Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 04:43 PM UTC

PDB ID	:	2F7X / pdb_00002f7x
Title	:	Protein Kinase A bound to (S)-2-(1H-Indol-3-yl)-1-[5-((E)-2-pyridin-4-yl-vinyl)-pyridin-3-yloxymethyl]-ethylamine
Authors	:	Li, Q.; Li, T.; Zhu, G.D.; Gong, J.; Claibone, A.; Dalton, C.; Luo, Y.; Johnson, E.F.; Shi, Y.; Liu, X.; Klinghofer, V.; Bauch, J.L.; Marsh, K.C.; Bouska, J.J.; Arries, S.; De Jong, R.; Oltersdorf, T.; Stoll, V.S.; Jakob, C.G.; Rosenberg, S.H.; Giranda, V.L.
Deposited on	:	2005-12-01
Resolution	:	1.90 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:

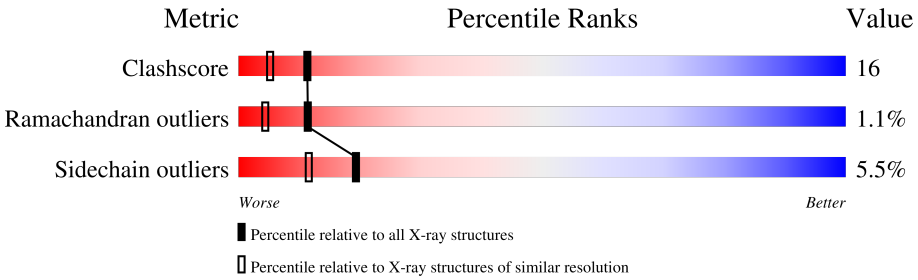
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	E	351	64% 27%
2	I	20	80% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3150 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.

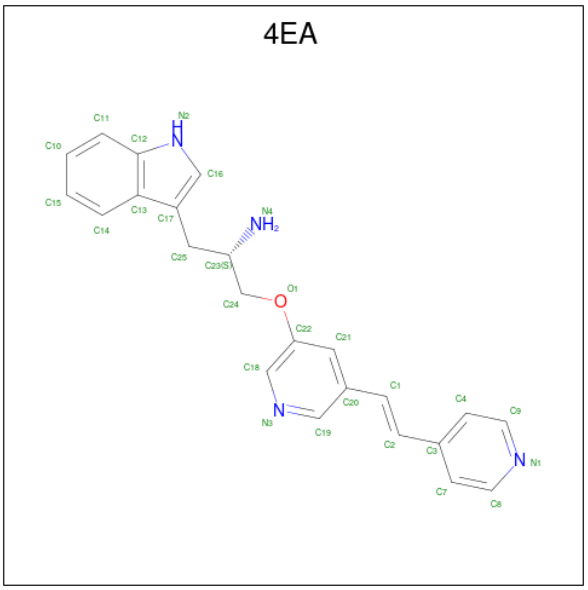
- Molecule 1 is a protein called cAMP-dependent protein kinase, alpha-catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	336	Total	C	N	O	S	0	0	0
			2770	1801	466	494	9			

- Molecule 2 is a protein called PKI, inhibitory peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	0	0
			157	94	32	31			

- Molecule 3 is (1S)-2-(1H-INDOL-3-YL)-1-[({5-[(E)-2-PYRIDIN-4-YLVINYL]PYRIDIN-3-YL}OXY)METHYL]ETHYLAMINE (CCD ID: 4EA) (formula: $C_{23}H_{22}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			28	23	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	173	Total O 173 173	0	0
4	I	22	Total O 22 22	0	0

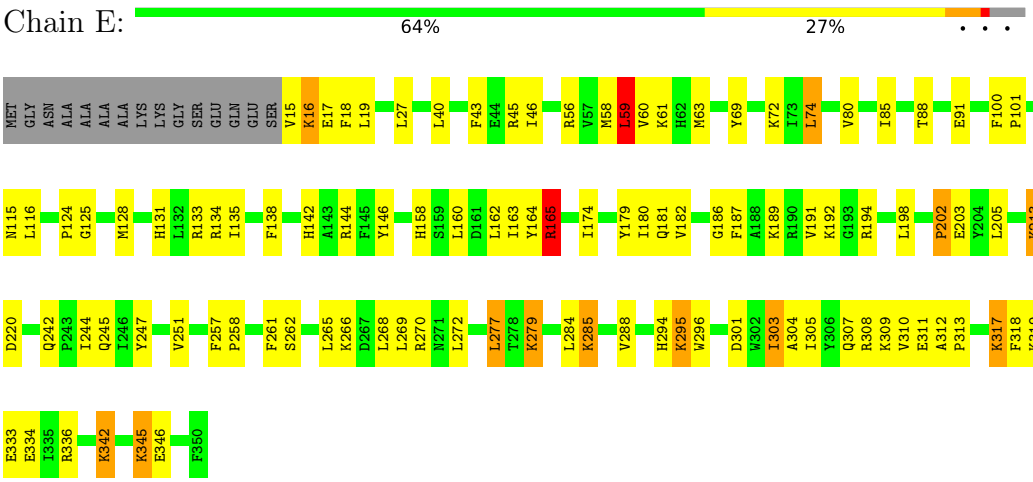
3 Residue-property plots (i)

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.

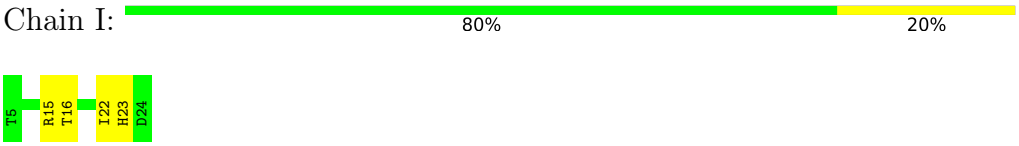
• Molecule 1: cAMP-dependent protein kinase, alpha-catalytic subunit

Chain E:



• Molecule 2: PKI, inhibitory peptide

Chain I:



4 Data and refinement statistics (i)

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, α, β, γ	72.84Å 74.40Å 80.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.90	Depositor
% Data completeness (in resolution range)	96.7 (19.99-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2000	Depositor
R, R_{free}	0.268 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3150	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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: 4EA

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	E	0.43	0/2842	0.91	10/3831 (0.3%)
2	I	0.48	0/159	0.84	0/212
All	All	0.44	0/3001	0.90	10/4043 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	213	LYS	N-CA-C	7.91	119.94	110.44
1	E	194	ARG	N-CA-C	6.50	120.10	110.48
1	E	63	MET	N-CA-C	6.34	118.19	111.28
1	E	192	LYS	N-CA-C	-6.34	98.87	109.07
1	E	59	LEU	N-CA-C	-6.11	99.70	109.96
1	E	115	ASN	N-CA-C	6.07	119.09	109.81
1	E	128	MET	N-CA-C	-6.00	104.74	111.28
1	E	124	PRO	N-CA-CB	5.65	109.13	103.48
1	E	342	LYS	N-CA-C	5.58	120.08	112.04
1	E	165	ARG	N-CA-C	5.08	119.06	112.86

There are no chirality outliers.

There are no planarity outliers.

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	E	2770	0	2757	95	0
2	I	157	0	146	3	0
3	E	28	0	22	0	0
4	E	173	0	0	3	0
4	I	22	0	0	0	0
All	All	3150	0	2925	95	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 16.

All (95) 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:E:279:LYS:HA	1:E:284:LEU:HD21	1.34	1.08
1:E:303:ILE:HG22	1:E:307:GLN:HE21	1.26	1.01
1:E:317:LYS:HE3	1:E:317:LYS:HA	1.41	1.00
1:E:131:HIS:HA	1:E:134:ARG:HH12	1.40	0.86
1:E:165:ARG:HD3	1:E:187:PHE:O	1.74	0.86
1:E:303:ILE:HD12	1:E:303:ILE:H	1.42	0.82
1:E:203:GLU:OE2	2:I:15:ARG:HD2	1.79	0.82
1:E:303:ILE:HG22	1:E:307:GLN:NE2	1.95	0.81
1:E:266:LYS:O	1:E:270:ARG:HG3	1.81	0.80
1:E:45:ARG:NE	1:E:58:MET:HE1	1.97	0.79
1:E:163:ILE:HG12	1:E:217:LYS:HG2	1.64	0.79
1:E:295:LYS:HD3	1:E:295:LYS:H	1.48	0.78
1:E:265:LEU:O	1:E:269:LEU:HD13	1.89	0.72
1:E:40:LEU:HD23	1:E:40:LEU:O	1.91	0.71
1:E:43:PHE:HB3	1:E:60:VAL:CG2	2.21	0.70
1:E:305:ILE:HD12	1:E:310:VAL:HG21	1.74	0.70
1:E:43:PHE:HB3	1:E:60:VAL:HG21	1.73	0.69
1:E:165:ARG:CD	1:E:187:PHE:O	2.39	0.69
1:E:205:LEU:HD11	2:I:22:ILE:HD11	1.76	0.67
1:E:74:LEU:HD22	1:E:74:LEU:N	2.10	0.67
1:E:17:GLU:H	1:E:17:GLU:CD	2.07	0.63
1:E:134:ARG:NH1	1:E:134:ARG:HB3	2.14	0.63
1:E:244:ILE:HG13	1:E:245:GLN:N	2.13	0.62
1:E:257:PHE:HB2	1:E:266:LYS:NZ	2.14	0.62
1:E:244:ILE:HG13	1:E:245:GLN:H	1.65	0.61
1:E:164:TYR:C	1:E:165:ARG:HG3	2.25	0.61
1:E:345:LYS:H	1:E:345:LYS:HD2	1.66	0.61
1:E:242:GLN:HB2	1:E:245:GLN:HG3	1.82	0.60
1:E:80:VAL:HG22	1:E:85:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:HIS:HA	1:E:134:ARG:NH1	2.14	0.59
1:E:319:LYS:HD2	1:E:319:LYS:N	2.18	0.59
1:E:294:HIS:CE1	1:E:295:LYS:HE3	2.38	0.58
1:E:131:HIS:O	1:E:135:ILE:HG13	2.04	0.58
1:E:345:LYS:HD2	1:E:345:LYS:N	2.19	0.57
1:E:258:PRO:HD2	1:E:261:PHE:CE2	2.41	0.56
1:E:46:ILE:HG21	1:E:59:LEU:HD13	1.89	0.55
1:E:134:ARG:CB	1:E:134:ARG:HH11	2.19	0.55
1:E:18:PHE:HD2	1:E:19:LEU:HD22	1.71	0.55
1:E:345:LYS:H	1:E:345:LYS:CD	2.20	0.55
1:E:46:ILE:HD11	1:E:61:LYS:HB2	1.88	0.54
1:E:40:LEU:HD23	1:E:40:LEU:C	2.33	0.54
1:E:69:TYR:CE1	1:E:107:GLU:HG3	2.43	0.53
1:E:15:VAL:O	1:E:19:LEU:HD23	2.08	0.53
1:E:46:ILE:HD12	1:E:59:LEU:HD22	1.90	0.53
1:E:279:LYS:HA	1:E:284:LEU:CD2	2.23	0.53
1:E:317:LYS:HE3	1:E:317:LYS:CA	2.27	0.53
1:E:295:LYS:H	1:E:295:LYS:CD	2.20	0.53
1:E:45:ARG:HH12	1:E:334:GLU:HA	1.74	0.52
1:E:295:LYS:HD3	1:E:295:LYS:N	2.22	0.50
1:E:158:HIS:HE1	1:E:220:ASP:OD2	1.95	0.50
1:E:133:ARG:NH1	2:I:16:THR:O	2.45	0.49
1:E:285:LYS:N	1:E:285:LYS:HD2	2.27	0.49
1:E:334:GLU:HB2	1:E:336:ARG:CZ	2.41	0.49
1:E:72:LYS:NZ	1:E:91:GLU:OE2	2.46	0.49
1:E:277:LEU:C	1:E:277:LEU:HD22	2.38	0.48
1:E:304:ALA:HA	1:E:309:LYS:HE2	1.94	0.48
1:E:279:LYS:CA	1:E:284:LEU:HD21	2.24	0.48
1:E:59:LEU:HD12	1:E:324:THR:CG2	2.44	0.48
1:E:16:LYS:HZ1	1:E:16:LYS:HA	1.79	0.47
1:E:125:GLY:HA3	1:E:174:ILE:O	2.15	0.47
1:E:134:ARG:HB3	1:E:134:ARG:HH11	1.79	0.47
1:E:284:LEU:HB2	4:E:407:HOH:O	2.14	0.47
1:E:213:LYS:O	1:E:214:GLY:O	2.32	0.47
1:E:257:PHE:HB2	1:E:266:LYS:HZ2	1.79	0.47
1:E:43:PHE:HB3	1:E:60:VAL:HG22	1.94	0.47
1:E:313:PRO:HB3	4:E:487:HOH:O	2.15	0.47
1:E:40:LEU:C	1:E:40:LEU:CD2	2.88	0.47
1:E:19:LEU:HD22	1:E:19:LEU:N	2.32	0.45
1:E:303:ILE:H	1:E:303:ILE:CD1	2.20	0.45
1:E:104:VAL:HG22	1:E:182:VAL:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:ARG:HH11	1:E:56:ARG:HB3	1.83	0.44
1:E:104:VAL:CG1	1:E:181:GLN:HB3	2.47	0.44
1:E:45:ARG:NH2	1:E:333:GLU:O	2.51	0.44
1:E:268:LEU:C	1:E:268:LEU:HD13	2.42	0.44
1:E:88:THR:HG21	1:E:116:LEU:CD1	2.48	0.43
1:E:144:ARG:HH21	1:E:296:TRP:CD1	2.35	0.43
1:E:180:ILE:HG22	1:E:181:GLN:N	2.33	0.43
1:E:312:ALA:HA	1:E:313:PRO:HD3	1.88	0.43
1:E:288:VAL:HG22	1:E:288:VAL:O	2.19	0.43
1:E:100:PHE:CD1	1:E:101:PRO:HD2	2.54	0.42
1:E:262:SER:O	1:E:266:LYS:HG3	2.19	0.42
1:E:318:PHE:HD1	1:E:320:GLY:H	1.67	0.42
1:E:186:GLY:HA3	4:E:425:HOH:O	2.19	0.42
1:E:247:TYR:O	1:E:251:VAL:HG22	2.19	0.42
1:E:301:ASP:HB3	1:E:304:ALA:HB3	2.02	0.41
1:E:242:GLN:HB2	1:E:245:GLN:CG	2.47	0.41
1:E:342:LYS:HA	1:E:342:LYS:HD3	1.86	0.41
1:E:189:LYS:HG2	1:E:191:VAL:CG2	2.50	0.41
1:E:319:LYS:N	1:E:319:LYS:CD	2.83	0.41
1:E:345:LYS:HG2	1:E:346:GLU:N	2.36	0.41
1:E:74:LEU:N	1:E:74:LEU:CD2	2.81	0.40
1:E:142:HIS:CD2	1:E:146:TYR:CE2	3.09	0.40
1:E:317:LYS:CE	1:E:318:PHE:H	2.35	0.40
1:E:138:PHE:HB3	1:E:142:HIS:HB3	2.04	0.40
1:E:179:TYR:CZ	1:E:308:ARG:HA	2.57	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	E	334/351 (95%)	316 (95%)	15 (4%)	3 (1%)	14 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	I	18/20 (90%)	17 (94%)	0	1 (6%)	1 0
All	All	352/371 (95%)	333 (95%)	15 (4%)	4 (1%)	11 4

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	214	GLY
1	E	279	LYS
2	I	23	HIS
1	E	202	PRO

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	E	296/306 (97%)	279 (94%)	17 (6%)	18 11
2	I	15/15 (100%)	15 (100%)	0	100 100
All	All	311/321 (97%)	294 (94%)	17 (6%)	19 11

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	16	LYS
1	E	27	LEU
1	E	59	LEU
1	E	74	LEU
1	E	160	LEU
1	E	162	LEU
1	E	165	ARG
1	E	198	LEU
1	E	202	PRO
1	E	272	LEU
1	E	277	LEU
1	E	285	LYS

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Mol	Chain	Res	Type
1	E	295	LYS
1	E	303	ILE
1	E	311	GLU
1	E	317	LYS
1	E	345	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	113	ASN
1	E	158	HIS
1	E	271	ASN
1	E	307	GLN
2	I	20	ASN

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)

1 ligand is 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	4EA	E	351	-	31,31,31	1.69	8 (25%)	38,41,41	0.71	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
3	4EA	E	351	-	-	0/14/14/14	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	351	4EA	C14-C13	4.67	1.47	1.39
3	E	351	4EA	C25-C23	2.72	1.57	1.53
3	E	351	4EA	C15-C14	2.57	1.43	1.38
3	E	351	4EA	C10-C11	2.48	1.43	1.38
3	E	351	4EA	C18-C22	2.44	1.41	1.38
3	E	351	4EA	C15-C10	2.32	1.43	1.38
3	E	351	4EA	C16-C17	2.30	1.40	1.36
3	E	351	4EA	C21-C22	2.14	1.42	1.39

There are no bond angle outliers.

There are no chirality outliers.

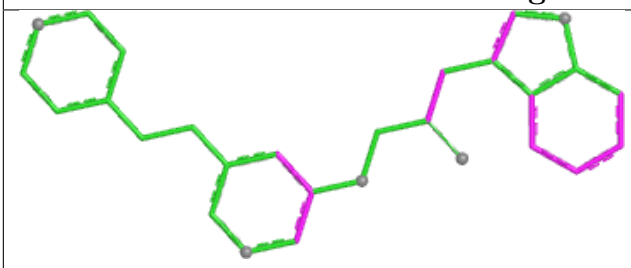
There are no torsion outliers.

There are no ring outliers.

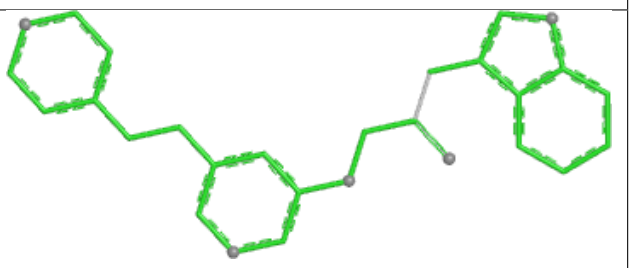
No monomer is involved in short contacts.

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.

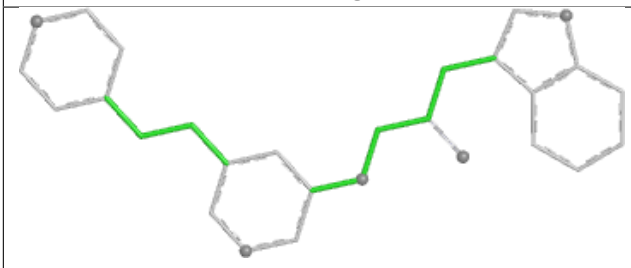
Ligand 4EA E 351



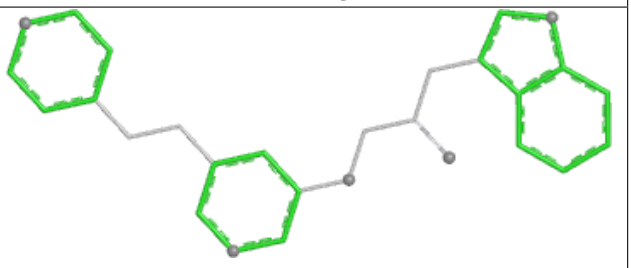
Bond lengths



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.