



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:16 PM UTC

PDB ID : 1P01 / pdb_00001p01
Title : Serine protease mechanism. structure of an inhibitory complex of ALPHA-LYTIC Protease and a tightly bound peptide boronic acid
Authors : Bone, R.; Agard, D.A.
Deposited on : 1989-04-24
Resolution : 2.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

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

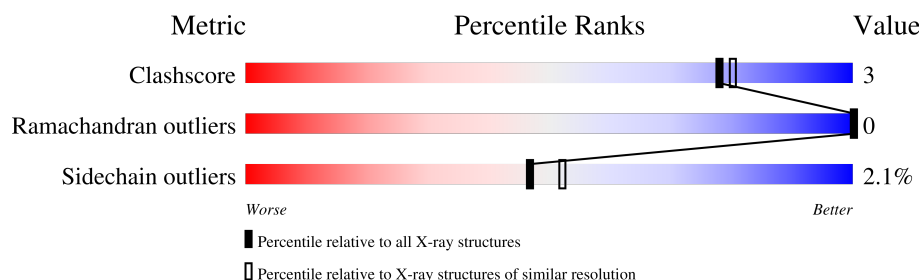
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	198	 57% 39% . .

2 Entry composition [i](#)

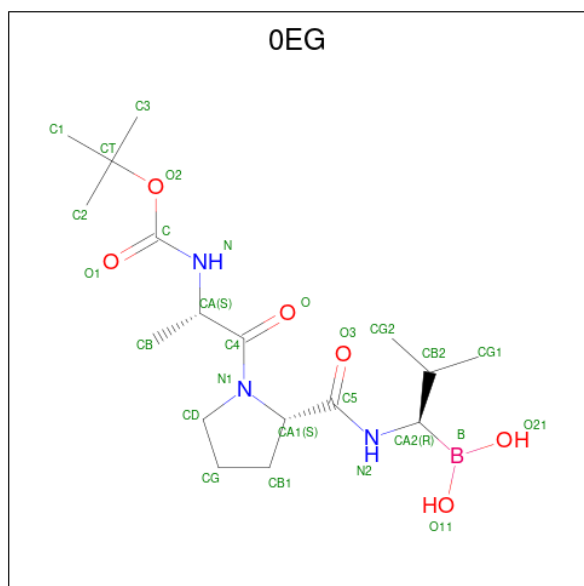
There are 4 unique types of molecules in this entry. The entry contains 1564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA-LYTIC PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			

- Molecule 2 is N-(tert-butoxycarbonyl)-L-alanyl-N-[(1R)-1-(dihydroxyboranyl)-2-methylpropyl]-L-prolinamide (CCD ID: 0EG) (formula: $C_{17}H_{32}BN_3O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			27	1	17	3	6		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



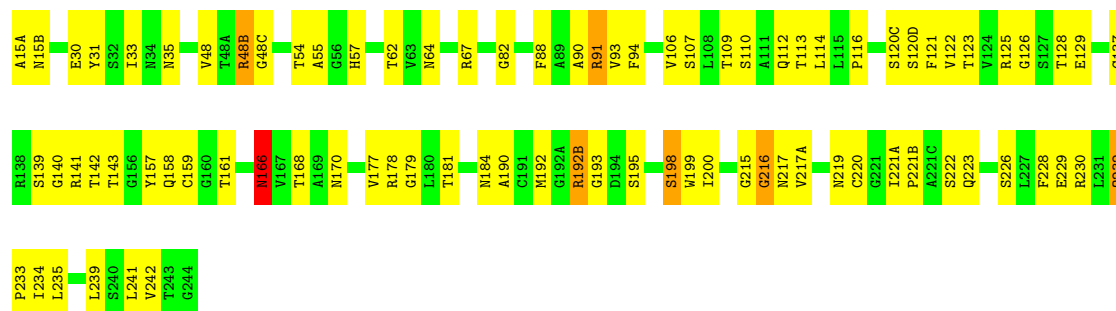
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		

Note EDS was not executed.

Chain A: 57% 39% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.34Å 66.34Å 80.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.138 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1564	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: SO4, OEG

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	1.53	7/1409 (0.5%)	2.62	115/1909 (6.0%)

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	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	GLY	N-CA	5.92	1.52	1.45
1	A	140	GLY	N-CA	5.52	1.51	1.45
1	A	234	ILE	CA-CB	5.43	1.60	1.54
1	A	168	THR	CA-CB	5.34	1.61	1.53
1	A	109	THR	N-CA	5.24	1.52	1.45
1	A	139	SER	C-O	5.24	1.30	1.23
1	A	178	ARG	NE-CZ	5.19	1.38	1.33

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48(B)	ARG	NE-CZ-NH1	-16.88	104.62	121.50
1	A	192(B)	ARG	NE-CZ-NH1	-13.71	107.79	121.50
1	A	91	ARG	NE-CZ-NH2	13.29	131.17	119.20
1	A	112	GLN	OE1-CD-NE2	-10.60	112.00	122.60
1	A	48(B)	ARG	NE-CZ-NH2	10.16	128.35	119.20
1	A	35	ASN	OD1-CG-ND2	9.39	131.99	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	SER	CB-CA-C	-9.02	91.30	110.32
1	A	110	SER	O-C-N	8.78	133.80	122.39
1	A	232	GLN	OE1-CD-NE2	-8.73	113.87	122.60
1	A	110	SER	CA-C-O	-8.67	109.00	119.49
1	A	107	SER	CA-CB-OG	-8.30	94.51	111.10
1	A	88	PHE	CA-C-O	-8.04	111.25	120.58
1	A	57	HIS	CA-C-O	-7.99	108.67	119.05
1	A	170	ASN	CA-CB-CG	-7.99	104.61	112.60
1	A	228	PHE	CA-CB-CG	7.84	121.64	113.80
1	A	113	THR	CA-CB-OG1	-7.75	97.97	109.60
1	A	106	VAL	CA-C-O	-7.74	112.28	120.48
1	A	166	ASN	CA-CB-CG	-7.69	104.91	112.60
1	A	64	ASN	CA-C-O	-7.61	109.04	119.16
1	A	125	ARG	NE-CZ-NH1	-7.57	113.93	121.50
1	A	223	GLN	CA-C-O	-7.49	110.75	119.59
1	A	192(B)	ARG	NE-CZ-NH2	7.40	125.86	119.20
1	A	198	SER	CA-C-O	-7.24	113.67	121.56
1	A	142	THR	O-C-N	7.17	130.65	122.19
1	A	116	PRO	CA-C-O	-7.15	116.02	121.31
1	A	139	SER	N-CA-CB	-6.97	98.65	111.13
1	A	91	ARG	NH1-CZ-NH2	-6.97	110.24	119.30
1	A	128	THR	CA-CB-OG1	-6.92	99.21	109.60
1	A	48	VAL	CA-C-O	-6.90	114.53	121.49
1	A	125	ARG	CA-C-O	-6.90	111.46	119.05
1	A	217(A)	VAL	CA-C-O	-6.89	113.85	121.23
1	A	161	THR	CA-CB-CG2	6.87	122.17	110.50
1	A	15(B)	ASN	OD1-CG-ND2	-6.87	115.73	122.60
1	A	199	TRP	N-CA-C	-6.83	97.13	108.34
1	A	200	ILE	CA-C-O	-6.77	114.22	121.19
1	A	158	GLN	CA-C-O	-6.69	113.28	121.11
1	A	88	PHE	O-C-N	6.69	131.38	122.96
1	A	216	GLY	O-C-N	6.68	130.33	123.92
1	A	158	GLN	OE1-CD-NE2	-6.52	116.08	122.60
1	A	242	VAL	CA-C-O	-6.45	113.50	120.85
1	A	112	GLN	CG-CD-OE1	6.44	133.68	120.80
1	A	228	PHE	O-C-N	6.33	131.02	123.24
1	A	142	THR	CA-C-O	-6.32	111.07	120.42
1	A	242	VAL	N-CA-CB	-6.28	103.69	110.53
1	A	120(D)	SER	N-CA-CB	-6.23	99.42	110.14
1	A	192(B)	ARG	CD-NE-CZ	-6.20	115.72	124.40
1	A	126	GLY	CA-C-O	-6.18	114.86	121.35
1	A	82	GLY	CA-C-O	-6.18	112.49	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ASN	CB-CG-ND2	6.17	125.65	116.40
1	A	122	VAL	N-CA-C	-6.17	99.54	108.17
1	A	67	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	A	230	ARG	CA-C-O	-6.10	114.48	121.19
1	A	168	THR	CA-CB-OG1	-6.08	100.47	109.60
1	A	143	THR	CA-CB-OG1	-6.07	100.50	109.60
1	A	31	TYR	N-CA-C	-6.05	99.88	109.07
1	A	221(A)	ILE	N-CA-CB	6.01	115.98	111.83
1	A	177	VAL	N-CA-CB	5.99	119.43	111.64
1	A	235	LEU	CA-C-O	-5.98	114.22	120.55
1	A	220	CYS	CA-C-O	-5.96	111.92	119.31
1	A	141	ARG	CA-C-O	-5.95	111.31	119.05
1	A	143	THR	CA-C-O	-5.94	112.61	119.56
1	A	15(A)	ALA	CA-C-O	-5.86	110.84	120.80
1	A	181	THR	CA-CB-OG1	-5.82	100.87	109.60
1	A	48(B)	ARG	NH1-CZ-NH2	5.82	126.86	119.30
1	A	177	VAL	N-CA-C	-5.80	99.28	107.75
1	A	190	ALA	N-CA-C	-5.71	102.45	110.50
1	A	120(C)	SER	CB-CA-C	-5.70	99.75	110.01
1	A	120(D)	SER	CA-C-O	-5.66	113.93	121.46
1	A	217	ASN	N-CA-CB	-5.60	103.01	110.57
1	A	55	ALA	CA-C-O	-5.60	114.67	121.05
1	A	142	THR	CA-C-N	-5.58	113.72	122.65
1	A	142	THR	C-N-CA	-5.58	113.72	122.65
1	A	241	LEU	N-CA-CB	-5.54	101.83	109.97
1	A	110	SER	CA-CB-OG	-5.53	100.04	111.10
1	A	114	LEU	CA-C-O	-5.52	114.75	121.05
1	A	241	LEU	CA-C-O	-5.52	114.98	121.16
1	A	193	GLY	N-CA-C	-5.49	107.37	113.79
1	A	120(C)	SER	CA-CB-OG	-5.48	100.14	111.10
1	A	15(B)	ASN	CA-C-O	-5.46	114.36	120.54
1	A	123	THR	O-C-N	5.43	129.40	123.04
1	A	192(B)	ARG	NH1-CZ-NH2	5.41	126.34	119.30
1	A	30	GLU	N-CA-CB	-5.41	102.07	110.29
1	A	121	PHE	CA-C-O	-5.41	114.78	121.06
1	A	222	SER	CA-C-O	-5.41	112.95	119.49
1	A	195	SER	O-C-N	5.40	129.56	122.97
1	A	226	SER	CA-C-O	-5.38	114.55	120.30
1	A	90	ALA	CA-C-O	-5.34	115.22	121.10
1	A	184	ASN	O-C-N	5.34	129.16	122.22
1	A	221(B)	PRO	CA-C-O	-5.34	115.16	121.67
1	A	30	GLU	CB-CG-CD	-5.32	103.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	TYR	CA-C-O	-5.31	114.68	120.36
1	A	48(C)	GLY	N-CA-C	-5.26	101.19	110.86
1	A	94	PHE	CA-C-O	-5.24	112.98	120.16
1	A	31	TYR	CA-C-O	-5.23	115.68	121.33
1	A	123	THR	CA-C-O	-5.22	114.73	120.69
1	A	184	ASN	CA-C-O	-5.22	113.64	119.95
1	A	15(B)	ASN	CA-C-N	-5.21	115.86	122.37
1	A	15(B)	ASN	C-N-CA	-5.21	115.86	122.37
1	A	120(D)	SER	O-C-N	5.20	129.61	122.59
1	A	94	PHE	O-C-N	5.20	127.30	121.32
1	A	33	ILE	CA-C-O	-5.19	114.99	120.39
1	A	219	ASN	N-CA-C	-5.19	105.67	112.41
1	A	200	ILE	O-C-N	5.17	128.69	123.00
1	A	91	ARG	CD-NE-CZ	5.15	131.62	124.40
1	A	216	GLY	CA-C-O	-5.15	115.95	121.35
1	A	232	GLN	CG-CD-NE2	5.14	124.12	116.40
1	A	64	ASN	O-C-N	5.12	127.25	121.87
1	A	54	THR	CA-C-O	-5.09	115.70	121.05
1	A	129	GLU	CG-CD-OE2	-5.09	106.69	118.40
1	A	15(A)	ALA	O-C-N	5.08	130.83	122.70
1	A	67	ARG	NE-CZ-NH2	-5.05	114.65	119.20
1	A	239	LEU	CA-C-O	-5.02	115.53	121.66
1	A	93	VAL	O-C-N	5.01	128.19	123.03
1	A	229	GLU	CA-CB-CG	5.01	124.12	114.10
1	A	62	THR	CA-CB-OG1	-5.00	102.09	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192(B)	ARG	Sidechain

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	A	1391	0	1360	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	32	0	0
3	A	5	0	0	1	0
4	A	141	0	0	2	0
All	All	1564	0	1392	8	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 3.

All (8) 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:166:ASN:HD22	1:A:179:GLY:HA2	1.58	0.67
1:A:48(B):ARG:HD2	4:A:354:HOH:O	2.03	0.57
1:A:137:CYS:HA	1:A:159:CYS:HA	1.94	0.49
1:A:232:GLN:N	1:A:233:PRO:HD2	2.29	0.48
1:A:192:MET:HE2	1:A:216:GLY:HA3	1.96	0.47
1:A:166:ASN:ND2	1:A:179:GLY:HA2	2.29	0.45
1:A:233:PRO:HB3	3:A:1:SO4:O4	2.18	0.43
1:A:48(B):ARG:NE	4:A:379:HOH:O	2.54	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 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	196/198 (99%)	188 (96%)	8 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	142/142 (100%)	139 (98%)	3 (2%)	47 52

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	166	ASN
1	A	198	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	166	ASN
1	A	182	GLN
1	A	217(B)	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

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
2	0EG	A	4	1	23,27,27	1.77	2 (8%)	31,39,39	2.07	5 (16%)
3	SO4	A	1	-	4,4,4	0.66	0	6,6,6	0.64	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
2	0EG	A	4	1	-	0/28/43/43	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4	0EG	O2-C	7.68	1.49	1.34
2	A	4	0EG	CB-CA	-2.02	1.47	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4	0EG	CB-CA-C4	-9.40	91.75	109.87
2	A	4	0EG	CT-O2-C	-2.36	117.38	120.97
2	A	4	0EG	O2-C-N	2.24	113.69	110.03
2	A	4	0EG	O-C4-CA	-2.17	115.68	120.15
2	A	4	0EG	O-C4-N1	2.00	124.98	121.38

There are no chirality outliers.

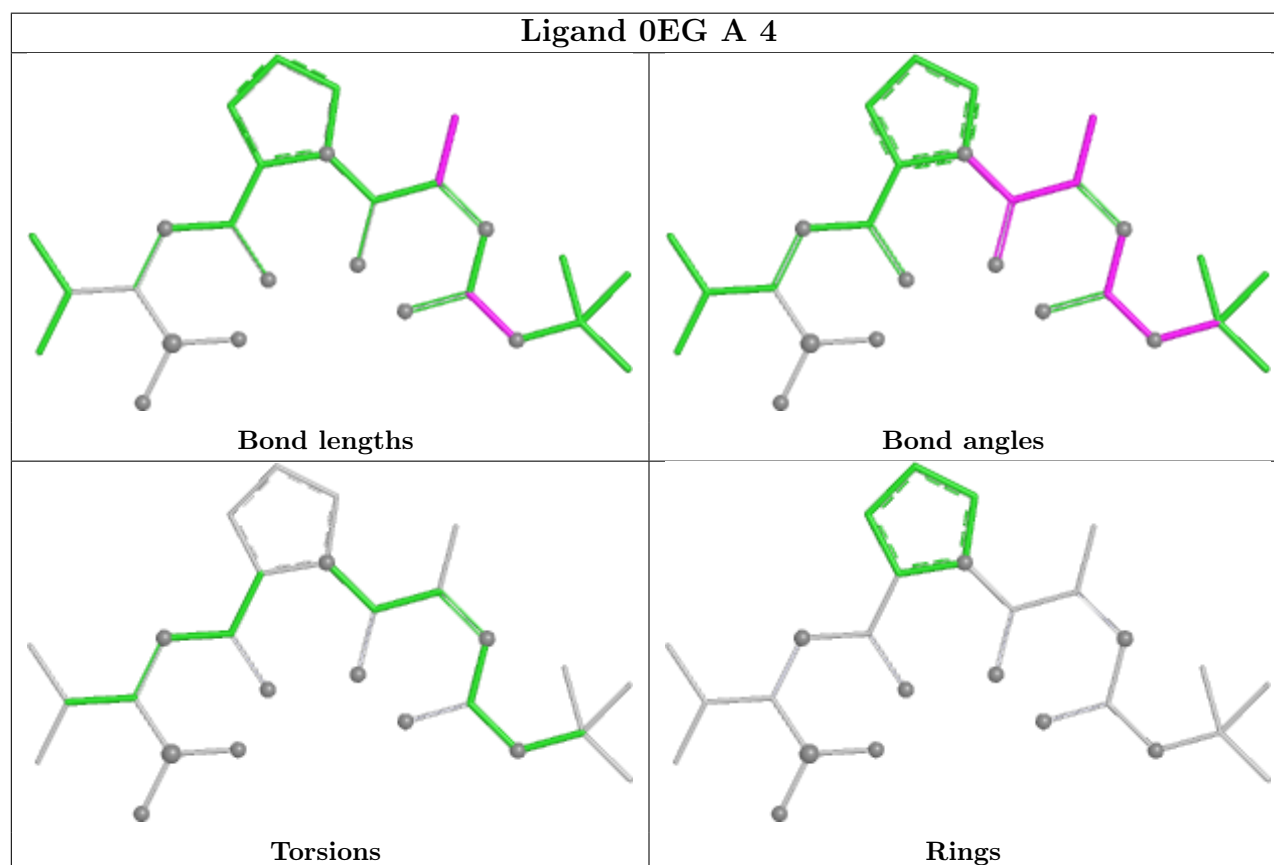
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	SO4	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 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 ⓘ

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.