



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:47 PM GMT

PDB ID : 3URA  
Title : Crystal Structure of PTE mutant H254G/H257W/L303T/K185R/I274N/A80V/S61T  
Authors : Tsai, P.; Fox, N.G.; Li, Y.; Barondeau, D.P.; Raushel, F.M.  
Deposited on : 2011-11-21  
Resolution : 1.88 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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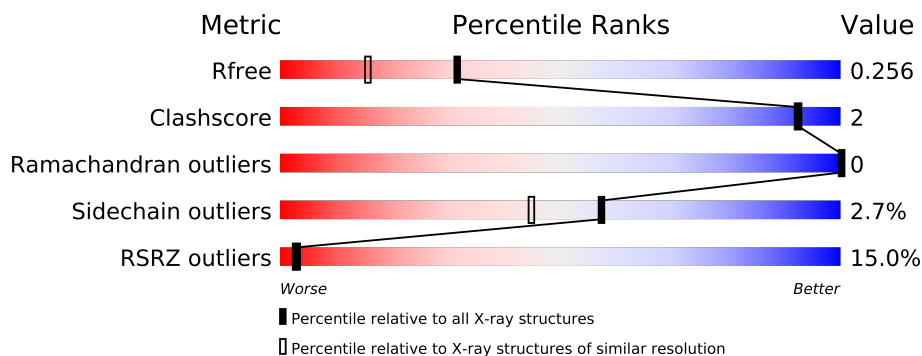
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 1.88 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))
$R_{free}$	66092	5260 (1.90-1.86)
Clashscore	79885	6268 (1.90-1.86)
Ramachandran outliers	78287	6195 (1.90-1.86)
Sidechain outliers	78261	6196 (1.90-1.86)
RSRZ outliers	66119	5262 (1.90-1.86)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	327	
1	B	327	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	IMD	A	1372	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5351 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2504	1582	444	471	7			
1	B	322	Total	C	N	O	S	0	0	0
			2467	1561	439	460	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	THR	SER	ENGINEERED MUTATION	UNP P0A434
A	80	VAL	ALA	ENGINEERED MUTATION	UNP P0A434
A	185	ARG	LYS	ENGINEERED MUTATION	UNP P0A434
A	254	GLY	HIS	ENGINEERED MUTATION	UNP P0A434
A	257	TRP	HIS	ENGINEERED MUTATION	UNP P0A434
A	274	ASN	ILE	ENGINEERED MUTATION	UNP P0A434
A	303	THR	LEU	ENGINEERED MUTATION	UNP P0A434
B	61	THR	SER	ENGINEERED MUTATION	UNP P0A434
B	80	VAL	ALA	ENGINEERED MUTATION	UNP P0A434
B	185	ARG	LYS	ENGINEERED MUTATION	UNP P0A434
B	254	GLY	HIS	ENGINEERED MUTATION	UNP P0A434
B	257	TRP	HIS	ENGINEERED MUTATION	UNP P0A434
B	274	ASN	ILE	ENGINEERED MUTATION	UNP P0A434
B	303	THR	LEU	ENGINEERED MUTATION	UNP P0A434

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Co	0	0
			2	2		
3	A	2	Total	Co	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	279	Total	O	0	0
			279	279		
4	B	92	Total	O	0	0
			92	92		

### 3 Residue-property plots

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.

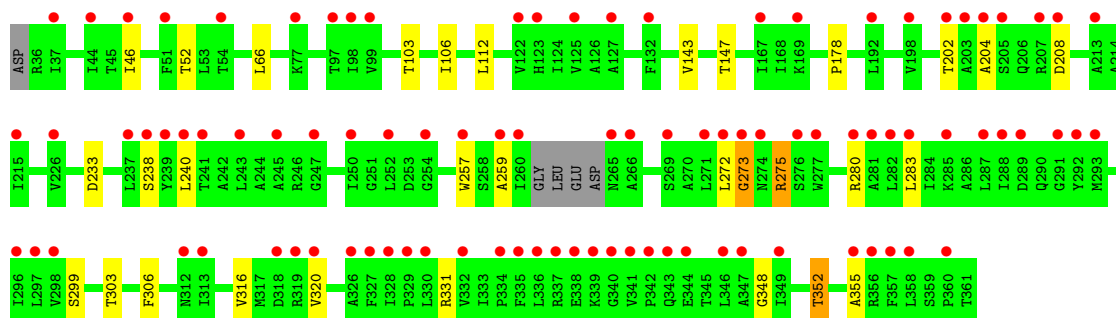
- Molecule 1: Parathion hydrolase

Chain A: 



- Molecule 1: Parathion hydrolase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.21Å 85.52Å 88.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.88 39.17 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-1.88) 99.2 (39.17-1.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.26 (at 1.88Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.253 0.235 , 0.256	Depositor DCC
$R_{free}$ test set	2662 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.2	EDS
Estimated twinning fraction	0.025 for -h,l,k 0.023 for -l,-k,-h 0.023 for k,h,-l 0.012 for k,l,h 0.012 for l,h,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 52140 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5351	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: CO, IMD, KCX

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	0.63	0/2539	0.76	2/3449 (0.1%)
1	B	0.62	0/2501	0.76	1/3396 (0.0%)
All	All	0.62	0/5040	0.76	3/6845 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ALA	N-CA-C	-6.55	93.32	111.00
1	B	273	GLY	N-CA-C	5.49	126.83	113.10
1	A	253	ASP	N-CA-C	5.04	124.62	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2504	0	2512	4	0
1	B	2467	0	2483	14	0
2	A	5	0	5	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
4	A	279	0	0	0	0
4	B	92	0	0	3	0
All	All	5351	0	5000	18	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (18) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:202:THR:HG23	1:B:208:ASP:HB2	1.79	0.64
1:B:275:ARG:HH12	1:B:280:ARG:HE	1.56	0.54
1:B:143:VAL:O	1:B:147:THR:HG23	2.08	0.53
1:B:283:LEU:HD13	4:B:1247:HOH:O	2.12	0.50
1:A:36:ARG:HH21	1:A:45:THR:HG23	1.76	0.49
1:B:46:ILE:HG23	1:B:355:ALA:HB1	1.95	0.48
1:B:259:ALA:HB3	1:B:273:GLY:O	2.15	0.46
1:B:257:TRP:O	1:B:280:ARG:NH1	2.49	0.46
1:B:348:GLY:HA2	1:B:352:THR:HG23	1.97	0.45
1:A:252:LEU:HD11	1:A:287:LEU:HD12	2.00	0.44
1:B:316:VAL:O	1:B:320:VAL:HG23	2.17	0.44
1:B:66:LEU:HD21	1:B:112:LEU:HD22	1.99	0.43
1:B:240:LEU:HD11	4:B:1247:HOH:O	2.18	0.42
1:A:259:ALA:HB2	1:A:272:LEU:HB2	2.02	0.41
1:B:204:ALA:HB3	1:B:233:ASP:HB2	2.03	0.41
1:A:61:THR:HG23	1:A:107:GLY:HA3	2.02	0.41
1:B:103:THR:H	1:B:106:ILE:HD12	1.85	0.40
1:B:238:SER:HB2	4:B:1282:HOH:O	2.21	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	324/327 (99%)	312 (96%)	12 (4%)	0	100	100
1	B	317/327 (97%)	297 (94%)	20 (6%)	0	100	100
All	All	641/654 (98%)	609 (95%)	32 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	262/262 (100%)	257 (98%)	5 (2%)	69	61
1	B	258/262 (98%)	249 (96%)	9 (4%)	48	32
All	All	520/524 (99%)	506 (97%)	14 (3%)	57	45

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	262	LEU
1	A	299	SER
1	A	306	PHE
1	A	361	THR
1	B	52	THR
1	B	178	PRO
1	B	272	LEU
1	B	275	ARG
1	B	299	SER
1	B	303	THR
1	B	306	PHE
1	B	331	ARG
1	B	352	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	155	GLN
1	B	290	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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$
1	KCX	A	169	1,3	11,11,12	5.43	2 (18%)	10,12,14	2.11	2 (20%)
1	KCX	B	169	1,3	11,11,12	5.09	3 (27%)	10,12,14	2.10	2 (20%)

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
1	KCX	A	169	1,3	-	0/8/10/12	0/0/0/0
1	KCX	B	169	1,3	-	0/8/10/12	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	KCX	O-C	17.63	1.23	1.11
1	B	169	KCX	O-C	16.42	1.22	1.11
1	B	169	KCX	CA-C	3.02	1.54	1.48
1	A	169	KCX	CA-C	2.72	1.53	1.48
1	B	169	KCX	OQ1-CX	2.04	1.25	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	KCX	C-CA-N	-4.63	109.20	113.83
1	A	169	KCX	OQ1-CX-NZ	-4.45	117.54	124.94
1	A	169	KCX	C-CA-N	-4.17	109.67	113.83
1	B	169	KCX	OQ1-CX-NZ	-4.13	118.07	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	IMD	A	1372	-	5,5,5	0.63	0	5,5,5	0.44	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	IMD	A	1372	-	-	0/0/0/0	0/1/1/1

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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	327/327 (100%)	0.09	4 (1%) 75 77	17, 26, 44, 63	0
1	B	322/327 (98%)	1.56	94 (29%) 1 1	26, 58, 76, 82	0
All	All	649/654 (99%)	0.82	98 (15%) 3 3	17, 39, 74, 82	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	ALA	5.8
1	B	259	ALA	5.7
1	B	241	THR	5.6
1	B	288	ILE	5.1
1	B	292	TYR	4.9
1	B	282	LEU	4.8
1	B	341	VAL	4.8
1	B	335	PHE	4.6
1	B	293	MET	4.5
1	A	361	THR	4.4
1	B	272	LEU	4.3
1	B	342	PRO	4.3
1	B	298	VAL	4.2
1	B	274	ASN	4.2
1	B	254	GLY	4.2
1	B	347	ALA	4.2
1	B	239	TYR	4.1
1	B	330	LEU	3.8
1	B	346	LEU	3.7
1	B	338	GLU	3.6
1	B	339	LYS	3.6
1	B	337	ARG	3.6
1	B	237	LEU	3.4
1	B	260	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	98	ILE	3.3
1	B	271	LEU	3.2
1	B	277	TRP	3.2
1	B	240	LEU	3.2
1	B	289	ASP	3.2
1	B	169	KCX	3.2
1	B	296	ILE	3.1
1	B	198	VAL	3.1
1	B	77	LYS	3.1
1	B	269	SER	3.1
1	B	204	ALA	3.1
1	B	266	ALA	3.0
1	B	297	LEU	3.0
1	B	291	GLY	3.0
1	B	213	ALA	3.0
1	B	340	GLY	2.9
1	B	281	ALA	2.9
1	B	127	ALA	2.8
1	B	287	LEU	2.8
1	B	319	ARG	2.8
1	B	205	SER	2.8
1	B	51	PHE	2.7
1	B	276	SER	2.7
1	B	252	LEU	2.7
1	B	312	ASN	2.7
1	B	125	VAL	2.7
1	B	328	ILE	2.7
1	B	257	TRP	2.6
1	B	283	LEU	2.6
1	B	343	GLN	2.6
1	B	327	PHE	2.6
1	B	326	ALA	2.6
1	B	336	LEU	2.6
1	B	54	THR	2.6
1	B	203	ALA	2.5
1	B	334	PRO	2.5
1	B	122	VAL	2.5
1	B	320	VAL	2.5
1	B	167	ILE	2.4
1	B	356	ARG	2.4
1	B	99	VAL	2.3
1	B	332	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	37	ILE	2.3
1	B	208	ASP	2.3
1	B	285	LYS	2.3
1	B	46	ILE	2.3
1	B	329	PRO	2.2
1	B	202	THR	2.2
1	B	247	GLY	2.2
1	B	207	ARG	2.2
1	A	125	VAL	2.2
1	A	312	ASN	2.2
1	B	250	ILE	2.2
1	B	360	PRO	2.2
1	B	132	PHE	2.2
1	B	243	LEU	2.2
1	B	349	ILE	2.1
1	B	123	HIS	2.1
1	B	318	ASP	2.1
1	B	97	THR	2.1
1	B	192	LEU	2.1
1	A	338	GLU	2.1
1	B	265	ASN	2.1
1	B	313	ILE	2.1
1	B	280	ARG	2.1
1	B	238	SER	2.1
1	B	358	LEU	2.1
1	B	44	ILE	2.0
1	B	226	VAL	2.0
1	B	273	GLY	2.0
1	B	357	PHE	2.0
1	B	355	ALA	2.0
1	B	215	ILE	2.0
1	B	344	GLU	2.0

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

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KCX	B	169	12/13	0.22	1.25	45,46,48,51	0
1	KCX	A	169	12/13	0.10	-0.46	14,17,22,23	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IMD	A	1372	5/5	0.23	8.80	33,33,35,36	0
3	CO	A	802	1/1	0.08	-1.46	21,21,21,21	0
3	CO	A	801	1/1	0.03	-4.50	22,22,22,22	0
3	CO	B	804	1/1	0.04	-6.06	57,57,57,57	0
3	CO	B	803	1/1	0.06	-8.03	48,48,48,48	0

### 6.5 Other polymers

There are no such residues in this entry.