



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:52 pm BST

PDB ID : 1YYY  
Title : Trypsin inhibitors with rigid tripeptidyl aldehydes  
Authors : Krishnan, R.; Zhang, E.; Hakansson, K.; Arni, R.K.; Tulinsky, A.; Lim-Wilby, M.S.L.; Levy, O.E.; Semple, J.E.; Brunck, T.K.  
Deposited on : 1998-06-03  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

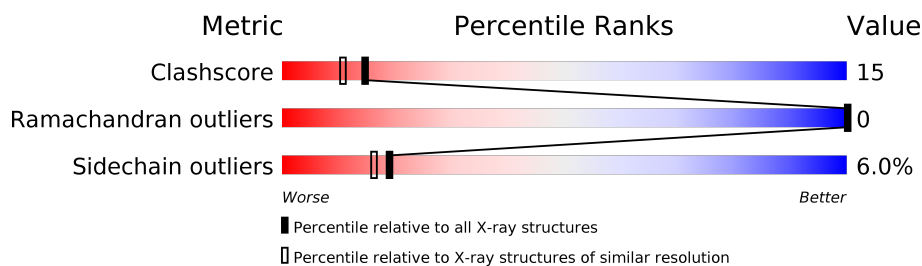
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	223	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1815 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.

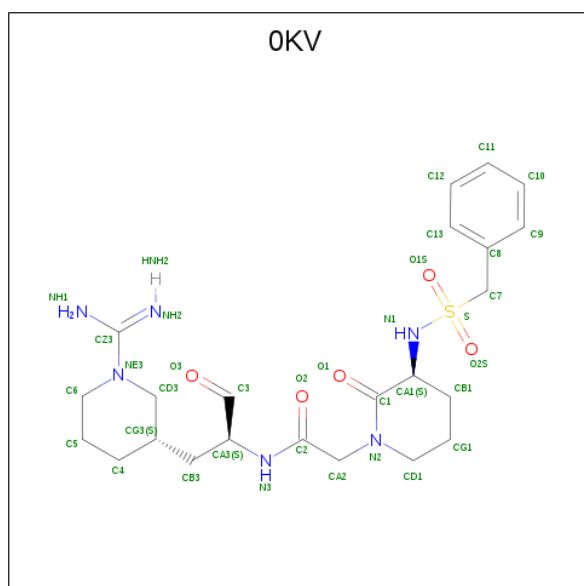
- Molecule 1 is a protein called TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2-{(3S)-3-[(benzylsulfonyl)amino]-2-oxopiperidin-1-yl}-N-{(2S)-1-[(3S)-1-carbamimidoylpiperidin-3-yl]-3-oxopropan-2-yl}acetamide (three-letter code: 0KV) (formula: C<sub>23</sub>H<sub>34</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1	1	Total	C	N	O	S	0	0
			28	16	6	5	1		

- Molecule 4 is water.

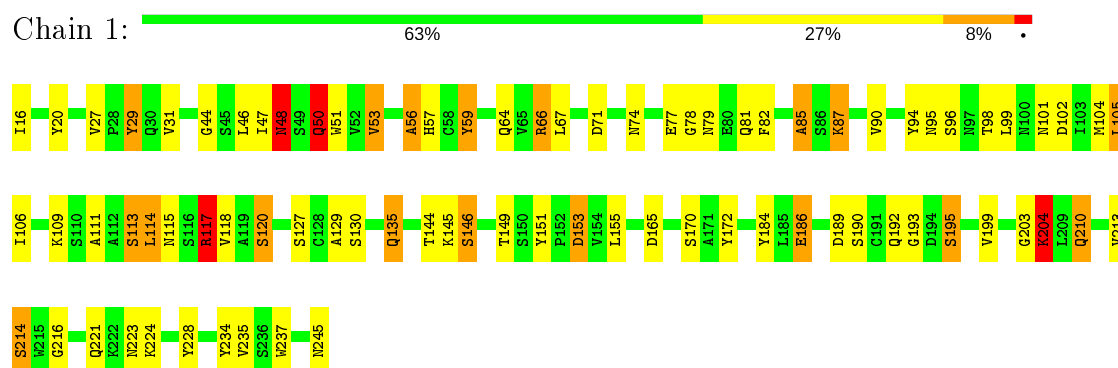
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	157	Total	O	0	0
			157	157		

### 3 Residue-property plots

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: TRYPSIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.76 Å 63.14 Å 69.29 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	72.0 (7.00-2.10)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.12	Depositor
Refinement program	PROFFT, X-PLOR	Depositor
R, $R_{free}$	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	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: CA, OKV

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	1	0.98	0/1660	1.99	45/2250 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	17

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	66	ARG	NE-CZ-NH1	16.70	128.65	120.30
1	1	117	ARG	NE-CZ-NH2	-14.77	112.92	120.30
1	1	165	ASP	CB-CG-OD1	13.58	130.52	118.30
1	1	94	TYR	CB-CG-CD2	-10.88	114.47	121.00
1	1	66	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	1	153	ASP	CB-CG-OD2	-9.54	109.71	118.30
1	1	117	ARG	CB-CA-C	-8.24	93.92	110.40
1	1	151	TYR	CB-CG-CD1	-7.56	116.47	121.00
1	1	130	SER	CB-CA-C	7.12	123.62	110.10
1	1	59	TYR	CB-CG-CD1	-6.74	116.95	121.00
1	1	117	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	1	104	MET	CG-SD-CE	6.47	110.56	100.20
1	1	153	ASP	CB-CG-OD1	6.44	124.09	118.30
1	1	145	LYS	CB-CA-C	-6.22	97.95	110.40
1	1	53	VAL	CG1-CB-CG2	-6.12	101.11	110.90
1	1	82	PHE	CB-CG-CD2	-5.94	116.64	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	118	VAL	CA-CB-CG1	-5.89	102.06	110.90
1	1	165	ASP	CB-CA-C	5.86	122.11	110.40
1	1	235	VAL	CA-CB-CG1	-5.85	102.12	110.90
1	1	146	SER	CB-CA-C	-5.83	99.02	110.10
1	1	203	GLY	CA-C-O	-5.78	110.20	120.60
1	1	50	GLN	CA-CB-CG	-5.72	100.81	113.40
1	1	105	LEU	CA-CB-CG	5.68	128.38	115.30
1	1	96	SER	N-CA-CB	5.66	119.00	110.50
1	1	170	SER	CB-CA-C	5.64	120.82	110.10
1	1	56	ALA	N-CA-CB	5.55	117.87	110.10
1	1	184	TYR	CD1-CE1-CZ	-5.53	114.82	119.80
1	1	190	SER	CB-CA-C	5.51	120.57	110.10
1	1	71	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	1	98	THR	O-C-N	5.43	131.40	122.70
1	1	48	ASN	N-CA-CB	5.39	120.31	110.60
1	1	109	LYS	CB-CG-CD	-5.38	97.61	111.60
1	1	85	ALA	CB-CA-C	5.35	118.12	110.10
1	1	172	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	1	189	ASP	CB-CG-OD2	5.19	122.97	118.30
1	1	170	SER	CA-C-N	5.15	128.52	117.20
1	1	113	SER	N-CA-CB	5.09	118.13	110.50
1	1	223	ASN	CB-CG-OD1	-5.08	111.44	121.60
1	1	127	SER	N-CA-CB	-5.07	102.89	110.50
1	1	20	TYR	CG-CD1-CE1	-5.05	117.26	121.30
1	1	102	ASP	CB-CG-OD1	5.05	122.84	118.30
1	1	214	SER	CB-CA-C	5.04	119.67	110.10
1	1	114	LEU	C-N-CA	5.04	134.29	121.70
1	1	237	TRP	CB-CG-CD1	-5.02	120.48	127.00
1	1	210	GLN	OE1-CD-NE2	-5.01	110.37	121.90

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	111	ALA	Mainchain
1	1	117	ARG	Sidechain,Mainchain
1	1	120	SER	Mainchain
1	1	129	ALA	Mainchain
1	1	135	GLN	Mainchain
1	1	155	LEU	Mainchain
1	1	186	GLU	Mainchain
1	1	193	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	1	195	SER	Mainchain
1	1	204	LYS	Mainchain
1	1	213	VAL	Mainchain
1	1	216	GLY	Mainchain
1	1	29	TYR	Sidechain
1	1	44	GLY	Mainchain
1	1	48	ASN	Mainchain
1	1	77	GLU	Mainchain

## 5.2 Too-close contacts ⓘ

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	1	1629	0	1588	50	0
2	1	1	0	0	0	0
3	1	28	0	26	10	0
4	1	157	0	0	9	0
All	All	1815	0	1614	50	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 15.

All (50) 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)
1:1:195:SER:OG	3:1:1:0KV:C3	1.70	1.37
1:1:67:LEU:HG	4:1:471:HOH:O	1.25	1.26
1:1:117:ARG:HD2	1:1:117:ARG:N	1.59	1.11
1:1:186:GLU:HG3	4:1:598:HOH:O	1.52	1.07
1:1:67:LEU:CG	4:1:471:HOH:O	1.89	0.98
1:1:81:GLN:HE22	1:1:113:SER:H	1.15	0.93
1:1:195:SER:HG	3:1:1:0KV:C3	1.68	0.91
1:1:67:LEU:CD1	4:1:471:HOH:O	2.15	0.91
1:1:48:ASN:HD22	1:1:50:GLN:H	1.18	0.91
1:1:31:VAL:HG12	1:1:67:LEU:HD23	1.67	0.76
1:1:195:SER:OG	3:1:1:0KV:CA3	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:195:SER:CB	3:1:1:0KV:C3	2.68	0.70
1:1:117:ARG:N	1:1:117:ARG:CD	2.49	0.70
1:1:81:GLN:NE2	1:1:113:SER:H	1.89	0.68
1:1:195:SER:HG	3:1:1:0KV:H3	1.55	0.64
1:1:64:GLN:NE2	1:1:66:ARG:HE	1.97	0.62
1:1:224:LYS:CE	4:1:626:HOH:O	2.47	0.62
1:1:195:SER:OG	3:1:1:0KV:O3	2.18	0.62
1:1:48:ASN:ND2	1:1:50:GLN:H	1.94	0.62
1:1:117:ARG:HD2	1:1:117:ARG:H	1.58	0.61
1:1:186:GLU:OE2	4:1:612:HOH:O	2.17	0.60
1:1:64:GLN:HE21	1:1:66:ARG:HE	1.49	0.58
1:1:74:ASN:ND2	1:1:153:ASP:OD1	2.36	0.58
1:1:64:GLN:HE22	1:1:66:ARG:HH21	1.51	0.58
1:1:224:LYS:HE3	4:1:626:HOH:O	2.06	0.56
1:1:27:VAL:HG13	1:1:29:TYR:CZ	2.42	0.54
1:1:59:TYR:C	1:1:59:TYR:CD1	2.82	0.54
1:1:81:GLN:HE22	1:1:113:SER:N	1.96	0.53
1:1:47:ILE:HD13	1:1:53:VAL:HG23	1.93	0.50
1:1:16:ILE:O	1:1:144:THR:HA	2.11	0.49
1:1:78:GLY:O	1:1:79:ASN:HB2	2.12	0.49
1:1:204:LYS:N	1:1:204:LYS:HD2	2.26	0.49
1:1:195:SER:OG	3:1:1:0KV:H3	1.92	0.48
1:1:56:ALA:HB1	1:1:90:VAL:HG13	1.97	0.47
1:1:47:ILE:HD13	1:1:53:VAL:CG2	2.45	0.46
1:1:85:ALA:HB1	1:1:106:ILE:HG23	1.98	0.46
1:1:48:ASN:HD21	1:1:51:TRP:HD1	1.62	0.45
1:1:47:ILE:C	1:1:120:SER:HB2	2.37	0.45
1:1:87:LYS:NZ	1:1:245:ASN:OD1	2.50	0.45
1:1:115:ASN:OD1	1:1:117:ARG:HB2	2.16	0.45
1:1:46:LEU:HD21	1:1:114:LEU:HD11	1.98	0.44
1:1:214:SER:O	3:1:1:0KV:HA2	2.18	0.43
1:1:195:SER:CB	3:1:1:0KV:O3	2.66	0.43
1:1:101:ASN:ND2	1:1:234:TYR:OH	2.44	0.43
1:1:221:GLN:HG3	4:1:481:HOH:O	2.18	0.42
1:1:46:LEU:O	1:1:120:SER:HA	2.20	0.42
1:1:57:HIS:NE2	3:1:1:0KV:H3	2.35	0.41
1:1:199:VAL:HG21	1:1:228:TYR:CD2	2.55	0.41
1:1:81:GLN:NE2	4:1:530:HOH:O	2.41	0.40
1:1:95:ASN:O	1:1:99:LEU:N	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1	221/223 (99%)	212 (96%)	9 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	1	184/184 (100%)	173 (94%)	11 (6%)	19	16

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	48	ASN
1	1	50	GLN
1	1	87	LYS
1	1	105	LEU
1	1	117	ARG
1	1	135	GLN
1	1	146	SER
1	1	149	THR
1	1	192	GLN
1	1	204	LYS
1	1	210	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	30	GLN
1	1	48	ASN
1	1	50	GLN
1	1	64	GLN
1	1	81	GLN
1	1	97	ASN
1	1	100	ASN
1	1	101	ASN
1	1	210	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
3	OKV	1	1	-	26,29,37	2.49	10 (38%)	30,39,51	4.25	16 (53%)

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	0KV	1	1	-	-	6/20/46/52	0/2/2/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	1	0KV	O3-C3	5.93	1.43	1.19
3	1	1	0KV	CZ3-NE3	4.63	1.45	1.35
3	1	1	0KV	CA1-N1	-4.01	1.42	1.47
3	1	1	0KV	C2-N3	3.55	1.41	1.34
3	1	1	0KV	CA2-N2	3.45	1.50	1.45
3	1	1	0KV	CA1-C1	3.43	1.57	1.52
3	1	1	0KV	CD3-NE3	3.36	1.50	1.46
3	1	1	0KV	C6-NE3	3.06	1.52	1.47
3	1	1	0KV	CA3-N3	2.68	1.50	1.46
3	1	1	0KV	O2-C2	2.29	1.27	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	1	0KV	CG3-CB3-CA3	-9.65	101.54	114.52
3	1	1	0KV	C4-CG3-CD3	9.62	119.56	108.68
3	1	1	0KV	CA2-C2-N3	-9.35	94.22	115.31
3	1	1	0KV	C2-CA2-N2	-8.90	92.34	113.60
3	1	1	0KV	CA3-N3-C2	-6.28	111.56	123.15
3	1	1	0KV	O3-C3-CA3	-5.45	110.49	124.78
3	1	1	0KV	CA2-N2-C1	-5.42	114.83	119.70
3	1	1	0KV	O1-C1-N2	3.72	126.88	122.49
3	1	1	0KV	O1-C1-CA1	-3.56	112.88	120.58
3	1	1	0KV	CB1-CG1-CD1	3.39	115.60	110.85
3	1	1	0KV	C1-CA1-N1	3.01	115.10	110.02
3	1	1	0KV	C3-CA3-N3	2.99	115.13	109.73
3	1	1	0KV	CG1-CB1-CA1	2.42	114.37	111.04
3	1	1	0KV	C5-C4-CG3	2.31	116.51	112.15
3	1	1	0KV	O2-C2-CA2	2.30	125.10	121.08
3	1	1	0KV	CB3-CG3-CD3	2.21	116.55	110.69

There are no chirality outliers.

All (6) torsion outliers are listed below:

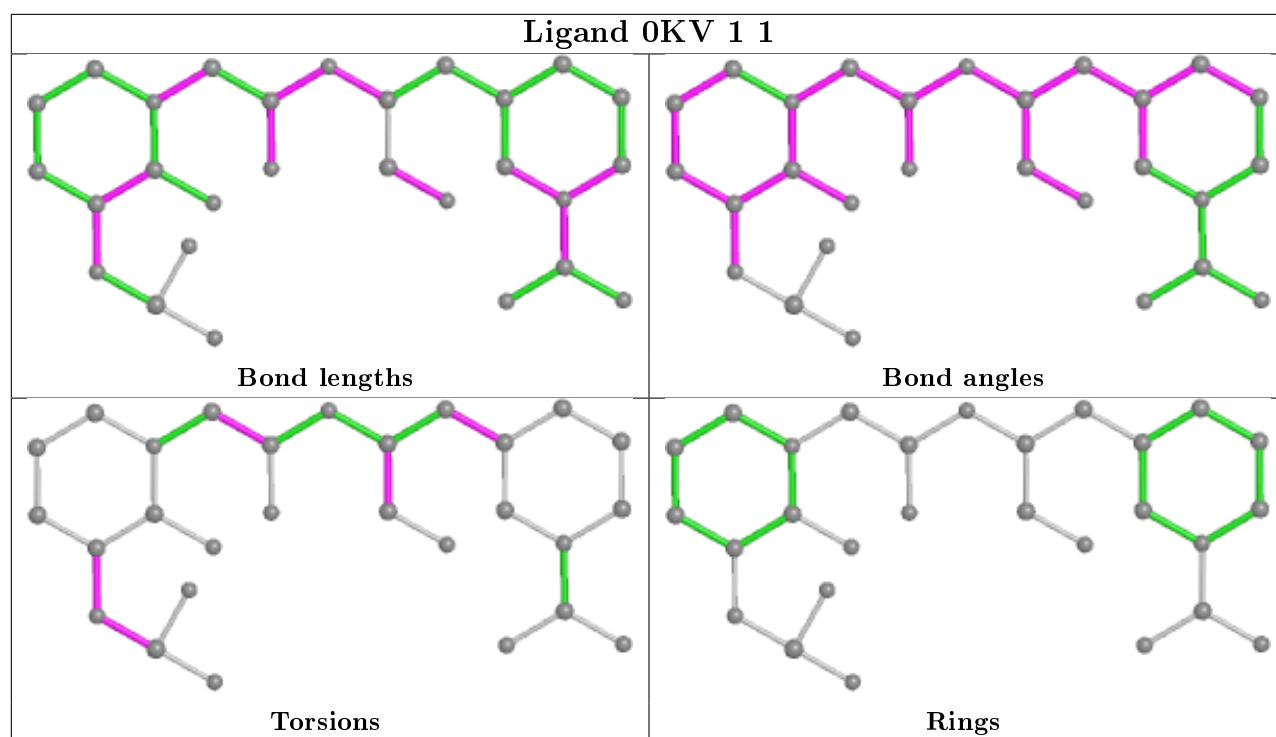
Mol	Chain	Res	Type	Atoms
3	1	1	0KV	CA1-N1-S-O1S
3	1	1	0KV	CA1-N1-S-O2S
3	1	1	0KV	O3-C3-CA3-CB3
3	1	1	0KV	CA3-CB3-CG3-CD3
3	1	1	0KV	O2-C2-CA2-N2
3	1	1	0KV	CB1-CA1-N1-S

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	1	0KV	10	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 than 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.



## 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.