



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 05:26 AM EDT

PDB ID : 1TYZ  
Title : Crystal structure of 1-Aminocyclopropane-1-carboxylate Deaminase from Pseudomonas  
Authors : Karthikeyan, S.; Zhou, Q.; Zhao, Z.; Kao, C.L.; Tao, Z.; Robinson, H.; Liu, H.W.; Zhang, H.  
Deposited on : 2004-07-08  
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 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

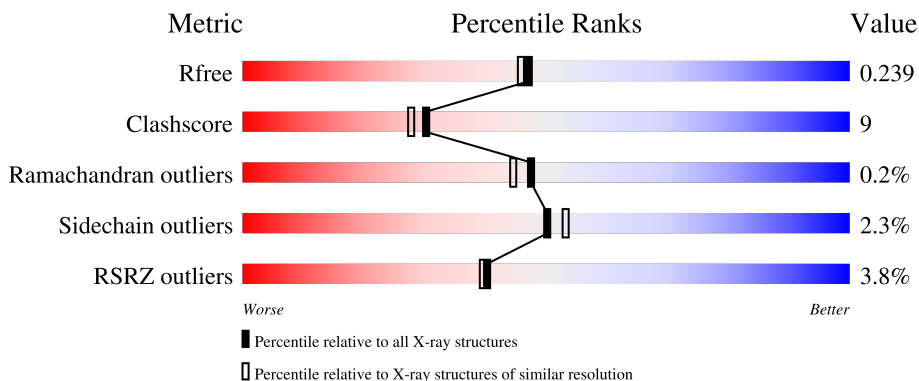
# 1 Overall quality at a glance i

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 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	338	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81%      14%      ..</p>
1	B	338	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">79%      17%      ..</p>
1	C	338	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">82%      17%      .</p>
1	D	338	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">79%      17%      ..</p>

## 2 Entry composition [i](#)

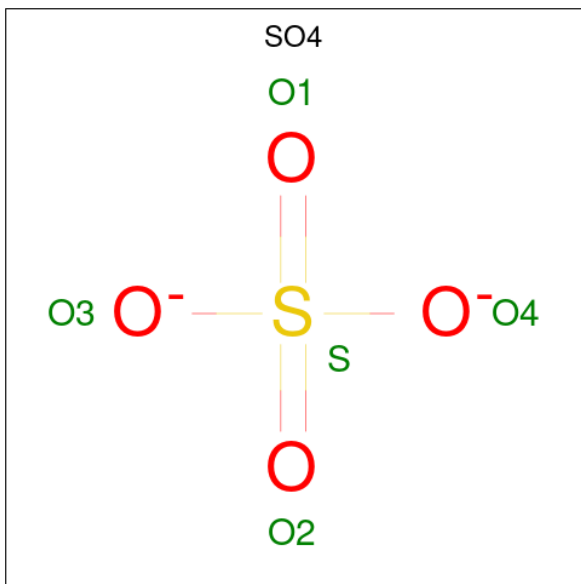
There are 4 unique types of molecules in this entry. The entry contains 10486 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-aminocyclopropane-1-carboxylate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	Total 2514	C 1576	N 451	O 472	S 15	0	0	0
1	B	329	Total 2499	C 1567	N 449	O 468	S 15	0	0	0
1	C	338	Total 2571	C 1614	N 461	O 481	S 15	0	0	0
1	D	329	Total 2499	C 1567	N 449	O 468	S 15	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



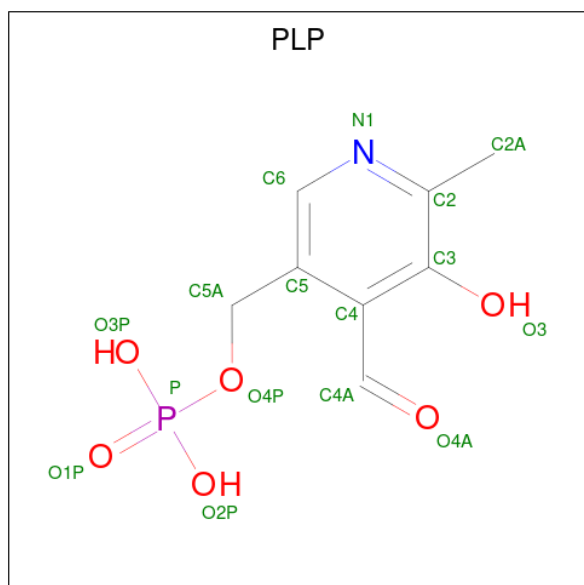
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	92	Total O 92 92	0	0
4	B	85	Total O 85 85	0	0
4	C	73	Total O 73 73	0	0

Continued on next page...

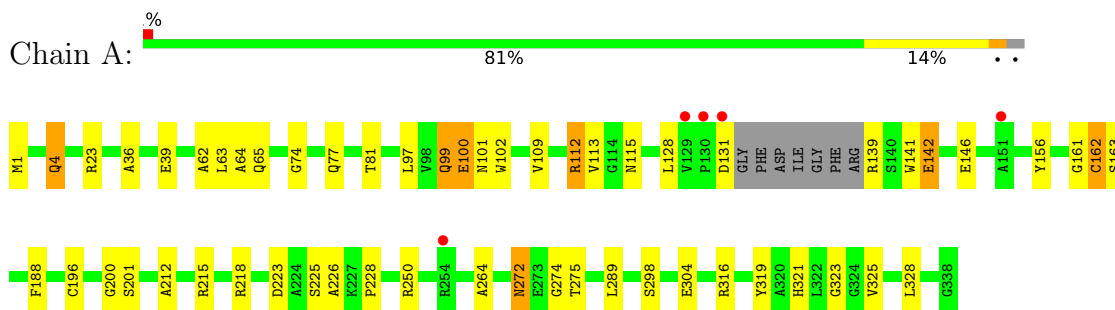
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	D	73	Total	O	0	0
			73	73		

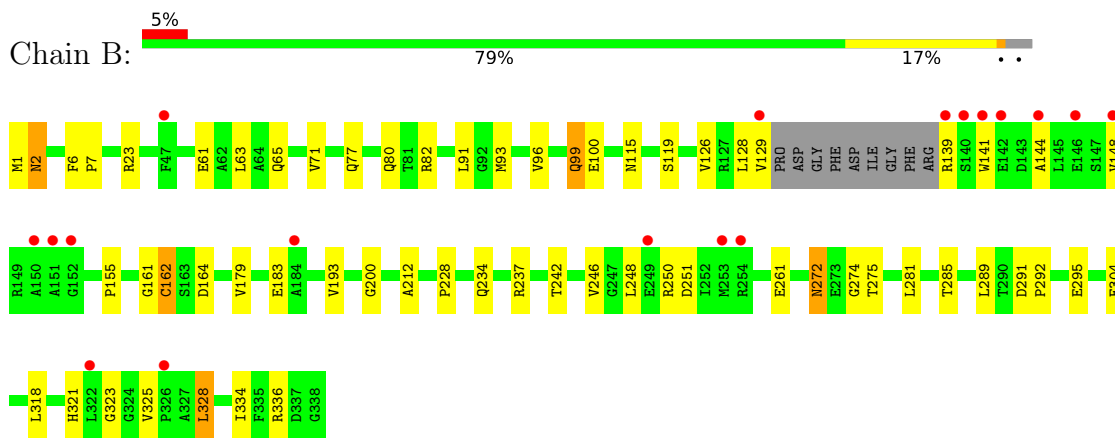
### 3 Residue-property plots [i](#)

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.

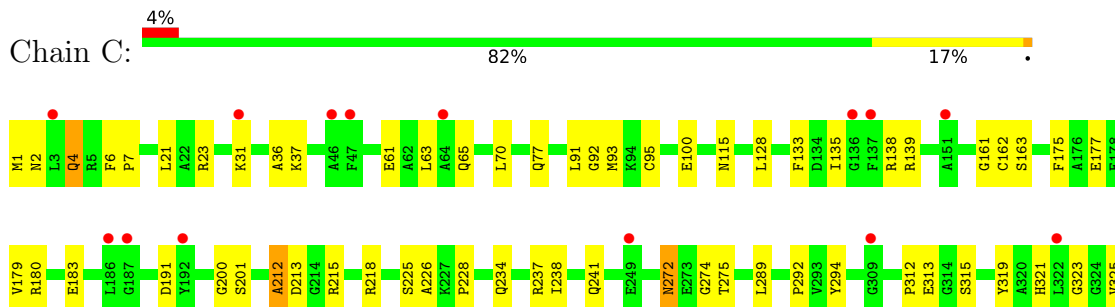
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

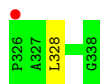


- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



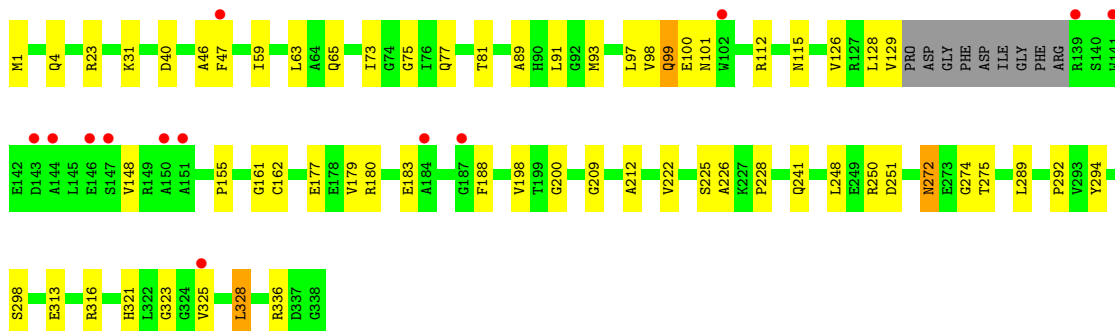
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





● Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain D: 4% 79% 17%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.72Å 68.65Å 350.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.73 – 2.00 39.73 – 1.99	Depositor EDS
% Data completeness (in resolution range)	86.5 (39.73-2.00) 85.9 (39.73-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.215 , 0.251 0.204 , 0.239	Depositor DCC
$R_{free}$ test set	4851 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtrriage
Anisotropy	0.265	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.033 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10486	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, 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	0.55	1/2561 (0.0%)	0.73	2/3461 (0.1%)
1	B	0.51	1/2545 (0.0%)	0.72	1/3438 (0.0%)
1	C	0.55	0/2621	0.74	1/3542 (0.0%)
1	D	0.50	0/2545	0.70	1/3438 (0.0%)
All	All	0.53	2/10272 (0.0%)	0.72	5/13879 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	CYS	CB-SG	-5.15	1.73	1.81
1	B	162	CYS	CB-SG	-5.11	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	GLY	N-CA-C	6.95	130.47	113.10
1	A	200	GLY	N-CA-C	6.90	130.35	113.10
1	B	200	GLY	N-CA-C	6.67	129.76	113.10
1	A	112	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	D	200	GLY	N-CA-C	6.23	128.68	113.10

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	2514	0	2485	42	0
1	B	2499	0	2475	50	0
1	C	2571	0	2539	53	0
1	D	2499	0	2474	46	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	7	1	0
3	C	15	0	7	0	0
3	D	15	0	7	0	0
4	A	92	0	0	0	0
4	B	85	0	0	2	0
4	C	73	0	0	3	0
4	D	73	0	0	2	0
All	All	10486	0	10001	188	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 9.

All (188) 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:4:GLN:NE2	1:A:4:GLN:H	1.63	0.96
1:B:100:GLU:HG3	1:B:129:VAL:HG21	1.45	0.96
1:A:139:ARG:HG3	1:A:142:GLU:H	1.32	0.93
1:D:1:MET:HE3	1:D:212:ALA:HB2	1.52	0.92
1:B:1:MET:HE1	1:B:212:ALA:HB2	1.55	0.87
1:C:272:ASN:HD22	1:C:274:GLY:H	1.20	0.86
1:D:1:MET:CE	1:D:212:ALA:HB2	2.10	0.82
1:A:4:GLN:H	1:A:4:GLN:HE21	1.23	0.81
1:B:272:ASN:HD22	1:B:274:GLY:H	1.28	0.81
1:A:139:ARG:HD2	1:A:141:TRP:HB3	1.62	0.81
1:B:1:MET:CE	1:B:212:ALA:HB2	2.11	0.80
1:B:139:ARG:HD2	1:B:141:TRP:HB3	1.63	0.79
1:A:272:ASN:HD22	1:A:274:GLY:H	1.30	0.79
1:B:77:GLN:HE22	1:B:115:ASN:H	1.32	0.77
1:C:272:ASN:HD22	1:C:274:GLY:N	1.84	0.74
1:B:100:GLU:HG3	1:B:129:VAL:CG2	2.17	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLN:HB2	1:A:128:LEU:HD23	1.71	0.73
1:B:334:ILE:HG12	4:B:541:HOH:O	1.90	0.71
1:D:272:ASN:HD22	1:D:274:GLY:H	1.37	0.71
1:B:321:HIS:HD2	1:B:323:GLY:H	1.39	0.70
1:C:234:GLN:O	1:C:238:ILE:HG13	1.92	0.70
1:A:4:GLN:NE2	1:A:4:GLN:N	2.38	0.69
1:D:289:LEU:O	1:D:321:HIS:HE1	1.76	0.67
1:C:161:GLY:O	1:C:162:CYS:HB2	1.93	0.67
1:C:4:GLN:H	1:C:4:GLN:CD	1.96	0.67
1:B:139:ARG:HD2	1:B:141:TRP:CB	2.24	0.67
1:D:179:VAL:O	1:D:183:GLU:HG3	1.95	0.67
1:C:21:LEU:HD11	1:C:36:ALA:HB2	1.77	0.66
1:B:91:LEU:HD13	1:B:93:MET:HE3	1.76	0.66
1:D:99:GLN:HB2	1:D:128:LEU:HD23	1.77	0.66
1:A:100:GLU:HG3	1:A:102:TRP:NE1	2.11	0.66
1:B:234:GLN:CD	1:B:237:ARG:HH21	1.99	0.66
1:A:161:GLY:O	1:A:162:CYS:HB2	1.96	0.66
1:C:1:MET:CE	1:C:212:ALA:HB2	2.26	0.66
1:C:191:ASP:O	1:C:218:ARG:HD2	1.96	0.66
1:D:228:PRO:HG3	4:D:522:HOH:O	1.95	0.66
1:C:77:GLN:HE22	1:C:115:ASN:H	1.42	0.65
1:B:139:ARG:HG2	1:B:139:ARG:HH11	1.61	0.64
1:B:272:ASN:HD22	1:B:274:GLY:N	1.98	0.62
1:A:1:MET:HE2	1:A:212:ALA:HB2	1.82	0.62
1:A:1:MET:CE	1:A:212:ALA:HB2	2.29	0.61
1:C:2:ASN:OD1	1:C:4:GLN:NE2	2.34	0.61
1:A:289:LEU:O	1:A:321:HIS:HE1	1.84	0.60
1:D:272:ASN:HD22	1:D:274:GLY:N	1.98	0.60
1:A:250:ARG:HH11	1:A:250:ARG:HG3	1.64	0.60
1:C:312:PRO:HG2	1:C:315:SER:OG	2.02	0.60
1:D:77:GLN:HE22	1:D:115:ASN:H	1.48	0.60
1:D:180:ARG:NH2	1:D:209:GLY:O	2.33	0.60
1:B:289:LEU:O	1:B:321:HIS:HE1	1.84	0.59
1:A:77:GLN:HE22	1:A:115:ASN:H	1.49	0.59
1:B:228:PRO:HG3	4:B:558:HOH:O	2.02	0.59
1:D:321:HIS:HD2	1:D:323:GLY:H	1.51	0.59
1:A:272:ASN:HD22	1:A:274:GLY:N	1.98	0.59
1:C:4:GLN:H	1:C:4:GLN:NE2	2.01	0.59
1:B:99:GLN:HG3	1:B:126:VAL:HG13	1.85	0.59
1:B:139:ARG:HG2	1:B:139:ARG:NH1	2.17	0.58
1:C:321:HIS:HD2	1:C:323:GLY:H	1.51	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:HG3	1:A:102:TRP:CE2	2.39	0.58
1:C:312:PRO:O	1:C:315:SER:OG	2.21	0.58
1:D:272:ASN:ND2	1:D:275:THR:H	2.02	0.57
1:C:1:MET:HE2	1:C:212:ALA:HB2	1.87	0.57
1:C:272:ASN:ND2	1:C:275:THR:H	2.01	0.57
1:B:99:GLN:HB2	1:B:128:LEU:HD23	1.86	0.56
1:D:161:GLY:O	1:D:162:CYS:HB2	2.06	0.55
1:C:179:VAL:O	1:C:183:GLU:HG3	2.06	0.55
1:D:222:VAL:HG11	1:D:298:SER:HA	1.88	0.55
1:D:31:LYS:HB3	1:D:313:GLU:HG3	1.89	0.55
1:A:321:HIS:HD2	1:A:323:GLY:H	1.55	0.54
1:D:250:ARG:HD3	1:D:251:ASP:O	2.07	0.54
1:A:215:ARG:O	1:A:218:ARG:HB2	2.08	0.54
1:A:163:SER:HA	1:A:201:SER:HB3	1.90	0.54
1:D:99:GLN:HG3	1:D:126:VAL:HG13	1.88	0.54
1:B:179:VAL:O	1:B:183:GLU:HG3	2.08	0.54
1:C:1:MET:HE3	1:C:212:ALA:HB2	1.89	0.53
1:C:213:ASP:OD1	1:C:215:ARG:HG3	2.08	0.53
1:B:321:HIS:CD2	1:B:323:GLY:H	2.24	0.53
1:C:61:GLU:O	1:C:65:GLN:HG3	2.10	0.52
1:D:198:VAL:HG21	1:D:294:TYR:CE1	2.44	0.52
1:B:161:GLY:O	1:B:162:CYS:HB2	2.09	0.52
1:A:63:LEU:O	1:A:65:GLN:O	2.27	0.52
1:C:63:LEU:O	1:C:65:GLN:O	2.27	0.52
1:C:289:LEU:O	1:C:321:HIS:HE1	1.93	0.52
1:C:133:PHE:CE1	1:C:138:ARG:HD3	2.45	0.52
1:C:237:ARG:HH11	1:C:241:GLN:HE22	1.57	0.52
1:A:139:ARG:CG	1:A:142:GLU:H	2.14	0.51
1:A:81:THR:HB	1:A:97:LEU:HD13	1.91	0.51
1:A:99:GLN:HB2	1:A:128:LEU:CD2	2.39	0.51
1:B:63:LEU:O	1:B:65:GLN:O	2.29	0.51
1:B:148:VAL:HG11	1:B:155:PRO:HB3	1.93	0.50
1:C:23:ARG:NH1	1:D:89:ALA:O	2.44	0.50
1:B:291:ASP:HB2	1:B:292:PRO:HD2	1.94	0.50
1:C:2:ASN:HA	1:C:4:GLN:HE22	1.75	0.50
1:D:188:PHE:HB2	1:D:316:ARG:NH1	2.26	0.50
1:D:198:VAL:HG21	1:D:294:TYR:HE1	1.76	0.50
1:D:250:ARG:CD	1:D:251:ASP:O	2.60	0.50
1:B:91:LEU:HD13	1:B:93:MET:CE	2.42	0.49
1:C:325:VAL:HG23	4:C:515:HOH:O	2.10	0.49
1:B:61:GLU:HG2	1:B:65:GLN:NE2	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:HG22	1:B:96:VAL:HB	1.94	0.49
1:D:59:ILE:HD12	1:D:91:LEU:CD1	2.43	0.49
1:C:92:GLY:HA2	1:D:23:ARG:CZ	2.43	0.49
1:C:294:TYR:OH	2:C:503:SO4:O1	2.30	0.48
1:C:228:PRO:HG3	4:C:550:HOH:O	2.13	0.48
1:D:40:ASP:HB3	1:D:323:GLY:HA2	1.94	0.48
1:B:164:ASP:CG	1:B:237:ARG:HH22	2.17	0.48
1:D:91:LEU:HD13	1:D:93:MET:HE2	1.95	0.48
1:B:292:PRO:HD3	1:B:328:LEU:CD1	2.44	0.48
1:D:23:ARG:HG2	1:D:23:ARG:HH11	1.78	0.48
1:D:148:VAL:HG11	1:D:155:PRO:HB3	1.94	0.48
1:C:100:GLU:OE1	1:C:135:ILE:HG12	2.15	0.47
1:A:36:ALA:HA	1:A:319:TYR:O	2.14	0.47
1:C:138:ARG:O	1:C:139:ARG:HB2	2.14	0.47
1:B:23:ARG:NH1	1:B:285:THR:HA	2.30	0.47
1:C:225:SER:O	1:C:226:ALA:HB3	2.14	0.47
1:A:74:GLY:HA2	1:A:102:TRP:CZ3	2.51	0.46
1:B:292:PRO:HD3	1:B:328:LEU:HD13	1.97	0.46
1:D:289:LEU:O	1:D:321:HIS:CE1	2.64	0.46
1:C:175:PHE:O	1:C:179:VAL:HG23	2.14	0.46
1:B:6:PHE:HA	1:B:7:PRO:HD3	1.79	0.46
1:C:272:ASN:ND2	1:C:274:GLY:N	2.61	0.46
1:B:91:LEU:CD1	1:B:93:MET:HE3	2.44	0.46
1:C:91:LEU:HD12	1:C:93:MET:HE2	1.98	0.46
1:A:225:SER:O	1:A:226:ALA:HB3	2.15	0.46
1:B:1:MET:HE2	1:B:248:LEU:HD13	1.97	0.45
1:B:250:ARG:HG2	1:B:251:ASP:N	2.31	0.45
1:C:6:PHE:HA	1:C:7:PRO:HD3	1.86	0.45
1:D:225:SER:O	1:D:226:ALA:HB3	2.16	0.45
1:A:289:LEU:O	1:A:321:HIS:CE1	2.69	0.45
1:C:91:LEU:CD1	1:C:93:MET:HE2	2.46	0.45
1:D:101:ASN:HB2	4:D:552:HOH:O	2.16	0.45
1:A:223:ASP:O	1:A:264:ALA:HB2	2.17	0.44
1:B:1:MET:HB2	1:B:246:VAL:O	2.18	0.44
1:B:2:ASN:HD22	1:B:2:ASN:H	1.65	0.44
1:C:91:LEU:HD12	1:C:93:MET:CE	2.47	0.44
1:C:321:HIS:CD2	1:C:323:GLY:H	2.33	0.44
1:B:1:MET:HE3	1:B:212:ALA:HB2	1.94	0.44
1:C:191:ASP:OD2	1:C:315:SER:HA	2.17	0.44
1:B:242:THR:O	1:B:246:VAL:HG22	2.17	0.44
1:C:36:ALA:HA	1:C:319:TYR:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:PRO:O	1:C:313:GLU:C	2.55	0.44
1:D:325:VAL:O	1:D:328:LEU:HB2	2.18	0.44
1:D:73:ILE:HG13	1:D:98:VAL:O	2.17	0.44
1:A:101:ASN:HD21	1:D:336:ARG:NH2	2.16	0.44
1:A:188:PHE:CE1	1:A:316:ARG:HD3	2.53	0.44
1:A:325:VAL:HG13	1:A:328:LEU:HD12	2.00	0.43
1:C:70:LEU:O	1:C:95:CYS:HA	2.18	0.43
1:C:163:SER:HA	1:C:201:SER:HB3	1.99	0.43
1:A:62:ALA:HA	1:A:156:TYR:CD1	2.53	0.43
1:A:112:ARG:HD3	4:C:539:HOH:O	2.17	0.43
1:B:2:ASN:O	1:B:2:ASN:ND2	2.51	0.43
1:D:63:LEU:O	1:D:65:GLN:O	2.36	0.43
1:C:139:ARG:HD3	1:C:139:ARG:HA	1.73	0.43
1:A:321:HIS:CD2	1:A:323:GLY:H	2.35	0.43
1:C:37:LYS:HD3	1:C:175:PHE:CE2	2.53	0.43
1:B:144:ALA:O	1:B:148:VAL:HG23	2.19	0.43
1:B:295:GLU:OE2	3:B:401:PLP:N1	2.52	0.43
1:B:193:VAL:HA	1:B:318:LEU:O	2.19	0.43
1:D:81:THR:HB	1:D:97:LEU:HD13	2.00	0.43
1:A:109:VAL:O	1:A:113:VAL:HG22	2.19	0.42
1:B:82:ARG:HA	1:B:119:SER:OG	2.19	0.42
1:B:325:VAL:O	1:B:328:LEU:HB2	2.19	0.42
1:C:133:PHE:CE2	1:C:138:ARG:NH1	2.87	0.42
1:D:183:GLU:HB3	1:D:188:PHE:O	2.19	0.42
1:C:180:ARG:HD3	1:C:213:ASP:OD2	2.19	0.42
1:D:99:GLN:HB2	1:D:128:LEU:CD2	2.46	0.42
1:D:250:ARG:HH11	1:D:250:ARG:HG3	1.83	0.42
1:A:196:CYS:HB2	1:A:298:SER:HB3	2.01	0.42
1:A:39:GLU:HB2	1:A:321:HIS:O	2.19	0.42
1:A:64:ALA:C	1:A:65:GLN:O	2.58	0.42
1:A:272:ASN:ND2	1:A:275:THR:H	2.17	0.42
1:D:248:LEU:HG	1:D:250:ARG:H	1.84	0.42
1:B:228:PRO:HB3	1:B:261:GLU:HG2	2.00	0.42
1:B:80:GLN:HB3	2:B:502:SO4:O3	2.20	0.41
1:D:46:ALA:O	1:D:47:PHE:HB2	2.18	0.41
1:B:336:ARG:HH11	1:B:336:ARG:HG2	1.85	0.41
1:A:226:ALA:C	1:A:228:PRO:HD3	2.41	0.41
1:A:250:ARG:HG3	1:A:250:ARG:NH1	2.34	0.41
1:C:133:PHE:CD2	1:C:138:ARG:NH1	2.89	0.41
1:D:292:PRO:HD3	1:D:328:LEU:CD1	2.50	0.41
1:D:59:ILE:HD12	1:D:91:LEU:HD11	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:ND2	1:B:275:THR:H	2.19	0.41
1:C:31:LYS:HB3	1:C:313:GLU:HG3	2.03	0.41
1:D:100:GLU:HG3	1:D:129:VAL:CG2	2.51	0.41
1:D:177:GLU:HA	1:D:180:ARG:NH1	2.36	0.41
1:D:75:GLY:HA2	1:D:100:GLU:O	2.21	0.41
1:C:292:PRO:HD3	1:C:328:LEU:HD23	2.03	0.40
1:C:237:ARG:NH1	1:C:241:GLN:HE22	2.20	0.40
1:A:188:PHE:CD1	1:A:188:PHE:C	2.95	0.40

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	327/338 (97%)	314 (96%)	13 (4%)	0	100	100
1	B	325/338 (96%)	316 (97%)	9 (3%)	0	100	100
1	C	336/338 (99%)	322 (96%)	13 (4%)	1 (0%)	41	37
1	D	325/338 (96%)	315 (97%)	9 (3%)	1 (0%)	41	37
All	All	1313/1352 (97%)	1267 (96%)	44 (3%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	212	ALA
1	D	4	GLN

### 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	258/264 (98%)	249 (96%)	9 (4%)	36	35
1	B	256/264 (97%)	250 (98%)	6 (2%)	50	53
1	C	263/264 (100%)	259 (98%)	4 (2%)	65	69
1	D	256/264 (97%)	251 (98%)	5 (2%)	55	58
All	All	1033/1056 (98%)	1009 (98%)	24 (2%)	50	53

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	23	ARG
1	A	99	GLN
1	A	100	GLU
1	A	131	ASP
1	A	142	GLU
1	A	146	GLU
1	A	272	ASN
1	A	304	GLU
1	B	2	ASN
1	B	99	GLN
1	B	272	ASN
1	B	281	LEU
1	B	304	GLU
1	B	328	LEU
1	C	4	GLN
1	C	128	LEU
1	C	177	GLU
1	C	272	ASN
1	D	99	GLN
1	D	112	ARG
1	D	241	GLN
1	D	272	ASN
1	D	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	4	GLN
1	A	77	GLN
1	A	99	GLN
1	A	101	ASN
1	A	241	GLN
1	A	272	ASN
1	A	308	ASN
1	A	321	HIS
1	B	2	ASN
1	B	65	GLN
1	B	77	GLN
1	B	99	GLN
1	B	272	ASN
1	B	321	HIS
1	C	2	ASN
1	C	4	GLN
1	C	77	GLN
1	C	230	GLN
1	C	241	GLN
1	C	272	ASN
1	C	308	ASN
1	C	321	HIS
1	D	2	ASN
1	D	77	GLN
1	D	99	GLN
1	D	230	GLN
1	D	241	GLN
1	D	272	ASN
1	D	308	ASN
1	D	321	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

8 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	PLP	C	401	1	15,15,16	1.62	4 (26%)	20,22,23	1.00	0
3	PLP	D	401	1	15,15,16	1.57	4 (26%)	20,22,23	0.85	0
3	PLP	A	401	1	15,15,16	1.94	3 (20%)	20,22,23	0.89	0
3	PLP	B	401	1	15,15,16	1.90	4 (26%)	20,22,23	1.03	1 (5%)
2	SO4	A	501	-	4,4,4	0.30	0	6,6,6	0.26	0
2	SO4	C	503	-	4,4,4	0.34	0	6,6,6	0.31	0
2	SO4	D	504	-	4,4,4	0.29	0	6,6,6	0.27	0
2	SO4	B	502	-	4,4,4	0.32	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
3	PLP	B	401	1	-	0/6/6/8	0/1/1/1
3	PLP	D	401	1	-	0/6/6/8	0/1/1/1
3	PLP	A	401	1	-	0/6/6/8	0/1/1/1
3	PLP	C	401	1	-	0/6/6/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PLP	C5-C4	5.14	1.46	1.40
3	B	401	PLP	C5-C4	4.07	1.45	1.40
3	B	401	PLP	C3-C2	3.71	1.44	1.40
3	C	401	PLP	C5-C4	3.39	1.44	1.40
3	B	401	PLP	C2A-C2	3.28	1.55	1.50
3	C	401	PLP	C2A-C2	3.10	1.55	1.50
3	D	401	PLP	C2A-C2	2.87	1.55	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	PLP	C3-C2	2.70	1.43	1.40
3	D	401	PLP	C5-C4	2.66	1.43	1.40
3	A	401	PLP	C6-C5	2.59	1.43	1.37
3	A	401	PLP	C2A-C2	2.44	1.54	1.50
3	C	401	PLP	C3-C2	2.28	1.43	1.40
3	D	401	PLP	C6-C5	2.23	1.42	1.37
3	B	401	PLP	C4A-C4	2.21	1.56	1.51
3	C	401	PLP	C6-C5	2.16	1.42	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	PLP	C6-N1-C2	2.01	122.88	119.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	PLP	1	0
2	C	503	SO4	1	0
2	B	502	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, 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	331/338 (97%)	0.11	5 (1%) 73 72	19, 33, 49, 70	0
1	B	329/338 (97%)	0.18	18 (5%) 25 24	21, 33, 55, 69	0
1	C	338/338 (100%)	0.28	15 (4%) 34 33	20, 36, 53, 63	0
1	D	329/338 (97%)	0.23	13 (3%) 38 37	22, 37, 57, 74	0
All	All	1327/1352 (98%)	0.20	51 (3%) 40 39	19, 34, 55, 74	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	150	ALA	4.4
1	A	129	VAL	4.0
1	A	130	PRO	3.7
1	D	150	ALA	3.2
1	B	140	SER	3.1
1	C	47	PHE	3.0
1	C	192	TYR	2.9
1	B	151	ALA	2.9
1	C	137	PHE	2.9
1	B	146	GLU	2.9
1	D	184	ALA	2.8
1	A	254	ARG	2.8
1	C	322	LEU	2.8
1	C	64	ALA	2.7
1	A	131	ASP	2.7
1	C	136	GLY	2.7
1	D	139	ARG	2.7
1	C	46	ALA	2.6
1	B	152	GLY	2.6
1	D	47	PHE	2.6
1	B	322	LEU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	147	SER	2.5
1	D	151	ALA	2.5
1	B	139	ARG	2.5
1	C	187	GLY	2.4
1	D	144	ALA	2.4
1	C	309	GLY	2.4
1	B	326	PRO	2.3
1	B	254	ARG	2.3
1	B	142	GLU	2.3
1	B	148	VAL	2.3
1	B	184	ALA	2.2
1	D	325	VAL	2.2
1	B	249	GLU	2.2
1	C	186	LEU	2.2
1	C	326	PRO	2.2
1	D	146	GLU	2.2
1	D	102	TRP	2.2
1	B	47	PHE	2.2
1	C	151	ALA	2.2
1	C	3	LEU	2.1
1	D	187	GLY	2.1
1	B	129	VAL	2.1
1	B	144	ALA	2.1
1	A	151	ALA	2.0
1	B	141	TRP	2.0
1	D	141	TRP	2.0
1	D	143	ASP	2.0
1	C	249	GLU	2.0
1	B	253	MET	2.0
1	C	31	LYS	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 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(Å <sup>2</sup> )	Q<0.9
2	SO4	C	503	5/5	0.86	0.20	59,60,63,64	0
2	SO4	B	502	5/5	0.88	0.17	75,75,76,76	0
2	SO4	D	504	5/5	0.89	0.15	65,66,67,67	0
2	SO4	A	501	5/5	0.92	0.15	68,68,69,70	0
3	PLP	A	401	15/16	0.97	0.16	24,26,28,30	0
3	PLP	B	401	15/16	0.97	0.13	23,26,28,28	0
3	PLP	C	401	15/16	0.97	0.15	22,27,29,29	0
3	PLP	D	401	15/16	0.98	0.12	26,29,31,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.