



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 02:16 am BST

PDB ID : 1EH4
Title : BINARY COMPLEX OF CASEIN KINASE-1 FROM S. POMBE WITH AN
ATP COMPETITIVE INHIBITOR, IC261
Authors : Mashhoon, N.; Demaggio, A.J.; Tereshko, V.; Bergmeier, S.C.; Egli, M.; Hoek-
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Deposited on : 2000-02-18
Resolution : 2.80 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 ⓘ symbol.

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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

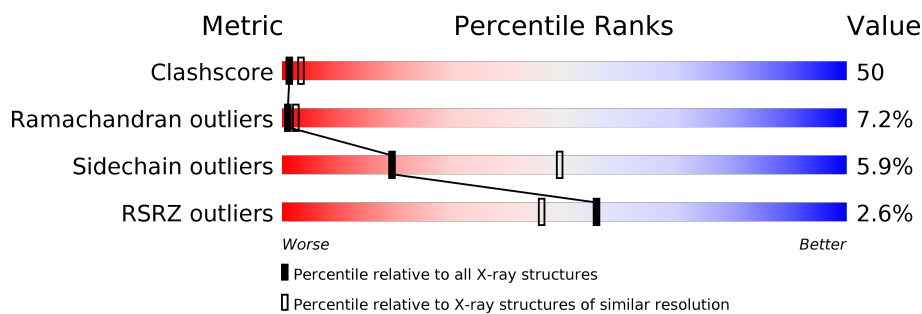
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	298	 3% 34% 54% 9% ..
1	B	298	 2% 36% 54% 7% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4918 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 CASEIN KINASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2385	1522	421	432	10			
1	B	293	Total	C	N	O	S	0	0	0
			2385	1522	421	432	10			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



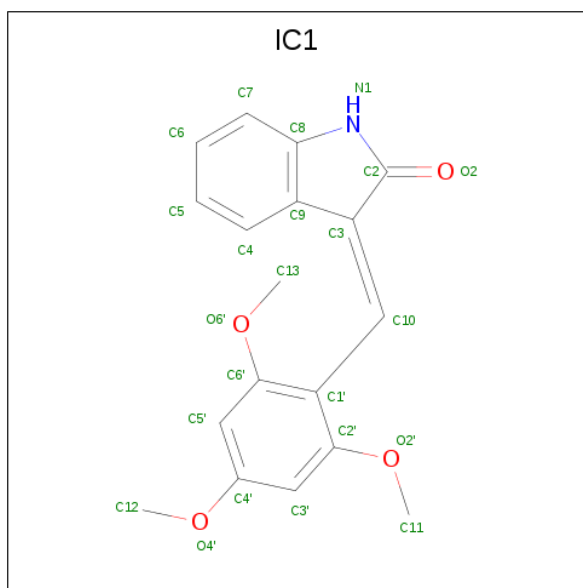
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 3-[(2,4,6-TRIMETHOXY-PHENYL)-METHYLENE]-INDOLIN-2-ONE (three-letter code: IC1) (formula: C₁₈H₁₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 23	C 18	N 1	O 4	0	0
3	B	1	Total 23	C 18	N 1	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	17	Total 17	O 17	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

[illegible]

Chain B:

29% 36% 54% 7%

Label	Color
Q199	Yellow
D200	Yellow
L201	Yellow
E202	Yellow
A203	Yellow
H206	Yellow
V207	Yellow
F208	Yellow
L212	Yellow
R213	Yellow
L216	Yellow
P217	Yellow
Q218	Yellow
Q219	Yellow
G220	Yellow
L221	Yellow
K222	Yellow
A223	Yellow
A224	Yellow
T225	Yellow
Q228	Yellow
K229	Yellow
I233	Yellow
K236	Yellow
S239	Yellow
T240	Yellow
P241	Yellow
L242	Yellow
R243	Yellow
E244	Yellow
F249	Yellow
P250	Yellow
E251	Yellow
E252	Yellow
F253	Yellow
Y259	Yellow
A260	Yellow
R261	Yellow
Y262	Yellow
L263	Yellow
A264	Yellow
F265	Yellow
D266	Yellow
A267	Yellow
T268	Yellow
P269	Yellow
L274	Yellow
Q275	Yellow
T276	Yellow
P277	Yellow
R130	Red
K133	Yellow
P134	Yellow
D135	Yellow
M136	Yellow
F137	Yellow
L138	Yellow
V139	Yellow
G140	Yellow
R141	Yellow
P142	Yellow
M143	Yellow
S144	Yellow
K145	Yellow
M146	Yellow
A147	Yellow
M148	Yellow
Y151	Yellow
V152	Yellow
V153	Yellow
D154	Yellow
F155	Yellow
G156	Yellow
M157	Yellow
V158	Yellow
K159	Yellow
F160	Yellow
Y161	Yellow
V165	Yellow
H169	Yellow
L170	Yellow
P171	Yellow
Y172	Yellow
R173	Yellow
E174	Yellow
K175	Yellow
P176	Yellow
M177	Yellow
L178	Yellow
S179	Yellow
G180	Yellow
T181	Yellow
A182	Yellow
R183	Yellow
Y184	Yellow
L187	Yellow
M188	Yellow
G192	Yellow
R193	Yellow
E194	Yellow
Q195	Yellow
S196	Yellow
R197	Yellow
P198	Yellow
L61	Yellow
L62	Yellow
G67	Yellow
I68	Yellow
P69	Yellow
N70	Yellow
V71	Yellow
Y72	Yellow
Y73	Yellow
Q76	Yellow
H80	Yellow
N81	Yellow
V82	Yellow
L83	Yellow
V84	Yellow
I85	Yellow
D86	Yellow
L87	Yellow
P90	Yellow
S91	Yellow
D94	Yellow
L95	Yellow
L96	Yellow
D97	Yellow
L98	Yellow
C99	Yellow
G100	Yellow
L101	Yellow
S104	Yellow
V105	Yellow
K106	Yellow
T107	Yellow
A108	Yellow
A109	Yellow
M110	Yellow
A111	Yellow
A112	Yellow
K113	Yellow
Q114	Yellow
M115	Yellow
L116	Yellow
A117	Yellow
R118	Yellow
V119	Yellow
Q120	Yellow
S121	Yellow
I122	Yellow
H123	Yellow
E124	Yellow
K125	Yellow
S126	Yellow
L127	Yellow
T128	Yellow
V129	Yellow
R130	Red
K133	Yellow
P134	Yellow
D135	Yellow
M136	Yellow
F137	Yellow
L138	Yellow
V139	Yellow
G140	Yellow
R141	Yellow
P142	Yellow
M143	Yellow
S144	Yellow
K145	Yellow
M146	Yellow
A147	Yellow
M148	Yellow
Y151	Yellow
V152	Yellow
V153	Yellow
D154	Yellow
F155	Yellow
G156	Yellow
M157	Yellow
V158	Yellow
K159	Yellow
F160	Yellow
Y161	Yellow
V165	Yellow
H169	Yellow
L170	Yellow
P171	Yellow
Y172	Yellow
R173	Yellow
E174	Yellow
K175	Yellow
P176	Yellow
M177	Yellow
L178	Yellow
S179	Yellow
G180	Yellow
T181	Yellow
A182	Yellow
R183	Yellow
Y184	Yellow
L187	Yellow
M188	Yellow
G192	Yellow
R193	Yellow
E194	Yellow
Q195	Yellow

K280	V281	R284	T287	D290	E291	N292	F293	L297	L298
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	113.50Å 113.50Å 110.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 98.29 – 2.82	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.00-2.80) 95.5 (98.29-2.82)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.82Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.224 , 0.304 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.103 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4918	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1197e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: IC1, SO4

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	0.41	0/2439	0.69	1/3289 (0.0%)
1	B	0.40	0/2439	0.68	0/3289
All	All	0.40	0/4878	0.68	1/6578 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	79	LEU	CA-CB-CG	5.28	127.44	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	130	ARG	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	2385	0	2371	229	0
1	B	2385	0	2371	257	0
2	A	30	0	0	1	0
2	B	25	0	0	1	0
3	A	23	0	17	5	0
3	B	23	0	17	8	0
4	A	30	0	0	3	0
4	B	17	0	0	2	0
All	All	4918	0	4776	479	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 50.

The worst 5 of 479 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:181:THR:HG22	4:A:404:HOH:O	1.45	1.13
1:A:138:LEU:HD21	3:A:300:IC1:H131	1.29	1.09
1:B:49:ALA:HB1	1:B:51:GLN:CD	1.77	1.05
1:B:44:PRO:HA	1:B:80:HIS:HA	1.37	1.02
1:B:49:ALA:HB1	1:B:51:GLN:CG	1.94	0.97

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	291/298 (98%)	217 (75%)	54 (19%)	20 (7%)	1	3
1	B	291/298 (98%)	216 (74%)	53 (18%)	22 (8%)	1	2
All	All	582/596 (98%)	433 (74%)	107 (18%)	42 (7%)	1	2

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	22	SER
1	A	23	PHE
1	A	25	VAL
1	A	51	GLN

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	A	255/259 (98%)	238 (93%)	17 (7%)	16	43
1	B	255/259 (98%)	242 (95%)	13 (5%)	24	55
All	All	510/518 (98%)	480 (94%)	30 (6%)	19	49

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	ASP
1	A	287	THR
1	B	213	ARG
1	A	284	ARG
1	B	11	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	238	GLN
1	B	120	GLN
1	A	206	HIS
1	B	31	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	IC1	A	300	-	25,25,25	2.15	1 (4%)	35,35,35	2.63	10 (28%)
2	SO4	A	302	-	4,4,4	0.29	0	6,6,6	0.13	0
2	SO4	B	309	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	B	310	-	4,4,4	0.34	0	6,6,6	0.12	0
2	SO4	A	306	-	4,4,4	0.32	0	6,6,6	0.30	0
2	SO4	A	301	-	4,4,4	0.34	0	6,6,6	0.13	0
2	SO4	A	305	-	4,4,4	0.23	0	6,6,6	0.17	0
2	SO4	B	308	-	4,4,4	0.33	0	6,6,6	0.22	0
2	SO4	A	304	-	4,4,4	0.42	0	6,6,6	0.13	0
2	SO4	B	311	-	4,4,4	0.45	0	6,6,6	0.16	0
3	IC1	B	400	-	25,25,25	2.21	1 (4%)	35,35,35	2.62	10 (28%)
2	SO4	A	303	-	4,4,4	0.27	0	6,6,6	0.10	0
2	SO4	B	307	-	4,4,4	0.41	0	6,6,6	0.13	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	IC1	A	300	-	-	4/10/22/22	0/3/3/3
3	IC1	B	400	-	-	2/10/22/22	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	IC1	C3-C2	-10.27	1.35	1.50
3	A	300	IC1	C3-C2	-9.97	1.35	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	IC1	C3-C2-N1	10.31	112.66	106.88
3	B	400	IC1	C3-C2-N1	10.18	112.58	106.88
3	B	400	IC1	C8-N1-C2	-5.92	107.66	111.38
3	A	300	IC1	C8-N1-C2	-5.81	107.73	111.38
3	A	300	IC1	O2'-C2'-C3'	-5.08	115.37	124.12

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	IC1	C1'-C2'-O2'-C11
3	B	400	IC1	C1'-C2'-O2'-C11
3	B	400	IC1	C3'-C2'-O2'-C11
3	A	300	IC1	C3'-C2'-O2'-C11
3	A	300	IC1	C3'-C4'-O4'-C12

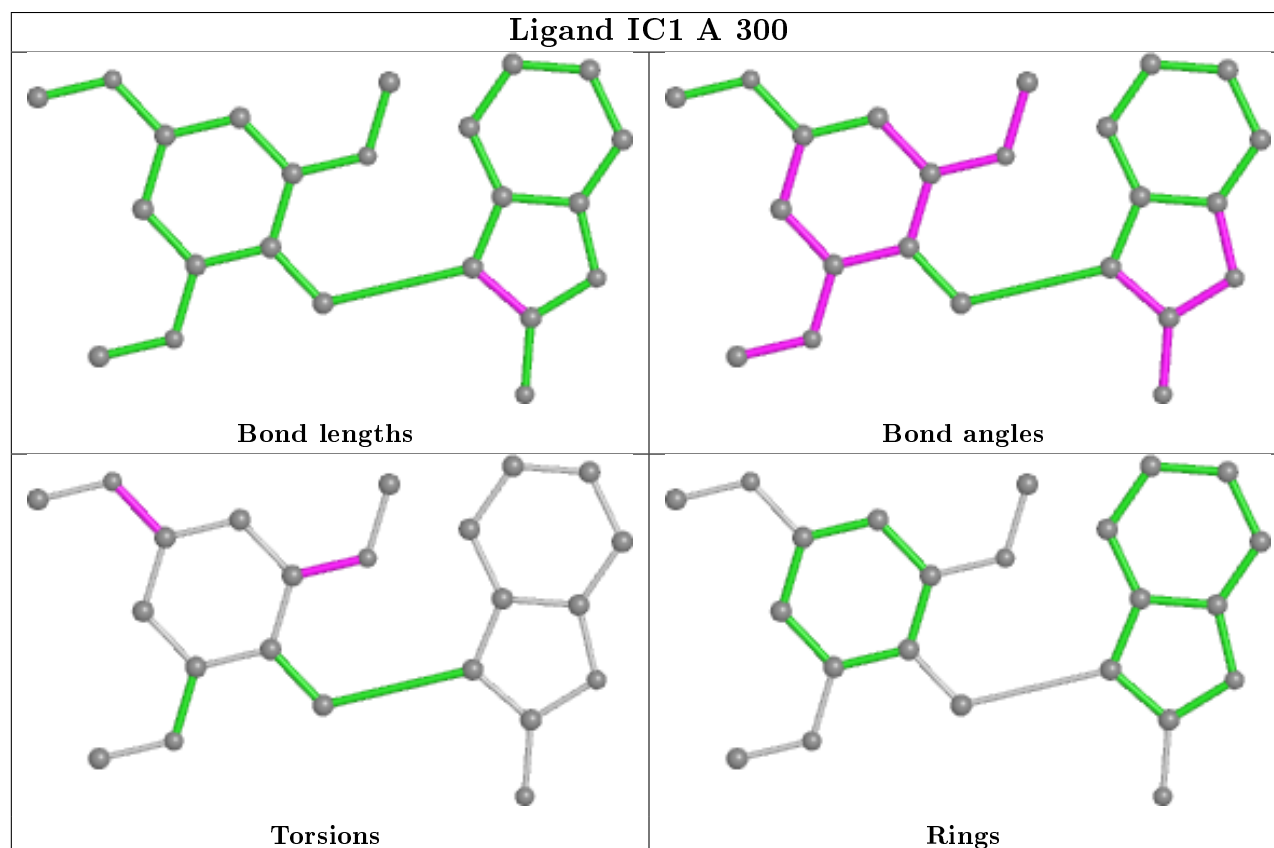
There are no ring outliers.

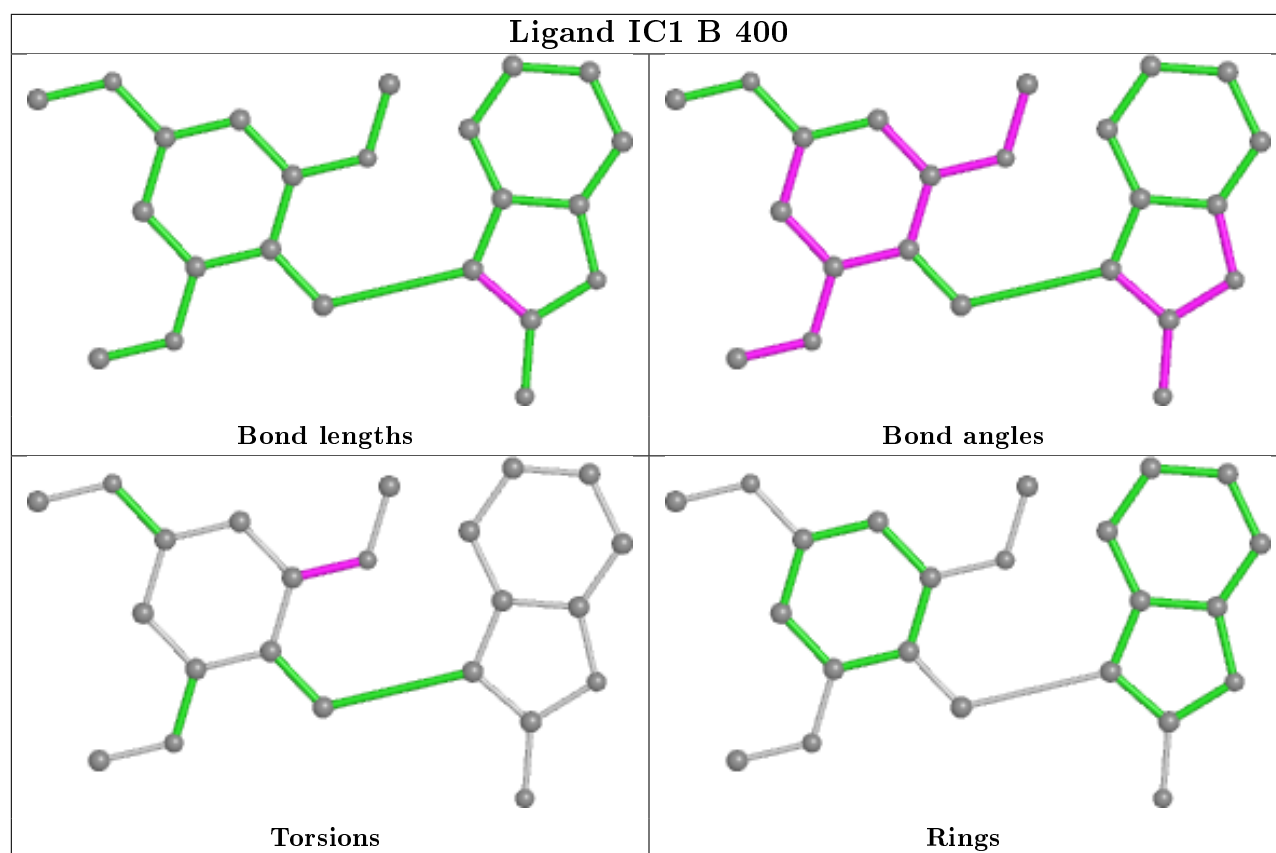
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300	IC1	5	0
2	B	311	SO4	1	0
3	B	400	IC1	8	0
2	A	303	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	293/298 (98%)	-0.15	8 (2%) 54 44	6, 19, 78, 99	0
1	B	293/298 (98%)	-0.18	7 (2%) 59 49	5, 21, 75, 91	0
All	All	586/596 (98%)	-0.16	15 (2%) 56 46	5, 20, 77, 99	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	ALA	5.8
1	B	223	ALA	4.2
1	B	176	LYS	3.8
1	A	174	GLU	3.3
1	A	48	ASP	3.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

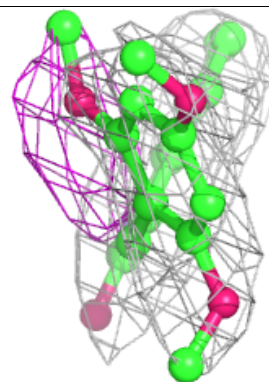
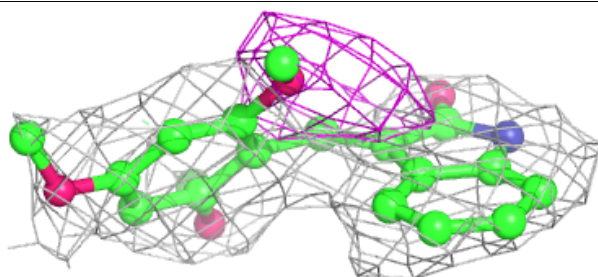
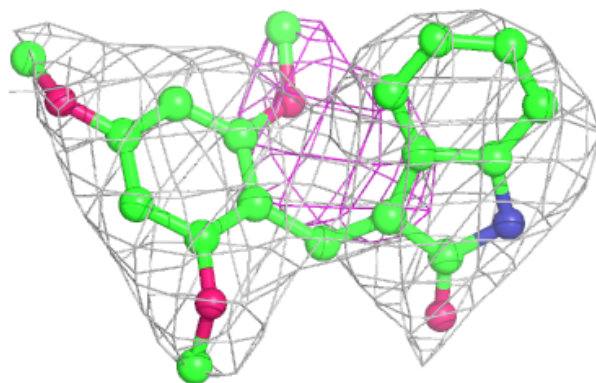
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	IC1	A	300	23/23	0.90	0.38	16,31,42,60	0
2	SO4	B	307	5/5	0.91	0.14	53,57,67,75	0
2	SO4	A	306	5/5	0.92	0.23	41,51,58,66	0
3	IC1	B	400	23/23	0.93	0.46	36,48,80,87	0
2	SO4	A	301	5/5	0.94	0.10	44,54,55,65	0
2	SO4	B	310	5/5	0.95	0.17	35,43,50,54	0
2	SO4	B	311	5/5	0.95	0.15	22,47,50,54	0
2	SO4	A	304	5/5	0.96	0.14	28,32,47,54	0
2	SO4	B	309	5/5	0.96	0.12	28,35,39,42	0
2	SO4	A	303	5/5	0.97	0.15	27,37,42,44	0
2	SO4	B	308	5/5	0.98	0.13	20,23,36,43	0
2	SO4	A	302	5/5	0.98	0.14	24,26,38,41	0
2	SO4	A	305	5/5	0.99	0.11	18,20,28,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

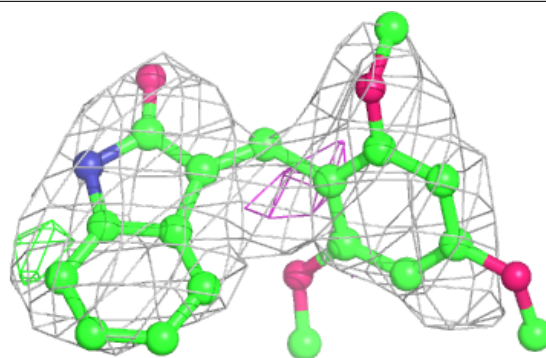
Electron density around IC1 A 300:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

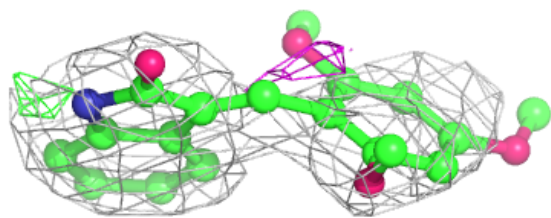


Electron density around IC1 B 400:

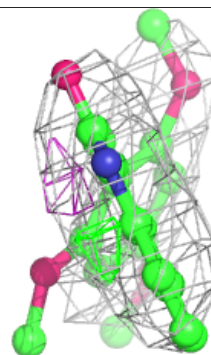
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



✓



△



△

6.5 Other polymers ⓘ

There are no such residues in this entry.