



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:23 PM UTC

PDB ID : 4FAD / pdb_00004fad
Title : Design and Synthesis of a Novel Pyrrolidinyl Pyrido Pyrimidinone Derivative as a Potent Inhibitor of PI3Ka and mTOR
Authors : Greasley, S.E.; Knighton, D.R.; LaFleur Rogers, C.M.
Deposited on : 2012-05-22
Resolution : 2.70 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

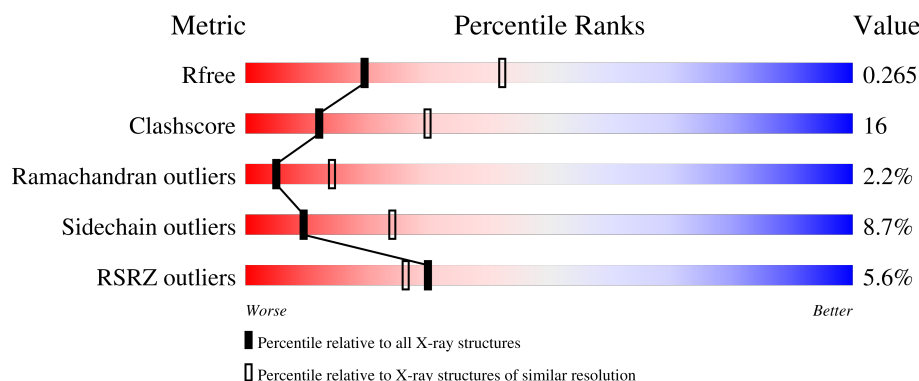
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	966	5% 54% 27% 5% 13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6813 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.

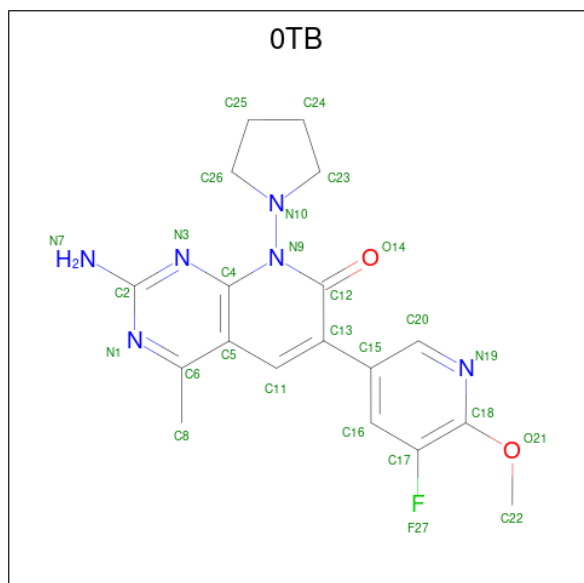
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6781	4363	1150	1233	35			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

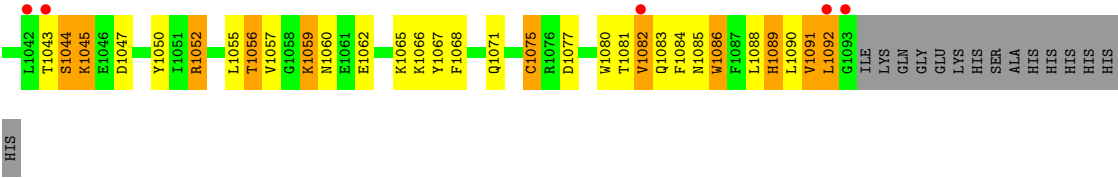
- Molecule 2 is 2-amino-6-(5-fluoro-6-methoxypyridin-3-yl)-4-methyl-8-(pyrrolidin-1-yl)pyrido [2,3-d]pyrimidin-7(8H)-one (CCD ID: 0TB) (formula: C₁₈H₁₉FN₆O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	18	1	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.55Å 67.26Å 107.60Å 90.00° 95.68° 90.00°	Depositor
Resolution (Å)	45.14 – 2.70 45.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.14-2.70) 99.6 (45.14-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.69Å)	Xtriage
Refinement program	CNS, BUSTER 2.11.1	Depositor
R, R_{free}	0.262 , 0.265 0.265 , 0.265	Depositor DCC
R_{free} test set	1453 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.5	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	0.92	EDS
Total number of atoms	6813	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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: 0TB

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	0.86	3/6925 (0.0%)	1.50	56/9368 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1039	MET	SD-CE	-7.50	1.60	1.79
1	A	1033	MET	SD-CE	-7.17	1.61	1.79
1	A	804	MET	SD-CE	-5.22	1.66	1.79

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	918	GLU	N-CA-C	-7.37	104.82	113.88
1	A	904	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	470	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	420	ILE	CA-C-N	6.37	130.80	120.60
1	A	420	ILE	C-N-CA	6.37	130.80	120.60
1	A	637	ASP	CA-C-N	6.24	128.96	120.54
1	A	637	ASP	C-N-CA	6.24	128.96	120.54
1	A	498	ASN	CA-C-N	5.85	128.92	120.38
1	A	498	ASN	C-N-CA	5.85	128.92	120.38
1	A	938	ALA	CA-C-N	5.72	127.88	120.44
1	A	938	ALA	C-N-CA	5.72	127.88	120.44
1	A	381	VAL	N-CA-C	5.70	116.08	108.27
1	A	948	HIS	N-CA-C	5.65	120.88	113.20
1	A	149	ALA	CA-C-N	5.64	128.41	120.28
1	A	149	ALA	C-N-CA	5.64	128.41	120.28
1	A	684	ARG	CA-C-N	5.59	126.15	120.00
1	A	684	ARG	C-N-CA	5.59	126.15	120.00
1	A	937	VAL	CA-C-N	5.56	128.05	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	937	VAL	C-N-CA	5.56	128.05	120.54
1	A	936	CYS	CA-C-N	5.48	127.41	120.72
1	A	936	CYS	C-N-CA	5.48	127.41	120.72
1	A	1012	ILE	CA-C-N	5.42	127.80	120.65
1	A	1012	ILE	C-N-CA	5.42	127.80	120.65
1	A	278	ASP	N-CA-C	-5.35	103.91	110.65
1	A	1056	THR	CB-CA-C	5.35	120.32	112.09
1	A	815	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	797	ALA	CA-C-N	5.29	127.42	120.60
1	A	797	ALA	C-N-CA	5.29	127.42	120.60
1	A	898	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	925	VAL	CA-C-N	5.27	127.61	120.65
1	A	925	VAL	C-N-CA	5.27	127.61	120.65
1	A	762	GLN	CA-C-N	5.24	127.64	120.46
1	A	762	GLN	C-N-CA	5.24	127.64	120.46
1	A	511	GLU	CA-C-N	5.20	128.62	120.82
1	A	511	GLU	C-N-CA	5.20	128.62	120.82
1	A	571	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	178	ARG	CA-C-N	5.17	125.72	119.98
1	A	178	ARG	C-N-CA	5.17	125.72	119.98
1	A	1086	TRP	CA-C-N	5.15	127.95	120.79
1	A	1086	TRP	C-N-CA	5.15	127.95	120.79
1	A	154	LEU	CA-C-N	5.15	127.44	120.38
1	A	154	LEU	C-N-CA	5.15	127.44	120.38
1	A	765	SER	CA-C-N	5.15	127.49	120.54
1	A	765	SER	C-N-CA	5.15	127.49	120.54
1	A	1044	SER	CA-C-N	5.15	131.38	121.54
1	A	1044	SER	C-N-CA	5.15	131.38	121.54
1	A	639	ASN	N-CA-C	5.12	116.67	111.14
1	A	798	ILE	CA-C-N	5.11	127.38	120.38
1	A	798	ILE	C-N-CA	5.11	127.38	120.38
1	A	839	ARG	CA-C-N	5.10	127.43	120.54
1	A	839	ARG	C-N-CA	5.10	127.43	120.54
1	A	1029	ILE	N-CA-CB	5.09	116.51	110.55
1	A	762	GLN	N-CA-C	-5.05	105.86	111.36
1	A	649	GLU	CB-CG-CD	5.03	121.16	112.60
1	A	840	GLN	CA-C-N	5.00	126.98	120.28
1	A	840	GLN	C-N-CA	5.00	126.98	120.28

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	6781	0	6820	213	0
2	A	27	0	19	0	0
3	A	5	0	0	0	0
All	All	6813	0	6839	213	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 16.

All (213) 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:1081:THR:O	1:A:1085:ASN:ND2	1.96	0.97
1:A:939:THR:HG22	1:A:945:GLY:HA2	1.50	0.92
1:A:149:ALA:HA	1:A:152:ARG:NH1	1.85	0.91
1:A:270:PHE:HB3	1:A:307:LEU:HD11	1.57	0.87
1:A:734:GLN:HE21	1:A:780:PRO:HB2	1.43	0.83
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	1.94	0.82
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.62	0.82
1:A:775:GLN:NE2	1:A:796:LEU:H	1.78	0.82
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.66	0.77
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.16	0.76
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.68	0.76
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.51	0.75
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.70	0.74
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.68	0.74
1:A:983:VAL:CG1	1:A:1082:VAL:HG11	2.17	0.73
1:A:807:LYS:HE3	1:A:807:LYS:H	1.53	0.73
1:A:918:GLU:O	1:A:921:PHE:HB3	1.90	0.71
1:A:1081:THR:C	1:A:1085:ASN:HD22	1.99	0.71
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.26	0.70
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.22	0.70
1:A:766:GLN:H	1:A:766:GLN:HE21	1.40	0.69
1:A:939:THR:HG22	1:A:945:GLY:CA	2.23	0.68
1:A:775:GLN:HE22	1:A:796:LEU:H	1.39	0.67
1:A:149:ALA:HA	1:A:152:ARG:HH11	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:VAL:HG12	1:A:1082:VAL:HG11	1.77	0.66
1:A:947:ARG:NH1	1:A:948:HIS:CE1	2.64	0.66
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.61	0.66
1:A:1089:HIS:ND1	1:A:1089:HIS:C	2.51	0.65
1:A:907:LEU:HD22	1:A:994:VAL:HG21	1.78	0.65
1:A:235:VAL:HG13	1:A:239:ASP:HB2	1.80	0.64
1:A:944:ILE:HB	1:A:968:ILE:HD12	1.78	0.64
1:A:947:ARG:HD3	1:A:968:ILE:HD13	1.80	0.64
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.79	0.64
1:A:472:ARG:HG3	1:A:472:ARG:HH11	1.62	0.64
1:A:359:ARG:O	1:A:420:ILE:HG12	1.99	0.63
1:A:843:LEU:HG	1:A:1034:MET:HG3	1.81	0.63
1:A:291:GLN:HE21	1:A:291:GLN:HA	1.63	0.63
1:A:497:PHE:O	1:A:1043:THR:HG21	1.99	0.63
1:A:1091:VAL:HG12	1:A:1091:VAL:O	1.99	0.62
1:A:949:ASN:HB2	1:A:1083:GLN:HE22	1.63	0.62
1:A:969:LEU:HD13	1:A:1039:MET:HE1	1.82	0.62
1:A:766:GLN:H	1:A:766:GLN:NE2	1.99	0.61
1:A:996:GLY:O	1:A:1003:SER:HB2	2.01	0.60
1:A:371:PRO:HG2	1:A:511:GLU:O	2.00	0.60
1:A:239:ASP:O	1:A:287:ILE:HG13	2.02	0.60
1:A:207:LEU:HD21	1:A:211:LEU:HB2	1.84	0.60
1:A:486:GLN:HG2	1:A:487:ILE:H	1.66	0.60
1:A:1081:THR:C	1:A:1085:ASN:ND2	2.59	0.60
1:A:847:ILE:HG22	1:A:851:MET:HE2	1.83	0.59
1:A:202:VAL:HG11	1:A:285:THR:HG21	1.85	0.59
1:A:387:ILE:HD12	1:A:418:ILE:HD13	1.84	0.59
1:A:270:PHE:HB3	1:A:307:LEU:CD1	2.32	0.59
1:A:916:PRO:HD2	1:A:920:LYS:HD2	1.85	0.59
1:A:184:ARG:HH11	1:A:719:ALA:HA	1.68	0.59
1:A:558:ILE:O	1:A:561:THR:HG22	2.03	0.59
1:A:955:THR:C	1:A:957:THR:H	2.11	0.58
1:A:271:VAL:HG21	1:A:282:VAL:HG13	1.86	0.58
1:A:1008:LYS:HG2	1:A:1012:ILE:HD11	1.84	0.58
1:A:241:PRO:HD3	1:A:285:THR:O	2.04	0.58
1:A:251:LYS:O	1:A:251:LYS:HD3	2.03	0.58
1:A:149:ALA:HA	1:A:152:ARG:HH12	1.65	0.58
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.85	0.58
1:A:764:ILE:O	1:A:768:LYS:HG2	2.04	0.57
1:A:568:THR:HG23	1:A:571:ASP:H	1.69	0.57
1:A:370:ILE:HD12	1:A:372:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:VAL:O	1:A:929:VAL:HG23	2.05	0.56
1:A:214:LYS:HD3	1:A:297:LEU:O	2.05	0.56
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.71	0.56
1:A:1091:VAL:O	1:A:1092:LEU:HG	2.06	0.56
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	1.87	0.56
1:A:734:GLN:O	1:A:738:VAL:HG23	2.06	0.56
1:A:921:PHE:O	1:A:925:VAL:HG23	2.06	0.56
1:A:170:ASP:OD1	1:A:172:GLU:HB2	2.06	0.55
1:A:739:ILE:O	1:A:743:GLN:HG3	2.06	0.55
1:A:640:VAL:O	1:A:643:ILE:HG12	2.06	0.55
1:A:733:THR:HG22	1:A:737:GLN:HE21	1.71	0.55
1:A:1009:PHE:HA	1:A:1012:ILE:HD12	1.88	0.55
1:A:273:ARG:HG3	1:A:274:VAL:N	2.21	0.54
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.37	0.54
1:A:801:CYS:HA	1:A:812:TRP:O	2.08	0.54
1:A:983:VAL:HG11	1:A:1082:VAL:HG11	1.89	0.54
1:A:998:SER:O	1:A:1000:LYS:N	2.41	0.54
1:A:896:VAL:HG21	1:A:899:THR:HB	1.91	0.53
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.44	0.53
1:A:1060:ASN:OD1	1:A:1062:GLU:HB2	2.08	0.53
1:A:418:ILE:HD12	1:A:418:ILE:H	1.72	0.53
1:A:948:HIS:HD2	1:A:1086:TRP:CZ3	2.27	0.53
1:A:246:GLN:O	1:A:250:THR:HB	2.08	0.53
1:A:734:GLN:NE2	1:A:780:PRO:HB2	2.20	0.53
1:A:767:LEU:HG	1:A:803:VAL:HG23	1.89	0.53
1:A:896:VAL:CG2	1:A:899:THR:HB	2.39	0.53
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.91	0.53
1:A:830:ILE:CG2	1:A:878:MET:HB2	2.39	0.53
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.90	0.52
1:A:905:GLU:HG3	1:A:993:PHE:CE2	2.44	0.52
1:A:184:ARG:NH1	1:A:719:ALA:HA	2.24	0.52
1:A:248:PHE:O	1:A:252:MET:HG3	2.10	0.52
1:A:615:GLU:O	1:A:619:GLN:HB2	2.09	0.52
1:A:625:GLY:O	1:A:629:GLN:HG3	2.10	0.52
1:A:1002:THR:HG22	1:A:1003:SER:H	1.75	0.52
1:A:653:ASP:OD2	1:A:688:ASN:ND2	2.42	0.52
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.90	0.51
1:A:689:LYS:HG2	1:A:728:MET:SD	2.49	0.51
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.92	0.51
1:A:887:THR:HG23	1:A:950:ASP:O	2.11	0.51
1:A:947:ARG:NH1	1:A:948:HIS:HE1	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:VAL:HG13	1:A:603:ILE:HG22	1.94	0.50
1:A:735:GLN:O	1:A:739:ILE:HG23	2.12	0.50
1:A:1056:THR:OG1	1:A:1059:LYS:HG3	2.12	0.49
1:A:472:ARG:HG3	1:A:472:ARG:NH1	2.27	0.49
1:A:272:LEU:HB3	1:A:305:VAL:CG1	2.42	0.49
1:A:887:THR:HG22	1:A:889:ALA:H	1.77	0.49
1:A:144:SER:HB3	1:A:147:SER:HB3	1.94	0.49
1:A:180:LEU:HD22	1:A:682:LEU:HD12	1.94	0.49
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.12	0.49
1:A:240:THR:HG23	1:A:243:ALA:HB3	1.94	0.48
1:A:354:LEU:HD22	1:A:529:LEU:HB2	1.94	0.48
1:A:274:VAL:HG23	1:A:279:GLU:O	2.14	0.48
1:A:746:THR:O	1:A:750:LYS:HB2	2.12	0.48
1:A:893:GLN:HA	1:A:896:VAL:O	2.14	0.48
1:A:287:ILE:N	1:A:287:ILE:HD12	2.29	0.48
1:A:320:LYS:HD2	1:A:320:LYS:H	1.79	0.47
1:A:1052:ARG:HG2	1:A:1052:ARG:HH11	1.79	0.47
1:A:389:HIS:O	1:A:392:GLN:HB3	2.15	0.47
1:A:365:ILE:HD12	1:A:383:VAL:HG11	1.96	0.47
1:A:706:SER:O	1:A:710:GLN:HB3	2.15	0.47
1:A:932:CYS:O	1:A:936:CYS:SG	2.70	0.47
1:A:987:LEU:HB3	1:A:1075:CYS:SG	2.54	0.47
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.97	0.47
1:A:767:LEU:O	1:A:771:LEU:HG	2.15	0.47
1:A:291:GLN:HA	1:A:291:GLN:NE2	2.30	0.46
1:A:969:LEU:HD13	1:A:1039:MET:CE	2.44	0.46
1:A:240:THR:HG23	1:A:243:ALA:CB	2.46	0.46
1:A:583:LEU:HD13	1:A:610:LEU:HD22	1.98	0.46
1:A:1017:TYR:OH	1:A:1056:THR:HG22	2.16	0.46
1:A:929:VAL:HG13	1:A:1009:PHE:HB2	1.98	0.46
1:A:236:SER:O	1:A:287:ILE:HD11	2.16	0.46
1:A:768:LYS:HE2	1:A:801:CYS:O	2.16	0.46
1:A:764:ILE:HG23	1:A:768:LYS:HE3	1.98	0.45
1:A:1024:THR:HA	1:A:1055:LEU:HD13	1.98	0.45
1:A:807:LYS:HE3	1:A:807:LYS:N	2.26	0.45
1:A:908:ASN:ND2	1:A:994:VAL:HA	2.30	0.45
1:A:271:VAL:CG2	1:A:282:VAL:HG13	2.46	0.45
1:A:568:THR:HG22	1:A:571:ASP:CG	2.41	0.45
1:A:690:ARG:NH1	1:A:789:PRO:HG2	2.31	0.45
1:A:799:GLU:H	1:A:799:GLU:HG3	1.61	0.45
1:A:811:LEU:HD23	1:A:813:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:HG13	1:A:170:ASP:H	1.81	0.45
1:A:947:ARG:NH2	1:A:964:ASP:O	2.50	0.45
1:A:364:LYS:HD2	1:A:413:TRP:CE2	2.52	0.45
1:A:198:MET:CB	1:A:282:VAL:HG21	2.48	0.44
1:A:732:PHE:O	1:A:736:VAL:HG23	2.18	0.44
1:A:203:THR:O	1:A:289:ASN:HB3	2.17	0.44
1:A:152:ARG:HH11	1:A:152:ARG:HB2	1.83	0.44
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.32	0.44
1:A:431:LEU:O	1:A:463:TYR:HA	2.18	0.43
1:A:1043:THR:C	1:A:1045:LYS:H	2.26	0.43
1:A:464:VAL:HB	1:A:484:MET:HG2	2.00	0.43
1:A:622:LEU:HD13	1:A:647:LYS:O	2.18	0.43
1:A:210:TYR:OH	1:A:856:GLU:HG3	2.18	0.43
1:A:896:VAL:HG13	1:A:900:GLY:H	1.82	0.43
1:A:944:ILE:HB	1:A:968:ILE:CD1	2.45	0.43
1:A:1029:ILE:O	1:A:1033:MET:HB2	2.17	0.43
1:A:547:MET:HE2	1:A:552:ARG:HA	2.00	0.43
1:A:278:ASP:OD2	1:A:792:LYS:NZ	2.52	0.43
1:A:601:GLN:HE21	1:A:601:GLN:HB2	1.45	0.43
1:A:598:TRP:CE3	1:A:604:VAL:HG22	2.54	0.43
1:A:486:GLN:HG2	1:A:487:ILE:N	2.31	0.43
1:A:847:ILE:HG21	1:A:942:LEU:HD21	2.00	0.43
1:A:874:ASP:O	1:A:876:ILE:HG22	2.19	0.43
1:A:935:TYR:O	1:A:939:THR:CB	2.67	0.43
1:A:246:GLN:HE21	1:A:246:GLN:HA	1.84	0.43
1:A:579:ARG:HB2	1:A:610:LEU:HD11	2.01	0.42
1:A:848:LEU:HD12	1:A:851:MET:CE	2.49	0.42
1:A:201:TRP:CE3	1:A:291:GLN:HB2	2.54	0.42
1:A:207:LEU:HD21	1:A:211:LEU:CB	2.50	0.42
1:A:424:PRO:HD2	1:A:427:ALA:HB2	2.02	0.42
1:A:945:GLY:O	1:A:986:VAL:HG23	2.20	0.42
1:A:1034:MET:HE3	1:A:1039:MET:SD	2.60	0.42
1:A:355:TRP:NE1	1:A:601:GLN:NE2	2.67	0.42
1:A:1029:ILE:HD11	1:A:1033:MET:HE3	2.00	0.42
1:A:745:VAL:O	1:A:749:ILE:HD13	2.20	0.42
1:A:207:LEU:HD23	1:A:208:PRO:O	2.20	0.42
1:A:466:LEU:HD11	1:A:476:ARG:HH11	1.84	0.42
1:A:562:ASP:OD2	1:A:1052:ARG:NH1	2.53	0.42
1:A:1080:TRP:O	1:A:1081:THR:C	2.62	0.42
1:A:1083:GLN:NE2	1:A:1083:GLN:HA	2.35	0.42
1:A:145:GLU:C	1:A:147:SER:H	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:HB2	1:A:517:SER:HB2	2.01	0.41
1:A:910:TRP:HE3	1:A:911:LEU:HD23	1.85	0.41
1:A:236:SER:O	1:A:238:ASP:N	2.53	0.41
1:A:701:SER:O	1:A:705:GLN:HG2	2.21	0.41
1:A:767:LEU:HD21	1:A:811:LEU:HG	2.01	0.41
1:A:147:SER:HB2	1:A:319:ARG:NH2	2.34	0.41
1:A:273:ARG:HG3	1:A:274:VAL:H	1.83	0.41
1:A:1043:THR:O	1:A:1047:ASP:HB2	2.20	0.41
1:A:546:GLU:HG3	1:A:547:MET:H	1.85	0.41
1:A:990:ASP:O	1:A:994:VAL:HG23	2.21	0.41
1:A:207:LEU:CD2	1:A:211:LEU:HB2	2.49	0.41
1:A:935:TYR:O	1:A:939:THR:HB	2.21	0.41
1:A:741:MET:O	1:A:745:VAL:HG23	2.21	0.41
1:A:434:TYR:HA	1:A:459:GLN:O	2.20	0.40
1:A:155:THR:HG23	1:A:161:ASP:HA	2.03	0.40
1:A:320:LYS:H	1:A:320:LYS:CD	2.34	0.40
1:A:768:LYS:O	1:A:772:GLU:HG2	2.21	0.40
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.56	0.40
1:A:1050:TYR:CD2	1:A:1050:TYR:C	2.98	0.40
1:A:152:ARG:NH1	1:A:152:ARG:HB2	2.36	0.40
1:A:430:ASN:OD1	1:A:432:GLN:NE2	2.52	0.40
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.46	0.40
1:A:184:ARG:HD3	1:A:719:ALA:O	2.21	0.40
1:A:1084:PHE:CZ	1:A:1088:LEU:HD21	2.56	0.40
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.03	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	819/966 (85%)	713 (87%)	88 (11%)	18 (2%)	5	14

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	521	ASP
1	A	548	PRO
1	A	984	PRO
1	A	999	GLY
1	A	1045	LYS
1	A	1092	LEU
1	A	237	PRO
1	A	282	VAL
1	A	896	VAL
1	A	902	PHE
1	A	968	ILE
1	A	1044	SER
1	A	904	ASP
1	A	956	GLU
1	A	752	LEU
1	A	283	GLY
1	A	1091	VAL
1	A	372	VAL

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	750/864 (87%)	685 (91%)	65 (9%)	9 24

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	152	ARG
1	A	165	VAL
1	A	168	VAL
1	A	195	LEU
1	A	214	LYS
1	A	223	VAL

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Mol	Chain	Res	Type
1	A	225	HIS
1	A	229	THR
1	A	235	VAL
1	A	240	THR
1	A	246	GLN
1	A	252	MET
1	A	282	VAL
1	A	287	ILE
1	A	298	LYS
1	A	320	LYS
1	A	354	LEU
1	A	359	ARG
1	A	366	ARG
1	A	370	ILE
1	A	409	LEU
1	A	418	ILE
1	A	458	VAL
1	A	472	ARG
1	A	518	ILE
1	A	544	ARG
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	626	LEU
1	A	646	GLN
1	A	682	LEU
1	A	717	LEU
1	A	729	LEU
1	A	739	ILE
1	A	766	GLN
1	A	767	LEU
1	A	778	GLN
1	A	799	GLU
1	A	807	LYS
1	A	808	LYS
1	A	823	LEU
1	A	832	PHE
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	886	THR

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Mol	Chain	Res	Type
1	A	896	VAL
1	A	898	ASN
1	A	904	ASP
1	A	907	LEU
1	A	948	HIS
1	A	1026	LEU
1	A	1039	MET
1	A	1052	ARG
1	A	1057	VAL
1	A	1059	LYS
1	A	1066	LYS
1	A	1075	CYS
1	A	1077	ASP
1	A	1082	VAL
1	A	1089	HIS
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	246	GLN
1	A	291	GLN
1	A	304	HIS
1	A	389	HIS
1	A	391	GLN
1	A	392	GLN
1	A	483	HIS
1	A	549	ASN
1	A	554	GLN
1	A	600	GLN
1	A	601	GLN
1	A	634	ASN
1	A	646	GLN
1	A	708	HIS
1	A	734	GLN
1	A	737	GLN
1	A	762	GLN
1	A	766	GLN
1	A	769	GLN
1	A	773	ASN
1	A	775	GLN

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Mol	Chain	Res	Type
1	A	834	HIS
1	A	840	GLN
1	A	893	GLN
1	A	908	ASN
1	A	948	HIS
1	A	959	ASN
1	A	1023	HIS
1	A	1083	GLN

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](#)

1 ligand is 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	0TB	A	1201	-	27,30,30	1.55	5 (18%)	34,44,44	2.52	6 (17%)

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	0TB	A	1201	-	-	2/6/17/17	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	0TB	C4-N9	4.35	1.43	1.39
2	A	1201	0TB	C2-N7	3.13	1.40	1.33
2	A	1201	0TB	C13-C12	2.80	1.50	1.46
2	A	1201	0TB	O21-C18	2.80	1.39	1.35
2	A	1201	0TB	C5-C4	-2.73	1.38	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	0TB	C22-O21-C18	-9.65	108.17	117.20
2	A	1201	0TB	O21-C18-C17	-6.30	111.74	117.17
2	A	1201	0TB	O14-C12-C13	-5.76	117.83	125.37
2	A	1201	0TB	O21-C18-N19	3.33	124.08	120.23
2	A	1201	0TB	N3-C4-N9	2.18	120.76	118.41
2	A	1201	0TB	C17-C18-N19	2.15	124.16	122.28

There are no chirality outliers.

All (2) torsion outliers are listed below:

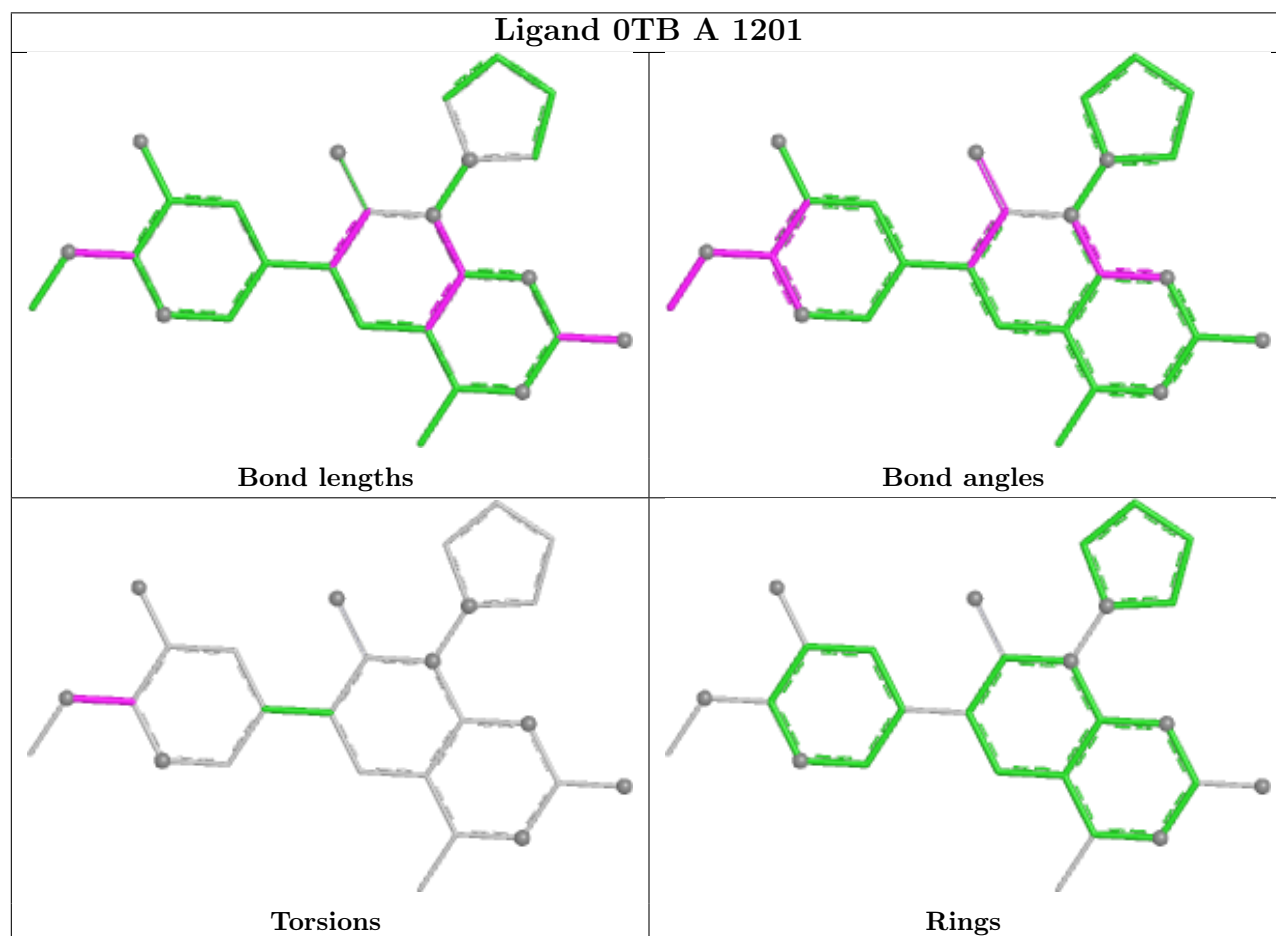
Mol	Chain	Res	Type	Atoms
2	A	1201	0TB	C17-C18-O21-C22
2	A	1201	0TB	N19-C18-O21-C22

There are no ring outliers.

No monomer is involved in short contacts.

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	839/966 (86%)	0.68	47 (5%) 30 26	41, 79, 118, 149	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	995	MET	4.3
1	A	899	THR	3.8
1	A	1042	LEU	3.4
1	A	1082	VAL	3.2
1	A	1092	LEU	3.1
1	A	898	ASN	3.1
1	A	272	LEU	3.0
1	A	779	LEU	2.9
1	A	529	LEU	2.8
1	A	224	ILE	2.8
1	A	823	LEU	2.8
1	A	202	VAL	2.8
1	A	911	LEU	2.6
1	A	895	THR	2.6
1	A	548	PRO	2.6
1	A	972	TYR	2.6
1	A	283	GLY	2.6
1	A	530	PRO	2.5
1	A	929	VAL	2.5
1	A	994	VAL	2.5
1	A	393	VAL	2.5
1	A	418	ILE	2.5
1	A	235	VAL	2.4
1	A	813	LEU	2.4
1	A	522	ASN	2.4
1	A	992	LEU	2.4
1	A	987	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	527	ILE	2.3
1	A	986	VAL	2.3
1	A	401	PRO	2.2
1	A	404	PHE	2.2
1	A	832	PHE	2.2
1	A	753	SER	2.2
1	A	767	LEU	2.2
1	A	968	ILE	2.2
1	A	288	LYS	2.2
1	A	311	PRO	2.1
1	A	318	VAL	2.1
1	A	760	SER	2.1
1	A	380	THR	2.1
1	A	774	LEU	2.1
1	A	1043	THR	2.1
1	A	435	CYS	2.1
1	A	1093	GLY	2.1
1	A	220	ILE	2.1
1	A	248	PHE	2.1
1	A	237	PRO	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.

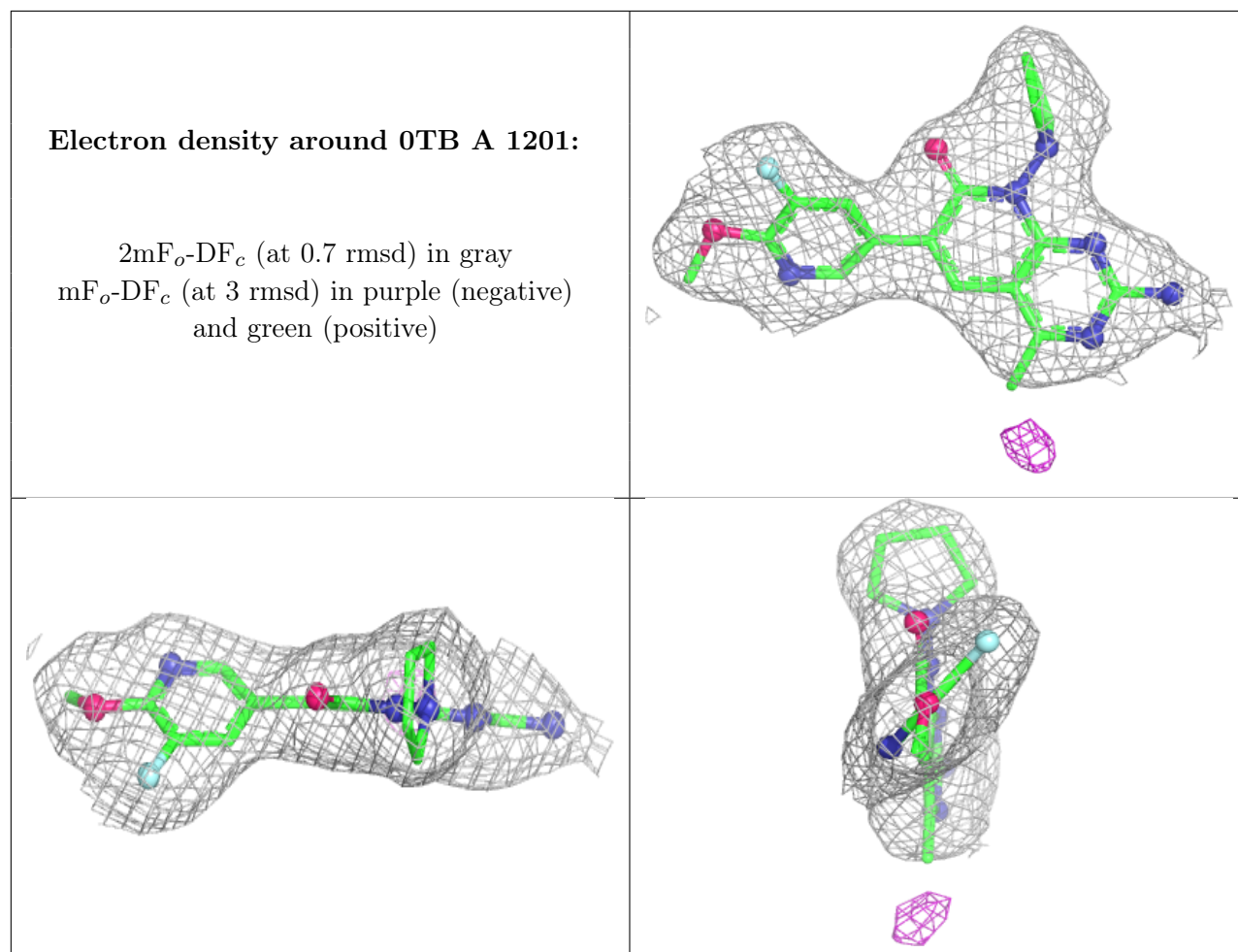
6.4 Ligands [i](#)

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	0TB	A	1201	27/27	0.94	0.08	52,54,55,55	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.