



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:09 PM UTC

PDB ID : 2D1J / pdb_00002d1j
Title : Factor Xa in complex with the inhibitor 2-[[4-[(5-chloroindol-2-yl)sulfonyl]piperazin-1-yl] carbonyl]thieno[3,2-b]pyridine n-oxide
Authors : Suzuki, M.
Deposited on : 2005-08-24
Resolution : 2.20 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

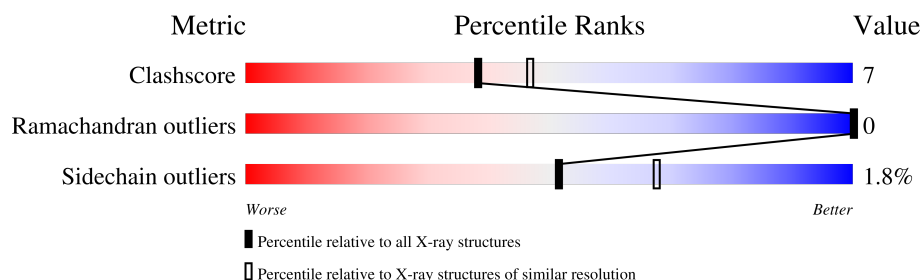
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	233	
2	B	54	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2293 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 Coagulation factor X, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1770	1130	298	328	14			

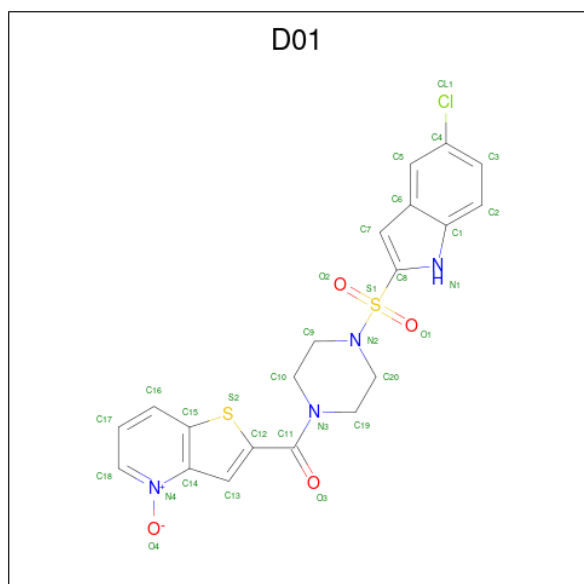
- Molecule 2 is a protein called Coagulation factor X, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	54	Total	C	N	O	S	0	0	0
			379	229	63	80	7			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is 2-({4-[(5-CHLORO-1H-INDOL-2-YL)SULFONYL]PIPERAZIN-1-YL}CARBONYL)THIENO[3,2-B]PYRIDINE 4-OXIDE (CCD ID: D01) (formula: C₂₀H₁₇ClN₄O₄S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			31	20	1	4	4	2		

- Molecule 5 is water.

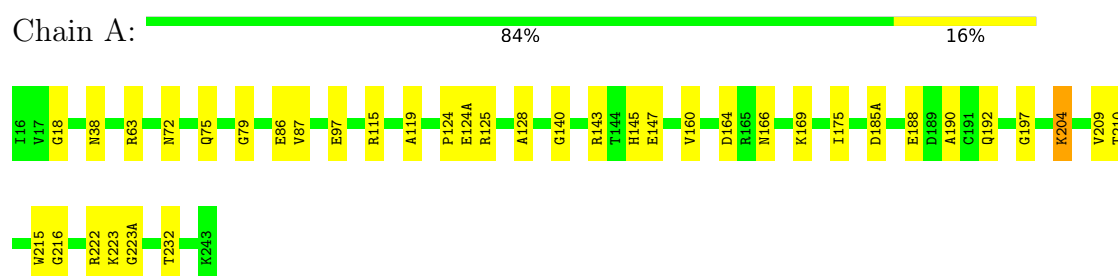
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total	O	0	0
			91	91		
5	B	20	Total	O	0	0
			20	20		

3 Residue-property plots

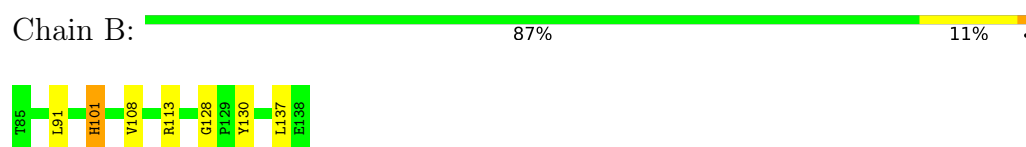
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 2: Coagulation factor X, light chain



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, α , β , γ	57.08Å 73.12Å 79.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20	Depositor
% Data completeness (in resolution range)	100.0 (25.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2293	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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, D01

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	1.13	2/1807 (0.1%)	1.22	10/2443 (0.4%)
2	B	1.14	0/385	1.44	4/524 (0.8%)
All	All	1.13	2/2192 (0.1%)	1.26	14/2967 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	VAL	CA-CB	5.98	1.61	1.54
1	A	140	GLY	N-CA	5.06	1.50	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	LYS	CA-C-N	-10.14	106.57	122.49
1	A	204	LYS	C-N-CA	-10.14	106.57	122.49
2	B	128	GLY	CA-C-N	-9.57	111.05	120.52
2	B	128	GLY	C-N-CA	-9.57	111.05	120.52
1	A	160	VAL	CA-C-N	-7.20	112.58	119.85
1	A	160	VAL	C-N-CA	-7.20	112.58	119.85
1	A	125	ARG	N-CA-C	6.55	118.11	110.97
2	B	130	TYR	CA-C-N	-6.54	113.55	120.03
2	B	130	TYR	C-N-CA	-6.54	113.55	120.03
1	A	190	ALA	N-CA-C	-6.12	101.91	110.35
1	A	160	VAL	N-CA-C	5.98	114.72	107.61
1	A	119	ALA	CA-C-N	-5.76	114.38	120.66
1	A	119	ALA	C-N-CA	-5.76	114.38	120.66
1	A	63	ARG	N-CA-C	-5.08	101.59	109.72

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	A	1770	0	1669	24	0
2	B	379	0	328	7	0
3	A	2	0	0	0	0
4	A	31	0	17	4	0
5	A	91	0	0	7	0
5	B	20	0	0	1	0
All	All	2293	0	2014	29	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 7.

All (29) 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:143:ARG:HD3	1:A:192:GLN:HB3	1.57	0.87
1:A:145:HIS:HB3	5:A:351:HOH:O	1.79	0.81
2:B:101:HIS:HD2	2:B:108:VAL:O	1.64	0.80
1:A:232:THR:HG23	5:A:311:HOH:O	1.92	0.69
1:A:185(A):ASP:OD1	1:A:223(A):GLY:HA2	2.00	0.60
2:B:101:HIS:CD2	2:B:108:VAL:O	2.50	0.60
1:A:124(A):GLU:HB3	5:A:322:HOH:O	2.04	0.57
1:A:124(A):GLU:OE1	2:B:101:HIS:HE1	1.90	0.54
1:A:72:ASN:ND2	1:A:75:GLN:HG2	2.23	0.54
1:A:38:ASN:O	1:A:38:ASN:CG	2.52	0.52
1:A:79:GLY:O	1:A:115:ARG:NH2	2.34	0.51
1:A:147:GLU:OE2	1:A:222:ARG:NH2	2.46	0.49
1:A:164:ASP:OD2	1:A:166:ASN:HB3	2.12	0.48
1:A:124(A):GLU:OE1	2:B:101:HIS:CE1	2.67	0.47
1:A:97:GLU:O	4:A:700:D01:H18	2.13	0.47
1:A:18:GLY:HA3	1:A:188:GLU:HG2	1.97	0.46
1:A:185(A):ASP:O	1:A:223:LYS:HA	2.15	0.46
2:B:113:ARG:HB2	5:B:396:HOH:O	2.15	0.46
2:B:101:HIS:CD2	2:B:101:HIS:N	2.81	0.45
1:A:215:TRP:CE3	4:A:700:D01:H16	2.51	0.44
1:A:169:LYS:HD3	5:A:505:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:HG2	1:A:87:VAL:HG23	2.00	0.43
1:A:197:GLY:HA3	5:A:304:HOH:O	2.20	0.41
2:B:137:LEU:HA	2:B:137:LEU:HD23	1.47	0.41
1:A:145:HIS:HE1	5:A:362:HOH:O	2.03	0.41
1:A:216:GLY:O	4:A:700:D01:H202	2.21	0.41
1:A:124:PRO:HB2	1:A:128:ALA:HB2	2.03	0.41
1:A:215:TRP:CZ3	4:A:700:D01:H16	2.57	0.40
1:A:204:LYS:O	5:A:404:HOH:O	2.22	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	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
2	B	52/54 (96%)	46 (88%)	6 (12%)	0	100	100
All	All	283/287 (99%)	267 (94%)	16 (6%)	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	176/198 (89%)	174 (99%)	2 (1%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	41/46 (89%)	39 (95%)	2 (5%)	22	29
All	All	217/244 (89%)	213 (98%)	4 (2%)	51	68

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	ILE
1	A	210	THR
2	B	91	LEU
2	B	101	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
2	B	101	HIS
2	B	135	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 [i](#)

Of 3 ligands modelled in this entry, 2 are 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	$\# Z > 2$
4	D01	A	700	-	29,35,35	1.75	7 (24%)	40,53,53	1.64	9 (22%)

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
4	D01	A	700	-	-	4/18/30/30	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	D01	C11-C12	-5.16	1.39	1.48
4	A	700	D01	C15-S2	-3.20	1.68	1.74
4	A	700	D01	O4-N4	-3.20	1.30	1.37
4	A	700	D01	O1-S1	3.06	1.46	1.43
4	A	700	D01	C6-C1	2.17	1.44	1.41
4	A	700	D01	C2-C1	-2.11	1.36	1.39
4	A	700	D01	C16-C15	2.01	1.43	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	D01	C12-C11-N3	4.23	124.28	119.10
4	A	700	D01	C15-S2-C12	3.82	96.53	90.97
4	A	700	D01	O3-C11-N3	-3.04	117.87	122.67
4	A	700	D01	C15-C14-C13	2.91	112.91	111.92
4	A	700	D01	C16-C15-S2	2.58	133.44	127.36
4	A	700	D01	O2-S1-O1	2.46	123.23	119.69
4	A	700	D01	C19-N3-C11	-2.19	115.37	122.74
4	A	700	D01	C20-N2-C9	-2.12	109.68	112.12
4	A	700	D01	C19-N3-C10	2.02	116.80	112.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

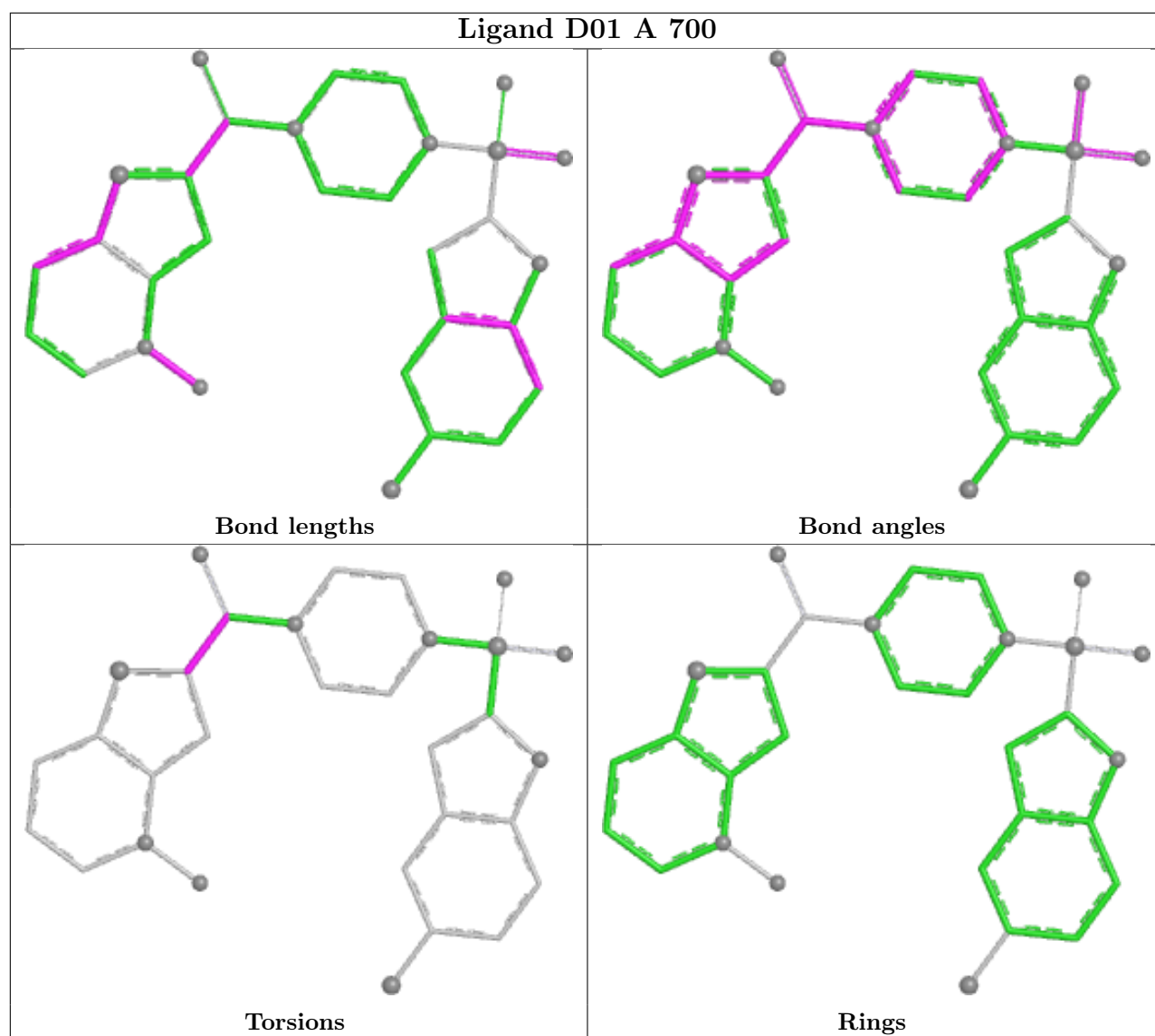
Mol	Chain	Res	Type	Atoms
4	A	700	D01	N3-C11-C12-S2
4	A	700	D01	O3-C11-C12-S2
4	A	700	D01	N3-C11-C12-C13
4	A	700	D01	O3-C11-C12-C13

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	D01	4	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.