



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:06 PM UTC

PDB ID : 4PP9 / pdb_00004pp9
Title : ITK kinase domain with compound 1 (N-[1-(3-CYANOBENZYL)-1H-PYRAZOL-4-YL]-2H-INDAZOLE-3-CARBOXAMIDE)
Authors : Eigenbrot, C.; Shia, S.
Deposited on : 2014-02-26
Resolution : 2.58 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

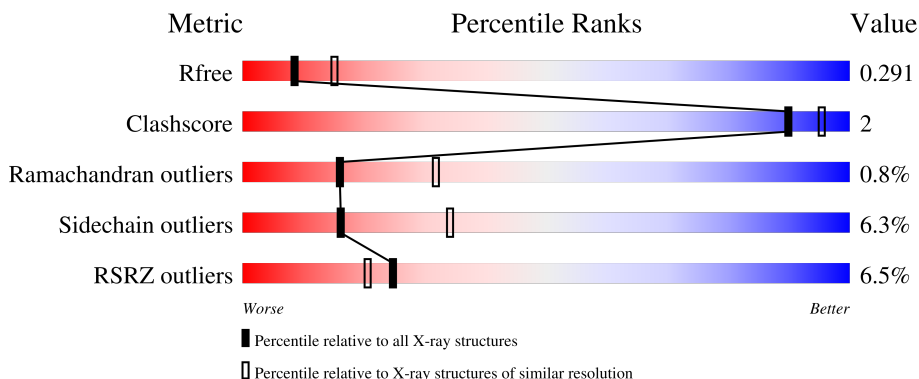
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


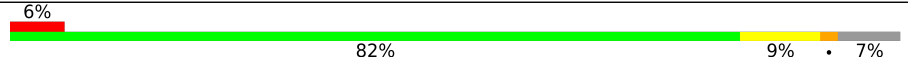
The reported resolution of this entry is 2.58 Å.

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))
R_{free}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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 $\leq 5\%$. 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	266	 6% 81% 10% • 8%
1	B	266	 6% 82% 9% • 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4068 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.

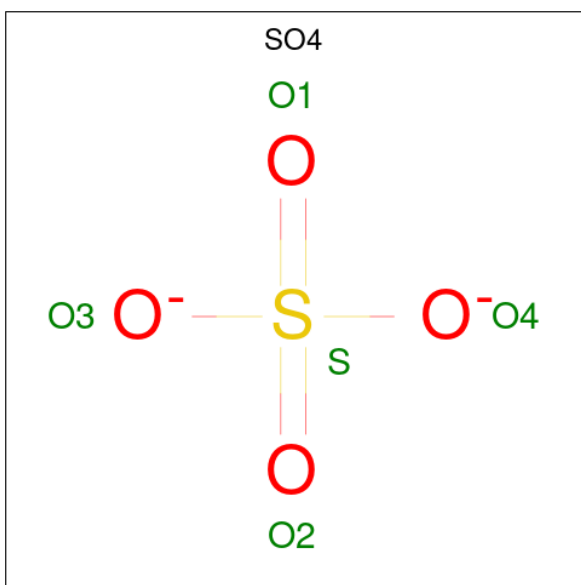
- Molecule 1 is a protein called Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	246	Total 1962	C 1252	N 327	O 367	S 16	0	0	0
1	B	247	Total 1970	C 1257	N 328	O 368	S 17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

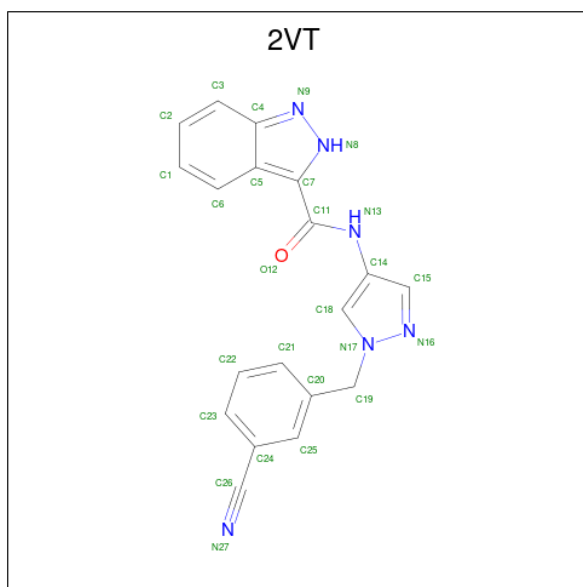
Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	expression tag	UNP Q08881
A	356	SER	-	expression tag	UNP Q08881
A	512	GLU	TYR	engineered mutation	UNP Q08881
B	355	GLY	-	expression tag	UNP Q08881
B	356	SER	-	expression tag	UNP Q08881
B	512	GLU	TYR	engineered mutation	UNP Q08881

- Molecule 2 is SULFATE ION (CCD ID: 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		

- Molecule 3 is N-[1-(3-cyanobenzyl)-1H-pyrazol-4-yl]-2H-indazole-3-carboxamide (CCD ID: 2VT) (formula: C₁₉H₁₄N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	6	1		
3	B	1	Total	C	N	O	0	0
			26	19	6	1		

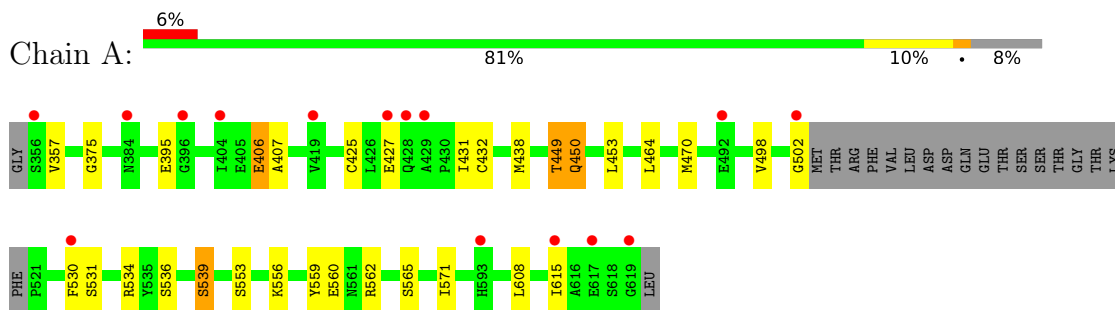
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	32	Total	O	0	0
			32	32		

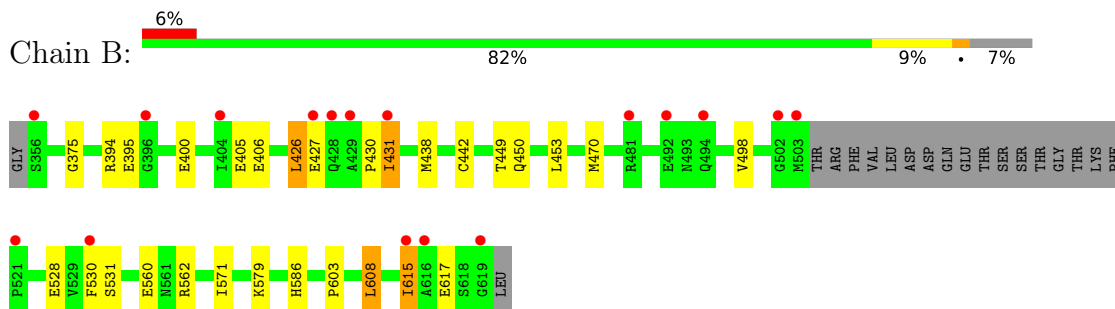
3 Residue-property plots [i](#)

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 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 ($RSRZ > 2$). 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.

- Molecule 1: Tyrosine-protein kinase ITK/TSK



- Molecule 1: Tyrosine-protein kinase ITK/TSK



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.04Å 104.09Å 57.31Å 90.00° 110.21° 90.00°	Depositor
Resolution (Å)	25.34 – 2.58 25.34 – 2.58	Depositor EDS
% Data completeness (in resolution range)	94.0 (25.34-2.58) 94.1 (25.34-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.57Å)	Xtrriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.223 , 0.284 0.230 , 0.291	Depositor DCC
R_{free} test set	919 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.866	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4068	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 2VT, 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	0.74	0/2006	1.35	7/2708 (0.3%)
1	B	0.75	0/2014	1.36	11/2718 (0.4%)
All	All	0.75	0/4020	1.35	18/5426 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	PHE	CA-CB-CG	9.99	123.79	113.80
1	A	530	PHE	CA-CB-CG	8.44	122.24	113.80
1	B	449	THR	N-CA-C	-6.00	102.45	110.55
1	B	400	GLU	CA-C-N	5.86	128.06	120.44
1	B	400	GLU	C-N-CA	5.86	128.06	120.44
1	B	430	PRO	CA-C-N	5.86	128.35	120.50
1	B	430	PRO	C-N-CA	5.86	128.35	120.50
1	A	449	THR	N-CA-C	-5.51	100.71	109.96
1	A	559	TYR	CA-C-N	5.45	131.95	121.54
1	A	559	TYR	C-N-CA	5.45	131.95	121.54
1	B	608	LEU	CA-C-N	5.32	127.41	120.28
1	B	608	LEU	C-N-CA	5.32	127.41	120.28
1	A	407	ALA	CA-C-N	5.30	127.39	120.28
1	A	407	ALA	C-N-CA	5.30	127.39	120.28
1	A	375	GLY	N-CA-C	5.27	118.10	111.09
1	B	442	CYS	CA-C-N	5.20	127.25	120.28
1	B	442	CYS	C-N-CA	5.20	127.25	120.28
1	B	375	GLY	N-CA-C	5.05	118.06	110.18

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	1962	0	1918	8	0
1	B	1970	0	1927	6	0
2	A	10	0	0	0	0
3	A	26	0	14	1	0
3	B	26	0	14	1	0
4	A	42	0	0	0	0
4	B	32	0	0	0	0
All	All	4068	0	3873	14	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 2.

All (14) 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:B:438:MET:H	3:B:701:2VT:H5	1.40	0.67
1:A:438:MET:H	3:A:703:2VT:H5	1.43	0.66
1:B:426:LEU:HA	1:B:431:ILE:HG13	1.80	0.64
1:B:586:HIS:HB3	1:B:615:ILE:HG12	1.83	0.61
1:A:406:GLU:HG3	1:A:502:GLY:HA3	1.83	0.61
1:A:470:MET:HE3	1:A:498:VAL:HG11	1.81	0.60
1:A:449:THR:O	1:A:450:GLN:HB2	2.08	0.52
1:A:553:SER:HB3	1:A:556:LYS:HB2	1.94	0.50
1:A:536:SER:H	1:A:539:SER:HB2	1.78	0.48
1:B:603:PRO:HG2	1:B:608:LEU:HG	1.95	0.47
1:B:450:GLN:HA	1:B:453:LEU:HD12	1.98	0.45
1:B:470:MET:HE3	1:B:498:VAL:HG11	1.98	0.44
1:A:425:CYS:HB3	1:A:432:CYS:SG	2.60	0.41
1:A:450:GLN:HA	1:A:453:LEU:HD12	2.02	0.41

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	242/266 (91%)	234 (97%)	7 (3%)	1 (0%)	30	49
1	B	243/266 (91%)	236 (97%)	4 (2%)	3 (1%)	10	22
All	All	485/532 (91%)	470 (97%)	11 (2%)	4 (1%)	16	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	395	GLU
1	B	560	GLU
1	A	560	GLU
1	B	394	ARG

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	215/233 (92%)	200 (93%)	15 (7%)	14	29
1	B	216/233 (93%)	204 (94%)	12 (6%)	19	38
All	All	431/466 (92%)	404 (94%)	27 (6%)	16	34

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	VAL
1	A	395	GLU

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Mol	Chain	Res	Type
1	A	406	GLU
1	A	427	GLU
1	A	431	ILE
1	A	450	GLN
1	A	464	LEU
1	A	531	SER
1	A	534	ARG
1	A	539	SER
1	A	562	ARG
1	A	565	SER
1	A	571	ILE
1	A	608	LEU
1	A	615	ILE
1	B	405	GLU
1	B	406	GLU
1	B	426	LEU
1	B	427	GLU
1	B	431	ILE
1	B	528	GLU
1	B	531	SER
1	B	562	ARG
1	B	571	ILE
1	B	579	LYS
1	B	615	ILE
1	B	617	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	ASN
1	A	420	GLN
1	A	440	HIS
1	A	487	ASN
1	A	493	ASN
1	B	384	ASN
1	B	420	GLN
1	B	589	GLN

5.3.3 RNA

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](#)

4 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	SO4	A	701	-	4,4,4	0.28	0	6,6,6	0.10	0
3	2VT	A	703	-	26,29,29	1.69	3 (11%)	29,40,40	1.51	6 (20%)
2	SO4	A	702	-	4,4,4	0.25	0	6,6,6	0.08	0
3	2VT	B	701	-	26,29,29	1.72	4 (15%)	29,40,40	1.60	6 (20%)

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	2VT	A	703	-	-	1/14/14/14	0/4/4/4
3	2VT	B	701	-	-	1/14/14/14	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	2VT	C7-C5	6.09	1.48	1.40
3	A	703	2VT	C7-C5	5.87	1.47	1.40
3	B	701	2VT	N8-N9	-3.59	1.29	1.36
3	A	703	2VT	N8-N9	-3.57	1.29	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	2VT	C4-N9	3.37	1.37	1.33
3	B	701	2VT	C4-N9	3.05	1.37	1.33
3	B	701	2VT	N17-N16	2.05	1.40	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	2VT	C4-N9-N8	4.78	111.30	106.29
3	A	703	2VT	C4-N9-N8	4.45	110.95	106.29
3	B	701	2VT	C7-C11-N13	3.72	121.55	115.82
3	A	703	2VT	C7-C11-N13	2.84	120.19	115.82
3	B	701	2VT	O12-C11-C7	-2.72	117.22	120.87
3	A	703	2VT	C18-N17-N16	-2.64	107.68	112.01
3	B	701	2VT	C18-N17-N16	-2.55	107.82	112.01
3	A	703	2VT	C1-C6-C5	-2.48	119.36	121.80
3	A	703	2VT	C15-N16-N17	2.41	108.36	104.68
3	B	701	2VT	C1-C6-C5	-2.34	119.50	121.80
3	B	701	2VT	C15-N16-N17	2.33	108.23	104.68
3	A	703	2VT	C19-N17-N16	2.14	124.90	121.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	2VT	C18-C14-N13-C11
3	B	701	2VT	C18-C14-N13-C11

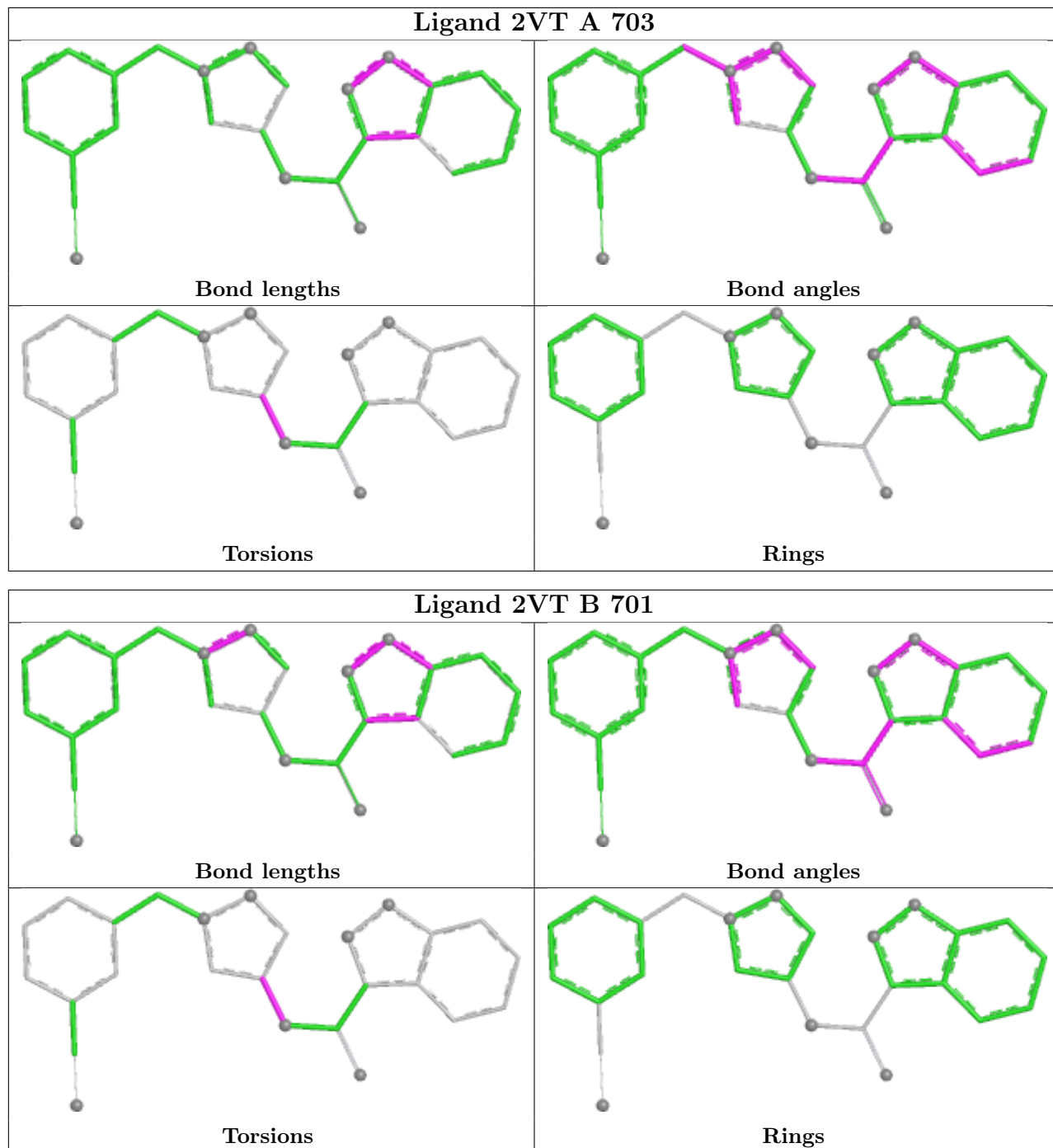
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	2VT	1	0
3	B	701	2VT	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

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	246/266 (92%)	0.67	15 (6%) 27 22	26, 41, 65, 105	0
1	B	247/266 (92%)	0.66	17 (6%) 23 19	27, 42, 67, 97	0
All	All	493/532 (92%)	0.66	32 (6%) 25 20	26, 42, 66, 105	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	GLY	5.0
1	A	619	GLY	4.8
1	B	503	MET	4.3
1	A	404	ILE	3.9
1	B	530	PHE	3.8
1	B	427	GLU	3.5
1	B	356	SER	3.4
1	A	384	ASN	3.4
1	A	530	PHE	3.3
1	B	404	ILE	3.3
1	A	615	ILE	3.2
1	A	356	SER	3.0
1	B	619	GLY	3.0
1	B	615	ILE	2.9
1	B	396	GLY	2.8
1	B	429	ALA	2.8
1	B	431	ILE	2.7
1	A	492	GLU	2.7
1	A	429	ALA	2.7
1	B	494	GLN	2.6
1	A	428	GLN	2.6
1	A	427	GLU	2.5
1	B	616	ALA	2.5
1	A	617	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	396	GLY	2.4
1	B	428	GLN	2.4
1	B	492	GLU	2.3
1	B	521	PRO	2.3
1	B	502	GLY	2.2
1	B	481	ARG	2.2
1	A	593	HIS	2.2
1	A	419	VAL	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

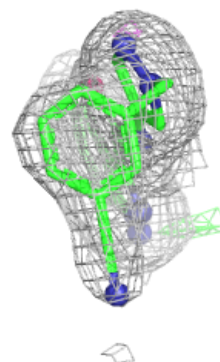
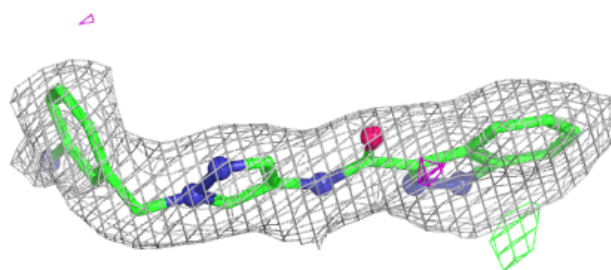
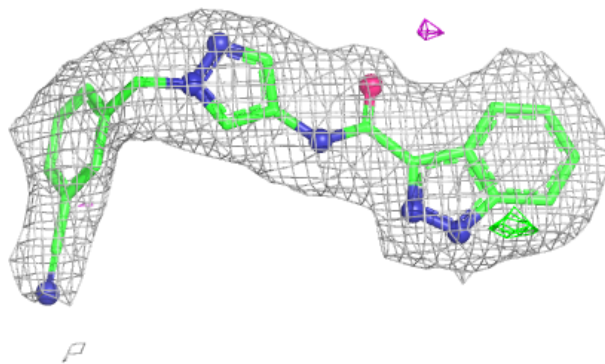
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	SO4	A	701	5/5	0.77	0.19	107,108,108,108	0
2	SO4	A	702	5/5	0.80	0.17	107,107,108,108	0
3	2VT	A	703	26/26	0.94	0.09	26,29,43,48	0
3	2VT	B	701	26/26	0.94	0.08	21,26,42,45	0

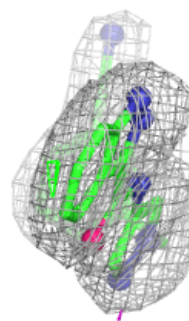
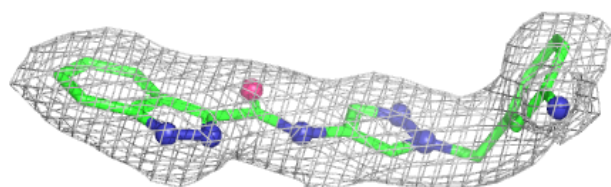
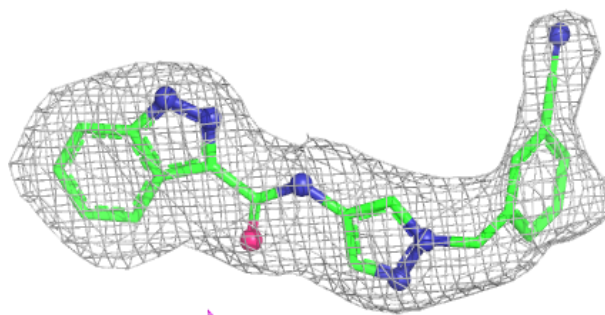
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2VT A 703:

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

**Electron density around 2VT B 701:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.