



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:17 AM UTC

PDB ID : 5UID / pdb\_00005uid  
Title : The crystal structure of an aminotransferase TlmJ from *Streptoalloteichus hindustanus*  
Authors : Tan, K.; Bigelow, L.; Bearden, J.; Phillips Jr., G.N.; Joachmiak, A.; Midwest Center for Structural Genomics (MCSG); Enzyme Discovery for Natural Product Biosynthesis (NatPro)  
Deposited on : 2017-01-13  
Resolution : 2.18 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

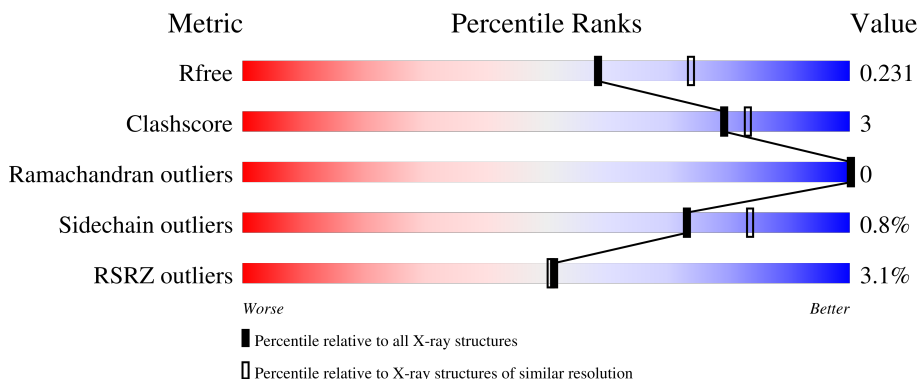
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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))
$R_{free}$	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	402	 2% 84% 7% 9%
1	B	402	 3% 86% 5% 9%
1	C	402	 3% 83% 7% 9%
1	D	402	 3% 84% 6% 9%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11670 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 Aminotransferase TlmJ.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S	Se			
1	A	367	2781	1752	491	521	1	9	7	0	1	0
1	B	367	2775	1746	490	522	1	9	7	0	0	0
1	C	367	2786	1752	495	522	1	9	7	0	0	0
1	D	366	2783	1753	490	523	1	9	7	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A4KUD2
A	-1	ASN	-	expression tag	UNP A4KUD2
A	0	ALA	-	expression tag	UNP A4KUD2
B	-2	SER	-	expression tag	UNP A4KUD2
B	-1	ASN	-	expression tag	UNP A4KUD2
B	0	ALA	-	expression tag	UNP A4KUD2
C	-2	SER	-	expression tag	UNP A4KUD2
C	-1	ASN	-	expression tag	UNP A4KUD2
C	0	ALA	-	expression tag	UNP A4KUD2
D	-2	SER	-	expression tag	UNP A4KUD2
D	-1	ASN	-	expression tag	UNP A4KUD2
D	0	ALA	-	expression tag	UNP A4KUD2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



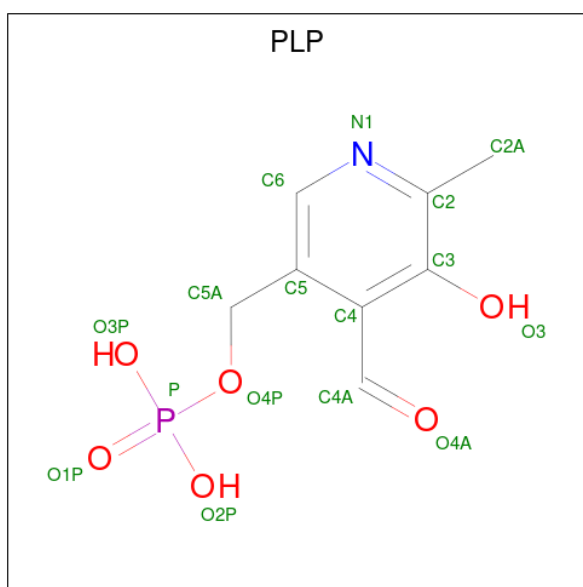
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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

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

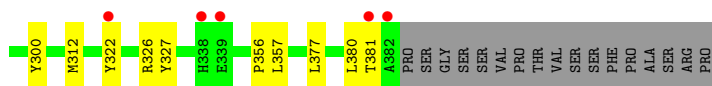


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	1	3		
3	D	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		
4	B	142	Total	O	0	0
			142	142		
4	C	128	Total	O	0	0
			128	128		
4	D	14	Total	O	0	0
			14	14		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.60Å 198.09Å 60.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 2.18 34.90 – 2.18	Depositor EDS
% Data completeness (in resolution range)	94.3 (34.90-2.18) 94.4 (34.90-2.18)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 2.18Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.190 , 0.233 0.190 , 0.231	Depositor DCC
$R_{free}$ test set	4194 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3375e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, LLP

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	0.11	0/2807	0.30	0/3803
1	B	0.11	0/2800	0.31	0/3793
1	C	0.11	0/2812	0.31	0/3808
1	D	0.12	0/2810	0.30	0/3809
All	All	0.11	0/11229	0.30	0/15213

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	2781	0	2715	18	0
1	B	2775	0	2716	11	0
1	C	2786	0	2732	18	0
1	D	2783	0	2724	14	0
2	A	25	0	0	0	0
2	B	45	0	0	1	0
2	C	40	0	0	0	0
2	D	15	0	0	0	0
3	A	12	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	12	0	8	0	0
4	A	112	0	0	2	0
4	B	142	0	0	0	0
4	C	128	0	0	0	0
4	D	14	0	0	0	0
All	All	11670	0	10903	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (60) 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:D:300:TYR:HB2	1:D:357:LEU:HD22	1.84	0.58
1:A:207:LYS:HE3	1:A:214:ALA:HB2	1.85	0.56
1:D:143:GLU:OE1	1:D:146:ARG:NH1	2.39	0.56
1:A:9:PRO:HB3	1:A:187:VAL:HG21	1.90	0.54
1:A:229:ARG:N	4:A:502:HOH:O	2.40	0.53
1:D:159:ALA:HB1	1:D:162:SER:HB2	1.91	0.53
1:D:312:MSE:HE2	1:D:380:LEU:HD12	1.90	0.53
1:C:265:ARG:NH1	1:C:268:GLU:OE2	2.36	0.52
1:A:6:VAL:HA	1:A:356:PRO:HA	1.91	0.52
1:B:300:TYR:HB2	1:B:357:LEU:HD22	1.91	0.52
1:A:159:ALA:HB1	1:A:162:SER:HB2	1.93	0.51
1:D:52:VAL:HG13	1:D:193:MSE:SE	2.61	0.51
1:C:9:PRO:HB3	1:C:187:VAL:HG21	1.92	0.51
1:C:13:GLU:OE2	1:D:20:ARG:NH2	2.40	0.51
1:B:6:VAL:HG23	1:B:322:TYR:HD2	1.75	0.51
1:B:9:PRO:HB3	1:B:187:VAL:HG21	1.92	0.51
1:D:4:ILE:O	1:D:322[B]:TYR:HB2	2.12	0.50
1:A:21:GLU:OE2	1:A:33:ARG:NH2	2.45	0.50
1:C:159:ALA:HB1	1:C:162:SER:HB2	1.94	0.49
1:A:6:VAL:HG23	1:A:322[A]:TYR:HD2	1.77	0.49
1:D:213:MSE:HE3	1:D:233:PHE:CG	2.48	0.49
1:B:159:ALA:HB1	1:B:162:SER:HB2	1.94	0.49
1:C:58:CYS:HB2	1:C:179:SER:HB2	1.95	0.49
1:A:312:MSE:CE	1:A:373:VAL:HA	2.43	0.48
1:B:6:VAL:HA	1:B:356:PRO:HA	1.96	0.47
1:A:300:TYR:HB2	1:A:357:LEU:HD22	1.95	0.47
1:C:312:MSE:HE2	1:C:380:LEU:HD12	1.97	0.47
1:A:265:ARG:NH1	1:A:268:GLU:OE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:VAL:HG13	1:C:193:MSE:SE	2.66	0.46
1:C:300:TYR:HB2	1:C:357:LEU:HD22	1.98	0.46
3:A:406:PLP:H5A2	1:B:190:ASP:H	1.82	0.45
1:D:79:LEU:O	1:D:100:PHE:HA	2.16	0.45
1:B:79:LEU:O	1:B:100:PHE:HA	2.16	0.45
1:A:283:LEU:HD11	1:A:302:VAL:HB	1.99	0.45
1:C:283:LEU:HB2	1:C:377:LEU:HD21	1.99	0.45
1:D:6:VAL:HA	1:D:356:PRO:HA	1.99	0.45
1:D:326:ARG:HA	1:D:327:TYR:HA	1.73	0.45
1:A:33:ARG:NH1	4:A:503:HOH:O	2.41	0.44
1:C:33:ARG:HB2	1:C:246:ASP:CG	2.42	0.44
1:D:6:VAL:HG23	1:D:322[A]:TYR:HD2	1.82	0.44
1:D:9:PRO:HB3	1:D:187:VAL:HG21	1.98	0.44
1:C:6:VAL:HG23	1:C:322:TYR:HB3	1.99	0.44
1:C:312:MSE:HE1	1:C:376:GLY:C	2.43	0.44
1:C:79:LEU:O	1:C:100:PHE:HA	2.17	0.44
1:C:181:ASP:OD2	1:C:184:LLP:HE3	2.18	0.44
1:A:4:ILE:O	1:A:322[B]:TYR:HB2	2.18	0.43
1:A:52:VAL:HG12	1:A:193:MSE:SE	2.68	0.43
1:C:108:LEU:HD22	1:C:131:TYR:CZ	2.54	0.43
1:A:274:ASP:O	1:A:278:SER:OG	2.27	0.42
1:C:6:VAL:HA	1:C:356:PRO:HA	2.00	0.42
1:B:97:ARG:NH1	2:B:407:SO4:O1	2.53	0.42
1:D:377:LEU:HD12	1:D:377:LEU:HA	1.87	0.41
1:A:40:ASP:HB3	1:A:256:LEU:HD23	2.03	0.41
1:B:261:GLU:HG3	1:B:264:ARG:HH2	1.86	0.41
1:A:181:ASP:OD1	1:A:184:LLP:HG3	2.19	0.41
1:B:33:ARG:HB2	1:B:246:ASP:CG	2.46	0.41
1:B:52:VAL:O	1:B:206:ARG:NH2	2.54	0.41
1:C:274:ASP:OD1	1:C:300:TYR:OH	2.38	0.40
1:C:326:ARG:HA	1:C:327:TYR:HA	1.73	0.40
1:A:173:GLY:O	1:A:197:ARG:HD3	2.22	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	363/402 (90%)	356 (98%)	7 (2%)	0	100	100
1	B	362/402 (90%)	355 (98%)	7 (2%)	0	100	100
1	C	362/402 (90%)	353 (98%)	9 (2%)	0	100	100
1	D	362/402 (90%)	355 (98%)	7 (2%)	0	100	100
All	All	1449/1608 (90%)	1419 (98%)	30 (2%)	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	280/301 (93%)	279 (100%)	1 (0%)	84	91
1	B	281/301 (93%)	281 (100%)	0	100	100
1	C	283/301 (94%)	278 (98%)	5 (2%)	51	65
1	D	282/301 (94%)	279 (99%)	3 (1%)	65	77
All	All	1126/1204 (94%)	1117 (99%)	9 (1%)	73	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ARG
1	C	52	VAL
1	C	177	VAL
1	C	183	MSE
1	C	322	TYR
1	C	377	LEU
1	D	52	VAL
1	D	177	VAL

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Mol	Chain	Res	Type
1	D	381	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	5	ASN
1	C	275	GLN
1	D	293	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](#)

4 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	LLP	D	184	1	23,24,25	2.55	6 (26%)	25,32,34	1.18	3 (12%)
1	LLP	B	184	1	23,24,25	2.53	6 (26%)	25,32,34	1.18	3 (12%)
1	LLP	A	184	1	23,24,25	2.54	6 (26%)	25,32,34	1.23	3 (12%)
1	LLP	C	184	1	23,24,25	2.53	6 (26%)	25,32,34	1.22	4 (16%)

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	LLP	D	184	1	-	5/16/17/19	0/1/1/1
1	LLP	B	184	1	-	4/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	184	1	-	8/16/17/19	0/1/1/1
1	LLP	C	184	1	-	6/16/17/19	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	184	LLP	C4-C4'	7.38	1.62	1.46
1	B	184	LLP	C4-C4'	7.38	1.62	1.46
1	A	184	LLP	C4-C4'	7.27	1.62	1.46
1	C	184	LLP	C4-C4'	7.26	1.62	1.46
1	B	184	LLP	C4'-NZ	5.19	1.44	1.27
1	D	184	LLP	C4'-NZ	5.17	1.44	1.27
1	C	184	LLP	C4'-NZ	5.11	1.44	1.27
1	A	184	LLP	C4'-NZ	5.08	1.44	1.27
1	A	184	LLP	C4-C5	-3.87	1.36	1.42
1	C	184	LLP	C2'-C2	3.86	1.56	1.50
1	D	184	LLP	C4-C5	-3.85	1.36	1.42
1	B	184	LLP	C2'-C2	3.79	1.56	1.50
1	A	184	LLP	C2'-C2	3.76	1.56	1.50
1	B	184	LLP	C4-C5	-3.72	1.36	1.42
1	D	184	LLP	C2'-C2	3.70	1.56	1.50
1	C	184	LLP	C4-C5	-3.69	1.36	1.42
1	A	184	LLP	C6-N1	3.09	1.40	1.34
1	D	184	LLP	C6-N1	3.03	1.40	1.34
1	C	184	LLP	C6-N1	2.98	1.40	1.34
1	B	184	LLP	C6-N1	2.94	1.40	1.34
1	C	184	LLP	C5'-C5	2.21	1.56	1.50
1	D	184	LLP	C5'-C5	2.09	1.56	1.50
1	A	184	LLP	C4-C3	-2.02	1.37	1.41
1	B	184	LLP	C5'-C5	2.01	1.56	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	LLP	C4-C4'-NZ	-3.01	110.17	124.04
1	C	184	LLP	C4-C4'-NZ	-2.97	110.35	124.04
1	D	184	LLP	C4-C4'-NZ	-2.94	110.46	124.04
1	B	184	LLP	C4-C4'-NZ	-2.85	110.89	124.04
1	A	184	LLP	CE-NZ-C4'	-2.83	109.66	118.72
1	D	184	LLP	CE-NZ-C4'	-2.54	110.57	118.72
1	B	184	LLP	C5-C6-N1	-2.52	119.74	123.83
1	A	184	LLP	C5-C6-N1	-2.48	119.79	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	LLP	CE-NZ-C4'	-2.48	110.77	118.72
1	B	184	LLP	CE-NZ-C4'	-2.45	110.86	118.72
1	C	184	LLP	C5-C6-N1	-2.45	119.85	123.83
1	D	184	LLP	C5-C6-N1	-2.31	120.07	123.83
1	C	184	LLP	C3-C4-C5	2.03	119.91	118.28

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	184	LLP	C4-C4'-NZ-CE
1	A	184	LLP	C5'-OP4-P-OP1
1	A	184	LLP	C5'-OP4-P-OP2
1	A	184	LLP	C5'-OP4-P-OP3
1	B	184	LLP	C4-C4'-NZ-CE
1	C	184	LLP	C4-C4'-NZ-CE
1	D	184	LLP	C4-C4'-NZ-CE
1	C	184	LLP	CG-CD-CE-NZ
1	C	184	LLP	C4-C5-C5'-OP4
1	B	184	LLP	CG-CD-CE-NZ
1	D	184	LLP	CG-CD-CE-NZ
1	B	184	LLP	CD-CE-NZ-C4'
1	C	184	LLP	CD-CE-NZ-C4'
1	D	184	LLP	CD-CE-NZ-C4'
1	A	184	LLP	CA-CB-CG-CD
1	A	184	LLP	CD-CE-NZ-C4'
1	A	184	LLP	C3-C4-C4'-NZ
1	B	184	LLP	C3-C4-C4'-NZ
1	C	184	LLP	C3-C4-C4'-NZ
1	D	184	LLP	C3-C4-C4'-NZ
1	A	184	LLP	C6-C5-C5'-OP4
1	C	184	LLP	C6-C5-C5'-OP4
1	D	184	LLP	C5'-OP4-P-OP3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	184	LLP	1	0
1	C	184	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

27 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	SO4	A	404	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	403	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	406	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	402	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	404	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	D	401	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	404	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	408	-	4,4,4	0.24	0	6,6,6	0.07	0
3	PLP	D	404	-	12,12,16	1.29	1 (8%)	15,16,23	1.28	1 (6%)
2	SO4	C	405	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	407	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	408	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	405	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	406	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	A	402	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	403	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	C	407	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	401	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	405	-	4,4,4	0.23	0	6,6,6	0.07	0
3	PLP	A	406	-	12,12,16	1.26	1 (8%)	15,16,23	1.20	1 (6%)
2	SO4	B	409	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	D	403	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	C	401	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	D	402	-	4,4,4	0.23	0	6,6,6	0.09	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	A	406	-	-	3/4/4/8	0/1/1/1
3	PLP	D	404	-	-	3/4/4/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	PLP	C2-N1	2.44	1.38	1.33
3	A	406	PLP	C2-N1	2.37	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	404	PLP	C3-C4-C4A	-3.13	115.53	119.84
3	A	406	PLP	C3-C4-C4A	-2.98	115.75	119.84

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	406	PLP	C3-C4-C4A-O4A
3	D	404	PLP	C3-C4-C4A-O4A
3	D	404	PLP	C4-C5-C5A-O4P
3	A	406	PLP	C4-C5-C5A-O4P
3	D	404	PLP	C6-C5-C5A-O4P
3	A	406	PLP	C6-C5-C5A-O4P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	407	SO4	1	0
3	A	406	PLP	1	0

## 5.7 Other polymers [i](#)

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	359/402 (89%)	-0.02	9 (2%) 58 57	18, 33, 58, 76	1 (0%)
1	B	359/402 (89%)	-0.10	12 (3%) 49 48	21, 30, 54, 82	0
1	C	359/402 (89%)	-0.04	12 (3%) 49 48	22, 31, 54, 91	0
1	D	358/402 (89%)	0.03	11 (3%) 51 51	17, 33, 58, 82	1 (0%)
All	All	1435/1608 (89%)	-0.03	44 (3%) 51 51	17, 32, 56, 91	2 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	ARG	5.9
1	D	382	ALA	4.6
1	A	381	THR	4.5
1	C	2	GLY	4.5
1	D	338	HIS	4.1
1	A	215	GLN	4.0
1	B	279	THR	4.0
1	B	338	HIS	3.9
1	D	229	ARG	3.9
1	B	2	GLY	3.8
1	A	229	ARG	3.7
1	C	322	TYR	3.6
1	C	279	THR	3.6
1	B	377	LEU	3.2
1	B	215	GLN	3.1
1	C	230	TRP	3.1
1	A	279	THR	3.1
1	D	339	GLU	3.1
1	D	230	TRP	3.0
1	C	215	GLN	2.9
1	B	322	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	279	THR	2.8
1	A	230	TRP	2.7
1	B	214	ALA	2.6
1	A	338	HIS	2.6
1	C	338	HIS	2.6
1	C	231	TRP	2.6
1	B	381	THR	2.6
1	D	322[A]	TYR	2.5
1	C	341	SER	2.5
1	C	229	ARG	2.4
1	A	281	ASP	2.4
1	C	381	THR	2.4
1	D	214	ALA	2.3
1	D	234	GLU	2.3
1	C	200	GLU	2.2
1	A	278	SER	2.2
1	A	2	GLY	2.2
1	B	230	TRP	2.2
1	D	231	TRP	2.2
1	D	381	THR	2.2
1	B	167	ARG	2.1
1	C	52	VAL	2.1
1	B	339	GLU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	D	184	24/25	0.96	0.07	24,28,33,36	0
1	LLP	B	184	24/25	0.97	0.07	17,24,29,35	0
1	LLP	A	184	24/25	0.97	0.06	20,27,32,35	0
1	LLP	C	184	24/25	0.98	0.06	20,27,35,41	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	B	407	5/5	0.65	0.17	109,109,112,113	5
2	SO4	B	406	5/5	0.66	0.23	110,110,110,112	5
2	SO4	D	402	5/5	0.67	0.18	96,97,97,100	5
2	SO4	C	405	5/5	0.69	0.15	91,94,96,96	0
2	SO4	A	405	5/5	0.70	0.20	77,78,84,86	5
2	SO4	B	402	5/5	0.72	0.16	87,91,91,92	0
2	SO4	C	407	5/5	0.74	0.16	83,86,87,91	5
2	SO4	A	404	5/5	0.77	0.15	113,114,114,116	0
2	SO4	A	402	5/5	0.80	0.15	90,92,94,95	5
2	SO4	D	403	5/5	0.80	0.14	91,93,96,98	0
2	SO4	A	401	5/5	0.83	0.13	72,73,75,79	0
2	SO4	B	408	5/5	0.83	0.14	84,89,91,92	5
2	SO4	B	404	5/5	0.84	0.10	80,80,81,84	0
2	SO4	A	403	5/5	0.84	0.14	50,59,63,73	5
2	SO4	B	409	5/5	0.85	0.16	74,78,80,81	5
3	PLP	A	406	12/16	0.85	0.20	60,63,66,71	0
2	SO4	C	408	5/5	0.86	0.22	104,105,105,106	5
2	SO4	C	403	5/5	0.86	0.12	72,76,78,81	0
2	SO4	D	401	5/5	0.87	0.11	84,84,84,85	0
2	SO4	C	406	5/5	0.87	0.19	101,103,104,105	5
3	PLP	D	404	12/16	0.87	0.19	60,70,77,80	0
2	SO4	B	405	5/5	0.88	0.17	85,86,89,89	0
2	SO4	C	401	5/5	0.89	0.11	77,77,79,81	0
2	SO4	C	402	5/5	0.89	0.09	71,72,79,82	0
2	SO4	C	404	5/5	0.90	0.12	95,95,96,99	0
2	SO4	B	403	5/5	0.91	0.10	74,78,81,82	0
2	SO4	B	401	5/5	0.95	0.11	53,62,66,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.