

Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 11:01 AM EDT

PDB ID : 3K5V

Title : Structure of Abl kinase in complex with imatinib and GNF-2 Authors : Cowan-Jacob, S.W.; Fendrich, G.; Rummel, G.; Strauss, A.

Deposited on : 2009-10-08

Resolution : 1.74 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

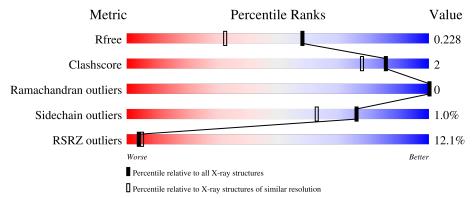
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.74 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 <=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	293	91%	7%	·
1	В	293	91%	5%	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5194 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 ABL1.

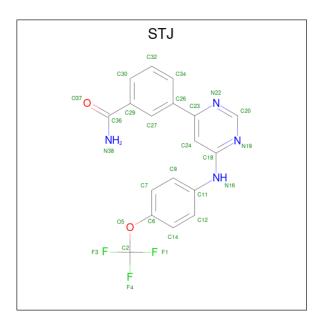
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	286	Total 2337	C 1501	N 377	O 441	S 18	0	3	0
1	В	283	Total 2299	C 1478	N 372	O 431	S 18	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLY	=	expression tag	UNP P00520
A	243	ALA	-	expression tag	UNP P00520
A	244	MET	-	expression tag	UNP P00520
A	245	ASP	ı	expression tag	UNP P00520
A	246	PRO	-	expression tag	UNP P00520
A	247	SER	-	expression tag	UNP P00520
В	242	GLY	-	expression tag	UNP P00520
В	243	ALA	-	expression tag	UNP P00520
В	244	MET	-	expression tag	UNP P00520
В	245	ASP	-	expression tag	UNP P00520
В	246	PRO	-	expression tag	UNP P00520
В	247	SER	-	expression tag	UNP P00520

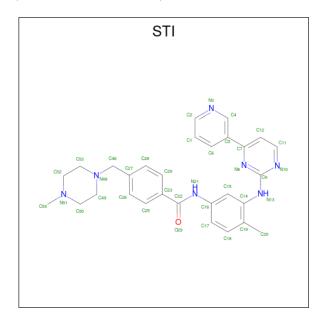
• Molecule 2 is 3-(6-{[4-(trifluoromethoxy)phenyl]amino}pyrimidin-4-yl)benzamide (three-letter code: STJ) (formula: $C_{18}H_{13}F_3N_4O_2$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
9	٨	1	Total	С	F	N	О	0	0	
2 A	1	27	18	3	4	2	U			
9	2 B	D	1	Total	С	F	N	О	0	0
2		1	27	18	3	4	2	U		

• Molecule 3 is 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRID IN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE (three-letter code: STI) (formula: $C_{29}H_{31}N_7O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	Λ	1	Total	С	N	О	0	0
3	A	1	37	29	7	1	0	0



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\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf
3	В	1	Total 37	C 29	N 7	O 1	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

• Molecule 5 is water.

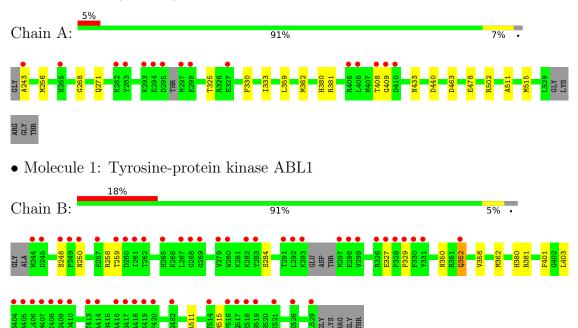
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	282	Total O 282 282	0	0
5	В	147	Total O 147 147	0	0



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: Tyrosine-protein kinase ABL1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	42.07Å 65.27Å 66.26Å	Donositor
a, b, c, α , β , γ	72.82° 80.25° 84.86°	Depositor
Resolution (Å)	38.95 - 1.74	Depositor
Resolution (A)	38.94 - 1.74	EDS
% Data completeness	95.4 (38.95-1.74)	Depositor
(in resolution range)	95.4 (38.94-1.74)	EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	3.28 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
D D.	0.199 , 0.231	Depositor
R, R_{free}	0.196 , 0.228	DCC
R_{free} test set	3247 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 58.8	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5194	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.79% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: CL, STI, STJ

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.56	0/2401	0.65	2/3248 (0.1%)	
1	В	0.42	0/2357	0.55	0/3188	
All	All	0.49	0/4758	0.61	2/6436 (0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	440	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	502	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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	2337	0	2283	9	0
1	В	2299	0	2247	9	0
2	A	27	0	13	1	0
2	В	27	0	13	1	0
3	A	37	0	31	1	0
3	В	37	0	31	0	0
4	A	1	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	282	0	0	2	0
5	В	147	0	0	2	0
All	All	5194	0	4618	21	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 2.

All (21) 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:511:ALA:O	1:B:515:MET:HB2	1.98	0.64
1:B:352:GLN:HG3	5:B:542:HOH:O	2.04	0.58
1:B:350:ASN:HB3	5:B:542:HOH:O	2.02	0.58
1:A:243:ALA:N	5:A:693:HOH:O	2.37	0.56
1:B:258:ARG:NH1	1:B:329:PRO:O	2.39	0.56
1:A:256:MET:SD	1:A:333:ILE:HD13	2.47	0.55
2:A:1:STJ:N19	2:A:1:STJ:H9	2.23	0.54
1:A:380:HIS:O	1:A:381:ARG:HB2	2.09	0.52
1:B:248:SER:OG	1:B:250:ASN:OD1	2.17	0.49
1:B:380:HIS:O	1:B:381:ARG:HB2	2.15	0.47
1:A:268:GLY:O	1:A:271:GLN:HG2	2.15	0.46
2:B:1:STJ:N19	2:B:1:STJ:H9	2.32	0.45
1:A:478:GLU:HG2	5:A:87:HOH:O	2.16	0.45
1:A:511:ALA:O	1:A:515:MET:HB2	2.17	0.44
1:B:258:ARG:NH2	1:B:327:GLU:O	2.51	0.44
1:A:408:THR:HG22	1:A:409:GLY:N	2.33	0.43
1:A:359:LEU:HA	1:A:362:MET:HE2	2.00	0.43
1:A:325:THR:HA	1:A:330:PHE:CD2	2.54	0.42
1:B:358:VAL:O	1:B:362:MET:HG3	2.19	0.42
1:B:401:PHE:HB2	1:B:403:LEU:HG	2.02	0.41
3:A:2:STI:O29	3:A:2:STI:H151	2.21	0.41

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	Perce	${f ntiles}$
1	A	$285/293 \ (97\%)$	276 (97%)	9 (3%)	0	100	100
1	В	$279/293 \; (95\%)$	269 (96%)	10 (4%)	0	100	100
All	All	564/586 (96%)	545 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	$254/255 \ (100\%)$	251 (99%)	3 (1%)	71	56	
1	В	$249/255 \ (98\%)$	246 (99%)	3 (1%)	71	56	
All	All	503/510 (99%)	497 (99%)	6 (1%)	76	56	

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	433[A]	ASN
1	A	433[B]	ASN
1	A	463	ASP
1	В	259	THR
1	В	284	SER
1	В	352	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	433	ASN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	Tuno	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	STJ	A	1	-	28,29,29	1.21	3 (10%)	37,41,41	1.72	8 (21%)
2	STJ	В	1	-	28,29,29	1.22	3 (10%)	37,41,41	1.69	7 (18%)
3	STI	A	2	-	40,41,41	1.10	2 (5%)	51,56,56	1.97	6 (11%)
3	STI	В	2	-	40,41,41	1.06	1 (2%)	51,56,56	1.83	6 (11%)

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	STJ	A	1	-	-	4/13/17/17	0/3/3/3
2	STJ	В	1	-	-	4/13/17/17	0/3/3/3
3	STI	A	2	-	-	1/16/30/30	0/5/5/5
3	STI	В	2	-	-	1/16/30/30	0/5/5/5



All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(A)
3	A	2	STI	C12-C11	3.13	1.40	1.36
3	В	2	STI	C12-C11	2.96	1.40	1.36
2	A	1	STJ	C20-N22	2.38	1.35	1.32
2	В	1	STJ	C20-N22	2.35	1.35	1.32
2	A	1	STJ	C11-N16	-2.30	1.35	1.40
2	В	1	STJ	O5-C2	2.25	1.44	1.31
3	A	2	STI	C4-N3	2.07	1.36	1.32
2	A	1	STJ	C32-C34	2.07	1.41	1.36
2	В	1	STJ	C27-C29	2.07	1.41	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	2	STI	C11-N10-C9	7.14	121.79	115.45
3	A	2	STI	N10-C9-N8	-7.01	119.75	126.52
3	В	2	STI	N10-C9-N8	-6.68	120.06	126.52
3	В	2	STI	C11-N10-C9	5.92	120.70	115.45
2	A	1	STJ	N22-C20-N19	-5.57	119.98	128.68
2	В	1	STJ	N22-C20-N19	-5.31	120.38	128.68
3	A	2	STI	C12-C11-N10	-4.79	119.09	123.81
2	В	1	STJ	C20-N22-C23	4.48	121.57	115.40
2	A	1	STJ	C20-N22-C23	4.28	121.30	115.40
3	В	2	STI	C9-N8-C7	3.99	122.10	115.60
3	В	2	STI	C12-C11-N10	-3.75	120.11	123.81
2	A	1	STJ	C29-C36-N38	3.69	122.18	117.75
2	В	1	STJ	C24-C23-N22	-3.67	118.52	121.54
3	A	2	STI	C9-N8-C7	3.50	121.30	115.60
2	В	1	STJ	C29-C36-N38	3.32	121.73	117.75
2	В	1	STJ	C24-C18-N19	-2.78	118.86	122.75
2	A	1	STJ	C24-C23-N22	-2.70	119.31	121.54
3	A	2	STI	C18-C19-C14	2.61	119.90	117.44
3	В	2	STI	C19-C14-N13	2.48	123.39	118.70
2	A	1	STJ	C24-C18-N19	-2.42	119.36	122.75
3	A	2	STI	C50-N51-C52	2.37	112.84	109.52
2	A	1	STJ	C27-C29-C36	-2.25	115.29	121.49
2	A	1	STJ	O37-C36-C29	-2.23	116.96	119.63
2	В	1	STJ	N16-C18-N19	2.13	123.30	116.81
2	A	1	STJ	N16-C18-N19	2.07	123.12	116.81
3	В	2	STI	C18-C19-C14	2.04	119.36	117.44
2	В	1	STJ	O37-C36-C29	-2.01	117.23	119.63

There are no chirality outliers.



All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	STI	C15-C14-N13-C9
3	В	2	STI	C15-C14-N13-C9
2	A	1	STJ	C27-C29-C36-O37
2	A	1	STJ	C27-C29-C36-N38
2	A	1	STJ	C30-C29-C36-N38
2	В	1	STJ	C27-C29-C36-O37
2	В	1	STJ	C27-C29-C36-N38
2	A	1	STJ	C30-C29-C36-O37
2	В	1	STJ	C30-C29-C36-O37
2	В	1	STJ	C30-C29-C36-N38

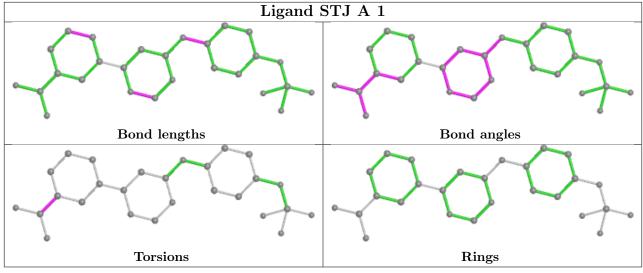
There are no ring outliers.

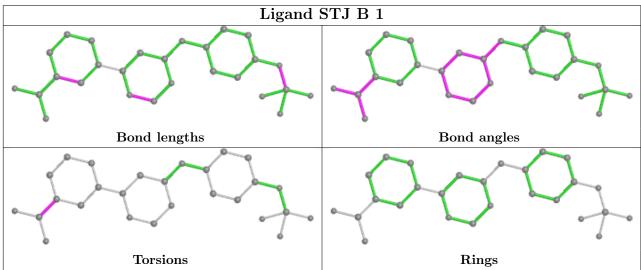
3 monomers are involved in 3 short contacts:

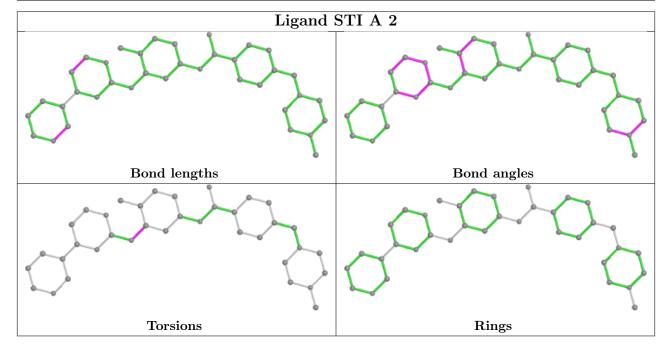
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	STJ	1	0
2	В	1	STJ	1	0
3	A	2	STI	1	0

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

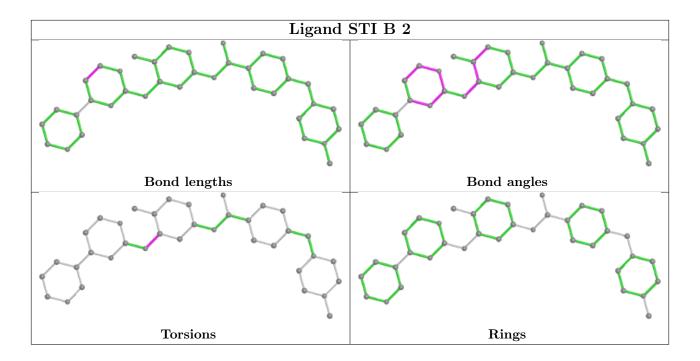












5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	$286/293 \ (97\%)$	0.32	15 (5%) 27 32	11, 23, 47, 64	0
1	В	283/293 (96%)	1.02	54 (19%) 1 1	19, 37, 61, 69	0
All	All	569/586 (97%)	0.67	69 (12%) 4 5	11, 30, 60, 69	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	406	LEU	8.6
1	В	407	MET	8.2
1	A	297	MET	6.9
1	В	408	THR	6.9
1	A	295	ASP	5.7
1	В	282	LYS	5.7
1	В	269	GLY	5.6
1	В	516	PHE	5.6
1	В	410	ASP	5.5
1	В	418	ALA	5.3
1	В	409	GLY	5.3
1	В	280	TRP	5.1
1	В	293	LYS	5.1
1	В	416	ALA	4.7
1	В	519	SER	4.5
1	В	327	GLU	4.3
1	В	292	LEU	4.3
1	В	518	GLU	4.3
1	В	249	PRO	4.1
1	A	408	THR	3.9
1	В	298	GLU	3.9
1	В	299	VAL	3.8
1	В	279	VAL	3.8
1	В	262	THR	3.7



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1 B 417 GLY 3.5 1 B 405 ARG 3.5 1 B 517 GLN 3.5 1 B 414 ALA 3.4 1 A 405 ARG 3.3 1 A 294 GLU 3.3 1 A 409 GLY 3.3 1 B 329 PRO 3.2 1 B 329 PRO 3.2 1 B 326 HIS 3.2 1 B 326 ARG 3.1 1 B 326 ARG 3.1 1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 268 GLY 3.1 1 B 352 GLN 3.0 1 B 352 GLN 3.0		nued fron Chain			
1 B 405 ARG 3.5 1 B 517 GLN 3.5 1 B 414 ALA 3.4 1 A 405 ARG 3.3 1 A 294 GLU 3.3 1 A 409 GLY 3.3 1 B 329 PRO 3.2 1 B 329 PRO 3.2 1 B 283 TYR 3.2 1 B 326 HIS 3.2 1 B 326 ARG 3.1 1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 268 GLY 3.1 1 B 352 GLN 3.0 1 B 352 GLN 3.0 1 B 352 GLN 3.0	Mol		Res	Type	RSRZ
1 B 517 GLN 3.5 1 B 414 ALA 3.4 1 A 405 ARG 3.3 1 A 294 GLU 3.3 1 A 409 GLY 3.3 1 B 329 PRO 3.2 1 B 329 PRO 3.2 1 B 283 TYR 3.2 1 B 265 HIS 3.2 1 B 326 ARG 3.1 1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 268 GLY 3.1 1 B 352 GLN 3.0 1 B 352 GLN 3.0 1 B 354 THR 3.0 1 B 354 THR 2.8					
1 B 414 ALA 3.4 1 A 405 ARG 3.3 1 A 294 GLU 3.3 1 A 409 GLY 3.3 1 B 329 PRO 3.2 1 B 329 PRO 3.2 1 B 283 TYR 3.2 1 B 265 HIS 3.2 1 B 326 ARG 3.1 1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 268 GLY 3.1 1 B 259 THR 3.1 1 B 352 GLN 3.0 1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 261 ILE 2.7					
1 A 405 ARG 3.3 1 A 294 GLU 3.3 1 A 409 GLY 3.3 1 B 329 PRO 3.2 1 B 329 PRO 3.2 1 B 283 TYR 3.2 1 A 265 HIS 3.2 1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 259 THR 3.1 1 B 352 GLN 3.0 1 B 352 GLN 3.0 1 B 354 THR 3.0 1 B 365 HIS 2.8 1 B 261 ILE 2.7 1 A 4					
1 A 294 GLU 3.3 1 A 409 GLY 3.3 1 B 329 PRO 3.2 1 B 283 TYR 3.2 1 A 265 HIS 3.2 1 B 326 ARG 3.1 1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 268 GLY 3.1 1 B 259 THR 3.1 1 B 259 THR 3.0 1 B 352 GLN 3.0 1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 514 THR 2.8 1 B 514 THR 2.8 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 2					
1 A 409 GLY 3.3 1 B 329 PRO 3.2 1 B 283 TYR 3.2 1 A 265 HIS 3.2 1 B 326 ARG 3.1 1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 268 GLY 3.1 1 B 259 THR 3.1 1 B 259 THR 3.0 1 B 352 GLN 3.0 1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 265 HIS 2.9 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 B 2					
1 B 329 PRO 3.2 1 B 283 TYR 3.2 1 A 265 HIS 3.2 1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 259 THR 3.1 1 B 413 THR 3.0 1 B 352 GLN 3.0 1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 265 HIS 2.9 1 B 514 THR 2.8 1 B 265 HIS 2.9 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 B 244 MET 2.6 1 B 2					
1 B 283 TYR 3.2 1 A 265 HIS 3.2 1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 259 THR 3.1 1 B 259 THR 3.0 1 B 352 GLN 3.0 1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 A 298 GLU 2.6 1 B 244 MET 2.6 1 B 2					
1 A 265 HIS 3.2 1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 259 THR 3.1 1 B 259 THR 3.0 1 B 352 GLN 3.0 1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 265 HIS 2.9 1 B 514 THR 2.8 1 B 265 HIS 2.9 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 248 SER 2.5 1 B 2					
1 B 326 ARG 3.1 1 B 268 GLY 3.1 1 B 259 THR 3.1 1 B 413 THR 3.0 1 B 352 GLN 3.0 1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 265 HIS 2.9 1 B 514 THR 2.8 1 B 265 HIS 2.9 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 282 LYS 2.7 1 A 298 GLU 2.6 1 A 298 GLU 2.6 1 B 244 MET 2.6 1 B 248 SER 2.6 1 B 248 SER 2.5 1 B 2					
1 B 268 GLY 3.1 1 B 259 THR 3.1 1 B 413 THR 3.0 1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 265 HIS 2.9 1 B 514 THR 2.8 1 A 410 ASP 2.8 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 A 298 GLU 2.6 1 B 244 MET 2.6 1 B 244 MET 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 4					
1 B 259 THR 3.1 1 B 413 THR 3.0 1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 514 THR 2.8 1 A 410 ASP 2.8 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 282 LYS 2.7 1 A 298 GLU 2.6 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 244 MET 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 B 413 THR 3.0 1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 514 THR 2.8 1 A 410 ASP 2.8 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 282 LYS 2.7 1 A 298 GLU 2.6 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 244 MET 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 B 352 GLN 3.0 1 B 265 HIS 2.9 1 B 514 THR 2.8 1 A 410 ASP 2.8 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 282 LYS 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 244 MET 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 B 265 HIS 2.9 1 B 514 THR 2.8 1 A 410 ASP 2.8 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 282 LYS 2.7 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 B 514 THR 2.8 1 A 410 ASP 2.8 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 282 LYS 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 A 410 ASP 2.8 1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 282 LYS 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 B 261 ILE 2.7 1 A 406 LEU 2.7 1 A 282 LYS 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 A 406 LEU 2.7 1 A 282 LYS 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 A 282 LYS 2.7 1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 A 243 ALA 2.7 1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 A 298 GLU 2.6 1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 A 293 LYS 2.6 1 B 244 MET 2.6 1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5	1				2.7
1 B 244 MET 2.6 1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 B 404 SER 2.6 1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 B 248 SER 2.5 1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					2.6
1 B 260 ASP 2.5 1 B 521 ILE 2.5 1 B 482 GLY 2.5					
1 B 521 ILE 2.5 1 B 482 GLY 2.5	1	В	248		
1 B 482 GLY 2.5	1				
	1	В	521	ILE	2.5
1 D 100 DITE 0.1	1	В	482	GLY	2.5
	1	В	420	PHE	2.4
1 B 250 ASN 2.4	1	В	250	ASN	2.4
1 B 267 LEU 2.3	1	В	267	LEU	2.3
1 B 328 PRO 2.3	1	В	328	PRO	2.3
1 A 283 TYR 2.3	1	A	283	TYR	2.3
1 B 291 THR 2.3	1	В	291	THR	2.3
1 B 526 GLU 2.3	1	В	526	GLU	2.3
1 A 327 GLU 2.2	1	A	327	GLU	2.2
1 B 331 TYR 2.2	1	В	331	TYR	2.2
1 B 257 GLU 2.1	1	В	257	GLU	2.1
1 B 419 LYS 2.1	1	В		LYS	2.1
1 D 220 DIIE 2.0	1	В	330	PHE	2.0



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Mol	Chain	Res	Type	RSRZ
1	В	245	ASP	2.0
1	В	297	MET	2.0
1	В	529	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

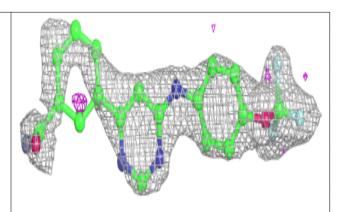
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	STJ	В	1	27/27	0.77	0.24	49,62,68,68	0
2	STJ	A	1	27/27	0.94	0.10	23,26,42,44	0
3	STI	В	2	37/37	0.96	0.09	24,27,32,34	0
3	STI	A	2	37/37	0.97	0.09	16,19,23,24	0
4	CL	A	5	1/1	0.97	0.09	33,33,33,33	0

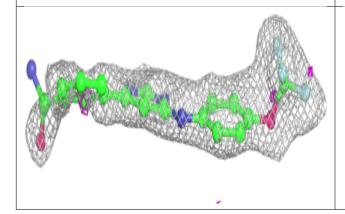
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

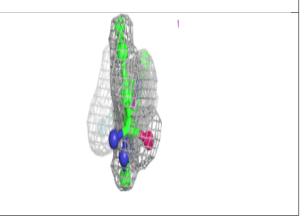


Electron density around STJ B 1:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

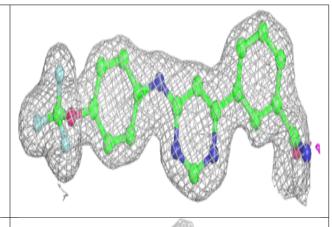


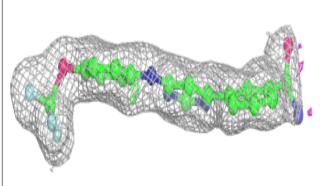


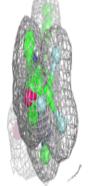


Electron density around STJ A 1:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



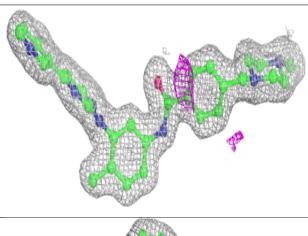


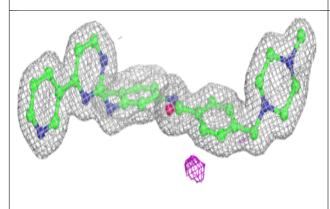


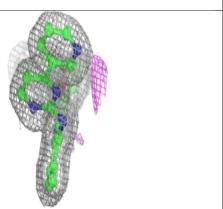


Electron density around STI B 2: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around STI A 2: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray

 mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

