



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:54 AM GMT

PDB ID : 3K5V
Title : Structure of Abl kinase in complex with imatinib and GNF-2
Authors : Cowan-Jacob, S.W.; Fendrich, G.; Rummel, G.; Strauss, A.
Deposited on : 2009-10-08
Resolution : 1.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

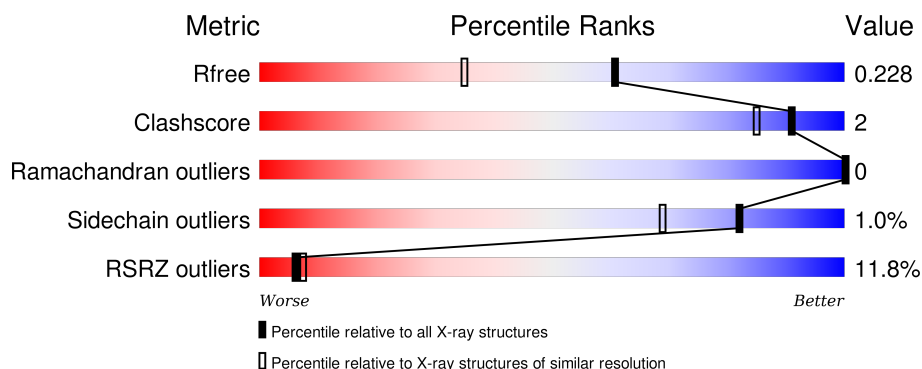
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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>5%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	B	293	<div> <div>18%</div> <div>91%</div> <div>5%</div> <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	STJ	B	1	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5194 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

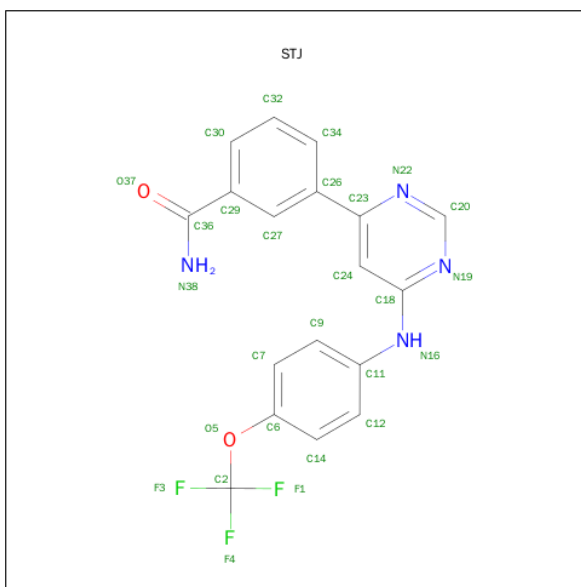
- Molecule 1 is a protein called Tyrosine-protein kinase ABL1.

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

There are 12 discrepancies between the modelled and reference sequences:

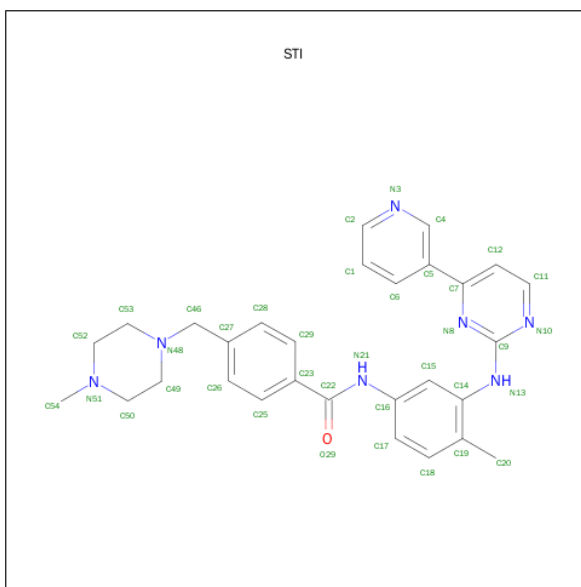
Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLY	-	EXPRESSION TAG	UNP P00520
A	243	ALA	-	EXPRESSION TAG	UNP P00520
A	244	MET	-	EXPRESSION TAG	UNP P00520
A	245	ASP	-	EXPRESSION TAG	UNP P00520
A	246	PRO	-	EXPRESSION TAG	UNP P00520
A	247	SER	-	EXPRESSION TAG	UNP P00520
B	242	GLY	-	EXPRESSION TAG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

- Molecule 2 is 3-(6-{[4-(TRIFLUOROMETHOXY)PHENYL]AMINO}PYRIMIDIN-4-YL)BENZAMIDE (three-letter code: STJ) (formula: C₁₈H₁₃F₃N₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	18	3	4	2		
2	B	1	Total	C	F	N	O	0	0
			27	18	3	4	2		

- 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: C₂₉H₃₁N₇O).



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

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

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

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

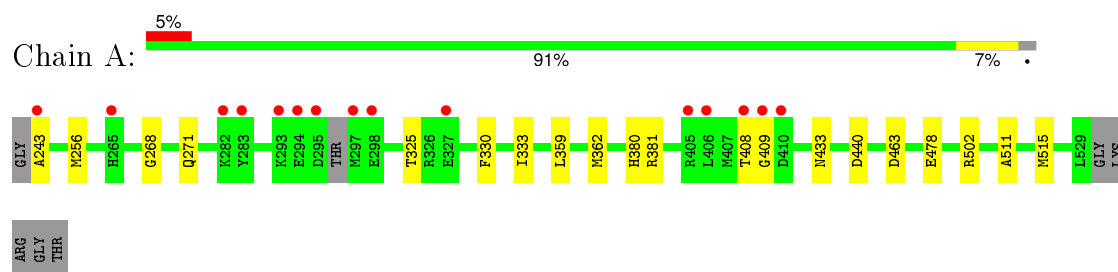
- Molecule 5 is water.

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

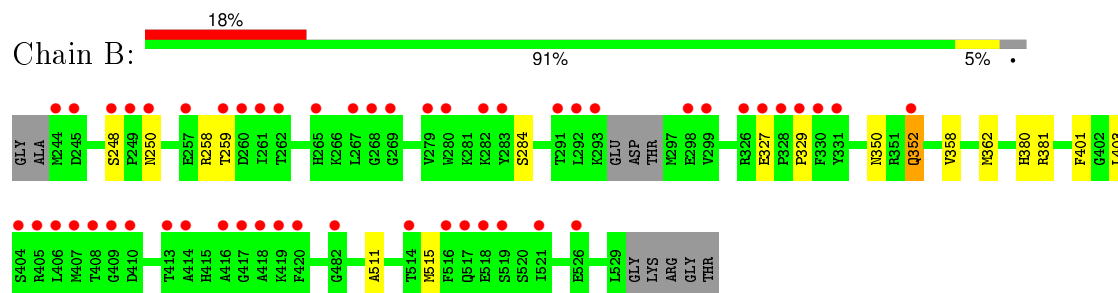
3 Residue-property plots [i](#)

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: Tyrosine-protein kinase ABL1



- Molecule 1: 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	42.07Å 65.27Å 66.26Å 72.82° 80.25° 84.86°	Depositor
Resolution (Å)	38.95 – 1.74 38.94 – 1.74	Depositor EDS
% Data completeness (in resolution range)	95.4 (38.95-1.74) 87.2 (38.94-1.74)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.199 , 0.231 0.196 , 0.228	Depositor DCC
R_{free} test set	3247 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 64929 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5194	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, STJ, 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	0.56	0/2401	0.65	2/3248 (0.1%)
1	B	0.42	0/2357	0.55	0/3188
All	All	0.49	0/4758	0.61	2/6436 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	502	ARG	NE-CZ-NH2	-5.38	117.61	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2337	0	2283	9	0
1	B	2299	0	2247	9	0
2	A	27	0	13	1	0
2	B	27	0	13	1	0
3	A	37	0	31	1	0
3	B	37	0	31	0	0
4	A	1	0	0	0	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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	285/293 (97%)	276 (97%)	9 (3%)	0	100	100
1	B	279/293 (95%)	269 (96%)	10 (4%)	0	100	100
All	All	564/586 (96%)	545 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/255 (100%)	251 (99%)	3 (1%)	78	62
1	B	249/255 (98%)	246 (99%)	3 (1%)	78	62
All	All	503/510 (99%)	497 (99%)	6 (1%)	82	62

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

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	STJ	A	1	-	25,29,29	1.06	1 (4%)	32,41,41	1.83	8 (25%)
3	STI	A	2	-	41,41,41	0.91	0	56,56,56	2.04	7 (12%)
2	STJ	B	1	-	25,29,29	1.02	0	32,41,41	1.75	7 (21%)
3	STI	B	2	-	41,41,41	0.88	0	56,56,56	1.93	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
2	STJ	A	1	-	-	0/14/17/17	0/3/3/3
3	STI	A	2	-	-	0/20/30/30	0/5/5/5
2	STJ	B	1	-	-	0/14/17/17	0/3/3/3
3	STI	B	2	-	-	0/20/30/30	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	STJ	C11-N16	-2.38	1.35	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	STI	N10-C9-N8	-6.49	119.75	126.67
3	B	2	STI	N10-C9-N8	-6.20	120.06	126.67
2	A	1	STJ	N22-C20-N19	-5.16	119.98	128.67
2	B	1	STJ	N22-C20-N19	-4.92	120.38	128.67
3	A	2	STI	C12-C11-N10	-4.21	119.09	123.90
2	B	1	STJ	C24-C18-N19	-3.76	118.86	123.06
3	B	2	STI	C12-C11-N10	-3.32	120.11	123.90
2	A	1	STJ	C24-C18-N19	-3.31	119.36	123.06
2	B	1	STJ	C24-C23-N22	-2.66	118.52	122.02
2	A	1	STJ	C27-C26-C23	-2.44	117.35	120.54
2	A	1	STJ	O37-C36-C29	-2.40	116.96	119.59
2	B	1	STJ	O37-C36-C29	-2.16	117.23	119.59
3	B	2	STI	C12-C7-N8	-2.14	119.06	122.01
3	B	2	STI	C14-N13-C9	-2.12	123.62	129.22
2	A	1	STJ	C24-C23-N22	-2.05	119.31	122.02
3	B	2	STI	C15-C14-N13	-2.02	116.97	121.31
2	A	1	STJ	N16-C18-N19	2.02	123.12	116.71
2	B	1	STJ	N16-C18-N19	2.08	123.30	116.71
3	B	2	STI	C19-C14-N13	2.08	123.39	118.70
3	B	2	STI	C2-N3-C4	2.14	120.78	116.84
3	A	2	STI	C2-N3-C4	2.18	120.85	116.84
3	B	2	STI	C18-C19-C14	2.51	119.36	117.39
3	A	2	STI	C50-N51-C52	2.52	112.84	109.53
3	A	2	STI	C18-C19-C14	3.19	119.90	117.39
2	B	1	STJ	C29-C36-N38	3.58	121.73	117.82
2	A	1	STJ	C20-N22-C23	3.96	121.30	115.74
2	A	1	STJ	C29-C36-N38	3.99	122.18	117.82
2	B	1	STJ	C20-N22-C23	4.15	121.57	115.74
3	B	2	STI	C11-N10-C9	5.99	120.70	115.49
3	A	2	STI	C7-N8-C9	6.44	121.30	116.49
3	A	2	STI	C11-N10-C9	7.25	121.79	115.49
3	B	2	STI	C7-N8-C9	7.51	122.10	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
2	A	1	STJ	1	0
3	A	2	STI	1	0
2	B	1	STJ	1	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, 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	286/293 (97%)	0.33	15 (5%) 31 36	11, 23, 47, 64	0
1	B	283/293 (96%)	1.03	52 (18%) 2 2	19, 37, 61, 69	0
All	All	569/586 (97%)	0.68	67 (11%) 6 7	11, 30, 60, 69	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	LEU	8.7
1	B	407	MET	8.1
1	A	297	MET	6.9
1	B	408	THR	6.9
1	A	295	ASP	5.7
1	B	269	GLY	5.7
1	B	282	LYS	5.6
1	B	516	PHE	5.5
1	B	410	ASP	5.5
1	B	418	ALA	5.3
1	B	409	GLY	5.3
1	B	280	TRP	5.1
1	B	293	LYS	5.0
1	B	416	ALA	4.7
1	B	519	SER	4.5
1	B	518	GLU	4.3
1	B	327	GLU	4.3
1	B	292	LEU	4.3
1	B	249	PRO	4.1
1	A	408	THR	3.9
1	B	298	GLU	3.9
1	B	299	VAL	3.8
1	B	279	VAL	3.7
1	B	262	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	414	ALA	3.6
1	B	417	GLY	3.5
1	B	405	ARG	3.5
1	B	517	GLN	3.4
1	A	294	GLU	3.3
1	A	405	ARG	3.3
1	A	409	GLY	3.3
1	B	329	PRO	3.2
1	A	265	HIS	3.2
1	B	283	TYR	3.2
1	B	326	ARG	3.1
1	B	268	GLY	3.1
1	B	259	THR	3.0
1	B	413	THR	3.0
1	B	352	GLN	3.0
1	B	265	HIS	2.9
1	A	410	ASP	2.9
1	B	514	THR	2.8
1	A	406	LEU	2.7
1	B	261	ILE	2.7
1	A	243	ALA	2.7
1	A	282	LYS	2.7
1	B	404	SER	2.6
1	A	298	GLU	2.6
1	A	293	LYS	2.6
1	B	482	GLY	2.6
1	B	244	MET	2.5
1	B	521	ILE	2.5
1	B	248	SER	2.5
1	B	260	ASP	2.5
1	B	267	LEU	2.5
1	B	420	PHE	2.4
1	A	283	TYR	2.3
1	B	250	ASN	2.3
1	B	328	PRO	2.3
1	B	526	GLU	2.3
1	B	291	THR	2.3
1	A	327	GLU	2.2
1	B	331	TYR	2.2
1	B	257	GLU	2.1
1	B	419	LYS	2.1
1	B	330	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	245	ASP	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	STJ	B	1	27/27	0.77	0.24	3.12	49,62,68,68	0
3	STI	A	2	37/37	0.97	0.09	-0.24	16,19,23,24	0
2	STJ	A	1	27/27	0.94	0.10	-0.31	23,26,42,44	0
3	STI	B	2	37/37	0.96	0.09	-0.76	24,27,32,34	0
4	CL	A	5	1/1	0.97	0.09	-0.76	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.