wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 09:23 pm BST

PDB ID	:	1LMW
Title	:	LMW U-PA Structure complexed with EGRCMK (GLU-GLY-ARG Chloromethyl Ketone)
Authors	:	Spraggon, G.S.; Phillips, C.; Nowak, U.K.; Ponting, C.P.; Saunders, D.; Dobson, C.M.; Stuart, D.I.; Jones, E.Y.
Deposited on	:	1995-07-26
Resolution	:	2.50 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 following versions of software and data (see references (1)) were used in the production of this report:

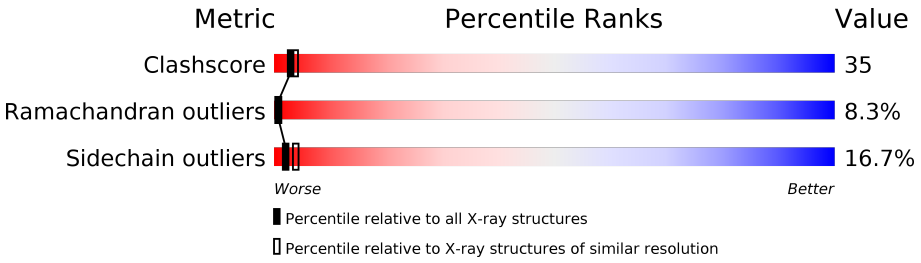
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 on 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	23	17% 22% 61%
1	C	23	22% 13% 65%
2	B	253	37% 45% 14%
2	D	253	37% 50% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4093 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.

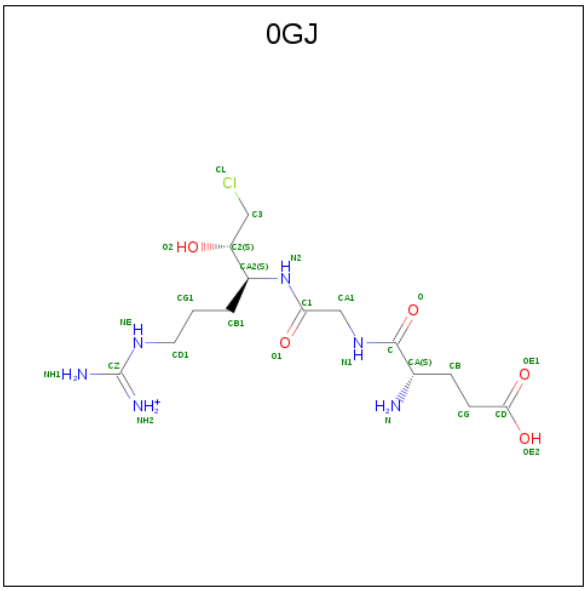
- Molecule 1 is a protein called UROKINASE-TYPE PLASMINOGEN ACTIVATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	9	Total	C	N	O	S	0	0	1
			62	37	14	10	1			
1	C	8	Total	C	N	O	S	0	0	0
			61	37	13	10	1			

- Molecule 2 is a protein called UROKINASE-TYPE PLASMINOGEN ACTIVATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			1960	1234	342	367	17			
2	D	248	Total	C	N	O	S	0	0	0
			1960	1234	342	367	17			

- Molecule 3 is L-alpha-glutamyl-N-{(1S)-4-{[amino(iminio)methyl]amino}-1-[(1S)-2-chloro-1-hydroxyethyl]butyl}glycinamide (three-letter code: 0GJ) (formula: $C_{14}H_{28}ClN_6O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			25	14	6	5		
3	D	1	Total	C	N	O	0	0
			25	14	6	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

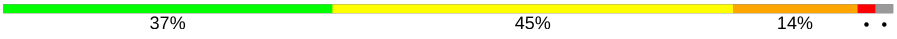
Chain A:

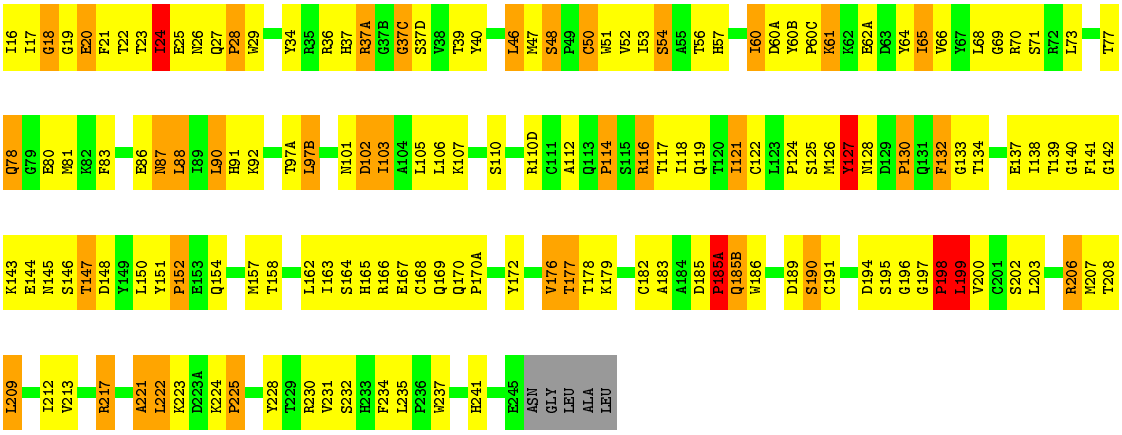
- Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain C:

- Molecule 2: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

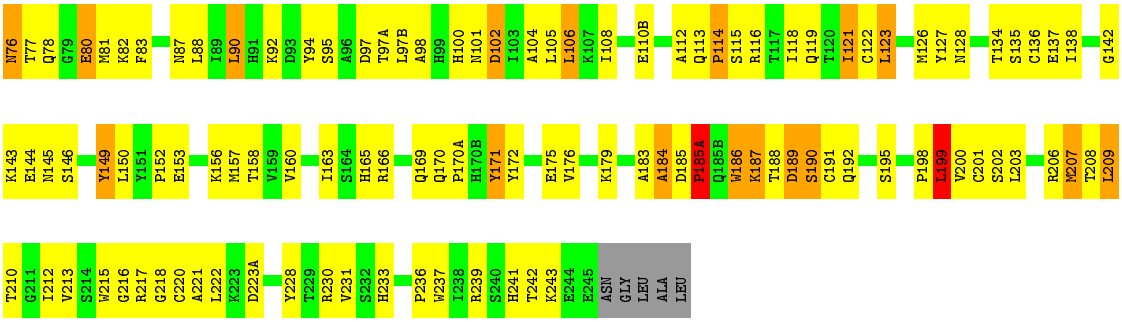
Chain B:





- Molecule 2: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain D:


N76 T77 Q78 G79 E80 M81 K82 F83
N87 L88 I89 L90 H91 K92 D93 Y94 S95 A96 D97 T97A L97B A98 H99 H100 N101 D102 I103 A104 L105 L106 K107 I108
E110B
A112 Q113 P114 S115 R116 T117 I118 Q119 T120 I121 C122 L123
M126 Y127 N128
T134 S135 C136 E137 I138
G142
K143 E144 N145 S146
Y149 L150 Y151 P152 E153
K156 M157 T158 V159 V160
I163 S164 H165 R166
Q169 Q170 P170A H170B Y171 Y172
E175 V176
K179
A183 A184 D185 P185A Q185B W186 K187 T188 D189 S190 C191 Q192
S195
P198 L199 V200 C201 S202 L203
R206 M207 T208 L209
T210 G211 I212 V213 S214 W215 G216 R217 G218 C220 A221 L222 K223 D223A
Y228 T229 R230 V231 S232 H233
P236 W237 I238 R239 S240 H241 T242 K243 E244 E245
ASN GLY LEU ALA LEU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	176.70Å 176.70Å 54.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.224 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4093	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0GJ

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	0.80	0/62	0.84	0/82
1	C	0.50	0/61	0.70	0/80
2	B	0.64	0/2009	0.90	4/2720 (0.1%)
2	D	0.63	0/2009	0.88	1/2720 (0.0%)
All	All	0.64	0/4141	0.89	5/5602 (0.1%)

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	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	199	LEU	N-CA-C	-7.49	90.79	111.00
2	D	199	LEU	N-CA-C	-6.66	93.02	111.00
2	B	198	PRO	N-CA-C	6.25	128.36	112.10
2	B	37(C)	GLY	N-CA-C	6.21	128.63	113.10
2	B	150	LEU	CA-CB-CG	6.10	129.32	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	57	HIS	Sidechain

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	62	0	68	9	0
1	C	61	0	68	3	0
2	B	1960	0	1901	148	8
2	D	1960	0	1901	127	8
3	B	25	0	24	1	0
3	D	25	0	24	0	0
All	All	4093	0	3986	280	9

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 35.

The worst 5 of 280 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)
2:B:121:ILE:HD13	2:B:209:LEU:HB2	1.49	0.95
2:B:145:ASN:HB3	2:B:148:ASP:HB2	1.52	0.91
2:B:202:SER:HA	2:B:207:MET:HA	1.55	0.88
2:B:37:HIS:HE1	2:B:39:THR:HG23	1.39	0.86
2:B:22:THR:HG21	2:B:157:MET:SD	2.16	0.85

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110(B):GLU:OE2	2:D:206:ARG:NH2[5_655]	1.72	0.48
2:B:127:TYR:O	2:D:166:ARG:NE[6_675]	1.76	0.44
2:B:127:TYR:CB	2:D:166:ARG:NH2[6_675]	1.96	0.24
2:B:127:TYR:CB	2:D:166:ARG:CZ[6_675]	1.97	0.23
2:B:127:TYR:CA	2:D:166:ARG:NH2[6_675]	1.98	0.22

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	7/23 (30%)	5 (71%)	2 (29%)	0	100 100
1	C	6/23 (26%)	6 (100%)	0	0	100 100
2	B	246/253 (97%)	179 (73%)	42 (17%)	25 (10%)	0 0
2	D	246/253 (97%)	181 (74%)	48 (20%)	17 (7%)	1 1
All	All	505/552 (92%)	371 (74%)	92 (18%)	42 (8%)	1 1

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	37(C)	GLY
2	B	60	ILE
2	B	92	LYS
2	B	127	TYR
2	D	24	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	7/22 (32%)	7 (100%)	0	100 100
1	C	7/22 (32%)	7 (100%)	0	100 100
2	B	217/220 (99%)	179 (82%)	38 (18%)	2 3
2	D	217/220 (99%)	180 (83%)	37 (17%)	2 3
All	All	448/484 (93%)	373 (83%)	75 (17%)	2 4

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	206	ARG
2	D	50	CYS
2	D	199	LEU
2	B	209	LEU
2	D	24	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	GLN
2	D	26	ASN
2	D	170	GLN
2	B	91	HIS
2	D	165	HIS

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 carbohydrates 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	$\#\|Z\|>2$
3	0GJ	B	1	2	20,24,25	0.73	1 (5%)	23,30,31	0.94	2 (8%)
3	0GJ	D	1	2	20,24,25	0.58	0	23,30,31	0.82	1 (4%)

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
3	0GJ	B	1	2	-	6/27/29/31	-
3	0GJ	D	1	2	-	5/27/29/31	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	0GJ	C3-C2	2.84	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	0GJ	O2-C2-C3	-2.83	101.37	109.74
3	B	1	0GJ	O2-C2-C3	-2.82	101.39	109.74
3	B	1	0GJ	CB1-CA2-C2	2.19	116.31	112.51

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	0GJ	N-CA-CB-CG
3	B	1	0GJ	O2-C2-CA2-CB1
3	D	1	0GJ	N-CA-CB-CG
3	D	1	0GJ	O2-C2-CA2-CB1
3	B	1	0GJ	C-CA-CB-CG

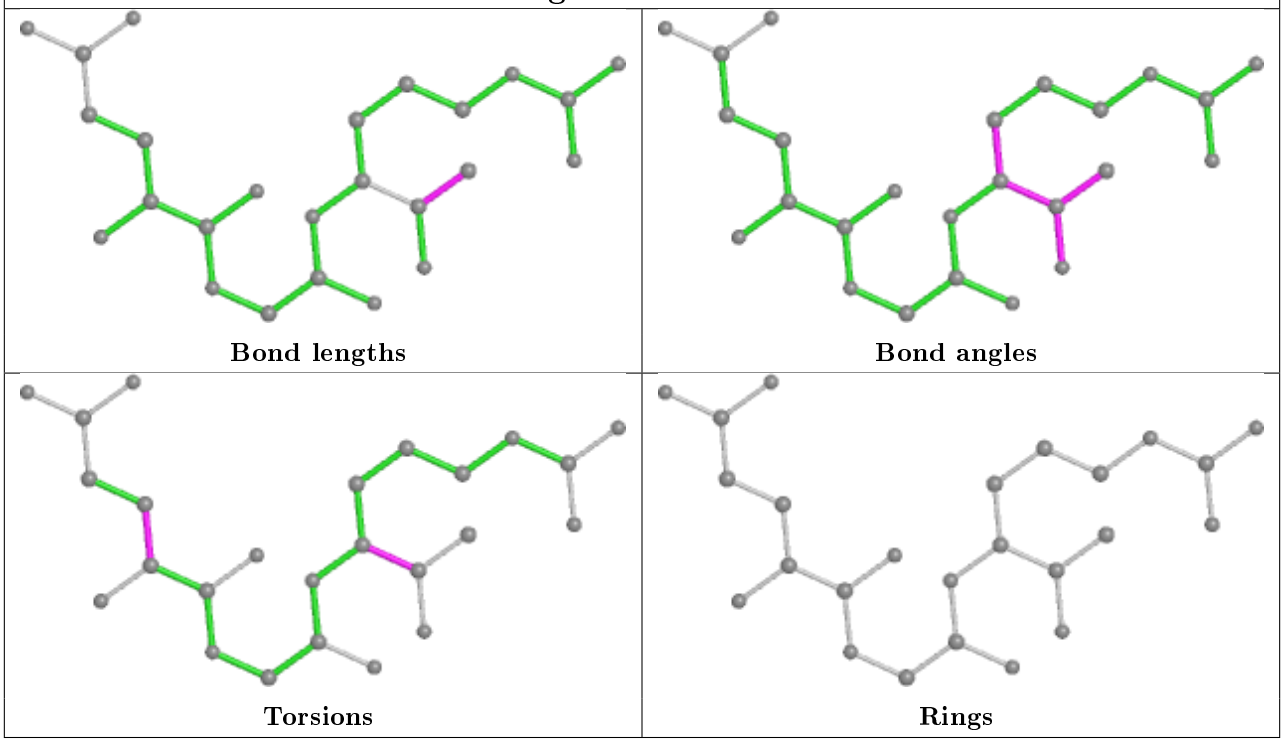
There are no ring outliers.

1 monomer is involved in 1 short contact:

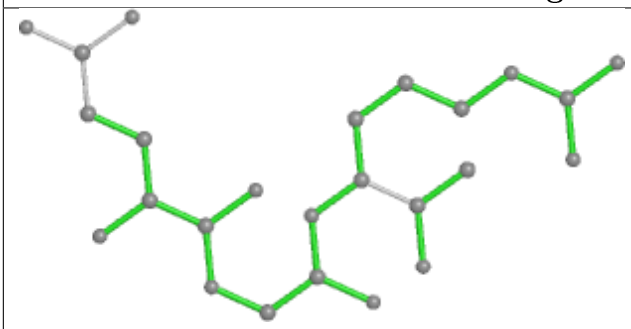
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	0GJ	1	0

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

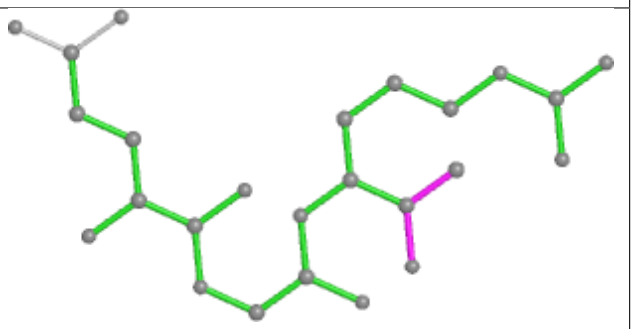
Ligand 0GJ B 1



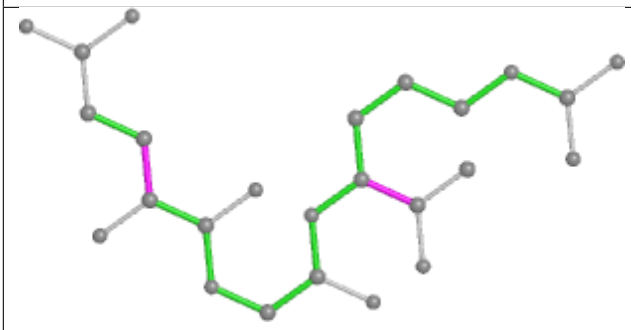
Ligand 0GJ D 1



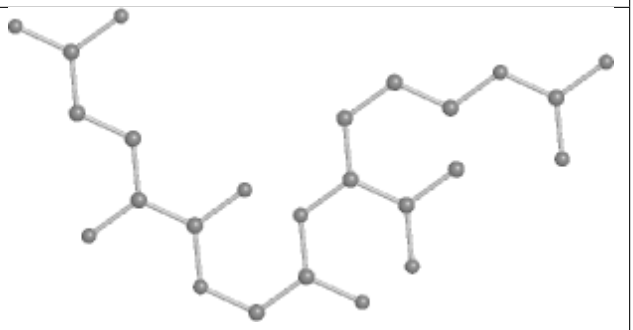
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.