



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:15 PM UTC

PDB ID : 2OIQ / pdb_00002oiq
Title : Crystal Structure of chicken c-Src kinase domain in complex with the cancer drug imatinib.
Authors : Seeliger, M.A.; Nagar, B.; Frank, F.; Cao, X.; Henderson, M.N.; Kuriyan, J.
Deposited on : 2007-01-11
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

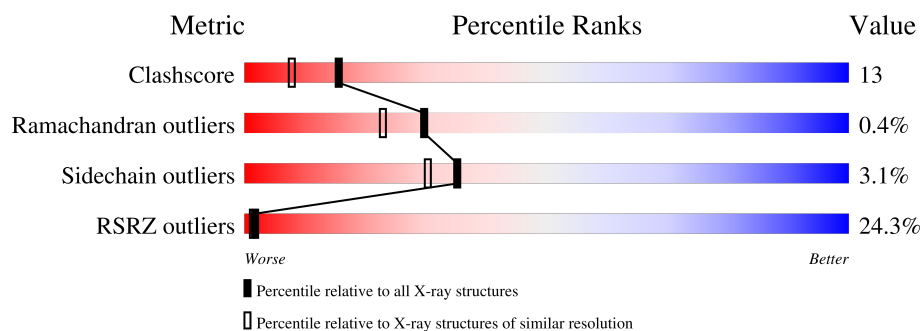
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	20% 68% 23% 7%
1	B	286	25% 65% 26% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4560 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.

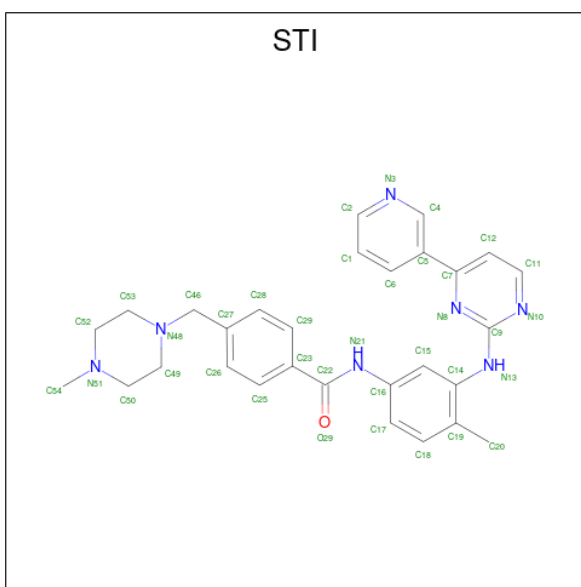
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2126	1365	355	389	17			
1	B	265	Total	C	N	O	S	0	0	0
			2135	1371	356	391	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	cloning artifact	UNP P00523
A	249	HIS	-	cloning artifact	UNP P00523
A	250	MET	-	initiating methionine	UNP P00523
B	248	GLY	-	cloning artifact	UNP P00523
B	249	HIS	-	cloning artifact	UNP P00523
B	250	MET	-	initiating methionine	UNP P00523

- Molecule 2 is 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE (CCD ID: STI) (formula: C₂₉H₃₁N₇O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	29	7	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

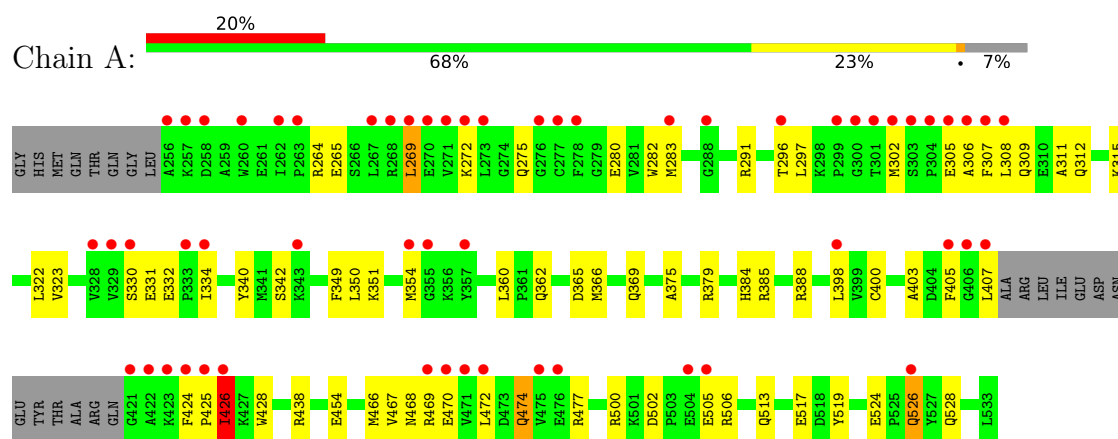
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total 136	O 136	0	0
4	B	114	Total 114	O 114	0	0

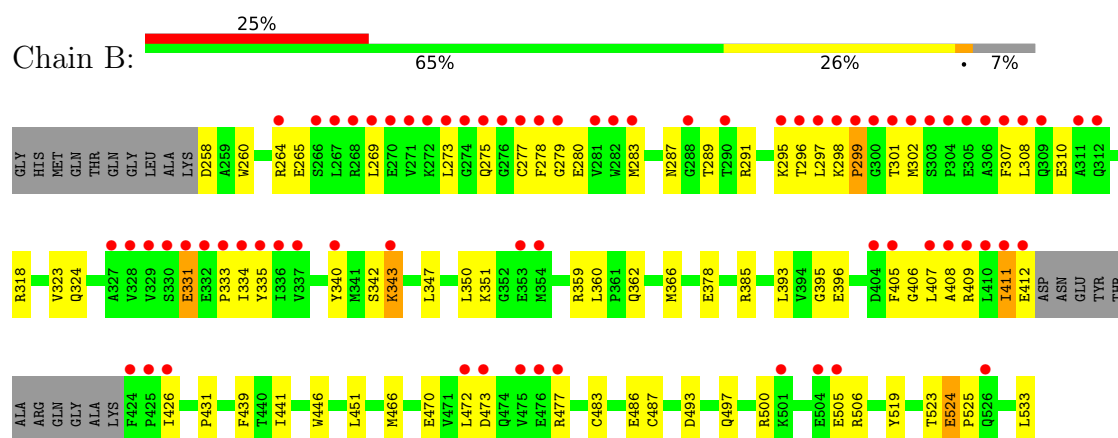
3 Residue-property plots [i](#)

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 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.

- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.08Å 63.37Å 74.47Å 78.99° 89.12° 90.10°	Depositor
Resolution (Å)	50.00 – 2.07 50.00 – 2.07	Depositor EDS
% Data completeness (in resolution range)	93.5 (50.00-2.07) 96.8 (50.00-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.263 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4560	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.42	0/2178	0.91	5/2947 (0.2%)
1	B	0.41	0/2187	0.88	5/2961 (0.2%)
All	All	0.42	0/4365	0.90	10/5908 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	SER	N-CA-C	7.22	120.99	111.75
1	B	524	GLU	CA-C-N	7.16	127.16	119.28
1	B	524	GLU	C-N-CA	7.16	127.16	119.28
1	A	519	TYR	N-CA-C	6.52	122.13	111.37
1	B	519	TYR	N-CA-C	6.31	121.77	111.37
1	A	330	SER	N-CA-C	5.44	119.79	113.20
1	A	474	GLN	N-CA-C	5.43	116.89	111.07
1	A	426	ILE	N-CA-C	5.40	116.78	110.62
1	A	506	ARG	N-CA-C	5.38	115.78	109.60
1	B	343	LYS	N-CA-C	5.10	118.53	112.72

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	2126	0	2115	58	0
1	B	2135	0	2122	57	0
2	A	37	0	31	0	0
3	A	12	0	16	0	0
4	A	136	0	0	1	0
4	B	114	0	0	3	0
All	All	4560	0	4284	115	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 13.

All (115) 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:500:ARG:HD3	1:B:505:GLU:HG2	1.52	0.91
1:A:500:ARG:HD3	1:A:505:GLU:HB3	1.55	0.89
1:A:275:GLN:HG2	1:A:280:GLU:HG2	1.55	0.87
1:B:426:ILE:HG12	1:B:472:LEU:HG	1.62	0.81
1:A:524:GLU:HG3	1:A:526:GLN:HE22	1.48	0.79
1:A:306:ALA:HA	1:A:309:GLN:HE21	1.48	0.77
1:B:278:PHE:HA	1:B:301:THR:HG21	1.71	0.72
1:A:526:GLN:CD	1:A:526:GLN:H	1.98	0.72
1:A:398:LEU:HD12	1:A:398:LEU:N	2.08	0.69
1:A:524:GLU:HG3	1:A:526:GLN:NE2	2.11	0.65
1:A:332:GLU:HA	1:A:334:ILE:HD12	1.78	0.64
1:A:524:GLU:CG	1:A:526:GLN:HE22	2.10	0.64
1:B:298:LYS:HB3	1:B:301:THR:OG1	1.98	0.63
1:A:305:GLU:O	1:A:309:GLN:HG3	1.99	0.63
1:A:323:VAL:HG21	1:A:403:ALA:HB2	1.80	0.63
1:A:283:MET:HG3	1:A:340:TYR:CE1	2.34	0.62
1:A:405:PHE:HB2	1:A:407:LEU:HG	1.82	0.62
1:A:388:ARG:NH1	1:A:425:PRO:HB3	2.13	0.62
1:A:477:ARG:HB2	1:A:477:ARG:NH1	2.15	0.62
1:B:323:VAL:HG21	1:B:393:LEU:HD12	1.82	0.62
1:B:264:ARG:NH2	1:B:331:GLU:O	2.33	0.61
1:A:311:ALA:O	1:A:315:LYS:HG3	2.01	0.60
1:A:351:LYS:HE3	4:B:534:HOH:O	2.03	0.58
1:B:287:ASN:O	1:B:289:THR:HG23	2.03	0.58
1:B:523:THR:C	1:B:525:PRO:HD3	2.28	0.58
1:B:493:ASP:O	1:B:497:GLN:HG3	2.03	0.58
1:B:359:ARG:H	1:B:362:GLN:NE2	2.02	0.58
1:B:343:LYS:HD3	1:B:395:GLY:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:HE2	1:A:275:GLN:HG3	1.87	0.57
1:A:502:ASP:HB3	1:A:505:GLU:HG3	1.86	0.56
1:B:359:ARG:H	1:B:362:GLN:HE21	1.51	0.56
1:A:467:VAL:HG22	1:A:470:GLU:HG2	1.87	0.56
1:B:385:ARG:HD3	1:B:407:LEU:O	2.06	0.56
1:B:277:CYS:O	1:B:301:THR:HG21	2.06	0.56
1:B:486:GLU:HG2	4:B:594:HOH:O	2.04	0.56
1:B:308:LEU:HD21	1:B:334:ILE:CG2	2.35	0.55
1:B:466:MET:HE3	1:B:470:GLU:HG2	1.88	0.55
1:B:278:PHE:CE1	1:B:295:LYS:HE3	2.42	0.55
1:B:409:ARG:HH21	1:B:439:PHE:HB2	1.72	0.54
1:A:296:THR:HG22	1:A:297:LEU:N	2.24	0.53
1:B:258:ASP:OD1	1:B:260:TRP:HB2	2.08	0.53
1:B:473:ASP:O	1:B:477:ARG:HG3	2.08	0.53
1:B:500:ARG:HD3	1:B:505:GLU:CG	2.33	0.53
1:A:264:ARG:NH2	1:A:331:GLU:O	2.42	0.52
1:A:291:ARG:HG3	1:A:291:ARG:HH11	1.75	0.51
1:A:388:ARG:HH12	1:A:425:PRO:HB3	1.75	0.51
1:A:477:ARG:HB2	1:A:477:ARG:HH11	1.76	0.51
1:B:405:PHE:HD1	1:B:408:ALA:CB	2.23	0.51
1:A:265:GLU:H	1:A:265:GLU:CD	2.19	0.50
1:B:297:LEU:HB2	1:B:307:PHE:CE2	2.47	0.50
1:B:405:PHE:HD1	1:B:408:ALA:HB2	1.76	0.50
1:B:483:CYS:SG	1:B:487:CYS:O	2.69	0.50
1:B:524:GLU:N	1:B:525:PRO:HD3	2.26	0.50
1:B:265:GLU:H	1:B:265:GLU:CD	2.20	0.49
1:B:264:ARG:HE	1:B:333:PRO:HG2	1.76	0.49
1:B:318:ARG:HD3	1:B:324:GLN:OE1	2.12	0.49
1:B:296:THR:HG22	1:B:297:LEU:N	2.27	0.49
1:B:283:MET:HE3	1:B:291:ARG:NH1	2.27	0.49
1:B:331:GLU:C	1:B:334:ILE:HD13	2.38	0.49
1:A:362:GLN:O	1:A:366:MET:HG3	2.12	0.49
1:A:513:GLN:O	1:A:517:GLU:HG3	2.12	0.48
1:A:524:GLU:OE2	1:A:526:GLN:NE2	2.46	0.48
1:A:269:LEU:HD22	1:A:269:LEU:N	2.28	0.48
1:B:331:GLU:HA	1:B:331:GLU:OE1	2.14	0.48
1:A:384:HIS:O	1:A:385:ARG:HB2	2.14	0.48
1:B:431:PRO:HG2	4:B:635:HOH:O	2.14	0.48
1:A:306:ALA:HA	1:A:309:GLN:NE2	2.22	0.48
1:A:466:MET:HA	1:A:470:GLU:OE1	2.13	0.48
1:A:323:VAL:CG2	1:A:403:ALA:HB2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLN:CD	1:A:526:GLN:N	2.68	0.47
1:A:308:LEU:O	1:A:312:GLN:HG2	2.15	0.47
1:B:409:ARG:NH2	1:B:439:PHE:O	2.48	0.46
1:A:269:LEU:HD12	1:A:282:TRP:CG	2.50	0.46
1:A:398:LEU:N	1:A:398:LEU:CD1	2.78	0.46
1:B:426:ILE:HG12	1:B:472:LEU:CG	2.41	0.46
1:B:269:LEU:N	1:B:269:LEU:HD12	2.31	0.46
1:B:347:LEU:O	1:B:351:LYS:HG2	2.16	0.46
1:B:301:THR:HG22	1:B:302:MET:HG3	1.97	0.45
1:B:278:PHE:CD1	1:B:279:GLY:N	2.84	0.45
1:A:365:ASP:O	1:A:369:GLN:HG3	2.17	0.45
1:A:477:ARG:HH11	1:A:477:ARG:CB	2.29	0.45
1:B:283:MET:HE3	1:B:291:ARG:HH11	1.80	0.45
1:B:310:GLU:HB2	1:B:406:GLY:HA2	1.99	0.44
1:B:378:GLU:HG3	1:B:441:ILE:HG12	1.98	0.44
1:A:469:ARG:HH11	1:A:469:ARG:HG2	1.82	0.44
1:B:497:GLN:O	1:B:506:ARG:HG3	2.18	0.44
1:B:451:LEU:O	1:B:451:LEU:HD23	2.17	0.43
1:A:302:MET:HE2	1:A:307:PHE:CA	2.48	0.43
1:B:362:GLN:O	1:B:366:MET:HG3	2.18	0.43
1:A:269:LEU:HD12	1:A:282:TRP:HB2	2.00	0.43
1:A:332:GLU:HB2	4:A:1118:HOH:O	2.19	0.43
1:B:385:ARG:HD2	1:B:409:ARG:HG2	2.00	0.43
1:B:273:LEU:HD11	1:B:340:TYR:HE1	1.84	0.42
1:A:332:GLU:CA	1:A:334:ILE:HD12	2.45	0.42
1:B:486:GLU:HB2	1:B:533:LEU:HD12	2.02	0.42
1:A:426:ILE:HD13	1:A:472:LEU:HD21	2.00	0.42
1:A:375:ALA:O	1:A:379:ARG:HG3	2.19	0.42
1:B:359:ARG:HB2	1:B:362:GLN:HE22	1.85	0.42
1:A:384:HIS:O	1:A:385:ARG:CB	2.68	0.41
1:B:279:GLY:HA3	1:B:296:THR:O	2.20	0.41
1:A:428:TRP:HE1	1:A:454:GLU:CD	2.28	0.41
1:A:466:MET:CE	1:A:474:GLN:HG3	2.50	0.41
1:A:269:LEU:N	1:A:269:LEU:CD2	2.83	0.41
1:A:349:PHE:CE1	1:A:354:MET:HG3	2.56	0.41
1:B:331:GLU:N	1:B:334:ILE:HD13	2.36	0.41
1:A:426:ILE:HG21	1:A:468:ASN:CG	2.46	0.41
1:B:334:ILE:O	1:B:335:TYR:HD2	2.02	0.41
1:B:411:ILE:O	1:B:412:GLU:HG3	2.21	0.41
1:B:446:TRP:CD1	1:B:446:TRP:C	2.98	0.41
1:A:426:ILE:O	1:A:426:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ILE:HG23	1:A:468:ASN:OD1	2.21	0.41
1:A:438:ARG:HB2	1:A:438:ARG:HH11	1.86	0.41
1:A:296:THR:CG2	1:A:297:LEU:N	2.84	0.40
1:A:366:MET:HE2	1:A:400:CYS:SG	2.62	0.40
1:B:275:GLN:HG2	1:B:280:GLU:HG2	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	261/286 (91%)	251 (96%)	9 (3%)	1 (0%)	30	23
1	B	261/286 (91%)	246 (94%)	14 (5%)	1 (0%)	30	23
All	All	522/572 (91%)	497 (95%)	23 (4%)	2 (0%)	30	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	PRO
1	A	342	SER

5.3.2 Protein sidechains [i](#)

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	228/245 (93%)	220 (96%)	8 (4%)	32	26
1	B	230/245 (94%)	224 (97%)	6 (3%)	40	37
All	All	458/490 (94%)	444 (97%)	14 (3%)	35	30

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	LEU
1	A	322	LEU
1	A	350	LEU
1	A	360	LEU
1	A	424	PHE
1	A	426	ILE
1	A	526	GLN
1	A	528	GLN
1	B	299	PRO
1	B	331	GLU
1	B	350	LEU
1	B	360	LEU
1	B	396	GLU
1	B	411	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	GLN
1	A	381	ASN
1	A	397	ASN
1	B	362	GLN
1	B	381	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
3	GOL	A	1002	-	5,5,5	0.31	0	5,5,5	0.34	0
2	STI	A	1001	-	41,41,41	2.49	25 (60%)	56,56,56	2.03	9 (16%)
3	GOL	A	1003	-	5,5,5	0.31	0	5,5,5	0.31	0

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
3	GOL	A	1002	-	-	0/4/4/4	-
2	STI	A	1001	-	-	2/20/30/30	0/5/5/5
3	GOL	A	1003	-	-	0/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	STI	C25-C23	5.21	1.47	1.39
2	A	1001	STI	C15-C16	4.10	1.46	1.39
2	A	1001	STI	C26-C25	3.99	1.45	1.38
2	A	1001	STI	C26-C27	3.83	1.46	1.38
2	A	1001	STI	C14-C19	3.68	1.48	1.40
2	A	1001	STI	C17-C18	3.49	1.44	1.38
2	A	1001	STI	C29-C23	3.49	1.44	1.39
2	A	1001	STI	C4-C5	3.41	1.45	1.39
2	A	1001	STI	C6-C5	3.24	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	STI	C28-C27	3.19	1.45	1.38
2	A	1001	STI	C1-C6	3.04	1.44	1.38
2	A	1001	STI	C9-N10	2.96	1.38	1.34
2	A	1001	STI	C50-N51	2.79	1.53	1.46
2	A	1001	STI	C17-C16	2.59	1.43	1.39
2	A	1001	STI	C2-N3	2.40	1.40	1.33
2	A	1001	STI	C52-N51	2.38	1.52	1.46
2	A	1001	STI	C49-N48	2.29	1.53	1.46
2	A	1001	STI	C12-C7	2.28	1.44	1.39
2	A	1001	STI	C20-C19	2.25	1.55	1.51
2	A	1001	STI	C7-N8	2.25	1.38	1.34
2	A	1001	STI	C1-C2	2.16	1.43	1.37
2	A	1001	STI	C11-N10	2.15	1.39	1.34
2	A	1001	STI	C12-C11	2.10	1.42	1.38
2	A	1001	STI	C18-C19	2.08	1.44	1.39
2	A	1001	STI	C4-N3	2.08	1.38	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	STI	C7-N8-C9	7.33	122.45	116.81
2	A	1001	STI	N10-C9-N8	-7.03	119.62	126.42
2	A	1001	STI	C11-N10-C9	6.67	120.99	115.42
2	A	1001	STI	C2-N3-C4	3.33	122.68	116.85
2	A	1001	STI	C12-C11-N10	-3.02	120.28	123.97
2	A	1001	STI	C27-C46-N48	2.54	118.35	113.15
2	A	1001	STI	C14-N13-C9	-2.31	122.18	129.22
2	A	1001	STI	N13-C9-N10	2.29	122.79	116.29
2	A	1001	STI	C20-C19-C14	2.01	123.50	121.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

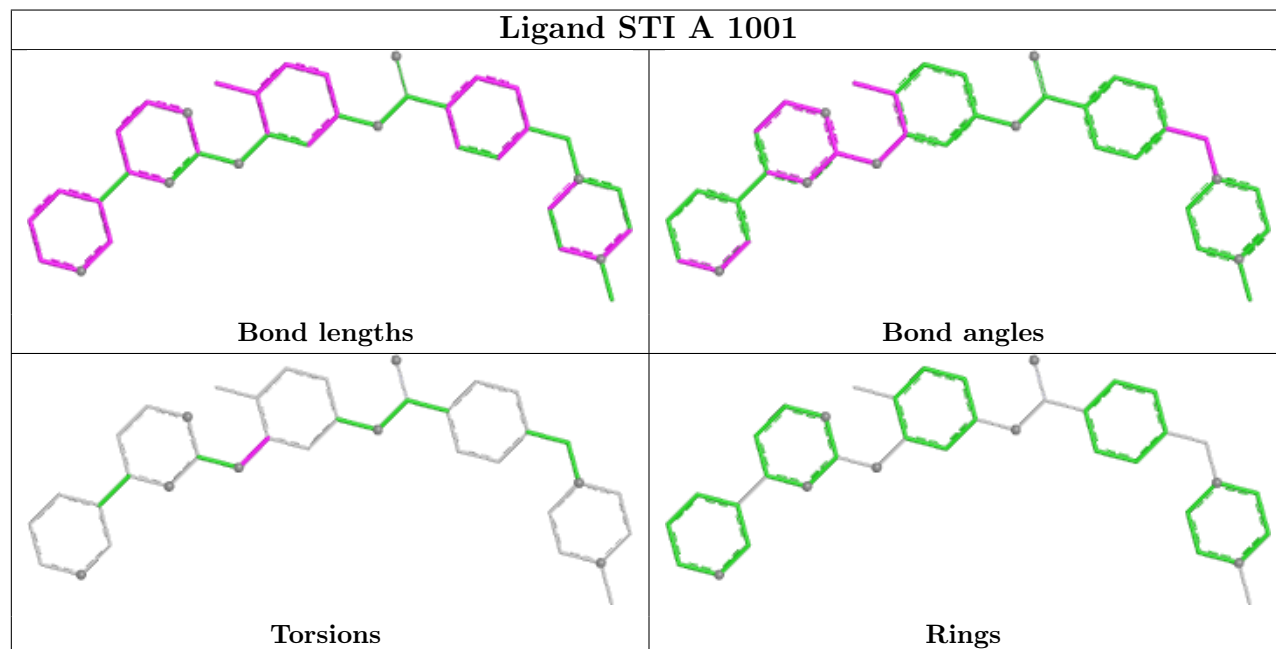
Mol	Chain	Res	Type	Atoms
2	A	1001	STI	C19-C14-N13-C9
2	A	1001	STI	C15-C14-N13-C9

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/286 (92%)	1.10	57 (21%) 2 2	21, 36, 66, 88	0
1	B	265/286 (92%)	1.34	72 (27%) 1 1	20, 37, 90, 104	0
All	All	530/572 (92%)	1.22	129 (24%) 2 1	20, 37, 80, 104	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	LEU	6.7
1	A	422	ALA	6.6
1	B	278	PHE	6.6
1	B	273	LEU	6.3
1	A	256	ALA	5.6
1	B	411	ILE	5.5
1	A	424	PHE	5.5
1	B	297	LEU	5.1
1	B	306	ALA	4.9
1	B	426	ILE	4.8
1	B	277	CYS	4.8
1	B	272	LYS	4.6
1	B	269	LEU	4.4
1	B	296	THR	4.3
1	A	426	ILE	4.3
1	B	307	PHE	4.3
1	B	328	VAL	4.2
1	B	409	ARG	4.2
1	A	476	GLU	4.1
1	A	269	LEU	4.0
1	B	303	SER	4.0
1	B	407	LEU	4.0
1	A	307	PHE	3.9
1	B	410	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	334	ILE	3.9
1	B	283	MET	3.9
1	B	472	LEU	3.9
1	B	274	GLY	3.8
1	A	423	LYS	3.8
1	B	405	PHE	3.8
1	B	271	VAL	3.7
1	B	282	TRP	3.6
1	B	267	LEU	3.6
1	B	302	MET	3.6
1	A	475	VAL	3.6
1	B	281	VAL	3.6
1	A	305	GLU	3.4
1	B	279	GLY	3.4
1	B	299	PRO	3.4
1	A	405	PHE	3.4
1	B	404	ASP	3.4
1	B	270	GLU	3.3
1	B	334	ILE	3.3
1	A	472	LEU	3.3
1	B	501	LYS	3.3
1	B	304	PRO	3.3
1	A	304	PRO	3.3
1	B	276	GLY	3.2
1	B	300	GLY	3.2
1	A	421	GLY	3.2
1	B	268	ARG	3.2
1	A	406	GLY	3.2
1	A	343	LYS	3.2
1	B	475	VAL	3.1
1	A	257	LYS	3.1
1	A	505	GLU	3.1
1	B	309	GLN	3.1
1	B	329	VAL	3.1
1	B	424	PHE	3.1
1	B	311	ALA	3.0
1	B	354	MET	3.0
1	A	306	ALA	3.0
1	B	332	GLU	3.0
1	A	354	MET	2.9
1	B	330	SER	2.9
1	B	353	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	505	GLU	2.8
1	A	355	GLY	2.8
1	B	476	GLU	2.8
1	A	425	PRO	2.8
1	A	526	GLN	2.8
1	A	357	TYR	2.8
1	B	305	GLU	2.8
1	A	277	CYS	2.8
1	A	283	MET	2.7
1	B	301	THR	2.7
1	A	300	GLY	2.7
1	B	288	GLY	2.7
1	A	268	ARG	2.7
1	A	398	LEU	2.7
1	B	337	VAL	2.7
1	A	273	LEU	2.7
1	B	308	LEU	2.7
1	B	275	GLN	2.6
1	B	408	ALA	2.6
1	B	425	PRO	2.6
1	B	335	TYR	2.6
1	B	477	ARG	2.6
1	B	336	ILE	2.6
1	A	504	GLU	2.5
1	B	331	GLU	2.5
1	A	299	PRO	2.5
1	B	340	TYR	2.5
1	A	263	PRO	2.5
1	A	330	SER	2.5
1	B	312	GLN	2.5
1	B	298	LYS	2.5
1	B	412	GLU	2.5
1	B	504	GLU	2.5
1	A	272	LYS	2.5
1	A	302	MET	2.4
1	A	301	THR	2.4
1	A	278	PHE	2.4
1	A	303	SER	2.4
1	B	295	LYS	2.3
1	A	267	LEU	2.3
1	B	526	GLN	2.3
1	A	288	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	271	VAL	2.3
1	A	471	VAL	2.3
1	B	333	PRO	2.3
1	A	276	GLY	2.3
1	A	262	ILE	2.2
1	A	258	ASP	2.2
1	A	270	GLU	2.2
1	A	469	ARG	2.2
1	B	264	ARG	2.2
1	A	333	PRO	2.2
1	A	329	VAL	2.2
1	A	470	GLU	2.1
1	B	343	LYS	2.1
1	A	296	THR	2.1
1	A	308	LEU	2.1
1	A	260	TRP	2.1
1	B	473	ASP	2.0
1	B	290	THR	2.0
1	A	328	VAL	2.0
1	B	266	SER	2.0
1	B	327	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

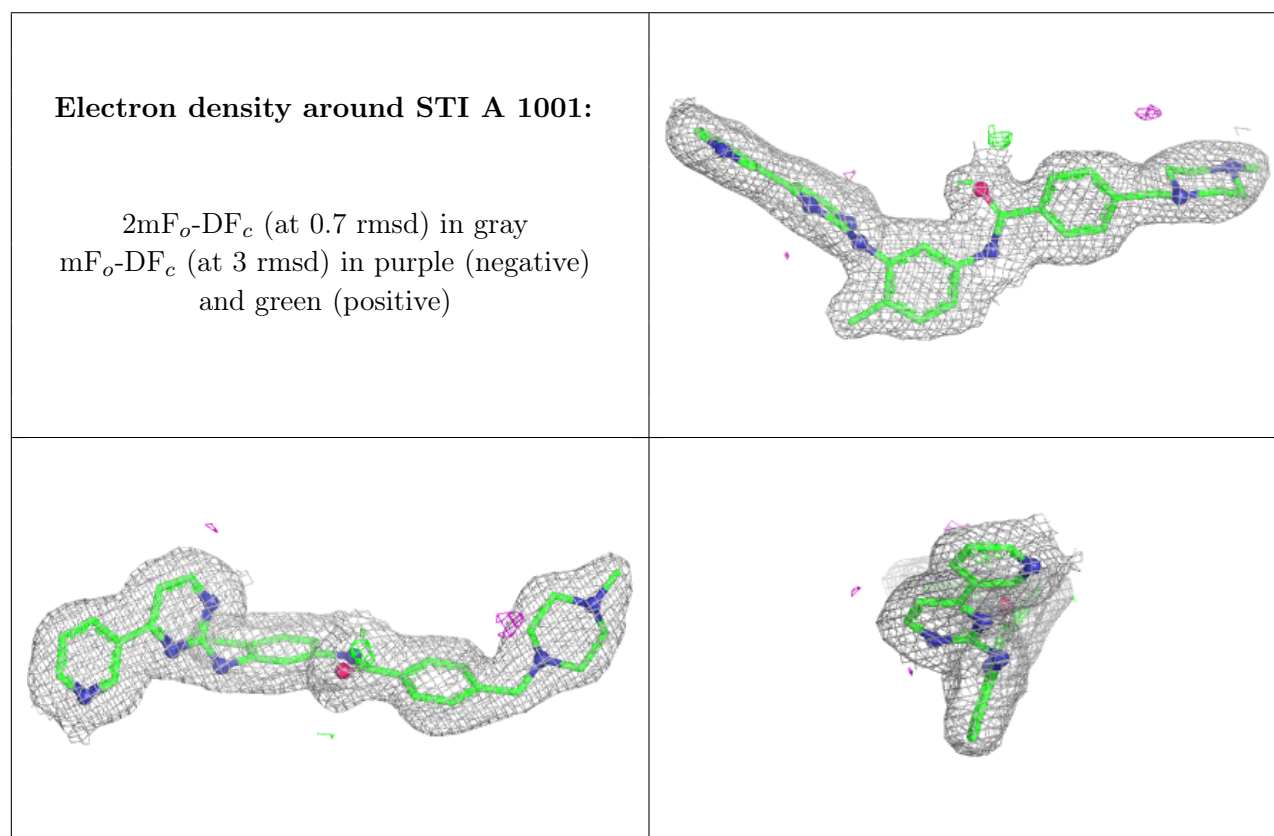
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1002	6/6	0.92	0.09	33,36,37,38	0
3	GOL	A	1003	6/6	0.92	0.11	45,46,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	STI	A	1001	37/37	0.93	0.09	26,33,40,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.