



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:53 pm GMT

PDB ID : 1IEP  
Title : CRYSTAL STRUCTURE OF THE C-ABL KINASE DOMAIN IN COMPLEX WITH STI-571.  
Authors : Nagar, B.; Bornmann, W.; Schindler, T.; Clarkson, B.; Kuriyan, J.  
Deposited on : 2001-04-10  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

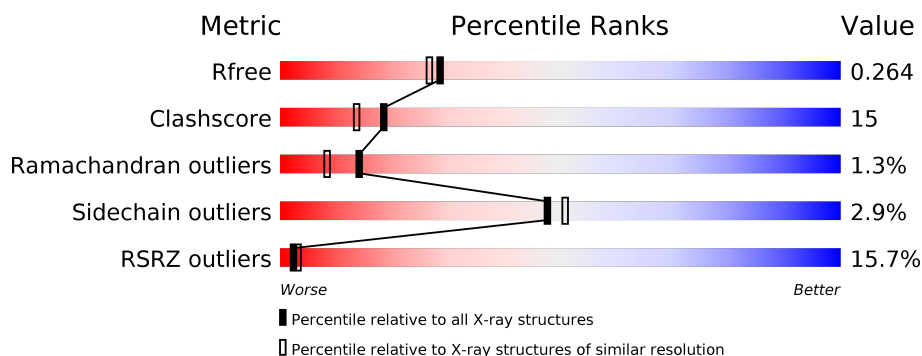
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>14%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>• 6%</div> </div> </div>
1	B	293	<div> <div>15%</div> <div> <div></div> <div>63%</div> <div>28%</div> <div>• 6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	B	6	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4710 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 ABL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2229	1435	362	414	18			
1	B	274	Total	C	N	O	S	0	0	0
			2229	1435	362	414	18			

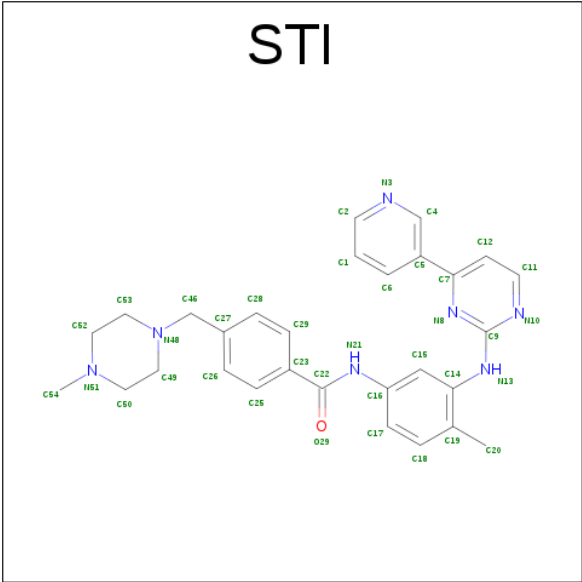
There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 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: C<sub>29</sub>H<sub>31</sub>N<sub>7</sub>O).



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

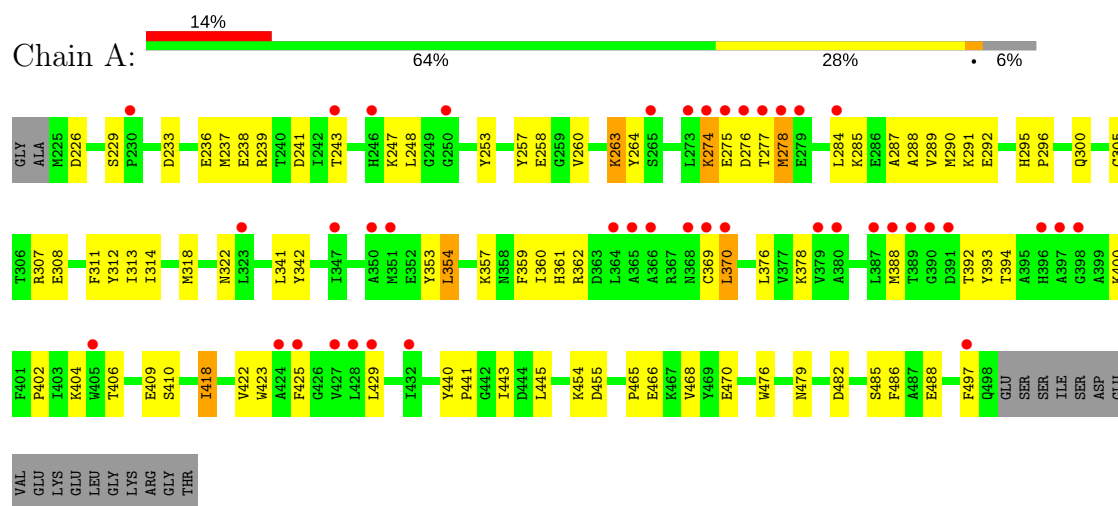
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total	O	0	0
			99	99		
4	B	73	Total	O	0	0
			73	73		

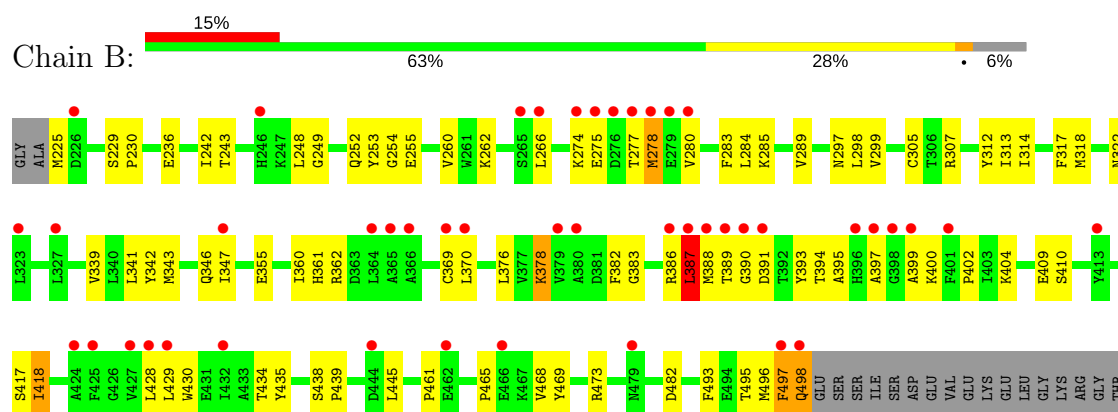
### 3 Residue-property plots [i](#)

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: PROTO-ONCOGENE TYROSINE-PROTEIN KINASE ABL



#### • Molecule 1: PROTO-ONCOGENE TYROSINE-PROTEIN KINASE ABL



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.89Å 147.37Å 153.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.14 – 2.10 29.14 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.14-2.10) 91.3 (29.14-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.231 , 0.262 0.230 , 0.264	Depositor DCC
$R_{free}$ test set	2917 reflections (8.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: STI, 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	0.30	0/2288	0.57	0/3098
1	B	0.30	0/2288	0.56	0/3098
All	All	0.30	0/4576	0.56	0/6196

There are no bond length outliers.

There are no bond angle outliers.

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	2229	0	2178	65	0
1	B	2229	0	2178	66	0
2	A	4	0	0	1	0
2	B	2	0	0	4	0
3	A	37	0	31	0	0
3	B	37	0	31	2	0
4	A	99	0	0	1	0
4	B	73	0	0	0	0
All	All	4710	0	4418	133	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 15.



All (133) 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:225:MET:HE2	1:B:307:ARG:HD2	1.52	0.89
1:A:253:TYR:OH	2:A:5:CL:CL	2.30	0.85
1:A:404:LYS:HE3	1:A:440:TYR:HB2	1.60	0.82
1:A:305:CYS:HB2	1:A:312:TYR:HB2	1.64	0.80
1:A:466:GLU:O	1:A:470:GLU:HG3	1.84	0.78
1:B:253:TYR:OH	2:B:6:CL:CL	2.39	0.78
1:B:305:CYS:HB2	1:B:312:TYR:HB2	1.67	0.77
1:A:388:MET:HG3	1:A:393:TYR:CE1	2.23	0.73
1:A:353:TYR:CZ	1:A:357:LYS:HD2	2.22	0.73
1:B:370:LEU:HD21	1:B:382:PHE:HZ	1.54	0.73
1:B:225:MET:CE	1:B:307:ARG:HD2	2.19	0.73
1:A:443:ILE:HD12	1:A:443:ILE:H	1.55	0.72
1:A:418:ILE:HD11	1:A:486:PHE:HD1	1.53	0.72
1:B:495:THR:C	1:B:497:PHE:H	1.96	0.69
1:B:387:LEU:HD12	1:B:388:MET:H	1.58	0.69
1:B:243:THR:HB	1:B:260:VAL:HB	1.74	0.68
1:B:361:HIS:O	1:B:362:ARG:HB2	1.94	0.68
1:B:387:LEU:HD12	1:B:388:MET:N	2.08	0.67
1:B:370:LEU:HD21	1:B:382:PHE:CZ	2.31	0.66
1:A:274:LYS:H	1:A:274:LYS:HD2	1.61	0.65
1:B:274:LYS:HG2	1:B:275:GLU:H	1.62	0.65
1:A:388:MET:HG3	1:A:393:TYR:HE1	1.62	0.64
1:B:248:LEU:HD11	1:B:317:PHE:HE1	1.61	0.64
1:A:342:TYR:HB2	1:A:497:PHE:HE2	1.62	0.64
1:B:394:THR:HG22	1:B:395:ALA:N	2.13	0.64
1:A:361:HIS:O	1:A:362:ARG:HB2	1.97	0.63
1:A:418:ILE:HD11	1:A:486:PHE:CD1	2.33	0.62
1:A:443:ILE:HD12	1:A:443:ILE:N	2.15	0.61
1:A:359:PHE:C	1:A:360:ILE:HD12	2.20	0.61
1:A:307:ARG:HE	1:A:307:ARG:HA	1.66	0.59
1:A:290:MET:CE	1:A:313:ILE:HD13	2.32	0.59
1:B:394:THR:CG2	1:B:395:ALA:N	2.66	0.59
1:B:342:TYR:O	1:B:346:GLN:HG3	2.03	0.59
1:B:339:VAL:O	1:B:343:MET:HG3	2.02	0.58
1:A:485:SER:OG	1:A:488:GLU:HG3	2.02	0.58
1:B:285:LYS:O	1:B:289:VAL:HG23	2.04	0.58
1:A:296:PRO:O	1:A:378:LYS:HE2	2.04	0.57
1:B:254:GLY:HA3	1:B:387:LEU:HD22	1.85	0.57
1:A:318:MET:HG3	1:A:370:LEU:HB3	1.87	0.57
1:B:275:GLU:C	1:B:277:THR:H	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:GLU:HG2	1:B:410:SER:N	2.21	0.56
1:B:465:PRO:HG2	1:B:468:VAL:CG2	2.36	0.56
1:B:297:ASN:HA	1:B:378:LYS:HG3	1.87	0.56
1:B:360:ILE:HD13	1:B:417:SER:HA	1.89	0.55
1:B:370:LEU:N	1:B:370:LEU:HD22	2.23	0.54
2:B:3:CL:CL	3:B:202:STI:H501	2.45	0.54
1:B:314:ILE:N	1:B:314:ILE:HD12	2.23	0.53
1:A:263:LYS:HD2	1:A:264:TYR:CE1	2.44	0.53
1:A:274:LYS:O	1:A:276:ASP:N	2.42	0.52
1:B:318:MET:HG3	1:B:370:LEU:CB	2.40	0.52
1:A:238:GLU:HB3	1:A:241:ASP:OD1	2.10	0.51
1:A:465:PRO:HG2	1:A:468:VAL:CG2	2.42	0.50
1:A:247:LYS:HG2	1:A:257:TYR:CE2	2.46	0.50
1:B:278:MET:SD	1:B:278:MET:N	2.83	0.50
1:A:406:THR:HG22	1:A:410:SER:HB2	1.94	0.50
1:B:383:GLY:O	1:B:386:ARG:HB3	2.12	0.50
1:B:465:PRO:HG2	1:B:468:VAL:HG23	1.94	0.49
1:A:290:MET:HE1	1:A:313:ILE:HD13	1.93	0.49
1:A:288:ALA:O	1:A:292:GLU:HG2	2.12	0.49
1:B:274:LYS:HG2	1:B:275:GLU:N	2.28	0.49
1:B:495:THR:C	1:B:497:PHE:N	2.65	0.49
1:B:394:THR:O	1:B:400:LYS:HA	2.12	0.49
1:B:249:GLY:O	1:B:252:GLN:HG2	2.13	0.49
1:A:295:HIS:CG	1:A:296:PRO:HD2	2.48	0.48
1:A:445:LEU:HD12	1:A:445:LEU:N	2.28	0.48
1:A:226:ASP:HB3	1:A:229:SER:HB2	1.95	0.48
1:B:391:ASP:OD2	1:B:445:LEU:HD11	2.13	0.48
1:A:239:ARG:NH2	1:A:308:GLU:O	2.47	0.48
1:A:300:GLN:HA	4:A:135:HOH:O	2.14	0.48
1:A:443:ILE:CD1	1:A:443:ILE:H	2.25	0.48
1:B:429:LEU:HD21	1:B:493:PHE:CZ	2.48	0.47
1:A:445:LEU:CD1	1:A:445:LEU:H	2.27	0.47
1:B:369:CYS:C	1:B:370:LEU:HD22	2.34	0.47
1:B:280:VAL:O	1:B:284:LEU:HG	2.14	0.47
1:B:347:ILE:HD13	1:B:428:LEU:HD21	1.97	0.47
1:B:242:ILE:CD1	1:B:314:ILE:HG12	2.45	0.47
1:A:342:TYR:HB2	1:A:497:PHE:CE2	2.48	0.46
1:B:386:ARG:O	1:B:386:ARG:HG2	2.15	0.46
1:A:237:MET:SD	1:A:314:ILE:HD13	2.56	0.46
1:B:355:GLU:HG3	1:B:418:ILE:HG13	1.97	0.46
1:B:394:THR:CG2	1:B:395:ALA:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:THR:OG1	1:B:390:GLY:N	2.49	0.46
1:B:248:LEU:HD11	1:B:317:PHE:CE1	2.48	0.46
1:A:441:PRO:O	1:A:443:ILE:HD12	2.16	0.46
1:A:290:MET:HE3	1:A:313:ILE:HD13	1.96	0.46
1:A:360:ILE:N	1:A:360:ILE:HD12	2.31	0.45
1:A:285:LYS:O	1:A:289:VAL:HG23	2.17	0.45
1:B:397:ALA:C	1:B:399:ALA:H	2.19	0.45
1:A:418:ILE:O	1:A:422:VAL:HG23	2.17	0.45
1:B:229:SER:HA	1:B:230:PRO:HD3	1.83	0.44
1:A:479:ASN:HB3	1:A:482:ASP:OD2	2.18	0.44
1:A:248:LEU:CD1	1:A:258:GLU:HB2	2.47	0.44
1:B:322:ASN:N	2:B:6:CL:CL	2.87	0.43
1:A:409:GLU:HG2	1:A:410:SER:N	2.32	0.43
1:A:445:LEU:HD12	1:A:445:LEU:H	1.82	0.43
1:A:322:ASN:HA	1:A:369:CYS:O	2.18	0.43
1:B:298:LEU:O	1:B:299:VAL:C	2.57	0.42
1:A:425:PHE:CZ	1:A:429:LEU:HD21	2.54	0.42
1:B:434:THR:O	1:B:435:TYR:HB2	2.18	0.42
1:B:469:TYR:CZ	1:B:473:ARG:HD3	2.54	0.42
1:A:277:THR:HG22	1:A:278:MET:N	2.34	0.42
1:A:354:LEU:HA	1:A:354:LEU:HD12	1.91	0.42
1:A:454:LYS:O	1:A:455:ASP:HB2	2.19	0.42
1:B:255:GLU:OE1	1:B:255:GLU:HA	2.20	0.42
1:A:287:ALA:O	1:A:291:LYS:HG3	2.19	0.42
1:A:284:LEU:HD11	1:A:311:PHE:CE1	2.55	0.42
2:B:6:CL:CL	3:B:202:STI:H11	2.57	0.42
1:A:423:TRP:CE3	1:A:476:TRP:HA	2.55	0.42
1:B:434:THR:HG22	1:B:461:PRO:HB3	2.01	0.42
1:A:248:LEU:HD13	1:A:258:GLU:HB2	2.02	0.42
1:A:392:THR:O	1:A:402:PRO:HA	2.19	0.41
1:A:418:ILE:HD13	1:A:418:ILE:O	2.20	0.41
1:B:438:SER:HA	1:B:439:PRO:HD3	1.91	0.41
1:A:233:ASP:HB3	1:A:236:GLU:HG2	2.02	0.41
1:B:430:TRP:NE1	1:B:461:PRO:HG3	2.35	0.41
1:B:498:GLN:OE1	1:B:498:GLN:HA	2.20	0.41
1:A:341:LEU:CD2	1:A:497:PHE:HA	2.51	0.41
1:A:393:TYR:HB3	1:A:400:LYS:HB3	2.03	0.41
1:B:225:MET:CE	1:B:236:GLU:HG3	2.50	0.41
1:B:318:MET:HG3	1:B:370:LEU:HB3	2.02	0.41
1:A:318:MET:HB2	1:A:370:LEU:HG	2.02	0.41
1:B:283:PHE:CZ	1:B:313:ILE:HG13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:TYR:CE2	1:B:402:PRO:HD3	2.56	0.41
1:A:243:THR:HB	1:A:260:VAL:HB	2.02	0.41
1:A:274:LYS:HB2	1:A:277:THR:OG1	2.21	0.41
1:B:429:LEU:HD21	1:B:493:PHE:HZ	1.85	0.41
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.91	0.41
1:B:360:ILE:CD1	1:B:417:SER:HA	2.49	0.41
1:B:225:MET:HE1	1:B:236:GLU:HG3	2.03	0.40
1:B:404:LYS:HE2	1:B:445:LEU:CD2	2.51	0.40
1:B:341:LEU:HG	1:B:497:PHE:CE1	2.56	0.40
1:A:305:CYS:O	1:A:311:PHE:HA	2.22	0.40
1:B:275:GLU:C	1:B:277:THR:N	2.72	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	272/293 (93%)	251 (92%)	17 (6%)	4 (2%)	12	6
1	B	272/293 (93%)	245 (90%)	24 (9%)	3 (1%)	17	11
All	All	544/586 (93%)	496 (91%)	41 (8%)	7 (1%)	14	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	GLU
1	A	263	LYS
1	A	274	LYS
1	B	262	LYS
1	B	496	MET
1	B	387	LEU
1	A	278	MET

### 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	240/255 (94%)	235 (98%)	5 (2%)	59	64
1	B	240/255 (94%)	231 (96%)	9 (4%)	38	38
All	All	480/510 (94%)	466 (97%)	14 (3%)	48	51

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

Mol	Chain	Res	Type
1	A	354	LEU
1	A	370	LEU
1	A	376	LEU
1	A	394	THR
1	A	418	ILE
1	B	266	LEU
1	B	278	MET
1	B	376	LEU
1	B	378	LYS
1	B	387	LEU
1	B	418	ILE
1	B	482	ASP
1	B	497	PHE
1	B	498	GLN

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

Mol	Chain	Res	Type
1	A	252	GLN

### 5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z  > 2$
3	STI	A	201	-	41,41,41	2.44	22 (53%)	56,56,56	2.02	8 (14%)
3	STI	B	202	-	41,41,41	2.44	24 (58%)	56,56,56	2.06	9 (16%)

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	STI	A	201	-	-	0/20/30/30	0/5/5/5
3	STI	B	202	-	-	0/20/30/30	0/5/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	STI	C9-N13	2.00	1.40	1.36
3	B	202	STI	C17-C16	2.04	1.42	1.39
3	A	201	STI	C20-C19	2.07	1.55	1.51
3	B	202	STI	C20-C19	2.09	1.55	1.51
3	B	202	STI	C1-C2	2.11	1.44	1.37
3	A	201	STI	C7-N8	2.11	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	STI	C12-C7	2.14	1.43	1.38
3	B	202	STI	C2-N3	2.20	1.40	1.33
3	B	202	STI	C49-N48	2.20	1.52	1.47
3	A	201	STI	C1-C2	2.22	1.44	1.37
3	A	201	STI	C17-C16	2.23	1.43	1.39
3	B	202	STI	C12-C7	2.34	1.44	1.38
3	A	201	STI	C2-N3	2.35	1.40	1.33
3	B	202	STI	C7-N8	2.39	1.38	1.34
3	A	201	STI	C49-N48	2.44	1.53	1.47
3	B	202	STI	C4-N3	2.50	1.39	1.34
3	A	201	STI	C4-N3	2.51	1.39	1.34
3	B	202	STI	C15-C14	2.58	1.43	1.39
3	B	202	STI	C52-N51	2.77	1.52	1.46
3	B	202	STI	C50-N51	2.83	1.52	1.46
3	A	201	STI	C52-N51	2.85	1.52	1.46
3	B	202	STI	C28-C27	3.07	1.45	1.38
3	A	201	STI	C1-C6	3.16	1.44	1.38
3	A	201	STI	C50-N51	3.19	1.53	1.46
3	B	202	STI	C26-C25	3.19	1.44	1.38
3	B	202	STI	C1-C6	3.21	1.45	1.38
3	A	201	STI	C6-C5	3.23	1.46	1.39
3	A	201	STI	C26-C25	3.26	1.44	1.38
3	B	202	STI	C6-C5	3.27	1.46	1.39
3	A	201	STI	C17-C18	3.28	1.44	1.38
3	B	202	STI	C17-C18	3.29	1.44	1.38
3	B	202	STI	C26-C27	3.34	1.45	1.38
3	A	201	STI	C28-C27	3.35	1.45	1.38
3	A	201	STI	C9-N10	3.37	1.38	1.34
3	B	202	STI	C29-C23	3.37	1.44	1.39
3	B	202	STI	C14-C19	3.46	1.47	1.40
3	B	202	STI	C4-C5	3.50	1.45	1.39
3	A	201	STI	C14-C19	3.53	1.47	1.40
3	A	201	STI	C29-C23	3.56	1.45	1.39
3	B	202	STI	C9-N10	3.61	1.39	1.34
3	A	201	STI	C4-C5	3.70	1.46	1.39
3	A	201	STI	C26-C27	3.70	1.46	1.38
3	A	201	STI	C15-C16	3.81	1.45	1.39
3	B	202	STI	C15-C16	4.40	1.46	1.39
3	B	202	STI	C25-C23	4.53	1.46	1.39
3	A	201	STI	C25-C23	4.64	1.47	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	STI	N10-C9-N8	-7.14	119.80	126.68
3	A	201	STI	N10-C9-N8	-7.00	119.94	126.68
3	A	201	STI	C12-C11-N10	-3.27	120.15	123.92
3	B	202	STI	C12-C11-N10	-3.01	120.44	123.92
3	B	202	STI	O29-C22-C23	-2.64	116.25	120.94
3	A	201	STI	C14-N13-C9	-2.58	120.74	129.51
3	A	201	STI	O29-C22-C23	-2.41	116.67	120.94
3	B	202	STI	C14-N13-C9	-2.05	122.53	129.51
3	A	201	STI	C27-C46-N48	2.12	117.25	113.17
3	B	202	STI	C20-C19-C14	2.32	123.73	121.33
3	B	202	STI	C27-C46-N48	2.41	117.80	113.17
3	A	201	STI	C2-N3-C4	3.25	122.52	116.83
3	B	202	STI	C2-N3-C4	3.39	122.78	116.83
3	B	202	STI	C11-N10-C9	6.49	120.84	115.43
3	A	201	STI	C11-N10-C9	6.73	121.05	115.43
3	A	201	STI	C7-N8-C9	7.36	121.80	116.55
3	B	202	STI	C7-N8-C9	7.68	122.03	116.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	STI	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	274/293 (93%)	0.80	41 (14%) 3 4	29, 48, 85, 110	0
1	B	274/293 (93%)	0.97	45 (16%) 2 3	37, 53, 94, 109	0
All	All	548/586 (93%)	0.88	86 (15%) 2 3	29, 51, 91, 110	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	MET	7.8
1	B	391	ASP	6.9
1	B	276	ASP	5.8
1	B	396	HIS	5.6
1	B	278	MET	5.4
1	A	274	LYS	5.4
1	A	428	LEU	4.8
1	A	389	THR	4.7
1	A	388	MET	4.4
1	A	275	GLU	4.4
1	B	364	LEU	4.3
1	B	365	ALA	4.3
1	B	497	PHE	4.3
1	B	498	GLN	4.3
1	A	391	ASP	4.2
1	B	390	GLY	4.1
1	B	369	CYS	4.1
1	A	276	ASP	4.1
1	B	389	THR	3.9
1	A	277	THR	3.9
1	B	399	ALA	3.9
1	B	366	ALA	3.8
1	A	364	LEU	3.8
1	A	427	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	425	PHE	3.8
1	B	428	LEU	3.7
1	B	379	VAL	3.6
1	B	424	ALA	3.6
1	A	398	GLY	3.5
1	B	387	LEU	3.5
1	A	379	VAL	3.4
1	A	265	SER	3.4
1	B	274	LYS	3.3
1	B	279	GLU	3.3
1	A	387	LEU	3.3
1	A	243	THR	3.2
1	B	275	GLU	3.2
1	A	425	PHE	3.2
1	B	323	LEU	3.2
1	A	365	ALA	3.1
1	A	366	ALA	3.1
1	A	369	CYS	3.1
1	A	278	MET	3.1
1	A	396	HIS	3.1
1	B	265	SER	3.0
1	A	497	PHE	3.0
1	B	386	ARG	2.9
1	B	401	PHE	2.9
1	A	424	ALA	2.9
1	A	323	LEU	2.8
1	A	273	LEU	2.8
1	A	397	ALA	2.8
1	B	398	GLY	2.7
1	B	413	TYR	2.7
1	B	427	VAL	2.7
1	A	429	LEU	2.7
1	B	380	ALA	2.6
1	A	250	GLY	2.6
1	A	350	ALA	2.6
1	B	277	THR	2.6
1	B	370	LEU	2.5
1	B	397	ALA	2.4
1	B	347	ILE	2.4
1	B	266	LEU	2.4
1	A	279	GLU	2.3
1	A	347	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	466	GLU	2.3
1	A	390	GLY	2.3
1	A	432	ILE	2.2
1	B	479	ASN	2.2
1	A	405	TRP	2.2
1	A	284	LEU	2.2
1	A	351	MET	2.2
1	B	444	ASP	2.2
1	A	370	LEU	2.1
1	B	462	GLU	2.1
1	B	246	HIS	2.1
1	A	230	PRO	2.1
1	B	280	VAL	2.1
1	A	368	ASN	2.1
1	B	432	ILE	2.1
1	B	226	ASP	2.1
1	A	380	ALA	2.1
1	A	246	HIS	2.1
1	B	327	LEU	2.0
1	B	429	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	STI	A	201	37/37	0.94	0.19	0.80	25,33,46,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	STI	B	202	37/37	0.94	0.19	0.36	34,42,52,54	0
2	CL	B	3	1/1	0.89	0.07	-	64,64,64,64	0
2	CL	A	2	1/1	0.95	0.06	-	64,64,64,64	0
2	CL	B	6	1/1	0.88	0.14	-	73,73,73,73	0
2	CL	A	5	1/1	0.98	0.14	-	49,49,49,49	0
2	CL	A	1	1/1	0.96	0.07	-	50,50,50,50	0
2	CL	A	4	1/1	0.95	0.12	-	86,86,86,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.