



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:44 PM UTC

PDB ID : 4QD6 / pdb_00004qd6
Title : ITK kinase domain in complex with inhibitor compound
Authors : McEwan, P.A.; Barker, J.J.; Eigenbrot, C.
Deposited on : 2014-05-13
Resolution : 2.45 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

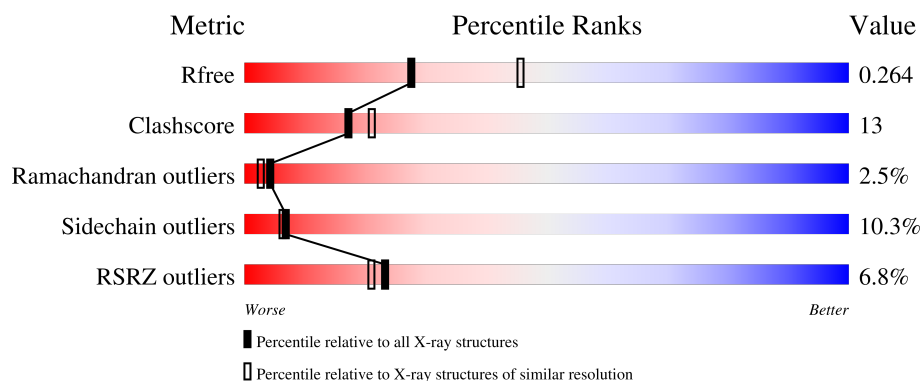
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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% 63% 24% 8%
1	B	266	7% 59% 26% 6% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3988 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.

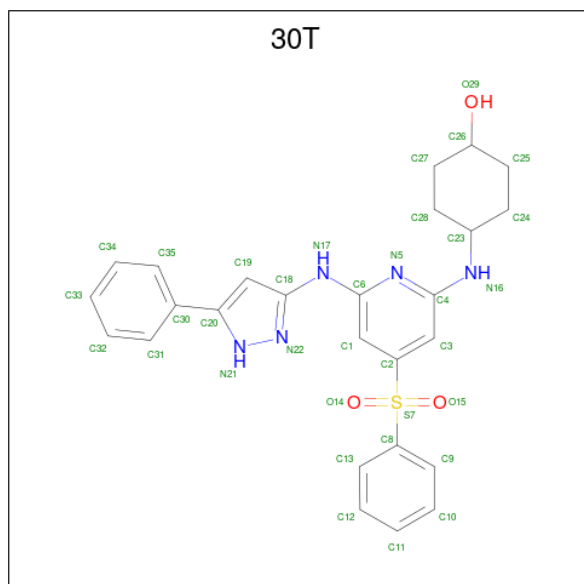
- Molecule 1 is a protein called Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1944	1242	322	364	16			
1	B	243	Total	C	N	O	S	0	2	0
			1955	1248	326	365	16			

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 trans-4-({6-[(5-phenyl-1H-pyrazol-3-yl)amino]-4-(phenylsulfonyl)pyridin-2-yl}amino)cyclohexanol (CCD ID: 30T) (formula: C₂₆H₂₇N₅O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	26	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			35	26	5	3	1		

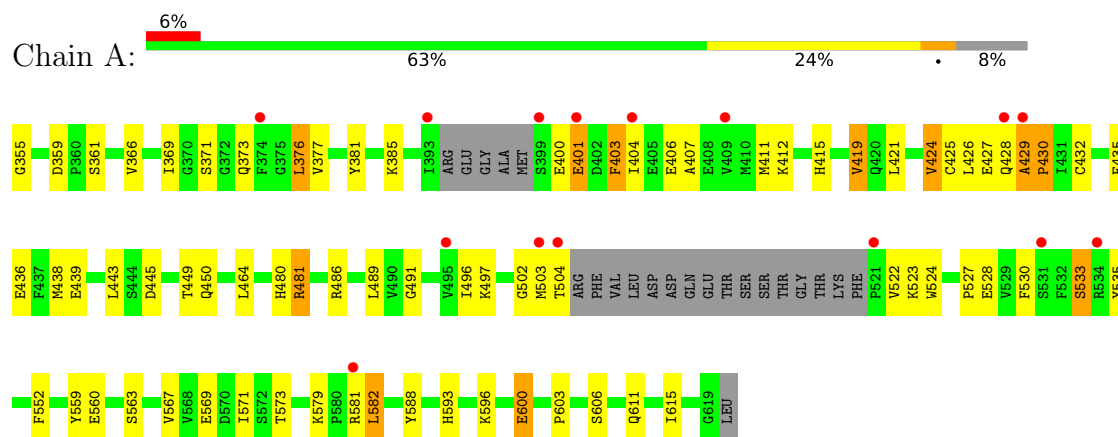
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	8	Total	O	0	0
			8	8		

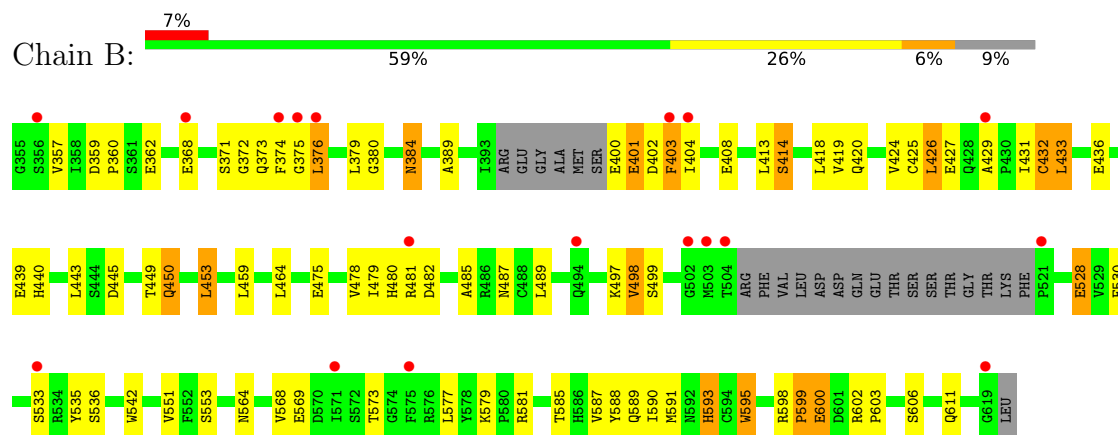
3 Residue-property plots

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 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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.06Å 94.32Å 156.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.76 – 2.45 80.76 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.4 (80.76-2.45) 98.4 (80.76-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.209 , 0.267 0.208 , 0.264	Depositor DCC
R_{free} test set	1137 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3988	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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 71.55 % 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 2.5782e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 30T

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	0.93	0/1987	1.17	4/2682 (0.1%)
1	B	0.97	2/1998 (0.1%)	1.20	7/2696 (0.3%)
All	All	0.95	2/3985 (0.1%)	1.19	11/5378 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	498	VAL	CA-CB	5.39	1.60	1.54
1	B	593	HIS	CA-C	5.01	1.59	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	LEU	N-CA-C	7.88	121.32	110.06
1	A	415	HIS	CA-C-N	-7.00	112.59	119.87
1	A	415	HIS	C-N-CA	-7.00	112.59	119.87
1	B	595	TRP	N-CA-C	6.56	121.44	113.17
1	A	533	SER	N-CA-C	5.93	123.43	110.80
1	B	389	ALA	N-CA-C	-5.60	99.89	109.24
1	A	559	TYR	N-CA-C	-5.58	103.54	111.24
1	B	432	CYS	N-CA-C	5.30	118.09	109.24
1	B	553	SER	N-CA-C	-5.24	106.73	113.02
1	B	579	LYS	CA-C-N	-5.23	114.59	120.14
1	B	579	LYS	C-N-CA	-5.23	114.59	120.14

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	1944	0	1900	48	0
1	B	1955	0	1911	51	0
2	A	35	0	27	3	0
2	B	35	0	27	5	0
3	A	11	0	0	1	0
3	B	8	0	0	1	0
All	All	3988	0	3865	99	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 13.

All (99) 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:503:MET:HB3	1:A:504:THR:HA	1.12	1.12
1:A:429:ALA:HB3	1:A:430:PRO:HD2	1.37	1.06
1:A:503:MET:CB	1:A:504:THR:HA	2.00	0.86
1:A:429:ALA:CB	1:A:430:PRO:HD2	2.10	0.81
1:A:503:MET:HB3	1:A:504:THR:CA	2.04	0.78
1:A:429:ALA:CB	1:A:430:PRO:CD	2.66	0.74
1:A:552:PHE:O	1:A:582:LEU:HD13	1.89	0.72
1:A:427:GLU:HB2	1:B:360:PRO:HG3	1.70	0.72
1:B:480:HIS:O	1:B:481[A]:ARG:HB2	1.88	0.72
1:A:377:VAL:HG21	2:B:701:30T:H15	1.71	0.71
1:A:366:VAL:HG21	1:A:381:TYR:CE1	2.25	0.71
1:A:429:ALA:O	1:A:430:PRO:C	2.34	0.69
1:A:429:ALA:HB3	1:A:430:PRO:CD	2.18	0.69
1:B:418:LEU:HD23	1:B:498:VAL:HB	1.74	0.68
1:B:445:ASP:O	1:B:449:THR:HG23	1.96	0.66
2:A:701:30T:H12	2:A:701:30T:H10	1.76	0.66
1:A:582:LEU:HD12	1:A:582:LEU:H	1.61	0.65
1:A:481:ARG:HG2	1:A:535:TYR:CD2	2.33	0.64
1:B:400:GLU:C	1:B:402:ASP:H	2.05	0.64
1:A:359:ASP:OD1	1:A:361:SER:OG	2.16	0.63
1:A:407:ALA:O	1:A:411:MET:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ASP:O	1:A:449:THR:HG23	1.98	0.63
1:B:373:GLN:C	1:B:375:GLY:H	2.05	0.63
1:B:587:VAL:HG12	1:B:591:MET:HE3	1.80	0.62
1:A:425:CYS:HB3	1:A:432:CYS:SG	2.40	0.61
1:B:384:ASN:H	1:B:384:ASN:HD22	1.47	0.61
1:A:563:SER:O	1:A:567:VAL:HG23	2.00	0.60
1:B:528:GLU:OE2	1:B:602:ARG:NH2	2.32	0.58
1:B:400:GLU:O	1:B:402:ASP:N	2.37	0.58
1:A:419:VAL:HG21	1:A:489:LEU:HD12	1.86	0.58
1:B:414:SER:HB2	1:B:420:GLN:HE22	1.68	0.57
1:B:577:LEU:O	1:B:588:TYR:OH	2.19	0.57
1:A:481:ARG:HG2	1:A:535:TYR:CE2	2.39	0.57
1:B:479:ILE:HB	1:B:481[B]:ARG:HE	1.69	0.57
1:B:542:TRP:CZ3	1:B:595:TRP:O	2.57	0.57
1:A:480:HIS:O	1:A:481:ARG:HB2	2.04	0.55
1:A:369:ILE:HG22	2:B:701:30T:H7	1.89	0.54
1:A:596:LYS:NZ	3:A:811:HOH:O	2.40	0.53
2:B:701:30T:H12	2:B:701:30T:H10	1.92	0.52
1:B:459:LEU:HB3	1:B:551:VAL:HG12	1.91	0.52
1:A:527:PRO:HA	1:A:530:PHE:CE1	2.45	0.52
1:A:376:LEU:HD23	1:A:376:LEU:N	2.25	0.51
1:A:428:GLN:HG2	1:B:360:PRO:CB	2.40	0.51
1:B:569:GLU:O	1:B:573:THR:HG23	2.11	0.50
1:A:593:HIS:CE1	1:A:603:PRO:HD3	2.46	0.50
1:B:373:GLN:C	1:B:375:GLY:N	2.68	0.50
1:B:379:LEU:HD12	1:B:380:GLY:H	1.75	0.50
1:A:438:MET:HE3	1:A:491:GLY:CA	2.42	0.49
1:A:371:SER:HA	1:A:376:LEU:HA	1.94	0.48
1:B:419:VAL:HG21	1:B:489:LEU:HD12	1.93	0.48
1:A:428:GLN:HG2	1:B:360:PRO:HB3	1.96	0.48
1:A:435:PHE:CD2	2:A:701:30T:H24	2.49	0.48
1:B:593:HIS:ND1	1:B:603:PRO:HD3	2.29	0.47
1:B:542:TRP:HZ3	1:B:595:TRP:O	1.97	0.47
1:B:450:GLN:HG3	1:B:453:LEU:HD23	1.95	0.47
1:B:590:ILE:HD11	1:B:611:GLN:NE2	2.30	0.47
1:B:425:CYS:O	1:B:432:CYS:HB2	2.15	0.47
1:B:481[B]:ARG:NH2	3:B:804:HOH:O	2.26	0.47
1:A:600:GLU:H	1:A:600:GLU:CD	2.22	0.47
2:A:701:30T:C19	2:A:701:30T:N5	2.77	0.47
1:A:523:LYS:HB2	1:A:524:TRP:CE3	2.50	0.46
1:A:366:VAL:CG2	1:A:381:TYR:CE1	2.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LEU:HD12	1:B:380:GLY:N	2.29	0.46
1:B:480:HIS:O	1:B:481[B]:ARG:HB2	2.15	0.46
1:B:479:ILE:HG22	1:B:481[B]:ARG:HG3	1.97	0.46
1:B:424:VAL:HG12	1:B:433:LEU:HD12	1.98	0.45
1:A:355:GLY:N	1:B:408:GLU:OE2	2.49	0.45
1:B:439:GLU:HB3	1:B:440:HIS:CD2	2.51	0.45
1:B:359:ASP:O	1:B:362:GLU:HG3	2.18	0.44
1:A:443:LEU:HD13	1:A:496:ILE:HD12	1.98	0.44
1:A:411:MET:HE2	1:A:411:MET:HB3	1.71	0.44
1:A:438:MET:CE	1:A:491:GLY:HA3	2.48	0.44
1:B:436:GLU:OE1	1:B:497:LYS:NZ	2.42	0.44
1:B:600:GLU:H	1:B:600:GLU:CD	2.26	0.43
1:B:564:ASN:O	1:B:568:VAL:HG23	2.18	0.43
1:B:482:ASP:O	1:B:487:ASN:ND2	2.45	0.43
1:A:376:LEU:HD23	1:A:376:LEU:H	1.84	0.43
1:B:413:LEU:HD11	1:B:478:VAL:HG21	2.01	0.43
2:B:701:30T:N5	2:B:701:30T:C19	2.82	0.43
1:A:436:GLU:OE1	1:A:497:LYS:NZ	2.37	0.42
1:B:375:GLY:O	1:B:376:LEU:CB	2.66	0.42
1:B:585:THR:O	1:B:589:GLN:HG3	2.19	0.42
1:B:375:GLY:O	1:B:376:LEU:HB3	2.20	0.42
2:B:701:30T:H27	2:B:701:30T:H16	2.02	0.42
1:B:372:GLY:H	1:B:376:LEU:H	1.66	0.42
1:B:481[A]:ARG:HG2	1:B:535:TYR:CD2	2.55	0.42
1:B:418:LEU:CD2	1:B:498:VAL:HB	2.47	0.41
1:B:419:VAL:HG21	1:B:499:SER:HB3	2.02	0.41
1:A:569:GLU:O	1:A:573:THR:HG23	2.20	0.41
1:B:590:ILE:O	1:B:591:MET:C	2.63	0.41
1:B:598:ARG:HA	1:B:599:PRO:HD2	1.74	0.41
1:A:593:HIS:ND1	1:A:603:PRO:HD3	2.36	0.41
1:B:443:LEU:HB3	1:B:485:ALA:O	2.19	0.41
1:A:403:PHE:O	1:A:406:GLU:HB2	2.20	0.41
1:A:424:VAL:HG23	1:B:357:VAL:HA	2.03	0.41
1:B:400:GLU:CD	1:B:400:GLU:N	2.79	0.41
1:A:611:GLN:O	1:A:615:ILE:HG13	2.21	0.40
1:A:579:LYS:HG3	1:A:588:TYR:HB2	2.02	0.40
1:A:400:GLU:HB2	1:A:401:GLU:H	1.72	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	238/266 (90%)	216 (91%)	15 (6%)	7 (3%)	3	2
1	B	239/266 (90%)	214 (90%)	20 (8%)	5 (2%)	5	4
All	All	477/532 (90%)	430 (90%)	35 (7%)	12 (2%)	4	3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	ALA
1	A	430	PRO
1	A	533	SER
1	B	401	GLU
1	B	403	PHE
1	A	481	ARG
1	A	502	GLY
1	B	376	LEU
1	B	429	ALA
1	A	385	LYS
1	A	439	GLU
1	B	599	PRO

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	214/233 (92%)	193 (90%)	21 (10%)	7 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	215/233 (92%)	192 (89%)	23 (11%)	6	6
All	All	429/466 (92%)	385 (90%)	44 (10%)	7	6

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	GLN
1	A	376	LEU
1	A	401	GLU
1	A	403	PHE
1	A	404	ILE
1	A	412	LYS
1	A	419	VAL
1	A	421	LEU
1	A	424	VAL
1	A	426	LEU
1	A	450	GLN
1	A	464	LEU
1	A	486	ARG
1	A	522	VAL
1	A	528	GLU
1	A	560	GLU
1	A	571	ILE
1	A	581	ARG
1	A	582	LEU
1	A	600	GLU
1	A	606	SER
1	B	368	GLU
1	B	371	SER
1	B	374	PHE
1	B	384	ASN
1	B	401	GLU
1	B	403	PHE
1	B	404	ILE
1	B	414	SER
1	B	426	LEU
1	B	427	GLU
1	B	431	ILE
1	B	433	LEU
1	B	450	GLN
1	B	453	LEU
1	B	464	LEU

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Mol	Chain	Res	Type
1	B	475	GLU
1	B	528	GLU
1	B	530	PHE
1	B	533	SER
1	B	536	SER
1	B	581	ARG
1	B	600	GLU
1	B	606	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	378	HIS
1	A	450	GLN
1	A	494	GLN
1	A	611	GLN
1	B	367	GLN
1	B	384	ASN
1	B	420	GLN
1	B	440	HIS
1	B	493	ASN
1	B	589	GLN
1	B	611	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	30T	B	701	-	39,39,39	2.75	6 (15%)	52,55,55	2.30	22 (42%)
2	30T	A	701	-	39,39,39	2.45	4 (10%)	52,55,55	3.06	19 (36%)

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	30T	B	701	-	-	2/24/34/34	0/5/5/5
2	30T	A	701	-	-	4/24/34/34	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	30T	C2-S7	-12.25	1.58	1.77
2	A	701	30T	C2-S7	-10.41	1.61	1.77
2	A	701	30T	C8-S7	-9.25	1.62	1.77
2	B	701	30T	C8-S7	-8.92	1.63	1.77
2	B	701	30T	N21-N22	3.88	1.44	1.36
2	B	701	30T	C18-N22	3.36	1.37	1.33
2	A	701	30T	C20-N21	-3.33	1.31	1.35
2	A	701	30T	C6-N17	-2.61	1.34	1.40
2	B	701	30T	C32-C31	2.46	1.43	1.38
2	B	701	30T	C20-N21	2.01	1.37	1.35

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	30T	C30-C20-N21	-9.87	109.33	122.62
2	A	701	30T	C18-N22-N21	9.40	110.55	103.71
2	A	701	30T	C19-C20-N21	6.46	114.32	106.18
2	A	701	30T	C8-S7-C2	5.34	114.15	104.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	30T	C20-N21-N22	-5.24	103.35	112.35
2	B	701	30T	O15-S7-O14	-5.08	108.97	119.25
2	B	701	30T	C30-C20-N21	-4.92	116.00	122.62
2	B	701	30T	C8-S7-C2	4.85	113.27	104.37
2	B	701	30T	C19-C20-N21	4.56	111.92	106.18
2	A	701	30T	C35-C30-C31	4.18	123.89	118.57
2	B	701	30T	C25-C24-C23	-4.01	107.09	111.49
2	A	701	30T	O15-S7-O14	-4.01	111.14	119.25
2	A	701	30T	O15-S7-C8	-4.00	103.04	107.96
2	A	701	30T	C27-C28-C23	3.95	115.82	111.49
2	A	701	30T	C32-C31-C30	-3.90	116.53	120.36
2	B	701	30T	C3-C2-S7	-3.85	114.02	119.15
2	B	701	30T	C1-C2-S7	3.80	124.20	119.15
2	A	701	30T	C30-C20-C19	3.45	136.34	131.03
2	B	701	30T	C20-N21-N22	-3.43	106.47	112.35
2	A	701	30T	C19-C18-N22	-3.28	109.79	112.14
2	A	701	30T	O15-S7-C2	3.26	111.97	107.96
2	B	701	30T	C10-C9-C8	3.16	122.18	118.95
2	B	701	30T	O14-S7-C8	3.14	111.82	107.96
2	A	701	30T	C12-C13-C8	3.01	122.02	118.95
2	A	701	30T	C19-C18-N17	3.01	138.81	127.85
2	A	701	30T	C3-C2-S7	2.92	123.04	119.15
2	A	701	30T	N17-C18-N22	-2.83	111.34	117.81
2	B	701	30T	N17-C6-N5	2.81	120.12	113.33
2	B	701	30T	C1-C6-N5	-2.80	117.54	123.35
2	B	701	30T	C6-N5-C4	2.63	122.20	117.93
2	A	701	30T	C31-C30-C20	-2.61	116.85	120.81
2	B	701	30T	C32-C31-C30	-2.57	117.84	120.36
2	B	701	30T	C18-N22-N21	2.47	105.50	103.71
2	B	701	30T	C34-C35-C30	2.40	122.72	120.36
2	B	701	30T	C13-C8-C9	-2.38	117.36	120.47
2	B	701	30T	O14-S7-C2	-2.36	105.06	107.96
2	B	701	30T	N16-C4-N5	2.18	120.18	117.03
2	B	701	30T	C6-C1-C2	2.09	119.44	117.23
2	A	701	30T	C34-C35-C30	-2.03	118.37	120.36
2	B	701	30T	C33-C32-C31	2.03	122.74	120.24
2	B	701	30T	C24-C23-N16	-2.02	107.52	110.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

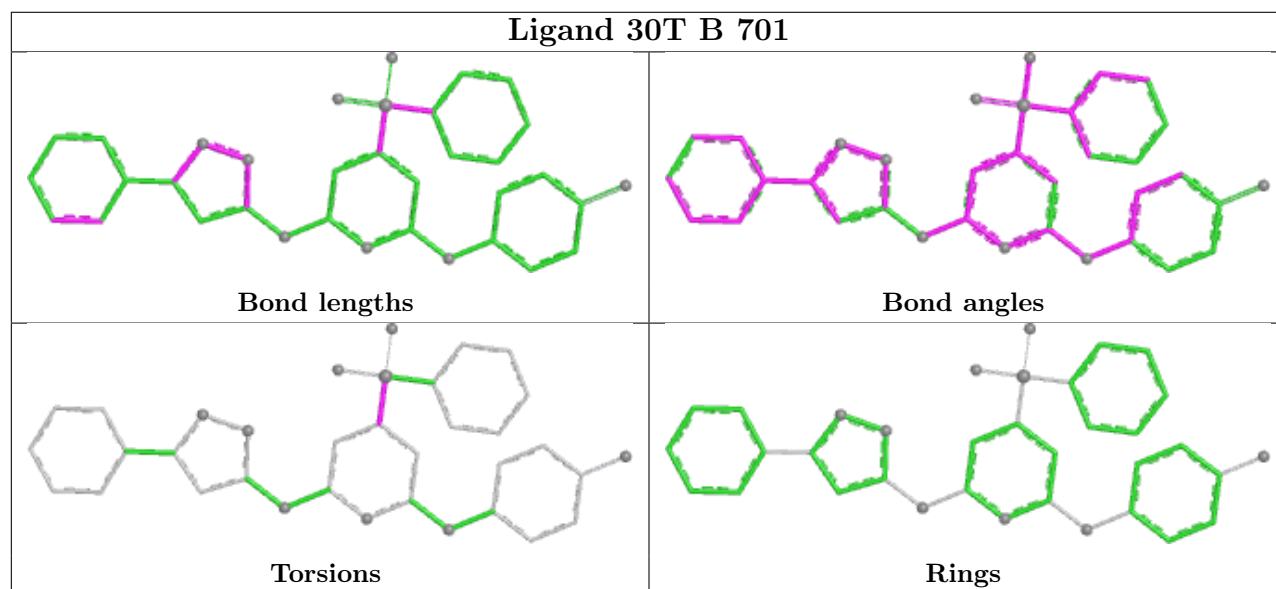
Mol	Chain	Res	Type	Atoms
2	B	701	30T	C3-C2-S7-O15
2	B	701	30T	C1-C2-S7-O15
2	A	701	30T	C13-C8-S7-O14
2	A	701	30T	C9-C8-S7-O14
2	A	701	30T	C3-C2-S7-O15
2	A	701	30T	C1-C2-S7-O15

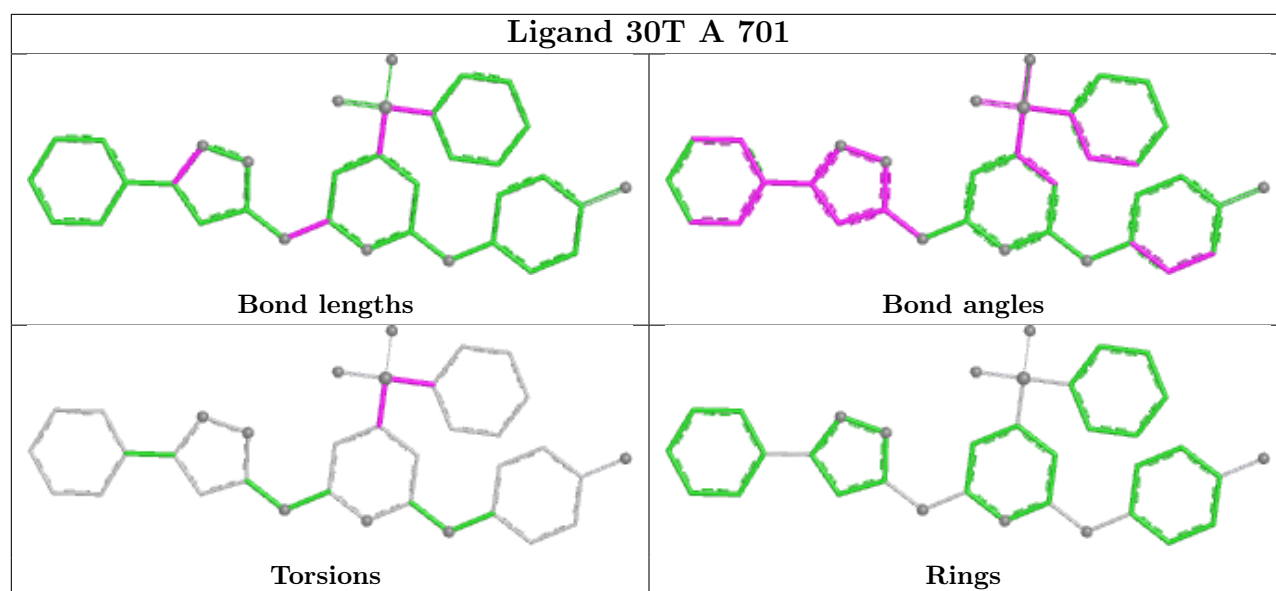
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	30T	5	0
2	A	701	30T	3	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	244/266 (91%)	0.17	15 (6%) 27 24	26, 50, 108, 159	0
1	B	243/266 (91%)	0.19	18 (7%) 20 18	27, 51, 104, 130	2 (0%)
All	All	487/532 (91%)	0.18	33 (6%) 23 21	26, 51, 107, 159	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	THR	4.9
1	A	504	THR	4.5
1	B	502	GLY	4.3
1	A	374	PHE	4.2
1	B	503	MET	4.0
1	A	521	PRO	3.9
1	B	374	PHE	3.8
1	B	481[A]	ARG	3.5
1	A	503	MET	3.4
1	B	429	ALA	3.2
1	B	494	GLN	3.0
1	B	403	PHE	2.9
1	B	376	LEU	2.9
1	B	619	GLY	2.7
1	B	571	ILE	2.6
1	A	399	SER	2.6
1	B	404	ILE	2.5
1	A	401	GLU	2.5
1	B	368	GLU	2.5
1	A	581	ARG	2.4
1	B	375	GLY	2.3
1	A	429	ALA	2.3
1	A	534	ARG	2.3
1	B	521	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	575	PHE	2.2
1	A	495	VAL	2.2
1	B	356[A]	SER	2.2
1	A	531	SER	2.2
1	A	428	GLN	2.1
1	A	404	ILE	2.1
1	A	409	VAL	2.1
1	B	533	SER	2.1
1	A	393	ILE	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](#)

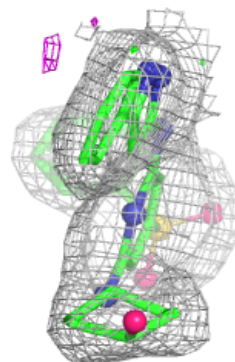
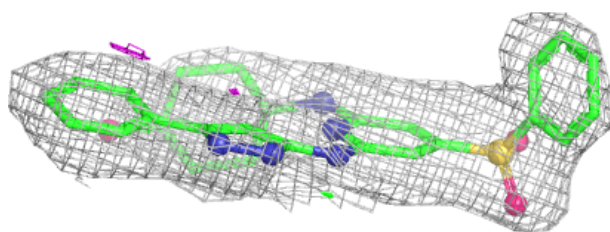
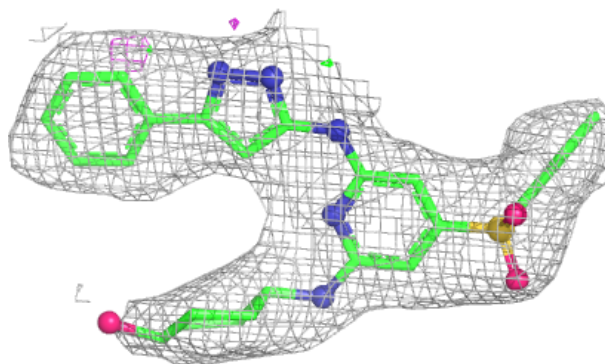
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	30T	A	701	35/35	0.92	0.10	31,60,78,83	0
2	30T	B	701	35/35	0.92	0.10	31,57,84,89	0

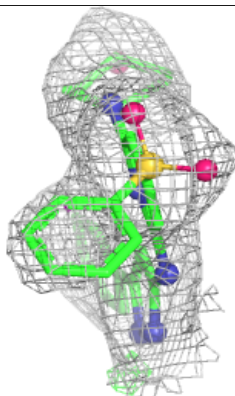
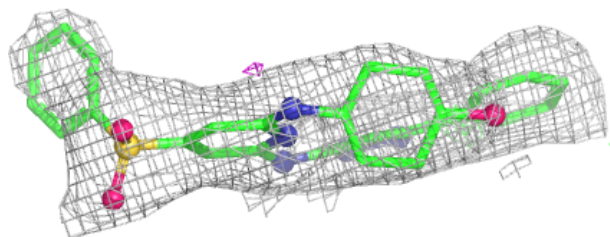
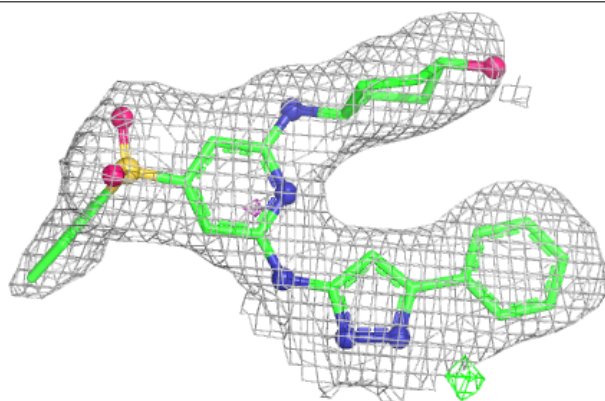
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 30T 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)

**Electron density around 30T 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.