Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:22 PM GMT

PDB ID	:	1OPJ
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
http://wwpdb.org/validation/2016/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:

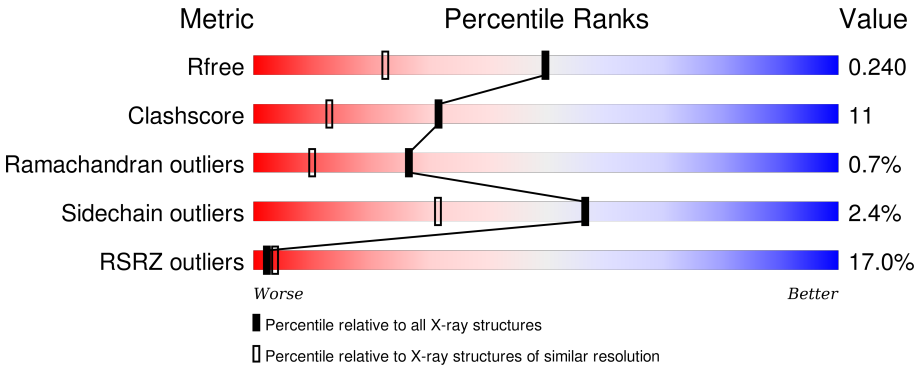
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.75 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}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	14% 81% 16%
1	B	293	19% 71% 26%

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
3	MYR	A	1	-	-	-	X
3	MYR	B	2	-	-	-	X

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			

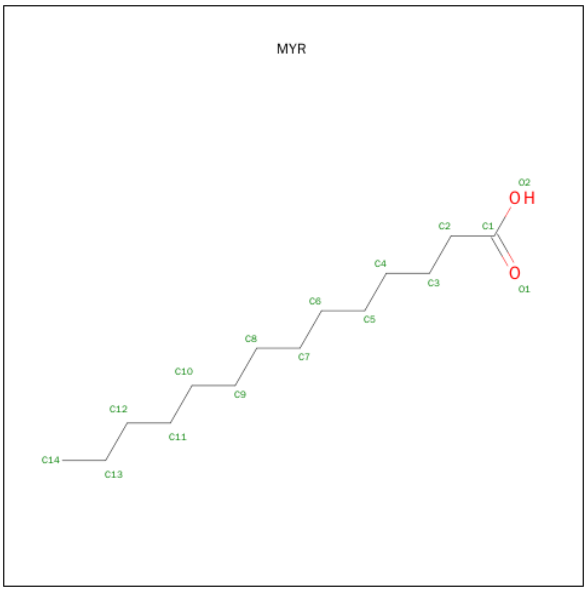
There are 12 discrepancies between the modelled and reference sequences:

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 (three-letter code: CL) (formula: Cl).

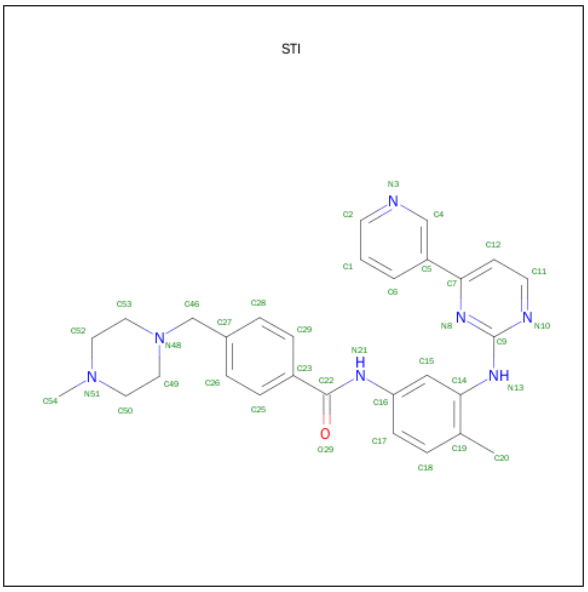
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 4 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: $C_{29}H_{31}N_7O$).



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

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

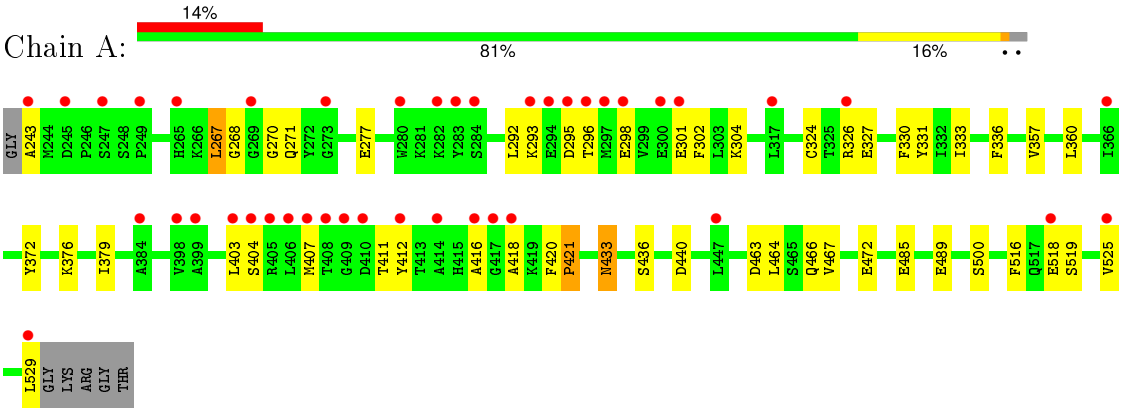
- Molecule 5 is water.

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

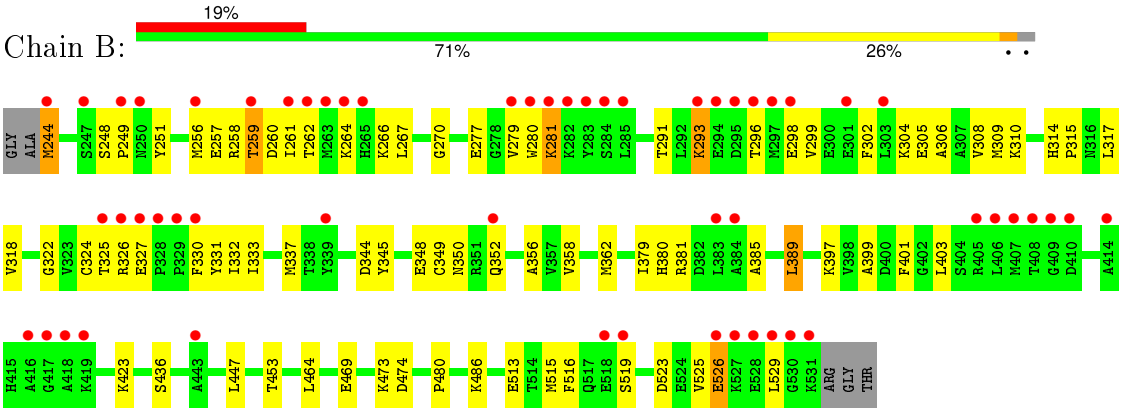
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 (i)

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 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (29.41-1.75) 83.8 (29.41-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.242 0.209 , 0.240	Depositor DCC
R_{free} test set	2886 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 61583 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MYR, 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	0.46	0/2387	0.69	3/3231 (0.1%)
1	B	0.37	0/2395	0.61	0/3240
All	All	0.42	0/4782	0.65	3/6471 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	421	PRO	N-CA-C	-5.73	97.20	112.10
1	A	331	TYR	CB-CA-C	-5.08	100.25	110.40
1	A	440	ASP	CB-CG-OD2	5.05	122.84	118.30

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	38	0
1	B	2336	0	2281	63	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	101	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 (101) 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:H	1:B:293:LYS:HD2	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	1.67	0.76
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:VAL:HG23	5:A:226:HOH:O	2.09	0.53
1:B:258:ARG:C	1:B:260:ASP:H	2.11	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: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: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:325:THR:HA	1:B:330:PHE:HD2	1.77	0.50
1:B:314:HIS:CG	1:B:315:PRO:HD2	2.47	0.50
1:B:267:LEU:CD2	1:B:277:GLU:HB2	2.41	0.49
1:B:244:MET:N	1:B:244:MET:SD	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:326:ARG:HB3	1:B:327:GLU:OE2	2.13	0.48
1:B:264:LYS:HE2	1:B:279:VAL:CG2	2.43	0.48
1:A:326:ARG:HA	1:A:326:ARG:NE	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:B:296:THR:C	1:B:298:GLU:H	2.18	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:A:268:GLY:O	1:A:271:GLN:HG2	2.14	0.47
1:B:453:THR:HG22	1:B:480:PRO:HB3	1.96	0.47
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:A:518:GLU:CD	1:A:518:GLU:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:385:ALA:N	1:B:447:LEU:HD13	2.32	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: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:B:256:MET:HG2	1:B:257:GLU:N	2.34	0.43
1:B:280:TRP:O	1:B:281:LYS:C	2.56	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: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:HG12	1:A:525:VAL:O	2.20	0.41
1:B:379:ILE:CD1	1:B:436:SER:HA	2.50	0.41
1:B:305:GLU:O	1:B:309:MET:HG3	2.21	0.41
1:A:379:ILE:HD13	1:A:436:SER:HA	2.02	0.41
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.91	0.41
1:A:326:ARG:HE	1:A:326:ARG:HA	1.86	0.40
1:B:266:LYS:CD	1:B:270:GLY:HA2	2.47	0.40
1:A:418:ALA:HB3	1:A:420:PHE:HE2	1.87	0.40
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%)	26	10
1	B	286/293 (98%)	263 (92%)	21 (7%)	2 (1%)	26	10
All	All	571/586 (97%)	534 (94%)	33 (6%)	4 (1%)	26	10

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%)	51	25
1	B	253/255 (99%)	248 (98%)	5 (2%)	63	39
All	All	505/510 (99%)	493 (98%)	12 (2%)	57	31

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	463	ASP
1	A	472	GLU
1	A	500	SER
1	B	244	MET
1	B	293	LYS

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Mol	Chain	Res	Type
1	B	389	LEU
1	B	513	GLU
1	B	526	GLU

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

Mol	Chain	Res	Type
1	A	433	ASN
1	A	496	GLN
1	A	517	GLN
1	B	271	GLN
1	B	510	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 carbohydrates 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	$\#\|Z\| > 2$
3	MYR	A	1	-	14,14,15	1.02	1 (7%)	12,13,15	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	STI	A	3	-	41,41,41	2.08	20 (48%)	56,56,56	1.96	8 (14%)
3	MYR	B	2	-	14,14,15	1.00	1 (7%)	12,13,15	0.32	0
4	STI	B	4	-	41,41,41	2.35	23 (56%)	56,56,56	2.05	10 (17%)

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	MYR	A	1	-	-	0/11/12/13	0/0/0/0
4	STI	A	3	-	-	0/20/30/30	0/5/5/5
3	MYR	B	2	-	-	0/11/12/13	0/0/0/0
4	STI	B	4	-	-	0/20/30/30	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4	STI	C4-N3	2.05	1.38	1.34
4	A	3	STI	C49-N48	2.05	1.52	1.46
4	B	4	STI	C15-C14	2.07	1.42	1.39
4	B	4	STI	C49-N48	2.10	1.52	1.46
4	A	3	STI	C12-C7	2.13	1.44	1.38
4	A	3	STI	C9-N13	2.13	1.40	1.36
4	B	4	STI	C1-C2	2.17	1.44	1.37
4	A	3	STI	C2-N3	2.18	1.40	1.33
4	B	4	STI	C2-N3	2.19	1.40	1.33
4	A	3	STI	C17-C16	2.30	1.43	1.39
4	B	4	STI	C12-C7	2.35	1.44	1.38
4	B	4	STI	C52-N51	2.35	1.51	1.46
4	A	3	STI	C26-C25	2.44	1.43	1.38
4	B	4	STI	C9-N13	2.44	1.40	1.36
4	A	3	STI	C52-N51	2.52	1.51	1.46
4	A	3	STI	C4-N3	2.64	1.40	1.34
4	A	3	STI	C6-C5	2.65	1.45	1.39
4	B	4	STI	C29-C23	2.68	1.43	1.39
4	B	4	STI	C17-C16	2.70	1.43	1.39
4	A	3	STI	C4-C5	2.73	1.44	1.39
4	B	4	STI	C1-C6	2.73	1.44	1.38
4	B	4	STI	C7-N8	2.73	1.38	1.34
4	A	3	STI	C1-C6	2.73	1.44	1.38
4	A	3	STI	C9-N10	2.74	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3	STI	C28-C27	2.82	1.44	1.38
4	B	4	STI	C6-C5	2.93	1.45	1.39
4	A	3	STI	C26-C27	2.95	1.45	1.38
4	B	4	STI	C26-C25	2.98	1.44	1.38
4	B	4	STI	C50-N51	3.01	1.53	1.46
4	B	4	STI	C28-C27	3.02	1.45	1.38
4	A	3	STI	C14-C19	3.10	1.46	1.40
4	A	3	STI	C15-C16	3.11	1.44	1.39
4	A	3	STI	C50-N51	3.16	1.53	1.46
4	B	4	STI	C17-C18	3.19	1.44	1.38
3	B	2	MYR	O1-C1	3.29	1.41	1.19
4	B	4	STI	C15-C16	3.34	1.45	1.39
4	B	4	STI	C26-C27	3.34	1.45	1.38
3	A	1	MYR	O1-C1	3.35	1.41	1.19
4	A	3	STI	C17-C18	3.36	1.44	1.38
4	A	3	STI	C29-C23	3.41	1.45	1.39
4	B	4	STI	C9-N10	3.50	1.39	1.34
4	A	3	STI	C25-C23	3.60	1.45	1.39
4	B	4	STI	C4-C5	3.74	1.46	1.39
4	B	4	STI	C14-C19	4.20	1.48	1.40
4	B	4	STI	C25-C23	4.26	1.46	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	4	STI	N10-C9-N8	-6.73	119.50	126.67
4	A	3	STI	N10-C9-N8	-6.61	119.62	126.67
4	A	3	STI	C12-C11-N10	-3.44	119.97	123.90
4	A	3	STI	C14-N13-C9	-3.14	120.93	129.22
4	B	4	STI	C12-C11-N10	-2.94	120.54	123.90
4	B	4	STI	O29-C22-C23	-2.77	116.24	120.97
4	B	4	STI	C14-N13-C9	-2.59	122.39	129.22
4	B	4	STI	C46-C27-C28	-2.03	116.95	120.78
4	A	3	STI	O29-C22-C23	-2.02	117.53	120.97
4	B	4	STI	N13-C9-N10	2.10	122.36	116.01
4	A	3	STI	N13-C9-N10	2.17	122.58	116.01
4	A	3	STI	C2-N3-C4	2.73	121.87	116.84
4	B	4	STI	C20-C19-C14	2.83	124.31	121.36
4	B	4	STI	C2-N3-C4	3.02	122.40	116.84
4	B	4	STI	C11-N10-C9	6.45	121.09	115.49
4	A	3	STI	C11-N10-C9	6.72	121.33	115.49
4	A	3	STI	C7-N8-C9	6.97	121.69	116.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	4	STI	C7-N8-C9	7.57	122.14	116.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	MYR	1	0
3	B	2	MYR	1	0
4	B	4	STI	1	0

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, 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>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	287/293 (97%)	0.87	42 (14%)	3	5	8, 21, 52, 69	0
1	B	288/293 (98%)	1.11	56 (19%)	1	2	14, 31, 62, 78	0
All	All	575/586 (98%)	0.99	98 (17%)	2	4	8, 26, 60, 78	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	530	GLY	13.1
1	B	295	ASP	8.7
1	A	295	ASP	8.6
1	A	409	GLY	8.1
1	A	406	LEU	7.7
1	B	417	GLY	7.2
1	B	297	MET	6.6
1	A	269	GLY	6.4
1	B	529	LEU	6.1
1	A	296	THR	6.0
1	A	297	MET	6.0
1	A	407	MET	5.9
1	A	410	ASP	5.8
1	A	405	ARG	5.8
1	B	408	THR	5.5
1	A	408	THR	5.4
1	B	282	LYS	5.1
1	B	294	GLU	5.0
1	A	414	ALA	4.9
1	B	296	THR	4.9
1	B	406	LEU	4.8
1	A	416	ALA	4.7
1	B	405	ARG	4.6
1	B	416	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	259	THR	4.5
1	B	265	HIS	4.3
1	B	531	LYS	4.1
1	A	243	ALA	4.0
1	A	404	SER	4.0
1	B	326	ARG	4.0
1	B	352	GLN	3.9
1	B	418	ALA	3.9
1	A	298	GLU	3.8
1	A	273	GLY	3.8
1	A	417	GLY	3.8
1	B	284	SER	3.7
1	A	282	LYS	3.7
1	B	298	GLU	3.7
1	B	280	TRP	3.5
1	B	328	PRO	3.5
1	B	526	GLU	3.5
1	A	265	HIS	3.3
1	B	293	LYS	3.3
1	B	414	ALA	3.3
1	A	317	LEU	3.3
1	B	410	ASP	3.2
1	B	407	MET	3.2
1	B	301	GLU	3.2
1	A	247	SER	3.1
1	A	294	GLU	3.1
1	A	398	VAL	3.1
1	B	249	PRO	3.1
1	B	244	MET	3.0
1	B	527	LYS	3.0
1	A	529	LEU	3.0
1	A	418	ALA	3.0
1	A	293	LYS	2.8
1	A	284	SER	2.8
1	B	303	LEU	2.8
1	A	300	GLU	2.8
1	B	518	GLU	2.8
1	B	409	GLY	2.8
1	B	327	GLU	2.8
1	A	326	ARG	2.7
1	B	443	ALA	2.7
1	B	285	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	263	MET	2.7
1	A	283	TYR	2.7
1	A	245	ASP	2.6
1	A	384	ALA	2.6
1	B	330	PHE	2.5
1	A	249	PRO	2.5
1	B	281	LYS	2.5
1	B	262	THR	2.5
1	B	256	MET	2.4
1	B	528	GLU	2.4
1	B	419	LYS	2.4
1	A	412	TYR	2.3
1	B	250	ASN	2.3
1	B	283	TYR	2.3
1	B	264	LYS	2.3
1	A	525	VAL	2.3
1	B	279	VAL	2.3
1	A	280	TRP	2.3
1	B	325	THR	2.3
1	A	447	LEU	2.2
1	B	383	LEU	2.2
1	A	399	ALA	2.2
1	A	301	GLU	2.2
1	B	519	SER	2.2
1	A	366	ILE	2.2
1	B	247	SER	2.1
1	B	329	PRO	2.1
1	B	384	ALA	2.1
1	A	518	GLU	2.1
1	A	403	LEU	2.1
1	B	261	ILE	2.1
1	B	339	TYR	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

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^{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	LLDF	B-factors(Å^2)	Q<0.9
3	MYR	A	1	15/16	0.72	0.26	4.13	31,36,55,55	0
3	MYR	B	2	15/16	0.56	0.30	2.91	37,46,56,56	0
4	STI	A	3	37/37	0.95	0.12	-0.17	13,17,21,21	0
4	STI	B	4	37/37	0.93	0.11	-0.29	22,27,32,35	0
2	CL	A	5	1/1	0.99	0.04	-	28,28,28,28	0
2	CL	B	6	1/1	0.99	0.06	-	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.