



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 10:35 AM GMT

PDB ID : 1SM2
Title : Crystal structure of the phosphorylated Interleukin-2 tyrosine kinase catalytic domain
Authors : Brown, K.; Long, J.M.; Vial, S.C.M.; Dedi, N.; Dunster, N.J.; Renwick, S.B.; Tanner, A.J.; Frantz, J.D.; Fleming, M.A.; Cheetham, G.M.T.
Deposited on : 2004-03-08
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

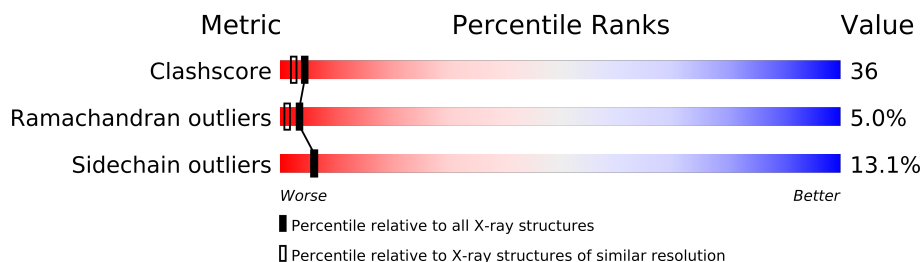
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

2 Entry composition i

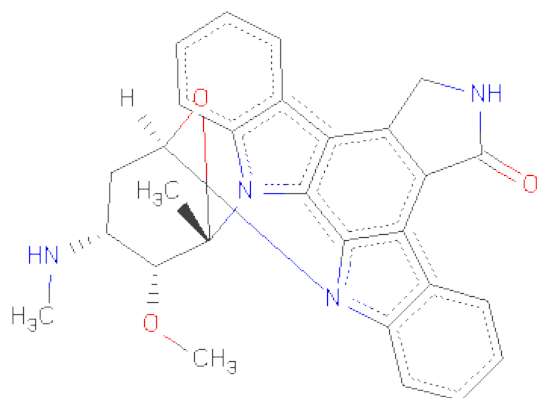
There are 3 unique types of molecules in this entry. The entry contains 4212 atoms, of which 0 are hydrogen and 0 are deuterium.

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	144	Total 144	O 144	0	0
3	B	107	Total 107	O 107	0	0

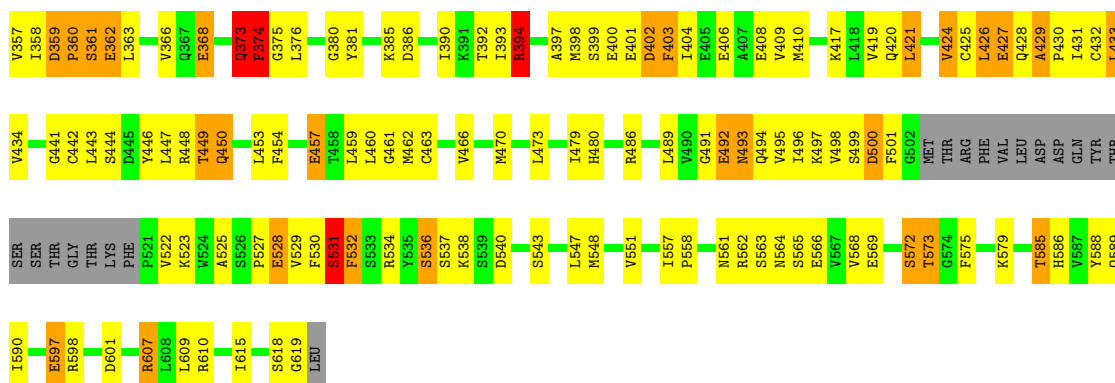
3 Residue-property plots

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.

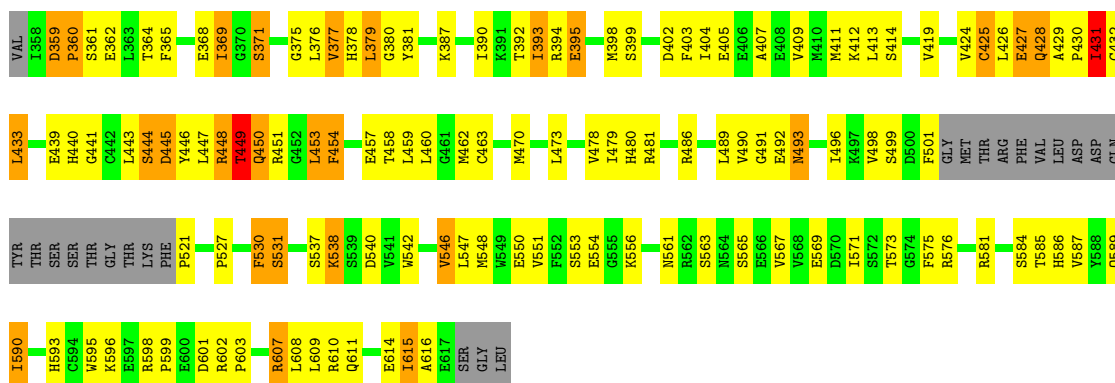
- Molecule 1: Tyrosine-protein kinase ITK/TSK

Chain A:



- Molecule 1: Tyrosine-protein kinase ITK/TSK

Chain B:



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, α , β , γ	125.10Å 74.40Å 78.90Å 90.00° 93.90° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	70.0 (20.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.214 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4212	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.77	3/2000 (0.1%)	0.72	2/2700 (0.1%)
1	B	0.75	2/1979 (0.1%)	0.74	1/2672 (0.0%)
All	All	0.76	5/3979 (0.1%)	0.73	3/5372 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	SER	CA-CB	-8.00	1.41	1.52
1	B	361	SER	CA-CB	-5.75	1.44	1.52
1	A	457	GLU	CA-CB	5.68	1.66	1.53
1	B	546	VAL	CA-CB	5.28	1.65	1.54
1	A	442	CYS	CB-SG	-5.23	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	PHE	N-CA-C	-6.09	94.56	111.00
1	B	530	PHE	CB-CA-C	-5.99	98.42	110.40
1	A	449	THR	N-CA-C	-5.36	96.52	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1956	0	1913	139	0
1	B	1935	0	1893	137	0
2	A	35	0	26	3	0
2	B	35	0	26	3	0
3	A	144	0	0	29	0
3	B	107	0	0	23	0
All	All	4212	0	3858	279	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (279) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:607:ARG:HB2	1:A:607:ARG:HH11	1.11	1.13
1:A:607:ARG:HB2	1:A:607:ARG:NH1	1.73	1.02
1:B:470:MET:HE3	1:B:498:VAL:HG21	1.42	1.01
1:B:593:HIS:HB2	3:B:10:HOH:O	1.67	0.94
1:B:590:ILE:O	3:B:10:HOH:O	1.94	0.86
1:B:486:ARG:HG3	2:B:621:STU:H281	1.59	0.83
1:B:449:THR:C	1:B:451:ARG:H	1.82	0.82
1:B:457:GLU:HG3	3:B:15:HOH:O	1.79	0.82
1:B:399:SER:HB2	1:B:402:ASP:HB2	1.60	0.81
1:B:393:ILE:HG23	1:B:394:ARG:N	1.95	0.81
1:B:403:PHE:CZ	1:B:433:LEU:HD13	2.15	0.81
1:B:561:ASN:HA	3:B:90:HOH:O	1.81	0.80
1:B:615:ILE:C	3:B:68:HOH:O	2.21	0.80
1:A:585:THR:O	1:A:589:GLN:HG3	1.83	0.78
1:B:407:ALA:O	1:B:411:MET:HG3	1.85	0.77
1:B:377:VAL:HA	1:B:390:ILE:O	1.86	0.76
1:B:445:ASP:O	1:B:449:THR:HG23	1.86	0.76
1:B:449:THR:O	1:B:451:ARG:N	2.19	0.76
1:B:470:MET:HE1	1:B:498:VAL:HG11	1.66	0.76
1:B:615:ILE:O	1:B:615:ILE:HG22	1.86	0.76
1:A:360:PRO:HG2	1:A:362:GLU:HG3	1.68	0.76
1:A:462:MET:HG2	1:A:496:ILE:HG13	1.69	0.74
1:B:369:ILE:HD13	1:B:379:LEU:HB2	1.69	0.74
1:A:536:SER:HB3	3:A:17:HOH:O	1.88	0.74
1:A:360:PRO:HA	1:A:427:GLU:HG3	1.68	0.73
1:B:427:GLU:O	1:B:429:ALA:N	2.22	0.73
1:B:424:VAL:HG12	1:B:433:LEU:HD12	1.71	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:369:ILE:HG22	1:B:377:VAL:CG2	2.19	0.72
1:A:424:VAL:HG13	1:A:433:LEU:CD1	2.17	0.72
1:B:459:LEU:HA	1:B:462:MET:HE3	1.72	0.71
1:A:375:GLY:HA3	1:A:392:THR:O	1.91	0.71
1:A:597:GLU:HG2	3:A:149:HOH:O	1.91	0.71
1:A:563:SER:HB3	1:A:566:GLU:HB2	1.74	0.70
1:A:424:VAL:HG13	1:A:433:LEU:HD12	1.72	0.70
1:A:361:SER:C	1:A:363:LEU:H	1.96	0.69
1:A:569:GLU:O	1:A:573:THR:HG23	1.92	0.69
1:A:406:GLU:HG3	3:A:173:HOH:O	1.93	0.69
1:B:586:HIS:HB3	1:B:615:ILE:HD13	1.75	0.69
1:B:413:LEU:HD11	1:B:478:VAL:HG21	1.75	0.69
1:A:615:ILE:O	1:A:619:GLY:N	2.25	0.69
1:B:419:VAL:HG21	1:B:489:LEU:HD12	1.73	0.69
1:A:598:ARG:HB2	1:A:601:ASP:OD2	1.93	0.68
1:B:593:HIS:HB3	3:B:27:HOH:O	1.91	0.68
1:A:362:GLU:HA	3:A:1:HOH:O	1.93	0.67
1:B:486:ARG:HH11	1:B:486:ARG:HB2	1.58	0.67
1:B:399:SER:HB2	1:B:402:ASP:CB	2.25	0.67
1:B:440:HIS:NE2	3:B:44:HOH:O	2.29	0.66
1:B:584:SER:OG	1:B:587:VAL:HG23	1.95	0.66
1:B:360:PRO:HD2	1:B:362:GLU:CD	2.17	0.66
1:B:607:ARG:HH11	1:B:607:ARG:HB2	1.61	0.65
1:A:460:LEU:HB3	3:A:2:HOH:O	1.95	0.65
1:B:459:LEU:HD23	1:B:462:MET:HE1	1.77	0.64
1:B:378:HIS:HD2	3:B:48:HOH:O	1.79	0.64
1:A:361:SER:O	3:A:1:HOH:O	2.14	0.64
1:B:491:GLY:C	1:B:493:ASN:H	2.00	0.64
1:B:585:THR:HG23	3:B:191:HOH:O	1.96	0.64
1:A:447:LEU:HD13	1:A:551:VAL:HA	1.80	0.64
1:B:538:LYS:HE2	1:B:602:ARG:O	1.98	0.64
1:A:421:LEU:HD12	1:A:434:VAL:O	1.97	0.64
1:B:590:ILE:HG13	1:B:615:ILE:HD12	1.79	0.63
1:A:500:ASP:HB3	3:A:13:HOH:O	1.98	0.63
1:A:609:LEU:HD23	1:A:610:ARG:NH1	2.14	0.62
1:A:480:HIS:CD2	1:A:501:PHE:HB3	2.34	0.62
1:B:581:ARG:NH2	3:B:131:HOH:O	2.32	0.62
1:A:459:LEU:HD23	1:A:462:MET:HE3	1.81	0.62
1:B:393:ILE:HG23	1:B:394:ARG:H	1.61	0.62
1:B:440:HIS:HB2	1:B:490:VAL:O	2.00	0.62
1:A:569:GLU:HB2	3:A:5:HOH:O	1.99	0.62
1:A:373:GLN:HG2	1:A:394:ARG:HD2	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:301:STU:H16	2:A:301:STU:H261	1.82	0.61
1:B:424:VAL:HG12	1:B:433:LEU:CD1	2.30	0.61
1:A:493:ASN:HB2	3:A:201:HOH:O	2.00	0.60
1:A:425:CYS:HB2	1:A:432:CYS:SG	2.41	0.60
1:B:603:PRO:HD3	3:B:27:HOH:O	2.01	0.60
1:B:448:ARG:HH11	1:B:448:ARG:HG2	1.67	0.60
1:B:393:ILE:HD11	1:B:398:MET:HB3	1.84	0.60
1:A:537:SER:HB3	3:A:200:HOH:O	2.02	0.59
1:A:486:ARG:HB3	3:A:108:HOH:O	2.02	0.59
1:A:470:MET:CE	1:A:473:LEU:HD12	2.32	0.59
1:A:462:MET:HG2	1:A:496:ILE:CG1	2.31	0.59
1:B:393:ILE:HG12	1:B:394:ARG:H	1.67	0.59
1:A:479:ILE:HD12	1:A:536:SER:C	2.23	0.59
1:B:585:THR:O	1:B:589:GLN:HG3	2.02	0.59
1:B:563:SER:O	1:B:567:VAL:HG23	2.03	0.59
1:B:403:PHE:HZ	1:B:433:LEU:HD13	1.66	0.58
1:A:532:PHE:N	1:A:532:PHE:CD1	2.71	0.58
1:B:448:ARG:HG2	1:B:448:ARG:NH1	2.19	0.58
1:A:523:LYS:HD3	1:A:558:PRO:O	2.04	0.58
1:A:563:SER:HB3	1:A:566:GLU:CB	2.33	0.58
1:B:399:SER:CB	1:B:402:ASP:HB2	2.34	0.57
1:B:599:PRO:HG2	3:B:97:HOH:O	2.04	0.57
1:B:365:PHE:CZ	1:B:390:ILE:HG21	2.39	0.57
1:A:400:GLU:O	1:A:404:ILE:HG13	2.03	0.57
1:A:463:CYS:SG	1:A:548:MET:HG2	2.44	0.57
1:B:360:PRO:HB3	3:B:104:HOH:O	2.04	0.57
1:A:466:VAL:HG13	1:A:498:VAL:CG2	2.34	0.57
1:B:527:PRO:HA	1:B:530:PHE:CD1	2.39	0.57
1:B:368:GLU:OE2	1:B:376:LEU:HD22	2.04	0.57
1:B:521:PRO:HA	3:B:107:HOH:O	2.05	0.57
1:A:563:SER:O	1:A:566:GLU:HB3	2.05	0.56
1:A:428:GLN:O	1:A:429:ALA:HB3	2.05	0.56
1:B:491:GLY:O	1:B:493:ASN:N	2.39	0.56
1:A:538:LYS:HE2	3:A:181:HOH:O	2.06	0.55
1:A:531:SER:HB2	1:A:532:PHE:CD1	2.42	0.55
1:A:447:LEU:CD1	1:A:551:VAL:HA	2.35	0.55
1:A:403:PHE:CZ	1:A:431:ILE:HG22	2.41	0.55
1:A:547:LEU:C	1:A:547:LEU:HD23	2.27	0.55
1:A:419:VAL:HG21	1:A:489:LEU:HD12	1.89	0.54
1:B:593:HIS:HA	1:B:596:LYS:HE2	1.89	0.54
1:B:486:ARG:NH1	1:B:486:ARG:HB2	2.22	0.54
1:B:399:SER:HB2	1:B:402:ASP:CG	2.28	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:409:VAL:HG13	1:A:410:MET:N	2.23	0.54
1:B:459:LEU:HD23	1:B:462:MET:CE	2.37	0.54
1:A:393:ILE:HD12	1:A:398:MET:CE	2.38	0.54
1:A:394:ARG:HB2	1:A:397:ALA:CB	2.38	0.54
1:A:406:GLU:O	1:A:409:VAL:HG12	2.07	0.54
1:A:373:GLN:CG	1:A:394:ARG:HD2	2.38	0.53
1:A:399:SER:OG	1:A:401:GLU:HG2	2.09	0.53
1:B:615:ILE:HD11	3:B:82:HOH:O	2.09	0.53
1:B:480:HIS:O	1:B:540:ASP:OD1	2.27	0.53
1:B:449:THR:C	1:B:451:ARG:N	2.50	0.53
1:A:394:ARG:HB2	1:A:397:ALA:HB2	1.90	0.52
1:A:429:ALA:HB1	1:A:430:PRO:HD2	1.91	0.52
1:A:385:LYS:HG3	1:A:386:ASP:N	2.23	0.52
1:A:427:GLU:HA	3:A:143:HOH:O	2.10	0.52
1:A:443:LEU:HD13	1:A:496:ILE:HD12	1.91	0.52
1:B:375:GLY:HA3	1:B:392:THR:O	2.10	0.52
1:A:373:GLN:HG2	1:A:394:ARG:HG3	1.91	0.52
1:B:615:ILE:O	1:B:615:ILE:CG2	2.57	0.52
1:A:531:SER:HA	3:A:163:HOH:O	2.09	0.52
1:A:522:VAL:HG13	1:A:530:PHE:CE2	2.44	0.51
1:B:614:GLU:C	1:B:616:ALA:H	2.14	0.51
1:A:360:PRO:HA	1:A:427:GLU:CG	2.41	0.51
1:A:459:LEU:O	1:A:462:MET:HB2	2.11	0.51
1:B:480:HIS:CD2	1:B:501:PHE:HB3	2.45	0.51
1:A:480:HIS:O	1:A:540:ASP:OD1	2.28	0.51
1:A:499:SER:OG	1:A:500:ASP:N	2.42	0.51
1:A:441:GLY:HA3	3:A:145:HOH:O	2.11	0.51
1:A:426:LEU:HD23	1:A:426:LEU:N	2.25	0.51
1:A:538:LYS:HE3	3:A:80:HOH:O	2.09	0.51
1:A:538:LYS:CE	3:A:80:HOH:O	2.59	0.51
1:A:393:ILE:HG12	1:A:431:ILE:O	2.10	0.51
1:B:470:MET:CE	1:B:473:LEU:HD12	2.41	0.50
1:B:426:LEU:HA	1:B:431:ILE:CD1	2.41	0.50
1:B:489:LEU:HD12	1:B:499:SER:HB3	1.92	0.50
1:A:426:LEU:C	1:A:428:GLN:H	2.14	0.50
1:B:546:VAL:O	1:B:550:GLU:HG3	2.11	0.50
1:B:521:PRO:HD2	3:B:126:HOH:O	2.11	0.50
1:B:369:ILE:HG22	1:B:377:VAL:HG22	1.91	0.50
1:A:470:MET:HE1	1:A:473:LEU:HD12	1.94	0.50
1:B:575:PHE:O	1:B:576:ARG:CD	2.60	0.50
1:B:581:ARG:HD2	3:B:34:HOH:O	2.11	0.49
1:A:450:GLN:HA	1:A:453:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:360:PRO:CB	3:B:104:HOH:O	2.59	0.49
1:B:598:ARG:HB2	1:B:601:ASP:OD2	2.12	0.49
1:A:419:VAL:HG23	1:A:498:VAL:O	2.11	0.49
1:A:441:GLY:HA2	2:A:301:STU:C3	2.42	0.49
1:A:360:PRO:O	1:A:361:SER:HB3	2.12	0.49
1:A:566:GLU:CA	3:A:5:HOH:O	2.59	0.49
1:A:361:SER:C	1:A:363:LEU:N	2.65	0.49
1:B:589:GLN:NE2	3:B:11:HOH:O	2.44	0.49
1:A:381:TYR:HA	1:A:386:ASP:O	2.13	0.49
1:A:561:ASN:HA	3:A:129:HOH:O	2.12	0.49
1:B:553:SER:OG	1:B:556:LYS:HB2	2.12	0.48
1:A:493:ASN:O	1:A:493:ASN:CG	2.51	0.48
1:A:527:PRO:HA	1:A:530:PHE:CD1	2.48	0.48
1:A:375:GLY:N	1:A:393:ILE:O	2.47	0.48
1:B:444:SER:O	1:B:448:ARG:HD2	2.14	0.48
1:B:587:VAL:HG21	3:B:39:HOH:O	2.14	0.48
1:B:586:HIS:HB3	1:B:615:ILE:CD1	2.43	0.47
1:B:426:LEU:HA	1:B:431:ILE:HD11	1.95	0.47
1:A:399:SER:HB3	1:A:402:ASP:HB2	1.96	0.47
1:A:586:HIS:HB2	3:A:184:HOH:O	2.13	0.47
1:B:393:ILE:HD11	1:B:398:MET:CB	2.43	0.47
1:B:491:GLY:C	1:B:493:ASN:N	2.67	0.47
2:A:301:STU:H4	2:A:301:STU:O5	2.15	0.47
1:A:359:ASP:O	1:A:427:GLU:HG3	2.14	0.47
1:A:563:SER:N	1:A:566:GLU:OE1	2.47	0.47
1:A:522:VAL:HG12	1:A:522:VAL:O	2.15	0.47
1:B:441:GLY:HA2	2:B:621:STU:C3	2.45	0.47
1:B:447:LEU:HD11	1:B:551:VAL:HG22	1.97	0.47
1:A:564:ASN:C	1:A:566:GLU:H	2.18	0.47
1:B:537:SER:O	1:B:540:ASP:HB2	2.15	0.47
1:A:417:LYS:O	1:A:497:LYS:HA	2.15	0.47
1:B:409:VAL:O	1:B:412:LYS:HB3	2.15	0.47
1:B:607:ARG:HB2	1:B:607:ARG:NH1	2.29	0.47
1:B:567:VAL:HG12	1:B:571:ILE:HD12	1.97	0.46
1:A:428:GLN:HG3	3:A:133:HOH:O	2.15	0.46
1:A:537:SER:O	1:A:540:ASP:HB2	2.15	0.46
1:A:461:GLY:N	3:A:2:HOH:O	2.38	0.46
1:A:534:ARG:HD3	3:A:158:HOH:O	2.14	0.46
1:B:443:LEU:HD13	1:B:496:ILE:HD12	1.97	0.46
1:B:575:PHE:O	1:B:576:ARG:HD3	2.16	0.46
1:B:470:MET:CE	1:B:498:VAL:HG21	2.31	0.46
1:B:393:ILE:HG12	1:B:394:ARG:N	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:562:ARG:NH1	1:A:575:PHE:CE2	2.84	0.46
1:A:373:GLN:HE21	1:A:394:ARG:HG3	1.81	0.46
1:B:446:TYR:CE1	1:B:451:ARG:HG3	2.51	0.46
1:B:590:ILE:HG13	1:B:615:ILE:CD1	2.45	0.45
1:A:569:GLU:O	1:A:573:THR:CG2	2.63	0.45
1:A:528:GLU:HG3	1:A:528:GLU:H	1.51	0.45
2:B:621:STU:H16	2:B:621:STU:H261	1.97	0.45
1:A:454:PHE:CG	1:A:459:LEU:HD21	2.52	0.45
1:A:419:VAL:HG21	1:A:499:SER:HB3	1.98	0.45
1:A:479:ILE:HD12	1:A:537:SER:N	2.31	0.45
1:B:447:LEU:HD22	1:B:554:GLU:HA	1.98	0.45
1:B:405:GLU:O	1:B:409:VAL:HG23	2.15	0.45
1:B:393:ILE:CG2	1:B:431:ILE:HG22	2.46	0.45
1:B:393:ILE:CG2	1:B:394:ARG:N	2.66	0.45
1:A:404:ILE:O	1:A:408:GLU:HG3	2.16	0.45
1:A:568:VAL:O	1:A:572:SER:HB2	2.15	0.45
1:B:463:CYS:SG	1:B:548:MET:HG2	2.57	0.45
1:A:428:GLN:O	1:A:429:ALA:CB	2.65	0.44
1:B:576:ARG:HG3	1:B:595:TRP:CE3	2.51	0.44
1:A:417:LYS:HA	1:A:417:LYS:HD3	1.87	0.44
1:A:373:GLN:HE21	1:A:397:ALA:HB2	1.81	0.44
1:B:547:LEU:C	1:B:547:LEU:HD23	2.38	0.44
1:A:615:ILE:O	1:A:619:GLY:CA	2.66	0.44
1:A:579:LYS:HB2	1:A:588:TYR:CG	2.52	0.44
1:B:425:CYS:HB2	1:B:432:CYS:SG	2.58	0.44
1:A:398:MET:CE	1:A:403:PHE:HB2	2.48	0.44
1:A:589:GLN:NE2	3:A:51:HOH:O	2.51	0.43
1:B:607:ARG:NH1	3:B:4:HOH:O	2.48	0.43
1:A:368:GLU:OE2	1:A:376:LEU:HD13	2.17	0.43
1:B:607:ARG:NH2	3:B:4:HOH:O	2.44	0.43
1:B:598:ARG:HD2	1:B:601:ASP:OD2	2.18	0.43
1:A:493:ASN:O	1:A:494:GLN:HB2	2.18	0.43
1:B:470:MET:CE	1:B:498:VAL:HG11	2.44	0.43
1:A:457:GLU:C	3:A:2:HOH:O	2.56	0.43
1:B:444:SER:O	1:B:448:ARG:CD	2.67	0.43
1:B:364:THR:O	1:B:380:GLY:CA	2.66	0.43
1:A:357:VAL:N	3:A:3:HOH:O	2.51	0.43
1:B:530:PHE:HB2	1:B:531:SER:H	1.59	0.43
1:A:562:ARG:HD2	3:A:112:HOH:O	2.19	0.43
1:B:428:GLN:HG3	1:B:428:GLN:H	1.71	0.43
1:B:453:LEU:HD12	1:B:453:LEU:H	1.83	0.43
1:A:398:MET:HE3	1:A:403:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:590:ILE:CD1	1:A:615:ILE:HD12	2.48	0.43
1:A:429:ALA:O	1:A:430:PRO:C	2.57	0.43
1:A:366:VAL:HG23	1:A:380:GLY:HA2	2.00	0.42
1:B:478:VAL:C	1:B:479:ILE:HD13	2.39	0.42
1:A:443:LEU:O	1:A:446:TYR:N	2.51	0.42
1:B:598:ARG:HA	1:B:599:PRO:HD2	1.89	0.42
1:B:443:LEU:HD13	1:B:496:ILE:CD1	2.49	0.42
1:A:566:GLU:HA	3:A:5:HOH:O	2.19	0.42
1:A:557:ILE:HA	1:A:558:PRO:HD2	1.98	0.42
1:A:492:GLU:O	1:A:495:VAL:HG23	2.20	0.42
1:B:575:PHE:O	1:B:576:ARG:HD2	2.18	0.42
1:A:586:HIS:CD2	3:A:184:HOH:O	2.73	0.42
1:B:608:LEU:HA	1:B:608:LEU:HD23	1.87	0.42
1:B:454:PHE:N	1:B:454:PHE:CD1	2.88	0.42
1:A:579:LYS:HB2	1:A:588:TYR:CD1	2.55	0.42
1:B:553:SER:O	1:B:554:GLU:HB2	2.20	0.42
1:A:357:VAL:O	1:A:357:VAL:HG22	2.20	0.42
1:A:393:ILE:O	1:A:394:ARG:CB	2.67	0.42
1:B:609:LEU:HD12	1:B:609:LEU:HA	1.90	0.42
1:A:547:LEU:O	1:A:547:LEU:HD23	2.20	0.41
1:B:542:TRP:HZ3	1:B:596:LYS:O	2.03	0.41
1:B:393:ILE:CG2	1:B:394:ARG:H	2.28	0.41
1:A:373:GLN:HG2	1:A:394:ARG:CD	2.49	0.41
1:A:466:VAL:HG13	1:A:498:VAL:HG21	2.02	0.41
1:B:375:GLY:HA2	1:B:394:ARG:HG3	2.02	0.41
1:B:404:ILE:HG12	1:B:426:LEU:HD13	2.02	0.41
1:B:569:GLU:O	1:B:573:THR:HG23	2.21	0.41
1:A:491:GLY:O	1:A:493:ASN:N	2.54	0.41
1:B:381:TYR:CD2	1:B:387:LYS:HA	2.55	0.41
1:B:590:ILE:CD1	1:B:611:GLN:HB3	2.51	0.41
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.87	0.41
1:B:448:ARG:NH1	3:B:29:HOH:O	2.53	0.40
1:A:447:LEU:HD11	1:A:551:VAL:HG22	2.02	0.40
1:A:492:GLU:O	1:A:493:ASN:OD1	2.39	0.40
1:B:444:SER:OG	1:B:445:ASP:N	2.55	0.40
1:B:392:THR:HG22	1:B:432:CYS:HB3	2.02	0.40
1:B:538:LYS:HG3	1:B:599:PRO:O	2.20	0.40
1:A:529:VAL:O	1:A:530:PHE:C	2.60	0.40
1:B:460:LEU:CD2	1:B:615:ILE:O	2.69	0.40
1:A:525:ALA:HB1	1:A:529:VAL:HB	2.03	0.40
1:A:403:PHE:CD2	1:A:403:PHE:C	2.94	0.40
1:B:371:SER:HB3	1:B:376:LEU:HD23	2.04	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	241/264 (91%)	204 (85%)	26 (11%)	11 (5%)	4	1
1	B	237/264 (90%)	208 (88%)	16 (7%)	13 (6%)	3	1
All	All	478/528 (90%)	412 (86%)	42 (9%)	24 (5%)	3	1

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	SER
1	A	374	PHE
1	A	394	ARG
1	A	492	GLU
1	B	360	PRO
1	B	393	ILE
1	B	428	GLN
1	B	430	PRO
1	B	450	GLN
1	B	492	GLU
1	B	615	ILE
1	A	493	ASN
1	B	449	THR
1	B	481	ARG
1	A	362	GLU
1	A	427	GLU
1	B	359	ASP
1	B	439	GLU
1	A	373	GLN
1	A	531	SER
1	B	395	GLU
1	A	429	ALA
1	A	360	PRO
1	B	431	ILE

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%)	184 (86%)	30 (14%)	5	5
1	B	212/232 (91%)	186 (88%)	26 (12%)	7	7
All	All	426/464 (92%)	370 (87%)	56 (13%)	6	6

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	ILE
1	A	359	ASP
1	A	368	GLU
1	A	373	GLN
1	A	374	PHE
1	A	390	ILE
1	A	394	ARG
1	A	402	ASP
1	A	403	PHE
1	A	420	GLN
1	A	421	LEU
1	A	424	VAL
1	A	426	LEU
1	A	433	LEU
1	A	444	SER
1	A	448	ARG
1	A	449	THR
1	A	450	GLN
1	A	500	ASP
1	A	528	GLU
1	A	531	SER
1	A	532	PHE
1	A	536	SER
1	A	565	SER
1	A	572	SER
1	A	573	THR
1	A	585	THR
1	A	597	GLU
1	A	607	ARG

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Mol	Chain	Res	Type
1	A	618	SER
1	B	359	ASP
1	B	369	ILE
1	B	371	SER
1	B	377	VAL
1	B	379	LEU
1	B	395	GLU
1	B	414	SER
1	B	425	CYS
1	B	427	GLU
1	B	431	ILE
1	B	433	LEU
1	B	444	SER
1	B	445	ASP
1	B	448	ARG
1	B	449	THR
1	B	450	GLN
1	B	453	LEU
1	B	454	PHE
1	B	458	THR
1	B	493	ASN
1	B	531	SER
1	B	538	LYS
1	B	565	SER
1	B	590	ILE
1	B	607	ARG
1	B	610	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	GLN
1	A	373	GLN
1	A	420	GLN
1	A	428	GLN
1	A	494	GLN
1	A	564	ASN
1	A	586	HIS
1	A	589	GLN
1	A	611	GLN
1	B	367	GLN
1	B	378	HIS

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Mol	Chain	Res	Type
1	B	428	GLN
1	B	589	GLN
1	B	611	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	-	40,42,42	2.07	15 (37%)	62,68,68	2.26	17 (27%)
2	STU	B	621	-	40,42,42	1.96	16 (40%)	62,68,68	3.28	21 (33%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STU	B	621	-	-	0/4/42/42	0/0/8/8

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	STU	C15-C16	4.44	1.46	1.36
2	B	621	STU	C3-C4	4.35	1.46	1.36
2	A	301	STU	C21-C22	4.15	1.58	1.53
2	B	621	STU	C10-C11	3.82	1.49	1.42
2	B	621	STU	C15-C16	3.67	1.45	1.36
2	A	301	STU	C14-C13	3.43	1.44	1.36
2	A	301	STU	C5-C20	3.30	1.46	1.41
2	A	301	STU	C10-C11	3.25	1.48	1.42
2	A	301	STU	C2-C1	3.18	1.43	1.36
2	A	301	STU	C9-N1	3.10	1.49	1.45
2	B	621	STU	C9-N1	3.08	1.49	1.45
2	A	301	STU	C3-C4	2.98	1.43	1.36
2	B	621	STU	C2-C1	2.94	1.43	1.36
2	B	621	STU	C7-C8	-2.91	1.44	1.49
2	B	621	STU	C19-C18	2.68	1.48	1.41
2	B	621	STU	C14-C13	2.66	1.42	1.36
2	A	301	STU	C19-C18	2.64	1.48	1.41
2	B	621	STU	C3-C2	2.42	1.44	1.37
2	B	621	STU	O4-C21	-2.38	1.39	1.44
2	B	621	STU	C12-C11	-2.35	1.36	1.45
2	B	621	STU	C26-C21	2.32	1.54	1.51
2	A	301	STU	C9-C10	2.31	1.54	1.50
2	A	301	STU	C11-C18	2.31	1.45	1.42
2	A	301	STU	C12-C11	-2.26	1.36	1.45
2	A	301	STU	C16-C17	2.24	1.45	1.41
2	A	301	STU	C7-C6	-2.18	1.39	1.43
2	A	301	STU	C3-C2	2.18	1.44	1.37
2	B	621	STU	C22-C23	-2.13	1.48	1.52
2	B	621	STU	C11-C18	2.08	1.45	1.42
2	B	621	STU	O6-C22	2.02	1.46	1.42
2	B	621	STU	C13-C12	2.01	1.45	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	621	STU	C26-C21-N2	17.21	120.41	111.09
2	B	621	STU	C28-N4-C23	10.99	119.95	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	STU	C26-C21-N2	8.30	115.58	111.09
2	A	301	STU	C6-C19-C18	-6.05	116.09	121.20
2	B	621	STU	C6-C5-C20	5.86	112.77	106.37
2	A	301	STU	C6-C5-C20	5.17	112.02	106.37
2	A	301	STU	C6-C7-C8	4.81	132.67	128.93
2	B	621	STU	C22-C21-N2	-4.76	105.80	112.78
2	B	621	STU	C6-C19-C18	-4.47	117.42	121.20
2	B	621	STU	C11-C12-C17	4.22	110.98	106.37
2	B	621	STU	C5-C6-C19	-4.08	98.85	106.05
2	A	301	STU	C5-C6-C19	-3.74	99.45	106.05
2	B	621	STU	C6-C7-C8	3.61	131.74	128.93
2	A	301	STU	C11-C12-C17	3.57	110.26	106.37
2	A	301	STU	C26-C21-C22	-3.25	105.13	112.87
2	B	621	STU	O4-C21-C22	3.20	117.50	109.80
2	A	301	STU	C13-C12-C17	3.15	123.38	119.39
2	A	301	STU	C13-C12-C11	-3.07	126.34	135.38
2	A	301	STU	C7-C8-N1	3.05	109.70	106.39
2	B	621	STU	O6-C22-C21	2.96	114.98	108.27
2	A	301	STU	C27-O6-C22	2.92	120.02	114.29
2	B	621	STU	C13-C12-C11	-2.90	126.85	135.38
2	B	621	STU	C10-C11-C12	2.77	139.25	132.94
2	A	301	STU	C4-C5-C6	-2.75	127.28	135.38
2	A	301	STU	C22-C21-N2	-2.68	108.85	112.78
2	B	621	STU	C21-C22-C23	-2.48	102.69	111.00
2	B	621	STU	C15-C14-C13	-2.45	116.89	120.47
2	B	621	STU	C3-C2-C1	-2.44	116.89	120.47
2	B	621	STU	C26-C21-C22	-2.43	107.08	112.87
2	B	621	STU	O4-C21-C26	-2.42	97.24	107.36
2	A	301	STU	C16-C17-C12	-2.28	117.44	120.73
2	A	301	STU	O6-C22-C21	2.28	113.44	108.27
2	B	621	STU	C4-C5-C6	-2.25	128.76	135.38
2	B	621	STU	C24-C25-N3	2.24	115.05	112.48
2	B	621	STU	C13-C12-C17	2.19	122.16	119.39
2	A	301	STU	C19-N3-C20	-2.09	102.08	106.19
2	A	301	STU	C9-N1-C8	-2.08	110.61	113.15
2	B	621	STU	C7-C6-C5	2.02	138.32	133.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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.