21	11:K:170:HIS:HA	1.83	0.43
2:B:26:LEU:HG	22:B:603:LHG:H383	2.01	0.43
6:F:43:PHE:HB2	24:F:714:AJP:C03	2.49	0.43
24:F:707:AJP:C13	24:F:714:AJP:C18	2.97	0.43
7:G:37:PHE:CB	24:G:301:AJP:C13	2.97	0.43
8:H:76:MET:SD	8:H:109:ASN:ND2	2.92	0.43
9:I:183:ARG:NH2	19:S:62:GLN:O	2.51	0.43
10:J:58:PHE:HB3	10:J:81:LEU:HD12	1.99	0.43
8:H:196:ASN:HB3	9:I:20:TYR:CZ	2.53	0.43
20:V:136:ARG:HH12	20:V:140:GLN:HG3	1.83	0.43
1:A:73:ILE:HD11	12:L:62:ALA:HB2	1.99	0.42
4:D:389:LEU:HD13	4:D:390:PRO:HD2	2.01	0.42
4:D:390:PRO:HA	4:D:395:PHE:HB3	2.01	0.42
11:K:60:MET:HG2	11:K:152:PRO:HB3	2.00	0.42
20:V:74:ASN:HB3	20:V:91:PHE:O	2.19	0.42
1:A:55:ILE:HD13	1:A:323:PHE:HD1	1.84	0.42
1:A:229:ARG:HB3	1:A:329:ARG:HD2	2.00	0.42
2:B:100:ARG:HH11	7:G:177:LEU:HD22	1.83	0.42
2:B:188:SER:OG	2:B:189:GLY:N	2.52	0.42
6:F:626:GLY:HA2	24:F:718:AJP:O82	2.11	0.42
1:A:300:PRO:HA	1:A:303:GLN:HB2	2.02	0.42
3:C:52:ARG:HH12	11:K:107:SER:N	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:424:ALA:HB1	6:F:187:PHE:HD1	1.84	0.42
7:G:131:SER:O	7:G:131:SER:OG	2.36	0.42
8:H:166:ALA:HB1	9:I:51:ARG:HH12	1.83	0.42
13:M:18:VAL:HG23	13:M:19:ASP:N	2.32	0.42
2:B:484:LEU:HD11	24:B:606:AJP:C12	2.29	0.42
3:C:112:PHE:CZ	3:C:116:LEU:HD11	2.55	0.42
4:D:213:LEU:HD23	24:D:613:AJP:O82	2.15	0.42
7:G:37:PHE:HB3	24:G:301:AJP:C13	2.49	0.42
1:A:212:GLN:NE2	1:A:355:ASN:OD1	2.51	0.42
1:A:234:LEU:O	1:A:238:GLU:N	2.36	0.42
1:A:346:LYS:N	1:A:346:LYS:HD3	2.34	0.42
22:B:604:LHG:H162	22:B:604:LHG:H132	1.94	0.42
24:D:612:AJP:C06	24:D:612:AJP:C02	2.90	0.42
6:F:2:GLU:HB3	6:F:3:PRO:HD3	2.00	0.42
6:F:29:PHE:HE2	24:F:707:AJP:C10	2.31	0.42
9:I:57:HIS:CE1	9:I:142:GLY:HA2	2.54	0.42
19:S:42:ILE:HG22	19:S:43:MET:N	2.34	0.42
6:F:36:LEU:HD21	24:F:714:AJP:C80	2.50	0.42
11:K:110:TYR:CZ	11:K:166:ILE:HG12	2.55	0.42
1:A:30:LEU:HD22	3:C:21:TYR:CE1	2.55	0.42
1:A:90:LEU:HD11	1:A:96:ARG:HA	2.02	0.42
24:B:607:AJP:C02	24:B:607:AJP:C06	2.93	0.42
7:G:75:LEU:O	7:G:79:MET:HG2	2.19	0.42
10:J:98:VAL:HG12	10:J:100:VAL:HG13	2.01	0.42
14:N:113:PHE:HE1	14:N:130:VAL:HG21	1.85	0.42
2:B:403:TRP:CZ2	24:D:610:AJP:C81	3.03	0.42
14:N:21:LEU:HD21	14:N:131:GLU:HG2	2.02	0.42
20:V:53:LEU:O	20:V:57:LYS:HG2	2.20	0.42
2:B:165:LYS:HG2	6:F:635:ALA:HB2	2.02	0.42
4:D:213:LEU:CD2	24:D:614:AJP:C83	2.98	0.42
20:V:48:ILE:HD12	20:V:48:ILE:HA	1.91	0.42
21:A:401:BCR:HC32	23:A:404:DGD:HBV2	2.02	0.42
2:B:111:GLU:OE2	7:G:166:ARG:NH2	2.39	0.42
2:B:413:LEU:HD13	24:B:616:AJP:C13	2.50	0.42
5:E:94:GLU:O	5:E:97:ASN:ND2	2.53	0.42
10:J:48:ALA:O	10:J:52:THR:HG23	2.19	0.42
11:K:112:ILE:HD11	11:K:162:LEU:HD22	2.01	0.42
12:L:54:PHE:O	12:L:58:LEU:HG	2.20	0.42
4:D:134:GLN:HE22	4:D:264:ARG:HE	1.68	0.41
6:F:349:HIS:HA	6:F:352:PHE:CE1	2.55	0.41
1:A:347:PHE:O	1:A:351:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:PRO:HD3	2:B:281:LEU:HD22	2.01	0.41
2:B:276:LEU:CB	24:B:615:AJP:C80	2.93	0.41
24:B:607:AJP:C83	24:B:607:AJP:C02	2.98	0.41
4:D:209:GLY:CA	24:D:613:AJP:C18	2.98	0.41
8:H:357:PRO:HG2	8:H:360:PHE:HB3	2.02	0.41
11:K:33:ASP:OD1	14:N:35:ARG:NH2	2.53	0.41
12:L:35:ARG:HD2	12:L:38:VAL:HB	2.01	0.41
14:N:74:ASP:OD1	14:N:74:ASP:N	2.46	0.41
14:N:118:GLN:HE22	20:V:109:ILE:HB	1.85	0.41
21:P:101:BCR:H15C	21:P:101:BCR:H351	1.82	0.41
20:V:76:VAL:HB	20:V:89:LEU:HB2	2.02	0.41
2:B:59:ILE:HB	2:B:60:PRO:HD3	2.01	0.41
2:B:403:TRP:CH2	24:D:610:AJP:C81	3.04	0.41
11:K:170:HIS:CD2	11:K:172:ASN:HB2	2.54	0.41
1:A:218:VAL:HG13	1:A:348:LEU:HD22	2.02	0.41
3:C:122:TYR:HE1	3:C:126:LYS:HZ2	1.68	0.41
19:S:79:PHE:HE2	19:S:88:VAL:HB	1.85	0.41
1:A:15:LEU:HD13	1:A:25:ALA:HB1	2.02	0.41
3:C:32:VAL:HA	3:C:35:LEU:HG	2.02	0.41
6:F:20:LEU:HD13	26:F:704:SQD:H192	2.02	0.41
6:F:559:THR:OG1	6:F:560:PRO:HD3	2.20	0.41
2:B:219:ILE:O	2:B:223:ILE:HG13	2.21	0.41
7:G:62:GLN:NE2	7:G:66:TYR:HD2	2.18	0.41
8:H:234:LEU:HB2	8:H:332:GLU:HB2	2.02	0.41
26:L:101:SQD:H282	26:L:101:SQD:H311	1.93	0.41
14:N:88:LEU:HD23	14:N:91:LEU:HD22	2.02	0.41
15:O:20:LEU:HD23	15:O:20:LEU:HA	1.90	0.41
21:P:101:BCR:H20C	21:P:101:BCR:H361	1.87	0.41
21:P:101:BCR:H371	21:P:101:BCR:H24C	1.78	0.41
20:V:67:VAL:HG22	20:V:80:TRP:CD1	2.55	0.41
2:B:290:ASN:ND2	2:B:417:THR:HB	2.35	0.41
2:B:378:LEU:HD12	2:B:378:LEU:HA	1.94	0.41
24:D:609:AJP:C21	17:Q:40:LEU:HD21	2.50	0.41
6:F:629:TYR:CZ	24:F:712:AJP:C15	2.90	0.41
4:D:111:LEU:HB2	16:P:40:ASN:HB3	2.02	0.41
4:D:119:LEU:HD21	4:D:152:LEU:HD23	2.01	0.41
6:F:356:LEU:HD22	6:F:405:ILE:HD11	2.02	0.41
6:F:403:LEU:O	6:F:407:GLY:N	2.51	0.41
24:F:707:AJP:C06	24:F:707:AJP:C02	2.91	0.41
8:H:49:ARG:HD3	11:K:124:PHE:CZ	2.56	0.41
8:H:226:ARG:NH1	8:H:268:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:O	1:A:263:VAL:HG13	2.20	0.41
21:A:401:BCR:H361	21:A:401:BCR:H20C	1.83	0.41
3:C:13:VAL:HG12	3:C:15:VAL:HG13	2.01	0.41
4:D:78:LEU:HG	4:D:137:LEU:HD23	2.03	0.41
4:D:435:LEU:HD11	6:F:179:PHE:CD2	2.56	0.41
4:D:488:TYR:O	4:D:492:THR:HG23	2.21	0.41
6:F:10:LEU:HD23	6:F:10:LEU:H	1.85	0.41
6:F:626:GLY:HA3	24:F:718:AJP:C08	2.50	0.41
8:H:357:PRO:HG3	8:H:394:ARG:NH1	2.36	0.41
14:N:55:LEU:HD12	14:N:112:GLU:HB2	2.03	0.41
18:R:27:ASP:O	18:R:30:GLU:HG3	2.20	0.41
2:B:34:ILE:CD1	24:B:611:AJP:C16	2.97	0.41
6:F:143:ASN:O	6:F:147:VAL:HG23	2.21	0.41
6:F:626:GLY:HA3	24:F:718:AJP:C10	2.49	0.41
22:A:402:LHG:H151	3:C:22:PHE:HE2	1.86	0.40
2:B:59:ILE:HD13	24:B:606:AJP:C17	2.51	0.40
2:B:283:ILE:CD1	24:B:616:AJP:C20	2.88	0.40
2:B:353:ARG:HD3	2:B:447:TYR:OH	2.21	0.40
4:D:294:LEU:HD12	21:F:701:BCR:HC41	2.03	0.40
4:D:474:ILE:H	4:D:474:ILE:HG13	1.72	0.40
6:F:225:LEU:HD13	24:F:708:AJP:C81	2.51	0.40
6:F:374:ASN:HB3	6:F:377:LEU:HB2	2.01	0.40
6:F:445:TYR:HA	6:F:448:ARG:HB3	2.03	0.40
21:F:701:BCR:H361	21:F:701:BCR:H20C	1.77	0.40
7:G:10:ILE:HA	24:G:304:AJP:C83	2.51	0.40
9:I:61:ASP:OD2	20:V:117:PHE:HA	2.22	0.40
10:J:38:MET:HG3	10:J:95:ARG:HB2	2.03	0.40
12:L:43:GLU:O	12:L:47:MET:HG3	2.21	0.40
2:B:225:ALA:O	2:B:229:HIS:HB3	2.22	0.40
2:B:462:VAL:HG23	22:B:604:LHG:H122	2.03	0.40
6:F:109:LEU:HD21	6:F:488:LEU:HD23	2.03	0.40
6:F:567:LYS:HE3	6:F:567:LYS:HB2	1.84	0.40
7:G:7:THR:O	7:G:11:THR:HG23	2.21	0.40
7:G:94:TRP:CZ3	24:G:306:AJP:C23	2.99	0.40
8:H:198:PRO:O	8:H:200:PHE:N	2.53	0.40
8:H:212:ARG:O	8:H:216:ILE:HG12	2.21	0.40
11:K:192:PRO:HG3	13:M:26:THR:HG21	2.04	0.40
14:N:9:PHE:HE2	14:N:37:LEU:HD11	1.85	0.40
1:A:340:LEU:O	1:A:343:LEU:HG	2.22	0.40
2:B:53:GLY:O	2:B:57:THR:HG23	2.21	0.40
2:B:361:GLU:OE1	2:B:441:SER:OG	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:243:GLN:NE2	6:F:331:VAL:HG21	2.37	0.40
6:F:625:GLU:O	6:F:628:LYS:HG3	2.22	0.40
26:F:704:SQD:H271	26:F:704:SQD:H241	1.92	0.40
8:H:82:THR:HG22	8:H:353:TRP:HZ2	1.86	0.40
18:R:19:VAL:HB	18:R:28:VAL:HG21	2.02	0.40
20:V:47:PHE:O	20:V:50:GLU:HG3	2.21	0.40
1:A:112:LEU:HD21	3:C:22:PHE:CE1	2.56	0.40
1:A:181:LEU:HD13	3:C:92:TYR:HD1	1.86	0.40
23:A:403:DGD:HB21	23:A:403:DGD:HB51	1.86	0.40
2:B:353:ARG:NE	2:B:449:GLU:OE1	2.39	0.40
4:D:13:PHE:HB3	4:D:14:PRO:HD3	2.04	0.40
4:D:209:GLY:HA3	24:D:613:AJP:C24	2.51	0.40
4:D:424:ALA:HB1	6:F:187:PHE:CD1	2.57	0.40
8:H:15:MET:N	8:H:28:LEU:O	2.46	0.40
8:H:78:ASN:HA	8:H:81:VAL:HG22	2.04	0.40
20:V:92:LEU:HB3	20:V:93:GLU:H	1.75	0.40
2:B:400:TRP:CD1	4:D:189:PHE:HZ	2.39	0.40
4:D:479:LEU:O	24:D:612:AJP:C81	2.70	0.40
6:F:71:GLN:HE21	24:F:711:AJP:C80	2.18	0.40
6:F:111:SER:HA	6:F:114:TYR:HB3	2.03	0.40
6:F:200:THR:HG22	6:F:202:THR:H	1.86	0.40
6:F:309:ALA:HB2	6:F:321:TYR:HB3	2.04	0.40
11:K:183:LEU:HD12	13:M:30:THR:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/372 (99%)	342 (93%)	27 (7%)	0	100	100
2	B	491/515 (95%)	472 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
4	D	502/529 (95%)	477 (95%)	25 (5%)	0	100	100
5	E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
6	F	643/656 (98%)	613 (95%)	30 (5%)	0	100	100
7	G	190/200 (95%)	183 (96%)	7 (4%)	0	100	100
8	H	391/394 (99%)	359 (92%)	32 (8%)	0	100	100
9	I	188/196 (96%)	177 (94%)	11 (6%)	0	100	100
10	J	154/168 (92%)	147 (96%)	7 (4%)	0	100	100
11	K	204/237 (86%)	193 (95%)	11 (5%)	0	100	100
12	L	71/76 (93%)	65 (92%)	6 (8%)	0	100	100
13	M	108/111 (97%)	100 (93%)	8 (7%)	0	100	100
14	N	146/150 (97%)	140 (96%)	6 (4%)	0	100	100
15	O	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
16	P	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
17	Q	42/45 (93%)	42 (100%)	0	0	100	100
18	R	95/98 (97%)	95 (100%)	0	0	100	100
19	S	60/110 (54%)	58 (97%)	2 (3%)	0	100	100
20	V	101/146 (69%)	93 (92%)	8 (8%)	0	100	100
All	All	4078/4350 (94%)	3863 (95%)	215 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/302 (99%)	300 (100%)	0	100	100
2	B	396/413 (96%)	396 (100%)	0	100	100
3	C	100/109 (92%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	404/424 (95%)	403 (100%)	1 (0%)	93	98
5	E	82/82 (100%)	82 (100%)	0	100	100
6	F	519/527 (98%)	517 (100%)	2 (0%)	91	95
7	G	159/166 (96%)	158 (99%)	1 (1%)	86	94
8	H	337/338 (100%)	336 (100%)	1 (0%)	92	96
9	I	166/172 (96%)	166 (100%)	0	100	100
10	J	138/148 (93%)	138 (100%)	0	100	100
11	K	175/196 (89%)	175 (100%)	0	100	100
12	L	61/63 (97%)	61 (100%)	0	100	100
13	M	95/96 (99%)	95 (100%)	0	100	100
14	N	119/120 (99%)	118 (99%)	1 (1%)	81	93
15	O	57/59 (97%)	57 (100%)	0	100	100
16	P	35/37 (95%)	35 (100%)	0	100	100
17	Q	31/32 (97%)	31 (100%)	0	100	100
18	R	85/86 (99%)	85 (100%)	0	100	100
19	S	55/97 (57%)	55 (100%)	0	100	100
20	V	83/118 (70%)	81 (98%)	2 (2%)	49	77
All	All	3397/3585 (95%)	3389 (100%)	8 (0%)	93	98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	162	ARG
6	F	187	PHE
6	F	628	LYS
7	G	31	ASN
8	H	330	ARG
14	N	107	ARG
20	V	122	ARG
20	V	136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	291	ASN
1	A	355	ASN
2	B	340	ASN
2	B	358	GLN
4	D	60	ASN
4	D	65	GLN
4	D	134	GLN
4	D	163	GLN
4	D	339	HIS
5	E	39	ASN
5	E	44	ASN
5	E	87	ASN
6	F	6	GLN
6	F	62	GLN
6	F	146	GLN
6	F	349	HIS
6	F	563	GLN
6	F	600	GLN
9	I	5	ASN
9	I	76	ASN
9	I	95	HIS
10	J	23	ASN
10	J	64	GLN
10	J	120	GLN
11	K	32	ASN
11	K	104	GLN
11	K	170	HIS
13	M	37	ASN
14	N	69	HIS
14	N	94	ASN
14	N	118	GLN
15	O	49	GLN
19	S	55	ASN
20	V	140	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

83 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	$\#\|Z\| > 2$
24	AJP	B	608	-	37,37,95	1.15	6 (16%)	58,62,149	2.13	16 (27%)
24	AJP	D	606	-	37,37,95	1.36	6 (16%)	58,62,149	2.23	18 (31%)
24	AJP	D	609	-	37,37,95	1.35	7 (18%)	58,62,149	2.34	13 (22%)
24	AJP	B	615	-	37,37,95	1.17	6 (16%)	58,62,149	2.13	16 (27%)
24	AJP	D	610	-	37,37,95	1.42	7 (18%)	58,62,149	2.26	21 (36%)
24	AJP	F	708	-	37,37,95	1.33	7 (18%)	58,62,149	2.24	19 (32%)
24	AJP	F	707	-	37,37,95	1.39	8 (21%)	58,62,149	2.20	18 (31%)
24	AJP	B	606	-	37,37,95	1.49	7 (18%)	58,62,149	2.38	19 (32%)
24	AJP	A	408	-	37,37,95	1.32	8 (21%)	58,62,149	2.23	19 (32%)
22	LHG	A	402	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
24	AJP	E	201	-	37,37,95	1.30	7 (18%)	58,62,149	2.23	17 (29%)
24	AJP	F	711	-	37,37,95	1.30	7 (18%)	58,62,149	2.24	17 (29%)
27	SF4	I	202	9	0,12,12	-	-	-		
24	AJP	B	616	-	37,37,95	1.33	7 (18%)	58,62,149	2.24	18 (31%)
24	AJP	D	603	-	37,37,95	1.55	8 (21%)	58,62,149	2.26	20 (34%)
24	AJP	B	609	-	37,37,95	1.27	7 (18%)	58,62,149	2.26	17 (29%)
24	AJP	G	307	-	37,37,95	1.25	5 (13%)	58,62,149	2.23	15 (25%)
24	AJP	B	610	-	37,37,95	1.28	8 (21%)	58,62,149	2.20	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	AJP	G	304	-	37,37,95	1.34	8 (21%)	58,62,149	2.21	19 (32%)
24	AJP	D	607	-	37,37,95	1.26	5 (13%)	58,62,149	2.30	17 (29%)
22	LHG	D	602	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
24	AJP	F	713	-	37,37,95	1.36	7 (18%)	58,62,149	2.24	18 (31%)
24	AJP	G	305	-	37,37,95	1.27	8 (21%)	58,62,149	2.19	17 (29%)
24	AJP	D	605	-	37,37,95	1.25	6 (16%)	58,62,149	2.19	18 (31%)
24	AJP	D	614	-	37,37,95	1.25	7 (18%)	58,62,149	2.22	18 (31%)
21	BCR	P	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	5 (8%)
24	AJP	F	712	-	37,37,95	1.16	4 (10%)	58,62,149	2.14	16 (27%)
24	AJP	A	409	-	37,37,95	1.21	5 (13%)	58,62,149	2.25	19 (32%)
24	AJP	F	716	-	37,37,95	1.54	8 (21%)	58,62,149	2.26	19 (32%)
24	AJP	Q	102	-	37,37,95	1.47	7 (18%)	58,62,149	2.37	18 (31%)
24	AJP	B	613	-	37,37,95	1.32	7 (18%)	58,62,149	2.17	19 (32%)
24	AJP	G	301	-	37,37,95	1.51	7 (18%)	58,62,149	2.32	20 (34%)
24	AJP	B	612	-	37,37,95	1.29	6 (16%)	58,62,149	2.33	18 (31%)
24	AJP	B	614	-	37,37,95	1.18	6 (16%)	58,62,149	2.11	16 (27%)
24	AJP	B	617	-	37,37,95	1.18	6 (16%)	58,62,149	2.19	18 (31%)
24	AJP	Q	104	-	37,37,95	1.26	7 (18%)	58,62,149	2.13	19 (32%)
22	LHG	B	603	-	48,48,48	0.61	0	51,54,54	1.25	6 (11%)
22	LHG	F	702	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
24	AJP	D	604	-	37,37,95	1.52	7 (18%)	58,62,149	2.45	20 (34%)
24	AJP	F	714	-	37,37,95	1.38	8 (21%)	58,62,149	2.24	18 (31%)
24	AJP	Q	101	-	37,37,95	1.23	7 (18%)	58,62,149	2.15	16 (27%)
22	LHG	D	601	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
24	AJP	Q	103	-	37,37,95	1.29	6 (16%)	58,62,149	2.24	18 (31%)
24	AJP	Q	105	-	37,37,95	1.16	5 (13%)	58,62,149	2.15	17 (29%)
22	LHG	H	401	-	48,48,48	0.58	0	51,54,54	1.25	6 (11%)
23	DGD	A	403	-	67,67,67	0.84	2 (2%)	81,81,81	1.42	12 (14%)
24	AJP	F	709	-	37,37,95	1.30	6 (16%)	58,62,149	2.21	20 (34%)
24	AJP	A	405	-	37,37,95	1.34	6 (16%)	58,62,149	2.22	16 (27%)
27	SF4	K	301	11	0,12,12	-	-	-		
26	SQD	L	101	-	53,54,54	0.96	5 (9%)	62,65,65	1.51	10 (16%)
24	AJP	F	710	-	37,37,95	1.34	4 (10%)	58,62,149	2.32	19 (32%)
24	AJP	G	306	-	37,37,95	1.40	7 (18%)	58,62,149	2.23	19 (32%)
26	SQD	F	704	-	53,54,54	0.95	4 (7%)	62,65,65	1.49	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	AJP	D	612	-	37,37,95	1.26	5 (13%)	58,62,149	2.24	18 (31%)
24	AJP	C	201	-	37,37,95	1.30	7 (18%)	58,62,149	2.18	16 (27%)
23	DGD	A	404	-	67,67,67	0.86	2 (2%)	81,81,81	1.42	11 (13%)
24	AJP	F	718	-	37,37,95	1.18	5 (13%)	58,62,149	2.29	16 (27%)
25	PQN	B	601	-	34,34,34	2.84	9 (26%)	42,45,45	2.04	6 (14%)
21	BCR	A	401	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
24	AJP	F	715	-	37,37,95	1.17	5 (13%)	58,62,149	2.21	15 (25%)
27	SF4	I	201	9	0,12,12	-	-	-		
24	AJP	F	706	-	37,37,95	1.30	6 (16%)	58,62,149	2.15	19 (32%)
24	AJP	B	607	-	37,37,95	1.28	6 (16%)	58,62,149	2.17	17 (29%)
24	AJP	Q	108	-	37,37,95	1.24	7 (18%)	58,62,149	2.18	16 (27%)
24	AJP	A	406	-	37,37,95	1.27	3 (8%)	58,62,149	2.26	19 (32%)
22	LHG	B	602	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
24	AJP	G	302	-	37,37,95	1.28	6 (16%)	58,62,149	2.22	18 (31%)
24	AJP	G	303	-	37,37,95	1.30	8 (21%)	58,62,149	2.42	16 (27%)
24	AJP	A	407	-	37,37,95	1.26	6 (16%)	58,62,149	2.25	17 (29%)
22	LHG	B	604	-	48,48,48	0.60	0	51,54,54	1.25	6 (11%)
24	AJP	Q	107	-	37,37,95	1.24	7 (18%)	58,62,149	2.18	18 (31%)
26	SQD	B	605	-	53,54,54	0.95	5 (9%)	62,65,65	1.48	9 (14%)
24	AJP	F	717	-	37,37,95	1.26	7 (18%)	58,62,149	2.38	18 (31%)
28	FES	R	101	18	0,4,4	-	-	-		
24	AJP	Q	106	-	37,37,95	1.11	6 (16%)	58,62,149	2.16	17 (29%)
22	LHG	F	703	-	48,48,48	0.58	1 (2%)	51,54,54	1.24	6 (11%)
21	BCR	F	701	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	6 (10%)
24	AJP	B	611	-	37,37,95	1.44	9 (24%)	58,62,149	2.40	19 (32%)
24	AJP	C	202	-	37,37,95	1.37	8 (21%)	58,62,149	2.21	17 (29%)
24	AJP	D	611	-	37,37,95	1.24	6 (16%)	58,62,149	2.24	16 (27%)
24	AJP	D	613	-	37,37,95	1.22	5 (13%)	58,62,149	2.33	19 (32%)
26	SQD	F	705	-	53,54,54	0.96	5 (9%)	62,65,65	1.49	9 (14%)
24	AJP	D	608	-	37,37,95	1.30	6 (16%)	58,62,149	2.29	19 (32%)

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
24	AJP	B	608	-	12/12/14/38	-	0/6/6/11
24	AJP	D	606	-	12/12/14/38	-	0/6/6/11
24	AJP	D	609	-	12/12/14/38	-	0/6/6/11
24	AJP	B	615	-	12/12/14/38	-	0/6/6/11
24	AJP	D	610	-	12/12/14/38	-	0/6/6/11
24	AJP	F	708	-	12/12/14/38	-	0/6/6/11
24	AJP	F	707	-	12/12/14/38	-	0/6/6/11
24	AJP	B	606	-	12/12/14/38	-	0/6/6/11
24	AJP	A	408	-	12/12/14/38	-	0/6/6/11
22	LHG	A	402	-	-	20/53/53/53	-
24	AJP	E	201	-	12/12/14/38	-	0/6/6/11
24	AJP	F	711	-	12/12/14/38	-	0/6/6/11
27	SF4	I	202	9	-	-	0/6/5/5
24	AJP	B	616	-	12/12/14/38	-	0/6/6/11
24	AJP	D	603	-	12/12/14/38	-	0/6/6/11
24	AJP	B	609	-	12/12/14/38	-	0/6/6/11
24	AJP	G	307	-	12/12/14/38	-	0/6/6/11
24	AJP	B	610	-	12/12/14/38	-	0/6/6/11
24	AJP	G	304	-	12/12/14/38	-	0/6/6/11
24	AJP	D	607	-	12/12/14/38	-	0/6/6/11
22	LHG	D	602	-	-	21/53/53/53	-
24	AJP	F	713	-	12/12/14/38	-	0/6/6/11
24	AJP	G	305	-	12/12/14/38	-	0/6/6/11
24	AJP	D	605	-	12/12/14/38	-	0/6/6/11
24	AJP	D	614	-	12/12/14/38	-	0/6/6/11
21	BCR	P	101	-	-	14/29/63/63	0/2/2/2
24	AJP	F	712	-	12/12/14/38	-	0/6/6/11
24	AJP	A	409	-	12/12/14/38	-	0/6/6/11
24	AJP	F	716	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	102	-	12/12/14/38	-	0/6/6/11
24	AJP	B	613	-	12/12/14/38	-	0/6/6/11
24	AJP	G	301	-	12/12/14/38	-	0/6/6/11
24	AJP	B	612	-	12/12/14/38	-	0/6/6/11
24	AJP	B	614	-	12/12/14/38	-	0/6/6/11
24	AJP	B	617	-	12/12/14/38	-	0/6/6/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AJP	Q	104	-	12/12/14/38	-	0/6/6/11
22	LHG	B	603	-	-	21/53/53/53	-
22	LHG	F	702	-	-	25/53/53/53	-
24	AJP	D	604	-	12/12/14/38	-	0/6/6/11
24	AJP	F	714	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	101	-	12/12/14/38	-	0/6/6/11
22	LHG	D	601	-	-	17/53/53/53	-
24	AJP	Q	103	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	105	-	12/12/14/38	-	0/6/6/11
22	LHG	H	401	-	-	25/53/53/53	-
23	DGD	A	403	-	-	18/55/95/95	0/2/2/2
24	AJP	F	709	-	12/12/14/38	-	0/6/6/11
24	AJP	A	405	-	12/12/14/38	-	0/6/6/11
27	SF4	K	301	11	-	-	0/6/5/5
26	SQD	L	101	-	-	19/49/69/69	0/1/1/1
24	AJP	F	710	-	12/12/14/38	-	0/6/6/11
24	AJP	G	306	-	12/12/14/38	-	0/6/6/11
26	SQD	F	704	-	-	20/49/69/69	0/1/1/1
24	AJP	D	612	-	12/12/14/38	-	0/6/6/11
24	AJP	C	201	-	12/12/14/38	-	0/6/6/11
23	DGD	A	404	-	-	19/55/95/95	0/2/2/2
24	AJP	F	718	-	12/12/14/38	-	0/6/6/11
25	PQN	B	601	-	-	7/23/43/43	0/2/2/2
21	BCR	A	401	-	-	10/29/63/63	0/2/2/2
24	AJP	F	715	-	12/12/14/38	-	0/6/6/11
27	SF4	I	201	9	-	-	0/6/5/5
24	AJP	F	706	-	12/12/14/38	-	0/6/6/11
24	AJP	B	607	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	108	-	12/12/14/38	-	0/6/6/11
24	AJP	A	406	-	12/12/14/38	-	0/6/6/11
22	LHG	B	602	-	-	27/53/53/53	-
24	AJP	G	302	-	12/12/14/38	-	0/6/6/11
24	AJP	G	303	-	12/12/14/38	-	0/6/6/11
24	AJP	A	407	-	12/12/14/38	-	0/6/6/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LHG	B	604	-	-	25/53/53/53	-
24	AJP	Q	107	-	12/12/14/38	-	0/6/6/11
26	SQD	B	605	-	-	14/49/69/69	0/1/1/1
24	AJP	F	717	-	12/12/14/38	-	0/6/6/11
28	FES	R	101	18	-	-	0/1/1/1
24	AJP	Q	106	-	12/12/14/38	-	0/6/6/11
22	LHG	F	703	-	-	24/53/53/53	-
21	BCR	F	701	-	-	11/29/63/63	0/2/2/2
24	AJP	B	611	-	12/12/14/38	-	0/6/6/11
24	AJP	C	202	-	12/12/14/38	-	0/6/6/11
24	AJP	D	611	-	12/12/14/38	-	0/6/6/11
24	AJP	D	613	-	12/12/14/38	-	0/6/6/11
26	SQD	F	705	-	-	16/49/69/69	0/1/1/1
24	AJP	D	608	-	12/12/14/38	-	0/6/6/11

All (432) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	PQN	C12-C13	8.24	1.52	1.33
25	B	601	PQN	O4-C4	8.17	1.40	1.23
25	B	601	PQN	O1-C1	8.10	1.40	1.23
25	B	601	PQN	C2-C1	-4.20	1.39	1.48
24	B	606	AJP	C16-C11	-4.04	1.48	1.54
24	D	603	AJP	C16-C11	-3.79	1.49	1.54
24	F	716	AJP	C16-C11	-3.77	1.49	1.54
24	D	604	AJP	C16-C11	-3.73	1.49	1.54
24	E	201	AJP	C16-C11	-3.69	1.49	1.54
24	F	710	AJP	C16-C11	-3.59	1.49	1.54
24	D	612	AJP	C16-C11	-3.48	1.49	1.54
24	F	708	AJP	C16-C11	-3.47	1.49	1.54
24	A	406	AJP	C16-C11	-3.47	1.49	1.54
24	F	712	AJP	C16-C11	-3.47	1.49	1.54
24	G	307	AJP	C16-C11	-3.46	1.49	1.54
24	F	706	AJP	C16-C11	-3.45	1.49	1.54
24	G	306	AJP	C07-C08	-3.43	1.47	1.53
24	C	201	AJP	C16-C11	-3.43	1.49	1.54
24	D	603	AJP	C07-C08	-3.42	1.47	1.53
24	Q	102	AJP	C07-C08	-3.41	1.47	1.53
24	A	405	AJP	C12-C11	-3.41	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	401	BCR	C1-C6	-3.41	1.49	1.53
21	P	101	BCR	C1-C6	-3.39	1.49	1.53
24	G	301	AJP	C20-C15	-3.39	1.49	1.56
24	F	716	AJP	C07-C08	-3.38	1.47	1.53
24	Q	108	AJP	C16-C11	-3.38	1.49	1.54
24	D	603	AJP	C12-C11	-3.37	1.49	1.56
24	D	604	AJP	C20-C15	-3.35	1.49	1.56
24	F	710	AJP	C07-C08	-3.35	1.48	1.53
24	F	716	AJP	C12-C11	-3.35	1.49	1.56
24	D	608	AJP	C16-C11	-3.33	1.49	1.54
24	F	714	AJP	C16-C11	-3.33	1.49	1.54
24	B	609	AJP	C16-C11	-3.33	1.49	1.54
21	F	701	BCR	C1-C6	-3.31	1.49	1.53
24	D	607	AJP	C16-C11	-3.31	1.49	1.54
24	G	301	AJP	C07-C08	-3.30	1.48	1.53
24	D	610	AJP	C20-C15	-3.29	1.50	1.56
24	D	608	AJP	C12-C11	-3.29	1.49	1.56
24	Q	103	AJP	C07-C08	-3.28	1.48	1.53
24	B	606	AJP	C07-C08	-3.28	1.48	1.53
24	A	406	AJP	C12-C11	-3.27	1.49	1.56
24	A	405	AJP	C07-C08	-3.27	1.48	1.53
24	D	610	AJP	C16-C11	-3.26	1.50	1.54
24	C	202	AJP	C07-C08	-3.25	1.48	1.53
24	F	707	AJP	C16-C11	-3.24	1.50	1.54
24	Q	102	AJP	C16-C11	-3.24	1.50	1.54
24	B	611	AJP	C12-C11	-3.24	1.49	1.56
24	B	616	AJP	C12-C11	-3.23	1.49	1.56
24	G	304	AJP	C07-C08	-3.23	1.48	1.53
24	D	606	AJP	C16-C11	-3.22	1.50	1.54
24	C	202	AJP	C16-C11	-3.21	1.50	1.54
24	B	607	AJP	C16-C11	-3.21	1.50	1.54
24	B	611	AJP	C07-C08	-3.20	1.48	1.53
24	D	606	AJP	C07-C08	-3.19	1.48	1.53
24	B	610	AJP	C16-C11	-3.19	1.50	1.54
24	F	709	AJP	C16-C11	-3.19	1.50	1.54
24	B	606	AJP	C12-C11	-3.18	1.49	1.56
24	D	605	AJP	C16-C11	-3.17	1.50	1.54
24	Q	102	AJP	C12-C11	-3.17	1.49	1.56
24	A	406	AJP	C07-C08	-3.17	1.48	1.53
24	B	616	AJP	C07-C08	-3.17	1.48	1.53
24	B	613	AJP	C07-C08	-3.17	1.48	1.53
24	G	306	AJP	C16-C11	-3.16	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	301	AJP	C13-C12	-3.16	1.48	1.54
24	G	302	AJP	C07-C08	-3.16	1.48	1.53
24	F	708	AJP	C12-C11	-3.15	1.49	1.56
26	B	605	SQD	O48-C23	3.15	1.42	1.33
26	F	704	SQD	O48-C23	3.15	1.42	1.33
26	F	705	SQD	O48-C23	3.13	1.42	1.33
24	F	713	AJP	C16-C11	-3.13	1.50	1.54
24	F	710	AJP	C12-C11	-3.13	1.49	1.56
24	D	604	AJP	C07-C08	-3.13	1.48	1.53
24	F	708	AJP	C07-C08	-3.13	1.48	1.53
26	L	101	SQD	O48-C23	3.12	1.42	1.33
24	B	611	AJP	C20-C15	-3.11	1.50	1.56
24	F	713	AJP	C07-C08	-3.11	1.48	1.53
24	Q	101	AJP	C16-C11	-3.11	1.50	1.54
24	D	608	AJP	C07-C08	-3.09	1.48	1.53
21	P	101	BCR	C30-C25	-3.09	1.49	1.53
24	G	305	AJP	C07-C08	-3.08	1.48	1.53
25	B	601	PQN	C3-C4	-3.07	1.39	1.47
24	G	301	AJP	C20-C19	-3.07	1.50	1.55
24	Q	102	AJP	C20-C19	-3.06	1.50	1.55
24	B	612	AJP	C13-C12	-3.04	1.48	1.54
24	D	604	AJP	C12-C11	-3.04	1.49	1.56
24	G	301	AJP	C12-C11	-3.01	1.50	1.56
24	Q	104	AJP	O09-C05	3.01	1.49	1.42
24	G	305	AJP	C16-C11	-3.01	1.50	1.54
24	A	407	AJP	C07-C08	-3.00	1.48	1.53
24	F	716	AJP	C20-C19	-3.00	1.50	1.55
24	B	606	AJP	C20-C19	-3.00	1.50	1.55
24	F	717	AJP	C20-C15	-2.99	1.50	1.56
24	G	305	AJP	C12-C11	-2.99	1.50	1.56
24	C	202	AJP	C12-C11	-2.99	1.50	1.56
24	F	714	AJP	C12-C11	-2.99	1.50	1.56
24	B	612	AJP	C16-C11	-2.98	1.50	1.54
24	D	603	AJP	C20-C19	-2.98	1.50	1.55
24	F	713	AJP	O09-C05	2.97	1.49	1.42
24	F	718	AJP	C16-C11	-2.97	1.50	1.54
24	D	606	AJP	C12-C11	-2.96	1.50	1.56
24	B	610	AJP	C07-C08	-2.96	1.48	1.53
24	A	405	AJP	C16-C11	-2.96	1.50	1.54
24	B	613	AJP	C12-C11	-2.96	1.50	1.56
24	D	603	AJP	C13-C12	-2.96	1.48	1.54
25	B	601	PQN	C5-C4	-2.95	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	610	AJP	O09-C05	2.95	1.49	1.42
24	B	607	AJP	C12-C11	-2.95	1.50	1.56
24	G	304	AJP	C20-C15	-2.95	1.50	1.56
24	G	304	AJP	C16-C11	-2.95	1.50	1.54
24	D	613	AJP	C07-C08	-2.94	1.48	1.53
24	D	603	AJP	C20-C15	-2.93	1.50	1.56
24	F	716	AJP	C13-C12	-2.93	1.48	1.54
24	A	407	AJP	C16-C11	-2.92	1.50	1.54
24	B	607	AJP	C07-C08	-2.91	1.48	1.53
24	D	611	AJP	C16-C11	-2.91	1.50	1.54
24	F	713	AJP	C12-C11	-2.90	1.50	1.56
24	G	306	AJP	C12-C07	-2.90	1.50	1.56
24	F	711	AJP	C16-C11	-2.90	1.50	1.54
24	A	408	AJP	C12-C11	-2.89	1.50	1.56
24	A	407	AJP	C12-C11	-2.88	1.50	1.56
24	B	615	AJP	C16-C11	-2.88	1.50	1.54
24	Q	107	AJP	C07-C08	-2.88	1.48	1.53
24	F	716	AJP	C20-C15	-2.88	1.50	1.56
26	F	704	SQD	O47-C7	2.87	1.42	1.34
24	A	408	AJP	C20-C15	-2.87	1.50	1.56
24	B	608	AJP	C07-C08	-2.87	1.48	1.53
24	D	611	AJP	C07-C08	-2.87	1.48	1.53
26	F	705	SQD	O47-C7	2.87	1.42	1.34
24	B	617	AJP	C16-C11	-2.87	1.50	1.54
26	L	101	SQD	O47-C7	2.87	1.42	1.34
24	A	409	AJP	C12-C11	-2.87	1.50	1.56
24	D	606	AJP	C20-C15	-2.86	1.50	1.56
24	F	715	AJP	C16-C11	-2.86	1.50	1.54
24	G	304	AJP	C12-C11	-2.86	1.50	1.56
24	F	707	AJP	C12-C11	-2.85	1.50	1.56
25	B	601	PQN	C10-C1	-2.85	1.42	1.48
24	G	306	AJP	C12-C11	-2.85	1.50	1.56
24	B	610	AJP	C12-C11	-2.85	1.50	1.56
26	B	605	SQD	O47-C7	2.85	1.42	1.34
24	A	408	AJP	C07-C08	-2.84	1.48	1.53
24	D	613	AJP	C16-C11	-2.84	1.50	1.54
24	A	408	AJP	C16-C11	-2.84	1.50	1.54
24	G	302	AJP	C12-C11	-2.84	1.50	1.56
24	G	303	AJP	C16-C11	-2.84	1.50	1.54
24	Q	103	AJP	C12-C11	-2.84	1.50	1.56
24	D	614	AJP	C07-C08	-2.83	1.48	1.53
24	F	709	AJP	C12-C11	-2.82	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	707	AJP	C20-C15	-2.82	1.50	1.56
24	D	604	AJP	C20-C19	-2.82	1.50	1.55
24	E	201	AJP	C07-C08	-2.81	1.48	1.53
24	D	605	AJP	C12-C11	-2.81	1.50	1.56
24	F	709	AJP	C07-C08	-2.81	1.48	1.53
24	G	303	AJP	C20-C15	-2.81	1.50	1.56
24	Q	108	AJP	C07-C08	-2.81	1.48	1.53
24	G	303	AJP	C13-C12	-2.81	1.49	1.54
24	C	201	AJP	C07-C08	-2.80	1.48	1.53
24	B	616	AJP	C20-C15	-2.80	1.51	1.56
24	B	613	AJP	C16-C11	-2.80	1.50	1.54
24	A	409	AJP	C16-C11	-2.79	1.50	1.54
24	G	306	AJP	C20-C15	-2.79	1.51	1.56
21	A	401	BCR	C30-C25	-2.79	1.49	1.53
24	D	605	AJP	C07-C08	-2.79	1.49	1.53
24	B	612	AJP	C12-C11	-2.79	1.50	1.56
24	B	609	AJP	C07-C08	-2.79	1.49	1.53
24	G	302	AJP	C16-C11	-2.78	1.50	1.54
24	Q	101	AJP	C07-C08	-2.78	1.49	1.53
24	Q	102	AJP	C20-C15	-2.78	1.51	1.56
24	D	607	AJP	C20-C15	-2.78	1.51	1.56
24	F	717	AJP	C16-C11	-2.77	1.50	1.54
24	F	714	AJP	C20-C15	-2.77	1.51	1.56
24	D	609	AJP	C16-C11	-2.77	1.50	1.54
24	D	610	AJP	C20-C19	-2.77	1.50	1.55
24	F	707	AJP	C07-C08	-2.77	1.49	1.53
24	F	706	AJP	C12-C11	-2.76	1.50	1.56
24	D	613	AJP	C12-C11	-2.76	1.50	1.56
24	G	301	AJP	C16-C11	-2.76	1.50	1.54
24	F	711	AJP	C07-C08	-2.75	1.49	1.53
24	B	616	AJP	C16-C11	-2.74	1.50	1.54
24	F	714	AJP	C07-C08	-2.74	1.49	1.53
24	Q	104	AJP	C20-C15	-2.74	1.51	1.56
24	E	201	AJP	C12-C11	-2.73	1.50	1.56
24	D	614	AJP	C16-C11	-2.72	1.50	1.54
24	D	612	AJP	C12-C11	-2.72	1.50	1.56
24	B	617	AJP	C07-C08	-2.72	1.49	1.53
24	F	711	AJP	C12-C11	-2.72	1.50	1.56
24	B	611	AJP	C21-C20	-2.71	1.50	1.54
25	B	601	PQN	C3-C2	2.71	1.40	1.35
24	B	615	AJP	C07-C08	-2.70	1.49	1.53
24	B	611	AJP	C16-C11	-2.70	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	105	AJP	C07-C08	-2.69	1.49	1.53
24	B	617	AJP	C12-C11	-2.69	1.50	1.56
24	Q	104	AJP	C07-C08	-2.69	1.49	1.53
24	D	614	AJP	C12-C11	-2.67	1.50	1.56
24	A	409	AJP	C07-C08	-2.67	1.49	1.53
24	F	707	AJP	C20-C19	-2.66	1.51	1.55
24	B	612	AJP	C07-C08	-2.66	1.49	1.53
24	F	714	AJP	O09-C05	2.66	1.48	1.42
24	Q	107	AJP	C12-C11	-2.66	1.50	1.56
24	B	613	AJP	O09-C05	2.66	1.48	1.42
24	B	613	AJP	C20-C15	-2.65	1.51	1.56
24	Q	105	AJP	C16-C11	-2.65	1.50	1.54
24	F	713	AJP	C12-C07	-2.64	1.50	1.56
24	D	613	AJP	C20-C15	-2.64	1.51	1.56
24	Q	107	AJP	C16-C11	-2.64	1.50	1.54
24	B	614	AJP	O09-C05	2.64	1.48	1.42
24	B	614	AJP	C16-C11	-2.64	1.50	1.54
24	D	609	AJP	C13-C12	-2.63	1.49	1.54
24	D	614	AJP	O09-C05	2.62	1.48	1.42
24	A	405	AJP	C20-C15	-2.62	1.51	1.56
24	F	711	AJP	C20-C19	-2.62	1.51	1.55
24	Q	106	AJP	C07-C08	-2.61	1.49	1.53
24	B	614	AJP	C12-C11	-2.61	1.50	1.56
24	B	611	AJP	C13-C12	-2.61	1.49	1.54
24	F	718	AJP	C07-C08	-2.61	1.49	1.53
24	B	609	AJP	O09-C05	2.60	1.48	1.42
24	C	201	AJP	C12-C11	-2.60	1.50	1.56
24	F	706	AJP	C07-C08	-2.59	1.49	1.53
24	Q	108	AJP	O09-C05	2.59	1.48	1.42
24	B	615	AJP	C12-C11	-2.57	1.50	1.56
24	F	718	AJP	C12-C11	-2.57	1.50	1.56
24	G	301	AJP	C12-C07	-2.57	1.50	1.56
24	F	708	AJP	C20-C15	-2.57	1.51	1.56
24	D	604	AJP	C21-C20	-2.57	1.50	1.54
24	Q	101	AJP	C12-C11	-2.57	1.50	1.56
24	D	612	AJP	C07-C08	-2.56	1.49	1.53
24	D	607	AJP	C12-C11	-2.56	1.50	1.56
21	F	701	BCR	C30-C25	-2.55	1.50	1.53
24	Q	104	AJP	C16-C11	-2.55	1.51	1.54
24	B	608	AJP	C12-C11	-2.55	1.50	1.56
24	C	202	AJP	C20-C15	-2.55	1.51	1.56
24	Q	107	AJP	C20-C15	-2.54	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	717	AJP	C12-C11	-2.54	1.50	1.56
24	Q	103	AJP	C20-C15	-2.54	1.51	1.56
24	B	616	AJP	O09-C05	2.54	1.48	1.42
24	B	612	AJP	C20-C15	-2.53	1.51	1.56
24	Q	103	AJP	C16-C11	-2.53	1.51	1.54
24	G	303	AJP	C12-C11	-2.53	1.50	1.56
24	D	610	AJP	C12-C07	-2.53	1.50	1.56
24	G	306	AJP	C20-C19	-2.53	1.51	1.55
24	D	607	AJP	C07-C08	-2.53	1.49	1.53
24	A	409	AJP	C20-C15	-2.52	1.51	1.56
24	F	713	AJP	C20-C15	-2.52	1.51	1.56
24	A	405	AJP	C13-C12	-2.52	1.49	1.54
24	D	609	AJP	C12-C11	-2.51	1.51	1.56
24	F	706	AJP	C20-C15	-2.51	1.51	1.56
24	B	609	AJP	C12-C11	-2.51	1.51	1.56
24	D	614	AJP	C20-C15	-2.51	1.51	1.56
24	B	614	AJP	C07-C08	-2.51	1.49	1.53
24	D	609	AJP	C20-C15	-2.50	1.51	1.56
24	Q	108	AJP	C12-C11	-2.50	1.51	1.56
24	B	608	AJP	C16-C11	-2.50	1.51	1.54
24	B	609	AJP	C20-C15	-2.50	1.51	1.56
24	D	609	AJP	C20-C19	-2.50	1.51	1.55
24	F	709	AJP	C20-C15	-2.49	1.51	1.56
24	D	611	AJP	O09-C05	2.49	1.48	1.42
24	D	610	AJP	C12-C11	-2.48	1.51	1.56
25	B	601	PQN	C10-C5	-2.48	1.36	1.40
24	F	717	AJP	C13-C12	-2.48	1.49	1.54
24	G	305	AJP	C20-C15	-2.47	1.51	1.56
24	Q	101	AJP	O09-C05	2.47	1.47	1.42
24	D	611	AJP	C12-C07	-2.47	1.51	1.56
24	F	707	AJP	C13-C12	-2.46	1.49	1.54
24	A	407	AJP	O09-C05	2.46	1.47	1.42
24	G	307	AJP	C12-C11	-2.46	1.51	1.56
24	Q	102	AJP	C21-C20	-2.46	1.50	1.54
24	D	604	AJP	C13-C12	-2.45	1.49	1.54
24	F	717	AJP	C07-C08	-2.45	1.49	1.53
24	D	606	AJP	C12-C07	-2.44	1.51	1.56
24	G	304	AJP	C12-C07	-2.43	1.51	1.56
24	B	615	AJP	C13-C12	-2.41	1.49	1.54
24	C	202	AJP	C21-C20	-2.41	1.50	1.54
24	Q	104	AJP	C12-C11	-2.40	1.51	1.56
24	D	605	AJP	C20-C15	-2.40	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	303	AJP	C07-C08	-2.40	1.49	1.53
24	F	714	AJP	C13-C12	-2.40	1.49	1.54
24	B	609	AJP	C12-C07	-2.40	1.51	1.56
24	G	302	AJP	C20-C15	-2.40	1.51	1.56
24	B	606	AJP	C24-C19	-2.40	1.49	1.53
24	B	611	AJP	C20-C19	-2.39	1.51	1.55
24	D	611	AJP	C12-C11	-2.39	1.51	1.56
24	Q	106	AJP	O09-C05	2.39	1.47	1.42
24	F	706	AJP	C12-C07	-2.39	1.51	1.56
24	D	605	AJP	O09-C05	2.39	1.47	1.42
24	B	613	AJP	C20-C19	-2.39	1.51	1.55
24	D	610	AJP	C07-C08	-2.38	1.49	1.53
24	B	613	AJP	C12-C07	-2.38	1.51	1.56
24	Q	103	AJP	C13-C12	-2.37	1.49	1.54
24	Q	105	AJP	O09-C05	2.37	1.47	1.42
24	D	613	AJP	C13-C12	-2.36	1.49	1.54
24	Q	107	AJP	O09-C05	2.36	1.47	1.42
24	B	608	AJP	C20-C15	-2.35	1.51	1.56
24	Q	103	AJP	O09-C05	2.35	1.47	1.42
24	B	617	AJP	C20-C15	-2.34	1.51	1.56
24	F	712	AJP	C07-C08	-2.34	1.49	1.53
24	F	715	AJP	C12-C11	-2.34	1.51	1.56
24	Q	108	AJP	C20-C19	-2.33	1.51	1.55
24	B	606	AJP	C20-C15	-2.33	1.51	1.56
24	G	307	AJP	C07-C08	-2.33	1.49	1.53
24	A	408	AJP	C13-C12	-2.32	1.50	1.54
24	A	408	AJP	O09-C05	2.32	1.47	1.42
24	Q	105	AJP	C12-C11	-2.31	1.51	1.56
24	A	408	AJP	C20-C19	-2.31	1.51	1.55
24	F	711	AJP	C20-C15	-2.31	1.51	1.56
24	Q	106	AJP	C12-C11	-2.31	1.51	1.56
24	F	712	AJP	C12-C11	-2.31	1.51	1.56
23	A	404	DGD	O2G-C2G	-2.31	1.40	1.46
24	Q	104	AJP	C12-C07	-2.30	1.51	1.56
24	G	302	AJP	O09-C05	2.29	1.47	1.42
24	A	408	AJP	C12-C07	-2.29	1.51	1.56
24	F	707	AJP	C21-C20	-2.29	1.50	1.54
23	A	403	DGD	O2G-C2G	-2.28	1.40	1.46
24	C	202	AJP	C20-C19	-2.28	1.51	1.55
24	E	201	AJP	C20-C15	-2.28	1.51	1.56
24	G	304	AJP	O09-C05	2.28	1.47	1.42
24	F	706	AJP	O09-C05	2.26	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	711	AJP	C13-C12	-2.26	1.50	1.54
24	Q	106	AJP	C16-C11	-2.26	1.51	1.54
24	D	605	AJP	C12-C07	-2.26	1.51	1.56
24	C	201	AJP	C20-C15	-2.25	1.52	1.56
24	D	607	AJP	C13-C12	-2.25	1.50	1.54
24	F	715	AJP	C07-C08	-2.25	1.49	1.53
24	F	718	AJP	C13-C12	-2.25	1.50	1.54
24	B	610	AJP	C20-C15	-2.24	1.52	1.56
24	B	615	AJP	C20-C15	-2.24	1.52	1.56
24	G	303	AJP	O09-C05	2.24	1.47	1.42
24	F	716	AJP	C21-C20	-2.24	1.50	1.54
24	D	609	AJP	C07-C08	-2.23	1.49	1.53
24	Q	105	AJP	C20-C15	-2.23	1.52	1.56
24	B	608	AJP	C12-C07	-2.22	1.51	1.56
24	D	608	AJP	C20-C15	-2.22	1.52	1.56
24	B	611	AJP	C12-C07	-2.22	1.51	1.56
24	D	611	AJP	C20-C19	-2.21	1.51	1.55
24	B	610	AJP	C20-C19	-2.21	1.51	1.55
24	C	202	AJP	C12-C07	-2.21	1.51	1.56
24	E	201	AJP	O09-C05	2.20	1.47	1.42
23	A	404	DGD	O1G-C1G	-2.20	1.40	1.45
24	G	306	AJP	C13-C12	-2.20	1.50	1.54
24	B	610	AJP	O09-C05	2.20	1.47	1.42
24	E	201	AJP	C12-C07	-2.19	1.51	1.56
24	Q	106	AJP	C20-C15	-2.18	1.52	1.56
24	G	307	AJP	C20-C19	-2.18	1.51	1.55
24	B	617	AJP	C12-C07	-2.18	1.51	1.56
24	G	304	AJP	C20-C19	-2.18	1.51	1.55
24	Q	108	AJP	C12-C07	-2.17	1.51	1.56
24	B	606	AJP	C12-C07	-2.16	1.51	1.56
24	D	603	AJP	C21-C20	-2.16	1.51	1.54
24	E	201	AJP	C20-C19	-2.16	1.51	1.55
24	B	614	AJP	C20-C15	-2.16	1.52	1.56
24	A	409	AJP	C13-C12	-2.15	1.50	1.54
24	D	606	AJP	C20-C19	-2.15	1.51	1.55
24	G	302	AJP	C12-C07	-2.15	1.51	1.56
23	A	403	DGD	O1G-C1G	-2.15	1.40	1.45
24	C	201	AJP	C21-C20	-2.14	1.51	1.54
24	F	708	AJP	C12-C07	-2.14	1.51	1.56
24	F	712	AJP	O09-C05	2.14	1.47	1.42
24	C	201	AJP	C13-C12	-2.14	1.50	1.54
24	A	407	AJP	C20-C19	-2.14	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	704	SQD	O2-C2	-2.14	1.37	1.43
24	C	202	AJP	C13-C12	-2.14	1.50	1.54
24	F	713	AJP	C20-C19	-2.14	1.51	1.55
24	G	307	AJP	C13-C12	-2.13	1.50	1.54
26	L	101	SQD	O2-C2	-2.13	1.38	1.43
24	F	709	AJP	C20-C19	-2.13	1.52	1.55
24	D	614	AJP	C12-C07	-2.13	1.51	1.56
24	D	612	AJP	C20-C19	-2.13	1.52	1.55
24	Q	104	AJP	C20-C19	-2.13	1.52	1.55
24	F	716	AJP	C12-C07	-2.13	1.51	1.56
26	F	705	SQD	O2-C2	-2.12	1.38	1.43
24	D	608	AJP	C20-C19	-2.12	1.52	1.55
24	G	305	AJP	C20-C19	-2.12	1.52	1.55
24	Q	101	AJP	C20-C19	-2.12	1.52	1.55
24	Q	101	AJP	C20-C15	-2.11	1.52	1.56
24	F	718	AJP	C20-C15	-2.11	1.52	1.56
24	B	610	AJP	C13-C12	-2.11	1.50	1.54
24	B	611	AJP	O09-C05	2.10	1.47	1.42
24	Q	107	AJP	C20-C19	-2.10	1.52	1.55
24	D	603	AJP	C12-C07	-2.10	1.51	1.56
22	A	402	LHG	O7-C5	-2.10	1.41	1.46
26	B	605	SQD	O2-C2	-2.10	1.38	1.43
22	D	602	LHG	O7-C5	-2.10	1.41	1.46
24	B	607	AJP	C20-C15	-2.10	1.52	1.56
24	F	707	AJP	C12-C07	-2.10	1.51	1.56
24	D	614	AJP	C13-C12	-2.10	1.50	1.54
24	D	612	AJP	C21-C20	-2.09	1.51	1.54
24	B	610	AJP	C12-C07	-2.09	1.51	1.56
24	B	617	AJP	O09-C05	2.09	1.47	1.42
24	Q	108	AJP	C20-C15	-2.09	1.52	1.56
24	Q	107	AJP	C12-C07	-2.08	1.51	1.56
24	B	608	AJP	O09-C05	2.08	1.47	1.42
24	F	715	AJP	C20-C15	-2.08	1.52	1.56
24	F	714	AJP	C21-C20	-2.07	1.51	1.54
24	D	608	AJP	O09-C05	2.07	1.47	1.42
24	G	303	AJP	C21-C20	-2.07	1.51	1.54
24	G	305	AJP	O09-C05	2.07	1.47	1.42
26	F	705	SQD	O4-C4	-2.07	1.38	1.43
24	F	708	AJP	C20-C19	-2.07	1.52	1.55
24	A	407	AJP	C12-C07	-2.06	1.51	1.56
24	F	715	AJP	C13-C12	-2.06	1.50	1.54
24	G	305	AJP	C12-C07	-2.06	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	201	AJP	C20-C19	-2.06	1.52	1.55
26	L	101	SQD	O3-C3	-2.06	1.38	1.43
24	G	304	AJP	C13-C12	-2.06	1.50	1.54
24	F	717	AJP	C12-C07	-2.06	1.51	1.56
24	F	711	AJP	C12-C07	-2.06	1.51	1.56
24	F	710	AJP	C20-C15	-2.06	1.52	1.56
22	D	601	LHG	O7-C5	-2.06	1.41	1.46
24	A	405	AJP	C20-C19	-2.06	1.52	1.55
26	F	705	SQD	O3-C3	-2.05	1.38	1.43
24	B	615	AJP	O09-C05	2.05	1.47	1.42
24	Q	101	AJP	C12-C07	-2.05	1.51	1.56
24	B	607	AJP	C12-C07	-2.05	1.51	1.56
24	B	614	AJP	C12-C07	-2.05	1.51	1.56
26	L	101	SQD	O4-C4	-2.05	1.38	1.43
24	G	305	AJP	C13-C12	-2.05	1.50	1.54
24	Q	102	AJP	C12-C07	-2.05	1.51	1.56
24	B	612	AJP	C12-C07	-2.03	1.52	1.56
26	F	704	SQD	O3-C3	-2.03	1.38	1.43
24	F	717	AJP	O09-C05	2.03	1.46	1.42
26	B	605	SQD	O3-C3	-2.03	1.38	1.43
24	B	609	AJP	C13-C12	-2.02	1.50	1.54
24	F	714	AJP	C20-C19	-2.02	1.52	1.55
24	D	609	AJP	O09-C05	2.02	1.46	1.42
24	B	616	AJP	C20-C19	-2.02	1.52	1.55
24	F	709	AJP	C13-C12	-2.02	1.50	1.54
26	B	605	SQD	O4-C4	-2.02	1.38	1.43
22	F	702	LHG	P-O6	2.01	1.67	1.59
24	G	303	AJP	C20-C19	-2.01	1.52	1.55
24	B	607	AJP	C20-C19	-2.01	1.52	1.55
24	Q	106	AJP	C12-C07	-2.01	1.52	1.56
22	F	703	LHG	P-O6	2.01	1.67	1.59
24	F	708	AJP	C13-C12	-2.00	1.50	1.54
24	B	616	AJP	C12-C07	-2.00	1.52	1.56

All (1197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	609	AJP	C12-C07-C08	-9.56	94.56	104.88
24	B	612	AJP	C12-C07-C08	-9.22	94.92	104.88
24	D	607	AJP	C12-C07-C08	-9.19	94.95	104.88
24	G	307	AJP	C12-C07-C08	-9.19	94.95	104.88
24	F	711	AJP	C12-C07-C08	-9.18	94.96	104.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	F	717	AJP	C12-C07-C08	-9.16	94.99	104.88
24	F	715	AJP	C12-C07-C08	-9.14	95.01	104.88
24	G	303	AJP	C12-C07-C08	-9.06	95.10	104.88
24	F	718	AJP	C12-C07-C08	-8.99	95.16	104.88
24	D	613	AJP	C12-C07-C08	-8.82	95.35	104.88
24	C	201	AJP	C12-C07-C08	-8.72	95.46	104.88
24	A	409	AJP	C12-C07-C08	-8.50	95.70	104.88
24	F	709	AJP	C12-C07-C08	-8.44	95.76	104.88
24	F	707	AJP	C12-C07-C08	-8.43	95.77	104.88
24	D	604	AJP	C12-C07-C08	-8.36	95.85	104.88
25	B	601	PQN	C11-C12-C13	-8.33	112.93	126.79
24	G	301	AJP	C12-C07-C08	-8.28	95.93	104.88
24	F	716	AJP	C12-C07-C08	-8.26	95.96	104.88
24	A	405	AJP	C12-C07-C08	-8.25	95.96	104.88
24	D	603	AJP	C12-C07-C08	-8.22	96.00	104.88
24	B	607	AJP	C12-C07-C08	-8.16	96.06	104.88
24	A	406	AJP	C12-C07-C08	-8.15	96.08	104.88
24	B	617	AJP	C12-C07-C08	-8.14	96.09	104.88
24	C	202	AJP	C12-C07-C08	-8.07	96.17	104.88
24	B	610	AJP	C12-C07-C08	-8.05	96.18	104.88
24	D	605	AJP	C12-C07-C08	-8.05	96.18	104.88
24	D	614	AJP	C12-C07-C08	-8.04	96.20	104.88
24	B	615	AJP	C12-C07-C08	-8.03	96.20	104.88
24	G	305	AJP	C12-C07-C08	-7.99	96.25	104.88
24	F	708	AJP	C12-C07-C08	-7.99	96.25	104.88
24	Q	102	AJP	C12-C07-C08	-7.98	96.26	104.88
24	B	614	AJP	C12-C07-C08	-7.96	96.28	104.88
24	F	714	AJP	C12-C07-C08	-7.95	96.29	104.88
24	B	608	AJP	C12-C07-C08	-7.92	96.32	104.88
24	D	612	AJP	C12-C07-C08	-7.92	96.32	104.88
24	B	606	AJP	C19-C24-C23	-7.91	105.73	114.46
24	Q	105	AJP	C12-C07-C08	-7.87	96.37	104.88
24	F	712	AJP	C12-C07-C08	-7.87	96.38	104.88
24	D	608	AJP	C12-C07-C08	-7.83	96.42	104.88
24	B	606	AJP	C12-C07-C08	-7.82	96.43	104.88
24	F	710	AJP	C12-C07-C08	-7.80	96.45	104.88
24	A	408	AJP	C12-C07-C08	-7.79	96.46	104.88
24	D	606	AJP	C12-C07-C08	-7.78	96.48	104.88
24	E	201	AJP	C12-C07-C08	-7.77	96.48	104.88
24	Q	107	AJP	C12-C07-C08	-7.76	96.50	104.88
24	F	706	AJP	C12-C07-C08	-7.74	96.51	104.88
24	G	306	AJP	C12-C07-C08	-7.71	96.55	104.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	304	AJP	C12-C07-C08	-7.70	96.56	104.88
24	B	611	AJP	C12-C07-C08	-7.66	96.60	104.88
24	G	302	AJP	C12-C07-C08	-7.63	96.64	104.88
24	Q	106	AJP	C12-C07-C08	-7.56	96.71	104.88
24	Q	104	AJP	C12-C07-C08	-7.56	96.71	104.88
24	Q	101	AJP	C12-C07-C08	-7.53	96.75	104.88
24	Q	103	AJP	C12-C07-C08	-7.45	96.83	104.88
24	B	609	AJP	C12-C07-C08	-7.42	96.87	104.88
24	B	613	AJP	C12-C07-C08	-7.40	96.88	104.88
24	B	611	AJP	C20-C15-C16	-7.33	104.72	112.42
24	B	616	AJP	C12-C07-C08	-7.33	96.97	104.88
24	D	610	AJP	C12-C07-C08	-7.15	97.15	104.88
24	Q	108	AJP	C12-C07-C08	-7.15	97.16	104.88
24	D	611	AJP	C12-C07-C08	-7.13	97.18	104.88
24	D	604	AJP	C20-C15-C16	-6.98	105.08	112.42
24	F	717	AJP	C20-C15-C16	-6.96	105.11	112.42
24	F	713	AJP	C12-C07-C08	-6.94	97.38	104.88
24	A	407	AJP	C12-C07-C08	-6.90	97.42	104.88
24	G	303	AJP	C20-C15-C16	-6.84	105.23	112.42
24	A	406	AJP	C19-C24-C23	-6.68	107.09	114.46
24	D	609	AJP	C19-C24-C23	-6.56	107.22	114.46
24	Q	102	AJP	C24-C19-C20	-6.46	105.80	112.66
24	D	608	AJP	C19-C24-C23	-6.33	107.48	114.46
24	B	606	AJP	C12-C11-C16	-6.18	104.94	113.82
24	F	710	AJP	C19-C24-C23	-6.16	107.67	114.46
24	F	712	AJP	C19-C24-C23	-6.14	107.68	114.46
24	D	609	AJP	C12-C11-C16	-6.10	105.07	113.82
24	F	715	AJP	C12-C11-C16	-6.10	105.07	113.82
24	D	613	AJP	C20-C15-C16	-6.00	106.12	112.42
25	B	601	PQN	C15-C13-C12	-5.98	109.01	121.12
24	A	407	AJP	C12-C11-C16	-5.98	105.24	113.82
24	D	612	AJP	C19-C24-C23	-5.94	107.91	114.46
24	F	708	AJP	C19-C24-C23	-5.90	107.95	114.46
24	F	711	AJP	C12-C11-C16	-5.90	105.35	113.82
24	D	606	AJP	C12-C11-C16	-5.89	105.37	113.82
24	D	605	AJP	C12-C11-C16	-5.87	105.40	113.82
24	A	407	AJP	C19-C24-C23	-5.84	108.01	114.46
24	D	607	AJP	C12-C11-C16	-5.78	105.52	113.82
24	Q	103	AJP	C12-C11-C16	-5.74	105.58	113.82
24	B	612	AJP	C20-C15-C16	-5.74	106.39	112.42
24	G	307	AJP	C12-C11-C16	-5.74	105.58	113.82
24	D	611	AJP	C19-C24-C23	-5.72	108.14	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	607	AJP	C12-C11-C16	-5.71	105.62	113.82
24	C	202	AJP	C12-C11-C16	-5.70	105.64	113.82
24	G	304	AJP	C19-C24-C23	-5.70	108.17	114.46
24	D	614	AJP	C12-C11-C16	-5.69	105.66	113.82
24	F	717	AJP	C12-C11-C16	-5.69	105.66	113.82
24	G	303	AJP	C12-C11-C16	-5.68	105.67	113.82
24	G	301	AJP	C19-C24-C23	-5.66	108.21	114.46
24	G	304	AJP	C12-C11-C16	-5.66	105.70	113.82
24	Q	106	AJP	C19-C24-C23	-5.64	108.23	114.46
24	E	201	AJP	C12-C11-C16	-5.64	105.73	113.82
24	G	301	AJP	C12-C11-C16	-5.62	105.75	113.82
24	Q	102	AJP	C12-C11-C16	-5.62	105.75	113.82
24	F	714	AJP	C12-C11-C16	-5.62	105.76	113.82
25	B	601	PQN	C14-C13-C12	-5.61	109.29	123.68
24	F	706	AJP	C12-C11-C16	-5.60	105.78	113.82
24	B	609	AJP	C05-C06-C07	-5.60	94.25	103.37
24	D	611	AJP	C05-C06-C07	-5.58	94.28	103.37
24	D	613	AJP	C12-C11-C16	-5.56	105.85	113.82
24	D	605	AJP	C19-C24-C23	-5.53	108.36	114.46
24	F	718	AJP	C19-C24-C23	-5.53	108.36	114.46
24	F	710	AJP	C12-C11-C16	-5.50	105.92	113.82
24	C	201	AJP	C12-C11-C16	-5.47	105.96	113.82
24	B	612	AJP	C12-C11-C16	-5.47	105.97	113.82
24	F	708	AJP	C12-C11-C16	-5.45	106.00	113.82
24	B	617	AJP	C12-C11-C16	-5.45	106.00	113.82
24	F	716	AJP	C20-C15-C16	-5.44	106.71	112.42
24	A	405	AJP	C12-C11-C16	-5.44	106.01	113.82
24	F	713	AJP	C12-C11-C16	-5.43	106.03	113.82
24	D	603	AJP	C20-C15-C16	-5.42	106.73	112.42
24	B	610	AJP	C12-C11-C16	-5.38	106.09	113.82
24	D	610	AJP	C05-C06-C07	-5.38	94.62	103.37
24	D	608	AJP	C12-C11-C16	-5.37	106.11	113.82
24	Q	108	AJP	C19-C24-C23	-5.32	108.59	114.46
24	F	713	AJP	C19-C24-C23	-5.31	108.60	114.46
24	G	305	AJP	C19-C24-C23	-5.29	108.62	114.46
24	F	713	AJP	C05-C06-C07	-5.29	94.76	103.37
24	B	613	AJP	C12-C11-C16	-5.28	106.24	113.82
24	Q	103	AJP	C19-C24-C23	-5.27	108.65	114.46
24	A	409	AJP	C20-C15-C16	-5.26	106.89	112.42
24	G	306	AJP	C12-C11-C16	-5.25	106.28	113.82
24	B	607	AJP	C19-C24-C23	-5.24	108.68	114.46
24	B	610	AJP	C19-C24-C23	-5.17	108.75	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	AJP	C20-C21-C22	-5.17	105.61	114.09
24	F	718	AJP	C20-C15-C16	-5.16	107.00	112.42
24	B	614	AJP	C12-C11-C16	-5.08	106.53	113.82
24	B	609	AJP	C12-C11-C16	-5.06	106.56	113.82
24	G	302	AJP	C19-C24-C23	-5.03	108.91	114.46
24	G	305	AJP	C12-C11-C16	-5.03	106.61	113.82
24	D	603	AJP	C12-C11-C16	-5.01	106.63	113.82
24	F	706	AJP	C19-C24-C23	-4.97	108.97	114.46
24	G	303	AJP	C24-C19-C20	-4.97	107.38	112.66
24	A	409	AJP	C12-C11-C16	-4.97	106.69	113.82
24	G	306	AJP	C19-C24-C23	-4.94	109.00	114.46
24	F	716	AJP	C12-C11-C16	-4.94	106.72	113.82
24	Q	107	AJP	C12-C11-C16	-4.94	106.73	113.82
24	D	612	AJP	C12-C11-C16	-4.94	106.73	113.82
24	Q	108	AJP	C12-C11-C16	-4.94	106.74	113.82
24	F	709	AJP	C20-C15-C16	-4.92	107.26	112.42
24	A	406	AJP	C12-C11-C16	-4.91	106.77	113.82
24	G	302	AJP	C12-C11-C16	-4.90	106.78	113.82
24	B	617	AJP	C19-C24-C23	-4.90	109.06	114.46
24	F	711	AJP	C19-C24-C23	-4.87	109.09	114.46
24	A	407	AJP	C05-C06-C07	-4.85	95.47	103.37
24	F	718	AJP	C12-C11-C16	-4.84	106.88	113.82
24	Q	101	AJP	C19-C24-C23	-4.80	109.16	114.46
24	G	301	AJP	C14-C13-C12	-4.80	104.54	112.78
24	A	407	AJP	C06-C07-C08	-4.78	95.64	104.34
24	B	608	AJP	C19-C24-C23	-4.75	109.22	114.46
24	C	202	AJP	C24-C19-C20	-4.74	107.62	112.66
24	A	408	AJP	C12-C11-C16	-4.74	107.02	113.82
24	D	604	AJP	C20-C21-C22	-4.71	106.37	114.09
24	A	408	AJP	C20-C15-C16	-4.70	107.49	112.42
24	Q	103	AJP	C20-C15-C16	-4.70	107.49	112.42
24	Q	101	AJP	C12-C11-C16	-4.68	107.10	113.82
24	B	616	AJP	C20-C15-C16	-4.66	107.53	112.42
24	D	607	AJP	C19-C24-C23	-4.66	109.32	114.46
24	B	616	AJP	C06-C07-C08	-4.64	95.90	104.34
24	Q	102	AJP	C20-C15-C16	-4.62	107.56	112.42
24	B	611	AJP	C12-C11-C16	-4.62	107.20	113.82
24	A	406	AJP	C06-C07-C08	-4.61	95.94	104.34
24	B	611	AJP	C06-C07-C08	-4.60	95.96	104.34
24	D	607	AJP	C20-C15-C16	-4.58	107.61	112.42
24	B	608	AJP	C12-C11-C16	-4.56	107.27	113.82
24	A	405	AJP	C20-C15-C16	-4.56	107.63	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	E	201	AJP	C19-C24-C23	-4.56	109.43	114.46
24	Q	108	AJP	C05-C06-C07	-4.54	95.99	103.37
24	B	615	AJP	C19-C24-C23	-4.53	109.46	114.46
24	F	714	AJP	C20-C15-C16	-4.52	107.67	112.42
24	F	715	AJP	C19-C24-C23	-4.52	109.47	114.46
24	B	614	AJP	C19-C24-C23	-4.50	109.49	114.46
24	D	608	AJP	C06-C07-C08	-4.47	96.20	104.34
24	D	612	AJP	C06-C07-C08	-4.46	96.21	104.34
24	C	202	AJP	C19-C24-C23	-4.46	109.54	114.46
24	G	307	AJP	C20-C15-C16	-4.44	107.75	112.42
24	C	202	AJP	C14-C15-C20	-4.42	108.82	113.91
24	B	612	AJP	C14-C13-C12	-4.42	105.21	112.78
23	A	403	DGD	O3G-C3G-C2G	-4.40	100.29	110.90
24	F	710	AJP	C06-C07-C08	-4.39	96.34	104.34
24	D	614	AJP	C20-C15-C16	-4.39	107.81	112.42
24	Q	104	AJP	C12-C11-C16	-4.38	107.53	113.82
24	B	612	AJP	C19-C24-C23	-4.36	109.65	114.46
24	A	405	AJP	C19-C24-C23	-4.34	109.68	114.46
24	D	614	AJP	C19-C24-C23	-4.33	109.68	114.46
24	Q	104	AJP	C19-C24-C23	-4.33	109.69	114.46
24	B	616	AJP	C05-C06-C07	-4.31	96.35	103.37
24	Q	102	AJP	C14-C15-C20	-4.31	108.94	113.91
24	C	201	AJP	C19-C24-C23	-4.30	109.72	114.46
24	Q	105	AJP	C19-C24-C23	-4.30	109.72	114.46
24	D	606	AJP	C14-C15-C20	-4.30	108.96	113.91
24	F	707	AJP	C12-C11-C16	-4.29	107.67	113.82
24	Q	101	AJP	C05-C06-C07	-4.29	96.39	103.37
26	L	101	SQD	O7-S-C6	4.28	112.03	106.94
24	B	616	AJP	C12-C11-C16	-4.28	107.68	113.82
24	B	616	AJP	C19-C24-C23	-4.27	109.75	114.46
24	F	709	AJP	C12-C11-C16	-4.26	107.70	113.82
24	F	712	AJP	C11-C12-C07	-4.26	92.91	100.19
24	G	306	AJP	C14-C15-C20	-4.25	109.02	113.91
24	B	611	AJP	C05-C06-C07	-4.24	96.46	103.37
24	F	717	AJP	C14-C13-C12	-4.24	105.51	112.78
24	D	609	AJP	C24-C19-C20	-4.24	108.16	112.66
24	Q	107	AJP	C19-C24-C23	-4.23	109.79	114.46
23	A	404	DGD	O3G-C3G-C2G	-4.22	100.70	110.90
24	A	407	AJP	C83-C06-C05	-4.22	107.22	114.92
22	A	402	LHG	O4-P-O5	4.21	133.05	112.24
22	D	601	LHG	O4-P-O5	4.20	132.98	112.24
22	F	702	LHG	O4-P-O5	4.20	132.98	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	602	LHG	O4-P-O5	4.19	132.98	112.24
22	F	703	LHG	O4-P-O5	4.19	132.98	112.24
24	Q	106	AJP	C12-C11-C16	-4.19	107.81	113.82
22	B	604	LHG	O4-P-O5	4.19	132.94	112.24
22	B	603	LHG	O4-P-O5	4.19	132.94	112.24
22	H	401	LHG	O4-P-O5	4.18	132.93	112.24
22	B	602	LHG	O4-P-O5	4.18	132.91	112.24
24	B	613	AJP	C05-C06-C07	-4.18	96.57	103.37
24	A	409	AJP	C19-C24-C23	-4.18	109.85	114.46
24	G	303	AJP	C14-C13-C12	-4.17	105.63	112.78
24	F	713	AJP	C06-C07-C08	-4.14	96.80	104.34
24	G	306	AJP	C24-C19-C20	-4.14	108.26	112.66
24	B	611	AJP	C14-C13-C12	-4.13	105.70	112.78
24	B	609	AJP	C83-C06-C05	-4.11	107.41	114.92
24	E	201	AJP	C05-C06-C07	-4.10	96.69	103.37
24	C	201	AJP	C24-C19-C20	-4.09	108.31	112.66
24	D	611	AJP	C11-C12-C07	-4.08	93.21	100.19
24	D	604	AJP	C12-C11-C16	-4.07	107.97	113.82
24	D	606	AJP	C19-C24-C23	-4.07	109.97	114.46
24	F	718	AJP	C14-C13-C12	-4.07	105.80	112.78
24	G	303	AJP	C14-C15-C20	-4.06	109.23	113.91
24	Q	106	AJP	C05-C06-C07	-4.06	96.76	103.37
24	Q	103	AJP	C06-C07-C08	-4.06	96.95	104.34
24	B	610	AJP	C14-C13-C12	-4.06	105.82	112.78
24	D	611	AJP	C12-C11-C16	-4.05	108.00	113.82
24	D	604	AJP	C85-O84-C05	-4.03	106.07	113.72
24	Q	107	AJP	C20-C15-C16	-4.03	108.18	112.42
24	B	609	AJP	C06-C07-C08	-4.03	97.00	104.34
24	B	615	AJP	C12-C11-C16	-4.02	108.05	113.82
24	D	607	AJP	C14-C15-C20	-4.01	109.29	113.91
24	D	603	AJP	C06-C07-C08	-4.01	97.04	104.34
24	Q	101	AJP	C06-C07-C08	-4.01	97.04	104.34
24	F	714	AJP	C14-C15-C20	-4.01	109.29	113.91
24	F	707	AJP	C19-C24-C23	-4.01	110.04	114.46
24	F	707	AJP	C20-C15-C16	-4.00	108.22	112.42
24	D	610	AJP	C19-C24-C23	-4.00	110.05	114.46
24	D	609	AJP	C14-C13-C12	-4.00	105.92	112.78
24	G	304	AJP	C14-C15-C20	-3.99	109.32	113.91
24	F	710	AJP	C05-C06-C07	-3.98	96.89	103.37
24	F	716	AJP	C06-C07-C08	-3.98	97.10	104.34
24	D	613	AJP	C14-C13-C12	-3.97	105.97	112.78
24	G	302	AJP	C06-C07-C08	-3.97	97.12	104.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	108	AJP	C06-C07-C08	-3.95	97.14	104.34
24	B	613	AJP	C19-C24-C23	-3.95	110.10	114.46
24	F	709	AJP	C06-C07-C08	-3.93	97.18	104.34
24	D	604	AJP	C06-C07-C08	-3.92	97.21	104.34
24	Q	105	AJP	C05-C06-C07	-3.92	96.99	103.37
24	F	715	AJP	C24-C19-C20	-3.92	108.50	112.66
26	F	705	SQD	O9-S-C6	3.92	111.59	106.94
24	Q	102	AJP	C19-C24-C23	-3.91	110.15	114.46
24	F	707	AJP	C24-C19-C20	-3.90	108.51	112.66
24	D	604	AJP	C21-C22-C23	-3.90	106.89	111.36
24	G	307	AJP	C24-C19-C20	-3.89	108.53	112.66
24	F	714	AJP	C14-C13-C12	-3.89	106.12	112.78
24	D	610	AJP	C11-C12-C07	-3.88	93.55	100.19
24	A	408	AJP	C14-C13-C12	-3.88	106.13	112.78
24	G	303	AJP	C20-C21-C22	-3.88	107.73	114.09
24	Q	102	AJP	C06-C07-C08	-3.87	97.29	104.34
24	D	612	AJP	C24-C19-C20	-3.87	108.55	112.66
24	F	713	AJP	C83-C06-C05	-3.87	107.86	114.92
26	F	704	SQD	O9-S-C6	3.86	111.53	106.94
24	A	408	AJP	C19-C24-C23	-3.85	110.21	114.46
24	D	608	AJP	C05-C06-C07	-3.85	97.11	103.37
24	E	201	AJP	C24-C19-C20	-3.84	108.58	112.66
26	F	705	SQD	O7-S-C6	3.84	111.51	106.94
24	D	604	AJP	C14-C13-C12	-3.84	106.19	112.78
26	F	704	SQD	O7-S-C6	3.84	111.50	106.94
24	F	709	AJP	C19-C24-C23	-3.83	110.24	114.46
24	F	707	AJP	C11-C12-C07	-3.83	93.65	100.19
24	Q	104	AJP	C05-C06-C07	-3.82	97.15	103.37
24	D	611	AJP	C83-C06-C05	-3.81	107.96	114.92
24	Q	105	AJP	C12-C11-C16	-3.80	108.36	113.82
26	B	605	SQD	O9-S-C6	3.80	111.46	106.94
26	B	605	SQD	O47-C7-C8	3.80	119.69	111.50
24	A	409	AJP	C14-C13-C12	-3.79	106.27	112.78
26	B	605	SQD	O7-S-C6	3.79	111.44	106.94
24	F	717	AJP	C19-C24-C23	-3.79	110.28	114.46
24	Q	104	AJP	C14-C13-C12	-3.79	106.29	112.78
26	L	101	SQD	O47-C7-C8	3.78	119.66	111.50
24	D	609	AJP	O09-C08-C10	3.78	117.96	110.17
24	F	712	AJP	C06-C07-C08	-3.77	97.47	104.34
24	B	615	AJP	C14-C13-C12	-3.77	106.32	112.78
24	B	616	AJP	C14-C15-C20	-3.76	109.58	113.91
24	Q	105	AJP	C06-C07-C08	-3.75	97.51	104.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	F	718	AJP	C06-C07-C08	-3.75	97.51	104.34
24	B	609	AJP	C14-C13-C12	-3.75	106.35	112.78
26	L	101	SQD	O9-S-O7	-3.75	100.98	113.95
24	D	610	AJP	C06-C07-C08	-3.75	97.52	104.34
24	B	615	AJP	C06-C07-C08	-3.74	97.54	104.34
24	B	608	AJP	C20-C15-C16	-3.74	108.50	112.42
24	G	307	AJP	C19-C24-C23	-3.72	110.35	114.46
24	G	302	AJP	C20-C15-C16	-3.72	108.51	112.42
24	D	609	AJP	C14-C15-C20	-3.72	109.63	113.91
24	E	201	AJP	C14-C15-C20	-3.71	109.64	113.91
24	F	711	AJP	C11-C16-C15	-3.70	102.77	109.23
24	F	708	AJP	C06-C07-C08	-3.70	97.61	104.34
24	A	405	AJP	C14-C13-C12	-3.70	106.44	112.78
24	G	301	AJP	C14-C15-C20	-3.69	109.66	113.91
24	D	614	AJP	C14-C13-C12	-3.68	106.46	112.78
24	A	408	AJP	C06-C07-C08	-3.68	97.65	104.34
24	B	615	AJP	C20-C15-C16	-3.67	108.56	112.42
24	A	405	AJP	C06-C07-C08	-3.67	97.66	104.34
26	F	704	SQD	O9-S-O7	-3.67	101.25	113.95
24	G	304	AJP	C05-C06-C07	-3.67	97.40	103.37
24	B	617	AJP	C21-C20-C19	3.66	111.27	107.14
24	B	608	AJP	C14-C13-C12	-3.65	106.52	112.78
24	C	202	AJP	C06-C07-C08	-3.65	97.70	104.34
26	B	605	SQD	O9-S-O7	-3.65	101.32	113.95
24	Q	105	AJP	C11-C12-C07	-3.65	93.96	100.19
24	F	714	AJP	C20-C21-C22	-3.64	108.11	114.09
24	F	711	AJP	O09-C08-C10	3.64	117.67	110.17
24	F	717	AJP	O09-C08-C10	3.64	117.66	110.17
26	F	705	SQD	O9-S-O7	-3.64	101.36	113.95
24	B	606	AJP	O09-C08-C10	3.64	117.65	110.17
24	D	611	AJP	C06-C07-C08	-3.63	97.73	104.34
24	B	609	AJP	C85-O84-C05	-3.62	106.85	113.72
26	F	705	SQD	O47-C7-C8	3.62	119.30	111.50
24	D	614	AJP	C05-C06-C07	-3.61	97.49	103.37
24	F	714	AJP	C19-C24-C23	-3.61	110.47	114.46
24	F	712	AJP	C12-C11-C16	-3.61	108.64	113.82
24	Q	106	AJP	C11-C12-C07	-3.60	94.04	100.19
24	B	607	AJP	C24-C19-C20	-3.60	108.84	112.66
24	B	609	AJP	C20-C15-C16	-3.59	108.65	112.42
24	F	714	AJP	C24-C19-C20	-3.59	108.85	112.66
24	Q	106	AJP	C06-C07-C08	-3.58	97.81	104.34
24	E	201	AJP	C06-C07-C08	-3.58	97.82	104.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	610	AJP	C12-C11-C16	-3.58	108.69	113.82
24	D	607	AJP	C24-C19-C20	-3.57	108.86	112.66
24	B	615	AJP	C11-C12-C07	-3.57	94.10	100.19
24	B	606	AJP	C06-C07-C08	-3.56	97.85	104.34
24	Q	103	AJP	C05-C06-C07	-3.56	97.57	103.37
24	D	610	AJP	C21-C22-C23	-3.56	107.28	111.36
24	Q	105	AJP	C20-C15-C16	-3.56	108.68	112.42
24	F	711	AJP	C06-C07-C08	-3.56	97.86	104.34
24	D	613	AJP	C19-C24-C23	-3.56	110.53	114.46
24	F	715	AJP	C20-C15-C16	-3.55	108.69	112.42
24	Q	108	AJP	C11-C12-C07	-3.55	94.12	100.19
24	D	604	AJP	C11-C12-C07	-3.55	94.12	100.19
24	B	613	AJP	C14-C15-C20	-3.55	109.83	113.91
24	A	408	AJP	C05-C06-C07	-3.55	97.60	103.37
24	B	617	AJP	C14-C13-C12	-3.54	106.70	112.78
24	B	616	AJP	C83-C06-C05	-3.54	108.45	114.92
24	G	307	AJP	C14-C13-C12	-3.54	106.71	112.78
24	D	603	AJP	C14-C13-C12	-3.54	106.71	112.78
24	G	305	AJP	C14-C15-C20	-3.53	109.84	113.91
24	B	616	AJP	C20-C21-C22	-3.53	108.30	114.09
24	B	612	AJP	O09-C08-C10	3.53	117.43	110.17
24	G	302	AJP	C05-C06-C07	-3.53	97.63	103.37
24	Q	103	AJP	C14-C13-C12	-3.53	106.73	112.78
24	D	612	AJP	C11-C12-C07	-3.52	94.17	100.19
24	C	201	AJP	C14-C15-C20	-3.52	109.86	113.91
24	G	304	AJP	C24-C19-C20	-3.51	108.93	112.66
24	B	610	AJP	C20-C15-C16	-3.51	108.73	112.42
24	F	706	AJP	C11-C12-C07	-3.51	94.19	100.19
24	B	608	AJP	O09-C08-C10	3.51	117.40	110.17
24	D	614	AJP	C20-C21-C22	-3.51	108.33	114.09
24	C	202	AJP	C05-C06-C07	-3.51	97.65	103.37
24	B	615	AJP	C05-C06-C07	-3.50	97.67	103.37
24	Q	104	AJP	C11-C12-C07	-3.50	94.21	100.19
24	D	606	AJP	C24-C19-C20	-3.50	108.94	112.66
24	F	716	AJP	C14-C13-C12	-3.50	106.79	112.78
24	Q	106	AJP	C14-C13-C12	-3.50	106.79	112.78
24	F	707	AJP	C14-C13-C12	-3.49	106.80	112.78
24	F	715	AJP	C14-C15-C20	-3.49	109.89	113.91
24	F	717	AJP	C14-C15-C20	-3.49	109.89	113.91
24	A	405	AJP	C14-C15-C20	-3.49	109.90	113.91
24	B	617	AJP	C20-C15-C16	-3.49	108.76	112.42
24	Q	104	AJP	O09-C08-C10	3.48	117.34	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	610	AJP	C20-C21-C22	-3.48	108.38	114.09
24	F	709	AJP	C20-C21-C22	-3.48	108.38	114.09
24	Q	105	AJP	C14-C13-C12	-3.48	106.82	112.78
24	B	613	AJP	C06-C07-C08	-3.48	98.01	104.34
24	B	606	AJP	C11-C12-C07	-3.47	94.26	100.19
24	B	611	AJP	C83-C06-C05	-3.46	108.59	114.92
24	Q	107	AJP	C14-C15-C20	-3.46	109.92	113.91
24	D	610	AJP	O09-C08-C10	3.46	117.30	110.17
24	F	718	AJP	O09-C08-C10	3.46	117.28	110.17
24	G	301	AJP	C21-C20-C19	3.45	111.02	107.14
24	D	603	AJP	C19-C24-C23	-3.44	110.66	114.46
24	D	603	AJP	C20-C21-C22	-3.44	108.44	114.09
24	B	607	AJP	C14-C15-C20	-3.44	109.95	113.91
26	F	704	SQD	O47-C7-C8	3.44	118.91	111.50
24	B	609	AJP	C19-C24-C23	-3.44	110.67	114.46
24	Q	101	AJP	C11-C12-C07	-3.43	94.33	100.19
24	F	710	AJP	C83-C06-C05	-3.43	108.66	114.92
24	Q	102	AJP	C20-C21-C22	-3.43	108.47	114.09
24	D	605	AJP	C21-C20-C19	3.42	110.99	107.14
24	F	707	AJP	C14-C15-C20	-3.41	109.98	113.91
24	G	305	AJP	C14-C13-C12	-3.41	106.93	112.78
24	C	201	AJP	C20-C15-C16	-3.41	108.84	112.42
24	D	607	AJP	C14-C13-C12	-3.41	106.93	112.78
24	G	301	AJP	O09-C08-C10	3.41	117.18	110.17
24	B	610	AJP	C06-C07-C08	-3.41	98.14	104.34
24	F	713	AJP	C14-C13-C12	-3.40	106.95	112.78
24	D	613	AJP	C20-C21-C22	-3.40	108.52	114.09
24	F	716	AJP	C20-C21-C22	-3.40	108.52	114.09
24	G	305	AJP	C11-C12-C07	-3.40	94.39	100.19
24	F	714	AJP	C05-C06-C07	-3.40	97.84	103.37
24	F	717	AJP	C20-C21-C22	-3.40	108.52	114.09
24	D	610	AJP	C21-C20-C19	3.40	110.97	107.14
24	F	715	AJP	C14-C13-C12	-3.39	106.97	112.78
24	Q	108	AJP	C83-C06-C05	-3.38	108.74	114.92
24	G	304	AJP	C14-C13-C12	-3.38	106.98	112.78
24	Q	107	AJP	C14-C13-C12	-3.38	106.99	112.78
24	A	407	AJP	C24-C19-C20	-3.37	109.07	112.66
24	Q	104	AJP	C14-C15-C20	-3.37	110.03	113.91
24	A	409	AJP	O09-C08-C10	3.37	117.11	110.17
24	G	306	AJP	C05-C06-C07	-3.37	97.89	103.37
24	F	716	AJP	C19-C24-C23	-3.37	110.75	114.46
24	D	608	AJP	C83-C06-C05	-3.36	108.78	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	606	AJP	C20-C15-C16	-3.36	108.89	112.42
24	A	409	AJP	C06-C07-C08	-3.36	98.23	104.34
24	Q	101	AJP	C83-C06-C05	-3.36	108.79	114.92
24	B	606	AJP	C24-C19-C20	-3.35	109.09	112.66
24	B	606	AJP	C11-C16-C15	-3.35	103.39	109.23
26	L	101	SQD	O9-S-C6	3.35	110.92	106.94
24	B	614	AJP	C20-C15-C16	-3.34	108.91	112.42
24	Q	103	AJP	C14-C15-C20	-3.34	110.06	113.91
24	F	716	AJP	C05-C06-C07	-3.34	97.93	103.37
24	B	613	AJP	O09-C08-C10	3.34	117.04	110.17
24	G	306	AJP	C14-C13-C12	-3.34	107.06	112.78
25	B	601	PQN	C14-C13-C15	-3.33	109.66	115.27
24	D	612	AJP	C05-C06-C07	-3.33	97.94	103.37
24	G	307	AJP	C06-C07-C08	-3.33	98.28	104.34
24	F	712	AJP	O09-C08-C10	3.33	117.02	110.17
24	D	603	AJP	C05-C06-C07	-3.32	97.96	103.37
24	G	305	AJP	C06-C07-C08	-3.32	98.29	104.34
24	Q	101	AJP	C24-C19-C20	-3.32	109.13	112.66
24	E	201	AJP	C83-C06-C05	-3.32	108.86	114.92
24	Q	103	AJP	C83-C06-C05	-3.32	108.86	114.92
24	B	608	AJP	C11-C12-C07	-3.32	94.53	100.19
24	G	304	AJP	C06-C07-C08	-3.31	98.31	104.34
24	D	606	AJP	O09-C08-C10	3.31	116.99	110.17
24	F	709	AJP	C14-C13-C12	-3.31	107.10	112.78
24	B	610	AJP	O09-C08-C10	3.31	116.98	110.17
24	F	714	AJP	C06-C07-C08	-3.31	98.32	104.34
24	Q	107	AJP	C20-C21-C22	-3.31	108.66	114.09
24	D	610	AJP	C20-C15-C16	-3.31	108.95	112.42
24	G	307	AJP	O09-C08-C10	3.31	116.98	110.17
24	D	610	AJP	C83-C06-C05	-3.31	108.88	114.92
24	G	305	AJP	O09-C08-C10	3.30	116.97	110.17
24	B	607	AJP	O09-C08-C10	3.30	116.97	110.17
24	Q	107	AJP	C06-C07-C08	-3.30	98.33	104.34
24	D	604	AJP	C21-C20-C19	3.30	110.86	107.14
24	Q	107	AJP	C05-C06-C07	-3.30	98.00	103.37
24	D	604	AJP	C05-C06-C07	-3.30	98.00	103.37
24	B	617	AJP	C06-C07-C08	-3.29	98.34	104.34
24	F	715	AJP	O09-C08-C10	3.29	116.95	110.17
24	D	614	AJP	C06-C07-C08	-3.29	98.34	104.34
24	B	614	AJP	C14-C13-C12	-3.29	107.14	112.78
24	D	606	AJP	C06-C07-C08	-3.28	98.36	104.34
24	A	408	AJP	C14-C15-C20	-3.28	110.13	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	302	AJP	C20-C21-C22	-3.28	108.72	114.09
24	D	608	AJP	C21-C20-C19	3.28	110.83	107.14
24	D	610	AJP	C14-C13-C12	-3.27	107.17	112.78
24	B	607	AJP	C06-C07-C08	-3.27	98.39	104.34
24	A	409	AJP	C20-C21-C22	-3.26	108.74	114.09
24	D	605	AJP	O09-C08-C10	3.26	116.88	110.17
24	G	306	AJP	C11-C12-C07	-3.26	94.62	100.19
24	G	306	AJP	O09-C08-C07	-3.26	96.24	104.06
24	D	613	AJP	C06-C07-C08	-3.25	98.42	104.34
24	D	607	AJP	O09-C08-C10	3.25	116.86	110.17
24	F	709	AJP	O09-C08-C10	3.25	116.86	110.17
24	Q	102	AJP	C05-C06-C07	-3.25	98.08	103.37
24	B	614	AJP	C05-C06-C07	-3.24	98.09	103.37
24	F	713	AJP	C14-C15-C20	-3.24	110.18	113.91
24	F	709	AJP	C11-C12-C07	-3.24	94.66	100.19
24	F	710	AJP	C20-C21-C22	-3.23	108.78	114.09
23	A	404	DGD	O6D-C1D-O3G	-3.23	102.32	109.97
24	B	612	AJP	C06-C07-C08	-3.23	98.46	104.34
24	D	613	AJP	C14-C15-C20	-3.23	110.19	113.91
26	B	605	SQD	C44-O6-C1	3.22	120.04	113.74
24	D	607	AJP	C06-C07-C08	-3.22	98.48	104.34
24	B	614	AJP	C06-C07-C08	-3.22	98.48	104.34
24	D	614	AJP	C14-C15-C20	-3.21	110.21	113.91
24	B	608	AJP	C06-C07-C08	-3.20	98.51	104.34
24	B	612	AJP	C20-C21-C22	-3.20	108.84	114.09
24	F	710	AJP	C85-O84-C05	-3.20	107.66	113.72
24	Q	105	AJP	C83-C06-C05	-3.19	109.09	114.92
24	G	301	AJP	C85-O84-C05	-3.19	107.68	113.72
24	D	605	AJP	C14-C13-C12	-3.19	107.32	112.78
24	G	302	AJP	C14-C13-C12	-3.19	107.32	112.78
24	C	201	AJP	C14-C13-C12	-3.18	107.32	112.78
24	A	409	AJP	C14-C15-C20	-3.18	110.24	113.91
24	B	609	AJP	C20-C21-C22	-3.18	108.87	114.09
24	Q	107	AJP	C11-C12-C07	-3.18	94.75	100.19
24	A	408	AJP	C11-C12-C07	-3.18	94.76	100.19
24	F	714	AJP	O09-C08-C10	3.18	116.71	110.17
24	G	302	AJP	C11-C12-C07	-3.18	94.76	100.19
24	B	610	AJP	C14-C15-C20	-3.17	110.26	113.91
24	Q	108	AJP	C14-C15-C20	-3.17	110.26	113.91
24	D	605	AJP	C14-C15-C20	-3.17	110.26	113.91
24	C	201	AJP	C06-C07-C08	-3.16	98.58	104.34
24	B	613	AJP	C11-C12-C07	-3.16	94.79	100.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	611	AJP	O09-C08-C10	3.16	116.67	110.17
23	A	403	DGD	O6D-C1D-O3G	-3.16	102.49	109.97
24	Q	106	AJP	C83-C06-C05	-3.15	109.16	114.92
24	G	303	AJP	O09-C08-C10	3.15	116.65	110.17
24	A	408	AJP	O09-C08-C10	3.15	116.65	110.17
24	F	708	AJP	C05-C06-C07	-3.15	98.25	103.37
24	G	306	AJP	C06-C07-C08	-3.15	98.61	104.34
24	B	614	AJP	C14-C15-C20	-3.14	110.29	113.91
24	F	707	AJP	O09-C08-C10	3.14	116.64	110.17
24	Q	101	AJP	C14-C15-C20	-3.14	110.30	113.91
24	F	708	AJP	C14-C13-C12	-3.14	107.40	112.78
24	D	606	AJP	C05-C06-C07	-3.13	98.27	103.37
24	B	616	AJP	O09-C08-C07	-3.13	96.55	104.06
24	D	611	AJP	C24-C19-C20	-3.13	109.33	112.66
24	Q	107	AJP	O09-C08-C10	3.13	116.61	110.17
24	Q	106	AJP	C21-C20-C19	3.12	110.66	107.14
24	B	615	AJP	C83-C06-C05	-3.12	109.22	114.92
24	G	302	AJP	C14-C15-C20	-3.12	110.32	113.91
24	G	306	AJP	O09-C08-C10	3.12	116.59	110.17
24	B	613	AJP	C11-C16-C15	-3.11	103.80	109.23
24	Q	104	AJP	C21-C20-C19	3.11	110.64	107.14
24	D	606	AJP	C20-C21-C22	-3.11	108.99	114.09
24	B	610	AJP	C05-C06-C07	-3.10	98.32	103.37
24	Q	102	AJP	C18-C17-C16	-3.10	107.03	112.14
24	B	611	AJP	O09-C08-C10	3.10	116.55	110.17
24	Q	103	AJP	C20-C21-C22	-3.10	109.00	114.09
24	B	615	AJP	C14-C15-C20	-3.10	110.34	113.91
24	B	616	AJP	O09-C08-C10	3.10	116.55	110.17
24	B	608	AJP	C14-C15-C20	-3.09	110.35	113.91
24	F	707	AJP	C06-C07-C08	-3.09	98.71	104.34
24	A	405	AJP	O09-C08-C10	3.08	116.52	110.17
24	Q	105	AJP	O09-C08-C10	3.08	116.51	110.17
24	G	305	AJP	C20-C15-C16	-3.08	109.19	112.42
24	F	710	AJP	C20-C15-C16	-3.08	109.19	112.42
24	B	616	AJP	C11-C12-C07	-3.08	94.94	100.19
24	F	713	AJP	O09-C08-C10	3.07	116.50	110.17
24	D	611	AJP	C14-C13-C12	-3.07	107.51	112.78
24	Q	105	AJP	C21-C20-C19	3.07	110.60	107.14
24	G	307	AJP	C20-C21-C22	-3.07	109.05	114.09
24	B	608	AJP	C21-C20-C19	3.07	110.60	107.14
24	B	607	AJP	C14-C13-C12	-3.07	107.52	112.78
24	E	201	AJP	C20-C15-C16	-3.07	109.20	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	F	708	AJP	C11-C12-C07	-3.06	94.96	100.19
24	F	711	AJP	C14-C13-C12	-3.06	107.54	112.78
24	B	615	AJP	C20-C21-C22	-3.06	109.07	114.09
23	A	403	DGD	O5D-C6D-C5D	-3.05	103.40	109.05
24	F	717	AJP	C21-C20-C19	3.05	110.58	107.14
24	F	712	AJP	C11-C16-C15	-3.04	103.92	109.23
24	G	305	AJP	C24-C19-C20	-3.04	109.42	112.66
24	B	606	AJP	O09-C08-C07	-3.04	96.76	104.06
24	D	603	AJP	C11-C12-C07	-3.04	95.00	100.19
24	B	614	AJP	O09-C08-C10	3.03	116.41	110.17
24	B	613	AJP	C83-C06-C05	-3.03	109.39	114.92
26	F	704	SQD	C44-O6-C1	3.03	119.66	113.74
24	B	609	AJP	C11-C12-C07	-3.03	95.02	100.19
24	G	303	AJP	C19-C24-C23	-3.02	111.12	114.46
24	B	606	AJP	C14-C15-C20	-3.02	110.43	113.91
24	B	617	AJP	O09-C08-C10	3.02	116.38	110.17
24	F	706	AJP	C14-C15-C20	-3.01	110.44	113.91
24	D	606	AJP	C11-C12-C07	-3.01	95.04	100.19
24	D	607	AJP	C20-C21-C22	-3.01	109.15	114.09
24	D	611	AJP	C14-C15-C20	-3.01	110.44	113.91
24	E	201	AJP	C85-O84-C05	-3.01	108.01	113.72
24	F	711	AJP	C14-C15-C20	-3.01	110.45	113.91
24	D	614	AJP	C21-C20-C19	3.01	110.53	107.14
24	B	609	AJP	C14-C15-C20	-3.00	110.45	113.91
24	A	405	AJP	C20-C21-C22	-3.00	109.17	114.09
24	D	606	AJP	C14-C13-C12	-2.99	107.64	112.78
24	G	302	AJP	C21-C20-C19	2.99	110.51	107.14
24	A	406	AJP	C11-C12-C07	-2.99	95.08	100.19
24	G	302	AJP	O09-C08-C10	2.99	116.31	110.17
24	A	406	AJP	C11-C16-C15	-2.99	104.02	109.23
24	B	614	AJP	C24-C19-C20	-2.98	109.49	112.66
24	F	709	AJP	O09-C08-C07	-2.98	96.90	104.06
24	B	610	AJP	C24-C19-C20	-2.98	109.49	112.66
24	C	201	AJP	C11-C12-C07	-2.98	95.11	100.19
24	D	611	AJP	C85-O84-C05	-2.98	108.08	113.72
24	F	706	AJP	O09-C08-C10	2.97	116.29	110.17
24	F	708	AJP	C14-C15-C20	-2.97	110.49	113.91
24	D	606	AJP	O09-C08-C07	-2.97	96.93	104.06
24	Q	108	AJP	C24-C19-C20	-2.97	109.50	112.66
24	F	716	AJP	C11-C12-C07	-2.97	95.12	100.19
24	B	617	AJP	C05-C06-C07	-2.96	98.55	103.37
24	Q	104	AJP	C20-C15-C16	-2.96	109.31	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407	AJP	C11-C16-C15	-2.96	104.06	109.23
24	B	613	AJP	C14-C13-C12	-2.96	107.71	112.78
24	A	408	AJP	C20-C21-C22	-2.96	109.24	114.09
24	Q	101	AJP	O09-C08-C10	2.96	116.25	110.17
24	D	603	AJP	C83-C06-C05	-2.95	109.53	114.92
24	A	408	AJP	C21-C20-C19	2.95	110.47	107.14
24	F	718	AJP	C21-C20-C19	2.95	110.47	107.14
24	D	612	AJP	C85-O84-C05	-2.95	108.12	113.72
24	G	301	AJP	C06-C07-C08	-2.95	98.97	104.34
24	Q	108	AJP	O09-C08-C10	2.95	116.25	110.17
24	C	201	AJP	O09-C08-C10	2.95	116.24	110.17
24	F	707	AJP	C20-C21-C22	-2.95	109.26	114.09
24	D	614	AJP	C83-C06-C05	-2.95	109.54	114.92
24	D	604	AJP	C19-C24-C23	-2.94	111.21	114.46
24	F	716	AJP	C83-C06-C05	-2.94	109.55	114.92
24	D	614	AJP	O09-C08-C10	2.94	116.23	110.17
24	B	614	AJP	C11-C12-C07	-2.94	95.16	100.19
24	G	302	AJP	C83-C06-C05	-2.94	109.55	114.92
24	A	406	AJP	C21-C20-C19	2.94	110.45	107.14
26	L	101	SQD	C44-O6-C1	2.94	119.48	113.74
24	B	610	AJP	C11-C12-C07	-2.93	95.18	100.19
24	F	706	AJP	C14-C13-C12	-2.93	107.76	112.78
24	D	605	AJP	C11-C12-C07	-2.93	95.19	100.19
24	F	706	AJP	C20-C21-C22	-2.92	109.29	114.09
24	D	609	AJP	C18-C17-C16	-2.92	107.33	112.14
24	G	307	AJP	C14-C15-C20	-2.92	110.55	113.91
24	B	609	AJP	O09-C08-C10	2.92	116.17	110.17
26	L	101	SQD	O8-S-C6	2.92	110.39	105.74
24	G	306	AJP	C85-O84-C05	-2.92	108.19	113.72
24	F	708	AJP	C21-C20-C19	2.91	110.42	107.14
24	F	713	AJP	C11-C12-C07	-2.91	95.22	100.19
24	Q	105	AJP	C20-C21-C22	-2.91	109.31	114.09
24	G	305	AJP	C05-C06-C07	-2.91	98.63	103.37
24	F	706	AJP	C05-C06-C07	-2.91	98.64	103.37
24	Q	104	AJP	C06-C07-C08	-2.90	99.06	104.34
24	A	406	AJP	O09-C08-C10	2.90	116.13	110.17
24	F	710	AJP	C11-C12-C07	-2.89	95.25	100.19
24	A	405	AJP	C05-C06-C07	-2.89	98.66	103.37
24	Q	107	AJP	C21-C20-C19	2.89	110.40	107.14
24	C	201	AJP	C20-C21-C22	-2.89	109.35	114.09
24	F	713	AJP	C21-C20-C19	2.89	110.39	107.14
24	E	201	AJP	C14-C13-C12	-2.88	107.83	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	AJP	C14-C15-C20	-2.88	110.59	113.91
24	B	606	AJP	C17-C18-C19	-2.88	106.06	111.84
24	Q	107	AJP	C24-C19-C20	-2.88	109.60	112.66
24	B	611	AJP	C21-C22-C23	-2.88	108.06	111.36
24	F	717	AJP	C06-C07-C08	-2.88	99.10	104.34
24	G	304	AJP	C83-C06-C05	-2.88	109.67	114.92
24	B	606	AJP	C05-C06-C07	-2.88	98.69	103.37
24	B	613	AJP	C20-C21-C22	-2.87	109.38	114.09
24	D	608	AJP	C11-C12-C07	-2.87	95.29	100.19
24	D	604	AJP	C83-C06-C05	-2.87	109.69	114.92
24	F	711	AJP	C24-C19-C20	-2.87	109.61	112.66
24	D	612	AJP	C83-C06-C05	-2.86	109.69	114.92
24	D	611	AJP	C04-C05-C06	-2.85	109.82	115.69
24	Q	106	AJP	O09-C08-C10	2.85	116.03	110.17
24	B	612	AJP	C24-C19-C20	-2.85	109.63	112.66
24	B	611	AJP	C14-C15-C20	-2.85	110.63	113.91
24	E	201	AJP	C11-C12-C07	-2.85	95.33	100.19
24	Q	108	AJP	O09-C08-C07	-2.85	97.24	104.06
24	Q	102	AJP	C83-C06-C05	-2.84	109.73	114.92
24	D	613	AJP	C05-C06-C07	-2.84	98.75	103.37
24	B	611	AJP	C21-C20-C19	2.84	110.34	107.14
24	B	607	AJP	C11-C12-C07	-2.83	95.36	100.19
21	P	101	BCR	C15-C14-C13	-2.83	123.27	127.31
24	A	407	AJP	C14-C15-C20	-2.83	110.65	113.91
24	C	202	AJP	C14-C13-C12	-2.83	107.94	112.78
24	F	710	AJP	C14-C15-C20	-2.82	110.66	113.91
24	B	609	AJP	C04-C05-C06	-2.82	109.88	115.69
24	F	708	AJP	O09-C08-C10	2.82	115.97	110.17
24	Q	102	AJP	O09-C08-C07	-2.82	97.30	104.06
24	F	717	AJP	C24-C19-C20	-2.81	109.67	112.66
24	F	709	AJP	C14-C15-C20	-2.80	110.68	113.91
24	D	613	AJP	C24-C19-C20	-2.80	109.68	112.66
24	B	612	AJP	C21-C20-C19	2.80	110.30	107.14
26	F	705	SQD	C44-O6-C1	2.80	119.20	113.74
24	F	706	AJP	C11-C16-C15	-2.79	104.35	109.23
24	B	614	AJP	C20-C21-C22	-2.79	109.51	114.09
24	D	609	AJP	C20-C15-C16	-2.79	109.49	112.42
24	B	617	AJP	C11-C12-C07	-2.79	95.43	100.19
24	F	716	AJP	C21-C20-C19	2.79	110.28	107.14
24	Q	104	AJP	C04-C05-C06	-2.78	109.97	115.69
24	A	405	AJP	C11-C12-C07	-2.78	95.44	100.19
24	G	301	AJP	C18-C19-C20	-2.78	107.31	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	F	706	AJP	C06-C07-C08	-2.78	99.28	104.34
26	F	704	SQD	O8-S-C6	2.78	110.17	105.74
24	D	608	AJP	O09-C08-C10	2.78	115.88	110.17
24	G	303	AJP	C18-C17-C16	-2.77	107.57	112.14
24	D	610	AJP	C14-C15-C20	-2.77	110.72	113.91
24	F	712	AJP	C05-C06-C07	-2.77	98.86	103.37
24	D	608	AJP	C20-C15-C16	-2.77	109.51	112.42
24	F	712	AJP	C21-C20-C19	2.77	110.25	107.14
23	A	403	DGD	CDB-CCB-CBB	-2.76	100.39	114.42
26	B	605	SQD	O8-S-C6	2.76	110.14	105.74
24	D	604	AJP	C18-C19-C20	-2.76	107.35	112.31
24	F	707	AJP	C05-C06-C07	-2.76	98.88	103.37
24	A	408	AJP	C83-C06-C05	-2.75	109.89	114.92
24	F	710	AJP	C14-C13-C12	-2.75	108.06	112.78
24	Q	101	AJP	C14-C13-C12	-2.75	108.06	112.78
24	F	709	AJP	C21-C20-C19	2.75	110.24	107.14
24	Q	106	AJP	C04-C05-C06	-2.75	110.04	115.69
24	A	406	AJP	C05-C06-C07	-2.75	98.90	103.37
24	Q	104	AJP	C83-C06-C05	-2.75	109.91	114.92
24	G	301	AJP	C05-C06-C07	-2.75	98.90	103.37
24	D	613	AJP	O09-C08-C10	2.74	115.81	110.17
24	Q	108	AJP	C11-C16-C15	-2.74	104.45	109.23
24	A	407	AJP	O09-C08-C10	2.74	115.81	110.17
24	A	407	AJP	C14-C13-C12	-2.74	108.09	112.78
24	F	718	AJP	C11-C12-C07	-2.74	95.52	100.19
24	Q	102	AJP	O09-C08-C10	2.73	115.79	110.17
24	B	611	AJP	O09-C08-C07	-2.73	97.51	104.06
24	G	304	AJP	C20-C15-C16	-2.73	109.55	112.42
24	G	305	AJP	C21-C20-C19	2.73	110.21	107.14
24	F	715	AJP	C06-C07-C08	-2.73	99.38	104.34
24	A	409	AJP	C11-C12-C07	-2.73	95.53	100.19
24	F	714	AJP	C83-C06-C05	-2.72	109.94	114.92
24	B	615	AJP	O09-C08-C10	2.72	115.78	110.17
24	B	608	AJP	O09-C08-C07	-2.72	97.53	104.06
24	Q	102	AJP	C14-C13-C12	-2.72	108.11	112.78
21	A	401	BCR	C15-C14-C13	-2.72	123.43	127.31
24	A	406	AJP	C24-C23-C22	-2.72	106.91	110.27
24	D	605	AJP	C11-C16-C15	-2.72	104.49	109.23
24	D	609	AJP	C04-C05-C06	-2.72	110.10	115.69
26	F	705	SQD	O8-S-C6	2.72	110.07	105.74
23	A	404	DGD	CDB-CCB-CBB	-2.71	100.65	114.42
24	D	614	AJP	C21-C22-C23	-2.71	108.25	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	302	AJP	C85-O84-C05	-2.71	108.58	113.72
21	A	401	BCR	C24-C23-C22	-2.71	122.14	126.23
22	F	702	LHG	O8-C23-C24	2.70	120.39	111.91
24	Q	101	AJP	C04-C05-C06	-2.70	110.13	115.69
24	C	202	AJP	C20-C15-C16	-2.70	109.58	112.42
24	D	612	AJP	O09-C08-C10	2.70	115.73	110.17
24	D	613	AJP	C85-O84-C05	-2.70	108.60	113.72
24	F	708	AJP	C85-O84-C05	-2.70	108.60	113.72
22	D	601	LHG	O8-C23-C24	2.70	120.37	111.91
24	D	610	AJP	C17-C16-C11	-2.70	108.40	112.32
24	D	605	AJP	C06-C07-C08	-2.70	99.43	104.34
24	C	202	AJP	C83-C06-C05	-2.69	110.00	114.92
24	B	608	AJP	C05-C06-C07	-2.69	98.99	103.37
24	F	710	AJP	O09-C08-C10	2.69	115.71	110.17
24	F	711	AJP	C04-C05-C06	-2.69	110.16	115.69
24	B	611	AJP	C17-C16-C15	-2.69	107.16	110.49
24	E	201	AJP	O09-C08-C10	2.69	115.70	110.17
24	Q	103	AJP	C21-C20-C19	2.69	110.17	107.14
24	B	616	AJP	C14-C13-C12	-2.69	108.17	112.78
24	G	301	AJP	C24-C19-C20	-2.69	109.81	112.66
24	D	608	AJP	C14-C13-C12	-2.68	108.18	112.78
24	D	609	AJP	C06-C07-C08	-2.68	99.46	104.34
24	C	201	AJP	C18-C17-C16	-2.68	107.72	112.14
24	D	612	AJP	C20-C21-C22	-2.67	109.70	114.09
24	D	603	AJP	C21-C20-C19	2.67	110.14	107.14
21	P	101	BCR	C24-C23-C22	-2.67	122.20	126.23
24	C	202	AJP	O09-C08-C10	2.67	115.66	110.17
24	D	608	AJP	C85-O84-C05	-2.66	108.67	113.72
24	D	613	AJP	C83-C06-C05	-2.66	110.06	114.92
24	B	617	AJP	C14-C15-C20	-2.66	110.85	113.91
24	D	608	AJP	C24-C23-C22	-2.65	106.98	110.27
21	F	701	BCR	C24-C23-C22	-2.65	122.22	126.23
24	A	405	AJP	C83-C06-C05	-2.65	110.08	114.92
24	G	301	AJP	C11-C16-C15	-2.65	104.61	109.23
24	A	405	AJP	C24-C19-C20	-2.65	109.84	112.66
24	F	713	AJP	C24-C19-C20	-2.65	109.85	112.66
24	C	202	AJP	O09-C08-C07	-2.64	97.72	104.06
24	B	607	AJP	C20-C15-C16	-2.64	109.64	112.42
24	B	606	AJP	C18-C17-C16	-2.64	107.79	112.14
24	F	714	AJP	C11-C12-C07	-2.64	95.69	100.19
24	F	706	AJP	C85-O84-C05	-2.63	108.73	113.72
24	F	718	AJP	C20-C21-C22	-2.63	109.77	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	605	AJP	C05-C06-C07	-2.63	99.09	103.37
24	F	718	AJP	C24-C19-C20	-2.62	109.87	112.66
24	B	614	AJP	C83-C06-C05	-2.62	110.13	114.92
24	Q	105	AJP	C14-C15-C20	-2.62	110.89	113.91
24	D	612	AJP	C18-C17-C16	-2.62	107.82	112.14
24	A	409	AJP	C24-C19-C20	-2.62	109.87	112.66
24	G	304	AJP	C11-C12-C07	-2.62	95.71	100.19
22	D	602	LHG	O8-C23-C24	2.62	120.13	111.91
24	D	613	AJP	C21-C20-C19	2.62	110.09	107.14
24	D	611	AJP	C11-C16-C15	-2.62	104.66	109.23
24	G	304	AJP	O09-C08-C10	2.62	115.56	110.17
22	B	603	LHG	O8-C23-C24	2.62	120.12	111.91
24	Q	105	AJP	C04-C05-C06	-2.61	110.31	115.69
24	B	607	AJP	C05-C06-C07	-2.61	99.12	103.37
24	F	712	AJP	C04-C05-C06	-2.61	110.32	115.69
24	G	304	AJP	O09-C08-C07	-2.61	97.80	104.06
24	D	610	AJP	C18-C19-C20	-2.61	107.62	112.31
24	B	613	AJP	C04-C05-C06	-2.61	110.33	115.69
24	Q	106	AJP	C14-C15-C20	-2.61	110.91	113.91
25	B	601	PQN	C2M-C2-C3	-2.60	120.15	124.40
24	Q	107	AJP	O09-C08-C07	-2.60	97.82	104.06
24	Q	103	AJP	O09-C08-C07	-2.60	97.82	104.06
22	A	402	LHG	O8-C23-C24	2.60	120.06	111.91
22	F	703	LHG	O8-C23-C24	2.60	120.06	111.91
24	G	303	AJP	C17-C16-C15	-2.60	107.27	110.49
24	A	407	AJP	C18-C17-C16	-2.60	107.86	112.14
24	G	301	AJP	C11-C12-C07	-2.59	95.76	100.19
24	D	607	AJP	O09-C08-C07	-2.59	97.84	104.06
24	Q	102	AJP	C15-C20-C19	2.59	112.22	108.58
24	D	606	AJP	C85-O84-C05	-2.59	108.81	113.72
24	G	307	AJP	C04-C05-C06	-2.59	110.36	115.69
24	F	710	AJP	C21-C20-C19	2.59	110.06	107.14
24	C	202	AJP	C11-C12-C07	-2.59	95.77	100.19
24	F	716	AJP	C14-C15-C20	-2.59	110.93	113.91
24	Q	102	AJP	C11-C12-C07	-2.58	95.78	100.19
24	D	603	AJP	C21-C22-C23	-2.58	108.40	111.36
24	F	709	AJP	C05-C06-C07	-2.58	99.17	103.37
24	F	714	AJP	C04-C05-C06	-2.58	110.39	115.69
24	B	608	AJP	C24-C19-C20	-2.58	109.92	112.66
22	B	604	LHG	O8-C23-C24	2.57	119.99	111.91
24	B	613	AJP	O09-C08-C07	-2.57	97.89	104.06
24	F	711	AJP	O09-C08-C07	-2.57	97.89	104.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	302	AJP	C21-C22-C23	-2.57	108.42	111.36
24	F	713	AJP	O09-C08-C07	-2.57	97.91	104.06
24	F	708	AJP	C20-C15-C16	-2.57	109.73	112.42
24	B	613	AJP	C24-C19-C20	-2.56	109.93	112.66
24	G	304	AJP	C21-C20-C19	2.56	110.03	107.14
22	F	702	LHG	C11-C10-C9	-2.56	101.42	114.42
24	D	603	AJP	C14-C15-C20	-2.56	110.96	113.91
24	F	715	AJP	C11-C12-C07	-2.56	95.81	100.19
24	D	607	AJP	C11-C12-C07	-2.56	95.82	100.19
24	Q	107	AJP	C21-C22-C23	-2.56	108.43	111.36
24	F	710	AJP	C04-C05-C06	-2.56	110.43	115.69
24	B	607	AJP	O09-C08-C07	-2.55	97.93	104.06
24	B	607	AJP	C20-C21-C22	-2.55	109.90	114.09
24	F	710	AJP	C21-C22-C23	-2.55	108.43	111.36
24	F	715	AJP	C20-C21-C22	-2.55	109.91	114.09
26	L	101	SQD	O48-C23-C24	2.55	119.89	111.91
22	H	401	LHG	C11-C10-C9	-2.54	101.50	114.42
24	F	718	AJP	C14-C15-C20	-2.54	110.98	113.91
24	G	303	AJP	C06-C07-C08	-2.54	99.72	104.34
24	A	409	AJP	C21-C20-C19	2.54	110.00	107.14
24	F	717	AJP	C04-C05-C06	-2.54	110.47	115.69
24	D	613	AJP	C11-C12-C07	-2.54	95.85	100.19
24	Q	104	AJP	C20-C21-C22	-2.54	109.93	114.09
24	A	406	AJP	C18-C19-C20	-2.54	107.75	112.31
24	D	610	AJP	C11-C16-C15	-2.54	104.80	109.23
24	A	407	AJP	C85-O84-C05	-2.54	108.91	113.72
24	D	612	AJP	C14-C15-C20	-2.53	111.00	113.91
24	G	301	AJP	C20-C15-C16	-2.53	109.77	112.42
24	G	302	AJP	O09-C08-C07	-2.53	98.00	104.06
24	A	409	AJP	C85-O84-C05	-2.53	108.93	113.72
24	Q	107	AJP	C83-C06-C05	-2.52	110.31	114.92
24	B	612	AJP	O09-C08-C07	-2.52	98.00	104.06
24	D	605	AJP	C20-C21-C22	-2.52	109.95	114.09
24	F	715	AJP	C04-C05-C06	-2.52	110.50	115.69
24	A	407	AJP	C04-C05-C06	-2.52	110.50	115.69
24	B	610	AJP	C83-C06-C05	-2.52	110.32	114.92
21	F	701	BCR	C15-C14-C13	-2.52	123.72	127.31
24	B	613	AJP	C21-C20-C19	2.52	109.97	107.14
24	Q	101	AJP	O09-C08-C07	-2.51	98.03	104.06
24	F	708	AJP	O09-C08-C07	-2.51	98.04	104.06
24	F	716	AJP	C21-C22-C23	-2.51	108.48	111.36
24	Q	103	AJP	C21-C22-C23	-2.51	108.49	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	602	LHG	C11-C10-C9	-2.51	101.70	114.42
24	B	613	AJP	C21-C22-C23	-2.50	108.49	111.36
24	D	612	AJP	C11-C16-C15	-2.50	104.86	109.23
24	Q	103	AJP	C24-C19-C20	-2.50	110.00	112.66
24	D	612	AJP	O09-C08-C07	-2.50	98.06	104.06
24	C	202	AJP	C18-C17-C16	-2.50	108.02	112.14
26	L	101	SQD	O5-C5-C4	2.50	114.23	109.69
24	Q	101	AJP	C20-C15-C16	-2.50	109.80	112.42
24	A	409	AJP	C05-C06-C07	-2.50	99.30	103.37
24	F	712	AJP	C17-C16-C11	-2.50	108.69	112.32
24	D	607	AJP	C04-C05-C06	-2.50	110.55	115.69
22	H	401	LHG	O8-C23-C24	2.50	119.74	111.91
24	B	615	AJP	C24-C19-C20	-2.50	110.01	112.66
24	A	406	AJP	C83-C06-C05	-2.50	110.36	114.92
24	D	608	AJP	C14-C15-C20	-2.50	111.04	113.91
26	F	705	SQD	O48-C23-C24	2.49	119.74	111.91
24	F	708	AJP	C83-C06-C05	-2.49	110.37	114.92
24	B	616	AJP	C21-C20-C19	2.49	109.94	107.14
21	P	101	BCR	C33-C5-C6	-2.49	121.73	124.53
24	Q	108	AJP	C14-C13-C12	-2.49	108.52	112.78
24	D	604	AJP	O09-C08-C10	2.48	115.28	110.17
21	A	401	BCR	C33-C5-C6	-2.48	121.74	124.53
24	A	406	AJP	O09-C08-C07	-2.48	98.11	104.06
22	D	602	LHG	C11-C10-C9	-2.48	101.83	114.42
24	A	407	AJP	O09-C08-C07	-2.48	98.11	104.06
24	Q	103	AJP	C18-C17-C16	-2.48	108.06	112.14
24	Q	105	AJP	C21-C22-C23	-2.47	108.52	111.36
24	A	407	AJP	C11-C12-C07	-2.47	95.96	100.19
24	B	617	AJP	C20-C21-C22	-2.47	110.03	114.09
24	G	302	AJP	C04-C05-C06	-2.47	110.61	115.69
24	F	715	AJP	C18-C17-C16	-2.47	108.07	112.14
22	A	402	LHG	C11-C10-C9	-2.47	101.88	114.42
24	B	617	AJP	C83-C06-C05	-2.47	110.41	114.92
24	G	307	AJP	C11-C12-C07	-2.47	95.97	100.19
24	E	201	AJP	C20-C21-C22	-2.47	110.04	114.09
24	G	302	AJP	C24-C19-C20	-2.46	110.04	112.66
24	B	617	AJP	O09-C08-C07	-2.46	98.15	104.06
24	F	706	AJP	O09-C08-C07	-2.46	98.16	104.06
22	D	601	LHG	C11-C10-C9	-2.46	101.94	114.42
24	F	709	AJP	C21-C22-C23	-2.46	108.54	111.36
24	Q	108	AJP	O84-C85-C02	-2.46	108.64	112.18
24	A	408	AJP	C24-C19-C20	-2.46	110.05	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	107	AJP	C04-C05-C06	-2.46	110.64	115.69
24	G	307	AJP	C18-C17-C16	-2.45	108.10	112.14
24	G	301	AJP	O09-C08-C07	-2.45	98.18	104.06
24	G	305	AJP	O09-C08-C07	-2.45	98.18	104.06
22	B	602	LHG	O8-C23-C24	2.45	119.59	111.91
24	B	610	AJP	O09-C08-C07	-2.45	98.19	104.06
24	B	614	AJP	C04-C05-C06	-2.44	110.67	115.69
24	D	608	AJP	C18-C19-C20	-2.44	107.93	112.31
24	B	612	AJP	C21-C22-C23	-2.44	108.56	111.36
24	D	614	AJP	C11-C12-C07	-2.44	96.03	100.19
24	B	616	AJP	C21-C22-C23	-2.44	108.57	111.36
24	A	409	AJP	C04-C05-C06	-2.43	110.69	115.69
24	F	711	AJP	C83-C06-C05	-2.43	110.48	114.92
24	F	717	AJP	C17-C16-C15	-2.43	107.48	110.49
24	F	718	AJP	C04-C05-C06	-2.43	110.70	115.69
24	D	611	AJP	O09-C08-C07	-2.43	98.24	104.06
22	B	602	LHG	C20-C19-C18	-2.43	102.11	114.42
24	G	305	AJP	C04-C05-C06	-2.43	110.70	115.69
22	A	402	LHG	C20-C19-C18	-2.42	102.11	114.42
22	B	604	LHG	C11-C10-C9	-2.42	102.12	114.42
24	Q	103	AJP	O09-C08-C10	2.42	115.16	110.17
24	F	709	AJP	C83-C06-C05	-2.42	110.50	114.92
24	D	614	AJP	C04-C05-C06	-2.42	110.71	115.69
24	B	613	AJP	C85-O84-C05	-2.42	109.13	113.72
24	B	609	AJP	C24-C19-C20	-2.42	110.09	112.66
24	D	607	AJP	C18-C17-C16	-2.42	108.16	112.14
24	C	202	AJP	C85-O84-C05	-2.42	109.14	113.72
24	F	709	AJP	C24-C19-C20	-2.42	110.09	112.66
24	A	408	AJP	O09-C08-C07	-2.42	98.27	104.06
26	F	705	SQD	O5-C5-C4	2.42	114.08	109.69
26	B	605	SQD	O5-C5-C4	2.41	114.08	109.69
24	Q	101	AJP	C85-O84-C05	-2.41	109.14	113.72
23	A	404	DGD	C3G-C2G-C1G	-2.41	106.09	111.79
21	P	101	BCR	C27-C26-C25	2.41	126.23	122.73
24	C	201	AJP	C05-C06-C07	-2.40	99.46	103.37
24	F	710	AJP	C24-C23-C22	-2.40	107.30	110.27
24	D	609	AJP	C11-C12-C07	-2.40	96.09	100.19
24	D	605	AJP	O09-C08-C07	-2.40	98.30	104.06
22	B	603	LHG	C11-C10-C9	-2.40	102.26	114.42
24	Q	106	AJP	C11-C16-C15	-2.40	105.05	109.23
24	E	201	AJP	O09-C08-C07	-2.40	98.31	104.06
24	F	712	AJP	O09-C08-C07	-2.39	98.32	104.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	102	AJP	C85-O84-C05	-2.39	109.18	113.72
22	F	703	LHG	C20-C19-C18	-2.39	102.28	114.42
26	B	605	SQD	O48-C23-C24	2.39	119.41	111.91
24	F	713	AJP	C04-C05-C06	-2.39	110.78	115.69
24	A	406	AJP	C17-C16-C11	-2.39	108.85	112.32
24	G	303	AJP	C04-C05-C06	-2.38	110.79	115.69
24	F	706	AJP	C04-C05-C06	-2.38	110.80	115.69
24	A	408	AJP	C04-C05-C06	-2.38	110.80	115.69
24	B	608	AJP	C04-C05-C06	-2.38	110.80	115.69
24	B	612	AJP	C04-C05-C06	-2.38	110.80	115.69
24	F	708	AJP	C04-C05-C06	-2.37	110.81	115.69
22	F	703	LHG	C11-C10-C9	-2.37	102.37	114.42
24	F	711	AJP	C11-C12-C07	-2.37	96.14	100.19
24	G	306	AJP	C11-C16-C15	-2.37	105.09	109.23
24	D	604	AJP	C17-C16-C11	-2.37	108.88	112.32
24	F	707	AJP	O09-C08-C07	-2.37	98.38	104.06
24	F	717	AJP	C21-C22-C23	-2.37	108.65	111.36
22	H	401	LHG	C20-C19-C18	-2.36	102.42	114.42
24	G	306	AJP	C21-C20-C19	2.36	109.80	107.14
22	B	603	LHG	C20-C19-C18	-2.36	102.43	114.42
22	D	601	LHG	C20-C19-C18	-2.36	102.43	114.42
24	D	610	AJP	C04-C05-C06	-2.36	110.84	115.69
24	G	306	AJP	C83-C06-C05	-2.36	110.61	114.92
24	B	606	AJP	C04-C05-C06	-2.36	110.84	115.69
24	B	606	AJP	C14-C15-C16	-2.36	108.36	111.75
26	F	704	SQD	O5-C5-C4	2.36	113.97	109.69
22	B	604	LHG	C20-C19-C18	-2.35	102.49	114.42
24	G	303	AJP	C11-C12-C07	-2.35	96.17	100.19
24	B	608	AJP	C20-C21-C22	-2.35	110.24	114.09
24	G	304	AJP	C11-C16-C15	-2.35	105.13	109.23
24	B	612	AJP	C17-C16-C15	-2.35	107.58	110.49
26	F	704	SQD	O6-C1-C2	2.35	111.97	108.30
24	B	617	AJP	C04-C05-C06	-2.34	110.87	115.69
24	D	607	AJP	C05-C06-C07	-2.34	99.56	103.37
24	Q	108	AJP	C04-C05-C06	-2.34	110.87	115.69
24	D	606	AJP	C83-C06-C05	-2.34	110.65	114.92
24	F	709	AJP	C04-C05-C06	-2.34	110.88	115.69
24	B	610	AJP	C20-C21-C22	-2.34	110.25	114.09
21	F	701	BCR	C33-C5-C6	-2.34	121.90	124.53
24	A	405	AJP	C21-C20-C19	2.34	109.77	107.14
24	A	408	AJP	C18-C19-C20	-2.33	108.11	112.31
24	B	614	AJP	O09-C08-C07	-2.33	98.46	104.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	608	AJP	C04-C05-C06	-2.33	110.89	115.69
24	B	617	AJP	C21-C22-C23	-2.33	108.69	111.36
24	C	202	AJP	C04-C05-C06	-2.33	110.89	115.69
24	D	614	AJP	C85-O84-C05	-2.33	109.30	113.72
24	G	306	AJP	C03-C02-C85	2.33	111.80	108.56
24	G	305	AJP	C85-O84-C05	-2.33	109.31	113.72
24	A	405	AJP	O09-C08-C07	-2.33	98.48	104.06
24	Q	104	AJP	O09-C08-C07	-2.32	98.49	104.06
24	C	201	AJP	C83-C06-C05	-2.32	110.67	114.92
24	Q	106	AJP	O84-C85-C02	-2.32	108.84	112.18
22	F	702	LHG	C20-C19-C18	-2.32	102.65	114.42
23	A	403	DGD	C3G-C2G-C1G	-2.32	106.31	111.79
26	L	101	SQD	O6-C1-C2	2.32	111.92	108.30
22	D	602	LHG	C20-C19-C18	-2.32	102.67	114.42
24	C	201	AJP	C04-C05-C06	-2.31	110.93	115.69
24	F	712	AJP	C83-C06-C05	-2.31	110.69	114.92
24	B	612	AJP	C83-C06-C05	-2.31	110.70	114.92
24	G	305	AJP	C83-C06-C05	-2.31	110.70	114.92
24	F	707	AJP	C83-C06-C05	-2.31	110.70	114.92
24	D	613	AJP	O84-C05-C04	-2.31	108.62	110.77
24	F	706	AJP	C24-C19-C20	-2.31	110.20	112.66
24	D	608	AJP	O09-C08-C07	-2.31	98.53	104.06
24	A	408	AJP	C21-C22-C23	-2.31	108.72	111.36
24	D	608	AJP	C11-C16-C15	-2.31	105.20	109.23
23	A	403	DGD	C3D-C4D-C5D	-2.31	106.12	110.24
24	D	604	AJP	C14-C15-C20	-2.30	111.26	113.91
21	A	401	BCR	C15-C16-C17	-2.30	118.75	123.47
24	D	605	AJP	C83-C06-C05	-2.30	110.71	114.92
24	B	613	AJP	C18-C19-C20	-2.30	108.17	112.31
24	F	707	AJP	C04-C05-C06	-2.30	110.96	115.69
24	B	615	AJP	C04-C05-C06	-2.30	110.97	115.69
24	B	616	AJP	C24-C19-C20	-2.29	110.22	112.66
24	B	607	AJP	C18-C17-C16	-2.29	108.36	112.14
24	Q	101	AJP	C20-C21-C22	-2.29	110.33	114.09
24	B	617	AJP	O84-C85-C02	-2.29	108.88	112.18
26	F	704	SQD	O48-C23-C24	2.29	119.09	111.91
24	F	717	AJP	O09-C08-C07	-2.29	98.57	104.06
24	B	611	AJP	C04-C05-C06	-2.29	110.98	115.69
24	B	606	AJP	C14-C13-C12	-2.29	108.86	112.78
24	Q	106	AJP	O09-C08-C07	-2.29	98.58	104.06
24	D	612	AJP	C14-C13-C12	-2.28	108.86	112.78
24	G	303	AJP	C05-C06-C07	-2.28	99.66	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	DGD	O2D-C2D-C1D	-2.28	104.52	110.05
24	B	607	AJP	C83-C06-C05	-2.28	110.76	114.92
24	B	610	AJP	C04-C05-C06	-2.27	111.02	115.69
24	F	718	AJP	C83-C06-C05	-2.27	110.77	114.92
24	E	201	AJP	C18-C17-C16	-2.27	108.40	112.14
24	D	605	AJP	C21-C22-C23	-2.27	108.76	111.36
24	A	409	AJP	O09-C08-C07	-2.27	98.62	104.06
24	D	613	AJP	C21-C22-C23	-2.27	108.76	111.36
24	D	610	AJP	O09-C08-C07	-2.27	98.62	104.06
24	G	301	AJP	C04-C05-C06	-2.26	111.03	115.69
24	D	605	AJP	C04-C05-C06	-2.26	111.04	115.69
24	F	716	AJP	C17-C16-C11	-2.26	109.03	112.32
24	F	713	AJP	C20-C21-C22	-2.26	110.38	114.09
24	D	605	AJP	C20-C15-C16	-2.26	110.05	112.42
22	H	401	LHG	C18-C17-C16	-2.26	102.95	114.42
24	B	609	AJP	O09-C08-C07	-2.26	98.64	104.06
24	B	616	AJP	C04-C05-C06	-2.26	111.05	115.69
23	A	404	DGD	O5D-C6D-C5D	-2.26	104.87	109.05
24	D	607	AJP	C21-C20-C19	2.25	109.68	107.14
23	A	404	DGD	CFB-CEB-CDB	-2.25	102.99	114.42
23	A	404	DGD	C3D-C4D-C5D	-2.25	106.22	110.24
22	B	603	LHG	C18-C17-C16	-2.25	103.00	114.42
24	F	706	AJP	C03-C02-C85	2.25	111.69	108.56
24	F	711	AJP	C18-C19-C20	-2.25	108.27	112.31
24	D	603	AJP	C17-C16-C11	-2.25	109.05	112.32
24	D	603	AJP	C18-C19-C20	-2.25	108.27	112.31
21	P	101	BCR	C15-C16-C17	-2.24	118.88	123.47
24	D	605	AJP	C18-C19-C20	-2.24	108.29	112.31
24	D	603	AJP	C24-C19-C18	-2.24	107.64	111.74
24	F	713	AJP	C11-C16-C15	-2.24	105.33	109.23
24	A	406	AJP	C17-C18-C19	-2.23	107.36	111.84
23	A	403	DGD	CFB-CEB-CDB	-2.23	103.09	114.42
24	F	711	AJP	C04-C03-C02	-2.23	107.10	111.81
24	A	409	AJP	C17-C16-C15	-2.23	107.72	110.49
22	D	601	LHG	C18-C17-C16	-2.23	103.10	114.42
24	A	409	AJP	C83-C06-C05	-2.23	110.86	114.92
22	B	604	LHG	C27-C26-C25	-2.22	103.13	114.42
22	A	402	LHG	C18-C17-C16	-2.22	103.13	114.42
21	F	701	BCR	C11-C10-C9	-2.22	124.14	127.31
24	G	304	AJP	C85-O84-C05	-2.22	109.50	113.72
24	A	406	AJP	C14-C13-C12	-2.22	108.97	112.78
24	F	712	AJP	C14-C13-C12	-2.22	108.97	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	202	AJP	C20-C21-C22	-2.22	110.45	114.09
22	B	604	LHG	C18-C17-C16	-2.22	103.18	114.42
24	B	607	AJP	C04-C05-C06	-2.22	111.14	115.69
24	G	304	AJP	C04-C05-C06	-2.22	111.14	115.69
24	F	718	AJP	C05-C06-C07	-2.21	99.77	103.37
22	F	702	LHG	C18-C17-C16	-2.21	103.19	114.42
24	F	708	AJP	C18-C19-C20	-2.21	108.33	112.31
22	D	601	LHG	C27-C26-C25	-2.21	103.20	114.42
24	F	716	AJP	C18-C19-C20	-2.21	108.33	112.31
24	F	712	AJP	C18-C19-C20	-2.21	108.34	112.31
21	A	401	BCR	C27-C26-C25	2.21	125.94	122.73
24	F	713	AJP	C20-C15-C16	-2.21	110.10	112.42
24	G	301	AJP	C83-C06-C05	-2.21	110.89	114.92
24	B	615	AJP	O09-C08-C07	-2.20	98.78	104.06
24	D	614	AJP	O09-C08-C07	-2.20	98.78	104.06
24	F	716	AJP	O09-C08-C10	2.20	114.69	110.17
22	D	602	LHG	C18-C17-C16	-2.20	103.27	114.42
24	Q	108	AJP	C21-C20-C19	2.20	109.61	107.14
24	B	608	AJP	C83-C06-C05	-2.20	110.91	114.92
24	B	612	AJP	C11-C12-C07	-2.19	96.44	100.19
22	H	401	LHG	C27-C26-C25	-2.19	103.29	114.42
24	Q	105	AJP	O09-C08-C07	-2.19	98.80	104.06
24	F	706	AJP	C83-C06-C05	-2.19	110.91	114.92
24	G	303	AJP	C83-C06-C05	-2.19	110.92	114.92
24	F	708	AJP	C11-C16-C15	-2.19	105.41	109.23
22	B	602	LHG	C18-C17-C16	-2.19	103.31	114.42
24	F	710	AJP	O09-C08-C07	-2.19	98.81	104.06
22	F	703	LHG	C27-C26-C25	-2.19	103.32	114.42
24	B	610	AJP	C18-C17-C16	-2.19	108.54	112.14
24	C	201	AJP	O09-C08-C07	-2.19	98.82	104.06
24	F	716	AJP	C24-C19-C18	-2.18	107.73	111.74
23	A	403	DGD	CBB-CAB-C9B	-2.18	103.34	114.42
24	D	603	AJP	O09-C08-C10	2.18	114.66	110.17
24	F	718	AJP	O09-C08-C07	-2.18	98.83	104.06
24	F	717	AJP	C11-C12-C07	-2.18	96.46	100.19
22	B	602	LHG	C27-C26-C25	-2.18	103.35	114.42
26	F	705	SQD	C1-O5-C5	2.18	117.96	113.69
24	B	611	AJP	C11-C12-C07	-2.18	96.47	100.19
23	A	404	DGD	CBB-CAB-C9B	-2.17	103.40	114.42
24	F	715	AJP	C83-C06-C05	-2.17	110.95	114.92
24	F	717	AJP	C83-C06-C05	-2.17	110.95	114.92
22	A	402	LHG	C27-C26-C25	-2.17	103.42	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	406	AJP	C04-C05-C06	-2.16	111.24	115.69
24	F	716	AJP	O09-C08-C07	-2.16	98.88	104.06
24	F	707	AJP	C81-C12-C07	2.16	116.89	111.63
22	F	702	LHG	C27-C26-C25	-2.16	103.47	114.42
24	B	609	AJP	C21-C20-C19	2.16	109.57	107.14
22	D	602	LHG	C27-C26-C25	-2.16	103.48	114.42
24	D	606	AJP	C18-C17-C16	-2.16	108.59	112.14
24	D	611	AJP	C17-C16-C11	-2.16	109.19	112.32
24	F	711	AJP	C20-C21-C22	-2.16	110.55	114.09
24	F	708	AJP	C20-C21-C22	-2.15	110.56	114.09
24	Q	105	AJP	C18-C19-C20	-2.15	108.45	112.31
24	B	616	AJP	C17-C16-C11	-2.15	109.20	112.32
22	F	703	LHG	C18-C17-C16	-2.15	103.53	114.42
24	G	305	AJP	C20-C21-C22	-2.15	110.57	114.09
24	G	307	AJP	C83-C06-C05	-2.15	111.00	114.92
24	G	306	AJP	C04-C05-C06	-2.14	111.28	115.69
24	G	306	AJP	C20-C21-C22	-2.14	110.57	114.09
24	B	606	AJP	C21-C20-C19	2.14	109.55	107.14
24	D	606	AJP	C04-C05-C06	-2.14	111.29	115.69
24	A	406	AJP	C03-C04-C05	-2.14	108.23	111.93
24	B	617	AJP	C18-C19-C20	-2.14	108.47	112.31
24	F	715	AJP	O09-C08-C07	-2.14	98.93	104.06
24	D	603	AJP	O09-C08-C07	-2.14	98.93	104.06
24	D	604	AJP	O09-C08-C07	-2.14	98.94	104.06
22	B	603	LHG	C27-C26-C25	-2.13	103.60	114.42
24	F	709	AJP	C04-C03-C02	-2.13	107.31	111.81
24	B	607	AJP	C85-O84-C05	-2.13	109.67	113.72
24	D	607	AJP	C83-C06-C05	-2.13	111.03	114.92
24	F	714	AJP	C18-C17-C16	-2.13	108.63	112.14
24	G	304	AJP	C20-C21-C22	-2.13	110.60	114.09
24	F	717	AJP	C05-C06-C07	-2.13	99.91	103.37
24	B	615	AJP	C21-C20-C19	2.12	109.53	107.14
24	D	609	AJP	C83-C06-C05	-2.12	111.05	114.92
24	D	606	AJP	C21-C20-C19	2.12	109.53	107.14
24	Q	104	AJP	C24-C19-C20	-2.12	110.41	112.66
24	F	716	AJP	C24-C19-C20	-2.11	110.41	112.66
24	G	307	AJP	O09-C08-C07	-2.11	99.00	104.06
24	Q	104	AJP	C85-O84-C05	-2.11	109.72	113.72
24	Q	107	AJP	C85-O84-C05	-2.11	109.72	113.72
24	A	406	AJP	O84-C85-C02	-2.10	109.15	112.18
24	B	612	AJP	C05-C06-C07	-2.10	99.95	103.37
24	D	603	AJP	C24-C19-C20	-2.10	110.43	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	613	AJP	C03-C04-C05	-2.10	108.31	111.93
24	A	407	AJP	C17-C18-C19	-2.09	107.64	111.84
24	F	707	AJP	C24-C19-C18	-2.09	107.90	111.74
24	E	201	AJP	C04-C05-C06	-2.09	111.39	115.69
24	Q	103	AJP	C04-C05-C06	-2.09	111.39	115.69
24	F	714	AJP	O84-C85-C02	-2.09	109.17	112.18
23	A	404	DGD	C5B-C4B-C3B	-2.09	103.81	114.42
24	D	612	AJP	C14-C15-C16	-2.09	108.74	111.75
24	F	711	AJP	C17-C18-C19	-2.09	107.65	111.84
23	A	403	DGD	CAB-C9B-C8B	-2.09	103.82	114.42
24	G	306	AJP	C81-C12-C07	2.09	116.71	111.63
24	F	714	AJP	O09-C08-C07	-2.09	99.06	104.06
25	B	601	PQN	C2M-C2-C1	2.09	119.73	116.27
24	Q	103	AJP	C11-C12-C07	-2.08	96.63	100.19
24	G	301	AJP	C24-C23-C22	-2.08	107.69	110.27
24	B	614	AJP	C21-C20-C19	2.08	109.48	107.14
23	A	404	DGD	CAB-C9B-C8B	-2.08	103.88	114.42
24	F	708	AJP	C24-C19-C20	-2.08	110.45	112.66
23	A	403	DGD	O6E-C1E-O5D	-2.07	105.06	109.97
24	A	408	AJP	C85-O84-C05	-2.07	109.78	113.72
24	D	614	AJP	C24-C19-C20	-2.07	110.46	112.66
26	B	605	SQD	O6-C1-C2	2.07	111.53	108.30
24	Q	104	AJP	C18-C19-C20	-2.06	108.60	112.31
24	F	712	AJP	C85-O84-C05	-2.06	109.81	113.72
24	B	611	AJP	C24-C19-C18	-2.06	107.96	111.74
24	D	608	AJP	C21-C22-C23	-2.06	109.00	111.36
24	F	706	AJP	C21-C20-C19	2.06	109.46	107.14
24	D	604	AJP	C24-C19-C18	-2.06	107.96	111.74
24	B	611	AJP	C85-O84-C05	-2.06	109.81	113.72
23	A	403	DGD	O2D-C2D-C1D	-2.06	105.04	110.05
24	F	710	AJP	C03-C02-C85	2.05	111.41	108.56
24	D	610	AJP	O84-C85-C02	-2.05	109.23	112.18
24	F	707	AJP	C17-C16-C11	-2.05	109.34	112.32
24	Q	106	AJP	C24-C19-C20	-2.04	110.49	112.66
24	B	606	AJP	C83-C06-C05	-2.03	111.20	114.92
24	Q	102	AJP	C17-C16-C15	-2.03	107.97	110.49
24	A	405	AJP	C04-C05-C06	-2.03	111.51	115.69
24	F	713	AJP	C18-C19-C20	-2.03	108.66	112.31
24	Q	104	AJP	C21-C22-C23	-2.03	109.03	111.36
24	F	706	AJP	C20-C15-C16	-2.03	110.29	112.42
24	D	613	AJP	C04-C05-C06	-2.03	111.52	115.69
26	L	101	SQD	C4-C3-C2	2.03	114.36	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	612	AJP	C04-C05-C06	-2.03	111.53	115.69
24	D	604	AJP	C04-C05-C06	-2.02	111.53	115.69
23	A	403	DGD	C5B-C4B-C3B	-2.02	104.14	114.42
24	B	606	AJP	C81-C12-C07	2.02	116.56	111.63
21	F	701	BCR	C27-C26-C25	2.02	125.67	122.73
21	F	701	BCR	C28-C27-C26	-2.02	110.46	114.08
24	F	714	AJP	C85-O84-C05	-2.02	109.88	113.72
24	D	610	AJP	C24-C23-C22	-2.02	107.77	110.27
24	G	301	AJP	C03-C02-C85	2.02	111.36	108.56
24	Q	106	AJP	C18-C19-C20	-2.01	108.69	112.31
24	D	603	AJP	O84-C85-C02	-2.01	109.28	112.18
24	F	709	AJP	C17-C16-C11	-2.01	109.40	112.32
24	B	611	AJP	C24-C19-C20	-2.01	110.52	112.66
24	G	304	AJP	C18-C17-C16	-2.01	108.83	112.14
24	F	709	AJP	C18-C19-C20	-2.01	108.70	112.31
24	A	409	AJP	C21-C22-C23	-2.01	109.06	111.36

All (720) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	AJP	C12
24	A	405	AJP	C20
24	A	405	AJP	C23
24	A	405	AJP	C11
24	A	405	AJP	C16
24	A	405	AJP	C22
24	A	405	AJP	C10
24	A	405	AJP	C02
24	A	405	AJP	C19
24	A	405	AJP	C05
24	A	405	AJP	C15
24	A	405	AJP	C07
24	A	406	AJP	C12
24	A	406	AJP	C20
24	A	406	AJP	C23
24	A	406	AJP	C11
24	A	406	AJP	C16
24	A	406	AJP	C22
24	A	406	AJP	C10
24	A	406	AJP	C02
24	A	406	AJP	C19
24	A	406	AJP	C05

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Mol	Chain	Res	Type	Atom
24	A	406	AJP	C15
24	A	406	AJP	C07
24	A	407	AJP	C12
24	A	407	AJP	C20
24	A	407	AJP	C23
24	A	407	AJP	C11
24	A	407	AJP	C16
24	A	407	AJP	C22
24	A	407	AJP	C10
24	A	407	AJP	C02
24	A	407	AJP	C19
24	A	407	AJP	C05
24	A	407	AJP	C15
24	A	407	AJP	C07
24	A	408	AJP	C12
24	A	408	AJP	C20
24	A	408	AJP	C23
24	A	408	AJP	C11
24	A	408	AJP	C16
24	A	408	AJP	C22
24	A	408	AJP	C10
24	A	408	AJP	C02
24	A	408	AJP	C19
24	A	408	AJP	C05
24	A	408	AJP	C15
24	A	408	AJP	C07
24	A	409	AJP	C12
24	A	409	AJP	C20
24	A	409	AJP	C23
24	A	409	AJP	C11
24	A	409	AJP	C16
24	A	409	AJP	C22
24	A	409	AJP	C10
24	A	409	AJP	C02
24	A	409	AJP	C19
24	A	409	AJP	C05
24	A	409	AJP	C15
24	A	409	AJP	C07
24	B	606	AJP	C12
24	B	606	AJP	C20
24	B	606	AJP	C23
24	B	606	AJP	C11

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Mol	Chain	Res	Type	Atom
24	B	606	AJP	C16
24	B	606	AJP	C22
24	B	606	AJP	C10
24	B	606	AJP	C02
24	B	606	AJP	C19
24	B	606	AJP	C05
24	B	606	AJP	C15
24	B	606	AJP	C07
24	B	607	AJP	C12
24	B	607	AJP	C20
24	B	607	AJP	C23
24	B	607	AJP	C11
24	B	607	AJP	C16
24	B	607	AJP	C22
24	B	607	AJP	C10
24	B	607	AJP	C02
24	B	607	AJP	C19
24	B	607	AJP	C05
24	B	607	AJP	C15
24	B	607	AJP	C07
24	B	608	AJP	C12
24	B	608	AJP	C20
24	B	608	AJP	C23
24	B	608	AJP	C11
24	B	608	AJP	C16
24	B	608	AJP	C22
24	B	608	AJP	C10
24	B	608	AJP	C02
24	B	608	AJP	C19
24	B	608	AJP	C05
24	B	608	AJP	C15
24	B	608	AJP	C07
24	B	609	AJP	C12
24	B	609	AJP	C20
24	B	609	AJP	C23
24	B	609	AJP	C11
24	B	609	AJP	C16
24	B	609	AJP	C22
24	B	609	AJP	C10
24	B	609	AJP	C02
24	B	609	AJP	C19
24	B	609	AJP	C05

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Mol	Chain	Res	Type	Atom
24	B	609	AJP	C15
24	B	609	AJP	C07
24	B	610	AJP	C12
24	B	610	AJP	C20
24	B	610	AJP	C23
24	B	610	AJP	C11
24	B	610	AJP	C16
24	B	610	AJP	C22
24	B	610	AJP	C10
24	B	610	AJP	C02
24	B	610	AJP	C19
24	B	610	AJP	C05
24	B	610	AJP	C15
24	B	610	AJP	C07
24	B	611	AJP	C12
24	B	611	AJP	C20
24	B	611	AJP	C23
24	B	611	AJP	C11
24	B	611	AJP	C16
24	B	611	AJP	C22
24	B	611	AJP	C10
24	B	611	AJP	C02
24	B	611	AJP	C19
24	B	611	AJP	C05
24	B	611	AJP	C15
24	B	611	AJP	C07
24	B	612	AJP	C12
24	B	612	AJP	C20
24	B	612	AJP	C23
24	B	612	AJP	C11
24	B	612	AJP	C16
24	B	612	AJP	C22
24	B	612	AJP	C10
24	B	612	AJP	C02
24	B	612	AJP	C19
24	B	612	AJP	C05
24	B	612	AJP	C15
24	B	612	AJP	C07
24	B	613	AJP	C12
24	B	613	AJP	C20
24	B	613	AJP	C23
24	B	613	AJP	C11

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Mol	Chain	Res	Type	Atom
24	B	613	AJP	C16
24	B	613	AJP	C22
24	B	613	AJP	C10
24	B	613	AJP	C02
24	B	613	AJP	C19
24	B	613	AJP	C05
24	B	613	AJP	C15
24	B	613	AJP	C07
24	B	614	AJP	C12
24	B	614	AJP	C20
24	B	614	AJP	C23
24	B	614	AJP	C11
24	B	614	AJP	C16
24	B	614	AJP	C22
24	B	614	AJP	C10
24	B	614	AJP	C02
24	B	614	AJP	C19
24	B	614	AJP	C05
24	B	614	AJP	C15
24	B	614	AJP	C07
24	B	615	AJP	C12
24	B	615	AJP	C20
24	B	615	AJP	C23
24	B	615	AJP	C11
24	B	615	AJP	C16
24	B	615	AJP	C22
24	B	615	AJP	C10
24	B	615	AJP	C02
24	B	615	AJP	C19
24	B	615	AJP	C05
24	B	615	AJP	C15
24	B	615	AJP	C07
24	B	616	AJP	C12
24	B	616	AJP	C20
24	B	616	AJP	C23
24	B	616	AJP	C11
24	B	616	AJP	C16
24	B	616	AJP	C22
24	B	616	AJP	C10
24	B	616	AJP	C02
24	B	616	AJP	C19
24	B	616	AJP	C05

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Mol	Chain	Res	Type	Atom
24	B	616	AJP	C15
24	B	616	AJP	C07
24	B	617	AJP	C12
24	B	617	AJP	C20
24	B	617	AJP	C23
24	B	617	AJP	C11
24	B	617	AJP	C16
24	B	617	AJP	C22
24	B	617	AJP	C10
24	B	617	AJP	C02
24	B	617	AJP	C19
24	B	617	AJP	C05
24	B	617	AJP	C15
24	B	617	AJP	C07
24	C	201	AJP	C12
24	C	201	AJP	C20
24	C	201	AJP	C23
24	C	201	AJP	C11
24	C	201	AJP	C16
24	C	201	AJP	C22
24	C	201	AJP	C10
24	C	201	AJP	C02
24	C	201	AJP	C19
24	C	201	AJP	C05
24	C	201	AJP	C15
24	C	201	AJP	C07
24	C	202	AJP	C12
24	C	202	AJP	C20
24	C	202	AJP	C23
24	C	202	AJP	C11
24	C	202	AJP	C16
24	C	202	AJP	C22
24	C	202	AJP	C10
24	C	202	AJP	C02
24	C	202	AJP	C19
24	C	202	AJP	C05
24	C	202	AJP	C15
24	C	202	AJP	C07
24	D	603	AJP	C12
24	D	603	AJP	C20
24	D	603	AJP	C23
24	D	603	AJP	C11

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Mol	Chain	Res	Type	Atom
24	D	603	AJP	C16
24	D	603	AJP	C22
24	D	603	AJP	C10
24	D	603	AJP	C02
24	D	603	AJP	C19
24	D	603	AJP	C05
24	D	603	AJP	C15
24	D	603	AJP	C07
24	D	604	AJP	C12
24	D	604	AJP	C20
24	D	604	AJP	C23
24	D	604	AJP	C11
24	D	604	AJP	C16
24	D	604	AJP	C22
24	D	604	AJP	C10
24	D	604	AJP	C02
24	D	604	AJP	C19
24	D	604	AJP	C05
24	D	604	AJP	C15
24	D	604	AJP	C07
24	D	605	AJP	C12
24	D	605	AJP	C20
24	D	605	AJP	C23
24	D	605	AJP	C11
24	D	605	AJP	C16
24	D	605	AJP	C22
24	D	605	AJP	C10
24	D	605	AJP	C02
24	D	605	AJP	C19
24	D	605	AJP	C05
24	D	605	AJP	C15
24	D	605	AJP	C07
24	D	606	AJP	C12
24	D	606	AJP	C20
24	D	606	AJP	C23
24	D	606	AJP	C11
24	D	606	AJP	C16
24	D	606	AJP	C22
24	D	606	AJP	C10
24	D	606	AJP	C02
24	D	606	AJP	C19
24	D	606	AJP	C05

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Mol	Chain	Res	Type	Atom
24	D	606	AJP	C15
24	D	606	AJP	C07
24	D	607	AJP	C12
24	D	607	AJP	C20
24	D	607	AJP	C23
24	D	607	AJP	C11
24	D	607	AJP	C16
24	D	607	AJP	C22
24	D	607	AJP	C10
24	D	607	AJP	C02
24	D	607	AJP	C19
24	D	607	AJP	C05
24	D	607	AJP	C15
24	D	607	AJP	C07
24	D	608	AJP	C12
24	D	608	AJP	C20
24	D	608	AJP	C23
24	D	608	AJP	C11
24	D	608	AJP	C16
24	D	608	AJP	C22
24	D	608	AJP	C10
24	D	608	AJP	C02
24	D	608	AJP	C19
24	D	608	AJP	C05
24	D	608	AJP	C15
24	D	608	AJP	C07
24	D	609	AJP	C12
24	D	609	AJP	C20
24	D	609	AJP	C23
24	D	609	AJP	C11
24	D	609	AJP	C16
24	D	609	AJP	C22
24	D	609	AJP	C10
24	D	609	AJP	C02
24	D	609	AJP	C19
24	D	609	AJP	C05
24	D	609	AJP	C15
24	D	609	AJP	C07
24	D	610	AJP	C12
24	D	610	AJP	C20
24	D	610	AJP	C23
24	D	610	AJP	C11

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Mol	Chain	Res	Type	Atom
24	D	610	AJP	C16
24	D	610	AJP	C22
24	D	610	AJP	C10
24	D	610	AJP	C02
24	D	610	AJP	C19
24	D	610	AJP	C05
24	D	610	AJP	C15
24	D	610	AJP	C07
24	D	611	AJP	C12
24	D	611	AJP	C20
24	D	611	AJP	C23
24	D	611	AJP	C11
24	D	611	AJP	C16
24	D	611	AJP	C22
24	D	611	AJP	C10
24	D	611	AJP	C02
24	D	611	AJP	C19
24	D	611	AJP	C05
24	D	611	AJP	C15
24	D	611	AJP	C07
24	D	612	AJP	C12
24	D	612	AJP	C20
24	D	612	AJP	C23
24	D	612	AJP	C11
24	D	612	AJP	C16
24	D	612	AJP	C22
24	D	612	AJP	C10
24	D	612	AJP	C02
24	D	612	AJP	C19
24	D	612	AJP	C05
24	D	612	AJP	C15
24	D	612	AJP	C07
24	D	613	AJP	C12
24	D	613	AJP	C20
24	D	613	AJP	C23
24	D	613	AJP	C11
24	D	613	AJP	C16
24	D	613	AJP	C22
24	D	613	AJP	C10
24	D	613	AJP	C02
24	D	613	AJP	C19
24	D	613	AJP	C05

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Mol	Chain	Res	Type	Atom
24	D	613	AJP	C15
24	D	613	AJP	C07
24	D	614	AJP	C12
24	D	614	AJP	C20
24	D	614	AJP	C23
24	D	614	AJP	C11
24	D	614	AJP	C16
24	D	614	AJP	C22
24	D	614	AJP	C10
24	D	614	AJP	C02
24	D	614	AJP	C19
24	D	614	AJP	C05
24	D	614	AJP	C15
24	D	614	AJP	C07
24	E	201	AJP	C12
24	E	201	AJP	C20
24	E	201	AJP	C23
24	E	201	AJP	C11
24	E	201	AJP	C16
24	E	201	AJP	C22
24	E	201	AJP	C10
24	E	201	AJP	C02
24	E	201	AJP	C19
24	E	201	AJP	C05
24	E	201	AJP	C15
24	E	201	AJP	C07
24	F	706	AJP	C12
24	F	706	AJP	C20
24	F	706	AJP	C23
24	F	706	AJP	C11
24	F	706	AJP	C16
24	F	706	AJP	C22
24	F	706	AJP	C10
24	F	706	AJP	C02
24	F	706	AJP	C19
24	F	706	AJP	C05
24	F	706	AJP	C15
24	F	706	AJP	C07
24	F	707	AJP	C12
24	F	707	AJP	C20
24	F	707	AJP	C23
24	F	707	AJP	C11

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Mol	Chain	Res	Type	Atom
24	F	707	AJP	C16
24	F	707	AJP	C22
24	F	707	AJP	C10
24	F	707	AJP	C02
24	F	707	AJP	C19
24	F	707	AJP	C05
24	F	707	AJP	C15
24	F	707	AJP	C07
24	F	708	AJP	C12
24	F	708	AJP	C20
24	F	708	AJP	C23
24	F	708	AJP	C11
24	F	708	AJP	C16
24	F	708	AJP	C22
24	F	708	AJP	C10
24	F	708	AJP	C02
24	F	708	AJP	C19
24	F	708	AJP	C05
24	F	708	AJP	C15
24	F	708	AJP	C07
24	F	709	AJP	C12
24	F	709	AJP	C20
24	F	709	AJP	C23
24	F	709	AJP	C11
24	F	709	AJP	C16
24	F	709	AJP	C22
24	F	709	AJP	C10
24	F	709	AJP	C02
24	F	709	AJP	C19
24	F	709	AJP	C05
24	F	709	AJP	C15
24	F	709	AJP	C07
24	F	710	AJP	C12
24	F	710	AJP	C20
24	F	710	AJP	C23
24	F	710	AJP	C11
24	F	710	AJP	C16
24	F	710	AJP	C22
24	F	710	AJP	C10
24	F	710	AJP	C02
24	F	710	AJP	C19
24	F	710	AJP	C05

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Mol	Chain	Res	Type	Atom
24	F	710	AJP	C15
24	F	710	AJP	C07
24	F	711	AJP	C12
24	F	711	AJP	C20
24	F	711	AJP	C23
24	F	711	AJP	C11
24	F	711	AJP	C16
24	F	711	AJP	C22
24	F	711	AJP	C10
24	F	711	AJP	C02
24	F	711	AJP	C19
24	F	711	AJP	C05
24	F	711	AJP	C15
24	F	711	AJP	C07
24	F	712	AJP	C12
24	F	712	AJP	C20
24	F	712	AJP	C23
24	F	712	AJP	C11
24	F	712	AJP	C16
24	F	712	AJP	C22
24	F	712	AJP	C10
24	F	712	AJP	C02
24	F	712	AJP	C19
24	F	712	AJP	C05
24	F	712	AJP	C15
24	F	712	AJP	C07
24	F	713	AJP	C12
24	F	713	AJP	C20
24	F	713	AJP	C23
24	F	713	AJP	C11
24	F	713	AJP	C16
24	F	713	AJP	C22
24	F	713	AJP	C10
24	F	713	AJP	C02
24	F	713	AJP	C19
24	F	713	AJP	C05
24	F	713	AJP	C15
24	F	713	AJP	C07
24	F	714	AJP	C12
24	F	714	AJP	C20
24	F	714	AJP	C23
24	F	714	AJP	C11

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Mol	Chain	Res	Type	Atom
24	F	714	AJP	C16
24	F	714	AJP	C22
24	F	714	AJP	C10
24	F	714	AJP	C02
24	F	714	AJP	C19
24	F	714	AJP	C05
24	F	714	AJP	C15
24	F	714	AJP	C07
24	F	715	AJP	C12
24	F	715	AJP	C20
24	F	715	AJP	C23
24	F	715	AJP	C11
24	F	715	AJP	C16
24	F	715	AJP	C22
24	F	715	AJP	C10
24	F	715	AJP	C02
24	F	715	AJP	C19
24	F	715	AJP	C05
24	F	715	AJP	C15
24	F	715	AJP	C07
24	F	716	AJP	C12
24	F	716	AJP	C20
24	F	716	AJP	C23
24	F	716	AJP	C11
24	F	716	AJP	C16
24	F	716	AJP	C22
24	F	716	AJP	C10
24	F	716	AJP	C02
24	F	716	AJP	C19
24	F	716	AJP	C05
24	F	716	AJP	C15
24	F	716	AJP	C07
24	F	717	AJP	C12
24	F	717	AJP	C20
24	F	717	AJP	C23
24	F	717	AJP	C11
24	F	717	AJP	C16
24	F	717	AJP	C22
24	F	717	AJP	C10
24	F	717	AJP	C02
24	F	717	AJP	C19
24	F	717	AJP	C05

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Mol	Chain	Res	Type	Atom
24	F	717	AJP	C15
24	F	717	AJP	C07
24	F	718	AJP	C12
24	F	718	AJP	C20
24	F	718	AJP	C23
24	F	718	AJP	C11
24	F	718	AJP	C16
24	F	718	AJP	C22
24	F	718	AJP	C10
24	F	718	AJP	C02
24	F	718	AJP	C19
24	F	718	AJP	C05
24	F	718	AJP	C15
24	F	718	AJP	C07
24	G	301	AJP	C12
24	G	301	AJP	C20
24	G	301	AJP	C23
24	G	301	AJP	C11
24	G	301	AJP	C16
24	G	301	AJP	C22
24	G	301	AJP	C10
24	G	301	AJP	C02
24	G	301	AJP	C19
24	G	301	AJP	C05
24	G	301	AJP	C15
24	G	301	AJP	C07
24	G	302	AJP	C12
24	G	302	AJP	C20
24	G	302	AJP	C23
24	G	302	AJP	C11
24	G	302	AJP	C16
24	G	302	AJP	C22
24	G	302	AJP	C10
24	G	302	AJP	C02
24	G	302	AJP	C19
24	G	302	AJP	C05
24	G	302	AJP	C15
24	G	302	AJP	C07
24	G	303	AJP	C12
24	G	303	AJP	C20
24	G	303	AJP	C23
24	G	303	AJP	C11

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Mol	Chain	Res	Type	Atom
24	G	303	AJP	C16
24	G	303	AJP	C22
24	G	303	AJP	C10
24	G	303	AJP	C02
24	G	303	AJP	C19
24	G	303	AJP	C05
24	G	303	AJP	C15
24	G	303	AJP	C07
24	G	304	AJP	C12
24	G	304	AJP	C20
24	G	304	AJP	C23
24	G	304	AJP	C11
24	G	304	AJP	C16
24	G	304	AJP	C22
24	G	304	AJP	C10
24	G	304	AJP	C02
24	G	304	AJP	C19
24	G	304	AJP	C05
24	G	304	AJP	C15
24	G	304	AJP	C07
24	G	305	AJP	C12
24	G	305	AJP	C20
24	G	305	AJP	C23
24	G	305	AJP	C11
24	G	305	AJP	C16
24	G	305	AJP	C22
24	G	305	AJP	C10
24	G	305	AJP	C02
24	G	305	AJP	C19
24	G	305	AJP	C05
24	G	305	AJP	C15
24	G	305	AJP	C07
24	G	306	AJP	C12
24	G	306	AJP	C20
24	G	306	AJP	C23
24	G	306	AJP	C11
24	G	306	AJP	C16
24	G	306	AJP	C22
24	G	306	AJP	C10
24	G	306	AJP	C02
24	G	306	AJP	C19
24	G	306	AJP	C05

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Mol	Chain	Res	Type	Atom
24	G	306	AJP	C15
24	G	306	AJP	C07
24	G	307	AJP	C12
24	G	307	AJP	C20
24	G	307	AJP	C23
24	G	307	AJP	C11
24	G	307	AJP	C16
24	G	307	AJP	C22
24	G	307	AJP	C10
24	G	307	AJP	C02
24	G	307	AJP	C19
24	G	307	AJP	C05
24	G	307	AJP	C15
24	G	307	AJP	C07
24	Q	101	AJP	C12
24	Q	101	AJP	C20
24	Q	101	AJP	C23
24	Q	101	AJP	C11
24	Q	101	AJP	C16
24	Q	101	AJP	C22
24	Q	101	AJP	C10
24	Q	101	AJP	C02
24	Q	101	AJP	C19
24	Q	101	AJP	C05
24	Q	101	AJP	C15
24	Q	101	AJP	C07
24	Q	102	AJP	C12
24	Q	102	AJP	C20
24	Q	102	AJP	C23
24	Q	102	AJP	C11
24	Q	102	AJP	C16
24	Q	102	AJP	C22
24	Q	102	AJP	C10
24	Q	102	AJP	C02
24	Q	102	AJP	C19
24	Q	102	AJP	C05
24	Q	102	AJP	C15
24	Q	102	AJP	C07
24	Q	103	AJP	C12
24	Q	103	AJP	C20
24	Q	103	AJP	C23
24	Q	103	AJP	C11

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Mol	Chain	Res	Type	Atom
24	Q	103	AJP	C16
24	Q	103	AJP	C22
24	Q	103	AJP	C10
24	Q	103	AJP	C02
24	Q	103	AJP	C19
24	Q	103	AJP	C05
24	Q	103	AJP	C15
24	Q	103	AJP	C07
24	Q	104	AJP	C12
24	Q	104	AJP	C20
24	Q	104	AJP	C23
24	Q	104	AJP	C11
24	Q	104	AJP	C16
24	Q	104	AJP	C22
24	Q	104	AJP	C10
24	Q	104	AJP	C02
24	Q	104	AJP	C19
24	Q	104	AJP	C05
24	Q	104	AJP	C15
24	Q	104	AJP	C07
24	Q	105	AJP	C12
24	Q	105	AJP	C20
24	Q	105	AJP	C23
24	Q	105	AJP	C11
24	Q	105	AJP	C16
24	Q	105	AJP	C22
24	Q	105	AJP	C10
24	Q	105	AJP	C02
24	Q	105	AJP	C19
24	Q	105	AJP	C05
24	Q	105	AJP	C15
24	Q	105	AJP	C07
24	Q	106	AJP	C12
24	Q	106	AJP	C20
24	Q	106	AJP	C23
24	Q	106	AJP	C11
24	Q	106	AJP	C16
24	Q	106	AJP	C22
24	Q	106	AJP	C10
24	Q	106	AJP	C02
24	Q	106	AJP	C19
24	Q	106	AJP	C05

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Mol	Chain	Res	Type	Atom
24	Q	106	AJP	C15
24	Q	106	AJP	C07
24	Q	107	AJP	C12
24	Q	107	AJP	C20
24	Q	107	AJP	C23
24	Q	107	AJP	C11
24	Q	107	AJP	C16
24	Q	107	AJP	C22
24	Q	107	AJP	C10
24	Q	107	AJP	C02
24	Q	107	AJP	C19
24	Q	107	AJP	C05
24	Q	107	AJP	C15
24	Q	107	AJP	C07
24	Q	108	AJP	C12
24	Q	108	AJP	C20
24	Q	108	AJP	C23
24	Q	108	AJP	C11
24	Q	108	AJP	C16
24	Q	108	AJP	C22
24	Q	108	AJP	C10
24	Q	108	AJP	C02
24	Q	108	AJP	C19
24	Q	108	AJP	C05
24	Q	108	AJP	C15
24	Q	108	AJP	C07

All (353) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	401	BCR	C1-C6-C7-C8
21	A	401	BCR	C23-C24-C25-C30
21	F	701	BCR	C7-C8-C9-C34
21	F	701	BCR	C21-C22-C23-C24
21	P	101	BCR	C1-C6-C7-C8
21	P	101	BCR	C20-C21-C22-C23
22	A	402	LHG	O1-C1-C2-C3
22	A	402	LHG	C2-C3-O3-P
22	A	402	LHG	C3-O3-P-O5
22	A	402	LHG	C3-O3-P-O6
22	B	602	LHG	C1-C2-C3-O3
22	B	602	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
22	B	602	LHG	C3-O3-P-O5
22	B	602	LHG	C4-O6-P-O5
22	B	603	LHG	O1-C1-C2-C3
22	B	603	LHG	C3-O3-P-O6
22	B	603	LHG	O7-C5-C6-O8
22	B	603	LHG	C8-C7-O7-C5
22	B	604	LHG	O1-C1-C2-C3
22	B	604	LHG	C3-O3-P-O5
22	B	604	LHG	C4-O6-P-O4
22	B	604	LHG	O9-C7-O7-C5
22	D	601	LHG	C3-O3-P-O5
22	D	601	LHG	C3-O3-P-O6
22	D	602	LHG	C1-C2-C3-O3
22	D	602	LHG	C3-O3-P-O5
22	D	602	LHG	C8-C7-O7-C5
22	F	702	LHG	O1-C1-C2-C3
22	F	702	LHG	C3-O3-P-O5
22	F	702	LHG	C4-O6-P-O5
22	F	702	LHG	O9-C7-O7-C5
22	F	702	LHG	C8-C7-O7-C5
22	F	702	LHG	C24-C23-O8-C6
22	F	703	LHG	O1-C1-C2-C3
22	F	703	LHG	C1-C2-C3-O3
22	F	703	LHG	C4-O6-P-O5
22	F	703	LHG	C24-C23-O8-C6
22	H	401	LHG	O1-C1-C2-C3
22	H	401	LHG	C4-O6-P-O5
26	B	605	SQD	O5-C1-O6-C44
26	B	605	SQD	O6-C44-C45-O47
26	F	704	SQD	O5-C1-O6-C44
26	F	704	SQD	C8-C7-O47-C45
26	F	705	SQD	O49-C7-O47-C45
26	F	705	SQD	C8-C7-O47-C45
26	L	101	SQD	O5-C1-O6-C44
26	L	101	SQD	C8-C7-O47-C45
26	L	101	SQD	O5-C5-C6-S
22	F	702	LHG	O10-C23-O8-C6
22	F	703	LHG	O10-C23-O8-C6
26	F	704	SQD	C24-C23-O48-C46
22	A	402	LHG	O10-C23-O8-C6
22	B	604	LHG	O10-C23-O8-C6
26	F	704	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
26	F	705	SQD	O10-C23-O48-C46
22	D	602	LHG	O9-C7-O7-C5
22	F	703	LHG	O9-C7-O7-C5
22	H	401	LHG	O9-C7-O7-C5
26	F	704	SQD	O49-C7-O47-C45
22	A	402	LHG	C24-C23-O8-C6
26	F	705	SQD	C24-C23-O48-C46
22	B	604	LHG	C8-C7-O7-C5
25	B	601	PQN	C12-C13-C15-C16
22	B	604	LHG	C24-C23-O8-C6
25	B	601	PQN	C11-C12-C13-C14
22	B	603	LHG	O9-C7-O7-C5
26	L	101	SQD	O49-C7-O47-C45
22	B	602	LHG	O10-C23-O8-C6
22	D	602	LHG	O2-C2-C3-O3
22	F	703	LHG	O2-C2-C3-O3
23	A	403	DGD	C4E-C5E-C6E-O5E
22	B	603	LHG	C32-C33-C34-C35
22	B	602	LHG	C24-C23-O8-C6
22	F	703	LHG	C27-C28-C29-C30
23	A	403	DGD	O6E-C5E-C6E-O5E
25	B	601	PQN	C19-C18-C20-C21
21	F	701	BCR	C37-C22-C23-C24
21	P	101	BCR	C7-C8-C9-C34
21	P	101	BCR	C7-C8-C9-C10
22	A	402	LHG	C23-C24-C25-C26
21	F	701	BCR	C14-C15-C16-C17
22	B	602	LHG	C7-C8-C9-C10
22	B	603	LHG	C23-C24-C25-C26
22	B	604	LHG	C7-C8-C9-C10
22	B	604	LHG	C23-C24-C25-C26
22	D	601	LHG	C7-C8-C9-C10
22	F	702	LHG	C7-C8-C9-C10
22	F	702	LHG	C23-C24-C25-C26
22	D	601	LHG	C23-C24-C25-C26
22	F	703	LHG	C23-C24-C25-C26
21	P	101	BCR	C10-C11-C12-C13
25	B	601	PQN	C20-C21-C22-C23
22	B	602	LHG	C3-O3-P-O6
22	B	602	LHG	C4-O6-P-O3
22	B	604	LHG	C4-O6-P-O3
22	D	602	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
22	F	703	LHG	C4-O6-P-O3
22	H	401	LHG	C7-C8-C9-C10
23	A	403	DGD	C1B-C2B-C3B-C4B
22	H	401	LHG	C24-C23-O8-C6
21	P	101	BCR	C9-C10-C11-C12
22	F	703	LHG	C8-C7-O7-C5
21	P	101	BCR	C20-C21-C22-C37
22	B	602	LHG	C32-C33-C34-C35
23	A	403	DGD	C4A-C5A-C6A-C7A
26	B	605	SQD	C27-C28-C29-C30
26	F	704	SQD	C12-C13-C14-C15
22	B	604	LHG	C9-C10-C11-C12
22	D	602	LHG	C31-C32-C33-C34
22	F	702	LHG	C32-C33-C34-C35
26	L	101	SQD	C12-C13-C14-C15
23	A	404	DGD	C4A-C5A-C6A-C7A
22	B	602	LHG	C23-C24-C25-C26
21	A	401	BCR	C16-C17-C18-C19
26	F	705	SQD	C2-C1-O6-C44
22	B	604	LHG	C32-C33-C34-C35
22	D	601	LHG	C32-C33-C34-C35
26	F	704	SQD	C17-C18-C19-C20
22	H	401	LHG	C24-C25-C26-C27
23	A	403	DGD	C4B-C5B-C6B-C7B
22	B	602	LHG	C27-C28-C29-C30
22	D	602	LHG	C30-C31-C32-C33
22	F	703	LHG	C32-C33-C34-C35
26	B	605	SQD	C12-C13-C14-C15
22	B	604	LHG	C29-C30-C31-C32
22	D	601	LHG	C30-C31-C32-C33
22	A	402	LHG	C29-C30-C31-C32
22	F	702	LHG	C16-C17-C18-C19
22	H	401	LHG	C23-C24-C25-C26
26	F	704	SQD	C7-C8-C9-C10
23	A	403	DGD	C6A-C7A-C8A-C9A
23	A	404	DGD	C5A-C6A-C7A-C8A
23	A	404	DGD	C7B-C8B-C9B-CAB
26	F	705	SQD	C9-C10-C11-C12
25	B	601	PQN	C26-C27-C28-C30
22	A	402	LHG	C24-C25-C26-C27
22	A	402	LHG	C27-C28-C29-C30
23	A	404	DGD	CEB-CFB-CGB-CHB

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Mol	Chain	Res	Type	Atoms
26	B	605	SQD	C28-C29-C30-C31
22	A	402	LHG	C11-C10-C9-C8
22	B	602	LHG	C10-C11-C12-C13
22	D	602	LHG	C27-C28-C29-C30
22	H	401	LHG	C29-C30-C31-C32
26	F	704	SQD	C26-C27-C28-C29
23	A	403	DGD	CEB-CFB-CGB-CHB
26	F	704	SQD	C27-C28-C29-C30
26	F	704	SQD	C28-C29-C30-C31
23	A	404	DGD	C5B-C6B-C7B-C8B
22	H	401	LHG	C8-C7-O7-C5
26	F	705	SQD	C12-C13-C14-C15
22	A	402	LHG	O1-C1-C2-O2
22	H	401	LHG	O1-C1-C2-O2
22	F	703	LHG	C9-C10-C11-C12
22	D	602	LHG	C32-C33-C34-C35
22	B	604	LHG	C11-C12-C13-C14
22	B	604	LHG	C28-C29-C30-C31
22	A	402	LHG	C32-C33-C34-C35
23	A	403	DGD	C7B-C8B-C9B-CAB
21	A	401	BCR	C5-C6-C7-C8
21	A	401	BCR	C23-C24-C25-C26
21	F	701	BCR	C23-C24-C25-C26
21	F	701	BCR	C23-C24-C25-C30
21	P	101	BCR	C5-C6-C7-C8
22	F	702	LHG	C30-C31-C32-C33
26	F	705	SQD	C11-C12-C13-C14
23	A	404	DGD	O1B-C1B-O2G-C2G
22	D	602	LHG	C23-C24-C25-C26
23	A	403	DGD	C5B-C6B-C7B-C8B
22	D	602	LHG	C15-C16-C17-C18
22	B	602	LHG	C24-C25-C26-C27
22	F	702	LHG	C13-C14-C15-C16
22	B	603	LHG	C14-C15-C16-C17
22	B	604	LHG	C17-C18-C19-C20
23	A	403	DGD	C2B-C1B-O2G-C2G
21	P	101	BCR	C14-C15-C16-C17
22	F	702	LHG	C27-C28-C29-C30
22	D	602	LHG	C29-C30-C31-C32
23	A	403	DGD	C6B-C7B-C8B-C9B
22	D	601	LHG	C11-C10-C9-C8
26	L	101	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	F	701	BCR	C7-C8-C9-C10
22	D	601	LHG	C31-C32-C33-C34
22	H	401	LHG	C32-C33-C34-C35
23	A	404	DGD	C6B-C7B-C8B-C9B
22	F	703	LHG	C28-C29-C30-C31
26	B	605	SQD	C9-C10-C11-C12
22	H	401	LHG	C11-C12-C13-C14
22	B	603	LHG	C1-C2-C3-O3
22	D	601	LHG	C29-C30-C31-C32
22	B	603	LHG	C4-C5-C6-O8
22	H	401	LHG	C4-C5-C6-O8
22	B	603	LHG	C27-C28-C29-C30
26	F	705	SQD	C14-C15-C16-C17
23	A	404	DGD	O6E-C5E-C6E-O5E
22	B	604	LHG	O1-C1-C2-O2
22	F	702	LHG	O1-C1-C2-O2
22	F	703	LHG	O1-C1-C2-O2
22	F	703	LHG	C6-C5-O7-C7
22	H	401	LHG	C6-C5-O7-C7
26	F	704	SQD	C46-C45-O47-C7
22	B	603	LHG	C31-C32-C33-C34
22	F	703	LHG	C30-C31-C32-C33
22	H	401	LHG	O6-C4-C5-O7
22	F	703	LHG	C24-C25-C26-C27
23	A	403	DGD	C2D-C1D-O3G-C3G
26	F	704	SQD	C2-C1-O6-C44
26	B	605	SQD	O47-C45-C46-O48
26	L	101	SQD	C29-C30-C31-C32
22	D	601	LHG	C28-C29-C30-C31
26	F	704	SQD	C14-C15-C16-C17
22	B	604	LHG	C27-C28-C29-C30
21	P	101	BCR	C6-C7-C8-C9
22	B	602	LHG	O6-C4-C5-C6
22	H	401	LHG	O6-C4-C5-C6
22	B	602	LHG	C15-C16-C17-C18
22	B	603	LHG	C28-C29-C30-C31
22	A	402	LHG	C33-C34-C35-C36
22	D	602	LHG	C2-C3-O3-P
26	L	101	SQD	C34-C35-C36-C37
22	B	602	LHG	C33-C34-C35-C36
22	F	703	LHG	C4-C5-C6-O8
22	B	602	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
23	A	404	DGD	C8A-C9A-CAA-CBA
22	H	401	LHG	C33-C34-C35-C36
22	B	603	LHG	O1-C1-C2-O2
23	A	404	DGD	CCA-CDA-CEA-CFA
26	L	101	SQD	C10-C11-C12-C13
22	F	703	LHG	O7-C5-C6-O8
23	A	403	DGD	O1G-C1G-C2G-O2G
26	F	704	SQD	O6-C44-C45-O47
26	F	705	SQD	O47-C45-C46-O48
23	A	404	DGD	C8B-C9B-CAB-CBB
22	A	402	LHG	C1-C2-C3-O3
22	B	603	LHG	C29-C30-C31-C32
26	B	605	SQD	C26-C27-C28-C29
21	F	701	BCR	C1-C6-C7-C8
21	F	701	BCR	C5-C6-C7-C8
21	P	101	BCR	C23-C24-C25-C26
21	P	101	BCR	C23-C24-C25-C30
22	B	604	LHG	C30-C31-C32-C33
22	B	602	LHG	C30-C31-C32-C33
22	B	602	LHG	C8-C7-O7-C5
25	B	601	PQN	C26-C27-C28-C29
22	A	402	LHG	C31-C32-C33-C34
26	F	704	SQD	C16-C17-C18-C19
21	P	101	BCR	C19-C20-C21-C22
22	H	401	LHG	C28-C29-C30-C31
21	A	401	BCR	C16-C17-C18-C36
22	B	602	LHG	C29-C30-C31-C32
22	D	601	LHG	C34-C35-C36-C37
23	A	404	DGD	O6D-C1D-O3G-C3G
22	D	602	LHG	C33-C34-C35-C36
26	B	605	SQD	O6-C44-C45-C46
26	B	605	SQD	C44-C45-C46-O48
26	F	704	SQD	O6-C44-C45-C46
26	L	101	SQD	O6-C44-C45-C46
22	B	602	LHG	O6-C4-C5-O7
23	A	404	DGD	C6A-C7A-C8A-C9A
22	D	601	LHG	O7-C5-C6-O8
22	H	401	LHG	O7-C5-C6-O8
23	A	404	DGD	C3B-C4B-C5B-C6B
22	H	401	LHG	C4-O6-P-O3
22	F	702	LHG	C5-C4-O6-P
22	B	602	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
22	B	603	LHG	C3-O3-P-O5
22	D	601	LHG	C3-O3-P-O4
22	D	602	LHG	C3-O3-P-O4
22	F	703	LHG	C4-O6-P-O4
22	B	603	LHG	C15-C16-C17-C18
22	D	601	LHG	C33-C34-C35-C36
22	B	604	LHG	O6-C4-C5-C6
26	F	704	SQD	C9-C10-C11-C12
26	F	704	SQD	C23-C24-C25-C26
25	B	601	PQN	C17-C18-C20-C21
22	B	603	LHG	O2-C2-C3-O3
26	L	101	SQD	C15-C16-C17-C18
23	A	403	DGD	O1G-C1G-C2G-C3G
22	A	402	LHG	C11-C12-C13-C14
22	B	604	LHG	C12-C13-C14-C15
22	B	602	LHG	C17-C18-C19-C20
22	B	603	LHG	C2-C3-O3-P
22	F	702	LHG	C11-C10-C9-C8
26	L	101	SQD	O47-C7-C8-C9
22	A	402	LHG	C8-C7-O7-C5
22	F	702	LHG	C15-C16-C17-C18
22	F	702	LHG	C4-C5-O7-C7
22	H	401	LHG	O10-C23-O8-C6
22	F	703	LHG	C33-C34-C35-C36
26	B	605	SQD	C14-C15-C16-C17
22	D	602	LHG	C4-O6-P-O3
22	F	702	LHG	C3-O3-P-O6
22	H	401	LHG	C3-O3-P-O6
22	D	601	LHG	C27-C28-C29-C30
23	A	404	DGD	C4B-C5B-C6B-C7B
22	F	702	LHG	C31-C32-C33-C34
26	F	705	SQD	O6-C44-C45-C46
26	F	705	SQD	C17-C18-C19-C20
22	F	703	LHG	C5-C4-O6-P
26	B	605	SQD	C16-C17-C18-C19
22	D	602	LHG	O6-C4-C5-O7
23	A	403	DGD	C2A-C3A-C4A-C5A
21	F	701	BCR	C35-C13-C14-C15
26	F	705	SQD	C44-C45-C46-O48
22	B	602	LHG	C9-C10-C11-C12
22	F	702	LHG	C6-C5-O7-C7
22	A	402	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	604	LHG	O6-C4-C5-O7
23	A	403	DGD	C8A-C9A-CAA-CBA
22	B	603	LHG	C17-C18-C19-C20
21	A	401	BCR	C12-C13-C14-C15
21	F	701	BCR	C12-C13-C14-C15
23	A	403	DGD	C9A-CAA-CBA-CCA
23	A	404	DGD	CAB-CBB-CCB-CDB
22	F	702	LHG	O6-C4-C5-C6
22	D	602	LHG	C10-C11-C12-C13
26	L	101	SQD	O49-C7-C8-C9
26	F	705	SQD	C10-C11-C12-C13
21	A	401	BCR	C35-C13-C14-C15
22	B	603	LHG	C11-C12-C13-C14
23	A	403	DGD	O2G-C1B-C2B-C3B
26	L	101	SQD	C7-C8-C9-C10
22	B	604	LHG	O7-C7-C8-C9
22	D	601	LHG	O8-C23-C24-C25
26	L	101	SQD	C11-C10-C9-C8
22	F	702	LHG	O6-C4-C5-O7
21	A	401	BCR	C20-C21-C22-C23
22	D	602	LHG	O7-C7-C8-C9
26	L	101	SQD	O48-C23-C24-C25
22	B	602	LHG	O1-C1-C2-O2
22	B	604	LHG	C34-C35-C36-C37
26	F	705	SQD	O47-C7-C8-C9
22	B	602	LHG	C5-C4-O6-P
22	A	402	LHG	O2-C2-C3-O3
26	L	101	SQD	C4-C5-C6-S
23	A	404	DGD	C2B-C1B-O2G-C2G
26	F	704	SQD	C24-C25-C26-C27
22	F	702	LHG	C28-C29-C30-C31
22	H	401	LHG	C16-C17-C18-C19
26	L	101	SQD	O10-C23-C24-C25
26	F	705	SQD	C16-C17-C18-C19
22	D	601	LHG	O10-C23-C24-C25
23	A	404	DGD	C9B-CAB-CBB-CCB
21	A	401	BCR	C6-C7-C8-C9
26	L	101	SQD	C2-C1-O6-C44
22	D	602	LHG	C4-O6-P-O4
22	H	401	LHG	C3-O3-P-O5
22	F	703	LHG	C29-C30-C31-C32
26	B	605	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	A	404	DGD	CBA-CCA-CDA-CEA
22	H	401	LHG	C1-C2-C3-O3
22	B	604	LHG	O9-C7-C8-C9
21	P	101	BCR	C17-C18-C19-C20
26	B	605	SQD	C24-C25-C26-C27

There are no ring outliers.

79 monomers are involved in 391 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	608	AJP	4	0
24	D	606	AJP	6	0
24	D	609	AJP	9	0
24	B	615	AJP	7	0
24	D	610	AJP	10	0
24	F	708	AJP	4	0
24	F	707	AJP	11	0
24	B	606	AJP	19	0
24	A	408	AJP	6	0
22	A	402	LHG	3	0
24	E	201	AJP	1	0
24	F	711	AJP	8	0
27	I	202	SF4	1	0
24	B	616	AJP	23	0
24	D	603	AJP	4	0
24	B	609	AJP	3	0
24	G	307	AJP	3	0
24	B	610	AJP	2	0
24	G	304	AJP	6	0
24	D	607	AJP	6	0
24	F	713	AJP	2	0
24	G	305	AJP	10	0
24	D	605	AJP	6	0
24	D	614	AJP	4	0
21	P	101	BCR	5	0
24	F	712	AJP	11	0
24	A	409	AJP	9	0
24	F	716	AJP	3	0
24	Q	102	AJP	7	0
24	B	613	AJP	1	0
24	G	301	AJP	10	0
24	B	612	AJP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	614	AJP	9	0
24	B	617	AJP	8	0
24	Q	104	AJP	1	0
22	B	603	LHG	2	0
22	F	702	LHG	1	0
24	D	604	AJP	9	0
24	F	714	AJP	8	0
24	Q	101	AJP	3	0
22	D	601	LHG	1	0
24	Q	103	AJP	1	0
24	Q	105	AJP	2	0
22	H	401	LHG	3	0
23	A	403	DGD	1	0
24	F	709	AJP	2	0
24	A	405	AJP	1	0
27	K	301	SF4	3	0
26	L	101	SQD	1	0
24	F	710	AJP	5	0
24	G	306	AJP	6	0
26	F	704	SQD	5	0
24	D	612	AJP	11	0
24	C	201	AJP	5	0
23	A	404	DGD	2	0
24	F	718	AJP	12	0
21	A	401	BCR	4	0
24	F	715	AJP	2	0
24	F	706	AJP	2	0
24	B	607	AJP	5	0
24	Q	108	AJP	1	0
24	A	406	AJP	2	0
24	G	302	AJP	6	0
24	G	303	AJP	5	0
24	A	407	AJP	10	0
22	B	604	LHG	2	0
24	Q	107	AJP	5	0
26	B	605	SQD	3	0
24	F	717	AJP	1	0
28	R	101	FES	2	0
24	Q	106	AJP	5	0
22	F	703	LHG	7	0
21	F	701	BCR	3	0
24	B	611	AJP	5	0

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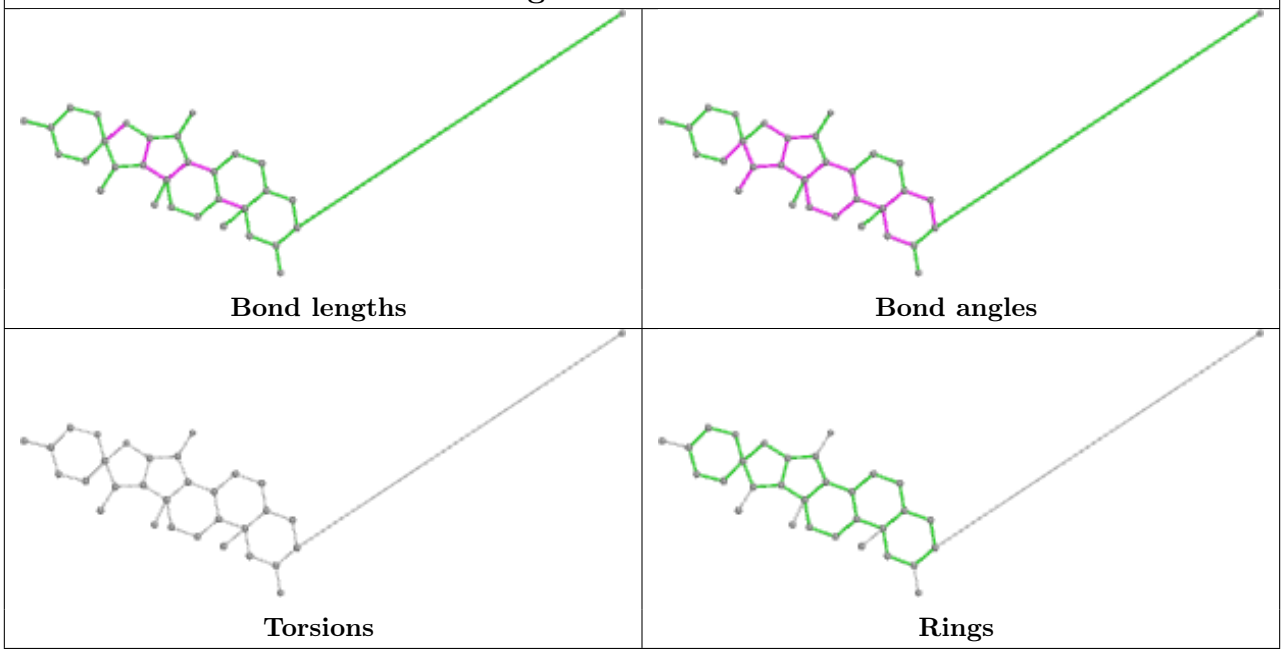
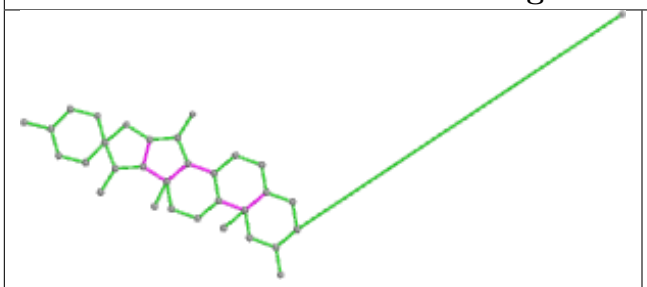
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	202	AJP	12	0
24	D	611	AJP	7	0
24	D	613	AJP	18	0
26	F	705	SQD	1	0
24	D	608	AJP	13	0

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.

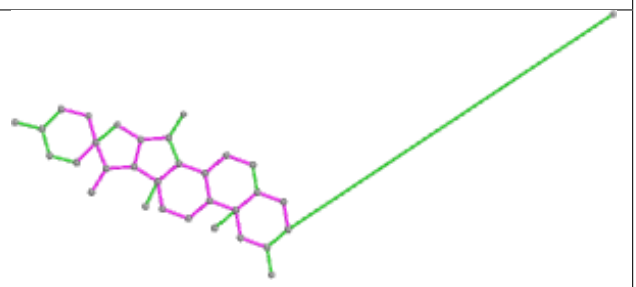
Ligand AJP B 608



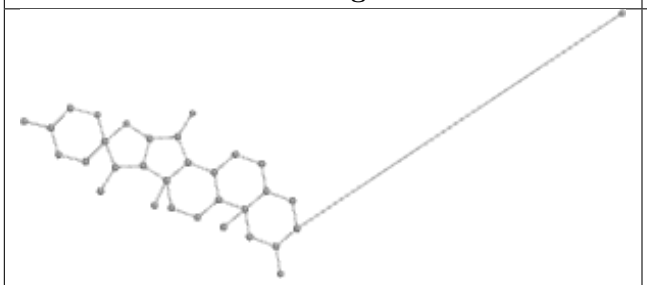
Ligand AJP D 606



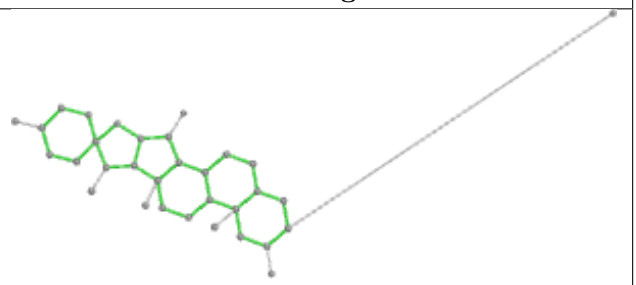
Bond lengths



Bond angles

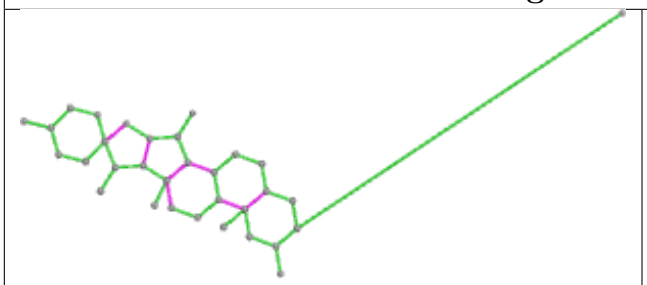


Torsions

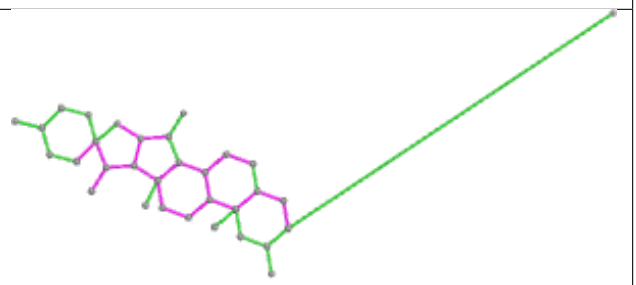


Rings

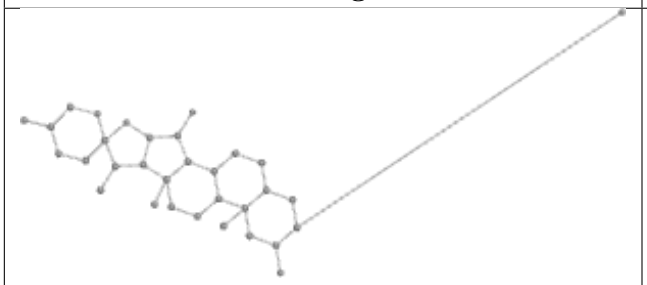
Ligand AJP D 609



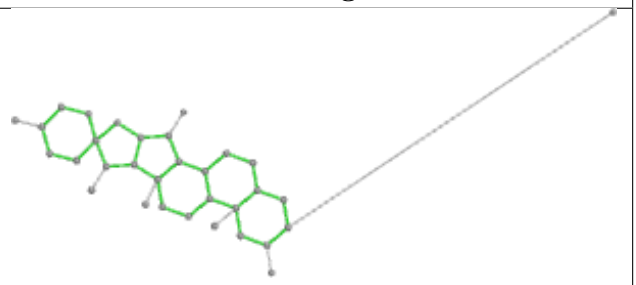
Bond lengths



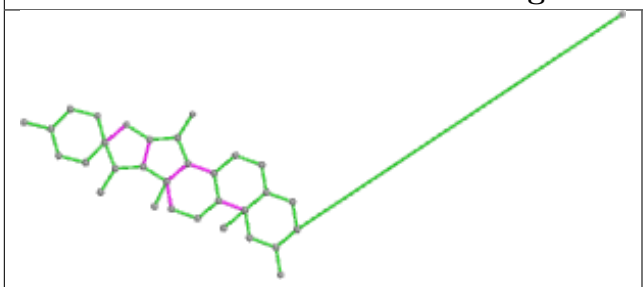
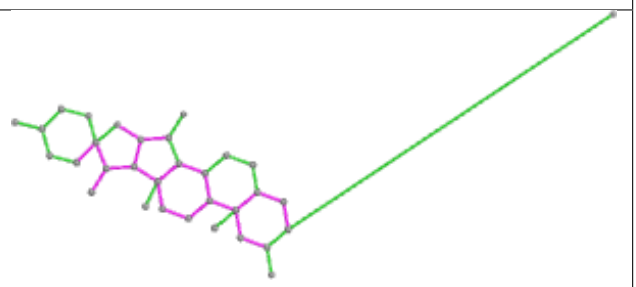
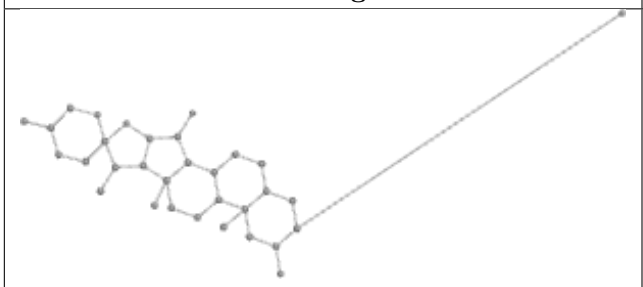
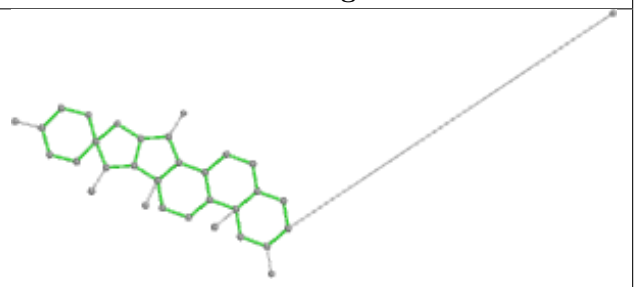
Bond angles



Torsions



Rings

Ligand AJP B 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

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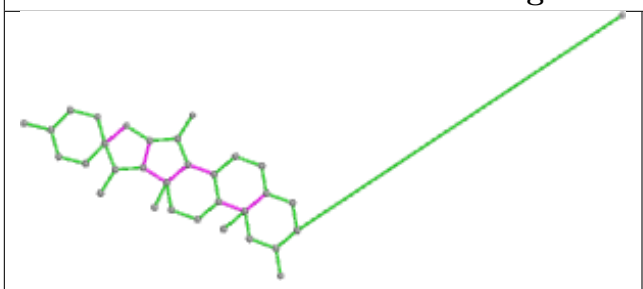
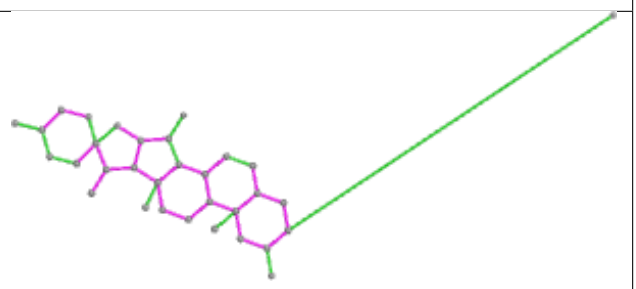
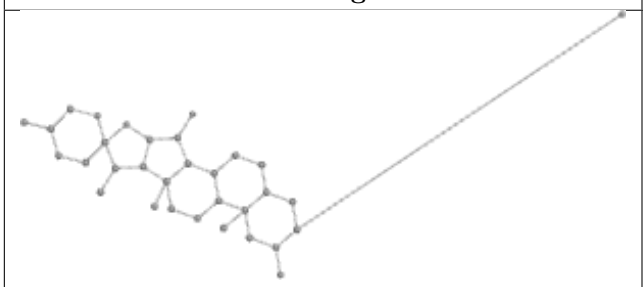
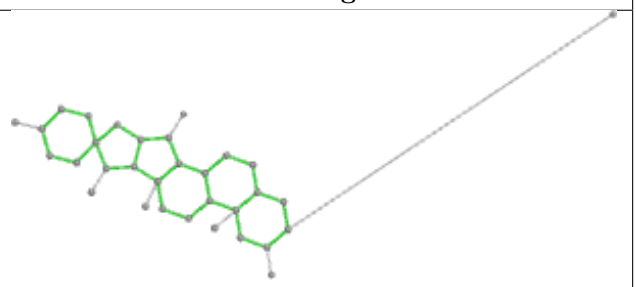
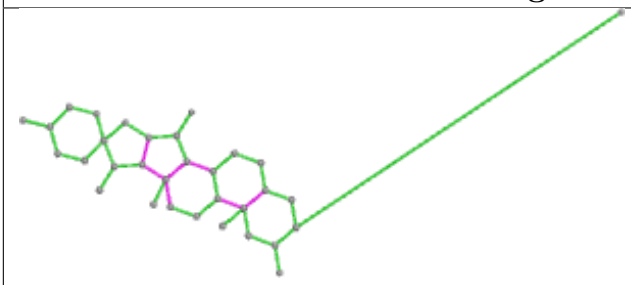
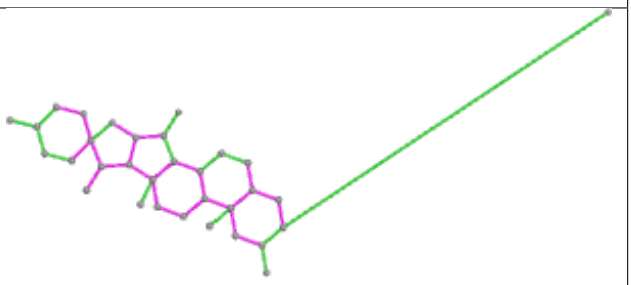
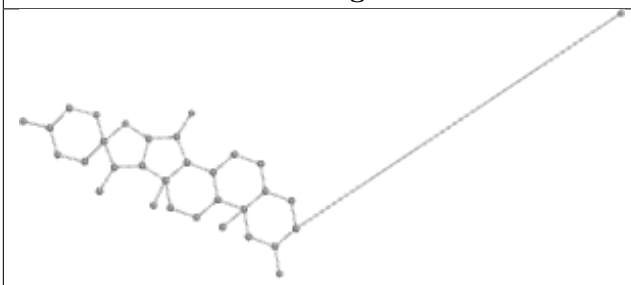
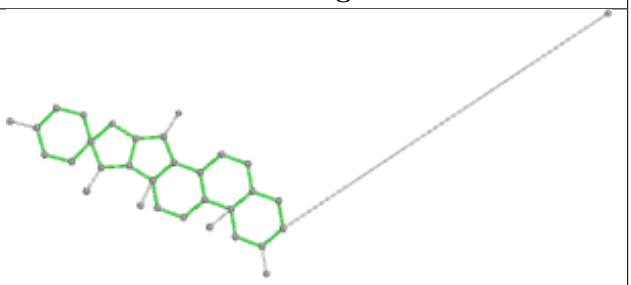
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AJP F 708	
 Bond lengths	 Bond angles
 Torsions	 Rings

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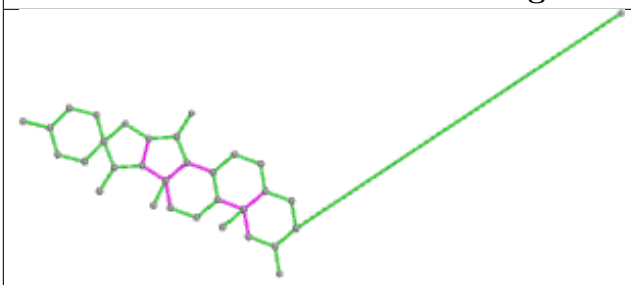
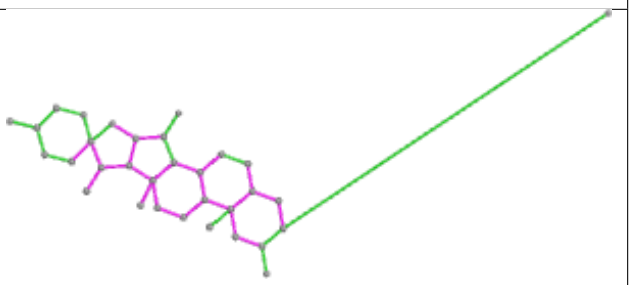
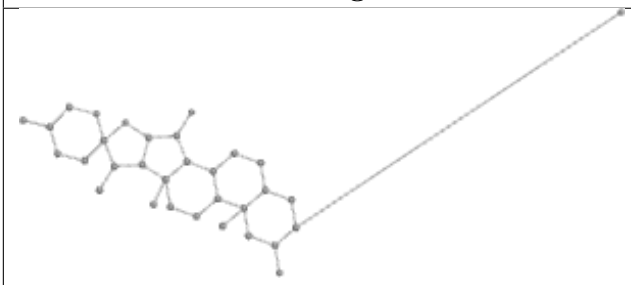
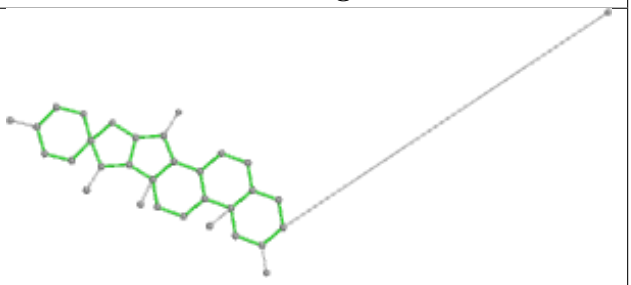
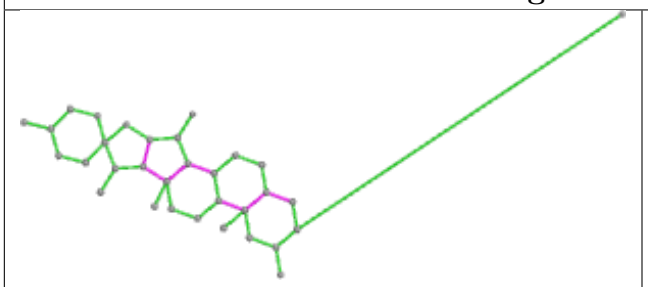
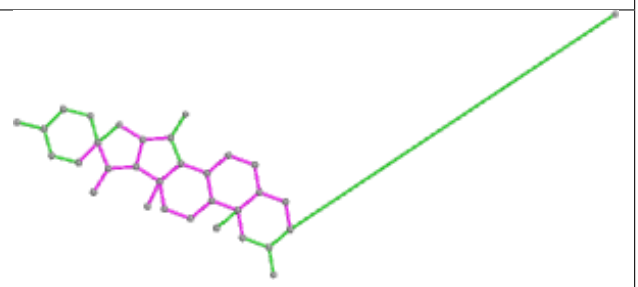
 Bond lengths	 Bond angles
 Torsions	 Rings

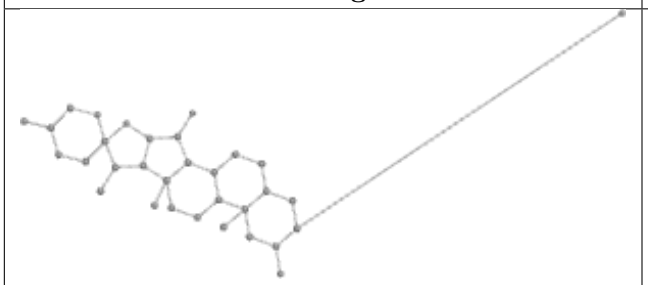
Ligand AJP B 606



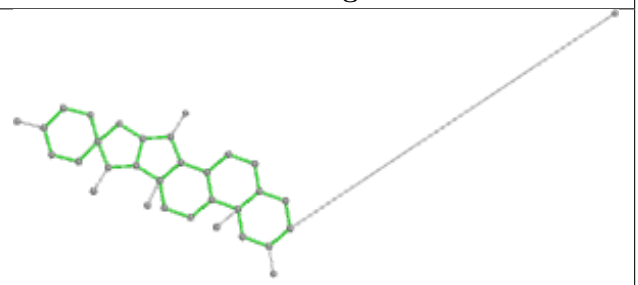
Bond lengths



Bond angles

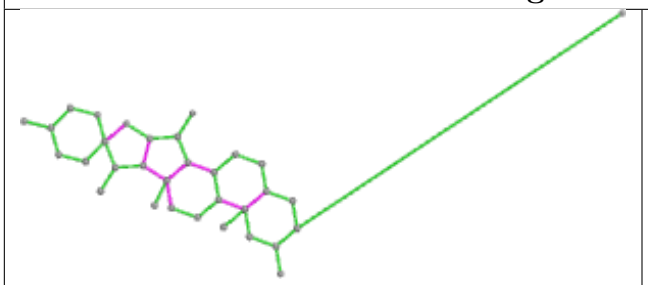


Torsions

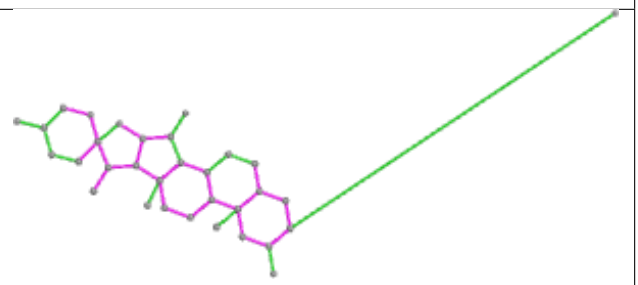


Rings

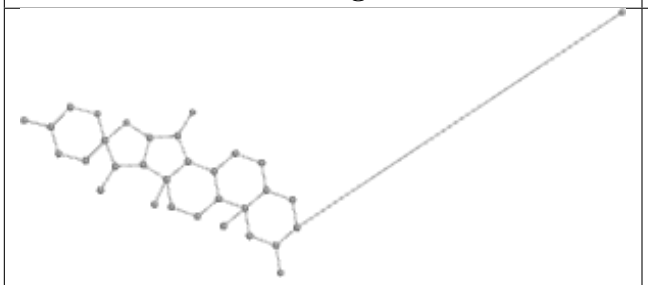
Ligand AJP A 408



Bond lengths



Bond angles



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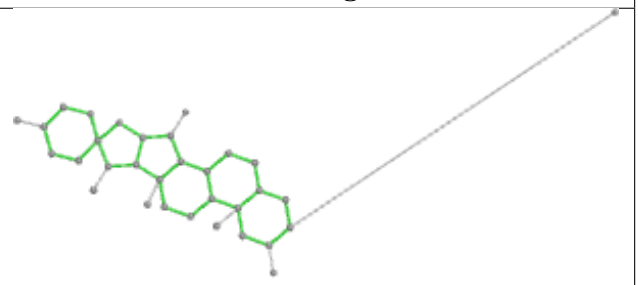
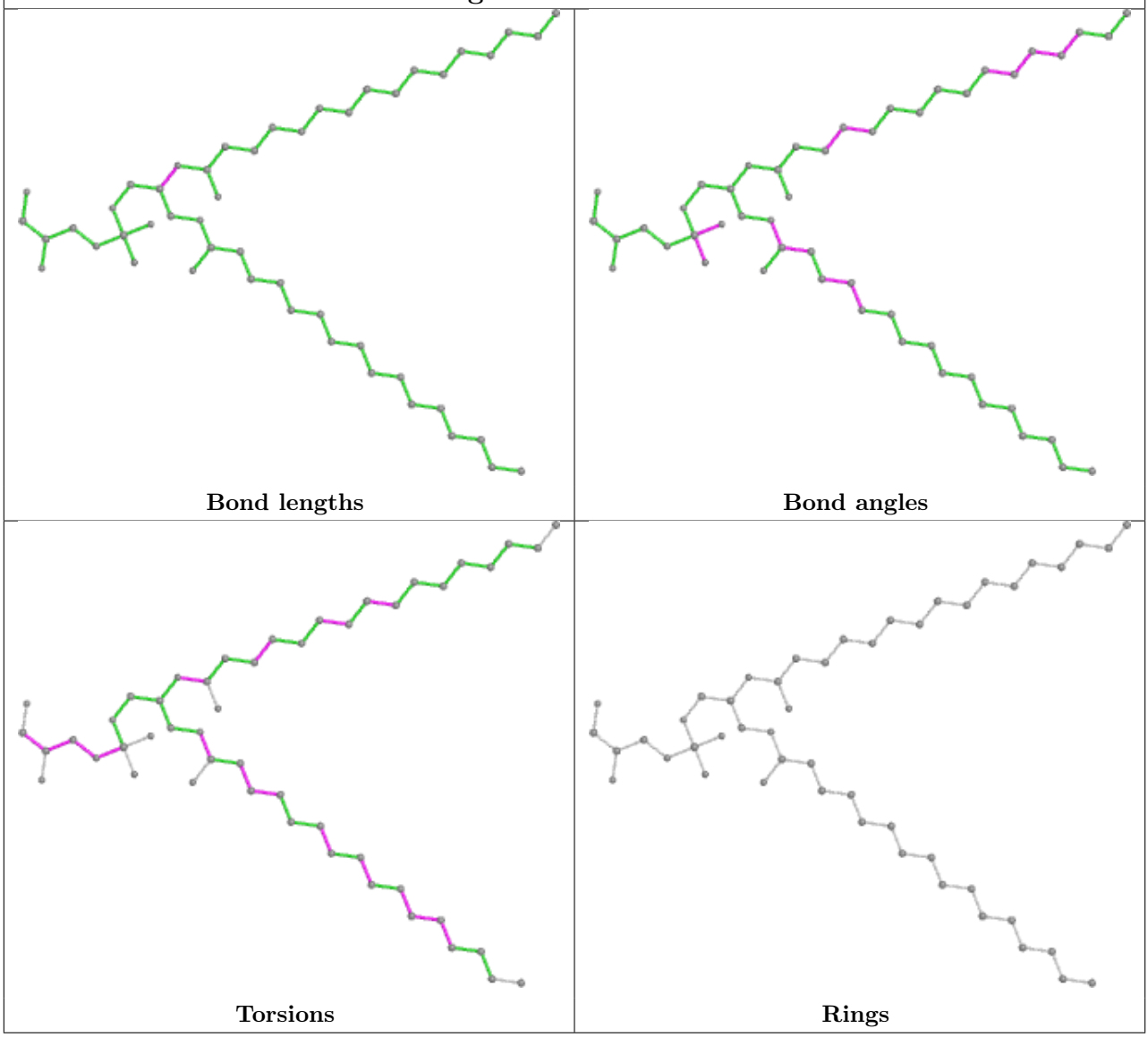
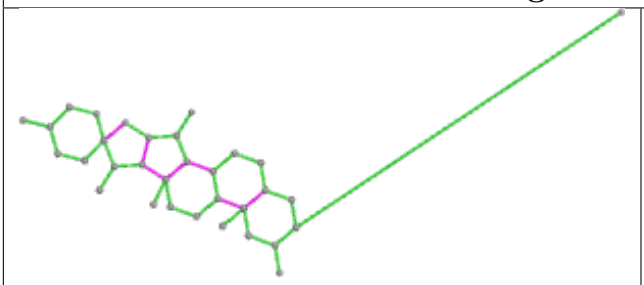
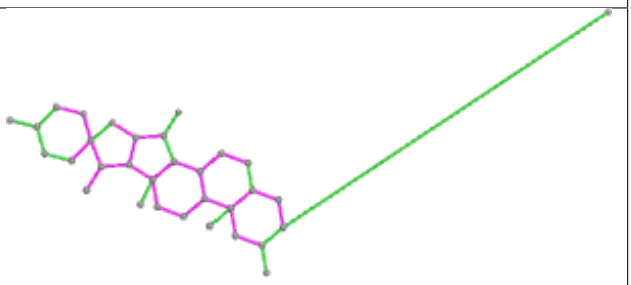
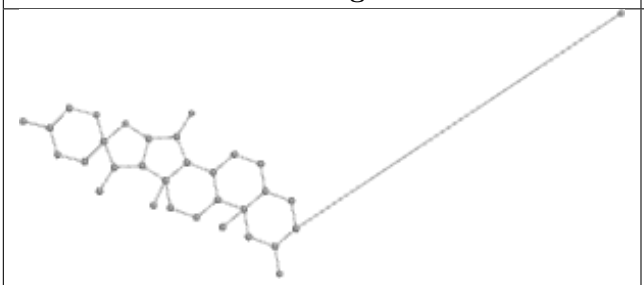
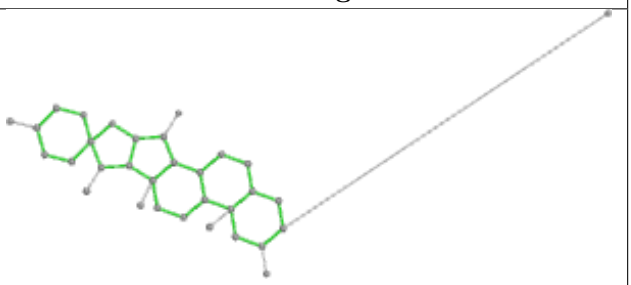


Rings

Ligand LHG A 402



Ligand AJP E 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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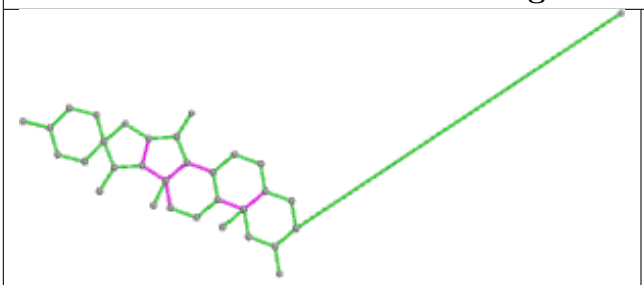
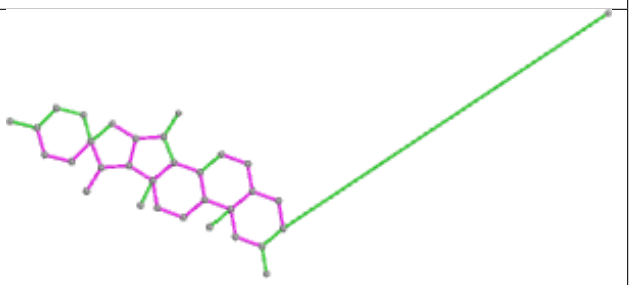
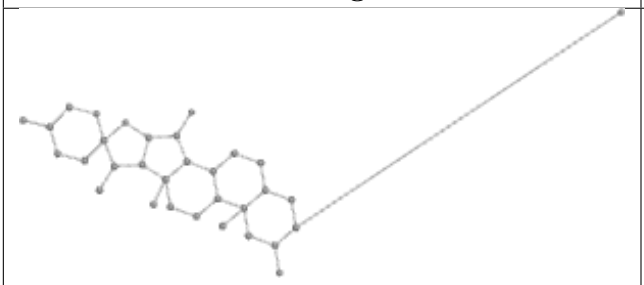
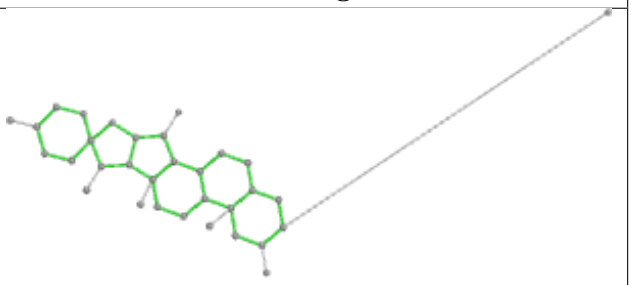
 Bond lengths	 Bond angles
 Torsions	 Rings

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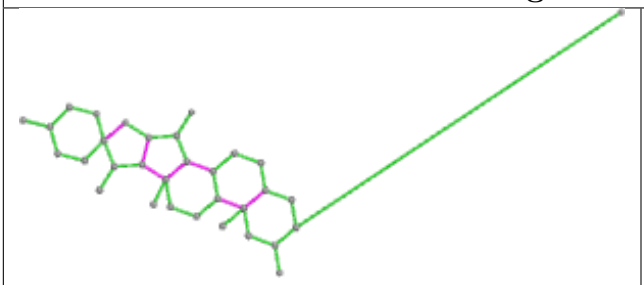
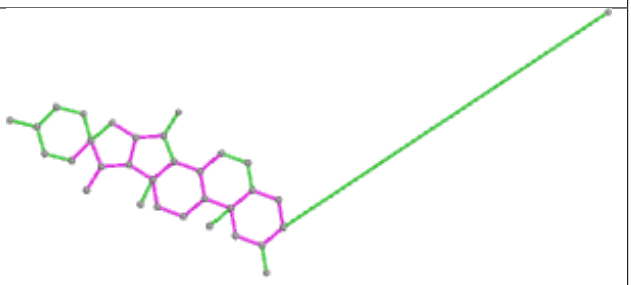
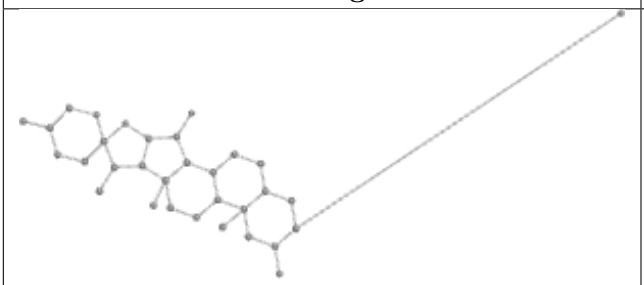
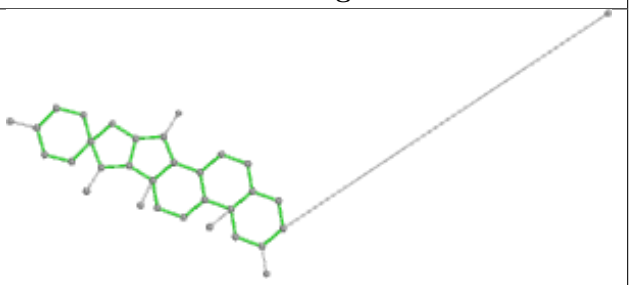
 Bond lengths	 Bond angles
 Torsions	 Rings

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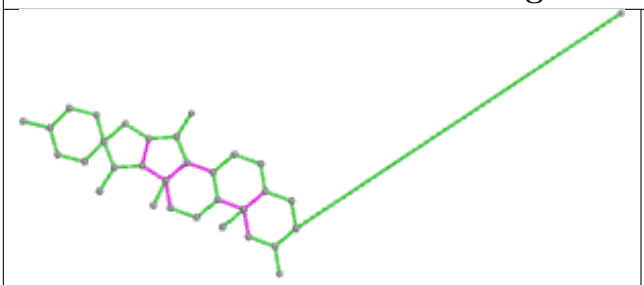
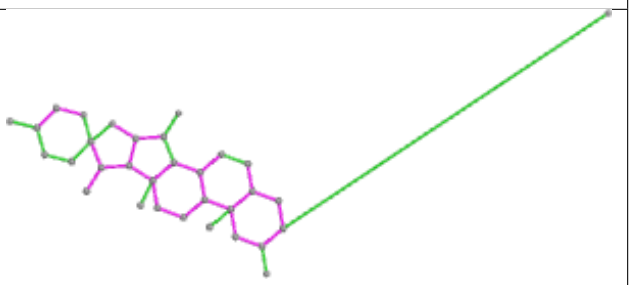
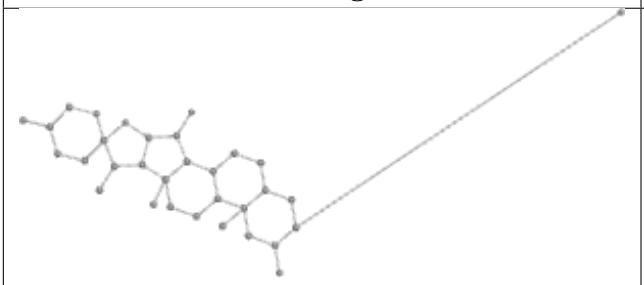
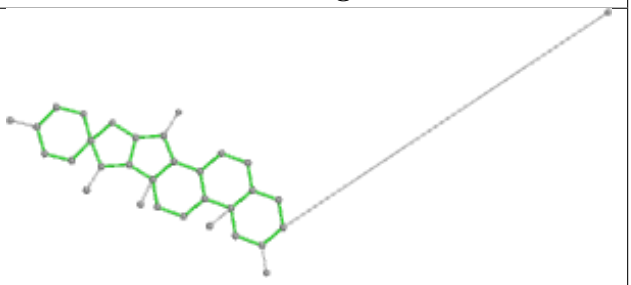
 Bond lengths	 Bond angles
 Torsions	 Rings

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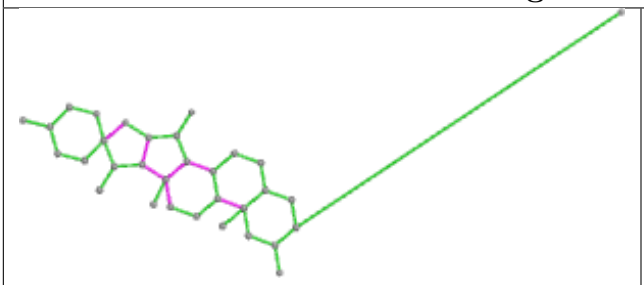
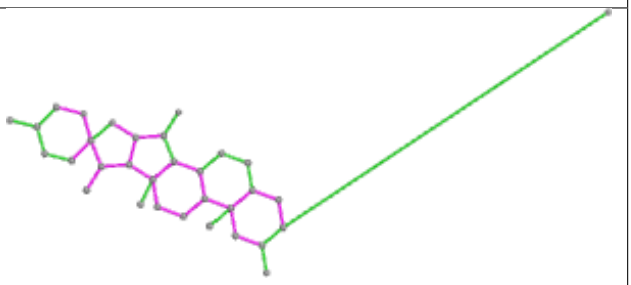
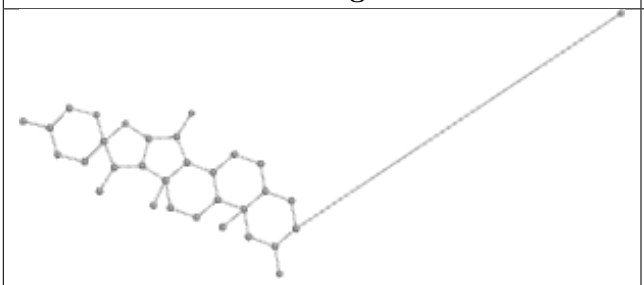
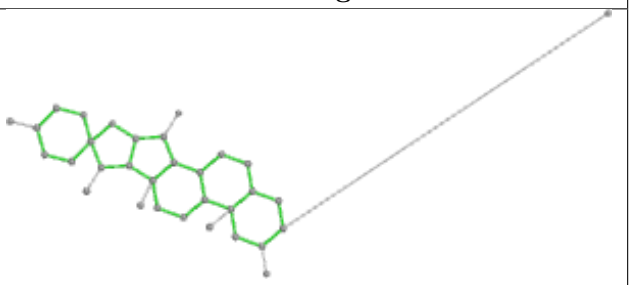
 Bond lengths	 Bond angles
 Torsions	 Rings

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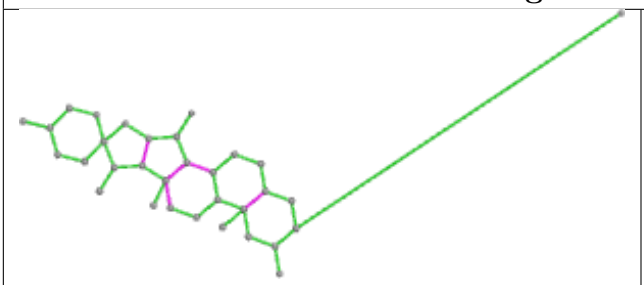
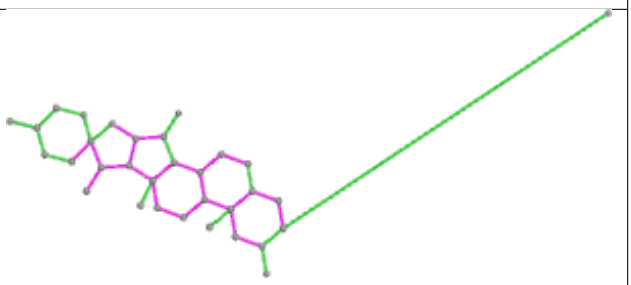
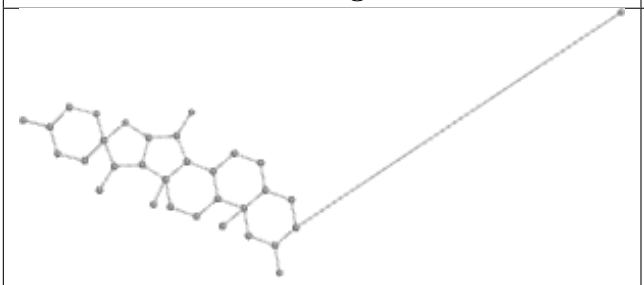
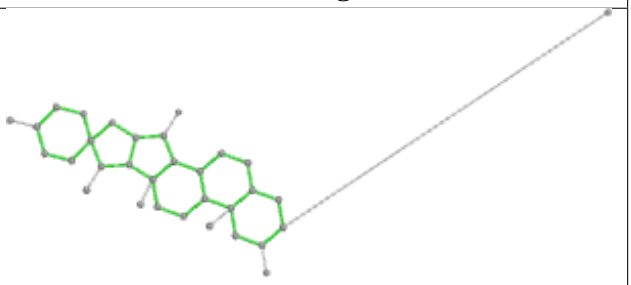
 Bond lengths	 Bond angles
 Torsions	 Rings

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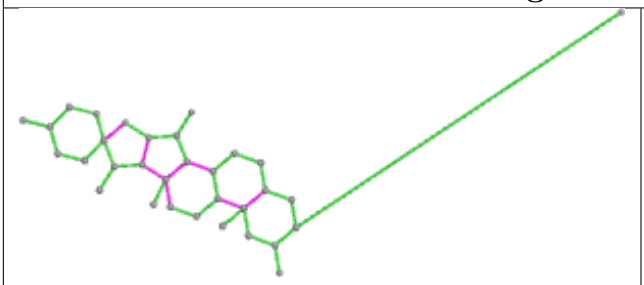
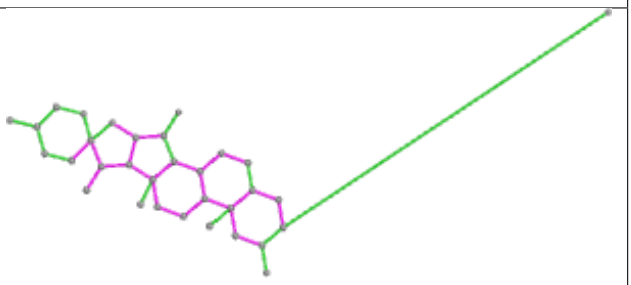
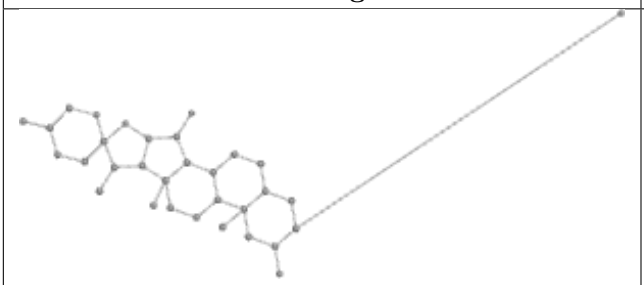
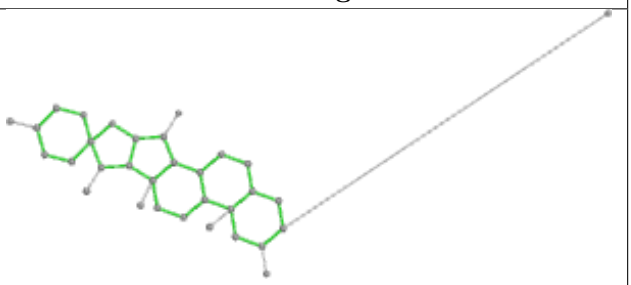
 Bond lengths	 Bond angles
 Torsions	 Rings

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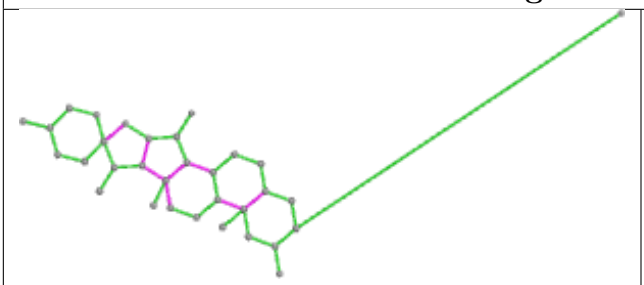
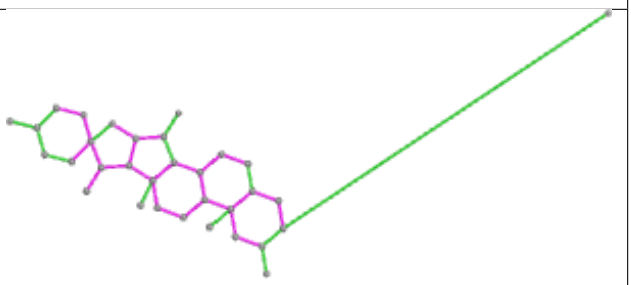
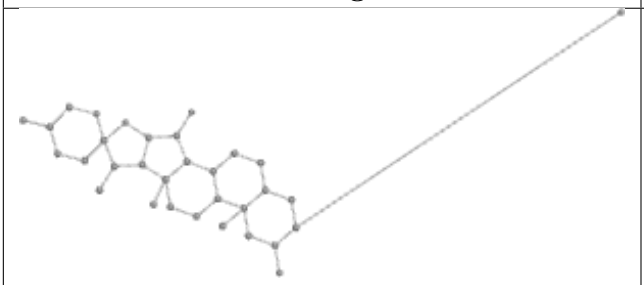
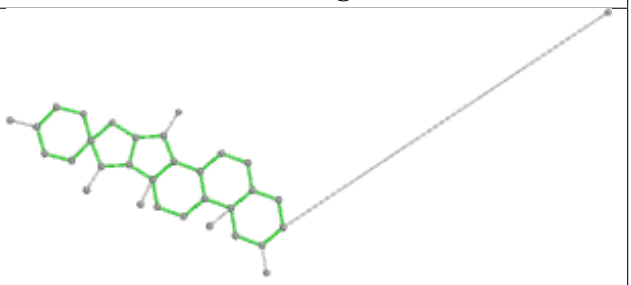
 Bond lengths	 Bond angles
 Torsions	 Rings

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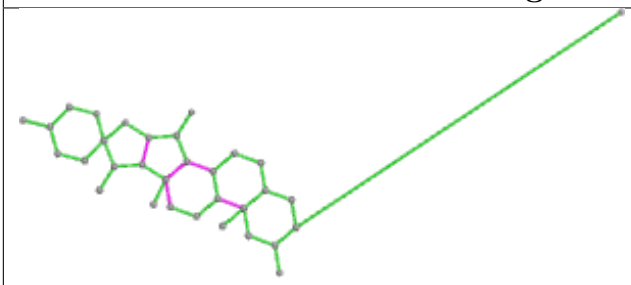
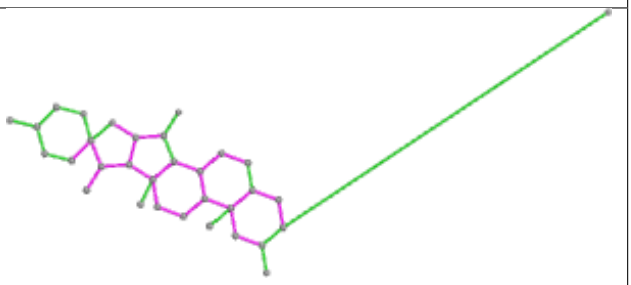
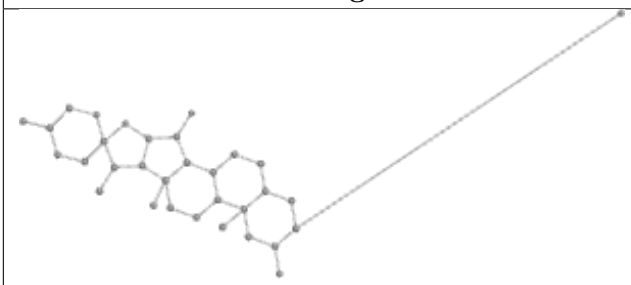
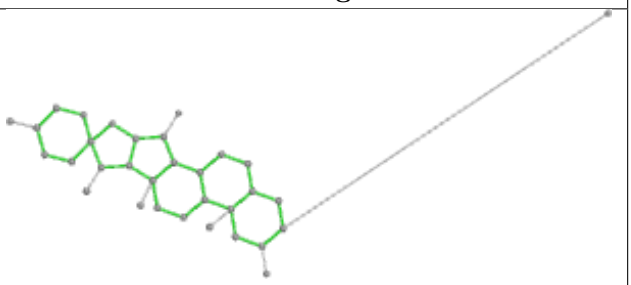
 Bond lengths	 Bond angles
 Torsions	 Rings

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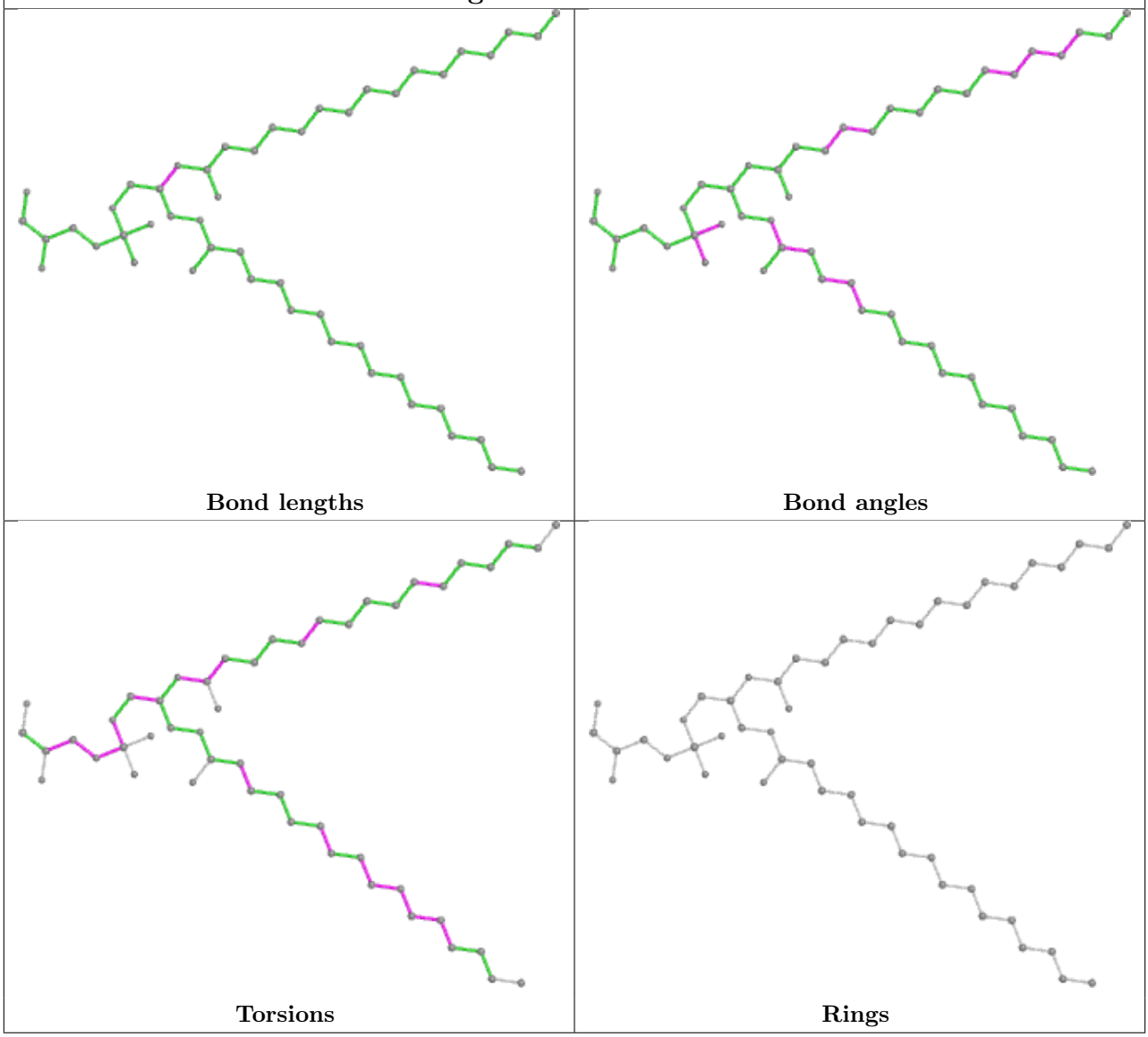
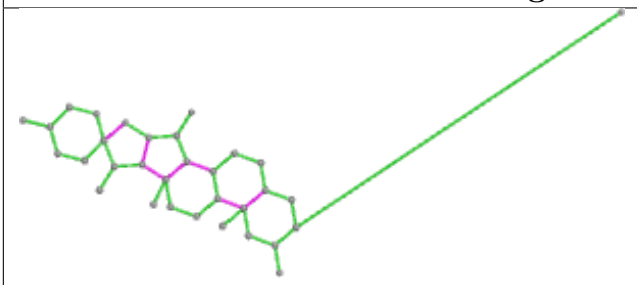
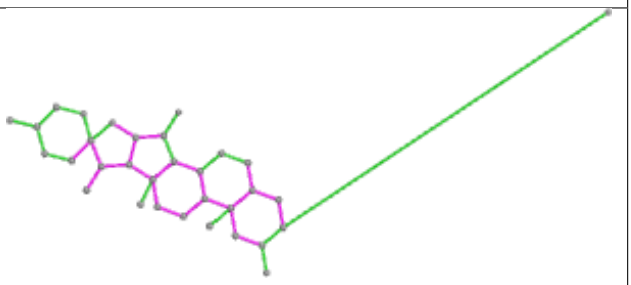
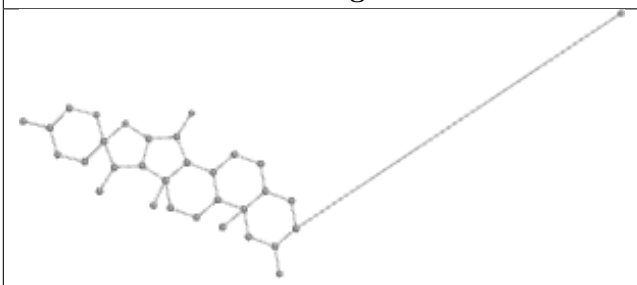
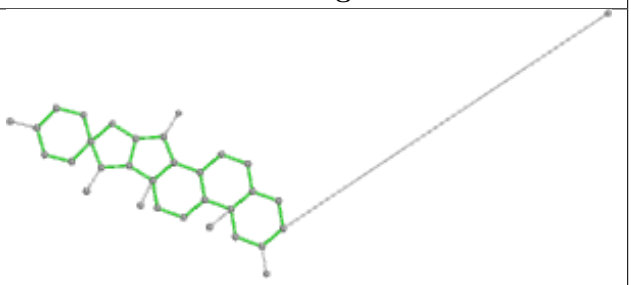


Ligand AJP F 713	
 Bond lengths	 Bond angles
 Torsions	 Rings

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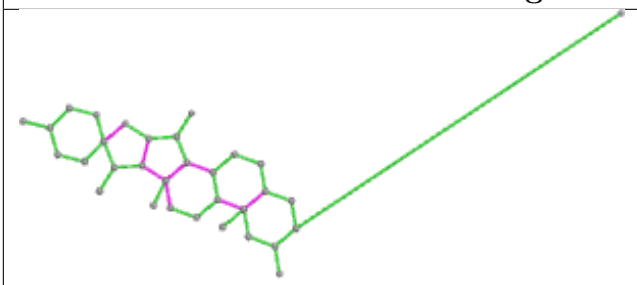
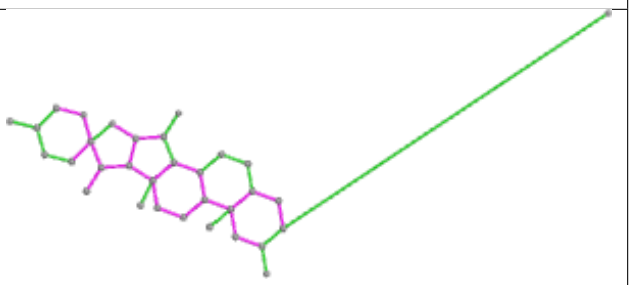
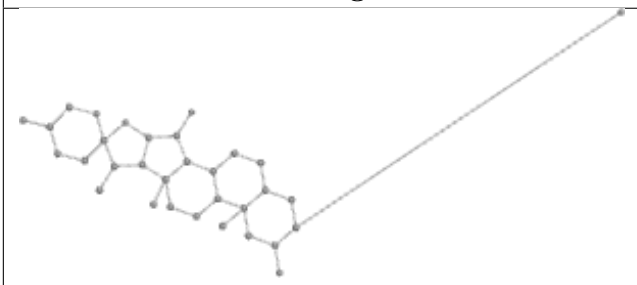
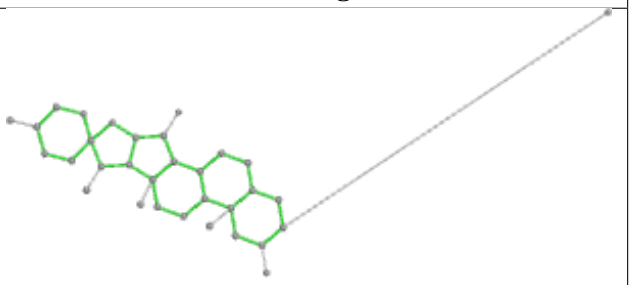
 Bond lengths	 Bond angles
 Torsions	 Rings

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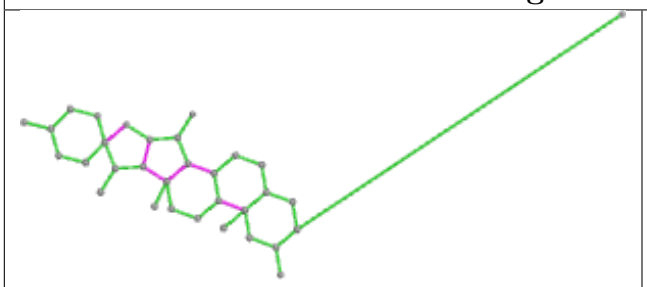
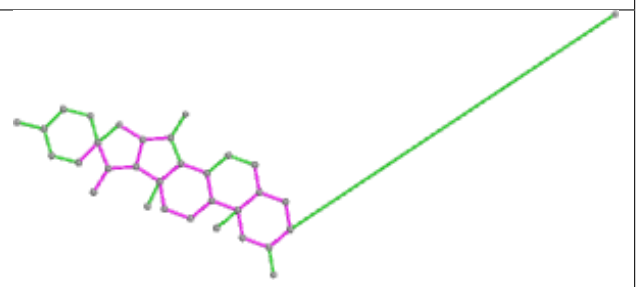
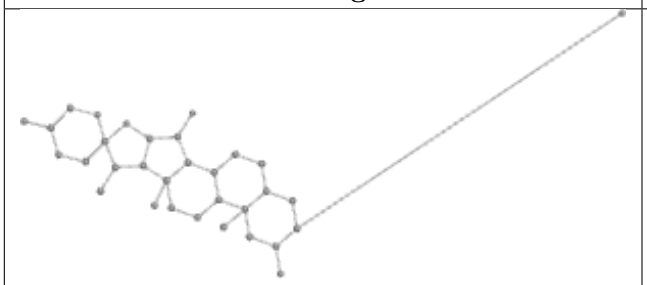


Bond lengths



Bond angles



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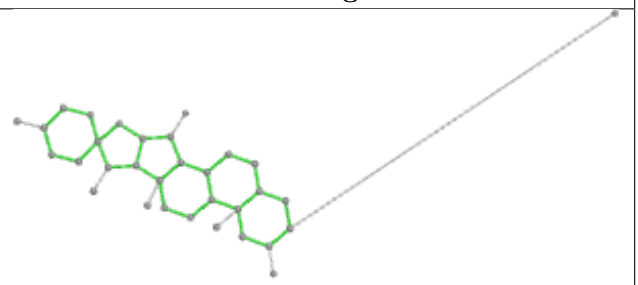

Rings

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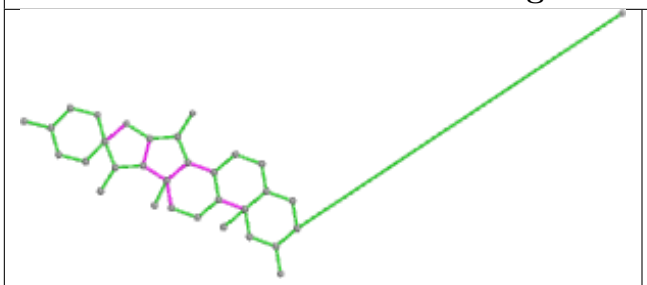

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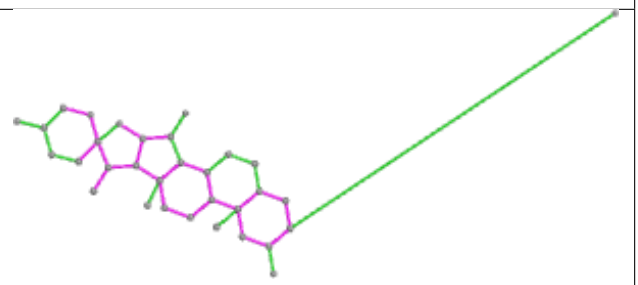

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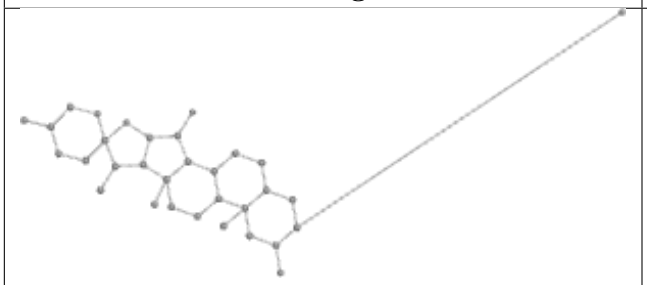

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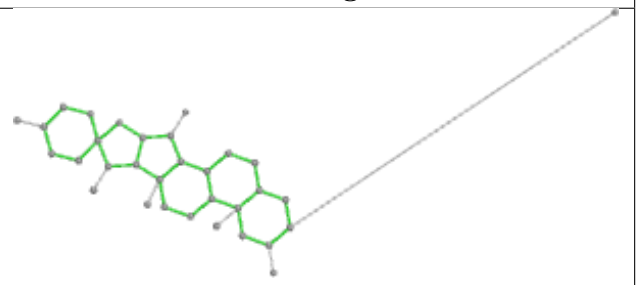
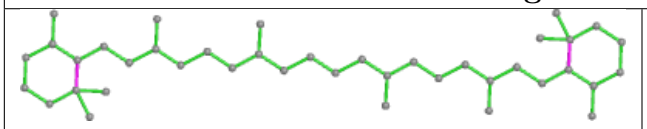


Rings

Ligand BCR P 101



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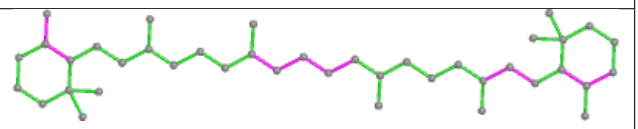

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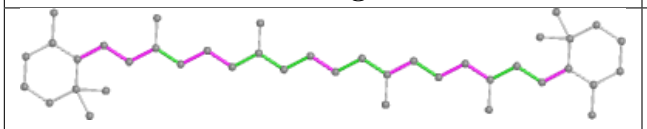

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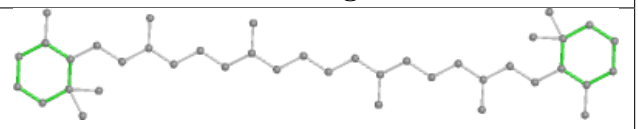

Rings

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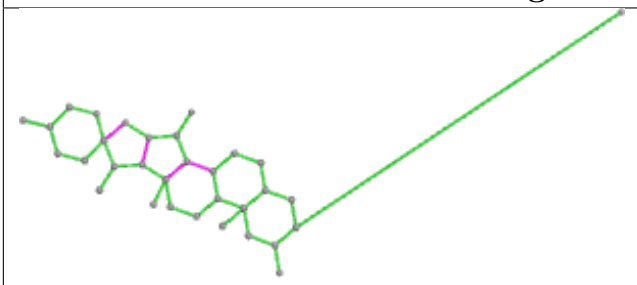
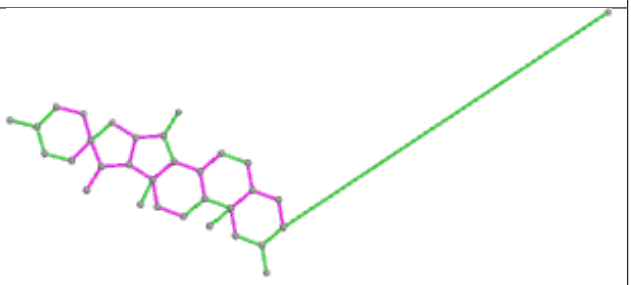
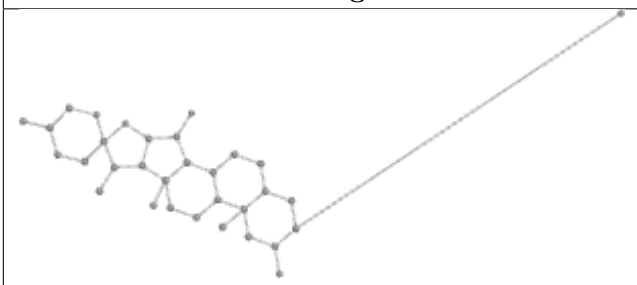
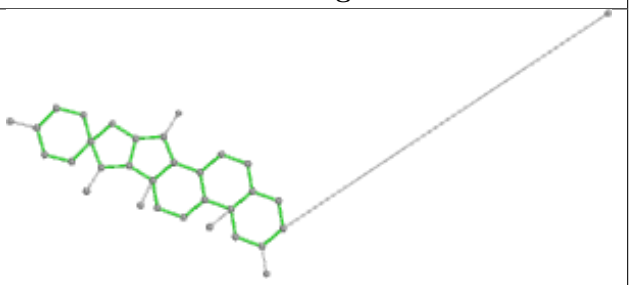
 Bond lengths	 Bond angles
 Torsions	 Rings

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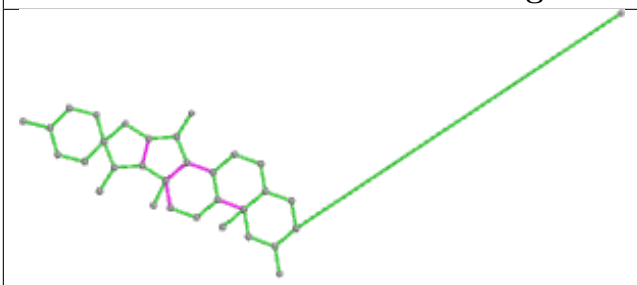
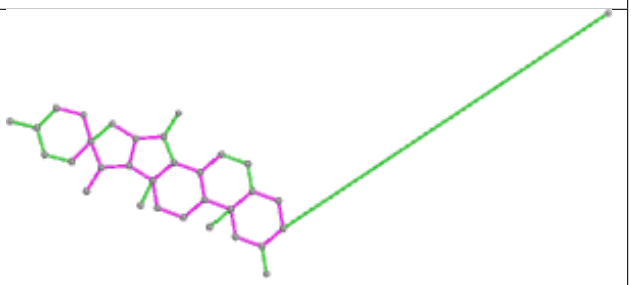
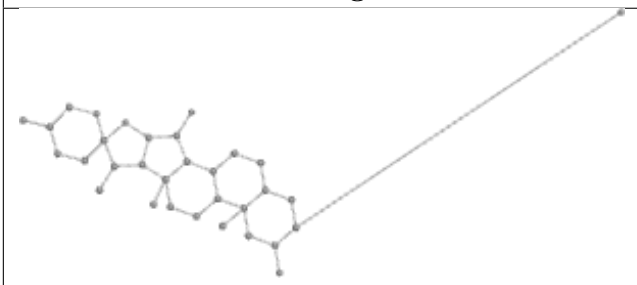
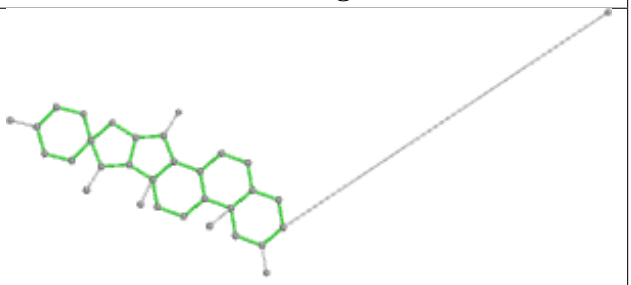
 Bond lengths	 Bond angles
 Torsions	 Rings

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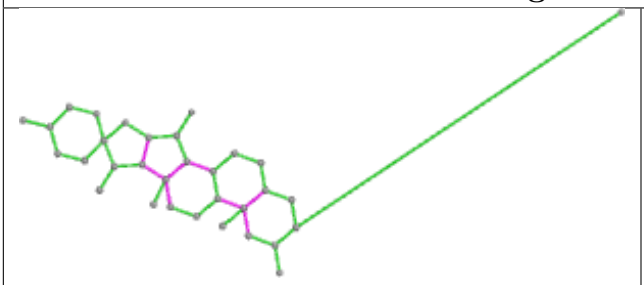
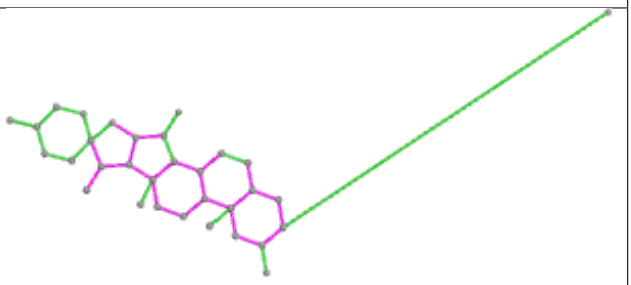
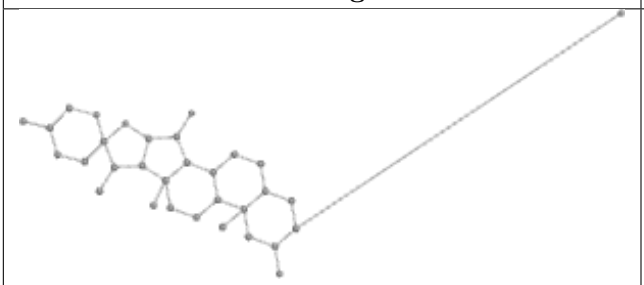
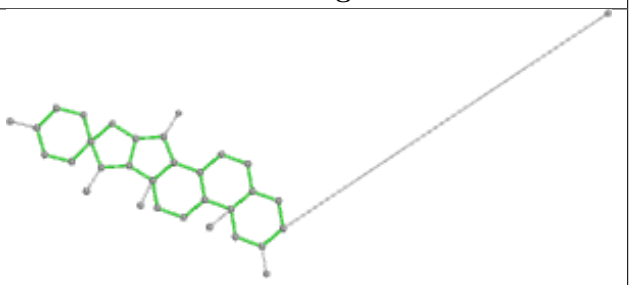
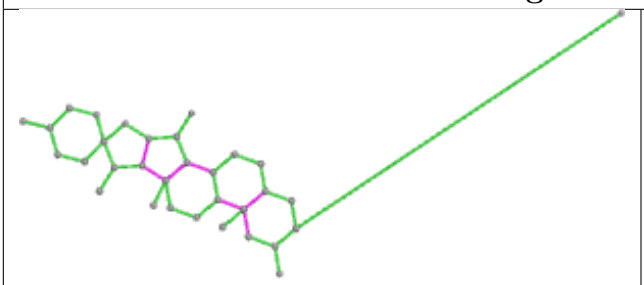
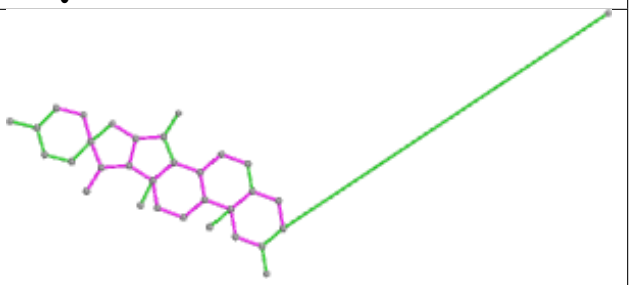
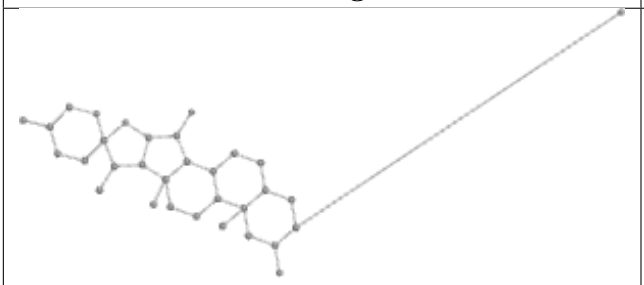
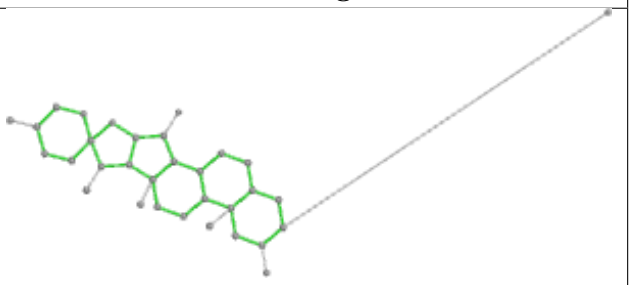
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AJP Q 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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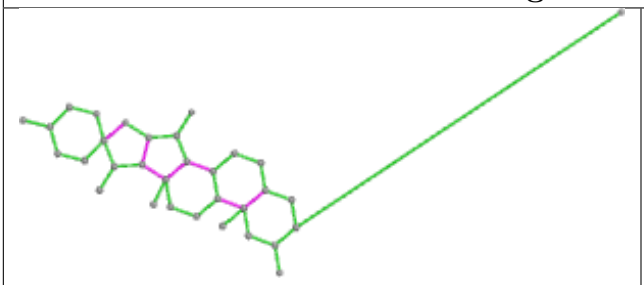
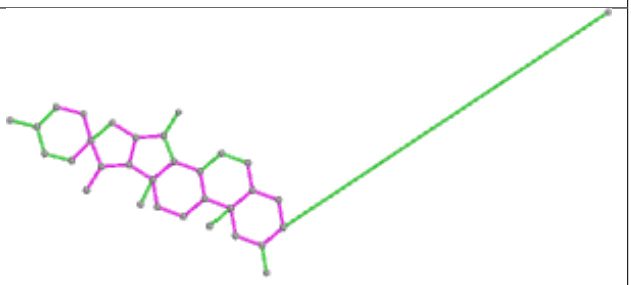
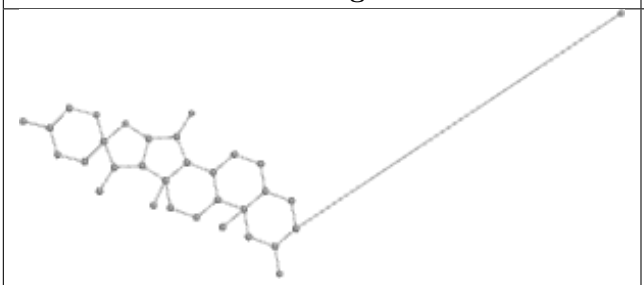
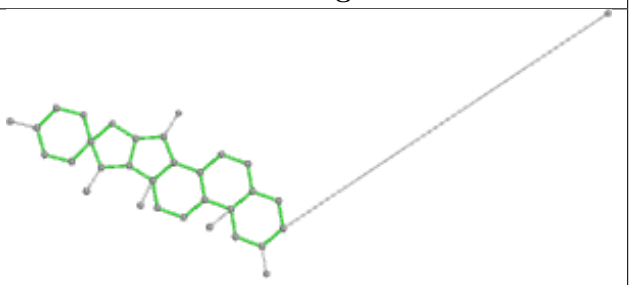
 Bond lengths	 Bond angles
 Torsions	 Rings

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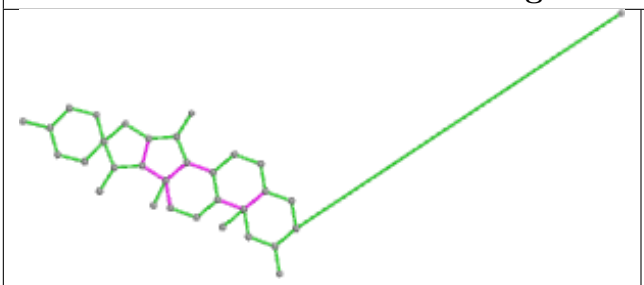
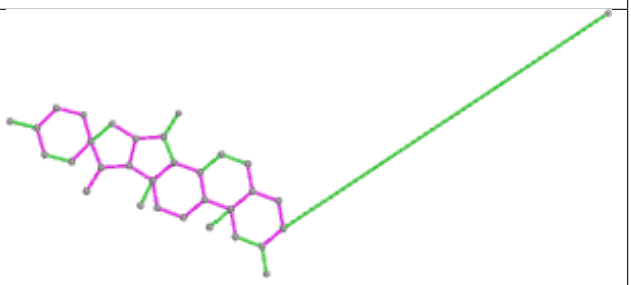
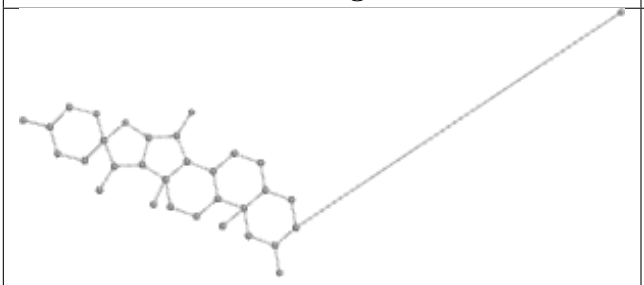
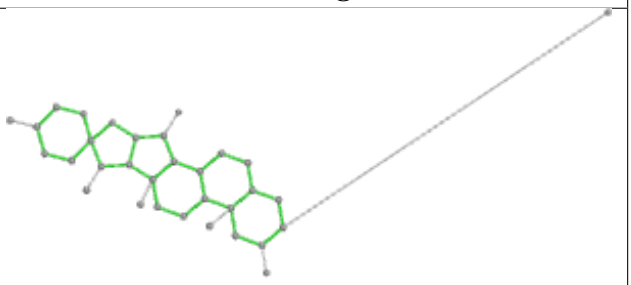
 Bond lengths	 Bond angles
 Torsions	 Rings

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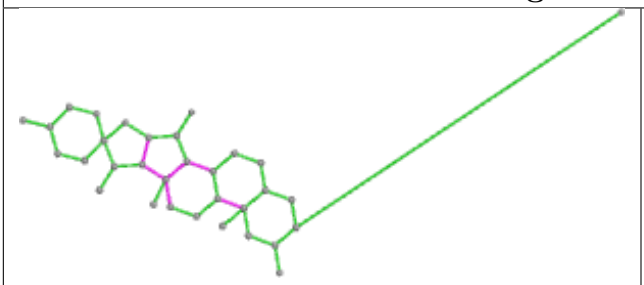
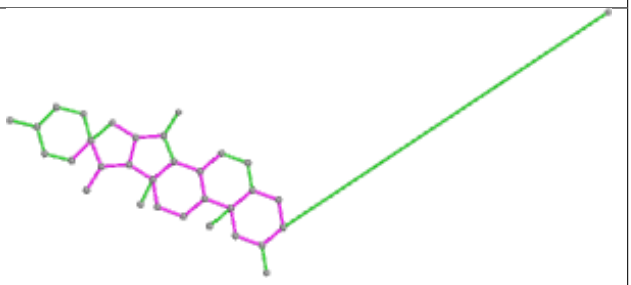
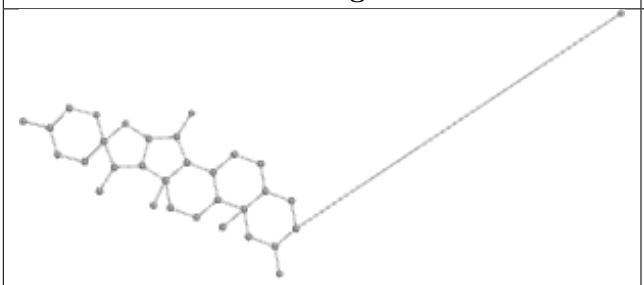
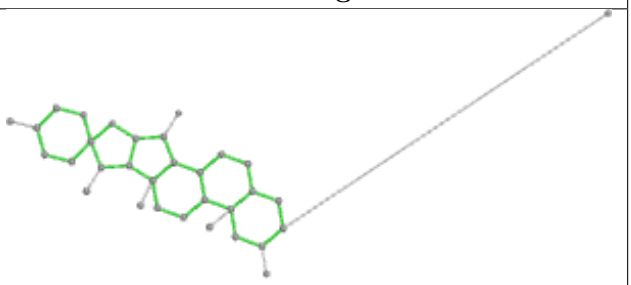
 Bond lengths	 Bond angles
 Torsions	 Rings

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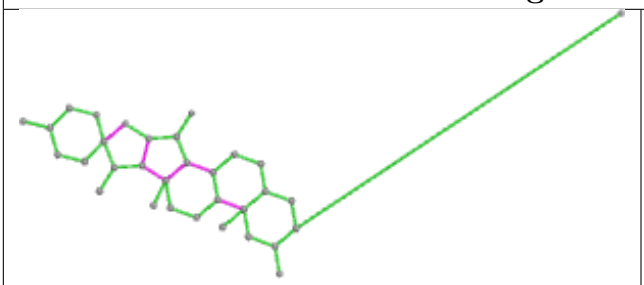
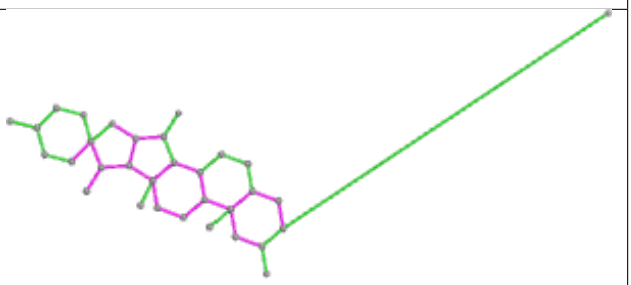
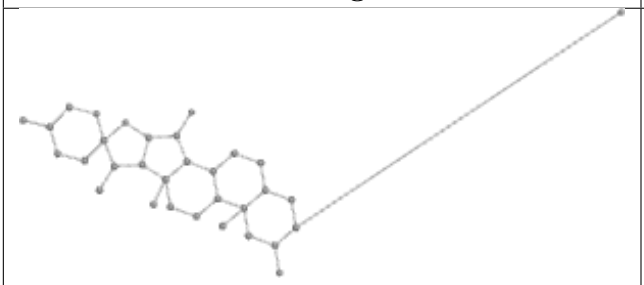
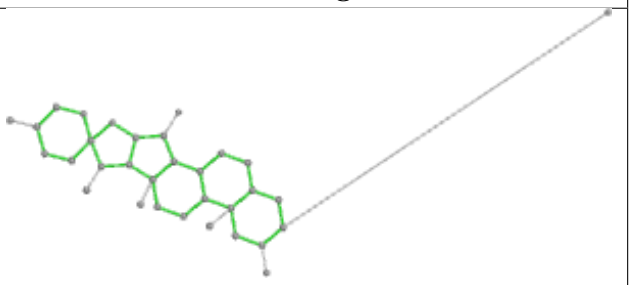
 Bond lengths	 Bond angles
 Torsions	 Rings

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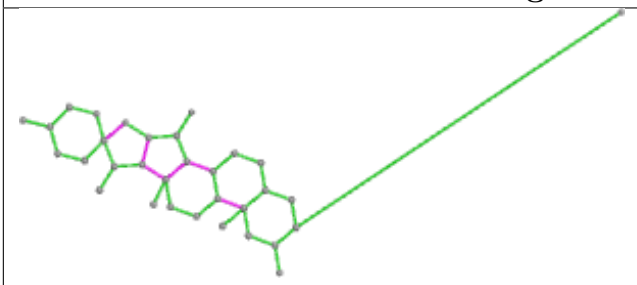
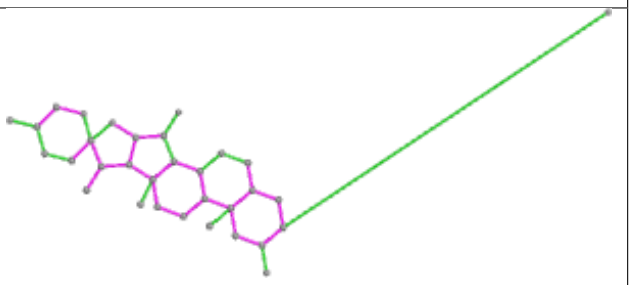
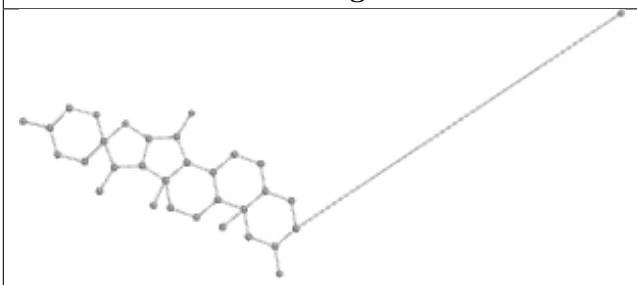
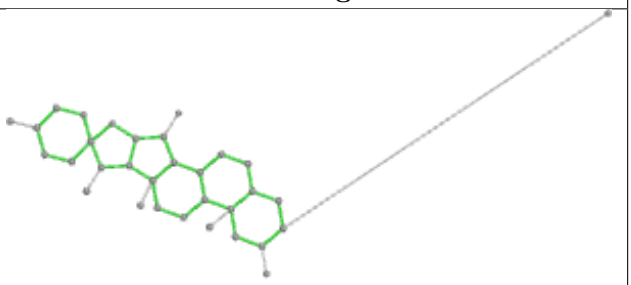
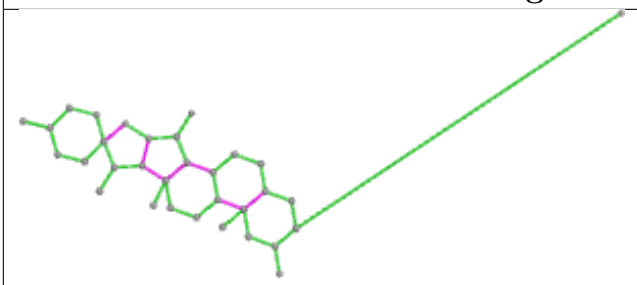
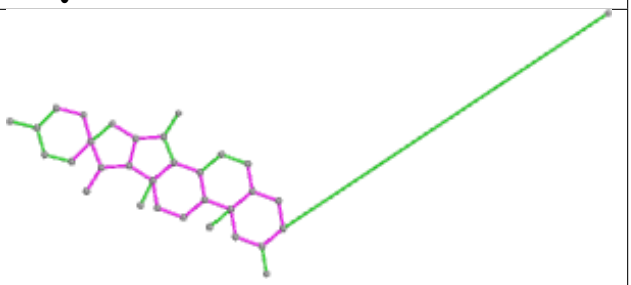
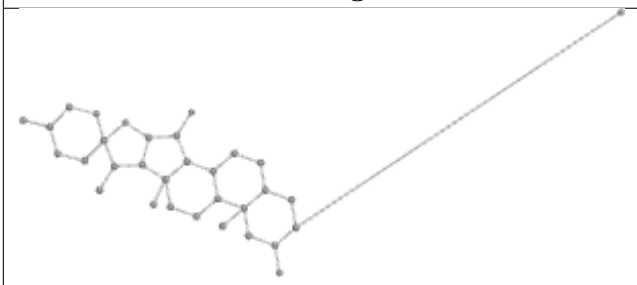
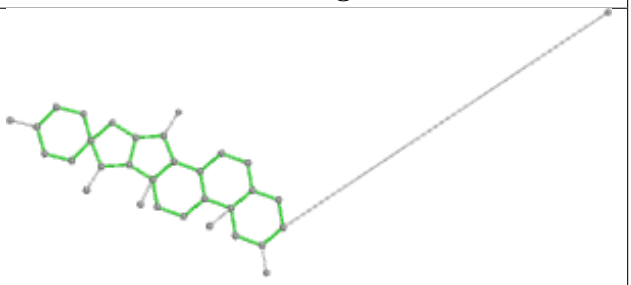
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AJP Q 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

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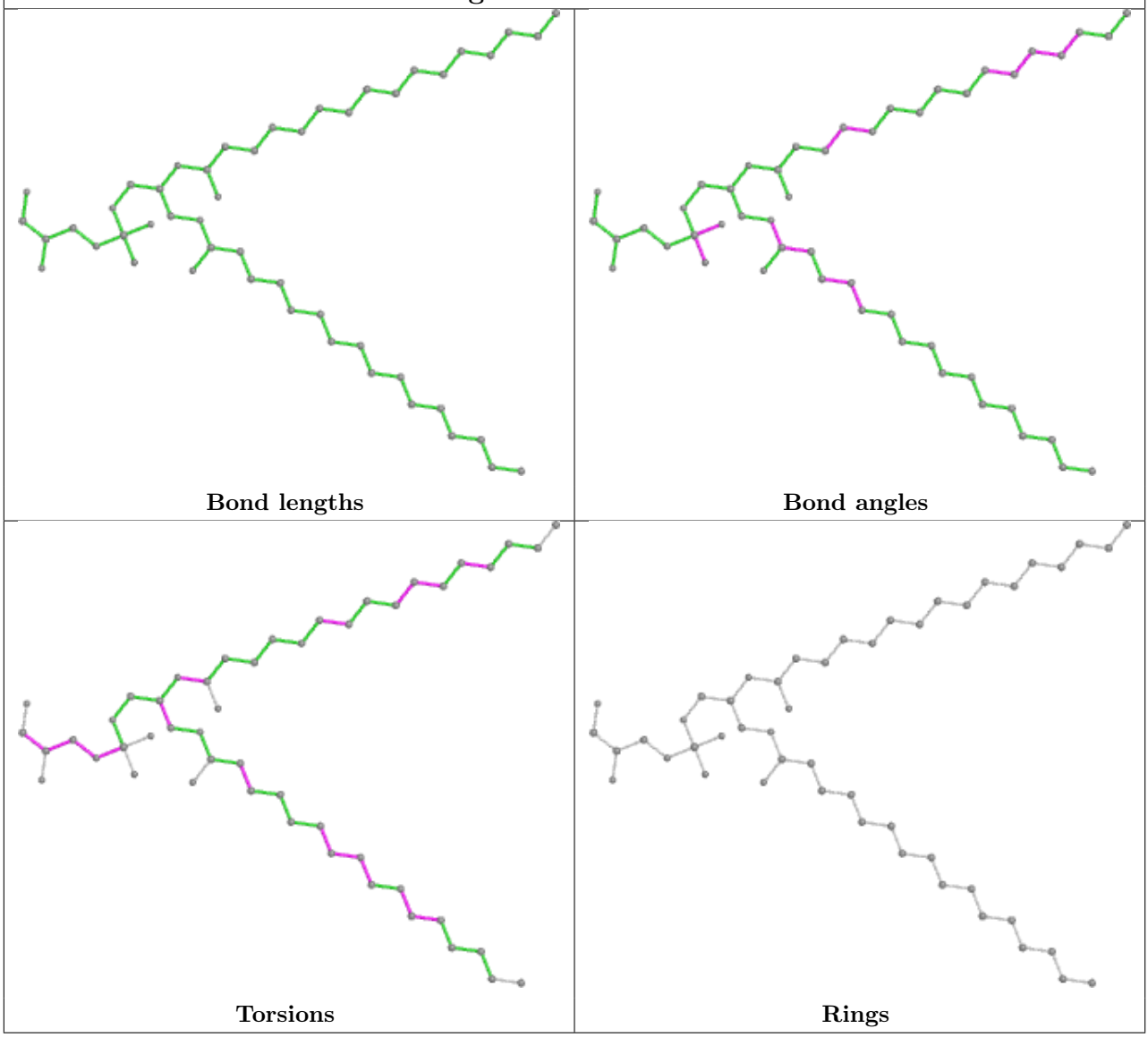
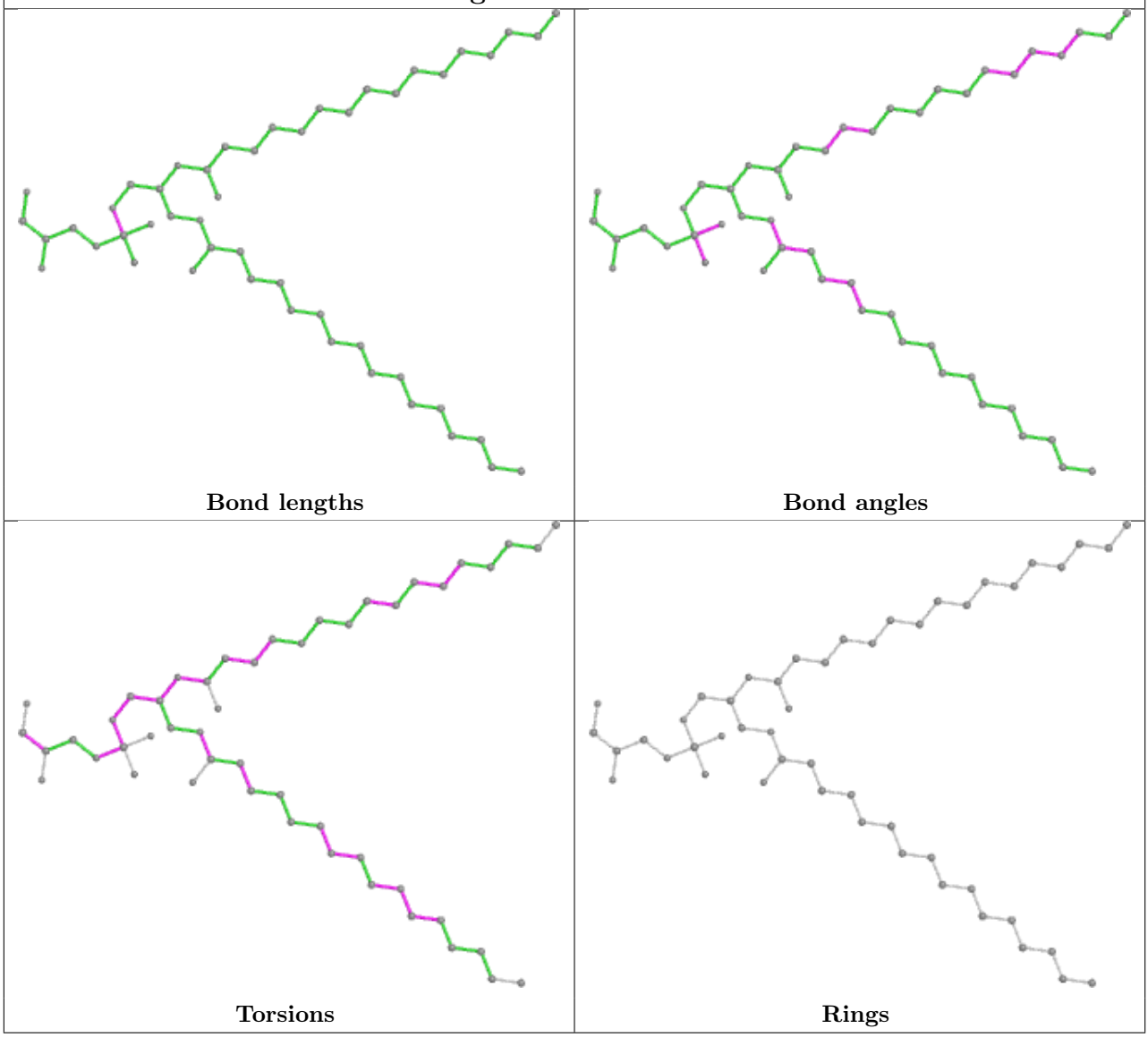
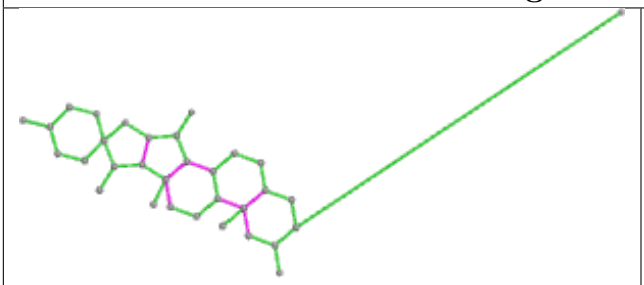
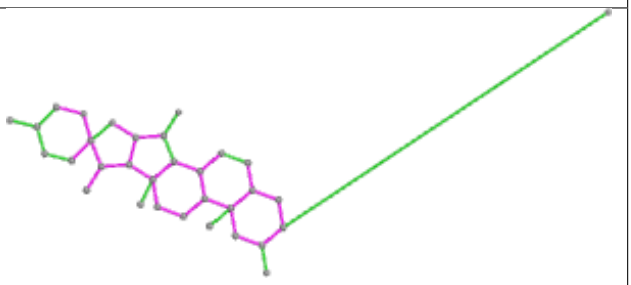
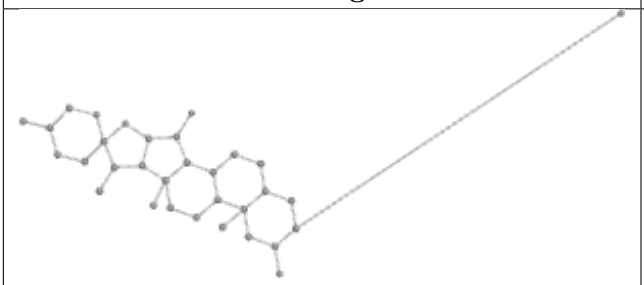
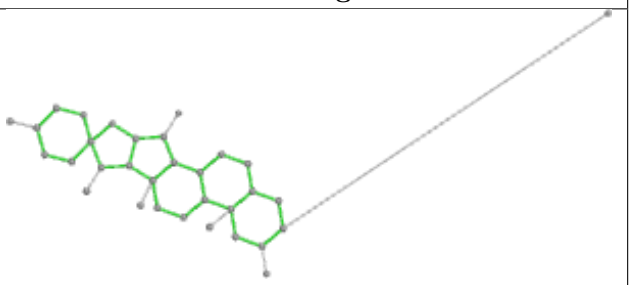


Ligand LHG F 702



Ligand AJP D 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

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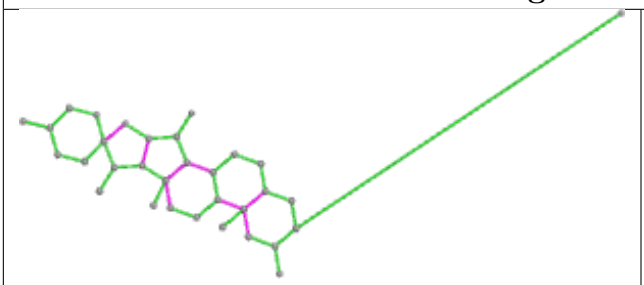
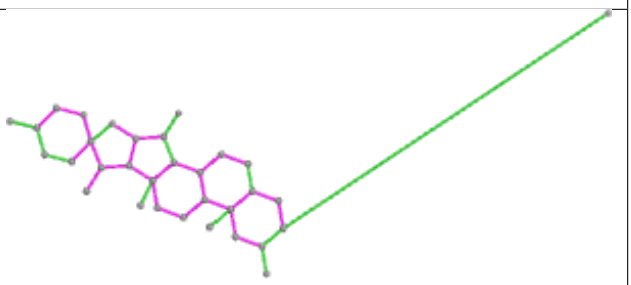
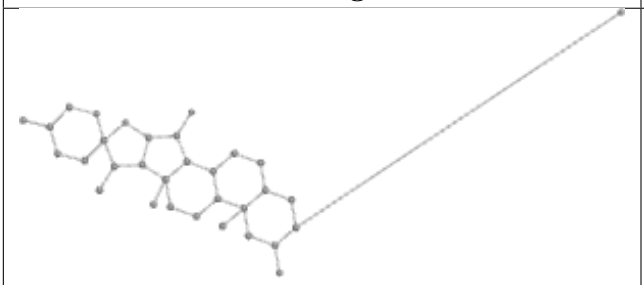
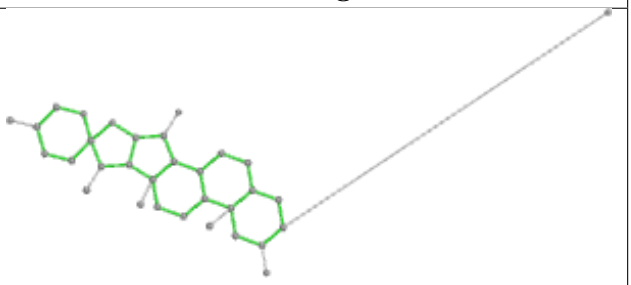
 Bond lengths	 Bond angles
 Torsions	 Rings

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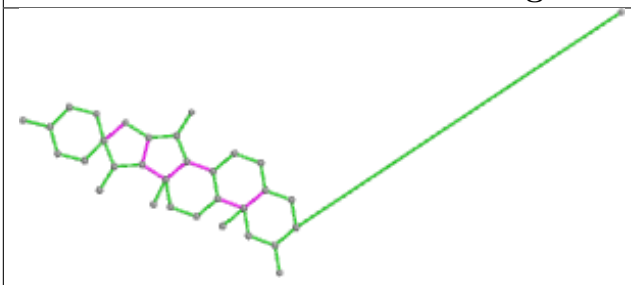
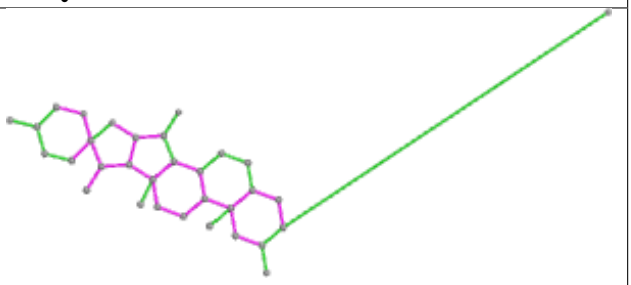
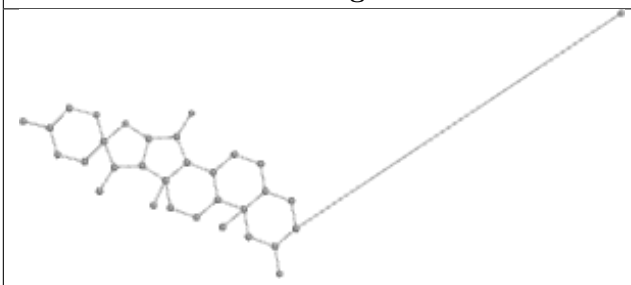
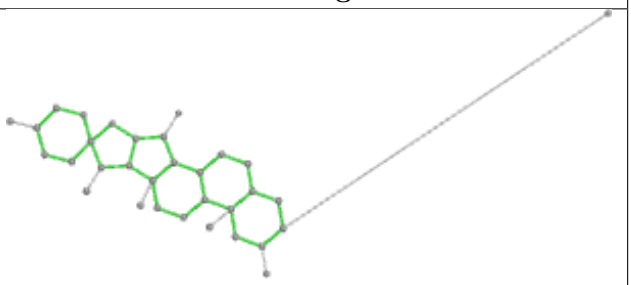
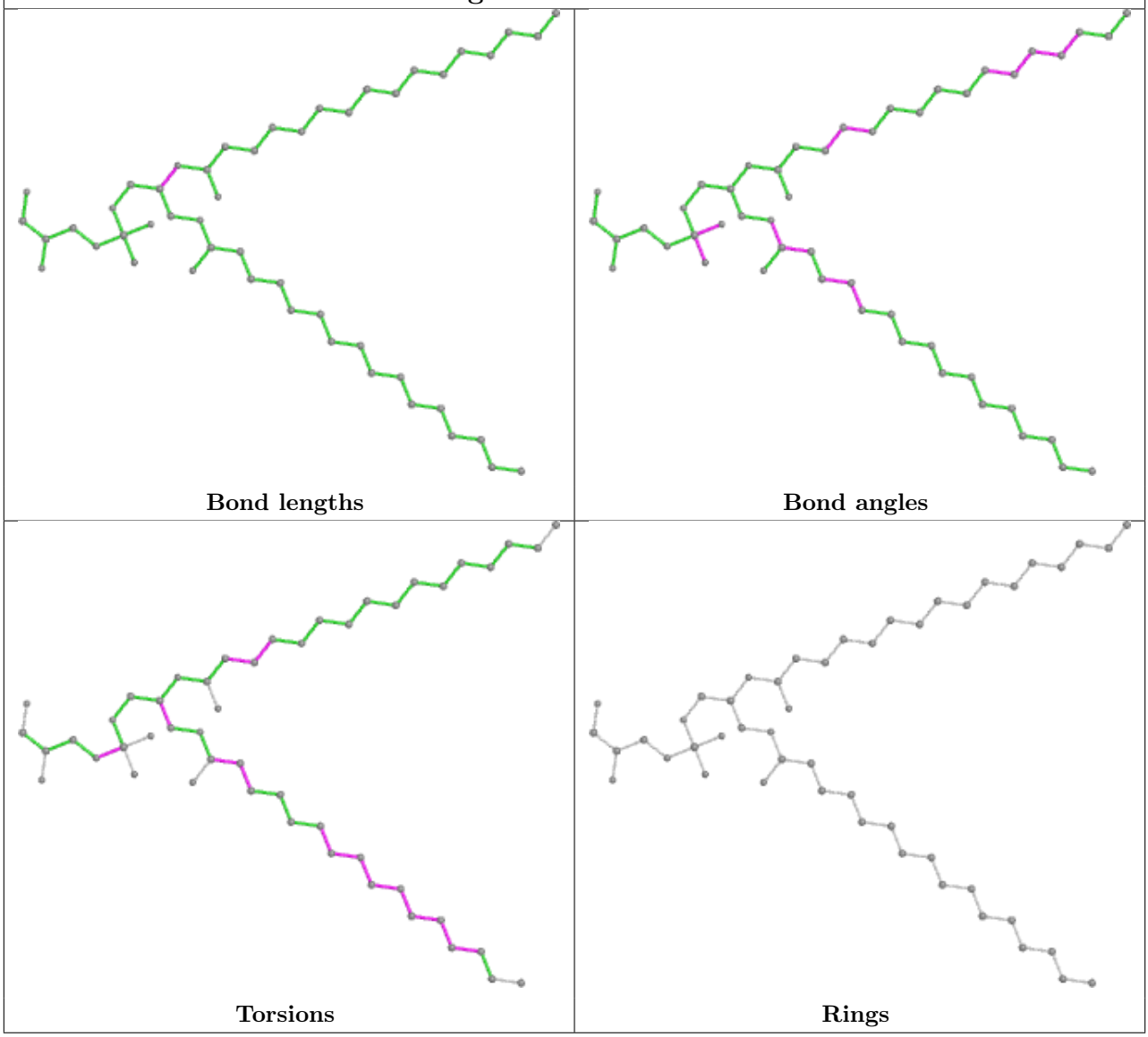
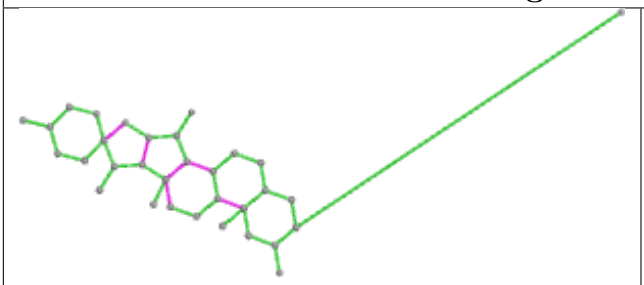
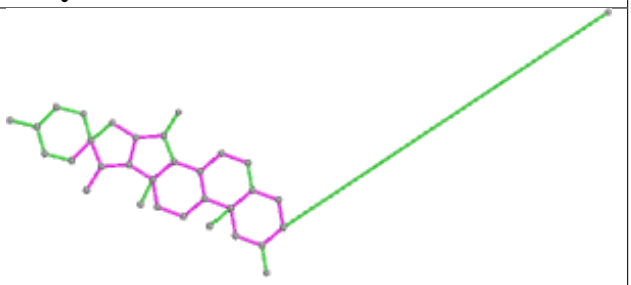
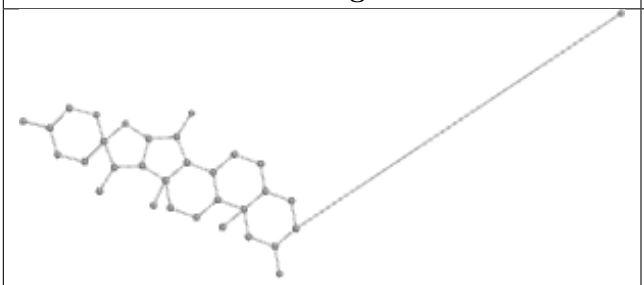
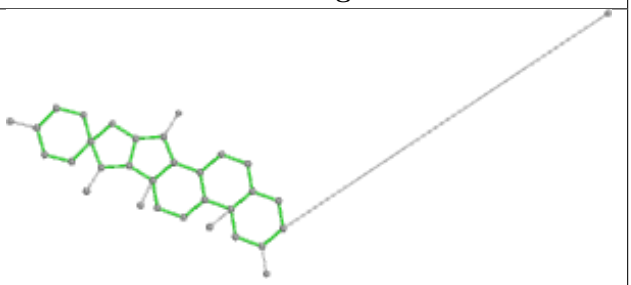
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG D 601



Ligand AJP Q 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

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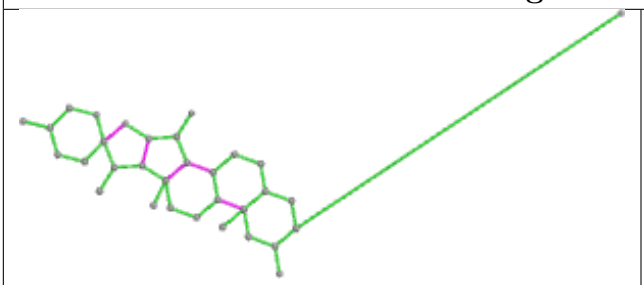
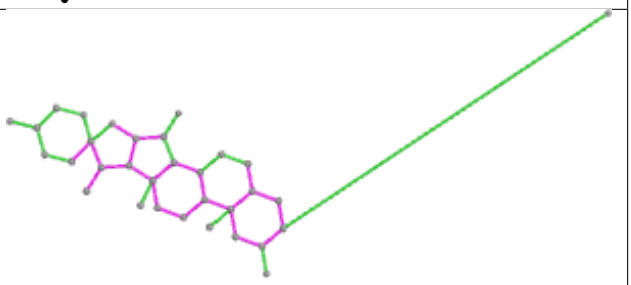
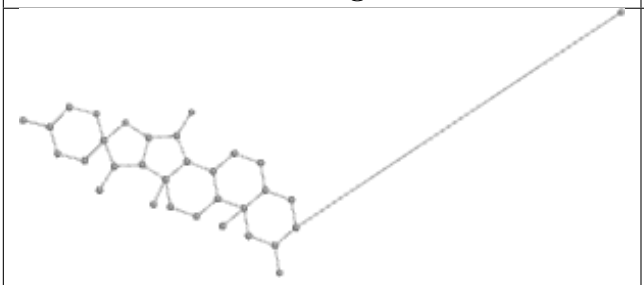
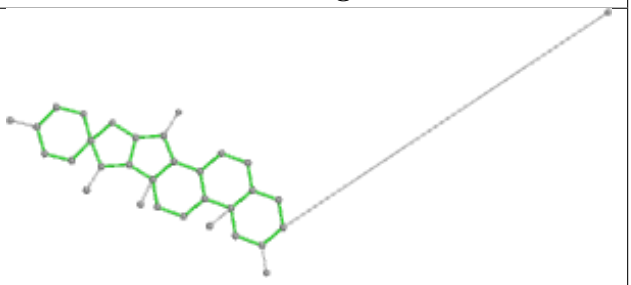
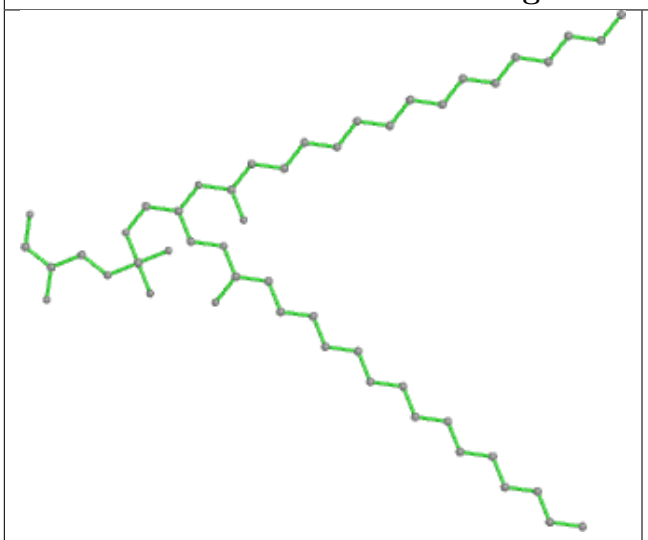
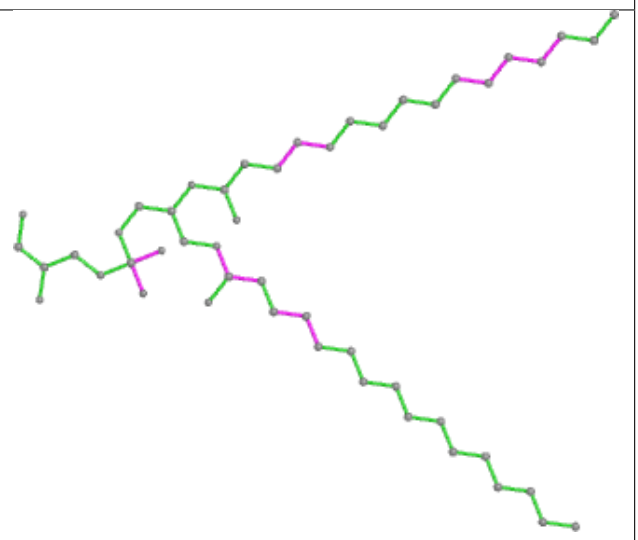
 Bond lengths	 Bond angles
 Torsions	 Rings

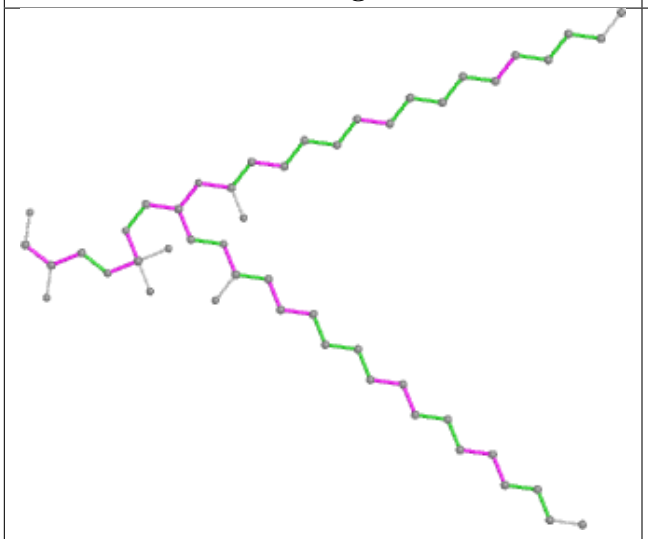
Ligand LHG H 401



Bond lengths



Bond angles



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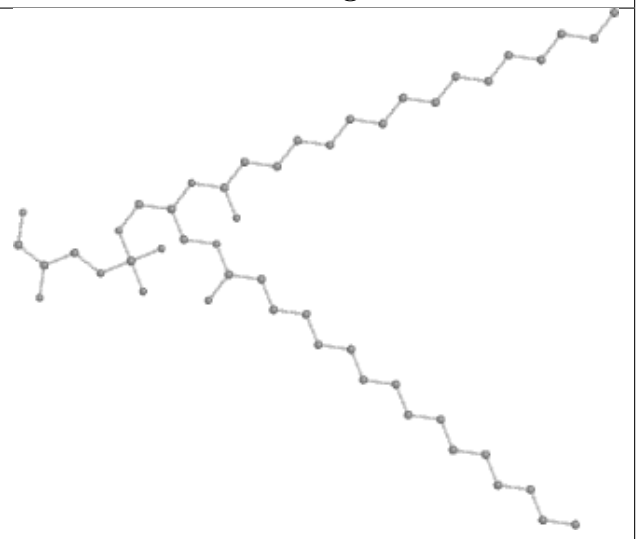
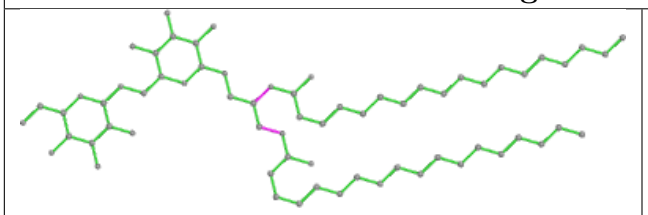
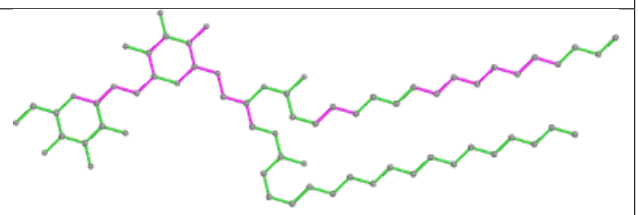


Rings

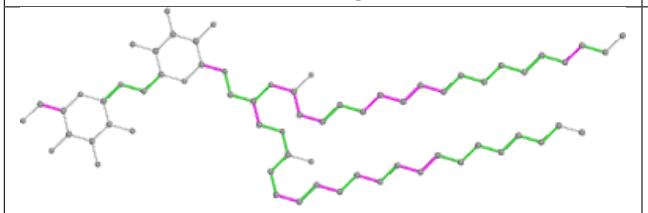
Ligand DGD A 403



Bond lengths



Bond angles



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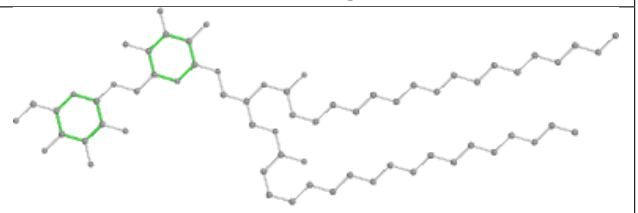
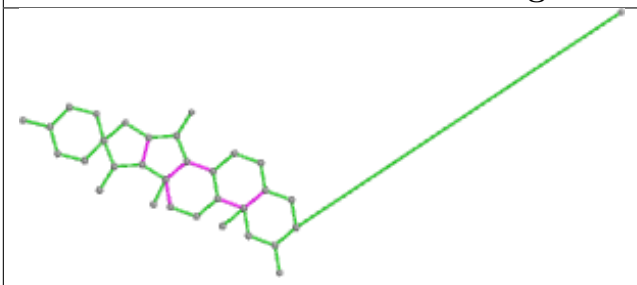
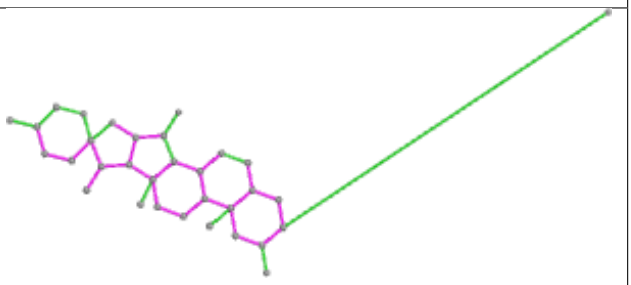
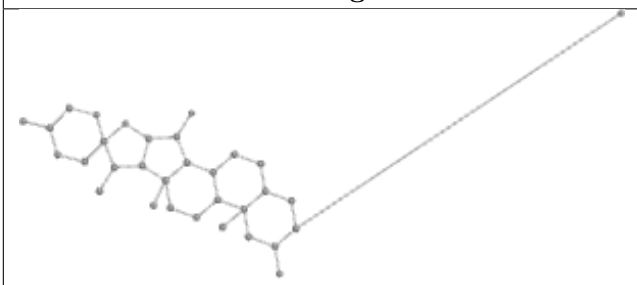
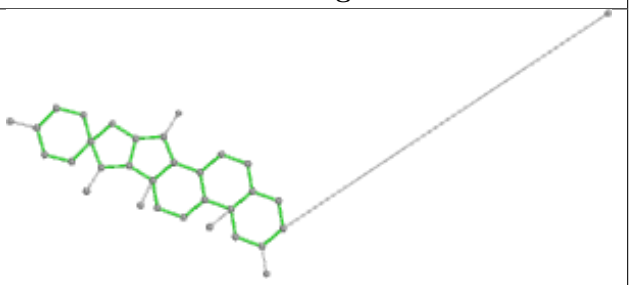
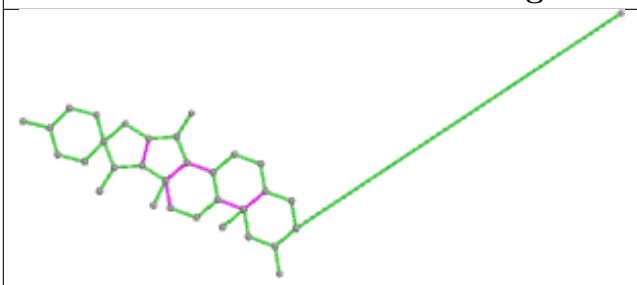
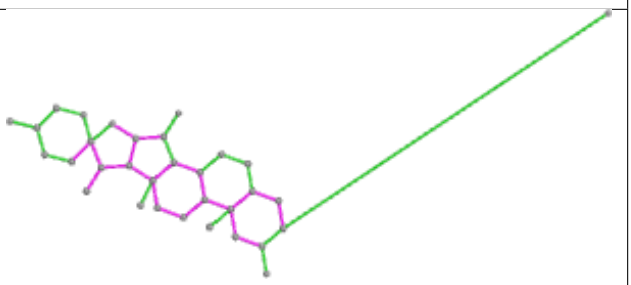
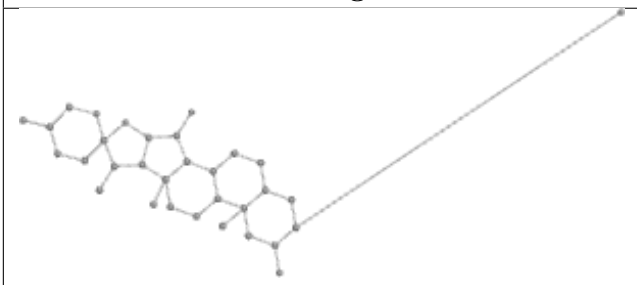
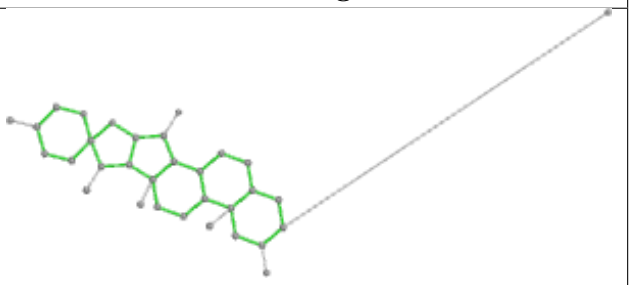
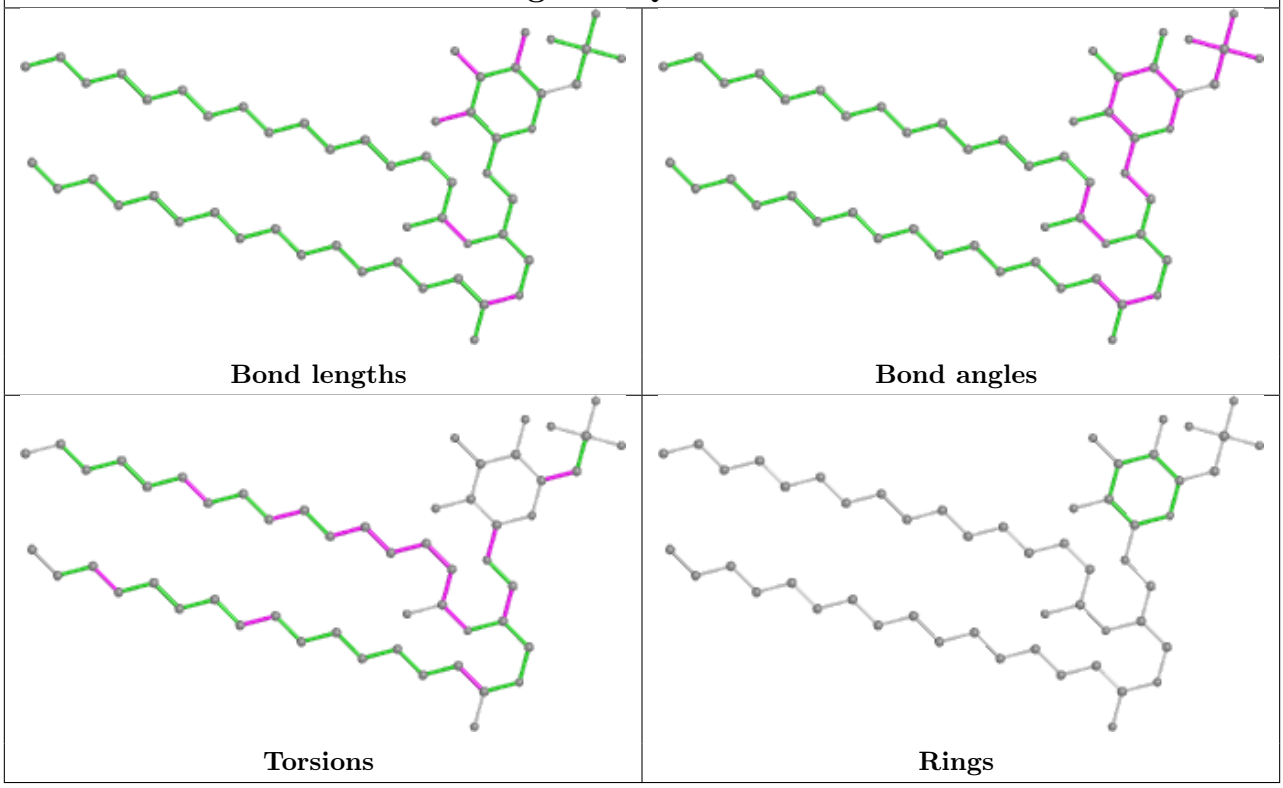


Rings

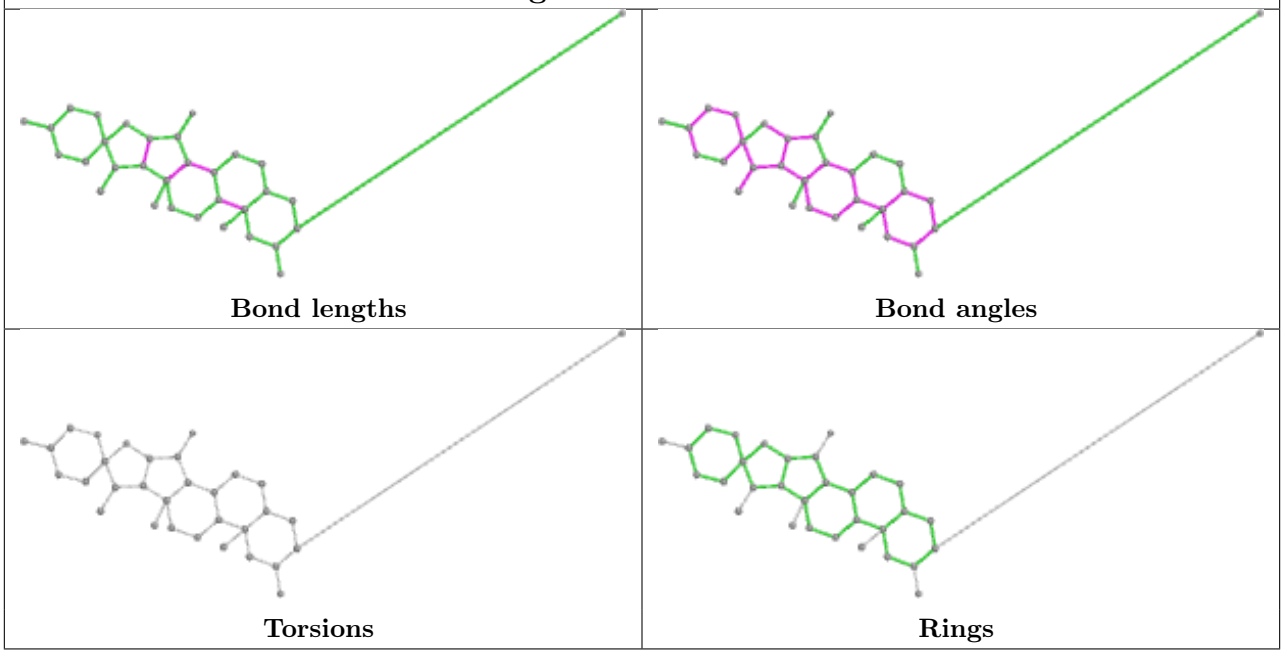
Ligand AJP F 709	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AJP A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

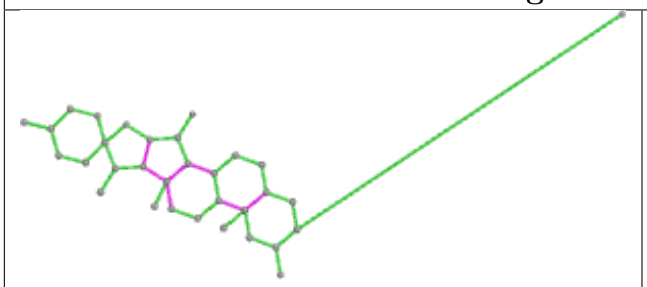
Ligand SQD L 101



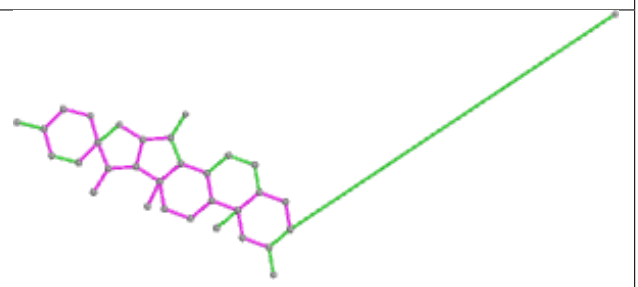
Ligand AJP F 710



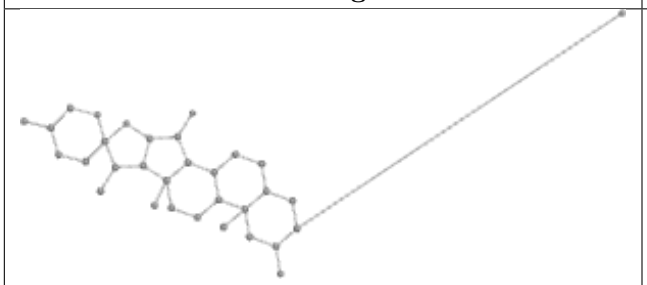
Ligand AJP G 306



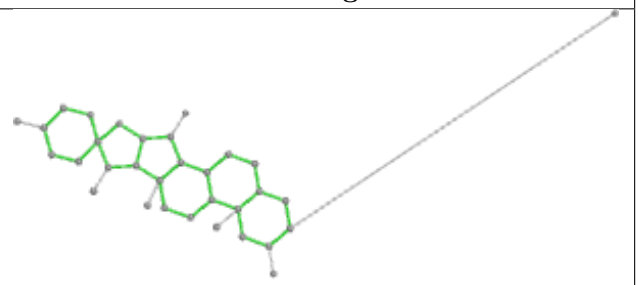
Bond lengths



Bond angles

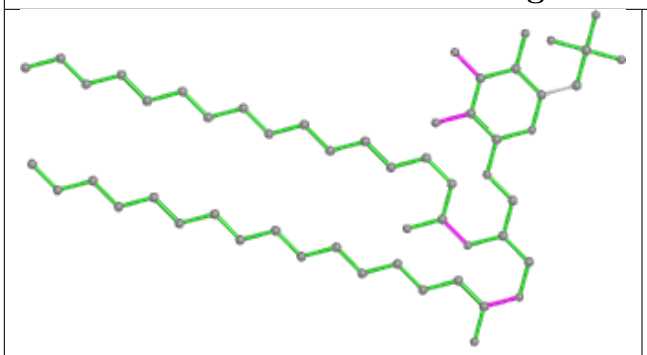


Torsions

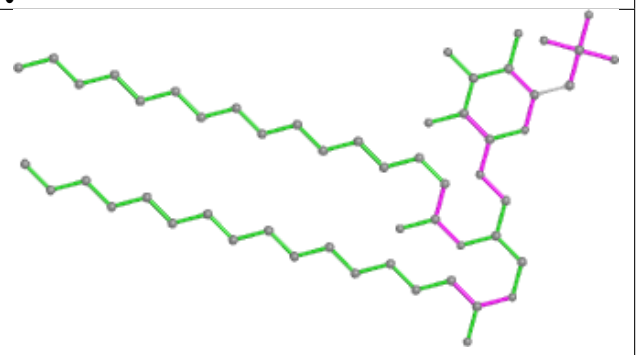


Rings

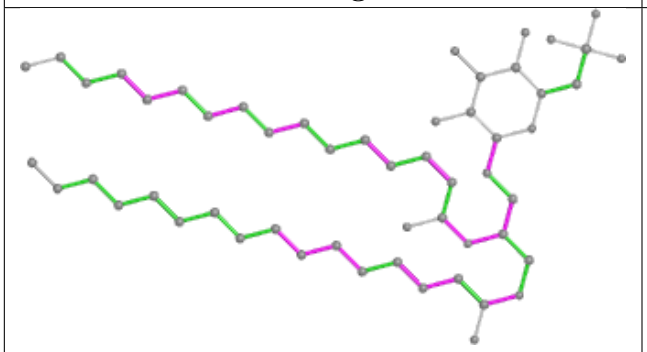
Ligand SQD F 704



Bond lengths



Bond angles



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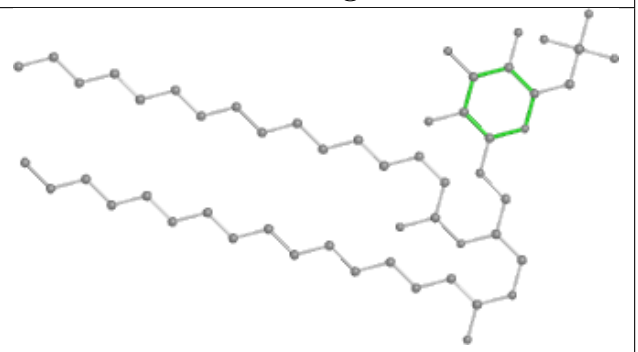
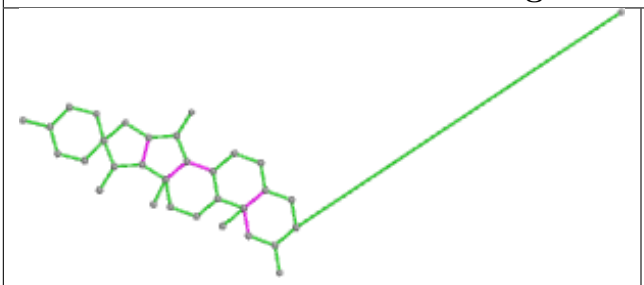
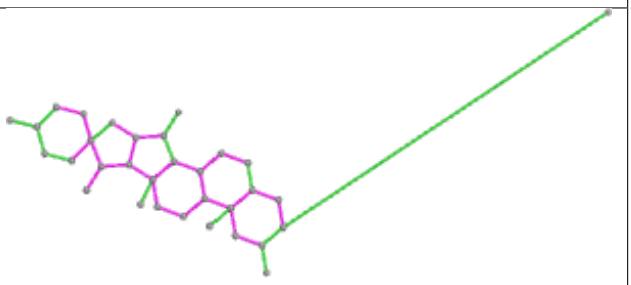
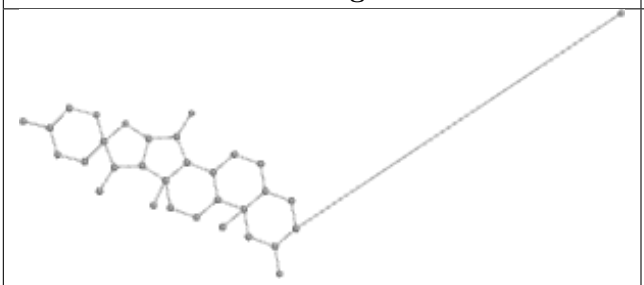
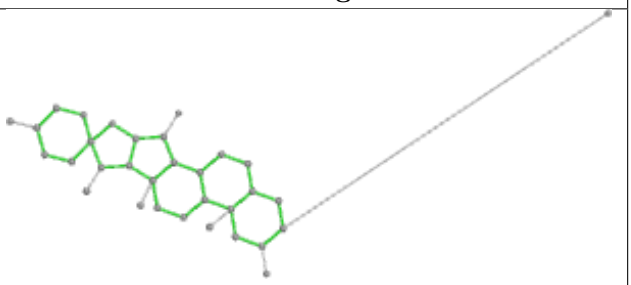


Rings

Ligand AJP D 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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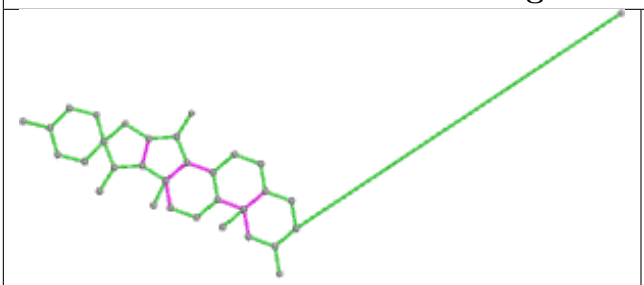
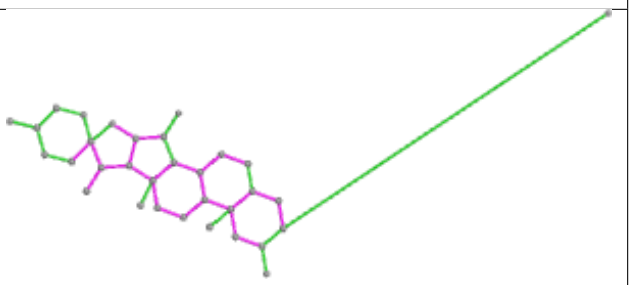
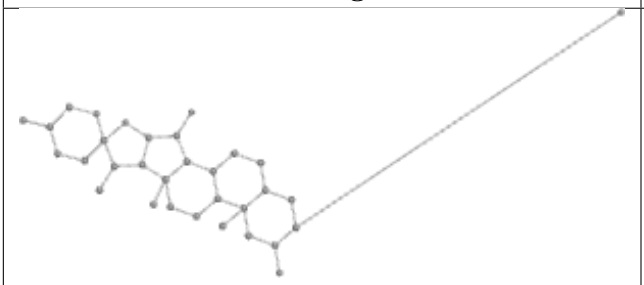
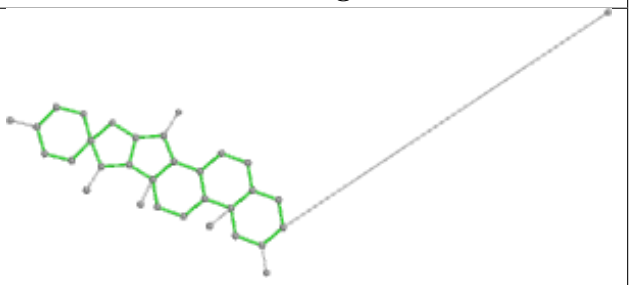
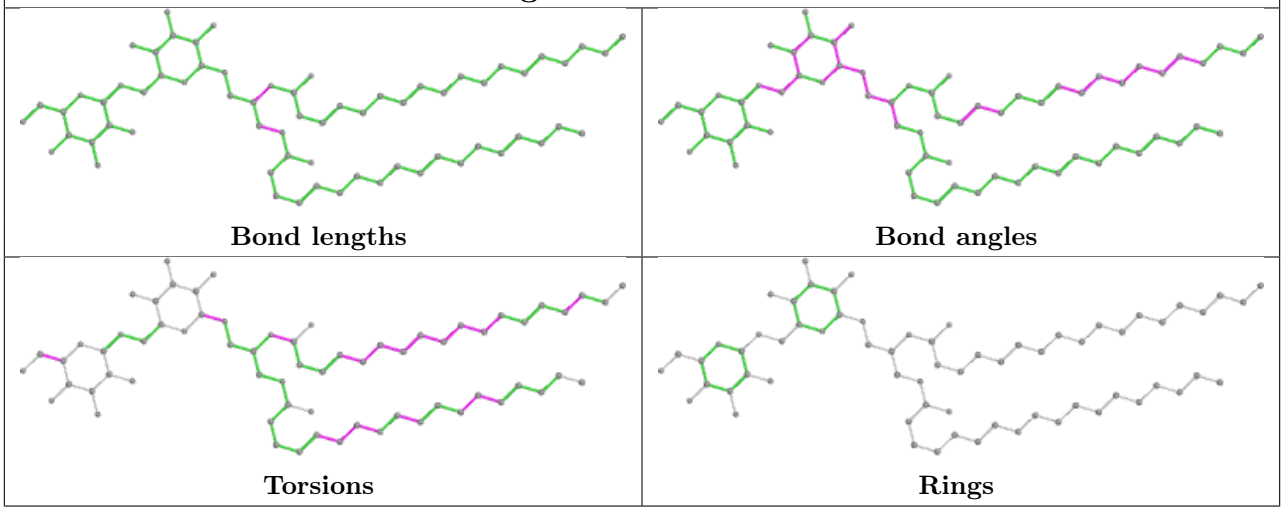
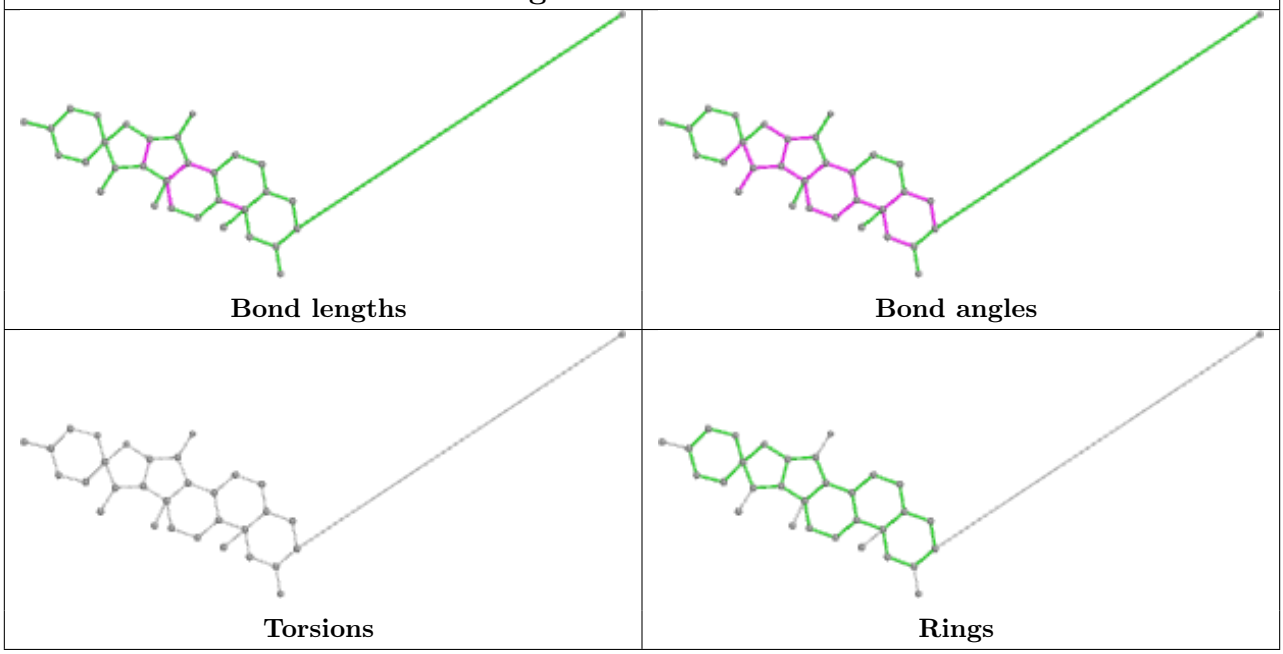
 Bond lengths	 Bond angles
 Torsions	 Rings

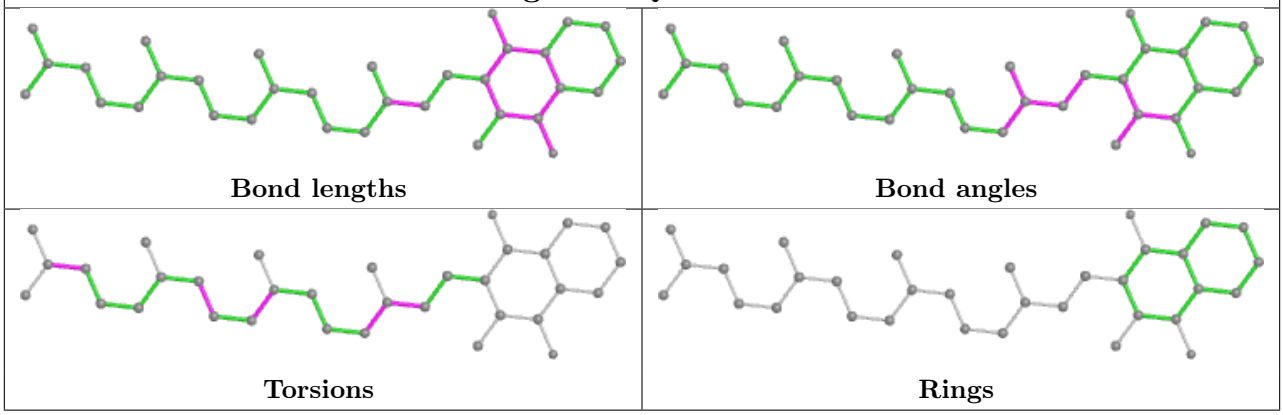
Ligand DGD A 404



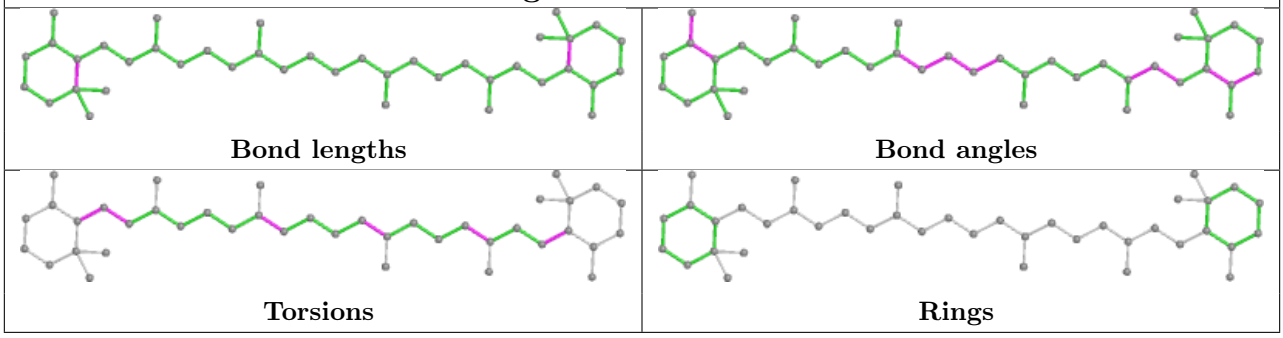
Ligand AJP F 718



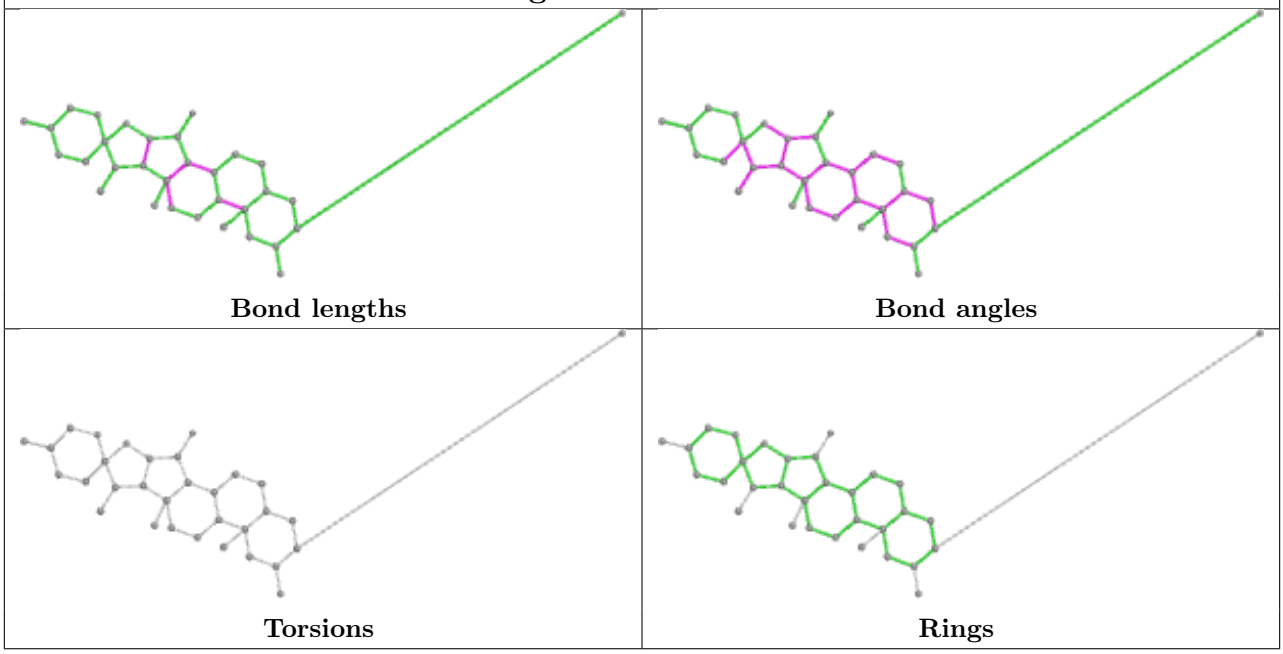
Ligand PQN B 601



Ligand BCR A 401



Ligand AJP F 715



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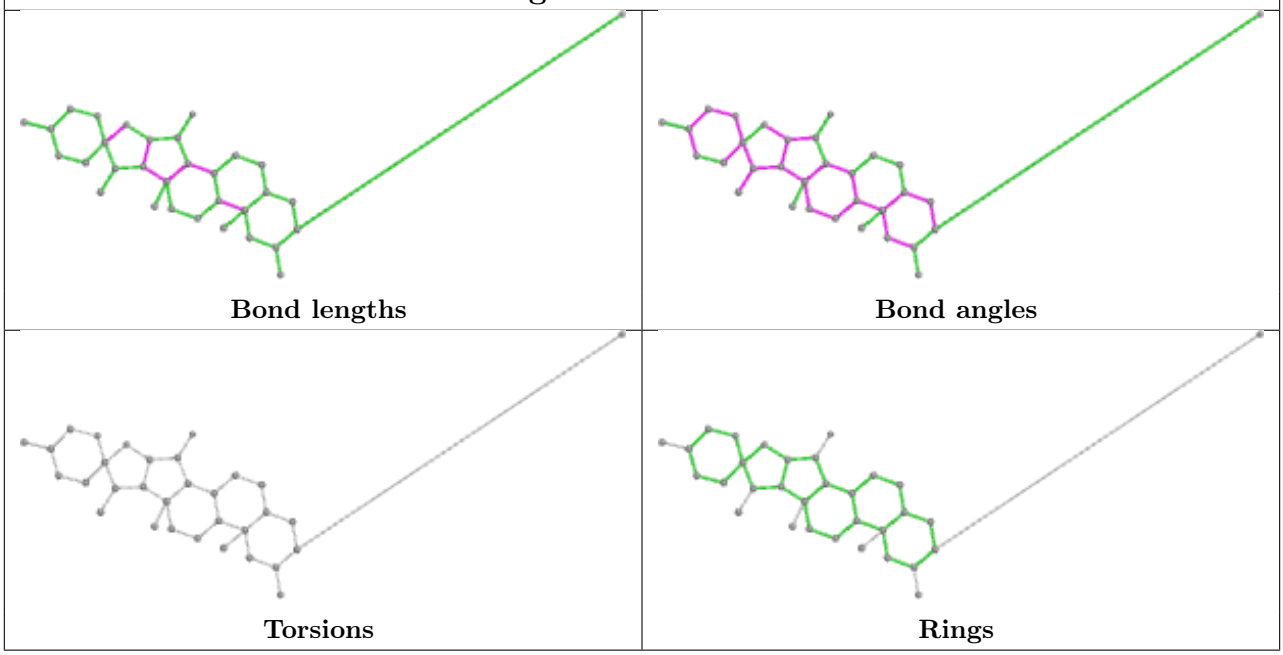

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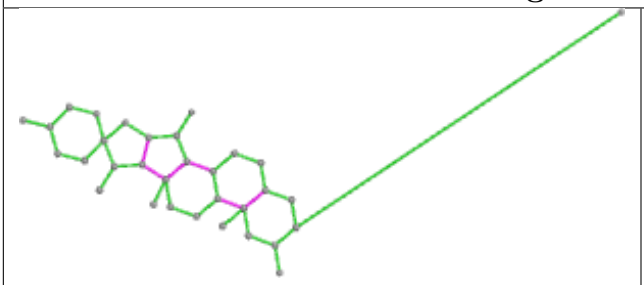
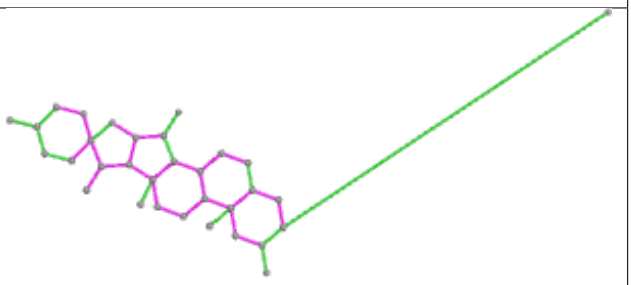
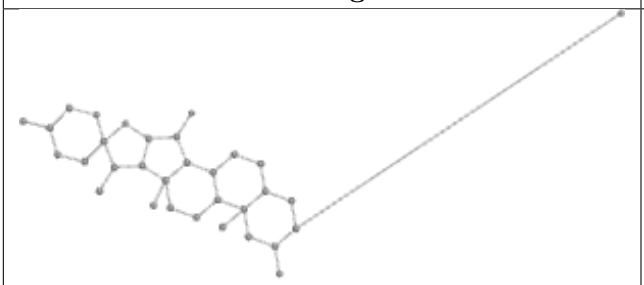
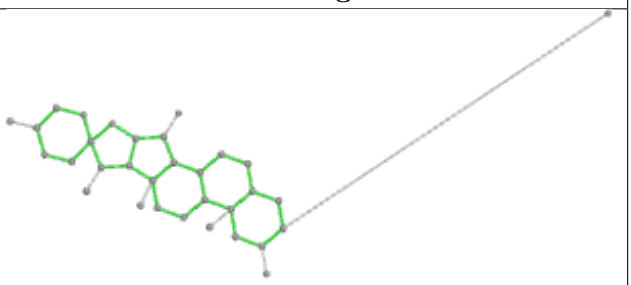
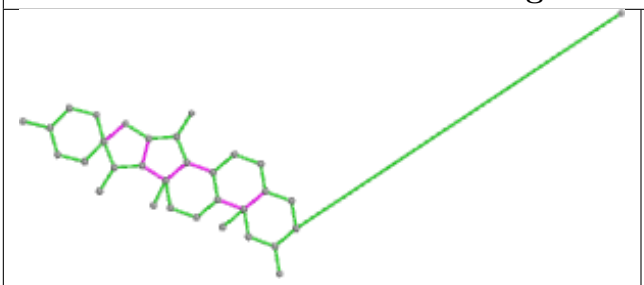
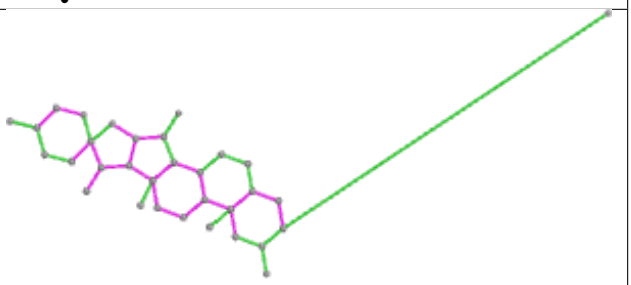
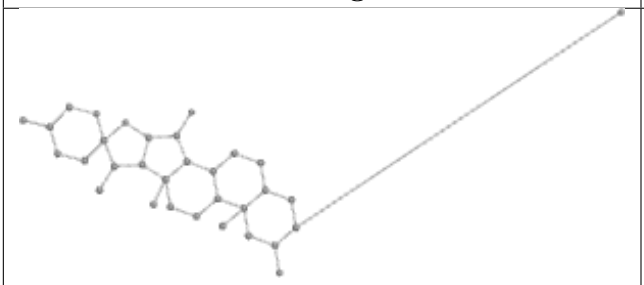
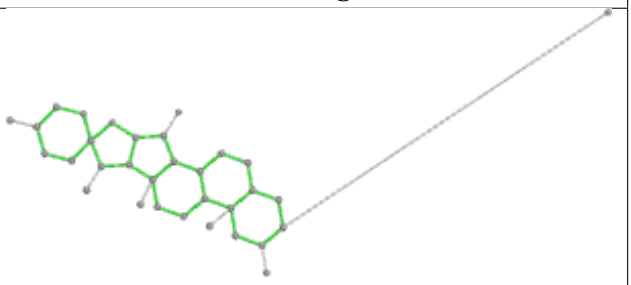
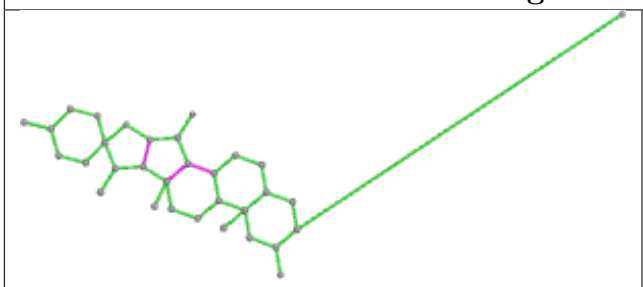
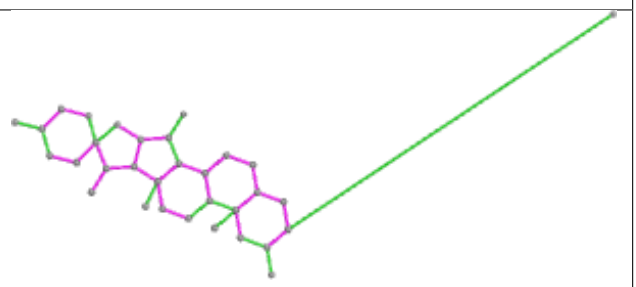
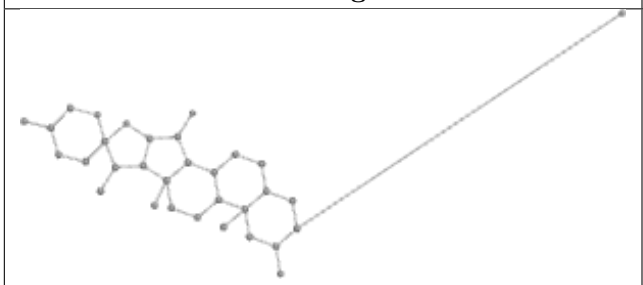
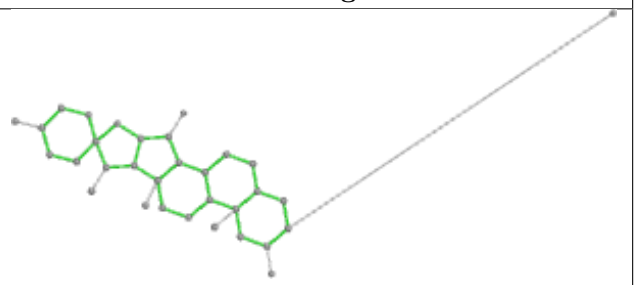
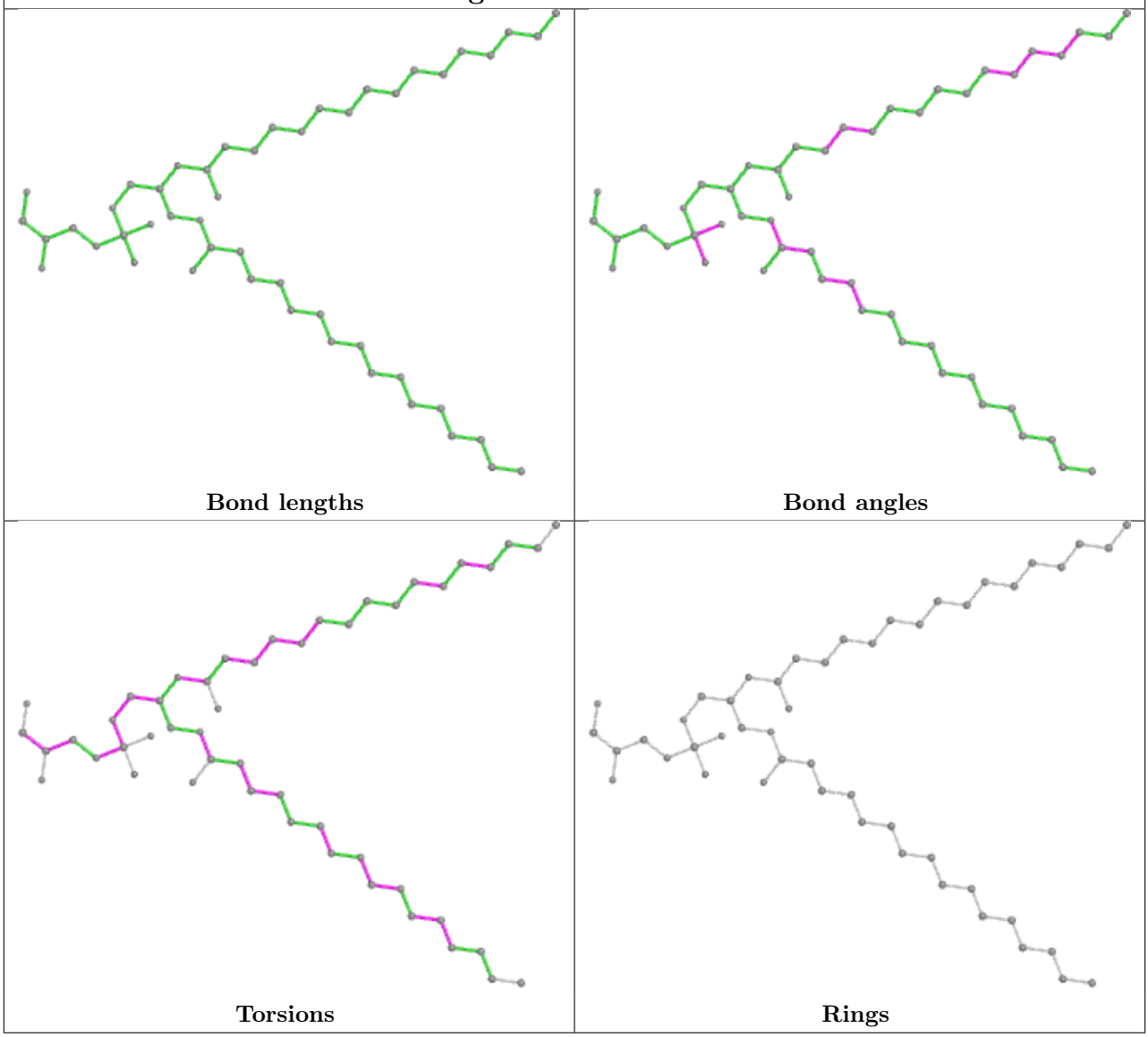
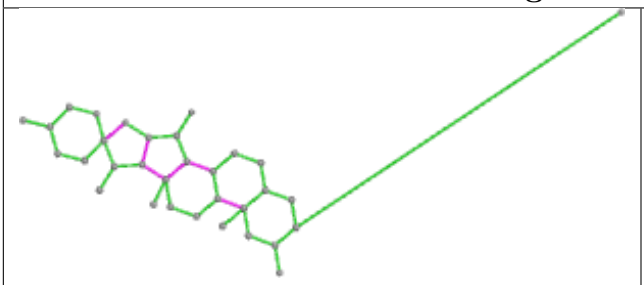
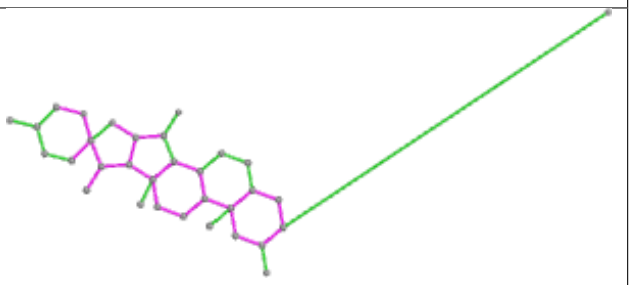
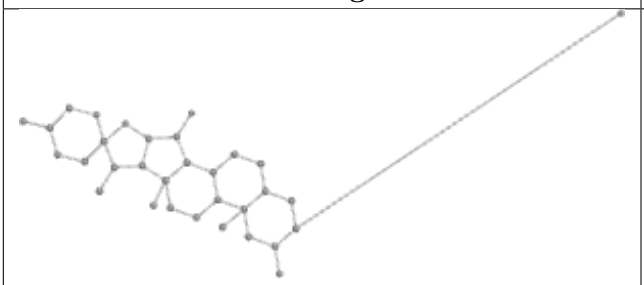
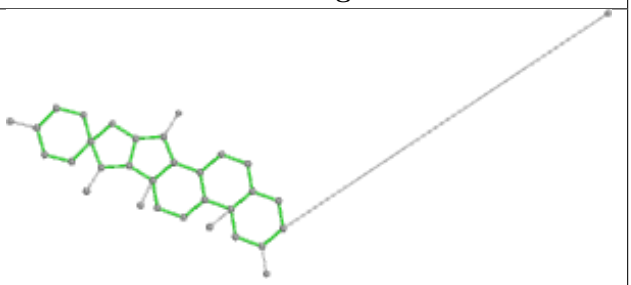
 Bond lengths	 Bond angles
 Torsions	 Rings

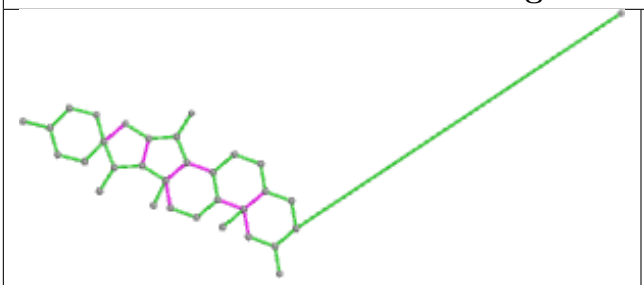
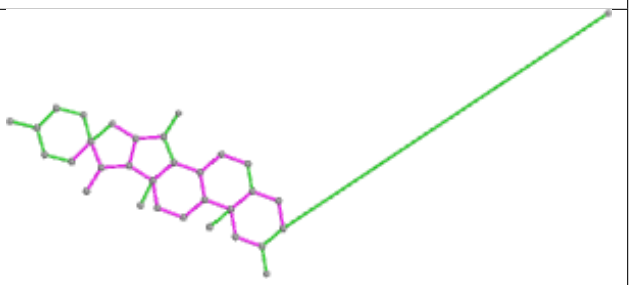
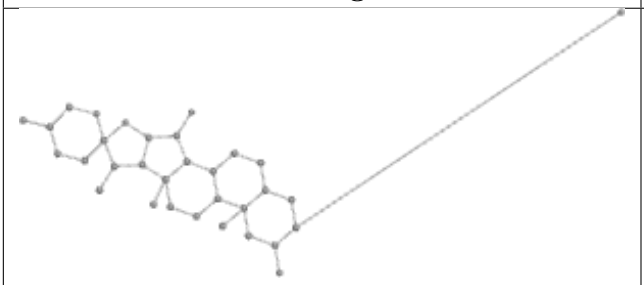
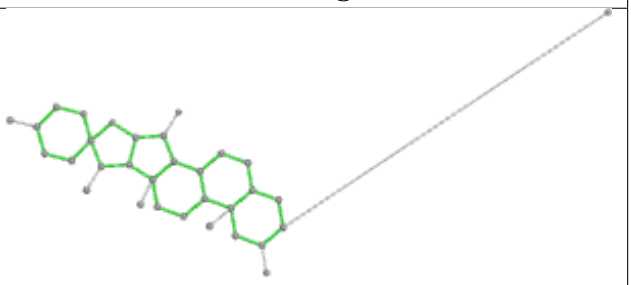
Ligand AJP Q 108	
 Bond lengths	 Bond angles
 Torsions	 Rings

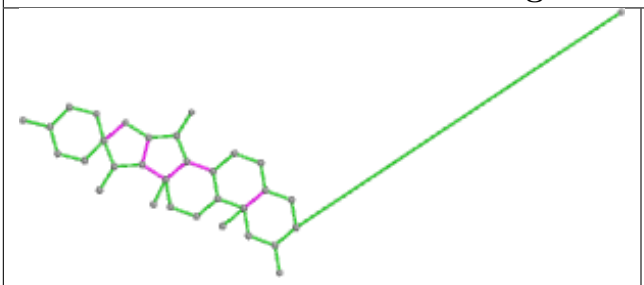
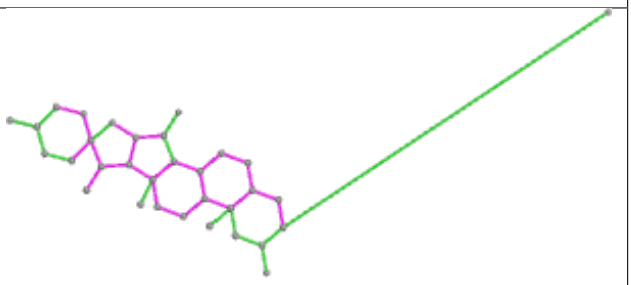
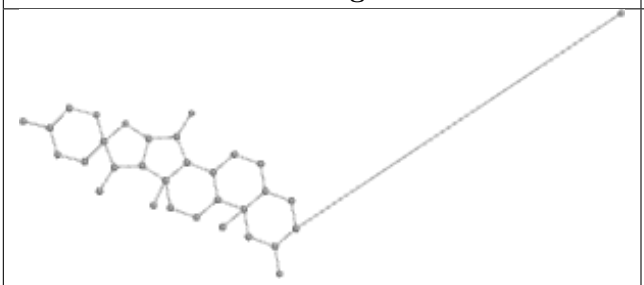
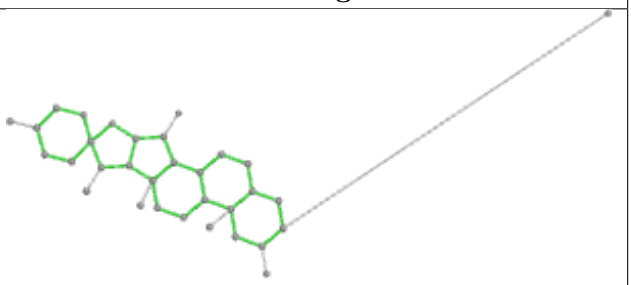
Ligand AJP A 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG B 602

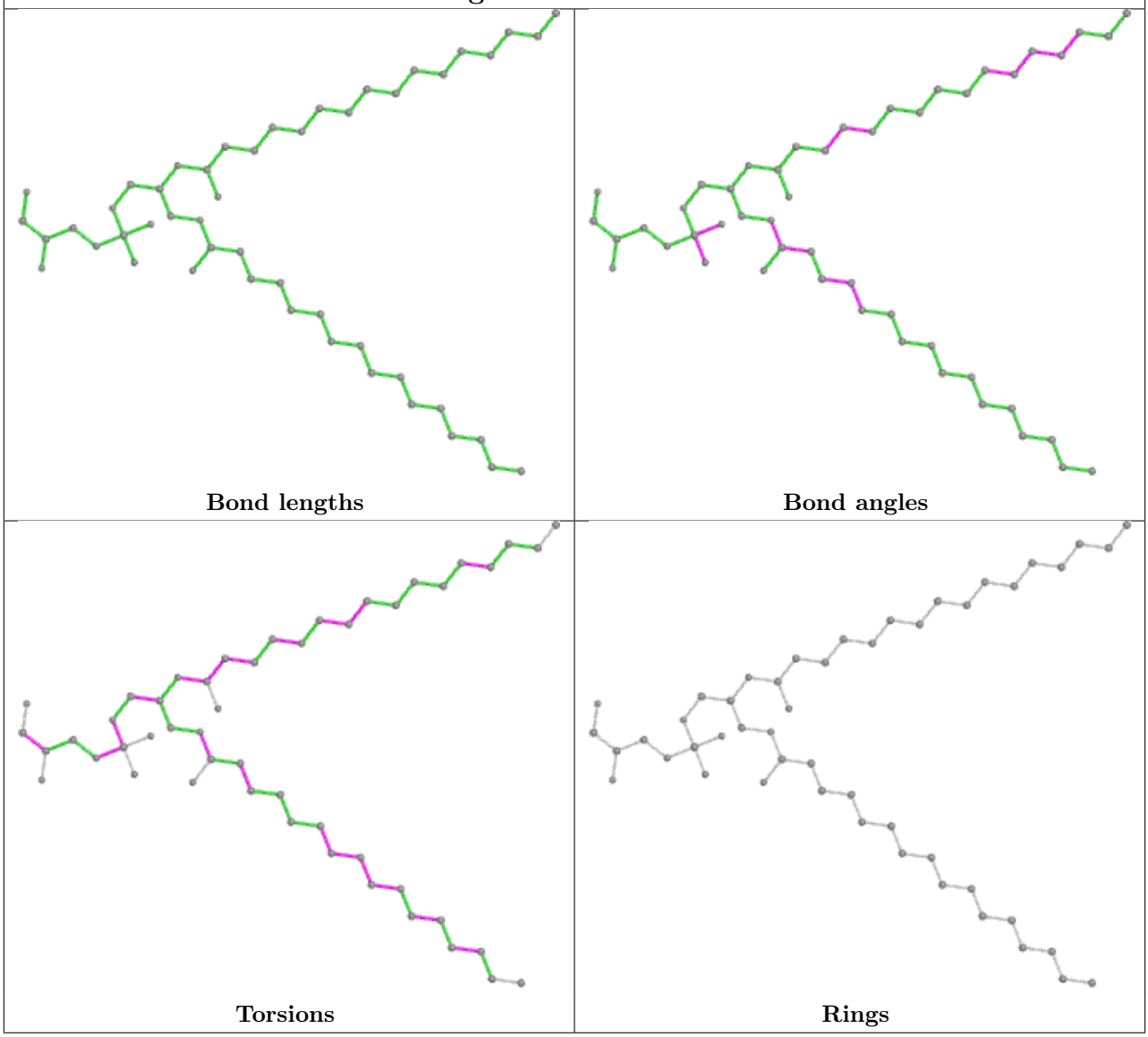


Ligand AJP G 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

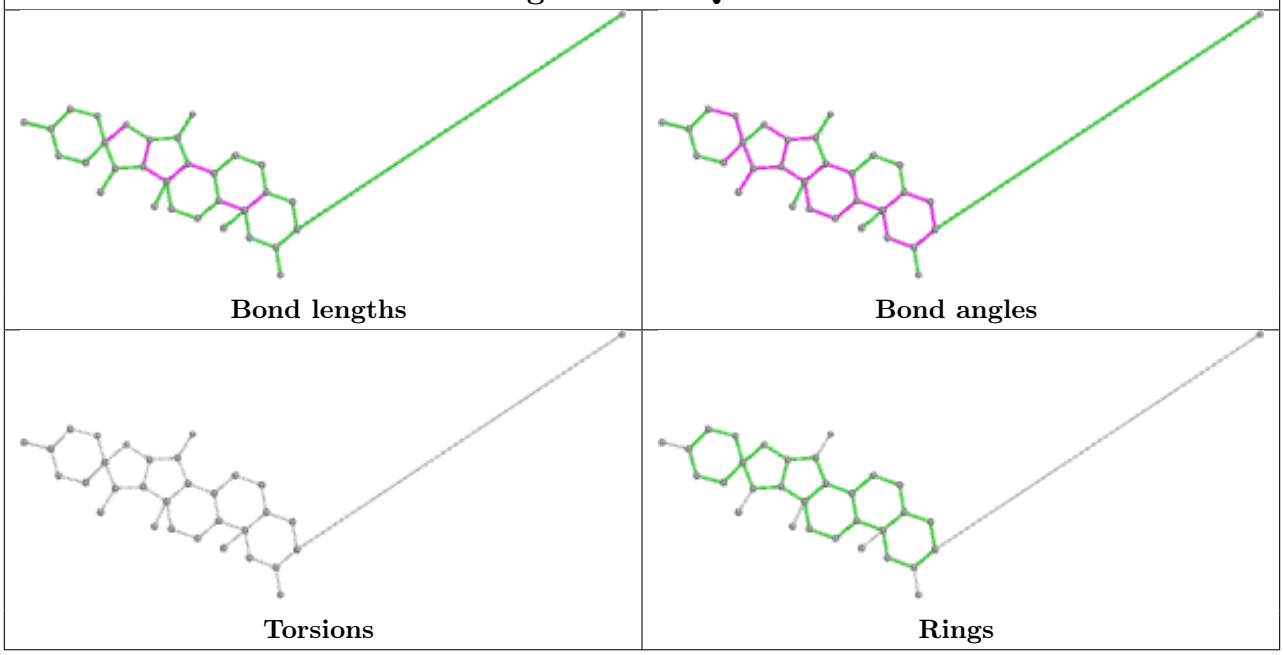
Ligand AJP G 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AJP A 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

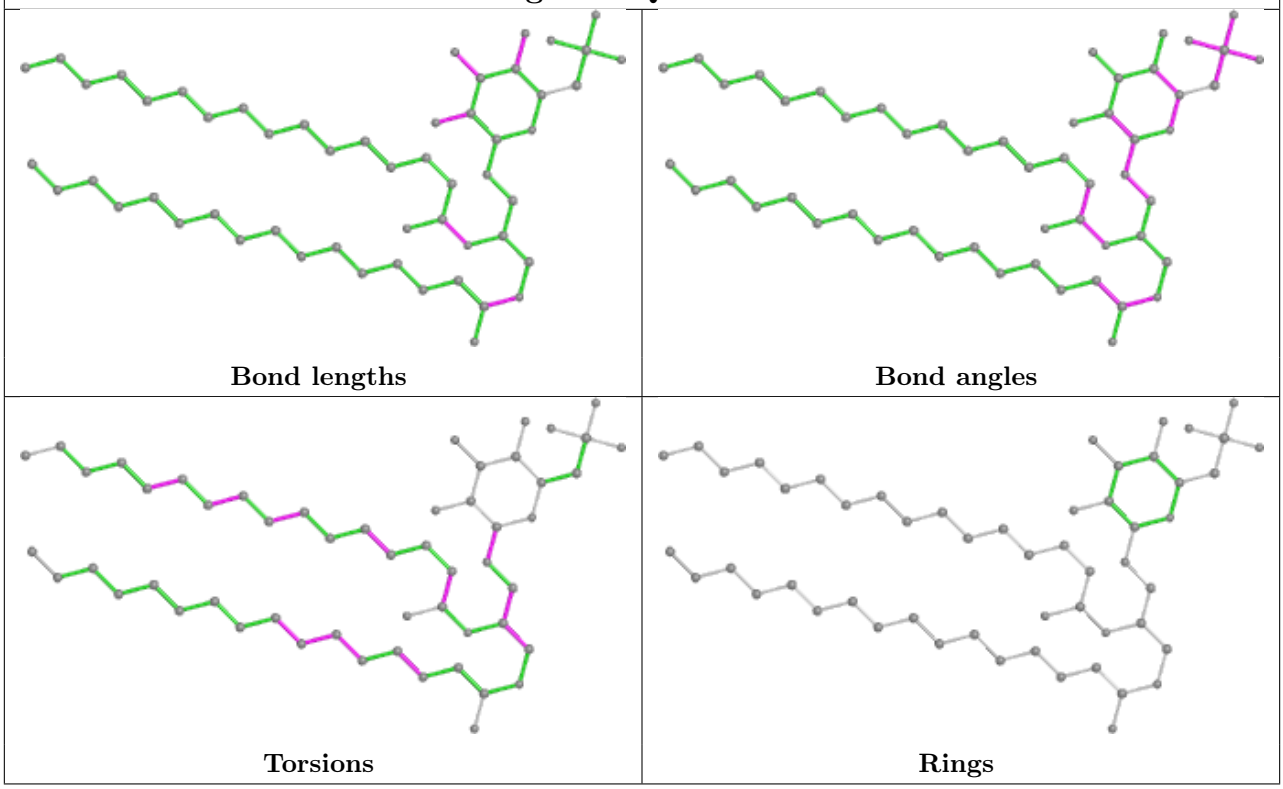
Ligand LHG B 604

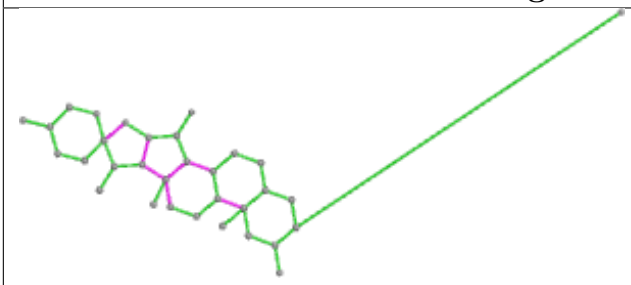
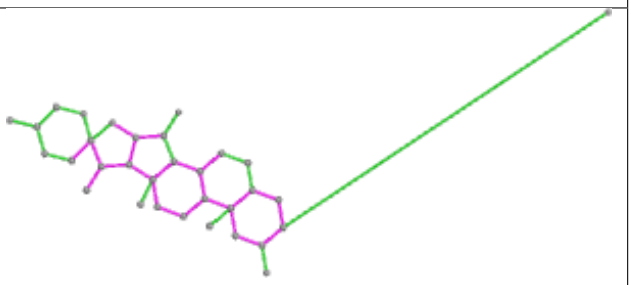
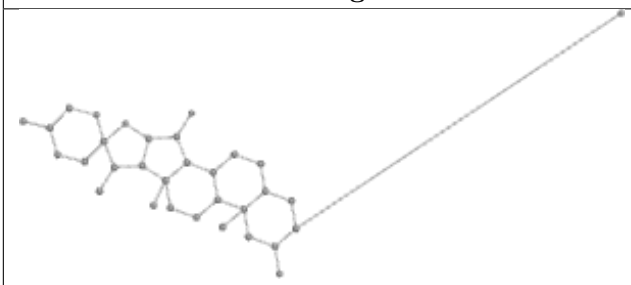
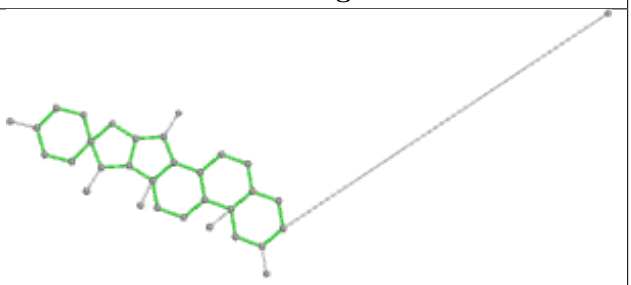


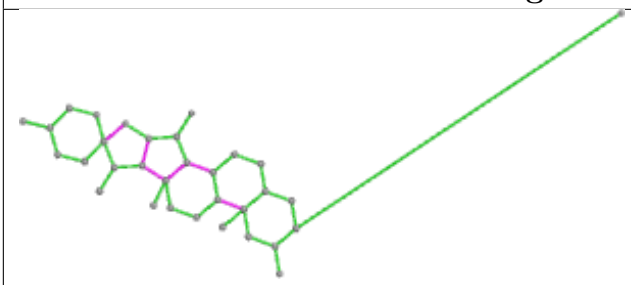
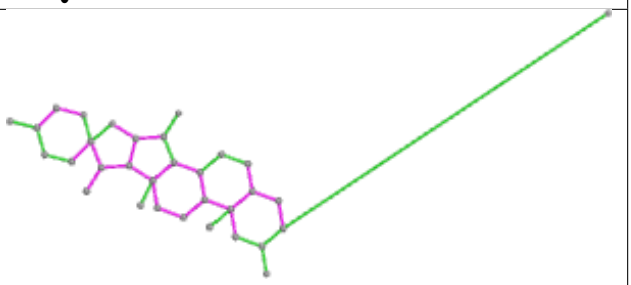
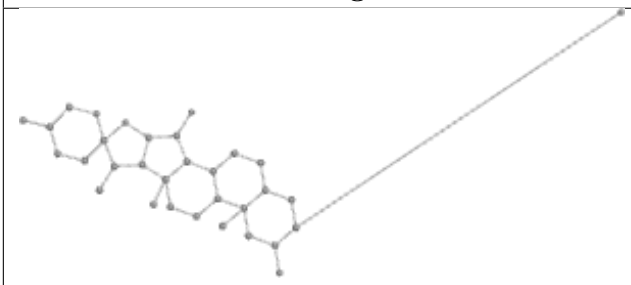
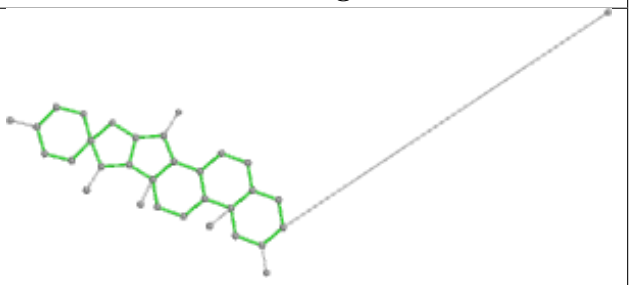
Ligand AJP Q 107



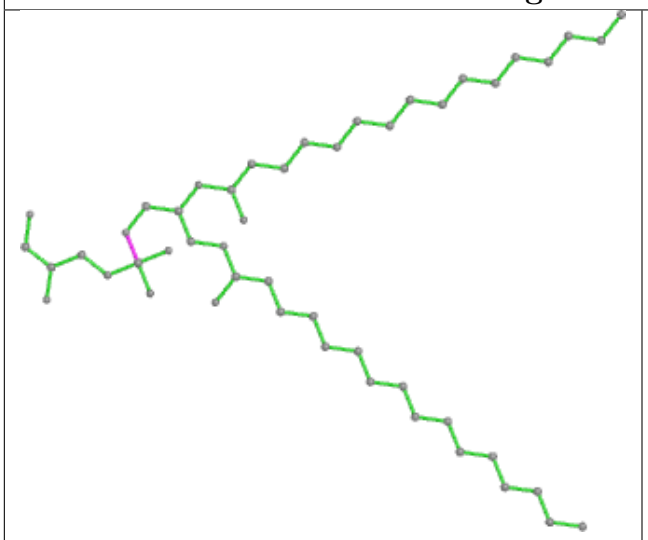
Ligand SQD B 605



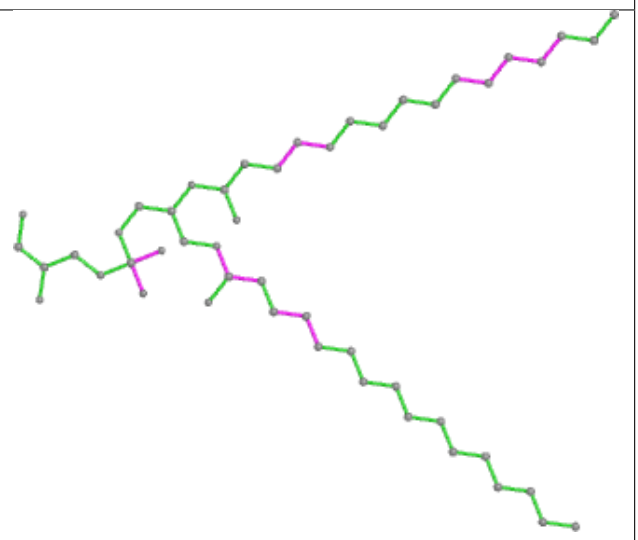
Ligand AJP F 717	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AJP Q 106	
 Bond lengths	 Bond angles
 Torsions	 Rings

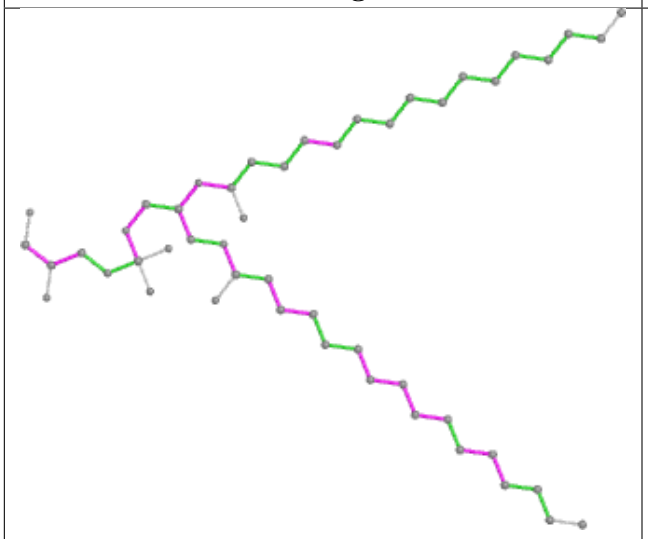
Ligand LHG F 703



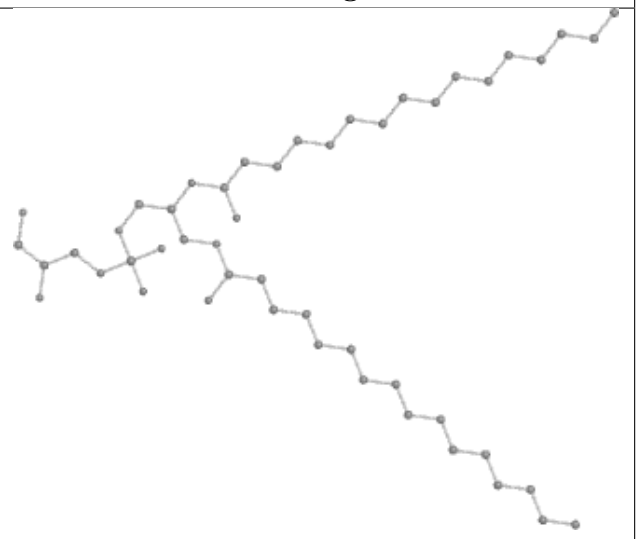
Bond lengths



Bond angles

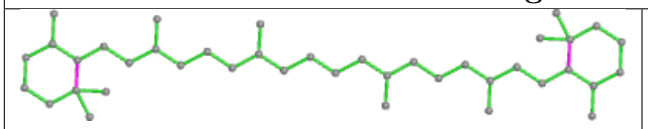


Torsions

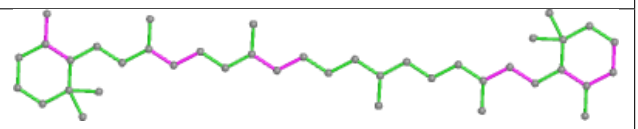


Rings

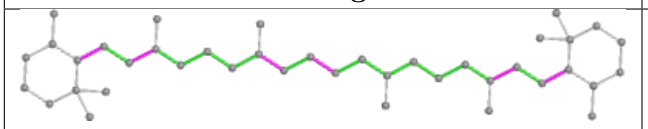
Ligand BCR F 701



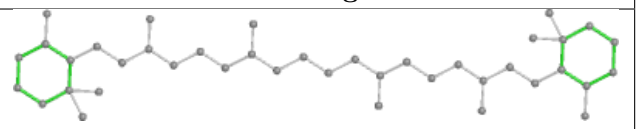
Bond lengths



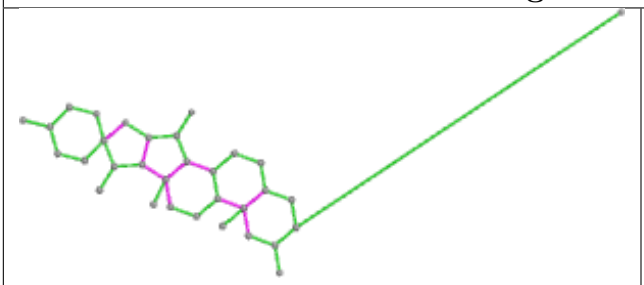
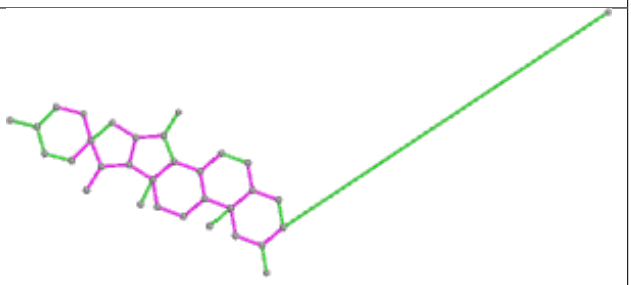
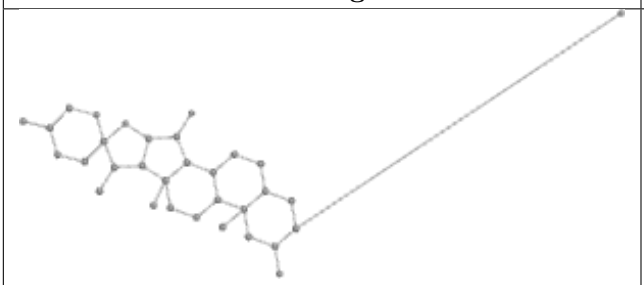
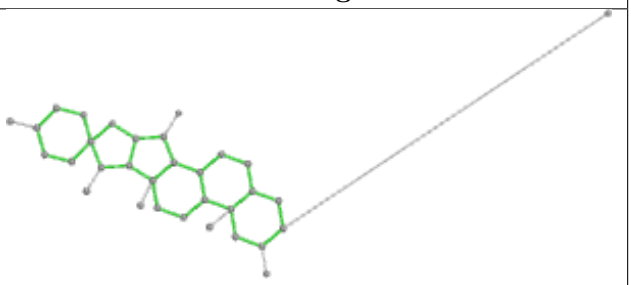
Bond angles

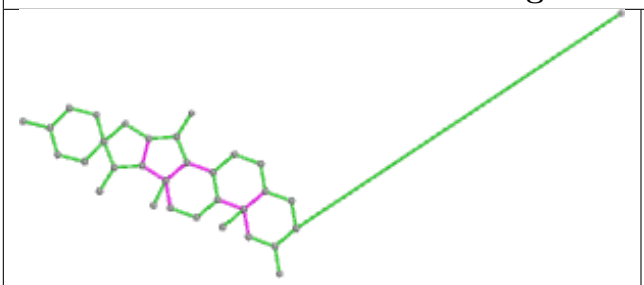
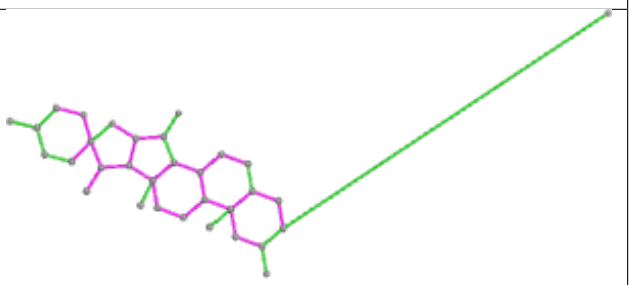
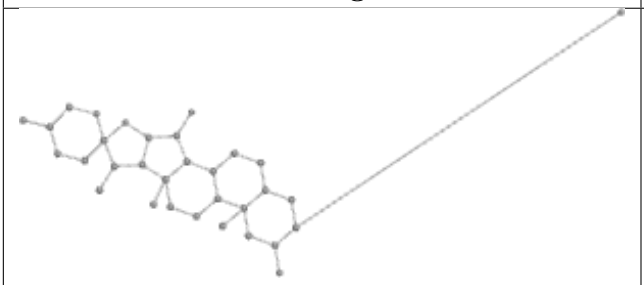
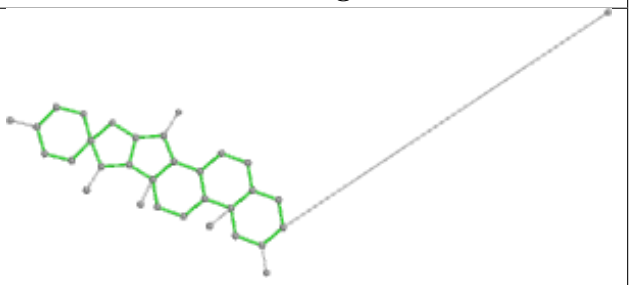


Torsions



Rings

Ligand AJP B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AJP C 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

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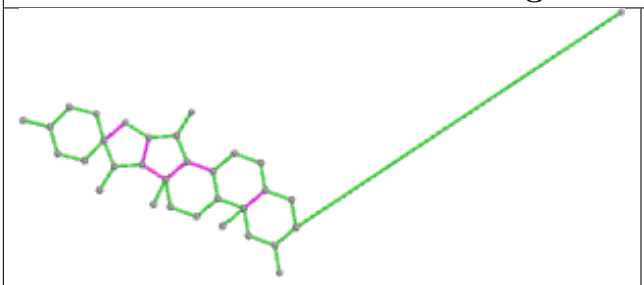
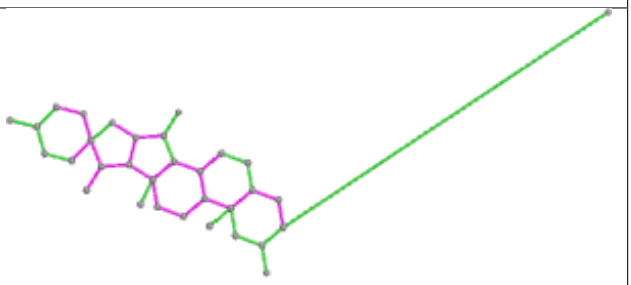
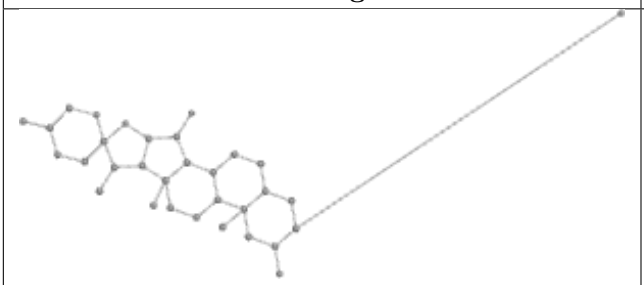
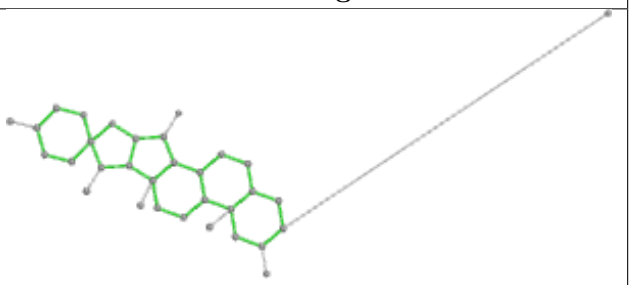
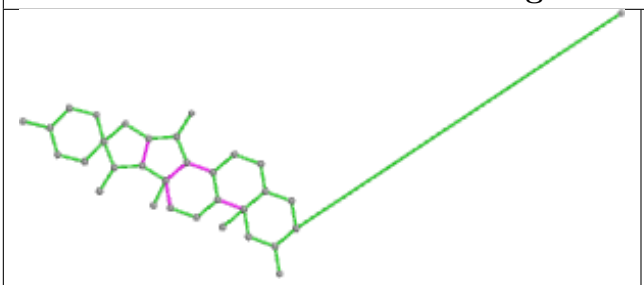
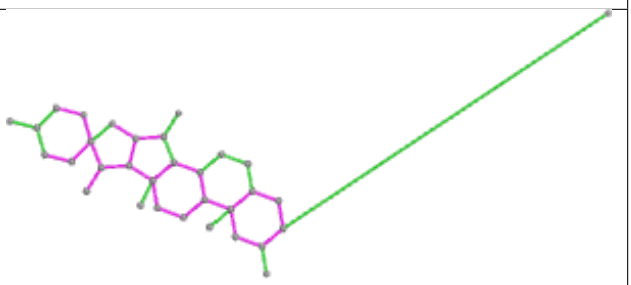
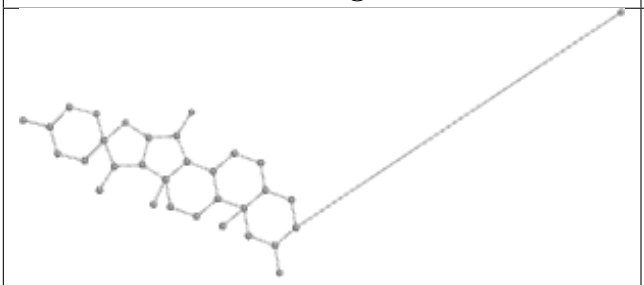
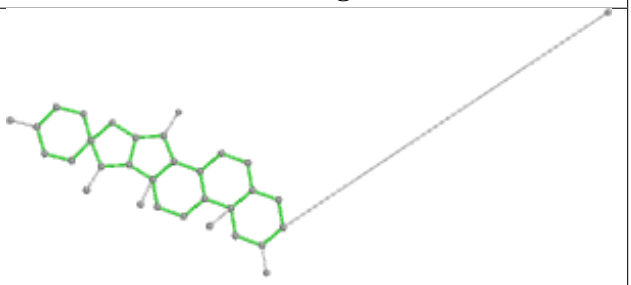
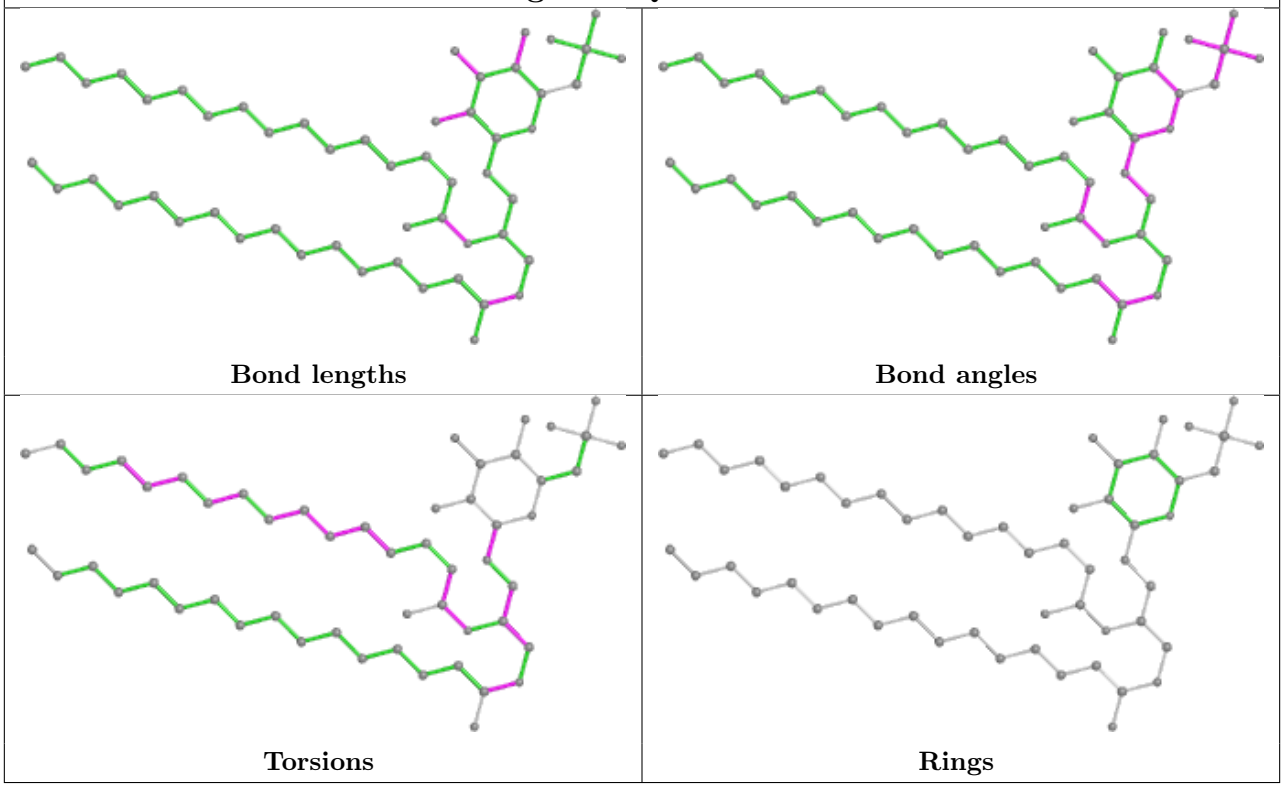
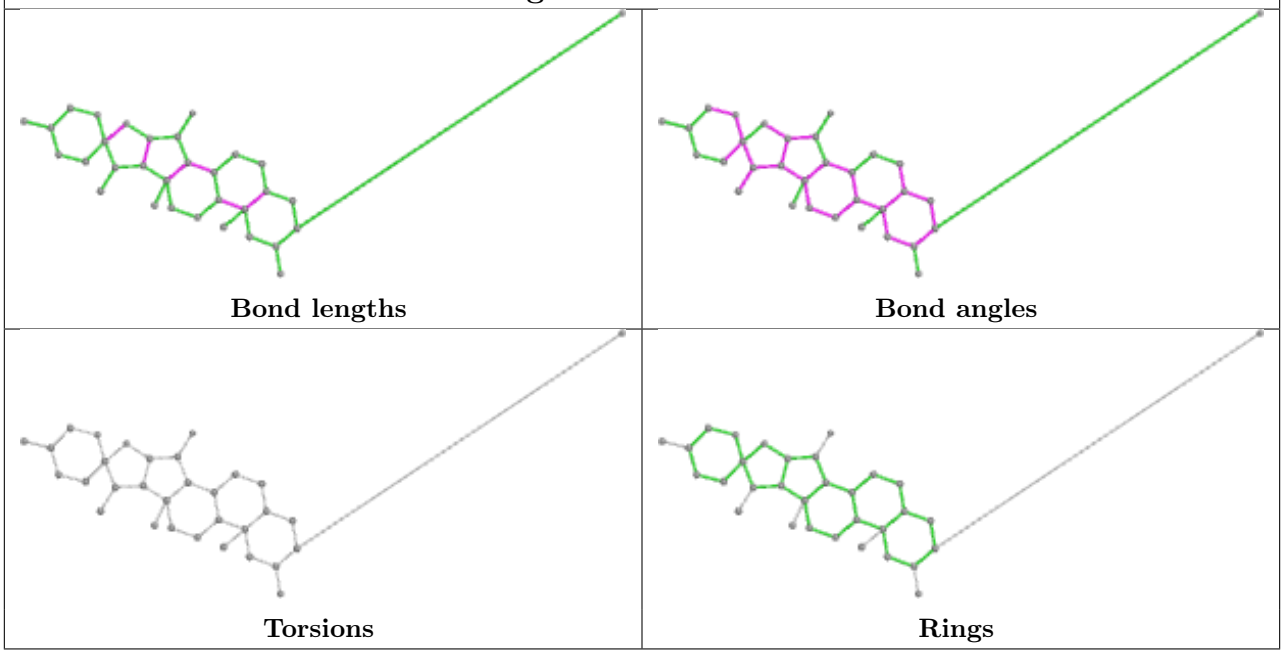
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AJP D 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD F 705



Ligand AJP D 608



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

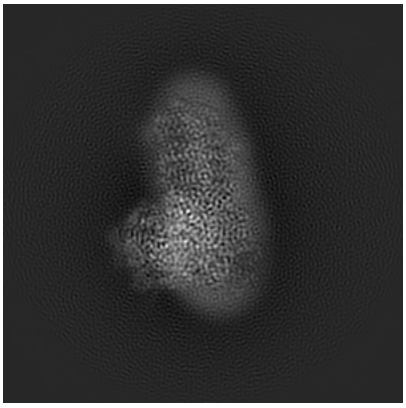
6 Map visualisation (i)

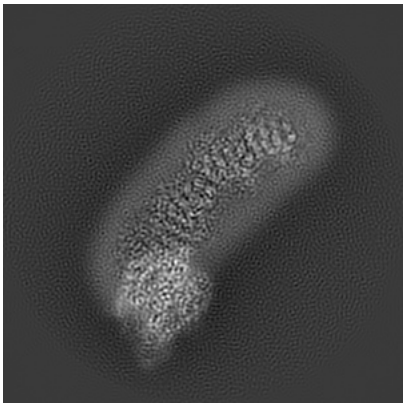
This section contains visualisations of the EMDB entry EMD-0849. These allow visual inspection of the internal detail of the map and identification of artifacts.

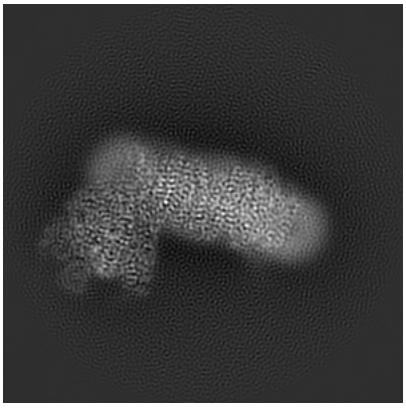
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

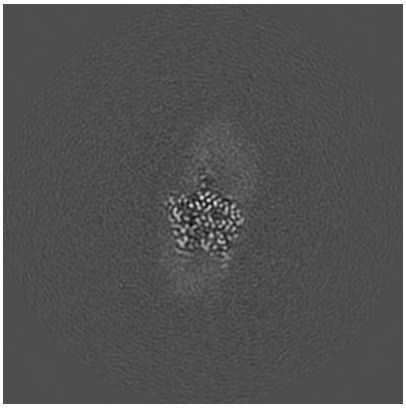

Y

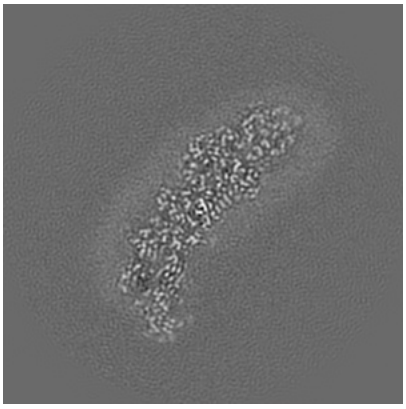

Z

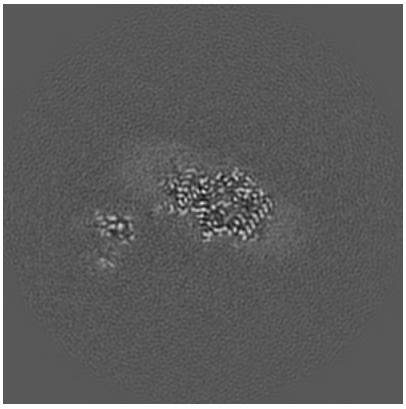
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 150

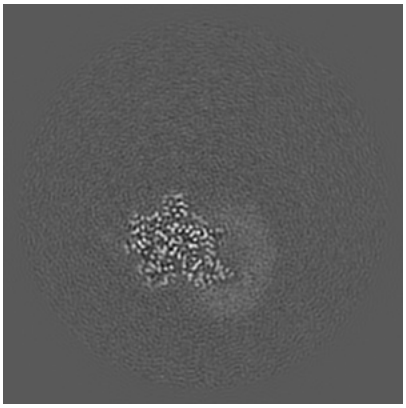

Y Index: 150

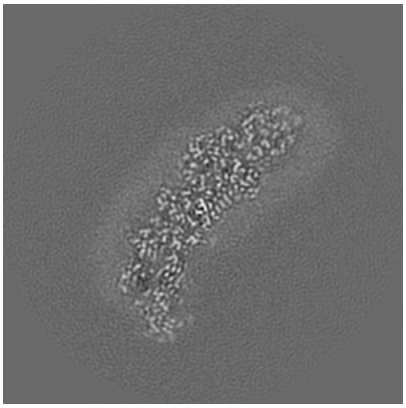

Z Index: 150

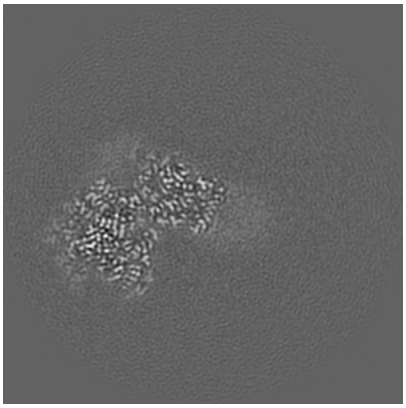
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 88

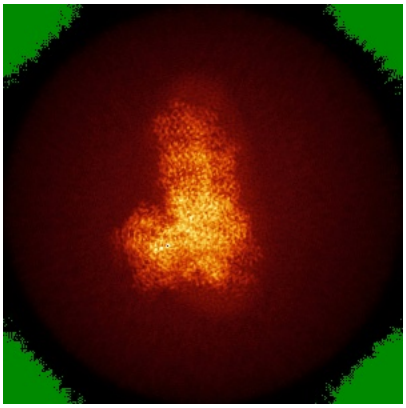

Y Index: 150

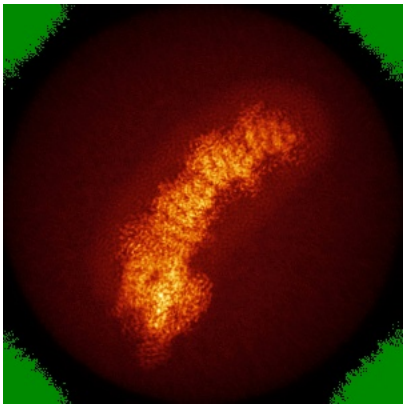

Z Index: 121

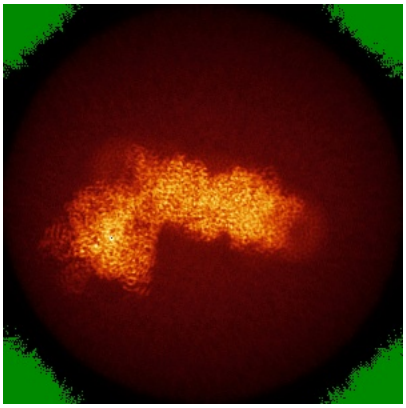
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

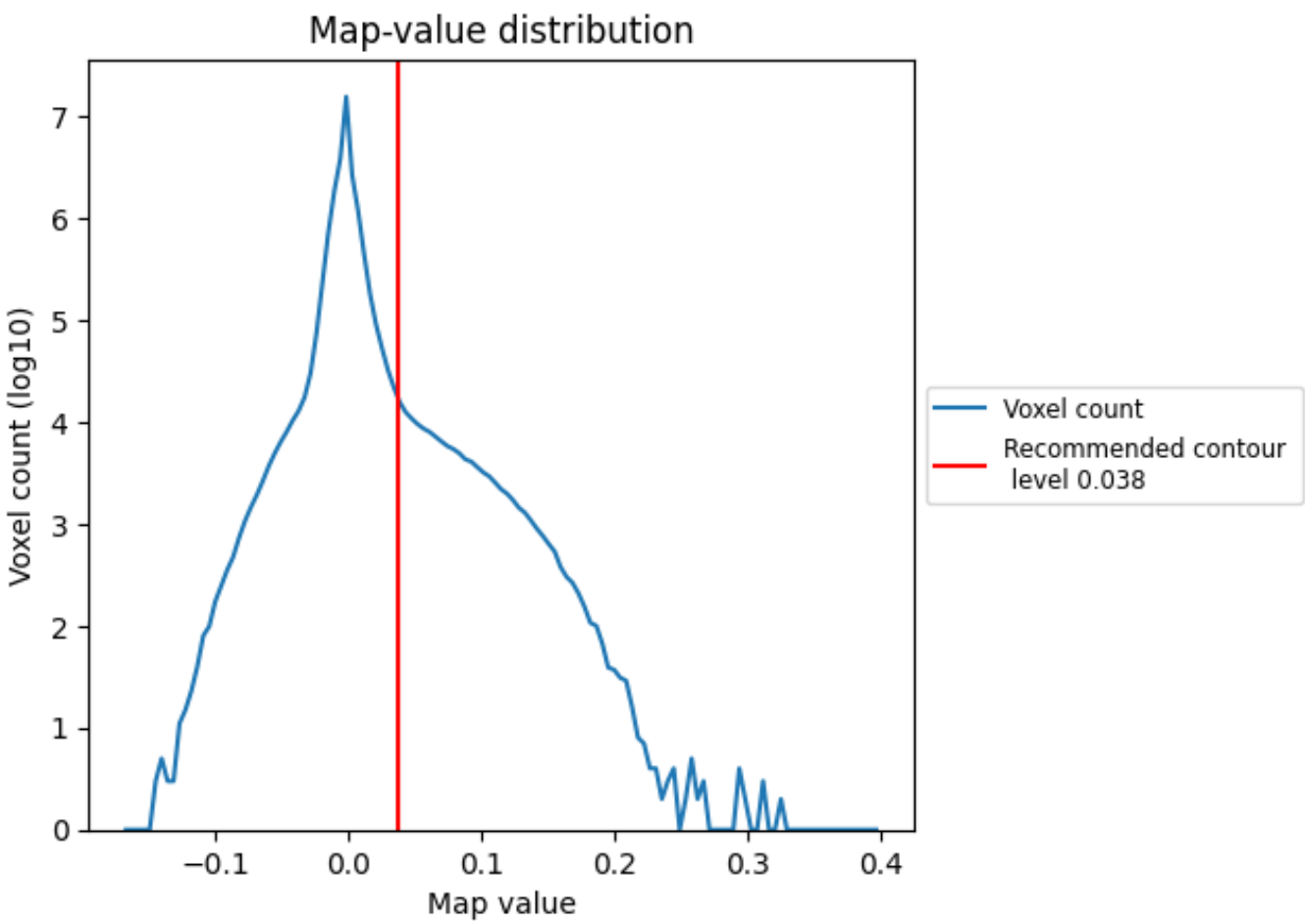
6.6 Mask visualisation (i)

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

7 Map analysis (i)

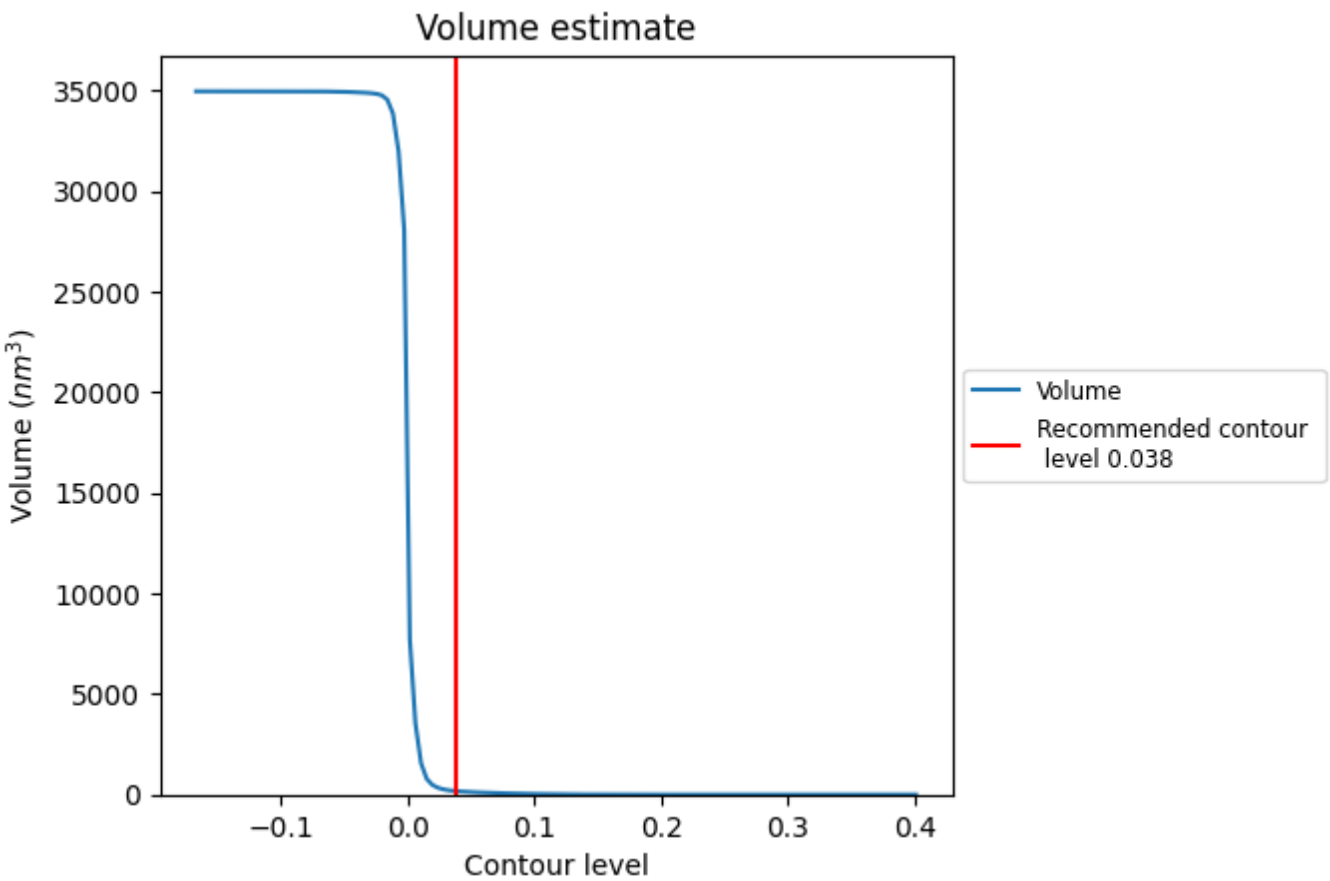
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

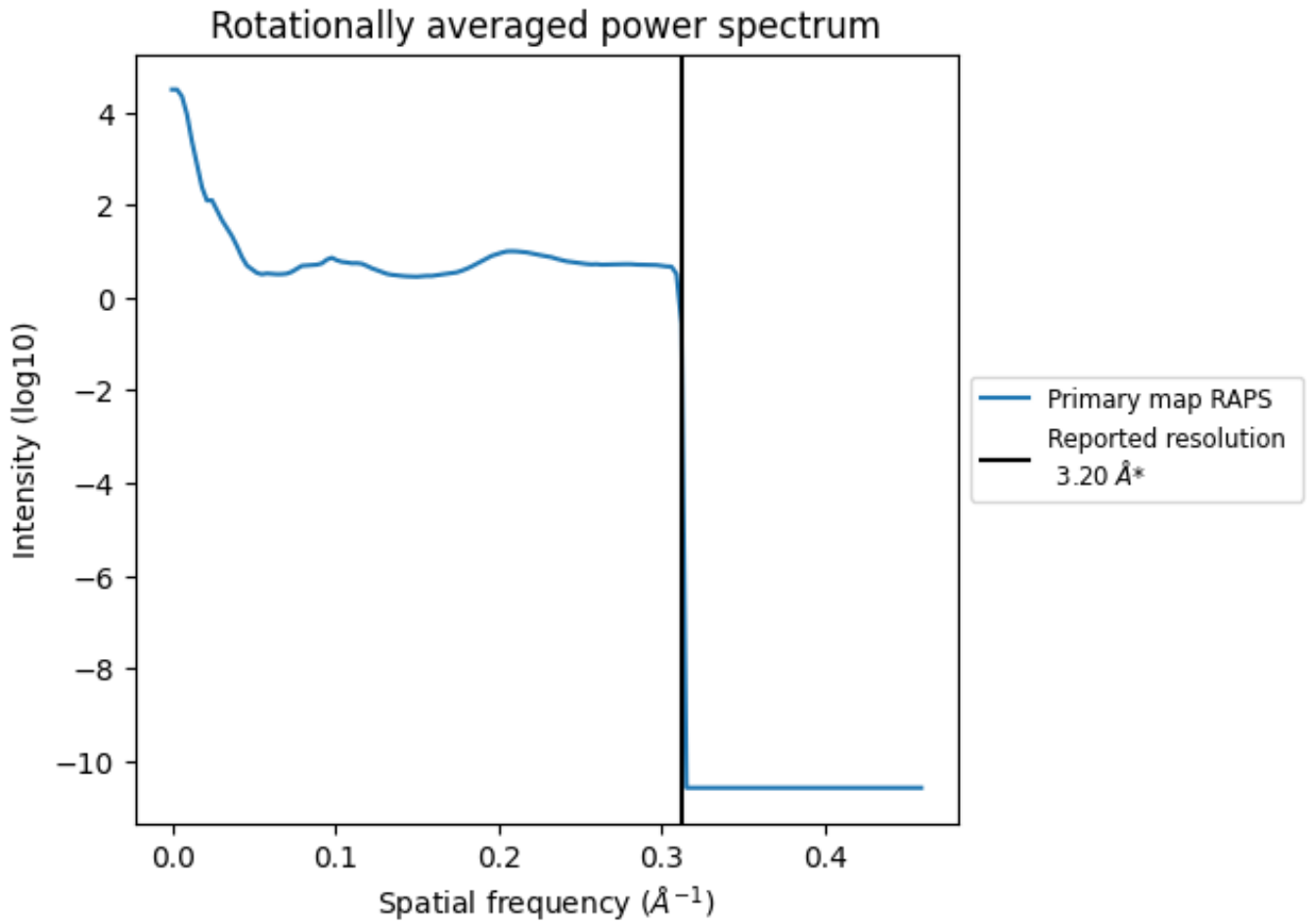
7.2 Volume estimate (i)



The volume at the recommended contour level is 172 nm^3; this corresponds to an approximate mass of 155 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 0.312 Å^{-1}

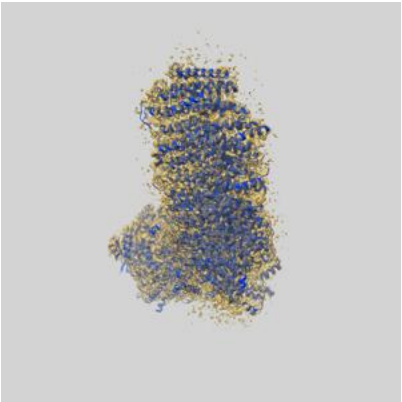
8 Fourier-Shell correlation (i)

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

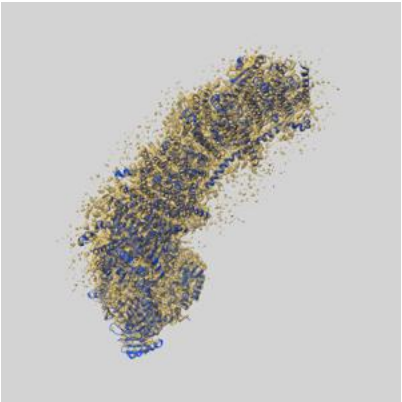
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0849 and PDB model 6L7O. Per-residue inclusion information can be found in section 3 on page 17.

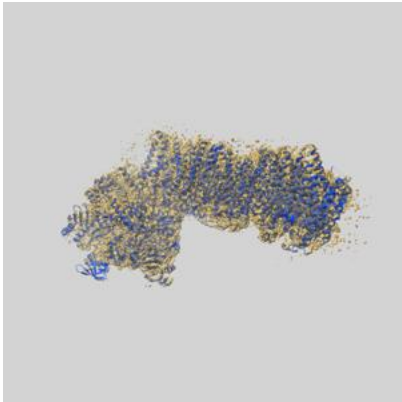
9.1 Map-model overlay (i)



X



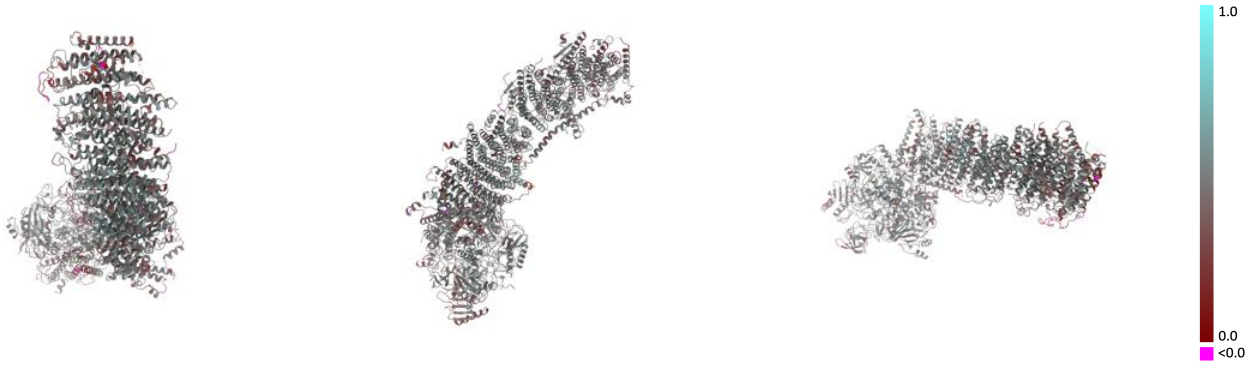
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

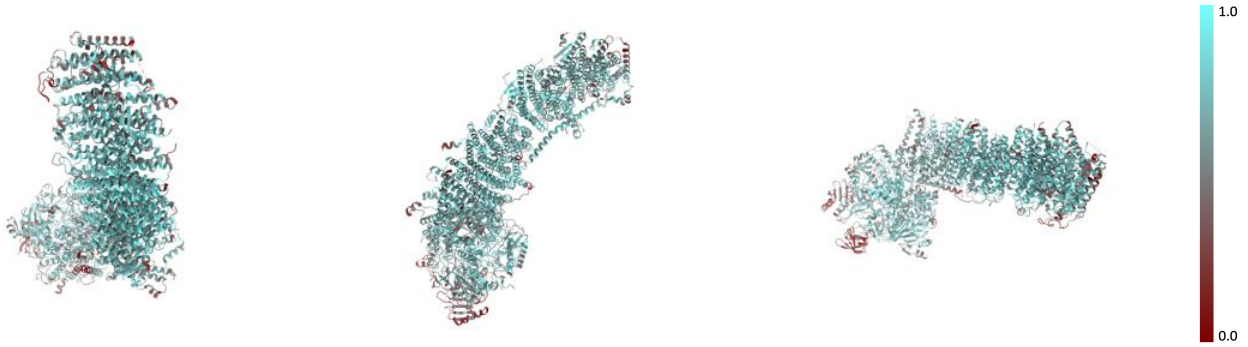
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

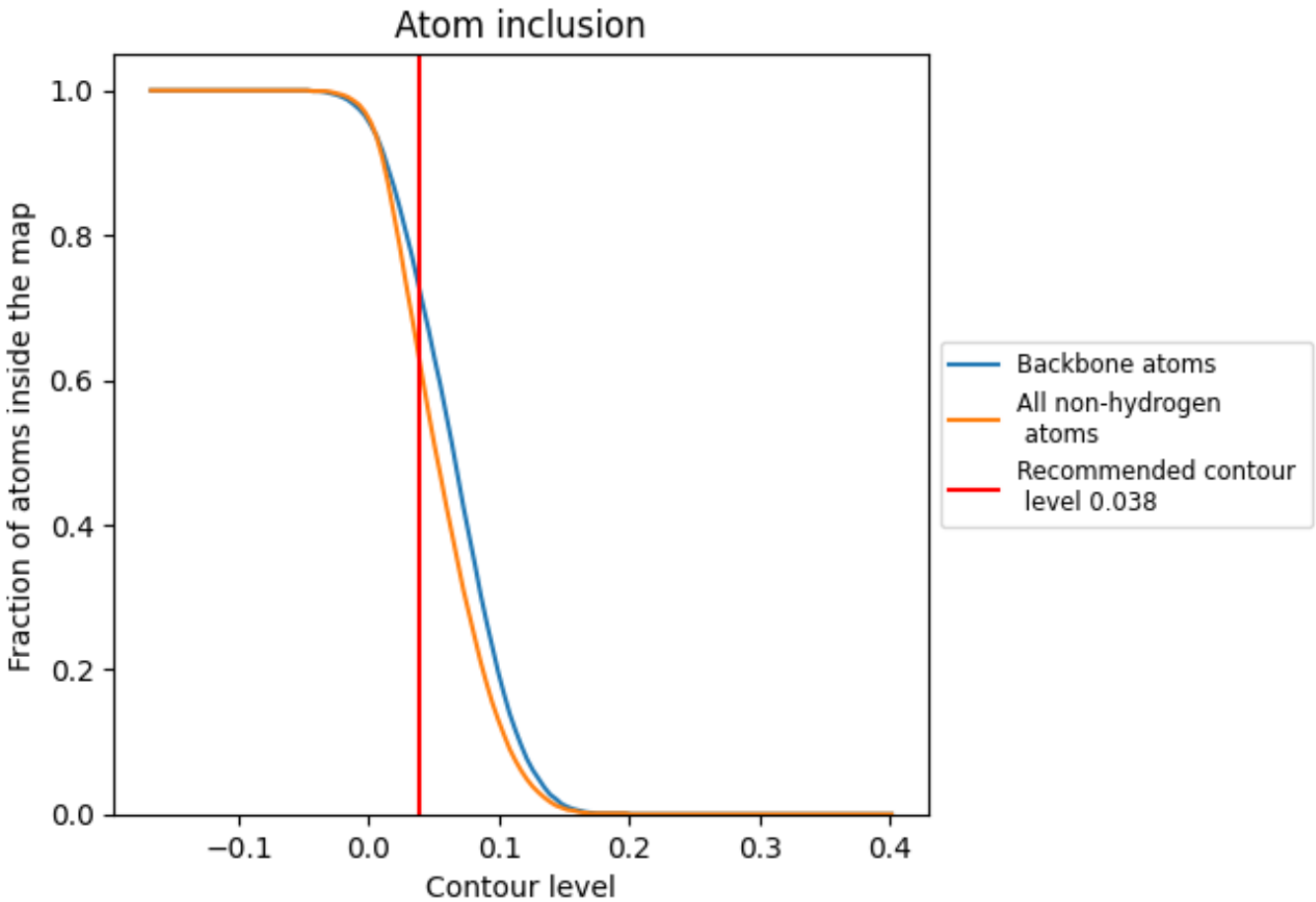
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.038).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.4330
A	0.6510	0.4290
B	0.6920	0.4540
C	0.6580	0.4240
D	0.7160	0.4480
E	0.7290	0.4560
F	0.6000	0.4130
G	0.6320	0.4350
H	0.6380	0.4150
I	0.6330	0.4280
J	0.6950	0.4530
K	0.7290	0.4760
L	0.6120	0.4340
M	0.6940	0.4610
N	0.6480	0.4380
O	0.6220	0.4420
P	0.6410	0.4420
Q	0.4630	0.3720
R	0.1930	0.3750
S	0.4230	0.4150
V	0.3120	0.3830