



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:41 PM UTC

PDB ID : 8DV7 / pdb_00008dv7
Title : Estrogen Receptor Alpha Ligand Binding Domain in Complex with (6'-hydroxy-1'-(4-(2-(1-propylpyrrolidin-3-yl)ethyl)phenyl)-1',4'-dihydro-2'-H</i>-spiro[cyclopropane-1,3'-isoquinolin]-2'-yl)(phenyl)methanone
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Deposited on : 2022-07-28
Resolution : 1.59 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](#) ①) 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

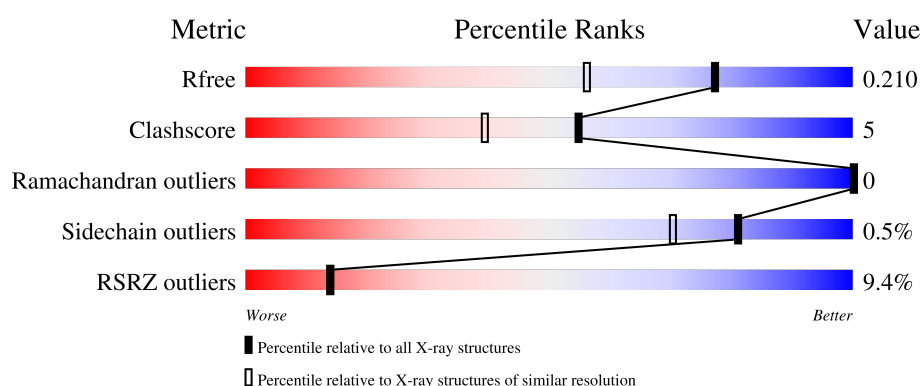
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	255	8% 84% 8% 8%
1	B	255	9% 67% 19% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4195 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.

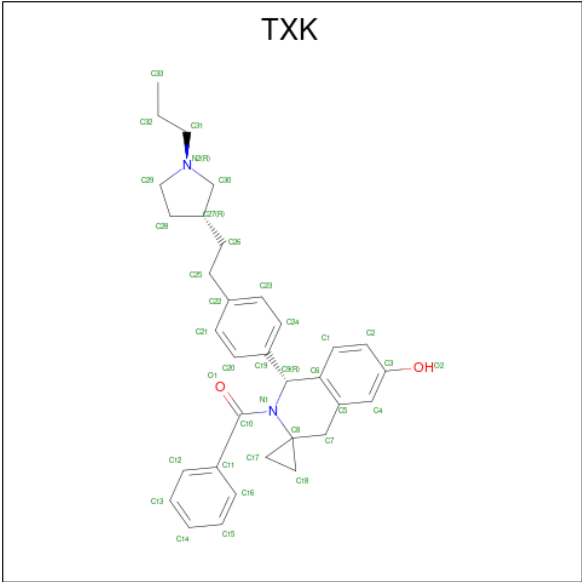
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	6	0
			1871	1203	317	335	16			
1	B	223	Total	C	N	O	S	0	7	0
			1808	1160	311	322	15			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	MET	-	initiating methionine	UNP P03372
A	381	SER	CYS	engineered mutation	UNP P03372
A	417	SER	CYS	engineered mutation	UNP P03372
A	530	SER	CYS	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	300	MET	-	initiating methionine	UNP P03372
B	381	SER	CYS	engineered mutation	UNP P03372
B	417	SER	CYS	engineered mutation	UNP P03372
B	530	SER	CYS	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is [(1'R)-6'-hydroxy-1'-(4-{2-[(3R)-1-propylpyrrolidin-3-yl]ethyl}phenyl)-1',4'-dihydro-2'H-spiro[cyclopropane-1,3'-isoquinolin]-2'-yl](phenyl)methanone (CCD ID: TXK) (formula: C₃₃H₃₈N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	33	2	2		
2	B	1	Total	C	N	O	0	0
			37	33	2	2		

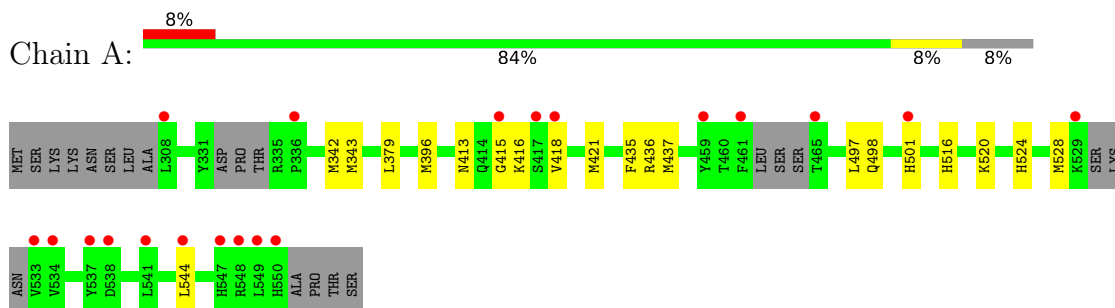
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	235	Total	O	0	0
			235	235		
3	B	207	Total	O	0	0
			207	207		

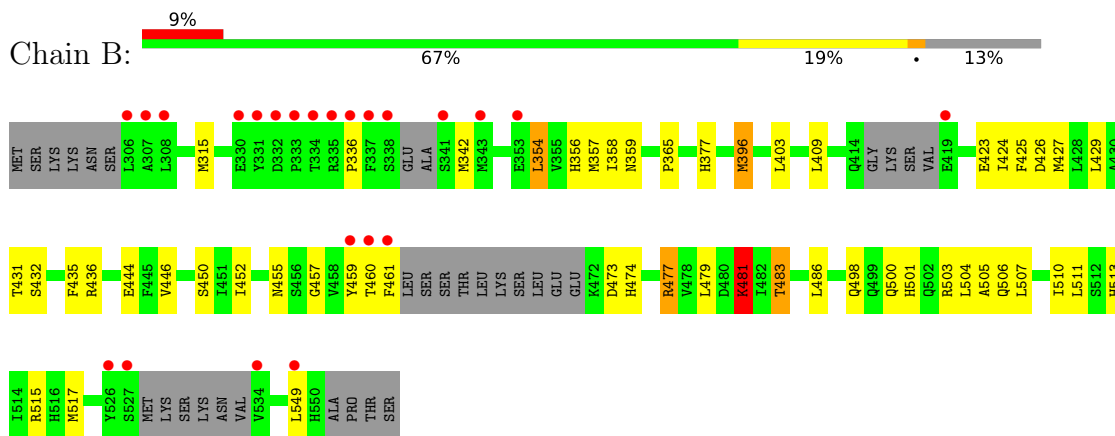
3 Residue-property plots [i](#)

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: Estrogen receptor



• Molecule 1: Estrogen receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.29Å 57.78Å 87.41Å 90.00° 103.01° 90.00°	Depositor
Resolution (Å)	41.13 – 1.59 41.13 – 1.59	Depositor EDS
% Data completeness (in resolution range)	85.6 (41.13-1.59) 85.6 (41.13-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.59Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.167 , 0.208 0.174 , 0.210	Depositor DCC
R_{free} test set	2785 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4195	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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: TXK

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	0.69	0/1905	0.83	0/2575
1	B	1.36	35/1845 (1.9%)	1.04	2/2493 (0.1%)
All	All	1.07	35/3750 (0.9%)	0.94	2/5068 (0.0%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	LEU	C-O	-8.59	1.13	1.24
1	B	457	GLY	C-O	-8.15	1.18	1.24
1	B	432	SER	C-O	-7.09	1.16	1.24
1	B	483	THR	C-O	-7.00	1.16	1.24
1	B	505	ALA	C-O	-6.92	1.16	1.24
1	B	423	GLU	C-O	-6.77	1.16	1.24
1	B	510	ILE	C-O	-6.14	1.16	1.24
1	B	503	ARG	C-O	-6.09	1.16	1.24
1	B	517	MET	C-O	-6.08	1.17	1.24
1	B	450	SER	C-O	-5.96	1.17	1.24
1	B	455	ASN	C-O	-5.81	1.16	1.24
1	B	515	ARG	C-O	-5.73	1.17	1.24
1	B	477	ARG	C-O	-5.71	1.17	1.24
1	B	396	MET	SD-CE	-5.70	1.65	1.79
1	B	429	LEU	C-O	-5.68	1.17	1.24
1	B	511	LEU	C-O	-5.66	1.17	1.24
1	B	425	PHE	C-O	-5.63	1.17	1.24
1	B	474	HIS	C-O	-5.62	1.17	1.24
1	B	336	PRO	C-O	-5.58	1.16	1.23
1	B	481	LYS	C-O	-5.56	1.17	1.24
1	B	446	VAL	C-O	-5.52	1.17	1.24
1	B	452	ILE	C-O	-5.49	1.18	1.24
1	B	500	GLN	C-O	-5.39	1.17	1.24
1	B	479	LEU	C-O	-5.30	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	506	GLN	C-O	-5.30	1.18	1.24
1	B	357	MET	C-O	-5.28	1.18	1.24
1	B	513	HIS	C-O	-5.28	1.17	1.24
1	B	444	GLU	C-O	-5.25	1.17	1.24
1	B	507	LEU	C-O	-5.22	1.17	1.24
1	B	435	PHE	C-O	-5.19	1.18	1.24
1	B	356	HIS	C-O	-5.14	1.17	1.24
1	B	504	LEU	C-O	-5.13	1.18	1.24
1	B	431	THR	C-O	-5.13	1.18	1.24
1	B	426	ASP	C-O	-5.12	1.18	1.24
1	B	486	LEU	C-O	-5.03	1.18	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	PRO	CB-CA-C	-6.16	103.73	111.56
1	B	473	ASP	CA-CB-CG	-5.62	106.97	112.60

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	1871	0	1877	20	0
1	B	1808	0	1816	19	0
2	A	37	0	0	1	0
2	B	37	0	0	0	0
3	A	235	0	0	1	0
3	B	207	0	0	3	0
All	All	4195	0	3693	36	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 (36) 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)
3:A:730:HOH:O	1:B:459:TYR:HE2	1.42	1.00
1:A:413:ASN:HD22	1:A:416:LYS:HE3	1.33	0.93
1:A:501:HIS:HD2	1:B:483:THR:HG22	1.43	0.82
1:A:498:GLN:HA	1:A:501:HIS:CE1	2.15	0.81
1:B:377[A]:HIS:CD2	1:B:461:PHE:CE1	2.72	0.78
1:A:413:ASN:ND2	1:A:416:LYS:HE3	2.08	0.66
1:A:415:GLY:C	1:A:421:MET:HE3	2.20	0.65
1:B:377[A]:HIS:HD2	1:B:461:PHE:CE1	2.17	0.61
1:A:379:LEU:HD12	1:A:544:LEU:HD11	1.83	0.61
1:B:460:THR:HG22	3:B:768:HOH:O	2.02	0.60
1:A:396:MET:O	1:A:436:ARG:HD3	2.03	0.58
1:A:524:HIS:CD2	1:A:528:MET:HE2	2.39	0.58
1:A:342:MET:HE1	1:A:421:MET:HE1	1.87	0.57
1:A:396:MET:HE3	1:A:435:PHE:O	2.05	0.56
1:B:315:MET:HE3	1:B:481:LYS:HG2	1.88	0.56
1:A:418:VAL:HB	1:A:421:MET:HE2	1.91	0.52
1:A:501:HIS:CD2	1:B:483:THR:HG22	2.33	0.51
1:A:396:MET:HE3	1:A:435:PHE:C	2.35	0.51
1:B:377[A]:HIS:CD2	1:B:461:PHE:CD1	2.99	0.50
1:B:396:MET:O	1:B:436:ARG:HD3	2.13	0.48
1:A:516:HIS:CE1	1:A:520:LYS:HE3	2.49	0.47
1:B:549:LEU:HD12	1:B:549:LEU:N	2.31	0.46
1:A:343:MET:HE2	1:A:528:MET:HE1	1.97	0.46
1:B:315:MET:HE3	1:B:481:LYS:CG	2.46	0.45
1:B:477:ARG:NE	3:B:708:HOH:O	2.49	0.45
1:A:437:MET:HE3	1:A:437:MET:HB3	1.86	0.43
1:B:354:LEU:O	1:B:358:ILE:HG12	2.18	0.43
1:B:498:GLN:HA	1:B:501[B]:HIS:CE1	2.53	0.43
1:A:501:HIS:HD2	1:B:483:THR:CG2	2.22	0.43
1:A:421:MET:HG3	2:A:601:TXK:C13	2.50	0.41
1:A:497:LEU:HD23	1:A:497:LEU:HA	1.94	0.41
1:B:403:LEU:HD13	1:B:409:LEU:HD13	2.03	0.41
1:B:359:ASN:CG	3:B:704:HOH:O	2.63	0.41
1:B:424:ILE:HA	1:B:427:MET:HE3	2.01	0.41
1:A:415:GLY:O	1:A:421:MET:HE3	2.22	0.40
1:B:315:MET:SD	1:B:365:PRO:HG2	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	231/255 (91%)	230 (100%)	1 (0%)	0	100	100
1	B	220/255 (86%)	216 (98%)	4 (2%)	0	100	100
All	All	451/510 (88%)	446 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	205/230 (89%)	205 (100%)	0	100	100
1	B	200/230 (87%)	198 (99%)	2 (1%)	68	50
All	All	405/460 (88%)	403 (100%)	2 (0%)	81	70

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	342	MET
1	B	481	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	A	413	ASN

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Mol	Chain	Res	Type
1	A	550	HIS
1	B	375	GLN
1	B	441	GLN
1	B	455	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](#)

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	TXK	B	601	-	41,42,42	4.90	27 (65%)	48,61,61	2.97	21 (43%)
2	TXK	A	601	-	41,42,42	4.73	27 (65%)	48,61,61	2.77	23 (47%)

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	TXK	B	601	-	-	5/20/52/52	0/6/6/6
2	TXK	A	601	-	-	3/20/52/52	0/6/6/6

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TXK	C1-C6	9.72	1.51	1.39
2	A	601	TXK	C31-N2	-9.70	1.25	1.47
2	A	601	TXK	C16-C11	9.54	1.53	1.39
2	B	601	TXK	C16-C11	9.38	1.53	1.39
2	B	601	TXK	C31-N2	-9.35	1.26	1.47
2	B	601	TXK	C24-C19	9.27	1.53	1.39
2	A	601	TXK	C21-C20	9.03	1.53	1.38
2	A	601	TXK	C24-C19	8.89	1.53	1.39
2	A	601	TXK	C1-C6	8.77	1.50	1.39
2	B	601	TXK	C2-C3	8.21	1.54	1.39
2	B	601	TXK	C13-C12	8.14	1.52	1.38
2	A	601	TXK	C8-N1	-8.08	1.38	1.51
2	B	601	TXK	C21-C20	7.80	1.51	1.38
2	A	601	TXK	C2-C3	7.48	1.53	1.39
2	A	601	TXK	C13-C12	7.45	1.51	1.38
2	B	601	TXK	C23-C22	7.43	1.53	1.38
2	B	601	TXK	C8-N1	-7.41	1.39	1.51
2	A	601	TXK	C23-C22	6.77	1.52	1.38
2	B	601	TXK	C14-C15	6.51	1.52	1.38
2	B	601	TXK	C7-C5	6.32	1.62	1.50
2	B	601	TXK	C4-C5	6.27	1.49	1.39
2	B	601	TXK	C18-C8	6.01	1.59	1.50
2	A	601	TXK	C10-N1	5.73	1.49	1.36
2	A	601	TXK	C14-C15	5.67	1.50	1.38
2	A	601	TXK	C4-C5	5.60	1.48	1.39
2	B	601	TXK	C10-N1	4.89	1.47	1.36
2	A	601	TXK	C7-C5	4.86	1.59	1.50
2	B	601	TXK	C30-N2	-4.83	1.39	1.47
2	B	601	TXK	C17-C8	4.62	1.57	1.50
2	A	601	TXK	C18-C8	4.37	1.57	1.50
2	A	601	TXK	C30-N2	-4.06	1.41	1.47
2	A	601	TXK	C12-C11	-4.06	1.33	1.39
2	A	601	TXK	C17-C8	3.81	1.56	1.50
2	A	601	TXK	C15-C16	-3.78	1.32	1.38
2	B	601	TXK	C12-C11	-3.69	1.33	1.39
2	B	601	TXK	C20-C19	-3.40	1.33	1.39
2	B	601	TXK	C14-C13	-3.26	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TXK	C5-C6	-3.04	1.35	1.40
2	A	601	TXK	C23-C24	-2.77	1.34	1.38
2	A	601	TXK	C29-N2	-2.62	1.42	1.47
2	A	601	TXK	C9-N1	-2.62	1.44	1.47
2	B	601	TXK	C11-C10	2.57	1.54	1.50
2	B	601	TXK	C6-C9	-2.51	1.49	1.51
2	A	601	TXK	C25-C22	2.42	1.58	1.51
2	B	601	TXK	C15-C16	-2.39	1.34	1.38
2	A	601	TXK	C2-C1	-2.37	1.35	1.38
2	A	601	TXK	C21-C22	-2.32	1.34	1.38
2	B	601	TXK	C29-N2	-2.28	1.42	1.47
2	B	601	TXK	C28-C27	-2.20	1.42	1.53
2	A	601	TXK	C5-C6	-2.18	1.36	1.40
2	B	601	TXK	C23-C24	-2.18	1.35	1.38
2	A	601	TXK	C28-C27	-2.08	1.42	1.53
2	B	601	TXK	O1-C10	-2.01	1.18	1.22
2	A	601	TXK	C11-C10	2.01	1.53	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	TXK	C13-C12-C11	-7.86	112.64	120.36
2	B	601	TXK	C13-C12-C11	-7.80	112.70	120.36
2	A	601	TXK	C16-C11-C12	6.46	126.78	118.57
2	B	601	TXK	C16-C11-C12	6.26	126.53	118.57
2	B	601	TXK	C3-C4-C5	-6.00	114.03	120.77
2	B	601	TXK	C4-C5-C6	5.93	126.96	119.49
2	A	601	TXK	C3-C4-C5	-5.68	114.39	120.77
2	B	601	TXK	C29-N2-C30	5.20	110.14	104.02
2	A	601	TXK	C4-C5-C6	5.17	126.01	119.49
2	B	601	TXK	C28-C27-C30	5.05	109.27	102.25
2	A	601	TXK	C23-C24-C19	-4.95	116.24	121.18
2	B	601	TXK	C14-C15-C16	-4.83	114.28	120.24
2	B	601	TXK	C5-C6-C9	4.42	128.87	121.32
2	B	601	TXK	C15-C14-C13	4.20	125.61	119.87
2	A	601	TXK	C5-C6-C9	4.16	128.43	121.32
2	A	601	TXK	C16-C11-C10	-4.13	109.68	120.28
2	B	601	TXK	C18-C17-C8	3.99	62.41	59.67
2	B	601	TXK	C7-C5-C4	-3.95	112.81	121.18
2	B	601	TXK	C16-C11-C10	-3.86	110.37	120.28
2	B	601	TXK	C1-C6-C9	-3.60	112.41	121.22
2	A	601	TXK	C20-C21-C22	-3.43	116.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	TXK	C1-C6-C9	-3.34	113.05	121.22
2	A	601	TXK	C14-C15-C16	-3.14	116.37	120.24
2	A	601	TXK	C7-C5-C4	-2.96	114.90	121.18
2	A	601	TXK	C15-C14-C13	2.94	123.90	119.87
2	B	601	TXK	O1-C10-N1	-2.88	117.71	121.84
2	A	601	TXK	C29-N2-C30	2.86	107.39	104.02
2	B	601	TXK	C25-C26-C27	-2.80	109.21	114.16
2	B	601	TXK	C26-C27-C28	-2.78	104.95	115.45
2	A	601	TXK	C23-C22-C21	2.73	122.30	118.23
2	A	601	TXK	C24-C19-C20	2.67	121.61	118.30
2	A	601	TXK	C26-C25-C22	-2.64	104.53	113.22
2	B	601	TXK	C26-C25-C22	-2.58	104.73	113.22
2	A	601	TXK	C18-C17-C8	2.52	61.40	59.67
2	A	601	TXK	C29-C28-C27	-2.49	98.79	104.33
2	A	601	TXK	C28-C27-C30	2.41	105.60	102.25
2	B	601	TXK	C2-C1-C6	-2.36	117.21	121.12
2	A	601	TXK	C31-N2-C30	-2.28	107.89	113.18
2	B	601	TXK	C20-C21-C22	-2.19	118.12	121.00
2	A	601	TXK	C31-N2-C29	-2.11	108.25	113.25
2	B	601	TXK	C1-C2-C3	2.10	122.10	119.88
2	B	601	TXK	C23-C24-C19	-2.10	119.09	121.18
2	A	601	TXK	C28-C29-N2	-2.01	101.18	104.76
2	A	601	TXK	C2-C1-C6	-2.01	117.80	121.12

There are no chirality outliers.

All (8) torsion outliers are listed below:

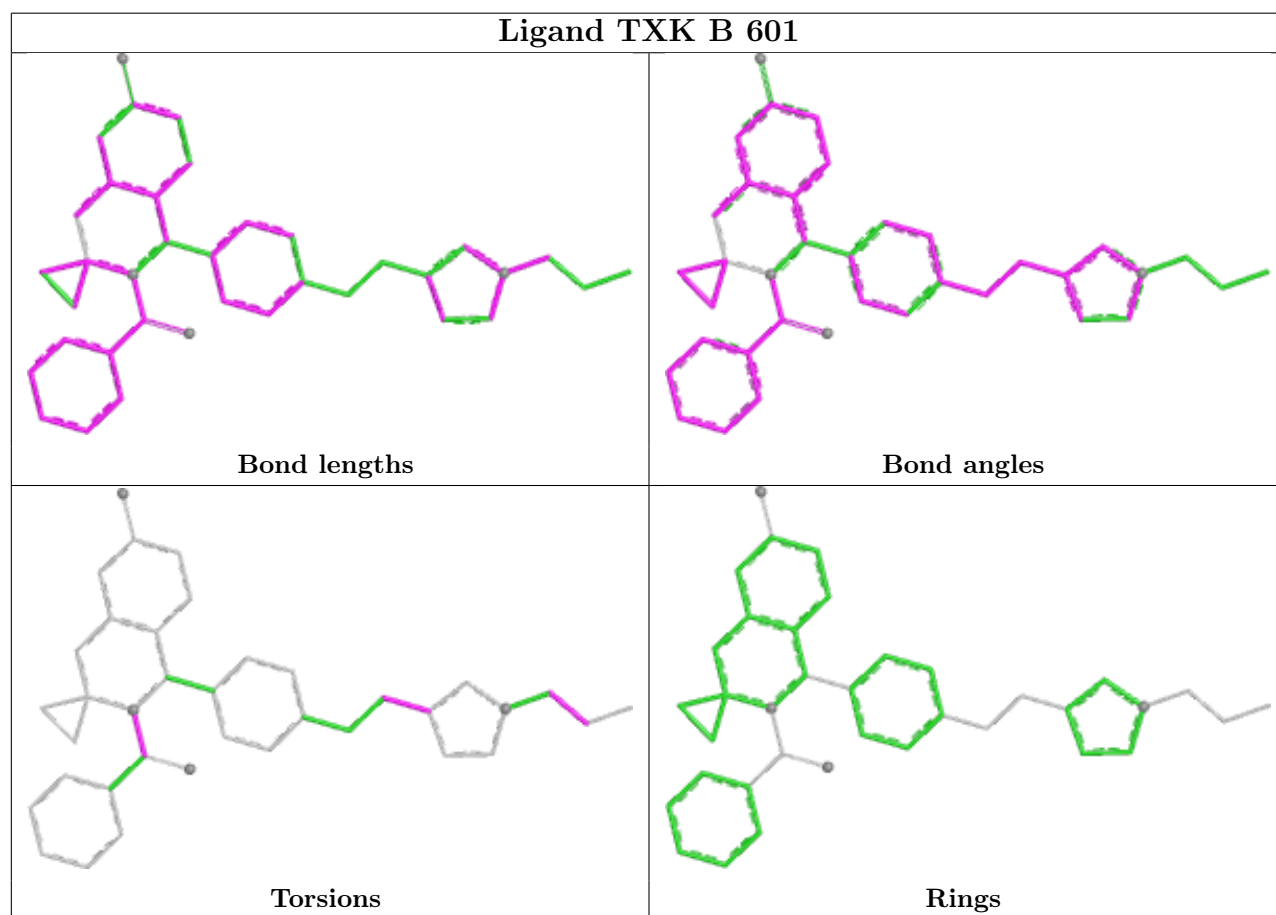
Mol	Chain	Res	Type	Atoms
2	A	601	TXK	C11-C10-N1-C8
2	A	601	TXK	O1-C10-N1-C8
2	B	601	TXK	C11-C10-N1-C8
2	B	601	TXK	O1-C10-N1-C8
2	A	601	TXK	C25-C26-C27-C30
2	B	601	TXK	C25-C26-C27-C30
2	B	601	TXK	C25-C26-C27-C28
2	B	601	TXK	N2-C31-C32-C33

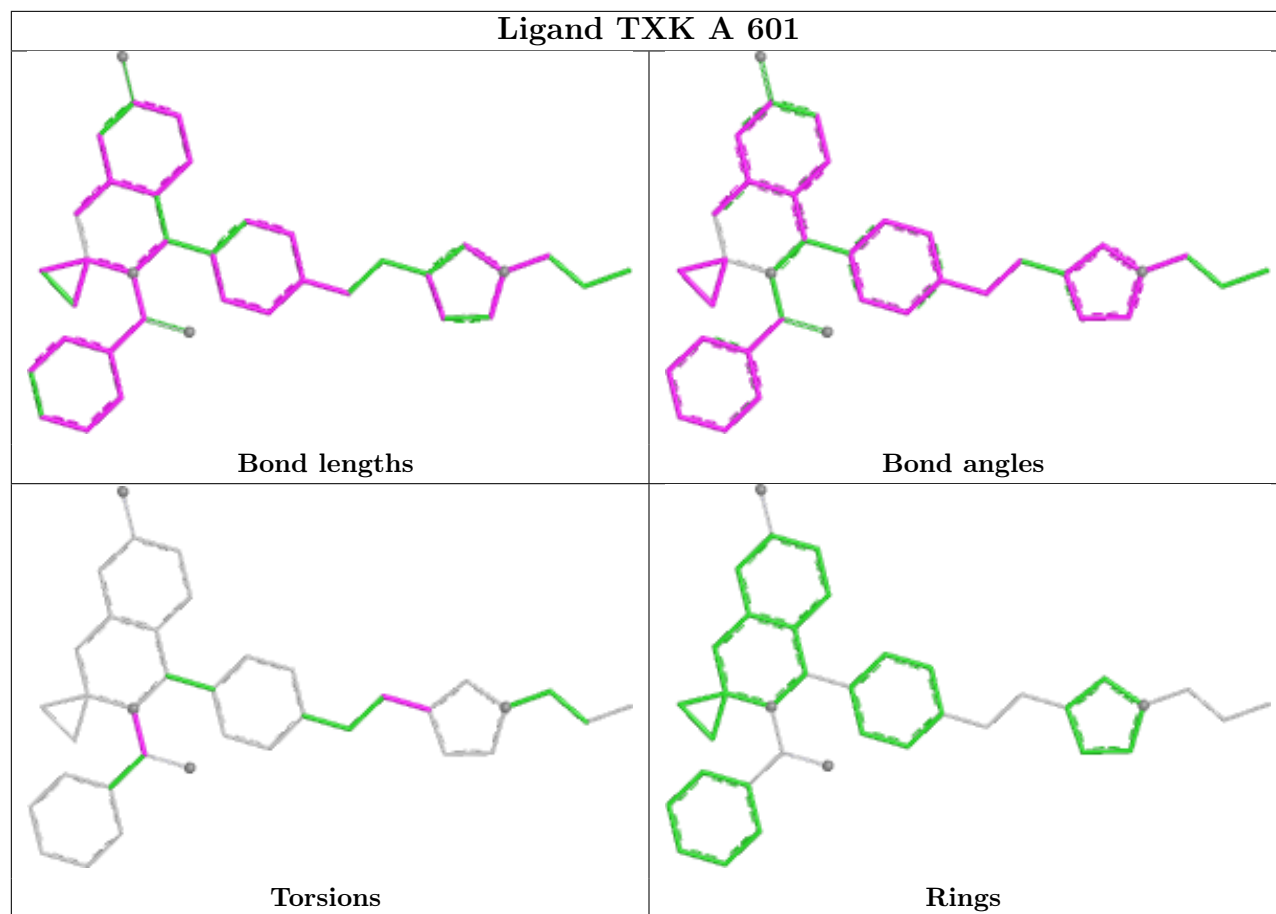
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TXK	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

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	234/255 (91%)	0.19	20 (8%)	16 16	5, 18, 43, 57	6 (2%)
1	B	223/255 (87%)	0.35	23 (10%)	12 12	5, 20, 49, 67	7 (3%)
All	All	457/510 (89%)	0.27	43 (9%)	14 14	5, 19, 46, 67	13 (2%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	VAL	6.5
1	B	461	PHE	5.6
1	B	338	SER	5.2
1	A	537	TYR	4.7
1	B	333	PRO	4.7
1	B	336	PRO	4.2
1	A	461	PHE	4.2
1	B	306	LEU	4.1
1	B	337	PHE	4.0
1	B	334	THR	3.9
1	B	331	TYR	3.8
1	B	307	ALA	3.7
1	B	419	GLU	3.7
1	B	459	TYR	3.7
1	A	549	LEU	3.6
1	A	459	TYR	3.4
1	B	343	MET	3.3
1	A	529	LYS	3.2
1	B	549	LEU	3.1
1	A	501	HIS	3.1
1	A	550	HIS	3.0
1	B	526	TYR	3.0
1	B	308	LEU	2.9
1	A	417	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	335	ARG	2.8
1	A	336	PRO	2.8
1	B	332	ASP	2.8
1	B	353	GLU	2.8
1	A	538	ASP	2.7
1	A	415	GLY	2.7
1	B	460	THR	2.7
1	B	330	GLU	2.7
1	A	418	VAL	2.6
1	B	341	SER	2.6
1	A	547	HIS	2.5
1	A	308	LEU	2.5
1	A	465	THR	2.5
1	A	544	LEU	2.4
1	A	534	VAL	2.4
1	A	548	ARG	2.3
1	A	541	LEU	2.2
1	B	527	SER	2.2
1	B	534	VAL	2.1

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.

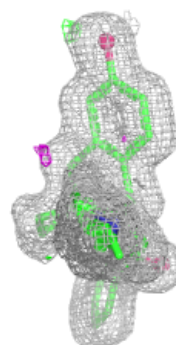
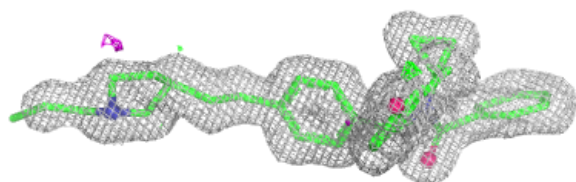
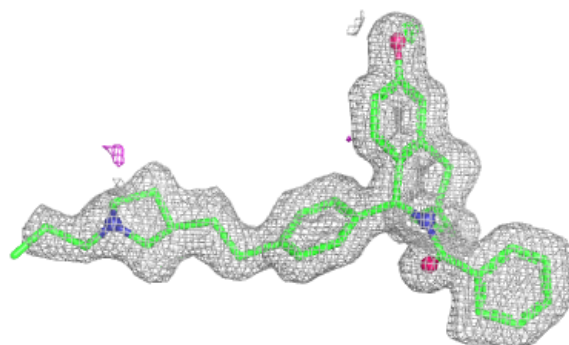
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TXK	A	601	37/37	0.96	0.07	9,13,33,48	0
2	TXK	B	601	37/37	0.96	0.07	10,14,29,50	0

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.

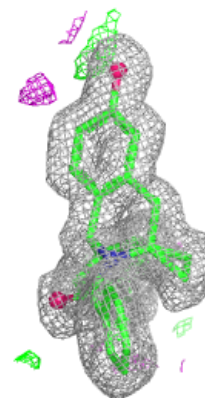
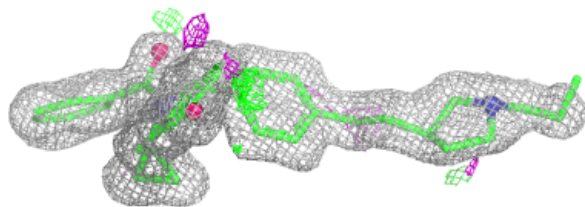
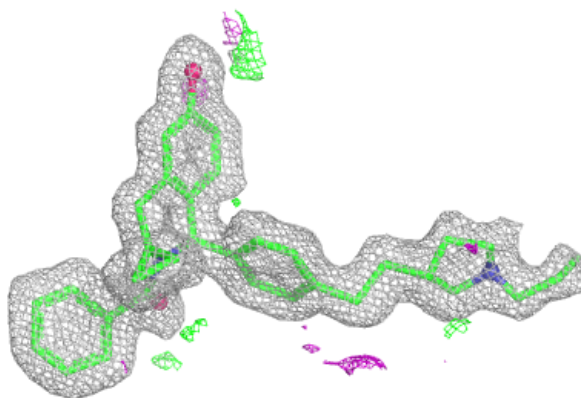
Electron density around TXK A 601:

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



Electron density around TXK B 601:

$2mF_o - DF_c$ (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.