



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:56 am BST

PDB ID : 6ILR
Title : Structure of Arabidopsis thaliana Ribokinase in unligand form
Authors : Kang, P.; Oh, J.; Rhee, S.
Deposited on : 2018-10-19
Resolution : 1.97 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

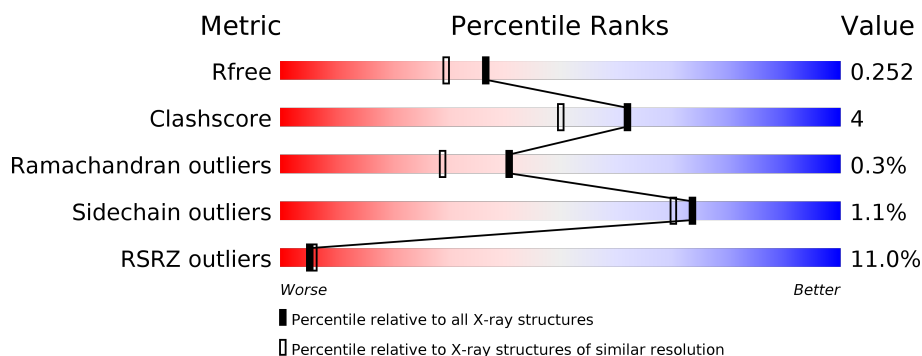
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 respectively. 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	313	<div> <div>14%</div> <div>87%</div> <div>12%</div> </div>
1	B	313	<div> <div>8%</div> <div>92%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4720 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.

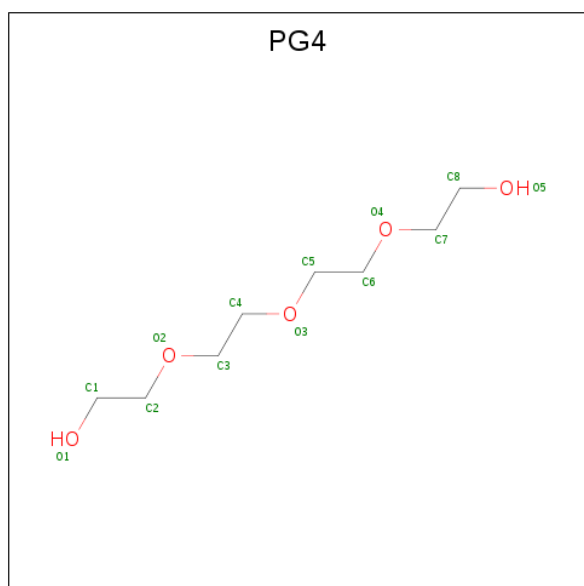
- Molecule 1 is a protein called Ribokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2266	1427	386	439	14			
1	B	313	Total	C	N	O	S	0	0	0
			2257	1423	387	433	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	MET	-	initiating methionine	UNP A1A6H3
B	67	MET	-	initiating methionine	UNP A1A6H3

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

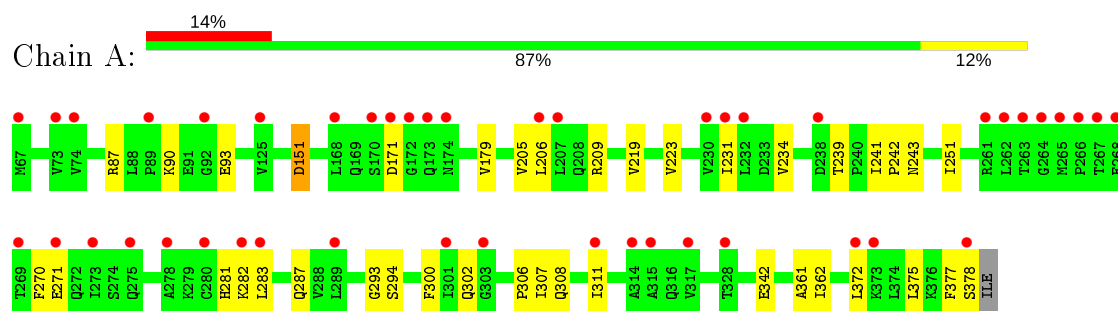
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	97	Total	O	0	0
			97	97		

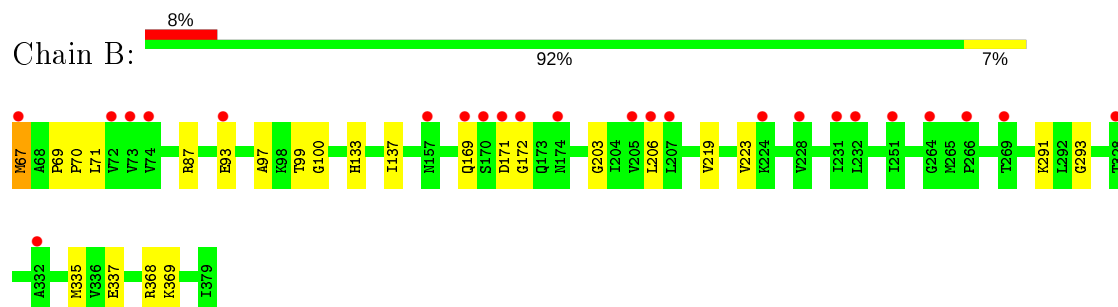
3 Residue-property plots [i](#)

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: Ribokinase



• Molecule 1: Ribokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.04Å 99.04Å 165.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.47 – 1.97 27.47 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (27.47-1.97) 90.3 (27.47-1.97)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.220 , 0.251 0.225 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4720	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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, 0.333 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: NA, PG4

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	0.31	0/2299	0.49	0/3121
1	B	0.31	0/2290	0.47	0/3111
All	All	0.31	0/4589	0.48	0/6232

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	2266	0	2295	24	0
1	B	2257	0	2280	16	0
2	A	13	0	18	2	0
2	B	13	0	18	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	72	0	0	2	0
4	B	97	0	0	2	0
All	All	4720	0	4611	40	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 (40) 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:293:GLY:HA2	2:A:401:PG4:H61	1.67	0.75
1:A:293:GLY:HA2	2:A:401:PG4:H42	1.74	0.68
1:A:206:LEU:HD23	1:A:231:ILE:HB	1.79	0.65
1:B:291:LYS:HB3	2:B:401:PG4:H32	1.77	0.65
1:A:219:VAL:O	1:A:223:VAL:HG22	2.01	0.59
1:B:337:GLU:OE2	1:B:368:ARG:NH2	2.32	0.59
1:A:209:ARG:NH2	1:A:239:THR:O	2.36	0.58
1:A:361:ALA:HB3	4:A:502:HOH:O	2.05	0.57
1:A:179:VAL:HG22	1:B:97:ALA:HB3	1.88	0.56
1:A:205:VAL:HG21	1:A:223:VAL:HG11	1.89	0.55
1:A:90:LYS:N	1:A:93:GLU:OE1	2.31	0.55
1:B:171:ASP:OD1	1:B:172:GLY:N	2.42	0.52
1:A:294:SER:HA	1:A:311:ILE:HD11	1.91	0.51
1:B:71:LEU:HD11	1:B:206:LEU:HG	1.93	0.51
1:A:151:ASP:OD1	1:A:151:ASP:N	2.45	0.50
1:B:369:LYS:NZ	4:B:505:HOH:O	2.45	0.50
1:A:281:HIS:CD2	1:A:302:GLN:HB2	2.48	0.49
1:B:219:VAL:O	1:B:223:VAL:HG23	2.13	0.49
1:B:293:GLY:HA2	2:B:401:PG4:H31	1.95	0.48
1:A:307:ILE:HG21	1:A:342:GLU:HG3	1.95	0.47
1:B:69:PRO:HB2	1:B:203:GLY:CA	2.44	0.47
1:A:87:ARG:NH1	1:A:93:GLU:OE2	2.28	0.47
1:A:372:LEU:HD23	1:A:375:LEU:HD12	1.96	0.46
1:B:87:ARG:NH2	1:B:93:GLU:OE2	2.37	0.46
1:A:362:ILE:HG12	4:A:502:HOH:O	2.17	0.44
1:A:241:ILE:HA	1:A:242:PRO:HD3	1.88	0.43
1:A:251:ILE:HG12	1:A:287:GLN:HB2	2.01	0.43
1:A:300:PHE:HD2	1:A:306:PRO:HG3	1.83	0.43
1:B:293:GLY:HA2	2:B:401:PG4:C5	2.49	0.43
1:A:282:LYS:HB3	1:A:283:LEU:HD12	2.02	0.42
1:B:99:THR:OG1	1:B:100:GLY:N	2.53	0.42
1:B:335:MET:SD	4:B:587:HOH:O	2.62	0.41
1:A:270:PHE:CZ	1:A:308:GLN:NE2	2.88	0.41
1:B:133:HIS:O	1:B:137:ILE:HG12	2.20	0.41
1:A:271:GLU:N	1:A:271:GLU:OE1	2.43	0.41
1:B:293:GLY:HA2	2:B:401:PG4:H52	2.02	0.41
2:B:401:PG4:H31	2:B:401:PG4:H51	1.85	0.41
1:B:67:MET:HE1	1:B:70:PRO:HB3	2.01	0.41
1:A:234:VAL:HG13	1:A:241:ILE:HD11	2.02	0.40
1:A:293:GLY:O	1:A:311:ILE:HD11	2.22	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	310/313 (99%)	298 (96%)	10 (3%)	2 (1%)	25	14
1	B	311/313 (99%)	305 (98%)	6 (2%)	0	100	100
All	All	621/626 (99%)	603 (97%)	16 (3%)	2 (0%)	41	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	A	377	PHE

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	240/248 (97%)	237 (99%)	3 (1%)	69	64
1	B	236/248 (95%)	234 (99%)	2 (1%)	81	80
All	All	476/496 (96%)	471 (99%)	5 (1%)	73	70

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	243	ASN
1	A	378	SER
1	B	67	MET
1	B	169	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	243	ASN

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	$\# Z > 2$
2	PG4	B	401	-	12,12,12	0.59	0	11,11,11	0.37	0
2	PG4	A	401	-	12,12,12	0.53	0	11,11,11	0.27	0

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	PG4	B	401	-	-	9/10/10/10	-
2	PG4	A	401	-	-	8/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PG4	O2-C3-C4-O3
2	A	401	PG4	O3-C5-C6-O4
2	B	401	PG4	C3-C4-O3-C5
2	A	401	PG4	O4-C7-C8-O5
2	A	401	PG4	C8-C7-O4-C6
2	B	401	PG4	O2-C3-C4-O3
2	B	401	PG4	C1-C2-O2-C3
2	A	401	PG4	C6-C5-O3-C4
2	B	401	PG4	C4-C3-O2-C2
2	A	401	PG4	C4-C3-O2-C2
2	B	401	PG4	C6-C5-O3-C4
2	A	401	PG4	C5-C6-O4-C7
2	B	401	PG4	O1-C1-C2-O2
2	A	401	PG4	O1-C1-C2-O2
2	B	401	PG4	C8-C7-O4-C6
2	B	401	PG4	O3-C5-C6-O4
2	B	401	PG4	C5-C6-O4-C7

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PG4	5	0
2	A	401	PG4	2	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, 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	312/313 (99%)	0.82	45 (14%) 2 2	26, 53, 86, 101	0
1	B	313/313 (100%)	0.57	24 (7%) 13 15	25, 44, 79, 96	0
All	All	625/626 (99%)	0.69	69 (11%) 5 6	25, 48, 84, 101	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	GLY	5.5
1	A	264	GLY	5.1
1	A	282	LYS	4.9
1	B	67	MET	4.8
1	B	172	GLY	4.7
1	A	283	LEU	4.5
1	A	92	GLY	4.5
1	A	172	GLY	4.2
1	A	67	MET	4.1
1	A	314	ALA	4.1
1	A	280	CYS	4.0
1	B	224	LYS	4.0
1	B	231	ILE	3.8
1	A	275	GLN	3.6
1	A	206	LEU	3.6
1	B	207	LEU	3.6
1	A	315	ALA	3.5
1	B	206	LEU	3.5
1	B	264	GLY	3.3
1	A	171	ASP	3.3
1	A	373	LYS	3.3
1	A	232	LEU	3.3
1	A	278	ALA	3.3
1	A	170	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	238	ASP	3.2
1	A	73	VAL	3.1
1	A	173	GLN	3.1
1	A	262	LEU	3.1
1	A	328	THR	3.0
1	A	74	VAL	3.0
1	A	378	SER	2.9
1	B	205	VAL	2.9
1	A	372	LEU	2.9
1	A	231	ILE	2.9
1	A	273	ILE	2.8
1	A	271	GLU	2.8
1	B	232	LEU	2.7
1	B	170	SER	2.7
1	A	168	LEU	2.7
1	A	289	LEU	2.7
1	A	207	LEU	2.6
1	A	266	PRO	2.6
1	B	228	VAL	2.6
1	B	266	PRO	2.6
1	B	328	THR	2.5
1	A	261	ARG	2.5
1	B	269	THR	2.5
1	B	174	ASN	2.4
1	A	311	ILE	2.4
1	B	251	ILE	2.4
1	A	267	THR	2.4
1	B	157	ASN	2.4
1	B	73	VAL	2.3
1	B	332	ALA	2.3
1	A	230	VAL	2.3
1	B	74	VAL	2.3
1	A	265	MET	2.2
1	A	269	THR	2.2
1	A	174	ASN	2.2
1	B	171	ASP	2.2
1	A	125	VAL	2.2
1	B	93	GLU	2.2
1	B	72	VAL	2.1
1	B	169	GLN	2.1
1	A	263	THR	2.1
1	A	317	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	268	GLU	2.1
1	A	301	ILE	2.1
1	A	89	PRO	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. 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	B-factors(\AA^2)	Q<0.9
2	PG4	B	401	13/13	0.79	0.18	40,59,71,74	0
2	PG4	A	401	13/13	0.87	0.15	53,65,74,74	0
3	NA	A	402	1/1	0.92	0.06	43,43,43,43	0
3	NA	B	402	1/1	0.97	0.10	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.