



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:30 AM EDT

PDB ID : 1OPJ / pdb_00001opj
Title : Structural basis for the auto-inhibition of c-Abl tyrosine kinase
Authors : Nagar, B.; Hantschel, O.; Young, M.A.; Scheffzek, K.; Veach, D.; Bornmann, W.; Clarkson, B.; Superti-Furga, G.; Kuriyan, J.
Deposited on : 2003-03-06
Resolution : 1.75 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

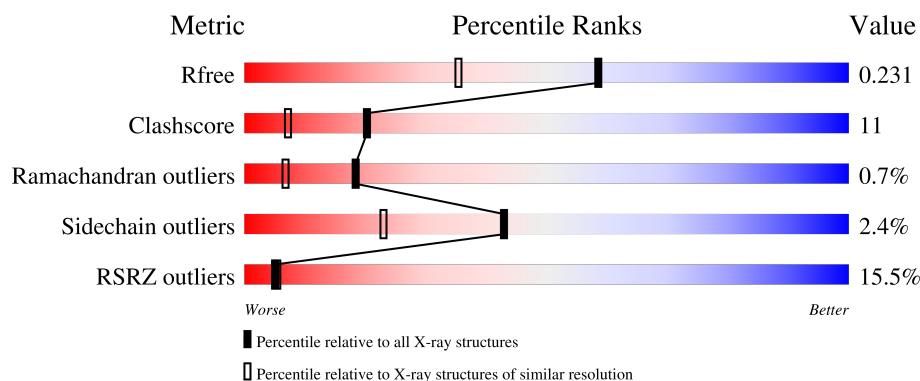
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	293	
1	B	293	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5001 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 ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2328	1494	376	440	18			
1	B	288	Total	C	N	O	S	0	0	0
			2336	1499	378	441	18			

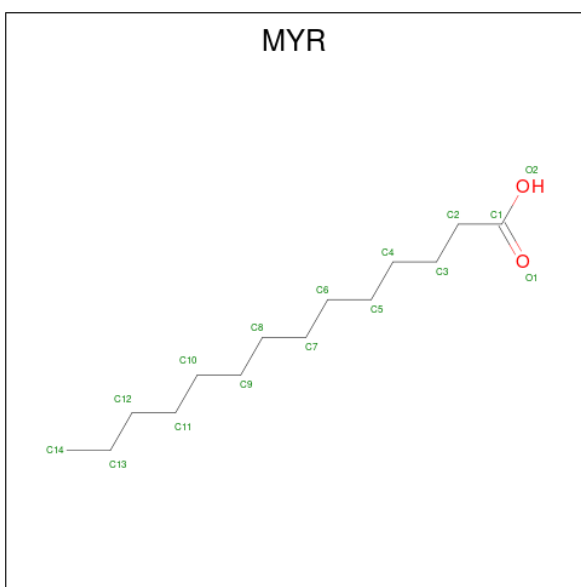
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLY	-	cloning artifact	UNP P00520
A	243	ALA	-	cloning artifact	UNP P00520
A	244	MET	-	cloning artifact	UNP P00520
A	245	ASP	-	cloning artifact	UNP P00520
A	246	PRO	-	cloning artifact	UNP P00520
A	247	SER	-	cloning artifact	UNP P00520
B	242	GLY	-	cloning artifact	UNP P00520
B	243	ALA	-	cloning artifact	UNP P00520
B	244	MET	-	cloning artifact	UNP P00520
B	245	ASP	-	cloning artifact	UNP P00520
B	246	PRO	-	cloning artifact	UNP P00520
B	247	SER	-	cloning artifact	UNP P00520

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

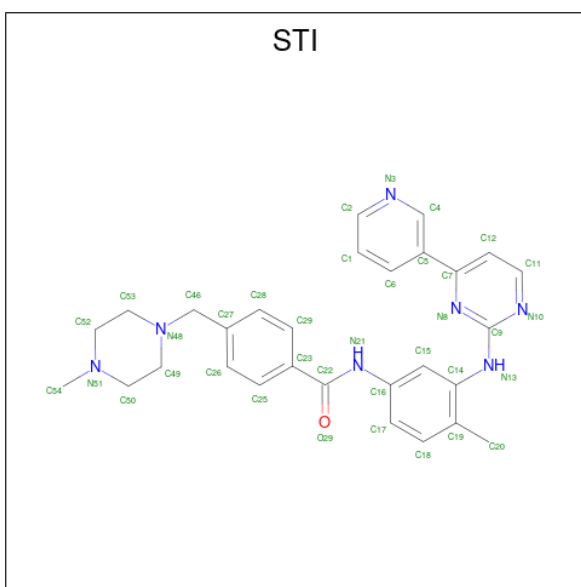
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	14	1		
3	B	1	Total	C	O	0	0
			15	14	1		

- Molecule 4 is 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE (CCD ID: STI) (formula: $C_{29}H_{31}N_7O$).



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

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

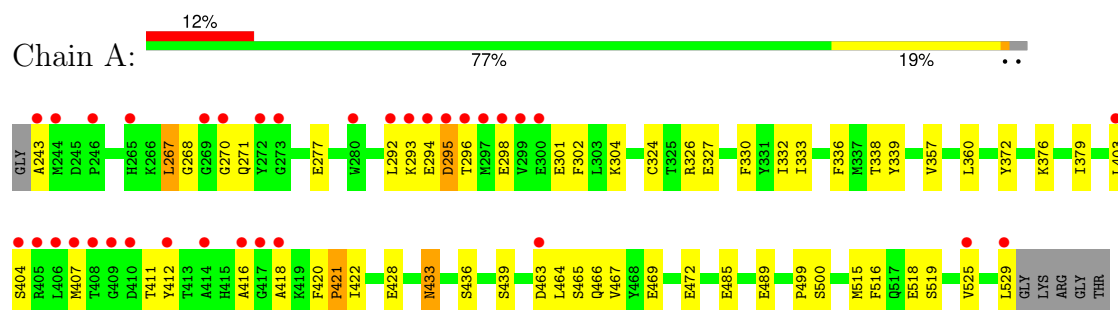
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total	O	0	0
			127	127		
5	B	104	Total	O	0	0
			104	104		

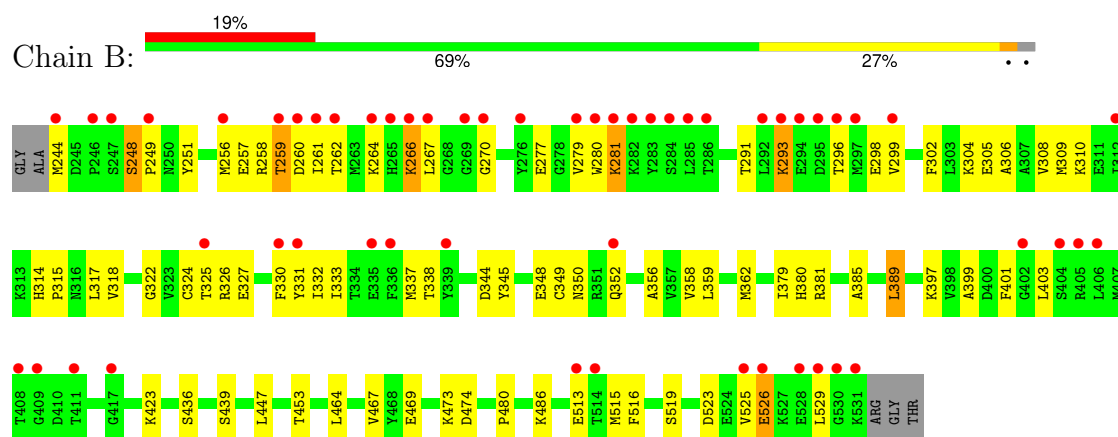
3 Residue-property plots [i](#)

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 ABL1



- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.84Å 63.51Å 64.05Å 67.91° 79.76° 84.88°	Depositor
Resolution (Å)	29.41 – 1.75 29.41 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.2 (29.41-1.75) 95.2 (29.41-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.242 0.200 , 0.231	Depositor DCC
R_{free} test set	3080 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5001	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: CL, STI, MYR

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	0.53	0/2387	0.94	7/3231 (0.2%)
1	B	0.40	0/2395	0.87	4/3240 (0.1%)
All	All	0.47	0/4782	0.90	11/6471 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ILE	N-CA-C	-6.57	98.04	107.77
1	A	515	MET	N-CA-C	6.31	118.96	111.33
1	B	248	SER	N-CA-C	6.04	116.55	109.60
1	A	338	THR	N-CA-C	5.97	121.22	111.37
1	B	467	VAL	N-CA-C	5.83	116.02	110.42
1	A	422	ILE	N-CA-C	5.76	117.19	110.62
1	A	439	SER	N-CA-C	-5.68	105.08	112.23
1	B	338	THR	N-CA-C	5.34	120.13	111.37
1	A	421	PRO	N-CA-C	-5.32	97.20	113.27
1	B	439	SER	N-CA-C	-5.26	105.60	112.23
1	A	339	TYR	N-CA-C	5.15	119.20	113.02

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	2328	0	2270	42	0
1	B	2336	0	2281	65	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	27	1	0
3	B	15	0	27	1	0
4	A	37	0	31	0	0
4	B	37	0	31	1	0
5	A	127	0	0	2	0
5	B	104	0	0	2	0
All	All	5001	0	4667	107	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 11.

All (107) 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:293:LYS:HD2	1:B:293:LYS:H	1.24	1.02
1:B:262:THR:OG1	1:B:281:LYS:HE3	1.82	0.79
1:B:256:MET:HE3	1:B:322:GLY:HA3	1.70	0.72
1:B:523:ASP:O	1:B:526:GLU:HG3	1.91	0.71
1:B:293:LYS:HD2	1:B:293:LYS:N	2.04	0.68
1:A:293:LYS:HB2	1:A:296:THR:HG21	1.75	0.68
1:B:266:LYS:HD3	1:B:270:GLY:HA2	1.74	0.67
1:A:267:LEU:HD13	1:A:277:GLU:HB2	1.77	0.66
1:A:333:ILE:HD12	1:A:333:ILE:N	2.10	0.66
1:B:296:THR:O	1:B:299:VAL:HG23	1.94	0.66
1:A:360:LEU:HA	3:A:1:MYR:H142	1.79	0.65
1:A:243:ALA:CB	1:A:326:ARG:HD2	2.27	0.65
1:A:407:MET:HG3	1:A:412:TYR:CE1	2.37	0.60
1:B:261:ILE:HD13	1:B:280:TRP:HA	1.84	0.59
1:A:243:ALA:HB3	1:A:326:ARG:HD2	1.83	0.59
1:A:407:MET:HG3	1:A:412:TYR:HE1	1.67	0.59
1:A:416:ALA:HB1	1:A:433:ASN:HD21	1.68	0.59
1:B:258:ARG:C	1:B:260:ASP:H	2.11	0.58
1:B:296:THR:HG22	1:B:298:GLU:H	1.70	0.57
1:A:516:PHE:HB3	1:A:519:SER:O	2.04	0.57
1:A:267:LEU:CD1	1:A:277:GLU:HB2	2.35	0.56
1:B:267:LEU:HD21	1:B:277:GLU:HB2	1.88	0.56
1:A:293:LYS:HB2	1:A:296:THR:CG2	2.35	0.56
1:B:380:HIS:O	1:B:381:ARG:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:PHE:CZ	1:B:332:ILE:HG13	2.42	0.55
1:B:244:MET:HG3	1:B:251:TYR:HA	1.90	0.54
1:B:469:GLU:HG3	5:B:224:HOH:O	2.08	0.54
1:B:486:LYS:HD2	5:B:202:HOH:O	2.06	0.54
1:A:403:LEU:HB3	1:A:407:MET:HG2	1.89	0.54
1:B:258:ARG:HG3	1:B:259:THR:N	2.23	0.53
1:A:357:VAL:HG23	5:A:226:HOH:O	2.09	0.53
1:B:359:LEU:HD23	1:B:362:MET:HE2	1.90	0.53
1:B:324:CYS:O	1:B:330:PHE:HA	2.08	0.53
1:B:379:ILE:HD13	1:B:436:SER:HA	1.91	0.53
1:A:411:THR:O	1:A:421:PRO:HA	2.08	0.53
1:A:298:GLU:HG2	1:A:301:GLU:HB2	1.91	0.52
1:B:315:PRO:O	1:B:397:LYS:HE2	2.09	0.52
1:B:296:THR:C	1:B:298:GLU:H	2.18	0.52
1:B:529:LEU:HD11	3:B:2:MYR:H42	1.92	0.52
1:B:262:THR:HG1	1:B:281:LYS:HE3	1.75	0.51
1:B:257:GLU:HB3	1:B:260:ASP:HB2	1.92	0.51
1:B:423:LYS:HE3	1:B:464:LEU:HD23	1.92	0.51
1:A:298:GLU:CG	1:A:301:GLU:HB2	2.41	0.51
1:A:518:GLU:N	1:A:518:GLU:CD	2.69	0.51
1:A:403:LEU:HB3	1:A:407:MET:CG	2.41	0.50
1:B:473:LYS:O	1:B:474:ASP:HB2	2.12	0.50
1:B:401:PHE:HB2	1:B:403:LEU:HG	1.94	0.50
1:B:314:HIS:CG	1:B:315:PRO:HD2	2.47	0.50
1:B:325:THR:HA	1:B:330:PHE:HD2	1.77	0.50
1:B:267:LEU:CD2	1:B:277:GLU:HB2	2.41	0.49
1:B:244:MET:SD	1:B:244:MET:N	2.86	0.49
1:B:257:GLU:HG3	1:B:259:THR:HG22	1.95	0.48
1:B:344:ASP:O	1:B:348:GLU:HG3	2.12	0.48
1:B:350:ASN:OD1	1:B:352:GLN:HB2	2.13	0.48
1:A:292:LEU:HD21	1:A:302:PHE:HB2	1.93	0.48
1:B:264:LYS:HE2	1:B:279:VAL:CG2	2.43	0.48
1:B:326:ARG:HB3	1:B:327:GLU:OE2	2.13	0.48
1:A:326:ARG:NE	1:A:326:ARG:HA	2.29	0.48
1:B:330:PHE:O	1:B:331:TYR:HD2	1.97	0.47
1:A:525:VAL:O	1:A:529:LEU:HG	2.14	0.47
1:A:268:GLY:O	1:A:271:GLN:HG2	2.14	0.47
1:B:280:TRP:O	1:B:281:LYS:C	2.56	0.47
1:B:291:THR:HG22	1:B:331:TYR:CD2	2.49	0.47
1:B:345:TYR:O	1:B:349:CYS:HB3	2.14	0.47
1:B:453:THR:HG22	1:B:480:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LYS:H	1:B:293:LYS:CD	1.99	0.47
1:B:304:LYS:O	1:B:308:VAL:HG23	2.15	0.47
1:B:306:ALA:O	1:B:310:LYS:HG3	2.16	0.46
1:B:257:GLU:O	1:B:260:ASP:HB3	2.16	0.46
1:A:485:GLU:O	1:A:489:GLU:HG3	2.16	0.45
1:A:267:LEU:HD11	1:A:336:PHE:HE1	1.80	0.45
1:B:515:MET:HG3	1:B:516:PHE:CD1	2.51	0.45
1:B:525:VAL:HG12	1:B:529:LEU:HD12	1.99	0.45
1:B:244:MET:CG	1:B:251:TYR:HA	2.47	0.45
1:B:248:SER:HA	1:B:249:PRO:HD3	1.80	0.44
1:B:337:MET:HG3	1:B:389:LEU:HB3	2.00	0.44
1:B:337:MET:O	4:B:4:STI:H21	2.18	0.44
1:B:385:ALA:N	1:B:447:LEU:HD13	2.32	0.44
1:B:314:HIS:HB3	1:B:317:LEU:HD12	2.00	0.44
1:B:358:VAL:O	1:B:362:MET:HG3	2.18	0.44
1:A:464:LEU:HA	1:A:467:VAL:HG23	2.00	0.43
1:A:466:GLN:NE2	5:A:62:HOH:O	2.48	0.43
1:A:404:SER:HA	1:A:412:TYR:CD2	2.53	0.43
1:A:243:ALA:HB2	1:A:326:ARG:HD2	1.99	0.43
1:A:463:ASP:OD1	1:A:465:SER:OG	2.29	0.43
1:B:256:MET:HG2	1:B:257:GLU:N	2.34	0.43
1:B:516:PHE:O	1:B:519:SER:O	2.36	0.43
1:A:372:TYR:CZ	1:A:376:LYS:HD2	2.54	0.42
1:B:258:ARG:C	1:B:260:ASP:N	2.77	0.42
1:B:423:LYS:HE3	1:B:464:LEU:CD2	2.49	0.42
1:A:333:ILE:N	1:A:333:ILE:CD1	2.81	0.42
1:B:318:VAL:HG21	1:B:399:ALA:HB2	2.02	0.41
1:A:416:ALA:CB	1:A:433:ASN:HD21	2.32	0.41
1:A:324:CYS:O	1:A:330:PHE:HA	2.20	0.41
1:B:333:ILE:HD12	1:B:333:ILE:N	2.35	0.41
1:A:525:VAL:O	1:A:525:VAL:HG12	2.20	0.41
1:B:305:GLU:O	1:B:309:MET:HG3	2.21	0.41
1:B:379:ILE:CD1	1:B:436:SER:HA	2.50	0.41
1:A:379:ILE:HD13	1:A:436:SER:HA	2.02	0.41
1:A:428:GLU:CD	1:A:499:PRO:HG3	2.45	0.41
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.91	0.41
1:A:326:ARG:HA	1:A:326:ARG:HE	1.86	0.40
1:A:294:GLU:O	1:A:295:ASP:C	2.64	0.40
1:A:418:ALA:HB3	1:A:420:PHE:HE2	1.87	0.40
1:B:266:LYS:CD	1:B:270:GLY:HA2	2.47	0.40
1:A:403:LEU:O	1:A:404:SER:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ALA:HB2	1:B:525:VAL:HG21	2.02	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	285/293 (97%)	271 (95%)	12 (4%)	2 (1%)	18	7
1	B	286/293 (98%)	263 (92%)	21 (7%)	2 (1%)	18	7
All	All	571/586 (97%)	534 (94%)	33 (6%)	4 (1%)	18	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281	LYS
1	A	270	GLY
1	A	295	ASP
1	B	259	THR

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	252/255 (99%)	245 (97%)	7 (3%)	38	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	253/255 (99%)	248 (98%)	5 (2%)	48	29
All	All	505/510 (99%)	493 (98%)	12 (2%)	43	23

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	LEU
1	A	304	LYS
1	A	327	GLU
1	A	433	ASN
1	A	469	GLU
1	A	472	GLU
1	A	500	SER
1	B	266	LYS
1	B	293	LYS
1	B	389	LEU
1	B	513	GLU
1	B	526	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	ASN
1	A	517	GLN
1	B	271	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

Of 6 ligands modelled in this entry, 2 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
4	STI	A	3	-	41,41,41	2.15	21 (51%)	56,56,56	1.96	8 (14%)
4	STI	B	4	-	41,41,41	2.40	23 (56%)	56,56,56	2.05	11 (19%)
3	MYR	A	1	-	13,14,15	1.09	1 (7%)	12,13,15	0.62	0
3	MYR	B	2	-	13,14,15	1.07	1 (7%)	12,13,15	0.61	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
4	STI	A	3	-	-	2/20/30/30	0/5/5/5
4	STI	B	4	-	-	2/20/30/30	0/5/5/5
3	MYR	A	1	-	-	5/12/12/13	-
3	MYR	B	2	-	-	7/12/12/13	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4	STI	C25-C23	4.74	1.46	1.39
4	A	3	STI	C25-C23	3.99	1.45	1.39
3	A	1	MYR	O1-C1	3.79	1.41	1.20
4	A	3	STI	C29-C23	3.77	1.45	1.39
4	B	4	STI	C14-C19	3.77	1.48	1.40
3	B	2	MYR	O1-C1	3.72	1.41	1.20
4	B	4	STI	C4-C5	3.71	1.46	1.39
4	A	3	STI	C17-C18	3.71	1.44	1.38
4	B	4	STI	C26-C27	3.54	1.45	1.38
4	B	4	STI	C17-C18	3.52	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4	STI	C15-C16	3.51	1.45	1.39
4	B	4	STI	C26-C25	3.29	1.44	1.38
4	A	3	STI	C1-C6	3.28	1.44	1.38
4	B	4	STI	C1-C6	3.28	1.44	1.38
4	A	3	STI	C15-C16	3.27	1.44	1.39
4	B	4	STI	C28-C27	3.20	1.45	1.38
4	B	4	STI	C9-N10	3.20	1.39	1.34
4	A	3	STI	C26-C27	3.12	1.45	1.38
4	B	4	STI	C6-C5	3.10	1.45	1.39
4	A	3	STI	C28-C27	2.98	1.44	1.38
4	B	4	STI	C29-C23	2.94	1.43	1.39
4	A	3	STI	C50-N51	2.89	1.53	1.46
4	A	3	STI	C6-C5	2.80	1.45	1.39
4	A	3	STI	C14-C19	2.76	1.46	1.40
4	B	4	STI	C50-N51	2.75	1.53	1.46
4	A	3	STI	C4-N3	2.69	1.40	1.34
4	A	3	STI	C26-C25	2.68	1.43	1.38
4	A	3	STI	C4-C5	2.67	1.44	1.39
4	B	4	STI	C17-C16	2.61	1.43	1.39
4	B	4	STI	C7-N8	2.49	1.38	1.34
4	A	3	STI	C9-N10	2.48	1.38	1.34
4	B	4	STI	C12-C7	2.43	1.44	1.39
4	B	4	STI	C2-N3	2.31	1.40	1.33
4	A	3	STI	C2-N3	2.31	1.40	1.33
4	A	3	STI	C52-N51	2.30	1.51	1.46
4	A	3	STI	C18-C19	2.27	1.44	1.39
4	B	4	STI	C1-C2	2.26	1.44	1.37
4	B	4	STI	C18-C19	2.22	1.44	1.39
4	A	3	STI	C17-C16	2.22	1.43	1.39
4	A	3	STI	C12-C7	2.20	1.44	1.39
4	B	4	STI	C52-N51	2.14	1.51	1.46
4	B	4	STI	C49-N48	2.14	1.52	1.46
4	A	3	STI	C49-N48	2.09	1.52	1.46
4	B	4	STI	C4-N3	2.09	1.38	1.34
4	A	3	STI	C1-C2	2.06	1.43	1.37
4	B	4	STI	C15-C14	2.05	1.42	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4	STI	N10-C9-N8	-7.16	119.50	126.42
4	A	3	STI	C11-N10-C9	7.07	121.33	115.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3	STI	N10-C9-N8	-7.03	119.62	126.42
4	B	4	STI	C7-N8-C9	6.92	122.14	116.81
4	B	4	STI	C11-N10-C9	6.79	121.09	115.42
4	A	3	STI	C7-N8-C9	6.34	121.69	116.81
4	A	3	STI	C12-C11-N10	-3.26	119.97	123.97
4	B	4	STI	C2-N3-C4	3.17	122.40	116.85
4	A	3	STI	C2-N3-C4	2.86	121.87	116.85
4	B	4	STI	C12-C11-N10	-2.80	120.54	123.97
4	B	4	STI	C20-C19-C14	2.72	124.31	121.23
4	A	3	STI	C14-N13-C9	-2.72	120.93	129.22
4	B	4	STI	C19-C14-N13	2.43	122.88	118.68
4	B	4	STI	O29-C22-C23	-2.35	116.24	120.90
4	B	4	STI	C14-N13-C9	-2.24	122.39	129.22
4	A	3	STI	N13-C9-N10	2.22	122.58	116.29
4	B	4	STI	N13-C9-N10	2.14	122.36	116.29
4	B	4	STI	C46-C27-C28	-2.06	116.95	120.75
4	A	3	STI	C46-C27-C28	-2.03	117.01	120.75

There are no chirality outliers.

All (16) torsion outliers are listed below:

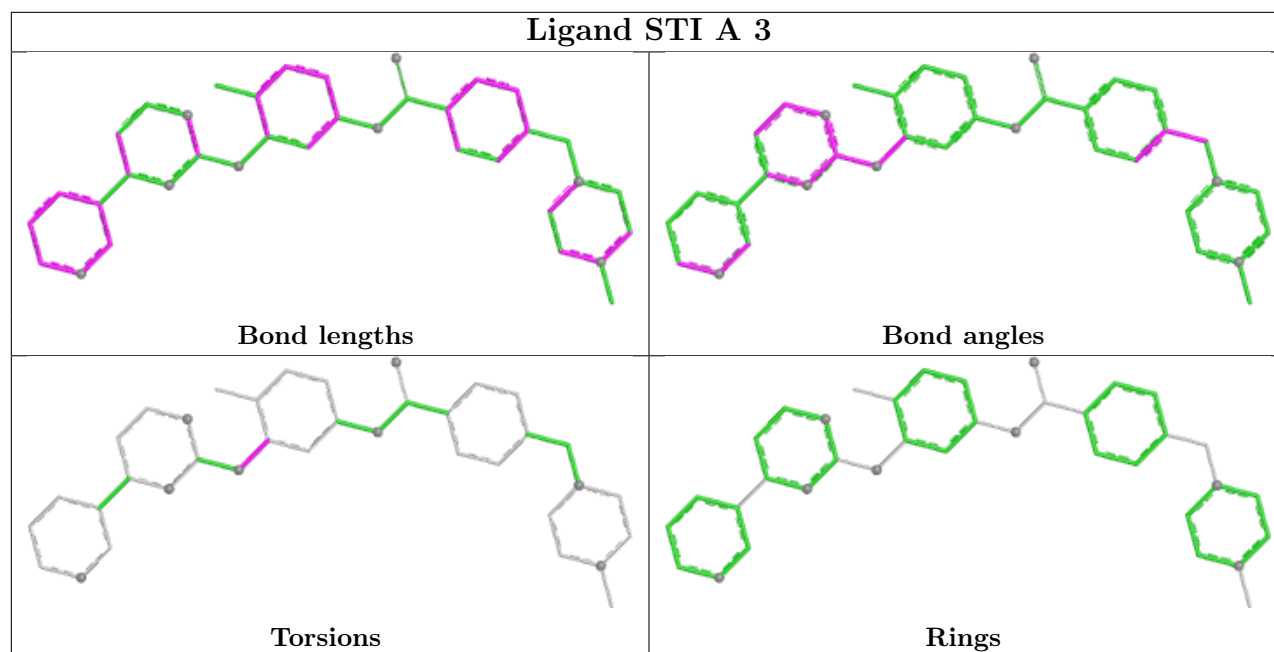
Mol	Chain	Res	Type	Atoms
3	A	1	MYR	O1-C1-C2-C3
3	B	2	MYR	C1-C2-C3-C4
4	A	3	STI	C19-C14-N13-C9
4	A	3	STI	C15-C14-N13-C9
4	B	4	STI	C19-C14-N13-C9
4	B	4	STI	C15-C14-N13-C9
3	B	2	MYR	C5-C6-C7-C8
3	B	2	MYR	C10-C11-C12-C13
3	B	2	MYR	C11-C10-C9-C8
3	B	2	MYR	C9-C10-C11-C12
3	A	1	MYR	C4-C5-C6-C7
3	B	2	MYR	C2-C3-C4-C5
3	A	1	MYR	C10-C11-C12-C13
3	A	1	MYR	C11-C12-C13-C14
3	A	1	MYR	C5-C6-C7-C8
3	B	2	MYR	C6-C7-C8-C9

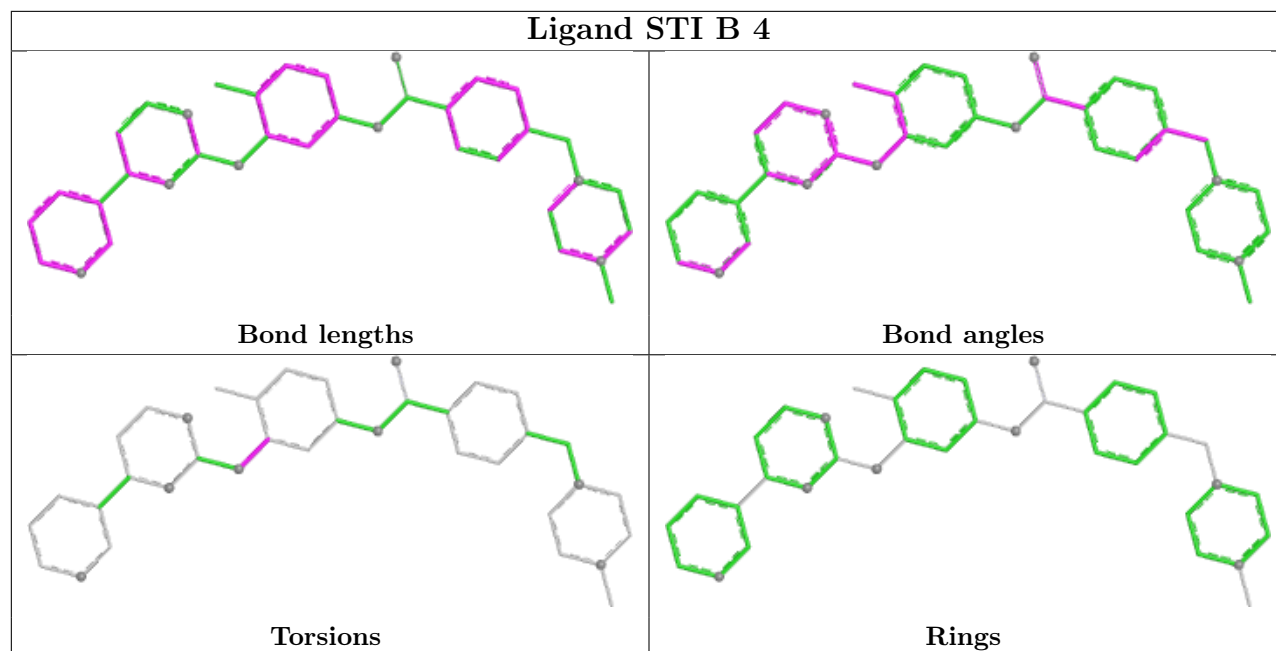
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4	STI	1	0
3	A	1	MYR	1	0
3	B	2	MYR	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 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	287/293 (97%)	0.46	34 (11%) 9 10	8, 21, 52, 69	0
1	B	288/293 (98%)	0.89	55 (19%) 3 3	14, 31, 62, 78	0
All	All	575/586 (98%)	0.68	89 (15%) 5 5	8, 26, 60, 78	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	529	LEU	5.7
1	A	243	ALA	5.3
1	A	406	LEU	5.1
1	A	529	LEU	4.6
1	A	409	GLY	4.6
1	A	295	ASP	4.5
1	B	279	VAL	4.3
1	B	282	LYS	4.1
1	B	531	LYS	4.0
1	B	530	GLY	4.0
1	B	408	THR	4.0
1	A	269	GLY	4.0
1	B	265	HIS	3.8
1	B	261	ILE	3.8
1	B	330	PHE	3.7
1	B	259	THR	3.6
1	B	283	TYR	3.6
1	B	417	GLY	3.4
1	A	296	THR	3.4
1	A	297	MET	3.4
1	B	244	MET	3.3
1	A	273	GLY	3.3
1	A	298	GLU	3.2
1	A	414	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	280	TRP	3.1
1	B	406	LEU	3.1
1	B	285	LEU	3.0
1	B	526	GLU	3.0
1	B	292	LEU	3.0
1	A	410	ASP	3.0
1	B	297	MET	3.0
1	A	270	GLY	3.0
1	A	417	GLY	3.0
1	B	256	MET	3.0
1	B	525	VAL	2.8
1	A	404	SER	2.8
1	B	299	VAL	2.8
1	A	403	LEU	2.8
1	B	264	LYS	2.7
1	A	292	LEU	2.7
1	B	312	ILE	2.7
1	B	409	GLY	2.7
1	B	352	GLN	2.7
1	B	513	GLU	2.7
1	B	286	THR	2.7
1	B	528	GLU	2.6
1	A	272	TYR	2.6
1	A	407	MET	2.6
1	B	249	PRO	2.6
1	A	405	ARG	2.6
1	B	295	ASP	2.5
1	A	246	PRO	2.5
1	A	416	ALA	2.5
1	A	418	ALA	2.5
1	A	280	TRP	2.5
1	B	262	THR	2.5
1	B	296	THR	2.5
1	B	293	LYS	2.5
1	A	294	GLU	2.5
1	B	331	TYR	2.5
1	B	335	GLU	2.5
1	A	408	THR	2.4
1	B	269	GLY	2.4
1	A	412	TYR	2.4
1	B	260	ASP	2.4
1	B	270	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	265	HIS	2.3
1	B	246	PRO	2.2
1	B	325	THR	2.2
1	A	244	MET	2.2
1	B	402	GLY	2.2
1	A	525	VAL	2.2
1	B	411	THR	2.2
1	A	300	GLU	2.2
1	B	339	TYR	2.2
1	B	404	SER	2.2
1	B	294	GLU	2.2
1	B	247	SER	2.2
1	B	284	SER	2.2
1	A	463	ASP	2.1
1	A	299	VAL	2.1
1	B	405	ARG	2.1
1	B	336	PHE	2.1
1	B	276	TYR	2.1
1	B	514	THR	2.1
1	B	267	LEU	2.0
1	B	281	LYS	2.0
1	A	293	LYS	2.0
1	B	266	LYS	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](#)

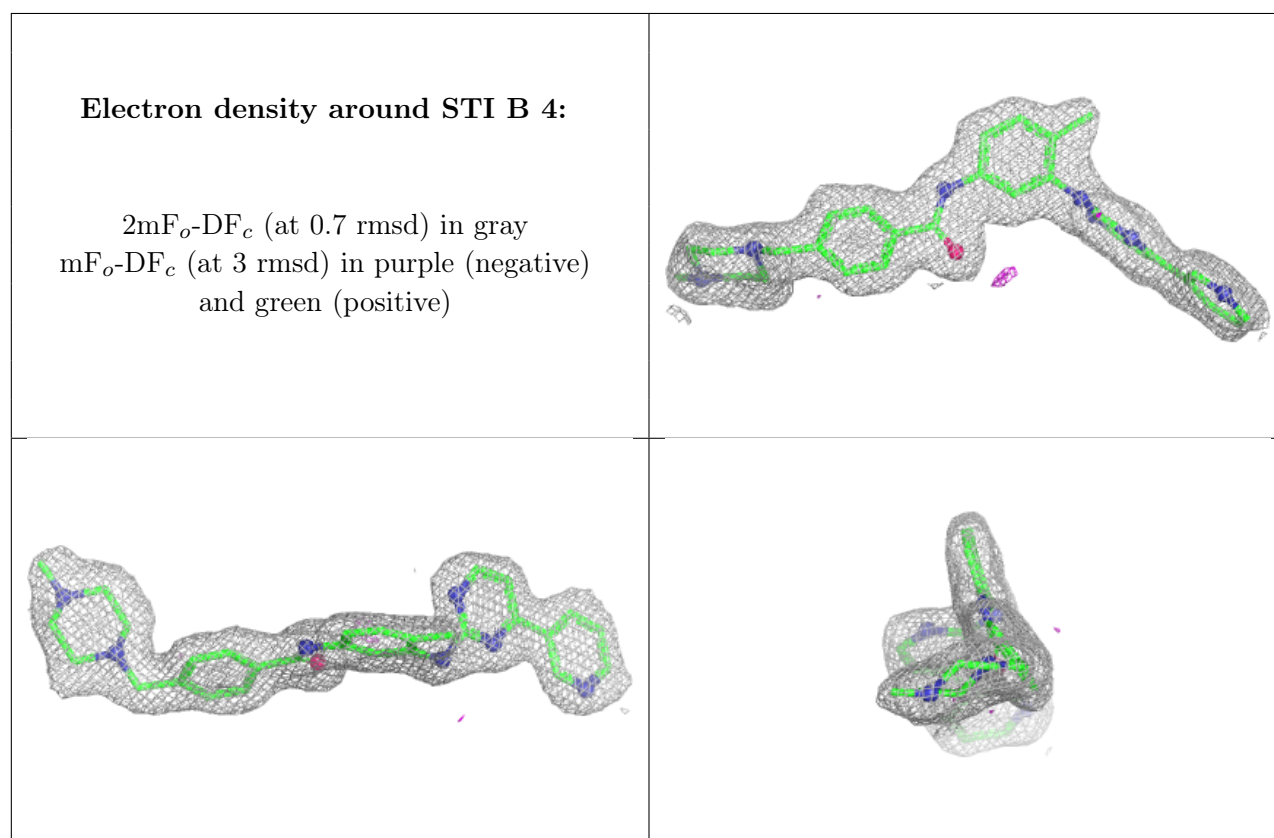
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

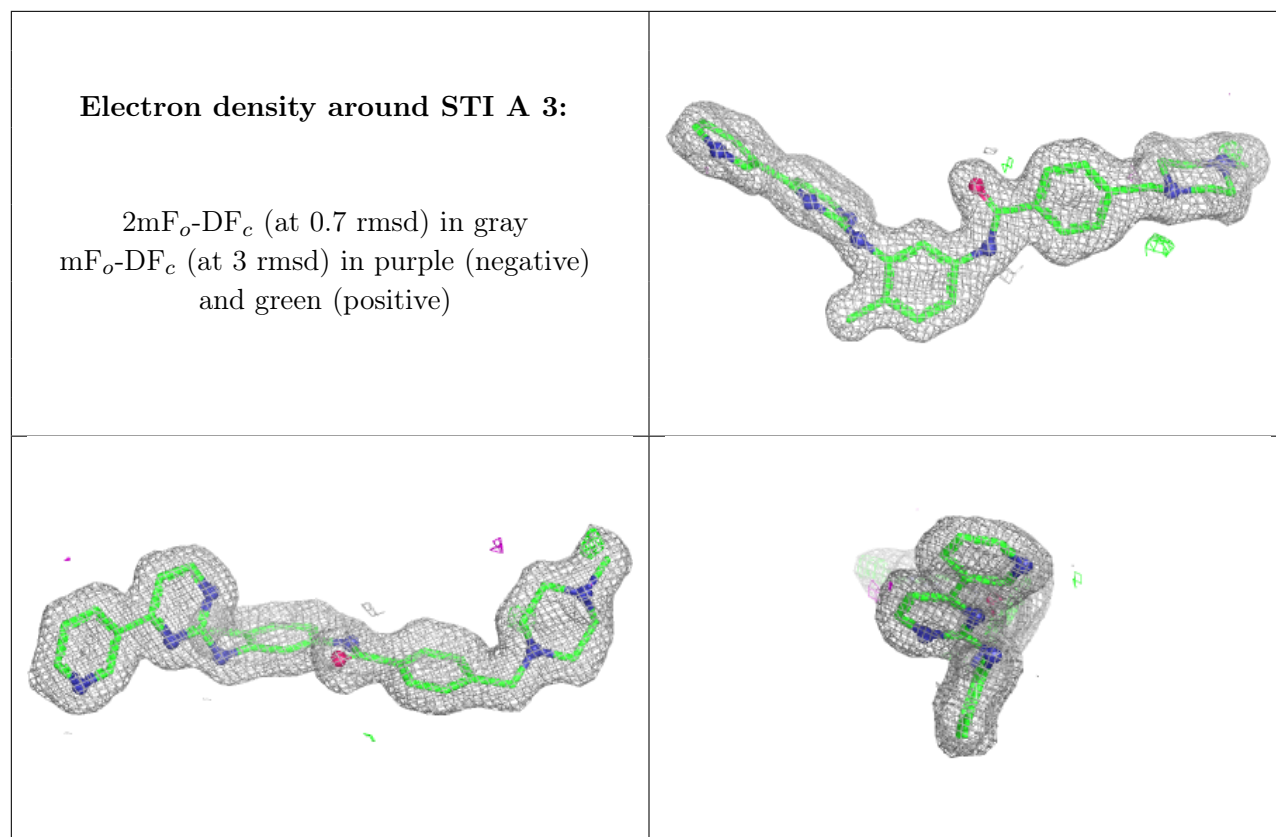
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MYR	B	2	15/16	0.82	0.18	37,46,56,56	0
3	MYR	A	1	15/16	0.84	0.18	31,36,55,55	0
4	STI	B	4	37/37	0.92	0.09	22,27,32,35	0
4	STI	A	3	37/37	0.95	0.06	13,17,21,21	0
2	CL	A	5	1/1	0.99	0.04	28,28,28,28	0
2	CL	B	6	1/1	0.99	0.04	37,37,37,37	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.