



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:11 AM UTC

PDB ID : 6WPP / pdb_00006wpp
Title : HUMAN NIK IN COMPLEX WITH LIGAND COMPOUND X
Authors : Shih, A.Y.; Hack, M.; Mirzadegan, T.
Deposited on : 2020-04-27
Resolution : 2.55 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) : 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

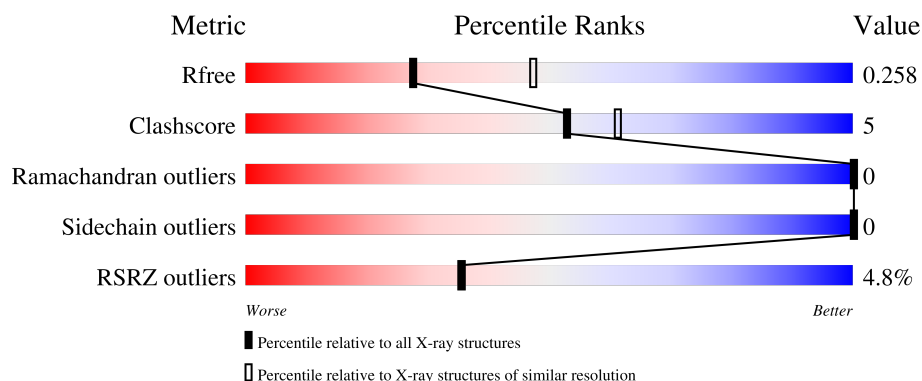
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	347	
1	B	347	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4989 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.

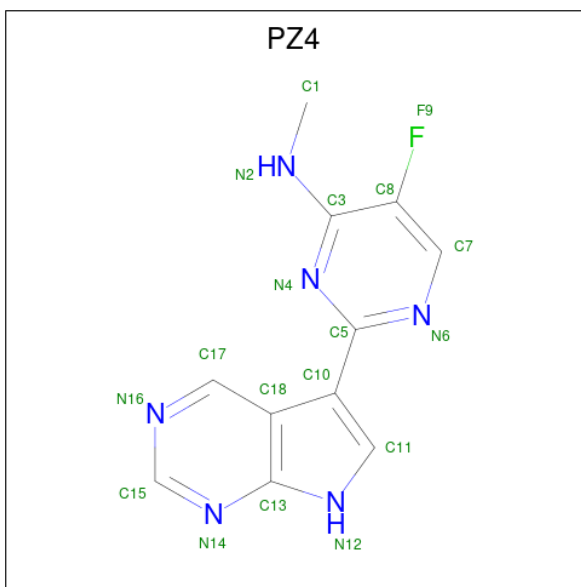
- Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	25	2	0
			2418	1518	437	445	18			
1	B	315	Total	C	N	O	S	48	0	0
			2417	1518	435	446	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	GLY	-	expression tag	UNP Q99558
A	341	PRO	-	expression tag	UNP Q99558
A	342	MET	-	expression tag	UNP Q99558
A	391	ALA	TYR	conflict	UNP Q99558
A	432	SER	ARG	conflict	UNP Q99558
A	464	ALA	TRP	conflict	UNP Q99558
B	340	GLY	-	expression tag	UNP Q99558
B	341	PRO	-	expression tag	UNP Q99558
B	342	MET	-	expression tag	UNP Q99558
B	391	ALA	TYR	conflict	UNP Q99558
B	432	SER	ARG	conflict	UNP Q99558
B	464	ALA	TRP	conflict	UNP Q99558

- Molecule 2 is 5-fluoro-N-methyl-2-(7H-pyrrolo[2,3-d]pyrimidin-5-yl)pyrimidin-4-amine (CCD ID: PZ4) (formula: C₁₁H₉FN₆) (labeled as "Ligand of Interest" by depositor).

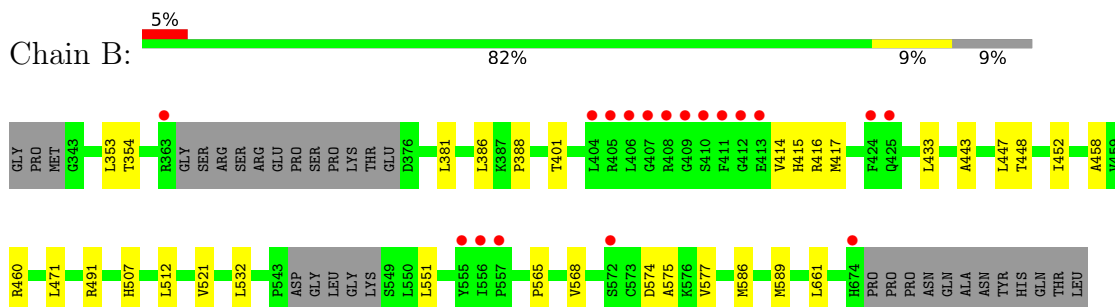


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	0	0
			18	11	1	6		
2	B	1	Total	C	F	N	0	0
			18	11	1	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	50	Total	O	0	0
			50	50		

- Molecule 1: Mitogen-activated protein kinase kinase kinase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.48Å 81.52Å 78.42Å 90.00° 111.43° 90.00°	Depositor
Resolution (Å)	73.00 – 2.55 73.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (73.00-2.55) 99.5 (73.00-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.256 0.203 , 0.258	Depositor DCC
R_{free} test set	1011 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4989	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.52% 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: PZ4

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	0.73	0/2472	0.76	0/3345
1	B	0.74	0/2470	0.77	0/3342
All	All	0.74	0/4942	0.77	0/6687

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2418	0	2392	25	0
1	B	2417	0	2398	26	0
2	A	18	0	0	1	0
2	B	18	0	0	2	0
3	A	68	0	0	0	0
3	B	50	0	0	0	0
All	All	4989	0	4790	47	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 5.

All (47) 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:353:LEU:HD11	1:B:458:ALA:HB3	1.47	0.96
1:A:353:LEU:HD11	1:A:458:ALA:HB3	1.66	0.78
1:B:447:LEU:HD13	1:B:452:ILE:HD13	1.73	0.70
1:A:448:THR:HG23	1:B:354:THR:HG21	1.73	0.70
1:B:447:LEU:HD12	1:B:452:ILE:HG21	1.80	0.62
1:A:564:ALA:O	1:A:567:VAL:HG22	2.00	0.61
1:B:433:LEU:HD11	1:B:460:ARG:HD2	1.82	0.60
1:A:354:THR:HG21	1:B:448:THR:HG21	1.83	0.60
1:B:416:ARG:NH1	1:B:471:LEU:HD21	2.19	0.56
1:B:386:LEU:HD22	1:B:417:MET:HE1	1.89	0.55
1:A:586:MET:HA	1:A:589:MET:HE3	1.90	0.54
1:B:447:LEU:CD1	1:B:452:ILE:HD13	2.39	0.53
1:A:447:LEU:HD12	1:A:452:ILE:HG21	1.91	0.53
1:B:414:VAL:HG21	2:B:701:PZ4:C3	2.39	0.53
1:B:551:LEU:HD23	1:B:574:ASP:HB3	1.93	0.51
1:B:443:ALA:O	1:B:447:LEU:HD11	2.12	0.49
1:B:381:LEU:HD12	1:B:388:PRO:HD3	1.95	0.49
1:B:401:THR:HG23	1:B:415:HIS:HB3	1.96	0.48
1:A:433:LEU:HD11	1:A:460:ARG:HD2	1.96	0.47
1:A:472:LEU:HD22	1:A:522:LEU:HB2	1.95	0.47
1:A:567:VAL:HG12	1:A:573:CYS:SG	2.55	0.47
1:A:344:SER:HB3	1:A:391:ALA:HB1	1.97	0.47
1:A:414:VAL:HG21	2:A:701:PZ4:C3	2.45	0.47
1:A:448:THR:CG2	1:B:354:THR:HG21	2.44	0.45
1:A:496:LEU:HD22	1:A:586:MET:HB2	1.98	0.45
1:B:386:LEU:CD2	1:B:417:MET:HE1	2.46	0.45
1:B:471:LEU:HD12	2:B:701:PZ4:N14	2.33	0.44
1:B:565:PRO:O	1:B:568:VAL:HG22	2.18	0.43
1:A:381:LEU:HD12	1:A:388:PRO:HD3	1.99	0.43
1:A:556:ILE:N	1:A:556:ILE:HD12	2.33	0.43
1:B:507:HIS:CG	1:B:575:ALA:HB1	2.53	0.43
1:B:512:LEU:HD21	1:B:577:VAL:HG23	2.00	0.43
1:A:448:THR:HG23	1:B:354:THR:CG2	2.43	0.43
1:A:447:LEU:CD1	1:A:452:ILE:HD13	2.49	0.42
1:A:353:LEU:HD13	1:A:380:VAL:HB	2.02	0.42
1:A:477:LEU:HD21	1:A:589:MET:SD	2.60	0.42
1:B:491:ARG:HD2	1:B:661:LEU:HD11	2.02	0.41
1:B:586:MET:HA	1:B:589:MET:HE3	2.02	0.41
1:B:512:LEU:HD21	1:B:577:VAL:CG2	2.50	0.41
1:A:521:VAL:HG22	1:A:532:LEU:HD23	2.02	0.41
1:A:443:ALA:O	1:A:447:LEU:HD11	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:VAL:HG22	1:B:532:LEU:HD23	2.03	0.40
1:A:512:LEU:HD23	1:A:514:GLY:N	2.37	0.40
1:A:399:TRP:CD2	1:A:417:MET:HE2	2.57	0.40
1:A:443:ALA:HA	1:A:511:ILE:HD13	2.04	0.40
1:B:447:LEU:HD13	1:B:452:ILE:CD1	2.47	0.40
1:A:452:ILE:HD11	1:A:506:LEU:HG	2.03	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	308/347 (89%)	300 (97%)	8 (3%)	0	100	100
1	B	309/347 (89%)	299 (97%)	10 (3%)	0	100	100
All	All	617/694 (89%)	599 (97%)	18 (3%)	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	258/285 (90%)	258 (100%)	0	100	100
1	B	258/285 (90%)	258 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	516/570 (90%)	516 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	466	ASN
1	A	537	HIS
1	B	349	GLN
1	B	351	HIS
1	B	403	GLN
1	B	484	GLN

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 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	PZ4	A	701	-	20,20,20	1.67	5 (25%)	22,28,28	3.47	12 (54%)
2	PZ4	B	701	-	20,20,20	1.47	4 (20%)	22,28,28	3.31	10 (45%)

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	PZ4	A	701	-	-	4/6/6/6	0/3/3/3
2	PZ4	B	701	-	-	2/6/6/6	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PZ4	C11-N12	-3.61	1.31	1.37
2	A	701	PZ4	C3-N2	3.28	1.38	1.34
2	B	701	PZ4	C11-N12	-3.17	1.32	1.37
2	B	701	PZ4	C3-N2	3.03	1.37	1.34
2	A	701	PZ4	C5-N4	2.87	1.37	1.34
2	A	701	PZ4	C11-C10	2.69	1.40	1.37
2	B	701	PZ4	C11-C10	2.67	1.40	1.37
2	A	701	PZ4	C13-N12	-2.40	1.33	1.36
2	B	701	PZ4	C5-N4	2.05	1.36	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PZ4	C13-N12-C11	8.93	112.69	108.48
2	B	701	PZ4	C13-N12-C11	8.55	112.51	108.48
2	B	701	PZ4	C18-C13-N14	-6.71	118.18	126.31
2	A	701	PZ4	C18-C13-N14	-6.15	118.86	126.31
2	A	701	PZ4	N6-C5-N4	-5.01	120.19	125.25
2	A	701	PZ4	C13-C18-C10	-4.82	104.55	106.22
2	A	701	PZ4	C17-N16-C15	4.81	121.48	115.80
2	B	701	PZ4	C17-N16-C15	4.80	121.46	115.80
2	B	701	PZ4	N12-C13-N14	4.55	134.06	126.69
2	A	701	PZ4	N12-C13-N14	3.93	133.06	126.69
2	B	701	PZ4	N6-C5-N4	-3.93	121.28	125.25
2	B	701	PZ4	C8-C7-N6	-3.44	119.78	122.68
2	A	701	PZ4	C18-C10-C5	3.16	130.41	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PZ4	C8-C7-N6	-2.99	120.16	122.68
2	A	701	PZ4	N16-C15-N14	-2.94	122.33	127.33
2	B	701	PZ4	C1-N2-C3	-2.92	120.14	122.85
2	B	701	PZ4	C13-C18-C10	-2.92	105.21	106.22
2	B	701	PZ4	C18-C17-N16	-2.91	118.35	123.95
2	B	701	PZ4	N16-C15-N14	-2.69	122.77	127.33
2	A	701	PZ4	C18-C17-N16	-2.49	119.15	123.95
2	A	701	PZ4	C3-N4-C5	2.44	120.79	116.45
2	A	701	PZ4	C8-C3-N4	-2.03	118.13	119.53

There are no chirality outliers.

All (6) torsion outliers are listed below:

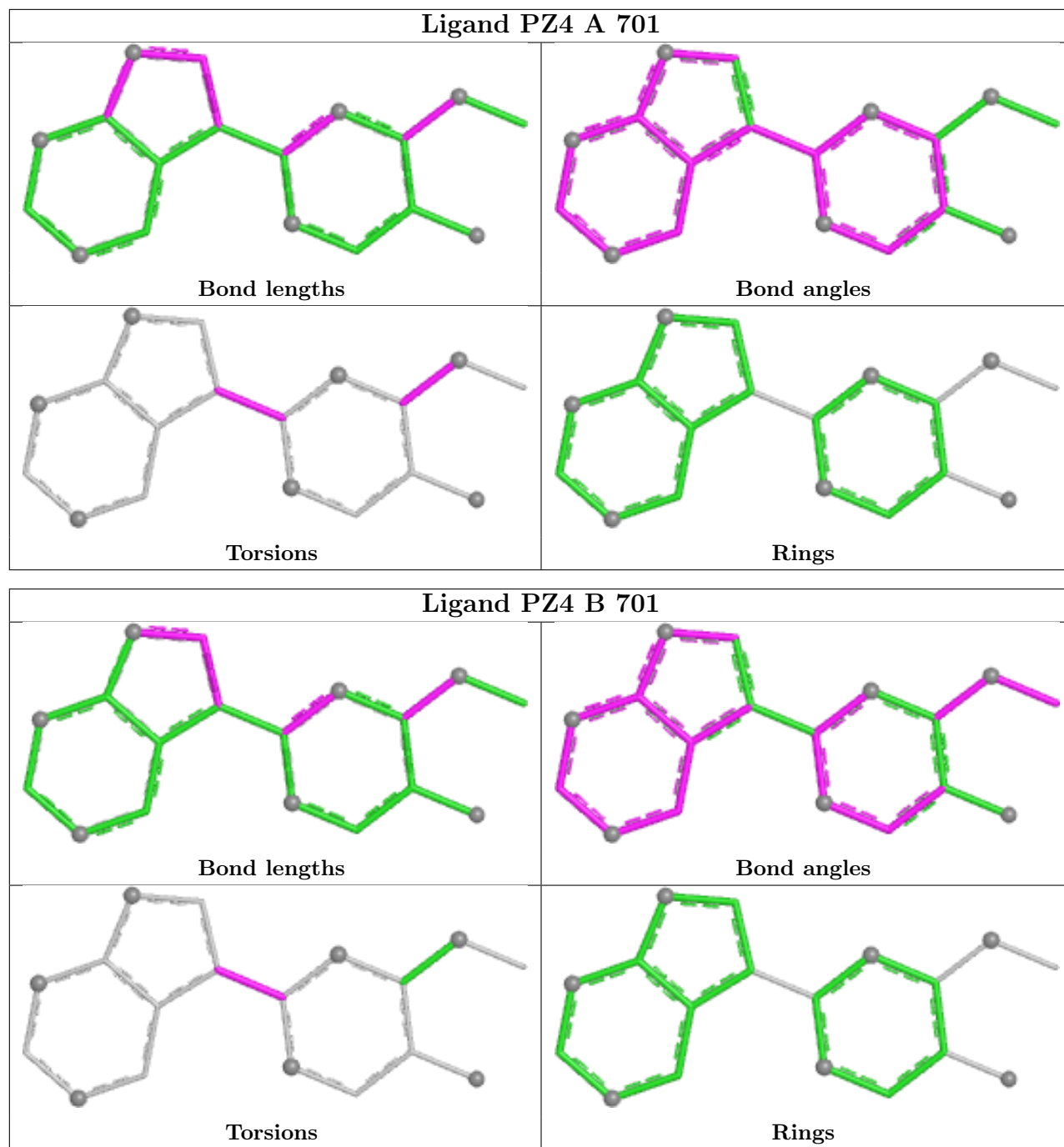
Mol	Chain	Res	Type	Atoms
2	A	701	PZ4	C8-C3-N2-C1
2	A	701	PZ4	N4-C3-N2-C1
2	A	701	PZ4	C11-C10-C5-N6
2	A	701	PZ4	C18-C10-C5-N6
2	B	701	PZ4	C11-C10-C5-N6
2	B	701	PZ4	C18-C10-C5-N6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	PZ4	1	0
2	B	701	PZ4	2	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 ⓘ

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	312/347 (89%)	0.19	12 (3%) 44 45	18, 39, 73, 115	10 (3%)
1	B	315/347 (90%)	0.38	18 (5%) 29 29	27, 45, 81, 141	13 (4%)
All	All	627/694 (90%)	0.29	30 (4%) 35 35	18, 42, 79, 141	23 (3%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	554	ASP	7.5
1	B	404	LEU	6.1
1	B	411	PHE	4.8
1	B	408	ARG	4.3
1	B	363	ARG	4.0
1	A	363	ARG	3.8
1	B	410	SER	3.8
1	A	553	GLY	3.6
1	A	555	TYR	3.5
1	B	409	GLY	3.4
1	A	411	PHE	3.3
1	B	405	ARG	3.3
1	B	424	PHE	2.9
1	B	407	GLY	2.8
1	B	413	GLU	2.7
1	A	552	THR	2.7
1	A	349	GLN	2.5
1	B	572	SER	2.5
1	B	406	LEU	2.5
1	B	556	ILE	2.4
1	B	555	TYR	2.4
1	A	543	PRO	2.4
1	A	355	SER	2.3
1	B	412	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	674	HIS	2.3
1	A	556	ILE	2.1
1	B	674	HIS	2.1
1	B	557	PRO	2.1
1	B	425	GLN	2.1
1	A	344	SER	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](#)

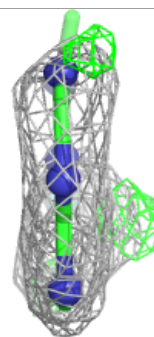
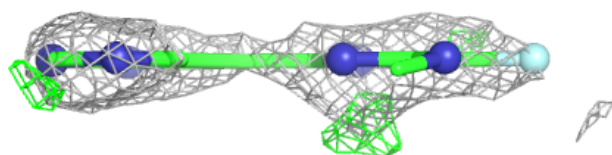
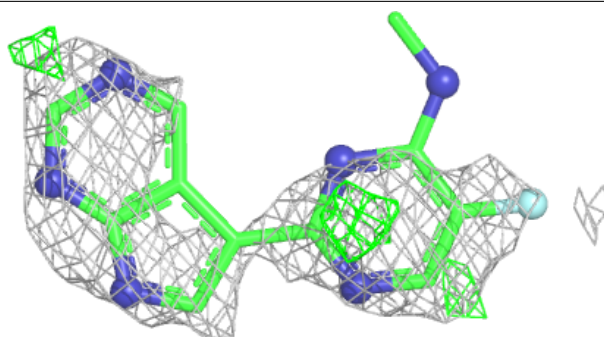
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PZ4	B	701	18/18	0.87	0.22	31,36,43,43	18
2	PZ4	A	701	18/18	0.94	0.07	27,32,39,44	0

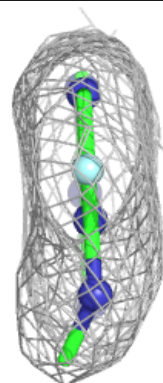
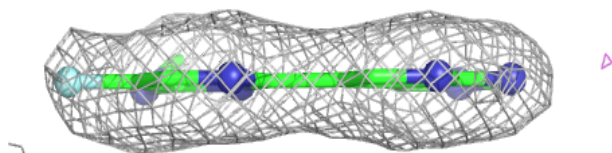
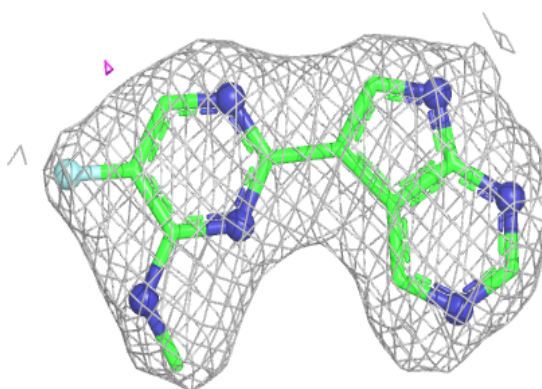
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PZ4 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)

**Electron density around PZ4 A 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.