



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:52 am BST

PDB ID : 5KR4  
Title : Directed Evolution of Transaminases By Ancestral Reconstruction. Using Old Proteins for New Chemistries  
Authors : Wilding, M.; Newman, J.; Peat, T.S.; Scott, C.  
Deposited on : 2016-07-06  
Resolution : 2.00 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](mailto: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

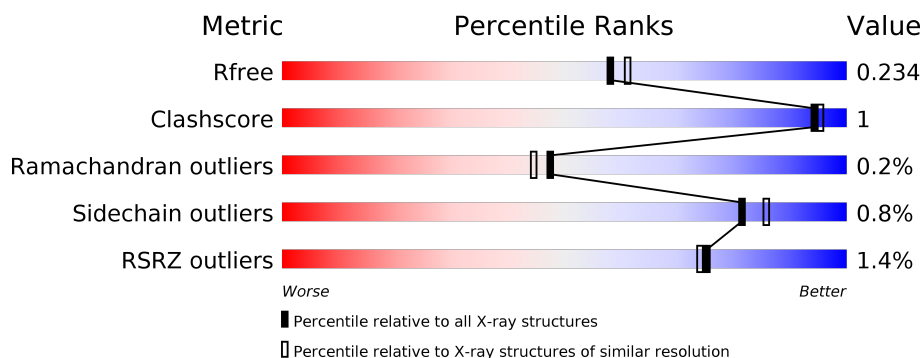
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	479	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>• 5%</div> </div> </div>
1	B	479	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>5% 5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7504 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 4-aminobutyrate transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	2	0
			3504	2227	608	653	16			
1	B	457	Total	C	N	O	S	0	3	0
			3511	2230	609	657	15			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

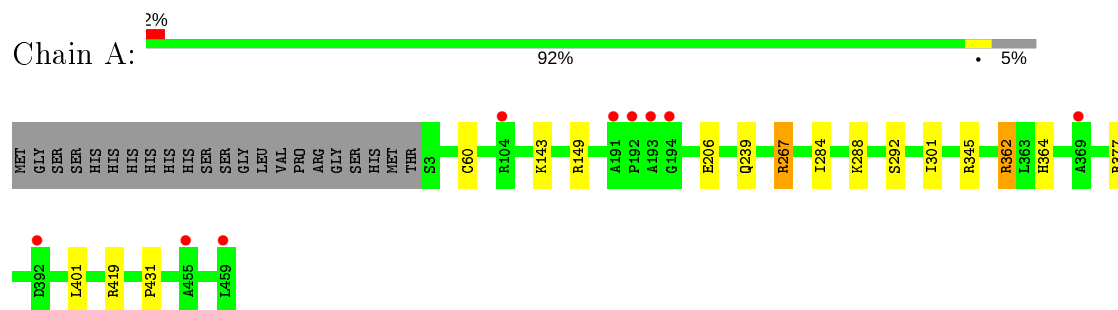
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	232	Total	O	0	0
			232	232		

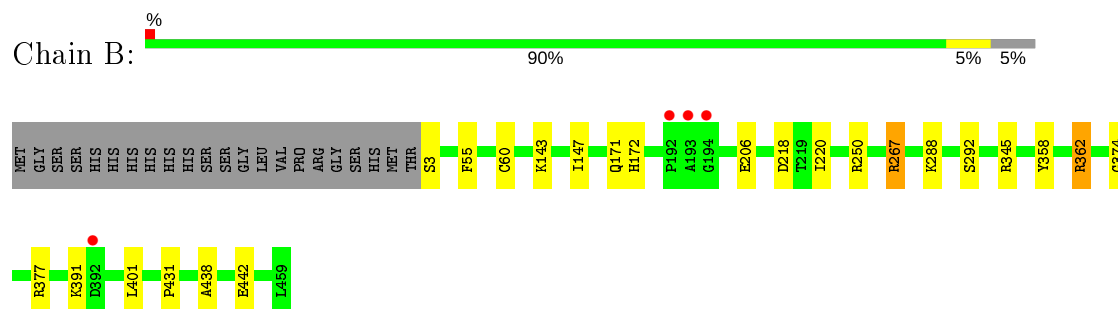
### 3 Residue-property plots [i](#)

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: 4-aminobutyrate transaminase



- Molecule 1: 4-aminobutyrate transaminase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.05Å 121.78Å 125.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.80 – 2.00 45.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.80-2.00) 99.2 (45.84-2.00)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.192 , 0.224 0.201 , 0.234	Depositor DCC
$R_{free}$ test set	3542 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7504	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: EDO, PLP

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	0.65	0/3589	0.79	8/4870 (0.2%)
1	B	0.67	0/3596	0.81	9/4881 (0.2%)
All	All	0.66	0/7185	0.80	17/9751 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	A	267	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	267	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	B	345	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	B	267	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	B	345	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	345	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	362	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	143	LYS	CD-CE-NZ	6.13	125.81	111.70
1	B	377	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	362	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	345	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	149	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	377	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	143	LYS	CD-CE-NZ	5.41	124.15	111.70
1	B	362	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	250	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	3504	0	3439	10	2
1	B	3511	0	3440	7	2
2	A	15	0	6	1	0
2	B	15	0	7	0	0
3	A	12	0	18	1	0
4	A	215	0	0	7	0
4	B	232	0	0	0	0
All	All	7504	0	6910	18	2

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 1.

All (18) 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)
2:A:501:PLP:O1P	4:A:601:HOH:O	2.07	0.71
1:B:374:GLY:HA2	1:B:391:LYS:HD3	1.79	0.63
1:A:267:ARG:NH2	1:A:431:PRO:O	2.43	0.51
1:B:267:ARG:NH2	1:B:431:PRO:O	2.45	0.49
1:A:362:ARG:HD2	4:A:780:HOH:O	2.13	0.48
1:A:206:GLU:HG3	4:A:683:HOH:O	2.13	0.47
1:B:171:GLN:HG2	1:B:172:HIS:CD2	2.51	0.46
1:A:267:ARG:CD	4:A:662:HOH:O	2.63	0.45
1:B:358:TYR:CZ	1:B:362:ARG:HD3	2.51	0.45
1:A:419:ARG:NH2	3:A:503:EDO:O2	2.45	0.45
1:A:60:CYS:O	1:A:292:SER:HA	2.17	0.44
1:B:60:CYS:O	1:B:292:SER:HA	2.17	0.44
1:A:267:ARG:HD3	4:A:662:HOH:O	2.20	0.42
1:A:364:HIS:HE1	4:A:642:HOH:O	2.02	0.42
1:B:438:ALA:O	1:B:442[A]:GLU:HG3	2.20	0.42
1:A:284:ILE:HB	1:A:301:ILE:HB	2.02	0.41
1:A:267:ARG:HD2	4:A:662:HOH:O	2.20	0.41
1:B:147:ILE:HD11	1:B:220:ILE:HD13	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:OE1	1:B:442[A]:GLU:OE1[3_654]	1.77	0.43
1:A:239:GLN:NE2	1:B:442[A]:GLU:OE2[3_654]	2.09	0.11

## 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	457/479 (95%)	438 (96%)	18 (4%)	1 (0%)	47	44
1	B	458/479 (96%)	438 (96%)	19 (4%)	1 (0%)	47	44
All	All	915/958 (96%)	876 (96%)	37 (4%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	LYS
1	B	288	LYS

### 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	356/373 (95%)	355 (100%)	1 (0%)	92	95
1	B	357/373 (96%)	351 (98%)	6 (2%)	60	65
All	All	713/746 (96%)	706 (99%)	7 (1%)	81	81

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

Mol	Chain	Res	Type
1	A	401	LEU
1	B	3	SER
1	B	55	PHE
1	B	206	GLU
1	B	218[A]	ASP
1	B	218[B]	ASP
1	B	401	LEU

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

Mol	Chain	Res	Type
1	A	171	GLN
1	B	171	GLN

### 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 ⓘ

5 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
2	PLP	A	501	-	15,15,16	2.56	5 (33%)	20,22,23	2.38	8 (40%)
3	EDO	A	503	-	3,3,3	0.54	0	2,2,2	0.56	0
3	EDO	A	502	-	3,3,3	0.58	0	2,2,2	0.73	0
3	EDO	A	504	-	3,3,3	0.53	0	2,2,2	0.55	0
2	PLP	B	500	-	15,15,16	3.13	5 (33%)	20,22,23	2.61	6 (30%)

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	PLP	A	501	-	-	1/6/6/8	0/1/1/1
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
2	PLP	B	500	-	-	2/6/6/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	PLP	C3-C2	9.50	1.50	1.40
2	A	501	PLP	C3-C2	7.19	1.48	1.40
2	B	500	PLP	C5-C4	4.92	1.45	1.40
2	A	501	PLP	C5-C4	3.95	1.44	1.40
2	B	500	PLP	P-O2P	-3.16	1.42	1.54
2	B	500	PLP	P-O4P	2.67	1.68	1.60
2	A	501	PLP	C3-C4	2.60	1.45	1.40
2	A	501	PLP	P-O2P	-2.47	1.45	1.54
2	B	500	PLP	C4A-C4	-2.21	1.47	1.51
2	A	501	PLP	C4A-C4	-2.01	1.47	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PLP	O2P-P-O4P	7.07	125.55	106.73
2	B	500	PLP	O4P-P-O1P	-5.52	90.99	106.47
2	A	501	PLP	O4P-P-O1P	-5.38	91.39	106.47
2	A	501	PLP	O2P-P-O4P	4.97	119.97	106.73
2	A	501	PLP	O3-C3-C2	4.40	127.09	117.49
2	B	500	PLP	O3-C3-C2	3.69	125.54	117.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PLP	O4P-C5A-C5	3.61	116.23	109.35
2	A	501	PLP	O3P-P-O4P	-2.97	98.83	106.73
2	A	501	PLP	C5A-C5-C6	2.88	124.11	119.37
2	A	501	PLP	O2P-P-O1P	2.68	121.18	110.68
2	A	501	PLP	O4P-C5A-C5	2.57	114.25	109.35
2	B	500	PLP	O3P-P-O4P	-2.52	100.03	106.73
2	B	500	PLP	O2P-P-O1P	2.25	119.48	110.68
2	A	501	PLP	C4-C3-C2	-2.18	116.86	120.07

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	PLP	C5A-O4P-P-O3P
3	A	503	EDO	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
2	A	501	PLP	C5A-O4P-P-O2P
2	B	500	PLP	C5A-O4P-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLP	1	0
3	A	503	EDO	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	457/479 (95%)	0.01	9 (1%) 65 63	12, 20, 38, 56	0
1	B	457/479 (95%)	-0.08	4 (0%) 84 83	12, 18, 34, 50	0
All	All	914/958 (95%)	-0.04	13 (1%) 75 74	12, 19, 36, 56	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	GLY	4.3
1	A	193	ALA	3.9
1	B	193	ALA	3.3
1	A	459	LEU	3.2
1	A	392	ASP	3.2
1	A	194	GLY	3.1
1	A	192	PRO	2.9
1	A	369	ALA	2.8
1	B	392	ASP	2.7
1	A	455	ALA	2.6
1	A	104	ARG	2.2
1	A	191	ALA	2.1
1	B	192	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

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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	A	504	4/4	0.77	0.18	32,35,36,36	0
2	PLP	A	501	15/16	0.83	0.47	8,11,11,12	15
3	EDO	A	502	4/4	0.85	0.14	25,26,26,29	0
2	PLP	B	500	15/16	0.85	0.39	8,11,12,13	15
3	EDO	A	503	4/4	0.92	0.28	33,33,33,35	0

## 6.5 Other polymers

There are no such residues in this entry.