



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:00 AM UTC

PDB ID : 1SM2 / pdb_00001sm2
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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

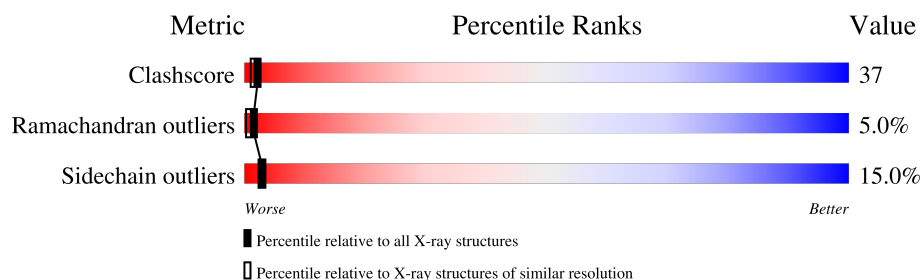
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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 $\leq 5\%$.

Note EDS was not executed.

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

2 Entry composition [i](#)

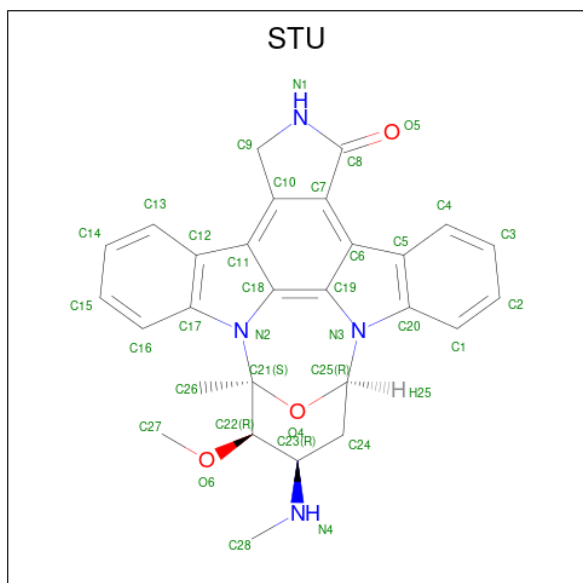
There are 3 unique types of molecules in this entry. The entry contains 4212 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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.

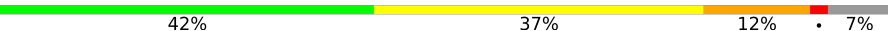
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	144	Total 144	O 144	0	0
3	B	107	Total 107	O 107	0	0

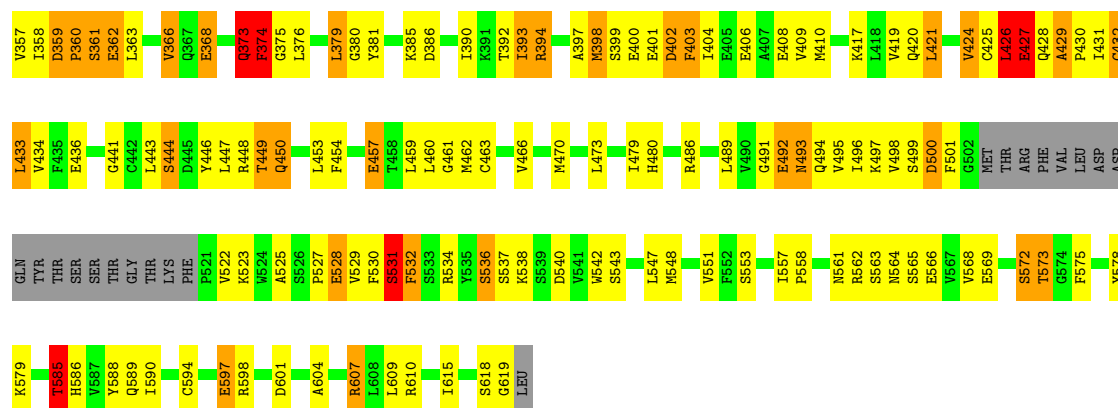
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

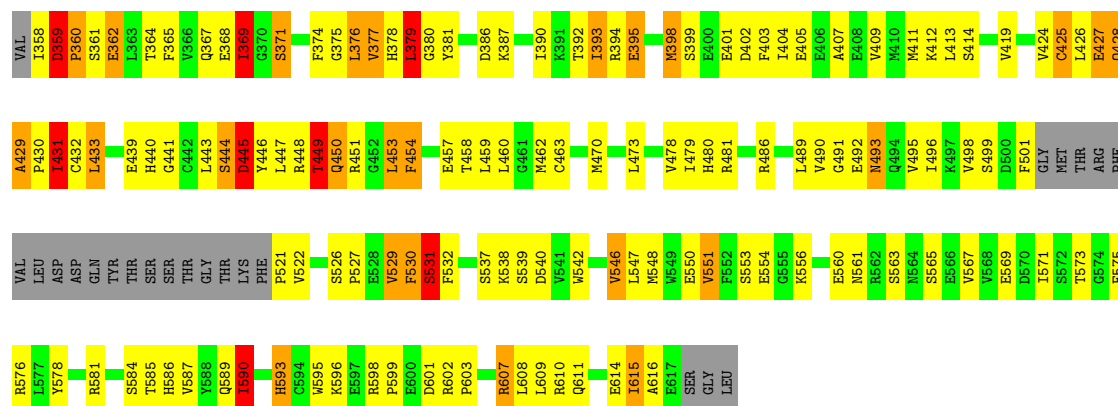
• Molecule 1: Tyrosine-protein kinase ITK/TSK

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 is therefore 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 [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	1.00	3/2000 (0.1%)	1.07	10/2700 (0.4%)
1	B	1.02	8/1979 (0.4%)	1.13	18/2672 (0.7%)
All	All	1.01	11/3979 (0.3%)	1.10	28/5372 (0.5%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	529	VAL	CA-CB	9.29	1.64	1.55
1	B	546	VAL	CA-CB	8.86	1.65	1.54
1	A	543	SER	CA-CB	-8.00	1.41	1.53
1	A	457	GLU	CA-CB	6.96	1.66	1.53
1	A	585	THR	CA-CB	6.08	1.63	1.53
1	B	367	GLN	CA-CB	-5.69	1.44	1.53
1	B	361	SER	CA-CB	-5.41	1.44	1.53
1	B	445	ASP	CA-CB	-5.41	1.45	1.53
1	B	590	ILE	C-O	-5.38	1.17	1.24
1	B	359	ASP	CA-CB	-5.10	1.45	1.53
1	B	522	VAL	CA-CB	-5.07	1.48	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	THR	N-CA-C	-10.02	96.52	110.35
1	B	531	SER	N-CA-C	8.71	120.85	111.36
1	B	369	ILE	N-CA-CB	-8.35	100.86	112.12
1	B	429	ALA	CA-C-N	7.79	129.58	119.84
1	B	429	ALA	C-N-CA	7.79	129.58	119.84
1	A	374	PHE	N-CA-C	-7.62	94.56	110.80
1	B	529	VAL	N-CA-C	-7.40	104.64	111.67
1	A	426	LEU	N-CA-C	-7.26	103.57	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	362	GLU	N-CA-C	-6.67	105.03	112.57
1	B	449	THR	N-CA-C	6.11	123.81	110.80
1	A	604	ALA	N-CA-C	-6.08	102.51	110.53
1	A	553	SER	N-CA-C	-6.05	105.76	113.02
1	B	530	PHE	CB-CA-C	-6.03	98.42	110.42
1	B	526	SER	N-CA-C	-5.91	101.69	110.20
1	B	359	ASP	CA-C-N	5.85	127.15	119.84
1	B	359	ASP	C-N-CA	5.85	127.15	119.84
1	A	432	CYS	N-CA-C	5.69	117.43	108.96
1	A	393	ILE	N-CA-C	5.62	121.03	109.34
1	B	379	LEU	N-CA-C	-5.61	100.14	109.46
1	B	367	GLN	N-CA-C	5.60	117.62	108.55
1	B	560	GLU	N-CA-C	5.51	116.98	110.97
1	A	436	GLU	N-CA-C	-5.43	102.85	110.50
1	B	593	HIS	N-CA-C	-5.42	105.92	112.54
1	B	431	ILE	N-CA-C	5.36	120.50	109.34
1	A	379	LEU	N-CA-C	-5.20	100.83	109.46
1	B	386	ASP	N-CA-C	5.18	117.68	109.24
1	A	594	CYS	N-CA-C	-5.00	106.02	111.82
1	B	532	PHE	N-CA-C	5.00	119.10	112.30

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	1956	0	1913	143	0
1	B	1935	0	1893	143	0
2	A	35	0	26	3	0
2	B	35	0	26	3	0
3	A	144	0	0	30	0
3	B	107	0	0	23	0
All	All	4212	0	3858	289	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 37.

All (289) 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:HH11	1:A:607:ARG:HB2	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	1.39	1.02
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:449:THR:C	1:B:451:ARG:H	1.82	0.85
1:B:615:ILE:C	3:B:68:HOH:O	2.21	0.84
1:B:486:ARG:HG3	2:B:621:STU:H281	1.59	0.83
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:459:LEU:HA	1:B:462:MET:HE3	1.66	0.78
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:A:360:PRO:HG2	1:A:362:GLU:HG3	1.68	0.76
1:B:615:ILE:HG22	1:B:615:ILE:O	1.86	0.76
1:A:462:MET:HG2	1:A:496:ILE:HG13	1.69	0.74
1:A:361:SER:C	1:A:363:LEU:H	1.96	0.74
1:A:536:SER:HB3	3:A:17:HOH:O	1.88	0.74
1:B:369:ILE:HD13	1:B:379:LEU:HB2	1.69	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
1:A:424:VAL:HG13	1:A:433:LEU:CD1	2.17	0.72
1:B:369:ILE:HG22	1:B:377:VAL:CG2	2.19	0.72
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:B:360:PRO:HD2	1:B:362:GLU:CD	2.17	0.70
1:A:424:VAL:HG13	1:A:433:LEU:HD12	1.72	0.70
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:413:LEU:HD11	1:B:478:VAL:HG21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:HIS:HB3	1:B:615:ILE:HD13	1.75	0.69
1:A:470:MET:HE1	1:A:473:LEU:HD12	1.74	0.69
1:B:491:GLY:C	1:B:493:ASN:H	2.00	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:HB2	1:B:486:ARG:HH11	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:374:PHE:HD2	1:B:398:MET:HE2	1.61	0.66
1:B:584:SER:OG	1:B:587:VAL:HG23	1.95	0.66
1:B:607:ARG:HB2	1:B:607:ARG:HH11	1.61	0.65
1:A:460:LEU:HB3	3:A:2:HOH:O	1.95	0.65
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: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:A:479:ILE:HD12	1:A:536:SER:C	2.23	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: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
2:A:301:STU:H261	2:A:301:STU:H16	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:393:ILE:HD11	1:B:398:MET:HB3	1.84	0.60
1:B:448:ARG:HG2	1:B:448:ARG:HH11	1.67	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:547:LEU:C	1:A:547:LEU:HD23	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:399:SER:HB2	1:B:402:ASP:CG	2.28	0.58
1:B:403:PHE:HZ	1:B:433:LEU:HD13	1.66	0.58
1:A:532:PHE:CD1	1:A:532:PHE:N	2.71	0.58
1:A:523:LYS:HD3	1:A:558:PRO:O	2.04	0.58
1:B:448:ARG:HG2	1:B:448:ARG:NH1	2.19	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:A:400:GLU:O	1:A:404:ILE:HG13	2.03	0.57
1:B:365:PHE:CZ	1:B:390:ILE:HG21	2.39	0.57
1:A:463:CYS:SG	1:A:548:MET:HG2	2.44	0.57
1:A:466:VAL:HG13	1:A:498:VAL:CG2	2.34	0.57
1:B:360:PRO:HB3	3:B:104:HOH:O	2.04	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:428:GLN:O	1:A:429:ALA:HB3	2.05	0.56
1:A:563:SER:O	1:A:566:GLU:HB3	2.05	0.56
1:B:614:GLU:C	1:B:616:ALA:H	2.14	0.56
1:B:374:PHE:CD2	1:B:398:MET:HE2	2.41	0.56
1:B:491:GLY:O	1:B:493:ASN:N	2.39	0.56
1:B:470:MET:HE1	1:B:498:VAL:HG11	1.88	0.55
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:419:VAL:HG21	1:A:489:LEU:HD12	1.89	0.54
1:A:426:LEU:C	1:A:428:GLN:H	2.14	0.54
1:B:593:HIS:HA	1:B:596:LYS:HE2	1.89	0.54
1:B:486:ARG:HB2	1:B:486:ARG:NH1	2.22	0.54
1:A:361:SER:C	1:A:363:LEU:N	2.65	0.54
1:A:409:VAL:HG13	1:A:410:MET:N	2.23	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:B:459:LEU:HD23	1:B:462:MET:CE	2.37	0.54
1:A:406:GLU:O	1:A:409:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:493:ASN:CG	1:A:493:ASN:O	2.51	0.53
1:B:480:HIS:O	1:B:540:ASP:OD1	2.27	0.53
1:B:615:ILE:HD11	3:B:82:HOH:O	2.09	0.53
1:A:385:LYS:HG3	1:A:386:ASP:N	2.23	0.52
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: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:A:564:ASN:C	1:A:566:GLU:H	2.18	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:426:LEU:N	1:A:426:LEU:HD23	2.25	0.51
1:A:441:GLY:HA3	3:A:145:HOH:O	2.11	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: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:426:LEU:HA	1:B:431:ILE:CD1	2.41	0.50
1:B:470:MET:CE	1:B:473:LEU:HD12	2.41	0.50
1:B:489:LEU:HD12	1:B:499:SER:HB3	1.92	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:B:575:PHE:O	1:B:576:ARG:CD	2.60	0.50
1:A:450:GLN:HA	1:A:453:LEU:HD12	1.93	0.49
1:B:581:ARG:HD2	3:B:34:HOH:O	2.11	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TYR:HA	1:A:386:ASP:O	2.13	0.49
1:B:547:LEU:C	1:B:547:LEU:HD23	2.38	0.49
1:B:589:GLN:NE2	3:B:11:HOH:O	2.44	0.49
1:A:561:ASN:HA	3:A:129:HOH:O	2.12	0.49
1:B:470:MET:HE1	1:B:473:LEU:HD12	1.95	0.48
1:B:553:SER:OG	1:B:556:LYS:HB2	2.12	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:459:LEU:HD23	1:B:462:MET:HE3	1.94	0.48
1:A:457:GLU:C	3:A:2:HOH:O	2.56	0.48
1:B:444:SER:O	1:B:448:ARG:HD2	2.14	0.48
1:B:470:MET:CE	1:B:498:VAL:HG11	2.44	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:A:399:SER:HB3	1:A:402:ASP:HB2	1.96	0.47
1:A:429:ALA:O	1:A:430:PRO:C	2.57	0.47
1:A:586:HIS:HB2	3:A:184:HOH:O	2.13	0.47
1:B:426:LEU:HA	1:B:431:ILE:HD11	1.95	0.47
1:B:393:ILE:HD11	1:B:398:MET:CB	2.43	0.47
2:A:301:STU:O5	2:A:301:STU:H4	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:B:478:VAL:C	1:B:479:ILE:HD13	2.39	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:417:LYS:O	1:A:497:LYS:HA	2.15	0.47
1:B:537:SER:O	1:B:540:ASP:HB2	2.15	0.47
1:A:522:VAL:HG12	1:A:522:VAL:O	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:A:428:GLN:HG3	3:A:133:HOH:O	2.15	0.46
1:B:567:VAL:HG12	1:B:571:ILE:HD12	1.97	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:A:562:ARG:NH1	1:A:575:PHE:CE2	2.84	0.46
1:B:393:ILE:HG12	1:B:394:ARG:N	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:GLU:H	1:A:528:GLU:HG3	1.51	0.45
1:A:569:GLU:O	1:A:573:THR:CG2	2.63	0.45
1:B:590:ILE:HG13	1:B:615:ILE:CD1	2.45	0.45
1:A:419:VAL:HG21	1:A:499:SER:HB3	1.98	0.45
1:A:454:PHE:CG	1:A:459:LEU:HD21	2.52	0.45
2:B:621:STU:H16	2:B:621:STU:H261	1.97	0.45
1:A:479:ILE:HD12	1:A:537:SER:N	2.31	0.45
1:A:529:VAL:O	1:A:530:PHE:C	2.60	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:394:ARG:N	2.66	0.45
1:B:393:ILE:CG2	1:B:431:ILE:HG22	2.46	0.45
1:B:491:GLY:C	1:B:493:ASN:N	2.67	0.45
1:A:403:PHE:CD2	1:A:403:PHE:C	2.94	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:A:417:LYS:HA	1:A:417:LYS:HD3	1.87	0.44
1:A:542:TRP:CD1	1:A:542:TRP:C	2.95	0.44
1:B:576:ARG:HG3	1:B:595:TRP:CE3	2.51	0.44
1:B:578:TYR:CD1	1:B:578:TYR:C	2.94	0.44
1:A:373:GLN:HE21	1:A:397:ALA:HB2	1.81	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:A:398:MET:CE	1:A:403:PHE:HB2	2.48	0.44
1:A:425:CYS:C	1:A:426:LEU:HD23	2.42	0.44
1:B:425:CYS:HB2	1:B:432:CYS:SG	2.58	0.44
1:A:368:GLU:OE2	1:A:376:LEU:HD13	2.17	0.43
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:493:ASN:O	1:A:494:GLN:HB2	2.18	0.43
1:B:598:ARG:HD2	1:B:601:ASP:OD2	2.18	0.43
1:B:607:ARG:NH2	3:B:4:HOH:O	2.44	0.43
1:A:578:TYR:C	1:A:578:TYR:CD1	2.96	0.43
1:B:364:THR:O	1:B:380:GLY:CA	2.66	0.43
1:B:444:SER:O	1:B:448:ARG:CD	2.67	0.43
1:A:357:VAL:N	3:A:3:HOH:O	2.51	0.43
1:A:562:ARG:HD2	3:A:112:HOH:O	2.19	0.43
1:B:530:PHE:HB2	1:B:531:SER:H	1.59	0.43
1:B:428:GLN:H	1:B:428:GLN:HG3	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:LEU:HD12	1:B:453:LEU:H	1.83	0.43
1:A:590:ILE:CD1	1:A:615:ILE:HD12	2.48	0.43
1:A:366:VAL:HG23	1:A:380:GLY:HA2	2.00	0.42
1:A:443:LEU:O	1:A:444:SER:C	2.62	0.42
1:A:361:SER:C	3:A:1:HOH:O	2.60	0.42
1:A:443:LEU:O	1:A:446:TYR:N	2.51	0.42
1:A:454:PHE:CE2	1:A:462:MET:HE1	2.55	0.42
1:B:426:LEU:O	1:B:427:GLU:C	2.63	0.42
1:B:443:LEU:HD13	1:B:496:ILE:CD1	2.49	0.42
1:B:598:ARG:HA	1:B:599:PRO:HD2	1.89	0.42
1:A:557:ILE:HA	1:A:558:PRO:HD2	1.98	0.42
1:A:566:GLU:HA	3:A:5:HOH:O	2.19	0.42
1:A:492:GLU:O	1:A:495:VAL:HG23	2.20	0.42
1:A:586:HIS:CD2	3:A:184:HOH:O	2.73	0.42
1:B:575:PHE:O	1:B:576:ARG:HD2	2.18	0.42
1:B:454:PHE:CD1	1:B:454:PHE:N	2.88	0.42
1:B:608:LEU:HD23	1:B:608:LEU:HA	1.87	0.42
1:A:579:LYS:HB2	1:A:588:TYR:CD1	2.55	0.42
1:A:357:VAL:O	1:A:357:VAL:HG22	2.20	0.42
1:B:553:SER:O	1:B:554:GLU:HB2	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:B:614:GLU:C	1:B:616:ALA:N	2.78	0.42
1:A:547:LEU:HD23	1:A:547:LEU:O	2.20	0.41
1:B:393:ILE:CG2	1:B:394:ARG:H	2.28	0.41
1:B:542:TRP:HZ3	1:B:596:LYS:O	2.03	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:529:VAL:O	1:B:530:PHE:C	2.63	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:427:GLU:O	1:B:428:GLN:C	2.64	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:A:433:LEU:HD12	1:A:433:LEU:HA	1.87	0.41
1:B:590:ILE:CD1	1:B:611:GLN:HB3	2.51	0.41
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:448:ARG:NH1	3:B:29:HOH:O	2.53	0.40
1:B:392:THR:HG22	1:B:432:CYS:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:SER:OG	1:B:445:ASP:N	2.55	0.40
1:B:538:LYS:HG3	1:B:599:PRO:O	2.20	0.40
1:A:525:ALA:HB1	1:A:529:VAL:HB	2.03	0.40
1:B:460:LEU:CD2	1:B:615:ILE:O	2.69	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 [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%)	26 (11%)	11 (5%)	2	1
1	B	237/264 (90%)	208 (88%)	16 (7%)	13 (6%)	1	0
All	All	478/528 (90%)	412 (86%)	42 (9%)	24 (5%)	1	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

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Mol	Chain	Res	Type
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%)	181 (85%)	33 (15%)	2	3
1	B	212/232 (91%)	181 (85%)	31 (15%)	3	3
All	All	426/464 (92%)	362 (85%)	64 (15%)	3	3

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	ILE
1	A	359	ASP
1	A	366	VAL
1	A	368	GLU
1	A	373	GLN
1	A	374	PHE
1	A	379	LEU
1	A	390	ILE
1	A	398	MET
1	A	402	ASP
1	A	403	PHE
1	A	420	GLN

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Mol	Chain	Res	Type
1	A	421	LEU
1	A	424	VAL
1	A	426	LEU
1	A	427	GLU
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
1	A	618	SER
1	B	358	ILE
1	B	359	ASP
1	B	369	ILE
1	B	371	SER
1	B	376	LEU
1	B	377	VAL
1	B	379	LEU
1	B	395	GLU
1	B	398	MET
1	B	401	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	449	THR
1	B	450	GLN
1	B	453	LEU
1	B	454	PHE

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Mol	Chain	Res	Type
1	B	458	THR
1	B	493	ASN
1	B	495	VAL
1	B	531	SER
1	B	539	SER
1	B	551	VAL
1	B	565	SER
1	B	590	ILE
1	B	607	ARG
1	B	610	ARG

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

Mol	Chain	Res	Type
1	A	367	GLN
1	A	373	GLN
1	A	415	HIS
1	A	420	GLN
1	A	428	GLN
1	A	494	GLN
1	A	586	HIS
1	A	589	GLN
1	A	611	GLN
1	B	367	GLN
1	B	378	HIS
1	B	428	GLN
1	B	494	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 oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	STU	B	621	-	39,42,42	2.39	19 (48%)	50,68,68	2.61	23 (46%)
2	STU	A	301	-	39,42,42	2.38	18 (46%)	50,68,68	2.41	20 (40%)

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

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	STU	C15-C16	4.63	1.46	1.38
2	B	621	STU	C12-C11	-4.54	1.36	1.46
2	B	621	STU	C3-C4	4.52	1.46	1.38
2	B	621	STU	C11-C10	4.48	1.49	1.40
2	A	301	STU	C12-C11	-4.39	1.36	1.46
2	B	621	STU	C22-C23	-4.21	1.48	1.53
2	A	301	STU	C16-C17	3.99	1.45	1.39
2	A	301	STU	C11-C10	3.94	1.48	1.40
2	A	301	STU	C9-C10	3.72	1.54	1.50
2	A	301	STU	C5-C20	3.71	1.46	1.41
2	B	621	STU	C15-C16	3.60	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	621	STU	C19-C18	3.46	1.48	1.40
2	A	301	STU	C19-C18	3.42	1.48	1.40
2	B	621	STU	C13-C12	3.36	1.45	1.40
2	A	301	STU	C9-N1	3.29	1.49	1.45
2	A	301	STU	C14-C13	3.28	1.44	1.38
2	B	621	STU	C9-N1	3.27	1.49	1.45
2	A	301	STU	C5-C6	-3.17	1.39	1.46
2	B	621	STU	C8-N1	3.07	1.37	1.35
2	B	621	STU	C3-C2	3.02	1.44	1.38
2	A	301	STU	C2-C1	2.94	1.43	1.38
2	B	621	STU	C16-C17	2.93	1.44	1.39
2	B	621	STU	C5-C6	-2.86	1.40	1.46
2	A	301	STU	C4-C5	2.85	1.44	1.40
2	A	301	STU	C3-C2	2.71	1.44	1.38
2	A	301	STU	C13-C12	2.67	1.44	1.40
2	A	301	STU	C3-C4	2.67	1.43	1.38
2	B	621	STU	C26-C21	2.63	1.54	1.51
2	B	621	STU	C2-C1	2.62	1.43	1.38
2	B	621	STU	C25-N3	2.61	1.47	1.45
2	B	621	STU	O6-C22	2.55	1.46	1.42
2	A	301	STU	C14-C15	2.39	1.43	1.38
2	B	621	STU	C1-C20	2.35	1.43	1.39
2	B	621	STU	C14-C15	2.31	1.43	1.38
2	B	621	STU	C14-C13	2.23	1.42	1.38
2	A	301	STU	C24-C23	-2.12	1.50	1.53
2	A	301	STU	C11-C18	2.12	1.45	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	621	STU	C6-C5-C20	6.23	112.77	106.49
2	A	301	STU	C6-C5-C20	5.49	112.02	106.49
2	B	621	STU	C5-C6-C19	-5.41	98.85	106.44
2	B	621	STU	C19-C18-N2	-5.35	126.83	131.38
2	B	621	STU	C18-C19-N3	-5.34	124.89	129.42
2	A	301	STU	C5-C6-C19	-4.98	99.45	106.44
2	A	301	STU	C6-C19-N3	4.97	117.91	109.61
2	B	621	STU	C6-C19-N3	4.84	117.69	109.61
2	B	621	STU	C28-N4-C23	4.66	119.95	114.39
2	B	621	STU	C11-C12-C17	4.46	110.98	106.49
2	A	301	STU	C19-N3-C20	-4.40	102.08	107.90
2	B	621	STU	C19-N3-C20	-4.07	102.52	107.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	STU	C18-C19-N3	-4.04	125.99	129.42
2	A	301	STU	C7-C6-C19	4.03	124.80	118.04
2	B	621	STU	C12-C11-C10	3.81	139.25	132.33
2	A	301	STU	C11-C12-C17	3.75	110.26	106.49
2	A	301	STU	C13-C12-C17	3.58	123.38	119.24
2	A	301	STU	C9-N1-C8	-3.57	110.61	113.86
2	A	301	STU	C16-C17-C12	-3.55	117.44	121.59
2	A	301	STU	C7-C8-N1	3.49	109.70	106.38
2	B	621	STU	C19-N3-C25	3.30	133.73	123.02
2	A	301	STU	C27-O6-C22	3.29	120.02	114.46
2	A	301	STU	C13-C12-C11	-3.01	126.34	133.49
2	B	621	STU	C7-C6-C19	2.85	122.82	118.04
2	B	621	STU	C13-C12-C11	-2.79	126.85	133.49
2	B	621	STU	C15-C14-C13	-2.72	116.89	120.24
2	A	301	STU	C12-C11-C10	2.71	137.26	132.33
2	B	621	STU	C3-C2-C1	-2.71	116.89	120.24
2	A	301	STU	C19-C18-N2	-2.69	129.09	131.38
2	A	301	STU	C19-N3-C25	2.67	131.70	123.02
2	A	301	STU	C4-C5-C6	-2.61	127.28	133.49
2	B	621	STU	C18-N2-C17	-2.61	104.21	107.37
2	B	621	STU	C13-C12-C17	2.53	122.16	119.24
2	B	621	STU	C16-C17-C12	-2.46	118.71	121.59
2	B	621	STU	C9-N1-C8	-2.38	111.69	113.86
2	A	301	STU	C6-C7-C10	-2.36	119.12	120.76
2	B	621	STU	C11-C18-N2	2.35	111.93	109.38
2	B	621	STU	C14-C15-C16	2.30	123.07	120.24
2	A	301	STU	C18-N2-C17	-2.27	104.62	107.37
2	B	621	STU	O5-C8-C7	-2.23	125.24	128.47
2	A	301	STU	C6-C19-C18	-2.16	116.09	121.25
2	B	621	STU	C18-C11-C10	-2.15	117.23	119.77
2	B	621	STU	C12-C11-C18	-2.08	103.51	106.44

There are no chirality outliers.

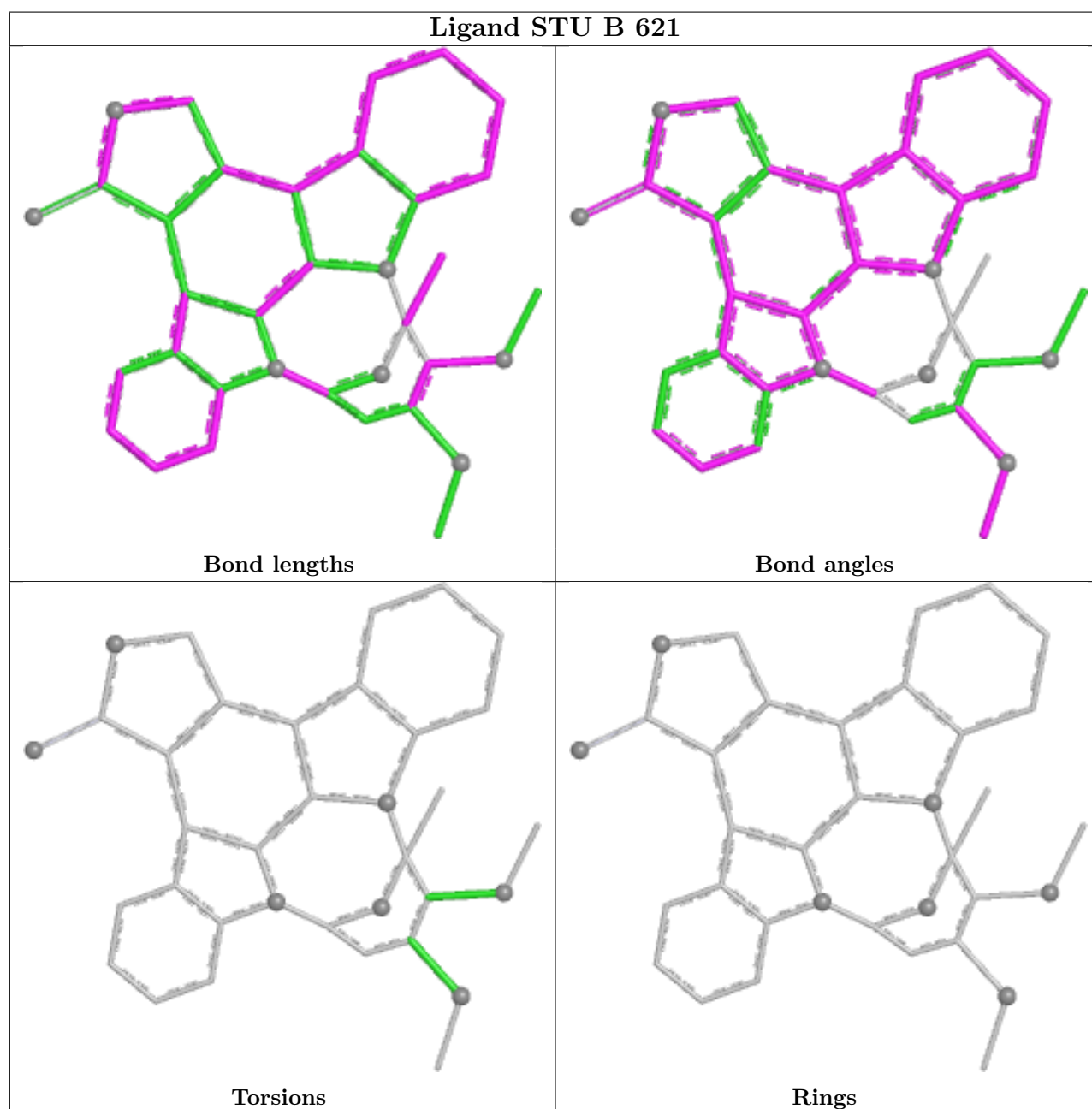
There are no torsion outliers.

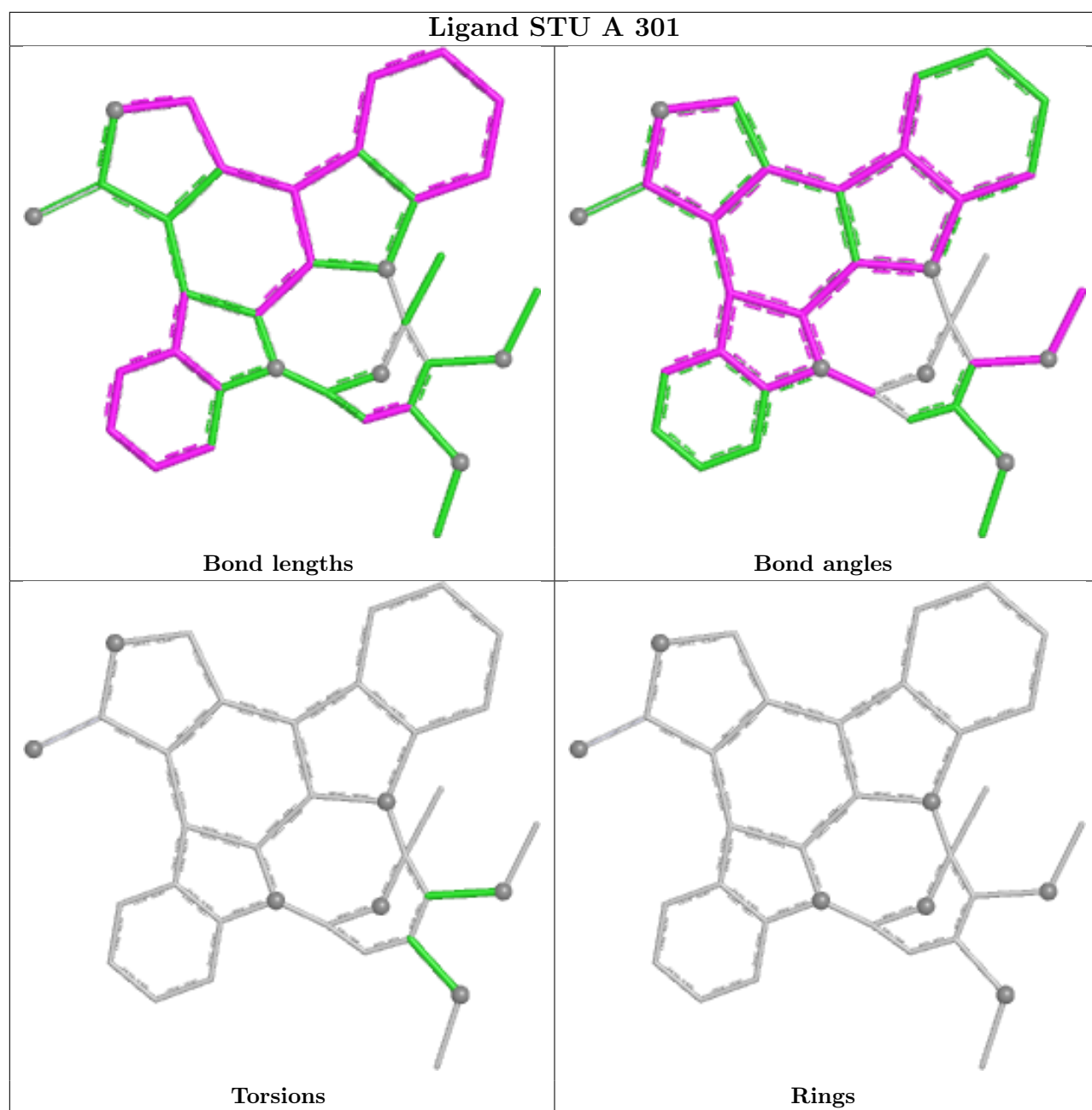
There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.