



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:50 PM BST

PDB ID : 4IVP
Title : Crystal structure of thymidine kinase from herpes simplex virus type 1 in complex with IN51/20
Authors : Pernot, L.; Novakovic, I.; Westermaier, Y.; Perozzo, R.; Raic-Malic, S.; Scapozza, L.
Deposited on : 2013-01-23
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

<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 : 2.13.1
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) : 2.13.1

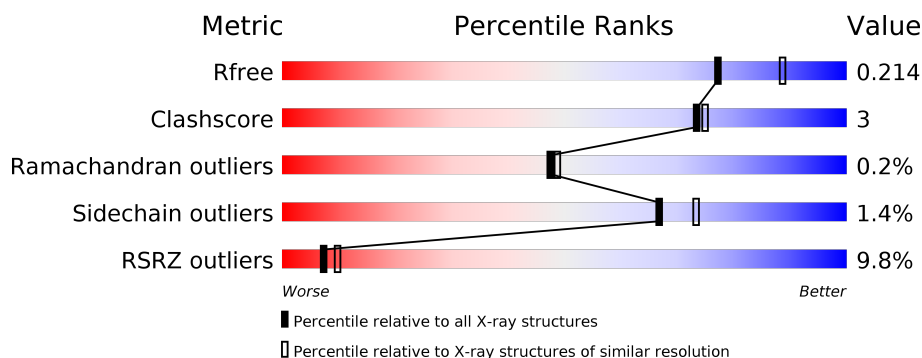
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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	331	<div> <div>7%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
1	B	331	<div> <div>11%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>

2 Entry composition [i](#)

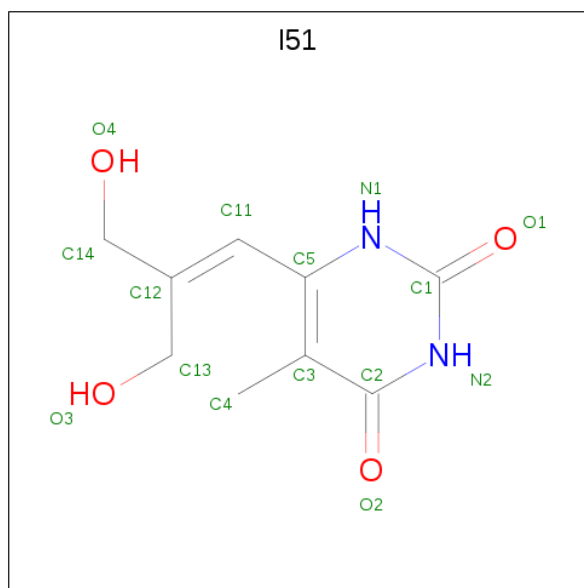
There are 4 unique types of molecules in this entry. The entry contains 5031 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thymidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	4	0
			2357	1505	405	428	19			
1	B	314	Total	C	N	O	S	0	5	0
			2406	1532	419	435	20			

- Molecule 2 is 6-[3-hydroxy-2-(hydroxymethyl)prop-1-en-1-yl]-5-methylpyrimidine-2,4(1H,3H)-dione (three-letter code: I51) (formula: C₉H₁₂N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	9	2	4		
2	B	1	Total	C	N	O	0	0
			15	9	2	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

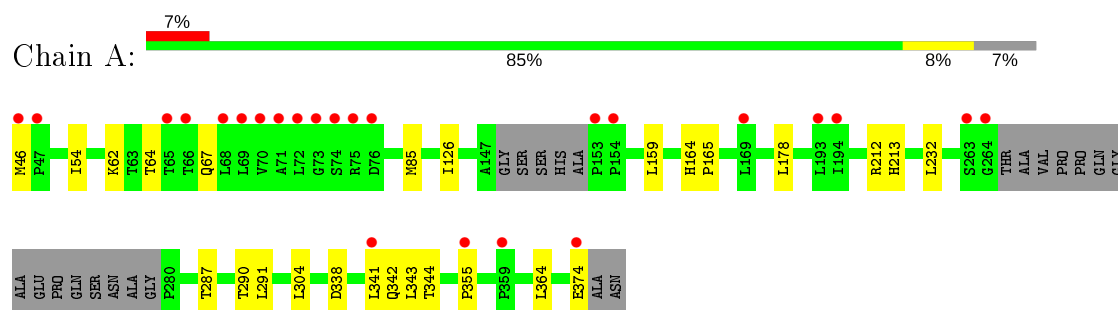
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	115	Total	O	0	0
			115	115		

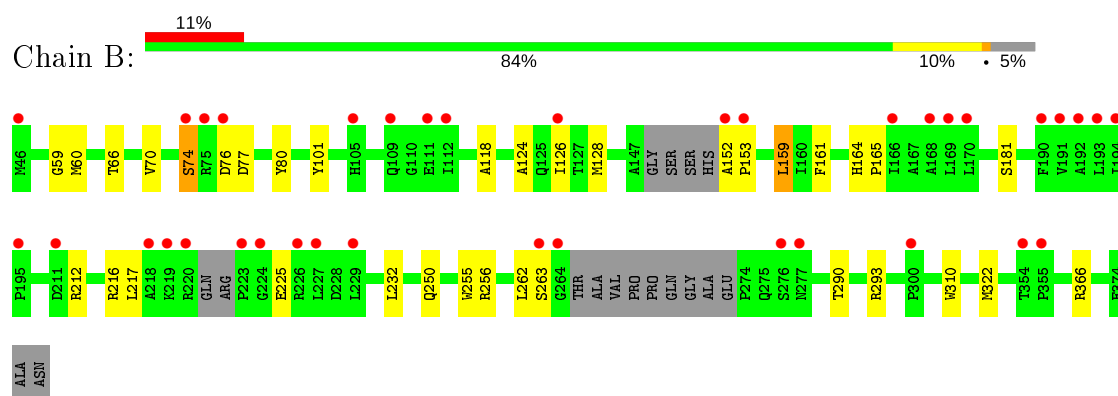
3 Residue-property plots [i](#)

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: Thymidine kinase



• Molecule 1: Thymidine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.00Å 117.83Å 108.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.87 – 2.10 39.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.87-2.10) 99.9 (39.87-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.24 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.178 , 0.214 0.179 , 0.214	Depositor DCC
R_{free} test set	2000 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5031	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 6.32% 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: I51, SO4

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	0.38	0/2427	0.56	0/3313
1	B	0.37	0/2480	0.53	0/3382
All	All	0.37	0/4907	0.54	0/6695

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	2357	0	2356	13	0
1	B	2406	0	2416	21	0
2	A	15	0	12	0	0
2	B	15	0	12	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	103	0	0	0	0
4	B	115	0	0	0	0
All	All	5031	0	4796	32	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 3.

All (32) 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:126:ILE:HD11	1:B:126:ILE:HD11	1.79	0.65
1:B:60:MET:O	1:B:216[B]:ARG:NH1	2.31	0.63
1:A:54:ILE:HG22	1:A:62:LYS:HG2	1.89	0.53
1:B:66:THR:HG21	1:B:80:TYR:CE1	2.43	0.53
1:B:101:TYR:CZ	1:B:225:GLU:HG3	2.45	0.51
1:A:341:LEU:O	1:A:344:THR:OG1	2.28	0.50
1:A:64:THR:O	1:A:67:GLN:HG2	2.13	0.49
1:B:159:LEU:HD13	1:B:161:PHE:CZ	2.47	0.48
1:B:217:LEU:HD22	1:B:232:LEU:HD13	1.95	0.48
1:B:76:ASP:HB3	1:B:366:ARG:HH22	1.79	0.48
1:A:46:MET:HE1	1:A:355:PRO:HG3	1.96	0.47
1:A:85:MET:HB3	1:A:374:GLU:HG3	1.95	0.47
1:A:364:LEU:HD22	1:B:310:TRP:CZ2	2.51	0.46
1:A:213:HIS:CE1	1:A:232:LEU:HD11	2.50	0.45
1:B:262:LEU:HB3	1:B:293:ARG:HD2	1.98	0.45
1:A:62:LYS:HB2	3:A:402:SO4:O3	2.16	0.45
1:A:178:LEU:HD21	1:A:291:LEU:HD22	1.97	0.45
1:B:59:GLY:HA3	1:B:217:LEU:HD13	1.99	0.44
1:B:70:VAL:HG21	1:B:80:TYR:HB2	2.00	0.44
1:B:152:ALA:HA	1:B:153:PRO:HD3	1.91	0.44
1:A:287:THR:O	1:A:290:THR:HG22	2.18	0.44
1:B:262:LEU:HD13	1:B:293:ARG:HD2	2.00	0.44
1:B:255:TRP:CE2	1:B:256:ARG:HG3	2.53	0.43
1:A:164:HIS:CG	1:A:165:PRO:HD2	2.52	0.43
1:B:74:SER:HB3	1:B:77:ASP:OD2	2.19	0.43
1:B:164:HIS:CG	1:B:165:PRO:HD2	2.54	0.42
1:B:118:ALA:HA	1:B:181:SER:O	2.20	0.42
1:A:338:ASP:O	1:A:342:GLN:HG2	2.20	0.41
1:B:290:THR:O	1:B:293:ARG:HD3	2.21	0.41
1:B:59:GLY:O	1:B:216[A]:ARG:HD3	2.21	0.41
1:B:250:GLN:NE2	1:B:322:MET:O	2.53	0.41
1:B:124:ALA:O	1:B:128:MET:HG2	2.20	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	307/331 (93%)	299 (97%)	8 (3%)	0	100	100
1	B	311/331 (94%)	302 (97%)	8 (3%)	1 (0%)	41	41
All	All	618/662 (93%)	601 (97%)	16 (3%)	1 (0%)	47	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	SER

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	248/264 (94%)	244 (98%)	4 (2%)	62	69
1	B	255/264 (97%)	252 (99%)	3 (1%)	71	77
All	All	503/528 (95%)	496 (99%)	7 (1%)	67	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LEU
1	A	212	ARG
1	A	304	LEU
1	A	343	LEU
1	B	74	SER

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Mol	Chain	Res	Type
1	B	159	LEU
1	B	212	ARG

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

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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	SO4	A	402	-	4,4,4	0.16	0	6,6,6	0.22	0
3	SO4	A	403	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	B	403	-	4,4,4	0.16	0	6,6,6	0.12	0
2	I51	B	401	-	14,15,15	2.15	5 (35%)	8,20,20	4.22	3 (37%)
2	I51	A	401	-	14,15,15	2.22	5 (35%)	8,20,20	4.20	3 (37%)
3	SO4	B	402	-	4,4,4	0.21	0	6,6,6	0.25	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	I51	A	401	-	-	5/8/8/8	0/1/1/1
2	I51	B	401	-	-	6/8/8/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	I51	C5-N1	5.16	1.40	1.35
2	B	401	I51	C5-N1	4.84	1.40	1.35
2	A	401	I51	C2-N2	4.48	1.40	1.33
2	B	401	I51	C2-N2	4.47	1.40	1.33
2	A	401	I51	C5-C3	-2.75	1.36	1.40
2	B	401	I51	C5-C3	-2.64	1.37	1.40
2	A	401	I51	C2-C3	2.14	1.46	1.41
2	B	401	I51	C2-C3	2.04	1.45	1.41
2	A	401	I51	C5-C11	2.02	1.48	1.41
2	B	401	I51	C5-C11	2.00	1.48	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	I51	C1-N1-C5	8.20	123.04	114.84
2	A	401	I51	C1-N1-C5	7.87	122.71	114.84
2	A	401	I51	C2-N2-C1	6.89	120.96	115.14
2	B	401	I51	C2-N2-C1	6.80	120.89	115.14
2	A	401	I51	C3-C2-N2	-5.23	118.14	125.25
2	B	401	I51	C3-C2-N2	-5.03	118.41	125.25

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	I51	C5-C11-C12-C13
2	B	401	I51	C11-C12-C13-O3
2	B	401	I51	C14-C12-C13-O3
2	B	401	I51	C11-C12-C14-O4
2	B	401	I51	C13-C12-C14-O4
2	A	401	I51	C11-C12-C13-O3
2	A	401	I51	C14-C12-C13-O3

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Mol	Chain	Res	Type	Atoms
2	A	401	I51	C11-C12-C14-O4
2	A	401	I51	C13-C12-C14-O4
2	B	401	I51	C12-C11-C5-C3
2	A	401	I51	C12-C11-C5-N1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	SO4	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	309/331 (93%)	0.21	24 (7%) 13 17	18, 29, 57, 94	0
1	B	314/331 (94%)	0.31	37 (11%) 4 5	18, 29, 59, 84	0
All	All	623/662 (94%)	0.26	61 (9%) 7 10	18, 29, 58, 94	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	LEU	10.2
1	A	73	GLY	8.1
1	A	69	LEU	6.4
1	A	264	GLY	5.9
1	B	277	ASN	5.6
1	B	227	LEU	5.3
1	B	263	SER	5.2
1	A	76	ASP	5.2
1	A	66	THR	5.1
1	A	75	ARG	5.0
1	B	264	GLY	5.0
1	B	223	PRO	4.9
1	A	74	SER	4.8
1	B	300	PRO	4.8
1	A	68	LEU	4.2
1	B	152	ALA	4.1
1	B	75	ARG	4.0
1	B	46	MET	3.8
1	A	71	ALA	3.7
1	B	153	PRO	3.7
1	A	70	VAL	3.7
1	B	169	LEU	3.6
1	B	355	PRO	3.5
1	B	109	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	65	THR	3.4
1	A	263	SER	3.3
1	B	220	ARG	3.2
1	B	193	LEU	3.2
1	B	226	ARG	3.1
1	B	74	SER	3.1
1	B	276	SER	3.0
1	A	193	LEU	2.9
1	B	219	LYS	2.9
1	A	374	GLU	2.9
1	B	194	ILE	2.8
1	A	154	PRO	2.8
1	B	224	GLY	2.7
1	B	111	GLU	2.7
1	A	153	PRO	2.6
1	B	112	ILE	2.6
1	A	355	PRO	2.5
1	B	168	ALA	2.5
1	B	192	ALA	2.5
1	B	190	PHE	2.5
1	B	76	ASP	2.4
1	A	47	PRO	2.3
1	A	341	LEU	2.3
1	B	354	THR	2.3
1	A	194	ILE	2.3
1	B	229	LEU	2.3
1	B	218	ALA	2.2
1	B	170	LEU	2.2
1	B	191	VAL	2.2
1	B	195	PRO	2.2
1	A	169	LEU	2.1
1	B	126	ILE	2.1
1	B	166	ILE	2.1
1	A	359	PRO	2.0
1	B	105	HIS	2.0
1	B	211	ASP	2.0
1	A	46	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	I51	A	401	15/15	0.93	0.16	21,27,43,45	0
2	I51	B	401	15/15	0.94	0.11	23,27,43,47	0
3	SO4	B	403	5/5	0.95	0.16	51,54,61,63	0
3	SO4	A	403	5/5	0.96	0.18	59,65,70,76	0
3	SO4	A	402	5/5	0.97	0.11	39,44,47,51	0
3	SO4	B	402	5/5	0.99	0.08	29,34,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.