



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2016 – 03:47 PM EDT

PDB ID : 5BYE
Title : Crystal structure of human ribokinase in P212121 spacegroup
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Deposited on : 2015-06-10
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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
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) : rb-20027674

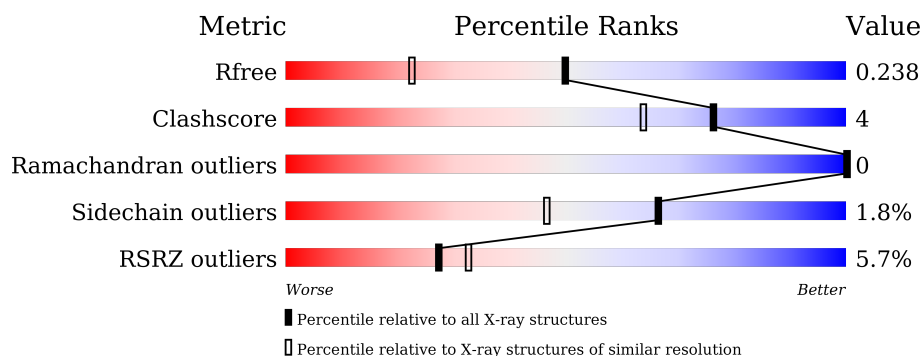
1 Overall quality at a glance

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}	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 $\leq 5\%$. 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	330	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	330	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5043 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 Ribokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	1	0
			2335	1474	387	459	15			
1	B	305	Total	C	N	O	S	0	0	0
			2264	1429	384	437	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	LEU	-	expression tag	UNP Q9H477
A	324	GLU	-	expression tag	UNP Q9H477
A	325	HIS	-	expression tag	UNP Q9H477
A	326	HIS	-	expression tag	UNP Q9H477
A	327	HIS	-	expression tag	UNP Q9H477
A	328	HIS	-	expression tag	UNP Q9H477
A	329	HIS	-	expression tag	UNP Q9H477
A	330	HIS	-	expression tag	UNP Q9H477
B	323	LEU	-	expression tag	UNP Q9H477
B	324	GLU	-	expression tag	UNP Q9H477
B	325	HIS	-	expression tag	UNP Q9H477
B	326	HIS	-	expression tag	UNP Q9H477
B	327	HIS	-	expression tag	UNP Q9H477
B	328	HIS	-	expression tag	UNP Q9H477
B	329	HIS	-	expression tag	UNP Q9H477
B	330	HIS	-	expression tag	UNP Q9H477

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

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

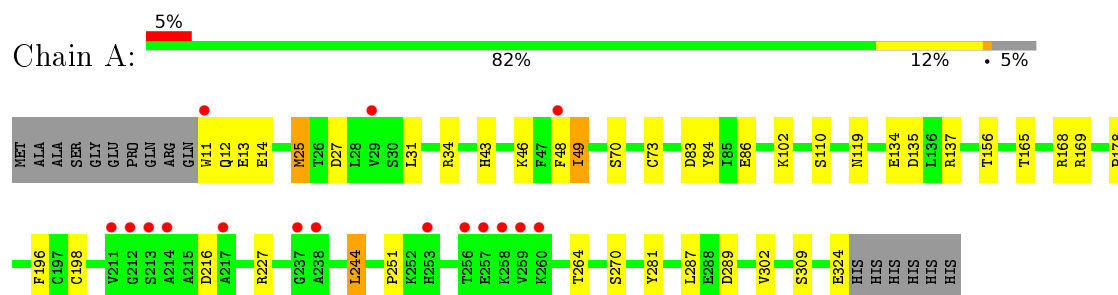
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	261	Total 264	O 264	0	3
4	B	176	Total 177	O 177	0	1

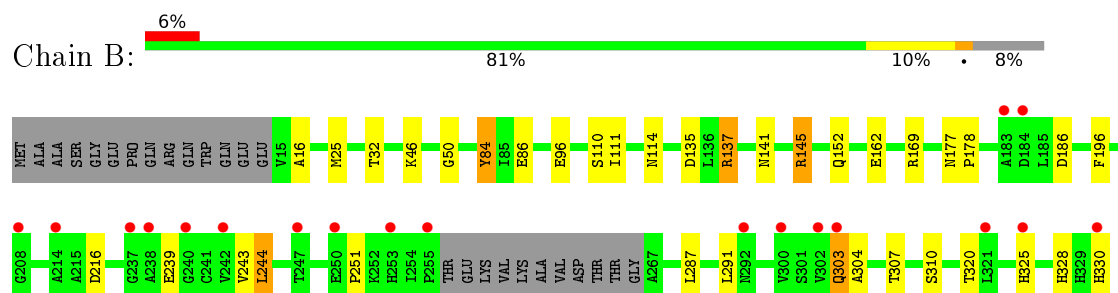
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: Ribokinase



• Molecule 1: Ribokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.25Å 65.48Å 180.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.74 – 1.75 47.74 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.74-1.75) 99.4 (47.74-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.190 , 0.229 0.201 , 0.238	Depositor DCC
R_{free} test set	3322 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5043	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: NA, 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	1.40	10/2370 (0.4%)	1.20	13/3222 (0.4%)
1	B	1.25	7/2302 (0.3%)	1.23	14/3130 (0.4%)
All	All	1.33	17/4672 (0.4%)	1.22	27/6352 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	ARG	CZ-NH1	6.82	1.42	1.33
1	B	84	TYR	CE1-CZ	-6.56	1.30	1.38
1	A	198	CYS	CB-SG	-6.28	1.71	1.82
1	A	134	GLU	CG-CD	5.82	1.60	1.51
1	A	86	GLU	CG-CD	5.81	1.60	1.51
1	B	145	ARG	CD-NE	-5.76	1.36	1.46
1	B	96	GLU	CD-OE1	5.64	1.31	1.25
1	A	156	THR	CB-CG2	-5.47	1.34	1.52
1	A	281	TYR	CD2-CE2	5.44	1.47	1.39
1	B	16	ALA	N-CA	5.37	1.57	1.46
1	A	73	CYS	CA-CB	-5.35	1.42	1.53
1	A	70	SER	CB-OG	-5.32	1.35	1.42
1	A	270	SER	CB-OG	5.21	1.49	1.42
1	A	119	ASN	N-CA	-5.19	1.35	1.46
1	A	324	GLU	CB-CG	5.15	1.61	1.52
1	B	86	GLU	CD-OE1	5.09	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	GLY	CA-C	5.01	1.59	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	ARG	NE-CZ-NH1	13.55	127.07	120.30
1	B	169	ARG	NE-CZ-NH2	-11.33	114.64	120.30
1	B	145	ARG	NE-CZ-NH2	10.15	125.38	120.30
1	B	145	ARG	NE-CZ-NH1	-9.25	115.67	120.30
1	B	137	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	186	ASP	CB-CG-OD1	8.18	125.66	118.30
1	A	83	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	244	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	169	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	B	244	LEU	CA-CB-CG	6.63	130.54	115.30
1	A	34	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	110	SER	CB-CA-C	6.19	121.86	110.10
1	A	289	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	B	25	MET	CG-SD-CE	-6.12	90.41	100.20
1	A	216	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	227	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	137	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	303	GLN	CA-CB-CG	5.56	125.63	113.40
1	A	168	ARG	CG-CD-NE	5.52	123.39	111.80
1	B	162	GLU	OE1-CD-OE2	-5.46	116.74	123.30
1	A	27	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	135	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	165	THR	CA-CB-CG2	-5.33	104.93	112.40
1	A	135	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	137	ARG	CG-CD-NE	-5.12	101.06	111.80
1	B	137	ARG	CG-CD-NE	5.04	122.38	111.80
1	B	216	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	HIS	Mainchain

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	2335	0	2338	18	0
1	B	2264	0	2249	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	264	0	0	6	0
4	B	177	0	0	3	0
All	All	5043	0	4587	35	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 4.

All (35) 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:13:GLU:HA	1:A:13:GLU:OE1	1.73	0.89
1:A:49:ILE:HG22	4:A:700:HOH:O	1.80	0.82
1:A:46:LYS:HG2	1:A:48:PHE:CZ	2.26	0.70
1:A:31:LEU:HG	1:A:48:PHE:HE2	1.55	0.70
1:A:244:LEU:HD23	1:A:251:PRO:HA	1.75	0.69
1:B:244:LEU:HD23	1:B:251:PRO:HA	1.75	0.67
1:B:244:LEU:CD2	1:B:251:PRO:HA	2.31	0.60
1:A:31:LEU:HG	1:A:48:PHE:CE2	2.39	0.56
1:A:244:LEU:CD2	1:A:251:PRO:HA	2.35	0.56
1:A:25[B]:MET:CE	4:A:625:HOH:O	2.56	0.54
1:B:137:ARG:HG2	1:B:137:ARG:HH11	1.74	0.53
1:A:46:LYS:NZ	4:A:504:HOH:O	2.41	0.52
1:A:46:LYS:HG2	1:A:48:PHE:CE2	2.44	0.52
1:B:320:THR:HG21	1:B:330:HIS:CD2	2.46	0.50
1:A:12:GLN:NE2	4:A:505:HOH:O	2.45	0.50
1:B:325:HIS:CE1	4:B:532:HOH:O	2.64	0.49
1:B:244:LEU:CD2	1:B:251:PRO:CA	2.92	0.48
1:B:141:ASN:HD21	1:B:145:ARG:HH11	1.63	0.47
1:A:178:PRO:HG3	1:A:196:PHE:CZ	2.51	0.46
1:A:244:LEU:CD2	1:A:251:PRO:CA	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:VAL:HG21	1:B:291:LEU:CD1	2.46	0.46
1:B:152:GLN:HA	1:B:177:ASN:O	2.17	0.44
1:A:25[B]:MET:HE1	4:A:625:HOH:O	2.16	0.43
1:B:178:PRO:HG3	1:B:196:PHE:CZ	2.54	0.43
1:A:13:GLU:CD	1:A:14:GLU:H	2.23	0.42
1:B:307:THR:HB	4:B:631:HOH:O	2.19	0.42
1:B:46:LYS:HE3	4:B:663:HOH:O	2.19	0.42
1:A:264:THR:HA	1:A:302:VAL:HG22	2.02	0.42
1:B:32:THR:O	1:B:114:ASN:HA	2.19	0.42
1:B:110:SER:C	1:B:111:ILE:HG13	2.39	0.41
1:B:239:GLU:HG3	1:B:239:GLU:O	2.20	0.41
1:A:11:TRP:O	1:A:12:GLN:C	2.59	0.41
1:B:328:HIS:HD2	1:B:330:HIS:H	1.68	0.41
1:A:25[B]:MET:HE2	4:A:625:HOH:O	2.18	0.40
1:B:304:ALA:HB3	1:B:310:SER:HB2	2.03	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	313/330 (95%)	304 (97%)	9 (3%)	0	100	100
1	B	301/330 (91%)	296 (98%)	5 (2%)	0	100	100
All	All	614/660 (93%)	600 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	251/266 (94%)	244 (97%)	7 (3%)	51	25
1	B	242/266 (91%)	239 (99%)	3 (1%)	78	62
All	All	493/532 (93%)	483 (98%)	10 (2%)	66	39

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25[A]	MET
1	A	25[B]	MET
1	A	49	ILE
1	A	84	TYR
1	A	102	LYS
1	A	287	LEU
1	A	309	SER
1	B	84	TYR
1	B	287	LEU
1	B	303	GLN

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

Mol	Chain	Res	Type
1	B	45	HIS
1	B	141	ASN
1	B	326	HIS
1	B	328	HIS
1	B	330	HIS

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	314/330 (95%)	0.32	16 (5%) 32 37	16, 27, 57, 81	0
1	B	305/330 (92%)	0.31	19 (6%) 24 29	16, 32, 71, 88	0
All	All	619/660 (93%)	0.32	35 (5%) 27 32	16, 29, 66, 88	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	VAL	6.3
1	A	238	ALA	5.5
1	A	258	LYS	4.8
1	B	325	HIS	4.6
1	A	256	THR	4.4
1	B	303	GLN	4.3
1	B	238	ALA	3.5
1	B	214	ALA	3.5
1	A	213	SER	3.4
1	A	212	GLY	3.4
1	B	255	PRO	3.3
1	A	211	VAL	3.3
1	A	237	GLY	3.2
1	B	237	GLY	3.2
1	B	240	GLY	3.1
1	A	214	ALA	2.9
1	B	330	HIS	2.9
1	A	253	HIS	2.8
1	A	217	ALA	2.8
1	B	242	VAL	2.7
1	B	302	VAL	2.7
1	A	11	TRP	2.6
1	B	300	VAL	2.5
1	B	292	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLU	2.4
1	B	184	ASP	2.4
1	B	250	GLU	2.3
1	B	208	GLY	2.3
1	A	260	LYS	2.3
1	B	321	LEU	2.2
1	B	253	HIS	2.1
1	A	48	PHE	2.1
1	B	247	THR	2.1
1	B	183	ALA	2.1
1	A	29	VAL	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	B	401	1/1	0.90	0.14	-0.52	45,45,45,45	0
2	NA	A	401	1/1	0.98	0.06	-2.15	27,27,27,27	0
3	CL	A	402	1/1	0.98	0.07	-	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.