



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 07:06 AM EDT

PDB ID : 5UID
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.

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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	:	2.37.1
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)	:	2.37.1

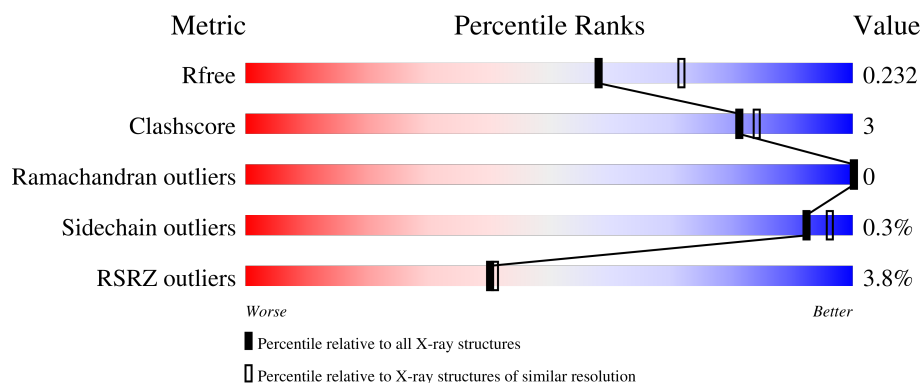
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


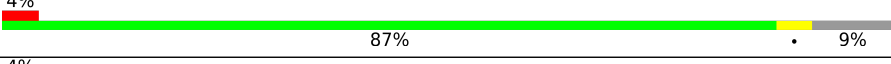


The reported resolution of this entry is 2.18 Å.

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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (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 ≥ 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	
1	B	402	
1	C	402	
1	D	402	

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
2	SO4	B	407	-	-	-	X

2 Entry composition

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

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 (three-letter code: SO4) (formula: O₄S).



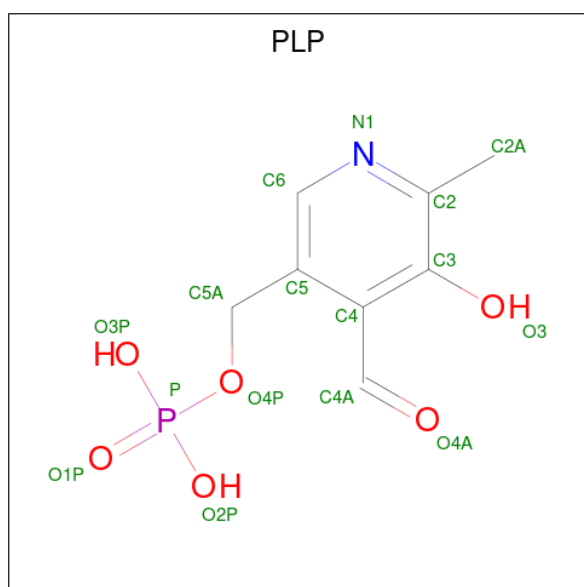
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O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

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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $\text{C}_8\text{H}_{10}\text{NO}_6\text{P}$).



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		

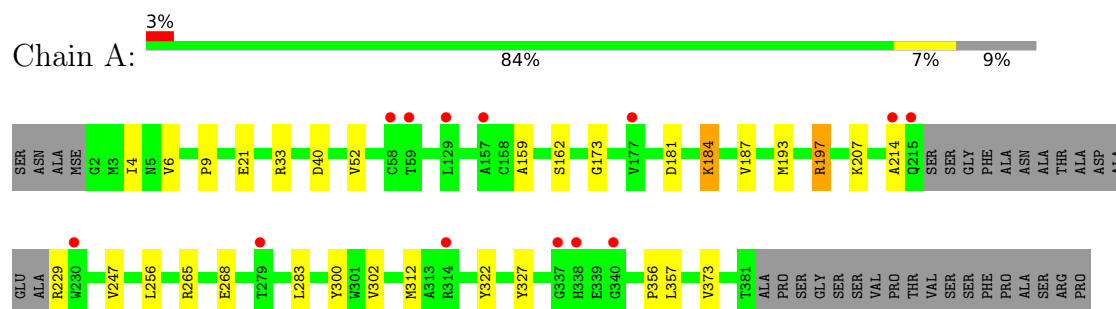
- Molecule 4 is water.

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		

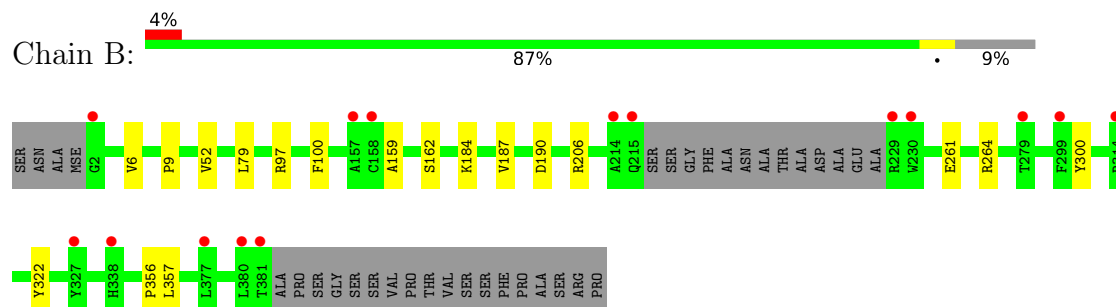
3 Residue-property plots [i](#)

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.

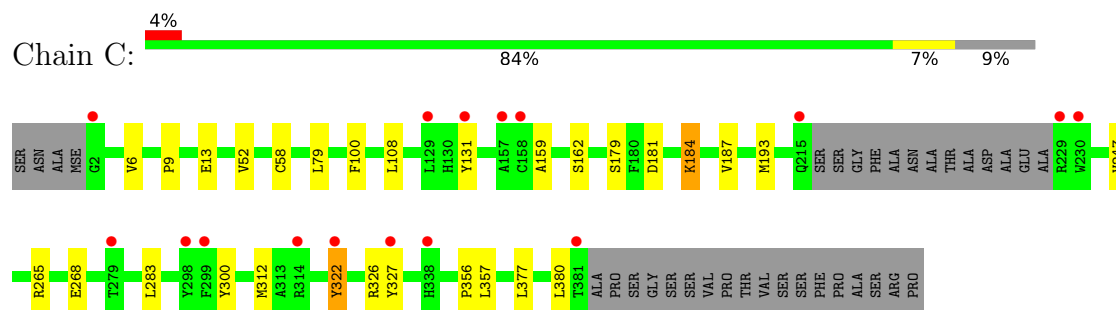
• Molecule 1: Aminotransferase TlmJ



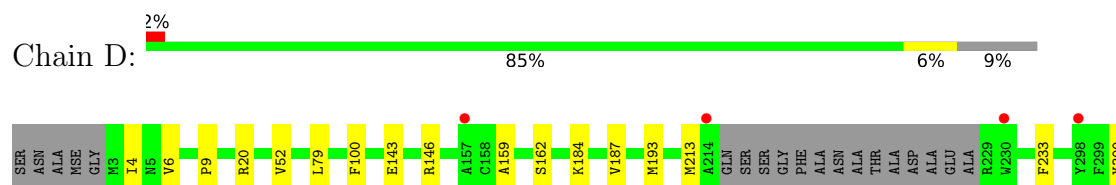
• Molecule 1: Aminotransferase TlmJ

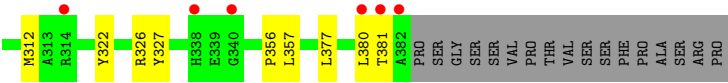


• Molecule 1: Aminotransferase TlmJ



• Molecule 1: Aminotransferase TlmJ





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.18Å)	Xtrriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.190 , 0.233 0.190 , 0.232	Depositor DCC
R_{free} test set	4189 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, LLP, 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	0.25	0/2807	0.43	0/3803
1	B	0.25	0/2800	0.43	0/3793
1	C	0.24	0/2812	0.42	0/3808
1	D	0.25	0/2810	0.43	0/3809
All	All	0.25	0/11229	0.43	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	2714	19	0
1	B	2775	0	2715	10	0
1	C	2786	0	2731	16	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	12	0	8	1	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	10900	58	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 (58) 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:247:VAL:HG12	3:A:406:PLP:H2A3	1.87	0.55
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:247:VAL:HG12	3:D:404:PLP:H2A3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:184:LLP:O3	1:A:327:TYR:OH	2.33	0.43
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:HH22	1.86	0.41
1:A:181:ASP:OD1	1:A:184:LLP:HG3	2.19	0.41
1:B:52:VAL:O	1:B:206:ARG:NH2	2.54	0.41
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 ⓘ

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%)	91	95
1	B	281/301 (93%)	281 (100%)	0	100	100
1	C	283/301 (94%)	282 (100%)	1 (0%)	91	95
1	D	282/301 (94%)	281 (100%)	1 (0%)	91	95
All	All	1126/1204 (94%)	1123 (100%)	3 (0%)	92	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ARG
1	C	322	TYR
1	D	381	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	293	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	B	184	1	23,24,25	2.65	5 (21%)	25,32,34	1.19	3 (12%)
1	LLP	C	184	1	23,24,25	2.64	6 (26%)	25,32,34	1.23	4 (16%)
1	LLP	A	184	1	23,24,25	2.66	7 (30%)	25,32,34	1.25	3 (12%)
1	LLP	D	184	1	23,24,25	2.67	7 (30%)	25,32,34	1.19	3 (12%)

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	B	184	1	-	4/16/17/19	0/1/1/1
1	LLP	C	184	1	-	6/16/17/19	0/1/1/1
1	LLP	A	184	1	-	8/16/17/19	0/1/1/1
1	LLP	D	184	1	-	5/16/17/19	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	184	LLP	C4-C4'	8.27	1.62	1.46
1	B	184	LLP	C4-C4'	8.27	1.62	1.46
1	A	184	LLP	C4-C4'	8.15	1.62	1.46
1	C	184	LLP	C4-C4'	8.14	1.62	1.46
1	B	184	LLP	C4'-NZ	5.14	1.44	1.27
1	D	184	LLP	C4'-NZ	5.13	1.44	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	184	LLP	C4'-NZ	5.07	1.44	1.27
1	A	184	LLP	C4'-NZ	5.03	1.44	1.27
1	A	184	LLP	C4-C5	-4.28	1.36	1.42
1	D	184	LLP	C4-C5	-4.25	1.36	1.42
1	B	184	LLP	C4-C5	-4.11	1.36	1.42
1	C	184	LLP	C4-C5	-4.08	1.36	1.42
1	C	184	LLP	C2'-C2	3.61	1.56	1.50
1	B	184	LLP	C2'-C2	3.54	1.56	1.50
1	A	184	LLP	C2'-C2	3.52	1.56	1.50
1	D	184	LLP	C2'-C2	3.46	1.56	1.50
1	A	184	LLP	C6-N1	2.98	1.40	1.34
1	D	184	LLP	C6-N1	2.93	1.40	1.34
1	C	184	LLP	C6-N1	2.87	1.40	1.34
1	B	184	LLP	C6-N1	2.84	1.40	1.34
1	C	184	LLP	C5'-C5	2.12	1.56	1.50
1	A	184	LLP	C3-C2	2.08	1.43	1.40
1	D	184	LLP	C3-C2	2.08	1.43	1.40
1	A	184	LLP	C4-C3	-2.02	1.37	1.40
1	D	184	LLP	C5'-C5	2.00	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	-3.08	110.17	124.31
1	C	184	LLP	C4-C4'-NZ	-3.04	110.35	124.31
1	D	184	LLP	C4-C4'-NZ	-3.02	110.46	124.31
1	A	184	LLP	CE-NZ-C4'	-3.01	109.66	118.90
1	B	184	LLP	C4-C4'-NZ	-2.92	110.89	124.31
1	D	184	LLP	CE-NZ-C4'	-2.71	110.57	118.90
1	C	184	LLP	CE-NZ-C4'	-2.65	110.77	118.90
1	B	184	LLP	CE-NZ-C4'	-2.62	110.86	118.90
1	B	184	LLP	C5-C6-N1	-2.45	119.74	123.82
1	A	184	LLP	C5-C6-N1	-2.42	119.79	123.82
1	C	184	LLP	C5-C6-N1	-2.38	119.85	123.82
1	D	184	LLP	C5-C6-N1	-2.25	120.07	123.82
1	C	184	LLP	C3-C4-C5	2.14	119.91	118.26

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

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Mol	Chain	Res	Type	Atoms
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	C	184	LLP	CD-CE-NZ-C4'
1	B	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	184	LLP	1	0
1	A	184	LLP	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	C	404	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	402	-	4,4,4	0.13	0	6,6,6	0.06	0
3	PLP	A	406	-	12,12,16	1.24	1 (8%)	15,16,23	1.17	1 (6%)
2	SO4	C	403	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	D	401	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	404	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	B	404	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	C	406	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	405	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	407	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	407	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	B	406	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	405	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	403	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	401	-	4,4,4	0.14	0	6,6,6	0.06	0
3	PLP	D	404	-	12,12,16	1.26	1 (8%)	15,16,23	1.24	1 (6%)
2	SO4	B	409	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	405	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	408	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	408	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	403	-	4,4,4	0.14	0	6,6,6	0.07	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	2.30	1.38	1.33
3	A	406	PLP	C2-N1	2.23	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	-3.08	115.53	119.90
3	A	406	PLP	C3-C4-C4A	-2.93	115.75	119.90

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	PLP	2	0
2	B	407	SO4	1	0
3	D	404	PLP	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, 95th 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 ²)	Q<0.9
1	A	359/402 (89%)	0.05	13 (3%) 42 43	24, 33, 58, 76	0
1	B	359/402 (89%)	-0.01	15 (4%) 36 37	21, 30, 54, 82	0
1	C	359/402 (89%)	0.03	16 (4%) 33 34	22, 31, 54, 91	0
1	D	358/402 (89%)	-0.02	10 (2%) 53 54	24, 33, 58, 82	0
All	All	1435/1608 (89%)	0.01	54 (3%) 40 41	21, 32, 56, 91	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	GLY	6.1
1	B	338	HIS	5.2
1	D	338	HIS	4.4
1	D	382	ALA	4.2
1	A	215	GLN	4.1
1	C	338	HIS	4.0
1	B	279	THR	3.9
1	C	230	TRP	3.7
1	C	314	ARG	3.4
1	C	158	CYS	3.4
1	D	381	THR	3.3
1	A	157	ALA	3.3
1	A	230	TRP	3.2
1	C	215	GLN	3.2
1	A	340	GLY	3.1
1	C	279	THR	3.1
1	D	230	TRP	3.1
1	B	230	TRP	3.1
1	B	380	LEU	3.0
1	B	229	ARG	2.9
1	C	157	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	279	THR	2.9
1	B	158	CYS	2.9
1	D	157	ALA	2.8
1	A	129	LEU	2.8
1	A	177	VAL	2.8
1	B	377	LEU	2.8
1	B	157	ALA	2.7
1	C	131	TYR	2.7
1	C	2	GLY	2.7
1	B	381	THR	2.7
1	B	214	ALA	2.5
1	C	129	LEU	2.5
1	D	214	ALA	2.5
1	B	314	ARG	2.5
1	D	380	LEU	2.4
1	D	340	GLY	2.4
1	C	322	TYR	2.4
1	C	381	THR	2.4
1	C	299	PHE	2.4
1	D	298	TYR	2.3
1	A	337	GLY	2.3
1	A	314	ARG	2.3
1	C	298	TYR	2.3
1	A	338	HIS	2.3
1	B	215	GLN	2.2
1	A	214	ALA	2.2
1	D	314	ARG	2.1
1	C	229	ARG	2.1
1	A	59	THR	2.1
1	B	327	TYR	2.1
1	C	327	TYR	2.1
1	B	299	PHE	2.0
1	A	58	CYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
1	LLP	B	184	24/25	0.96	0.21	17,24,29,35	0
1	LLP	D	184	24/25	0.96	0.19	24,28,33,36	0
1	LLP	A	184	24/25	0.97	0.20	20,27,32,35	0
1	LLP	C	184	24/25	0.98	0.22	20,27,35,41	0

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, 95th 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(\AA^2)	Q<0.9
2	SO4	C	405	5/5	0.76	0.25	91,94,96,96	0
3	PLP	A	406	12/16	0.76	0.31	60,63,66,71	0
2	SO4	A	403	5/5	0.78	0.26	50,59,63,73	5
2	SO4	B	406	5/5	0.78	0.29	110,110,110,112	5
2	SO4	B	407	5/5	0.79	0.42	109,109,112,113	5
2	SO4	C	406	5/5	0.81	0.25	101,103,104,105	5
2	SO4	D	402	5/5	0.83	0.32	96,97,97,100	5
2	SO4	C	407	5/5	0.84	0.29	83,86,87,91	5
2	SO4	A	405	5/5	0.85	0.28	77,78,84,86	5
2	SO4	D	403	5/5	0.85	0.21	91,93,96,98	0
2	SO4	C	408	5/5	0.85	0.30	104,105,105,106	5
3	PLP	D	404	12/16	0.85	0.24	60,70,77,80	0
2	SO4	B	402	5/5	0.86	0.21	87,91,91,92	0
2	SO4	B	405	5/5	0.86	0.20	85,86,89,89	0
2	SO4	B	408	5/5	0.86	0.24	84,89,91,92	5
2	SO4	B	409	5/5	0.86	0.29	74,78,80,81	5
2	SO4	A	404	5/5	0.89	0.21	113,114,114,116	0
2	SO4	A	402	5/5	0.91	0.16	90,92,94,95	5
2	SO4	C	403	5/5	0.93	0.20	72,76,78,81	0
2	SO4	C	404	5/5	0.93	0.19	95,95,96,99	0
2	SO4	C	401	5/5	0.94	0.15	77,77,79,81	0
2	SO4	C	402	5/5	0.94	0.24	71,72,79,82	0
2	SO4	B	403	5/5	0.95	0.16	74,78,81,82	0
2	SO4	A	401	5/5	0.95	0.13	72,73,75,79	0
2	SO4	B	404	5/5	0.96	0.19	80,80,81,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	D	401	5/5	0.96	0.10	84,84,84,85	0
2	SO4	B	401	5/5	0.98	0.18	53,62,66,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.