



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 01:56 am BST

PDB ID : 4CHI / pdb\_00004chi  
Title : (R)-selective amine transaminase from *Aspergillus fumigatus* at 1.27 Å resolution  
Authors : Thomsen, M.; Palm, G.J.; Hinrichs, W.  
Deposited on : 2013-12-02  
Resolution : 1.27 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 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

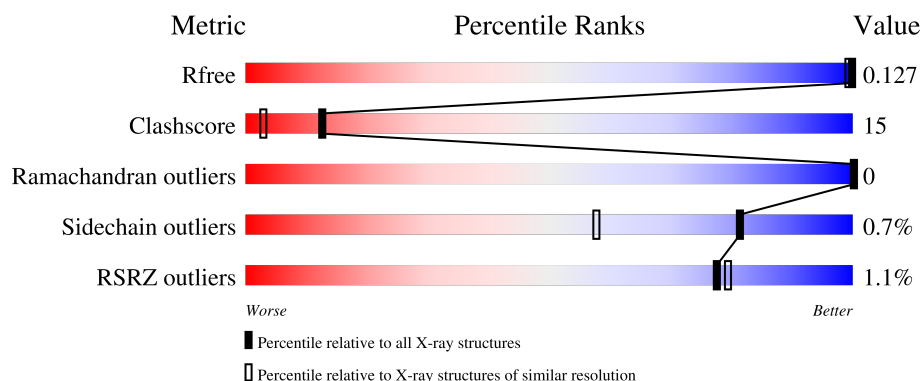
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.27 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))
$R_{free}$	164625	2484 (1.30-1.26)
Clashscore	180529	2694 (1.30-1.26)
Ramachandran outliers	177936	2628 (1.30-1.26)
Sidechain outliers	177891	2627 (1.30-1.26)
RSRZ outliers	164620	2481 (1.30-1.26)

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  $\geq 3$ , 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	332	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	332	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	K	A	501	-	-	X	-
7	CL	A	504	-	-	X	-
7	CL	B	504	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7037 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.

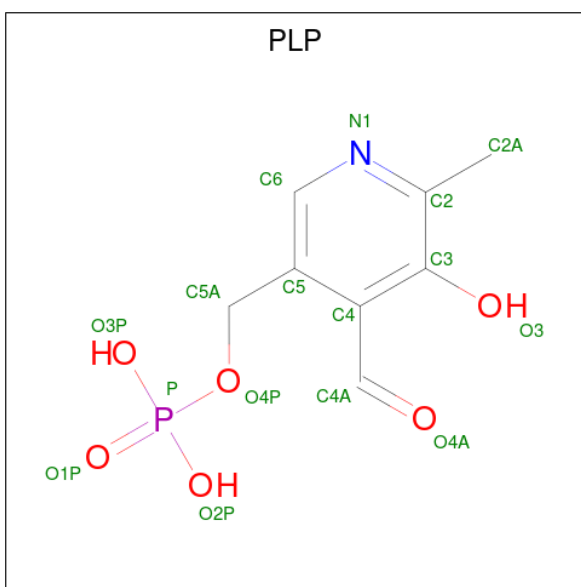
- Molecule 1 is a protein called BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	72	0
			2971	1935	478	540	18			
1	B	319	Total	C	N	O	S	0	66	0
			2939	1919	471	531	18			

There are 18 discrepancies between the modelled and reference sequences:

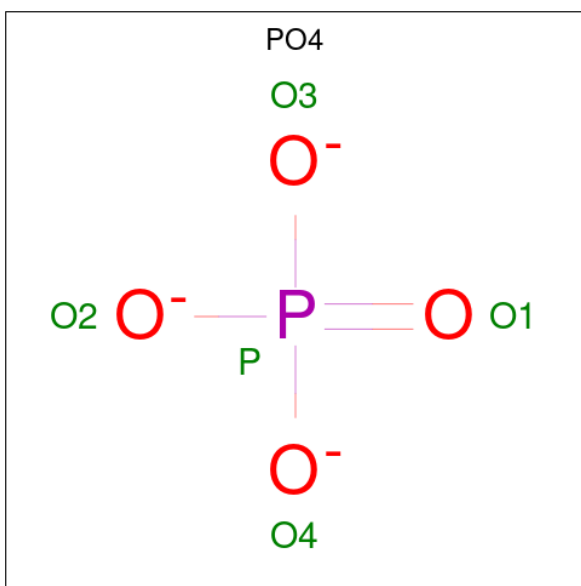
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	SER	-	expression tag	UNP Q4WH08
A	325	GLY	-	expression tag	UNP Q4WH08
A	326	SER	-	expression tag	UNP Q4WH08
A	327	HIS	-	expression tag	UNP Q4WH08
A	328	HIS	-	expression tag	UNP Q4WH08
A	329	HIS	-	expression tag	UNP Q4WH08
A	330	HIS	-	expression tag	UNP Q4WH08
A	331	HIS	-	expression tag	UNP Q4WH08
A	332	HIS	-	expression tag	UNP Q4WH08
B	324	SER	-	expression tag	UNP Q4WH08
B	325	GLY	-	expression tag	UNP Q4WH08
B	326	SER	-	expression tag	UNP Q4WH08
B	327	HIS	-	expression tag	UNP Q4WH08
B	328	HIS	-	expression tag	UNP Q4WH08
B	329	HIS	-	expression tag	UNP Q4WH08
B	330	HIS	-	expression tag	UNP Q4WH08
B	331	HIS	-	expression tag	UNP Q4WH08
B	332	HIS	-	expression tag	UNP Q4WH08

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			30	16	2	10	2		
2	B	1	Total	C	N	O	P	0	1
			30	16	2	10	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			7	3	4		
4	B	1	Total	C	O	0	1
			7	3	4		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	K	0	1
			3	3		
6	B	2	Total	K	0	1
			3	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total 2	Cl 2	0	0
7	B	2	Total 2	Cl 2	0	0

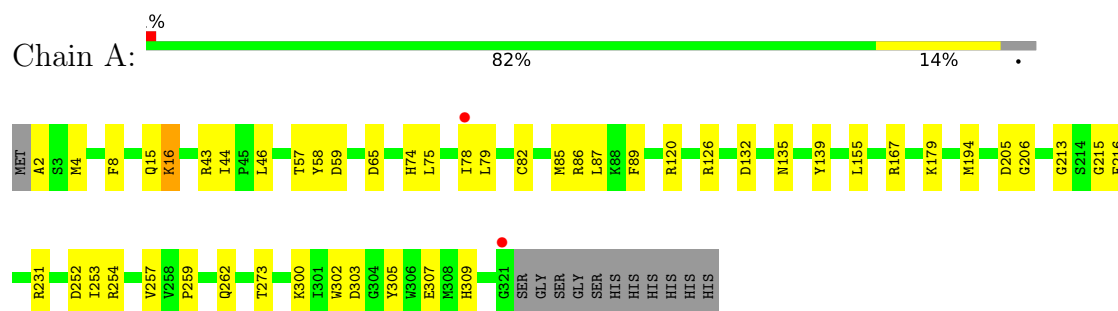
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	559	Total 559	O 559	0	45
8	B	472	Total 472	O 472	0	28

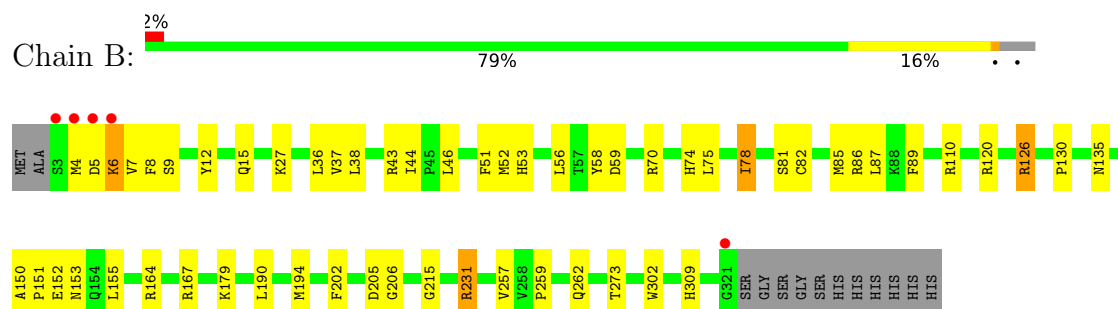
### 3 Residue-property plots

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: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE



#### • Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.37Å 120.94Å 135.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.88 – 1.27 47.88 – 1.27	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.88-1.27) 100.0 (47.88-1.27)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.103 , 0.127 0.103 , 0.127	Depositor DCC
$R_{free}$ test set	10976 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	7037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: GOL, NA, CL, K, PO4, 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	0.72	0/3215	0.89	5/4355 (0.1%)
1	B	0.69	0/3166	0.94	13/4290 (0.3%)
All	All	0.71	0/6381	0.91	18/8645 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231[A]	ARG	NE-CZ-NH2	9.35	124.97	120.30
1	B	231[B]	ARG	NE-CZ-NH2	9.35	124.97	120.30
1	B	78[A]	ILE	CG1-CB-CG2	-8.03	93.73	111.40
1	B	78[B]	ILE	CG1-CB-CG2	-8.03	93.73	111.40
1	B	78[C]	ILE	CG1-CB-CG2	-8.03	93.73	111.40
1	B	231[A]	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	B	231[B]	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	A	120[A]	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	120[B]	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	126[A]	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	126[B]	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	110	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	202	PHE	CB-CG-CD1	5.60	124.72	120.80
1	A	120[A]	ARG	NE-CZ-NH2	-5.54	117.53	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120[B]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	65	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	164	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	B	120	ARG	NE-CZ-NH2	-5.19	117.71	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	ARG	Sidechain

## 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	2971	0	3100	105	0
1	B	2939	0	3057	84	0
2	A	30	0	12	3	0
2	B	30	0	12	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	7	0	4	0	0
4	B	7	0	4	2	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
6	A	3	0	0	4	0
6	B	3	0	0	1	0
7	A	2	0	0	6	0
7	B	2	0	0	9	0
8	A	559	0	0	35	1
8	B	472	0	0	26	1
All	All	7037	0	6189	183	1

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 15.

All (183) 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:194[B]:MET:SD	1:B:130[B]:PRO:HG3	1.43	1.56
1:B:78[A]:ILE:HG21	7:B:504:CL:CL	1.49	1.49
1:A:78[A]:ILE:HG21	7:A:504:CL:CL	1.53	1.45
1:A:4[A]:MET:SD	1:A:155[A]:LEU:HD23	1.66	1.35
1:A:194[B]:MET:SD	1:B:130[B]:PRO:CG	2.13	1.34
1:B:78[A]:ILE:CG2	7:B:504:CL:CL	2.12	1.34
1:B:4[A]:MET:SD	1:B:155[A]:LEU:HD23	1.69	1.31
1:B:155[A]:LEU:HG	8:B:1383:HOH:O	1.33	1.27
1:B:4[A]:MET:SD	1:B:155[A]:LEU:CD2	2.24	1.26
1:A:194[B]:MET:HE2	8:A:1219:HOH:O	1.32	1.24
1:A:78[A]:ILE:CG2	7:A:504:CL:CL	2.24	1.22
1:A:259[B]:PRO:HD2	1:A:262[B]:GLN:CD	1.60	1.22
1:A:2[B]:ALA:O	1:A:303[B]:ASP:OD2	1.57	1.21
1:B:262[A]:GLN:OE1	8:B:1434:HOH:O	1.56	1.18
1:A:259[B]:PRO:HD2	1:A:262[B]:GLN:OE1	0.98	1.16
1:A:259[B]:PRO:CD	1:A:262[B]:GLN:OE1	1.93	1.16
1:B:4[A]:MET:HE1	8:B:1440:HOH:O	1.45	1.15
1:A:194[B]:MET:CE	8:A:1219:HOH:O	1.90	1.09
1:A:57[B]:THR:CG2	1:A:85[B]:MET:SD	2.41	1.08
1:A:231[B]:ARG:NE	8:A:1517:HOH:O	1.64	1.08
1:A:132[B]:ASP:OD2	8:A:1397:HOH:O	1.72	1.07
1:A:253[B]:ILE:C	1:A:253[B]:ILE:HD12	1.74	1.07
1:A:262[A]:GLN:OE1	8:A:1494:HOH:O	1.73	1.06
8:A:1521:HOH:O	1:B:194[C]:MET:SD	2.13	1.06
1:A:194[A]:MET:SD	8:A:1516:HOH:O	2.15	1.05
1:B:78[C]:ILE:HG21	7:B:504:CL:CL	1.95	1.04
1:A:262[B]:GLN:CD	8:A:1502:HOH:O	1.97	1.03
1:A:4[A]:MET:SD	1:A:155[A]:LEU:CD2	2.47	1.02
1:B:27[A]:LYS:HB2	8:B:1370:HOH:O	1.57	1.02
1:A:253[B]:ILE:HD12	1:A:253[B]:ILE:O	1.60	1.00
1:B:78[B]:ILE:HD11	7:B:503:CL:CL	0.43	0.97
1:B:4[B]:MET:HA	1:B:302:TRP:CH2	1.98	0.97
1:A:57[B]:THR:HG22	1:A:85[B]:MET:SD	2.05	0.95
1:A:82[B]:CYS:SG	8:A:1509[B]:HOH:O	2.19	0.95
1:A:2[B]:ALA:O	1:A:303[B]:ASP:CG	2.05	0.94
5:B:500:NA:NA	8:B:1468:HOH:O	0.50	0.94
1:A:75:LEU:HD23	7:A:504:CL:CL	2.05	0.94
1:B:82[A]:CYS:SG	6:B:501:K:K	2.20	0.93
1:B:78[A]:ILE:HG23	7:B:504:CL:CL	2.04	0.92
1:A:82[A]:CYS:SG	6:A:501:K:K	2.23	0.89
1:B:4[A]:MET:SD	1:B:155[A]:LEU:HD21	2.12	0.89
1:A:303[B]:ASP:OD1	8:A:1515:HOH:O	1.88	0.88

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206[B]:GLY:O	8:B:1360:HOH:O	1.91	0.88
1:A:194[B]:MET:SD	1:B:130[B]:PRO:HG2	2.14	0.88
1:A:135[B]:ASN:ND2	8:A:1407:HOH:O	2.05	0.87
5:A:500:NA:NA	8:A:1066:HOH:O	0.42	0.87
1:A:57[B]:THR:HG23	1:A:85[B]:MET:SD	2.16	0.85
1:B:262[A]:GLN:NE2	8:B:1348:HOH:O	2.00	0.84
1:B:78[C]:ILE:CG2	7:B:504:CL:CL	2.62	0.84
1:A:252[B]:ASP:OD1	8:A:1556:HOH:O	1.94	0.84
1:B:59:ASP:HB2	1:B:78[A]:ILE:HG22	1.58	0.83
1:B:309[B]:HIS:HE1	8:B:1059:HOH:O	1.62	0.83
1:A:75:LEU:O	1:A:78[A]:ILE:HG13	1.79	0.82
1:B:51:PHE:C	1:B:52[C]:MET:CA	2.49	0.80
1:A:206[B]:GLY:O	8:A:1394:HOH:O	1.98	0.80
1:A:59:ASP:HB2	1:A:78[A]:ILE:HG22	1.65	0.79
1:A:259[B]:PRO:CD	1:A:262[B]:GLN:CD	2.47	0.79
1:B:75:LEU:HD23	7:B:504:CL:CL	2.20	0.78
1:B:36:LEU:C	1:B:37[B]:VAL:CA	2.53	0.77
1:A:194[B]:MET:HE3	8:B:1272:HOH:O	1.86	0.76
1:B:37[B]:VAL:CA	1:B:38:LEU:N	2.49	0.75
1:A:78[A]:ILE:HD13	1:A:89:PHE:CE1	2.20	0.75
1:A:87[A]:LEU:O	6:A:502[A]:K:K	1.98	0.75
1:A:262[B]:GLN:NE2	8:A:1495:HOH:O	2.17	0.74
1:A:253[B]:ILE:C	1:A:253[B]:ILE:CD1	2.47	0.72
1:B:52[C]:MET:CA	1:B:53:HIS:N	2.52	0.71
1:B:78[A]:ILE:HG12	7:B:504:CL:CL	2.25	0.71
1:B:15[B]:GLN:NE2	8:B:1320:HOH:O	2.18	0.71
1:A:78[A]:ILE:HG23	7:A:504:CL:CL	2.25	0.71
1:B:82[B]:CYS:SG	1:B:87:LEU:O	2.50	0.69
1:B:4[A]:MET:HG2	1:B:8[A]:PHE:CE2	2.28	0.68
1:A:15[B]:GLN:OE1	8:A:1430:HOH:O	2.09	0.67
1:A:74:HIS:O	1:A:78[A]:ILE:HG23	1.96	0.66
1:B:78[A]:ILE:HD13	1:B:89:PHE:CE1	2.31	0.66
1:B:75:LEU:O	1:B:78[A]:ILE:HG13	1.96	0.65
1:B:135[B]:ASN:ND2	8:B:1378:HOH:O	2.28	0.65
1:B:262[A]:GLN:CD	8:B:1434:HOH:O	2.14	0.63
1:B:6[A]:LYS:HD3	1:B:7:VAL:HG23	1.80	0.63
1:A:253[B]:ILE:O	1:A:253[B]:ILE:CD1	2.43	0.62
1:A:46:LEU:HD13	1:B:44[A]:ILE:HD11	1.81	0.62
1:A:259[B]:PRO:HD2	1:A:262[B]:GLN:NE2	2.14	0.60
1:A:259[B]:PRO:CD	1:A:262[B]:GLN:NE2	2.64	0.60
1:A:78[A]:ILE:HD13	1:A:89:PHE:CD1	2.37	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2[B]:ALA:N	1:A:307[B]:GLU:HG2	2.16	0.59
1:B:150:ALA:HB3	1:B:153[B]:ASN:HD22	1.68	0.59
1:B:273[B]:THR:OG1	2:B:400[B]:PLP:H5A2	2.02	0.58
1:A:135[B]:ASN:ND2	8:A:1235:HOH:O	2.32	0.58
1:B:205[B]:ASP:CB	8:B:1138[B]:HOH:O	2.50	0.58
1:A:259[B]:PRO:HG2	1:A:262[B]:GLN:NE2	2.17	0.58
1:A:262[B]:GLN:OE1	8:A:1502:HOH:O	2.14	0.58
1:B:259[B]:PRO:HD2	1:B:262[B]:GLN:CD	2.24	0.58
1:B:59:ASP:CB	1:B:78[A]:ILE:HG22	2.30	0.58
1:A:4[A]:MET:HG3	1:A:8:PHE:CE2	2.39	0.58
1:A:59:ASP:CB	1:A:78[A]:ILE:HG22	2.32	0.56
1:A:205[B]:ASP:CB	8:A:1164[B]:HOH:O	2.53	0.56
1:B:126[B]:ARG:HB2	8:B:1114:HOH:O	2.06	0.55
1:A:257[B]:VAL:HG13	8:A:1229[B]:HOH:O	2.06	0.55
1:B:6[B]:LYS:NZ	8:B:1410:HOH:O	2.39	0.55
1:A:231[B]:ARG:HG3	8:A:1414:HOH:O	2.07	0.54
1:A:78[B]:ILE:HG21	7:A:504:CL:CL	2.45	0.54
1:A:273[A]:THR:OG1	2:A:400[A]:PLP:H5A2	2.08	0.53
1:B:205[B]:ASP:HB2	8:B:1138[B]:HOH:O	2.07	0.52
1:B:78[A]:ILE:CD1	1:B:89:PHE:CE1	2.93	0.52
1:B:58:TYR:CE1	1:B:179[A]:LYS:HG2	2.45	0.52
1:B:190:LEU:O	1:B:194[C]:MET:HG3	2.10	0.52
1:A:2[B]:ALA:N	1:A:307[B]:GLU:OE2	2.44	0.51
1:A:262[B]:GLN:NE2	8:A:1502:HOH:O	2.34	0.50
1:A:78[A]:ILE:C	1:A:78[A]:ILE:HD12	2.31	0.50
1:A:194[B]:MET:HE3	8:A:1219:HOH:O	1.82	0.50
1:A:58:TYR:CE1	1:A:179[A]:LYS:HG2	2.47	0.50
1:B:309[B]:HIS:CE1	8:B:1059:HOH:O	2.46	0.50
1:B:4[B]:MET:HA	1:B:302:TRP:HH2	1.68	0.49
1:B:86[A]:ARG:HD3	8:B:1256:HOH:O	2.13	0.49
1:A:78[A]:ILE:HD12	1:A:79:LEU:N	2.27	0.49
1:B:86[B]:ARG:CD	4:B:403[B]:GOL:O2	2.60	0.49
1:B:4[A]:MET:HG2	1:B:8[A]:PHE:CD2	2.47	0.49
1:A:206[B]:GLY:HA3	8:A:1394:HOH:O	2.12	0.49
1:A:15[A]:GLN:NE2	1:A:15[A]:GLN:HA	2.28	0.48
1:A:194[C]:MET:HG2	8:A:1187:HOH:O	2.13	0.48
1:A:194[B]:MET:SD	1:B:130[B]:PRO:CD	2.97	0.48
1:B:215:GLY:HA2	2:B:400[B]:PLP:C3	2.43	0.48
1:B:7:VAL:HG12	1:B:8[B]:PHE:CD1	2.48	0.48
1:A:205[B]:ASP:HB2	8:A:1164[B]:HOH:O	2.10	0.48
1:B:5[B]:ASP:O	1:B:9[B]:SER:OG	2.26	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:HIS:O	1:B:78[A]:ILE:HG23	2.14	0.48
1:A:16[A]:LYS:CE	1:A:16[A]:LYS:HA	2.44	0.48
1:B:4[A]:MET:SD	1:B:155[A]:LEU:CG	3.01	0.48
1:A:82[A]:CYS:HG	6:A:501:K:K	1.89	0.48
1:A:262[A]:GLN:HG3	8:A:1502:HOH:O	2.14	0.48
1:B:257[C]:VAL:HG13	8:B:1452:HOH:O	2.13	0.48
1:A:305:TYR:CZ	1:A:309[B]:HIS:HE1	2.31	0.47
1:A:44[B]:ILE:HD12	1:A:139:TYR:CZ	2.49	0.47
1:B:8[A]:PHE:CE1	1:B:151:PRO:HB3	2.50	0.47
1:A:231[B]:ARG:CG	8:A:1414:HOH:O	2.61	0.47
1:B:6[A]:LYS:HE2	1:B:6[A]:LYS:HB2	1.71	0.47
1:B:206[B]:GLY:HA3	8:B:1360:HOH:O	2.15	0.47
1:A:257[B]:VAL:HG22	1:A:257[B]:VAL:O	2.13	0.47
1:B:6[B]:LYS:HE2	8:B:1428:HOH:O	2.13	0.47
6:A:502[B]:K:K	8:A:1520:HOH:O	0.40	0.47
1:B:78[C]:ILE:HG22	7:B:504:CL:CL	2.50	0.47
1:B:4[A]:MET:HA	1:B:302:TRP:CH2	2.49	0.46
1:A:215:GLY:HA2	2:A:400[B]:PLP:C3	2.46	0.45
8:A:1521:HOH:O	1:B:194[B]:MET:CE	0.75	0.45
1:A:2[B]:ALA:CA	1:A:307[B]:GLU:OE2	2.65	0.45
1:A:259[B]:PRO:CG	1:A:262[B]:GLN:NE2	2.79	0.45
1:B:231[A]:ARG:NH2	8:B:1191:HOH:O	2.49	0.45
1:A:46:LEU:CD1	1:B:44[A]:ILE:HD11	2.46	0.44
1:A:78[A]:ILE:CD1	1:A:89:PHE:CD1	3.00	0.44
1:A:126[A]:ARG:HG3	8:A:1549:HOH:O	2.18	0.44
1:A:300[B]:LYS:HE2	1:A:300[B]:LYS:HB2	1.70	0.44
1:B:86[B]:ARG:HG3	4:B:403[B]:GOL:O2	2.17	0.44
1:A:253[B]:ILE:HD12	1:A:254:ARG:N	2.26	0.43
1:B:56:LEU:C	1:B:56:LEU:HD12	2.38	0.43
1:A:206[B]:GLY:C	8:A:1394:HOH:O	2.49	0.43
1:B:194[C]:MET:HG2	8:B:1131:HOH:O	2.19	0.43
1:B:206[B]:GLY:C	8:B:1360:HOH:O	2.48	0.43
1:B:81:SER:O	1:B:85[B]:MET:HG3	2.18	0.43
1:A:78[A]:ILE:CD1	1:A:89:PHE:CE1	2.96	0.43
1:A:16[A]:LYS:CE	1:A:16[A]:LYS:CA	2.97	0.42
1:A:2[B]:ALA:O	1:A:303[B]:ASP:OD1	2.34	0.42
1:A:4[A]:MET:HG3	1:A:8:PHE:CD2	2.53	0.42
1:B:259[B]:PRO:CD	1:B:262[B]:GLN:NE2	2.83	0.42
1:A:194[B]:MET:HE1	1:B:86[B]:ARG:NH2	2.35	0.42
1:A:44[B]:ILE:HD12	1:A:139:TYR:CE1	2.55	0.42
1:A:15[A]:GLN:HB3	1:A:16[A]:LYS:HE3	2.01	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1521:HOH:O	1:B:194[B]:MET:HE2	0.72	0.42
1:A:44[B]:ILE:HD11	1:B:46:LEU:HD13	2.02	0.41
1:A:213:GLY:HA3	1:A:216:PHE:CZ	2.55	0.41
1:A:2[B]:ALA:HB2	1:A:307[B]:GLU:OE2	2.20	0.41
1:B:259[B]:PRO:HB3	8:B:1386:HOH:O	2.21	0.41
1:A:254:ARG:NH1	8:A:1540:HOH:O	2.52	0.41
1:B:215:GLY:HA2	2:B:400[B]:PLP:O3	2.21	0.41
1:B:205[B]:ASP:HB3	8:B:1138[B]:HOH:O	2.16	0.41
1:A:43:ARG:HB3	1:B:43:ARG:HB3	2.03	0.41
1:A:305:TYR:CE2	1:A:309[B]:HIS:HE1	2.39	0.41
1:B:12[B]:TYR:OH	1:B:152:GLU:HG2	2.21	0.41
1:A:16[A]:LYS:HE3	1:A:16[A]:LYS:CA	2.51	0.41
1:A:86[B]:ARG:HD3	8:A:1301:HOH:O	2.19	0.41
1:A:215:GLY:HA2	2:A:400[B]:PLP:O3	2.21	0.40
1:A:78[B]:ILE:CG2	7:A:504:CL:CL	3.05	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1451:HOH:O	8:B:1410:HOH:O[6_554]	2.07	0.13

## 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	394/332 (119%)	386 (98%)	8 (2%)	0	100	100
1	B	389/332 (117%)	376 (97%)	13 (3%)	0	100	100
All	All	783/664 (118%)	762 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.



### 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	348/284 (122%)	345 (99%)	3 (1%)	75	49
1	B	344/284 (121%)	341 (99%)	3 (1%)	75	49
All	All	692/568 (122%)	686 (99%)	6 (1%)	81	49

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16[A]	LYS
1	A	16[B]	LYS
1	A	167	ARG
1	B	6[A]	LYS
1	B	6[B]	LYS
1	B	167	ARG

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

Mol	Chain	Res	Type
1	A	223	ASN
1	B	223	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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	PLP	A	400[A]	1	15,15,16	2.69	4 (26%)	20,22,23	1.88	8 (40%)
4	GOL	B	403[A]	-	5,5,5	0.49	0	5,5,5	0.99	0
2	PLP	A	400[B]	-	15,15,16	2.30	3 (20%)	20,22,23	1.53	3 (15%)
3	PO4	B	402	-	4,4,4	0.75	0	6,6,6	0.84	0
2	PLP	B	400[A]	1	15,15,16	2.51	4 (26%)	20,22,23	1.77	6 (30%)
3	PO4	A	402	-	4,4,4	0.74	0	6,6,6	0.88	0
4	GOL	A	403[A]	-	5,5,5	0.81	0	5,5,5	1.18	0
4	GOL	B	403[B]	-	5,5,5	0.43	0	5,5,5	1.52	1 (20%)
2	PLP	B	400[B]	-	15,15,16	2.32	4 (26%)	20,22,23	1.14	0
4	GOL	A	403[B]	-	5,5,5	0.74	0	5,5,5	1.70	1 (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
2	PLP	A	400[A]	1	-	1/6/6/8	0/1/1/1
4	GOL	B	403[A]	-	-	1/4/4/4	-
2	PLP	A	400[B]	-	-	1/6/6/8	0/1/1/1
4	GOL	B	403[B]	-	-	2/4/4/4	-
2	PLP	B	400[A]	1	-	0/6/6/8	0/1/1/1
4	GOL	A	403[A]	-	-	1/4/4/4	-
2	PLP	B	400[B]	-	-	0/6/6/8	0/1/1/1
4	GOL	A	403[B]	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400[A]	PLP	C5-C4	7.18	1.48	1.40
2	B	400[A]	PLP	C5-C4	6.25	1.47	1.40
2	A	400[B]	PLP	C3-C2	5.95	1.46	1.40
2	B	400[B]	PLP	C3-C2	5.67	1.46	1.40
2	B	400[A]	PLP	C3-C2	5.48	1.46	1.40
2	A	400[A]	PLP	C3-C2	5.20	1.46	1.40
2	B	400[B]	PLP	C5-C4	5.08	1.46	1.40
2	A	400[B]	PLP	C5-C4	4.92	1.45	1.40
2	B	400[A]	PLP	C3-C4	3.26	1.46	1.40
2	A	400[A]	PLP	C3-C4	3.16	1.46	1.40
2	B	400[B]	PLP	C3-C4	2.91	1.46	1.40
2	A	400[B]	PLP	C3-C4	2.82	1.46	1.40
2	A	400[A]	PLP	C4A-C4	-2.63	1.46	1.51
2	B	400[B]	PLP	C4A-C4	-2.26	1.46	1.51
2	B	400[A]	PLP	C4A-C4	-2.25	1.47	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400[A]	PLP	C2A-C2-C3	-4.25	115.64	120.89
2	B	400[A]	PLP	C2A-C2-C3	-4.16	115.75	120.89
2	A	400[B]	PLP	C6-C5-C4	3.95	121.27	118.16
2	A	400[A]	PLP	C6-C5-C4	3.30	120.76	118.16
2	A	400[B]	PLP	C3-C4-C5	-3.16	115.33	118.74
4	A	403[B]	GOL	O2-C2-C3	2.97	122.19	109.12
2	B	400[A]	PLP	O2P-P-O4P	-2.95	98.89	106.73
4	B	403[B]	GOL	O2-C2-C3	2.68	120.93	109.12
2	B	400[A]	PLP	C4-C3-C2	-2.63	116.18	120.07
2	B	400[A]	PLP	C6-C5-C4	2.54	120.16	118.16
2	A	400[A]	PLP	O3P-P-O2P	2.52	117.25	107.64
2	A	400[A]	PLP	C3-C4-C5	-2.43	116.12	118.74
2	B	400[A]	PLP	O3-C3-C4	2.42	124.48	118.10
2	A	400[A]	PLP	C3-C2-N1	2.35	123.80	120.77
2	A	400[B]	PLP	C4A-C4-C3	2.30	124.39	120.50
2	B	400[A]	PLP	O3P-P-O2P	2.16	115.88	107.64
2	A	400[A]	PLP	C4-C3-C2	-2.14	116.90	120.07
2	A	400[A]	PLP	O2P-P-O4P	-2.11	101.12	106.73
2	A	400[A]	PLP	O3-C3-C4	2.10	123.63	118.10

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403[B]	GOL	O2-C2-C3-O3
4	B	403[B]	GOL	O2-C2-C3-O3
4	A	403[A]	GOL	O1-C1-C2-O2
2	A	400[B]	PLP	C4-C5-C5A-O4P
4	A	403[B]	GOL	O1-C1-C2-O2
4	B	403[A]	GOL	O1-C1-C2-O2
2	A	400[A]	PLP	C5A-O4P-P-O2P
4	B	403[B]	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400[A]	PLP	1	0
2	A	400[B]	PLP	2	0
4	B	403[B]	GOL	2	0
2	B	400[B]	PLP	3	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	320/332 (96%)	-0.59	2 (0%) 85 88	4, 11, 23, 53	72 (22%)
1	B	319/332 (96%)	-0.54	5 (1%) 70 71	4, 11, 26, 145	66 (20%)
All	All	639/664 (96%)	-0.57	7 (1%) 77 79	4, 11, 24, 145	138 (21%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	SER	7.4
1	B	321	GLY	3.6
1	B	4[A]	MET	3.5
1	B	5[A]	ASP	2.9
1	B	6[A]	LYS	2.5
1	A	321	GLY	2.5
1	A	78[A]	ILE	2.4

### 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 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, 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( $\text{\AA}^2$ )	Q<0.9
7	CL	A	504	1/1	0.82	0.48	33,33,33,33	1
7	CL	B	504	1/1	0.91	0.17	28,28,28,28	1
4	GOL	B	403[A]	6/6	0.92	0.13	11,17,20,27	6
4	GOL	B	403[B]	6/6	0.92	0.13	11,17,18,20	6
4	GOL	A	403[A]	6/6	0.94	0.10	18,20,27,28	6
4	GOL	A	403[B]	6/6	0.94	0.10	18,20,23,27	6
7	CL	B	503	1/1	0.97	0.10	27,27,27,27	1
7	CL	A	503	1/1	0.97	0.08	17,17,17,17	1
5	NA	B	500	1/1	0.99	0.04	16,16,16,16	1
6	K	B	502[A]	1/1	0.99	0.06	17,17,17,17	1
6	K	B	502[B]	1/1	0.99	0.06	207,207,207,207	1
2	PLP	A	400[A]	15/16	0.99	0.05	11,15,20,30	15
2	PLP	A	400[B]	15/16	0.99	0.05	4,6,9,11	15
2	PLP	B	400[A]	15/16	0.99	0.05	11,13,18,23	15
2	PLP	B	400[B]	15/16	0.99	0.05	5,9,13,13	15
6	K	B	501	1/1	1.00	0.01	11,11,11,11	0
3	PO4	B	402	5/5	1.00	0.02	6,9,10,18	5
5	NA	A	500	1/1	1.00	0.02	13,13,13,13	1
3	PO4	A	402	5/5	1.00	0.02	6,7,9,10	5
6	K	A	501	1/1	1.00	0.03	11,11,11,11	1
6	K	A	502[A]	1/1	1.00	0.02	9,9,9,9	1
6	K	A	502[B]	1/1	1.00	0.02	20,20,20,20	1

## 6.5 Other polymers

There are no such residues in this entry.