



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:08 am BST

PDB ID : 3MS9
Title : ABL kinase in complex with imatinib and a fragment (FRAG1) in the myristate pocket
Authors : Cowan-Jacob, S.W.; Rummel, G.; Fendrich, G.
Deposited on : 2010-04-29
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

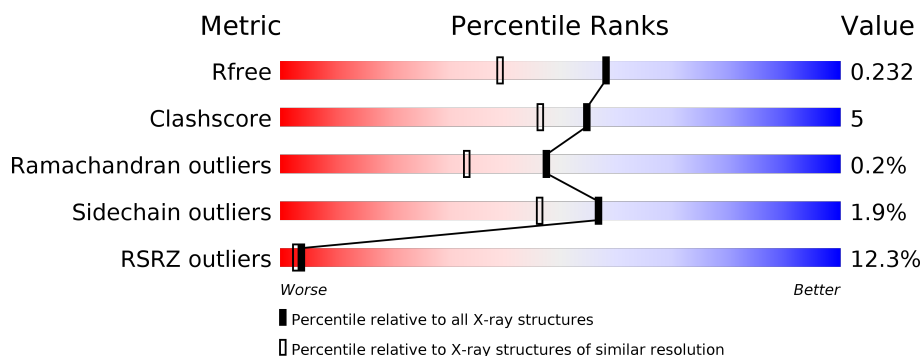
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	293	<div> <div>12%</div> <div>79%</div> <div>11%</div> <div>10%</div> </div>
1	B	293	<div> <div>11%</div> <div>76%</div> <div>16%</div> <div>7%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4955 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.

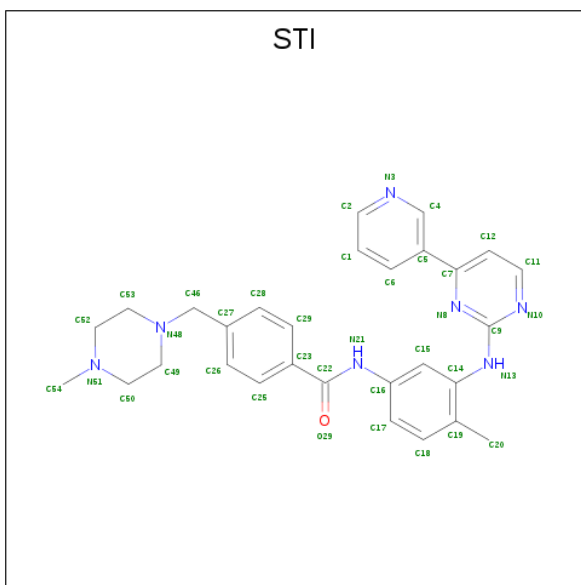
- Molecule 1 is a protein called Tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	6	0
			2195	1416	357	406	16			
1	B	272	Total	C	N	O	S	0	1	0
			2213	1426	360	409	18			

There are 12 discrepancies between the modelled and reference sequences:

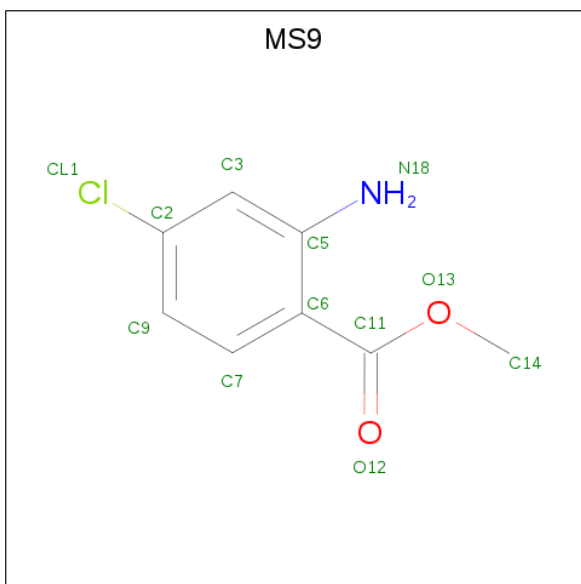
Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLY	-	EXPRESSION TAG	UNP P00520
A	224	ALA	-	EXPRESSION TAG	UNP P00520
A	225	MET	-	EXPRESSION TAG	UNP P00520
A	226	ASP	-	EXPRESSION TAG	UNP P00520
A	227	PRO	-	EXPRESSION TAG	UNP P00520
A	228	SER	-	EXPRESSION TAG	UNP P00520
B	223	GLY	-	EXPRESSION TAG	UNP P00520
B	224	ALA	-	EXPRESSION TAG	UNP P00520
B	225	MET	-	EXPRESSION TAG	UNP P00520
B	226	ASP	-	EXPRESSION TAG	UNP P00520
B	227	PRO	-	EXPRESSION TAG	UNP P00520
B	228	SER	-	EXPRESSION TAG	UNP P00520

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



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

- Molecule 3 is methyl 2-amino-4-chlorobenzoate (three-letter code: MS9) (formula: $C_8H_8ClNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			12	8	1	1	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			12	8	1	1	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	A	4	Total	Cl	0	0
			4	4		

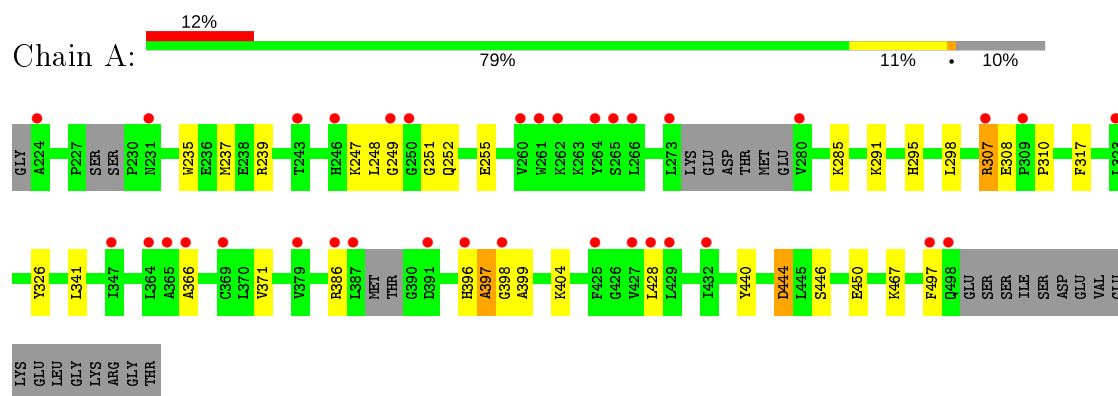
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	226	Total	O	0	0
			226	226		
5	B	217	Total	O	0	0
			217	217		

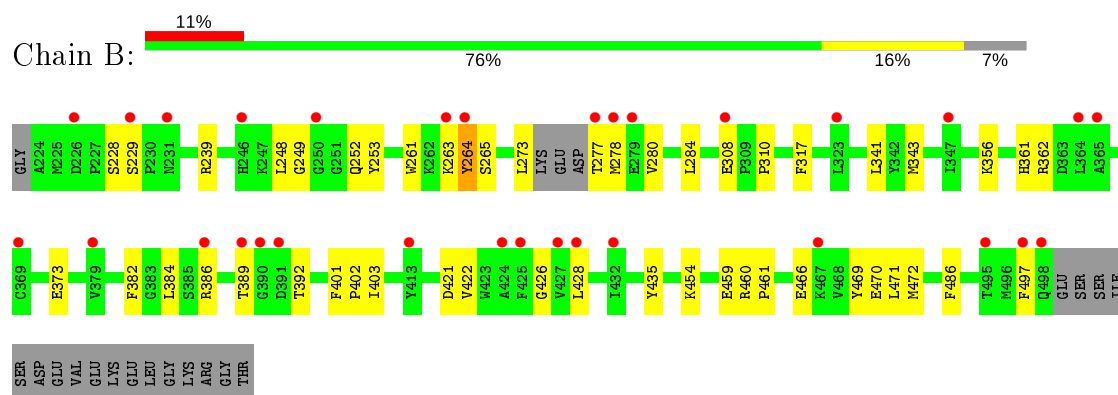
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



• Molecule 1: Tyrosine-protein kinase ABL1



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	115.78Å 147.35Å 152.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.92 – 1.80 29.27 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (33.92-1.80) 98.3 (29.27-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.234 0.183 , 0.232	Depositor DCC
R_{free} test set	2942 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4955	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: STI, MS9, CL

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	1.26	2/2260 (0.1%)	1.02	2/3058 (0.1%)
1	B	1.27	7/2271 (0.3%)	1.03	5/3075 (0.2%)
All	All	1.26	9/4531 (0.2%)	1.02	7/6133 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	486	PHE	CE2-CZ	6.67	1.50	1.37
1	B	469	TYR	CD2-CE2	6.16	1.48	1.39
1	B	422	VAL	CB-CG2	5.92	1.65	1.52
1	B	454	LYS	CD-CE	5.69	1.65	1.51
1	A	371	VAL	CB-CG2	5.64	1.64	1.52
1	B	426	GLY	N-CA	5.26	1.53	1.46
1	B	435	TYR	CE1-CZ	5.26	1.45	1.38
1	B	469	TYR	CD1-CE1	5.15	1.47	1.39
1	A	326	TYR	CD2-CE2	5.02	1.46	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	MET	CG-SD-CE	-10.31	83.70	100.20
1	B	454	LYS	CD-CE-NZ	-7.27	94.99	111.70
1	B	421	ASP	CB-CG-OD1	6.24	123.92	118.30
1	B	472	MET	CG-SD-CE	-6.10	90.43	100.20
1	A	444[A]	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	A	444[B]	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	B	428	LEU	CB-CG-CD2	-5.42	101.79	111.00

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	2195	0	2137	24	0
1	B	2213	0	2160	22	0
2	A	37	0	31	0	0
2	B	37	0	31	0	0
3	A	12	0	8	0	0
3	B	12	0	8	0	0
4	A	4	0	0	0	0
4	B	2	0	0	1	0
5	A	226	0	0	7	0
5	B	217	0	0	2	0
All	All	4955	0	4375	46	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 5.

All (46) 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:237:MET:HB3	5:A:561:HOH:O	1.63	0.96
1:A:249:GLY:O	1:A:252:GLN:HG2	1.87	0.75
1:B:466:GLU:O	1:B:470:GLU:HG3	1.88	0.74
1:B:253:TYR:OH	4:B:6:CL:CL	2.40	0.74
1:A:239:ARG:NH1	1:A:310:PRO:O	2.19	0.73
1:B:249:GLY:O	1:B:252:GLN:HG2	1.91	0.71
1:A:444[B]:ASP:OD1	1:A:446:SER:OG	2.16	0.64
1:B:261:TRP:HE1	1:B:263:LYS:NZ	1.96	0.62
1:B:362:ARG:NH2	5:B:594:HOH:O	2.33	0.60
1:B:261:TRP:HE1	1:B:263:LYS:HZ3	1.46	0.60
1:A:404:LYS:HE2	1:A:440:TYR:HB2	1.85	0.58
1:A:248:LEU:HD11	1:A:317:PHE:HE1	1.69	0.57
1:A:397:ALA:C	1:A:399:ALA:H	2.06	0.57
1:B:239:ARG:NH2	1:B:310:PRO:O	2.34	0.56
1:B:361:HIS:O	1:B:362:ARG:HB2	2.07	0.54
1:B:459:GLU:HG2	5:B:129:HOH:O	2.09	0.53
1:B:248:LEU:HD11	1:B:317:PHE:HE1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.76	0.50
1:A:396:HIS:CE1	5:A:81:HOH:O	2.64	0.49
1:A:450[B]:GLU:HG3	5:A:541:HOH:O	2.13	0.48
1:B:280:VAL:O	1:B:284:LEU:HG	2.13	0.48
1:A:341:LEU:HD21	1:A:497:PHE:HA	1.94	0.48
1:A:467:LYS:HG2	5:A:524:HOH:O	2.14	0.48
1:B:264:TYR:CD1	1:B:264:TYR:N	2.82	0.48
1:A:285:LYS:HD3	5:A:591:HOH:O	2.14	0.47
1:A:295:HIS:HB3	1:A:298:LEU:HD12	1.97	0.47
1:B:273:LEU:HB3	1:B:277:THR:HG21	1.97	0.47
1:B:356:LYS:HB3	1:B:356:LYS:HE3	1.59	0.46
1:A:285:LYS:HE2	5:A:135:HOH:O	2.15	0.46
1:B:401:PHE:HB2	1:B:403:ILE:HD13	1.99	0.45
1:A:247:LYS:CE	1:A:255:GLU:OE2	2.64	0.45
1:A:397:ALA:O	1:A:399:ALA:N	2.49	0.45
1:A:247:LYS:NZ	1:A:255:GLU:OE2	2.47	0.45
1:B:382:PHE:HB2	1:B:384:LEU:HG	1.99	0.45
1:A:397:ALA:C	1:A:399:ALA:N	2.68	0.44
1:A:386:ARG:NH2	1:A:398:GLY:O	2.50	0.43
1:B:248:LEU:HA	1:B:248:LEU:HD12	1.74	0.43
1:B:341:LEU:HD21	1:B:497:PHE:HA	2.00	0.43
1:B:228:SER:O	1:B:229:SER:C	2.56	0.43
1:A:251:GLY:HA2	5:A:88:HOH:O	2.19	0.42
1:A:366:ALA:N	1:A:428:LEU:HD13	2.35	0.42
1:B:460:ARG:HA	1:B:461:PRO:HD3	1.93	0.41
1:A:235:TRP:CD1	1:A:291:LYS:HG2	2.55	0.41
1:A:396:HIS:O	1:A:397:ALA:C	2.59	0.41
1:B:392:THR:O	1:B:402:PRO:HA	2.21	0.40
1:B:239:ARG:NH1	1:B:308:GLU:OE2	2.55	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	263/293 (90%)	253 (96%)	9 (3%)	1 (0%)	34	21
1	B	269/293 (92%)	258 (96%)	11 (4%)	0	100	100
All	All	532/586 (91%)	511 (96%)	20 (4%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	ALA

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	235/255 (92%)	233 (99%)	2 (1%)	78	75
1	B	237/255 (93%)	230 (97%)	7 (3%)	41	27
All	All	472/510 (92%)	463 (98%)	9 (2%)	57	46

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	ARG
1	A	308	GLU
1	B	264	TYR
1	B	265	SER
1	B	278	MET
1	B	373	GLU
1	B	386	ARG
1	B	389	THR
1	B	471	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	ASN

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Mol	Chain	Res	Type
1	A	490	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	STI	B	1	-	41,41,41	1.34	8 (19%)	56,56,56	2.11	17 (30%)
2	STI	A	1	-	41,41,41	1.18	3 (7%)	56,56,56	1.88	13 (23%)
3	MS9	B	516	-	12,12,12	1.53	2 (16%)	15,16,16	1.71	4 (26%)
3	MS9	A	516	-	12,12,12	1.73	5 (41%)	15,16,16	1.34	2 (13%)

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	STI	B	1	-	-	2/20/30/30	0/5/5/5
2	STI	A	1	-	-	2/20/30/30	0/5/5/5
3	MS9	B	516	-	-	0/6/6/6	0/1/1/1
3	MS9	A	516	-	-	0/6/6/6	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	516	MS9	C3-C2	3.17	1.43	1.38
2	A	1	STI	C50-N51	3.03	1.52	1.46
2	A	1	STI	C4-C5	2.74	1.44	1.39
2	B	1	STI	C11-N10	2.71	1.40	1.34
2	B	1	STI	C29-C23	2.65	1.43	1.39
3	A	516	MS9	C7-C6	2.62	1.44	1.39
3	A	516	MS9	C3-C5	2.56	1.43	1.40
3	A	516	MS9	C9-C7	2.54	1.43	1.38
3	A	516	MS9	O13-C11	2.53	1.39	1.33
2	B	1	STI	C18-C19	2.51	1.45	1.39
2	B	1	STI	C15-C14	2.44	1.43	1.39
2	A	1	STI	C52-N51	2.42	1.51	1.46
2	B	1	STI	C15-C16	2.42	1.43	1.39
3	A	516	MS9	C9-C2	2.33	1.42	1.38
3	B	516	MS9	C3-C5	2.23	1.43	1.40
2	B	1	STI	C20-C19	2.09	1.55	1.51
2	B	1	STI	C54-N51	2.07	1.51	1.46
2	B	1	STI	C26-C27	2.01	1.43	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	STI	C7-N8-C9	6.38	121.94	116.69
2	A	1	STI	C11-N10-C9	4.68	119.60	115.45
2	A	1	STI	N10-C9-N8	-4.40	122.38	126.55
2	A	1	STI	C7-N8-C9	4.36	120.28	116.69
2	B	1	STI	C46-C27-C26	-4.29	112.69	120.77
2	B	1	STI	C18-C19-C14	4.14	121.35	117.44
2	A	1	STI	C12-C11-N10	-4.12	118.84	123.96
2	B	1	STI	C28-C27-C26	3.69	123.97	118.17
2	B	1	STI	C17-C18-C19	-3.66	116.42	121.97
3	A	516	MS9	C14-O13-C11	-3.60	108.90	115.83
2	B	1	STI	N10-C9-N8	-3.57	123.16	126.55
2	B	1	STI	C25-C26-C27	-3.31	116.47	121.03
2	A	1	STI	C14-N13-C9	-3.28	119.70	129.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	STI	C18-C17-C16	-3.28	116.51	120.30
2	B	1	STI	C18-C17-C16	3.27	124.07	120.30
2	A	1	STI	C11-C12-C7	3.23	120.27	117.22
3	B	516	MS9	C7-C6-C5	3.22	122.34	118.93
2	B	1	STI	C14-N13-C9	-3.16	120.07	129.60
3	B	516	MS9	O13-C11-C6	3.03	117.32	112.30
2	B	1	STI	C54-N51-C52	-2.91	106.30	110.66
2	B	1	STI	C12-C7-C5	2.90	127.59	121.93
2	A	1	STI	C15-C14-C19	-2.89	116.40	119.77
2	A	1	STI	C18-C19-C14	2.83	120.11	117.44
2	B	1	STI	C12-C11-N10	-2.81	120.47	123.96
2	B	1	STI	C12-C7-N8	-2.79	118.35	121.97
2	B	1	STI	C23-C22-N21	2.67	121.79	115.92
2	A	1	STI	C12-C7-N8	-2.62	118.58	121.97
2	A	1	STI	C12-C7-C5	2.60	126.99	121.93
2	A	1	STI	C23-C22-N21	2.58	121.60	115.92
3	A	516	MS9	O13-C11-C6	2.45	116.36	112.30
2	B	1	STI	C54-N51-C50	2.32	114.13	110.66
2	B	1	STI	C11-C12-C7	2.29	119.39	117.22
3	B	516	MS9	O13-C11-O12	2.28	127.92	123.45
2	A	1	STI	C16-N21-C22	2.13	132.10	126.58
2	B	1	STI	C2-N3-C4	2.05	120.39	116.85
3	B	516	MS9	O12-C11-C6	-2.03	114.76	121.57

There are no chirality outliers.

All (4) torsion outliers are listed below:

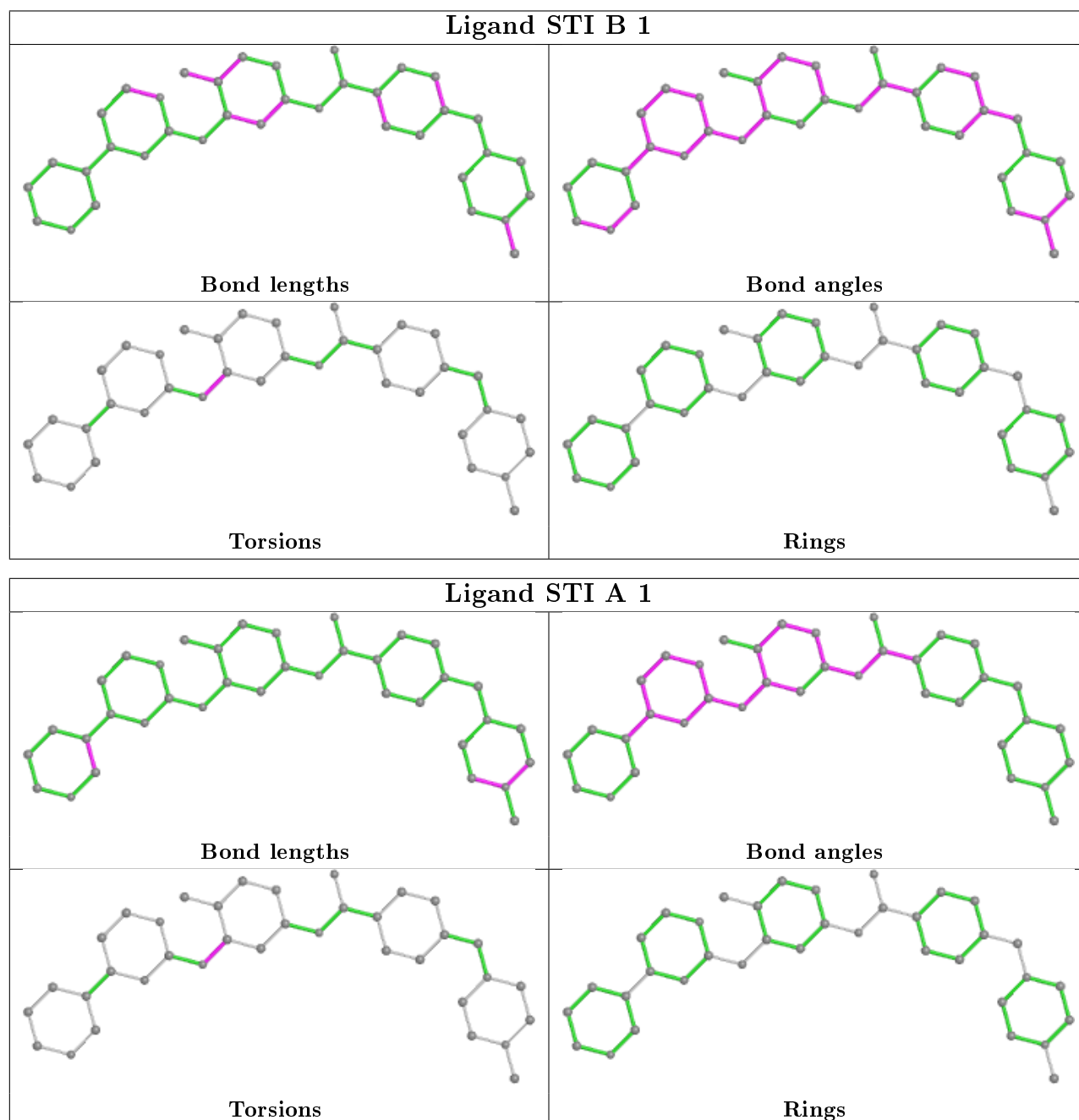
Mol	Chain	Res	Type	Atoms
2	B	1	STI	C15-C14-N13-C9
2	A	1	STI	C15-C14-N13-C9
2	A	1	STI	C19-C14-N13-C9
2	B	1	STI	C19-C14-N13-C9

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 ⓘ

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 ⓘ

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	265/293 (90%)	0.44	35 (13%)	3 2	16, 28, 51, 59	0
1	B	272/293 (92%)	0.47	31 (11%)	5 3	16, 27, 53, 76	0
All	All	537/586 (91%)	0.46	66 (12%)	4 3	16, 27, 51, 76	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	MET	7.7
1	B	277	THR	6.0
1	B	389	THR	5.2
1	A	497	PHE	4.6
1	B	498	GLN	4.6
1	B	391	ASP	4.5
1	B	497	PHE	4.2
1	A	265	SER	3.9
1	B	428	LEU	3.6
1	A	391	ASP	3.5
1	A	307	ARG	3.5
1	A	498	GLN	3.3
1	A	364	LEU	3.3
1	A	246	HIS	3.3
1	A	243	THR	3.2
1	A	273	LEU	3.2
1	B	364	LEU	3.2
1	B	226	ASP	3.2
1	A	428	LEU	3.1
1	B	279	GLU	3.1
1	A	386	ARG	3.1
1	B	390	GLY	3.1
1	A	387	LEU	3.1
1	A	250	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	413	TYR	2.9
1	B	246	HIS	2.8
1	A	369	CYS	2.8
1	A	398	GLY	2.7
1	A	309	PRO	2.7
1	A	261	TRP	2.7
1	A	266	LEU	2.7
1	A	396	HIS	2.6
1	A	379	VAL	2.6
1	B	427	VAL	2.6
1	A	249	GLY	2.6
1	B	369	CYS	2.5
1	B	425	PHE	2.5
1	A	323	LEU	2.5
1	B	347	ILE	2.5
1	A	260	VAL	2.5
1	B	386	ARG	2.5
1	A	425	PHE	2.5
1	A	224	ALA	2.4
1	B	379	VAL	2.4
1	B	495	THR	2.4
1	A	427	VAL	2.4
1	B	323	LEU	2.4
1	A	432	ILE	2.4
1	B	264	TYR	2.4
1	A	264	TYR	2.3
1	A	365	ALA	2.3
1	A	280	VAL	2.3
1	B	432	ILE	2.3
1	A	231	ASN	2.3
1	A	262	LYS	2.2
1	A	366	ALA	2.2
1	B	250	GLY	2.2
1	A	347	ILE	2.2
1	B	263	LYS	2.1
1	B	365	ALA	2.1
1	B	424	ALA	2.1
1	A	429	LEU	2.1
1	B	308	GLU	2.1
1	B	467	LYS	2.1
1	B	231	ASN	2.1
1	B	229	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

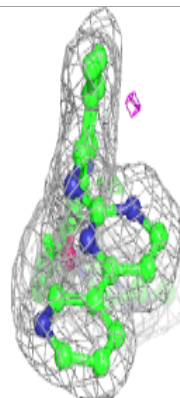
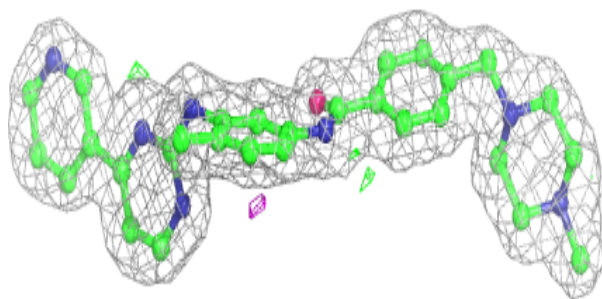
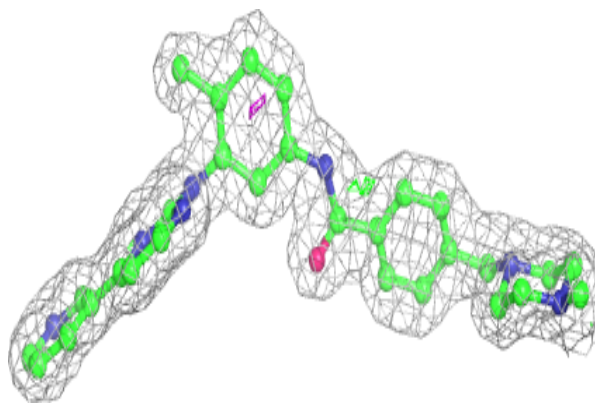
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	B	6	1/1	0.92	0.11	40,40,40,40	0
4	CL	A	5	1/1	0.93	0.11	44,44,44,44	0
4	CL	A	4	1/1	0.94	0.13	67,67,67,67	0
2	STI	B	1	37/37	0.95	0.12	18,22,25,29	0
3	MS9	B	516	12/12	0.95	0.09	23,25,28,34	0
3	MS9	A	516	12/12	0.96	0.10	21,24,30,31	0
2	STI	A	1	37/37	0.96	0.12	21,24,28,28	0
4	CL	A	517	1/1	0.97	0.06	40,40,40,40	0
4	CL	B	3	1/1	0.97	0.07	38,38,38,38	0
4	CL	A	2	1/1	0.98	0.09	39,39,39,39	0

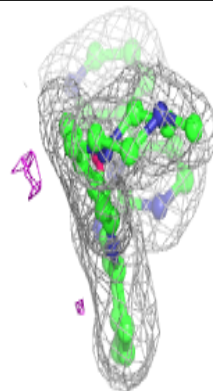
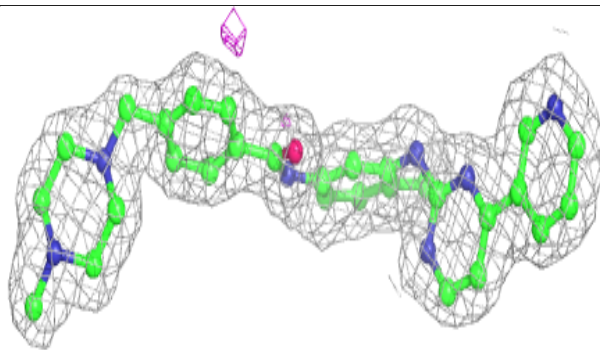
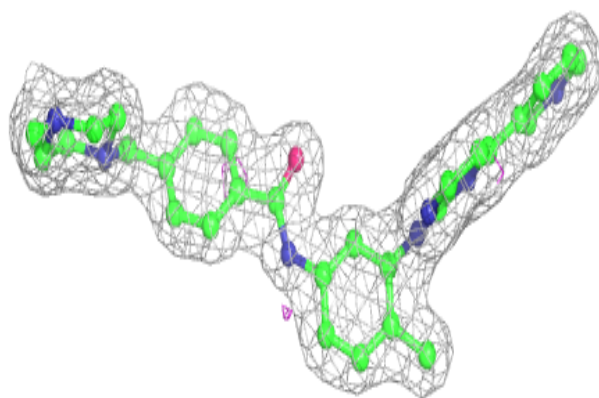
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STI B 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around STI A 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.