wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 07:04 AM EDT

PDB ID	:	1NU9
Title	:	Staphylocoagulase-Prethrombin-2 complex
Authors	:	Friedrich, R.; Bode, W.; Fuentes-Prior, P.; Panizzi, P.; Bock, P.E.
Deposited on	:	2003-01-31
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

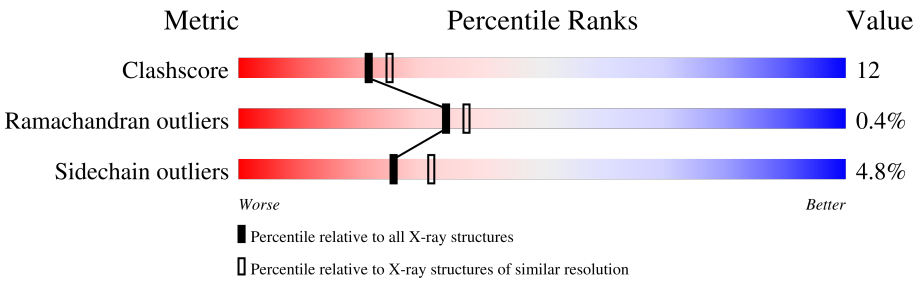
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	291	72% 24% •
1	D	291	73% 24% •
2	C	281	77% 20% •
2	F	281	81% 17% •

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
3	0ZJ	A	299	X	-	-	-
3	0ZJ	D	299	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10253 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

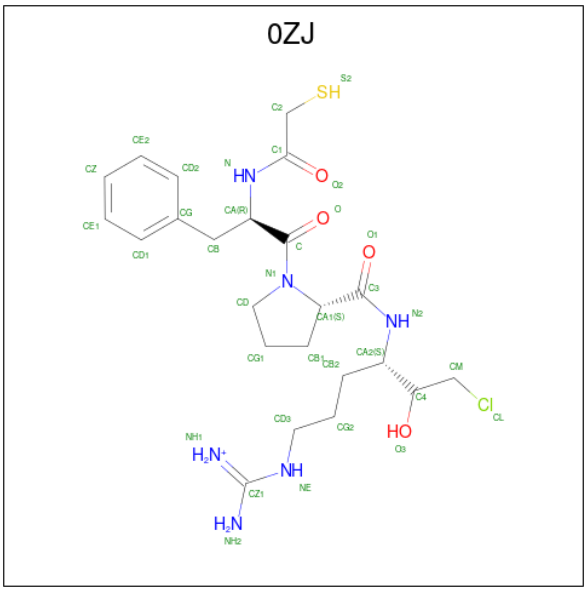
- Molecule 1 is a protein called Thrombin light and heavy chains.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	2341	1488	413	425	15	19	0	0
1	D	290	2341	1488	413	425	15	35	0	0

- Molecule 2 is a protein called Staphylocoagulase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	281	2338	1477	386	470	5	27	0	0
2	F	281	2338	1477	386	470	5	20	0	0

- Molecule 3 is N-(sulfanylacetyl)-D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (three-letter code: 0ZJ) (formula: $C_{23}H_{36}ClN_6O_4S$).

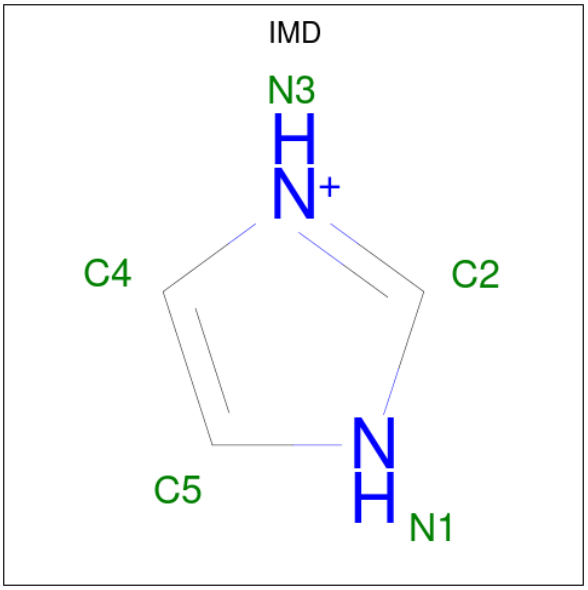


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	34	23	6	4	1	0	0
3	D	1	34	23	6	4	1	0	0

- Molecule 4 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
4	C	2	2	2	0	0
4	F	2	2	2	0	0

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	C	1	5	3	2	0	0
5	C	1	5	3	2	0	0
5	C	1	5	3	2	0	0
5	F	1	5	3	2	0	0
5	F	1	5	3	2	0	0
5	F	1	5	3	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	160	160	160	0	0
			Total	O		
6	C	250	250	250	0	0
			Total	O		
6	D	148	148	148	0	0
			Total	O		
6	F	235	235	235	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

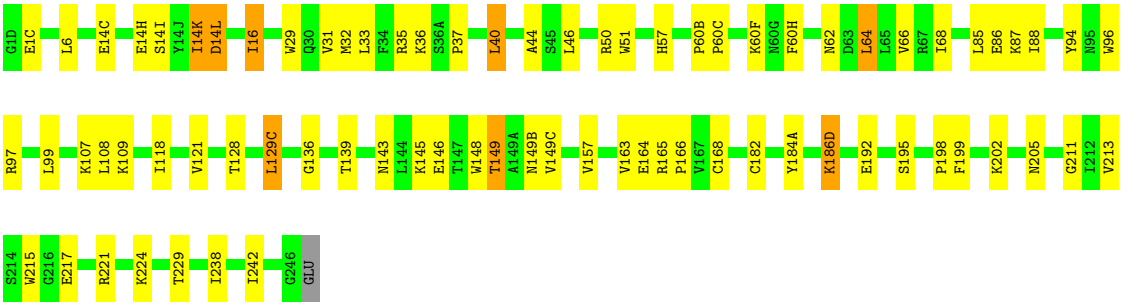
Note EDS was not executed.

• Molecule 1: Thrombin light and heavy chains

Chain A:

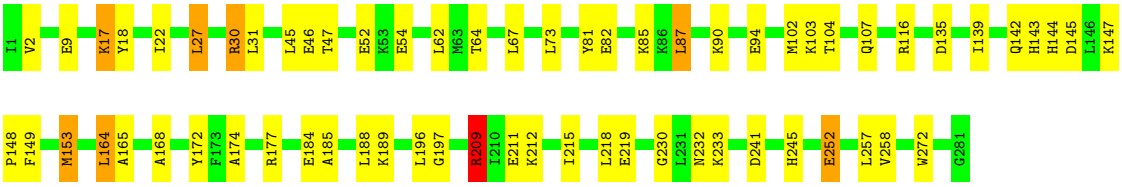
• Molecule 1: Thrombin light and heavy chains

Chain D:



• Molecule 2: Staphylocoagulase

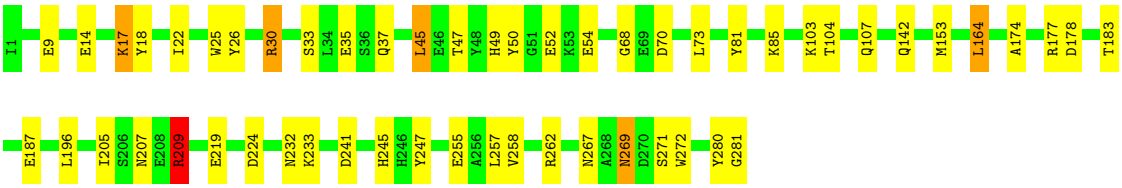
Chain C:



• Molecule 2: Staphylocoagulase

Chain F:

81%
17%


I1
E9
E14
K17
Y18
I22
W25
Y26
R30
S33
L34
E35
S36
Q37
L45
E46
T47
Y48
H49
Y50
G51
E52
K53
E54
G68
E69
D70
L73
Y81
K85
K103
T104
Q107
Q142
M153
L164
A174
R177
D178
T183
E187
L196
I205
S206
N207
E208
R209
E219
D224
N232
K233
D241
H245
H246
Y247
E255
A256
L257
V258
R262
N267
A268
N269
D270
S271
W272
Y280
G281

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	181.16Å 102.34Å 135.54Å 90.00° 129.91° 90.00°	Depositor
Resolution (Å)	19.98 – 2.20	Depositor
% Data completeness (in resolution range)	91.1 (19.98-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10253	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HG, 0ZJ, IMD

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	0.53	0/2399	0.77	2/3239 (0.1%)
1	D	0.53	0/2399	0.77	0/3239
2	C	0.54	0/2380	0.68	1/3194 (0.0%)
2	F	0.54	0/2380	0.66	3/3194 (0.1%)
All	All	0.54	0/9558	0.72	6/12866 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	LEU	CA-CB-CG	6.18	129.52	115.30
1	A	199	PHE	N-CA-C	-5.22	96.91	111.00
2	F	205	ILE	N-CA-C	-5.15	97.10	111.00
2	F	224	ASP	CB-CG-OD2	5.14	122.93	118.30
2	C	209	ARG	NE-CZ-NH1	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2341	0	2312	67	0
1	D	2341	0	2312	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2338	0	2303	46	0
2	F	2338	0	2303	45	0
3	A	34	0	31	4	0
3	D	34	0	31	3	0
4	C	2	0	0	0	0
4	F	2	0	0	1	0
5	C	15	0	15	2	0
5	F	15	0	15	2	0
6	A	160	0	0	3	0
6	C	250	0	0	5	0
6	D	148	0	0	3	0
6	F	235	0	0	4	0
All	All	10253	0	9322	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 222 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:NH1	1:A:107:LYS:HE2	1.73	1.03
1:A:14(K):ILE:HG12	1:A:14(L):ASP:H	1.27	0.96
2:F:104:THR:H	2:F:107:GLN:HE21	1.13	0.93
2:C:241:ASP:H	2:C:245:HIS:HD2	1.22	0.86
2:C:52:GLU:HG3	2:C:209:ARG:HH11	1.38	0.85

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 X-ray entries followed by that with respect to entries of similar resolution.

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	288/291 (99%)	272 (94%)	14 (5%)	2 (1%)	22	22
1	D	288/291 (99%)	268 (93%)	17 (6%)	3 (1%)	15	14
2	C	279/281 (99%)	274 (98%)	5 (2%)	0	100	100
2	F	279/281 (99%)	274 (98%)	5 (2%)	0	100	100
All	All	1134/1144 (99%)	1088 (96%)	41 (4%)	5 (0%)	34	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	14(K)	ILE
1	A	15	ARG
1	D	1(C)	GLU
1	A	14(L)	ASP
1	D	16	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	252/253 (100%)	240 (95%)	12 (5%)	25	32
1	D	252/253 (100%)	240 (95%)	12 (5%)	25	32
2	C	259/259 (100%)	245 (95%)	14 (5%)	22	26
2	F	259/259 (100%)	248 (96%)	11 (4%)	30	38
All	All	1022/1024 (100%)	973 (95%)	49 (5%)	25	32

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	14(I)	SER
1	D	149	THR
1	D	14(L)	ASP
1	D	46	LEU
1	D	198	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	119	ASN
2	F	269	ASN
2	F	245	HIS
2	C	245	HIS
2	F	107	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	IMD	C	2005	-	3,5,5	0.63	0	4,5,5	0.45	0
5	IMD	F	2000	-	3,5,5	0.58	0	4,5,5	0.50	0
5	IMD	C	2003	-	3,5,5	0.58	0	4,5,5	0.44	0
5	IMD	F	2004	-	3,5,5	0.61	0	4,5,5	0.44	0
3	0ZJ	D	299	4,1	33,35,36	1.43	1 (3%)	40,46,47	1.01	2 (5%)
5	IMD	C	2001	-	3,5,5	0.61	0	4,5,5	0.47	0
3	0ZJ	A	299	4,1	33,35,36	1.52	2 (6%)	40,46,47	0.99	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	IMD	F	2002	-	3,5,5	0.63	0	4,5,5	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	C	2005	-	-	-	0/1/1/1
5	IMD	F	2000	-	-	-	0/1/1/1
5	IMD	C	2003	-	-	-	0/1/1/1
5	IMD	F	2004	-	-	-	0/1/1/1
3	0ZJ	D	299	4,1	1/1/9/12	2/35/47/49	0/2/2/2
5	IMD	C	2001	-	-	-	0/1/1/1
3	0ZJ	A	299	4,1	1/1/9/12	3/35/47/49	0/2/2/2
5	IMD	F	2002	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	299	0ZJ	O3-C4	-7.00	1.24	1.43
3	D	299	0ZJ	O3-C4	-6.71	1.24	1.43
3	A	299	0ZJ	CD2-CG	2.20	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	299	0ZJ	O3-C4-CM	4.29	122.45	109.74
3	A	299	0ZJ	O3-C4-CM	4.06	121.78	109.74
3	D	299	0ZJ	C-CA-N	-2.12	103.87	108.81
3	A	299	0ZJ	C-CA-N	-2.10	103.89	108.81

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	299	0ZJ	C4
3	D	299	0ZJ	C4

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	299	0ZJ	CM-C4-CA2-N2
3	A	299	0ZJ	CM-C4-CA2-CB2
3	D	299	0ZJ	CM-C4-CA2-N2
3	D	299	0ZJ	CM-C4-CA2-CB2
3	A	299	0ZJ	O-C-N1-CD

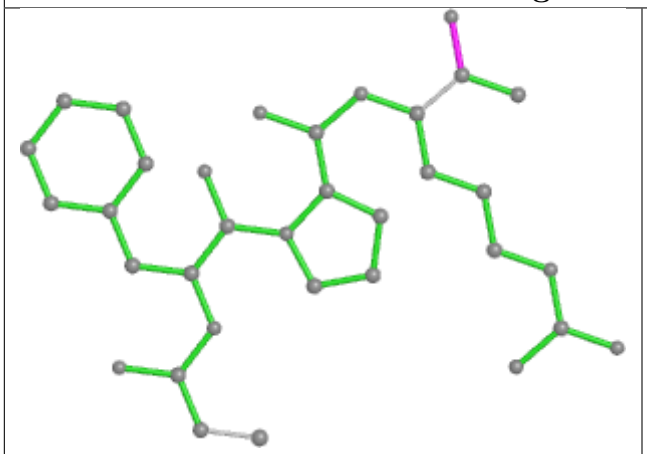
There are no ring outliers.

6 monomers are involved in 11 short contacts:

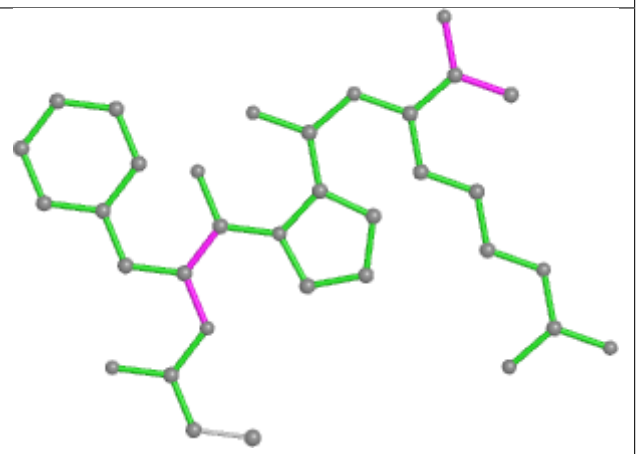
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2000	IMD	1	0
5	C	2003	IMD	1	0
5	F	2004	IMD	1	0
3	D	299	0ZJ	3	0
5	C	2001	IMD	1	0
3	A	299	0ZJ	4	0

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.

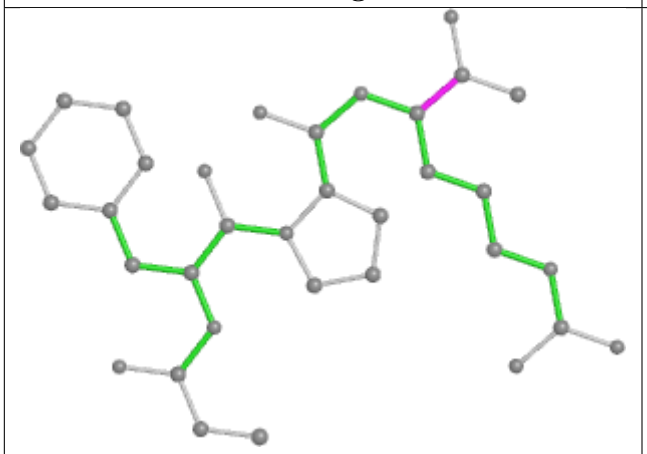
Ligand 0ZJ D 299



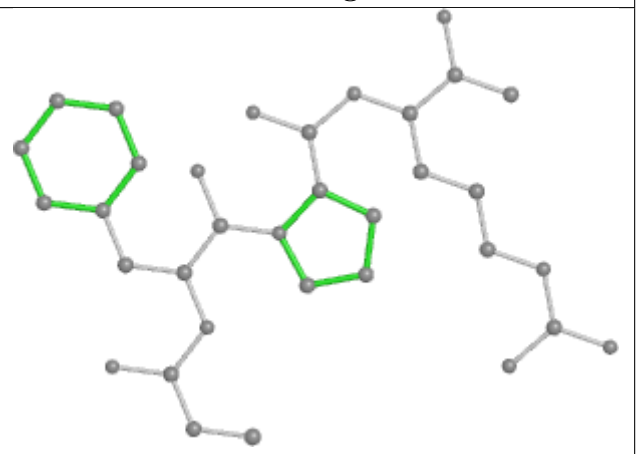
Bond lengths



Bond angles

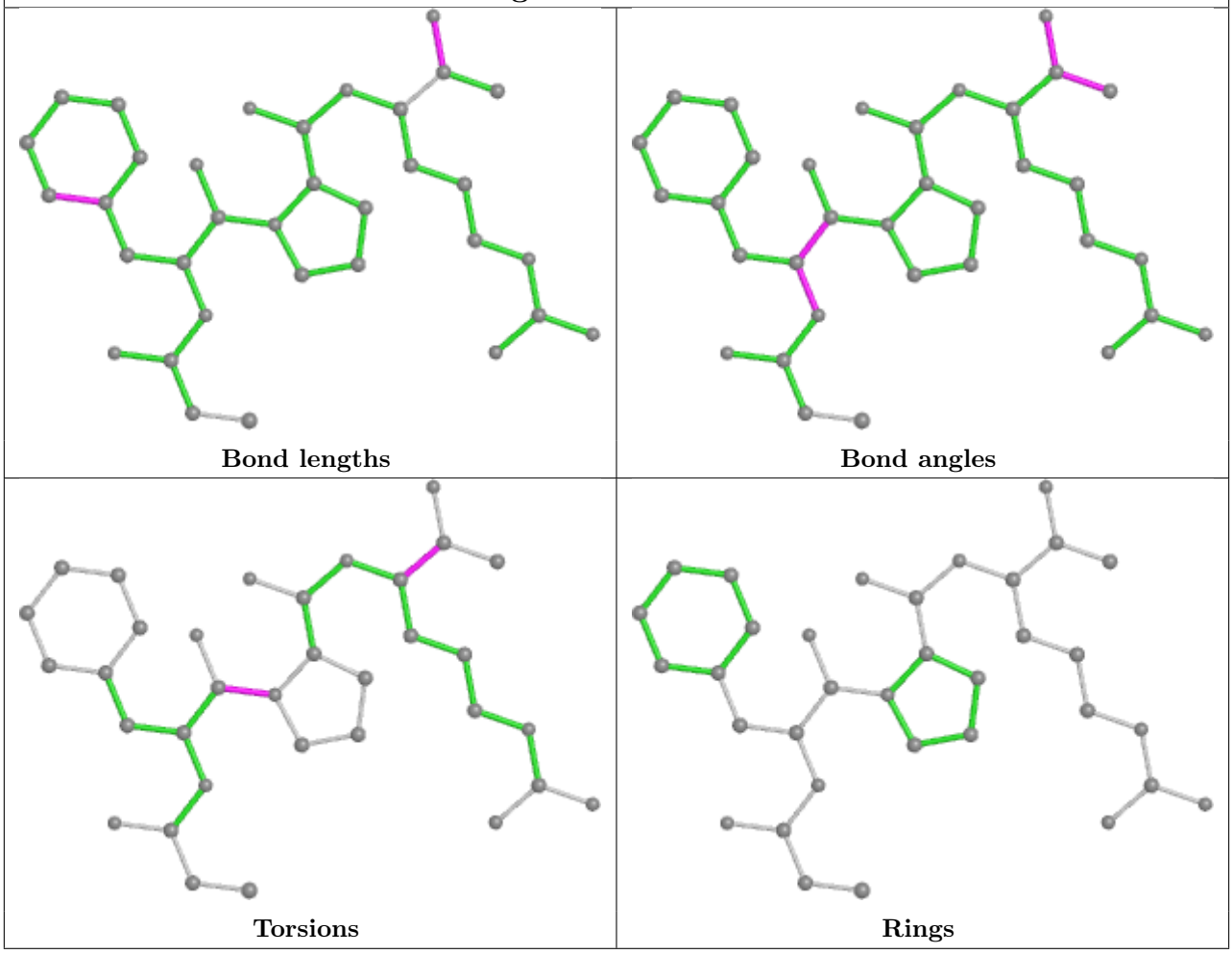


Torsions



Rings

Ligand 0ZJ A 299



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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.