



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:01 PM UTC

PDB ID : 4OLI / pdb_00004oli
Title : The pseudokinase/kinase protein from JAK-family member TYK2
Authors : Eigenbrot, C.; Ultsch, M.; Wallweber, H.
Deposited on : 2014-01-23
Resolution : 2.80 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

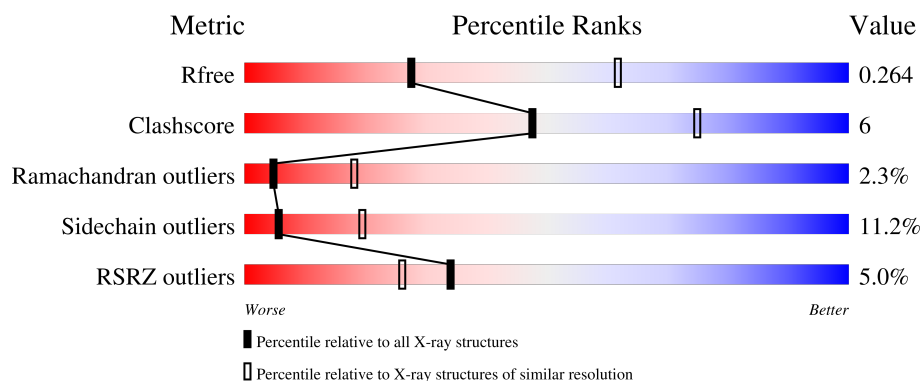
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	645	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4396 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 Non-receptor tyrosine-protein kinase TYK2.

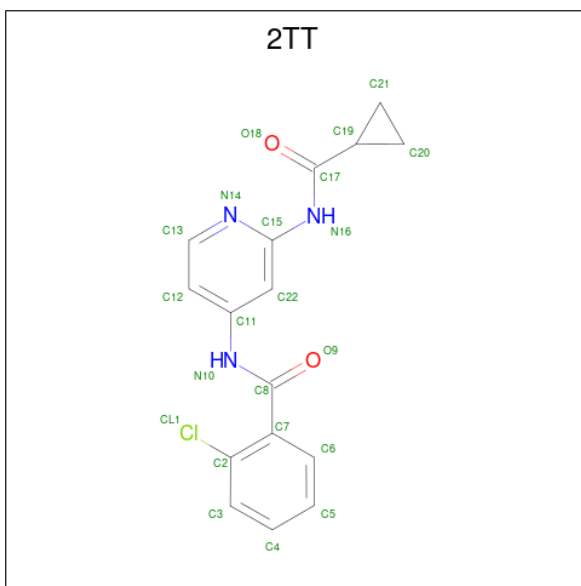
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4344	2770	764	785	25			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	543	MET	-	expression tag	UNP P29597
A	544	SER	-	expression tag	UNP P29597
A	545	TYR	-	expression tag	UNP P29597
A	546	TYR	-	expression tag	UNP P29597
A	547	HIS	-	expression tag	UNP P29597
A	548	HIS	-	expression tag	UNP P29597
A	549	HIS	-	expression tag	UNP P29597
A	550	HIS	-	expression tag	UNP P29597
A	551	HIS	-	expression tag	UNP P29597
A	552	HIS	-	expression tag	UNP P29597
A	553	ASP	-	expression tag	UNP P29597
A	554	TYR	-	expression tag	UNP P29597
A	555	ASP	-	expression tag	UNP P29597
A	556	ILE	-	expression tag	UNP P29597
A	557	PRO	-	expression tag	UNP P29597
A	558	THR	-	expression tag	UNP P29597
A	559	THR	-	expression tag	UNP P29597
A	560	GLU	-	expression tag	UNP P29597
A	561	ASN	-	expression tag	UNP P29597
A	562	LEU	-	expression tag	UNP P29597
A	563	TYR	-	expression tag	UNP P29597
A	564	PHE	-	expression tag	UNP P29597
A	565	GLN	-	expression tag	UNP P29597
A	1016	SER	ALA	SEE REMARK 999	UNP P29597
A	1023	ASN	ASP	engineered mutation	UNP P29597

- Molecule 2 is 2-chloro-N-{2-[(cyclopropylcarbonyl)amino]pyridin-4-yl}benzamide (CCD ID:

2TT) (formula: C₁₆H₁₄ClN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		
2	A	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		

- Molecule 3 is water.

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

- Molecule 1: Non-receptor tyrosine-protein kinase TYK2



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	111.02Å 111.02Å 123.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.09 – 2.80 46.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.09-2.80) 99.5 (46.09-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.201 , 0.257 0.211 , 0.264	Depositor DCC
R_{free} test set	1077 reflections (5.81%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4396	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2TT

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	0.88	0/4451	1.49	41/6026 (0.7%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	ALA	N-CA-C	-7.88	103.11	112.89
1	A	1032	ASP	CA-CB-CG	7.38	119.97	112.60
1	A	1080	TYR	CA-C-N	6.55	131.07	120.60
1	A	1080	TYR	C-N-CA	6.55	131.07	120.60
1	A	845	THR	CA-C-N	6.42	128.78	120.44
1	A	845	THR	C-N-CA	6.42	128.78	120.44
1	A	968	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	909	GLY	N-CA-C	6.12	119.37	110.63
1	A	723	SER	CA-C-N	6.07	128.74	120.54
1	A	723	SER	C-N-CA	6.07	128.74	120.54
1	A	763	GLY	CA-C-N	5.92	132.85	121.54
1	A	763	GLY	C-N-CA	5.92	132.85	121.54
1	A	1108	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	840	GLN	N-CA-C	-5.81	106.17	113.20
1	A	894	LYS	CA-C-N	5.73	127.96	120.28
1	A	894	LYS	C-N-CA	5.73	127.96	120.28
1	A	809	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	802	ALA	CA-C-N	5.53	127.69	120.28
1	A	802	ALA	C-N-CA	5.53	127.69	120.28
1	A	983	LEU	N-CA-C	5.53	119.87	113.18
1	A	1059	GLU	N-CA-C	5.44	122.40	110.80
1	A	991	PRO	CA-C-N	5.43	128.94	121.33
1	A	991	PRO	C-N-CA	5.43	128.94	121.33
1	A	1167	PRO	CA-C-N	5.41	127.58	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1167	PRO	C-N-CA	5.41	127.58	120.60
1	A	716	GLN	CA-C-N	5.33	127.42	120.28
1	A	716	GLN	C-N-CA	5.33	127.42	120.28
1	A	1148	MET	CA-C-N	5.33	127.68	120.44
1	A	1148	MET	C-N-CA	5.33	127.68	120.44
1	A	824	GLU	CA-C-N	5.29	127.37	120.28
1	A	824	GLU	C-N-CA	5.29	127.37	120.28
1	A	605	GLU	N-CA-C	-5.28	103.06	110.50
1	A	647	SER	N-CA-C	5.22	116.60	109.18
1	A	690	VAL	CA-C-N	5.12	128.50	120.82
1	A	690	VAL	C-N-CA	5.12	128.50	120.82
1	A	580	SER	N-CA-C	5.11	117.74	108.69
1	A	1051	GLY	CA-C-N	5.07	128.28	120.82
1	A	1051	GLY	C-N-CA	5.07	128.28	120.82
1	A	812	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	1165	LEU	CA-C-N	5.03	124.36	120.33
1	A	1165	LEU	C-N-CA	5.03	124.36	120.33

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	4344	0	4302	47	0
2	A	44	0	27	5	0
3	A	8	0	0	0	0
All	All	4396	0	4329	49	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 6.

All (49) 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:711:LYS:HD3	1:A:807:ILE:HG22	1.71	0.72
1:A:1164:ASN:O	1:A:1168:ILE:HD13	1.96	0.65
2:A:1201:2TT:O18	2:A:1201:2TT:H14	2.01	0.61
1:A:658:THR:HG23	1:A:760:PRO:HD2	1.83	0.61
1:A:1031:LEU:HA	1:A:1037:VAL:HG22	1.83	0.60
1:A:986:LEU:HD12	1:A:1029:VAL:HB	1.87	0.57
1:A:1147:LEU:HA	1:A:1150:ASN:HD22	1.70	0.57
1:A:708:MET:O	1:A:712:MET:HG2	2.06	0.56
1:A:641:LEU:HB3	1:A:684:ILE:HD13	1.88	0.54
1:A:764:LEU:C	1:A:766:ALA:H	2.15	0.54
1:A:597:GLN:N	2:A:1201:2TT:H1	2.24	0.53
1:A:836:PRO:HD3	1:A:845:THR:HG21	1.90	0.53
1:A:896:TYR:HB2	1:A:916:TYR:CE1	2.44	0.53
1:A:916:TYR:CE2	1:A:918:PRO:HG3	2.44	0.53
1:A:894:LYS:HA	1:A:897:LEU:HD12	1.92	0.52
1:A:997:LEU:HD11	1:A:1141:PRO:HG3	1.92	0.50
1:A:844:LEU:HD11	1:A:862:ILE:HG23	1.94	0.50
1:A:1005:GLN:HB3	1:A:1169:LEU:HB3	1.93	0.49
1:A:584:VAL:HG21	1:A:686:VAL:HG21	1.94	0.49
1:A:1031:LEU:HB2	1:A:1037:VAL:HG13	1.95	0.49
1:A:1054:TYR:HB3	1:A:1079:TYR:CE1	2.47	0.49
1:A:1172:VAL:O	1:A:1175:LYS:HB2	2.13	0.48
1:A:698:TRP:CE2	1:A:702:GLU:HG3	2.48	0.48
1:A:1056:ARG:NH1	1:A:1077:LYS:HE3	2.28	0.48
1:A:997:LEU:HD11	1:A:1141:PRO:CG	2.44	0.48
1:A:1084:VAL:HG11	1:A:1160:PRO:O	2.13	0.47
1:A:1002:LEU:O	1:A:1006:GLN:HG3	2.15	0.47
1:A:698:TRP:CZ2	1:A:702:GLU:HG3	2.50	0.47
1:A:764:LEU:HA	1:A:767:LEU:HD13	1.97	0.45
1:A:596:GLY:C	2:A:1201:2TT:H1	2.42	0.44
1:A:584:VAL:HB	1:A:677:CYS:HB2	1.99	0.44
1:A:769:ARG:O	1:A:773:VAL:HG23	2.18	0.44
1:A:1040:GLY:HA3	2:A:1202:2TT:CL1	2.55	0.44
1:A:1109:LEU:O	1:A:1112:ILE:HG13	2.17	0.44
1:A:664:GLN:HB3	1:A:983:LEU:HD21	2.00	0.44
1:A:987:ARG:HA	1:A:1098:CYS:SG	2.57	0.44
1:A:1025:ALA:O	1:A:1029:VAL:HG23	2.18	0.43
1:A:712:MET:HE1	1:A:841:LEU:HD13	2.01	0.43
1:A:780:ALA:HB3	1:A:783:CYS:SG	2.58	0.43
1:A:586:GLN:HE21	1:A:587:LYS:H	1.66	0.43
1:A:839:PRO:HD2	1:A:841:LEU:H	1.83	0.43
2:A:1201:2TT:H5	2:A:1201:2TT:H2	1.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:LEU:HD21	1:A:745:LEU:HD23	2.01	0.42
1:A:648:HIS:HD2	1:A:651:ILE:HG12	1.85	0.42
1:A:603:VAL:HG22	1:A:642:LYS:HG3	2.02	0.41
1:A:666:SER:HB2	1:A:982:PRO:HG3	2.02	0.41
1:A:858:SER:O	1:A:862:ILE:HG12	2.21	0.41
1:A:956:HIS:HE1	1:A:958:HIS:CD2	2.39	0.40
1:A:966:CYS:HB3	1:A:975:GLN:HB2	2.02	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	525/645 (81%)	484 (92%)	29 (6%)	12 (2%)	5	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	764	LEU
1	A	839	PRO
1	A	994	SER
1	A	1059	GLU
1	A	763	GLY
1	A	968	ASP
1	A	970	GLY
1	A	1120	THR
1	A	837	SER
1	A	908	PHE
1	A	920	ASN
1	A	972	LYS

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	475/563 (84%)	422 (89%)	53 (11%)	6 19

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	579	LEU
1	A	580	SER
1	A	586	GLN
1	A	587	LYS
1	A	591	GLN
1	A	593	SER
1	A	600	ARG
1	A	607	ARG
1	A	637	LEU
1	A	647	SER
1	A	648	HIS
1	A	651	ILE
1	A	661	LEU
1	A	682	GLU
1	A	684	ILE
1	A	686	VAL
1	A	749	GLU
1	A	764	LEU
1	A	770	GLU
1	A	797	LYS
1	A	816	GLN
1	A	833	LEU
1	A	837	SER
1	A	838	CYS
1	A	845	THR
1	A	861	THR
1	A	869	LEU
1	A	890	THR
1	A	894	LYS
1	A	898	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	925	GLU
1	A	950	ILE
1	A	972	LYS
1	A	995	ILE
1	A	999	GLN
1	A	1002	LEU
1	A	1009	GLU
1	A	1029	VAL
1	A	1030	LEU
1	A	1031	LEU
1	A	1032	ASP
1	A	1037	VAL
1	A	1052	HIS
1	A	1057	VAL
1	A	1086	SER
1	A	1090	THR
1	A	1109	LEU
1	A	1111	LEU
1	A	1119	MET
1	A	1124	LEU
1	A	1126	GLU
1	A	1136	ARG
1	A	1170	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	586	GLN
1	A	597	GLN
1	A	674	HIS
1	A	727	ASN
1	A	734	ASN
1	A	840	GLN
1	A	847	GLN
1	A	870	GLN
1	A	958	HIS
1	A	969	GLN
1	A	993	HIS
1	A	1006	GLN
1	A	1018	HIS
1	A	1150	ASN
1	A	1164	ASN

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	2TT	A	1202	-	24,24,24	0.66	0	32,33,33	1.42	5 (15%)
2	2TT	A	1201	-	24,24,24	0.87	0	32,33,33	1.71	12 (37%)

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	2TT	A	1202	-	-	4/16/18/18	0/3/3/3
2	2TT	A	1201	-	-	3/16/18/18	0/3/3/3

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1202	2TT	C13-N14-C15	4.10	123.06	117.21
2	A	1201	2TT	C13-N14-C15	3.25	121.86	117.21
2	A	1201	2TT	C22-C15-N14	-3.08	118.88	122.92
2	A	1202	2TT	C12-C13-N14	-3.01	120.28	123.97
2	A	1202	2TT	C22-C15-N14	-2.79	119.26	122.92
2	A	1202	2TT	C20-C19-C17	2.68	119.86	117.24
2	A	1201	2TT	N16-C15-N14	2.65	122.81	114.87
2	A	1201	2TT	C22-C11-N10	-2.49	112.03	120.13
2	A	1201	2TT	O18-C17-C19	-2.45	118.41	122.19
2	A	1201	2TT	C6-C7-C2	2.35	120.55	117.79
2	A	1202	2TT	C2-C7-C8	-2.32	118.81	122.56
2	A	1201	2TT	C12-C11-N10	2.29	128.11	120.41
2	A	1201	2TT	C5-C4-C3	2.17	122.91	120.24
2	A	1201	2TT	C7-C8-N10	-2.11	111.66	116.03
2	A	1201	2TT	C21-C19-C17	2.08	119.27	117.24
2	A	1201	2TT	C12-C13-N14	-2.08	121.43	123.97
2	A	1201	2TT	C3-C2-C7	-2.03	119.12	121.36

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1202	2TT	N16-C17-C19-C21
2	A	1202	2TT	O18-C17-C19-C20
2	A	1202	2TT	O18-C17-C19-C21
2	A	1201	2TT	C2-C7-C8-O9
2	A	1201	2TT	C2-C7-C8-N10
2	A	1201	2TT	C12-C11-N10-C8
2	A	1202	2TT	N16-C17-C19-C20

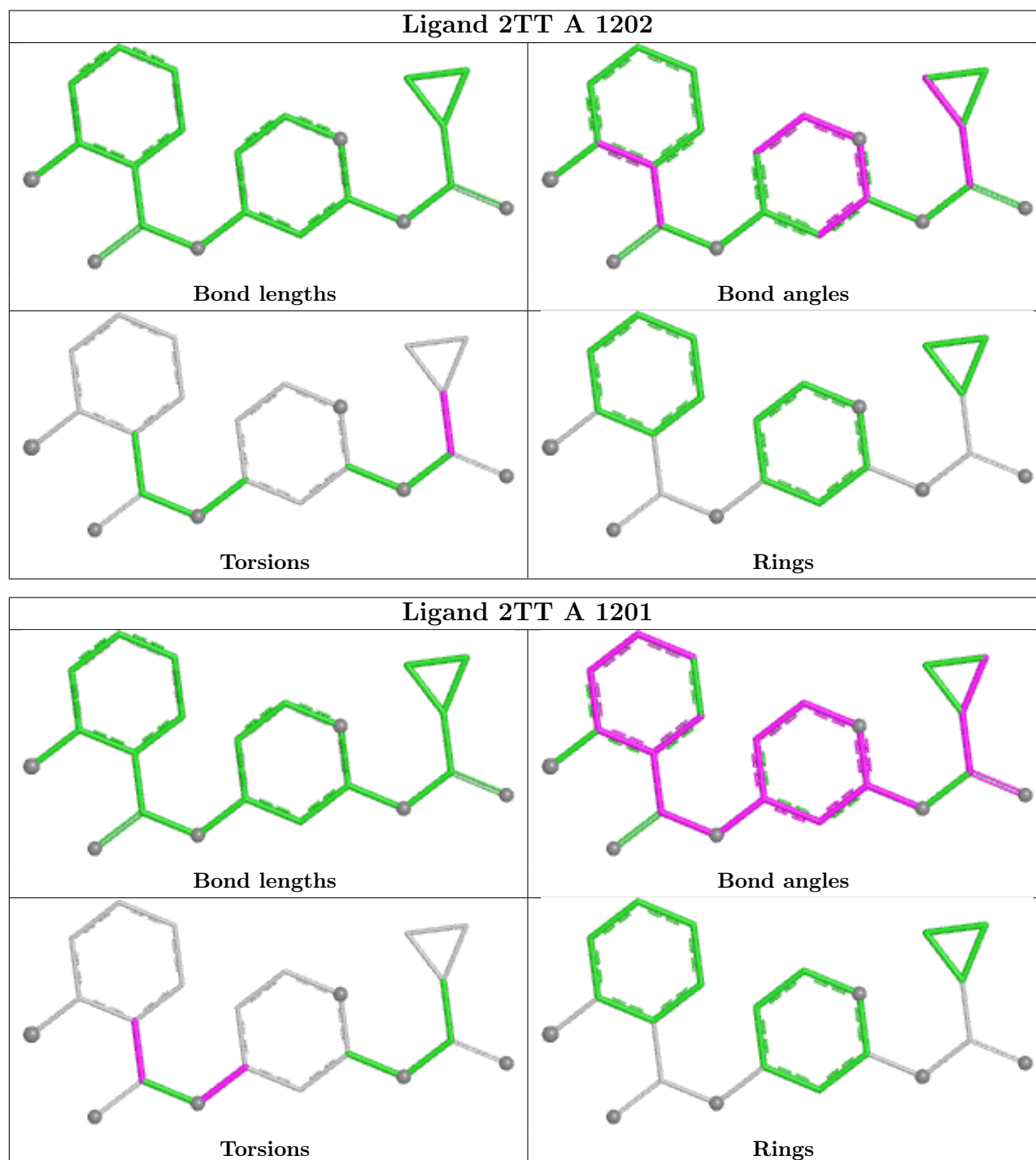
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1202	2TT	1	0
2	A	1201	2TT	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	539/645 (83%)	0.29	27 (5%) 34 26	37, 81, 127, 168	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	ARG	5.6
1	A	791	LEU	3.8
1	A	1037	VAL	3.4
1	A	932	LEU	3.2
1	A	871	PRO	3.2
1	A	890	THR	3.1
1	A	656	TYR	3.0
1	A	889	PRO	3.0
1	A	1011	MET	2.9
1	A	837	SER	2.9
1	A	1058	ARG	2.8
1	A	1066	PHE	2.7
1	A	1112	ILE	2.6
1	A	838	CYS	2.6
1	A	1176	TYR	2.5
1	A	1003	PHE	2.5
1	A	1119	MET	2.5
1	A	1113	GLY	2.5
1	A	1031	LEU	2.4
1	A	960	ILE	2.4
1	A	940	HIS	2.3
1	A	993	HIS	2.2
1	A	1120	THR	2.2
1	A	1001	LEU	2.2
1	A	1127	LEU	2.1
1	A	786	GLY	2.1
1	A	998	ALA	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](#)

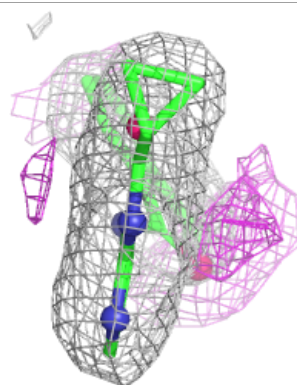
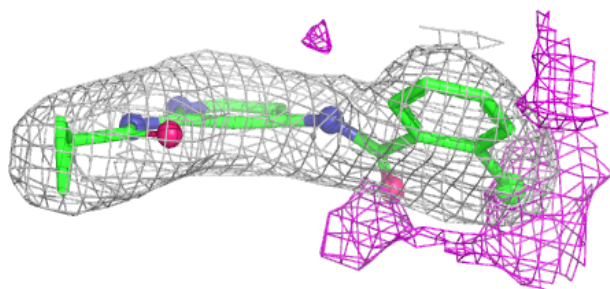
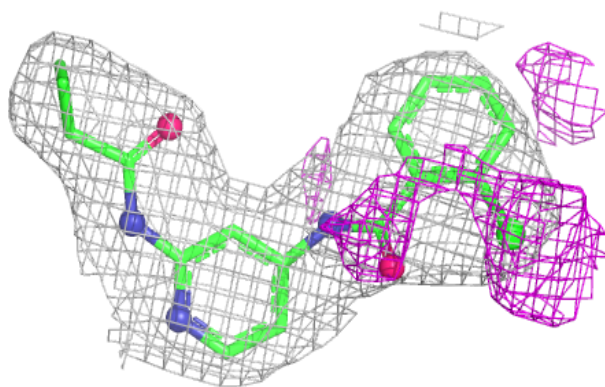
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	2TT	A	1201	22/22	0.94	0.09	32,42,60,67	0
2	2TT	A	1202	22/22	0.94	0.10	72,81,86,87	0

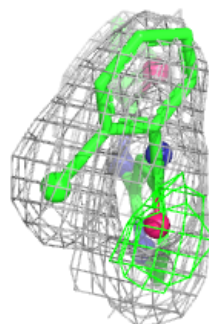
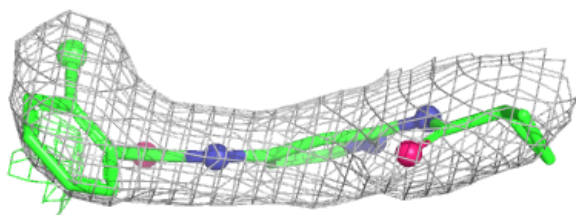
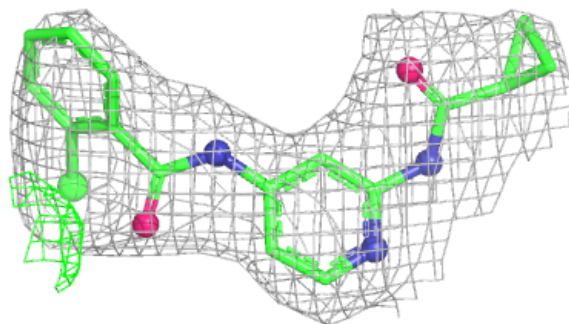
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2TT A 1201:

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

**Electron density around 2TT A 1202:**

$2mF_o-DF_c$ (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.