



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:19 am BST

PDB ID : 3PPZ  
Title : Crystal structure of CTR1 kinase domain in complex with staurosporine  
Authors : Mayerhofer, H.; Panneerselvam, S.; Mueller-Dieckmann, J.  
Deposited on : 2010-11-25  
Resolution : 2.99 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

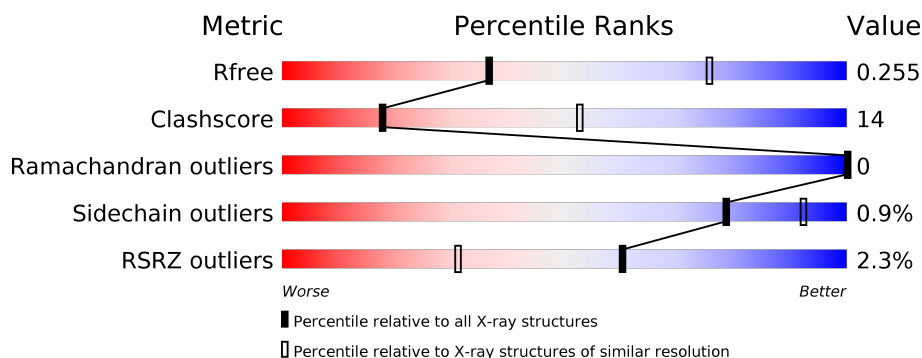
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	309	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>27%</div> <div>14%</div> </div> </div>
1	B	309	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>20%</div> <div>• 14%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4319 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 Serine/threonine-protein kinase CTR1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	P	S	0	0	0
			2132	1350	379	388	3	12			
1	B	267	Total	C	N	O	P	S	0	0	0
			2152	1362	383	392	3	12			

There are 54 discrepancies between the modelled and reference sequences:

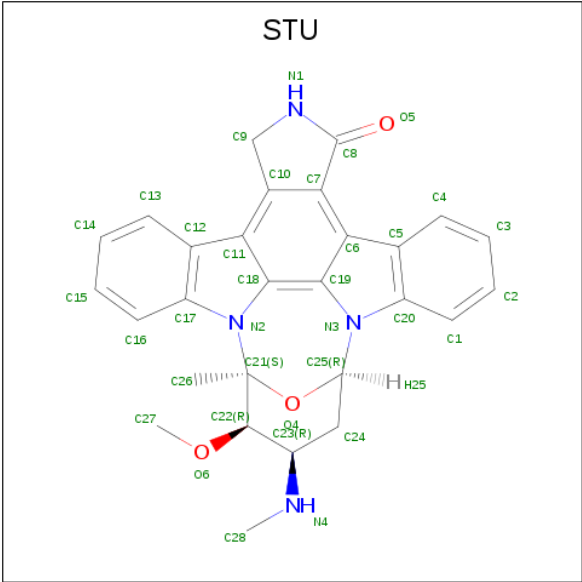
Chain	Residue	Modelled	Actual	Comment	Reference
A	513	MET	-	EXPRESSION TAG	UNP Q05609
A	514	LYS	-	EXPRESSION TAG	UNP Q05609
A	515	HIS	-	EXPRESSION TAG	UNP Q05609
A	516	HIS	-	EXPRESSION TAG	UNP Q05609
A	517	HIS	-	EXPRESSION TAG	UNP Q05609
A	518	HIS	-	EXPRESSION TAG	UNP Q05609
A	519	HIS	-	EXPRESSION TAG	UNP Q05609
A	520	HIS	-	EXPRESSION TAG	UNP Q05609
A	521	PRO	-	EXPRESSION TAG	UNP Q05609
A	522	MET	-	EXPRESSION TAG	UNP Q05609
A	523	SER	-	EXPRESSION TAG	UNP Q05609
A	524	ASP	-	EXPRESSION TAG	UNP Q05609
A	525	TYR	-	EXPRESSION TAG	UNP Q05609
A	526	ASP	-	EXPRESSION TAG	UNP Q05609
A	527	ILE	-	EXPRESSION TAG	UNP Q05609
A	528	PRO	-	EXPRESSION TAG	UNP Q05609
A	529	THR	-	EXPRESSION TAG	UNP Q05609
A	530	THR	-	EXPRESSION TAG	UNP Q05609
A	531	GLU	-	EXPRESSION TAG	UNP Q05609
A	532	ASN	-	EXPRESSION TAG	UNP Q05609
A	533	LEU	-	EXPRESSION TAG	UNP Q05609
A	534	TYR	-	EXPRESSION TAG	UNP Q05609
A	535	PHE	-	EXPRESSION TAG	UNP Q05609
A	536	GLN	-	EXPRESSION TAG	UNP Q05609
A	537	GLY	-	EXPRESSION TAG	UNP Q05609

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	538	ALA	-	EXPRESSION TAG	UNP Q05609
A	539	MET	-	EXPRESSION TAG	UNP Q05609
B	513	MET	-	EXPRESSION TAG	UNP Q05609
B	514	LYS	-	EXPRESSION TAG	UNP Q05609
B	515	HIS	-	EXPRESSION TAG	UNP Q05609
B	516	HIS	-	EXPRESSION TAG	UNP Q05609
B	517	HIS	-	EXPRESSION TAG	UNP Q05609
B	518	HIS	-	EXPRESSION TAG	UNP Q05609
B	519	HIS	-	EXPRESSION TAG	UNP Q05609
B	520	HIS	-	EXPRESSION TAG	UNP Q05609
B	521	PRO	-	EXPRESSION TAG	UNP Q05609
B	522	MET	-	EXPRESSION TAG	UNP Q05609
B	523	SER	-	EXPRESSION TAG	UNP Q05609
B	524	ASP	-	EXPRESSION TAG	UNP Q05609
B	525	TYR	-	EXPRESSION TAG	UNP Q05609
B	526	ASP	-	EXPRESSION TAG	UNP Q05609
B	527	ILE	-	EXPRESSION TAG	UNP Q05609
B	528	PRO	-	EXPRESSION TAG	UNP Q05609
B	529	THR	-	EXPRESSION TAG	UNP Q05609
B	530	THR	-	EXPRESSION TAG	UNP Q05609
B	531	GLU	-	EXPRESSION TAG	UNP Q05609
B	532	ASN	-	EXPRESSION TAG	UNP Q05609
B	533	LEU	-	EXPRESSION TAG	UNP Q05609
B	534	TYR	-	EXPRESSION TAG	UNP Q05609
B	535	PHE	-	EXPRESSION TAG	UNP Q05609
B	536	GLN	-	EXPRESSION TAG	UNP Q05609
B	537	GLY	-	EXPRESSION TAG	UNP Q05609
B	538	ALA	-	EXPRESSION TAG	UNP Q05609
B	539	MET	-	EXPRESSION TAG	UNP Q05609

- Molecule 2 is STAUROSPORINE (three-letter code: STU) (formula:  $C_{28}H_{26}N_4O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	4	3		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.27Å 95.27Å 179.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 2.99 46.05 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.20-2.99) 98.4 (46.05-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.201 , 0.256 0.212 , 0.255	Depositor DCC
$R_{free}$ test set	882 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TPO, STU, SEP

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	0.27	0/2147	0.40	0/2905
1	B	0.26	0/2168	0.40	0/2933
All	All	0.26	0/4315	0.40	0/5838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	2132	0	2134	66	0
1	B	2152	0	2155	50	0
2	A	35	0	26	6	0
All	All	4319	0	4315	117	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 14.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:LEU:HD13	1:B:728:SER:O	1.71	0.89
2:A:1:STU:H16	2:A:1:STU:H261	1.58	0.84
1:A:554:LYS:HB3	1:A:555:GLU:OE1	1.77	0.84
1:A:554:LYS:HB2	1:A:567:ARG:O	1.85	0.77
1:A:619:PRO:HD2	1:A:620:ASN:OD1	1.85	0.77
1:A:609:VAL:HG21	1:A:693:CYS:HB2	1.67	0.76
1:A:639:LYS:O	1:A:639:LYS:HG3	1.83	0.76
1:B:709:LYS:HD3	1:B:709:LYS:H	1.52	0.75
1:B:706:LEU:CD1	1:B:728:SER:O	2.34	0.75
1:A:708:SER:O	1:A:709:LYS:HB2	1.87	0.74
1:B:789:THR:HG21	1:B:794:LYS:HB2	1.69	0.74
1:B:579:ILE:HA	1:B:622:SER:HB3	1.70	0.73
1:B:556:LYS:HE3	1:B:564:THR:HG23	1.71	0.70
1:A:708:SER:O	1:A:709:LYS:CB	2.40	0.68
1:B:605:HIS:CD2	1:B:607:ASN:H	2.12	0.67
1:A:685:ASP:HB3	1:A:689:THR:H	1.60	0.65
1:A:693:CYS:SG	1:A:694:ASP:N	2.69	0.65
1:A:548:TRP:CG	1:A:620:ASN:ND2	2.65	0.65
1:A:548:TRP:CD2	1:A:620:ASN:ND2	2.65	0.65
1:B:706:LEU:HD12	1:B:706:LEU:N	2.12	0.64
1:A:606:PRO:O	1:A:691:LYS:HE3	1.99	0.63
1:A:628:LEU:HD12	1:A:683:LEU:HB2	1.80	0.62
2:A:1:STU:C16	2:A:1:STU:H261	2.29	0.62
1:A:605:HIS:CD2	1:A:607:ASN:H	2.18	0.61
1:A:714:THR:O	1:A:718:MET:HG3	2.01	0.60
1:A:633:LEU:HD21	1:A:744:LEU:HD21	1.83	0.60
1:A:604:ARG:HD3	1:B:611:PHE:O	2.01	0.60
1:A:602:ARG:HH21	1:B:543:ASP:HB2	1.67	0.60
1:A:611:PHE:O	1:B:604:ARG:HD2	2.03	0.59
1:A:679:SER:HB2	1:A:680:PRO:HD3	1.85	0.58
1:A:640:SER:OG	1:A:641:GLY:N	2.30	0.58
1:A:726:GLU:HB2	1:A:727:PRO:HD2	1.84	0.58
1:B:714:THR:O	1:B:718:MET:HG3	2.03	0.58
1:B:669:ASN:OD1	1:B:669:ASN:N	2.36	0.58
1:B:679:SER:HB2	1:B:680:PRO:HD3	1.84	0.58
1:B:704:TPO:HG22	1:B:704:TPO:O1P	2.05	0.57
1:A:592:GLU:HG3	1:A:595:ARG:NH2	2.20	0.57
1:B:685:ASP:HB3	1:B:689:THR:H	1.69	0.57
1:A:582:GLU:HG3	1:A:619:PRO:HB2	1.86	0.56
1:B:706:LEU:H	1:B:706:LEU:HD12	1.69	0.56
1:A:555:GLU:OE1	1:A:555:GLU:N	2.30	0.56
1:A:798:PHE:O	1:A:802:MET:HG3	2.06	0.56

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:GLU:O	1:A:600:MET:HG3	2.07	0.55
1:A:675:ARG:HH22	1:A:710:SEP:HB3	1.71	0.55
1:A:609:VAL:CG2	1:A:693:CYS:HB2	2.35	0.54
1:B:706:LEU:CD1	1:B:706:LEU:H	2.22	0.53
1:A:592:GLU:HG3	1:A:595:ARG:HH21	1.75	0.52
1:B:650:ARG:O	1:B:654:MET:HG3	2.09	0.52
1:B:666:HIS:CE1	1:B:730:GLU:HB2	2.45	0.51
1:A:635:ARG:O	1:A:639:LYS:HB3	2.10	0.51
1:A:579:ILE:H	1:A:579:ILE:HD12	1.76	0.51
1:A:701:LYS:HE3	1:A:730:GLU:OE1	2.11	0.51
1:A:806:ARG:N	1:A:807:PRO:HD2	2.25	0.50
1:B:584:ASP:HB3	1:B:589:ARG:HG2	1.92	0.50
1:A:605:HIS:CG	1:A:606:PRO:HD2	2.47	0.50
1:B:656:TYR:CE2	1:B:660:LYS:HD3	2.47	0.50
1:A:637:LEU:HD21	1:A:744:LEU:HD23	1.94	0.50
1:A:755:ASN:HB2	1:A:756:PRO:HD2	1.93	0.49
1:B:704:TPO:O3P	1:B:704:TPO:HG21	2.11	0.49
1:A:662:MET:HB3	1:A:798:PHE:CE2	2.47	0.49
2:A:1:STU:H283	2:A:1:STU:H272	1.95	0.48
1:B:706:LEU:CD1	1:B:706:LEU:N	2.76	0.48
1:A:656:TYR:CE2	1:A:660:LYS:HD3	2.49	0.47
1:B:682:LEU:HD11	1:B:740:ILE:HD13	1.96	0.47
1:A:665:LEU:O	1:A:668:ARG:HG2	2.14	0.46
1:B:670:PRO:HG2	1:B:700:LEU:HD23	1.97	0.46
1:A:595:ARG:HH22	1:A:699:ARG:NH2	2.14	0.46
1:B:646:LEU:HD22	1:B:650:ARG:HD2	1.98	0.46
1:A:790:ASN:O	1:A:792:PRO:HD3	2.17	0.45
1:A:579:ILE:HA	1:A:622:SER:HG	1.81	0.45
1:A:611:PHE:HA	1:A:625:THR:HG22	1.98	0.45
1:A:706:LEU:HD12	1:A:728:SER:OG	2.16	0.45
1:A:589:ARG:HA	1:A:592:GLU:HB3	1.98	0.45
1:B:662:MET:CE	1:B:677:LEU:HD13	2.47	0.45
1:B:654:MET:HB3	1:B:690:VAL:HG21	1.98	0.45
1:A:597:VAL:O	1:A:601:LYS:HG3	2.17	0.44
1:A:753:ASN:C	1:A:754:LEU:HD12	2.38	0.44
2:A:1:STU:C16	2:A:1:STU:C26	2.96	0.44
1:A:555:GLU:OE2	1:A:567:ARG:HD3	2.17	0.44
1:B:709:LYS:HD3	1:B:709:LYS:N	2.27	0.44
1:A:544:MET:CE	1:B:604:ARG:HG3	2.47	0.44
1:B:628:LEU:HD12	1:B:683:LEU:CB	2.48	0.44
1:B:628:LEU:HD12	1:B:683:LEU:HB3	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:ASN:HB2	1:B:756:PRO:HD2	2.00	0.43
1:B:806:ARG:HB3	1:B:807:PRO:HD3	1.99	0.43
1:B:668:ARG:HD2	1:B:668:ARG:HA	1.55	0.43
1:A:565:VAL:HG11	2:A:1:STU:H263	2.01	0.43
1:B:590:VAL:O	1:B:593:PHE:HB3	2.19	0.42
1:B:632:SER:OG	1:B:635:ARG:HG2	2.18	0.42
1:B:804:LEU:O	1:B:808:LEU:HD13	2.19	0.42
1:A:628:LEU:HB3	1:A:684:VAL:O	2.19	0.42
1:B:603:LEU:HD21	1:B:672:ILE:HD12	2.00	0.42
1:A:721:GLU:HG2	1:A:722:VAL:N	2.34	0.42
1:A:630:ARG:HB2	1:A:684:VAL:HB	2.02	0.42
1:B:715:PRO:HA	1:B:718:MET:HE3	2.01	0.42
1:A:669:ASN:HA	1:A:670:PRO:HA	1.84	0.41
1:A:595:ARG:NH2	1:A:699:ARG:NH2	2.67	0.41
1:B:621:LEU:HD12	1:B:621:LEU:H	1.85	0.41
1:A:546:ILE:HA	1:A:547:PRO:HD3	1.90	0.41
1:B:621:LEU:HD12	1:B:621:LEU:N	2.35	0.41
1:B:662:MET:HE1	1:B:692:VAL:HG11	2.02	0.41
1:B:674:HIS:HD2	1:B:676:ASP:H	1.66	0.41
1:A:618:PRO:CB	1:A:619:PRO:HA	2.51	0.41
1:A:675:ARG:NH2	1:A:710:SEP:HB3	2.35	0.41
1:A:678:LYS:HE2	1:A:681:ASN:ND2	2.35	0.41
1:A:662:MET:HB3	1:A:798:PHE:CD2	2.55	0.41
1:B:754:LEU:HD12	1:B:754:LEU:N	2.36	0.41
1:A:654:MET:O	1:A:658:VAL:HG23	2.21	0.41
1:B:683:LEU:HD13	1:B:693:CYS:SG	2.61	0.41
1:B:598:ALA:O	1:B:602:ARG:HG3	2.21	0.41
1:A:708:SER:OG	1:A:710:SEP:O3P	2.30	0.41
1:B:755:ASN:OD1	1:B:758:GLN:HG3	2.21	0.41
1:A:718:MET:HE3	1:A:718:MET:HB2	1.93	0.40
1:A:806:ARG:N	1:A:807:PRO:CD	2.84	0.40
2:A:1:STU:H283	2:A:1:STU:H22	1.81	0.40
1:A:565:VAL:HG23	1:A:577:VAL:O	2.20	0.40
1:B:605:HIS:HA	1:B:606:PRO:HD3	1.95	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	260/309 (84%)	248 (95%)	12 (5%)	0	100	100
1	B	260/309 (84%)	246 (95%)	14 (5%)	0	100	100
All	All	520/618 (84%)	494 (95%)	26 (5%)	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	227/268 (85%)	226 (100%)	1 (0%)	91	97
1	B	231/268 (86%)	228 (99%)	3 (1%)	69	89
All	All	458/536 (85%)	454 (99%)	4 (1%)	78	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	620	ASN
1	B	668	ARG
1	B	694	ASP
1	B	709	LYS

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

Mol	Chain	Res	Type
1	A	566	HIS
1	A	605	HIS
1	A	645	GLN
1	B	605	HIS
1	B	645	GLN
1	B	674	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	TPO	A	704	1	8,10,11	1.07	0	10,14,16	1.91	1 (10%)
1	TPO	B	704	1	8,10,11	1.13	0	10,14,16	1.45	2 (20%)
1	SEP	B	710	1	8,9,10	1.56	1 (12%)	8,12,14	1.65	2 (25%)
1	SEP	A	710	1	8,9,10	1.31	1 (12%)	8,12,14	1.69	2 (25%)
1	SEP	B	707	1	8,9,10	1.55	1 (12%)	8,12,14	1.53	2 (25%)
1	SEP	A	707	1	8,9,10	1.36	1 (12%)	8,12,14	2.95	3 (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
1	TPO	A	704	1	-	3/9/11/13	-
1	TPO	B	704	1	-	5/9/11/13	-
1	SEP	B	710	1	-	0/5/8/10	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	710	1	-	5/5/8/10	-
1	SEP	B	707	1	-	5/5/8/10	-
1	SEP	A	707	1	-	4/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	710	SEP	P-O1P	3.38	1.61	1.50
1	B	707	SEP	P-O1P	3.37	1.61	1.50
1	A	707	SEP	P-O1P	3.00	1.60	1.50
1	A	710	SEP	P-O1P	2.87	1.59	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	707	SEP	OG-CB-CA	6.24	114.22	108.14
1	A	704	TPO	P-OG1-CB	-5.47	106.68	123.21
1	A	707	SEP	P-OG-CB	-4.67	105.43	118.30
1	B	704	TPO	P-OG1-CB	-3.48	112.71	123.21
1	B	710	SEP	OG-CB-CA	3.21	111.27	108.14
1	A	710	SEP	P-OG-CB	-3.19	109.52	118.30
1	A	710	SEP	OG-CB-CA	2.94	111.00	108.14
1	B	710	SEP	P-OG-CB	-2.77	110.67	118.30
1	B	707	SEP	P-OG-CB	-2.72	110.80	118.30
1	B	707	SEP	OG-CB-CA	2.71	110.79	108.14
1	A	707	SEP	OG-P-O1P	2.23	112.73	106.47
1	B	704	TPO	CG2-CB-CA	-2.13	108.97	113.16

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	704	TPO	CB-OG1-P-O2P
1	B	704	TPO	N-CA-CB-CG2
1	B	704	TPO	N-CA-CB-OG1
1	B	704	TPO	C-CA-CB-CG2
1	B	704	TPO	O-C-CA-CB
1	B	704	TPO	CG2-CB-OG1-P
1	A	710	SEP	N-CA-CB-OG
1	A	710	SEP	CB-OG-P-O3P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	B	707	SEP	CB-OG-P-O2P
1	B	707	SEP	CB-OG-P-O3P
1	A	707	SEP	N-CA-CB-OG
1	A	707	SEP	CB-OG-P-O2P
1	A	707	SEP	CB-OG-P-O3P
1	B	707	SEP	CB-OG-P-O1P
1	A	707	SEP	CB-OG-P-O1P
1	A	710	SEP	CB-OG-P-O2P
1	B	707	SEP	CA-CB-OG-P
1	A	704	TPO	C-CA-CB-CG2
1	B	707	SEP	N-CA-CB-OG
1	A	710	SEP	CB-OG-P-O1P
1	A	710	SEP	CA-CB-OG-P
1	A	704	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	704	TPO	2	0
1	A	710	SEP	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	STU	A	1	-	30,42,42	1.04	2 (6%)	31,68,68	2.25	9 (29%)

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	STU	A	1	-	-	1/4/42/42	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	STU	O4-C25	-2.34	1.39	1.43
2	A	1	STU	C10-C11	-2.02	1.39	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	STU	C9-N1-C8	-6.00	108.08	113.85
2	A	1	STU	C27-O6-C22	-4.99	105.82	114.44
2	A	1	STU	C10-C9-N1	4.22	106.06	101.76
2	A	1	STU	C7-C8-N1	3.87	110.28	106.37
2	A	1	STU	O5-C8-C7	-3.65	124.99	129.32
2	A	1	STU	C26-C21-C22	-3.53	105.77	112.64
2	A	1	STU	C14-C13-C12	-2.35	116.92	120.86
2	A	1	STU	C3-C4-C5	-2.31	116.99	120.86
2	A	1	STU	C13-C12-C17	2.28	122.27	119.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	STU	C24-C23-N4-C28

There are no ring outliers.

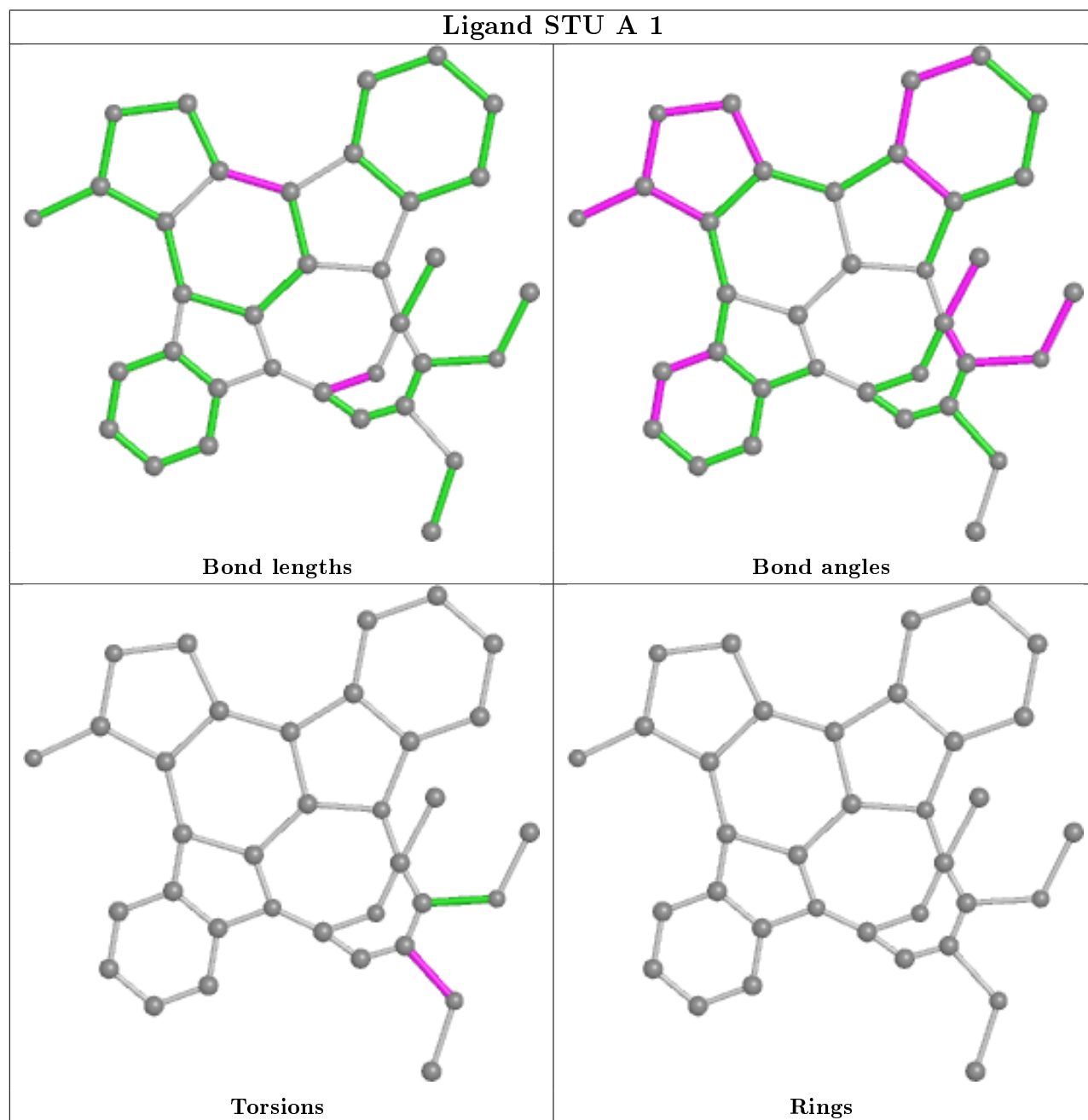
1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	STU	6	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/309 (85%)	0.07	7 (2%) 54 26	19, 51, 125, 215	0
1	B	264/309 (85%)	-0.04	5 (1%) 66 37	25, 52, 112, 168	0
All	All	528/618 (85%)	0.01	12 (2%) 60 31	19, 52, 120, 215	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	711	ALA	4.6
1	A	590	VAL	4.1
1	A	582	GLU	4.1
1	B	712	ALA	3.8
1	A	562	PHE	2.8
1	B	713	GLY	2.7
1	A	591	ASN	2.5
1	A	589	ARG	2.4
1	B	644	GLU	2.3
1	A	561	SER	2.2
1	B	693	CYS	2.2
1	B	775	ASN	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
1	SEP	B	707	10/11	0.71	0.32	156,161,164,164	0
1	SEP	A	710	10/11	0.78	0.22	125,127,139,140	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SEP	B	710	10/11	0.78	0.34	121,127,189,190	0
1	SEP	A	707	10/11	0.83	0.19	118,143,149,151	0
1	TPO	A	704	11/12	0.89	0.24	69,90,102,102	0
1	TPO	B	704	11/12	0.96	0.19	60,88,99,100	0

## 6.3 Carbohydrates [i](#)

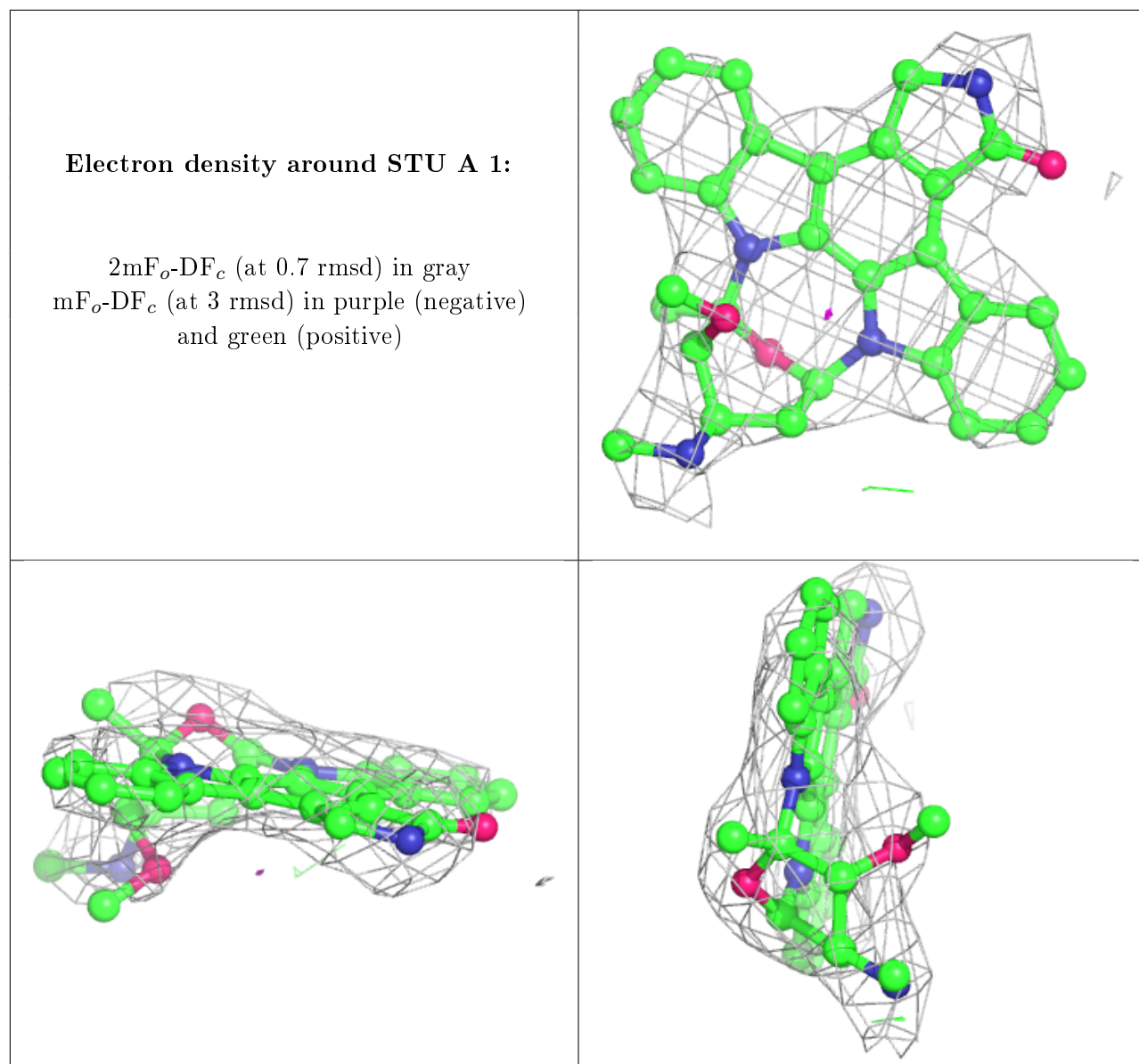
There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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	STU	A	1	35/35	0.93	0.29	73,73,73,73	35

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.