



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:19 PM GMT

PDB ID : 3QRI
Title : The crystal structure of human abl1 kinase domain in complex with DCC-2036
Authors : Chan, W.W.; Wise, S.C.; Kaufman, M.D.; Ahn, Y.M.; Ensinger, C.L.; Haack, T.; Hood, M.M.; Jones, J.; Lord, J.W.; Lu, W.P.; Miller, D.; Patt, W.C.; Smith, B.D.; Petillo, P.A.; Rutkoski, T.J.; Telikepalli, H.; Vogeti, L.; Yao, T.; Chun, L.; Clark, R.; Evangelista, P.; Gavrilescu, L.C.; Lazarides, K.; Zaleskas, V.M.; Stewart, L.J.; Van Etten, R.A.; Flynn, D.L.
Deposited on : 2011-02-18
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
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

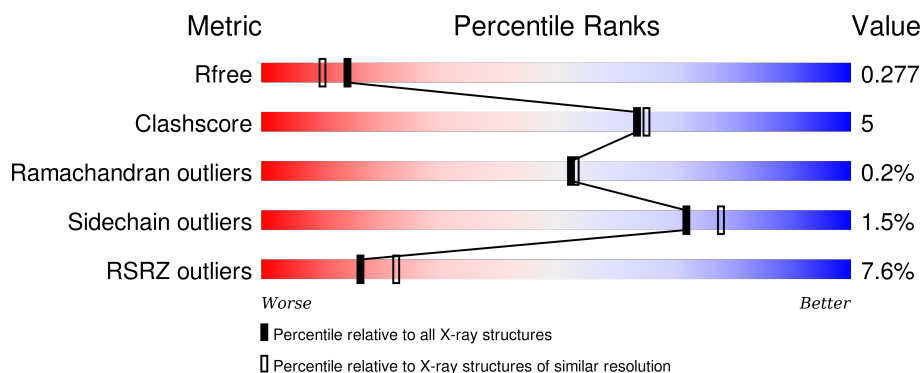
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 ≥ 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	277	<div> <div>9%</div> <div>89%</div> <div>10%</div> </div>
1	B	277	<div> <div>5%</div> <div>83%</div> <div>10%</div> <div>5%</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	NA	A	1	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4863 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	275	Total	C	N	O	S	0	6	0
			2254	1454	365	414	21			
1	B	262	Total	C	N	O	S	0	4	0
			2125	1376	344	387	18			

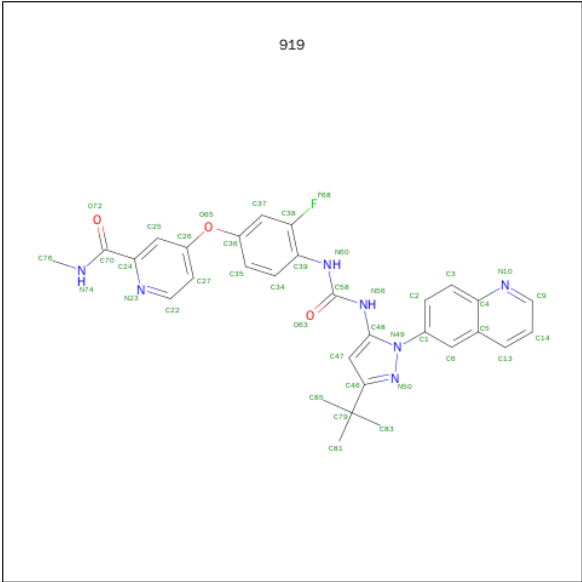
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	THR	-	EXPRESSION TAG	UNP P00519
A	224	SER	-	EXPRESSION TAG	UNP P00519
A	225	MET	-	EXPRESSION TAG	UNP P00519
A	226	ASP	-	EXPRESSION TAG	UNP P00519
A	227	PRO	-	EXPRESSION TAG	UNP P00519
A	228	SER	-	EXPRESSION TAG	UNP P00519
B	223	THR	-	EXPRESSION TAG	UNP P00519
B	224	SER	-	EXPRESSION TAG	UNP P00519
B	225	MET	-	EXPRESSION TAG	UNP P00519
B	226	ASP	-	EXPRESSION TAG	UNP P00519
B	227	PRO	-	EXPRESSION TAG	UNP P00519
B	228	SER	-	EXPRESSION TAG	UNP P00519

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		

- Molecule 3 is 4-[4-({[3-TERT-BUTYL-1-(QUINOLIN-6-YL)-1H-PYRAZOL-5-YL]CARBAMOYL}AMINO)-3-FLUOROPHENOXY]-N-METHYLPYRIDINE-2-CARBOXAMIDE (three-letter code: 919) (formula: C₃₀H₂₈FN₇O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			41	30	1	7	3		
3	B	1	Total	C	F	N	O	0	0
			41	30	1	7	3		

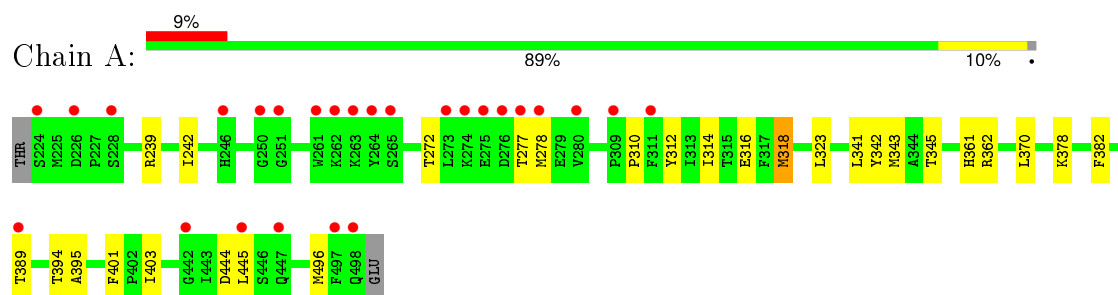
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	207	Total	O	0	0
			207	207		
4	B	193	Total	O	0	0
			193	193		

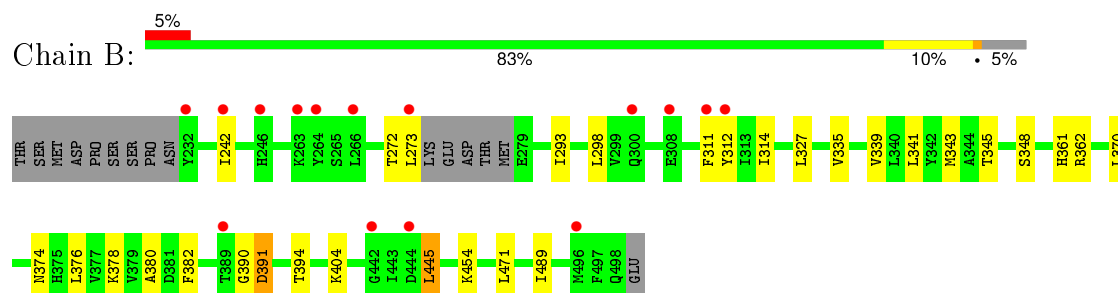
3 Residue-property plots [i](#)

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 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.26Å 59.70Å 79.43Å 90.00° 108.71° 90.00°	Depositor
Resolution (Å)	57.08 – 2.10 57.08 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (57.08-2.10) 97.2 (57.08-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.213 , 0.272 0.219 , 0.277	Depositor DCC
R_{free} test set	1540 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30533 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4863	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.80 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.0354e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 919

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	0.45	0/2330	0.63	0/3154
1	B	0.45	0/2191	0.64	0/2968
All	All	0.45	0/4521	0.63	0/6122

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	2254	0	2217	23	0
1	B	2125	0	2077	22	0
2	A	2	0	0	0	0
3	A	41	0	28	0	0
3	B	41	0	28	2	0
4	A	207	0	0	1	0
4	B	193	0	0	2	0
All	All	4863	0	4350	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:HD11	1:A:314:ILE:HD13	1.49	0.94
1:A:318[A]:MET:HA	1:A:318[A]:MET:HE2	1.62	0.81
1:A:318[A]:MET:CE	1:A:318[A]:MET:HA	2.12	0.79
1:B:374:ASN:HB3	4:B:578:HOH:O	1.84	0.76
1:B:376:LEU:HD21	1:B:378:LYS:NZ	2.09	0.68
1:A:242:ILE:HD11	1:A:314:ILE:CD1	2.24	0.67
1:A:242:ILE:CD1	1:A:314:ILE:HD13	2.23	0.66
1:B:335:VAL:HG13	1:B:343[B]:MET:HE3	1.79	0.65
1:A:316:GLU:OE2	1:A:378:LYS:NZ	2.30	0.63
1:A:242:ILE:CD1	1:A:314:ILE:CD1	2.77	0.63
1:A:401:PHE:HB2	1:A:403:ILE:HD13	1.79	0.62
1:B:404:LYS:HE3	1:B:445:LEU:HD12	1.82	0.61
1:B:341:LEU:O	1:B:345[B]:THR:HG23	2.02	0.59
1:A:239:ARG:NH1	1:A:310:PRO:O	2.34	0.58
1:B:314:ILE:N	1:B:314:ILE:HD12	2.18	0.58
1:A:342:TYR:O	1:A:345[B]:THR:HG22	2.04	0.57
1:A:361:HIS:O	1:A:362:ARG:HB2	2.05	0.56
1:B:376:LEU:HD21	1:B:378:LYS:HZ1	1.70	0.56
1:B:272:THR:HG22	1:B:312:TYR:CD2	2.41	0.56
1:A:394:THR:HG21	1:A:445:LEU:HD23	1.89	0.54
1:B:361:HIS:O	1:B:362:ARG:HB2	2.10	0.52
1:A:272:THR:HG22	1:A:312:TYR:CD2	2.44	0.52
1:A:394:THR:CG2	1:A:445:LEU:HD23	2.39	0.52
1:B:390:GLY:CA	1:B:391:ASP:CB	2.89	0.51
1:A:394:THR:OG1	1:A:395:ALA:N	2.44	0.51
1:A:362:ARG:NH2	4:A:503:HOH:O	2.44	0.50
1:B:471:LEU:HD11	1:B:489:ILE:HD13	1.94	0.49
1:B:339:VAL:HG12	1:B:343[B]:MET:HE3	1.94	0.48
1:B:454:LYS:NZ	4:B:568:HOH:O	2.45	0.48
1:A:341:LEU:HD11	1:A:496:MET:HE3	1.95	0.48
3:B:2:919:H34	3:B:2:919:O63	2.15	0.47
1:A:370:LEU:HD21	1:A:382:PHE:CZ	2.50	0.46
1:B:380:ALA:HB1	3:B:2:919:H34	1.98	0.46
1:B:242:ILE:CD1	1:B:314:ILE:HG12	2.46	0.45
1:A:277:THR:O	1:A:277:THR:HG22	2.17	0.45
1:B:293:ILE:CG2	1:B:298:LEU:HD13	2.47	0.45
1:B:272:THR:HG22	1:B:312:TYR:CE2	2.52	0.45
1:A:370:LEU:HD21	1:A:382:PHE:HZ	1.81	0.45
1:B:327:LEU:HD21	1:B:343[A]:MET:HE1	1.99	0.44
1:B:293:ILE:HG23	1:B:298:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LEU:HD21	1:B:343[A]:MET:CE	2.49	0.43
1:B:370:LEU:HD21	1:B:382:PHE:HZ	1.84	0.42
1:B:273:LEU:HD23	1:B:311:PHE:HD2	1.86	0.41
1:A:242:ILE:CD1	1:A:314:ILE:HD11	2.51	0.41
1:A:341:LEU:HD11	1:A:496:MET:CE	2.49	0.41
1:A:323:LEU:CD1	1:A:343[A]:MET:CE	2.97	0.41

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	279/277 (101%)	265 (95%)	14 (5%)	0	100	100
1	B	262/277 (95%)	254 (97%)	7 (3%)	1 (0%)	39	37
All	All	541/554 (98%)	519 (96%)	21 (4%)	1 (0%)	52	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	391	ASP

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	244/243 (100%)	239 (98%)	5 (2%)	63	68
1	B	225/243 (93%)	222 (99%)	3 (1%)	76	82
All	All	469/486 (96%)	461 (98%)	8 (2%)	72	74

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	MET
1	A	318[A]	MET
1	A	318[B]	MET
1	A	389	THR
1	A	444	ASP
1	B	348	SER
1	B	394	THR
1	B	445	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	919	A	500	-	44,45,45	1.11	3 (6%)	57,65,65	2.01	11 (19%)
3	919	B	2	-	44,45,45	1.17	2 (4%)	57,65,65	2.09	13 (22%)

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	919	A	500	-	-	0/26/28/28	0/5/5/5
3	919	B	2	-	-	0/26/28/28	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	919	C1-N49	-4.20	1.35	1.44
3	A	500	919	C1-N49	-4.17	1.35	1.44
3	B	2	919	C39-N60	-2.65	1.36	1.41
3	A	500	919	C39-N60	-2.46	1.37	1.41
3	A	500	919	C5-C4	-2.32	1.38	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	919	C2-C1-C6	-7.30	114.89	121.50
3	B	2	919	C2-C1-C6	-7.23	114.95	121.50
3	B	2	919	C47-C46-C79	-5.60	122.25	129.15
3	B	2	919	C1-N49-C48	-4.92	123.36	129.02
3	A	500	919	C47-C46-C79	-4.64	123.44	129.15
3	A	500	919	C25-C24-N23	-3.19	119.55	123.30
3	A	500	919	C14-C9-N10	-3.19	118.94	123.94
3	A	500	919	C27-C22-N23	-2.87	120.62	123.90
3	B	2	919	C25-C24-N23	-2.81	120.00	123.30
3	B	2	919	C14-C9-N10	-2.54	119.96	123.94
3	B	2	919	C27-C22-N23	-2.49	121.05	123.90
3	B	2	919	O63-C58-N60	-2.07	120.45	123.58
3	A	500	919	C3-C2-C1	2.06	123.28	119.98
3	B	2	919	C79-C46-N50	2.23	122.94	120.58
3	B	2	919	N60-C58-N56	2.34	116.20	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	919	C9-N10-C4	2.48	121.08	116.87
3	A	500	919	C9-N10-C4	2.53	121.16	116.87
3	B	2	919	C22-N23-C24	3.17	121.17	116.92
3	B	2	919	C36-O65-C26	3.29	127.00	118.81
3	A	500	919	F68-C38-C39	3.43	120.94	117.50
3	A	500	919	C22-N23-C24	3.53	121.66	116.92
3	A	500	919	C36-O65-C26	4.33	129.58	118.81
3	A	500	919	C6-C1-N49	5.77	126.16	119.13
3	B	2	919	C6-C1-N49	6.32	126.83	119.13

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	2	919	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, 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	275/277 (99%)	0.61	26 (9%)	10 14	18, 31, 48, 57	0
1	B	262/277 (94%)	0.55	15 (5%)	27 35	21, 32, 52, 57	0
All	All	537/554 (96%)	0.58	41 (7%)	17 23	18, 31, 51, 57	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	389	THR	6.6
1	A	442	GLY	6.1
1	B	389	THR	5.2
1	A	278	MET	5.2
1	A	265	SER	5.1
1	A	277	THR	5.1
1	A	276	ASP	4.2
1	B	232	TYR	3.8
1	B	263	LYS	3.8
1	B	311	PHE	3.7
1	A	264	TYR	3.5
1	A	262	LYS	3.4
1	B	264	TYR	3.4
1	A	311	PHE	3.2
1	A	263	LYS	3.1
1	B	308	GLU	3.0
1	A	497	PHE	3.0
1	B	312	TYR	2.9
1	B	442	GLY	2.8
1	B	246	HIS	2.7
1	A	250	GLY	2.7
1	A	309	PRO	2.6
1	B	273	LEU	2.6
1	A	228	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	280	VAL	2.5
1	A	224	SER	2.4
1	A	246	HIS	2.4
1	B	300	GLN	2.3
1	A	275	GLU	2.3
1	B	242	ILE	2.3
1	A	274	LYS	2.2
1	A	226	ASP	2.2
1	A	445	LEU	2.2
1	A	273	LEU	2.2
1	A	261	TRP	2.1
1	A	251	GLY	2.1
1	B	266	LEU	2.1
1	B	444	ASP	2.1
1	A	447	GLN	2.1
1	A	498	GLN	2.1
1	B	496	MET	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	NA	A	1	1/1	0.78	0.31	9.01	52,52,52,52	0
3	919	B	2	41/41	0.89	0.15	0.10	28,32,34,35	0
3	919	A	500	41/41	0.92	0.14	-0.16	25,28,30,32	0
2	NA	A	2	1/1	0.86	0.17	-	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.