wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2026 – 01:04 AM UTC

PDB ID	:	1DX5 / pdb_00001dx5
Title	:	Crystal structure of the thrombin-thrombomodulin complex
Authors	:	Fuentes-Prior, P.; Iwanaga, Y.; Huber, R.; Pagila, R.; Rumennik, G.; Seto, M.; Morser, J.; Light, D.R.; Bode, W.
Deposited on	:	1999-12-20
Resolution	:	2.30 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 (i)) were used in the production of this report:

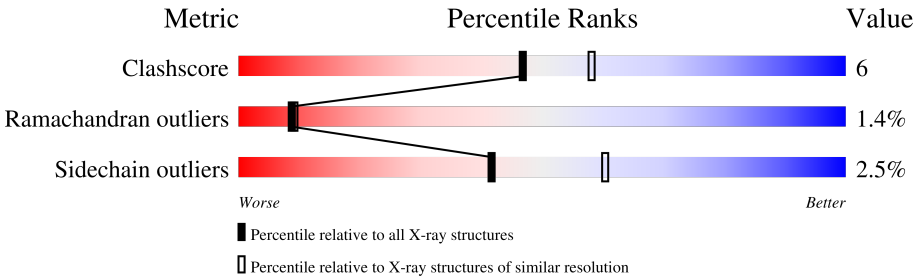
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	36	89% 8% ·
1	B	36	86% 14%
1	C	36	86% 11% ·
1	D	36	86% 11% ·
2	I	118	87% 12% ·
2	J	118	84% 14% ·
2	K	118	90% 9% ·
2	L	118	87% 12% ·

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Mol	Chain	Length	Quality of chain
3	M	259	78% 20%
3	N	259	80% 18%
3	O	259	83% 16%
3	P	259	80% 18%

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
7	NAG	M	301	X	-	-	-
7	NAG	N	301	X	-	-	-
7	NAG	O	301	X	-	-	-
7	NAG	P	301	X	-	-	-
8	0GJ	M	305	X	-	-	-
8	0GJ	N	305	X	-	-	-
8	0GJ	O	305	X	-	-	-
8	0GJ	P	306	X	-	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14018 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	36	Total	C	N	O	S	46	0	0
			287	177	48	61	1			
1	B	36	Total	C	N	O	S	38	0	0
			287	177	48	61	1			
1	C	36	Total	C	N	O	S	47	0	0
			287	177	48	61	1			
1	D	36	Total	C	N	O	S	39	0	0
			287	177	48	61	1			

- Molecule 2 is a protein called Thrombomodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	118	Total	C	N	O	S	61	0	0
			874	531	142	182	19			
2	J	118	Total	C	N	O	S	81	0	0
			874	531	142	182	19			
2	K	118	Total	C	N	O	S	74	0	0
			874	531	142	182	19			
2	L	118	Total	C	N	O	S	69	0	0
			874	531	142	182	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	364	ASP	ASN	conflict	UNP P07204
I	456	GLY	ARG	conflict	UNP P07204
I	457	GLN	HIS	conflict	UNP P07204
J	364	ASP	ASN	conflict	UNP P07204
J	456	GLY	ARG	conflict	UNP P07204
J	457	GLN	HIS	conflict	UNP P07204
K	364	ASP	ASN	conflict	UNP P07204
K	456	GLY	ARG	conflict	UNP P07204

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Chain	Residue	Modelled	Actual	Comment	Reference
K	457	GLN	HIS	conflict	UNP P07204
L	364	ASP	ASN	conflict	UNP P07204
L	456	GLY	ARG	conflict	UNP P07204
L	457	GLN	HIS	conflict	UNP P07204

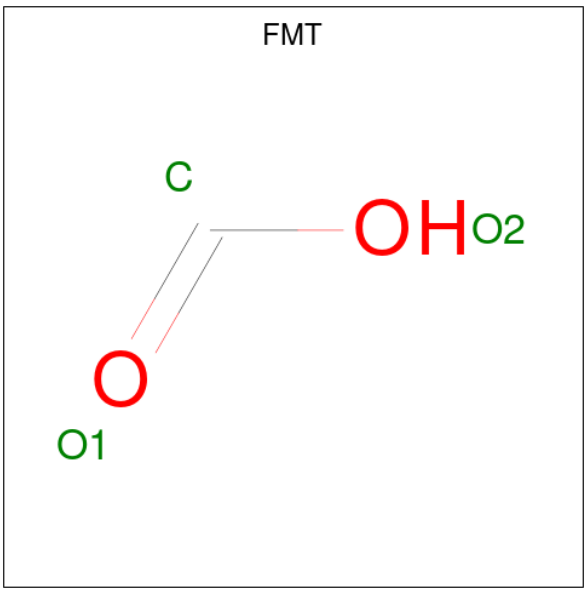
- Molecule 3 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	259	Total	C	N	O	S	72	0	0
			2094	1336	370	374	14			
3	N	259	Total	C	N	O	S	70	0	0
			2094	1336	370	374	14			
3	O	259	Total	C	N	O	S	76	0	0
			2094	1336	370	374	14			
3	P	259	Total	C	N	O	S	69	0	0
			2094	1336	370	374	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	60I	ILE	THR	conflict	UNP P00734
N	60I	ILE	THR	conflict	UNP P00734
O	60I	ILE	THR	conflict	UNP P00734
P	60I	ILE	THR	conflict	UNP P00734

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total C O 3 1 2	0	0
4	J	1	Total C O 3 1 2	0	0
4	K	1	Total C O 3 1 2	0	0
4	L	1	Total C O 3 1 2	0	0
4	P	1	Total C O 3 1 2	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

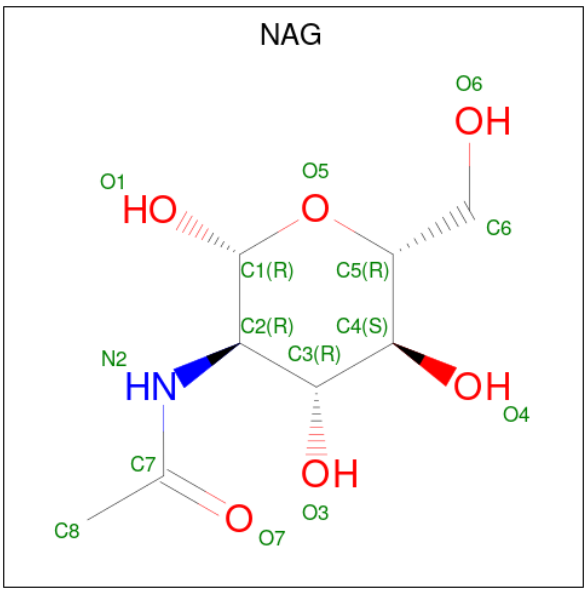
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total Ca 1 1	0	0
5	J	1	Total Ca 1 1	0	0
5	K	1	Total Ca 1 1	0	0
5	L	1	Total Ca 1 1	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total Na 1 1	0	0
6	J	1	Total Na 1 1	0	0
6	K	1	Total Na 1 1	0	0
6	L	1	Total Na 1 1	0	0
6	M	1	Total Na 1 1	0	0
6	N	1	Total Na 1 1	0	0
6	O	1	Total Na 1 1	0	0
6	P	1	Total Na 1 1	0	0

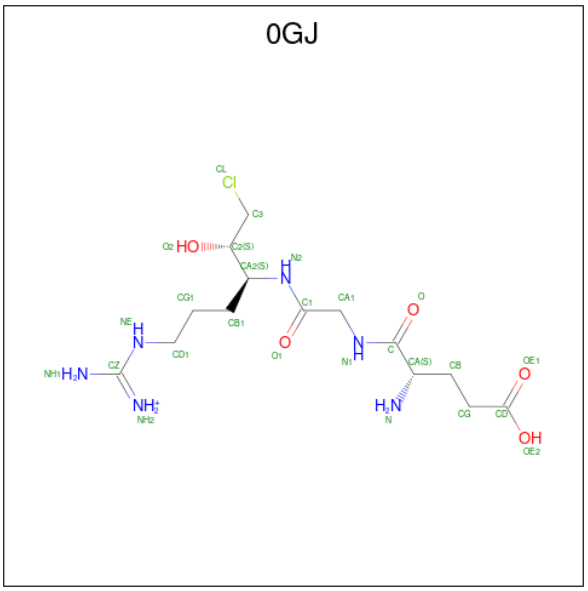
- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	1	0
			14	8	1	5		
7	N	1	Total	C	N	O	1	0
			14	8	1	5		
7	O	1	Total	C	N	O	1	0
			14	8	1	5		
7	P	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is L-alpha-glutamyl-N-{(1S)-4-{[amino(iminio)methyl]amino}-1-[(1S)-2-chloro-1-hydroxyethyl]butyl}glycinamide (CCD ID: 0GJ) (formula: $C_{14}H_{28}ClN_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total C N O 9 5 1 3	0	0
8	M	1	Total C N O 4 2 1 1	0	0
8	M	1	Total C N O 11 6 4 1	0	0
8	M	1	Total C 1 1	0	0
8	N	1	Total C N O 9 5 1 3	0	0
8	N	1	Total C N O 4 2 1 1	0	0
8	N	1	Total C N O 11 6 4 1	0	0
8	N	1	Total C 1 1	0	0
8	O	1	Total C N O 9 5 1 3	0	0
8	O	1	Total C N O 4 2 1 1	0	0
8	O	1	Total C N O 11 6 4 1	0	0
8	O	1	Total C 1 1	0	0
8	P	1	Total C N O 9 5 1 3	0	0
8	P	1	Total C N O 4 2 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	P	1	Total C N O 11 6 4 1	0	0
8	P	1	Total C 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	13	Total O 13 13	0	0
9	B	14	Total O 14 14	0	0
9	C	17	Total O 17 17	0	0
9	D	4	Total O 4 4	0	0
9	I	67	Total O 67 67	0	0
9	J	66	Total O 66 66	0	0
9	K	63	Total O 63 63	0	0
9	L	60	Total O 60 60	0	0
9	M	131	Total O 131 131	0	0
9	N	133	Total O 133 133	0	0
9	O	123	Total O 123 123	0	0
9	P	124	Total O 124 124	0	0

3 Residue-property plots

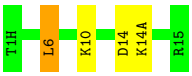
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Chain A:

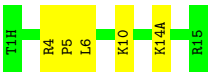




- Molecule 1: Thrombin light chain

Chain B:

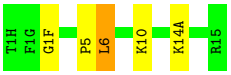




- Molecule 1: Thrombin light chain

Chain C:

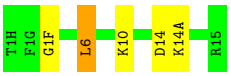




- Molecule 1: Thrombin light chain

Chain D:





- Molecule 2: Thrombomodulin

Chain I:

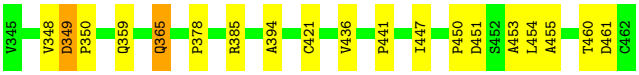




- Molecule 2: Thrombomodulin

Chain J:





• Molecule 2: Thrombomodulin

Chain K:

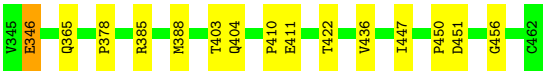




• Molecule 2: Thrombomodulin

Chain L:

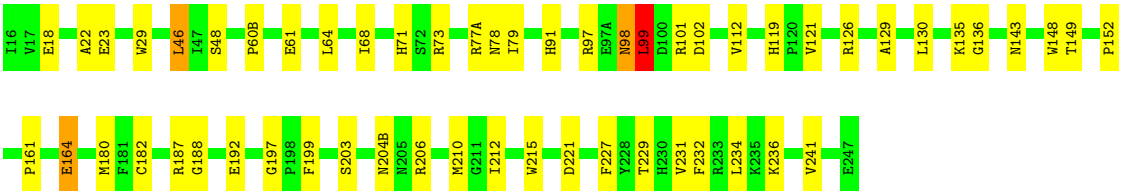




• Molecule 3: Thrombin heavy chain

Chain M:

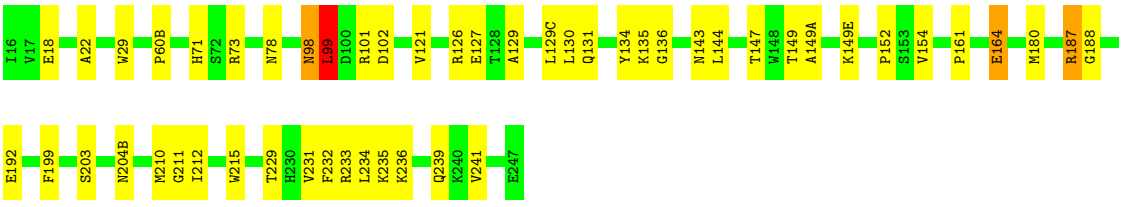




• Molecule 3: Thrombin heavy chain

Chain N:

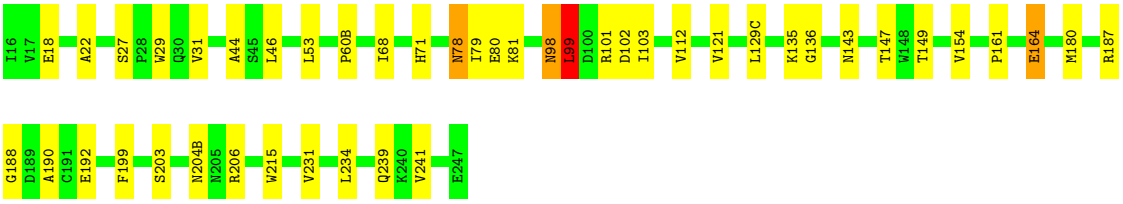




• Molecule 3: Thrombin heavy chain

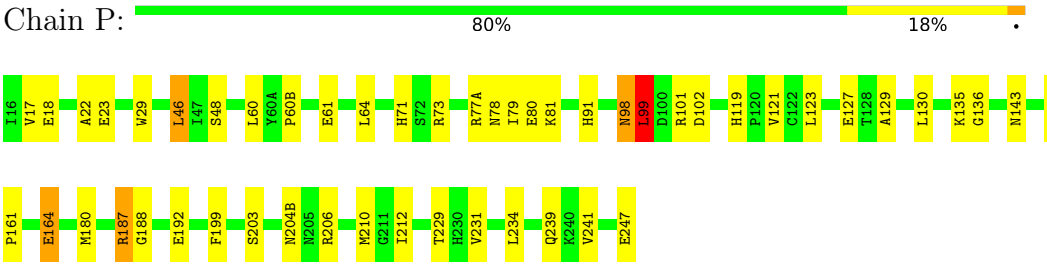
Chain O:





• Molecule 3: Thrombin heavy chain

Chain P:


80%
18%
I16
V17
E18
A22
E23
W29
L46
I47
S48
L60
Y60A
P60B
E61
L64
H71
S72
R73
R77A
N78
I79
E80
K81
H91
N98
L99
D100
R101
D102
H119
P120
V121
C122
L123
E127
T128
A129
L130
K135
G136
N143
T149
P152
P161
E164
M180
R187
G188
E192
F199
S203
N204B
N205
R206
M210
G211
I212
T229
H230
V231
L234
Q239
K240
V241
E247

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	214.40Å 214.40Å 131.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	99.7 (10.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.200 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14018	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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: CA, FMT, NA, NAG, 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	0.76	0/290	0.84	1/384 (0.3%)
1	B	0.76	0/290	0.87	1/384 (0.3%)
1	C	0.75	0/290	0.88	1/384 (0.3%)
1	D	0.77	0/290	0.85	1/384 (0.3%)
2	I	0.84	0/896	0.99	1/1222 (0.1%)
2	J	0.82	0/896	0.99	3/1222 (0.2%)
2	K	0.83	0/896	1.00	1/1222 (0.1%)
2	L	0.81	0/896	0.97	2/1222 (0.2%)
3	M	0.72	0/2149	0.98	9/2904 (0.3%)
3	N	0.72	0/2149	0.97	7/2904 (0.2%)
3	O	0.73	0/2149	0.99	10/2904 (0.3%)
3	P	0.72	0/2149	0.98	10/2904 (0.3%)
All	All	0.75	0/13340	0.97	47/18040 (0.3%)

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	365	GLN	N-CA-C	-8.06	103.23	113.23
1	A	14(A)	LYS	N-CA-C	8.03	120.75	111.11
1	B	14(A)	LYS	N-CA-C	7.89	120.58	111.11
1	C	14(A)	LYS	N-CA-C	7.80	120.76	111.33
1	D	14(A)	LYS	N-CA-C	7.70	119.67	111.28

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	287	0	278	2	0
1	B	287	0	278	2	0
1	C	287	0	278	3	0
1	D	287	0	278	3	0
2	I	874	0	754	6	0
2	J	874	0	754	8	0
2	K	874	0	754	5	0
2	L	874	0	754	8	0
3	M	2094	0	2066	28	0
3	N	2094	0	2066	26	0
3	O	2094	0	2066	20	0
3	P	2094	0	2066	33	0
4	I	3	0	1	0	0
4	J	3	0	1	0	0
4	K	3	0	1	0	0
4	L	3	0	1	0	0
4	P	3	0	1	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
7	M	14	0	13	0	0
7	N	14	0	13	0	0
7	O	14	0	13	0	0
7	P	14	0	13	2	0
8	M	25	0	21	0	0
8	N	25	0	21	0	0
8	O	25	0	21	0	0
8	P	25	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	13	0	0	0	0
9	B	14	0	0	0	0
9	C	17	0	0	0	0
9	D	4	0	0	0	0
9	I	67	0	0	1	0
9	J	66	0	0	2	0
9	K	63	0	0	0	0
9	L	60	0	0	0	0
9	M	131	0	0	4	0
9	N	133	0	0	1	0
9	O	123	0	0	0	0
9	P	124	0	0	3	0
All	All	14018	0	12533	137	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 6.

The worst 5 of 137 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:P:60:LEU:HD11	7:P:301:NAG:H82	1.57	0.85
2:I:448:CYS:SG	2:I:457:GLN:NE2	2.56	0.78
3:P:247:GLU:HG2	9:P:404:HOH:O	1.86	0.76
1:C:1(F):GLY:HA3	3:O:239:GLN:HE21	1.58	0.67
3:O:18:GLU:HB2	3:O:188:GLY:HA2	1.80	0.64

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	34/36 (94%)	32 (94%)	2 (6%)	0	100 100
1	B	34/36 (94%)	32 (94%)	2 (6%)	0	100 100
1	C	34/36 (94%)	32 (94%)	2 (6%)	0	100 100
1	D	34/36 (94%)	32 (94%)	2 (6%)	0	100 100
2	I	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	7 7
2	J	116/118 (98%)	105 (90%)	6 (5%)	5 (4%)	2 1
2	K	116/118 (98%)	107 (92%)	6 (5%)	3 (3%)	4 3
2	L	116/118 (98%)	105 (90%)	7 (6%)	4 (3%)	3 2
3	M	257/259 (99%)	243 (95%)	12 (5%)	2 (1%)	16 20
3	N	257/259 (99%)	241 (94%)	13 (5%)	3 (1%)	10 12
3	O	257/259 (99%)	243 (95%)	12 (5%)	2 (1%)	16 20
3	P	257/259 (99%)	245 (95%)	11 (4%)	1 (0%)	30 38
All	All	1628/1652 (98%)	1524 (94%)	82 (5%)	22 (1%)	9 9

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	346	GLU
2	K	346	GLU
2	L	346	GLU
2	L	451	ASP
3	M	149	THR

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	31/31 (100%)	30 (97%)	1 (3%)	34 51
1	B	31/31 (100%)	30 (97%)	1 (3%)	34 51
1	C	31/31 (100%)	30 (97%)	1 (3%)	34 51
1	D	31/31 (100%)	30 (97%)	1 (3%)	34 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	I	100/100 (100%)	99 (99%)	1 (1%)	68 82
2	J	100/100 (100%)	100 (100%)	0	100 100
2	K	100/100 (100%)	99 (99%)	1 (1%)	68 82
2	L	100/100 (100%)	99 (99%)	1 (1%)	68 82
3	M	225/225 (100%)	218 (97%)	7 (3%)	35 52
3	N	225/225 (100%)	218 (97%)	7 (3%)	35 52
3	O	225/225 (100%)	218 (97%)	7 (3%)	35 52
3	P	225/225 (100%)	217 (96%)	8 (4%)	31 47
All	All	1424/1424 (100%)	1388 (98%)	36 (2%)	42 60

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	46	LEU
3	P	241	VAL
3	P	61	GLU
3	P	127	GLU
3	M	180	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	204(B)	ASN
3	P	204(B)	ASN
3	N	78	ASN
3	O	244	GLN
3	N	71	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 12 are monoatomic and 4 are modelled with single atom - leaving 21 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	$\#\|Z\| > 2$
8	0GJ	O	304	8	3,3,25	0.54	0	1,2,31	0.01	0
7	NAG	P	301	3	14,14,15	0.83	0	17,19,21	1.08	2 (11%)
8	0GJ	P	306	8,3	10,10,25	1.46	1 (10%)	9,11,31	0.84	0
4	FMT	P	303	-	2,2,2	1.16	0	1,1,1	1.65	0
8	0GJ	M	305	8,3	10,10,25	1.46	1 (10%)	9,11,31	0.90	0
4	FMT	J	501	6	2,2,2	1.22	0	1,1,1	1.68	0
8	0GJ	P	304	8	7,8,25	2.16	1 (14%)	4,9,31	1.09	0
7	NAG	O	301	3	14,14,15	0.72	0	17,19,21	1.08	3 (17%)
4	FMT	L	501	6	2,2,2	1.24	0	1,1,1	1.69	0
8	0GJ	O	303	8	7,8,25	2.04	1 (14%)	4,9,31	1.00	0
4	FMT	I	501	6	2,2,2	1.21	0	1,1,1	1.69	0
7	NAG	M	301	3	14,14,15	0.81	0	17,19,21	1.03	1 (5%)
8	0GJ	N	303	8	7,8,25	2.08	1 (14%)	4,9,31	0.97	0
8	0GJ	P	305	8	3,3,25	0.49	0	1,2,31	0.25	0
7	NAG	N	301	3	14,14,15	0.83	0	17,19,21	1.00	1 (5%)
8	0GJ	N	305	8,3	10,10,25	1.46	1 (10%)	9,11,31	0.88	0
8	0GJ	M	303	8	7,8,25	2.04	1 (14%)	4,9,31	1.05	0
8	0GJ	M	304	8	3,3,25	0.56	0	1,2,31	0.23	0
8	0GJ	N	304	8	3,3,25	0.48	0	1,2,31	0.20	0
4	FMT	K	501	6	2,2,2	1.24	0	1,1,1	1.67	0
8	0GJ	O	305	8,3	10,10,25	1.45	1 (10%)	9,11,31	0.83	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
8	0GJ	O	304	8	-	0/0/1/31	-
8	0GJ	P	304	8	-	0/6/7/31	-
8	0GJ	N	303	8	-	1/6/7/31	-
8	0GJ	M	304	8	-	0/0/1/31	-
8	0GJ	N	304	8	-	0/0/1/31	-
7	NAG	P	301	3	1/1/5/7	2/6/23/26	0/1/1/1
8	0GJ	P	306	8,3	1/1/2/10	2/9/9/31	-
7	NAG	O	301	3	1/1/5/7	0/6/23/26	0/1/1/1
8	0GJ	P	305	8	-	0/0/1/31	-
7	NAG	N	301	3	1/1/5/7	0/6/23/26	0/1/1/1
8	0GJ	O	303	8	-	0/6/7/31	-
8	0GJ	N	305	8,3	1/1/2/10	2/9/9/31	-
8	0GJ	O	305	8,3	1/1/2/10	2/9/9/31	-
8	0GJ	M	305	8,3	1/1/2/10	1/9/9/31	-
8	0GJ	M	303	8	-	0/6/7/31	-
7	NAG	M	301	3	1/1/5/7	2/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	304	0GJ	CG-CD	5.18	1.62	1.50
8	N	303	0GJ	CG-CD	4.97	1.62	1.50
8	M	303	0GJ	CG-CD	4.87	1.61	1.50
8	O	303	0GJ	CG-CD	4.86	1.61	1.50
8	M	305	0GJ	O2-C2	-4.51	1.23	1.42

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	301	NAG	C8-C7-N2	-2.24	112.41	116.12
7	P	301	NAG	C1-O5-C5	2.19	115.12	112.19
7	P	301	NAG	C2-N2-C7	-2.17	119.99	122.90
7	O	301	NAG	C1-O5-C5	2.14	115.06	112.19
7	O	301	NAG	C2-N2-C7	-2.07	120.12	122.90

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	M	301	NAG	C1
7	N	301	NAG	C1
7	O	301	NAG	C1
7	P	301	NAG	C1
8	M	305	0GJ	C2

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	301	NAG	C3-C2-N2-C7
7	P	301	NAG	C3-C2-N2-C7
8	N	305	0GJ	O2-C2-CA2-CB1
8	O	305	0GJ	O2-C2-CA2-CB1
8	P	306	0GJ	O2-C2-CA2-CB1

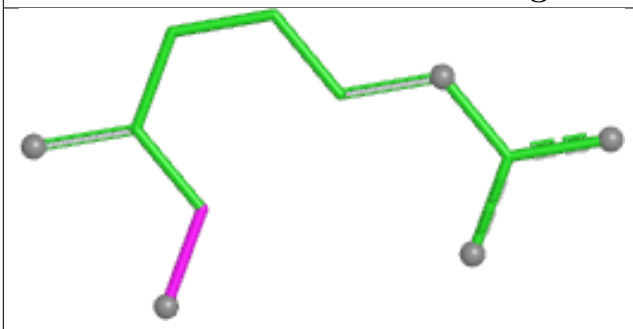
There are no ring outliers.

1 monomer is involved in 2 short contacts:

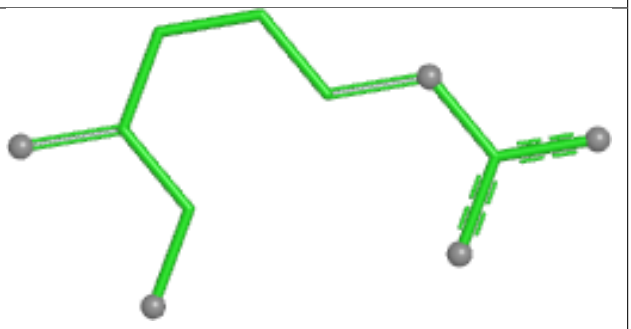
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	301	NAG	2	0

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.

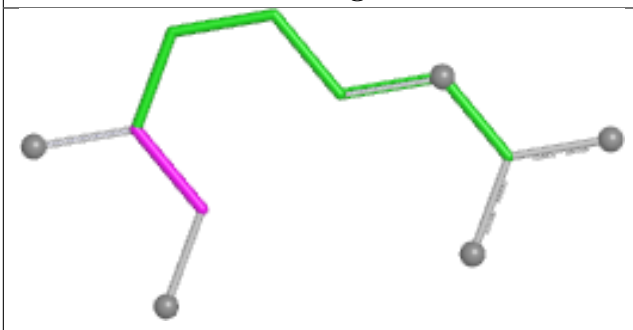
Ligand 0GJ P 306



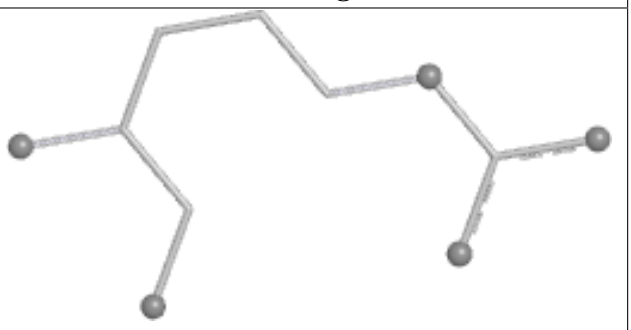
Bond lengths



Bond angles

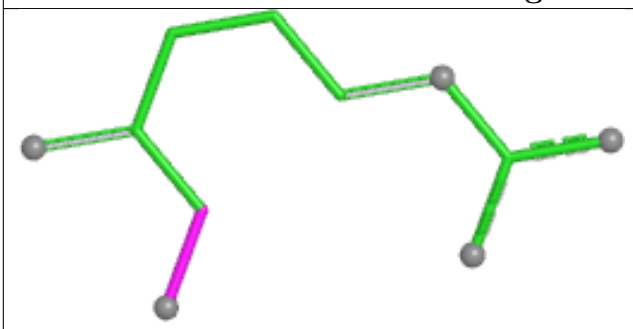


Torsions

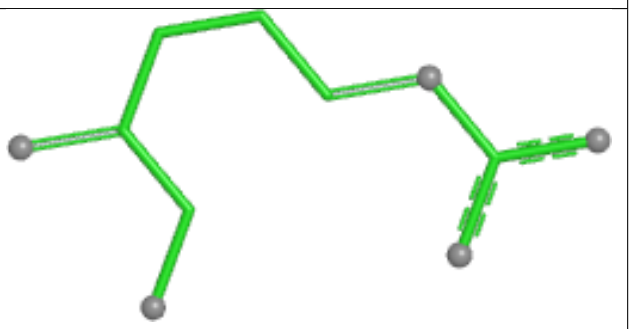


Rings

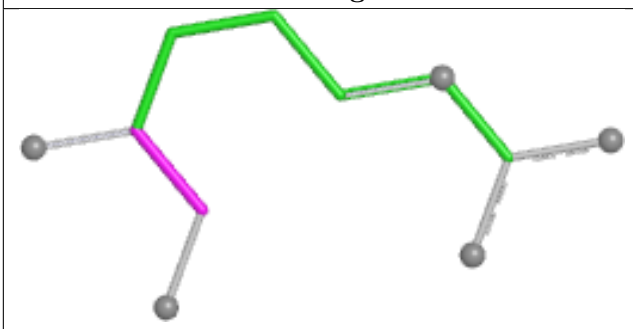
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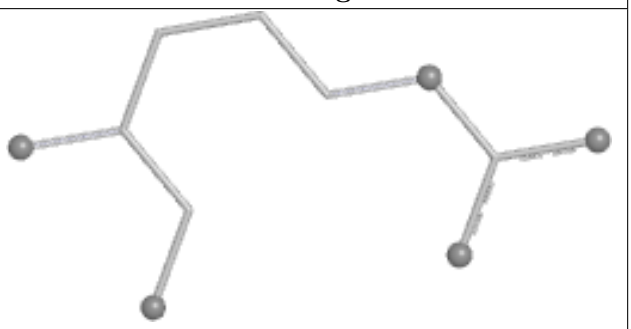
Bond lengths



Bond angles

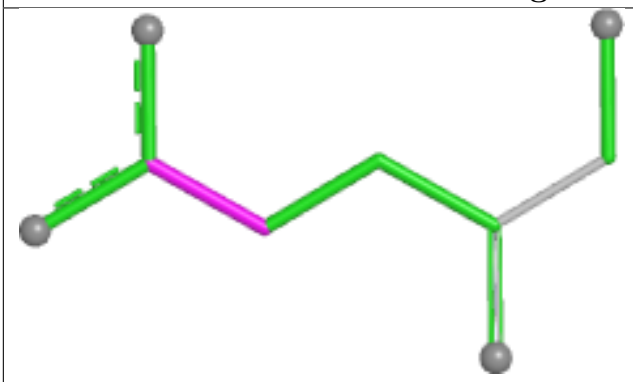


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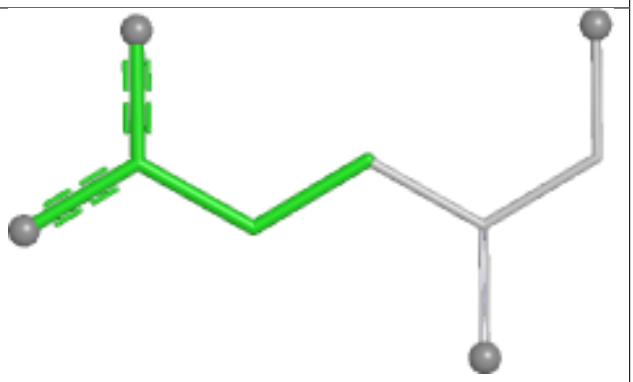


Rings

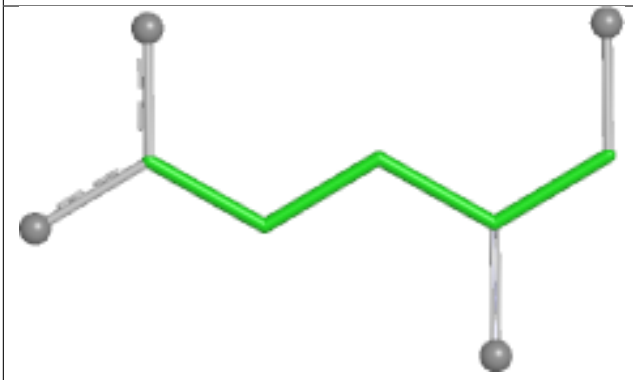
Ligand 0GJ P 304



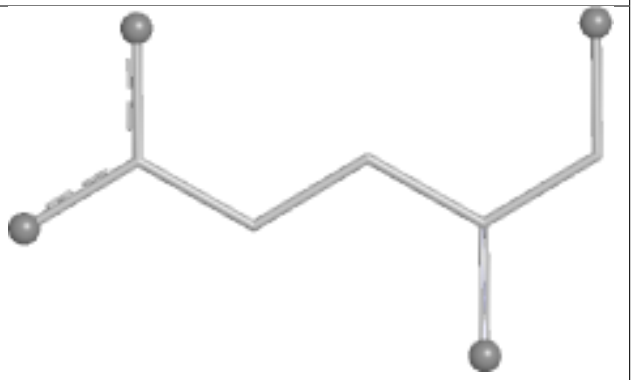
Bond lengths



Bond angles

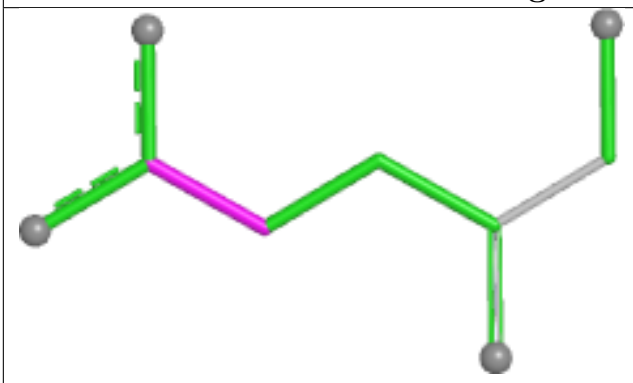


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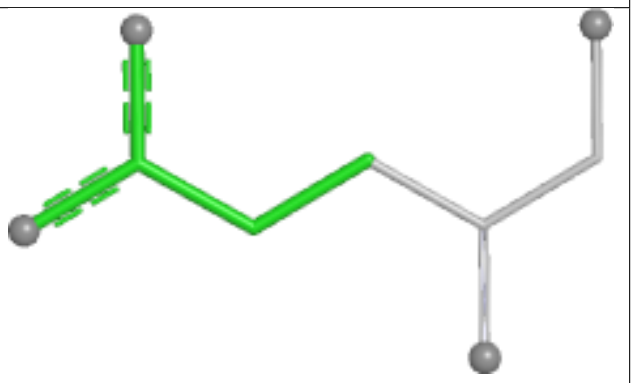


Rings

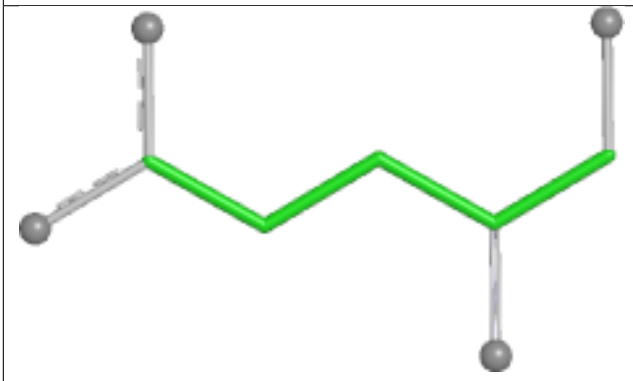
Ligand 0GJ O 303



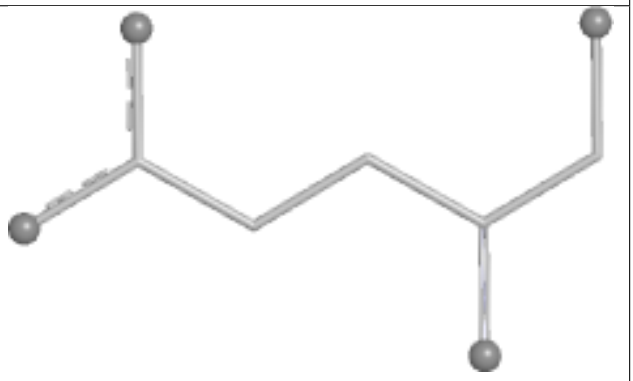
Bond lengths



Bond angles

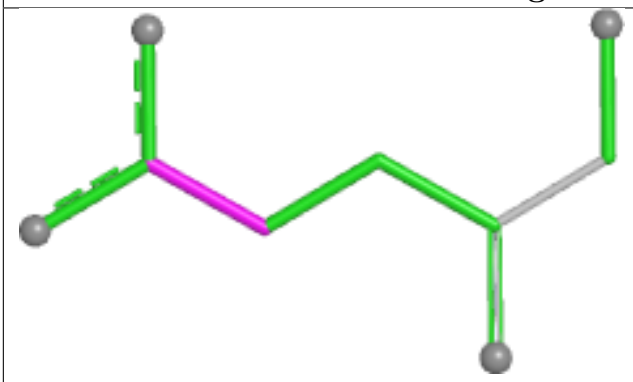


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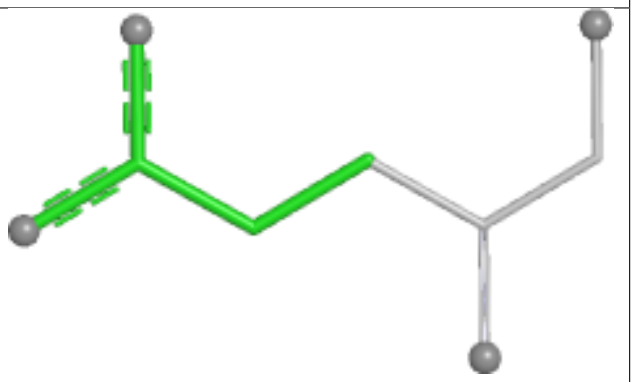


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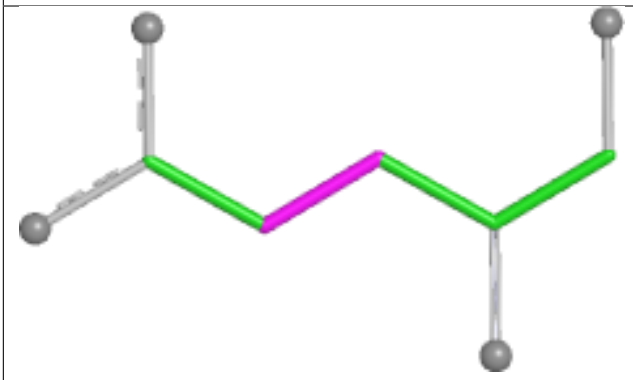
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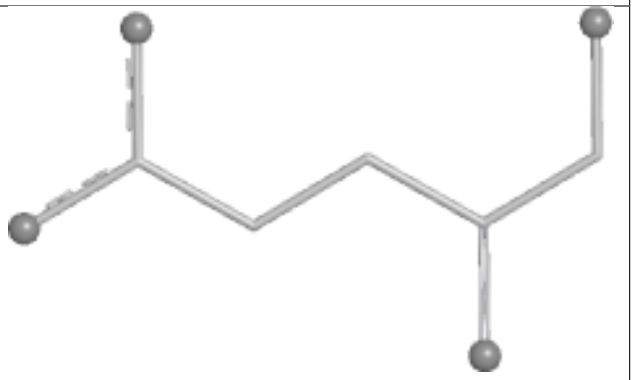
Bond lengths



Bond angles

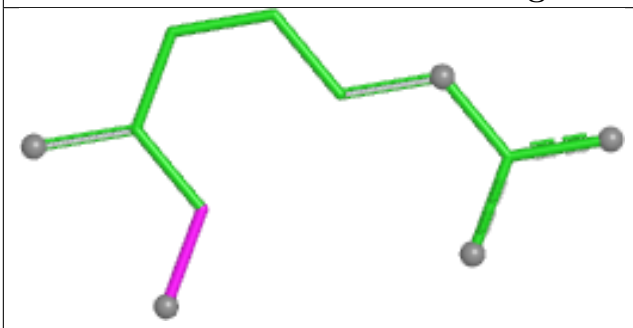


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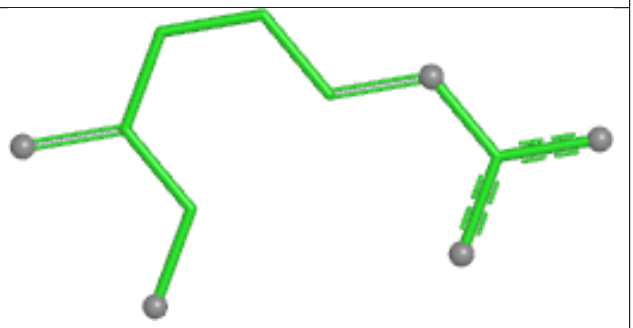


Rings

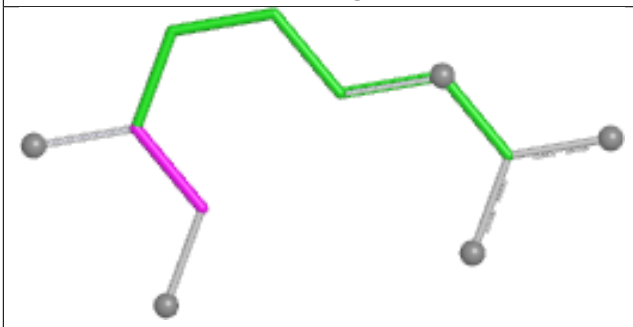
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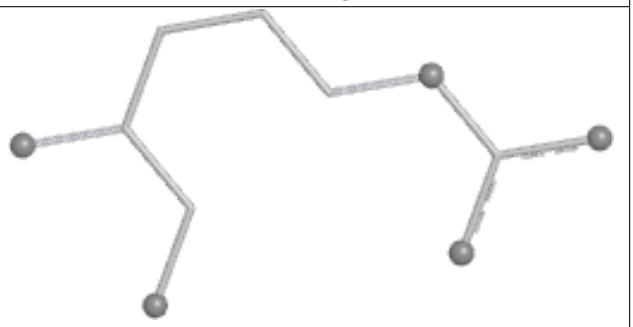
Bond lengths



Bond angles

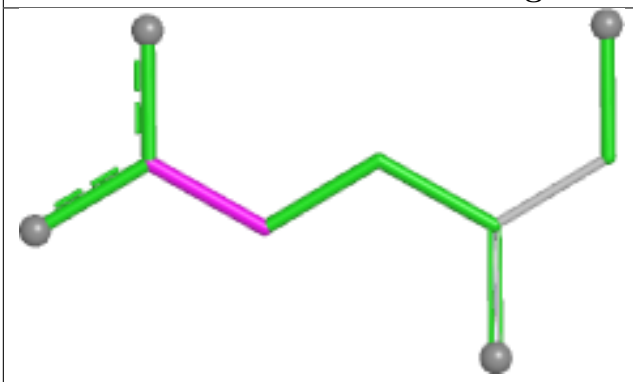


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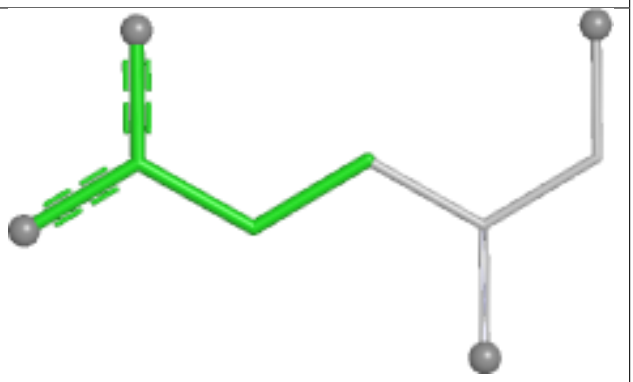


Rings

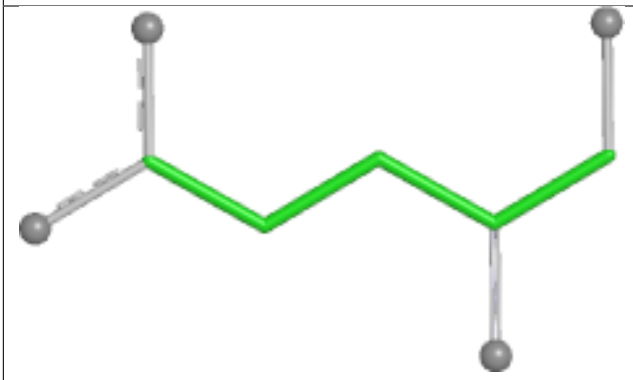
Ligand 0GJ M 303



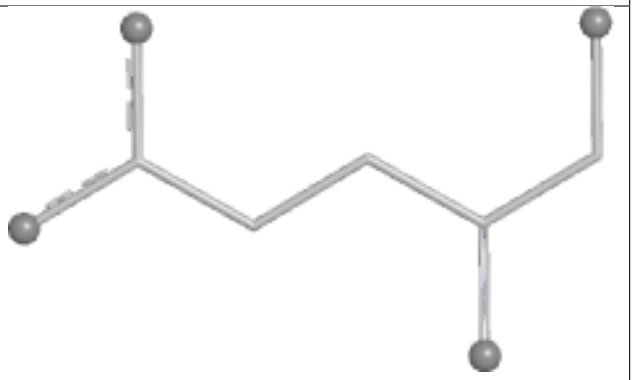
Bond lengths



Bond angles

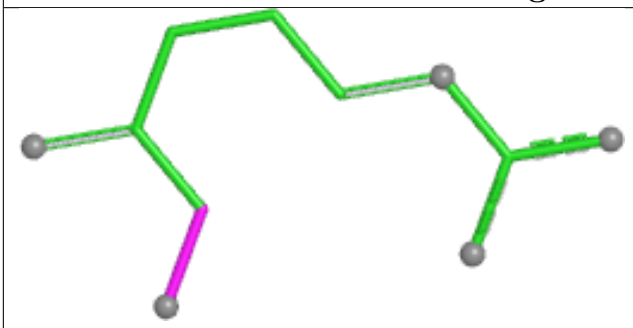


Torsions

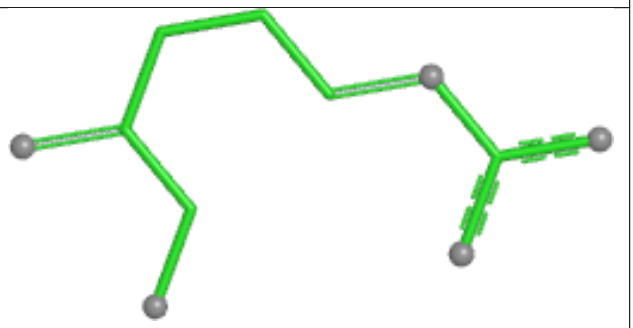


Rings

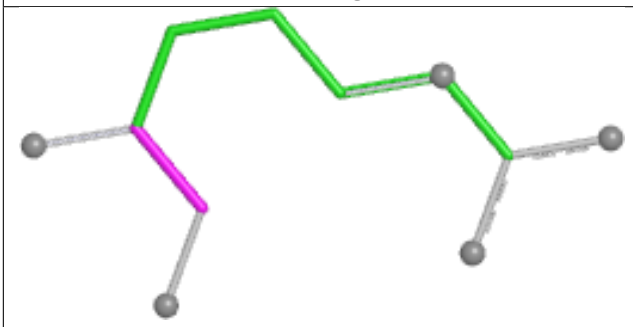
Ligand 0GJ O 305



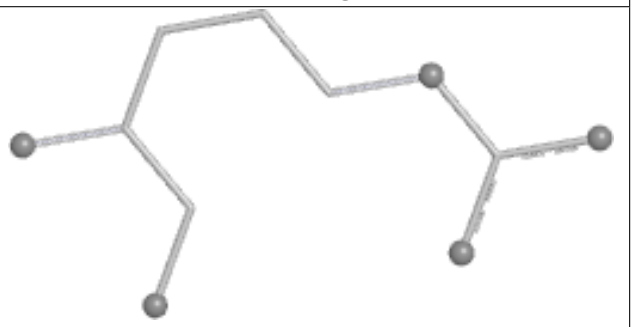
Bond lengths



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 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.