



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:13 PM GMT

PDB ID : 1SNU  
Title : CRYSTAL STRUCTURE OF THE UNPHOSPHORYLATED  
INTERLEUKIN-2 TYROSINE KINASE CATALYTIC DOMAIN  
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Deposited on : 2004-03-12  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

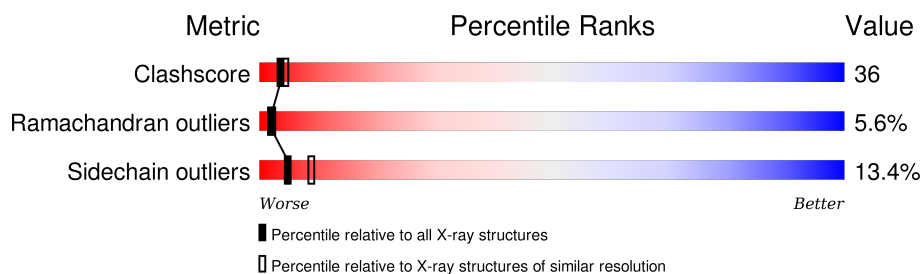
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	

## 2 Entry composition [i](#)

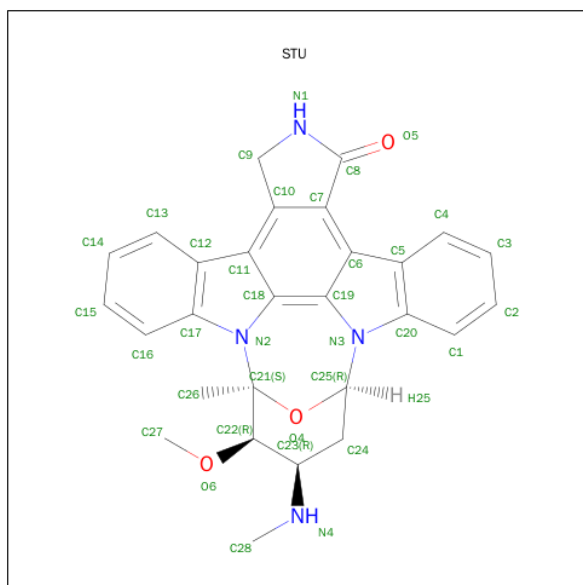
There are 3 unique types of molecules in this entry. The entry contains 4158 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	245	Total	C	N	O	S	0	0	0
			1956	1249	326	365	16			
1	B	241	Total	C	N	O	S	0	0	0
			1935	1237	322	360	16			

- 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		
2	B	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 3 is water.

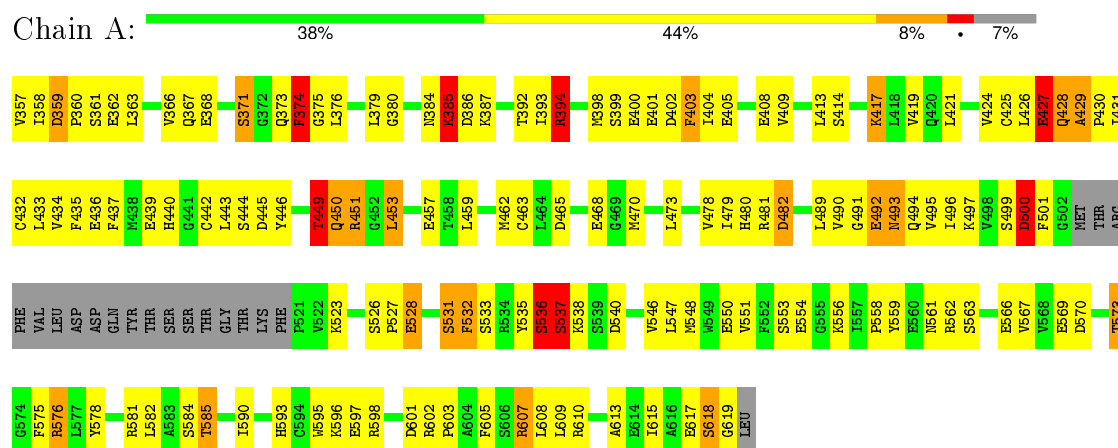
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total 116	O 116	0	0
3	B	81	Total 81	O 81	0	0

### 3 Residue-property plots

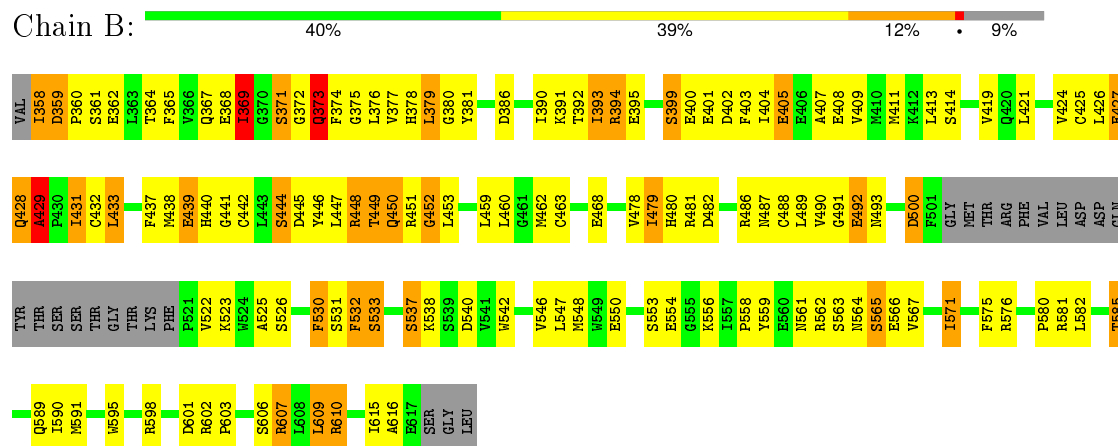
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: Tyrosine-protein kinase ITK/TSK



#### • Molecule 1: Tyrosine-protein kinase ITK/TSK



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.40 Å   74.20 Å   78.80 Å 90.00°   94.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	72.4 (20.00-2.50)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNX	Depositor
R, $R_{free}$	0.237 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.76	0/2000	0.77	1/2700 (0.0%)
1	B	0.75	0/1979	0.78	3/2672 (0.1%)
All	All	0.75	0/3979	0.77	4/5372 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	PHE	CB-CA-C	-6.14	98.11	110.40
1	B	369	ILE	N-CA-CB	-5.89	97.25	110.80
1	B	429	ALA	N-CA-C	-5.81	95.31	111.00
1	A	449	THR	N-CA-C	-5.66	95.71	111.00

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	1956	0	1913	146	1
1	B	1935	0	1893	131	0
2	A	35	0	26	3	0
2	B	35	0	26	9	0
3	A	116	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	81	0	0	10	0
All	All	4158	0	3858	281	1

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 36.

All (281) 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:607:ARG:HB2	1:A:607:ARG:HH11	1.14	1.07
1:B:360:PRO:HB2	3:B:75:HOH:O	1.61	0.98
1:A:609:LEU:HD23	3:A:34:HOH:O	1.66	0.94
1:B:393:ILE:HG22	1:B:394:ARG:N	1.86	0.90
1:B:393:ILE:HG22	1:B:394:ARG:H	1.36	0.88
1:A:607:ARG:HB2	1:A:607:ARG:NH1	1.90	0.87
1:B:393:ILE:HD11	1:B:403:PHE:CE1	2.11	0.85
1:A:536:SER:O	1:A:537:SER:HB2	1.76	0.85
1:A:428:GLN:HG3	3:A:100:HOH:O	1.77	0.84
1:B:419:VAL:HG21	1:B:489:LEU:HD12	1.61	0.83
1:A:375:GLY:HA3	1:A:392:THR:O	1.78	0.82
1:A:385:LYS:HA	1:A:385:LYS:HE2	1.61	0.81
1:B:460:LEU:HD21	1:B:615:ILE:O	1.81	0.81
1:A:401:GLU:HG3	1:A:402:ASP:N	1.99	0.78
1:A:451:ARG:NH2	1:A:556:LYS:HG3	2.03	0.74
1:B:459:LEU:HA	1:B:462:MET:HE3	1.70	0.73
1:B:575:PHE:O	1:B:576:ARG:HD3	1.89	0.73
1:A:500:ASP:HB3	3:A:10:HOH:O	1.90	0.72
1:A:426:LEU:C	1:A:428:GLN:H	1.93	0.72
1:A:526:SER:HB2	1:A:528:GLU:OE2	1.90	0.72
1:A:492:GLU:O	1:A:495:VAL:HG23	1.90	0.71
1:A:419:VAL:HG21	1:A:489:LEU:HD12	1.73	0.71
1:A:569:GLU:O	1:A:573:THR:HG23	1.91	0.70
1:B:403:PHE:CZ	1:B:433:LEU:HD13	2.27	0.69
1:A:430:PRO:HG3	3:A:125:HOH:O	1.92	0.69
1:A:399:SER:HB2	1:A:402:ASP:HB2	1.75	0.69
1:A:360:PRO:HG2	1:A:362:GLU:HG3	1.74	0.69
1:B:378:HIS:HD2	3:B:36:HOH:O	1.76	0.68
1:B:365:PHE:CZ	1:B:390:ILE:HG21	2.28	0.68
1:B:607:ARG:HH11	1:B:607:ARG:HB2	1.58	0.68
1:B:424:VAL:HG12	1:B:433:LEU:HD12	1.76	0.68
1:B:449:THR:O	1:B:450:GLN:HB2	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:VAL:HG23	1:A:380:GLY:HA2	1.76	0.68
1:B:375:GLY:HA3	1:B:392:THR:O	1.94	0.67
1:B:369:ILE:HG22	1:B:377:VAL:CG2	2.23	0.67
1:A:424:VAL:HG13	1:A:433:LEU:HD12	1.77	0.66
1:A:373:GLN:HG2	1:A:394:ARG:HG3	1.78	0.66
1:A:531:SER:HB2	1:A:532:PHE:CD1	2.30	0.65
1:A:492:GLU:H	1:A:492:GLU:CD	1.98	0.65
1:A:610:ARG:CZ	3:A:34:HOH:O	2.44	0.65
1:A:450:GLN:HG3	1:A:453:LEU:HD12	1.77	0.65
1:A:553:SER:HB2	1:A:556:LYS:HB2	1.80	0.64
1:B:492:GLU:O	1:B:493:ASN:OD1	2.15	0.64
1:B:491:GLY:O	1:B:493:ASN:N	2.31	0.63
1:B:393:ILE:HD11	1:B:403:PHE:CD1	2.33	0.63
1:B:459:LEU:HD23	1:B:462:MET:HE1	1.79	0.63
1:B:565:SER:O	3:B:67:HOH:O	2.16	0.62
1:B:407:ALA:O	1:B:411:MET:HG3	1.98	0.62
1:B:444:SER:HB2	1:B:486:ARG:HA	1.81	0.62
1:A:470:MET:CE	1:A:473:LEU:HD12	2.30	0.62
1:B:372:GLY:O	1:B:374:PHE:N	2.33	0.62
1:B:459:LEU:HD11	1:B:582:LEU:HD13	1.80	0.62
1:A:404:ILE:O	1:A:408:GLU:HG3	2.00	0.61
1:B:358:ILE:HG22	1:B:424:VAL:H	1.66	0.61
1:B:424:VAL:HG12	1:B:433:LEU:CD1	2.30	0.61
1:B:427:GLU:O	1:B:428:GLN:HB2	2.00	0.61
1:A:442:CYS:HA	1:A:489:LEU:HD23	1.82	0.61
1:A:470:MET:HE1	1:A:473:LEU:HD12	1.84	0.60
1:B:581:ARG:NH2	3:B:98:HOH:O	2.33	0.60
1:A:360:PRO:HG2	1:A:362:GLU:CG	2.31	0.60
1:B:598:ARG:HB2	1:B:601:ASP:OD2	2.01	0.60
1:A:615:ILE:HG23	1:A:619:GLY:O	2.02	0.60
1:A:531:SER:HB2	1:A:532:PHE:CE1	2.37	0.59
1:B:394:ARG:HG3	1:B:395:GLU:N	2.18	0.59
1:B:440:HIS:HB2	1:B:490:VAL:O	2.02	0.59
1:B:369:ILE:HD11	1:B:379:LEU:HG	1.85	0.59
1:B:547:LEU:C	1:B:547:LEU:HD23	2.23	0.59
1:A:442:CYS:SG	1:A:445:ASP:HB2	2.42	0.59
1:B:492:GLU:H	1:B:492:GLU:CD	2.07	0.59
1:B:364:THR:O	1:B:380:GLY:HA2	2.03	0.58
1:B:493:ASN:O	1:B:493:ASN:OD1	2.20	0.58
1:B:487:ASN:HA	2:B:621:STU:H272	1.86	0.58
1:A:532:PHE:N	1:A:532:PHE:CD1	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ALA:HB1	1:A:430:PRO:HD2	1.85	0.57
1:A:570:ASP:O	1:A:575:PHE:HB3	2.04	0.57
1:A:575:PHE:O	1:A:576:ARG:HD3	2.04	0.57
1:A:457:GLU:HG3	3:A:182:HOH:O	2.03	0.57
1:A:373:GLN:HG3	1:A:394:ARG:HD2	1.87	0.57
1:A:393:ILE:HG12	1:A:431:ILE:O	2.04	0.57
1:B:391:LYS:NZ	2:B:621:STU:H15	2.20	0.57
1:A:479:ILE:HD12	1:A:536:SER:O	2.05	0.57
1:A:424:VAL:HG13	1:A:433:LEU:CD1	2.35	0.57
1:A:413:LEU:HD11	1:A:478:VAL:HG21	1.86	0.56
2:A:301:STU:H4	2:A:301:STU:O5	2.05	0.56
1:A:425:CYS:HB2	1:A:432:CYS:SG	2.45	0.56
1:B:393:ILE:CG2	1:B:394:ARG:N	2.59	0.56
1:B:576:ARG:HG3	1:B:595:TRP:CE3	2.41	0.56
1:A:449:THR:O	1:A:450:GLN:CB	2.54	0.56
1:B:428:GLN:O	1:B:429:ALA:HB3	2.06	0.56
1:A:421:LEU:HD12	1:A:434:VAL:O	2.07	0.55
1:A:421:LEU:HD13	1:A:435:PHE:CD2	2.42	0.55
1:B:400:GLU:O	1:B:404:ILE:HG13	2.06	0.55
1:A:360:PRO:O	1:A:362:GLU:N	2.40	0.55
1:A:425:CYS:C	1:A:426:LEU:HD23	2.28	0.55
1:A:399:SER:HB2	1:A:402:ASP:H	1.72	0.54
1:A:491:GLY:O	1:A:493:ASN:N	2.39	0.54
1:A:547:LEU:C	1:A:547:LEU:HD23	2.27	0.54
1:A:500:ASP:OD2	2:A:301:STU:H273	2.08	0.54
1:A:556:LYS:NZ	3:A:153:HOH:O	2.40	0.54
1:B:563:SER:O	1:B:567:VAL:HG23	2.08	0.54
1:A:494:GLN:HE21	1:A:494:GLN:HA	1.72	0.53
1:A:421:LEU:HD11	1:A:433:LEU:HG	1.89	0.53
1:A:400:GLU:O	1:A:404:ILE:HG13	2.08	0.53
1:A:387:LYS:HE2	1:A:437:PHE:CE2	2.44	0.53
1:A:375:GLY:N	1:A:393:ILE:O	2.42	0.53
1:A:538:LYS:NZ	1:A:602:ARG:O	2.37	0.53
1:B:368:GLU:CD	1:B:376:LEU:HD22	2.28	0.53
1:B:525:ALA:O	1:B:530:PHE:HE2	1.92	0.53
1:B:447:LEU:HD22	1:B:554:GLU:HA	1.91	0.53
2:A:301:STU:H16	2:A:301:STU:H261	1.91	0.53
1:B:358:ILE:O	1:B:424:VAL:O	2.28	0.52
1:B:369:ILE:CD1	1:B:379:LEU:HB2	2.40	0.52
1:B:607:ARG:HB2	1:B:607:ARG:NH1	2.22	0.52
1:A:440:HIS:HB2	1:A:490:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ILE:HD12	1:A:398:MET:CE	2.39	0.52
1:A:443:LEU:HD13	1:A:496:ILE:HD12	1.91	0.52
1:B:590:ILE:CD1	1:B:615:ILE:HD12	2.39	0.52
1:A:367:GLN:NE2	3:A:126:HOH:O	2.41	0.52
1:B:392:THR:OG1	3:B:36:HOH:O	2.18	0.52
1:B:532:PHE:O	1:B:533:SER:C	2.47	0.51
1:B:500:ASP:OD2	2:B:621:STU:H273	2.10	0.51
1:A:585:THR:HG22	3:A:136:HOH:O	2.10	0.51
1:A:379:LEU:HD11	1:A:387:LYS:HE3	1.91	0.51
1:B:585:THR:O	1:B:589:GLN:HG3	2.09	0.51
1:B:360:PRO:HG2	1:B:362:GLU:CD	2.30	0.51
1:A:427:GLU:C	1:A:428:GLN:HG2	2.31	0.51
1:B:522:VAL:HB	1:B:564:ASN:OD1	2.11	0.51
1:B:562:ARG:NH1	1:B:575:PHE:CE2	2.78	0.51
1:A:399:SER:CB	1:A:402:ASP:HB2	2.41	0.51
1:A:463:CYS:SG	1:A:548:MET:HG2	2.51	0.50
1:B:580:PRO:HB2	3:B:11:HOH:O	2.10	0.50
1:A:363:LEU:HD11	1:A:425:CYS:SG	2.51	0.50
1:A:428:GLN:O	1:A:429:ALA:HB3	2.12	0.50
1:A:401:GLU:CG	1:A:402:ASP:N	2.73	0.50
1:B:525:ALA:O	1:B:530:PHE:CE2	2.65	0.50
1:B:375:GLY:HA2	1:B:393:ILE:O	2.11	0.50
1:A:492:GLU:O	1:A:495:VAL:CG2	2.59	0.50
1:B:369:ILE:HG22	1:B:377:VAL:HG23	1.91	0.50
1:A:359:ASP:HB3	1:A:425:CYS:SG	2.52	0.50
1:A:426:LEU:HD22	1:A:431:ILE:CG2	2.41	0.50
1:B:393:ILE:CG2	1:B:394:ARG:H	2.10	0.50
1:B:442:CYS:SG	2:B:621:STU:H282	2.52	0.50
1:A:523:LYS:HD3	1:A:558:PRO:O	2.12	0.50
1:A:617:GLU:O	1:A:618:SER:CB	2.60	0.49
1:B:360:PRO:HG2	1:B:362:GLU:CG	2.42	0.49
1:B:448:ARG:HH11	1:B:448:ARG:HB2	1.77	0.49
1:B:426:LEU:C	1:B:428:GLN:H	2.16	0.49
1:B:479:ILE:CD1	1:B:479:ILE:N	2.75	0.49
1:A:593:HIS:ND1	1:A:596:LYS:HE2	2.28	0.49
1:A:493:ASN:O	1:A:493:ASN:OD1	2.29	0.49
1:A:426:LEU:HD23	1:A:426:LEU:N	2.26	0.49
1:A:393:ILE:HD12	1:A:398:MET:HE3	1.95	0.49
2:B:621:STU:O5	2:B:621:STU:H4	2.13	0.49
1:A:449:THR:O	1:A:450:GLN:HB2	2.13	0.49
1:B:451:ARG:O	1:B:453:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:PHE:CE2	1:B:433:LEU:HD13	2.48	0.48
1:A:436:GLU:HG3	1:A:436:GLU:O	2.13	0.48
1:B:425:CYS:HB2	1:B:432:CYS:SG	2.53	0.48
1:A:576:ARG:NH2	1:A:595:TRP:O	2.43	0.48
1:B:606:SER:HB2	1:B:610:ARG:HH12	1.78	0.48
1:B:403:PHE:HZ	1:B:433:LEU:HD13	1.78	0.48
1:A:417:LYS:O	1:A:497:LYS:HA	2.14	0.48
1:A:403:PHE:HZ	1:A:426:LEU:HD21	1.78	0.48
1:B:404:ILE:O	1:B:408:GLU:HB2	2.14	0.48
1:B:391:LYS:HZ1	2:B:621:STU:H15	1.78	0.47
1:B:523:LYS:HD3	1:B:558:PRO:O	2.14	0.47
1:A:426:LEU:C	1:A:428:GLN:N	2.65	0.47
1:B:575:PHE:O	1:B:576:ARG:CD	2.61	0.47
1:A:499:SER:O	1:A:501:PHE:N	2.47	0.47
1:B:373:GLN:O	1:B:374:PHE:CD1	2.67	0.47
1:A:494:GLN:NE2	1:A:494:GLN:HA	2.28	0.47
1:B:563:SER:HB3	1:B:566:GLU:HB2	1.96	0.47
1:B:610:ARG:HD3	3:B:3:HOH:O	2.14	0.47
1:A:493:ASN:O	1:A:493:ASN:CG	2.52	0.47
1:A:605:PHE:HA	1:A:608:LEU:HB2	1.96	0.47
1:A:384:ASN:O	1:A:386:ASP:N	2.47	0.47
1:B:369:ILE:HD12	1:B:379:LEU:HB2	1.95	0.47
1:A:417:LYS:HE2	1:A:465:ASP:OD1	2.14	0.47
1:B:381:TYR:HA	1:B:386:ASP:O	2.14	0.47
1:B:444:SER:O	1:B:448:ARG:HD3	2.15	0.47
1:B:427:GLU:O	1:B:428:GLN:CB	2.63	0.46
1:A:607:ARG:NH1	3:A:193:HOH:O	2.48	0.46
1:B:486:ARG:HG3	2:B:621:STU:H281	1.97	0.46
1:A:443:LEU:HD13	1:A:496:ILE:CD1	2.46	0.46
1:B:405:GLU:O	1:B:409:VAL:HG23	2.15	0.46
1:B:532:PHE:N	1:B:532:PHE:CD1	2.84	0.46
1:B:603:PRO:HB3	1:B:607:ARG:HG2	1.98	0.46
1:B:445:ASP:O	1:B:449:THR:HG23	2.16	0.46
1:B:480:HIS:O	1:B:540:ASP:OD1	2.34	0.46
1:B:546:VAL:O	1:B:550:GLU:HG3	2.16	0.46
1:A:535:TYR:N	1:A:535:TYR:CD1	2.83	0.46
1:A:581:ARG:CG	3:A:7:HOH:O	2.64	0.46
1:B:575:PHE:C	1:B:576:ARG:HD3	2.36	0.46
1:A:371:SER:HB3	1:A:376:LEU:HD22	1.97	0.46
1:B:392:THR:HG22	1:B:432:CYS:HB3	1.98	0.45
1:A:499:SER:OG	1:A:500:ASP:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:PRO:HB2	3:A:64:HOH:O	2.14	0.45
1:A:481:ARG:O	1:A:482:ASP:HB2	2.16	0.45
1:A:494:GLN:O	1:A:496:ILE:HG12	2.16	0.45
1:A:610:ARG:NH1	3:A:34:HOH:O	2.50	0.45
1:A:459:LEU:HA	1:A:462:MET:HE3	1.98	0.45
1:A:373:GLN:O	1:A:374:PHE:HB2	2.15	0.45
1:B:463:CYS:SG	1:B:548:MET:HG2	2.56	0.45
1:A:526:SER:CB	1:A:528:GLU:OE2	2.61	0.45
1:A:446:TYR:O	1:A:449:THR:O	2.35	0.45
1:A:602:ARG:HA	1:A:603:PRO:HD3	1.81	0.45
1:A:563:SER:O	1:A:566:GLU:HB3	2.16	0.45
1:B:591:MET:HE2	1:B:595:TRP:CH2	2.52	0.45
1:A:426:LEU:O	1:A:428:GLN:N	2.49	0.45
1:A:431:ILE:HG13	1:A:431:ILE:H	1.58	0.45
1:B:428:GLN:O	1:B:429:ALA:CB	2.65	0.45
1:A:417:LYS:NZ	1:A:468:GLU:OE1	2.50	0.44
1:A:451:ARG:HG3	1:A:554:GLU:HB3	1.99	0.44
1:B:537:SER:O	1:B:540:ASP:HB2	2.17	0.44
1:B:449:THR:O	1:B:450:GLN:CB	2.59	0.44
1:A:387:LYS:HE2	1:A:437:PHE:CD2	2.52	0.44
1:A:494:GLN:HE21	1:A:494:GLN:CA	2.30	0.44
1:B:369:ILE:HG22	1:B:377:VAL:HG21	1.99	0.44
1:A:421:LEU:HD13	1:A:435:PHE:CE2	2.53	0.44
1:B:479:ILE:HD13	1:B:479:ILE:N	2.33	0.44
1:B:615:ILE:HD11	3:B:62:HOH:O	2.17	0.44
1:A:607:ARG:CB	1:A:607:ARG:NH1	2.71	0.44
1:A:385:LYS:CA	1:A:385:LYS:HE2	2.41	0.44
1:A:576:ARG:HG3	1:A:595:TRP:CE3	2.53	0.43
1:A:398:MET:SD	1:A:403:PHE:HB2	2.58	0.43
1:B:360:PRO:O	1:B:362:GLU:N	2.52	0.43
1:B:561:ASN:HA	3:B:68:HOH:O	2.19	0.43
1:B:360:PRO:HG2	1:B:362:GLU:HG3	2.00	0.43
1:A:429:ALA:O	1:A:430:PRO:C	2.55	0.43
1:A:582:LEU:HA	1:A:582:LEU:HD23	1.86	0.43
1:B:562:ARG:HG2	3:B:137:HOH:O	2.18	0.43
1:A:563:SER:O	1:A:567:VAL:N	2.47	0.43
1:B:486:ARG:NH1	1:B:486:ARG:HB2	2.34	0.43
1:B:451:ARG:NH2	1:B:556:LYS:HG3	2.34	0.43
1:A:590:ILE:HD12	1:A:615:ILE:HD12	2.02	0.42
1:B:446:TYR:CD2	1:B:490:VAL:HG21	2.55	0.42
1:B:364:THR:O	1:B:380:GLY:CA	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ASN:C	1:A:495:VAL:H	2.23	0.42
1:B:559:TYR:OH	1:B:571:ILE:HD11	2.19	0.42
1:A:598:ARG:HB2	1:A:601:ASP:OD2	2.19	0.42
1:A:375:GLY:CA	1:A:393:ILE:O	2.67	0.42
1:B:413:LEU:HD11	1:B:478:VAL:HG21	2.02	0.42
1:A:492:GLU:O	1:A:493:ASN:OD1	2.37	0.42
1:A:480:HIS:O	1:A:540:ASP:OD1	2.38	0.42
1:B:377:VAL:HA	1:B:390:ILE:O	2.19	0.42
1:B:426:LEU:C	1:B:428:GLN:N	2.73	0.42
1:A:546:VAL:O	1:A:550:GLU:HG3	2.20	0.42
1:A:581:ARG:HG3	3:A:7:HOH:O	2.19	0.42
1:B:526:SER:HB3	1:B:542:TRP:CB	2.50	0.42
1:A:578:TYR:CD1	1:A:578:TYR:C	2.92	0.42
1:B:486:ARG:HH11	1:B:486:ARG:HB2	1.83	0.42
1:A:403:PHE:HZ	1:A:426:LEU:CD2	2.33	0.41
1:A:613:ALA:O	1:A:617:GLU:HG3	2.20	0.41
1:B:399:SER:OG	1:B:402:ASP:HB2	2.20	0.41
1:A:357:VAL:N	3:A:2:HOH:O	2.53	0.41
1:A:413:LEU:HD13	1:A:473:LEU:CD2	2.50	0.41
1:B:538:LYS:NZ	1:B:602:ARG:O	2.46	0.41
1:A:358:ILE:H	1:A:358:ILE:HG12	1.59	0.41
1:A:499:SER:C	1:A:501:PHE:N	2.73	0.41
1:B:441:GLY:HA2	2:B:621:STU:C3	2.50	0.41
1:B:421:LEU:HD11	1:B:433:LEU:HG	2.00	0.41
1:A:428:GLN:HB3	1:A:428:GLN:HE21	1.68	0.41
1:B:468:GLU:HG3	1:B:609:LEU:HD11	2.01	0.41
1:B:442:CYS:HA	1:B:488:CYS:O	2.21	0.41
1:B:438:MET:O	1:B:440:HIS:N	2.51	0.41
1:B:371:SER:HB3	1:B:376:LEU:HD23	2.01	0.41
1:B:553:SER:OG	1:B:556:LYS:HB2	2.21	0.41
1:B:439:GLU:O	1:B:439:GLU:HG3	2.21	0.41
1:A:584:SER:N	3:A:149:HOH:O	2.44	0.41
1:A:403:PHE:CZ	1:A:426:LEU:HD21	2.56	0.41
2:B:621:STU:H16	2:B:621:STU:H261	2.02	0.41
1:B:429:ALA:O	1:B:431:ILE:N	2.54	0.41
1:B:452:GLY:N	1:B:554:GLU:OE2	2.53	0.41
1:B:367:GLN:O	1:B:378:HIS:HA	2.20	0.41
1:B:369:ILE:HD12	1:B:379:LEU:N	2.36	0.41
1:B:437:PHE:CE2	1:B:439:GLU:HA	2.56	0.41
1:A:459:LEU:HB3	1:A:551:VAL:HG12	2.02	0.40
1:A:561:ASN:O	1:A:562:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:GLU:O	1:A:409:VAL:HG12	2.20	0.40
1:A:532:PHE:O	1:A:533:SER:C	2.60	0.40
1:B:426:LEU:HD22	1:B:431:ILE:HD13	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:GLU:OE2	1:A:408:GLU:OE2[2_555]	1.95	0.25

## 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	241/264 (91%)	204 (85%)	24 (10%)	13 (5%)	2	2
1	B	237/264 (90%)	201 (85%)	22 (9%)	14 (6%)	2	2
All	All	478/528 (90%)	405 (85%)	46 (10%)	27 (6%)	2	2

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PHE
1	A	394	ARG
1	A	482	ASP
1	A	492	GLU
1	A	500	ASP
1	A	618	SER
1	B	373	GLN
1	B	393	ILE
1	B	429	ALA
1	B	439	GLU

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Mol	Chain	Res	Type
1	B	492	GLU
1	A	361	SER
1	A	537	SER
1	B	428	GLN
1	B	452	GLY
1	B	616	ALA
1	A	385	LYS
1	A	439	GLU
1	A	536	SER
1	B	361	SER
1	B	482	ASP
1	B	394	ARG
1	B	481	ARG
1	A	427	GLU
1	A	429	ALA
1	B	359	ASP
1	B	533	SER

### 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	214/232 (92%)	185 (86%)	29 (14%)	5	8
1	B	212/232 (91%)	184 (87%)	28 (13%)	5	9
All	All	426/464 (92%)	369 (87%)	57 (13%)	5	9

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	359	ASP
1	A	368	GLU
1	A	371	SER
1	A	374	PHE
1	A	385	LYS
1	A	394	ARG

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Mol	Chain	Res	Type
1	A	403	PHE
1	A	414	SER
1	A	417	LYS
1	A	427	GLU
1	A	428	GLN
1	A	444	SER
1	A	449	THR
1	A	450	GLN
1	A	451	ARG
1	A	453	LEU
1	A	493	ASN
1	A	500	ASP
1	A	528	GLU
1	A	531	SER
1	A	532	PHE
1	A	536	SER
1	A	537	SER
1	A	559	TYR
1	A	573	THR
1	A	576	ARG
1	A	585	THR
1	A	597	GLU
1	A	607	ARG
1	B	358	ILE
1	B	359	ASP
1	B	369	ILE
1	B	371	SER
1	B	373	GLN
1	B	379	LEU
1	B	399	SER
1	B	401	GLU
1	B	405	GLU
1	B	414	SER
1	B	427	GLU
1	B	431	ILE
1	B	433	LEU
1	B	444	SER
1	B	448	ARG
1	B	449	THR
1	B	450	GLN
1	B	479	ILE
1	B	500	ASP

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Mol	Chain	Res	Type
1	B	531	SER
1	B	532	PHE
1	B	537	SER
1	B	565	SER
1	B	571	ILE
1	B	585	THR
1	B	607	ARG
1	B	609	LEU
1	B	610	ARG

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

Mol	Chain	Res	Type
1	A	367	GLN
1	A	373	GLN
1	A	428	GLN
1	A	487	ASN
1	A	494	GLN
1	A	589	GLN
1	A	611	GLN
1	B	367	GLN
1	B	373	GLN
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 carbohydrates 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	STU	A	301	-	27,42,42	2.98	18 (66%)	23,68,68	2.32	8 (34%)
2	STU	B	621	-	27,42,42	2.15	12 (44%)	23,68,68	2.12	9 (39%)

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	301	-	-	0/4/42/42	0/0/8/8
2	STU	B	621	-	-	0/4/42/42	0/0/8/8

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	STU	C7-C6	-2.55	1.39	1.43
2	A	301	STU	C7-C8	-2.08	1.41	1.49
2	B	621	STU	C24-C25	2.04	1.54	1.51
2	B	621	STU	C14-C15	2.20	1.43	1.38
2	B	621	STU	C13-C12	2.22	1.45	1.41
2	B	621	STU	C5-C20	2.31	1.45	1.41
2	A	301	STU	C24-C23	2.45	1.57	1.53
2	B	621	STU	C2-C1	2.47	1.42	1.36
2	A	301	STU	C4-C5	2.63	1.46	1.41
2	A	301	STU	C3-C4	2.67	1.42	1.36
2	A	301	STU	C14-C15	2.67	1.44	1.38
2	A	301	STU	C3-C2	2.72	1.45	1.38
2	A	301	STU	C10-C11	2.74	1.47	1.42
2	B	621	STU	C3-C2	2.88	1.45	1.38
2	B	621	STU	C11-C18	2.90	1.46	1.42
2	A	301	STU	C26-C21	3.00	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	STU	C14-C13	3.17	1.43	1.36
2	B	621	STU	C14-C13	3.18	1.44	1.36
2	A	301	STU	O6-C22	3.19	1.48	1.42
2	B	621	STU	C19-C18	3.30	1.49	1.41
2	A	301	STU	C2-C1	3.40	1.44	1.36
2	B	621	STU	C15-C16	3.44	1.44	1.36
2	A	301	STU	C11-C18	3.60	1.47	1.42
2	B	621	STU	C10-C11	3.65	1.48	1.42
2	A	301	STU	C15-C16	3.73	1.45	1.36
2	A	301	STU	C5-C20	3.90	1.47	1.41
2	B	621	STU	C3-C4	4.13	1.46	1.36
2	A	301	STU	C19-C18	4.78	1.53	1.41
2	A	301	STU	C24-C25	5.58	1.60	1.51
2	A	301	STU	C22-C23	6.44	1.59	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	621	STU	C6-C19-C18	-3.49	116.51	121.69
2	A	301	STU	C6-C19-C18	-3.46	116.55	121.69
2	B	621	STU	O5-C8-C7	-2.64	124.20	128.62
2	A	301	STU	O5-C8-C7	-2.60	124.28	128.62
2	B	621	STU	C15-C14-C13	-2.49	116.83	120.45
2	B	621	STU	O4-C21-C26	-2.27	96.23	106.42
2	A	301	STU	C1-C20-N3	-2.25	129.48	132.18
2	B	621	STU	C1-C20-N3	-2.21	129.52	132.18
2	B	621	STU	C16-C17-C12	-2.07	117.75	120.73
2	A	301	STU	C3-C4-C5	-2.03	117.28	120.79
2	A	301	STU	C13-C12-C17	2.67	122.77	119.39
2	B	621	STU	C13-C12-C17	3.00	123.19	119.39
2	B	621	STU	C11-C12-C17	3.44	110.13	106.37
2	A	301	STU	C6-C5-C20	4.29	111.06	106.37
2	A	301	STU	C11-C12-C17	4.99	111.82	106.37
2	A	301	STU	C27-O6-C22	5.33	124.59	114.39
2	B	621	STU	C6-C5-C20	5.43	112.31	106.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	STU	3	0
2	B	621	STU	9	0

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.