Full wwPDB EM Validation Report

Nov 13, 2024 – 10:23 AM JST

PDB ID	:	8J20
EMDB ID	:	EMD-35940
Title	:	Cryo-EM structure of FFAR3 bound with valeric acid and AR420626
Authors	:	Tai, L.; Li, F.; Sun, X.; Tang, W.; Wang, J.
Deposited on	:	2023-04-14
Resolution	:	3.20 Å(reported)

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

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

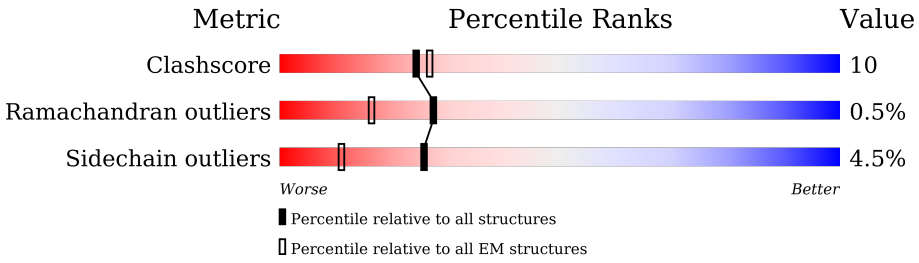
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	377	62% 27% • 10%
2	B	297	58% 18% •• 22%
3	C	354	49% 14% 37%
4	D	314	63% 22% • 13%
5	E	71	69% 10% • 20%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8832 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 Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	340	2610	1609	469	511	21	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P62873
A	2	HIS	-	expression tag	UNP P62873
A	3	HIS	-	expression tag	UNP P62873
A	4	HIS	-	expression tag	UNP P62873
A	5	HIS	-	expression tag	UNP P62873
A	6	HIS	-	expression tag	UNP P62873
A	7	HIS	-	expression tag	UNP P62873
A	8	GLY	-	expression tag	UNP P62873
A	9	SER	-	expression tag	UNP P62873
A	10	LEU	-	expression tag	UNP P62873
A	11	LEU	-	expression tag	UNP P62873
A	12	GLN	-	expression tag	UNP P62873
A	352	GLY	-	expression tag	UNP P62873
A	353	SER	-	expression tag	UNP P62873
A	354	SER	-	expression tag	UNP P62873
A	355	GLY	-	expression tag	UNP P62873
A	356	GLY	-	expression tag	UNP P62873
A	357	GLY	-	expression tag	UNP P62873
A	358	GLY	-	expression tag	UNP P62873
A	359	SER	-	expression tag	UNP P62873
A	360	GLY	-	expression tag	UNP P62873
A	361	GLY	-	expression tag	UNP P62873
A	362	GLY	-	expression tag	UNP P62873
A	363	GLY	-	expression tag	UNP P62873
A	364	SER	-	expression tag	UNP P62873
A	365	SER	-	expression tag	UNP P62873
A	366	GLY	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
A	367	VAL	-	expression tag	UNP P62873
A	368	SER	-	expression tag	UNP P62873
A	369	GLY	-	expression tag	UNP P62873
A	370	TRP	-	expression tag	UNP P62873
A	371	ARG	-	expression tag	UNP P62873
A	372	LEU	-	expression tag	UNP P62873
A	373	PHE	-	expression tag	UNP P62873
A	374	LYS	-	expression tag	UNP P62873
A	375	LYS	-	expression tag	UNP P62873
A	376	ILE	-	expression tag	UNP P62873
A	377	SER	-	expression tag	UNP P62873

- Molecule 2 is a protein called scFV16.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	231	Total	C	N	O	S	0	0
			1775	1125	294	346	10		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	223	Total	C	N	O	S	0	0
			1791	1142	298	337	14		

- Molecule 4 is a protein called Free fatty acid receptor 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	274	Total	C	N	O	S	0	0
			2188	1461	359	358	10		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	GLY	variant	UNP O14843
D	9	PHE	TYR	conflict	UNP O14843
D	11	PRO	SER	conflict	UNP O14843
D	16	LEU	PHE	conflict	UNP O14843
D	23	PHE	LEU	conflict	UNP O14843
D	38	ILE	VAL	variant	UNP O14843
D	44	ARG	GLN	variant	UNP O14843
D	59	LEU	ALA	conflict	UNP O14843
D	77	SER	ASN	variant	UNP O14843

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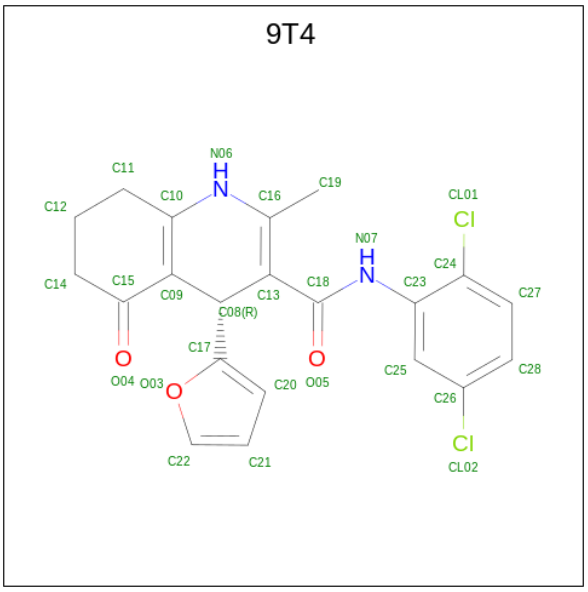
Chain	Residue	Modelled	Actual	Comment	Reference
D	94	LEU	ILE	conflict	UNP O14843
D	119	TYR	HIS	variant	UNP O14843
D	175	GLU	LYS	conflict	UNP O14843
D	194	GLY	VAL	conflict	UNP O14843
D	198	LEU	ILE	conflict	UNP O14843
D	215	ALA	GLY	conflict	UNP O14843
D	220	ARG	GLN	conflict	UNP O14843
D	227	VAL	LEU	variant	UNP O14843
D	251	GLN	CYS	conflict	UNP O14843
D	256	VAL	ALA	variant	UNP O14843
D	259	SER	ILE	conflict	UNP O14843
D	262	LEU	THR	conflict	UNP O14843
D	274	LEU	PHE	conflict	UNP O14843
D	300	PRO	GLN	conflict	UNP O14843

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

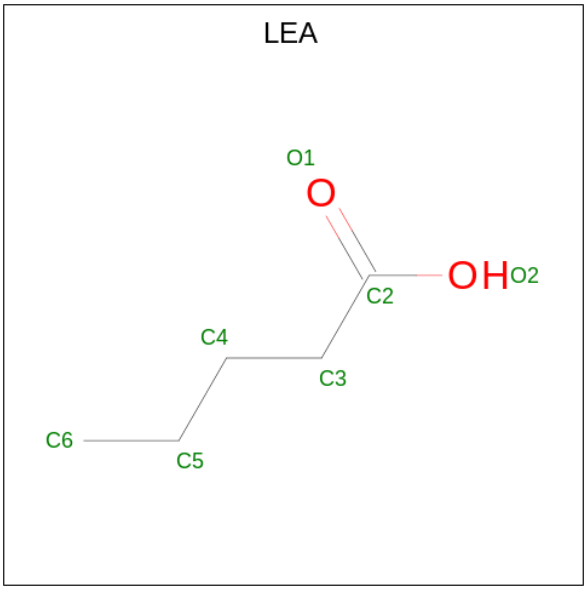
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	57	433	271	75	84	3	0	0

- Molecule 6 is (4R)-N-[2,5-bis(chloranyl)phenyl]-4-(furan-2-yl)-2-methyl-5-oxidanylidene-4,6,7,8-tetrahydro-1H-quinoline-3-carboxamide (three-letter code: 9T4) (formula: $C_{21}H_{18}Cl_2N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	Cl	N	O	0
			28	21	2	2	3	

- Molecule 7 is PENTANOIC ACID (three-letter code: LEA) (formula: $C_5H_{10}O_2$) (labeled as "Ligand of Interest" by depositor).



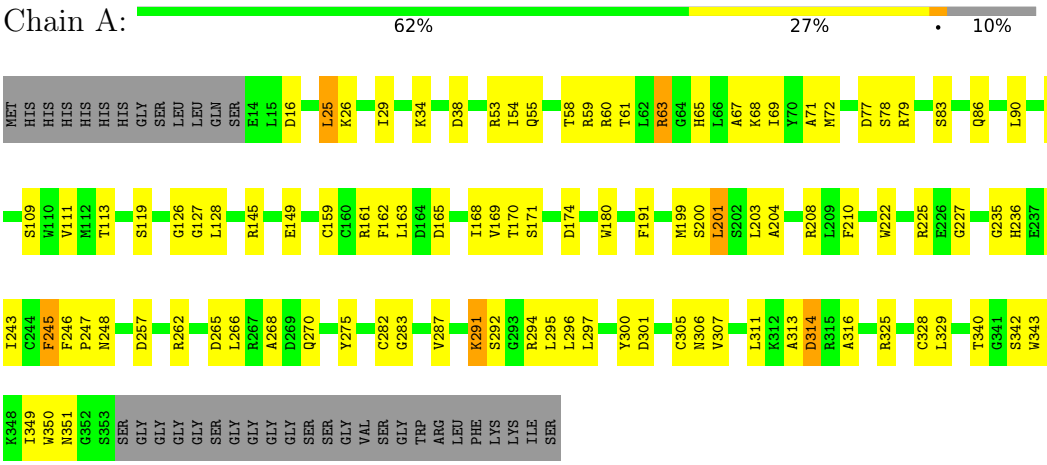
Mol	Chain	Residues	Atoms			AltConf
7	D	1	Total	C	O	0
			7	5	2	

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. 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. 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.

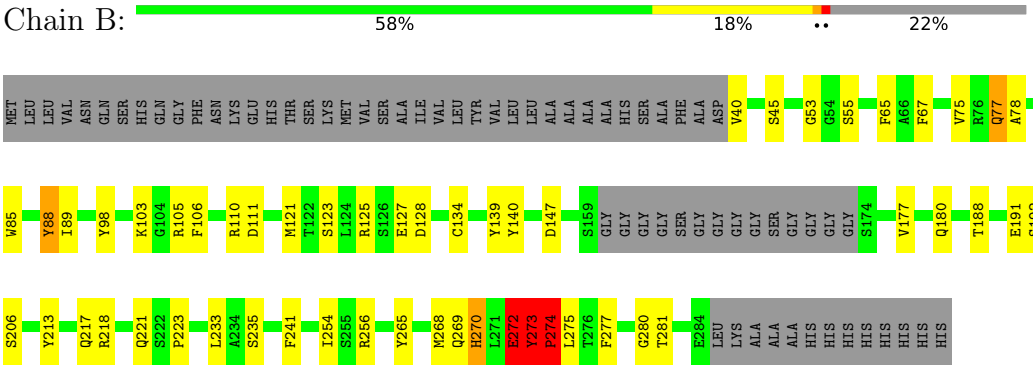
• Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain A:



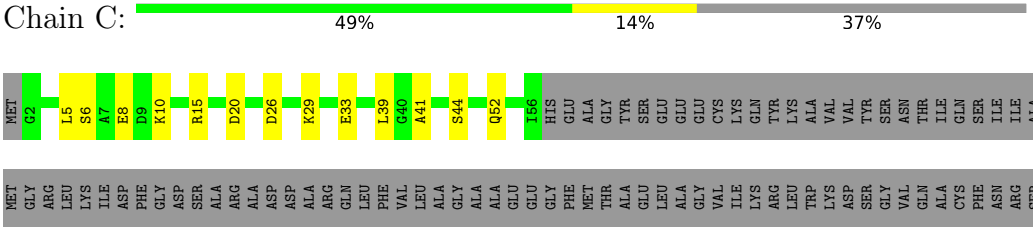
• Molecule 2: scFV16

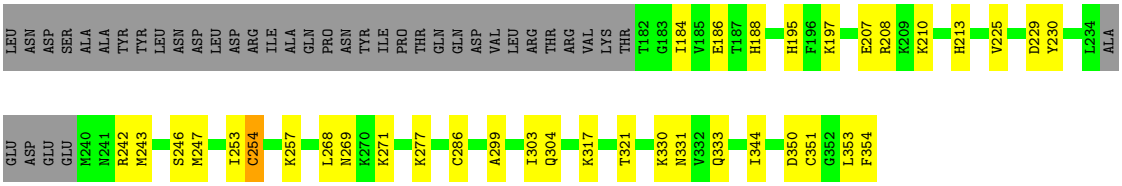
Chain B:



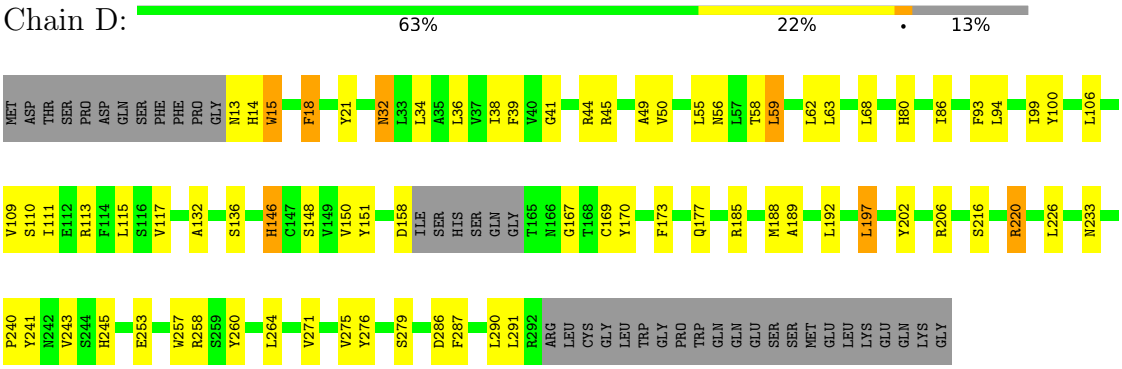
• Molecule 3: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain C:

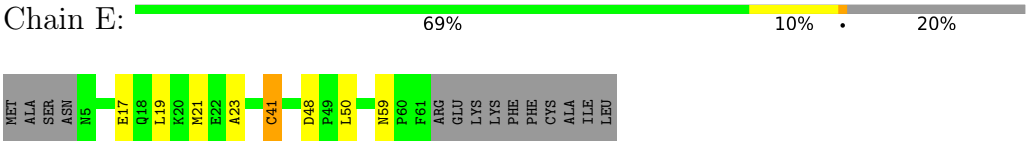




• Molecule 4: Free fatty acid receptor 3



• Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121800	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LEA, 9T4

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	0.24	0/2657	0.55	1/3602 (0.0%)
2	B	0.26	0/1819	0.57	3/2466 (0.1%)
3	C	0.24	0/1820	0.45	0/2440
4	D	0.25	0/2250	0.54	1/3073 (0.0%)
5	E	0.24	0/439	0.42	0/594
All	All	0.25	0/8985	0.53	5/12175 (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
2	B	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	59	LEU	CA-CB-CG	7.63	132.84	115.30
1	A	201	LEU	CA-CB-CG	7.45	132.44	115.30
2	B	273	TYR	N-CA-C	6.96	129.78	111.00
2	B	272	GLU	C-N-CA	5.35	135.07	121.70
2	B	274	PRO	CB-CA-C	5.03	124.57	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	272	GLU	Peptide
2	B	273	TYR	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	2610	0	2513	72	0
2	B	1775	0	1706	35	0
3	C	1791	0	1794	31	0
4	D	2188	0	2251	51	0
5	E	433	0	441	9	0
6	D	28	0	0	4	0
7	D	7	0	9	2	0
All	All	8832	0	8714	184	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 10.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:LEU:HD21	4:D:94:LEU:HD12	1.55	0.89
1:A:161:ARG:HB3	1:A:203:LEU:HD22	1.56	0.86
1:A:29:ILE:HD11	5:E:23:ALA:HA	1.69	0.75
1:A:169:VAL:HG13	1:A:201:LEU:HD21	1.70	0.72
1:A:297:LEU:HG	1:A:307:VAL:HG22	1.74	0.69
2:B:55:SER:HA	2:B:121:MET:O	1.93	0.69
4:D:185:ARG:HH22	4:D:258:ARG:HH12	1.43	0.67
3:C:44:SER:O	3:C:269:ASN:ND2	2.31	0.65
3:C:5:LEU:HB3	3:C:10:LYS:HG2	1.80	0.64
3:C:351:CYS:HA	4:D:50:VAL:HG11	1.81	0.61
3:C:186:GLU:OE1	3:C:197:LYS:NZ	2.33	0.61
4:D:275:VAL:O	4:D:279:SER:HB2	2.00	0.60
1:A:72:MET:HG2	1:A:328:CYS:HB2	1.83	0.60
2:B:270:HIS:HA	2:B:275:LEU:HD22	1.84	0.60
1:A:101:VAL:O	3:C:15:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:PHE:HE1	1:A:266:LEU:HD11	1.66	0.59
2:B:205:HIS:CD2	2:B:206:SER:H	2.20	0.59
1:A:342:SER:OG	1:A:344:ASP:OD1	2.21	0.59
1:A:295:LEU:HD22	5:E:50:LEU:HB3	1.85	0.59
2:B:125:ARG:HG3	2:B:127:GLU:HG2	1.83	0.59
4:D:233:ASN:HD21	4:D:271:VAL:HG11	1.68	0.58
1:A:340:THR:HG1	1:A:350:TRP:HE1	1.51	0.58
3:C:243:MET:O	3:C:247:MET:HG2	2.04	0.58
2:B:213:TYR:HB2	2:B:268:MET:HB3	1.86	0.58
4:D:56:ASN:HD22	4:D:136:SER:HB2	1.69	0.58
1:A:111:VAL:HA	1:A:127:GLY:HA3	1.85	0.58
4:D:93:PHE:HD2	4:D:94:LEU:HD22	1.69	0.57
2:B:177:VAL:HG22	2:B:200:SER:HB3	1.85	0.57
1:A:26:LYS:HG2	5:E:19:LEU:HD11	1.85	0.57
1:A:242:ALA:HB1	1:A:287:VAL:H	1.70	0.57
2:B:78:ALA:HB3	2:B:81:LYS:HB2	1.85	0.57
1:A:161:ARG:HG3	1:A:203:LEU:HB2	1.86	0.56
2:B:111:ASP:OD1	2:B:111:ASP:N	2.38	0.56
2:B:105:ARG:NH2	2:B:128:ASP:OD2	2.39	0.56
2:B:213:TYR:HE1	2:B:270:HIS:HB2	1.70	0.56
3:C:344:ILE:HG23	4:D:117:VAL:HG22	1.88	0.56
4:D:59:LEU:HA	4:D:62:LEU:HD23	1.86	0.56
2:B:241:PHE:HD1	2:B:254:ILE:HD12	1.70	0.56
1:A:351:ASN:ND2	5:E:59:ASN:OD1	2.39	0.56
1:A:246:PHE:O	1:A:248:ASN:N	2.39	0.55
4:D:146:HIS:HB3	4:D:188:MET:HE3	1.88	0.55
4:D:216:SER:O	4:D:220:ARG:NH2	2.40	0.55
1:A:208:ARG:HE	1:A:225:ARG:HE	1.54	0.55
1:A:294:ARG:HD2	5:E:41:CYS:SG	2.47	0.55
3:C:254:CYS:O	3:C:317:LYS:NZ	2.39	0.55
2:B:218:ARG:HB2	2:B:221:GLN:HB2	1.88	0.54
4:D:150:VAL:HG21	7:D:402:LEA:H52	1.89	0.54
1:A:305:CYS:SG	1:A:306:ASN:N	2.81	0.54
4:D:197:LEU:HA	6:D:401:9T4:CL02	2.45	0.54
4:D:55:LEU:O	4:D:59:LEU:HD23	2.08	0.54
2:B:269:GLN:HE21	2:B:275:LEU:HA	1.73	0.54
4:D:189:ALA:HB2	4:D:245:HIS:CE1	2.44	0.53
2:B:67:PHE:O	2:B:110:ARG:NH2	2.41	0.53
4:D:158:ASP:OD1	4:D:158:ASP:N	2.40	0.53
1:A:201:LEU:HD23	1:A:201:LEU:O	2.08	0.53
4:D:100:TYR:HD1	4:D:192:LEU:HD12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:SER:HA	4:D:151:TYR:CE2	2.44	0.53
5:E:17:GLU:O	5:E:21:MET:HG3	2.09	0.52
2:B:265:TYR:O	2:B:280:GLY:HA2	2.09	0.52
4:D:80:HIS:NE2	4:D:167:GLY:O	2.43	0.51
1:A:282:CYS:HB2	1:A:301:ASP:HB2	1.92	0.51
4:D:58:THR:O	4:D:62:LEU:HD22	2.10	0.51
1:A:287:VAL:HG13	1:A:296:LEU:HD11	1.92	0.51
3:C:33:GLU:OE1	3:C:195:HIS:ND1	2.43	0.51
4:D:113:ARG:NH1	6:D:401:9T4:O04	2.41	0.51
4:D:240:PRO:HA	4:D:243:VAL:HG22	1.93	0.51
1:A:25:LEU:HB3	5:E:19:LEU:HD13	1.91	0.51
3:C:230:TYR:HB2	3:C:286:CYS:HB2	1.91	0.51
2:B:192:SER:HA	2:B:254:ILE:O	2.11	0.51
3:C:225:VAL:HG13	3:C:268:LEU:HD13	1.92	0.51
4:D:197:LEU:HD23	6:D:401:9T4:CL02	2.49	0.50
1:A:54:ILE:HD12	1:A:316:ALA:HB1	1.94	0.50
1:A:307:VAL:HG12	1:A:316:ALA:HB3	1.93	0.50
2:B:77:GLN:HG3	2:B:83:LEU:HA	1.94	0.49
1:A:171:SER:HB3	1:A:201:LEU:HD13	1.92	0.49
1:A:101:VAL:HG13	2:B:140:TYR:HB2	1.94	0.49
1:A:78:SER:O	1:A:78:SER:OG	2.27	0.49
4:D:41:GLY:O	4:D:45:ARG:HG2	2.13	0.49
1:A:297:LEU:HB3	1:A:329:LEU:HD11	1.94	0.48
1:A:16:ASP:N	1:A:16:ASP:OD1	2.44	0.48
1:A:71:ALA:HB3	1:A:347:LEU:HD21	1.95	0.48
4:D:260:TYR:O	4:D:264:LEU:HG	2.13	0.48
1:A:200:SER:HB2	1:A:243:ILE:HB	1.95	0.48
4:D:148:SER:HA	4:D:151:TYR:CD2	2.49	0.48
1:A:25:LEU:HD13	5:E:19:LEU:HB3	1.96	0.47
3:C:207:GLU:HB3	3:C:210:LYS:HG2	1.95	0.47
1:A:235:GLY:O	1:A:262:ARG:NE	2.46	0.47
2:B:106:PHE:HE1	2:B:121:MET:HG2	1.80	0.47
4:D:13:ASN:OD1	4:D:14:HIS:N	2.46	0.47
4:D:185:ARG:HH22	4:D:258:ARG:NH1	2.12	0.47
3:C:29:LYS:HB2	3:C:29:LYS:NZ	2.29	0.47
4:D:173:PHE:HB3	4:D:177:GLN:NE2	2.29	0.47
2:B:98:TYR:HB2	2:B:103:LYS:HD3	1.97	0.46
1:A:113:THR:HB	1:A:126:GLY:H	1.79	0.46
2:B:75:VAL:HG13	2:B:85:TRP:HA	1.97	0.46
4:D:86:ILE:H	4:D:86:ILE:HD12	1.80	0.46
1:A:161:ARG:HD3	1:A:161:ARG:HA	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:TYR:CD1	3:C:8:GLU:HG2	2.49	0.46
4:D:38:ILE:H	4:D:38:ILE:HD12	1.80	0.46
1:A:238:SER:OG	1:A:239:ASP:N	2.48	0.46
2:B:241:PHE:CD1	2:B:254:ILE:HD12	2.49	0.46
1:A:301:ASP:HA	1:A:325:ARG:HG3	1.97	0.45
2:B:147:ASP:N	2:B:147:ASP:OD1	2.47	0.45
4:D:56:ASN:ND2	4:D:136:SER:HB2	2.31	0.45
1:A:292:SER:HB3	5:E:48:ASP:HB2	1.98	0.45
1:A:67:ALA:HB1	1:A:86:GLN:HB2	1.99	0.45
1:A:53:ARG:HH21	1:A:55:GLN:HE22	1.65	0.45
2:B:217:GLN:NE2	2:B:223:PRO:HG3	2.31	0.45
1:A:161:ARG:O	1:A:168:ILE:HG13	2.17	0.45
3:C:6:SER:O	3:C:8:GLU:N	2.50	0.45
1:A:54:ILE:HD13	1:A:295:LEU:HD21	1.99	0.44
2:B:272:GLU:O	2:B:274:PRO:HB2	2.17	0.44
1:A:58:THR:HA	1:A:350:TRP:HA	1.99	0.44
1:A:69:ILE:HD13	1:A:347:LEU:HG	1.98	0.44
1:A:128:LEU:HD11	3:C:184:ILE:HD11	1.99	0.44
1:A:191:PHE:HB3	1:A:222:TRP:CE3	2.52	0.44
1:A:291:LYS:HB2	1:A:291:LYS:HE2	1.74	0.44
3:C:210:LYS:O	3:C:213:HIS:NE2	2.51	0.44
3:C:353:LEU:HD11	6:D:401:9T4:C21	2.48	0.44
1:A:25:LEU:HD23	1:A:25:LEU:HA	1.85	0.44
2:B:180:GLN:OE1	2:B:281:THR:OG1	2.32	0.44
1:A:58:THR:HB	1:A:350:TRP:CD2	2.52	0.44
1:A:60:ARG:HG3	1:A:349:ILE:HD12	2.00	0.44
2:B:40:VAL:HG23	2:B:65:PHE:CD1	2.53	0.44
4:D:39:PHE:HB3	4:D:55:LEU:HD13	1.98	0.44
2:B:89:ILE:HD13	2:B:110:ARG:HG3	1.98	0.44
3:C:277:LYS:HG2	3:C:277:LYS:O	2.18	0.44
1:A:163:LEU:HD13	1:A:203:LEU:HD21	2.00	0.43
3:C:304:GLN:HG3	3:C:321:THR:HG21	1.99	0.43
4:D:15:TRP:HA	4:D:18:PHE:CD1	2.53	0.43
1:A:79:ARG:NE	1:A:94:ASP:OD1	2.47	0.43
2:B:53:GLY:HA2	2:B:123:SER:HA	2.00	0.43
4:D:68:LEU:HD23	4:D:68:LEU:HA	1.86	0.43
4:D:257:TRP:HB3	4:D:260:TYR:HE1	1.83	0.43
3:C:52:GLN:OE1	3:C:331:ASN:ND2	2.50	0.43
4:D:56:ASN:HA	4:D:59:LEU:HD23	2.00	0.43
4:D:36:LEU:HD13	4:D:62:LEU:HD21	2.01	0.43
1:A:236:HIS:CE1	1:A:262:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.85	0.43
3:C:230:TYR:HB2	3:C:286:CYS:CB	2.49	0.43
4:D:202:TYR:CZ	4:D:206:ARG:HD2	2.53	0.43
1:A:68:LYS:HB3	1:A:343:TRP:CD1	2.53	0.43
1:A:265:ASP:HB3	1:A:268:ALA:HB3	2.00	0.42
3:C:188:HIS:HB3	3:C:195:HIS:CE1	2.54	0.42
4:D:15:TRP:HA	4:D:18:PHE:HD1	1.84	0.42
1:A:119:SER:OG	1:A:165:ASP:OD1	2.37	0.42
1:A:163:LEU:HD22	1:A:203:LEU:HD21	2.01	0.42
4:D:49:ALA:HB1	4:D:132:ALA:HB2	2.00	0.42
3:C:330:LYS:HG2	3:C:333:GLN:HB3	2.02	0.42
2:B:188:THR:HG23	2:B:191:GLU:HB2	2.02	0.42
4:D:226:LEU:HD23	4:D:226:LEU:HA	1.88	0.42
4:D:286:ASP:O	4:D:290:LEU:HD22	2.20	0.42
2:B:269:GLN:NE2	2:B:275:LEU:HA	2.34	0.42
3:C:299:ALA:O	3:C:303:ILE:HG13	2.20	0.42
1:A:191:PHE:HE1	1:A:227:GLY:HA2	1.85	0.42
1:A:34:LYS:HE3	1:A:34:LYS:HB3	1.87	0.41
3:C:208:ARG:HH11	3:C:208:ARG:HG3	1.85	0.41
1:A:60:ARG:NH1	1:A:95:SER:O	2.52	0.41
1:A:170:THR:OG1	1:A:180:TRP:NE1	2.41	0.41
4:D:111:ILE:O	4:D:115:LEU:HD12	2.19	0.41
1:A:72:MET:HE2	1:A:328:CYS:C	2.41	0.41
1:A:314:ASP:N	1:A:314:ASP:OD1	2.53	0.41
2:B:85:TRP:HZ2	2:B:88:TYR:HB3	1.85	0.41
2:B:106:PHE:CE1	2:B:121:MET:HG2	2.55	0.41
3:C:271:LYS:HE3	3:C:271:LYS:HB3	1.84	0.41
1:A:174:ASP:OD1	1:A:174:ASP:N	2.54	0.41
3:C:41:ALA:HB2	3:C:246:SER:HB2	2.02	0.41
4:D:100:TYR:HE2	4:D:241:TYR:HE2	1.68	0.41
1:A:61:THR:HG22	1:A:63:ARG:HG2	2.03	0.41
1:A:257:ASP:O	1:A:283:GLY:HA2	2.21	0.41
3:C:257:LYS:H	3:C:257:LYS:HG2	1.64	0.41
4:D:32:ASN:HB2	4:D:62:LEU:CD1	2.50	0.41
1:A:65:HIS:CD2	1:A:83:SER:HG	2.37	0.40
1:A:83:SER:O	1:A:90:LEU:HD23	2.21	0.40
4:D:287:PHE:CE1	4:D:291:LEU:HD21	2.55	0.40
1:A:59:ARG:O	1:A:60:ARG:HG2	2.21	0.40
2:B:83:LEU:HD13	2:B:277:PHE:CZ	2.57	0.40
4:D:34:LEU:HD11	4:D:287:PHE:HE1	1.86	0.40
4:D:106:LEU:HA	4:D:109:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:TYR:CE2	1:A:306:ASN:HB2	2.56	0.40
3:C:39:LEU:HD13	3:C:253:ILE:HG13	2.02	0.40
3:C:229:ASP:HB3	3:C:242:ARG:HB2	2.03	0.40
4:D:99:ILE:HD13	4:D:99:ILE:HA	1.84	0.40
4:D:185:ARG:HH21	7:D:402:LEA:C2	2.35	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	338/377 (90%)	309 (91%)	25 (7%)	4 (1%)	11 43
2	B	227/297 (76%)	216 (95%)	9 (4%)	2 (1%)	14 49
3	C	217/354 (61%)	210 (97%)	7 (3%)	0	100 100
4	D	270/314 (86%)	262 (97%)	8 (3%)	0	100 100
5	E	55/71 (78%)	55 (100%)	0	0	100 100
All	All	1107/1413 (78%)	1052 (95%)	49 (4%)	6 (0%)	27 60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	ALA
2	B	273	TYR
2	B	274	PRO
1	A	159	CYS
1	A	204	ALA
1	A	247	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	282/308 (92%)	266 (94%)	16 (6%)	17 50
2	B	196/239 (82%)	188 (96%)	8 (4%)	26 59
3	C	198/305 (65%)	193 (98%)	5 (2%)	42 71
4	D	239/274 (87%)	226 (95%)	13 (5%)	18 51
5	E	46/58 (79%)	45 (98%)	1 (2%)	47 73
All	All	961/1184 (81%)	918 (96%)	43 (4%)	26 56

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	38	ASP
1	A	63	ARG
1	A	77	ASP
1	A	109	SER
1	A	145	ARG
1	A	149	GLU
1	A	162	PHE
1	A	199	MET
1	A	210	PHE
1	A	245	PHE
1	A	270	GLN
1	A	275	TYR
1	A	291	LYS
1	A	314	ASP
1	A	346	PHE
2	B	45	SER
2	B	77	GLN
2	B	88	TYR
2	B	134	CYS
2	B	233	LEU
2	B	235	SER
2	B	256	ARG

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Mol	Chain	Res	Type
2	B	270	HIS
3	C	20	ASP
3	C	26	ASP
3	C	254	CYS
3	C	350	ASP
3	C	354	PHE
4	D	15	TRP
4	D	18	PHE
4	D	21	TYR
4	D	32	ASN
4	D	44	ARG
4	D	110	SER
4	D	146	HIS
4	D	169	CYS
4	D	170	TYR
4	D	197	LEU
4	D	220	ARG
4	D	253	GLU
4	D	276	TYR
5	E	41	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	77	GLN
2	B	205	HIS
2	B	217	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
7	LEA	D	402	-	6,6,6	1.02	0	6,6,6	1.16	1 (16%)
6	9T4	D	401	-	27,31,31	5.70	20 (74%)	41,45,45	2.10	11 (26%)

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
7	LEA	D	402	-	-	1/4/4/4	-
6	9T4	D	401	-	-	0/8/42/42	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	401	9T4	C16-C13	14.03	1.52	1.35
6	D	401	9T4	C10-C09	12.70	1.52	1.36
6	D	401	9T4	C25-C26	8.72	1.52	1.38
6	D	401	9T4	C25-C23	8.55	1.52	1.39
6	D	401	9T4	C28-C26	8.11	1.53	1.38
6	D	401	9T4	C28-C27	8.01	1.53	1.38
6	D	401	9T4	C27-C24	6.95	1.53	1.38
6	D	401	9T4	C23-C24	5.75	1.53	1.39
6	D	401	9T4	C10-N06	5.42	1.46	1.37
6	D	401	9T4	C18-N07	4.76	1.45	1.35
6	D	401	9T4	C08-C09	4.37	1.58	1.52
6	D	401	9T4	C15-C09	4.32	1.53	1.45
6	D	401	9T4	C16-N06	4.12	1.44	1.38
6	D	401	9T4	C18-C13	3.30	1.53	1.49
6	D	401	9T4	C11-C10	2.57	1.54	1.49
6	D	401	9T4	O05-C18	-2.52	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	401	9T4	C24-CL01	2.14	1.78	1.73
6	D	401	9T4	C23-N07	2.10	1.45	1.41
6	D	401	9T4	C14-C15	2.08	1.53	1.50
6	D	401	9T4	O04-C15	-2.08	1.18	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	401	9T4	C19-C16-C13	-7.39	120.22	127.62
6	D	401	9T4	C11-C10-C09	-4.78	117.79	123.49
6	D	401	9T4	C19-C16-N06	4.47	118.77	113.45
6	D	401	9T4	C11-C10-N06	3.16	120.20	115.34
6	D	401	9T4	C13-C18-N07	3.10	120.09	115.81
6	D	401	9T4	C16-N06-C10	-2.62	120.25	122.43
6	D	401	9T4	C18-C13-C16	-2.33	118.18	123.09
6	D	401	9T4	C23-N07-C18	-2.22	120.61	126.80
7	D	402	LEA	O1-C2-C3	-2.21	115.97	123.08
6	D	401	9T4	C13-C08-C09	2.16	113.38	109.78
6	D	401	9T4	C21-C20-C17	2.14	107.99	106.91
6	D	401	9T4	C13-C16-N06	2.07	120.99	119.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	402	LEA	C2-C3-C4-C5

There are no ring outliers.

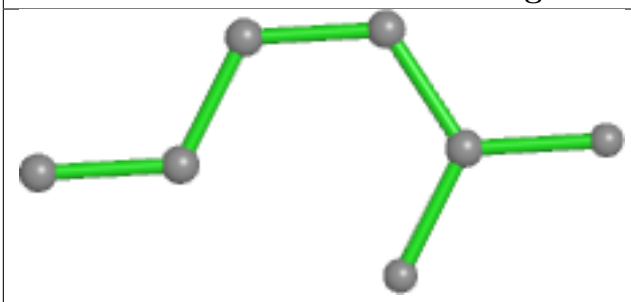
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	402	LEA	2	0
6	D	401	9T4	4	0

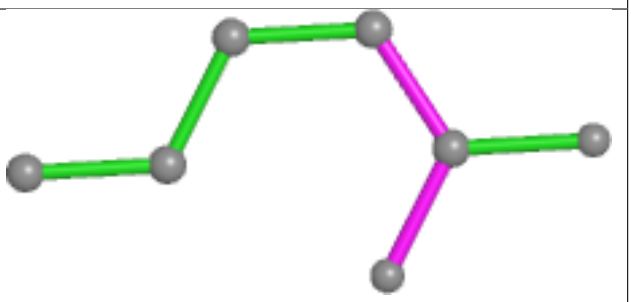
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

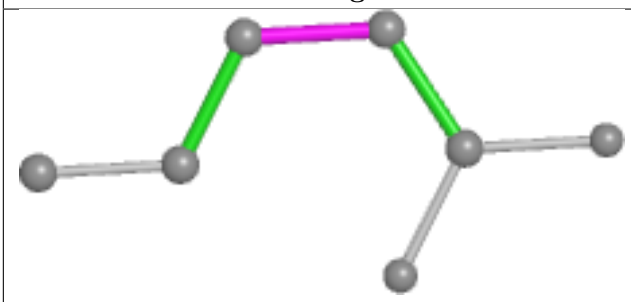
Ligand LEA D 402



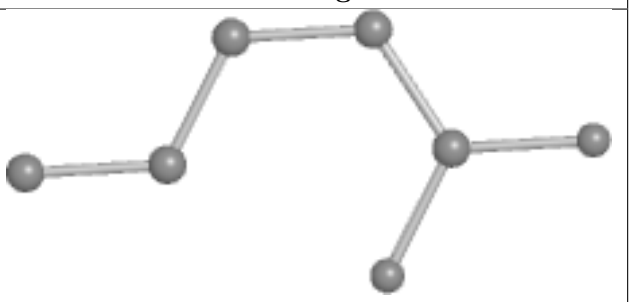
Bond lengths



Bond angles

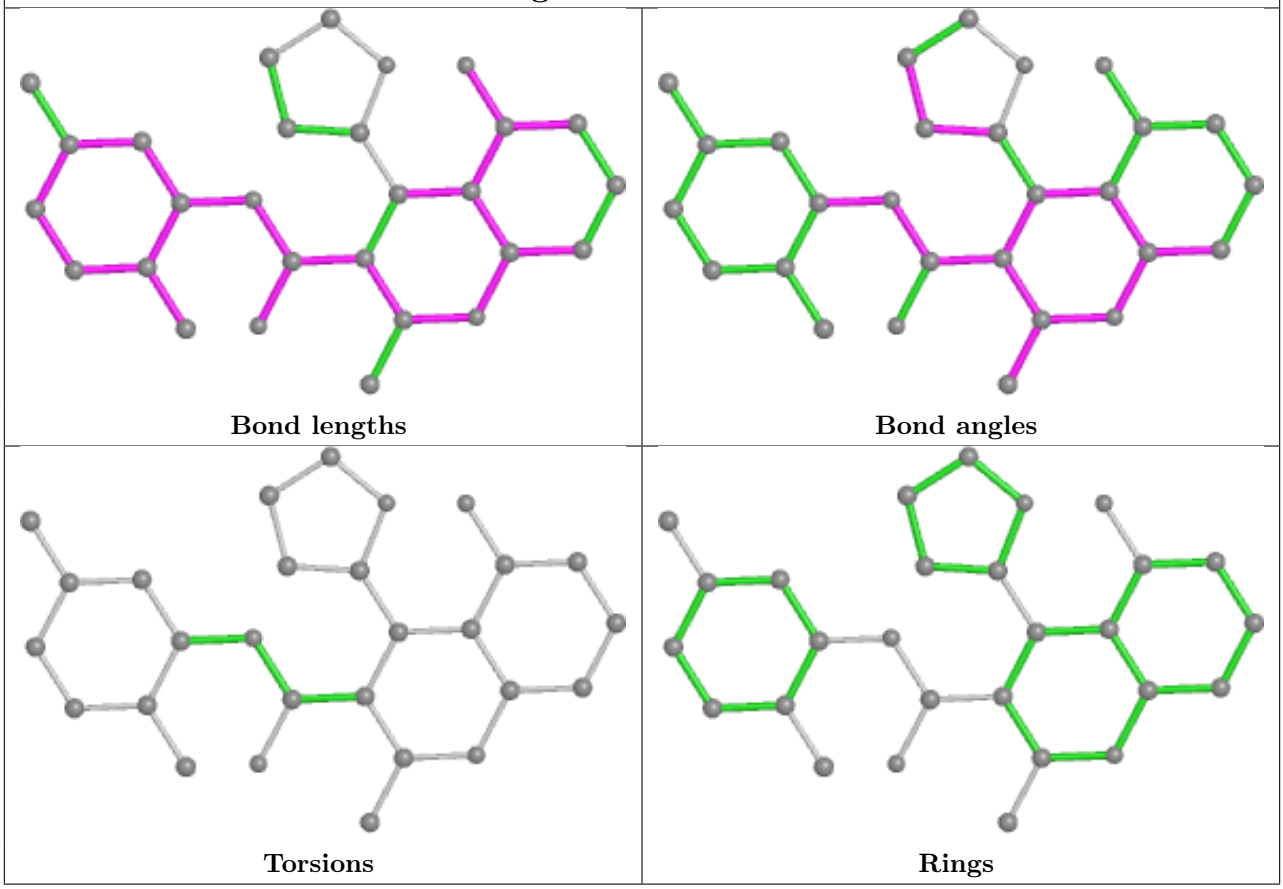


Torsions



Rings

Ligand 9T4 D 401



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.