



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:59 AM UTC

PDB ID : 6ILR / pdb_00006ilr
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

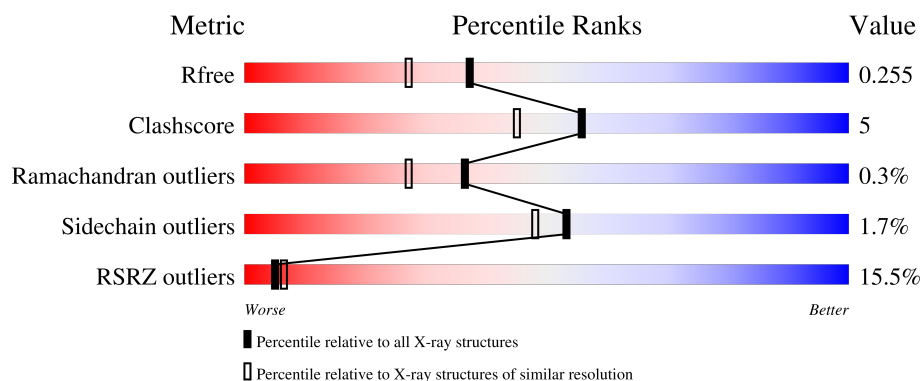
1 Overall quality at a glance

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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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 of 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	17% 86% 12%
1	B	313	14% 92% 8%

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.

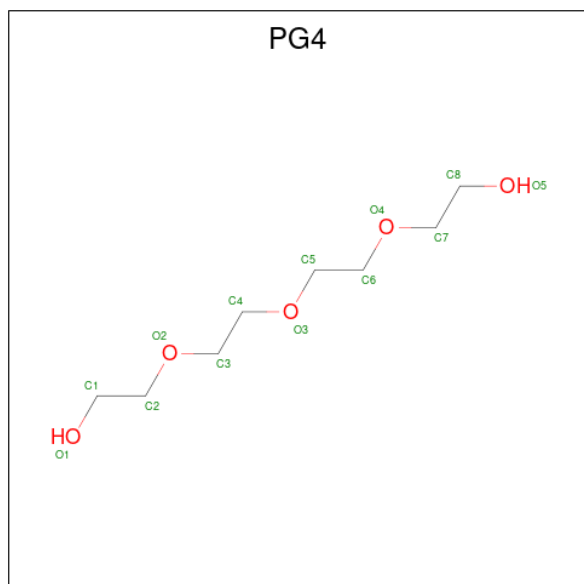
- Molecule 1 is a protein called Ribokinase.

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 (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

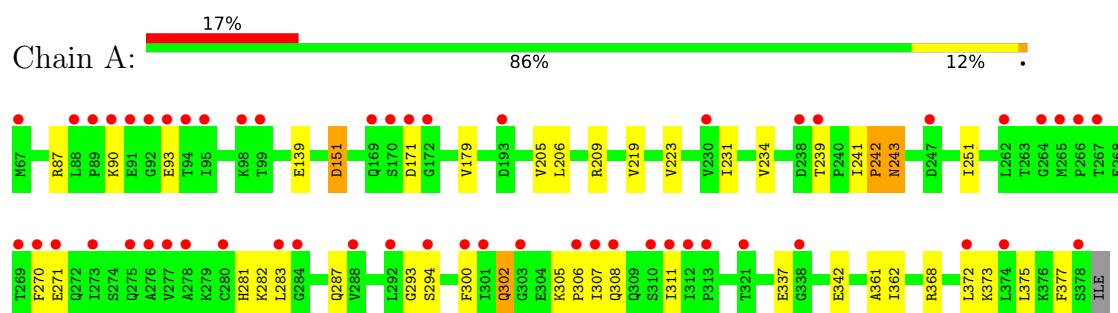
- Molecule 4 is water.

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

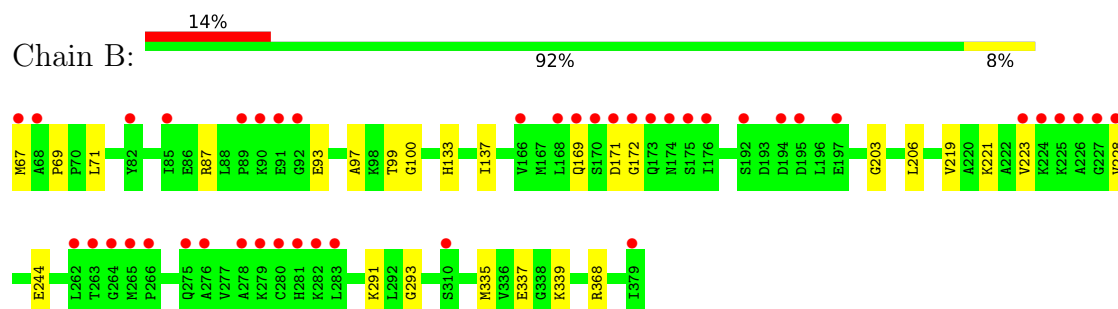
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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) 90.2 (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 0.226 , 0.255	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 , 47.5	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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/2299	0.81	4/3121 (0.1%)
1	B	0.42	0/2290	0.75	0/3111
All	All	0.42	0/4589	0.78	4/6232 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	LYS	CA-C-N	5.54	126.76	119.84
1	A	305	LYS	C-N-CA	5.54	126.76	119.84
1	A	243	ASN	N-CA-C	-5.47	106.56	113.18
1	A	242	PRO	CA-C-O	-5.35	115.31	121.36

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	2266	0	2295	26	0
1	B	2257	0	2280	17	0
2	A	13	0	18	2	0
2	B	13	0	18	5	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	43	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 (43) 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:90:LYS:N	1:A:93:GLU:OE1	2.31	0.55
1:A:205:VAL:HG21	1:A:223:VAL:HG11	1.89	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: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:B:339:LYS:NZ	4:B:508:HOH:O	2.47	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:337:GLU:CD	1:A:368:ARG:HH22	2.26	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:221:LYS:NZ	1:B:244:GLU:OE2	2.40	0.41
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:B:87:ARG:HH22	1:B:93:GLU:CD	2.27	0.41
1:A:271:GLU:H	1:A:271:GLU:CD	2.23	0.41
1:A:271:GLU:OE1	1:A:271:GLU:N	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: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

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	310/313 (99%)	298 (96%)	10 (3%)	2 (1%)	21	12
1	B	311/313 (99%)	305 (98%)	6 (2%)	0	100	100
All	All	621/626 (99%)	603 (97%)	16 (3%)	2 (0%)	36	27

All (2) Ramachandran outliers are listed below:

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

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	240/248 (97%)	235 (98%)	5 (2%)	47	40
1	B	236/248 (95%)	233 (99%)	3 (1%)	61	57
All	All	476/496 (96%)	468 (98%)	8 (2%)	53	48

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

Mol	Chain	Res	Type
1	A	139	GLU
1	A	151	ASP
1	A	243	ASN
1	A	302	GLN
1	A	373	LYS
1	B	67	MET
1	B	169	GLN
1	B	228	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	173	GLN
1	A	243	ASN
1	B	149	HIS
1	B	302	GLN
1	B	341	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	401	-	12,12,12	0.53	0	11,11,11	0.27	0
2	PG4	B	401	-	12,12,12	0.59	0	11,11,11	0.37	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	A	401	-	-	8/10/10/10	-
2	PG4	B	401	-	-	9/10/10/10	-

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

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

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PG4	2	0
2	B	401	PG4	5	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	312/313 (99%)	0.99	54 (17%) 4 4	26, 53, 86, 101	0
1	B	313/313 (100%)	0.75	43 (13%) 6 9	25, 44, 79, 96	0
All	All	625/626 (99%)	0.87	97 (15%) 5 6	25, 48, 84, 101	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	224	LYS	7.0
1	A	92	GLY	5.2
1	A	280	CYS	4.4
1	A	283	LEU	4.3
1	B	90	LYS	4.3
1	A	378	SER	4.2
1	B	379	ILE	4.2
1	B	68	ALA	3.9
1	B	173	GLN	3.8
1	B	67	MET	3.7
1	B	175	SER	3.6
1	A	273	ILE	3.6
1	A	301	ILE	3.6
1	B	283	LEU	3.5
1	B	195	ASP	3.5
1	A	303	GLY	3.5
1	B	227	GLY	3.5
1	A	307	ILE	3.4
1	B	228	VAL	3.4
1	B	264	GLY	3.3
1	B	91	GLU	3.3
1	A	88	LEU	3.3
1	A	89	PRO	3.3
1	A	294	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	271	GLU	3.2
1	A	171	ASP	3.2
1	B	176	ILE	3.2
1	A	169	GLN	3.2
1	A	247	ASP	3.2
1	A	91	GLU	3.2
1	B	174	ASN	3.1
1	A	67	MET	3.0
1	B	262	LEU	2.9
1	A	310	SER	2.9
1	B	82	TYR	2.9
1	B	170	SER	2.9
1	A	172	GLY	2.9
1	A	170	SER	2.8
1	A	95	ILE	2.8
1	A	277	VAL	2.8
1	A	270	PHE	2.8
1	A	90	LYS	2.8
1	B	172	GLY	2.8
1	B	282	LYS	2.8
1	A	239	THR	2.8
1	B	168	LEU	2.8
1	A	311	ILE	2.8
1	A	284	GLY	2.7
1	A	300	PHE	2.7
1	A	266	PRO	2.7
1	B	85	ILE	2.7
1	A	308	GLN	2.7
1	B	225	LYS	2.7
1	B	166	VAL	2.7
1	B	169	GLN	2.6
1	A	238	ASP	2.6
1	B	275	GLN	2.6
1	A	288	VAL	2.6
1	B	278	ALA	2.6
1	A	94	THR	2.6
1	B	265	MET	2.6
1	B	194	ASP	2.5
1	B	171	ASP	2.5
1	A	276	ALA	2.5
1	B	223	VAL	2.5
1	A	264	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	197	GLU	2.4
1	A	269	THR	2.4
1	B	89	PRO	2.4
1	A	193	ASP	2.4
1	B	92	GLY	2.4
1	A	374	LEU	2.4
1	A	230	VAL	2.3
1	A	267	THR	2.3
1	B	263	THR	2.3
1	A	278	ALA	2.3
1	B	279	LYS	2.3
1	A	99	THR	2.3
1	B	226	ALA	2.2
1	A	312	ILE	2.2
1	A	98	LYS	2.2
1	A	262	LEU	2.2
1	A	306	PRO	2.2
1	A	321	THR	2.2
1	A	338	GLY	2.2
1	B	266	PRO	2.2
1	B	192	SER	2.2
1	A	372	LEU	2.2
1	B	276	ALA	2.2
1	A	93	GLU	2.1
1	B	281	HIS	2.1
1	A	275	GLN	2.0
1	A	313	PRO	2.0
1	A	292	LEU	2.0
1	B	280	CYS	2.0
1	B	310	SER	2.0
1	A	265	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PG4	B	401	13/13	0.82	0.17	40,59,71,74	0
2	PG4	A	401	13/13	0.88	0.13	53,65,74,74	0
3	NA	A	402	1/1	0.94	0.09	43,43,43,43	0
3	NA	B	402	1/1	0.96	0.13	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.