Full wwPDB EM Validation Report ⓘ

May 19, 2024 – 09:11 PM JST

PDB ID	:	6L7P
EMDB ID	:	EMD-0850
Title	:	cryo-EM structure of cyanobacteria NDH-1LdelV complex
Authors	:	Zhang, C.; Shuai, J.; Wu, J.; Lei, M.
Deposited on	:	2019-11-02
Resolution	:	3.60 Å(reported)

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

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

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

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

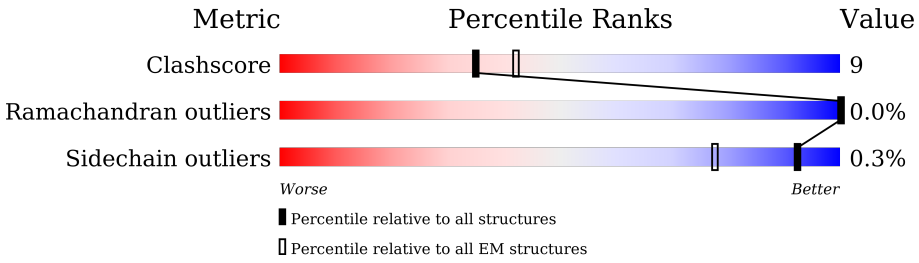
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	9% 87% 11%
2	B	515	83% 13%
3	C	132	16% 82% 10% 8%
4	D	529	83% 12% 5%
5	E	101	84% 16%
6	F	656	9% 87% 12%
7	G	200	8% 84% 12%
8	H	394	9% 84% 16%

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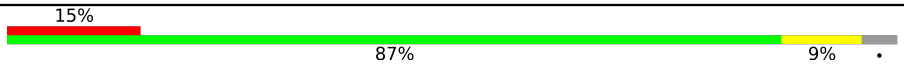
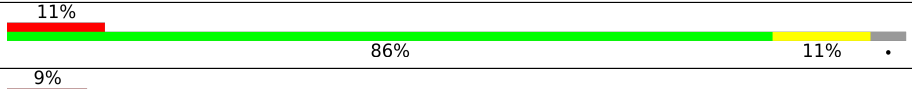
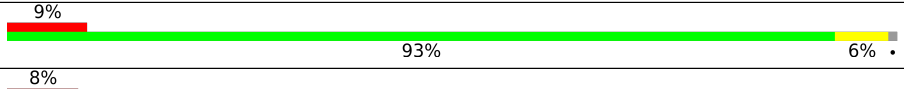
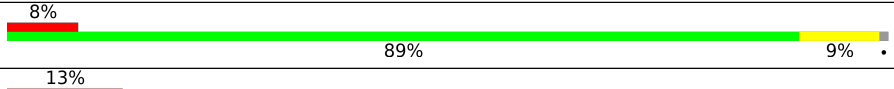
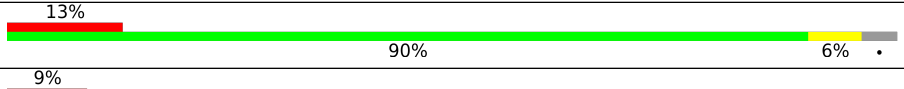
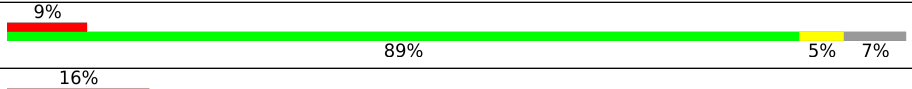
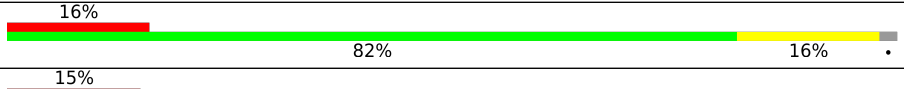
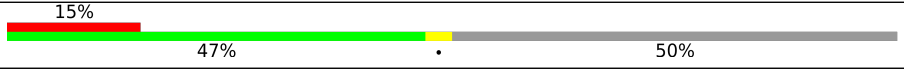
Mol	Chain	Length	Quality of chain
9	I	196	
10	J	168	
11	K	237	
12	L	76	
13	M	111	
14	N	150	
15	O	70	
16	P	44	
17	Q	45	
18	S	110	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	BCR	D	602	-	-	X	-
22	AJP	A	406	X	-	-	-
22	AJP	A	407	X	-	-	-
22	AJP	A	408	X	-	-	-
22	AJP	B	604	X	-	-	-
22	AJP	B	605	X	-	-	-
22	AJP	B	606	X	-	-	-
22	AJP	B	607	X	-	-	-
22	AJP	B	608	X	-	-	-
22	AJP	B	609	X	-	-	-
22	AJP	B	610	X	-	-	-
22	AJP	B	611	X	-	-	-
22	AJP	B	612	X	-	-	-
22	AJP	B	613	X	-	-	-
22	AJP	B	614	X	-	-	-
22	AJP	C	201	X	-	-	-
22	AJP	C	202	X	-	X	-
22	AJP	D	607	X	-	-	-
22	AJP	D	608	X	-	-	-
22	AJP	D	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	AJP	D	610	X	-	-	-
22	AJP	D	611	X	-	-	-
22	AJP	D	612	X	-	-	-
22	AJP	D	613	X	-	-	-
22	AJP	D	614	X	-	-	-
22	AJP	D	615	X	-	-	-
22	AJP	D	616	X	-	-	-
22	AJP	F	704	X	-	-	-
22	AJP	F	705	X	-	-	-
22	AJP	F	706	X	-	-	-
22	AJP	F	707	X	-	-	-
22	AJP	F	708	X	-	-	-
22	AJP	F	709	X	-	-	-
22	AJP	F	710	X	-	-	-
22	AJP	F	711	X	-	-	-
22	AJP	F	712	X	-	-	-
22	AJP	G	302	X	-	-	-
22	AJP	G	303	X	-	-	-
22	AJP	G	304	X	-	-	-
22	AJP	G	305	X	-	-	-
22	AJP	G	306	X	-	-	-
22	AJP	G	307	X	-	-	-
22	AJP	Q	101	X	-	-	-
22	AJP	Q	102	X	-	-	-
22	AJP	Q	103	X	-	-	-
25	SF4	I	202	-	-	X	-
25	SF4	K	301	-	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 32798 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	365	2820	1896	438	476	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	492	3723	2471	577	659	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	646	4997	3314	795	850	38	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1454	969	228	253	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	189	Total	C	N	O	S	0	0
			1516	967	260	276	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	200	Total	C	N	O	S	0	0
			1550	996	269	272	13		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	67	Total	C	N	O	0	0
			533	346	90	97		

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

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

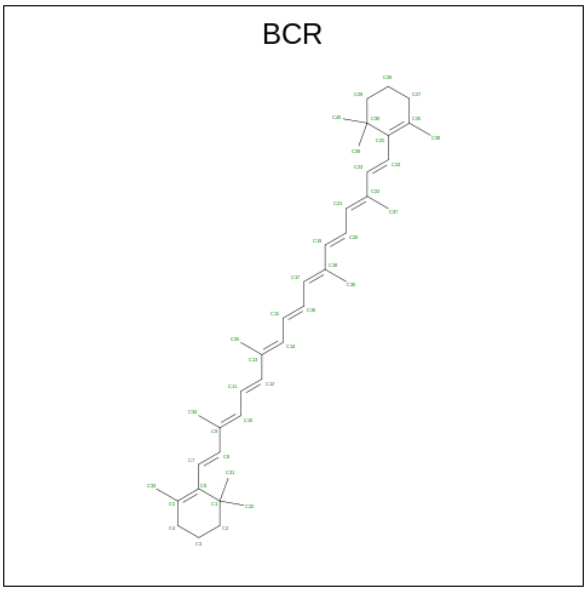
- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit Q.

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

- Molecule 18 is a protein called Tlr0636 protein.

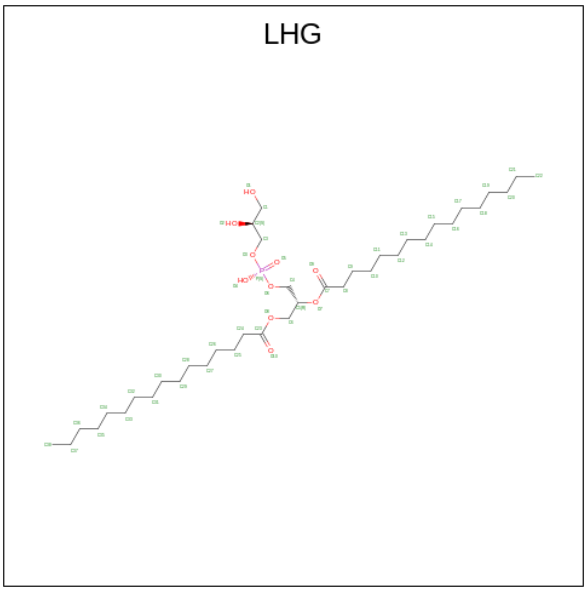
Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	55	Total	C	N	O	S	0	0
			432	280	69	82	1		

- Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



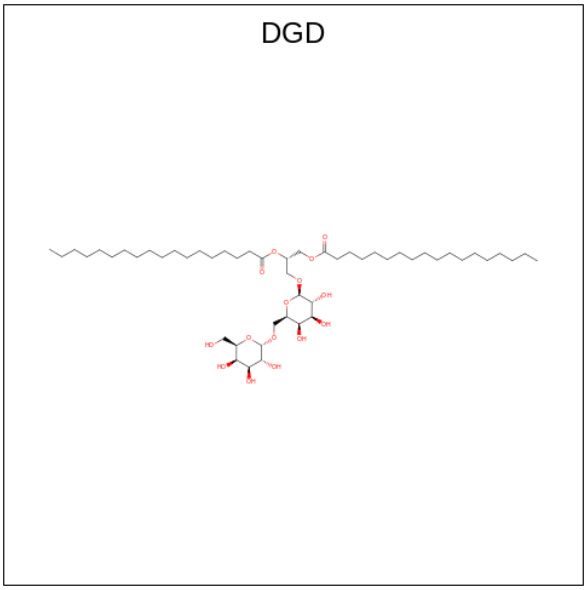
Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C 40 40	0
19	D	1	Total C 40 40	0
19	D	1	Total C 40 40	0

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



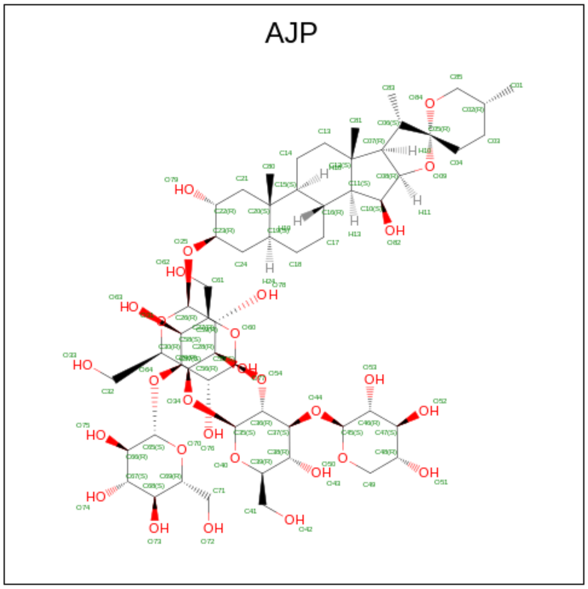
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	D	1	Total	C	O	P	0
			49	38	10	1	
20	D	1	Total	C	O	P	0
			49	38	10	1	
20	F	1	Total	C	O	P	0
			49	38	10	1	
20	F	1	Total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

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 22 is Digitonin (three-letter code: AJP) (formula: $C_{56}H_{92}O_{29}$).



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

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

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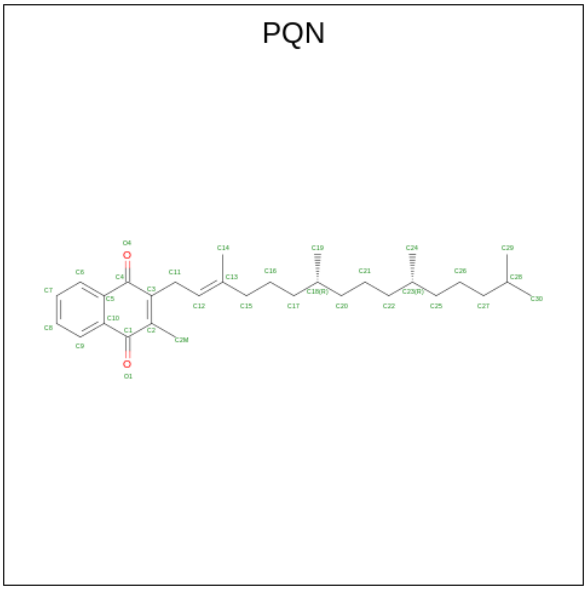
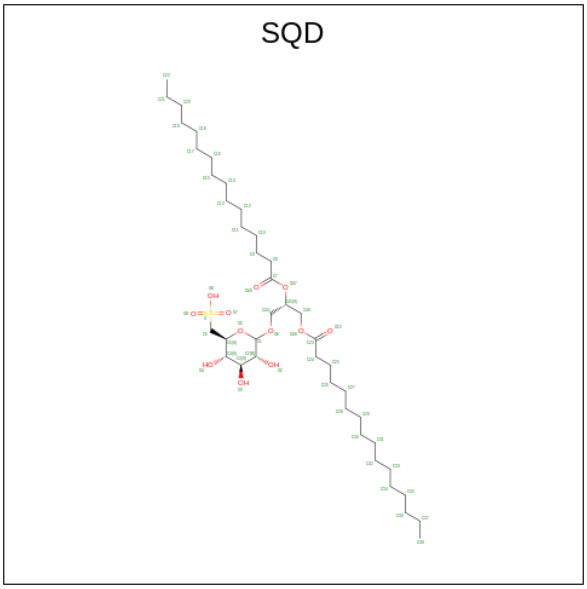
Mol	Chain	Residues	Atoms	AltConf
22	F	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	G	1	Total C O 32 27 5	0
22	Q	1	Total C O 32 27 5	0
22	Q	1	Total C O 32 27 5	0
22	Q	1	Total C O 32 27 5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

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



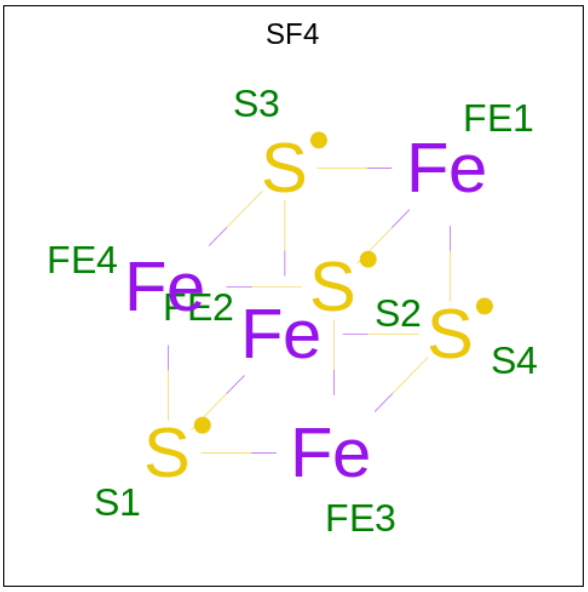
Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C O 33 31 2	0

- Molecule 24 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
24	D	1	Total	C	O	S	0
			54	41	12	1	
24	D	1	Total	C	O	S	0
			54	41	12	1	
24	F	1	Total	C	O	S	0
			54	41	12	1	
24	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



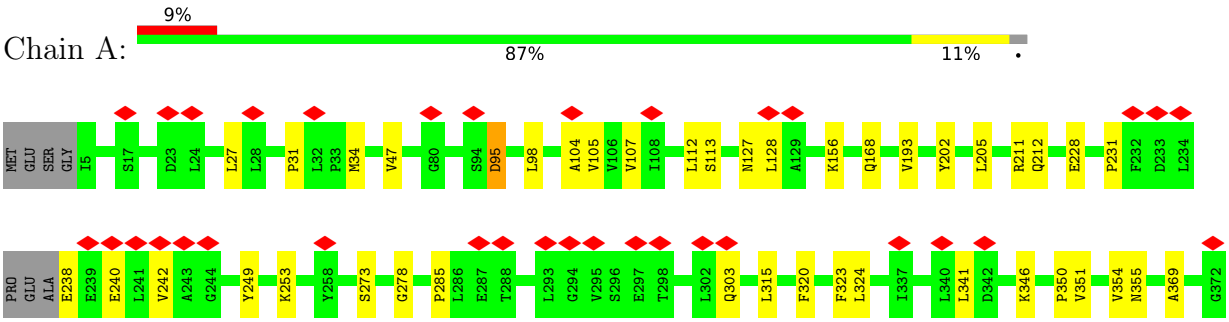
Mol	Chain	Residues	Atoms			AltConf
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	K	1	Total	Fe	S	0
			8	4	4	

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.

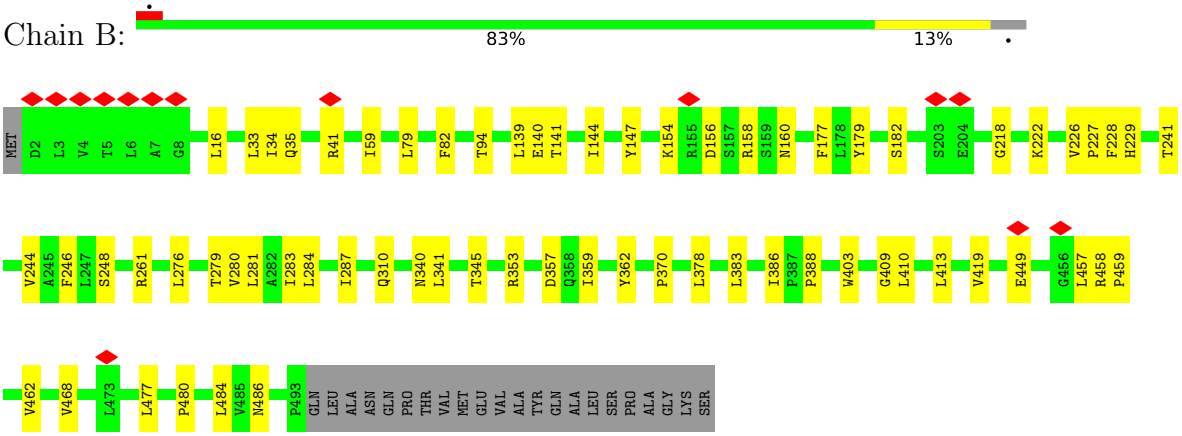
• Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1

Chain A:



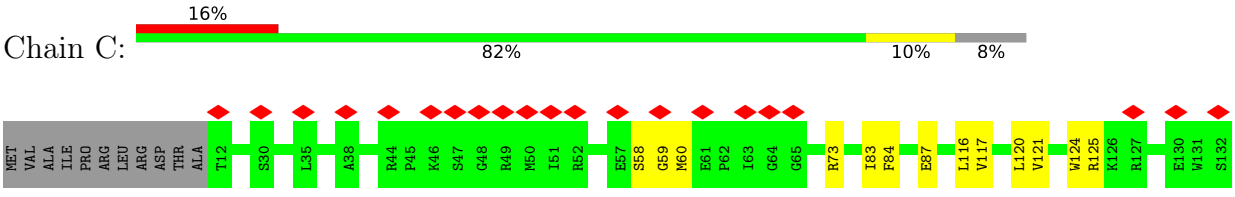
• Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2

Chain B:



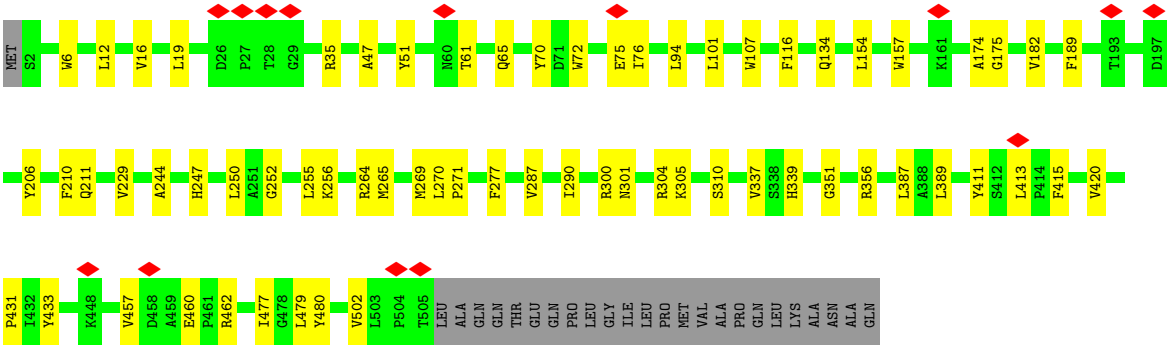
• Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3

Chain C:

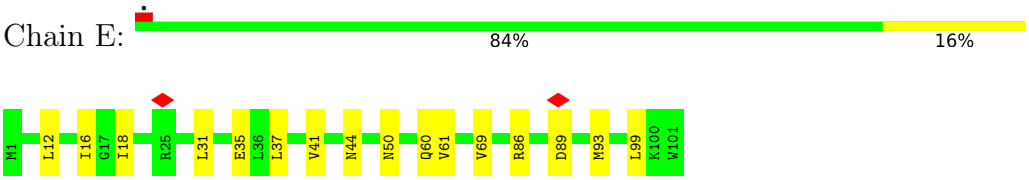


• Molecule 4: NAD(P)H-quinone oxidoreductase chain 4 1

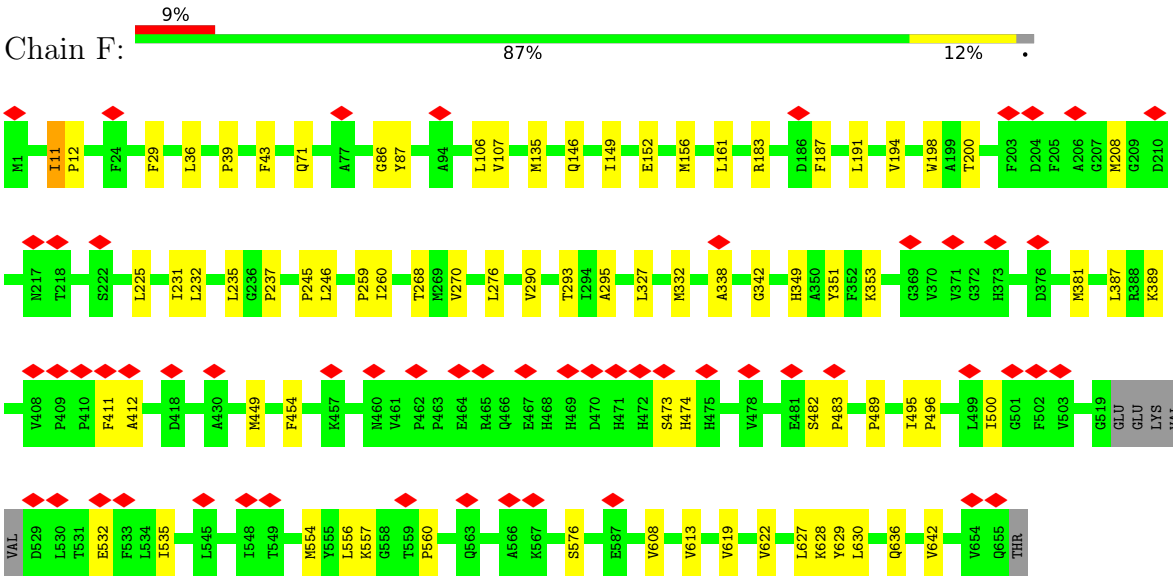
Chain D:



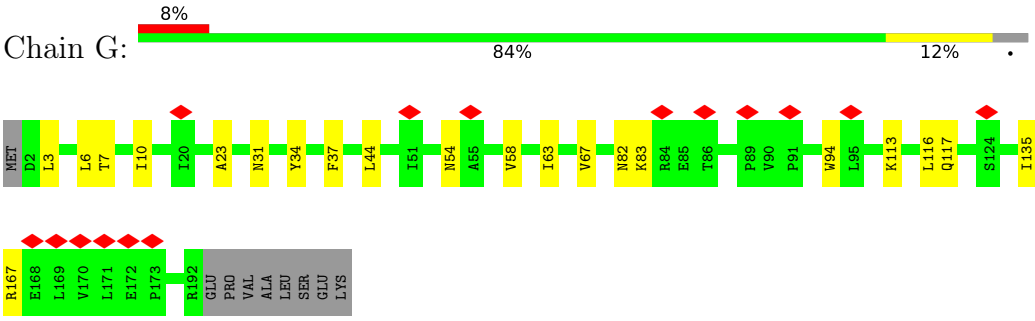
• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L



• Molecule 6: NADH dehydrogenase subunit 5

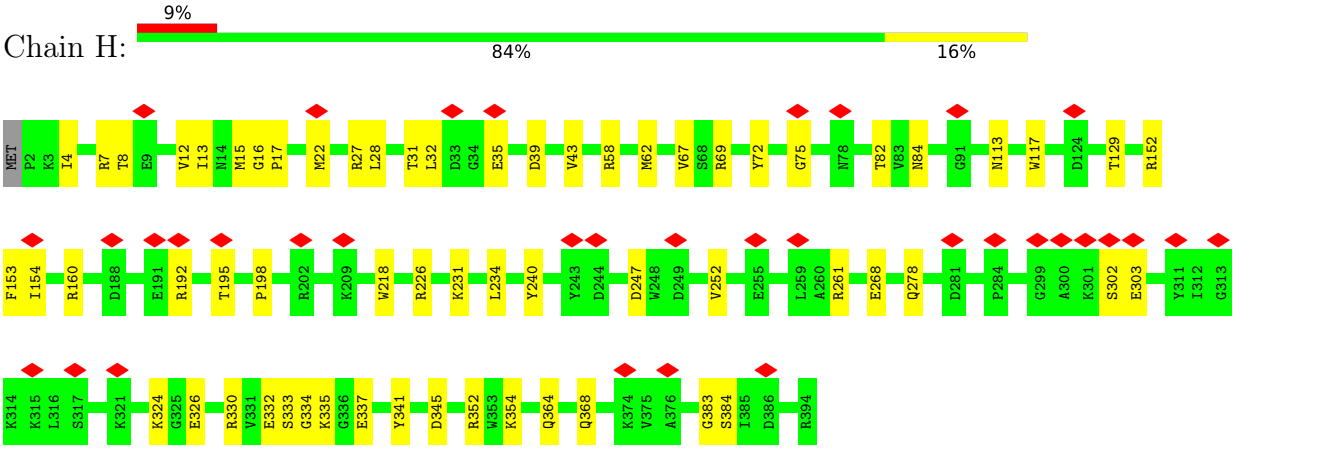


• Molecule 7: NADH-quinone oxidoreductase subunit J



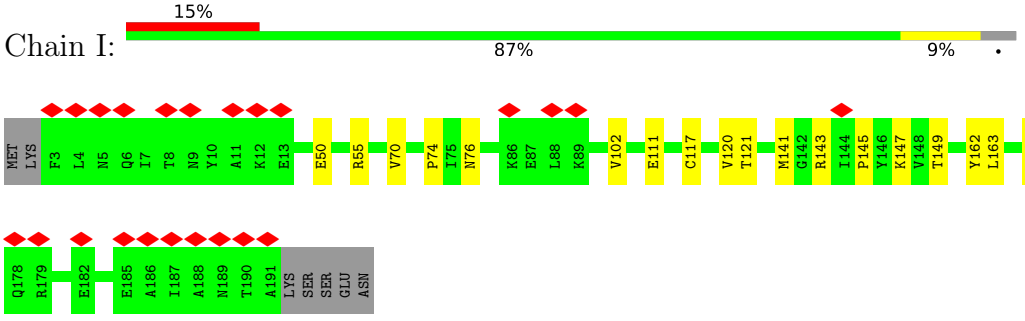
• Molecule 8: NAD(P)H-quinone oxidoreductase subunit H

Chain H:



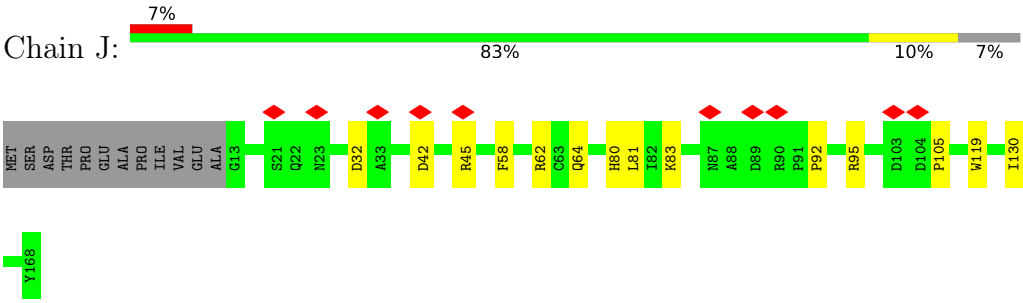
• Molecule 9: NAD(P)H-quinone oxidoreductase subunit I

Chain I:



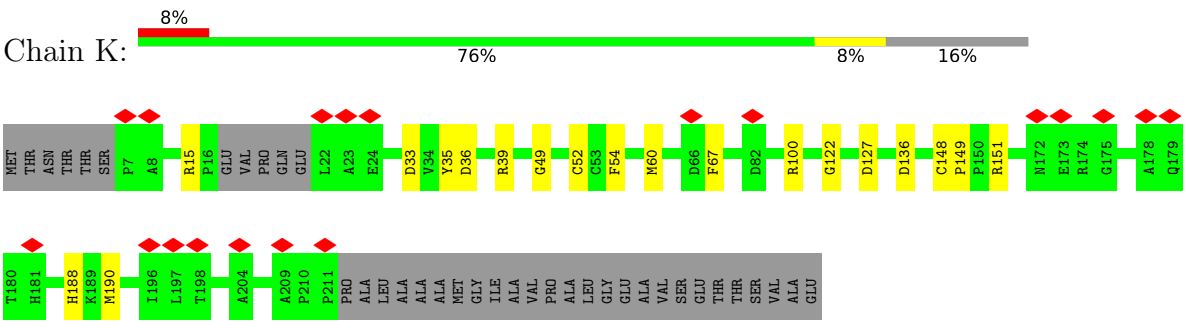
• Molecule 10: NAD(P)H-quinone oxidoreductase subunit J

Chain J:



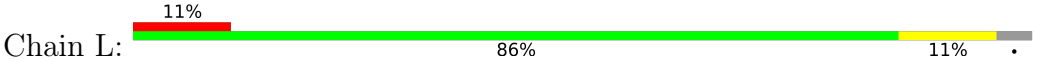
• Molecule 11: NAD(P)H-quinone oxidoreductase subunit K

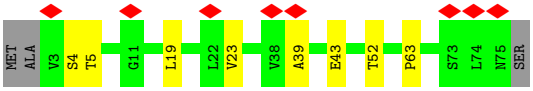
Chain K:



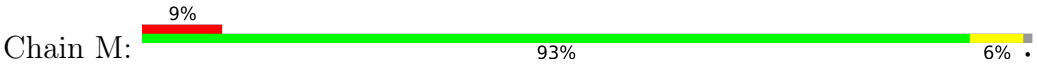
• Molecule 12: NAD(P)H-quinone oxidoreductase subunit L

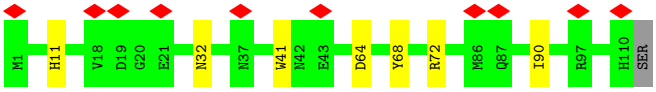
Chain L:



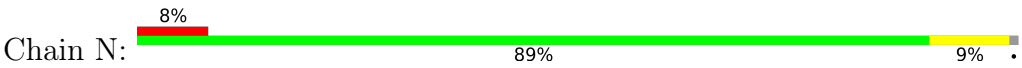


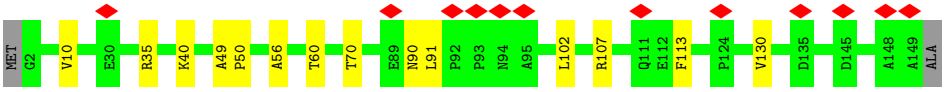
• Molecule 13: NAD(P)H-quinone oxidoreductase subunit M



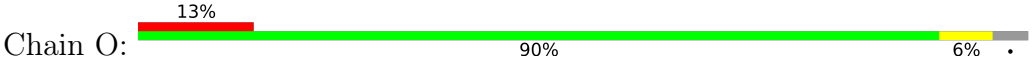


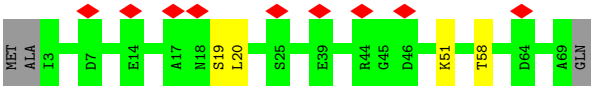
• Molecule 14: NAD(P)H-quinone oxidoreductase subunit N



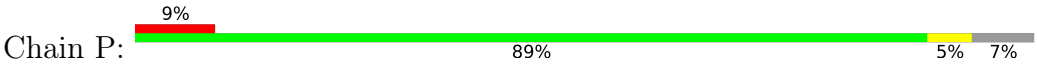


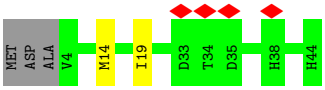
• Molecule 15: NAD(P)H-quinone oxidoreductase subunit O



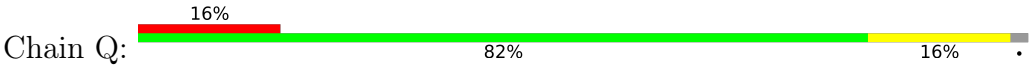


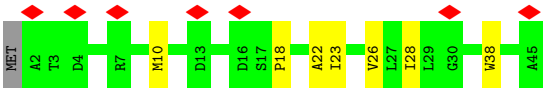
• Molecule 16: NAD(P)H-quinone oxidoreductase subunit P



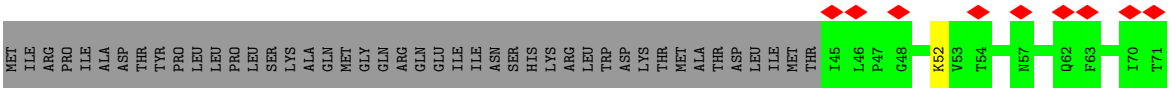


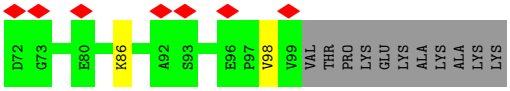
• Molecule 17: NAD(P)H-quinone oxidoreductase subunit Q





• Molecule 18: Tlr0636 protein




D72
G73
E80
K86
A92
S93
E96
P97
V98
V99
VAL
THR
PRO
LYS
GLU
LYS
ALA
LYS
ALA
LYS
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	439946	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	0.529	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0403	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, PQN, AJP, DGD, LHG, SQD, 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	0.28	0/2891	0.54	2/3950 (0.1%)
2	B	0.28	0/3809	0.49	0/5197
3	C	0.30	0/1008	0.52	0/1375
4	D	0.28	0/4003	0.50	1/5464 (0.0%)
5	E	0.27	0/793	0.46	0/1077
6	F	0.28	0/5146	0.48	0/7010
7	G	0.27	0/1486	0.46	0/2038
8	H	0.26	0/3260	0.47	0/4417
9	I	0.26	0/1554	0.46	0/2108
10	J	0.24	0/1314	0.46	1/1789 (0.1%)
11	K	0.26	0/1589	0.48	0/2160
12	L	0.30	0/610	0.49	0/835
13	M	0.24	0/895	0.44	0/1214
14	N	0.25	0/1197	0.46	0/1628
15	O	0.24	0/545	0.45	0/741
16	P	0.34	0/330	0.56	0/448
17	Q	0.26	0/341	0.38	0/464
18	S	0.26	0/441	0.47	0/601
All	All	0.27	0/31212	0.48	4/42516 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
8	H	0	1
14	N	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	LEU	CA-CB-CG	6.73	130.77	115.30
4	D	270	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	112	LEU	CA-CB-CG	5.53	128.02	115.30
10	J	42	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	GLU	Peptide
8	H	129	THR	Peptide
14	N	91	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2820	0	2953	48	0
2	B	3723	0	3857	88	0
3	C	978	0	1008	43	0
4	D	3896	0	4040	75	0
5	E	783	0	837	15	0
6	F	4997	0	5026	69	0
7	G	1454	0	1540	43	0
8	H	3177	0	3157	42	0
9	I	1516	0	1484	14	0
10	J	1278	0	1233	11	0
11	K	1550	0	1588	16	0
12	L	590	0	603	5	0
13	M	879	0	860	4	0
14	N	1165	0	1176	8	0
15	O	533	0	544	2	0
16	P	321	0	317	3	0
17	Q	332	0	331	7	0
18	S	432	0	430	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	40	0	56	18	0
19	D	80	0	112	40	0
20	A	98	0	144	1	0
20	B	98	0	146	2	0
20	D	98	0	148	2	0
20	F	98	0	144	0	0
20	G	49	0	74	2	0
21	A	132	0	191	2	0
22	A	96	0	0	15	0
22	B	352	0	0	86	0
22	C	64	0	0	29	0
22	D	320	0	0	63	0
22	F	288	0	0	46	0
22	G	192	0	0	36	0
22	Q	96	0	0	11	0
23	B	33	0	46	1	0
24	D	108	0	156	10	0
24	F	54	0	78	2	0
24	L	54	0	78	1	0
25	I	16	0	0	2	0
25	K	8	0	0	3	0
All	All	32798	0	32357	565	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (565) 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)
3:C:124:TRP:CZ3	22:C:202:AJP:C81	1.81	1.59
4:D:277:PHE:HE2	22:D:613:AJP:C81	1.08	1.57
2:B:287:ILE:CD1	22:B:614:AJP:C83	1.83	1.52
4:D:277:PHE:CE2	22:D:613:AJP:C81	1.93	1.51
1:A:323:PHE:CE2	19:A:401:BCR:H20C	1.45	1.50
2:B:280:VAL:CG2	22:B:613:AJP:C81	1.94	1.46
2:B:280:VAL:HG22	22:B:613:AJP:C81	1.42	1.44
3:C:124:TRP:HH2	22:C:201:AJP:C13	1.32	1.42
2:B:484:LEU:HD11	22:B:604:AJP:C13	1.47	1.40
4:D:413:LEU:HD23	22:D:612:AJP:C80	1.50	1.39
6:F:29:PHE:CE2	22:F:705:AJP:O82	1.79	1.34
2:B:283:ILE:CD1	22:B:614:AJP:C80	2.03	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:708:AJP:C03	22:Q:102:AJP:C13	2.04	1.33
7:G:7:THR:CG2	22:G:303:AJP:C83	2.09	1.30
3:C:124:TRP:CH2	22:C:201:AJP:C13	2.14	1.30
6:F:39:PRO:HB3	22:F:712:AJP:C83	1.59	1.30
2:B:283:ILE:HD13	22:B:614:AJP:C80	1.64	1.27
3:C:124:TRP:HZ3	22:C:202:AJP:C81	1.25	1.26
3:C:121:VAL:HG22	22:C:202:AJP:C13	1.63	1.26
2:B:484:LEU:CD1	22:B:604:AJP:C13	2.15	1.24
17:Q:18:PRO:HB3	22:Q:102:AJP:C18	1.66	1.23
4:D:413:LEU:CD2	22:D:612:AJP:C80	2.14	1.23
2:B:59:ILE:CD1	22:B:604:AJP:O82	1.85	1.22
3:C:124:TRP:CE3	22:C:202:AJP:C81	2.22	1.22
7:G:116:LEU:HD13	22:G:306:AJP:C14	1.70	1.21
7:G:116:LEU:CD1	22:G:306:AJP:C14	2.17	1.21
2:B:287:ILE:HD11	22:B:614:AJP:C83	1.49	1.19
7:G:10:ILE:HD13	22:G:304:AJP:C83	1.73	1.19
1:A:324:LEU:HD13	19:A:401:BCR:H371	1.24	1.16
6:F:39:PRO:CB	22:F:712:AJP:C83	2.23	1.16
2:B:59:ILE:HG23	22:B:604:AJP:C18	1.73	1.16
4:D:47:ALA:HB1	22:D:611:AJP:C01	1.78	1.14
4:D:277:PHE:CZ	22:D:613:AJP:C80	2.29	1.14
19:D:602:BCR:H343	19:D:602:BCR:H321	1.25	1.14
7:G:7:THR:HG22	22:G:303:AJP:C83	1.75	1.12
7:G:116:LEU:CD1	22:G:306:AJP:C13	2.28	1.11
2:B:287:ILE:HD12	22:B:614:AJP:C83	1.81	1.09
6:F:198:TRP:CE3	22:F:706:AJP:C10	2.35	1.09
3:C:124:TRP:CE3	22:C:202:AJP:C80	2.36	1.09
1:A:323:PHE:HE2	19:A:401:BCR:C20	1.65	1.08
19:D:601:BCR:H12C	19:D:601:BCR:H341	1.31	1.08
4:D:16:VAL:HG11	22:D:609:AJP:C01	1.84	1.06
1:A:323:PHE:CE2	19:A:401:BCR:C20	2.38	1.06
7:G:37:PHE:HB3	22:G:302:AJP:C83	1.86	1.05
1:A:324:LEU:HD13	19:A:401:BCR:C37	1.90	1.02
2:B:59:ILE:HD13	22:B:604:AJP:O82	1.57	1.00
6:F:36:LEU:HD11	22:F:712:AJP:C80	1.91	1.00
3:C:125:ARG:HD2	22:C:202:AJP:O79	1.62	0.99
2:B:280:VAL:HG23	22:B:613:AJP:C81	1.91	0.98
7:G:94:TRP:HZ3	22:G:307:AJP:O25	1.44	0.98
6:F:198:TRP:CZ3	22:F:706:AJP:C07	2.47	0.97
19:A:401:BCR:H23C	19:A:401:BCR:H392	1.45	0.97
4:D:6:TRP:CH2	22:D:615:AJP:C13	2.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:7:THR:HG21	22:G:303:AJP:C83	1.92	0.96
3:C:124:TRP:CH2	22:C:201:AJP:C14	2.48	0.96
19:D:602:BCR:H321	19:D:602:BCR:C34	1.96	0.95
22:B:612:AJP:O79	22:D:614:AJP:C18	2.14	0.95
2:B:484:LEU:HD13	22:B:605:AJP:O82	1.66	0.94
4:D:47:ALA:CB	22:D:611:AJP:C01	2.44	0.94
4:D:182:VAL:CG1	22:D:614:AJP:C83	2.44	0.94
6:F:71:GLN:NE2	22:F:709:AJP:C80	2.32	0.93
4:D:6:TRP:HH2	22:D:615:AJP:C13	1.82	0.92
7:G:116:LEU:HD12	22:G:306:AJP:C13	2.00	0.91
1:A:324:LEU:CD1	19:A:401:BCR:H371	2.02	0.90
3:C:124:TRP:CZ3	22:C:202:AJP:C80	2.54	0.90
19:D:601:BCR:H383	19:D:601:BCR:H23C	1.54	0.90
2:B:287:ILE:HD13	22:B:614:AJP:C83	2.00	0.90
3:C:124:TRP:CZ3	22:C:202:AJP:C16	2.54	0.90
4:D:290:ILE:HG21	19:D:602:BCR:H323	1.52	0.90
2:B:59:ILE:HD11	22:B:604:AJP:O82	1.71	0.90
3:C:124:TRP:HH2	22:C:201:AJP:C14	1.85	0.90
4:D:70:TYR:CE2	22:D:608:AJP:C80	2.56	0.89
7:G:10:ILE:HG12	22:G:305:AJP:C81	2.01	0.89
22:B:609:AJP:C24	3:C:125:ARG:HH22	1.86	0.89
17:Q:18:PRO:CB	22:Q:102:AJP:C18	2.51	0.88
7:G:116:LEU:HD11	22:G:306:AJP:C13	2.04	0.88
3:C:124:TRP:CD2	22:C:202:AJP:C80	2.57	0.87
2:B:477:LEU:HD22	22:B:607:AJP:C03	2.06	0.86
4:D:16:VAL:HG21	22:D:609:AJP:C03	2.05	0.86
19:D:602:BCR:H363	24:D:605:SQD:C16	2.06	0.85
2:B:34:ILE:HD11	22:B:609:AJP:C81	2.06	0.84
19:D:602:BCR:H343	19:D:602:BCR:C32	2.06	0.83
4:D:182:VAL:HG12	22:D:614:AJP:C83	2.08	0.83
6:F:225:LEU:HB3	22:F:706:AJP:C04	2.08	0.83
1:A:323:PHE:CD2	19:A:401:BCR:H20C	2.13	0.83
6:F:39:PRO:HB2	22:F:712:AJP:C83	2.08	0.82
19:D:602:BCR:H363	24:D:605:SQD:H161	1.62	0.82
2:B:283:ILE:HD12	22:B:614:AJP:C80	2.09	0.82
4:D:16:VAL:CG1	22:D:609:AJP:C01	2.58	0.82
4:D:479:LEU:O	22:D:616:AJP:C83	2.27	0.82
3:C:124:TRP:CZ2	22:C:201:AJP:C14	2.63	0.81
4:D:182:VAL:HG11	22:D:614:AJP:C83	2.08	0.81
19:D:602:BCR:C36	24:D:605:SQD:H152	2.09	0.81
7:G:116:LEU:CD1	22:G:306:AJP:C15	2.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:VAL:HG22	22:B:613:AJP:C83	2.12	0.80
7:G:116:LEU:HD13	22:G:306:AJP:C15	2.12	0.79
2:B:283:ILE:CG2	22:B:614:AJP:C81	2.60	0.79
4:D:277:PHE:CD2	22:D:613:AJP:C81	2.63	0.79
6:F:198:TRP:HZ3	22:F:706:AJP:C07	1.92	0.79
1:A:202:TYR:HE1	22:A:408:AJP:C80	1.96	0.79
4:D:413:LEU:HD21	22:D:612:AJP:C80	2.09	0.79
7:G:10:ILE:CD1	22:G:304:AJP:C83	2.60	0.78
6:F:29:PHE:CD2	22:F:705:AJP:O82	2.36	0.78
7:G:7:THR:CB	22:G:303:AJP:C83	2.61	0.78
3:C:124:TRP:HZ3	22:C:202:AJP:C16	1.96	0.78
19:D:602:BCR:H363	24:D:605:SQD:H152	1.66	0.78
22:F:708:AJP:C03	22:Q:102:AJP:C14	2.61	0.78
3:C:121:VAL:CG2	22:C:202:AJP:C13	2.56	0.77
2:B:35:GLN:CG	22:B:610:AJP:C14	2.62	0.77
2:B:484:LEU:HD12	22:B:604:AJP:C13	2.13	0.77
19:D:601:BCR:C8	19:D:601:BCR:H311	2.14	0.77
1:A:350:PRO:HB3	22:C:202:AJP:C04	2.15	0.76
22:B:609:AJP:C24	3:C:125:ARG:NH2	2.48	0.76
2:B:283:ILE:HD11	22:B:614:AJP:C80	2.09	0.76
6:F:29:PHE:HE2	22:F:705:AJP:O82	1.65	0.76
2:B:82:PHE:CD2	22:B:604:AJP:C85	2.69	0.76
3:C:124:TRP:CE3	22:C:202:AJP:C14	2.70	0.75
22:G:304:AJP:C13	22:G:305:AJP:O82	2.35	0.75
1:A:202:TYR:CE1	22:A:408:AJP:C80	2.70	0.75
7:G:94:TRP:CZ3	22:G:307:AJP:O25	2.36	0.75
22:D:610:AJP:O82	22:D:615:AJP:C83	2.35	0.74
4:D:290:ILE:HG21	19:D:602:BCR:HC31	1.70	0.74
19:D:602:BCR:H363	24:D:605:SQD:C15	2.18	0.74
2:B:283:ILE:HG23	22:B:614:AJP:C81	2.17	0.73
3:C:125:ARG:CD	22:C:202:AJP:O79	2.35	0.73
4:D:70:TYR:HE2	22:D:608:AJP:C80	1.98	0.73
4:D:290:ILE:CG2	19:D:602:BCR:HC31	2.18	0.73
19:D:601:BCR:H341	19:D:601:BCR:C12	2.06	0.73
4:D:480:TYR:CE2	22:D:616:AJP:C80	2.72	0.72
4:D:6:TRP:CH2	22:D:615:AJP:C14	2.73	0.72
22:F:708:AJP:C04	22:Q:102:AJP:C14	2.68	0.71
7:G:7:THR:HB	22:G:303:AJP:C83	2.20	0.71
8:H:330:ARG:HE	10:J:62:ARG:HH22	1.39	0.71
19:D:602:BCR:H23C	19:D:602:BCR:C40	2.21	0.71
4:D:6:TRP:HH2	22:D:615:AJP:C14	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:71:GLN:HE21	22:F:709:AJP:C21	2.04	0.70
19:A:401:BCR:H321	19:A:401:BCR:HC8	1.74	0.70
2:B:59:ILE:HD12	22:B:604:AJP:C17	2.21	0.70
2:B:287:ILE:HD11	22:B:614:AJP:C06	2.21	0.70
4:D:277:PHE:CE1	22:D:613:AJP:C80	2.75	0.70
2:B:59:ILE:CG2	22:B:604:AJP:C18	2.62	0.70
22:B:609:AJP:C10	3:C:121:VAL:HG11	2.22	0.70
19:D:602:BCR:H23C	19:D:602:BCR:H403	1.72	0.69
19:D:601:BCR:H12C	19:D:601:BCR:C34	2.18	0.69
2:B:59:ILE:HG23	22:B:604:AJP:C17	2.22	0.69
22:B:608:AJP:C03	4:D:19:LEU:HD22	2.22	0.69
7:G:10:ILE:HA	22:G:305:AJP:C83	2.23	0.69
22:B:609:AJP:C18	3:C:125:ARG:NH2	2.55	0.69
1:A:285:PRO:HG2	22:A:408:AJP:C14	2.23	0.69
2:B:283:ILE:HG21	22:B:614:AJP:C81	2.23	0.68
6:F:198:TRP:CZ3	22:F:706:AJP:C11	2.76	0.68
7:G:10:ILE:CG1	22:G:305:AJP:C81	2.70	0.68
22:B:612:AJP:C03	22:B:614:AJP:C13	2.72	0.68
7:G:116:LEU:HD12	22:G:306:AJP:C15	2.23	0.67
1:A:323:PHE:CD2	19:A:401:BCR:C20	2.75	0.67
1:A:211:ARG:NH2	22:A:407:AJP:C17	2.58	0.67
6:F:198:TRP:CZ3	22:F:706:AJP:C10	2.79	0.66
6:F:630:LEU:HD13	22:F:710:AJP:C83	2.25	0.66
2:B:484:LEU:CD1	22:B:605:AJP:O82	2.41	0.66
4:D:72:TRP:CD1	22:D:607:AJP:C17	2.79	0.65
2:B:35:GLN:CD	22:B:610:AJP:C14	2.65	0.65
19:D:602:BCR:H20C	24:D:605:SQD:H312	1.77	0.65
4:D:12:LEU:HD21	22:D:607:AJP:C04	2.27	0.64
19:D:602:BCR:H321	19:D:602:BCR:C9	2.27	0.64
2:B:413:LEU:HD22	22:B:614:AJP:C13	2.27	0.63
3:C:124:TRP:HE3	22:C:202:AJP:C14	2.11	0.63
4:D:72:TRP:NE1	22:D:607:AJP:C10	2.60	0.63
19:A:401:BCR:H392	19:A:401:BCR:C23	2.20	0.63
4:D:12:LEU:HD11	22:D:607:AJP:C83	2.29	0.62
6:F:71:GLN:HE22	22:F:709:AJP:C80	2.10	0.62
2:B:283:ILE:HD11	22:B:614:AJP:C21	2.28	0.62
22:D:607:AJP:C80	22:D:608:AJP:C81	2.77	0.62
4:D:277:PHE:CE2	22:D:613:AJP:C80	2.82	0.62
4:D:72:TRP:NE1	22:D:607:AJP:C11	2.63	0.62
2:B:59:ILE:CD1	22:B:604:AJP:C17	2.77	0.62
22:B:613:AJP:C13	22:B:614:AJP:C80	2.78	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:69:ARG:HG2	25:K:301:SF4:S2	2.39	0.62
1:A:127:ASN:HD22	1:A:193:VAL:HG21	1.65	0.62
1:A:285:PRO:HD3	22:A:408:AJP:C13	2.30	0.62
19:D:602:BCR:H403	19:D:602:BCR:C23	2.31	0.61
2:B:35:GLN:OE1	22:B:610:AJP:C13	2.48	0.61
5:E:12:LEU:CD1	22:G:307:AJP:C01	2.79	0.60
6:F:629:TYR:HB2	22:F:710:AJP:C81	2.31	0.60
8:H:69:ARG:NH2	11:K:148:CYS:SG	2.75	0.60
4:D:420:VAL:HG11	6:F:194:VAL:HG11	1.82	0.60
17:Q:22:ALA:HB2	22:Q:102:AJP:O82	2.02	0.60
4:D:244:ALA:HB2	4:D:351:GLY:HA3	1.83	0.59
6:F:270:VAL:HG13	6:F:327:LEU:HD21	1.83	0.59
19:D:601:BCR:H23C	19:D:601:BCR:C38	2.30	0.59
19:D:602:BCR:H311	19:D:602:BCR:H342	1.85	0.59
19:D:602:BCR:H362	24:D:605:SQD:H152	1.83	0.59
2:B:386:ILE:HG22	2:B:388:PRO:HD2	1.84	0.59
2:B:226:VAL:HG11	2:B:284:LEU:HB3	1.85	0.59
19:D:602:BCR:H321	19:D:602:BCR:C8	2.32	0.58
12:L:63:PRO:HB3	24:L:101:SQD:H82	1.85	0.58
3:C:60:MET:HG3	8:H:27:ARG:HH11	1.67	0.58
2:B:477:LEU:HD22	22:B:607:AJP:C04	2.33	0.58
1:A:346:LYS:HE3	3:C:124:TRP:HE1	1.68	0.57
6:F:198:TRP:CE3	22:F:706:AJP:C11	2.86	0.57
4:D:411:TYR:HB3	4:D:415:PHE:HB3	1.85	0.57
8:H:27:ARG:HB3	8:H:43:VAL:HB	1.85	0.57
5:E:12:LEU:HD12	22:G:307:AJP:C01	2.35	0.57
1:A:285:PRO:CD	22:A:408:AJP:C13	2.82	0.56
1:A:354:VAL:HG12	22:C:202:AJP:C01	2.36	0.56
22:D:610:AJP:O82	22:D:615:AJP:C81	2.54	0.56
5:E:50:ASN:OD1	7:G:54:ASN:ND2	2.39	0.56
22:Q:103:AJP:C83	22:Q:103:AJP:C81	2.84	0.56
22:B:609:AJP:C18	3:C:125:ARG:HH21	2.17	0.56
22:B:612:AJP:C81	22:B:612:AJP:C83	2.84	0.56
22:C:202:AJP:C81	22:C:202:AJP:C83	2.84	0.56
3:C:124:TRP:HE3	22:C:202:AJP:C81	2.10	0.56
22:F:706:AJP:C81	22:F:706:AJP:C83	2.85	0.55
22:A:407:AJP:C81	22:A:407:AJP:C83	2.85	0.55
22:D:611:AJP:C83	22:D:611:AJP:C81	2.85	0.55
22:F:704:AJP:C81	22:F:704:AJP:C83	2.85	0.55
22:Q:102:AJP:C81	22:Q:102:AJP:C83	2.84	0.55
1:A:354:VAL:CG1	22:C:202:AJP:C01	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:406:AJP:C81	22:A:406:AJP:C83	2.85	0.55
22:B:614:AJP:C83	22:B:614:AJP:C81	2.85	0.55
19:D:601:BCR:H383	19:D:601:BCR:C23	2.33	0.55
22:G:302:AJP:C83	22:G:302:AJP:C81	2.85	0.55
22:B:611:AJP:C81	22:B:611:AJP:C83	2.85	0.55
22:C:201:AJP:C83	22:C:201:AJP:C81	2.85	0.55
22:D:615:AJP:C83	22:D:615:AJP:C81	2.85	0.55
22:F:710:AJP:C83	22:F:710:AJP:C81	2.84	0.55
22:G:303:AJP:C83	22:G:303:AJP:C81	2.84	0.55
22:B:606:AJP:C81	22:B:606:AJP:C83	2.85	0.55
22:D:608:AJP:C81	22:D:608:AJP:C83	2.85	0.55
22:D:613:AJP:C81	22:D:613:AJP:C83	2.85	0.55
22:F:708:AJP:C83	22:F:708:AJP:C81	2.84	0.55
22:G:304:AJP:C83	22:G:304:AJP:C81	2.85	0.55
22:G:305:AJP:C81	22:G:305:AJP:C83	2.84	0.55
22:F:705:AJP:C81	22:F:705:AJP:C83	2.85	0.55
22:F:712:AJP:C83	22:F:712:AJP:C81	2.85	0.55
9:I:102:VAL:HG12	11:K:122:GLY:H	1.71	0.55
22:D:614:AJP:C83	22:D:614:AJP:C81	2.85	0.55
6:F:11:ILE:HG23	6:F:12:PRO:HD3	1.89	0.55
22:A:408:AJP:C81	22:A:408:AJP:C83	2.84	0.55
2:B:34:ILE:HD11	22:B:609:AJP:C16	2.36	0.55
22:B:607:AJP:C81	22:B:607:AJP:C83	2.85	0.55
22:B:609:AJP:C81	22:B:609:AJP:C83	2.85	0.55
22:D:610:AJP:C81	22:D:610:AJP:C83	2.84	0.55
22:F:709:AJP:C81	22:F:709:AJP:C83	2.85	0.55
22:G:307:AJP:C83	22:G:307:AJP:C81	2.85	0.55
2:B:276:LEU:HB2	22:B:613:AJP:C80	2.37	0.55
22:B:604:AJP:C81	22:B:604:AJP:C83	2.84	0.55
22:B:605:AJP:C81	22:B:605:AJP:C83	2.85	0.55
22:B:608:AJP:C81	22:B:608:AJP:C83	2.85	0.55
22:D:607:AJP:C83	22:D:607:AJP:C81	2.85	0.55
22:D:609:AJP:C83	22:D:609:AJP:C81	2.85	0.55
22:D:612:AJP:C81	22:D:612:AJP:C83	2.85	0.55
22:F:707:AJP:C81	22:F:707:AJP:C83	2.85	0.55
22:Q:101:AJP:C83	22:Q:101:AJP:C81	2.85	0.54
22:B:610:AJP:C83	22:B:610:AJP:C81	2.85	0.54
22:D:616:AJP:C83	22:D:616:AJP:C81	2.85	0.54
22:G:306:AJP:C81	22:G:306:AJP:C83	2.85	0.54
22:F:711:AJP:C81	22:F:711:AJP:C83	2.85	0.54
22:B:613:AJP:C81	22:B:613:AJP:C83	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D:611:AJP:C01	16:P:19:ILE:CD1	2.86	0.54
5:E:93:MET:HG2	6:F:636:GLN:HE22	1.73	0.54
6:F:71:GLN:HE21	22:F:709:AJP:C80	2.16	0.54
9:I:163:LEU:HD13	9:I:167:VAL:HB	1.88	0.54
2:B:156:ASP:O	2:B:160:ASN:ND2	2.41	0.54
22:B:605:AJP:C14	22:B:606:AJP:O82	2.55	0.54
22:B:604:AJP:C83	22:B:604:AJP:C02	2.85	0.54
22:F:709:AJP:C83	22:F:709:AJP:C02	2.85	0.54
19:D:601:BCR:C8	19:D:601:BCR:C31	2.85	0.54
22:D:611:AJP:C83	22:D:611:AJP:C02	2.85	0.54
6:F:86:GLY:H	6:F:146:GLN:HE22	1.54	0.54
2:B:409:GLY:HA2	22:B:612:AJP:C83	2.37	0.53
6:F:29:PHE:CZ	22:F:705:AJP:C17	2.92	0.53
8:H:326:GLU:OE2	10:J:95:ARG:NH1	2.41	0.53
11:K:188:HIS:HD2	11:K:190:MET:H	1.56	0.53
1:A:211:ARG:HH22	22:A:407:AJP:C17	2.21	0.53
13:M:41:TRP:HA	13:M:90:ILE:HD12	1.90	0.53
8:H:261:ARG:NH2	8:H:384:SER:OG	2.42	0.53
9:I:147:LYS:HG3	9:I:149:THR:H	1.72	0.53
6:F:198:TRP:HE3	22:F:706:AJP:C10	2.16	0.53
5:E:16:ILE:HG21	7:G:23:ALA:HB1	1.90	0.53
11:K:36:ASP:OD2	14:N:35:ARG:NH1	2.42	0.53
1:A:27:LEU:HD12	7:G:3:LEU:HD21	1.91	0.53
1:A:238:GLU:N	1:A:242:VAL:O	2.42	0.53
3:C:124:TRP:CH2	22:C:202:AJP:C80	2.92	0.52
1:A:351:VAL:HG12	22:C:201:AJP:C02	2.38	0.52
6:F:152:GLU:OE1	6:F:183:ARG:NH1	2.42	0.52
22:B:612:AJP:C06	22:B:612:AJP:C02	2.86	0.52
1:A:228:GLU:HA	1:A:231:PRO:HG2	1.91	0.52
22:B:606:AJP:C06	22:B:606:AJP:C02	2.85	0.52
3:C:124:TRP:CE2	22:C:202:AJP:C80	2.93	0.52
4:D:210:PHE:CE2	22:D:614:AJP:C21	2.92	0.52
4:D:387:LEU:HD22	4:D:431:PRO:HB3	1.91	0.52
2:B:480:PRO:HD3	22:B:607:AJP:C01	2.39	0.52
1:A:369:ALA:HB1	22:A:407:AJP:C11	2.40	0.52
2:B:177:PHE:HB2	2:B:218:GLY:HA3	1.92	0.52
1:A:320:PHE:HD1	19:A:401:BCR:H19C	1.74	0.52
4:D:72:TRP:HE1	22:D:607:AJP:C10	2.24	0.51
19:D:601:BCR:C38	19:D:601:BCR:C23	2.88	0.51
19:A:401:BCR:H321	19:A:401:BCR:C8	2.40	0.51
2:B:82:PHE:HD2	22:B:604:AJP:C85	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:606:AJP:C83	22:B:606:AJP:C02	2.88	0.51
9:I:143:ARG:NH1	14:N:50:PRO:O	2.43	0.51
2:B:283:ILE:HD13	22:B:614:AJP:C14	2.41	0.51
22:B:608:AJP:C06	22:B:608:AJP:C02	2.85	0.51
3:C:83:ILE:HG21	7:G:158:LEU:HD22	1.91	0.51
19:D:602:BCR:C40	19:D:602:BCR:C23	2.86	0.51
4:D:460:GLU:OE1	4:D:462:ARG:NH1	2.44	0.51
2:B:403:TRP:HZ2	22:D:614:AJP:C81	2.24	0.51
4:D:134:GLN:HE22	4:D:264:ARG:HE	1.57	0.51
22:D:610:AJP:C83	22:D:610:AJP:C02	2.88	0.51
7:G:37:PHE:CB	22:G:302:AJP:C83	2.76	0.51
7:G:82:ASN:ND2	8:H:4:ILE:O	2.44	0.51
8:H:333:SER:OG	8:H:334:GLY:N	2.44	0.51
22:F:711:AJP:C06	22:F:711:AJP:C02	2.85	0.51
8:H:72:TYR:HB2	11:K:52:CYS:HB3	1.93	0.51
10:J:64:GLN:NE2	10:J:132:TYR:OH	2.43	0.51
11:K:35:TYR:OH	11:K:39:ARG:NH2	2.44	0.51
2:B:179:TYR:HD1	5:E:41:VAL:HG12	1.76	0.50
4:D:477:ILE:HD11	19:D:601:BCR:H312	1.93	0.50
12:L:39:ALA:HB1	12:L:43:GLU:HB3	1.93	0.50
2:B:409:GLY:CA	22:B:612:AJP:C83	2.89	0.50
7:G:63:ILE:O	7:G:67:VAL:HB	2.10	0.50
2:B:353:ARG:NH1	2:B:449:GLU:O	2.45	0.50
2:B:459:PRO:HA	2:B:462:VAL:HG12	1.94	0.50
4:D:35:ARG:NH1	4:D:107:TRP:O	2.44	0.50
2:B:357:ASP:N	2:B:357:ASP:OD1	2.45	0.50
2:B:486:ASN:ND2	4:D:75:GLU:OE2	2.45	0.50
3:C:59:GLY:HA3	8:H:17:PRO:HD2	1.94	0.50
10:J:62:ARG:HB3	10:J:80:HIS:HB3	1.93	0.50
2:B:280:VAL:HG13	22:B:613:AJP:C83	2.42	0.50
22:B:604:AJP:C02	22:B:604:AJP:C06	2.87	0.50
4:D:265:MET:O	4:D:269:MET:HB2	2.12	0.50
4:D:389:LEU:HD21	6:F:156:MET:HG3	1.93	0.50
17:Q:38:TRP:NE1	22:Q:101:AJP:C83	2.74	0.50
2:B:35:GLN:HG3	22:B:610:AJP:C14	2.40	0.49
22:F:710:AJP:C02	22:F:710:AJP:C06	2.85	0.49
19:D:602:BCR:H333	17:Q:28:ILE:CD1	2.43	0.49
4:D:229:VAL:HG11	4:D:287:VAL:HG12	1.93	0.49
22:D:609:AJP:C83	22:D:609:AJP:C02	2.90	0.49
6:F:495:ILE:HG13	6:F:496:PRO:HD3	1.94	0.49
22:B:612:AJP:C04	22:B:614:AJP:C11	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:206:TYR:HB2	4:D:211:GLN:HG3	1.94	0.49
4:D:206:TYR:HD2	4:D:211:GLN:HE21	1.59	0.49
6:F:200:THR:HG21	6:F:208:MET:HA	1.95	0.49
11:K:49:GLY:HA3	11:K:54:PHE:HB2	1.93	0.49
2:B:353:ARG:HH21	2:B:457:LEU:HD13	1.78	0.49
3:C:60:MET:O	11:K:100:ARG:NH1	2.46	0.49
11:K:15:ARG:HB3	14:N:90:ASN:HB2	1.95	0.49
2:B:283:ILE:CD1	22:B:614:AJP:C14	2.91	0.49
22:D:610:AJP:C02	22:D:610:AJP:C06	2.86	0.49
6:F:87:TYR:HD2	22:F:709:AJP:C83	2.26	0.49
5:E:61:VAL:HG22	7:G:135:ILE:HG13	1.95	0.49
6:F:473:SER:OG	6:F:474:HIS:N	2.46	0.48
7:G:83:LYS:HE3	8:H:7:ARG:HG2	1.95	0.48
8:H:192:ARG:HA	8:H:195:THR:HG22	1.95	0.48
2:B:16:LEU:HD21	20:G:301:LHG:H241	1.95	0.48
9:I:70:VAL:O	9:I:76:ASN:ND2	2.46	0.48
2:B:35:GLN:HG2	22:B:610:AJP:C14	2.44	0.48
2:B:403:TRP:HD1	4:D:189:PHE:HD2	1.61	0.48
4:D:116:PHE:HB2	4:D:157:TRP:HH2	1.78	0.48
22:D:609:AJP:C02	22:D:609:AJP:C06	2.85	0.48
22:G:304:AJP:C06	22:G:304:AJP:C02	2.86	0.48
8:H:84:ASN:ND2	8:H:240:TYR:OH	2.46	0.48
2:B:226:VAL:O	2:B:229:HIS:ND1	2.47	0.48
8:H:152:ARG:HH21	11:K:151:ARG:HE	1.61	0.48
13:M:11:HIS:HB2	13:M:32:ASN:HB3	1.94	0.48
8:H:234:LEU:HB2	8:H:332:GLU:HB2	1.95	0.48
8:H:341:TYR:HB3	8:H:354:LYS:HB3	1.96	0.48
1:A:31:PRO:HA	1:A:34:MET:HB2	1.96	0.48
19:D:602:BCR:H372	6:F:235:LEU:HD11	1.96	0.48
6:F:43:PHE:HB2	22:F:712:AJP:C03	2.43	0.48
9:I:120:VAL:HB	18:S:86:LYS:HA	1.96	0.48
13:M:68:TYR:OH	13:M:72:ARG:NH1	2.47	0.48
4:D:252:GLY:O	4:D:256:LYS:NZ	2.44	0.48
5:E:86:ARG:HH22	7:G:167:ARG:HG2	1.79	0.48
1:A:320:PHE:CD1	19:A:401:BCR:H19C	2.49	0.47
7:G:31:ASN:HB3	7:G:34:TYR:HD2	1.78	0.47
9:I:121:THR:HG23	9:I:145:PRO:HB3	1.96	0.47
10:J:32:ASP:N	10:J:32:ASP:OD1	2.45	0.47
5:E:60:GLN:HB3	7:G:58:VAL:HG21	1.96	0.47
7:G:6:LEU:HD11	22:G:304:AJP:C22	2.45	0.47
2:B:34:ILE:CD1	22:B:609:AJP:C16	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:ILE:HG13	7:G:158:LEU:HD13	1.97	0.47
4:D:480:TYR:HD2	22:D:616:AJP:C81	2.27	0.47
6:F:29:PHE:CE2	22:F:705:AJP:C10	2.90	0.47
6:F:627:LEU:HD23	22:F:710:AJP:C04	2.45	0.47
15:O:19:SER:OG	15:O:20:LEU:N	2.48	0.47
4:D:356:ARG:NH2	4:D:457:VAL:O	2.47	0.47
6:F:619:VAL:HA	6:F:622:VAL:HG22	1.97	0.47
8:H:15:MET:HB3	8:H:28:LEU:HB3	1.97	0.47
2:B:279:THR:HG22	2:B:410:LEU:HD11	1.97	0.47
22:D:610:AJP:C13	22:D:611:AJP:C81	2.93	0.47
1:A:249:TYR:HB3	1:A:253:LYS:HB2	1.96	0.47
8:H:337:GLU:OE2	10:J:62:ARG:NH2	2.47	0.47
3:C:58:SER:HB2	8:H:16:GLY:HA3	1.97	0.47
4:D:255:LEU:HB2	4:D:256:LYS:HZ2	1.79	0.47
7:G:31:ASN:HB3	7:G:34:TYR:CD2	2.50	0.47
2:B:248:SER:OG	2:B:340:ASN:ND2	2.48	0.46
8:H:247:ASP:HB2	8:H:278:GLN:HE22	1.80	0.46
1:A:211:ARG:HH21	22:A:407:AJP:C10	2.28	0.46
14:N:49:ALA:HB2	14:N:102:LEU:HB3	1.96	0.46
4:D:72:TRP:CD1	22:D:607:AJP:C11	2.99	0.46
6:F:338:ALA:O	6:F:342:GLY:N	2.44	0.46
17:Q:23:ILE:HA	17:Q:26:VAL:HG12	1.96	0.46
11:K:136:ASP:N	11:K:136:ASP:OD1	2.48	0.46
21:A:405:DGD:HA31	21:A:405:DGD:HB92	1.96	0.46
3:C:73:ARG:HH12	8:H:35:GLU:HB3	1.80	0.46
19:A:401:BCR:C23	19:A:401:BCR:C39	2.91	0.46
22:B:609:AJP:C10	3:C:121:VAL:CG1	2.93	0.46
4:D:290:ILE:HG22	19:D:602:BCR:HC31	1.97	0.46
2:B:139:LEU:HD11	2:B:222:LYS:HG3	1.98	0.46
3:C:124:TRP:HZ2	22:C:201:AJP:C14	2.20	0.46
2:B:227:PRO:HD3	2:B:281:LEU:HD22	1.98	0.46
6:F:295:ALA:HA	6:F:332:MET:HA	1.98	0.46
6:F:349:HIS:O	6:F:353:LYS:HB2	2.16	0.46
8:H:13:ILE:HD12	8:H:32:LEU:HD21	1.97	0.46
4:D:247:HIS:HA	4:D:250:LEU:HB2	1.98	0.45
1:A:351:VAL:HA	1:A:354:VAL:HG22	1.98	0.45
22:B:612:AJP:O79	22:D:614:AJP:C24	2.64	0.45
1:A:273:SER:O	1:A:278:GLY:N	2.44	0.45
14:N:56:ALA:O	14:N:60:THR:OG1	2.33	0.45
8:H:226:ARG:NH1	8:H:268:GLU:OE1	2.49	0.45
8:H:113:ASN:HD21	8:H:335:LYS:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:70:VAL:HG12	9:I:76:ASN:HD22	1.82	0.45
2:B:310:GLN:HE22	2:B:383:LEU:HG	1.82	0.45
4:D:271:PRO:HG2	4:D:502:VAL:HG11	1.98	0.45
6:F:107:VAL:HG13	6:F:259:PRO:HB3	1.98	0.45
2:B:228:PHE:HD1	6:F:642:VAL:HG22	1.81	0.45
2:B:484:LEU:HD12	22:B:604:AJP:C14	2.46	0.45
6:F:245:PRO:HB2	6:F:246:LEU:HD12	1.98	0.45
1:A:168:GLN:HA	1:A:341:LEU:HD21	1.99	0.45
22:D:611:AJP:C01	16:P:19:ILE:HD11	2.46	0.45
24:F:703:SQD:H383	24:F:703:SQD:H202	1.98	0.45
22:G:304:AJP:C83	22:G:304:AJP:C02	2.95	0.45
10:J:105:PRO:HB2	10:J:130:ILE:HA	1.99	0.45
19:D:601:BCR:H311	19:D:601:BCR:HC8	1.95	0.44
20:D:604:LHG:H372	16:P:14:MET:HE2	1.99	0.44
24:D:606:SQD:H152	6:F:613:VAL:HG13	1.99	0.44
6:F:135:MET:HG2	6:F:268:THR:HG22	1.99	0.44
1:A:323:PHE:CD2	19:A:401:BCR:C19	3.00	0.44
8:H:22:MET:HA	11:K:54:PHE:HE2	1.82	0.44
8:H:218:TRP:NE1	8:H:368:GLN:OE1	2.50	0.44
19:A:401:BCR:HC8	19:A:401:BCR:C32	2.45	0.44
3:C:87:GLU:HG3	3:C:116:LEU:HG	1.98	0.44
4:D:47:ALA:HB2	22:D:611:AJP:C01	2.41	0.44
8:H:153:PHE:HD2	8:H:154:ILE:HG12	1.81	0.44
8:H:231:LYS:HE2	8:H:252:VAL:HG21	2.00	0.44
12:L:4:SER:OG	12:L:5:THR:N	2.50	0.44
6:F:557:LYS:HA	6:F:557:LYS:HD3	1.76	0.44
8:H:58:ARG:NH1	11:K:127:ASP:OD2	2.49	0.44
8:H:117:TRP:NE1	8:H:383:GLY:O	2.47	0.44
9:I:55:ARG:HH12	9:I:141:MET:HA	1.83	0.44
4:D:75:GLU:HB3	4:D:76:ILE:H	1.58	0.44
1:A:95:ASP:OD2	1:A:95:ASP:N	2.51	0.44
20:A:403:LHG:H211	7:G:44:LEU:HB3	2.00	0.44
7:G:31:ASN:CB	7:G:34:TYR:HD2	2.31	0.44
4:D:154:LEU:HD11	4:D:250:LEU:HD11	2.00	0.43
4:D:210:PHE:HE2	22:D:614:AJP:C21	2.31	0.43
19:D:601:BCR:H272	24:F:703:SQD:H122	2.00	0.43
7:G:113:LYS:O	7:G:117:GLN:HB2	2.18	0.43
2:B:94:THR:HG21	2:B:246:PHE:HB2	2.01	0.43
10:J:83:LYS:HD2	10:J:92:PRO:HD2	2.00	0.43
1:A:202:TYR:CE2	22:A:407:AJP:C80	3.01	0.43
6:F:554:MET:HA	6:F:560:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:67:VAL:HG21	8:H:82:THR:HG21	2.00	0.43
2:B:419:VAL:HG22	4:D:174:ALA:HB1	2.00	0.43
4:D:477:ILE:HD11	19:D:601:BCR:C31	2.48	0.43
22:D:616:AJP:C06	22:D:616:AJP:C02	2.90	0.43
14:N:113:PHE:HE1	14:N:130:VAL:HG21	1.83	0.43
8:H:352:ARG:HH22	10:J:152:LEU:HD21	1.84	0.43
14:N:10:VAL:HG21	14:N:40:LYS:HG3	2.00	0.43
6:F:161:LEU:HD22	6:F:260:ILE:HD12	1.99	0.43
8:H:75:GLY:HA3	8:H:154:ILE:HG22	2.00	0.43
8:H:160:ARG:NH2	9:I:111:GLU:OE1	2.40	0.43
2:B:370:PRO:HB3	20:D:603:LHG:HC62	2.01	0.43
8:H:302:SER:OG	8:H:303:GLU:N	2.52	0.43
10:J:58:PHE:HB3	10:J:81:LEU:HD12	2.00	0.43
4:D:51:TYR:HE1	22:D:611:AJP:O82	2.02	0.43
22:F:705:AJP:C06	22:F:705:AJP:C02	2.91	0.43
11:K:149:PRO:HB3	25:K:301:SF4:S1	2.59	0.43
1:A:104:ALA:HA	1:A:107:VAL:HG12	2.00	0.42
2:B:144:ILE:HD13	2:B:147:TYR:HD2	1.83	0.42
22:B:605:AJP:C02	22:B:605:AJP:C06	2.93	0.42
19:D:602:BCR:C34	19:D:602:BCR:H311	2.48	0.42
6:F:198:TRP:CZ3	22:F:706:AJP:C08	3.01	0.42
11:K:60:MET:HB3	11:K:67:PHE:HB2	2.01	0.42
13:M:64:ASP:N	13:M:64:ASP:OD2	2.45	0.42
1:A:113:SER:O	1:A:113:SER:OG	2.34	0.42
23:B:601:PQN:H2M1	23:B:601:PQN:H111	1.80	0.42
22:B:609:AJP:C01	3:C:117:VAL:HG12	2.48	0.42
4:D:175:GLY:HA3	24:D:606:SQD:H341	2.01	0.42
19:D:602:BCR:C32	19:D:602:BCR:C8	2.96	0.42
2:B:140:GLU:HG2	5:E:69:VAL:HG13	2.01	0.42
22:B:609:AJP:C19	3:C:125:ARG:NH2	2.82	0.42
4:D:61:THR:HB	4:D:65:GLN:HE22	1.83	0.42
4:D:305:LYS:HE2	4:D:433:TYR:HB2	2.01	0.42
12:L:19:LEU:HA	12:L:23:VAL:HG22	2.02	0.42
18:S:52:LYS:HE3	18:S:98:VAL:HG21	2.01	0.42
6:F:146:GLN:HA	6:F:149:ILE:HB	2.01	0.42
2:B:158:ARG:HA	5:E:99:LEU:HD11	2.01	0.42
6:F:237:PRO:HD3	6:F:276:LEU:HD23	2.00	0.42
8:H:31:THR:HB	8:H:39:ASP:HB2	2.01	0.42
1:A:205:LEU:O	22:A:407:AJP:O82	2.37	0.42
19:D:602:BCR:H382	6:F:231:ILE:HG23	2.01	0.42
6:F:387:LEU:HB2	6:F:454:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ARG:HD3	20:B:602:LHG:HC31	2.02	0.42
4:D:300:ARG:HH21	17:Q:10:MET:HG2	1.85	0.42
22:F:705:AJP:C13	22:F:712:AJP:C18	2.97	0.42
1:A:303:GLN:HB3	21:A:405:DGD:HD62	2.02	0.42
4:D:301:ASN:HD22	4:D:304:ARG:HG3	1.84	0.42
1:A:323:PHE:HE2	19:A:401:BCR:H20C	0.69	0.42
2:B:79:LEU:HD23	2:B:261:ARG:HH11	1.85	0.42
9:I:50:GLU:OE2	9:I:162:TYR:OH	2.37	0.42
6:F:411:PHE:HB3	6:F:412:ALA:H	1.76	0.42
20:G:301:LHG:H101	20:G:301:LHG:H131	1.79	0.42
11:K:33:ASP:OD1	14:N:35:ARG:NH2	2.52	0.41
2:B:141:THR:HA	7:G:153:LEU:HD13	2.02	0.41
2:B:359:ILE:O	2:B:362:TYR:HB2	2.19	0.41
19:D:602:BCR:C36	24:D:605:SQD:H161	2.42	0.41
6:F:225:LEU:HD22	22:F:706:AJP:C02	2.50	0.41
8:H:62:MET:HE3	9:I:74:PRO:HA	2.00	0.41
9:I:117:CYS:SG	25:I:202:SF4:S4	3.18	0.41
1:A:285:PRO:CG	22:A:408:AJP:C14	2.94	0.41
6:F:556:LEU:HD12	6:F:556:LEU:HA	1.89	0.41
8:H:324:LYS:HG3	8:H:345:ASP:HA	2.02	0.41
9:I:117:CYS:HB3	25:I:202:SF4:S4	2.61	0.41
2:B:241:THR:HA	2:B:244:VAL:HG12	2.03	0.41
2:B:341:LEU:O	2:B:345:THR:OG1	2.38	0.41
22:B:605:AJP:C83	22:B:605:AJP:C02	2.98	0.41
5:E:89:ASP:OD1	5:E:89:ASP:N	2.51	0.41
1:A:98:LEU:HD21	7:G:37:PHE:HE2	1.85	0.41
2:B:182:SER:OG	5:E:44:ASN:ND2	2.50	0.41
2:B:154:LYS:HD2	2:B:154:LYS:HA	1.79	0.41
3:C:84:PHE:HZ	3:C:120:LEU:HB2	1.86	0.41
1:A:47:VAL:HG11	12:L:52:THR:HG23	2.03	0.41
6:F:106:LEU:HD22	6:F:489:PRO:HB3	2.01	0.41
6:F:532:GLU:HA	6:F:535:ILE:HG12	2.01	0.41
6:F:290:VAL:HA	6:F:293:THR:HG22	2.02	0.41
1:A:105:VAL:HG21	22:G:302:AJP:C85	2.51	0.41
1:A:156:LYS:NZ	8:H:12:VAL:O	2.54	0.41
2:B:458:ARG:HD3	20:B:603:LHG:HC42	2.03	0.41
4:D:101:LEU:HD23	4:D:101:LEU:HA	1.90	0.41
4:D:310:SER:HA	4:D:339:HIS:CE1	2.55	0.41
5:E:18:ILE:HG13	5:E:37:LEU:HD21	2.03	0.41
6:F:353:LYS:HD3	6:F:353:LYS:HA	1.93	0.41
6:F:629:TYR:CB	22:F:710:AJP:C81	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:LEU:HD13	3:C:121:VAL:HG12	2.03	0.40
22:B:609:AJP:C01	3:C:117:VAL:CG1	3.00	0.40
6:F:351:TYR:HD2	6:F:500:ILE:HD13	1.86	0.40
6:F:576:SER:O	6:F:576:SER:OG	2.39	0.40
6:F:608:VAL:HG22	22:Q:102:AJP:C83	2.51	0.40
8:H:69:ARG:CG	25:K:301:SF4:S2	3.09	0.40
8:H:364:GLN:HE21	10:J:119:TRP:HB2	1.86	0.40
6:F:389:LYS:H	6:F:389:LYS:HG2	1.75	0.40
7:G:116:LEU:HD13	22:G:306:AJP:C21	2.51	0.40
15:O:51:LYS:HG3	15:O:58:THR:HG22	2.03	0.40
22:D:607:AJP:C81	22:D:608:AJP:O82	2.69	0.40
6:F:191:LEU:HB3	6:F:232:LEU:HD13	2.02	0.40
6:F:381:MET:HE3	6:F:449:MET:HG2	2.02	0.40
2:B:378:LEU:HD23	2:B:468:VAL:HG13	2.02	0.40
4:D:94:LEU:HD22	4:D:337:VAL:HG22	2.03	0.40
1:A:212:GLN:NE2	1:A:355:ASN:OD1	2.55	0.40
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.93	0.40
5:E:31:LEU:O	5:E:35:GLU:HG2	2.21	0.40
6:F:482:SER:HA	6:F:483:PRO:HD3	1.97	0.40
7:G:149:LEU:HD23	7:G:149:LEU:HA	1.95	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	361/372 (97%)	335 (93%)	26 (7%)	0	100	100
2	B	490/515 (95%)	470 (96%)	20 (4%)	0	100	100
3	C	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
4	D	502/529 (95%)	475 (95%)	27 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
6	F	642/656 (98%)	605 (94%)	37 (6%)	0	100	100
7	G	189/200 (94%)	182 (96%)	7 (4%)	0	100	100
8	H	391/394 (99%)	356 (91%)	34 (9%)	1 (0%)	41	75
9	I	187/196 (95%)	175 (94%)	12 (6%)	0	100	100
10	J	154/168 (92%)	140 (91%)	14 (9%)	0	100	100
11	K	196/237 (83%)	182 (93%)	14 (7%)	0	100	100
12	L	71/76 (93%)	65 (92%)	6 (8%)	0	100	100
13	M	108/111 (97%)	98 (91%)	10 (9%)	0	100	100
14	N	146/150 (97%)	136 (93%)	10 (7%)	0	100	100
15	O	65/70 (93%)	55 (85%)	10 (15%)	0	100	100
16	P	39/44 (89%)	31 (80%)	8 (20%)	0	100	100
17	Q	42/45 (93%)	41 (98%)	1 (2%)	0	100	100
18	S	53/110 (48%)	53 (100%)	0	0	100	100
All	All	3854/4106 (94%)	3598 (93%)	255 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	198	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/302 (98%)	296 (100%)	1 (0%)	92	97
2	B	395/413 (96%)	395 (100%)	0	100	100
3	C	100/109 (92%)	100 (100%)	0	100	100
4	D	404/424 (95%)	404 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	82/82 (100%)	82 (100%)	0	100 100
6	F	518/527 (98%)	515 (99%)	3 (1%)	86 94
7	G	158/166 (95%)	158 (100%)	0	100 100
8	H	337/338 (100%)	336 (100%)	1 (0%)	92 97
9	I	165/172 (96%)	165 (100%)	0	100 100
10	J	138/148 (93%)	136 (99%)	2 (1%)	67 85
11	K	169/196 (86%)	169 (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%)	117 (98%)	2 (2%)	60 82
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	S	48/97 (50%)	48 (100%)	0	100 100
All	All	3209/3381 (95%)	3200 (100%)	9 (0%)	92 97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASP
6	F	11	ILE
6	F	187	PHE
6	F	628	LYS
8	H	8	THR
10	J	45	ARG
10	J	155	ASP
14	N	70	THR
14	N	107	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	355	ASN
2	B	160	ASN
2	B	340	ASN

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Mol	Chain	Res	Type
4	D	134	GLN
4	D	163	GLN
5	E	39	ASN
5	E	56	GLN
6	F	6	GLN
6	F	62	GLN
6	F	146	GLN
6	F	265	HIS
6	F	379	GLN
8	H	84	ASN
8	H	156	ASN
8	H	196	ASN
8	H	278	GLN
9	I	76	ASN
10	J	64	GLN
10	J	120	GLN
11	K	104	GLN
11	K	188	HIS
13	M	23	HIS
13	M	37	ASN
15	O	49	GLN
16	P	44	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

66 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	$\#\|Z\| > 2$
22	AJP	D	615	-	37,37,95	1.24	6 (16%)	58,62,149	2.24	16 (27%)
22	AJP	B	608	-	37,37,95	1.27	8 (21%)	58,62,149	2.20	17 (29%)
25	SF4	I	201	9	0,12,12	-	-	-		
20	LHG	F	702	-	48,48,48	0.57	0	51,54,54	1.25	6 (11%)
20	LHG	B	603	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)
22	AJP	D	609	-	37,37,95	1.25	6 (16%)	58,62,149	2.19	18 (31%)
20	LHG	G	301	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)
22	AJP	B	604	-	37,37,95	1.50	7 (18%)	58,62,149	2.38	19 (32%)
22	AJP	B	609	-	37,37,95	1.44	9 (24%)	58,62,149	2.40	19 (32%)
22	AJP	A	406	-	37,37,95	1.34	6 (16%)	58,62,149	2.22	16 (27%)
22	AJP	D	608	-	37,37,95	1.51	7 (18%)	58,62,149	2.46	21 (36%)
22	AJP	F	707	-	37,37,95	1.31	6 (16%)	58,62,149	2.21	19 (32%)
22	AJP	F	709	-	37,37,95	1.30	7 (18%)	58,62,149	2.24	17 (29%)
22	AJP	Q	103	-	37,37,95	1.29	6 (16%)	58,62,149	2.25	18 (31%)
22	AJP	G	306	-	37,37,95	1.27	8 (21%)	58,62,149	2.20	17 (29%)
24	SQD	D	606	-	53,54,54	0.94	5 (9%)	62,65,65	1.53	11 (17%)
20	LHG	F	701	-	48,48,48	0.58	0	51,54,54	1.24	6 (11%)
22	AJP	B	606	-	37,37,95	1.16	7 (18%)	58,62,149	2.12	16 (27%)
22	AJP	D	607	-	37,37,95	1.55	7 (18%)	58,62,149	2.27	20 (34%)
22	AJP	D	614	-	37,37,95	1.43	7 (18%)	58,62,149	2.25	21 (36%)
22	AJP	B	610	-	37,37,95	1.29	7 (18%)	58,62,149	2.32	18 (31%)
22	AJP	Q	102	-	37,37,95	1.48	7 (18%)	58,62,149	2.37	18 (31%)
22	AJP	G	303	-	37,37,95	1.27	7 (18%)	58,62,149	2.22	18 (31%)
22	AJP	D	616	-	37,37,95	1.27	5 (13%)	58,62,149	2.23	17 (29%)
22	AJP	C	201	-	37,37,95	1.29	7 (18%)	58,62,149	2.19	16 (27%)
22	AJP	F	708	-	37,37,95	1.33	4 (10%)	58,62,149	2.33	21 (36%)
22	AJP	D	610	-	37,37,95	1.37	6 (16%)	58,62,149	2.22	18 (31%)
22	AJP	Q	101	-	37,37,95	1.23	6 (16%)	58,62,149	2.15	16 (27%)
23	PQN	B	601	-	34,34,34	2.85	9 (26%)	42,45,45	1.98	5 (11%)
25	SF4	I	202	9	0,12,12	-	-	-		
22	AJP	F	710	-	37,37,95	1.18	6 (16%)	58,62,149	2.11	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	AJP	D	612	-	37,37,95	1.30	6 (16%)	58,62,149	2.29	19 (32%)
24	SQD	L	101	-	53,54,54	0.95	5 (9%)	62,65,65	1.56	10 (16%)
24	SQD	D	605	-	53,54,54	0.95	5 (9%)	62,65,65	1.52	11 (17%)
22	AJP	C	202	-	37,37,95	1.37	8 (21%)	58,62,149	2.21	17 (29%)
25	SF4	K	301	11	0,12,12	-	-	-		
22	AJP	G	305	-	37,37,95	1.34	8 (21%)	58,62,149	2.21	19 (32%)
22	AJP	B	607	-	37,37,95	1.27	7 (18%)	58,62,149	2.26	17 (29%)
22	AJP	G	307	-	37,37,95	1.39	7 (18%)	58,62,149	2.23	20 (34%)
22	AJP	A	407	-	37,37,95	1.27	3 (8%)	58,62,149	2.26	19 (32%)
22	AJP	F	711	-	37,37,95	1.35	7 (18%)	58,62,149	2.24	18 (31%)
22	AJP	B	614	-	37,37,95	1.33	7 (18%)	58,62,149	2.23	18 (31%)
22	AJP	D	613	-	37,37,95	1.36	7 (18%)	58,62,149	2.34	13 (22%)
22	AJP	F	712	-	37,37,95	1.37	8 (21%)	58,62,149	2.25	18 (31%)
22	AJP	G	302	-	37,37,95	1.52	7 (18%)	58,62,149	2.31	20 (34%)
20	LHG	B	602	-	48,48,48	0.61	0	51,54,54	1.25	6 (11%)
22	AJP	D	611	-	37,37,95	1.26	5 (13%)	58,62,149	2.30	17 (29%)
21	DGD	A	404	-	67,67,67	0.89	2 (2%)	81,81,81	1.39	11 (13%)
19	BCR	A	401	-	41,41,41	1.74	8 (19%)	56,56,56	1.60	10 (17%)
22	AJP	B	612	-	37,37,95	1.18	6 (16%)	58,62,149	2.12	16 (27%)
22	AJP	F	705	-	37,37,95	1.39	8 (21%)	58,62,149	2.19	18 (31%)
19	BCR	D	601	-	41,41,41	1.69	8 (19%)	56,56,56	1.65	12 (21%)
24	SQD	F	703	-	53,54,54	0.95	5 (9%)	62,65,65	1.56	12 (19%)
22	AJP	F	706	-	37,37,95	1.33	7 (18%)	58,62,149	2.23	19 (32%)
21	DGD	A	405	-	67,67,67	0.91	3 (4%)	81,81,81	1.42	12 (14%)
20	LHG	A	402	-	48,48,48	0.58	0	51,54,54	1.24	6 (11%)
22	AJP	B	605	-	37,37,95	1.28	5 (13%)	58,62,149	2.16	17 (29%)
19	BCR	D	602	-	41,41,41	1.72	8 (19%)	56,56,56	1.67	11 (19%)
20	LHG	D	603	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
22	AJP	B	611	-	37,37,95	1.32	7 (18%)	58,62,149	2.17	19 (32%)
20	LHG	A	403	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	5 (9%)
22	AJP	F	704	-	37,37,95	1.30	6 (16%)	58,62,149	2.16	19 (32%)
22	AJP	G	304	-	37,37,95	1.29	8 (21%)	58,62,149	2.42	17 (29%)
22	AJP	A	408	-	37,37,95	1.25	6 (16%)	58,62,149	2.25	17 (29%)
20	LHG	D	604	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
22	AJP	B	613	-	37,37,95	1.16	5 (13%)	58,62,149	2.14	16 (27%)

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
22	AJP	D	615	-	12/12/14/38	-	0/6/6/11
22	AJP	B	608	-	12/12/14/38	-	0/6/6/11
25	SF4	I	201	9	-	-	0/6/5/5
20	LHG	F	702	-	-	21/53/53/53	-
20	LHG	B	603	-	-	20/53/53/53	-
22	AJP	D	609	-	12/12/14/38	-	0/6/6/11
22	AJP	B	604	-	12/12/14/38	-	0/6/6/11
22	AJP	B	609	-	12/12/14/38	-	0/6/6/11
22	AJP	D	608	-	12/12/14/38	-	0/6/6/11
22	AJP	A	406	-	12/12/14/38	-	0/6/6/11
22	AJP	F	707	-	12/12/14/38	-	0/6/6/11
22	AJP	F	709	-	12/12/14/38	-	0/6/6/11
22	AJP	Q	103	-	12/12/14/38	-	0/6/6/11
20	LHG	G	301	-	-	22/53/53/53	-
22	AJP	G	306	-	12/12/14/38	-	0/6/6/11
24	SQD	D	606	-	-	16/49/69/69	0/1/1/1
20	LHG	F	701	-	-	26/53/53/53	-
22	AJP	B	606	-	12/12/14/38	-	0/6/6/11
22	AJP	D	607	-	12/12/14/38	-	0/6/6/11
22	AJP	D	614	-	12/12/14/38	-	0/6/6/11
22	AJP	B	610	-	12/12/14/38	-	0/6/6/11
22	AJP	Q	102	-	12/12/14/38	-	0/6/6/11
22	AJP	G	303	-	12/12/14/38	-	0/6/6/11
22	AJP	D	616	-	12/12/14/38	-	0/6/6/11
22	AJP	C	201	-	12/12/14/38	-	0/6/6/11
22	AJP	F	708	-	12/12/14/38	-	0/6/6/11
22	AJP	D	610	-	12/12/14/38	-	0/6/6/11
22	AJP	Q	101	-	12/12/14/38	-	0/6/6/11
23	PQN	B	601	-	-	9/23/43/43	0/2/2/2
25	SF4	I	202	9	-	-	0/6/5/5
22	AJP	F	710	-	12/12/14/38	-	0/6/6/11
22	AJP	D	612	-	12/12/14/38	-	0/6/6/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	SQD	L	101	-	-	18/49/69/69	0/1/1/1
24	SQD	D	605	-	-	18/49/69/69	0/1/1/1
22	AJP	C	202	-	12/12/14/38	-	0/6/6/11
25	SF4	K	301	11	-	-	0/6/5/5
22	AJP	G	305	-	12/12/14/38	-	0/6/6/11
22	AJP	B	607	-	12/12/14/38	-	0/6/6/11
22	AJP	G	307	-	12/12/14/38	-	0/6/6/11
22	AJP	A	407	-	12/12/14/38	-	0/6/6/11
22	AJP	F	711	-	12/12/14/38	-	0/6/6/11
22	AJP	B	614	-	12/12/14/38	-	0/6/6/11
22	AJP	D	613	-	12/12/14/38	-	0/6/6/11
22	AJP	F	712	-	12/12/14/38	-	0/6/6/11
22	AJP	G	302	-	12/12/14/38	-	0/6/6/11
22	AJP	D	611	-	12/12/14/38	-	0/6/6/11
20	LHG	B	602	-	-	26/53/53/53	-
19	BCR	A	401	-	-	23/29/63/63	0/2/2/2
21	DGD	A	404	-	-	18/55/95/95	0/2/2/2
22	AJP	B	612	-	12/12/14/38	-	0/6/6/11
22	AJP	F	705	-	12/12/14/38	-	0/6/6/11
19	BCR	D	601	-	-	26/29/63/63	0/2/2/2
24	SQD	F	703	-	-	21/49/69/69	0/1/1/1
22	AJP	F	706	-	12/12/14/38	-	0/6/6/11
21	DGD	A	405	-	-	20/55/95/95	0/2/2/2
20	LHG	A	402	-	-	21/53/53/53	-
22	AJP	B	605	-	12/12/14/38	-	0/6/6/11
19	BCR	D	602	-	-	19/29/63/63	0/2/2/2
20	LHG	D	603	-	-	25/53/53/53	-
22	AJP	B	611	-	12/12/14/38	-	0/6/6/11
22	AJP	F	704	-	12/12/14/38	-	0/6/6/11
22	AJP	G	304	-	12/12/14/38	-	0/6/6/11
20	LHG	A	403	-	-	17/53/53/53	-
22	AJP	A	408	-	12/12/14/38	-	0/6/6/11
20	LHG	D	604	-	-	23/53/53/53	-
22	AJP	B	613	-	12/12/14/38	-	0/6/6/11

All (353) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	PQN	C12-C13	8.31	1.52	1.33
23	B	601	PQN	O4-C4	8.17	1.40	1.23
23	B	601	PQN	O1-C1	8.12	1.40	1.23
19	A	401	BCR	C10-C9	4.19	1.41	1.35
19	D	602	BCR	C21-C22	4.17	1.41	1.35
19	A	401	BCR	C14-C13	4.15	1.41	1.35
22	B	604	AJP	C16-C11	-4.10	1.48	1.54
23	B	601	PQN	C2-C1	-4.09	1.39	1.48
19	D	601	BCR	C21-C22	4.08	1.41	1.35
19	A	401	BCR	C21-C22	4.06	1.41	1.35
19	D	602	BCR	C10-C9	4.05	1.41	1.35
19	D	602	BCR	C17-C18	3.99	1.41	1.35
19	A	401	BCR	C17-C18	3.97	1.41	1.35
19	D	602	BCR	C14-C13	3.90	1.41	1.35
22	D	607	AJP	C16-C11	-3.78	1.49	1.54
19	D	601	BCR	C17-C18	3.70	1.40	1.35
19	D	601	BCR	C14-C13	3.69	1.40	1.35
22	D	608	AJP	C16-C11	-3.67	1.49	1.54
19	D	601	BCR	C10-C9	3.66	1.40	1.35
22	F	708	AJP	C16-C11	-3.54	1.49	1.54
22	D	616	AJP	C16-C11	-3.50	1.49	1.54
22	C	201	AJP	C16-C11	-3.46	1.49	1.54
22	A	406	AJP	C12-C11	-3.44	1.49	1.56
22	D	607	AJP	C07-C08	-3.43	1.47	1.53
22	A	407	AJP	C16-C11	-3.43	1.49	1.54
22	F	706	AJP	C16-C11	-3.42	1.49	1.54
22	Q	102	AJP	C07-C08	-3.42	1.47	1.53
22	G	302	AJP	C20-C15	-3.42	1.49	1.56
22	B	607	AJP	C16-C11	-3.39	1.49	1.54
22	F	704	AJP	C16-C11	-3.39	1.49	1.54
22	D	607	AJP	C12-C11	-3.39	1.49	1.56
22	F	712	AJP	C16-C11	-3.36	1.49	1.54
22	D	611	AJP	C16-C11	-3.35	1.49	1.54
22	D	614	AJP	C20-C15	-3.34	1.50	1.56
22	G	307	AJP	C07-C08	-3.33	1.48	1.53
22	D	608	AJP	C20-C15	-3.33	1.50	1.56
22	D	614	AJP	C16-C11	-3.33	1.49	1.54
22	D	612	AJP	C16-C11	-3.32	1.49	1.54
22	A	407	AJP	C12-C11	-3.32	1.49	1.56
22	Q	102	AJP	C16-C11	-3.30	1.50	1.54
22	B	604	AJP	C07-C08	-3.30	1.48	1.53
22	B	609	AJP	C12-C11	-3.29	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	202	AJP	C07-C08	-3.27	1.48	1.53
22	B	605	AJP	C16-C11	-3.27	1.50	1.54
22	B	609	AJP	C07-C08	-3.27	1.48	1.53
22	A	406	AJP	C07-C08	-3.27	1.48	1.53
22	G	302	AJP	C07-C08	-3.26	1.48	1.53
22	F	708	AJP	C07-C08	-3.25	1.48	1.53
22	F	705	AJP	C16-C11	-3.25	1.50	1.54
22	D	612	AJP	C12-C11	-3.25	1.49	1.56
22	D	610	AJP	C16-C11	-3.25	1.50	1.54
22	D	609	AJP	C16-C11	-3.23	1.50	1.54
22	D	610	AJP	C07-C08	-3.22	1.48	1.53
22	G	307	AJP	C16-C11	-3.22	1.50	1.54
22	F	707	AJP	C16-C11	-3.21	1.50	1.54
22	G	302	AJP	C13-C12	-3.20	1.48	1.54
22	B	614	AJP	C07-C08	-3.20	1.48	1.53
22	A	407	AJP	C07-C08	-3.19	1.48	1.53
22	B	604	AJP	C12-C11	-3.19	1.49	1.56
22	C	202	AJP	C16-C11	-3.19	1.50	1.54
22	F	708	AJP	C12-C11	-3.18	1.49	1.56
22	Q	103	AJP	C07-C08	-3.18	1.48	1.53
22	F	706	AJP	C12-C11	-3.17	1.49	1.56
22	B	614	AJP	C12-C11	-3.17	1.49	1.56
24	D	605	SQD	O48-C23	3.16	1.42	1.33
22	Q	102	AJP	C12-C11	-3.16	1.49	1.56
24	L	101	SQD	O48-C23	3.16	1.42	1.33
24	D	606	SQD	O48-C23	3.14	1.42	1.33
22	F	706	AJP	C07-C08	-3.14	1.48	1.53
22	G	305	AJP	C07-C08	-3.14	1.48	1.53
22	B	611	AJP	C07-C08	-3.11	1.48	1.53
22	G	302	AJP	C20-C19	-3.11	1.50	1.55
22	B	608	AJP	C16-C11	-3.11	1.50	1.54
22	D	608	AJP	C07-C08	-3.11	1.48	1.53
22	B	610	AJP	C13-C12	-3.11	1.48	1.54
24	F	703	SQD	O48-C23	3.11	1.42	1.33
22	G	306	AJP	C07-C08	-3.10	1.48	1.53
22	D	612	AJP	C07-C08	-3.08	1.48	1.53
22	Q	101	AJP	C16-C11	-3.08	1.50	1.54
22	B	609	AJP	C20-C15	-3.07	1.50	1.56
22	B	610	AJP	C16-C11	-3.07	1.50	1.54
22	G	303	AJP	C07-C08	-3.07	1.48	1.53
22	Q	102	AJP	C20-C19	-3.07	1.50	1.55
22	F	711	AJP	C07-C08	-3.05	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	202	AJP	C12-C11	-3.04	1.49	1.56
23	B	601	PQN	C3-C4	-3.03	1.39	1.47
22	G	305	AJP	C16-C11	-3.02	1.50	1.54
19	D	601	BCR	C8-C9	-3.01	1.39	1.45
22	G	306	AJP	C16-C11	-3.00	1.50	1.54
22	D	608	AJP	C12-C11	-3.00	1.50	1.56
23	B	601	PQN	C5-C4	-3.00	1.42	1.48
22	B	604	AJP	C20-C19	-2.98	1.50	1.55
22	F	711	AJP	C16-C11	-2.98	1.50	1.54
22	A	408	AJP	C07-C08	-2.98	1.48	1.53
22	D	607	AJP	C13-C12	-2.97	1.48	1.54
22	F	712	AJP	C12-C11	-2.97	1.50	1.56
22	G	306	AJP	C12-C11	-2.97	1.50	1.56
22	D	610	AJP	C12-C11	-2.97	1.50	1.56
22	D	615	AJP	C16-C11	-2.97	1.50	1.54
22	B	611	AJP	C12-C11	-2.97	1.50	1.56
22	F	711	AJP	O09-C05	2.96	1.49	1.42
22	D	614	AJP	O09-C05	2.95	1.49	1.42
22	F	709	AJP	C16-C11	-2.94	1.50	1.54
22	G	302	AJP	C12-C11	-2.94	1.50	1.56
22	G	305	AJP	C20-C15	-2.94	1.50	1.56
22	D	607	AJP	C20-C19	-2.93	1.50	1.55
22	B	605	AJP	C12-C11	-2.93	1.50	1.56
24	F	703	SQD	O47-C7	2.92	1.42	1.34
22	A	406	AJP	C16-C11	-2.92	1.50	1.54
22	A	408	AJP	C16-C11	-2.92	1.50	1.54
22	F	711	AJP	C12-C11	-2.92	1.50	1.56
23	B	601	PQN	C10-C1	-2.91	1.42	1.48
22	B	608	AJP	C07-C08	-2.90	1.48	1.53
22	G	303	AJP	C12-C11	-2.90	1.50	1.56
19	D	601	BCR	C23-C22	-2.90	1.39	1.45
22	A	408	AJP	C12-C11	-2.90	1.50	1.56
22	G	307	AJP	C12-C07	-2.89	1.50	1.56
22	G	302	AJP	C16-C11	-2.89	1.50	1.54
22	B	605	AJP	C07-C08	-2.89	1.48	1.53
22	F	707	AJP	C07-C08	-2.89	1.48	1.53
22	B	606	AJP	C07-C08	-2.89	1.48	1.53
22	D	610	AJP	C20-C15	-2.89	1.50	1.56
22	B	613	AJP	C16-C11	-2.88	1.50	1.54
24	D	605	SQD	O47-C7	2.88	1.42	1.34
24	L	101	SQD	O47-C7	2.87	1.42	1.34
22	F	705	AJP	C12-C11	-2.86	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	AJP	C12-C11	-2.85	1.50	1.56
19	A	401	BCR	C23-C22	-2.85	1.39	1.45
24	D	606	SQD	O47-C7	2.84	1.42	1.34
22	G	307	AJP	C12-C11	-2.84	1.50	1.56
22	D	608	AJP	C20-C19	-2.84	1.50	1.55
22	Q	103	AJP	C12-C11	-2.84	1.50	1.56
22	B	614	AJP	C20-C15	-2.83	1.50	1.56
19	D	602	BCR	C8-C9	-2.83	1.39	1.45
22	G	305	AJP	C12-C11	-2.82	1.50	1.56
22	G	307	AJP	C20-C15	-2.82	1.50	1.56
22	G	304	AJP	C20-C15	-2.82	1.50	1.56
22	D	607	AJP	C20-C15	-2.82	1.50	1.56
22	D	615	AJP	C07-C08	-2.82	1.48	1.53
19	D	602	BCR	C23-C22	-2.81	1.39	1.45
22	Q	101	AJP	C07-C08	-2.81	1.48	1.53
22	G	304	AJP	C16-C11	-2.81	1.50	1.54
22	B	611	AJP	C16-C11	-2.81	1.50	1.54
22	F	707	AJP	C12-C11	-2.81	1.50	1.56
22	D	609	AJP	C12-C11	-2.80	1.50	1.56
22	F	704	AJP	C12-C11	-2.80	1.50	1.56
23	B	601	PQN	C3-C2	2.80	1.40	1.35
22	C	201	AJP	C07-C08	-2.79	1.49	1.53
22	F	709	AJP	C07-C08	-2.79	1.49	1.53
22	D	613	AJP	C16-C11	-2.78	1.50	1.54
22	B	609	AJP	C21-C20	-2.76	1.50	1.54
22	F	705	AJP	C20-C15	-2.76	1.51	1.56
22	D	614	AJP	C20-C19	-2.75	1.50	1.55
22	B	610	AJP	C12-C11	-2.75	1.50	1.56
22	Q	102	AJP	C20-C15	-2.75	1.51	1.56
22	F	705	AJP	C07-C08	-2.75	1.49	1.53
22	D	611	AJP	C20-C15	-2.75	1.51	1.56
22	B	614	AJP	C16-C11	-2.75	1.50	1.54
22	D	609	AJP	C07-C08	-2.74	1.49	1.53
22	G	303	AJP	C16-C11	-2.74	1.50	1.54
22	F	710	AJP	C16-C11	-2.74	1.50	1.54
22	B	607	AJP	C07-C08	-2.74	1.49	1.53
22	F	712	AJP	C20-C15	-2.73	1.51	1.56
22	D	616	AJP	C12-C11	-2.72	1.50	1.56
22	G	304	AJP	C13-C12	-2.72	1.49	1.54
19	A	401	BCR	C8-C9	-2.71	1.40	1.45
22	B	613	AJP	C07-C08	-2.69	1.49	1.53
22	B	611	AJP	C20-C15	-2.67	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	616	AJP	C07-C08	-2.67	1.49	1.53
22	B	611	AJP	O09-C05	2.67	1.48	1.42
22	F	712	AJP	C07-C08	-2.66	1.49	1.53
22	F	711	AJP	C12-C07	-2.66	1.50	1.56
22	B	612	AJP	C16-C11	-2.66	1.50	1.54
22	F	709	AJP	C12-C11	-2.66	1.50	1.56
22	F	712	AJP	O09-C05	2.65	1.48	1.42
22	B	609	AJP	C16-C11	-2.65	1.50	1.54
22	D	613	AJP	C13-C12	-2.65	1.49	1.54
22	Q	103	AJP	C20-C15	-2.64	1.51	1.56
22	F	710	AJP	O09-C05	2.63	1.48	1.42
22	F	706	AJP	C20-C15	-2.62	1.51	1.56
22	B	610	AJP	C07-C08	-2.62	1.49	1.53
22	F	705	AJP	C20-C19	-2.62	1.51	1.55
22	D	614	AJP	C12-C07	-2.61	1.50	1.56
22	Q	103	AJP	C16-C11	-2.60	1.50	1.54
22	G	302	AJP	C12-C07	-2.60	1.50	1.56
22	B	612	AJP	O09-C05	2.60	1.48	1.42
22	B	612	AJP	C07-C08	-2.59	1.49	1.53
22	B	606	AJP	C12-C11	-2.59	1.50	1.56
22	D	611	AJP	C07-C08	-2.59	1.49	1.53
22	Q	101	AJP	C12-C11	-2.59	1.50	1.56
22	F	710	AJP	C07-C08	-2.59	1.49	1.53
22	B	609	AJP	C13-C12	-2.58	1.49	1.54
22	B	607	AJP	O09-C05	2.58	1.48	1.42
22	A	406	AJP	C20-C15	-2.57	1.51	1.56
22	F	709	AJP	C20-C19	-2.57	1.51	1.55
22	B	610	AJP	C20-C15	-2.57	1.51	1.56
22	B	614	AJP	O09-C05	2.57	1.48	1.42
22	F	704	AJP	C07-C08	-2.56	1.49	1.53
22	D	608	AJP	C21-C20	-2.56	1.50	1.54
22	D	611	AJP	C12-C11	-2.56	1.50	1.56
22	D	615	AJP	O09-C05	2.56	1.48	1.42
22	C	201	AJP	C12-C11	-2.56	1.50	1.56
22	B	613	AJP	C12-C11	-2.55	1.50	1.56
22	D	613	AJP	C20-C19	-2.55	1.51	1.55
22	B	607	AJP	C12-C11	-2.55	1.50	1.56
22	D	613	AJP	C20-C15	-2.55	1.51	1.56
22	B	606	AJP	C16-C11	-2.54	1.51	1.54
22	B	612	AJP	C12-C11	-2.53	1.50	1.56
22	F	710	AJP	C12-C11	-2.52	1.51	1.56
22	A	406	AJP	C13-C12	-2.51	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	AJP	C20-C15	-2.51	1.51	1.56
22	G	304	AJP	C12-C11	-2.51	1.51	1.56
22	F	711	AJP	C20-C15	-2.50	1.51	1.56
22	D	614	AJP	C12-C11	-2.50	1.51	1.56
22	D	613	AJP	C12-C11	-2.50	1.51	1.56
22	D	615	AJP	C12-C07	-2.49	1.51	1.56
22	G	307	AJP	C20-C19	-2.49	1.51	1.55
22	C	202	AJP	C20-C15	-2.49	1.51	1.56
22	G	306	AJP	C20-C15	-2.48	1.51	1.56
22	A	408	AJP	O09-C05	2.47	1.47	1.42
22	F	707	AJP	C20-C15	-2.47	1.51	1.56
22	B	611	AJP	C20-C19	-2.46	1.51	1.55
22	Q	102	AJP	C21-C20	-2.46	1.50	1.54
22	G	303	AJP	C20-C15	-2.45	1.51	1.56
22	F	705	AJP	C13-C12	-2.45	1.49	1.54
22	B	607	AJP	C12-C07	-2.45	1.51	1.56
22	Q	101	AJP	O09-C05	2.44	1.47	1.42
22	D	609	AJP	O09-C05	2.43	1.47	1.42
22	F	704	AJP	C12-C07	-2.43	1.51	1.56
22	D	610	AJP	C12-C07	-2.42	1.51	1.56
22	B	613	AJP	C13-C12	-2.42	1.49	1.54
22	B	604	AJP	C24-C19	-2.42	1.49	1.53
19	A	401	BCR	C19-C18	-2.41	1.40	1.45
21	A	405	DGD	C3D-C2D	2.41	1.58	1.52
22	D	608	AJP	C13-C12	-2.40	1.49	1.54
22	C	202	AJP	C21-C20	-2.40	1.50	1.54
22	D	614	AJP	C07-C08	-2.39	1.49	1.53
22	B	609	AJP	C20-C19	-2.39	1.51	1.55
22	F	704	AJP	C20-C15	-2.38	1.51	1.56
22	G	304	AJP	C07-C08	-2.38	1.49	1.53
22	B	611	AJP	C12-C07	-2.38	1.51	1.56
22	D	615	AJP	C12-C11	-2.37	1.51	1.56
22	G	305	AJP	C12-C07	-2.37	1.51	1.56
22	B	604	AJP	C20-C15	-2.36	1.51	1.56
22	F	709	AJP	C20-C15	-2.36	1.51	1.56
19	D	601	BCR	C12-C13	-2.36	1.40	1.45
22	D	609	AJP	C20-C15	-2.36	1.51	1.56
23	B	601	PQN	C10-C5	-2.34	1.36	1.40
22	F	712	AJP	C13-C12	-2.34	1.49	1.54
22	Q	103	AJP	O09-C05	2.33	1.47	1.42
22	B	606	AJP	C20-C15	-2.33	1.51	1.56
22	F	704	AJP	O09-C05	2.32	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	103	AJP	C13-C12	-2.31	1.50	1.54
22	D	611	AJP	C13-C12	-2.31	1.50	1.54
22	D	609	AJP	C12-C07	-2.29	1.51	1.56
21	A	405	DGD	O2G-C2G	-2.29	1.40	1.46
22	F	705	AJP	C21-C20	-2.28	1.50	1.54
22	G	303	AJP	O09-C05	2.27	1.47	1.42
22	B	608	AJP	C20-C19	-2.27	1.51	1.55
22	G	305	AJP	C20-C19	-2.26	1.51	1.55
19	D	602	BCR	C12-C13	-2.26	1.41	1.45
21	A	404	DGD	O2G-C2G	-2.25	1.41	1.46
19	D	601	BCR	C19-C18	-2.24	1.41	1.45
22	D	613	AJP	C07-C08	-2.24	1.49	1.53
22	C	202	AJP	C12-C07	-2.23	1.51	1.56
22	G	304	AJP	O09-C05	2.23	1.47	1.42
22	B	606	AJP	C12-C07	-2.22	1.51	1.56
19	A	401	BCR	C12-C13	-2.22	1.41	1.45
22	D	612	AJP	C20-C15	-2.22	1.52	1.56
22	D	607	AJP	C21-C20	-2.22	1.50	1.54
22	B	609	AJP	C12-C07	-2.22	1.51	1.56
22	G	305	AJP	O09-C05	2.22	1.47	1.42
21	A	405	DGD	O1G-C1G	-2.22	1.40	1.45
22	F	709	AJP	C13-C12	-2.21	1.50	1.54
22	F	711	AJP	C20-C19	-2.20	1.51	1.55
22	C	201	AJP	C20-C15	-2.20	1.52	1.56
22	C	202	AJP	C20-C19	-2.20	1.51	1.55
22	B	613	AJP	C20-C15	-2.20	1.52	1.56
22	B	608	AJP	C20-C15	-2.20	1.52	1.56
22	D	615	AJP	C20-C19	-2.18	1.51	1.55
22	G	307	AJP	C13-C12	-2.18	1.50	1.54
22	Q	101	AJP	C20-C19	-2.18	1.51	1.55
22	B	608	AJP	C13-C12	-2.17	1.50	1.54
22	B	608	AJP	O09-C05	2.16	1.47	1.42
24	D	606	SQD	O2-C2	-2.16	1.37	1.43
22	A	406	AJP	C20-C19	-2.16	1.51	1.55
22	B	609	AJP	O09-C05	2.16	1.47	1.42
24	D	605	SQD	O2-C2	-2.15	1.37	1.43
22	F	706	AJP	C12-C07	-2.15	1.51	1.56
19	D	602	BCR	C19-C18	-2.15	1.41	1.45
24	L	101	SQD	O2-C2	-2.14	1.37	1.43
24	F	703	SQD	O2-C2	-2.14	1.37	1.43
22	B	604	AJP	C12-C07	-2.14	1.51	1.56
22	F	712	AJP	C21-C20	-2.13	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	705	AJP	C12-C07	-2.13	1.51	1.56
22	B	605	AJP	C20-C15	-2.12	1.52	1.56
21	A	404	DGD	O1G-C1G	-2.12	1.40	1.45
22	G	303	AJP	C12-C07	-2.12	1.51	1.56
22	G	306	AJP	C20-C19	-2.12	1.52	1.55
22	B	606	AJP	O09-C05	2.11	1.47	1.42
22	C	201	AJP	C13-C12	-2.11	1.50	1.54
22	F	707	AJP	C20-C19	-2.11	1.52	1.55
22	Q	101	AJP	C20-C15	-2.11	1.52	1.56
22	B	605	AJP	C12-C07	-2.10	1.51	1.56
22	C	202	AJP	C13-C12	-2.10	1.50	1.54
22	A	408	AJP	C20-C19	-2.10	1.52	1.55
22	D	610	AJP	C20-C19	-2.10	1.52	1.55
24	L	101	SQD	O4-C4	-2.09	1.38	1.43
22	D	616	AJP	C21-C20	-2.09	1.51	1.54
22	Q	102	AJP	C12-C07	-2.09	1.51	1.56
22	G	306	AJP	C13-C12	-2.09	1.50	1.54
22	D	612	AJP	O09-C05	2.09	1.47	1.42
22	A	408	AJP	C12-C07	-2.09	1.51	1.56
20	D	604	LHG	O7-C5	-2.08	1.41	1.46
22	G	305	AJP	C13-C12	-2.08	1.50	1.54
24	D	605	SQD	O4-C4	-2.08	1.38	1.43
22	C	201	AJP	C21-C20	-2.08	1.51	1.54
22	D	612	AJP	C20-C19	-2.08	1.52	1.55
22	B	612	AJP	C12-C07	-2.08	1.51	1.56
24	F	703	SQD	O4-C4	-2.07	1.38	1.43
22	F	710	AJP	C12-C07	-2.07	1.51	1.56
22	B	610	AJP	C12-C07	-2.07	1.51	1.56
22	D	613	AJP	O09-C05	2.07	1.47	1.42
22	B	612	AJP	C20-C15	-2.07	1.52	1.56
22	F	710	AJP	C20-C15	-2.07	1.52	1.56
22	B	608	AJP	C12-C07	-2.07	1.51	1.56
22	B	614	AJP	C20-C19	-2.06	1.52	1.55
22	G	306	AJP	O09-C05	2.06	1.47	1.42
20	D	603	LHG	P-O6	2.05	1.67	1.59
22	F	712	AJP	C20-C19	-2.05	1.52	1.55
20	G	301	LHG	O7-C5	-2.05	1.41	1.46
22	G	304	AJP	C21-C20	-2.04	1.51	1.54
24	F	703	SQD	O3-C3	-2.04	1.38	1.43
24	L	101	SQD	O3-C3	-2.04	1.38	1.43
22	C	201	AJP	C20-C19	-2.04	1.52	1.55
22	B	614	AJP	C12-C07	-2.04	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	709	AJP	C12-C07	-2.04	1.51	1.56
24	D	605	SQD	O3-C3	-2.04	1.38	1.43
22	F	706	AJP	C20-C19	-2.04	1.52	1.55
20	A	403	LHG	O7-C5	-2.03	1.41	1.46
22	D	616	AJP	C20-C19	-2.03	1.52	1.55
22	G	304	AJP	C20-C19	-2.03	1.52	1.55
22	B	610	AJP	C20-C19	-2.03	1.52	1.55
22	B	606	AJP	C13-C12	-2.02	1.50	1.54
24	D	606	SQD	O4-C4	-2.02	1.38	1.43
22	F	708	AJP	C20-C15	-2.02	1.52	1.56
22	F	707	AJP	C13-C12	-2.02	1.50	1.54
22	G	303	AJP	C20-C19	-2.01	1.52	1.55
22	G	306	AJP	C12-C07	-2.01	1.52	1.56
24	D	606	SQD	O3-C3	-2.01	1.38	1.43
20	B	603	LHG	P-O6	2.01	1.67	1.59
22	F	706	AJP	C13-C12	-2.01	1.50	1.54
22	B	607	AJP	C13-C12	-2.00	1.50	1.54

All (943) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	613	AJP	C12-C07-C08	-9.65	94.45	104.88
22	B	610	AJP	C12-C07-C08	-9.22	94.92	104.88
22	F	709	AJP	C12-C07-C08	-9.16	94.98	104.88
22	D	611	AJP	C12-C07-C08	-9.15	94.99	104.88
22	G	304	AJP	C12-C07-C08	-9.04	95.12	104.88
22	C	201	AJP	C12-C07-C08	-8.70	95.48	104.88
23	B	601	PQN	C11-C12-C13	-8.49	112.66	126.79
22	D	608	AJP	C12-C07-C08	-8.42	95.78	104.88
22	F	705	AJP	C12-C07-C08	-8.38	95.82	104.88
22	F	707	AJP	C12-C07-C08	-8.36	95.85	104.88
22	D	607	AJP	C12-C07-C08	-8.32	95.89	104.88
22	G	302	AJP	C12-C07-C08	-8.28	95.94	104.88
22	A	406	AJP	C12-C07-C08	-8.23	95.99	104.88
22	B	605	AJP	C12-C07-C08	-8.22	96.00	104.88
22	A	407	AJP	C12-C07-C08	-8.12	96.11	104.88
22	D	609	AJP	C12-C07-C08	-8.06	96.18	104.88
22	G	306	AJP	C12-C07-C08	-8.04	96.19	104.88
22	B	613	AJP	C12-C07-C08	-8.03	96.20	104.88
22	F	712	AJP	C12-C07-C08	-8.03	96.20	104.88
22	B	608	AJP	C12-C07-C08	-8.03	96.20	104.88
22	F	706	AJP	C12-C07-C08	-8.03	96.20	104.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	202	AJP	C12-C07-C08	-8.01	96.23	104.88
22	B	604	AJP	C19-C24-C23	-7.95	105.69	114.46
22	B	612	AJP	C12-C07-C08	-7.94	96.30	104.88
22	B	606	AJP	C12-C07-C08	-7.94	96.30	104.88
22	Q	102	AJP	C12-C07-C08	-7.93	96.31	104.88
22	F	710	AJP	C12-C07-C08	-7.92	96.32	104.88
22	F	708	AJP	C12-C07-C08	-7.86	96.39	104.88
22	D	612	AJP	C12-C07-C08	-7.84	96.41	104.88
22	B	604	AJP	C12-C07-C08	-7.81	96.45	104.88
22	G	307	AJP	C12-C07-C08	-7.79	96.47	104.88
22	D	616	AJP	C12-C07-C08	-7.78	96.48	104.88
22	F	704	AJP	C12-C07-C08	-7.76	96.49	104.88
22	D	610	AJP	C12-C07-C08	-7.74	96.52	104.88
22	G	305	AJP	C12-C07-C08	-7.71	96.55	104.88
22	G	303	AJP	C12-C07-C08	-7.66	96.61	104.88
22	B	609	AJP	C12-C07-C08	-7.63	96.64	104.88
22	Q	103	AJP	C12-C07-C08	-7.56	96.71	104.88
22	Q	101	AJP	C12-C07-C08	-7.53	96.75	104.88
22	B	607	AJP	C12-C07-C08	-7.49	96.79	104.88
22	B	611	AJP	C12-C07-C08	-7.46	96.82	104.88
22	B	609	AJP	C20-C15-C16	-7.33	104.72	112.42
22	B	614	AJP	C12-C07-C08	-7.17	97.13	104.88
22	D	615	AJP	C12-C07-C08	-7.16	97.14	104.88
22	D	614	AJP	C12-C07-C08	-7.10	97.21	104.88
22	D	608	AJP	C20-C15-C16	-7.03	105.04	112.42
22	A	408	AJP	C12-C07-C08	-6.93	97.39	104.88
22	F	711	AJP	C12-C07-C08	-6.91	97.42	104.88
22	G	304	AJP	C20-C15-C16	-6.79	105.29	112.42
22	A	407	AJP	C19-C24-C23	-6.66	107.11	114.46
22	D	613	AJP	C19-C24-C23	-6.60	107.18	114.46
22	Q	102	AJP	C24-C19-C20	-6.42	105.84	112.66
22	D	612	AJP	C19-C24-C23	-6.37	107.43	114.46
22	B	604	AJP	C12-C11-C16	-6.16	104.98	113.82
22	F	708	AJP	C19-C24-C23	-6.15	107.67	114.46
22	D	613	AJP	C12-C11-C16	-6.12	105.03	113.82
22	A	408	AJP	C12-C11-C16	-6.00	105.22	113.82
22	D	616	AJP	C19-C24-C23	-5.96	107.88	114.46
22	F	709	AJP	C12-C11-C16	-5.95	105.28	113.82
22	F	706	AJP	C19-C24-C23	-5.92	107.93	114.46
22	A	408	AJP	C19-C24-C23	-5.91	107.94	114.46
22	D	610	AJP	C12-C11-C16	-5.88	105.38	113.82
22	D	609	AJP	C12-C11-C16	-5.85	105.43	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	611	AJP	C12-C11-C16	-5.80	105.50	113.82
22	D	615	AJP	C19-C24-C23	-5.79	108.07	114.46
22	G	304	AJP	C12-C11-C16	-5.77	105.53	113.82
22	B	610	AJP	C20-C15-C16	-5.77	106.36	112.42
22	Q	103	AJP	C12-C11-C16	-5.74	105.58	113.82
22	G	305	AJP	C19-C24-C23	-5.72	108.15	114.46
22	G	305	AJP	C12-C11-C16	-5.69	105.65	113.82
22	B	605	AJP	C12-C11-C16	-5.67	105.68	113.82
22	C	202	AJP	C12-C11-C16	-5.67	105.68	113.82
23	B	601	PQN	C15-C13-C12	-5.62	109.75	121.12
22	G	302	AJP	C19-C24-C23	-5.61	108.27	114.46
22	F	712	AJP	C12-C11-C16	-5.60	105.78	113.82
22	Q	102	AJP	C12-C11-C16	-5.59	105.80	113.82
22	B	607	AJP	C05-C06-C07	-5.59	94.27	103.37
22	D	609	AJP	C19-C24-C23	-5.58	108.30	114.46
22	G	302	AJP	C12-C11-C16	-5.58	105.82	113.82
22	F	704	AJP	C12-C11-C16	-5.55	105.85	113.82
22	F	708	AJP	C12-C11-C16	-5.54	105.86	113.82
22	D	615	AJP	C05-C06-C07	-5.51	94.40	103.37
22	C	201	AJP	C12-C11-C16	-5.50	105.92	113.82
22	F	711	AJP	C12-C11-C16	-5.46	105.98	113.82
22	F	706	AJP	C12-C11-C16	-5.45	106.00	113.82
22	A	406	AJP	C12-C11-C16	-5.44	106.01	113.82
23	B	601	PQN	C14-C13-C12	-5.43	109.75	123.68
22	B	610	AJP	C12-C11-C16	-5.42	106.04	113.82
22	B	608	AJP	C12-C11-C16	-5.42	106.05	113.82
22	D	607	AJP	C20-C15-C16	-5.41	106.73	112.42
22	D	612	AJP	C12-C11-C16	-5.40	106.07	113.82
22	D	614	AJP	C05-C06-C07	-5.37	94.62	103.37
22	G	306	AJP	C19-C24-C23	-5.35	108.56	114.46
22	F	711	AJP	C19-C24-C23	-5.35	108.56	114.46
22	Q	103	AJP	C19-C24-C23	-5.31	108.60	114.46
22	F	711	AJP	C05-C06-C07	-5.29	94.76	103.37
22	B	611	AJP	C12-C11-C16	-5.26	106.28	113.82
22	G	307	AJP	C12-C11-C16	-5.23	106.32	113.82
22	B	605	AJP	C19-C24-C23	-5.19	108.73	114.46
22	B	609	AJP	C20-C21-C22	-5.18	105.59	114.09
22	B	608	AJP	C19-C24-C23	-5.16	108.77	114.46
22	F	710	AJP	C12-C11-C16	-5.14	106.44	113.82
22	B	612	AJP	C12-C11-C16	-5.09	106.51	113.82
22	G	303	AJP	C19-C24-C23	-5.06	108.88	114.46
22	B	607	AJP	C12-C11-C16	-5.03	106.60	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	306	AJP	C12-C11-C16	-5.01	106.63	113.82
22	G	304	AJP	C24-C19-C20	-4.99	107.36	112.66
22	D	607	AJP	C12-C11-C16	-4.98	106.68	113.82
22	F	704	AJP	C19-C24-C23	-4.97	108.98	114.46
22	G	307	AJP	C19-C24-C23	-4.95	109.00	114.46
22	A	407	AJP	C12-C11-C16	-4.94	106.74	113.82
22	F	707	AJP	C20-C15-C16	-4.93	107.25	112.42
22	D	616	AJP	C12-C11-C16	-4.92	106.75	113.82
22	A	408	AJP	C05-C06-C07	-4.91	95.38	103.37
22	G	303	AJP	C12-C11-C16	-4.88	106.81	113.82
22	F	709	AJP	C19-C24-C23	-4.84	109.12	114.46
22	Q	101	AJP	C19-C24-C23	-4.83	109.14	114.46
22	A	408	AJP	C06-C07-C08	-4.79	95.62	104.34
22	D	608	AJP	C20-C21-C22	-4.77	106.26	114.09
22	B	606	AJP	C19-C24-C23	-4.73	109.24	114.46
22	C	202	AJP	C24-C19-C20	-4.73	107.63	112.66
22	G	302	AJP	C14-C13-C12	-4.73	104.67	112.78
24	L	101	SQD	O7-S-C6	4.70	112.53	106.94
22	Q	101	AJP	C12-C11-C16	-4.68	107.10	113.82
22	D	611	AJP	C19-C24-C23	-4.67	109.31	114.46
22	B	614	AJP	C06-C07-C08	-4.66	95.86	104.34
22	A	407	AJP	C06-C07-C08	-4.64	95.90	104.34
22	Q	102	AJP	C20-C15-C16	-4.63	107.56	112.42
22	B	613	AJP	C19-C24-C23	-4.61	109.37	114.46
22	Q	103	AJP	C20-C15-C16	-4.61	107.58	112.42
22	B	609	AJP	C12-C11-C16	-4.60	107.22	113.82
22	A	406	AJP	C20-C15-C16	-4.59	107.60	112.42
22	B	609	AJP	C06-C07-C08	-4.57	96.01	104.34
22	B	614	AJP	C20-C15-C16	-4.57	107.62	112.42
22	B	606	AJP	C12-C11-C16	-4.54	107.30	113.82
22	D	611	AJP	C20-C15-C16	-4.54	107.66	112.42
22	F	712	AJP	C20-C15-C16	-4.51	107.68	112.42
22	D	612	AJP	C06-C07-C08	-4.49	96.17	104.34
22	B	612	AJP	C19-C24-C23	-4.48	109.52	114.46
22	C	202	AJP	C14-C15-C20	-4.47	108.76	113.91
22	F	710	AJP	C19-C24-C23	-4.46	109.53	114.46
22	D	616	AJP	C06-C07-C08	-4.44	96.25	104.34
22	F	708	AJP	C06-C07-C08	-4.44	96.26	104.34
22	C	202	AJP	C19-C24-C23	-4.42	109.59	114.46
22	B	610	AJP	C14-C13-C12	-4.39	105.26	112.78
22	Q	102	AJP	C14-C15-C20	-4.35	108.90	113.91
22	B	610	AJP	C19-C24-C23	-4.32	109.69	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	614	AJP	C05-C06-C07	-4.31	96.36	103.37
22	B	614	AJP	C12-C11-C16	-4.30	107.64	113.82
22	D	610	AJP	C14-C15-C20	-4.30	108.95	113.91
22	C	201	AJP	C19-C24-C23	-4.30	109.71	114.46
22	Q	101	AJP	C05-C06-C07	-4.28	96.40	103.37
21	A	404	DGD	O3G-C3G-C2G	-4.27	100.59	110.90
22	A	406	AJP	C19-C24-C23	-4.26	109.76	114.46
22	B	609	AJP	C05-C06-C07	-4.26	96.44	103.37
22	G	307	AJP	C14-C15-C20	-4.26	109.01	113.91
22	F	705	AJP	C12-C11-C16	-4.25	107.73	113.82
22	B	614	AJP	C19-C24-C23	-4.23	109.79	114.46
22	F	707	AJP	C12-C11-C16	-4.23	107.75	113.82
20	A	403	LHG	O4-P-O5	4.21	133.03	112.24
20	B	602	LHG	O4-P-O5	4.20	133.02	112.24
19	D	602	BCR	C37-C22-C21	-4.20	117.04	122.92
22	D	613	AJP	C24-C19-C20	-4.20	108.20	112.66
22	G	304	AJP	C14-C13-C12	-4.20	105.58	112.78
20	F	701	LHG	O4-P-O5	4.19	132.96	112.24
20	F	702	LHG	O4-P-O5	4.19	132.96	112.24
22	B	611	AJP	C05-C06-C07	-4.19	96.55	103.37
22	A	408	AJP	C83-C06-C05	-4.19	107.27	114.92
20	G	301	LHG	O4-P-O5	4.18	132.93	112.24
20	D	604	LHG	O4-P-O5	4.18	132.92	112.24
20	B	603	LHG	O4-P-O5	4.18	132.92	112.24
19	D	601	BCR	C34-C9-C10	-4.18	117.06	122.92
20	A	402	LHG	O4-P-O5	4.18	132.91	112.24
19	A	401	BCR	C34-C9-C10	-4.18	117.07	122.92
22	G	307	AJP	C24-C19-C20	-4.17	108.23	112.66
20	D	603	LHG	O4-P-O5	4.17	132.84	112.24
22	B	607	AJP	C83-C06-C05	-4.16	107.33	114.92
22	B	609	AJP	C14-C13-C12	-4.16	105.65	112.78
22	F	711	AJP	C06-C07-C08	-4.15	96.78	104.34
22	D	608	AJP	C12-C11-C16	-4.13	107.89	113.82
22	C	201	AJP	C24-C19-C20	-4.12	108.28	112.66
22	D	611	AJP	C14-C15-C20	-4.11	109.17	113.91
19	D	601	BCR	C37-C22-C21	-4.10	117.17	122.92
19	A	401	BCR	C37-C22-C21	-4.10	117.18	122.92
22	F	705	AJP	C20-C15-C16	-4.09	108.12	112.42
22	Q	103	AJP	C06-C07-C08	-4.09	96.90	104.34
22	B	608	AJP	C14-C13-C12	-4.08	105.78	112.78
19	D	602	BCR	C34-C9-C10	-4.07	117.22	122.92
22	D	615	AJP	C12-C11-C16	-4.06	108.00	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	615	AJP	C11-C12-C07	-4.05	93.27	100.19
22	G	304	AJP	C14-C15-C20	-4.04	109.26	113.91
21	A	405	DGD	O3G-C3G-C2G	-4.04	101.16	110.90
22	B	607	AJP	C06-C07-C08	-4.04	96.99	104.34
22	F	712	AJP	C14-C15-C20	-4.02	109.28	113.91
22	G	303	AJP	C06-C07-C08	-4.01	97.03	104.34
22	D	614	AJP	C19-C24-C23	-3.98	110.07	114.46
22	D	607	AJP	C06-C07-C08	-3.98	97.10	104.34
22	F	708	AJP	C05-C06-C07	-3.98	96.89	103.37
22	D	613	AJP	C14-C13-C12	-3.98	105.96	112.78
22	D	608	AJP	C85-O84-C05	-3.98	106.18	113.72
22	Q	101	AJP	C06-C07-C08	-3.97	97.10	104.34
22	D	610	AJP	C19-C24-C23	-3.97	110.08	114.46
22	B	613	AJP	C12-C11-C16	-3.96	108.14	113.82
22	F	707	AJP	C06-C07-C08	-3.95	97.15	104.34
22	D	608	AJP	C21-C22-C23	-3.95	106.83	111.36
22	B	611	AJP	C19-C24-C23	-3.94	110.12	114.46
22	Q	102	AJP	C19-C24-C23	-3.93	110.13	114.46
22	D	608	AJP	C06-C07-C08	-3.93	97.19	104.34
22	G	305	AJP	C14-C15-C20	-3.93	109.39	113.91
22	F	705	AJP	C19-C24-C23	-3.92	110.13	114.46
22	D	616	AJP	C24-C19-C20	-3.92	108.50	112.66
22	G	304	AJP	C20-C21-C22	-3.90	107.69	114.09
19	A	401	BCR	C15-C16-C17	3.89	131.44	123.47
22	F	705	AJP	C24-C19-C20	-3.88	108.53	112.66
22	F	711	AJP	C83-C06-C05	-3.88	107.83	114.92
22	D	608	AJP	C14-C13-C12	-3.88	106.13	112.78
22	F	712	AJP	C14-C13-C12	-3.87	106.14	112.78
24	D	605	SQD	O7-S-C6	3.86	111.53	106.94
22	D	614	AJP	C11-C12-C07	-3.86	93.59	100.19
22	D	615	AJP	C83-C06-C05	-3.86	107.88	114.92
24	L	101	SQD	O47-C7-C8	3.85	119.81	111.50
22	Q	102	AJP	C06-C07-C08	-3.85	97.33	104.34
22	D	612	AJP	C05-C06-C07	-3.85	97.11	103.37
24	L	101	SQD	O9-S-O7	-3.84	100.65	113.95
22	F	707	AJP	C19-C24-C23	-3.83	110.23	114.46
24	D	606	SQD	O47-C7-C8	3.82	119.72	111.50
24	D	606	SQD	O9-S-C6	3.81	111.47	106.94
19	D	602	BCR	C15-C16-C17	3.81	131.28	123.47
22	F	705	AJP	C11-C12-C07	-3.80	93.69	100.19
22	B	607	AJP	C14-C13-C12	-3.80	106.27	112.78
22	D	614	AJP	C06-C07-C08	-3.79	97.44	104.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	614	AJP	C14-C15-C20	-3.79	109.55	113.91
24	D	606	SQD	O7-S-C6	3.78	111.44	106.94
22	B	606	AJP	C20-C15-C16	-3.78	108.45	112.42
19	A	401	BCR	C16-C15-C14	3.77	131.20	123.47
22	D	613	AJP	O09-C08-C10	3.76	117.91	110.17
24	F	703	SQD	O7-S-C6	3.75	111.39	106.94
22	G	303	AJP	C20-C15-C16	-3.73	108.50	112.42
19	D	601	BCR	C16-C15-C14	3.73	131.11	123.47
22	A	406	AJP	C14-C13-C12	-3.72	106.40	112.78
22	B	613	AJP	C06-C07-C08	-3.72	97.58	104.34
19	D	602	BCR	C16-C15-C14	3.71	131.08	123.47
24	D	605	SQD	O9-S-C6	3.70	111.34	106.94
22	D	613	AJP	C14-C15-C20	-3.70	109.65	113.91
24	F	703	SQD	O9-S-O7	-3.70	101.16	113.95
22	F	706	AJP	C06-C07-C08	-3.69	97.62	104.34
22	B	613	AJP	C14-C13-C12	-3.69	106.46	112.78
22	G	302	AJP	C14-C15-C20	-3.68	109.67	113.91
22	G	305	AJP	C05-C06-C07	-3.67	97.39	103.37
22	B	613	AJP	C20-C15-C16	-3.67	108.57	112.42
22	F	709	AJP	C11-C16-C15	-3.67	102.83	109.23
22	B	604	AJP	O09-C08-C10	3.67	117.72	110.17
22	F	712	AJP	C20-C21-C22	-3.66	108.09	114.09
22	D	615	AJP	C06-C07-C08	-3.65	97.69	104.34
19	D	601	BCR	C15-C16-C17	3.65	130.95	123.47
24	D	606	SQD	O9-S-O7	-3.65	101.33	113.95
22	A	406	AJP	C06-C07-C08	-3.64	97.72	104.34
22	F	712	AJP	C19-C24-C23	-3.63	110.45	114.46
24	D	605	SQD	O9-S-O7	-3.63	101.38	113.95
22	F	712	AJP	C24-C19-C20	-3.63	108.81	112.66
22	B	606	AJP	C14-C13-C12	-3.63	106.56	112.78
22	C	202	AJP	C06-C07-C08	-3.62	97.75	104.34
22	B	607	AJP	C85-O84-C05	-3.61	106.87	113.72
24	F	703	SQD	O9-S-C6	3.61	111.23	106.94
22	B	605	AJP	C24-C19-C20	-3.61	108.82	112.66
22	F	709	AJP	O09-C08-C10	3.60	117.58	110.17
22	D	611	AJP	C24-C19-C20	-3.59	108.84	112.66
22	B	608	AJP	C20-C15-C16	-3.58	108.66	112.42
22	F	709	AJP	C06-C07-C08	-3.58	97.83	104.34
24	D	605	SQD	O47-C7-C8	3.57	119.19	111.50
22	D	608	AJP	C11-C12-C07	-3.56	94.10	100.19
22	B	607	AJP	C20-C15-C16	-3.56	108.68	112.42
22	Q	103	AJP	C05-C06-C07	-3.56	97.58	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	614	AJP	C12-C11-C16	-3.56	108.72	113.82
22	B	614	AJP	C20-C21-C22	-3.56	108.26	114.09
19	D	602	BCR	C36-C18-C17	-3.55	117.95	122.92
22	C	201	AJP	C14-C15-C20	-3.55	109.83	113.91
22	G	306	AJP	C14-C15-C20	-3.54	109.83	113.91
22	D	607	AJP	C14-C13-C12	-3.53	106.72	112.78
22	B	604	AJP	C06-C07-C08	-3.53	97.91	104.34
22	Q	103	AJP	C14-C13-C12	-3.53	106.72	112.78
22	B	614	AJP	C83-C06-C05	-3.53	108.48	114.92
19	D	601	BCR	C35-C13-C14	-3.53	117.98	122.92
22	B	613	AJP	C05-C06-C07	-3.53	97.63	103.37
22	G	303	AJP	C05-C06-C07	-3.53	97.63	103.37
22	D	614	AJP	C21-C22-C23	-3.52	107.33	111.36
22	F	705	AJP	C14-C13-C12	-3.51	106.76	112.78
22	B	613	AJP	C11-C12-C07	-3.51	94.19	100.19
19	D	601	BCR	C36-C18-C17	-3.50	118.01	122.92
22	D	616	AJP	C11-C12-C07	-3.50	94.21	100.19
22	F	704	AJP	C11-C12-C07	-3.50	94.21	100.19
22	D	614	AJP	C20-C21-C22	-3.50	108.35	114.09
22	B	611	AJP	C14-C15-C20	-3.50	109.88	113.91
22	D	610	AJP	C24-C19-C20	-3.50	108.94	112.66
24	F	703	SQD	C44-O6-C1	3.50	120.57	113.74
22	C	202	AJP	C05-C06-C07	-3.50	97.68	103.37
22	B	604	AJP	C11-C12-C07	-3.49	94.23	100.19
22	B	610	AJP	O09-C08-C10	3.49	117.35	110.17
22	B	607	AJP	C19-C24-C23	-3.48	110.62	114.46
22	D	614	AJP	O09-C08-C10	3.48	117.33	110.17
22	B	606	AJP	O09-C08-C10	3.48	117.33	110.17
22	B	611	AJP	C06-C07-C08	-3.48	98.01	104.34
19	D	602	BCR	C35-C13-C14	-3.48	118.05	122.92
22	A	406	AJP	C14-C15-C20	-3.47	109.91	113.91
22	D	607	AJP	C20-C21-C22	-3.47	108.40	114.09
22	B	609	AJP	C83-C06-C05	-3.47	108.59	114.92
22	G	305	AJP	C24-C19-C20	-3.46	108.98	112.66
22	F	707	AJP	C20-C21-C22	-3.46	108.42	114.09
22	G	302	AJP	C21-C20-C19	3.45	111.03	107.14
22	D	614	AJP	C21-C20-C19	3.45	111.02	107.14
22	Q	102	AJP	C20-C21-C22	-3.44	108.45	114.09
22	C	201	AJP	C20-C15-C16	-3.44	108.81	112.42
22	Q	101	AJP	C11-C12-C07	-3.43	94.33	100.19
22	F	712	AJP	C05-C06-C07	-3.43	97.79	103.37
22	Q	101	AJP	C83-C06-C05	-3.42	108.67	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	306	AJP	C14-C13-C12	-3.42	106.92	112.78
22	F	705	AJP	C14-C15-C20	-3.41	109.98	113.91
22	G	305	AJP	C14-C13-C12	-3.41	106.93	112.78
22	D	607	AJP	C19-C24-C23	-3.41	110.70	114.46
22	D	609	AJP	C21-C20-C19	3.40	110.97	107.14
22	B	605	AJP	C14-C15-C20	-3.40	109.99	113.91
22	F	708	AJP	C83-C06-C05	-3.40	108.71	114.92
22	G	306	AJP	C11-C12-C07	-3.39	94.39	100.19
22	G	302	AJP	O09-C08-C10	3.39	117.15	110.17
22	D	612	AJP	C83-C06-C05	-3.39	108.73	114.92
22	B	608	AJP	C06-C07-C08	-3.39	98.17	104.34
19	A	401	BCR	C35-C13-C14	-3.39	118.18	122.92
22	A	408	AJP	C24-C19-C20	-3.38	109.06	112.66
22	G	307	AJP	C05-C06-C07	-3.38	97.86	103.37
22	D	611	AJP	C14-C13-C12	-3.38	106.98	112.78
22	B	604	AJP	C24-C19-C20	-3.38	109.07	112.66
22	F	711	AJP	C14-C13-C12	-3.37	107.00	112.78
22	Q	103	AJP	C14-C15-C20	-3.37	110.03	113.91
19	A	401	BCR	C36-C18-C17	-3.37	118.20	122.92
22	D	610	AJP	C20-C15-C16	-3.37	108.89	112.42
22	B	604	AJP	C11-C16-C15	-3.36	103.36	109.23
22	G	307	AJP	C14-C13-C12	-3.36	107.03	112.78
22	D	610	AJP	O09-C08-C10	3.36	117.08	110.17
22	B	608	AJP	O09-C08-C10	3.35	117.07	110.17
22	B	612	AJP	C20-C15-C16	-3.35	108.91	112.42
22	D	608	AJP	C21-C20-C19	3.34	110.91	107.14
22	B	611	AJP	O09-C08-C10	3.34	117.05	110.17
22	D	607	AJP	C05-C06-C07	-3.34	97.94	103.37
22	G	305	AJP	C06-C07-C08	-3.34	98.27	104.34
22	F	707	AJP	C14-C13-C12	-3.34	107.06	112.78
22	D	616	AJP	C05-C06-C07	-3.33	97.96	103.37
22	F	712	AJP	C06-C07-C08	-3.32	98.29	104.34
22	D	614	AJP	C83-C06-C05	-3.31	108.87	114.92
22	G	303	AJP	C20-C21-C22	-3.31	108.66	114.09
19	D	602	BCR	C19-C18-C17	3.31	124.01	118.94
22	Q	103	AJP	C83-C06-C05	-3.31	108.88	114.92
22	G	306	AJP	C06-C07-C08	-3.30	98.33	104.34
22	D	612	AJP	C21-C20-C19	3.30	110.86	107.14
22	Q	101	AJP	C24-C19-C20	-3.29	109.16	112.66
22	F	710	AJP	C20-C15-C16	-3.29	108.96	112.42
22	Q	102	AJP	C05-C06-C07	-3.29	98.01	103.37
22	G	306	AJP	O09-C08-C10	3.29	116.94	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	612	AJP	C05-C06-C07	-3.29	98.01	103.37
22	F	710	AJP	C14-C13-C12	-3.29	107.15	112.78
22	B	605	AJP	C06-C07-C08	-3.28	98.37	104.34
22	G	307	AJP	O09-C08-C07	-3.28	96.20	104.06
22	B	612	AJP	C14-C13-C12	-3.28	107.16	112.78
22	B	606	AJP	C11-C12-C07	-3.28	94.59	100.19
22	F	710	AJP	C05-C06-C07	-3.27	98.04	103.37
22	B	610	AJP	C06-C07-C08	-3.27	98.39	104.34
22	F	707	AJP	O09-C08-C10	3.26	116.89	110.17
22	D	610	AJP	C06-C07-C08	-3.26	98.40	104.34
22	D	611	AJP	O09-C08-C10	3.26	116.89	110.17
22	D	609	AJP	O09-C08-C10	3.26	116.89	110.17
22	F	710	AJP	C06-C07-C08	-3.25	98.42	104.34
22	D	614	AJP	C14-C13-C12	-3.25	107.20	112.78
22	B	605	AJP	O09-C08-C10	3.25	116.86	110.17
22	D	608	AJP	C05-C06-C07	-3.24	98.09	103.37
22	F	707	AJP	C11-C12-C07	-3.24	94.65	100.19
24	D	606	SQD	C44-O6-C1	3.24	120.07	113.74
22	C	201	AJP	C14-C13-C12	-3.24	107.22	112.78
22	B	612	AJP	C14-C15-C20	-3.23	110.19	113.91
22	F	710	AJP	C14-C15-C20	-3.23	110.19	113.91
22	B	612	AJP	C06-C07-C08	-3.23	98.47	104.34
22	B	610	AJP	C20-C21-C22	-3.22	108.80	114.09
19	D	602	BCR	C12-C13-C14	3.22	123.88	118.94
22	D	614	AJP	C20-C15-C16	-3.22	109.04	112.42
22	F	711	AJP	C14-C15-C20	-3.22	110.20	113.91
22	G	307	AJP	C11-C12-C07	-3.22	94.69	100.19
22	B	606	AJP	C06-C07-C08	-3.21	98.49	104.34
22	F	708	AJP	C20-C21-C22	-3.19	108.85	114.09
22	D	611	AJP	C06-C07-C08	-3.19	98.53	104.34
22	C	201	AJP	C06-C07-C08	-3.19	98.54	104.34
22	F	708	AJP	C20-C15-C16	-3.19	109.07	112.42
22	G	303	AJP	C14-C13-C12	-3.18	107.32	112.78
22	B	607	AJP	C20-C21-C22	-3.18	108.87	114.09
22	B	611	AJP	C11-C12-C07	-3.18	94.76	100.19
22	D	615	AJP	O09-C08-C10	3.17	116.70	110.17
21	A	405	DGD	O6D-C1D-O3G	-3.17	102.47	109.97
22	G	304	AJP	O09-C08-C10	3.17	116.69	110.17
22	D	609	AJP	C14-C15-C20	-3.16	110.27	113.91
22	D	609	AJP	C14-C13-C12	-3.16	107.36	112.78
22	F	706	AJP	C05-C06-C07	-3.16	98.23	103.37
22	F	708	AJP	C85-O84-C05	-3.16	107.73	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	303	AJP	C11-C12-C07	-3.15	94.81	100.19
22	Q	101	AJP	C14-C15-C20	-3.15	110.28	113.91
22	F	712	AJP	O09-C08-C10	3.15	116.65	110.17
21	A	404	DGD	O5D-C6D-C5D	-3.15	103.22	109.05
22	G	307	AJP	C06-C07-C08	-3.15	98.61	104.34
22	B	614	AJP	O09-C08-C10	3.14	116.63	110.17
19	D	601	BCR	C12-C13-C14	3.14	123.76	118.94
22	B	614	AJP	C11-C12-C07	-3.14	94.83	100.19
22	F	706	AJP	C14-C13-C12	-3.14	107.40	112.78
19	A	401	BCR	C19-C18-C17	3.14	123.75	118.94
22	F	705	AJP	O09-C08-C10	3.13	116.62	110.17
22	G	307	AJP	O09-C08-C10	3.13	116.62	110.17
22	B	611	AJP	C11-C16-C15	-3.13	103.77	109.23
22	B	608	AJP	C14-C15-C20	-3.13	110.31	113.91
22	G	306	AJP	C20-C15-C16	-3.13	109.14	112.42
22	B	613	AJP	C20-C21-C22	-3.12	108.97	114.09
22	G	302	AJP	C85-O84-C05	-3.12	107.80	113.72
22	B	613	AJP	C83-C06-C05	-3.12	109.22	114.92
22	F	705	AJP	C06-C07-C08	-3.12	98.67	104.34
22	B	614	AJP	O09-C08-C07	-3.10	96.61	104.06
22	B	609	AJP	O09-C08-C10	3.10	116.56	110.17
24	F	703	SQD	O47-C7-C8	3.10	118.19	111.50
22	B	608	AJP	C05-C06-C07	-3.10	98.32	103.37
24	L	101	SQD	O9-S-C6	3.09	110.62	106.94
22	B	604	AJP	C14-C15-C20	-3.09	110.35	113.91
19	A	401	BCR	C12-C13-C14	3.09	123.69	118.94
22	D	610	AJP	C05-C06-C07	-3.09	98.34	103.37
22	Q	103	AJP	C20-C21-C22	-3.09	109.02	114.09
22	Q	102	AJP	C18-C17-C16	-3.09	107.06	112.14
22	G	304	AJP	C19-C24-C23	-3.08	111.06	114.46
22	D	615	AJP	C14-C13-C12	-3.08	107.49	112.78
22	B	606	AJP	C21-C20-C19	3.08	110.61	107.14
22	A	406	AJP	O09-C08-C10	3.08	116.51	110.17
22	F	704	AJP	C14-C15-C20	-3.08	110.37	113.91
22	G	303	AJP	C14-C15-C20	-3.08	110.37	113.91
22	F	709	AJP	C14-C13-C12	-3.07	107.52	112.78
22	F	706	AJP	C11-C12-C07	-3.07	94.95	100.19
22	D	615	AJP	C24-C19-C20	-3.07	109.40	112.66
22	F	711	AJP	O09-C08-C10	3.06	116.48	110.17
19	D	601	BCR	C19-C18-C17	3.06	123.64	118.94
22	B	604	AJP	O09-C08-C07	-3.06	96.71	104.06
22	D	610	AJP	C20-C21-C22	-3.06	109.07	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	606	AJP	C14-C15-C20	-3.05	110.39	113.91
22	B	605	AJP	C14-C13-C12	-3.05	107.55	112.78
22	A	406	AJP	C20-C21-C22	-3.05	109.09	114.09
22	B	613	AJP	C14-C15-C20	-3.04	110.41	113.91
22	A	407	AJP	C11-C12-C07	-3.04	95.00	100.19
22	D	615	AJP	C14-C15-C20	-3.04	110.41	113.91
22	D	611	AJP	C20-C21-C22	-3.04	109.11	114.09
22	F	709	AJP	C14-C15-C20	-3.03	110.42	113.91
22	B	612	AJP	C24-C19-C20	-3.03	109.44	112.66
22	D	610	AJP	C14-C13-C12	-3.03	107.58	112.78
22	G	303	AJP	C21-C20-C19	3.03	110.55	107.14
22	D	615	AJP	C85-O84-C05	-3.01	108.01	113.72
22	B	611	AJP	C83-C06-C05	-3.01	109.43	114.92
22	B	612	AJP	O09-C08-C10	3.01	116.36	110.17
22	D	607	AJP	C11-C12-C07	-3.00	95.06	100.19
22	C	201	AJP	C11-C12-C07	-3.00	95.06	100.19
22	F	710	AJP	C11-C12-C07	-3.00	95.06	100.19
22	B	608	AJP	C24-C19-C20	-3.00	109.47	112.66
24	D	605	SQD	C1-O5-C5	3.00	119.58	113.69
22	B	611	AJP	C14-C13-C12	-2.99	107.65	112.78
22	F	710	AJP	O09-C08-C10	2.99	116.33	110.17
22	G	303	AJP	O09-C08-C10	2.99	116.33	110.17
22	G	306	AJP	C24-C19-C20	-2.99	109.48	112.66
22	B	607	AJP	C14-C15-C20	-2.98	110.48	113.91
22	D	610	AJP	C11-C12-C07	-2.98	95.10	100.19
22	A	407	AJP	C11-C16-C15	-2.98	104.03	109.23
22	F	704	AJP	C20-C21-C22	-2.97	109.21	114.09
22	Q	101	AJP	O09-C08-C10	2.97	116.29	110.17
22	B	612	AJP	C11-C12-C07	-2.97	95.12	100.19
23	B	601	PQN	C14-C13-C15	-2.97	110.28	115.27
22	B	607	AJP	C11-C12-C07	-2.97	95.12	100.19
22	F	710	AJP	C24-C19-C20	-2.97	109.50	112.66
22	C	201	AJP	O09-C08-C10	2.97	116.27	110.17
22	F	704	AJP	O09-C08-C10	2.96	116.27	110.17
22	D	607	AJP	C83-C06-C05	-2.95	109.52	114.92
22	D	616	AJP	C85-O84-C05	-2.95	108.12	113.72
22	A	407	AJP	C21-C20-C19	2.95	110.46	107.14
22	G	303	AJP	C83-C06-C05	-2.95	109.53	114.92
22	D	608	AJP	C19-C24-C23	-2.95	111.21	114.46
22	D	610	AJP	O09-C08-C07	-2.95	96.99	104.06
22	C	201	AJP	C20-C21-C22	-2.94	109.26	114.09
19	D	601	BCR	C30-C25-C26	-2.94	118.47	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	L	101	SQD	O8-S-C6	2.94	110.42	105.74
22	G	302	AJP	C06-C07-C08	-2.93	99.00	104.34
22	F	707	AJP	O09-C08-C07	-2.93	97.02	104.06
22	F	704	AJP	C14-C13-C12	-2.93	107.75	112.78
22	A	408	AJP	C11-C16-C15	-2.93	104.11	109.23
22	G	306	AJP	C05-C06-C07	-2.93	98.60	103.37
22	F	711	AJP	C11-C12-C07	-2.93	95.19	100.19
22	F	705	AJP	C20-C21-C22	-2.93	109.29	114.09
22	F	704	AJP	C05-C06-C07	-2.92	98.62	103.37
22	A	406	AJP	C05-C06-C07	-2.92	98.62	103.37
22	B	608	AJP	C11-C12-C07	-2.92	95.21	100.19
22	D	609	AJP	C11-C12-C07	-2.91	95.21	100.19
22	D	613	AJP	C18-C17-C16	-2.91	107.35	112.14
22	D	612	AJP	C11-C12-C07	-2.91	95.22	100.19
22	B	609	AJP	C21-C22-C23	-2.91	108.03	111.36
21	A	404	DGD	O6D-C1D-O3G	-2.91	103.09	109.97
22	F	706	AJP	C14-C15-C20	-2.91	110.56	113.91
22	B	607	AJP	O09-C08-C10	2.90	116.13	110.17
22	D	608	AJP	C83-C06-C05	-2.89	109.64	114.92
22	D	616	AJP	C83-C06-C05	-2.89	109.64	114.92
22	B	604	AJP	C05-C06-C07	-2.89	98.67	103.37
22	F	708	AJP	C11-C12-C07	-2.88	95.27	100.19
22	G	307	AJP	C85-O84-C05	-2.87	108.27	113.72
22	F	706	AJP	C21-C20-C19	2.87	110.38	107.14
22	F	711	AJP	C21-C20-C19	2.87	110.37	107.14
22	G	305	AJP	C83-C06-C05	-2.87	109.68	114.92
22	F	704	AJP	C11-C16-C15	-2.86	104.24	109.23
22	F	709	AJP	C24-C19-C20	-2.86	109.62	112.66
22	A	407	AJP	O09-C08-C10	2.86	116.05	110.17
24	F	703	SQD	C4-C3-C2	2.86	115.81	110.82
22	F	710	AJP	C20-C21-C22	-2.86	109.41	114.09
22	B	609	AJP	C14-C15-C20	-2.85	110.63	113.91
22	B	604	AJP	C17-C18-C19	-2.85	106.13	111.84
22	B	611	AJP	C20-C21-C22	-2.85	109.42	114.09
24	F	703	SQD	O8-S-C6	2.84	110.27	105.74
22	Q	102	AJP	C83-C06-C05	-2.84	109.73	114.92
22	B	609	AJP	C21-C20-C19	2.83	110.33	107.14
22	C	202	AJP	C14-C13-C12	-2.83	107.93	112.78
22	B	612	AJP	C20-C21-C22	-2.83	109.45	114.09
22	F	706	AJP	O09-C08-C10	2.83	115.99	110.17
22	F	707	AJP	C14-C15-C20	-2.82	110.66	113.91
19	D	602	BCR	C23-C22-C21	2.82	123.26	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Q	102	AJP	O09-C08-C07	-2.82	97.31	104.06
24	L	101	SQD	C4-C3-C2	2.81	115.73	110.82
22	B	605	AJP	C11-C12-C07	-2.81	95.39	100.19
22	F	708	AJP	C14-C15-C20	-2.81	110.68	113.91
22	B	607	AJP	C04-C05-C06	-2.80	109.92	115.69
22	B	610	AJP	C14-C15-C20	-2.80	110.68	113.91
22	D	615	AJP	C04-C05-C06	-2.80	109.92	115.69
22	A	408	AJP	C14-C15-C20	-2.80	110.68	113.91
22	F	708	AJP	C14-C13-C12	-2.80	107.98	112.78
21	A	405	DGD	CDB-CCB-CBB	-2.79	100.27	114.42
22	F	707	AJP	C21-C20-C19	2.79	110.28	107.14
22	Q	101	AJP	C14-C13-C12	-2.78	108.02	112.78
22	F	712	AJP	C83-C06-C05	-2.77	109.85	114.92
22	B	610	AJP	C21-C20-C19	2.77	110.26	107.14
22	F	704	AJP	C06-C07-C08	-2.77	99.29	104.34
22	G	302	AJP	C05-C06-C07	-2.77	98.86	103.37
22	B	613	AJP	O09-C08-C10	2.76	115.86	110.17
20	A	403	LHG	O8-C23-C24	2.76	120.58	111.91
22	A	406	AJP	C11-C12-C07	-2.76	95.48	100.19
22	F	705	AJP	C05-C06-C07	-2.76	98.88	103.37
19	A	401	BCR	C23-C22-C21	2.75	123.17	118.94
21	A	404	DGD	CDB-CCB-CBB	-2.75	100.44	114.42
22	D	613	AJP	C20-C15-C16	-2.75	109.53	112.42
19	A	401	BCR	C8-C9-C10	2.75	123.16	118.94
22	A	407	AJP	C05-C06-C07	-2.75	98.90	103.37
22	B	610	AJP	C24-C19-C20	-2.75	109.74	112.66
22	G	304	AJP	C18-C17-C16	-2.74	107.62	112.14
22	D	612	AJP	O09-C08-C10	2.74	115.81	110.17
22	C	202	AJP	C20-C15-C16	-2.74	109.54	112.42
22	Q	102	AJP	O09-C08-C10	2.74	115.81	110.17
22	G	302	AJP	C18-C19-C20	-2.74	107.39	112.31
22	A	408	AJP	C14-C13-C12	-2.74	108.08	112.78
22	D	607	AJP	C21-C20-C19	2.73	110.22	107.14
24	D	606	SQD	O8-S-C6	2.73	110.09	105.74
22	A	408	AJP	O09-C08-C10	2.73	115.79	110.17
24	D	605	SQD	C44-O6-C1	2.73	119.07	113.74
22	D	608	AJP	C18-C19-C20	-2.73	107.41	112.31
22	B	606	AJP	O09-C08-C07	-2.73	97.52	104.06
22	B	609	AJP	O09-C08-C07	-2.72	97.53	104.06
22	D	616	AJP	O09-C08-C10	2.72	115.77	110.17
22	D	609	AJP	C06-C07-C08	-2.72	99.39	104.34
22	C	202	AJP	C83-C06-C05	-2.72	109.96	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	303	AJP	C85-O84-C05	-2.71	108.57	113.72
22	D	614	AJP	C14-C15-C20	-2.71	110.79	113.91
22	A	406	AJP	C24-C19-C20	-2.71	109.78	112.66
22	Q	102	AJP	C14-C13-C12	-2.71	108.14	112.78
22	C	202	AJP	O09-C08-C10	2.71	115.74	110.17
22	C	201	AJP	C18-C17-C16	-2.71	107.68	112.14
24	D	605	SQD	O8-S-C6	2.70	110.05	105.74
22	D	612	AJP	C85-O84-C05	-2.70	108.60	113.72
22	D	613	AJP	C04-C05-C06	-2.70	110.14	115.69
22	F	708	AJP	O09-C08-C10	2.70	115.73	110.17
22	B	614	AJP	C14-C13-C12	-2.70	108.16	112.78
22	G	305	AJP	C20-C15-C16	-2.69	109.59	112.42
22	D	612	AJP	C14-C13-C12	-2.69	108.16	112.78
22	D	612	AJP	C20-C15-C16	-2.69	109.59	112.42
20	F	701	LHG	O8-C23-C24	2.69	120.35	111.91
22	D	609	AJP	C11-C16-C15	-2.69	104.54	109.23
22	F	709	AJP	C04-C05-C06	-2.69	110.16	115.69
22	Q	103	AJP	C21-C20-C19	2.69	110.17	107.14
22	D	613	AJP	C06-C07-C08	-2.68	99.46	104.34
22	D	614	AJP	C17-C16-C11	-2.68	108.43	112.32
24	D	606	SQD	C4-C3-C2	2.67	115.49	110.82
22	G	306	AJP	C21-C20-C19	2.67	110.15	107.14
22	B	606	AJP	C05-C06-C07	-2.67	99.03	103.37
22	Q	101	AJP	C04-C05-C06	-2.66	110.21	115.69
20	F	702	LHG	O8-C23-C24	2.66	120.26	111.91
22	A	407	AJP	C24-C23-C22	-2.66	106.98	110.27
22	D	615	AJP	C11-C16-C15	-2.66	104.59	109.23
24	D	606	SQD	C1-O5-C5	2.66	118.91	113.69
24	L	101	SQD	C44-O6-C1	2.66	118.93	113.74
24	F	703	SQD	C1-O5-C5	2.66	118.90	113.69
19	D	601	BCR	C23-C22-C21	2.65	123.01	118.94
22	F	706	AJP	C85-O84-C05	-2.65	108.69	113.72
22	G	305	AJP	C11-C12-C07	-2.64	95.67	100.19
22	G	305	AJP	O09-C08-C10	2.64	115.61	110.17
22	D	607	AJP	C14-C15-C20	-2.64	110.87	113.91
22	F	712	AJP	C11-C12-C07	-2.64	95.68	100.19
22	B	604	AJP	C18-C17-C16	-2.64	107.79	112.14
22	Q	103	AJP	O09-C08-C07	-2.64	97.73	104.06
22	A	406	AJP	C83-C06-C05	-2.64	110.10	114.92
22	G	305	AJP	O09-C08-C07	-2.64	97.73	104.06
22	B	611	AJP	C04-C05-C06	-2.64	110.27	115.69
22	G	302	AJP	C24-C19-C20	-2.64	109.86	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	704	AJP	C85-O84-C05	-2.63	108.72	113.72
22	B	611	AJP	O09-C08-C07	-2.63	97.75	104.06
22	Q	102	AJP	C15-C20-C19	2.63	112.27	108.58
20	D	603	LHG	O8-C23-C24	2.63	120.16	111.91
22	D	616	AJP	C20-C21-C22	-2.62	109.79	114.09
22	D	612	AJP	C24-C23-C22	-2.62	107.03	110.27
22	C	202	AJP	O09-C08-C07	-2.62	97.78	104.06
19	D	602	BCR	C30-C25-C26	-2.62	118.93	122.61
24	L	101	SQD	C1-O5-C5	2.61	118.82	113.69
22	F	711	AJP	C24-C19-C20	-2.61	109.89	112.66
22	G	302	AJP	C11-C16-C15	-2.60	104.69	109.23
22	B	609	AJP	C17-C16-C15	-2.60	107.27	110.49
22	D	614	AJP	C18-C19-C20	-2.60	107.64	112.31
22	F	707	AJP	C05-C06-C07	-2.60	99.14	103.37
22	B	611	AJP	C24-C19-C20	-2.60	109.90	112.66
22	F	706	AJP	C20-C15-C16	-2.60	109.69	112.42
22	G	303	AJP	C21-C22-C23	-2.60	108.38	111.36
22	B	605	AJP	C05-C06-C07	-2.59	99.15	103.37
19	D	602	BCR	C8-C9-C10	2.59	122.92	118.94
22	B	605	AJP	C20-C15-C16	-2.59	109.70	112.42
22	D	611	AJP	O09-C08-C07	-2.59	97.85	104.06
22	D	609	AJP	C05-C06-C07	-2.58	99.16	103.37
22	D	610	AJP	C85-O84-C05	-2.58	108.82	113.72
22	B	612	AJP	C83-C06-C05	-2.58	110.20	114.92
22	Q	101	AJP	C20-C15-C16	-2.58	109.71	112.42
20	D	604	LHG	O8-C23-C24	2.58	120.00	111.91
22	F	710	AJP	C83-C06-C05	-2.58	110.21	114.92
22	D	611	AJP	C11-C12-C07	-2.58	95.79	100.19
22	D	616	AJP	C18-C17-C16	-2.58	107.89	112.14
22	A	408	AJP	C04-C05-C06	-2.58	110.39	115.69
22	G	302	AJP	C11-C12-C07	-2.57	95.80	100.19
22	F	709	AJP	O09-C08-C07	-2.57	97.90	104.06
22	F	708	AJP	C21-C20-C19	2.57	110.03	107.14
22	B	606	AJP	C24-C19-C20	-2.57	109.93	112.66
22	F	708	AJP	C04-C05-C06	-2.57	110.42	115.69
24	D	605	SQD	C4-C3-C2	2.56	115.30	110.82
22	A	408	AJP	C18-C17-C16	-2.56	107.92	112.14
22	G	305	AJP	C21-C20-C19	2.56	110.03	107.14
22	F	711	AJP	O09-C08-C07	-2.56	97.92	104.06
20	B	602	LHG	O8-C23-C24	2.56	119.93	111.91
21	A	405	DGD	C3G-C2G-C1G	-2.55	105.75	111.79
22	F	708	AJP	C21-C22-C23	-2.55	108.43	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	304	AJP	C17-C16-C15	-2.55	107.33	110.49
22	Q	102	AJP	C11-C12-C07	-2.55	95.83	100.19
22	C	202	AJP	C11-C12-C07	-2.54	95.85	100.19
22	D	607	AJP	C21-C22-C23	-2.54	108.45	111.36
22	B	605	AJP	C20-C21-C22	-2.54	109.93	114.09
22	B	613	AJP	C24-C19-C20	-2.54	109.96	112.66
22	G	304	AJP	C06-C07-C08	-2.53	99.73	104.34
22	B	614	AJP	C21-C20-C19	2.53	109.99	107.14
22	D	614	AJP	C11-C16-C15	-2.53	104.81	109.23
22	G	303	AJP	O09-C08-C07	-2.53	97.99	104.06
22	A	408	AJP	C85-O84-C05	-2.53	108.92	113.72
22	F	712	AJP	C04-C05-C06	-2.53	110.49	115.69
20	A	402	LHG	O8-C23-C24	2.53	119.85	111.91
22	A	407	AJP	C18-C19-C20	-2.53	107.77	112.31
24	L	101	SQD	O5-C5-C4	2.53	114.28	109.69
22	B	611	AJP	C21-C20-C19	2.52	109.98	107.14
22	B	611	AJP	C21-C22-C23	-2.52	108.47	111.36
20	D	604	LHG	C11-C10-C9	-2.52	101.62	114.42
22	Q	101	AJP	O09-C08-C07	-2.52	98.01	104.06
22	B	610	AJP	O09-C08-C07	-2.52	98.01	104.06
20	F	701	LHG	C11-C10-C9	-2.52	101.63	114.42
22	B	605	AJP	O09-C08-C07	-2.52	98.02	104.06
24	F	703	SQD	O48-C23-C24	2.51	119.80	111.91
22	F	706	AJP	O09-C08-C07	-2.51	98.04	104.06
22	Q	103	AJP	C24-C19-C20	-2.51	109.99	112.66
22	F	706	AJP	C83-C06-C05	-2.51	110.34	114.92
20	B	603	LHG	O8-C23-C24	2.50	119.76	111.91
22	A	408	AJP	C11-C12-C07	-2.50	95.92	100.19
22	G	303	AJP	C24-C19-C20	-2.50	110.00	112.66
22	G	303	AJP	C04-C05-C06	-2.50	110.55	115.69
20	A	402	LHG	C11-C10-C9	-2.50	101.74	114.42
22	A	408	AJP	O09-C08-C07	-2.50	98.07	104.06
20	D	603	LHG	C11-C10-C9	-2.50	101.75	114.42
22	D	612	AJP	C14-C15-C20	-2.49	111.04	113.91
20	F	702	LHG	C11-C10-C9	-2.49	101.78	114.42
20	A	403	LHG	C11-C10-C9	-2.49	101.78	114.42
22	B	612	AJP	C04-C05-C06	-2.48	110.59	115.69
22	A	407	AJP	O09-C08-C07	-2.48	98.12	104.06
22	D	611	AJP	C04-C05-C06	-2.48	110.60	115.69
22	B	608	AJP	C83-C06-C05	-2.48	110.40	114.92
20	G	301	LHG	O8-C23-C24	2.48	119.67	111.91
21	A	405	DGD	O2D-C2D-C1D	-2.47	104.03	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	609	AJP	C20-C21-C22	-2.47	110.03	114.09
24	L	101	SQD	O48-C23-C24	2.47	119.67	111.91
22	F	710	AJP	C04-C05-C06	-2.47	110.60	115.69
22	B	611	AJP	C85-O84-C05	-2.47	109.03	113.72
22	D	616	AJP	C11-C16-C15	-2.47	104.92	109.23
22	F	707	AJP	C21-C22-C23	-2.47	108.53	111.36
22	G	302	AJP	C20-C15-C16	-2.47	109.83	112.42
20	B	602	LHG	C11-C10-C9	-2.47	101.90	114.42
22	G	306	AJP	O09-C08-C07	-2.47	98.14	104.06
22	A	407	AJP	C83-C06-C05	-2.46	110.42	114.92
22	B	610	AJP	C21-C22-C23	-2.46	108.54	111.36
22	C	202	AJP	C18-C17-C16	-2.46	108.09	112.14
22	D	616	AJP	O09-C08-C07	-2.46	98.17	104.06
20	B	603	LHG	C11-C10-C9	-2.45	101.97	114.42
22	D	608	AJP	O09-C08-C10	2.45	115.22	110.17
24	D	605	SQD	O48-C23-C24	2.45	119.61	111.91
22	Q	103	AJP	C21-C22-C23	-2.45	108.55	111.36
22	F	709	AJP	C83-C06-C05	-2.45	110.44	114.92
22	Q	103	AJP	C18-C17-C16	-2.45	108.10	112.14
22	F	704	AJP	O09-C08-C07	-2.45	98.19	104.06
22	G	302	AJP	O09-C08-C07	-2.44	98.20	104.06
22	D	616	AJP	C14-C15-C20	-2.44	111.10	113.91
22	Q	101	AJP	C85-O84-C05	-2.44	109.09	113.72
20	B	603	LHG	C20-C19-C18	-2.44	102.06	114.42
22	F	704	AJP	C04-C05-C06	-2.43	110.69	115.69
22	B	608	AJP	O09-C08-C07	-2.43	98.23	104.06
20	F	702	LHG	C20-C19-C18	-2.43	102.09	114.42
22	D	608	AJP	C17-C16-C11	-2.42	108.81	112.32
22	C	201	AJP	C05-C06-C07	-2.41	99.44	103.37
24	D	605	SQD	O5-C5-C4	2.41	114.08	109.69
19	D	601	BCR	C8-C9-C10	2.41	122.64	118.94
20	A	402	LHG	C20-C19-C18	-2.41	102.19	114.42
22	F	707	AJP	C24-C19-C20	-2.41	110.10	112.66
22	B	610	AJP	C04-C05-C06	-2.41	110.74	115.69
24	D	606	SQD	O48-C23-C24	2.41	119.46	111.91
20	D	603	LHG	C20-C19-C18	-2.41	102.20	114.42
22	D	613	AJP	C11-C12-C07	-2.41	96.08	100.19
22	C	202	AJP	C85-O84-C05	-2.40	109.16	113.72
22	A	406	AJP	C21-C20-C19	2.40	109.85	107.14
22	D	615	AJP	O09-C08-C07	-2.40	98.30	104.06
24	D	606	SQD	O5-C5-C4	2.40	114.06	109.69
22	F	707	AJP	C83-C06-C05	-2.40	110.53	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Q	103	AJP	O09-C08-C10	2.40	115.11	110.17
22	F	709	AJP	C11-C12-C07	-2.40	96.09	100.19
20	D	604	LHG	C20-C19-C18	-2.40	102.26	114.42
22	G	306	AJP	C04-C05-C06	-2.40	110.76	115.69
22	D	612	AJP	C18-C19-C20	-2.39	108.01	112.31
22	F	707	AJP	C04-C05-C06	-2.39	110.78	115.69
20	G	301	LHG	C20-C19-C18	-2.39	102.29	114.42
22	D	609	AJP	O09-C08-C07	-2.39	98.33	104.06
22	G	304	AJP	C11-C12-C07	-2.38	96.12	100.19
22	B	614	AJP	C21-C22-C23	-2.38	108.63	111.36
22	F	705	AJP	O09-C08-C07	-2.38	98.35	104.06
22	F	711	AJP	C04-C05-C06	-2.38	110.81	115.69
20	G	301	LHG	C11-C10-C9	-2.37	102.38	114.42
20	F	701	LHG	C20-C19-C18	-2.37	102.39	114.42
22	G	307	AJP	C11-C16-C15	-2.37	105.09	109.23
22	D	611	AJP	C05-C06-C07	-2.37	99.51	103.37
22	G	307	AJP	C21-C20-C19	2.37	109.81	107.14
22	B	608	AJP	C20-C21-C22	-2.37	110.21	114.09
22	F	704	AJP	C24-C19-C20	-2.36	110.15	112.66
22	A	407	AJP	C17-C16-C11	-2.36	108.89	112.32
22	Q	102	AJP	C85-O84-C05	-2.36	109.24	113.72
20	A	403	LHG	C20-C19-C18	-2.36	102.45	114.42
22	F	706	AJP	C04-C05-C06	-2.36	110.85	115.69
21	A	404	DGD	C3D-C4D-C5D	-2.35	106.04	110.24
22	B	606	AJP	C20-C21-C22	-2.35	110.23	114.09
22	D	614	AJP	C04-C05-C06	-2.35	110.86	115.69
22	G	304	AJP	C04-C05-C06	-2.35	110.86	115.69
22	B	604	AJP	C04-C05-C06	-2.35	110.86	115.69
22	B	612	AJP	O09-C08-C07	-2.35	98.43	104.06
22	B	607	AJP	C24-C19-C20	-2.34	110.17	112.66
22	G	306	AJP	C83-C06-C05	-2.34	110.64	114.92
22	D	611	AJP	C18-C17-C16	-2.34	108.28	112.14
24	F	703	SQD	O6-C1-C2	2.34	111.95	108.30
22	C	201	AJP	C04-C05-C06	-2.34	110.89	115.69
22	B	604	AJP	C14-C15-C16	-2.33	108.39	111.75
22	B	606	AJP	C04-C05-C06	-2.33	110.90	115.69
22	A	406	AJP	O09-C08-C07	-2.33	98.47	104.06
22	D	609	AJP	C21-C22-C23	-2.33	108.69	111.36
22	F	708	AJP	C24-C23-C22	-2.33	107.39	110.27
22	F	710	AJP	O09-C08-C07	-2.32	98.49	104.06
22	F	705	AJP	C04-C05-C06	-2.32	110.92	115.69
20	B	602	LHG	C20-C19-C18	-2.32	102.64	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	307	AJP	C83-C06-C05	-2.32	110.68	114.92
22	D	610	AJP	C83-C06-C05	-2.32	110.69	114.92
24	F	703	SQD	O5-C5-C4	2.32	113.90	109.69
22	B	610	AJP	C17-C16-C15	-2.31	107.62	110.49
22	D	612	AJP	C04-C05-C06	-2.31	110.94	115.69
22	B	611	AJP	C18-C19-C20	-2.31	108.16	112.31
22	G	307	AJP	C03-C02-C85	2.31	111.77	108.56
22	Q	101	AJP	C20-C21-C22	-2.31	110.30	114.09
22	G	305	AJP	C11-C16-C15	-2.31	105.20	109.23
22	G	306	AJP	C85-O84-C05	-2.31	109.35	113.72
22	D	612	AJP	O09-C08-C07	-2.30	98.53	104.06
22	B	605	AJP	C83-C06-C05	-2.30	110.71	114.92
22	C	202	AJP	C04-C05-C06	-2.30	110.96	115.69
22	G	302	AJP	C04-C05-C06	-2.30	110.96	115.69
22	D	609	AJP	C83-C06-C05	-2.30	110.72	114.92
22	B	613	AJP	C04-C05-C06	-2.30	110.97	115.69
21	A	404	DGD	C3G-C2G-C1G	-2.29	106.36	111.79
22	F	705	AJP	C83-C06-C05	-2.29	110.73	114.92
22	B	609	AJP	C04-C05-C06	-2.29	110.98	115.69
21	A	405	DGD	CFB-CEB-CDB	-2.29	102.81	114.42
22	B	610	AJP	C83-C06-C05	-2.29	110.74	114.92
22	C	201	AJP	C83-C06-C05	-2.28	110.75	114.92
22	B	605	AJP	C18-C17-C16	-2.28	108.38	112.14
22	F	711	AJP	C20-C21-C22	-2.28	110.35	114.09
22	G	304	AJP	C05-C06-C07	-2.28	99.66	103.37
22	F	711	AJP	C20-C15-C16	-2.28	110.03	112.42
22	B	608	AJP	C04-C05-C06	-2.27	111.02	115.69
22	B	604	AJP	C14-C13-C12	-2.27	108.89	112.78
22	B	607	AJP	O09-C08-C07	-2.27	98.62	104.06
22	D	612	AJP	C11-C16-C15	-2.26	105.28	109.23
22	D	616	AJP	C14-C13-C12	-2.26	108.90	112.78
20	B	603	LHG	C18-C17-C16	-2.26	102.95	114.42
22	D	608	AJP	C14-C15-C20	-2.26	111.31	113.91
22	D	609	AJP	C18-C19-C20	-2.26	108.25	112.31
22	F	711	AJP	C11-C16-C15	-2.26	105.29	109.23
22	F	709	AJP	C04-C03-C02	-2.26	107.05	111.81
22	D	607	AJP	C17-C16-C11	-2.26	109.04	112.32
20	D	603	LHG	C27-C26-C25	-2.25	103.01	114.42
22	B	614	AJP	C04-C05-C06	-2.25	111.07	115.69
22	D	609	AJP	C04-C05-C06	-2.25	111.07	115.69
22	D	607	AJP	C18-C19-C20	-2.24	108.27	112.31
20	A	402	LHG	C18-C17-C16	-2.24	103.03	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	304	AJP	C83-C06-C05	-2.24	110.82	114.92
22	B	614	AJP	C24-C19-C20	-2.24	110.28	112.66
22	F	706	AJP	C18-C19-C20	-2.24	108.28	112.31
24	D	606	SQD	O6-C1-C2	2.24	111.80	108.30
22	A	407	AJP	C14-C13-C12	-2.24	108.94	112.78
22	D	609	AJP	C20-C15-C16	-2.24	110.07	112.42
22	B	605	AJP	C04-C05-C06	-2.24	111.09	115.69
20	F	702	LHG	C27-C26-C25	-2.23	103.09	114.42
22	F	704	AJP	C03-C02-C85	2.23	111.66	108.56
22	D	614	AJP	O09-C08-C07	-2.23	98.71	104.06
22	B	613	AJP	O09-C08-C07	-2.23	98.71	104.06
21	A	404	DGD	CFB-CEB-CDB	-2.23	103.10	114.42
20	G	301	LHG	C27-C26-C25	-2.23	103.10	114.42
22	G	305	AJP	C04-C05-C06	-2.23	111.10	115.69
22	A	407	AJP	C17-C18-C19	-2.23	107.37	111.84
22	C	202	AJP	C20-C21-C22	-2.23	110.44	114.09
22	B	606	AJP	C83-C06-C05	-2.22	110.86	114.92
22	F	709	AJP	C18-C19-C20	-2.22	108.32	112.31
21	A	405	DGD	C3D-C4D-C5D	-2.21	106.29	110.24
22	D	611	AJP	C21-C20-C19	2.21	109.63	107.14
22	F	706	AJP	C11-C16-C15	-2.21	105.37	109.23
22	F	708	AJP	O09-C08-C07	-2.21	98.77	104.06
22	D	607	AJP	C24-C19-C18	-2.21	107.69	111.74
22	B	610	AJP	C11-C12-C07	-2.20	96.42	100.19
20	B	602	LHG	C18-C17-C16	-2.20	103.26	114.42
20	D	604	LHG	C18-C17-C16	-2.20	103.27	114.42
22	G	302	AJP	C83-C06-C05	-2.20	110.91	114.92
22	B	613	AJP	C21-C20-C19	2.20	109.61	107.14
21	A	405	DGD	C1E-O6E-C5E	2.19	117.99	113.69
22	A	407	AJP	C04-C05-C06	-2.19	111.19	115.69
22	G	305	AJP	C85-O84-C05	-2.19	109.57	113.72
22	A	407	AJP	C03-C04-C05	-2.19	108.16	111.93
20	A	402	LHG	C27-C26-C25	-2.19	103.33	114.42
21	A	405	DGD	CBB-CAB-C9B	-2.18	103.35	114.42
22	D	607	AJP	O09-C08-C07	-2.18	98.84	104.06
20	B	603	LHG	C27-C26-C25	-2.18	103.38	114.42
22	F	704	AJP	C83-C06-C05	-2.17	110.95	114.92
20	G	301	LHG	C18-C17-C16	-2.17	103.39	114.42
21	A	404	DGD	CBB-CAB-C9B	-2.17	103.39	114.42
23	B	601	PQN	C2M-C2-C3	-2.17	120.86	124.40
22	C	201	AJP	O09-C08-C07	-2.17	98.86	104.06
22	B	609	AJP	C11-C12-C07	-2.17	96.48	100.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	602	LHG	C27-C26-C25	-2.17	103.41	114.42
20	D	604	LHG	C27-C26-C25	-2.16	103.45	114.42
22	D	612	AJP	C21-C22-C23	-2.16	108.88	111.36
22	G	307	AJP	C04-C05-C06	-2.16	111.25	115.69
20	A	403	LHG	C18-C17-C16	-2.16	103.47	114.42
22	F	709	AJP	C20-C21-C22	-2.15	110.56	114.09
20	F	701	LHG	C27-C26-C25	-2.15	103.49	114.42
22	B	605	AJP	C85-O84-C05	-2.15	109.64	113.72
22	B	614	AJP	C17-C16-C11	-2.15	109.20	112.32
22	D	607	AJP	O09-C08-C10	2.15	114.59	110.17
22	F	706	AJP	C20-C21-C22	-2.15	110.57	114.09
22	F	705	AJP	C81-C12-C07	2.14	116.85	111.63
22	D	615	AJP	C17-C16-C11	-2.14	109.21	112.32
20	F	702	LHG	C18-C17-C16	-2.14	103.55	114.42
22	D	611	AJP	C83-C06-C05	-2.14	111.01	114.92
22	D	613	AJP	C83-C06-C05	-2.14	111.01	114.92
22	F	704	AJP	C20-C15-C16	-2.14	110.18	112.42
20	D	603	LHG	C18-C17-C16	-2.14	103.58	114.42
19	D	601	BCR	C1-C6-C5	-2.14	119.60	122.61
21	A	405	DGD	O5D-C6D-C5D	-2.14	105.10	109.05
22	B	608	AJP	C18-C17-C16	-2.13	108.63	112.14
22	A	408	AJP	C17-C18-C19	-2.13	107.58	111.84
22	F	707	AJP	C04-C03-C02	-2.13	107.32	111.81
22	G	305	AJP	C20-C21-C22	-2.13	110.60	114.09
22	F	710	AJP	C21-C20-C19	2.12	109.53	107.14
22	D	610	AJP	C18-C17-C16	-2.12	108.64	112.14
22	D	610	AJP	C04-C05-C06	-2.12	111.33	115.69
22	Q	103	AJP	C04-C05-C06	-2.12	111.33	115.69
24	F	703	SQD	C45-O47-C7	2.12	123.01	117.79
22	G	307	AJP	C20-C21-C22	-2.12	110.61	114.09
22	B	604	AJP	C21-C20-C19	2.12	109.52	107.14
22	A	407	AJP	O84-C85-C02	-2.12	109.13	112.18
22	F	712	AJP	O09-C08-C07	-2.12	98.99	104.06
20	F	701	LHG	C18-C17-C16	-2.12	103.68	114.42
22	D	608	AJP	O09-C08-C07	-2.12	98.99	104.06
22	F	712	AJP	C18-C17-C16	-2.11	108.66	112.14
22	D	607	AJP	C24-C19-C20	-2.11	110.42	112.66
22	D	616	AJP	C14-C15-C16	-2.11	108.72	111.75
22	F	709	AJP	C17-C18-C19	-2.10	107.62	111.84
22	G	306	AJP	C20-C21-C22	-2.10	110.65	114.09
21	A	404	DGD	CAB-C9B-C8B	-2.09	103.80	114.42
22	F	705	AJP	C17-C16-C11	-2.09	109.28	112.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	607	AJP	C21-C20-C19	2.09	109.49	107.14
22	D	610	AJP	C21-C20-C19	2.09	109.49	107.14
21	A	405	DGD	CAB-C9B-C8B	-2.09	103.82	114.42
22	B	610	AJP	C05-C06-C07	-2.08	99.98	103.37
21	A	404	DGD	O2D-C2D-C1D	-2.08	104.99	110.05
22	G	307	AJP	C81-C12-C07	2.08	116.70	111.63
22	F	705	AJP	C24-C19-C18	-2.08	107.93	111.74
24	D	605	SQD	O6-C1-C2	2.08	111.55	108.30
22	B	609	AJP	C24-C19-C18	-2.08	107.93	111.74
22	B	609	AJP	C85-O84-C05	-2.08	109.78	113.72
22	F	712	AJP	O84-C85-C02	-2.07	109.19	112.18
22	F	704	AJP	C21-C20-C19	2.07	109.47	107.14
22	A	406	AJP	C04-C05-C06	-2.07	111.43	115.69
21	A	405	DGD	C5B-C4B-C3B	-2.07	103.92	114.42
22	B	612	AJP	C21-C20-C19	2.07	109.47	107.14
22	F	708	AJP	C18-C17-C16	-2.06	108.75	112.14
22	Q	102	AJP	C17-C16-C15	-2.05	107.95	110.49
22	D	608	AJP	C24-C19-C18	-2.05	107.98	111.74
22	Q	103	AJP	C11-C12-C07	-2.05	96.69	100.19
22	B	604	AJP	C83-C06-C05	-2.03	111.20	114.92
22	F	712	AJP	C85-O84-C05	-2.03	109.86	113.72
22	G	307	AJP	C20-C15-C16	-2.03	110.29	112.42
22	G	302	AJP	C24-C23-C22	-2.03	107.76	110.27
22	D	608	AJP	C81-C12-C07	2.03	116.56	111.63
22	F	708	AJP	C03-C02-C85	2.03	111.38	108.56
21	A	404	DGD	C5B-C4B-C3B	-2.03	104.14	114.42
22	D	614	AJP	O84-C85-C02	-2.03	109.26	112.18
22	F	708	AJP	C18-C19-C20	-2.02	108.67	112.31
22	B	609	AJP	C24-C19-C20	-2.02	110.51	112.66
22	D	607	AJP	O84-C85-C02	-2.02	109.27	112.18
22	F	707	AJP	C18-C19-C20	-2.02	108.68	112.31
22	G	304	AJP	C80-C20-C15	-2.02	108.40	111.18
22	D	608	AJP	C04-C05-C06	-2.02	111.54	115.69
22	F	711	AJP	C18-C19-C20	-2.01	108.69	112.31
22	D	614	AJP	C24-C23-C22	-2.01	107.78	110.27
22	B	604	AJP	C81-C12-C07	2.01	116.53	111.63
22	F	706	AJP	C24-C19-C20	-2.01	110.52	112.66
22	G	305	AJP	C18-C17-C16	-2.01	108.83	112.14
22	G	302	AJP	C81-C12-C07	2.01	116.52	111.63
22	B	608	AJP	C21-C20-C19	2.00	109.39	107.14

All (528) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	406	AJP	C12
22	A	406	AJP	C02
22	A	406	AJP	C22
22	A	406	AJP	C07
22	A	406	AJP	C20
22	A	406	AJP	C10
22	A	406	AJP	C05
22	A	406	AJP	C16
22	A	406	AJP	C15
22	A	406	AJP	C19
22	A	406	AJP	C23
22	A	406	AJP	C11
22	A	407	AJP	C12
22	A	407	AJP	C02
22	A	407	AJP	C22
22	A	407	AJP	C07
22	A	407	AJP	C20
22	A	407	AJP	C10
22	A	407	AJP	C05
22	A	407	AJP	C16
22	A	407	AJP	C15
22	A	407	AJP	C19
22	A	407	AJP	C23
22	A	407	AJP	C11
22	A	408	AJP	C12
22	A	408	AJP	C02
22	A	408	AJP	C22
22	A	408	AJP	C07
22	A	408	AJP	C20
22	A	408	AJP	C10
22	A	408	AJP	C05
22	A	408	AJP	C16
22	A	408	AJP	C15
22	A	408	AJP	C19
22	A	408	AJP	C23
22	A	408	AJP	C11
22	B	604	AJP	C12
22	B	604	AJP	C02
22	B	604	AJP	C22
22	B	604	AJP	C07
22	B	604	AJP	C20
22	B	604	AJP	C10
22	B	604	AJP	C05

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Mol	Chain	Res	Type	Atom
22	B	604	AJP	C16
22	B	604	AJP	C15
22	B	604	AJP	C19
22	B	604	AJP	C23
22	B	604	AJP	C11
22	B	605	AJP	C12
22	B	605	AJP	C02
22	B	605	AJP	C22
22	B	605	AJP	C07
22	B	605	AJP	C20
22	B	605	AJP	C10
22	B	605	AJP	C05
22	B	605	AJP	C16
22	B	605	AJP	C15
22	B	605	AJP	C19
22	B	605	AJP	C23
22	B	605	AJP	C11
22	B	606	AJP	C12
22	B	606	AJP	C02
22	B	606	AJP	C22
22	B	606	AJP	C07
22	B	606	AJP	C20
22	B	606	AJP	C10
22	B	606	AJP	C05
22	B	606	AJP	C16
22	B	606	AJP	C15
22	B	606	AJP	C19
22	B	606	AJP	C23
22	B	606	AJP	C11
22	B	607	AJP	C12
22	B	607	AJP	C02
22	B	607	AJP	C22
22	B	607	AJP	C07
22	B	607	AJP	C20
22	B	607	AJP	C10
22	B	607	AJP	C05
22	B	607	AJP	C16
22	B	607	AJP	C15
22	B	607	AJP	C19
22	B	607	AJP	C23
22	B	607	AJP	C11
22	B	608	AJP	C12

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Mol	Chain	Res	Type	Atom
22	B	608	AJP	C02
22	B	608	AJP	C22
22	B	608	AJP	C07
22	B	608	AJP	C20
22	B	608	AJP	C10
22	B	608	AJP	C05
22	B	608	AJP	C16
22	B	608	AJP	C15
22	B	608	AJP	C19
22	B	608	AJP	C23
22	B	608	AJP	C11
22	B	609	AJP	C12
22	B	609	AJP	C02
22	B	609	AJP	C22
22	B	609	AJP	C07
22	B	609	AJP	C20
22	B	609	AJP	C10
22	B	609	AJP	C05
22	B	609	AJP	C16
22	B	609	AJP	C15
22	B	609	AJP	C19
22	B	609	AJP	C23
22	B	609	AJP	C11
22	B	610	AJP	C12
22	B	610	AJP	C02
22	B	610	AJP	C22
22	B	610	AJP	C07
22	B	610	AJP	C20
22	B	610	AJP	C10
22	B	610	AJP	C05
22	B	610	AJP	C16
22	B	610	AJP	C15
22	B	610	AJP	C19
22	B	610	AJP	C23
22	B	610	AJP	C11
22	B	611	AJP	C12
22	B	611	AJP	C02
22	B	611	AJP	C22
22	B	611	AJP	C07
22	B	611	AJP	C20
22	B	611	AJP	C10
22	B	611	AJP	C05

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Mol	Chain	Res	Type	Atom
22	B	611	AJP	C16
22	B	611	AJP	C15
22	B	611	AJP	C19
22	B	611	AJP	C23
22	B	611	AJP	C11
22	B	612	AJP	C12
22	B	612	AJP	C02
22	B	612	AJP	C22
22	B	612	AJP	C07
22	B	612	AJP	C20
22	B	612	AJP	C10
22	B	612	AJP	C05
22	B	612	AJP	C16
22	B	612	AJP	C15
22	B	612	AJP	C19
22	B	612	AJP	C23
22	B	612	AJP	C11
22	B	613	AJP	C12
22	B	613	AJP	C02
22	B	613	AJP	C22
22	B	613	AJP	C07
22	B	613	AJP	C20
22	B	613	AJP	C10
22	B	613	AJP	C05
22	B	613	AJP	C16
22	B	613	AJP	C15
22	B	613	AJP	C19
22	B	613	AJP	C23
22	B	613	AJP	C11
22	B	614	AJP	C12
22	B	614	AJP	C02
22	B	614	AJP	C22
22	B	614	AJP	C07
22	B	614	AJP	C20
22	B	614	AJP	C10
22	B	614	AJP	C05
22	B	614	AJP	C16
22	B	614	AJP	C15
22	B	614	AJP	C19
22	B	614	AJP	C23
22	B	614	AJP	C11
22	C	201	AJP	C12

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Mol	Chain	Res	Type	Atom
22	C	201	AJP	C02
22	C	201	AJP	C22
22	C	201	AJP	C07
22	C	201	AJP	C20
22	C	201	AJP	C10
22	C	201	AJP	C05
22	C	201	AJP	C16
22	C	201	AJP	C15
22	C	201	AJP	C19
22	C	201	AJP	C23
22	C	201	AJP	C11
22	C	202	AJP	C12
22	C	202	AJP	C02
22	C	202	AJP	C22
22	C	202	AJP	C07
22	C	202	AJP	C20
22	C	202	AJP	C10
22	C	202	AJP	C05
22	C	202	AJP	C16
22	C	202	AJP	C15
22	C	202	AJP	C19
22	C	202	AJP	C23
22	C	202	AJP	C11
22	D	607	AJP	C12
22	D	607	AJP	C02
22	D	607	AJP	C22
22	D	607	AJP	C07
22	D	607	AJP	C20
22	D	607	AJP	C10
22	D	607	AJP	C05
22	D	607	AJP	C16
22	D	607	AJP	C15
22	D	607	AJP	C19
22	D	607	AJP	C23
22	D	607	AJP	C11
22	D	608	AJP	C12
22	D	608	AJP	C02
22	D	608	AJP	C22
22	D	608	AJP	C07
22	D	608	AJP	C20
22	D	608	AJP	C10
22	D	608	AJP	C05

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Mol	Chain	Res	Type	Atom
22	D	608	AJP	C16
22	D	608	AJP	C15
22	D	608	AJP	C19
22	D	608	AJP	C23
22	D	608	AJP	C11
22	D	609	AJP	C12
22	D	609	AJP	C02
22	D	609	AJP	C22
22	D	609	AJP	C07
22	D	609	AJP	C20
22	D	609	AJP	C10
22	D	609	AJP	C05
22	D	609	AJP	C16
22	D	609	AJP	C15
22	D	609	AJP	C19
22	D	609	AJP	C23
22	D	609	AJP	C11
22	D	610	AJP	C12
22	D	610	AJP	C02
22	D	610	AJP	C22
22	D	610	AJP	C07
22	D	610	AJP	C20
22	D	610	AJP	C10
22	D	610	AJP	C05
22	D	610	AJP	C16
22	D	610	AJP	C15
22	D	610	AJP	C19
22	D	610	AJP	C23
22	D	610	AJP	C11
22	D	611	AJP	C12
22	D	611	AJP	C02
22	D	611	AJP	C22
22	D	611	AJP	C07
22	D	611	AJP	C20
22	D	611	AJP	C10
22	D	611	AJP	C05
22	D	611	AJP	C16
22	D	611	AJP	C15
22	D	611	AJP	C19
22	D	611	AJP	C23
22	D	611	AJP	C11
22	D	612	AJP	C12

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Mol	Chain	Res	Type	Atom
22	D	612	AJP	C02
22	D	612	AJP	C22
22	D	612	AJP	C07
22	D	612	AJP	C20
22	D	612	AJP	C10
22	D	612	AJP	C05
22	D	612	AJP	C16
22	D	612	AJP	C15
22	D	612	AJP	C19
22	D	612	AJP	C23
22	D	612	AJP	C11
22	D	613	AJP	C12
22	D	613	AJP	C02
22	D	613	AJP	C22
22	D	613	AJP	C07
22	D	613	AJP	C20
22	D	613	AJP	C10
22	D	613	AJP	C05
22	D	613	AJP	C16
22	D	613	AJP	C15
22	D	613	AJP	C19
22	D	613	AJP	C23
22	D	613	AJP	C11
22	D	614	AJP	C12
22	D	614	AJP	C02
22	D	614	AJP	C22
22	D	614	AJP	C07
22	D	614	AJP	C20
22	D	614	AJP	C10
22	D	614	AJP	C05
22	D	614	AJP	C16
22	D	614	AJP	C15
22	D	614	AJP	C19
22	D	614	AJP	C23
22	D	614	AJP	C11
22	D	615	AJP	C12
22	D	615	AJP	C02
22	D	615	AJP	C22
22	D	615	AJP	C07
22	D	615	AJP	C20
22	D	615	AJP	C10
22	D	615	AJP	C05

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Mol	Chain	Res	Type	Atom
22	D	615	AJP	C16
22	D	615	AJP	C15
22	D	615	AJP	C19
22	D	615	AJP	C23
22	D	615	AJP	C11
22	D	616	AJP	C12
22	D	616	AJP	C02
22	D	616	AJP	C22
22	D	616	AJP	C07
22	D	616	AJP	C20
22	D	616	AJP	C10
22	D	616	AJP	C05
22	D	616	AJP	C16
22	D	616	AJP	C15
22	D	616	AJP	C19
22	D	616	AJP	C23
22	D	616	AJP	C11
22	F	704	AJP	C12
22	F	704	AJP	C02
22	F	704	AJP	C22
22	F	704	AJP	C07
22	F	704	AJP	C20
22	F	704	AJP	C10
22	F	704	AJP	C05
22	F	704	AJP	C16
22	F	704	AJP	C15
22	F	704	AJP	C19
22	F	704	AJP	C23
22	F	704	AJP	C11
22	F	705	AJP	C12
22	F	705	AJP	C02
22	F	705	AJP	C22
22	F	705	AJP	C07
22	F	705	AJP	C20
22	F	705	AJP	C10
22	F	705	AJP	C05
22	F	705	AJP	C16
22	F	705	AJP	C15
22	F	705	AJP	C19
22	F	705	AJP	C23
22	F	705	AJP	C11
22	F	706	AJP	C12

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Mol	Chain	Res	Type	Atom
22	F	706	AJP	C02
22	F	706	AJP	C22
22	F	706	AJP	C07
22	F	706	AJP	C20
22	F	706	AJP	C10
22	F	706	AJP	C05
22	F	706	AJP	C16
22	F	706	AJP	C15
22	F	706	AJP	C19
22	F	706	AJP	C23
22	F	706	AJP	C11
22	F	707	AJP	C12
22	F	707	AJP	C02
22	F	707	AJP	C22
22	F	707	AJP	C07
22	F	707	AJP	C20
22	F	707	AJP	C10
22	F	707	AJP	C05
22	F	707	AJP	C16
22	F	707	AJP	C15
22	F	707	AJP	C19
22	F	707	AJP	C23
22	F	707	AJP	C11
22	F	708	AJP	C12
22	F	708	AJP	C02
22	F	708	AJP	C22
22	F	708	AJP	C07
22	F	708	AJP	C20
22	F	708	AJP	C10
22	F	708	AJP	C05
22	F	708	AJP	C16
22	F	708	AJP	C15
22	F	708	AJP	C19
22	F	708	AJP	C23
22	F	708	AJP	C11
22	F	709	AJP	C12
22	F	709	AJP	C02
22	F	709	AJP	C22
22	F	709	AJP	C07
22	F	709	AJP	C20
22	F	709	AJP	C10
22	F	709	AJP	C05

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Mol	Chain	Res	Type	Atom
22	F	709	AJP	C16
22	F	709	AJP	C15
22	F	709	AJP	C19
22	F	709	AJP	C23
22	F	709	AJP	C11
22	F	710	AJP	C12
22	F	710	AJP	C02
22	F	710	AJP	C22
22	F	710	AJP	C07
22	F	710	AJP	C20
22	F	710	AJP	C10
22	F	710	AJP	C05
22	F	710	AJP	C16
22	F	710	AJP	C15
22	F	710	AJP	C19
22	F	710	AJP	C23
22	F	710	AJP	C11
22	F	711	AJP	C12
22	F	711	AJP	C02
22	F	711	AJP	C22
22	F	711	AJP	C07
22	F	711	AJP	C20
22	F	711	AJP	C10
22	F	711	AJP	C05
22	F	711	AJP	C16
22	F	711	AJP	C15
22	F	711	AJP	C19
22	F	711	AJP	C23
22	F	711	AJP	C11
22	F	712	AJP	C12
22	F	712	AJP	C02
22	F	712	AJP	C22
22	F	712	AJP	C07
22	F	712	AJP	C20
22	F	712	AJP	C10
22	F	712	AJP	C05
22	F	712	AJP	C16
22	F	712	AJP	C15
22	F	712	AJP	C19
22	F	712	AJP	C23
22	F	712	AJP	C11
22	G	302	AJP	C12

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Mol	Chain	Res	Type	Atom
22	G	302	AJP	C02
22	G	302	AJP	C22
22	G	302	AJP	C07
22	G	302	AJP	C20
22	G	302	AJP	C10
22	G	302	AJP	C05
22	G	302	AJP	C16
22	G	302	AJP	C15
22	G	302	AJP	C19
22	G	302	AJP	C23
22	G	302	AJP	C11
22	G	303	AJP	C12
22	G	303	AJP	C02
22	G	303	AJP	C22
22	G	303	AJP	C07
22	G	303	AJP	C20
22	G	303	AJP	C10
22	G	303	AJP	C05
22	G	303	AJP	C16
22	G	303	AJP	C15
22	G	303	AJP	C19
22	G	303	AJP	C23
22	G	303	AJP	C11
22	G	304	AJP	C12
22	G	304	AJP	C02
22	G	304	AJP	C22
22	G	304	AJP	C07
22	G	304	AJP	C20
22	G	304	AJP	C10
22	G	304	AJP	C05
22	G	304	AJP	C16
22	G	304	AJP	C15
22	G	304	AJP	C19
22	G	304	AJP	C23
22	G	304	AJP	C11
22	G	305	AJP	C12
22	G	305	AJP	C02
22	G	305	AJP	C22
22	G	305	AJP	C07
22	G	305	AJP	C20
22	G	305	AJP	C10
22	G	305	AJP	C05

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Mol	Chain	Res	Type	Atom
22	G	305	AJP	C16
22	G	305	AJP	C15
22	G	305	AJP	C19
22	G	305	AJP	C23
22	G	305	AJP	C11
22	G	306	AJP	C12
22	G	306	AJP	C02
22	G	306	AJP	C22
22	G	306	AJP	C07
22	G	306	AJP	C20
22	G	306	AJP	C10
22	G	306	AJP	C05
22	G	306	AJP	C16
22	G	306	AJP	C15
22	G	306	AJP	C19
22	G	306	AJP	C23
22	G	306	AJP	C11
22	G	307	AJP	C12
22	G	307	AJP	C02
22	G	307	AJP	C22
22	G	307	AJP	C07
22	G	307	AJP	C20
22	G	307	AJP	C10
22	G	307	AJP	C05
22	G	307	AJP	C16
22	G	307	AJP	C15
22	G	307	AJP	C19
22	G	307	AJP	C23
22	G	307	AJP	C11
22	Q	101	AJP	C12
22	Q	101	AJP	C02
22	Q	101	AJP	C22
22	Q	101	AJP	C07
22	Q	101	AJP	C20
22	Q	101	AJP	C10
22	Q	101	AJP	C05
22	Q	101	AJP	C16
22	Q	101	AJP	C15
22	Q	101	AJP	C19
22	Q	101	AJP	C23
22	Q	101	AJP	C11
22	Q	102	AJP	C12

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Mol	Chain	Res	Type	Atom
22	Q	102	AJP	C02
22	Q	102	AJP	C22
22	Q	102	AJP	C07
22	Q	102	AJP	C20
22	Q	102	AJP	C10
22	Q	102	AJP	C05
22	Q	102	AJP	C16
22	Q	102	AJP	C15
22	Q	102	AJP	C19
22	Q	102	AJP	C23
22	Q	102	AJP	C11
22	Q	103	AJP	C12
22	Q	103	AJP	C02
22	Q	103	AJP	C22
22	Q	103	AJP	C07
22	Q	103	AJP	C20
22	Q	103	AJP	C10
22	Q	103	AJP	C05
22	Q	103	AJP	C16
22	Q	103	AJP	C15
22	Q	103	AJP	C19
22	Q	103	AJP	C23
22	Q	103	AJP	C11

All (389) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	401	BCR	C1-C6-C7-C8
19	A	401	BCR	C5-C6-C7-C8
19	A	401	BCR	C10-C11-C12-C13
19	A	401	BCR	C11-C12-C13-C14
19	A	401	BCR	C11-C12-C13-C35
19	A	401	BCR	C16-C17-C18-C19
19	A	401	BCR	C16-C17-C18-C36
19	A	401	BCR	C18-C19-C20-C21
19	A	401	BCR	C20-C21-C22-C37
19	A	401	BCR	C21-C22-C23-C24
19	A	401	BCR	C37-C22-C23-C24
19	A	401	BCR	C22-C23-C24-C25
19	D	601	BCR	C7-C8-C9-C10
19	D	601	BCR	C9-C10-C11-C12
19	D	601	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
19	D	601	BCR	C12-C13-C14-C15
19	D	601	BCR	C35-C13-C14-C15
19	D	601	BCR	C14-C15-C16-C17
19	D	601	BCR	C15-C16-C17-C18
19	D	601	BCR	C18-C19-C20-C21
19	D	601	BCR	C20-C21-C22-C23
19	D	601	BCR	C20-C21-C22-C37
19	D	601	BCR	C22-C23-C24-C25
19	D	601	BCR	C23-C24-C25-C26
19	D	602	BCR	C1-C6-C7-C8
19	D	602	BCR	C5-C6-C7-C8
19	D	602	BCR	C6-C7-C8-C9
19	D	602	BCR	C7-C8-C9-C10
19	D	602	BCR	C7-C8-C9-C34
19	D	602	BCR	C10-C11-C12-C13
19	D	602	BCR	C12-C13-C14-C15
19	D	602	BCR	C35-C13-C14-C15
19	D	602	BCR	C14-C15-C16-C17
19	D	602	BCR	C18-C19-C20-C21
19	D	602	BCR	C23-C24-C25-C26
19	D	602	BCR	C23-C24-C25-C30
20	A	402	LHG	O1-C1-C2-C3
20	A	402	LHG	C3-O3-P-O4
20	A	403	LHG	C3-O3-P-O5
20	A	403	LHG	C3-O3-P-O6
20	B	602	LHG	O1-C1-C2-C3
20	B	602	LHG	C3-O3-P-O4
20	B	602	LHG	O9-C7-O7-C5
20	B	602	LHG	C8-C7-O7-C5
20	B	603	LHG	C4-O6-P-O4
20	B	603	LHG	C5-C4-O6-P
20	B	603	LHG	O9-C7-O7-C5
20	B	603	LHG	C8-C7-O7-C5
20	D	603	LHG	C1-C2-C3-O3
20	D	603	LHG	C3-O3-P-O4
20	D	603	LHG	C4-O6-P-O5
20	D	604	LHG	C3-O3-P-O5
20	D	604	LHG	C4-O6-P-O4
20	D	604	LHG	C8-C7-O7-C5
20	F	701	LHG	C4-O6-P-O5
20	G	301	LHG	O1-C1-C2-C3
20	G	301	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
20	G	301	LHG	C4-O6-P-O3
20	G	301	LHG	O7-C5-C6-O8
24	D	605	SQD	C8-C7-O47-C45
24	D	605	SQD	C5-C6-S-O7
24	D	606	SQD	O5-C1-O6-C44
24	D	606	SQD	O6-C44-C45-O47
24	F	703	SQD	C2-C1-O6-C44
24	F	703	SQD	O5-C1-O6-C44
24	F	703	SQD	C5-C6-S-O7
24	F	703	SQD	C5-C6-S-O8
24	F	703	SQD	C5-C6-S-O9
24	L	101	SQD	O49-C7-O47-C45
24	L	101	SQD	O5-C5-C6-S
20	D	604	LHG	O10-C23-O8-C6
20	D	603	LHG	C24-C23-O8-C6
20	F	701	LHG	C24-C23-O8-C6
20	F	702	LHG	C24-C23-O8-C6
24	D	605	SQD	C24-C23-O48-C46
20	A	402	LHG	O10-C23-O8-C6
20	B	602	LHG	O10-C23-O8-C6
20	B	603	LHG	O10-C23-O8-C6
20	D	603	LHG	O10-C23-O8-C6
20	F	701	LHG	O10-C23-O8-C6
20	F	702	LHG	O10-C23-O8-C6
24	D	605	SQD	O10-C23-O48-C46
24	F	703	SQD	O10-C23-O48-C46
24	L	101	SQD	O10-C23-O48-C46
20	A	402	LHG	O9-C7-O7-C5
20	D	604	LHG	O9-C7-O7-C5
20	F	701	LHG	O9-C7-O7-C5
20	F	702	LHG	O9-C7-O7-C5
24	D	605	SQD	O49-C7-O47-C45
20	A	402	LHG	C24-C23-O8-C6
20	B	602	LHG	C24-C23-O8-C6
24	F	703	SQD	C24-C23-O48-C46
24	L	101	SQD	C24-C23-O48-C46
24	L	101	SQD	C8-C7-O47-C45
20	B	603	LHG	C24-C23-O8-C6
20	D	604	LHG	C24-C23-O8-C6
23	B	601	PQN	C11-C12-C13-C14
19	A	401	BCR	C13-C14-C15-C16
19	A	401	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
20	D	603	LHG	O2-C2-C3-O3
20	D	603	LHG	C8-C7-O7-C5
20	A	402	LHG	C2-C3-O3-P
20	A	403	LHG	C2-C3-O3-P
20	B	602	LHG	C2-C3-O3-P
20	G	301	LHG	C29-C30-C31-C32
20	A	403	LHG	C29-C30-C31-C32
20	A	403	LHG	C24-C23-O8-C6
19	D	601	BCR	C13-C14-C15-C16
19	D	602	BCR	C15-C16-C17-C18
19	D	602	BCR	C19-C20-C21-C22
21	A	404	DGD	C2D-C1D-O3G-C3G
19	A	401	BCR	C36-C18-C19-C20
19	D	601	BCR	C37-C22-C23-C24
19	D	602	BCR	C37-C22-C23-C24
19	D	601	BCR	C21-C22-C23-C24
19	D	602	BCR	C21-C22-C23-C24
20	B	603	LHG	C23-C24-C25-C26
20	D	604	LHG	C23-C24-C25-C26
20	B	602	LHG	C23-C24-C25-C26
20	D	603	LHG	C23-C24-C25-C26
20	F	701	LHG	C7-C8-C9-C10
24	L	101	SQD	C23-C24-C25-C26
23	B	601	PQN	C23-C25-C26-C27
20	F	702	LHG	C23-C24-C25-C26
20	G	301	LHG	C23-C24-C25-C26
20	A	403	LHG	O10-C23-O8-C6
19	D	602	BCR	C13-C14-C15-C16
20	F	701	LHG	C23-C24-C25-C26
21	A	404	DGD	C1B-C2B-C3B-C4B
20	A	402	LHG	C3-O3-P-O6
20	B	602	LHG	C3-O3-P-O6
20	B	603	LHG	C3-O3-P-O6
20	B	603	LHG	C4-O6-P-O3
20	D	603	LHG	C3-O3-P-O6
20	D	604	LHG	C4-O6-P-O3
20	F	701	LHG	C4-O6-P-O3
24	F	703	SQD	O49-C7-O47-C45
20	B	603	LHG	C32-C33-C34-C35
20	A	402	LHG	C8-C7-O7-C5
20	F	701	LHG	C8-C7-O7-C5
20	F	702	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
19	A	401	BCR	C11-C10-C9-C34
21	A	404	DGD	C6A-C7A-C8A-C9A
20	A	402	LHG	C28-C29-C30-C31
20	B	602	LHG	C32-C33-C34-C35
20	F	701	LHG	C27-C28-C29-C30
21	A	404	DGD	C4A-C5A-C6A-C7A
21	A	405	DGD	C4A-C5A-C6A-C7A
24	D	606	SQD	C27-C28-C29-C30
20	B	603	LHG	C4-C5-O7-C7
20	A	403	LHG	C33-C34-C35-C36
20	G	301	LHG	C28-C29-C30-C31
24	F	703	SQD	C9-C10-C11-C12
20	F	702	LHG	C24-C25-C26-C27
19	A	401	BCR	C11-C10-C9-C8
19	A	401	BCR	C20-C21-C22-C23
20	A	403	LHG	C32-C33-C34-C35
20	B	602	LHG	C27-C28-C29-C30
21	A	404	DGD	CEB-CFB-CGB-CHB
23	B	601	PQN	C26-C27-C28-C30
24	D	606	SQD	C12-C13-C14-C15
20	A	402	LHG	C31-C32-C33-C34
20	A	402	LHG	C32-C33-C34-C35
20	A	403	LHG	C28-C29-C30-C31
20	D	604	LHG	C28-C29-C30-C31
20	F	701	LHG	C17-C18-C19-C20
20	G	301	LHG	C32-C33-C34-C35
21	A	404	DGD	C4B-C5B-C6B-C7B
19	D	601	BCR	C7-C8-C9-C34
20	B	602	LHG	C26-C27-C28-C29
20	D	603	LHG	C32-C33-C34-C35
20	D	604	LHG	C30-C31-C32-C33
20	F	701	LHG	C12-C13-C14-C15
20	F	702	LHG	C27-C28-C29-C30
20	A	403	LHG	O1-C1-C2-C3
20	D	603	LHG	O1-C1-C2-C3
20	D	604	LHG	O1-C1-C2-C3
19	D	601	BCR	C11-C12-C13-C14
21	A	405	DGD	O1B-C1B-O2G-C2G
20	G	301	LHG	C24-C25-C26-C27
20	B	602	LHG	C24-C25-C26-C27
20	F	701	LHG	C15-C16-C17-C18
20	F	701	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	D	606	SQD	C28-C29-C30-C31
20	D	604	LHG	C27-C28-C29-C30
21	A	405	DGD	C5A-C6A-C7A-C8A
24	F	703	SQD	C12-C13-C14-C15
20	A	402	LHG	C30-C31-C32-C33
24	D	605	SQD	C9-C10-C11-C12
20	F	702	LHG	C7-C8-C9-C10
20	F	702	LHG	C32-C33-C34-C35
20	D	603	LHG	C29-C30-C31-C32
20	D	604	LHG	C11-C10-C9-C8
21	A	405	DGD	C7B-C8B-C9B-CAB
23	B	601	PQN	C26-C27-C28-C29
20	F	701	LHG	C32-C33-C34-C35
20	A	403	LHG	C27-C28-C29-C30
20	A	402	LHG	O1-C1-C2-O2
20	B	602	LHG	O1-C1-C2-O2
20	G	301	LHG	O1-C1-C2-O2
21	A	405	DGD	C5B-C6B-C7B-C8B
20	F	702	LHG	O2-C2-C3-O3
19	D	601	BCR	C23-C24-C25-C30
21	A	404	DGD	C6B-C7B-C8B-C9B
21	A	404	DGD	C7B-C8B-C9B-CAB
24	F	703	SQD	C8-C7-O47-C45
20	D	603	LHG	O9-C7-O7-C5
20	B	602	LHG	C12-C13-C14-C15
20	D	603	LHG	C28-C29-C30-C31
21	A	404	DGD	C5B-C6B-C7B-C8B
20	D	603	LHG	C11-C10-C9-C8
20	G	301	LHG	C8-C7-O7-C5
21	A	404	DGD	C2B-C1B-O2G-C2G
20	B	602	LHG	O2-C2-C3-O3
24	D	605	SQD	C2-C1-O6-C44
20	A	403	LHG	C11-C12-C13-C14
20	B	602	LHG	C7-C8-C9-C10
20	A	402	LHG	C24-C25-C26-C27
21	A	405	DGD	C6B-C7B-C8B-C9B
21	A	405	DGD	CEB-CFB-CGB-CHB
24	D	605	SQD	C11-C12-C13-C14
24	D	605	SQD	C12-C13-C14-C15
20	D	603	LHG	C4-O6-P-O3
24	L	101	SQD	C9-C10-C11-C12
24	L	101	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	A	405	DGD	C2B-C1B-O2G-C2G
20	D	604	LHG	C4-C5-C6-O8
20	F	702	LHG	C4-C5-C6-O8
24	D	606	SQD	O6-C44-C45-C46
21	A	405	DGD	O6E-C5E-C6E-O5E
20	B	603	LHG	C11-C10-C9-C8
20	D	604	LHG	O1-C1-C2-O2
20	A	403	LHG	C24-C25-C26-C27
20	G	301	LHG	C14-C15-C16-C17
19	D	601	BCR	C11-C10-C9-C34
19	D	601	BCR	C16-C17-C18-C36
20	B	603	LHG	C28-C29-C30-C31
20	A	402	LHG	C6-C5-O7-C7
20	F	701	LHG	C6-C5-O7-C7
20	F	702	LHG	C6-C5-O7-C7
20	G	301	LHG	C27-C28-C29-C30
24	D	606	SQD	C9-C10-C11-C12
21	A	405	DGD	CCA-CDA-CEA-CFA
19	D	601	BCR	C11-C10-C9-C8
24	D	606	SQD	C26-C27-C28-C29
20	G	301	LHG	C12-C13-C14-C15
21	A	405	DGD	C8B-C9B-CAB-CBB
23	B	601	PQN	C21-C22-C23-C24
20	F	701	LHG	C30-C31-C32-C33
24	F	703	SQD	C25-C26-C27-C28
20	A	403	LHG	C30-C31-C32-C33
19	D	601	BCR	C6-C7-C8-C9
20	G	301	LHG	C30-C31-C32-C33
24	L	101	SQD	C12-C13-C14-C15
20	B	603	LHG	C27-C28-C29-C30
24	L	101	SQD	C28-C29-C30-C31
20	D	603	LHG	C2-C3-O3-P
20	F	701	LHG	C29-C30-C31-C32
20	A	403	LHG	C11-C10-C9-C8
20	F	701	LHG	C10-C11-C12-C13
20	A	402	LHG	C4-C5-C6-O8
20	G	301	LHG	C4-C5-C6-O8
24	D	605	SQD	O6-C44-C45-C46
24	D	605	SQD	C44-C45-C46-O48
24	F	703	SQD	O6-C44-C45-C46
24	L	101	SQD	O6-C44-C45-C46
21	A	405	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
20	D	604	LHG	C32-C33-C34-C35
20	D	603	LHG	O1-C1-C2-O2
20	F	702	LHG	C29-C30-C31-C32
21	A	405	DGD	C8A-C9A-CAA-CBA
20	B	602	LHG	O6-C4-C5-O7
20	A	402	LHG	O7-C5-C6-O8
21	A	404	DGD	O1G-C1G-C2G-O2G
24	D	606	SQD	O47-C45-C46-O48
20	B	602	LHG	C1-C2-C3-O3
20	G	301	LHG	C11-C10-C9-C8
24	F	703	SQD	C10-C11-C12-C13
20	F	701	LHG	C11-C12-C13-C14
20	F	701	LHG	C5-C4-O6-P
20	F	702	LHG	C11-C10-C9-C8
19	A	401	BCR	C17-C18-C19-C20
24	D	605	SQD	C14-C15-C16-C17
23	B	601	PQN	C21-C22-C23-C25
20	D	603	LHG	C30-C31-C32-C33
19	A	401	BCR	C9-C10-C11-C12
24	F	703	SQD	C14-C15-C16-C17
24	F	703	SQD	C44-C45-O47-C7
20	G	301	LHG	O9-C7-O7-C5
20	B	603	LHG	C4-C5-C6-O8
21	A	404	DGD	O1G-C1G-C2G-C3G
20	F	701	LHG	C11-C10-C9-C8
19	D	601	BCR	C16-C17-C18-C19
20	D	604	LHG	O7-C5-C6-O8
20	F	702	LHG	O7-C5-C6-O8
24	D	605	SQD	O47-C45-C46-O48
24	L	101	SQD	C4-C5-C6-S
19	A	401	BCR	C15-C16-C17-C18
20	B	602	LHG	C4-O6-P-O3
21	A	405	DGD	C3B-C4B-C5B-C6B
20	D	603	LHG	C27-C28-C29-C30
20	B	602	LHG	C4-O6-P-O4
20	B	603	LHG	C3-O3-P-O5
20	D	603	LHG	C4-O6-P-O4
20	F	701	LHG	C4-O6-P-O4
20	F	702	LHG	C3-O3-P-O4
20	G	301	LHG	C4-O6-P-O4
21	A	405	DGD	C9B-CAB-CBB-CCB
24	D	606	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	D	603	LHG	C33-C34-C35-C36
20	B	603	LHG	O7-C5-C6-O8
24	D	605	SQD	O6-C44-C45-O47
20	D	603	LHG	C10-C11-C12-C13
24	L	101	SQD	C45-C44-O6-C1
24	D	605	SQD	C17-C18-C19-C20
20	A	403	LHG	O1-C1-C2-O2
20	B	602	LHG	C33-C34-C35-C36
24	L	101	SQD	C17-C18-C19-C20
20	D	604	LHG	C1-C2-C3-O3
20	G	301	LHG	C33-C34-C35-C36
20	F	701	LHG	C13-C14-C15-C16
23	B	601	PQN	C25-C26-C27-C28
24	F	703	SQD	O6-C44-C45-O47
20	F	701	LHG	C3-O3-P-O6
20	F	702	LHG	C3-O3-P-O6
21	A	404	DGD	C2A-C3A-C4A-C5A
20	B	603	LHG	C13-C14-C15-C16
24	D	606	SQD	C44-C45-C46-O48
19	D	601	BCR	C19-C20-C21-C22
24	F	703	SQD	C17-C18-C19-C20
24	F	703	SQD	C11-C12-C13-C14
20	D	604	LHG	C2-C3-O3-P
20	D	604	LHG	C34-C35-C36-C37
24	D	606	SQD	C16-C17-C18-C19
20	F	702	LHG	O6-C4-C5-C6
20	B	602	LHG	C28-C29-C30-C31
20	F	702	LHG	C17-C18-C19-C20
24	F	703	SQD	C11-C10-C9-C8
20	F	701	LHG	C28-C29-C30-C31
20	F	702	LHG	C33-C34-C35-C36
21	A	404	DGD	C8A-C9A-CAA-CBA
20	A	402	LHG	C11-C10-C9-C8
21	A	405	DGD	C6A-C7A-C8A-C9A
20	D	604	LHG	C24-C25-C26-C27
20	B	603	LHG	C30-C31-C32-C33
19	A	401	BCR	C23-C24-C25-C30
19	D	601	BCR	C1-C6-C7-C8
19	D	602	BCR	C9-C10-C11-C12
24	D	605	SQD	C10-C11-C12-C13
24	D	606	SQD	C24-C25-C26-C27
20	F	702	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	F	703	SQD	C16-C17-C18-C19
20	B	602	LHG	C29-C30-C31-C32
21	A	404	DGD	CCB-CDB-CEB-CFB
20	B	603	LHG	C33-C34-C35-C36
20	G	301	LHG	O8-C23-C24-C25
21	A	404	DGD	O2G-C1B-C2B-C3B
20	D	603	LHG	C34-C35-C36-C37
24	D	605	SQD	O47-C7-C8-C9
20	A	402	LHG	C29-C30-C31-C32
23	B	601	PQN	C12-C13-C15-C16
20	B	602	LHG	O6-C4-C5-C6
23	B	601	PQN	C20-C21-C22-C23
21	A	404	DGD	O6D-C1D-O3G-C3G
21	A	405	DGD	C2B-C3B-C4B-C5B
20	A	402	LHG	O9-C7-C8-C9
24	D	605	SQD	C5-C6-S-O8
24	D	606	SQD	O47-C7-C8-C9
21	A	405	DGD	C4B-C5B-C6B-C7B
20	D	604	LHG	O10-C23-C24-C25
21	A	405	DGD	O1A-C1A-O1G-C1G
20	F	701	LHG	C3-O3-P-O5
20	G	301	LHG	O10-C23-C24-C25
19	A	401	BCR	C23-C24-C25-C26
19	D	601	BCR	C5-C6-C7-C8
24	L	101	SQD	O10-C23-C24-C25
20	D	604	LHG	O9-C7-C8-C9
24	D	606	SQD	C15-C16-C17-C18
24	D	606	SQD	C5-C6-S-O7
21	A	404	DGD	C9A-CAA-CBA-CCA
20	B	602	LHG	C10-C11-C12-C13
20	A	403	LHG	O8-C23-C24-C25
21	A	405	DGD	O2G-C1B-C2B-C3B
24	L	101	SQD	O48-C23-C24-C25
19	D	602	BCR	C17-C18-C19-C20
20	D	603	LHG	O10-C23-C24-C25
24	L	101	SQD	O49-C7-C8-C9
24	L	101	SQD	O47-C7-C8-C9
20	A	402	LHG	O7-C7-C8-C9

There are no ring outliers.

61 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	D	615	AJP	7	0
22	B	608	AJP	3	0
20	B	603	LHG	1	0
22	D	609	AJP	6	0
20	G	301	LHG	2	0
22	B	604	AJP	17	0
22	B	609	AJP	13	0
22	A	406	AJP	1	0
22	D	608	AJP	5	0
22	F	707	AJP	1	0
22	F	709	AJP	7	0
22	Q	103	AJP	1	0
22	G	306	AJP	10	0
24	D	606	SQD	2	0
22	B	606	AJP	4	0
22	D	607	AJP	10	0
22	D	614	AJP	9	0
22	B	610	AJP	6	0
22	Q	102	AJP	8	0
22	G	303	AJP	6	0
22	D	616	AJP	5	0
22	C	201	AJP	8	0
22	F	708	AJP	4	0
22	D	610	AJP	6	0
22	Q	101	AJP	2	0
23	B	601	PQN	1	0
25	I	202	SF4	2	0
22	F	710	AJP	6	0
22	D	612	AJP	4	0
24	L	101	SQD	1	0
24	D	605	SQD	8	0
22	C	202	AJP	21	0
25	K	301	SF4	3	0
22	G	305	AJP	5	0
22	B	607	AJP	4	0
22	G	307	AJP	5	0
22	A	407	AJP	7	0
22	F	711	AJP	2	0
22	B	614	AJP	20	0
22	D	613	AJP	7	0
22	F	712	AJP	7	0
22	G	302	AJP	4	0
20	B	602	LHG	1	0

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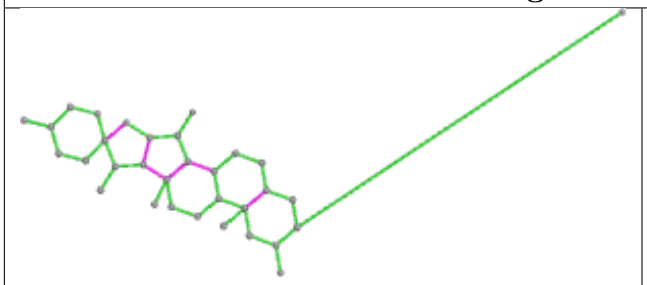
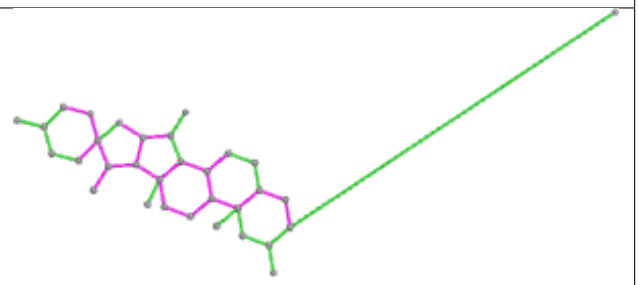
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	D	611	AJP	9	0
19	A	401	BCR	18	0
22	B	612	AJP	8	0
22	F	705	AJP	8	0
19	D	601	BCR	13	0
24	F	703	SQD	2	0
22	F	706	AJP	11	0
21	A	405	DGD	2	0
22	B	605	AJP	6	0
19	D	602	BCR	27	0
20	D	603	LHG	1	0
22	B	611	AJP	1	0
20	A	403	LHG	1	0
22	F	704	AJP	1	0
22	G	304	AJP	7	0
22	A	408	AJP	7	0
20	D	604	LHG	1	0
22	B	613	AJP	8	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.

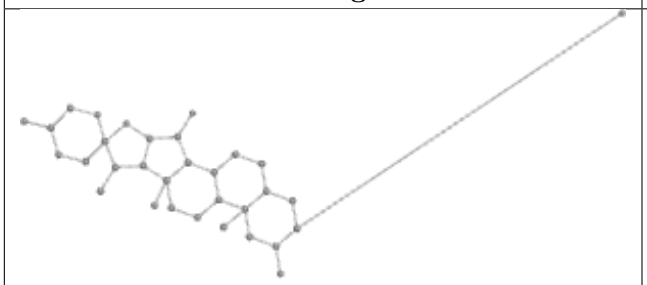
Ligand AJP D 615



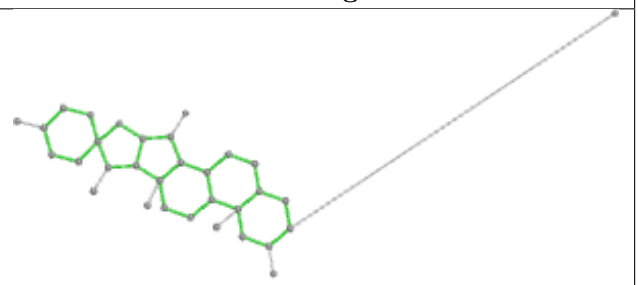
Bond lengths



Bond angles

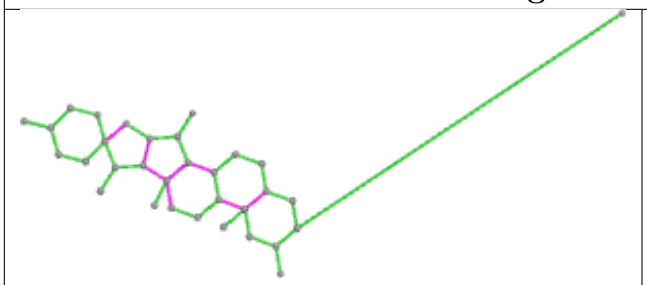


Torsions



Rings

Ligand AJP B 608



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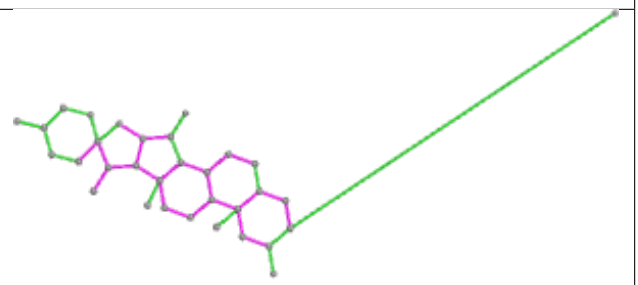
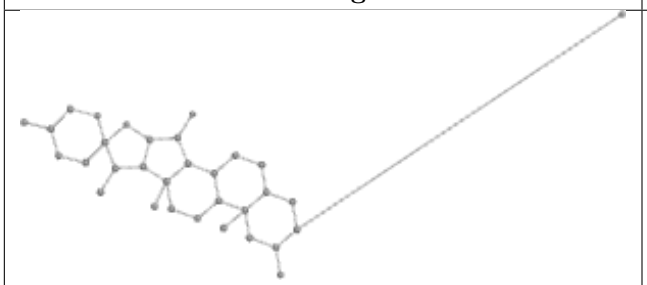
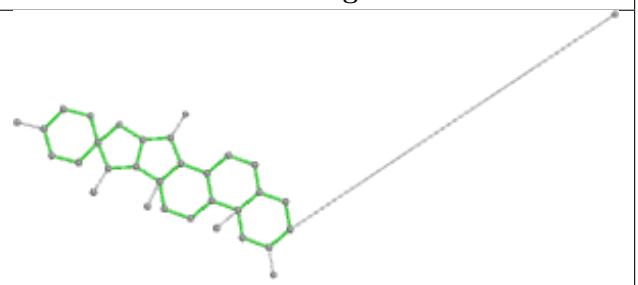


Bond angles

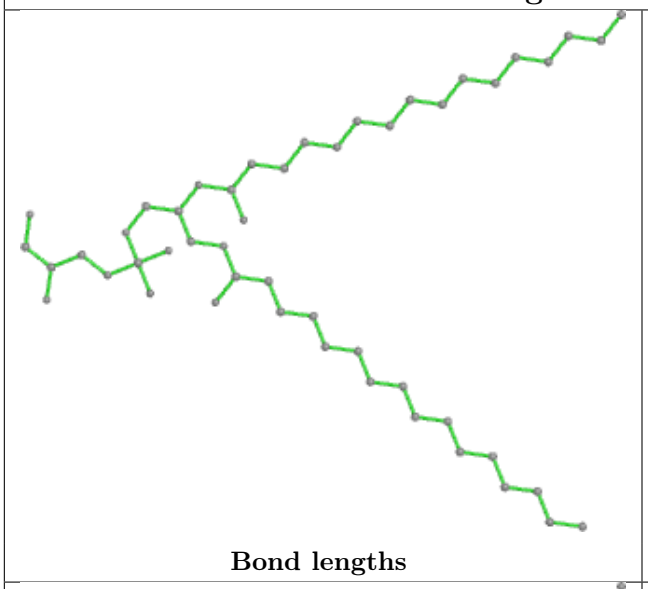


Torsions

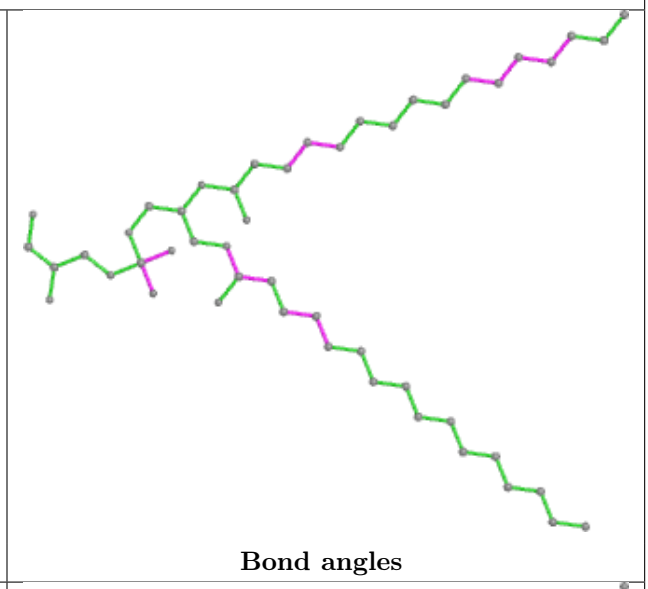


Rings

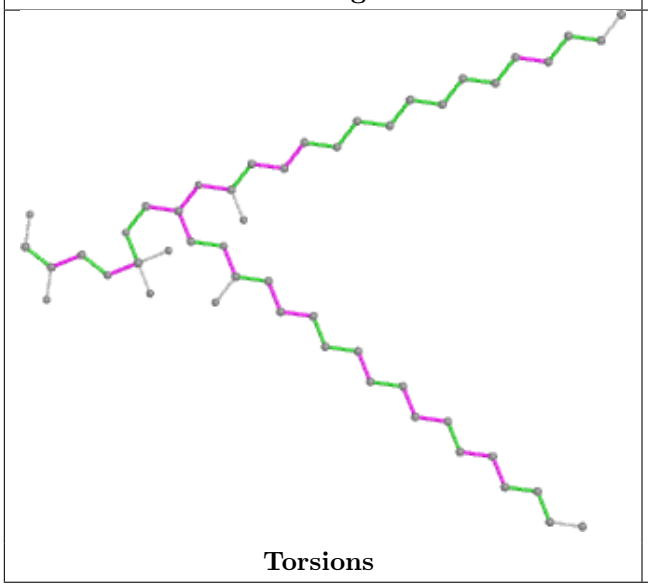
Ligand LHG F 702



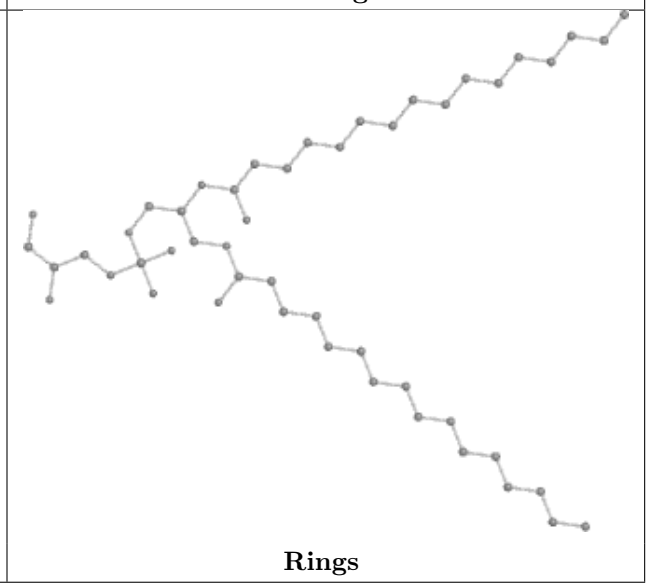
Bond lengths



Bond angles

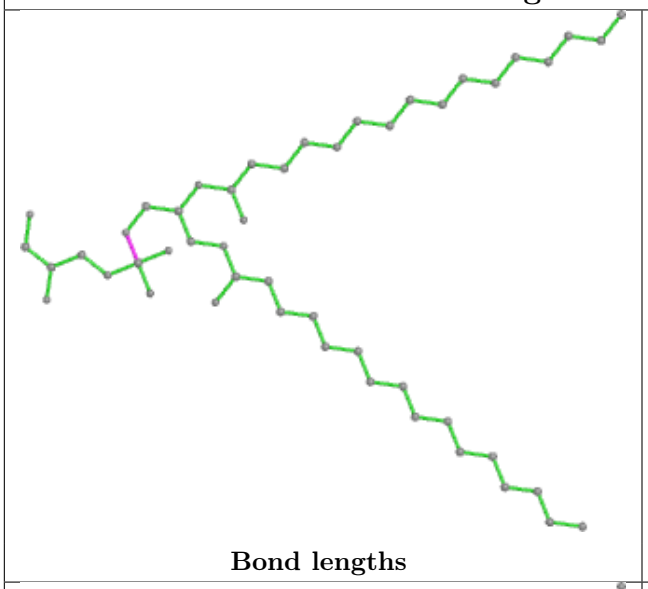


Torsions

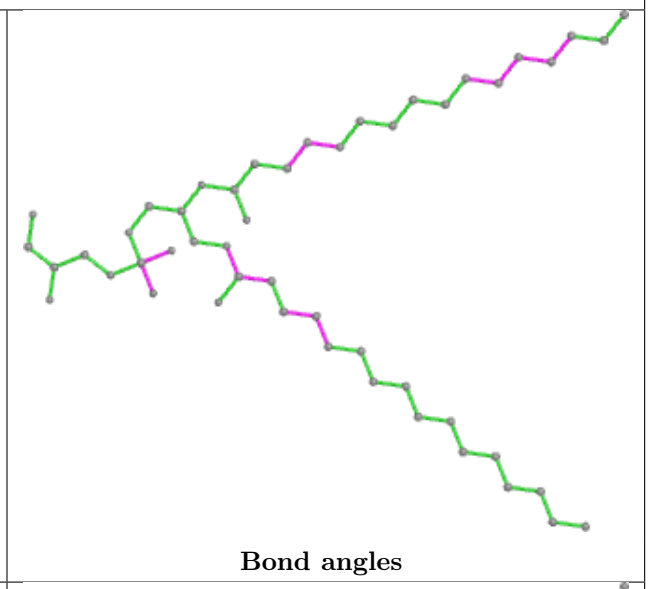


Rings

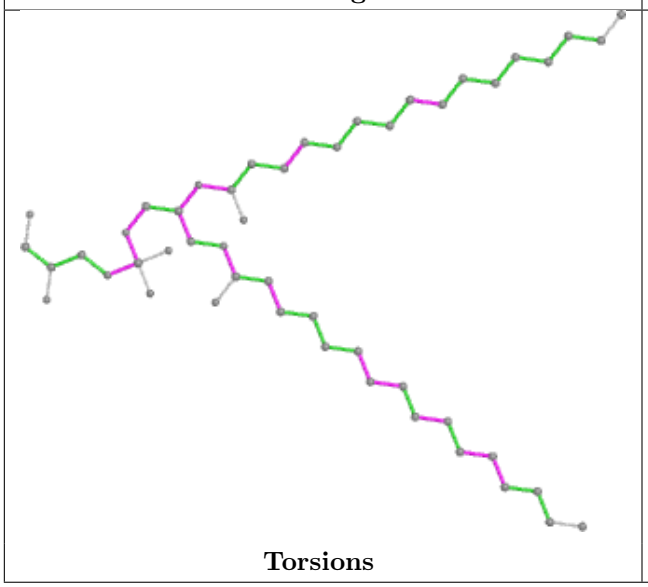
Ligand LHG B 603



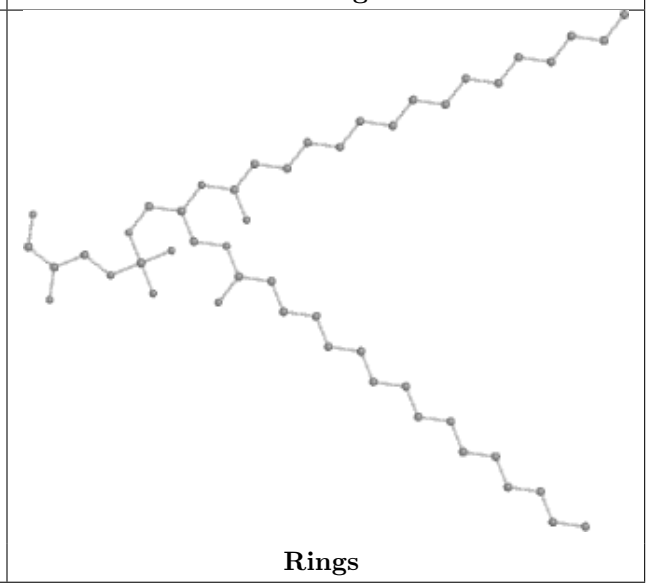
Bond lengths



Bond angles

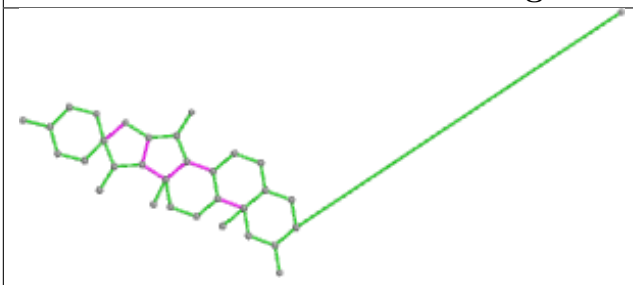


Torsions



Rings

Ligand AJP D 609



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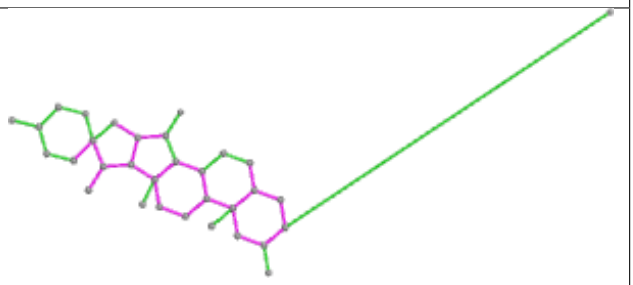
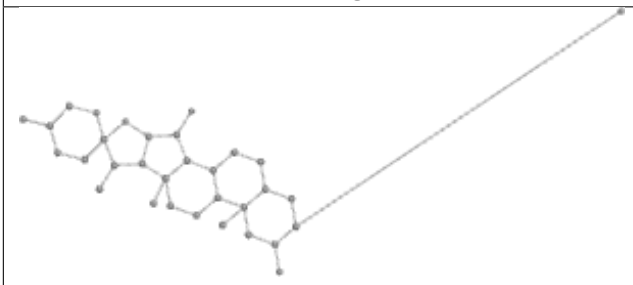


Bond angles



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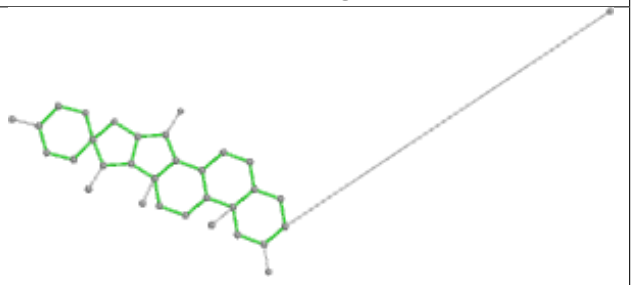
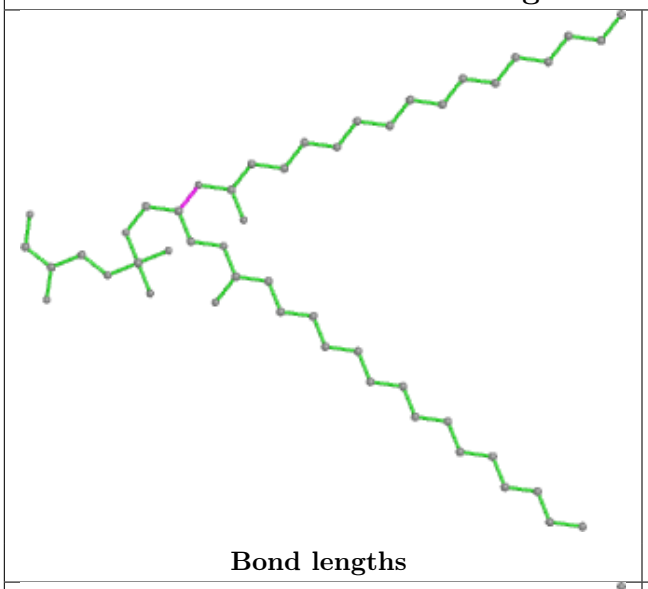


Rings

Ligand LHG G 301



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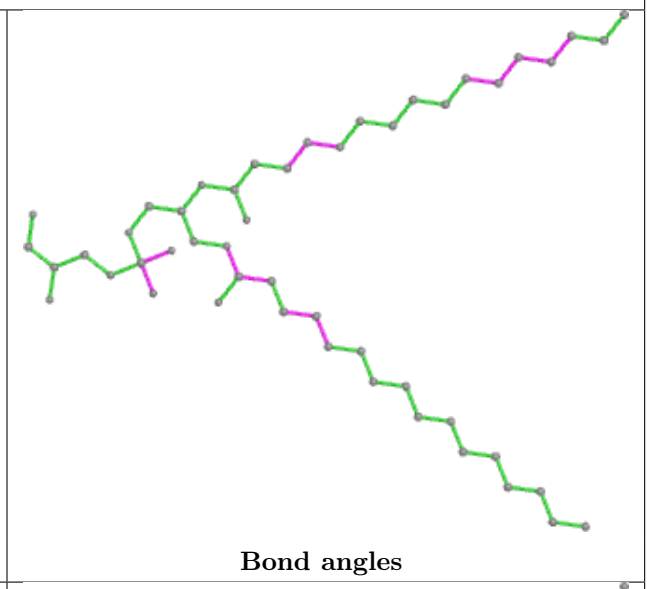
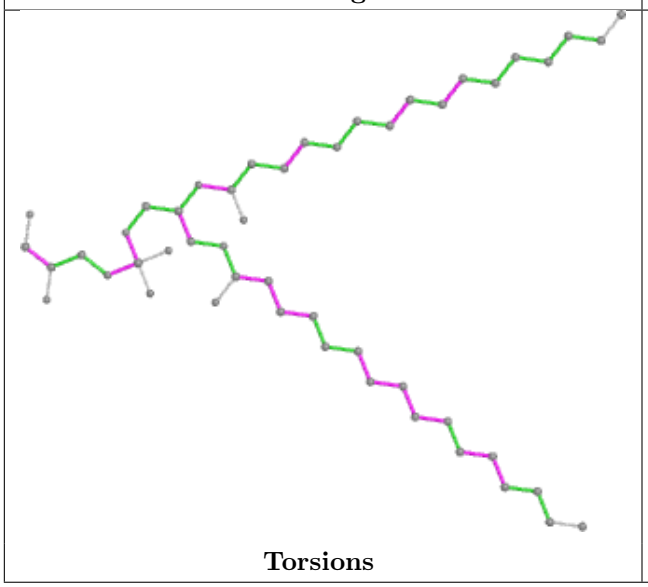
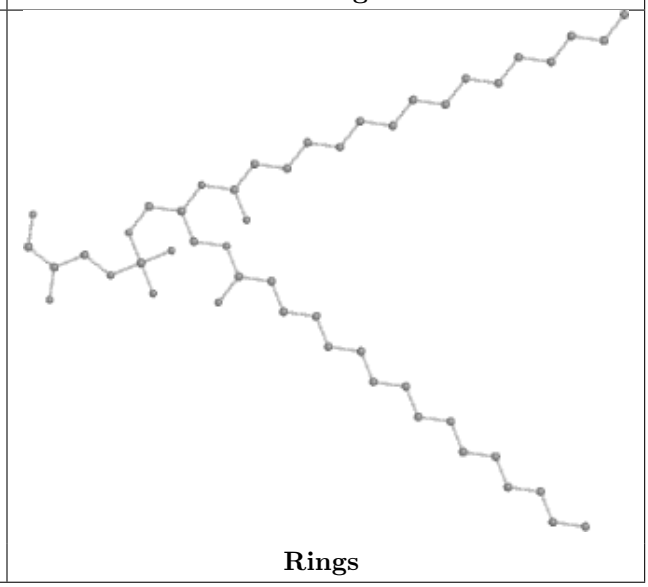


Bond angles

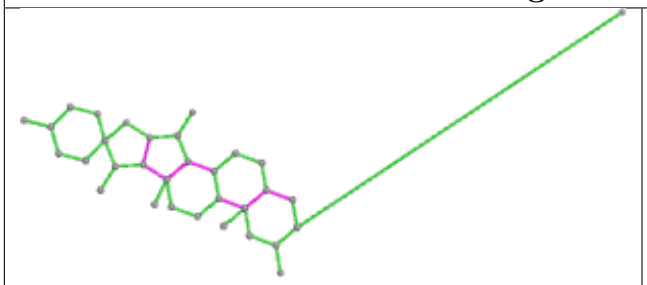


Torsions



Rings

Ligand AJP B 604



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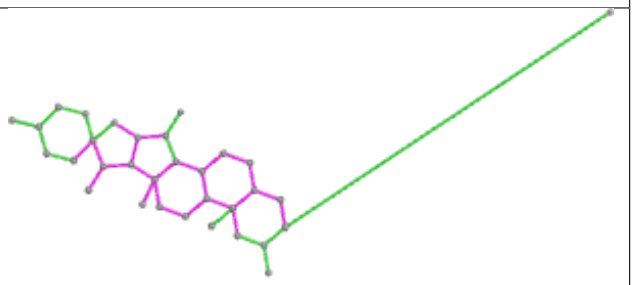
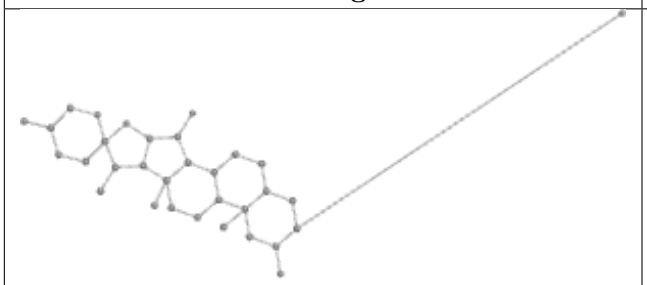


Bond angles



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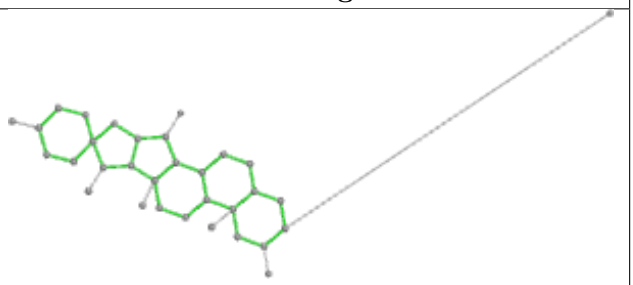
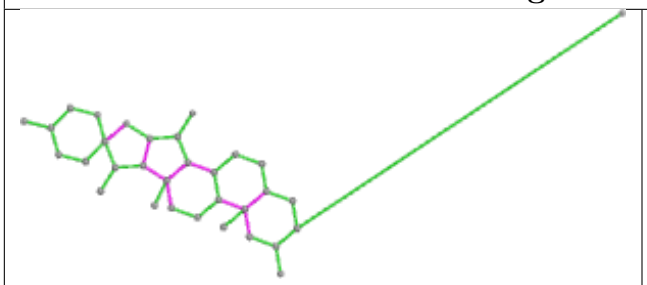


Rings

Ligand AJP B 609



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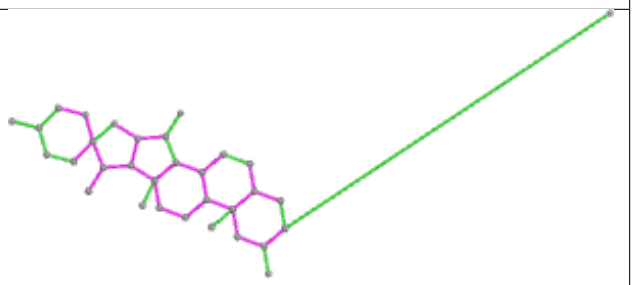
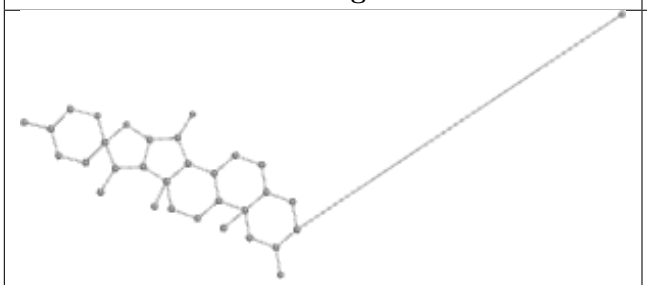
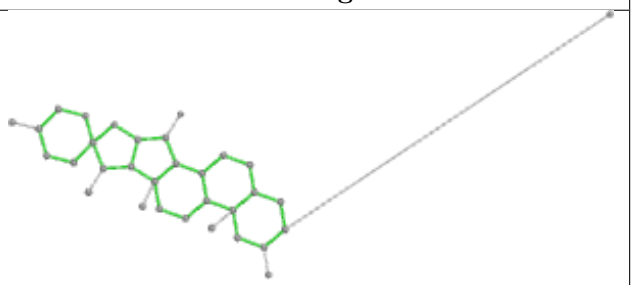


Bond angles

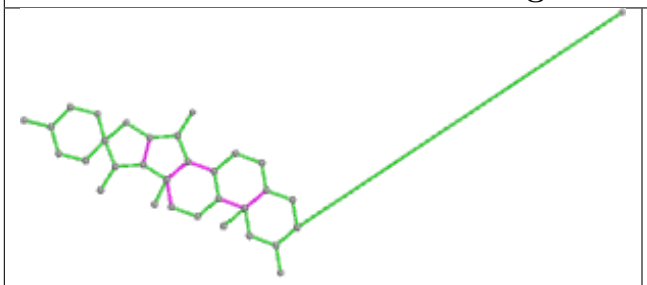


Torsions

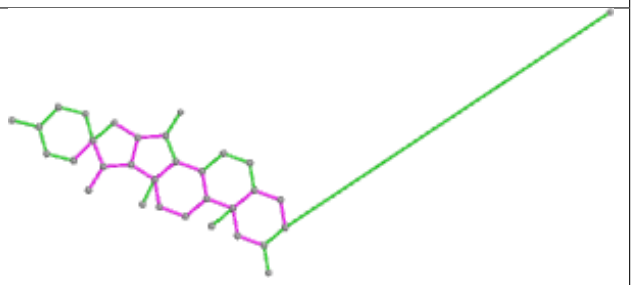


Rings

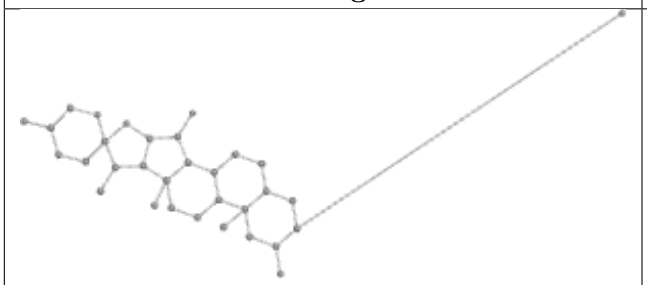
Ligand AJP A 406



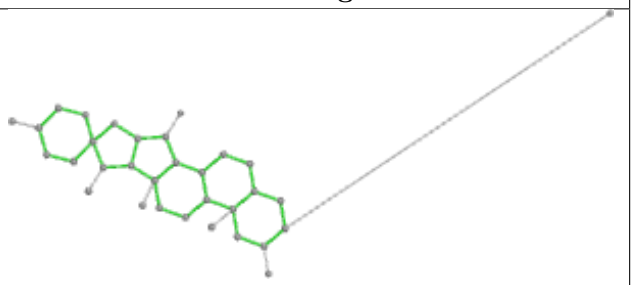
Bond lengths



Bond angles

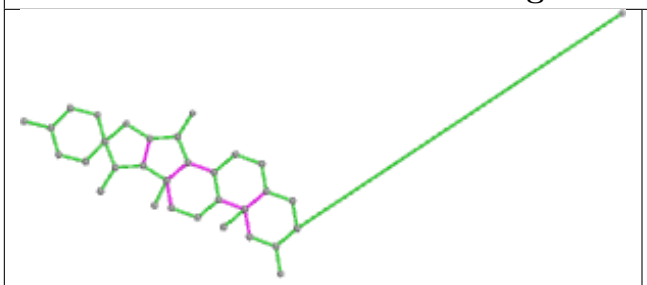


Torsions



Rings

Ligand AJP D 608



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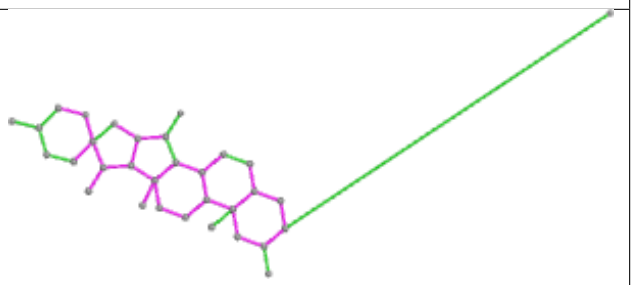
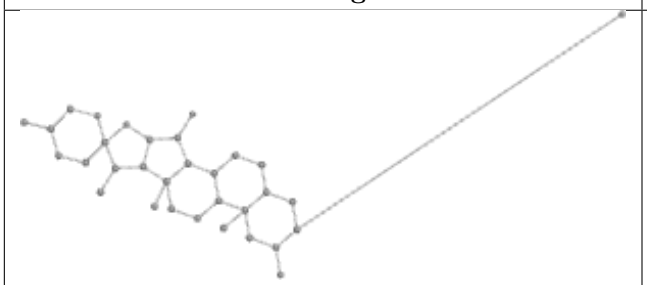
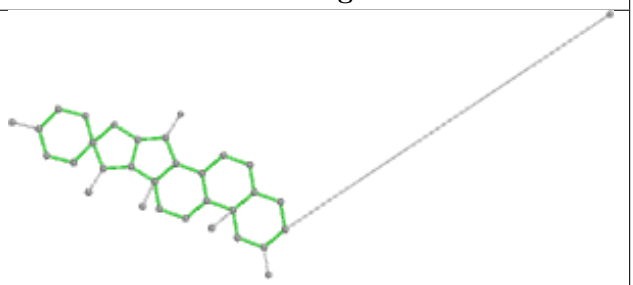


Bond angles

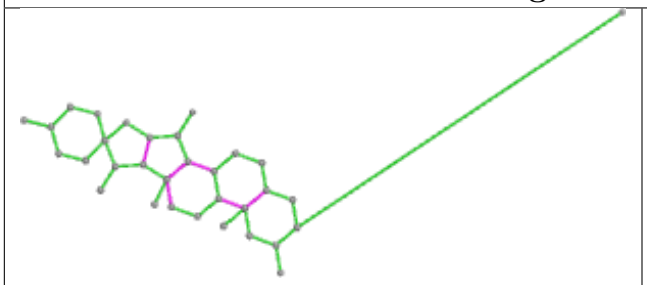


Torsions



Rings

Ligand AJP F 707



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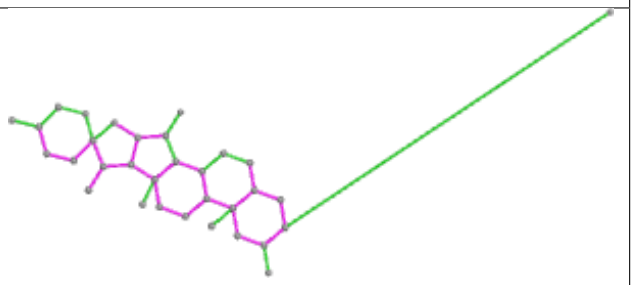
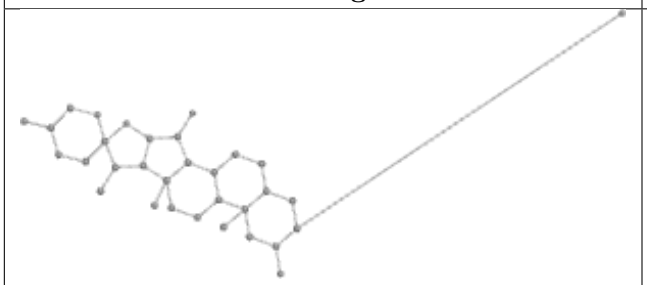


Bond angles



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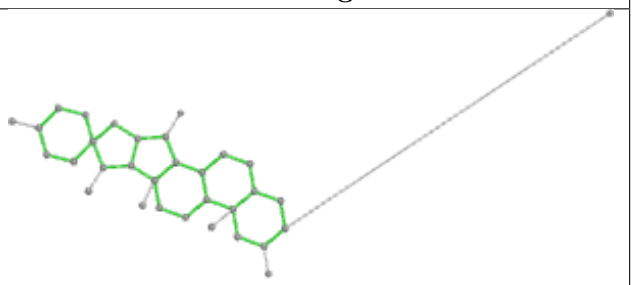
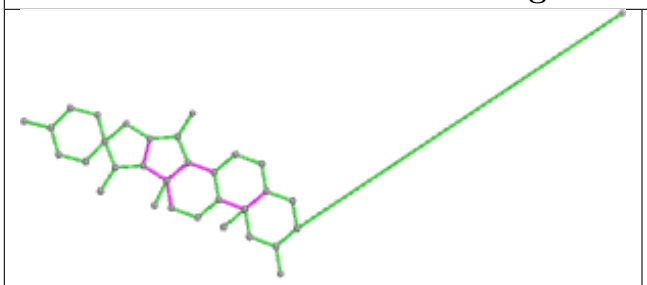


Rings

Ligand AJP F 709



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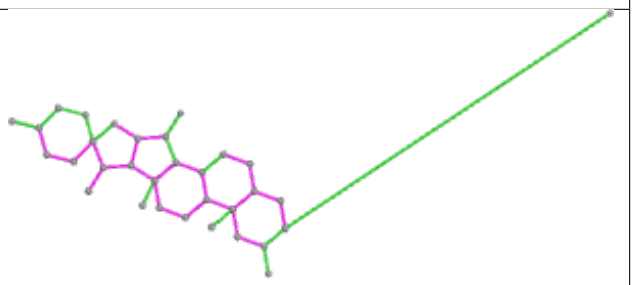
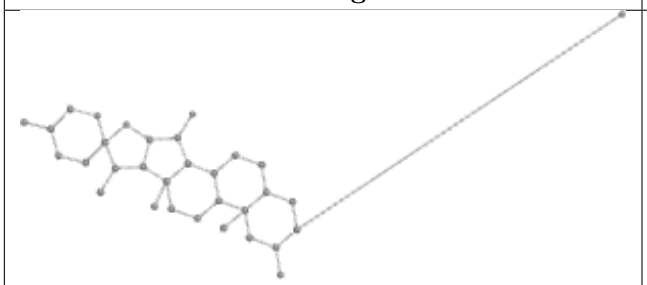
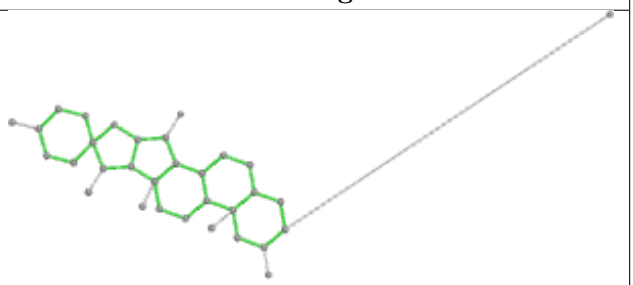


Bond angles

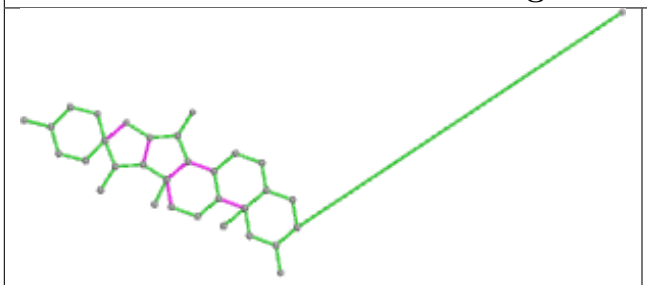


Torsions

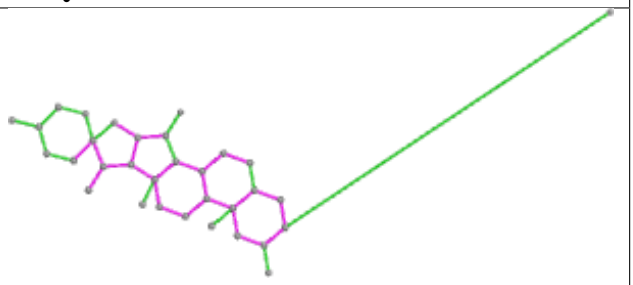


Rings

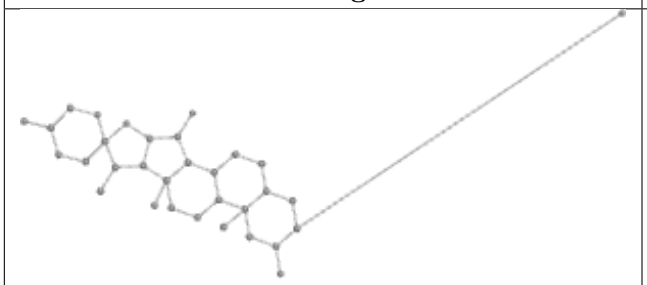
Ligand AJP Q 103



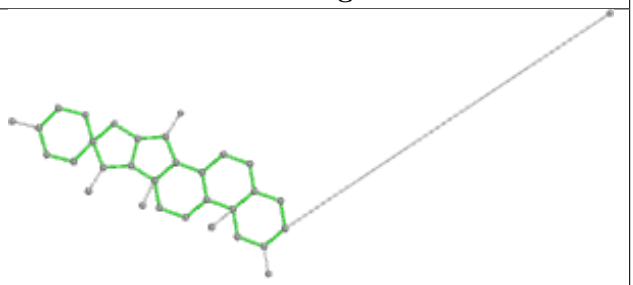
Bond lengths



Bond angles

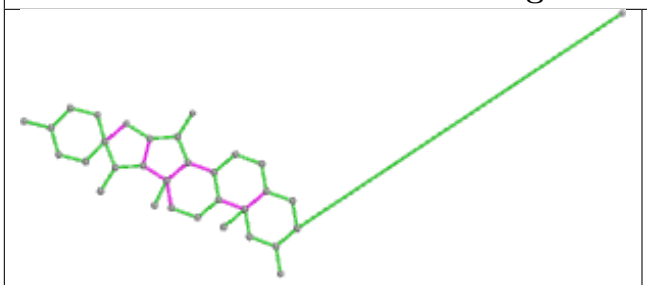


Torsions

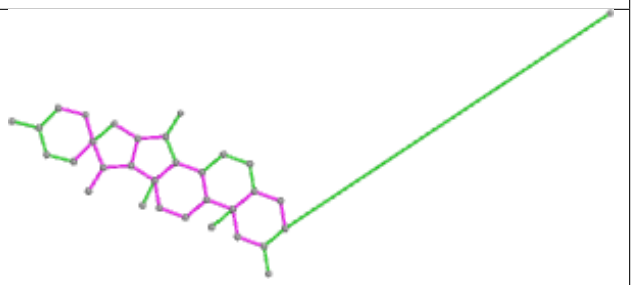


Rings

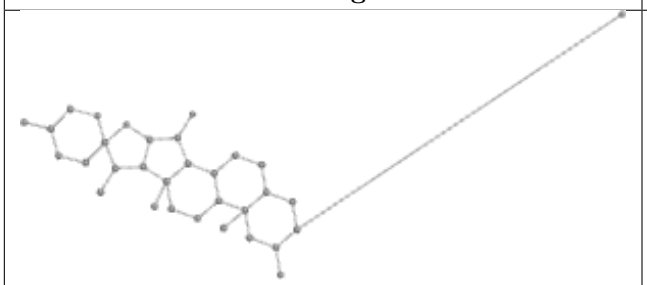
Ligand AJP G 306



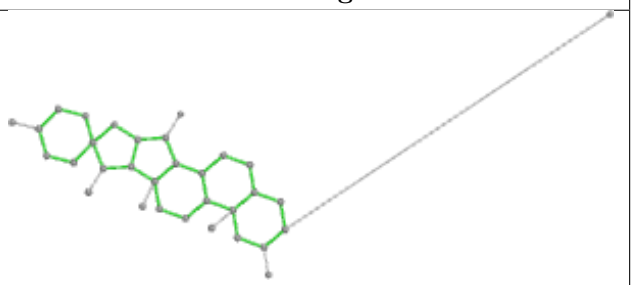
Bond lengths



Bond angles

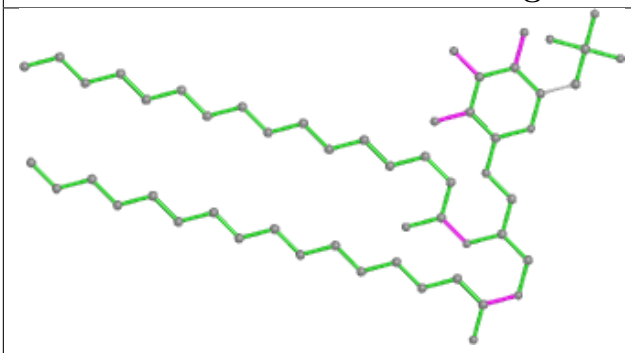


Torsions



Rings

Ligand SQD D 606



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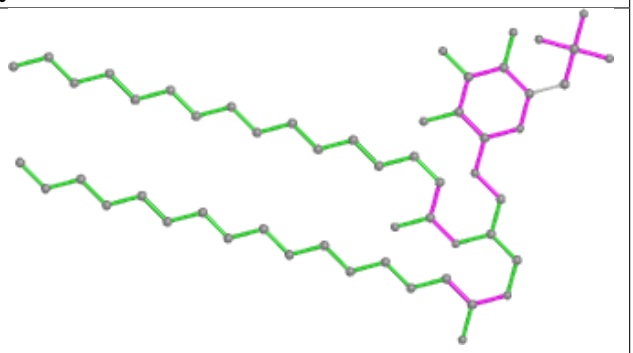
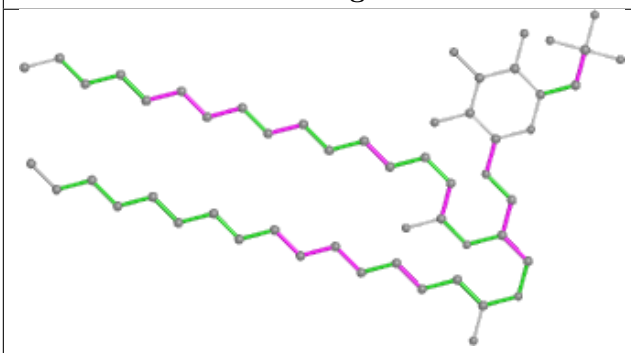
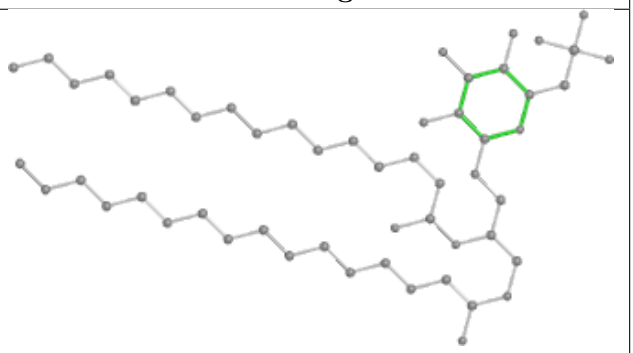


Bond angles

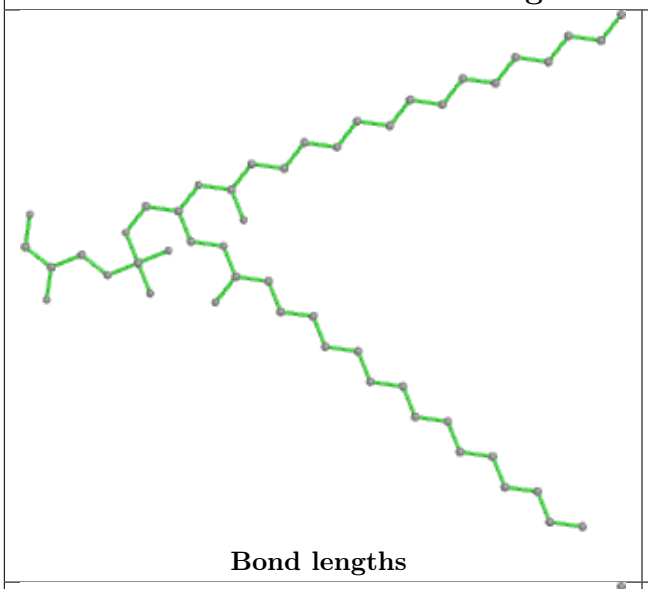


Torsions



Rings

Ligand LHG F 701



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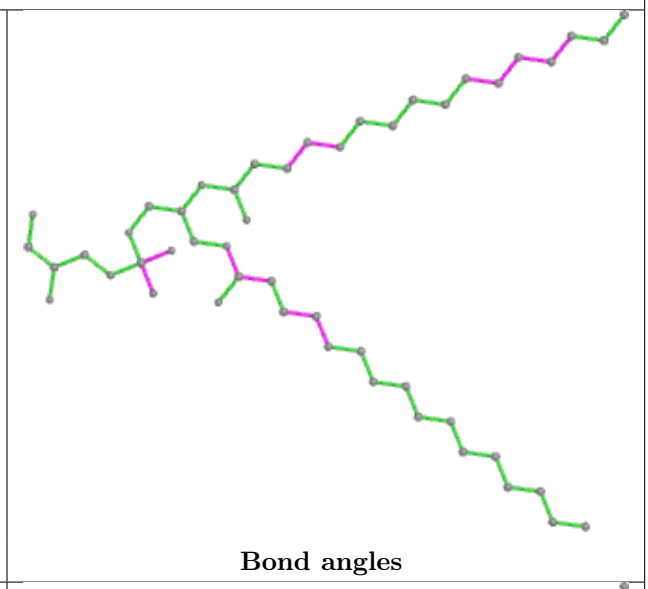
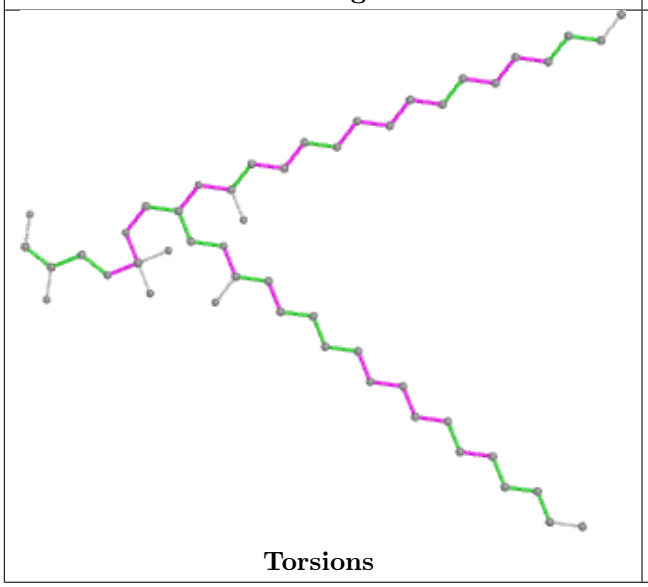
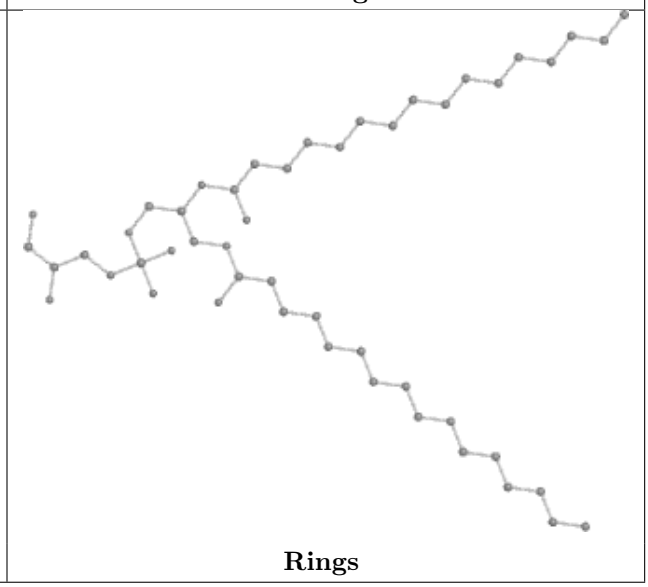


Bond angles

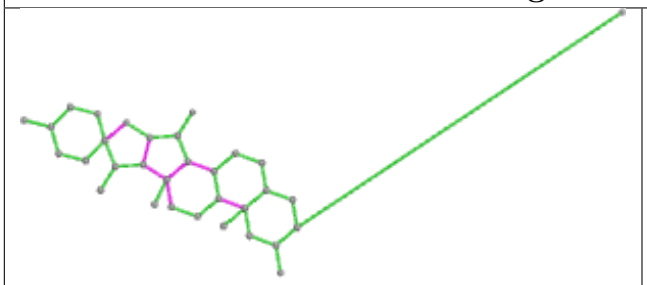


Torsions



Rings

Ligand AJP B 606



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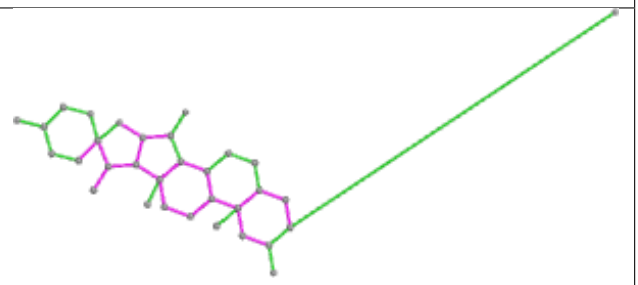
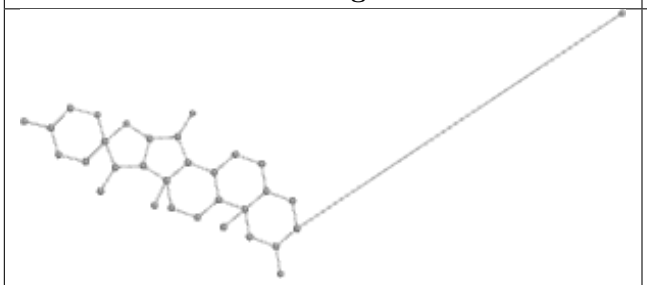
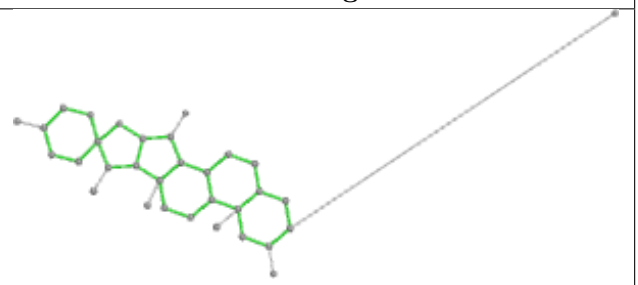


Bond angles

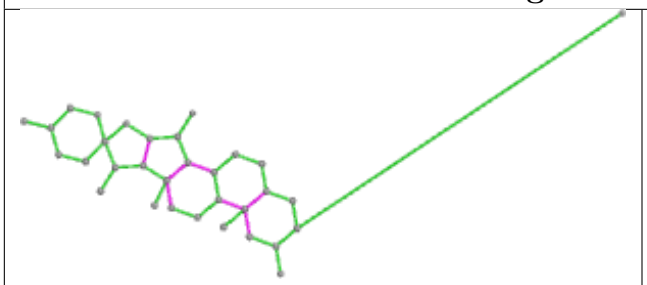


Torsions



Rings

Ligand AJP D 607



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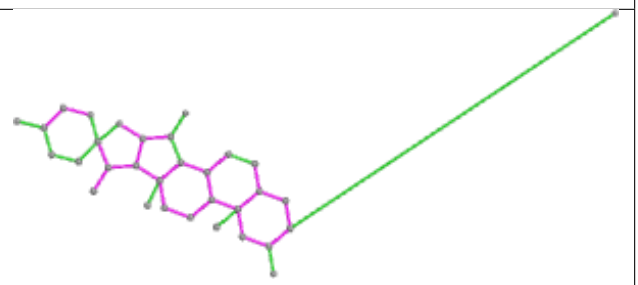
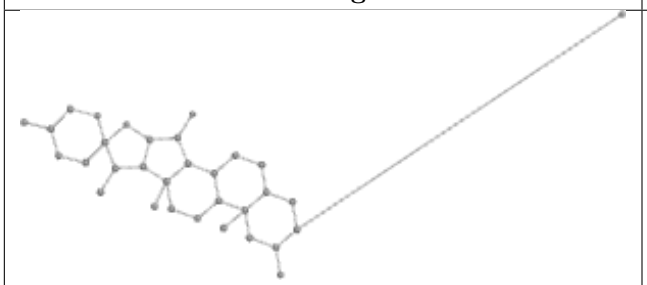
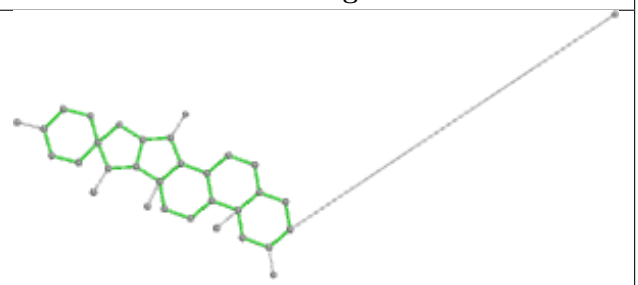


Bond angles

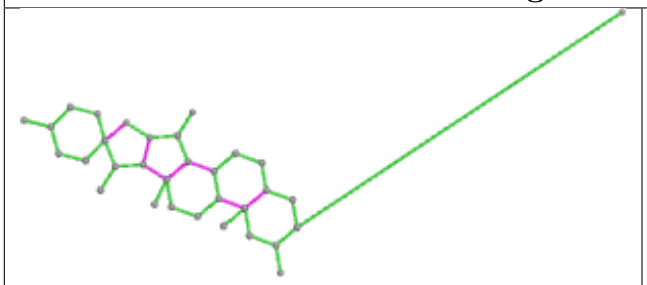


Torsions



Rings

Ligand AJP D 614



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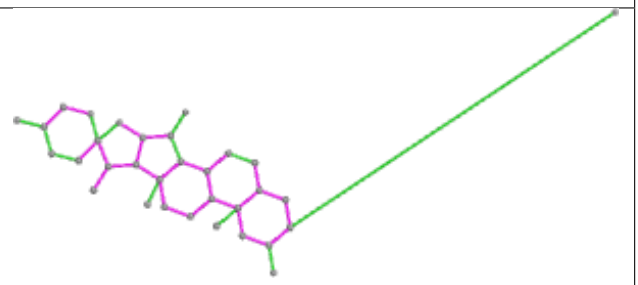
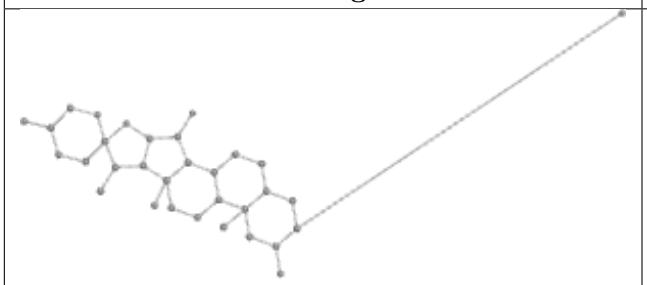
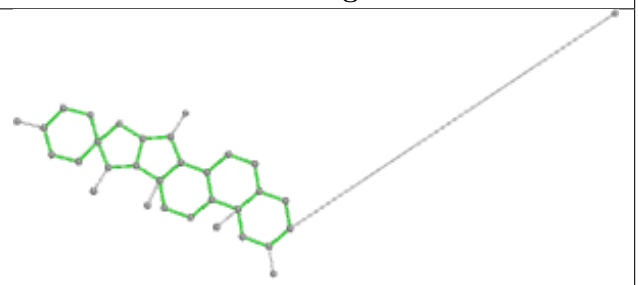


Bond angles

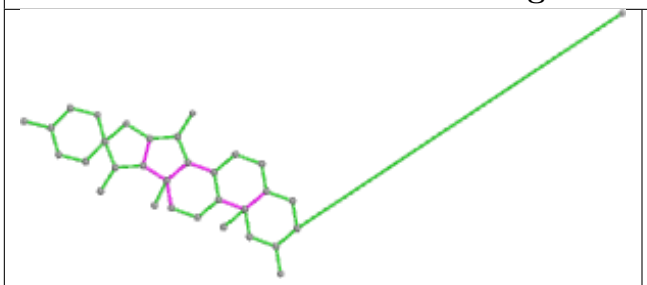


Torsions



Rings

Ligand AJP B 610



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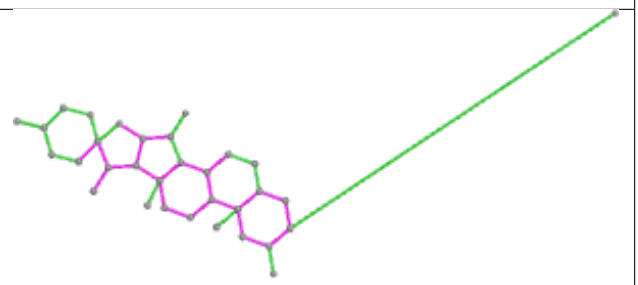
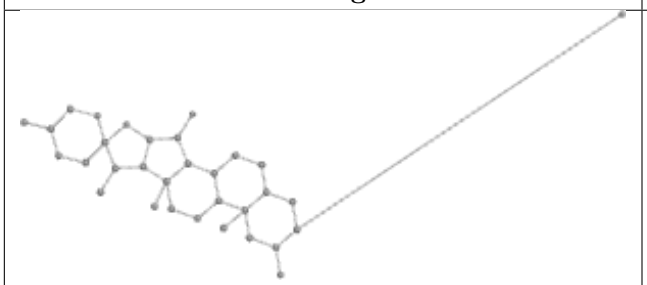
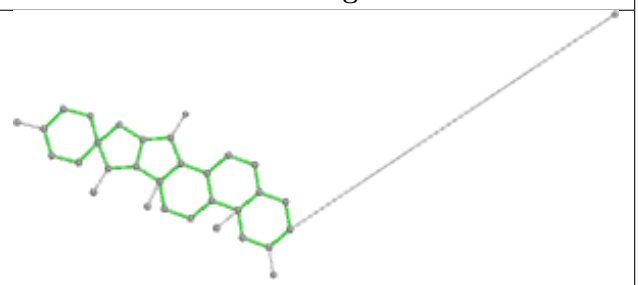


Bond angles

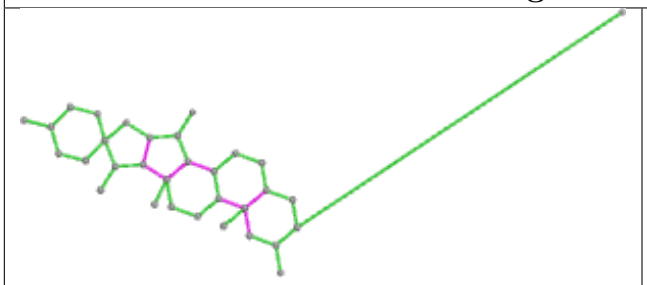


Torsions



Rings

Ligand AJP Q 102



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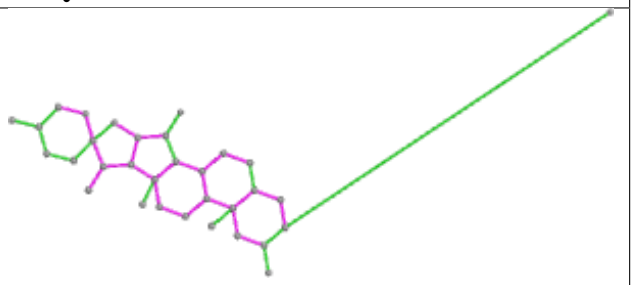
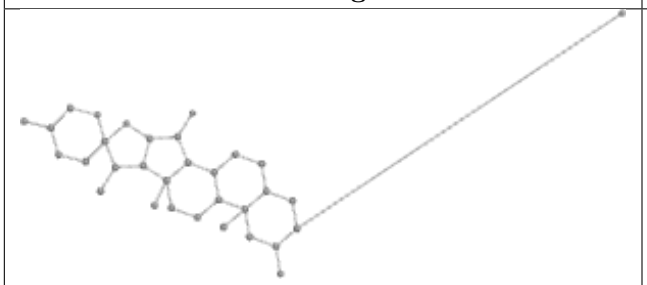
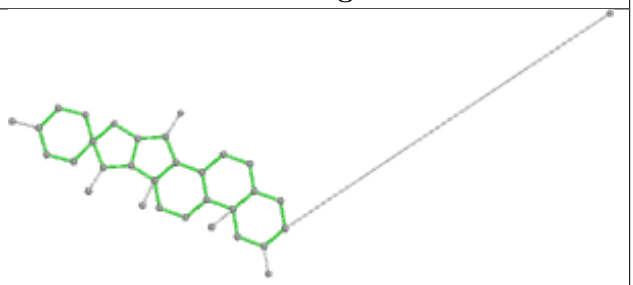


Bond angles

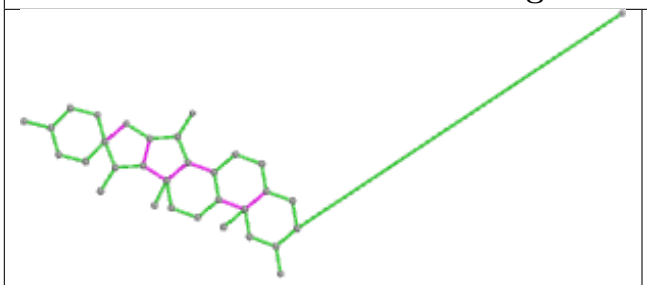


Torsions



Rings

Ligand AJP G 303



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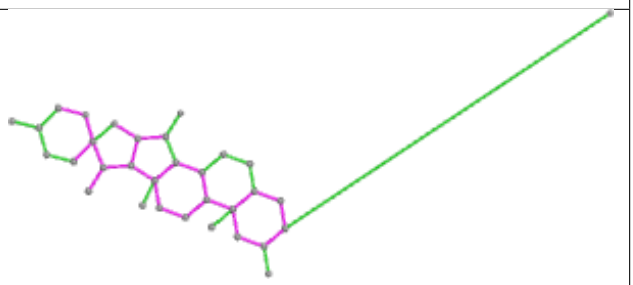
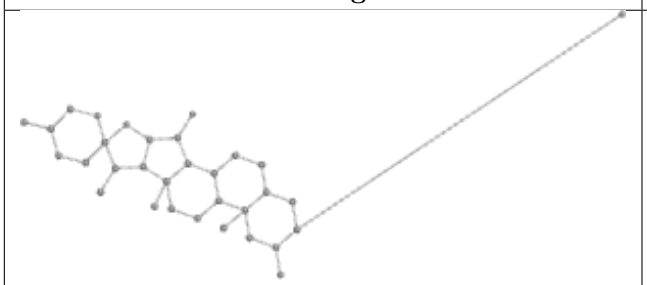
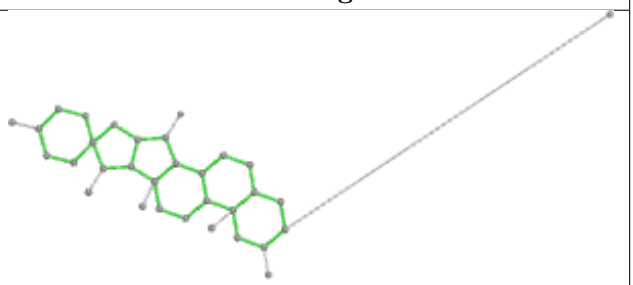


Bond angles

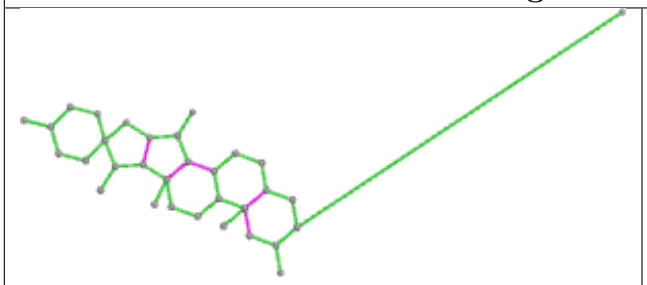


Torsions

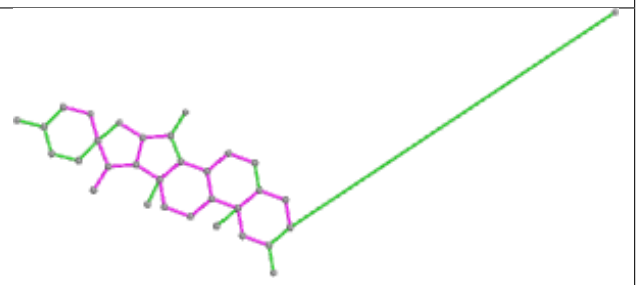


Rings

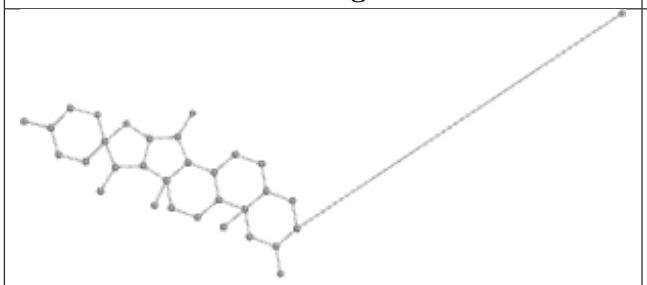
Ligand AJP D 616



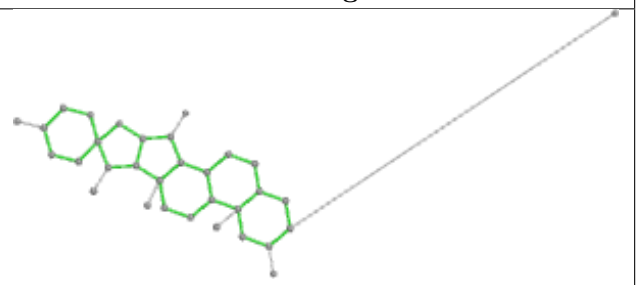
Bond lengths



Bond angles

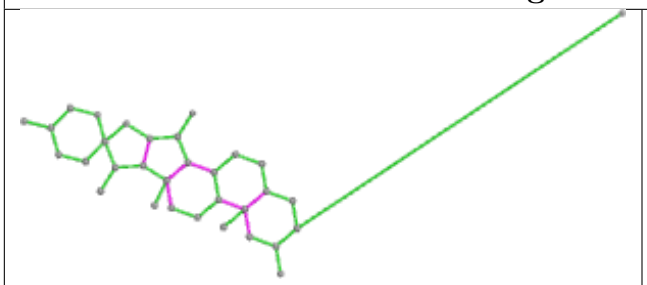


Torsions



Rings

Ligand AJP C 201



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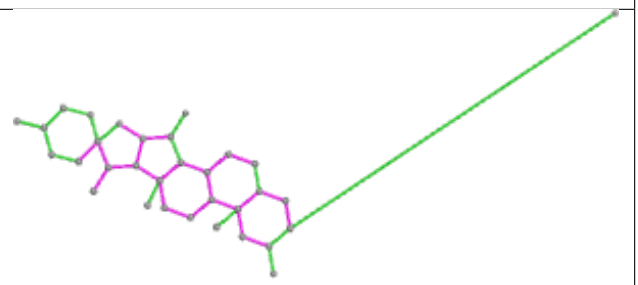
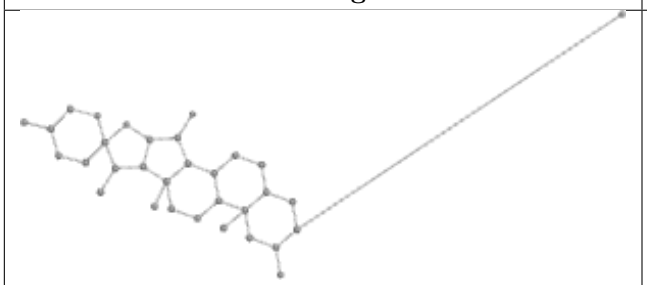
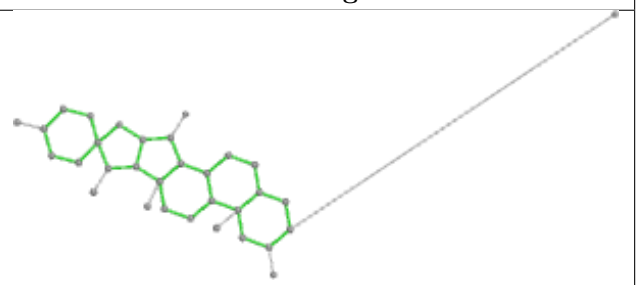


Bond angles

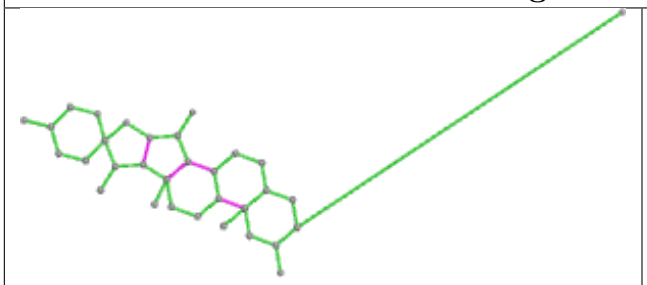


Torsions



Rings

Ligand AJP F 708



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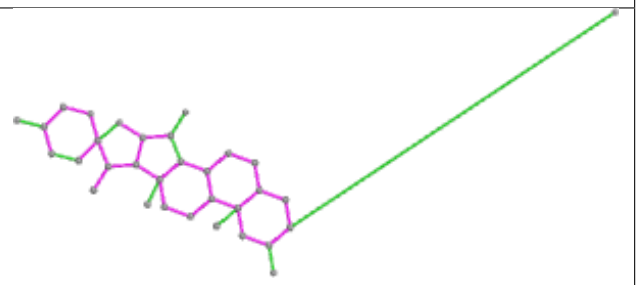
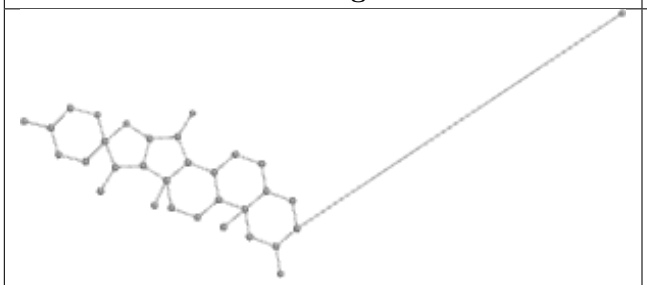


Bond angles



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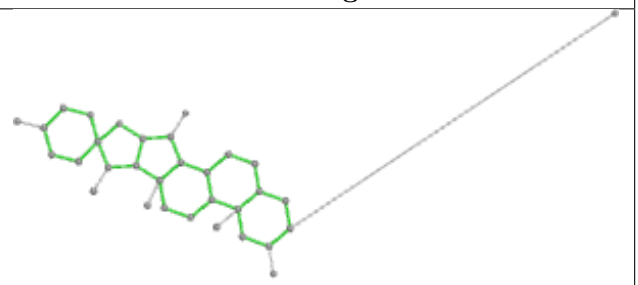
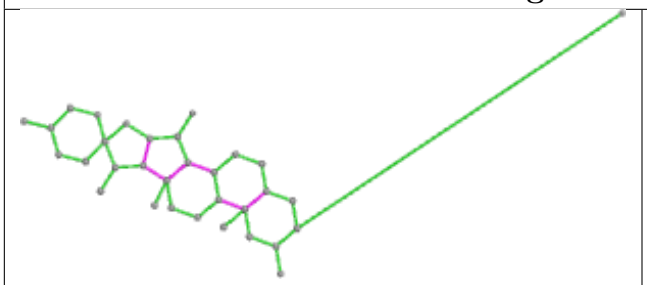
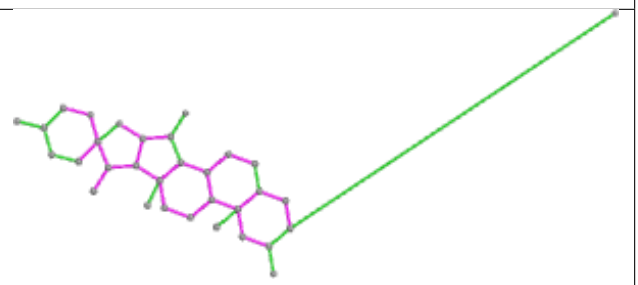


Rings

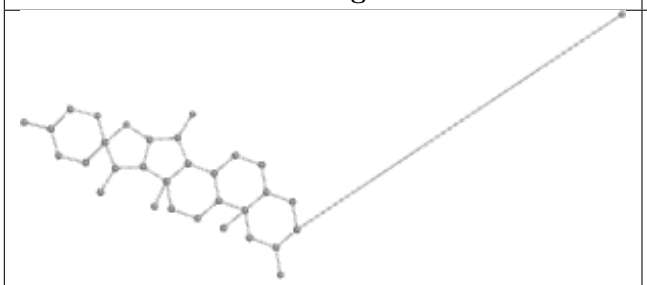
Ligand AJP D 610



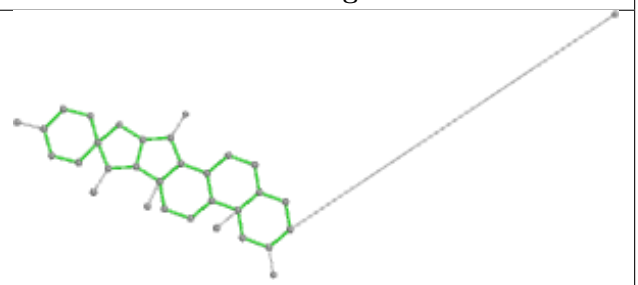
Bond lengths



Bond angles

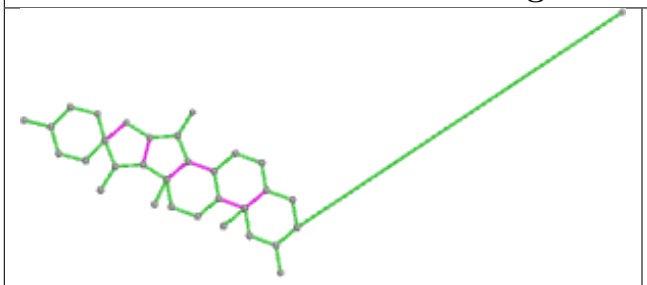


Torsions

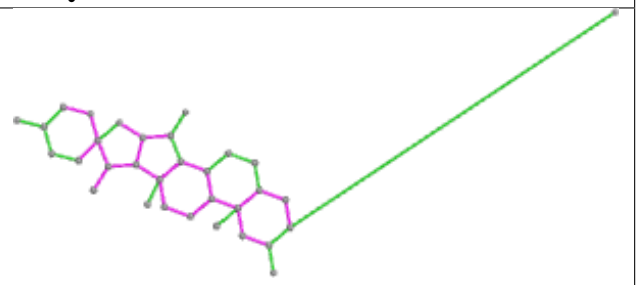


Rings

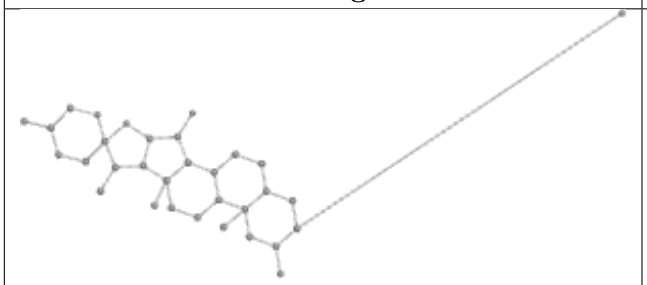
Ligand AJP Q 101



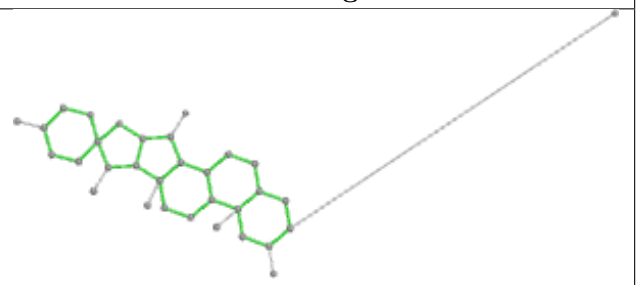
Bond lengths



Bond angles

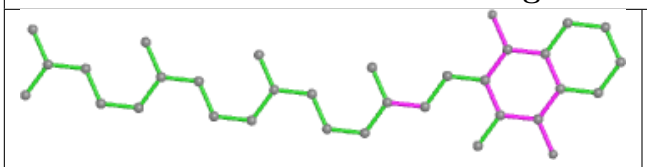


Torsions

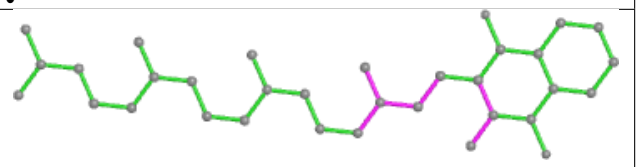


Rings

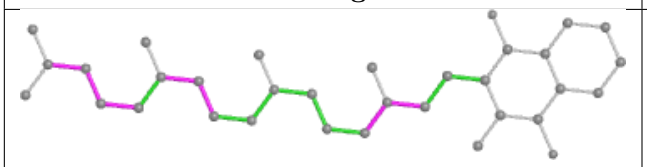
Ligand PQN B 601



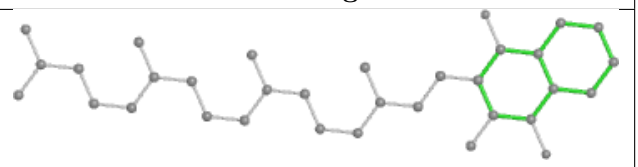
Bond lengths



Bond angles

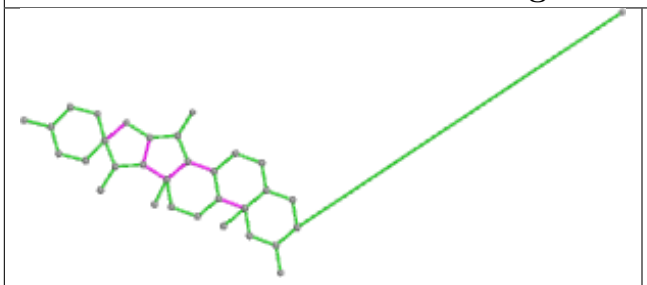


Torsions

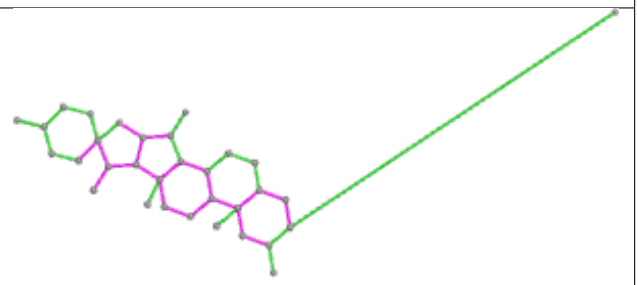


Rings

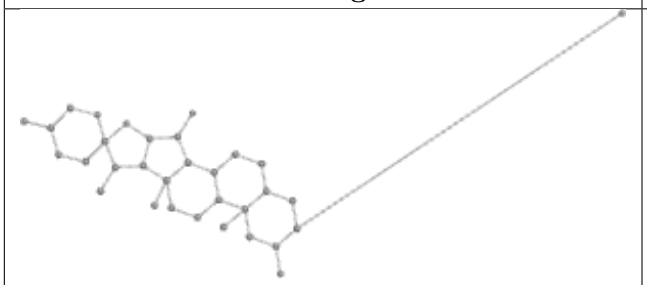
Ligand AJP F 710



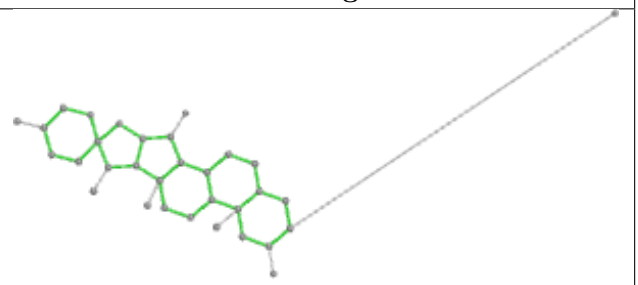
Bond lengths



Bond angles

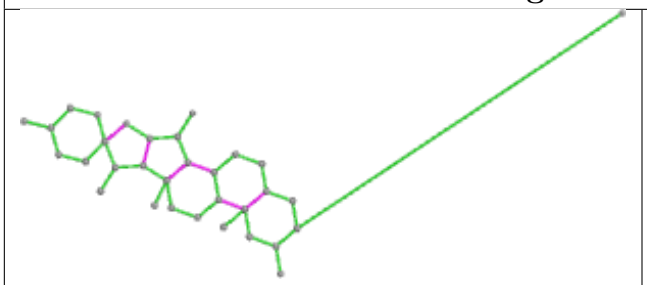


Torsions

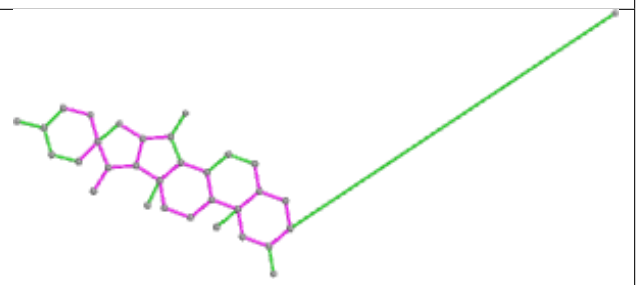


Rings

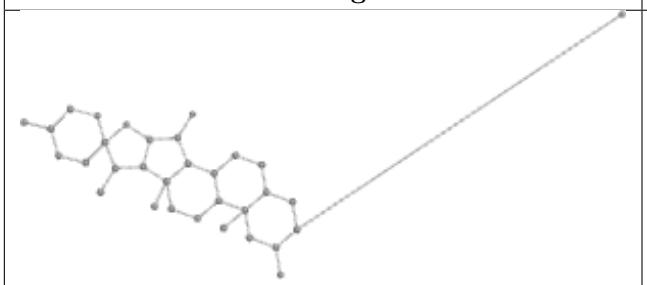
Ligand AJP D 612



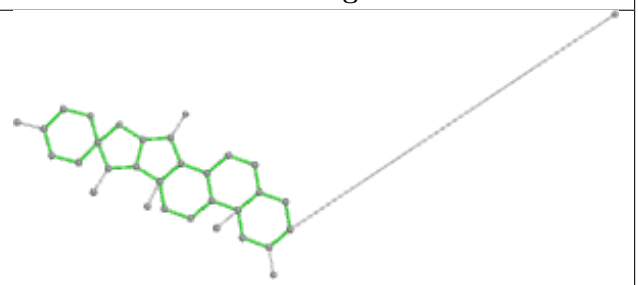
Bond lengths



Bond angles

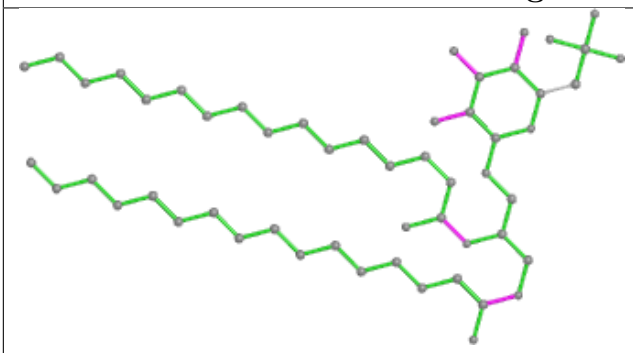


Torsions

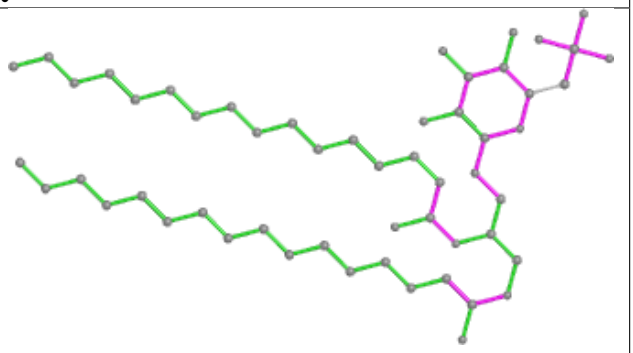


Rings

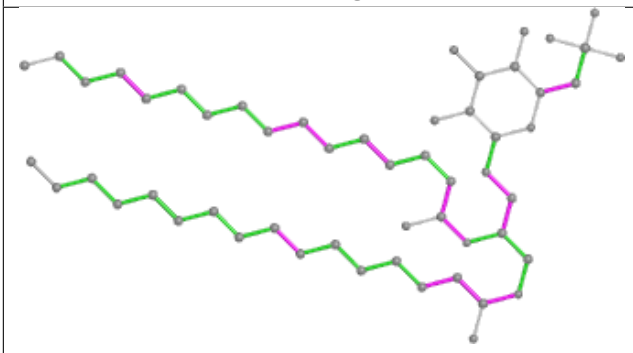
Ligand SQD L 101



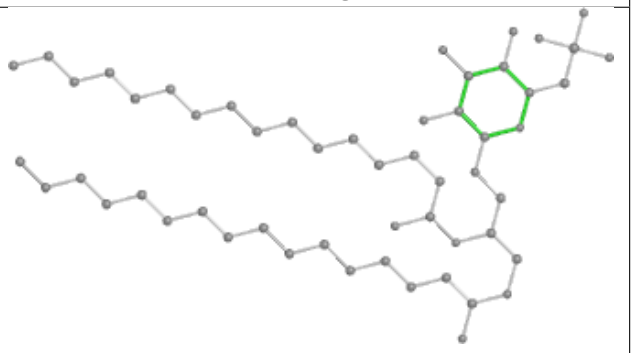
Bond lengths



Bond angles

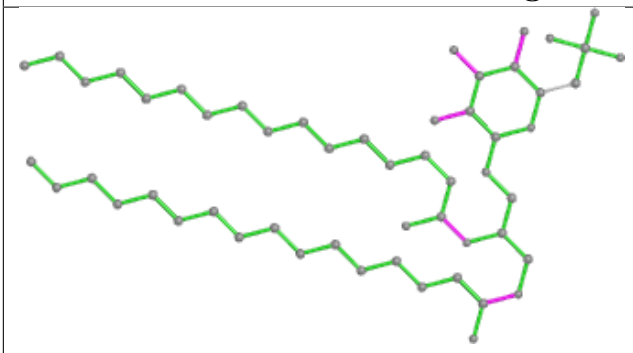


Torsions

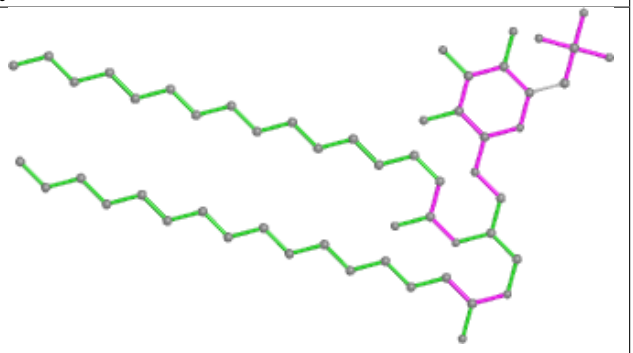


Rings

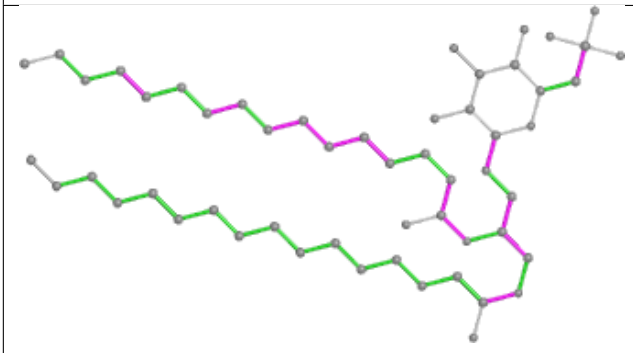
Ligand SQD D 605



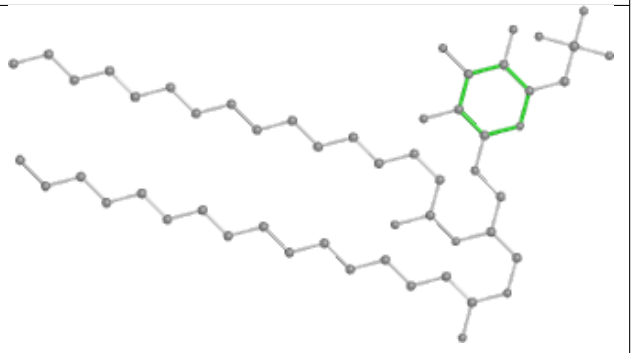
Bond lengths



Bond angles

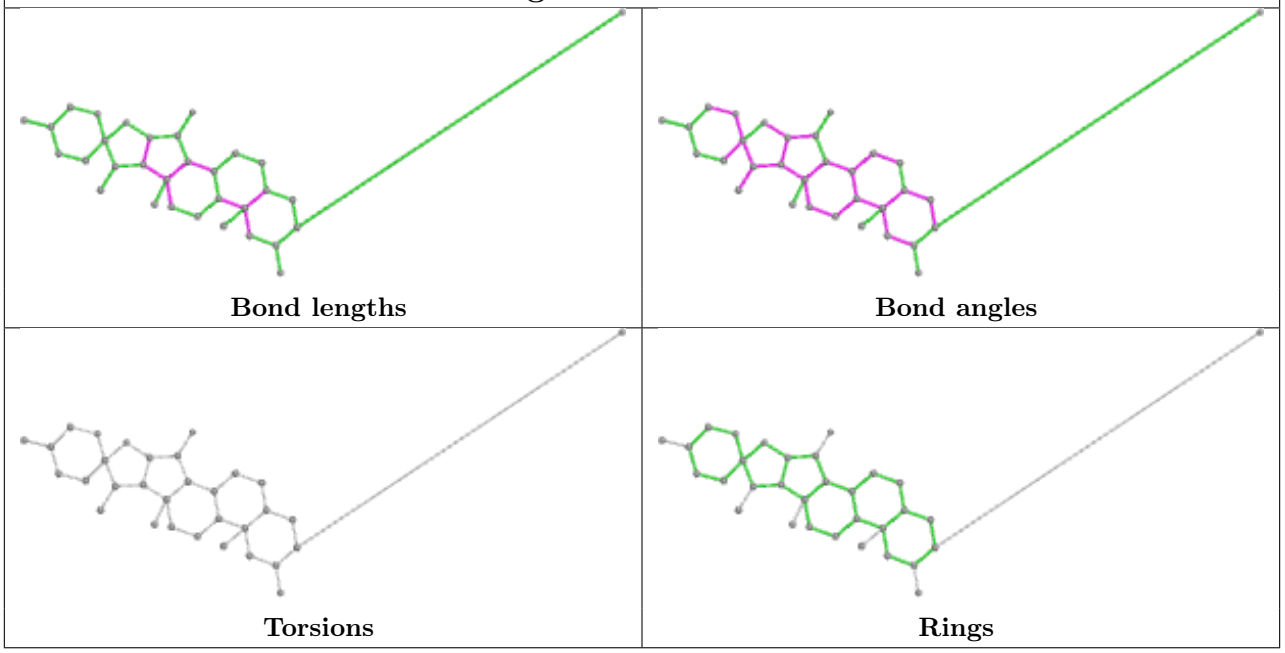


Torsions

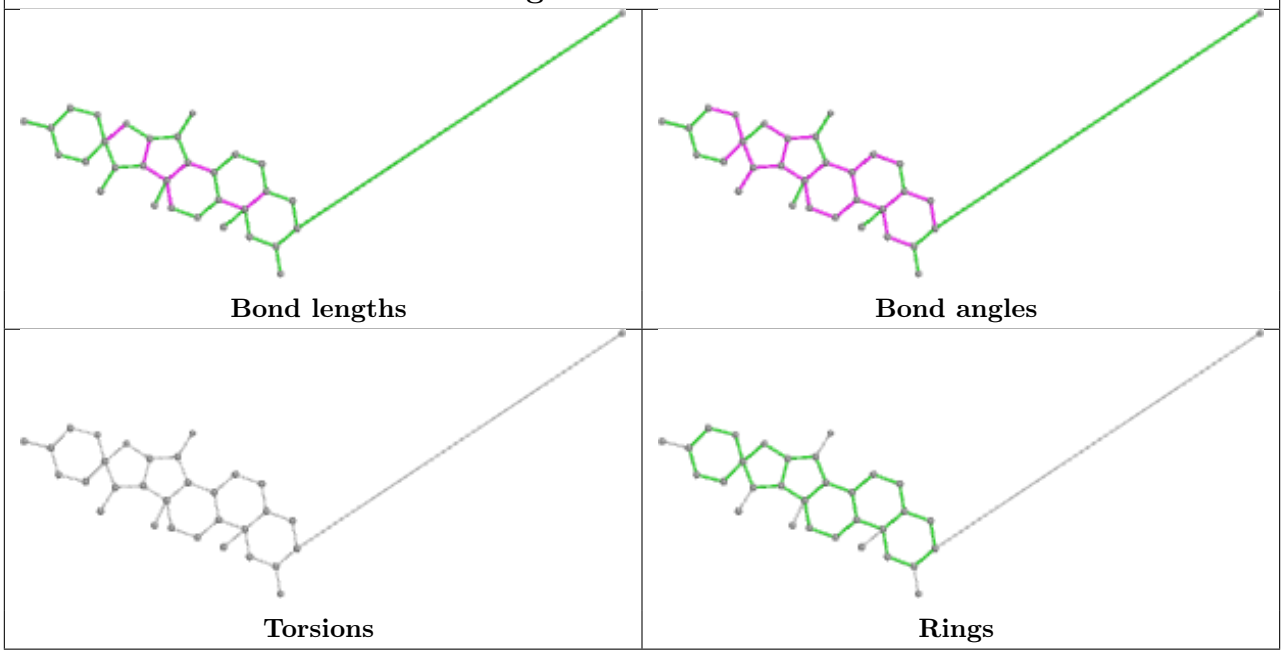


Rings

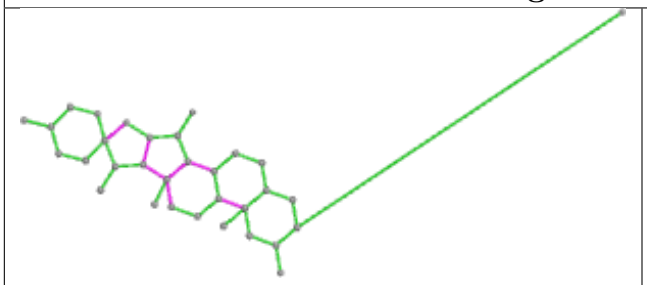
Ligand AJP C 202



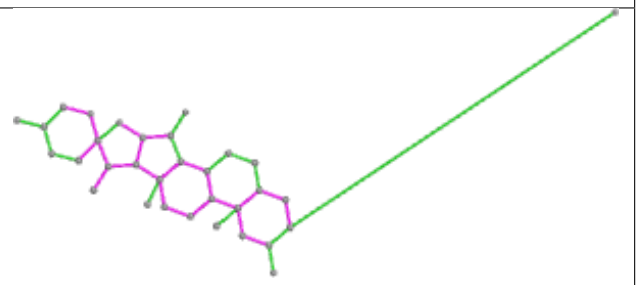
Ligand AJP G 305



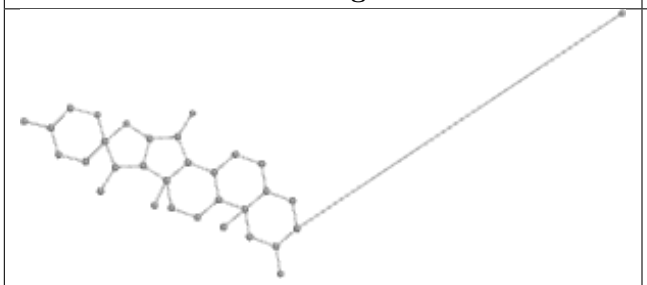
Ligand AJP B 607



Bond lengths



Bond angles



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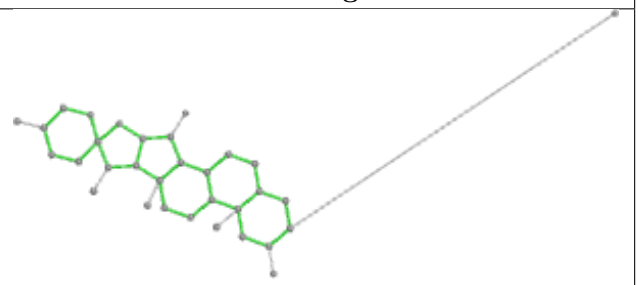
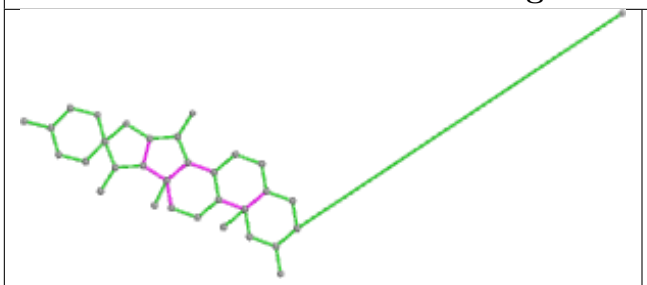
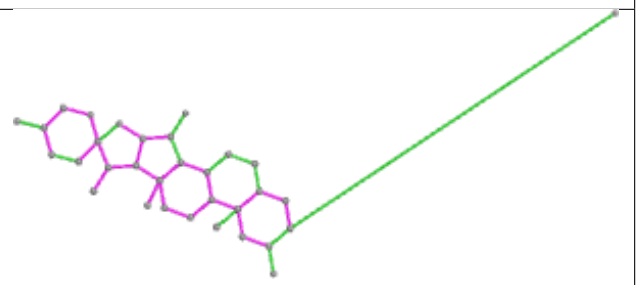


Rings

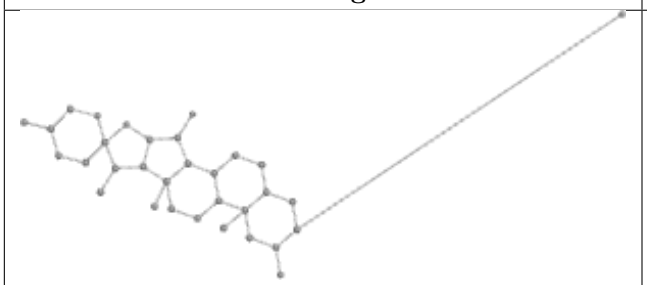
Ligand AJP G 307



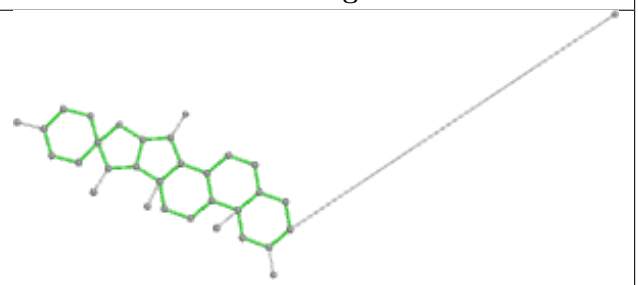
Bond lengths



Bond angles

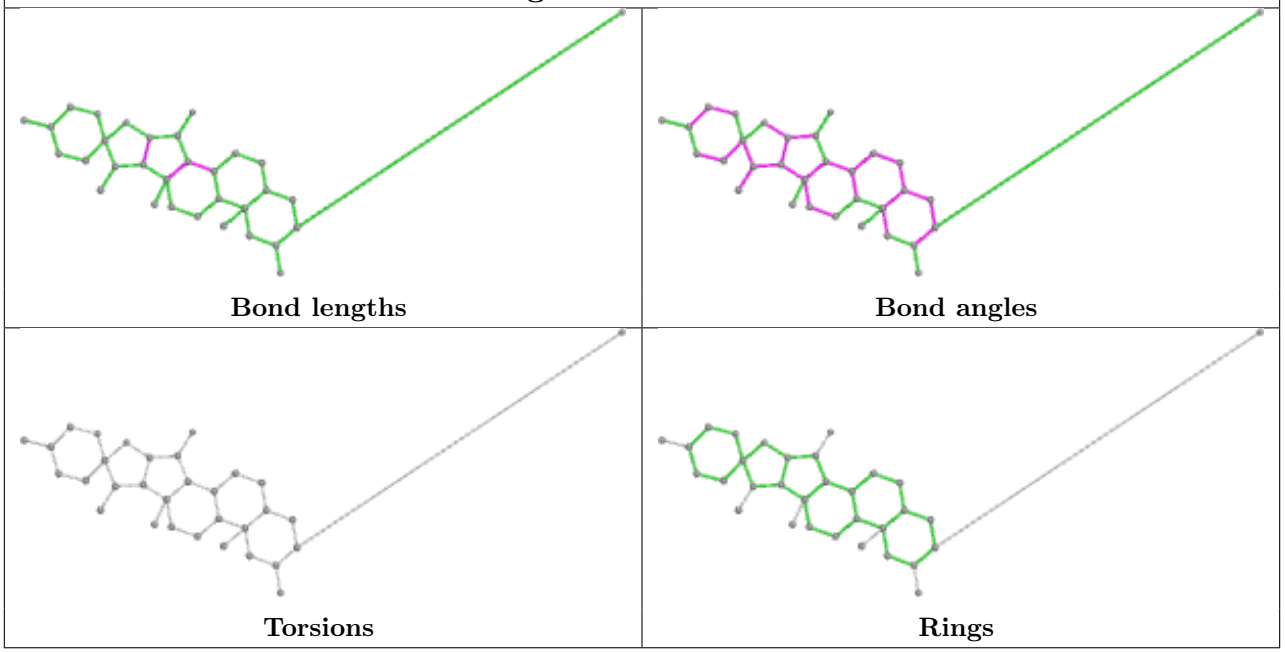


Torsions

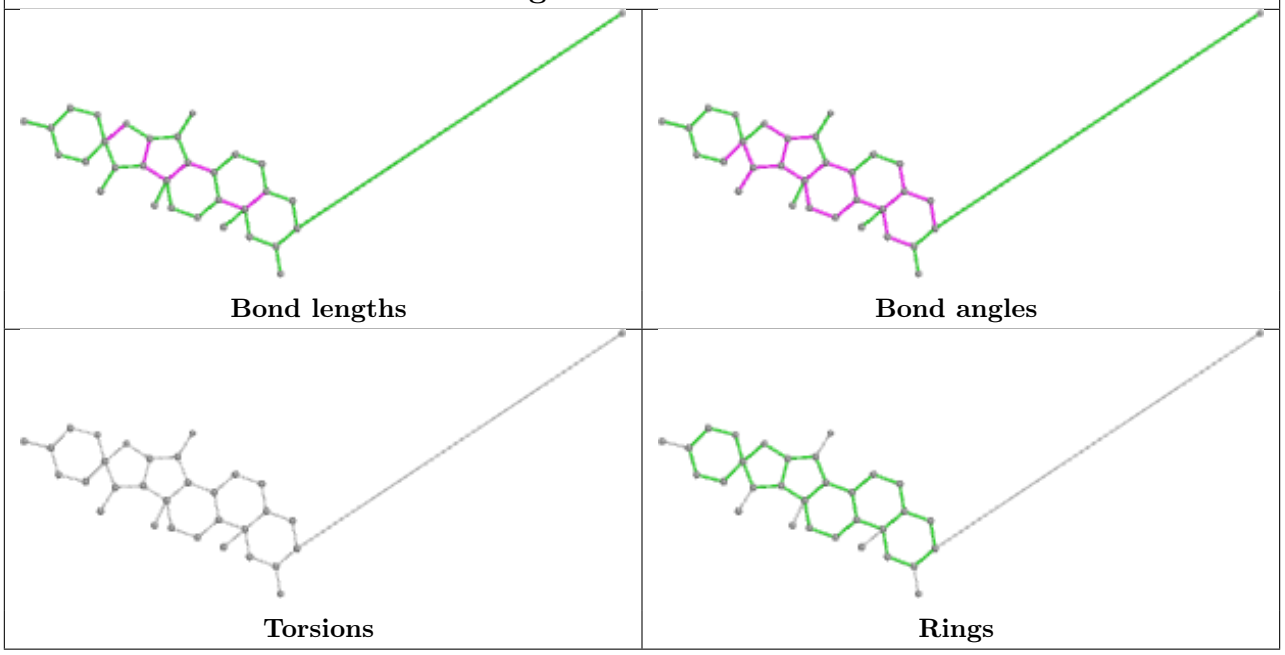


Rings

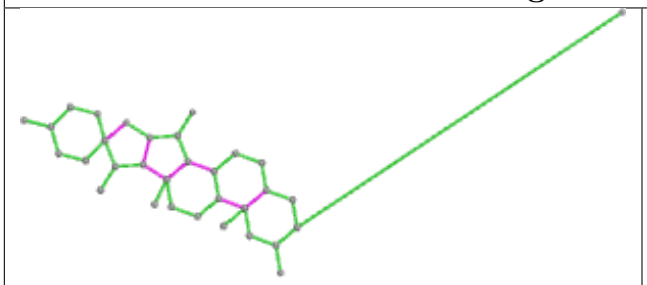
Ligand AJP A 407



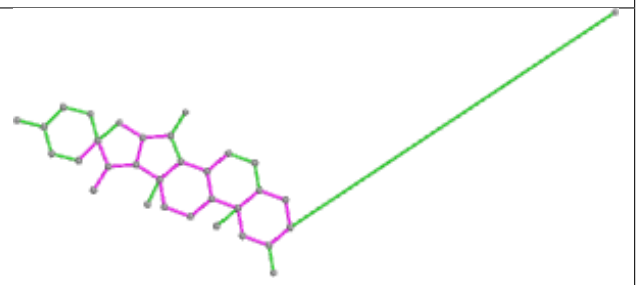
Ligand AJP F 711



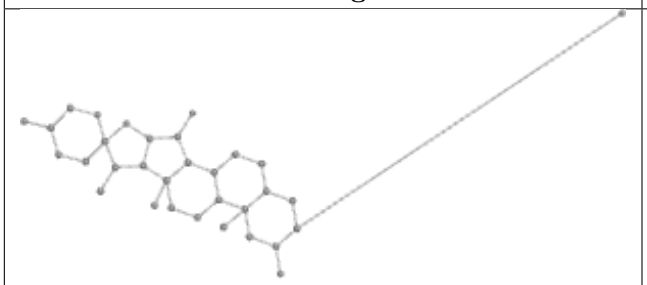
Ligand AJP B 614



Bond lengths



Bond angles



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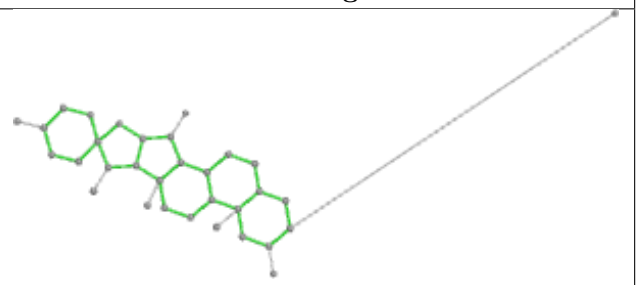
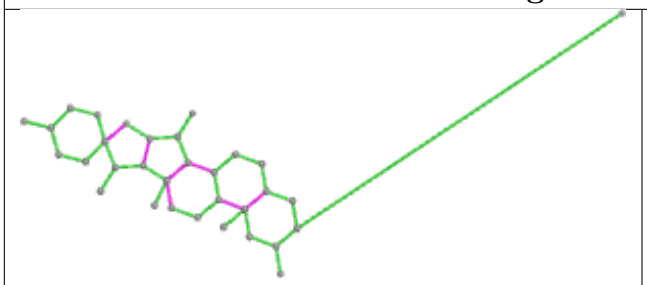
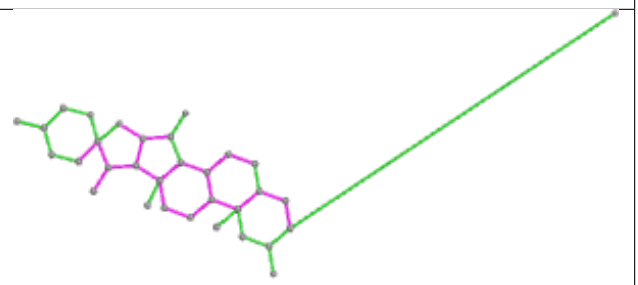


Rings

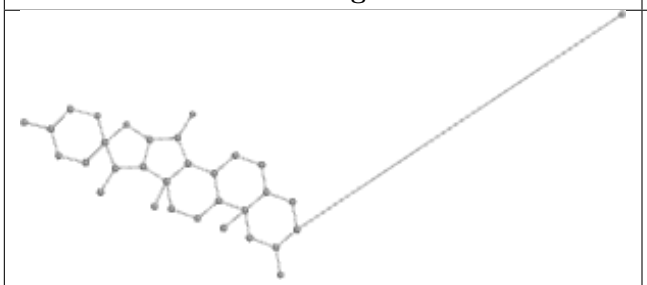
Ligand AJP D 613



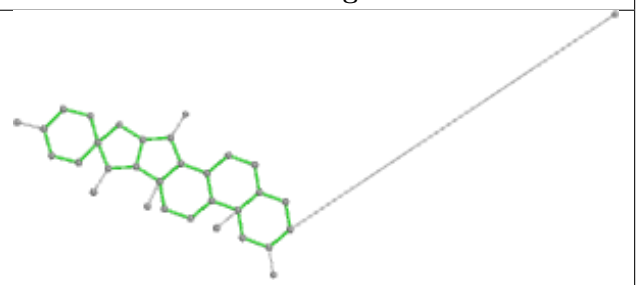
Bond lengths



Bond angles

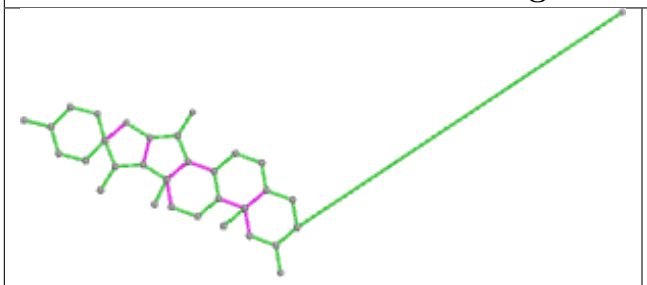


Torsions

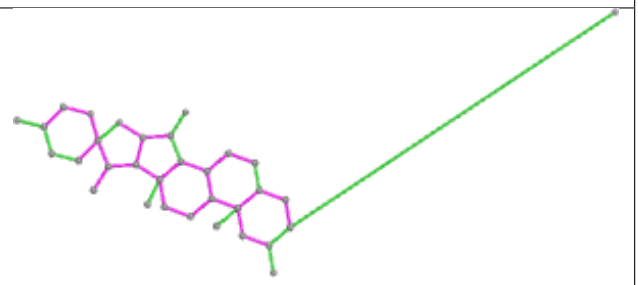


Rings

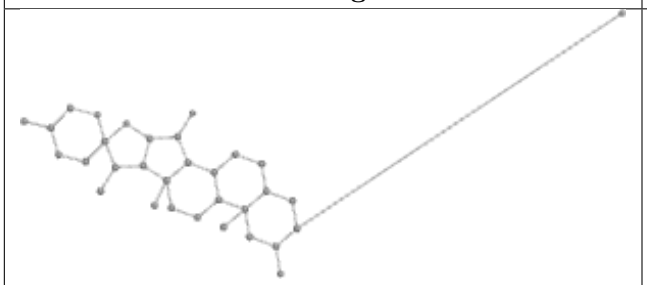
Ligand AJP F 712



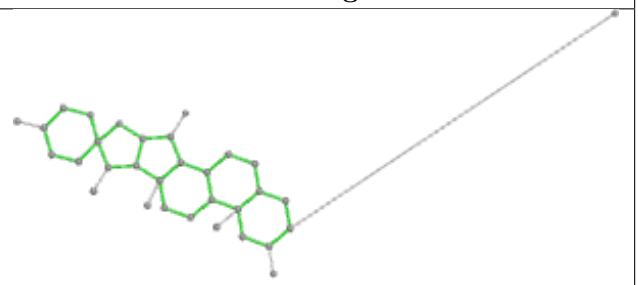
Bond lengths



Bond angles

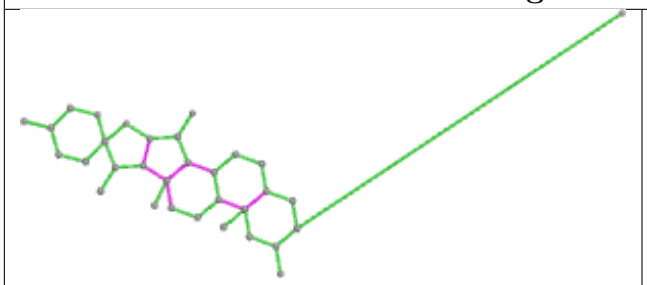


Torsions



Rings

Ligand AJP G 302



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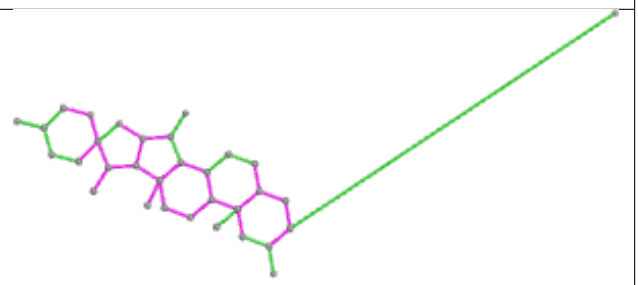
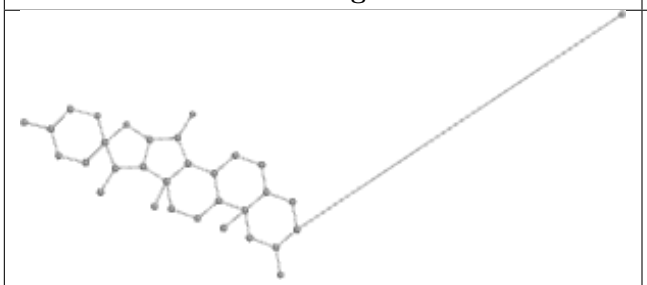
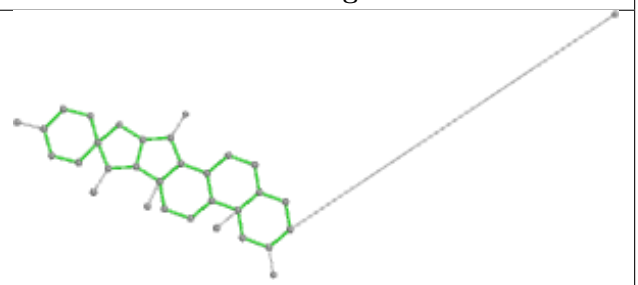


Bond angles

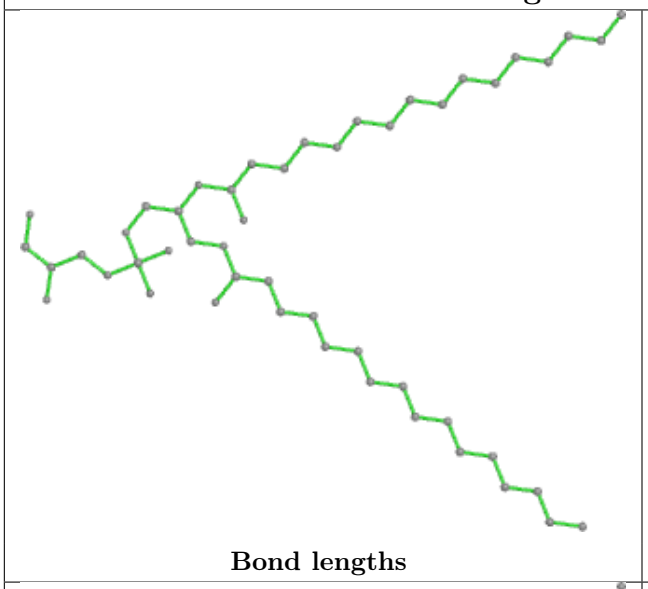


Torsions

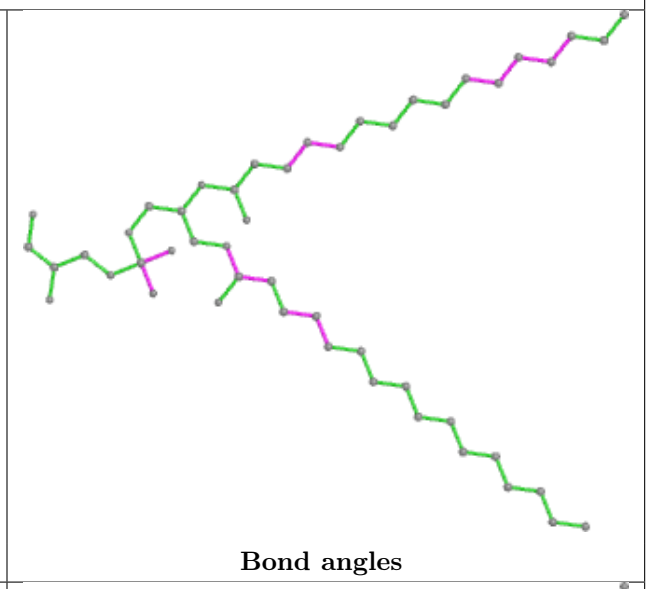


Rings

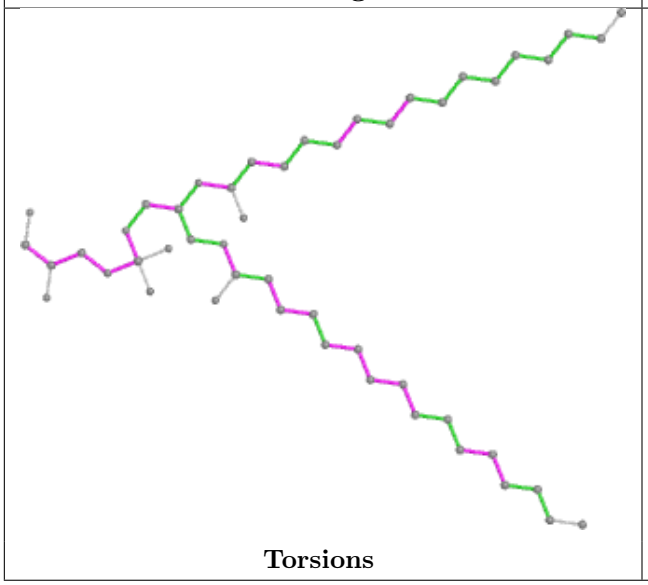
Ligand LHG B 602



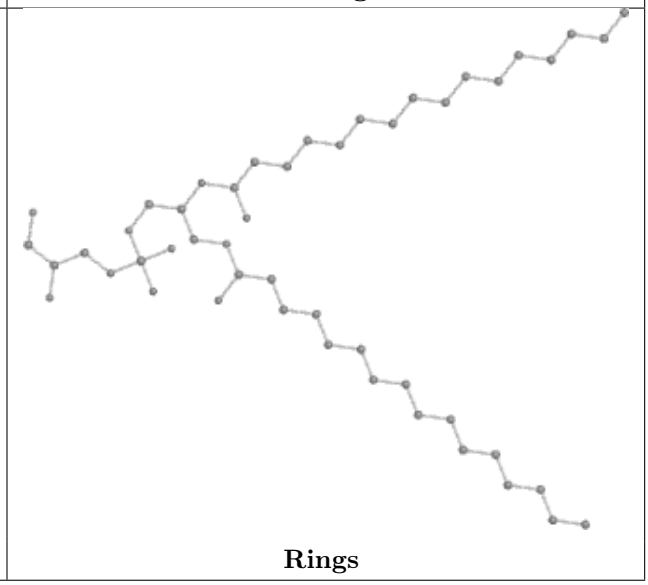
Bond lengths



Bond angles

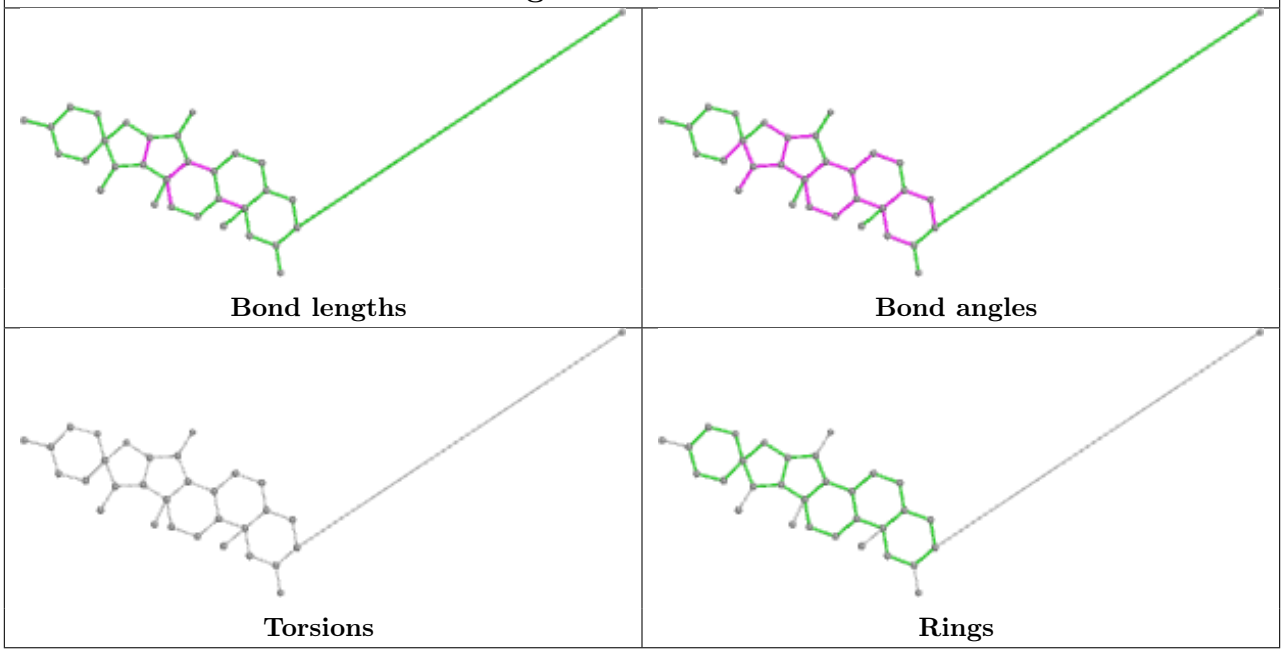


Torsions

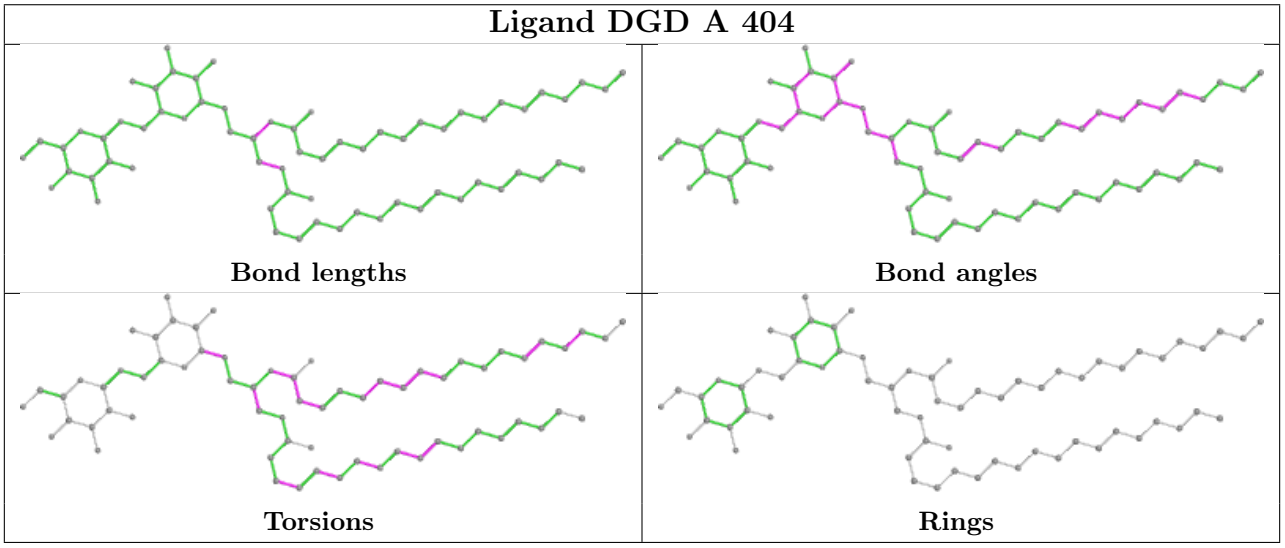


Rings

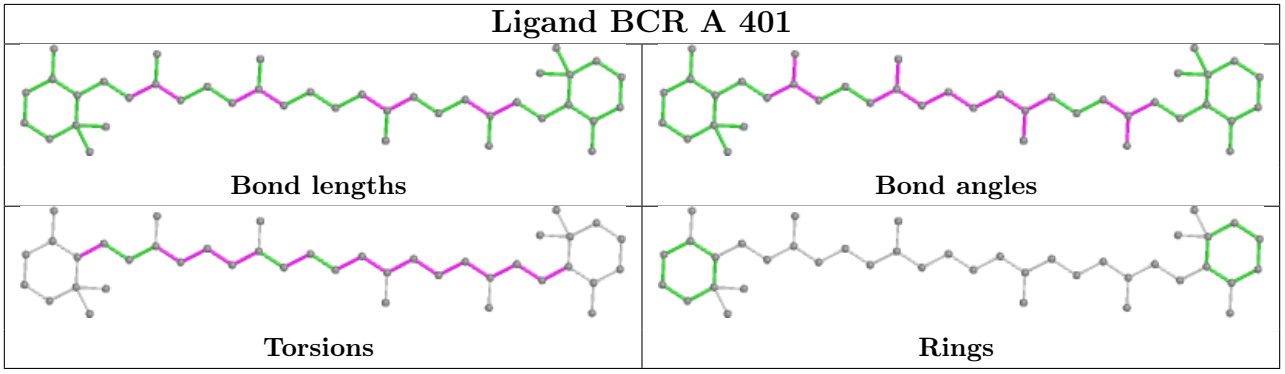
Ligand AJP D 611



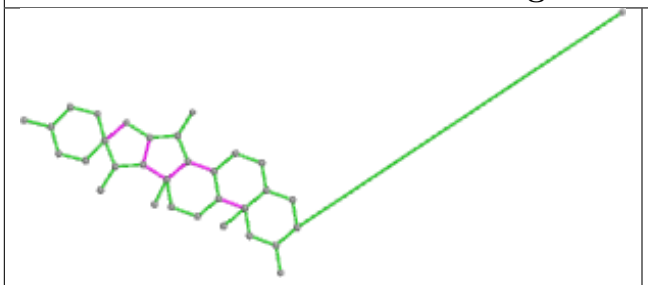
Ligand DGD A 404



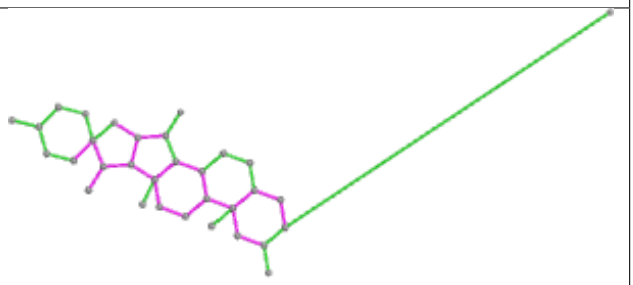
Ligand BCR A 401



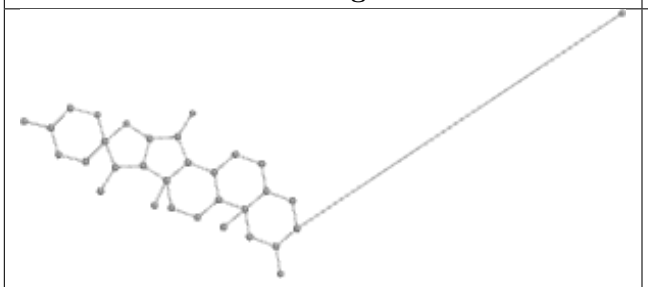
Ligand AJP B 612



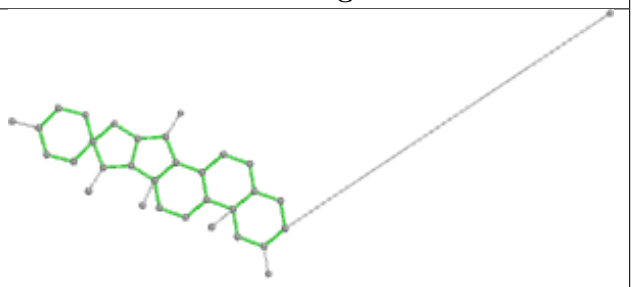
Bond lengths



Bond angles

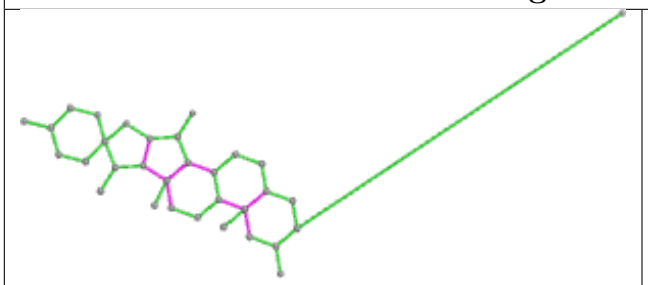


Torsions

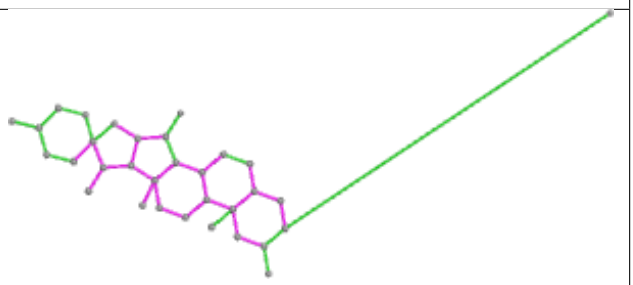


Rings

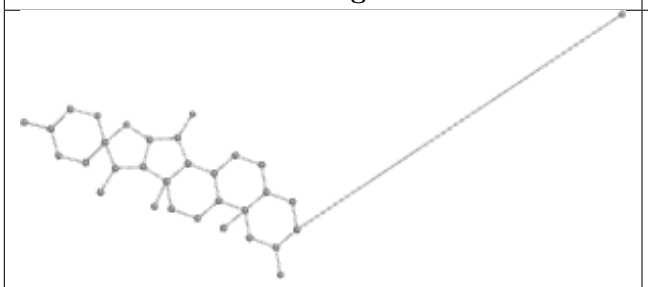
Ligand AJP F 705



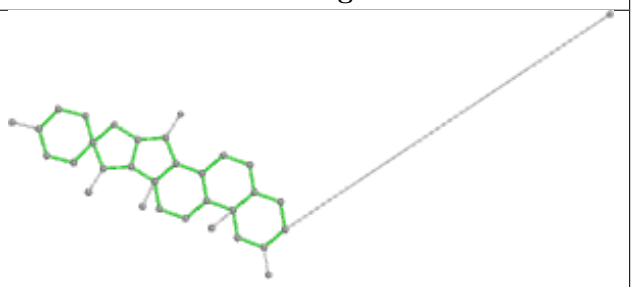
Bond lengths



Bond angles

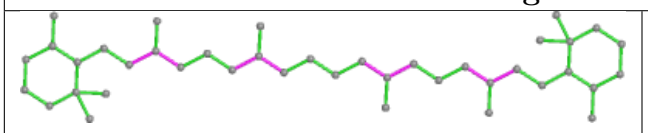


Torsions

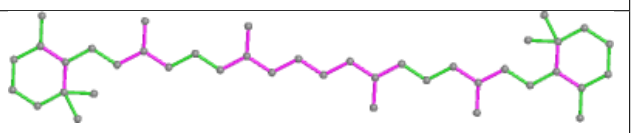


Rings

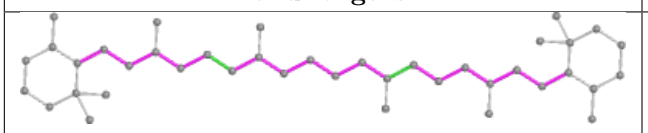
Ligand BCR D 601



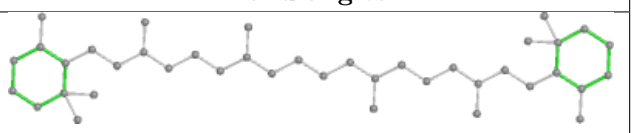
Bond lengths



Bond angles

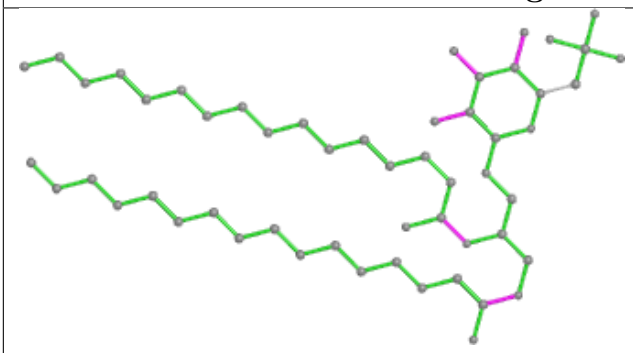


Torsions

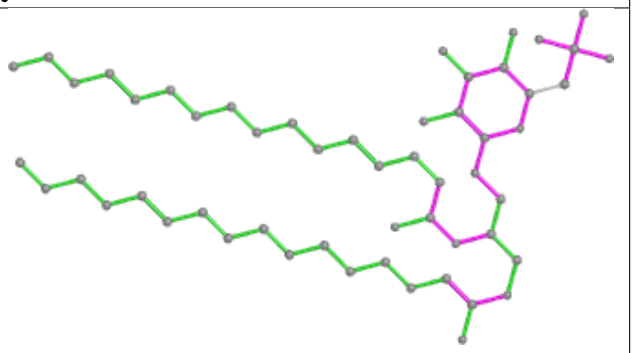


Rings

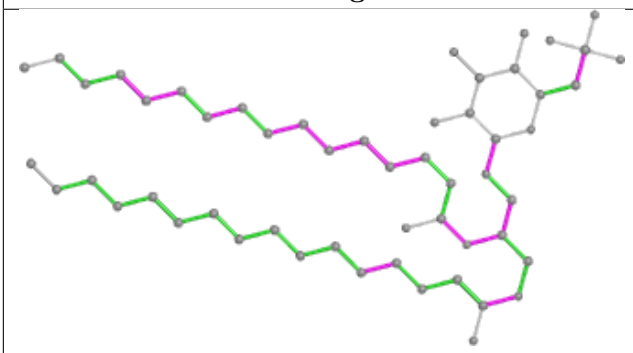
Ligand SQD F 703



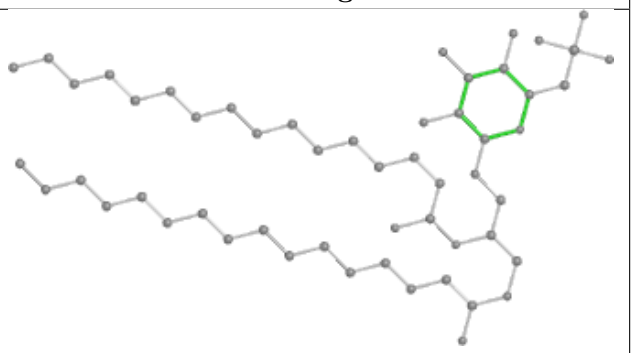
Bond lengths



Bond angles

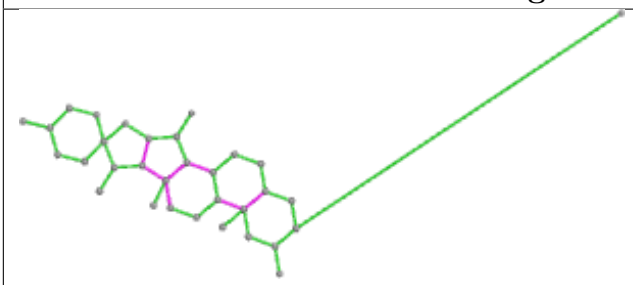


Torsions

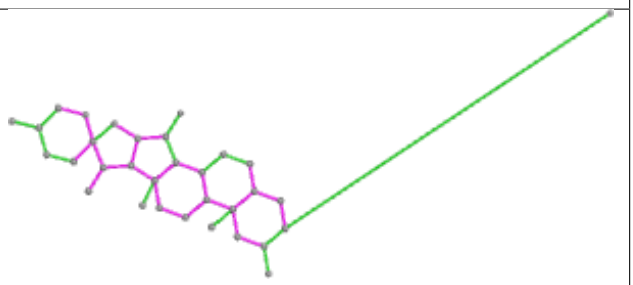


Rings

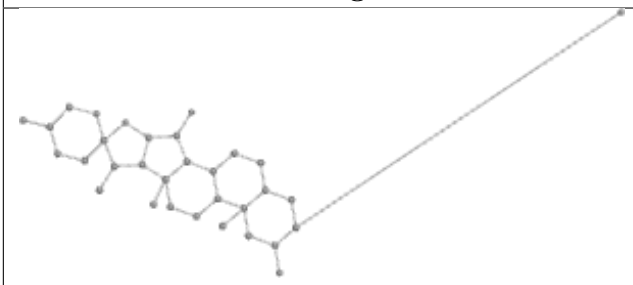
Ligand AJP F 706



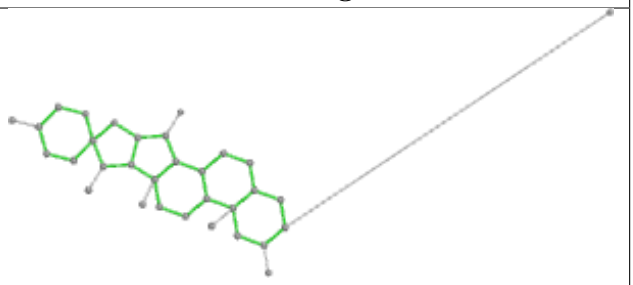
Bond lengths



Bond angles

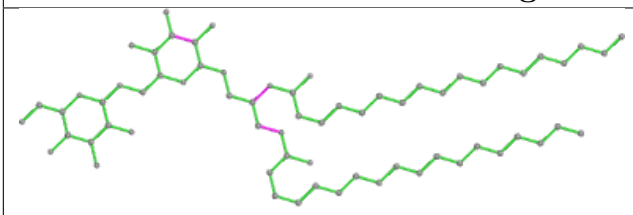


Torsions

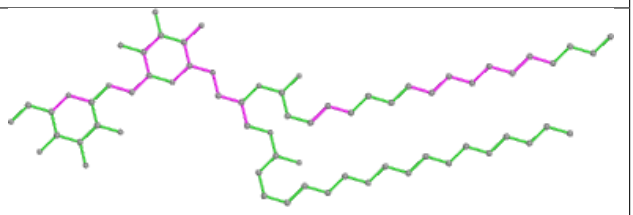


Rings

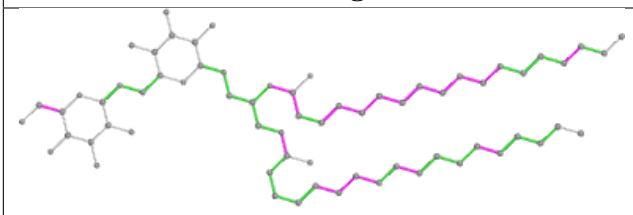
Ligand DGD A 405



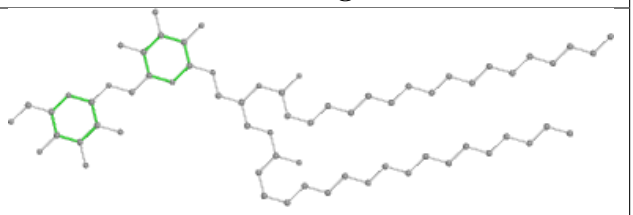
Bond lengths



Bond angles

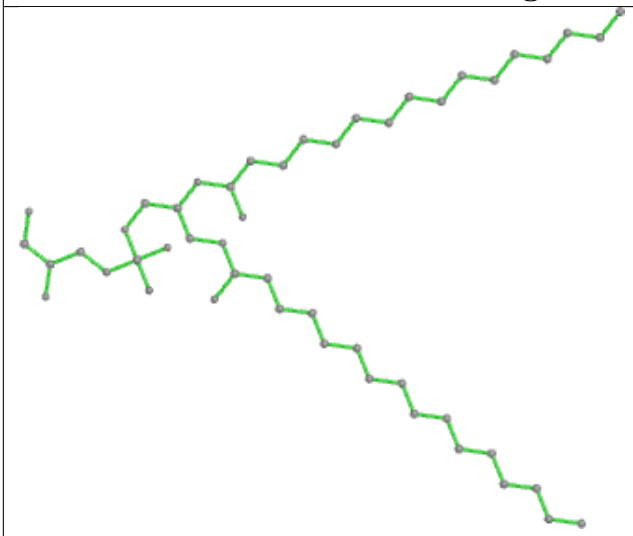


Torsions

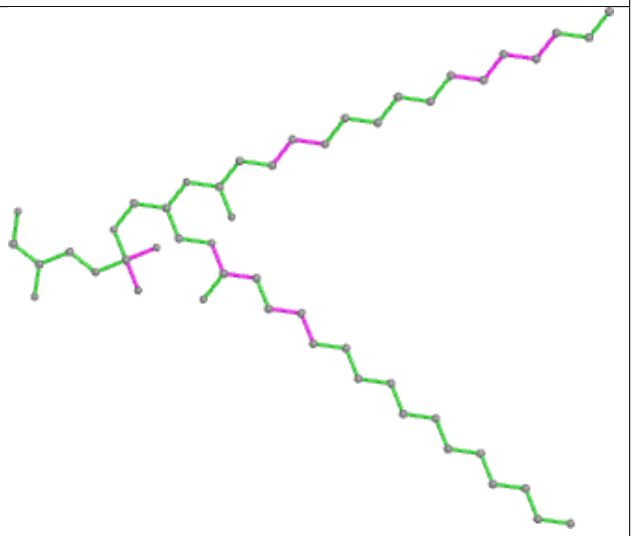


Rings

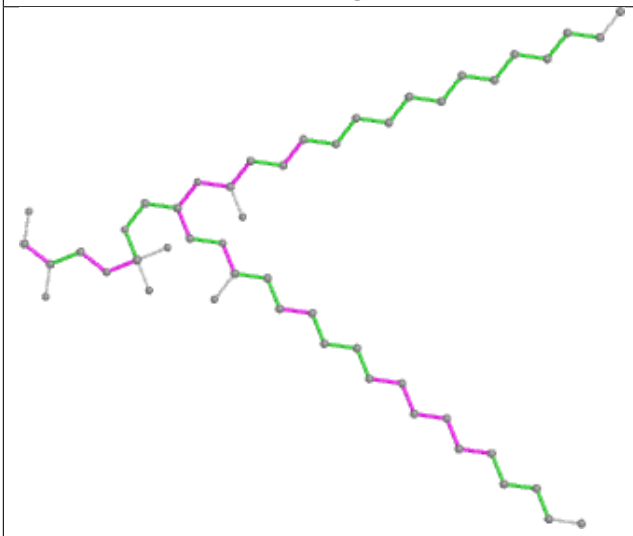
Ligand LHG A 402



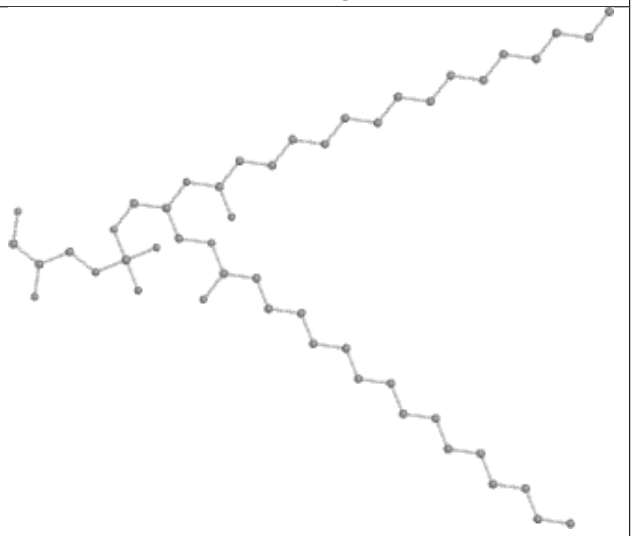
Bond lengths



Bond angles

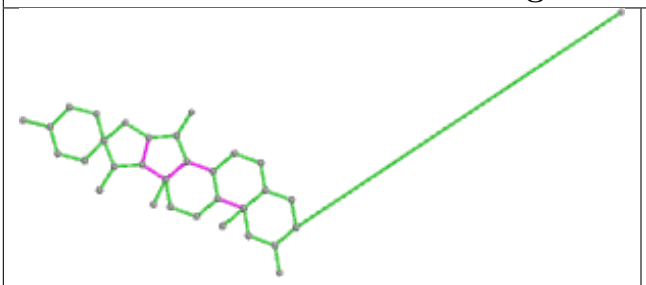


Torsions

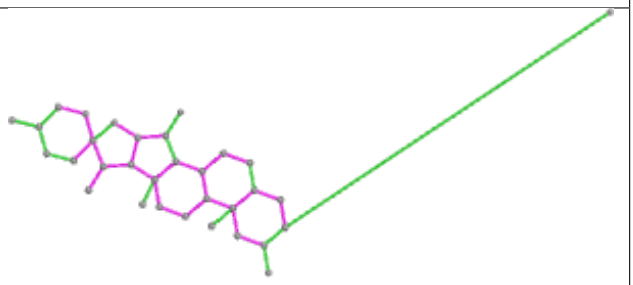


Rings

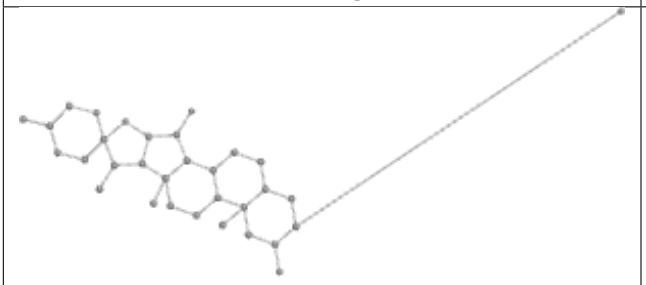
Ligand AJP B 605



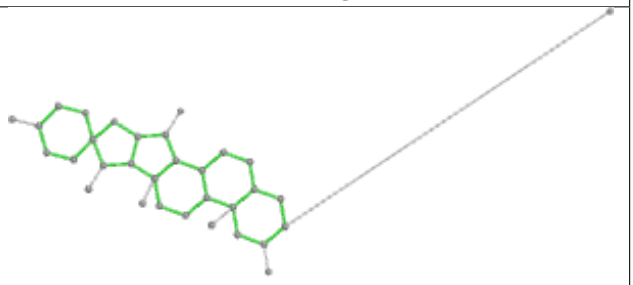
Bond lengths



Bond angles

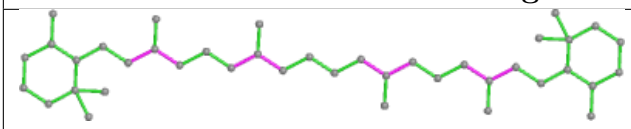


Torsions

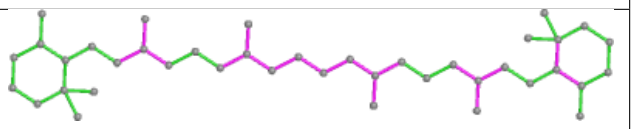


Rings

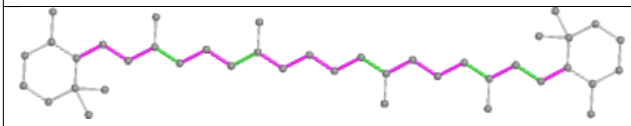
Ligand BCR D 602



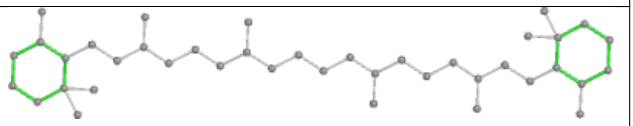
Bond lengths



Bond angles

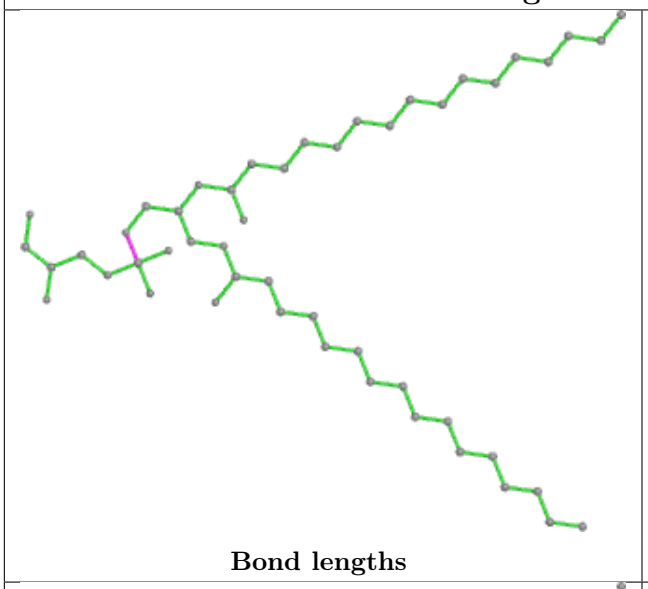


Torsions

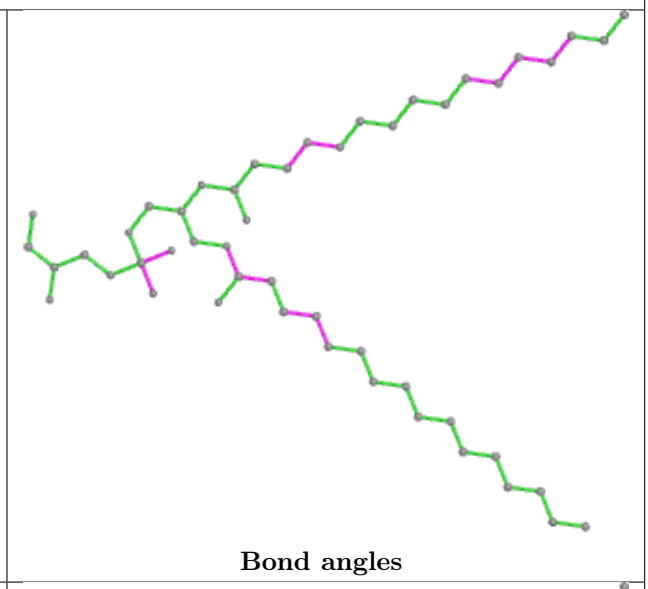


Rings

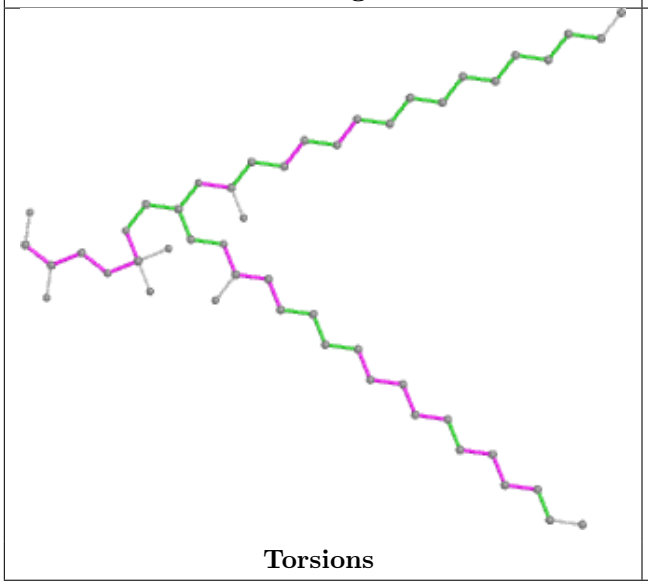
Ligand LHG D 603



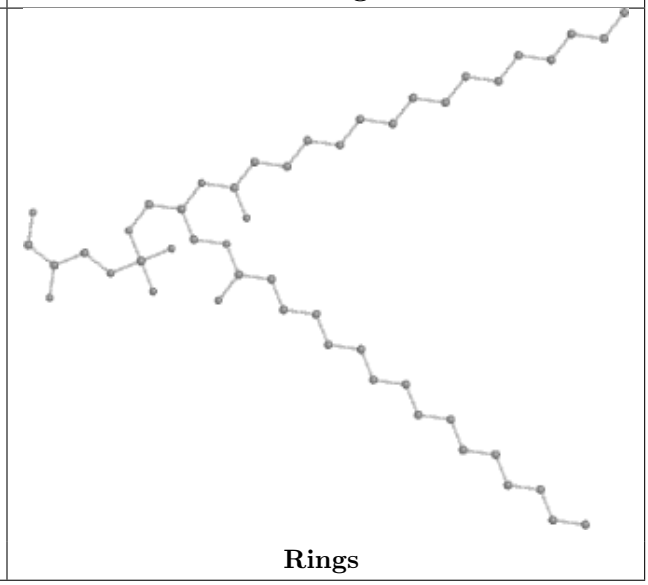
Bond lengths



Bond angles

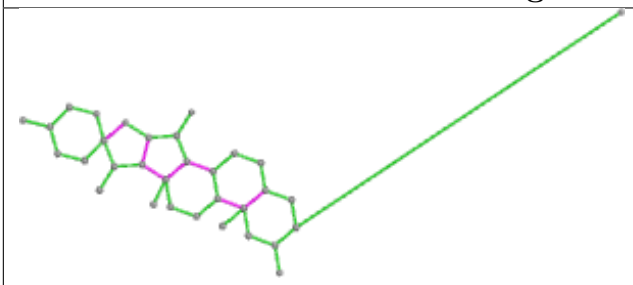


Torsions

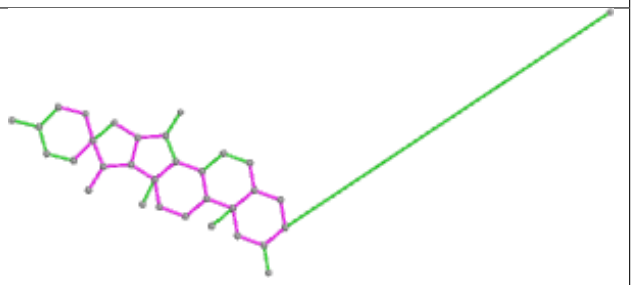


Rings

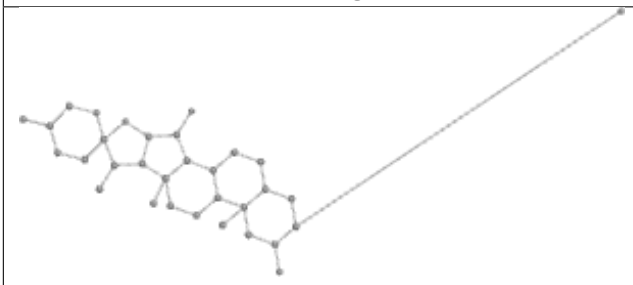
Ligand AJP B 611



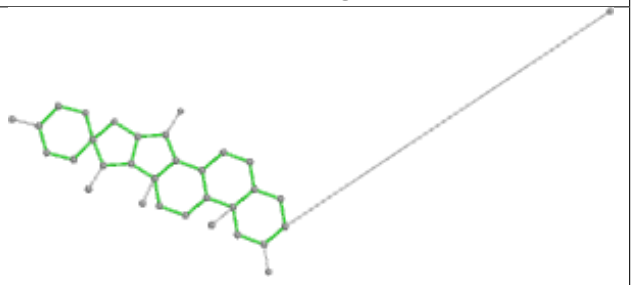
Bond lengths



Bond angles

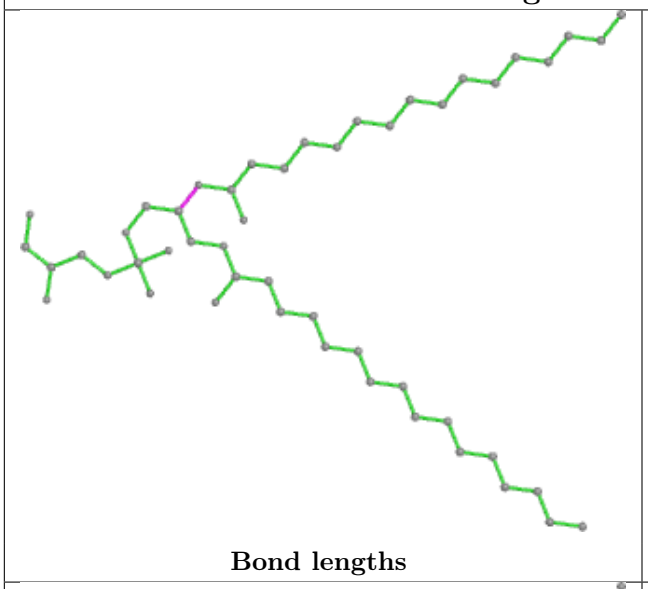


Torsions

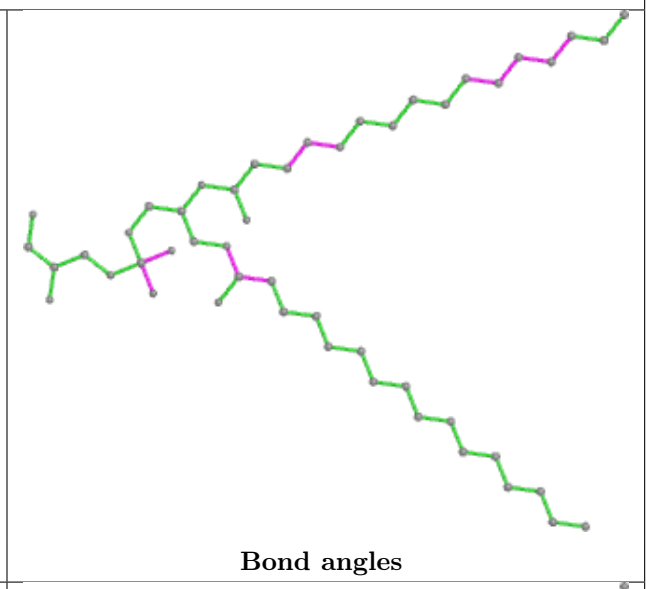


Rings

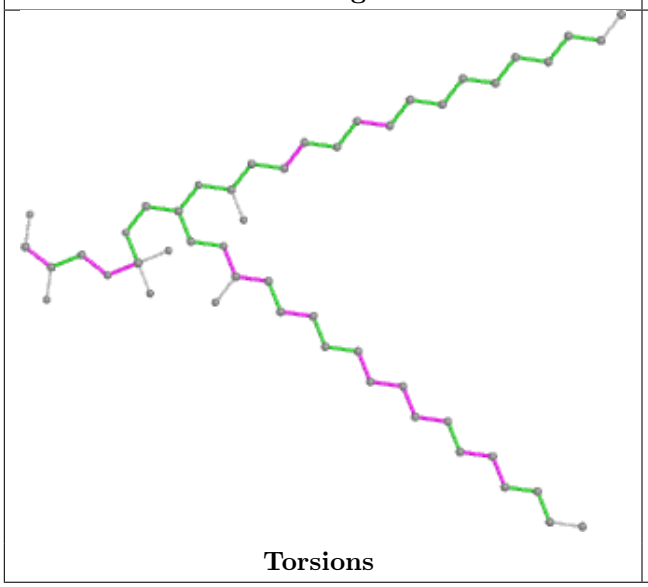
Ligand LHG A 403



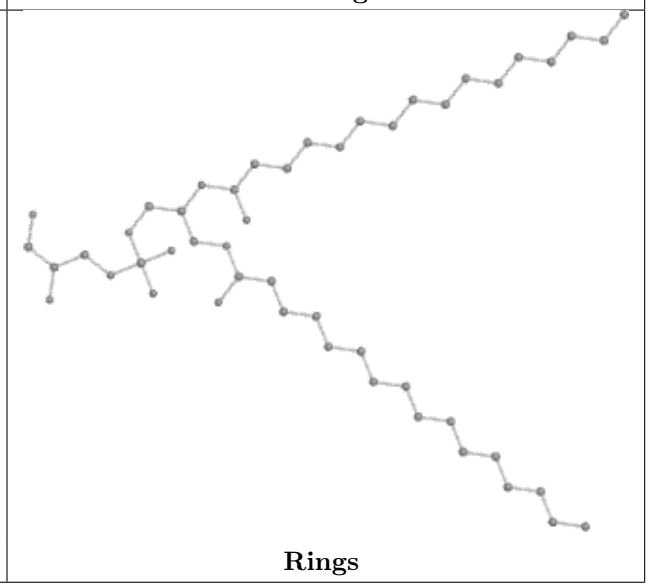
Bond lengths



Bond angles

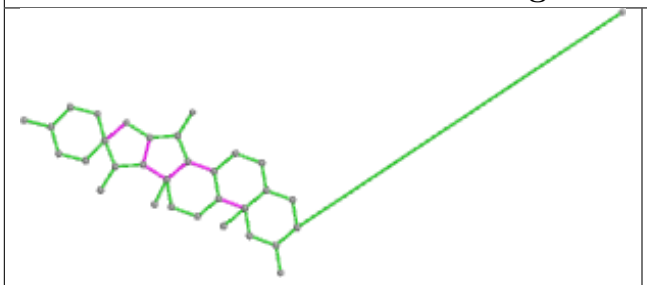


Torsions

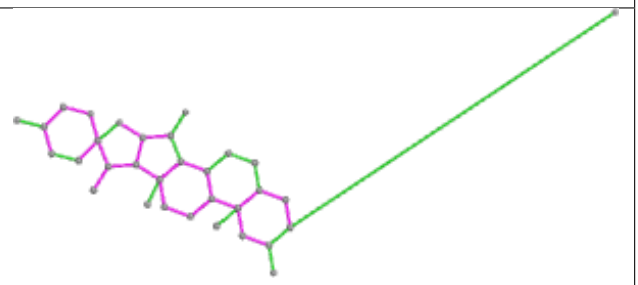


Rings

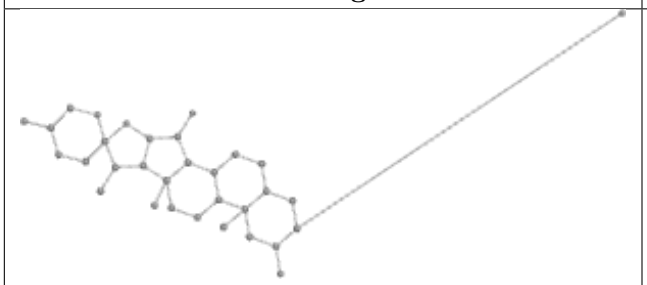
Ligand AJP F 704



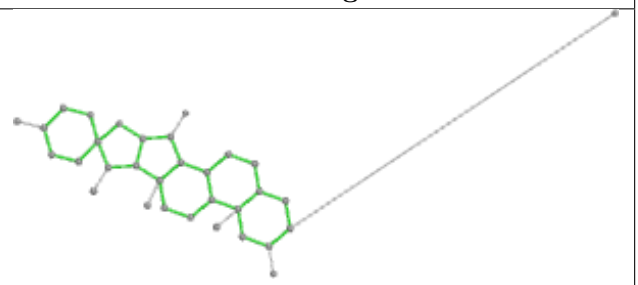
Bond lengths



Bond angles

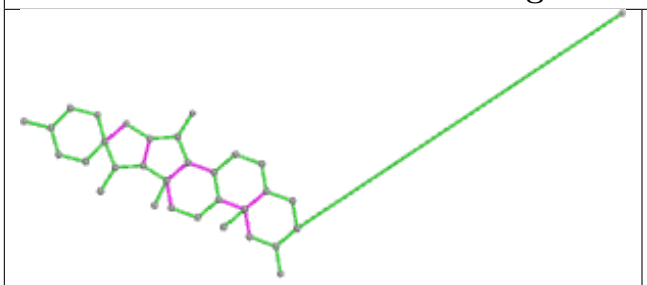


Torsions

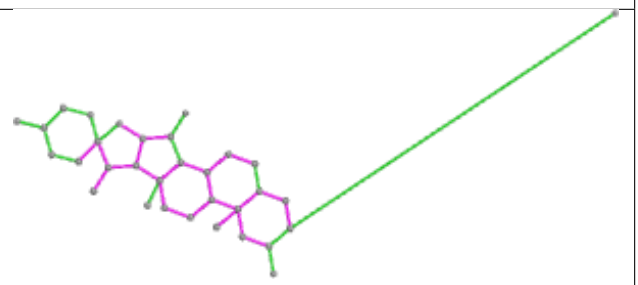


Rings

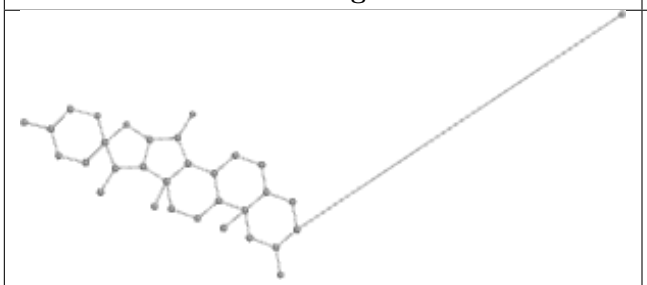
Ligand AJP G 304



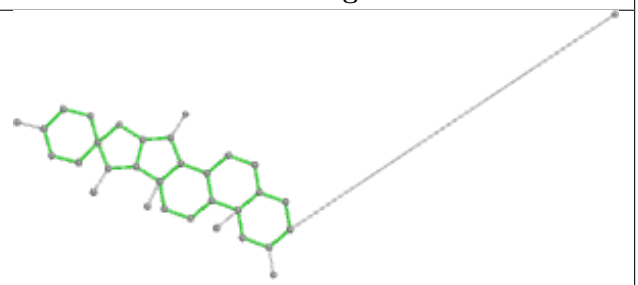
Bond lengths



Bond angles

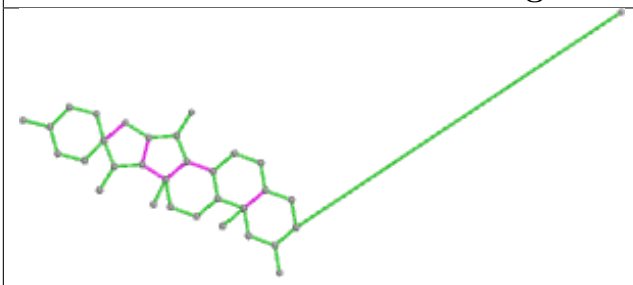


Torsions

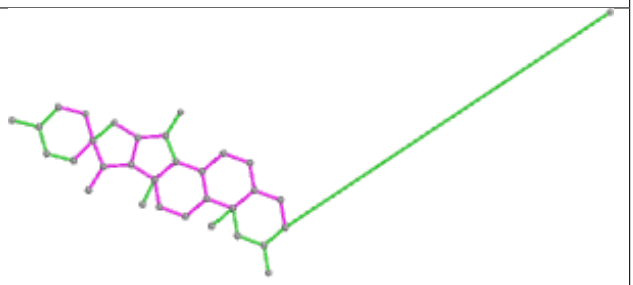


Rings

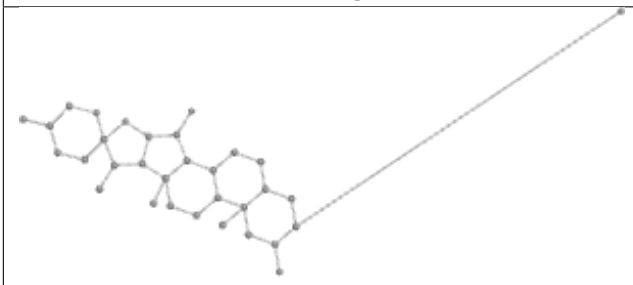
Ligand AJP A 408



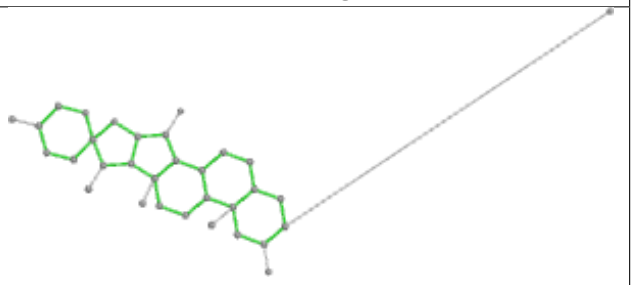
Bond lengths



Bond angles

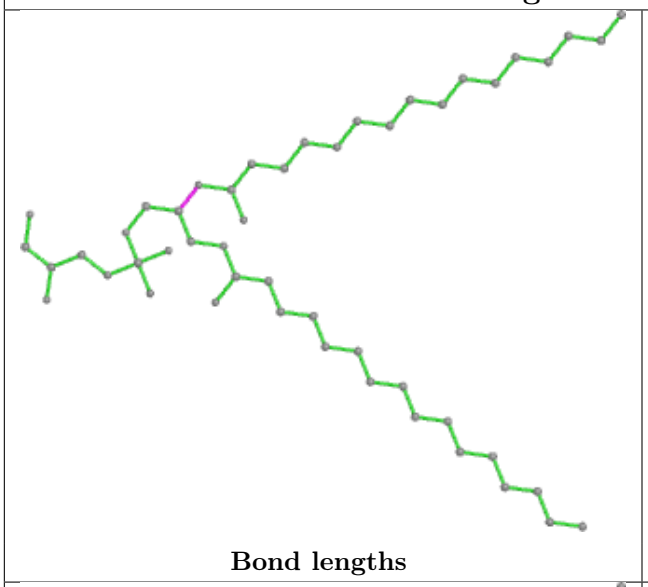


Torsions

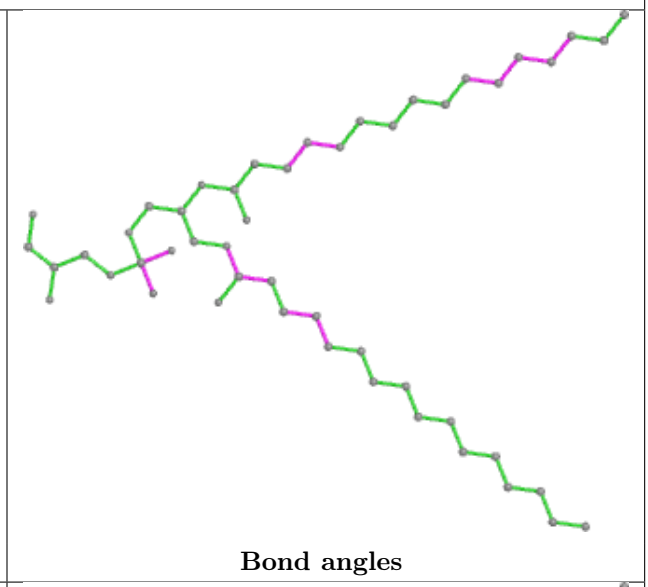


Rings

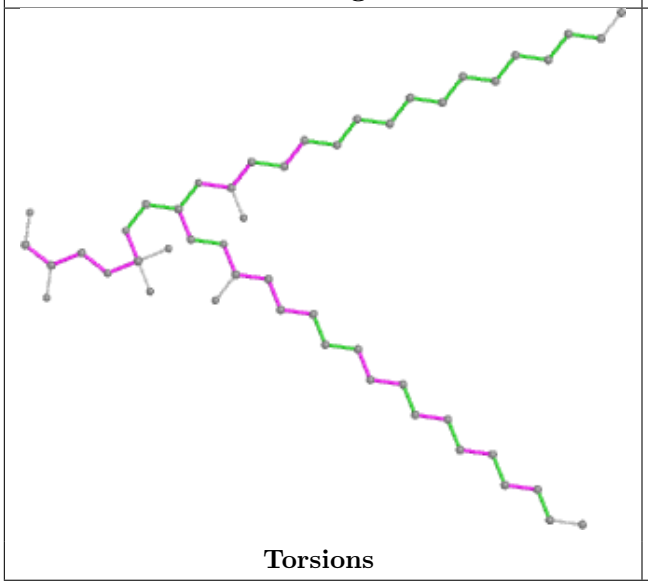
Ligand LHG D 604



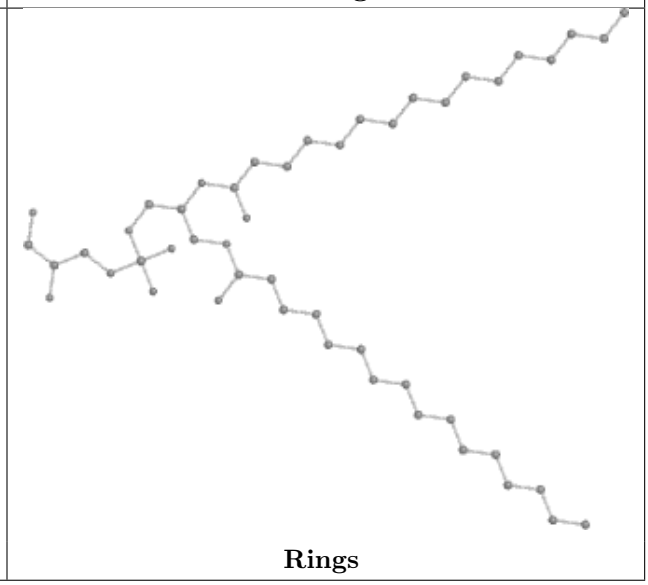
Bond lengths



Bond angles

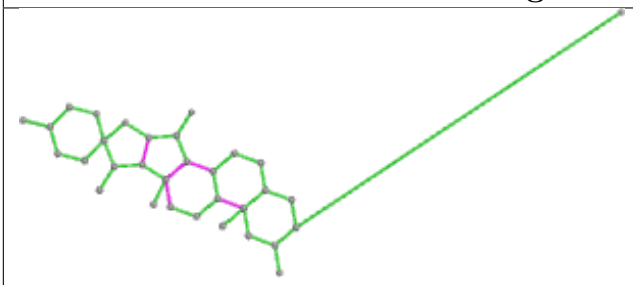


Torsions

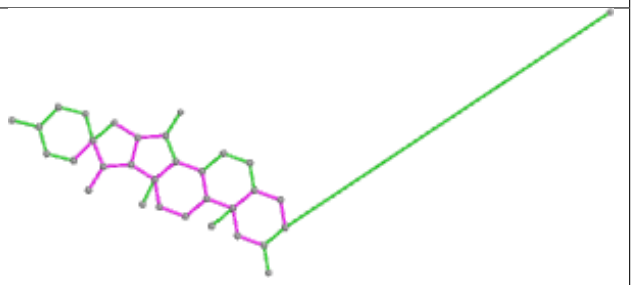


Rings

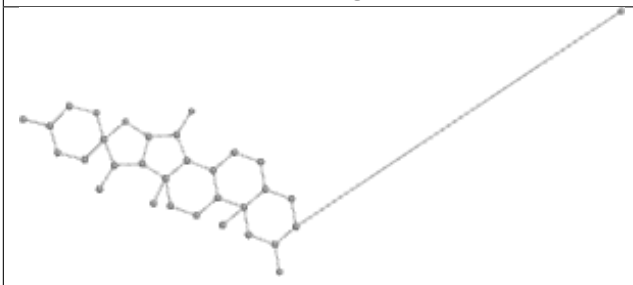
Ligand AJP B 613



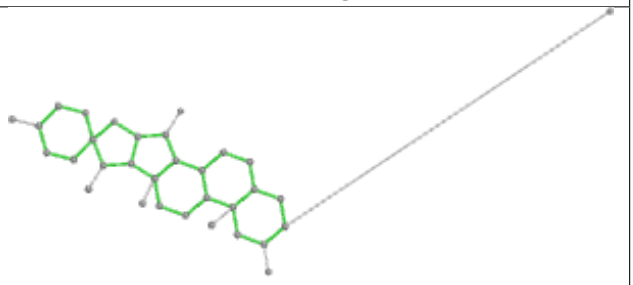
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

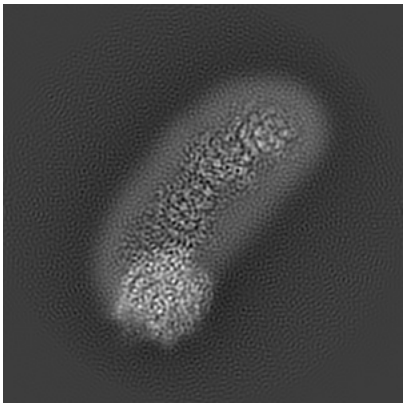
This section contains visualisations of the EMDB entry EMD-0850. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

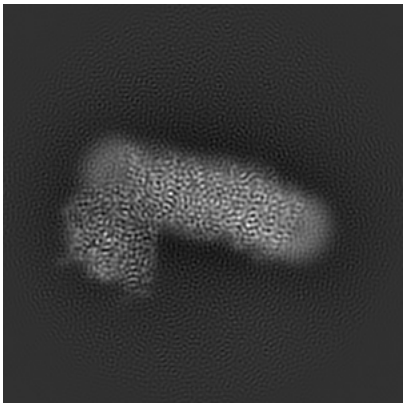
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

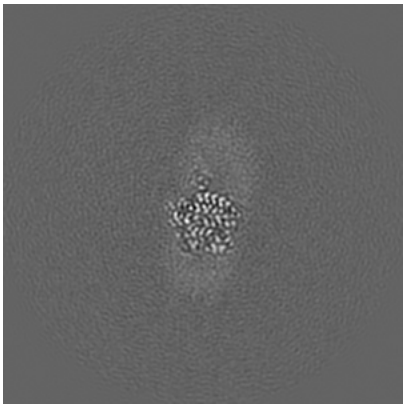


Z

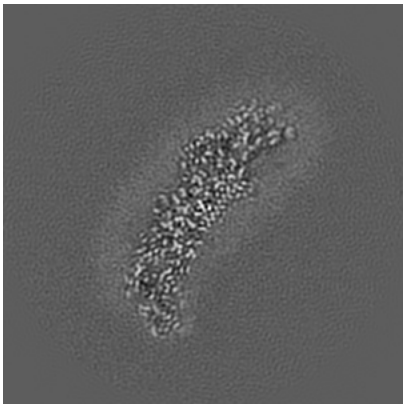
The images above show the map projected in three orthogonal directions.

6.2 Central slices

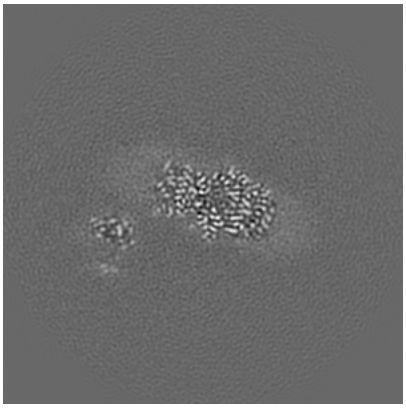
6.2.1 Primary map



X Index: 150



Y Index: 150

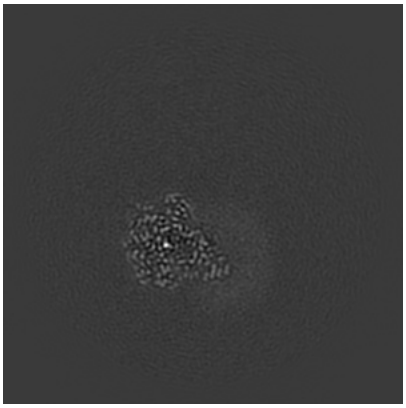


Z Index: 150

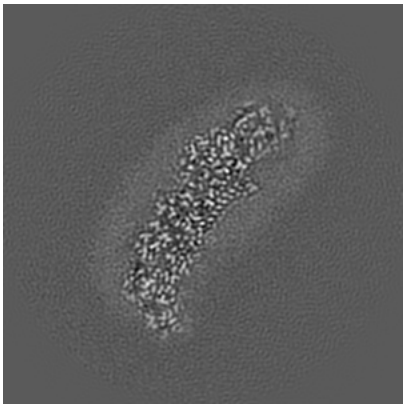
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

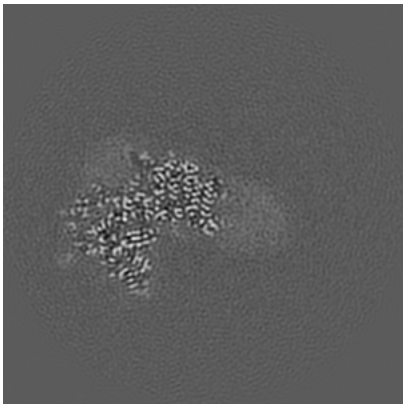
6.3.1 Primary map



X Index: 80



Y Index: 152

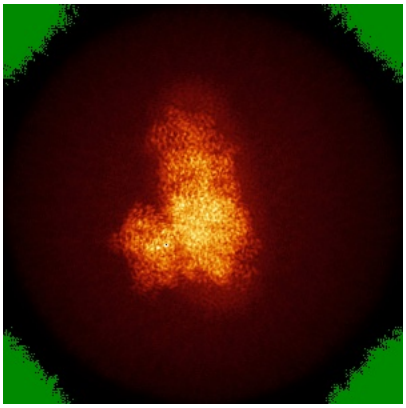


Z Index: 127

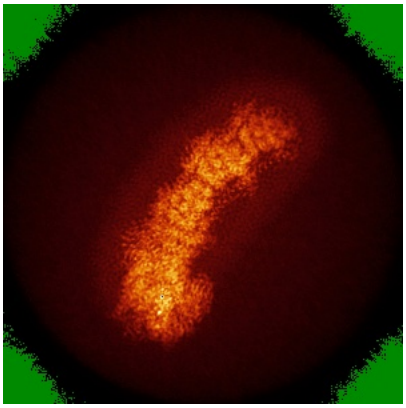
The images above show the largest variance slices of the map in three orthogonal directions.

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

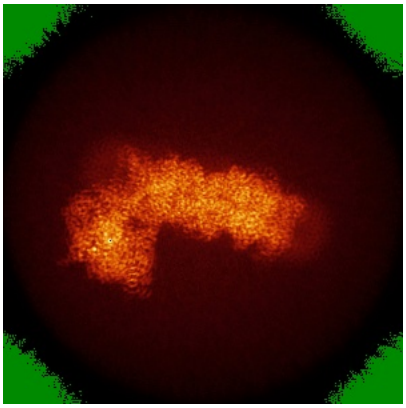
6.4.1 Primary map



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 0.0403. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

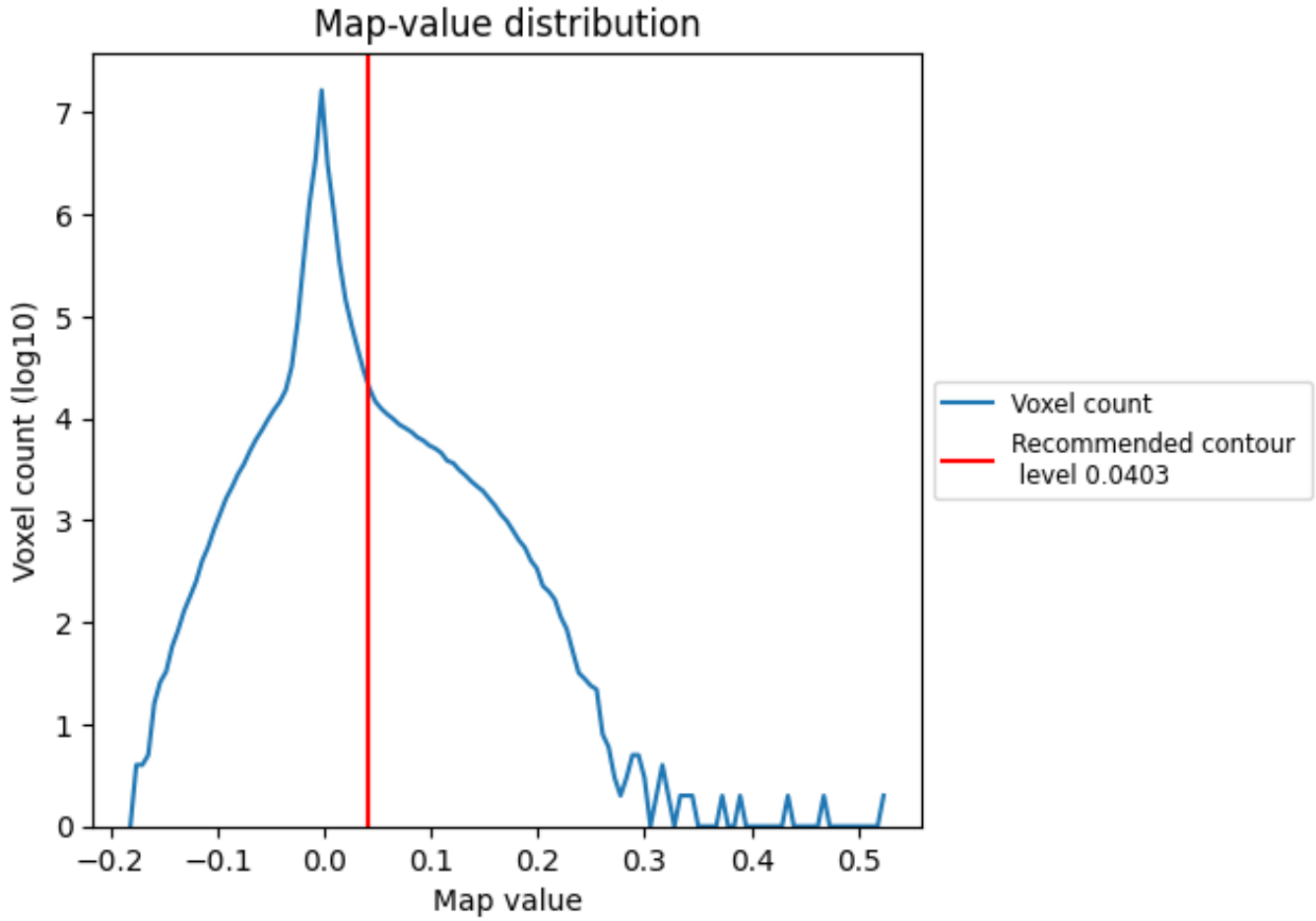
6.6 Mask visualisation (i)

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

7 Map analysis

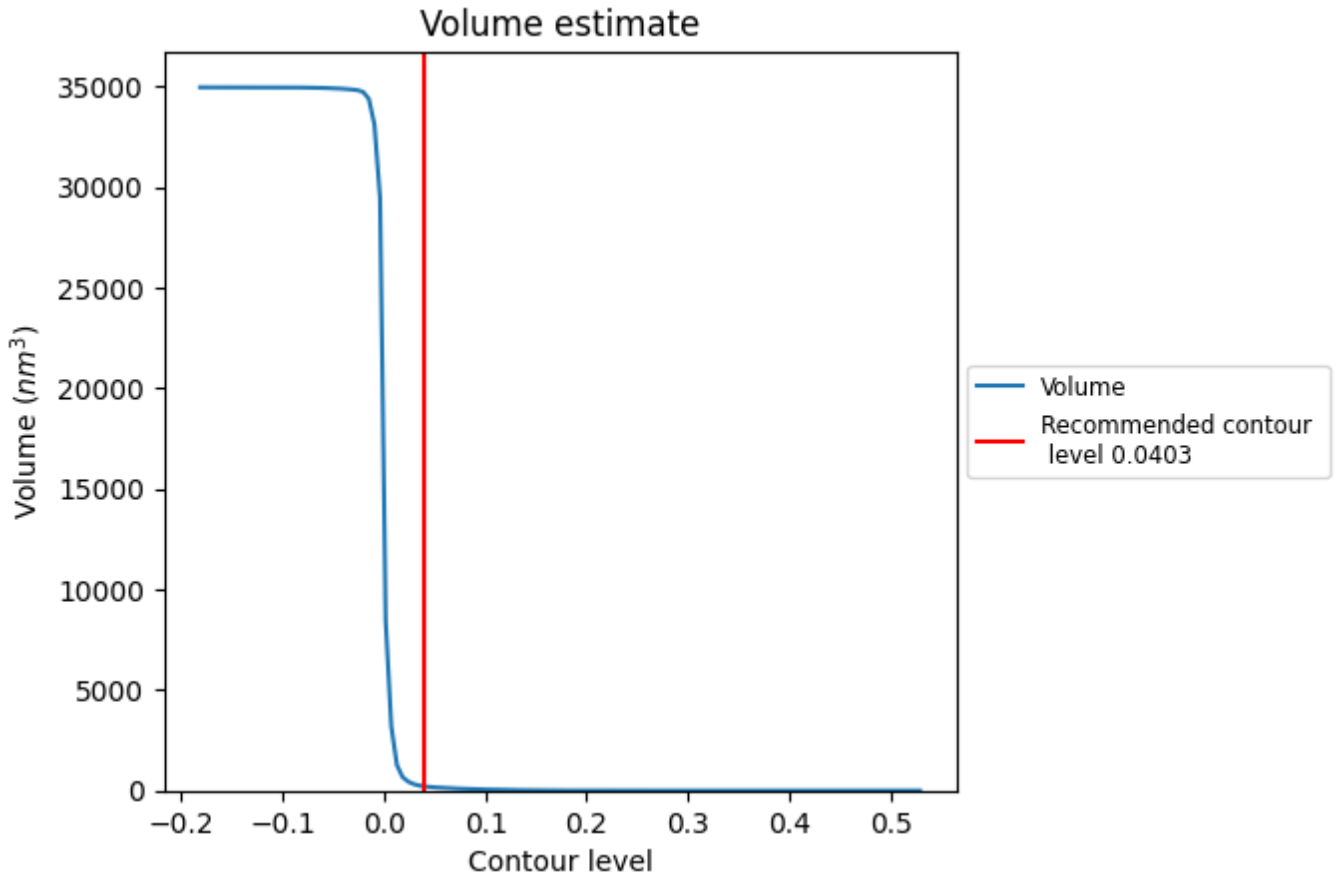
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

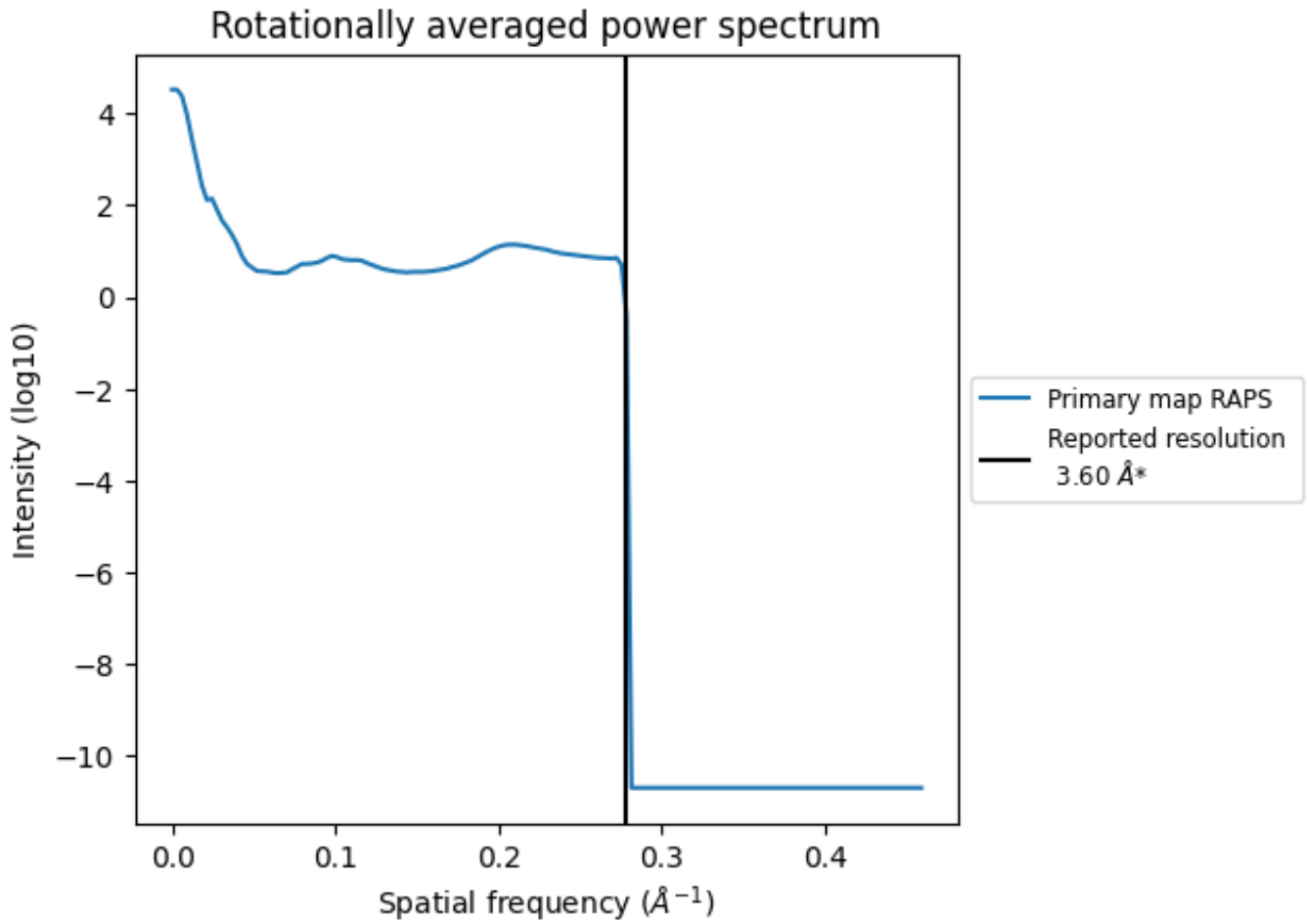
7.2 Volume estimate



The volume at the recommended contour level is 204 nm^3; this corresponds to an approximate mass of 185 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 0.278 Å^{-1}

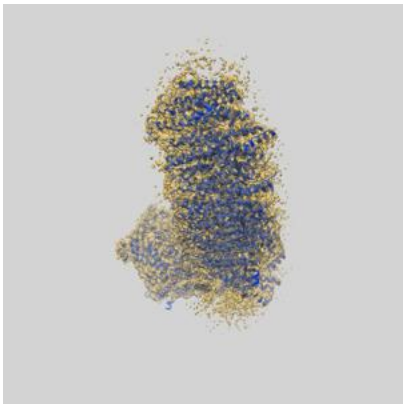
8 Fourier-Shell correlation (i)

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

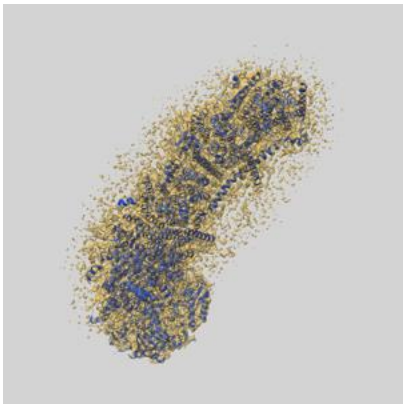
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0850 and PDB model 6L7P. Per-residue inclusion information can be found in section 3 on page 15.

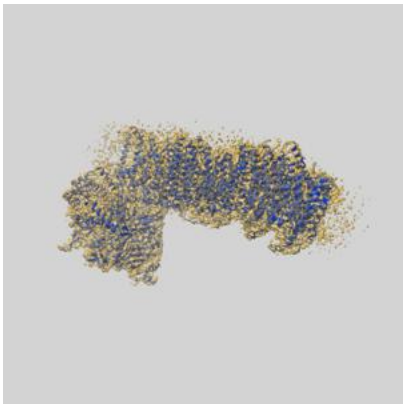
9.1 Map-model overlay



X



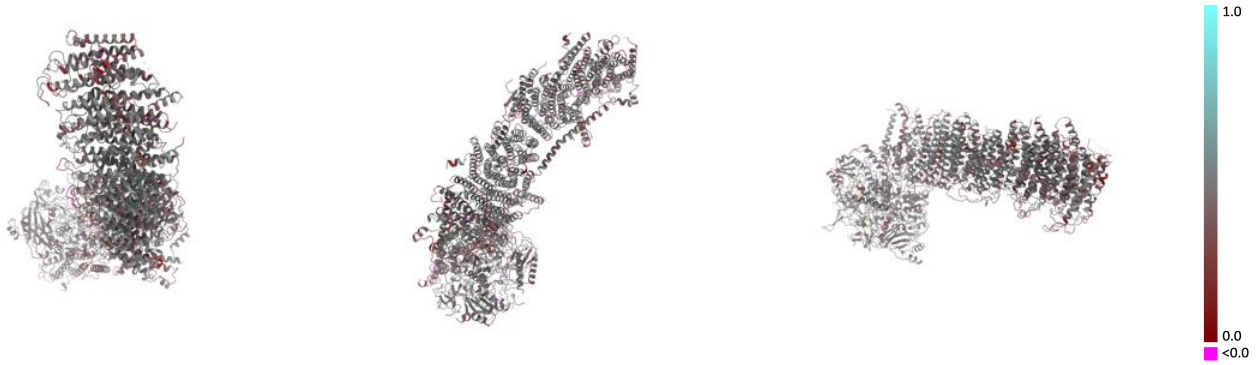
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0403 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.

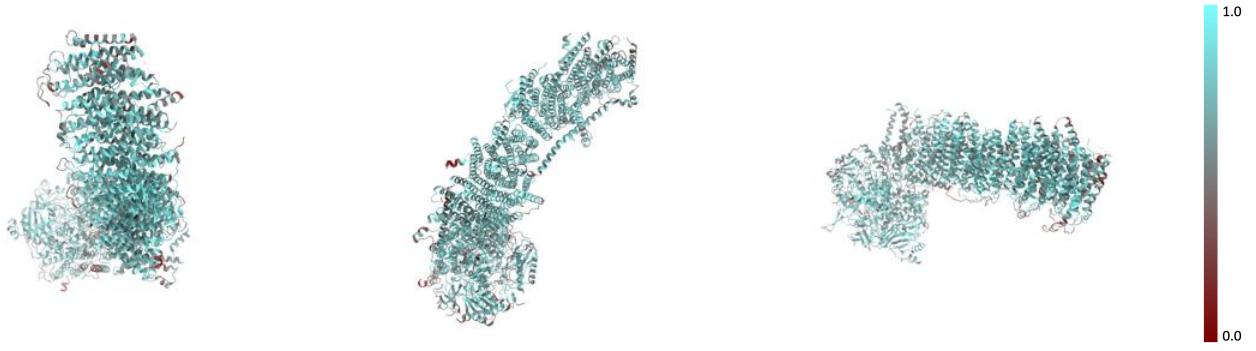
9.2 Q-score mapped to coordinate model



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.

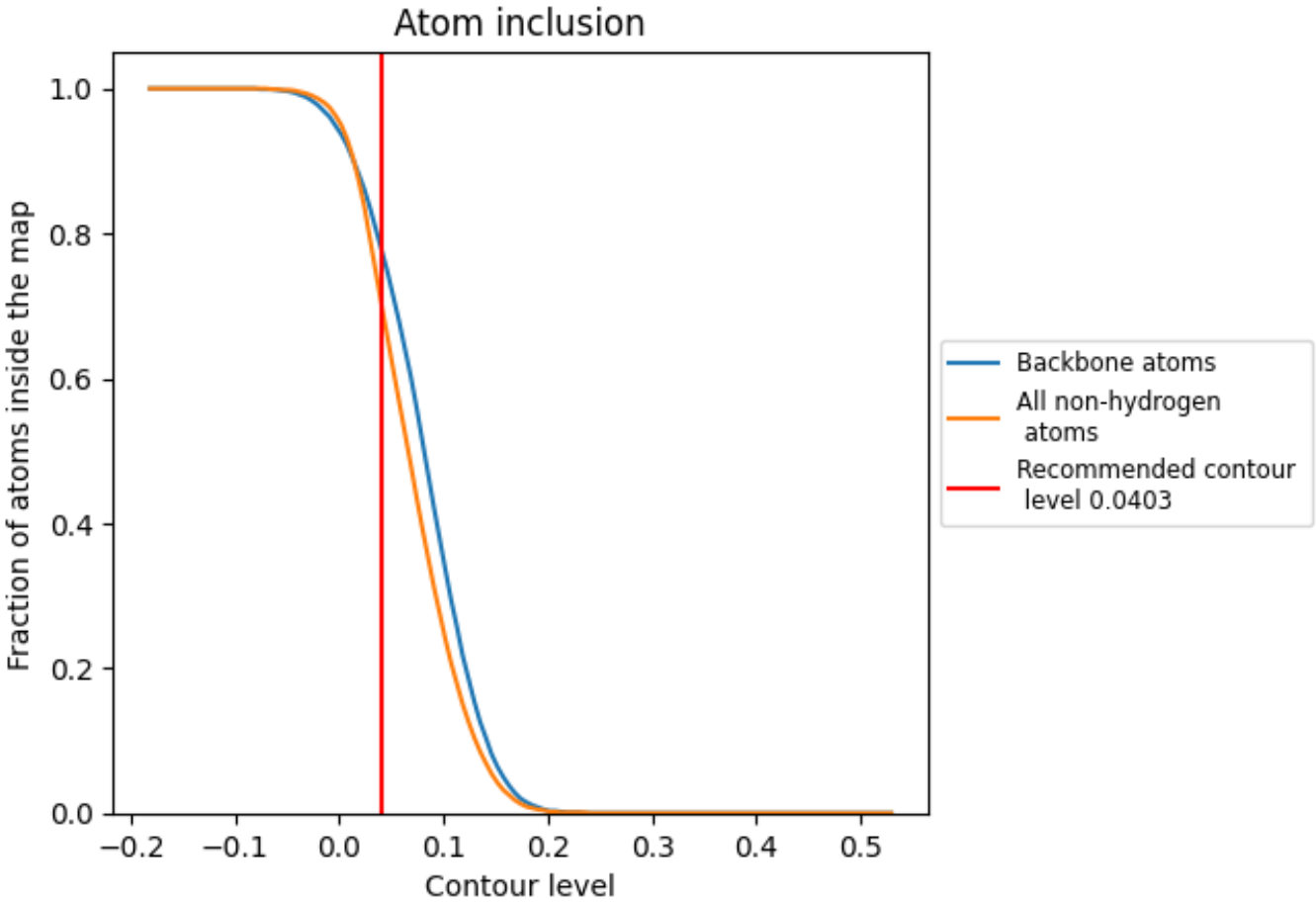
9.3 Atom inclusion mapped to coordinate model



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 (0.0403).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0403) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.4260
A	0.6860	0.4140
B	0.7410	0.4430
C	0.6350	0.4060
D	0.7570	0.4430
E	0.7660	0.4240
F	0.6770	0.4120
G	0.7020	0.4330
H	0.6910	0.4080
I	0.6620	0.4210
J	0.7260	0.4430
K	0.7200	0.4380
L	0.6710	0.4060
M	0.7030	0.4370
N	0.6900	0.4290
O	0.6540	0.4310
P	0.7190	0.4130
Q	0.6380	0.4110
S	0.5390	0.4240