



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2017 – 10:29 PM EST

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.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

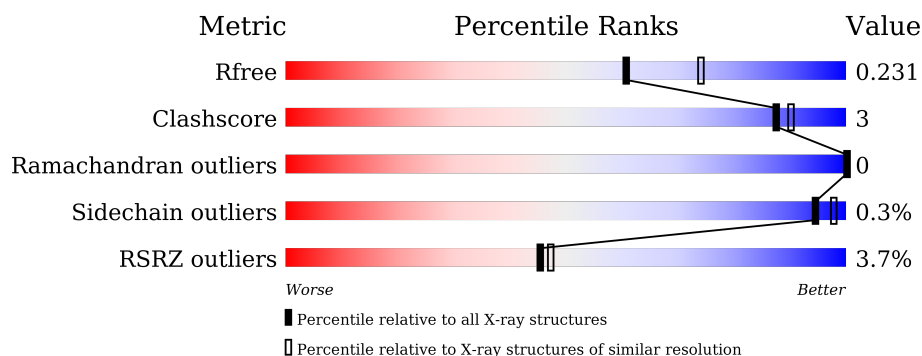
1 Overall quality at a glance

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}	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>9%</div> </div> </div>
1	B	402	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	402	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>9%</div> </div> </div>
1	D	402	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>9%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	405	-	-	-	X
2	SO4	B	407	-	-	-	X
2	SO4	C	405	-	-	-	X
2	SO4	C	406	-	-	-	X
3	PLP	A	406	-	-	-	X
3	PLP	D	404	-	-	-	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.

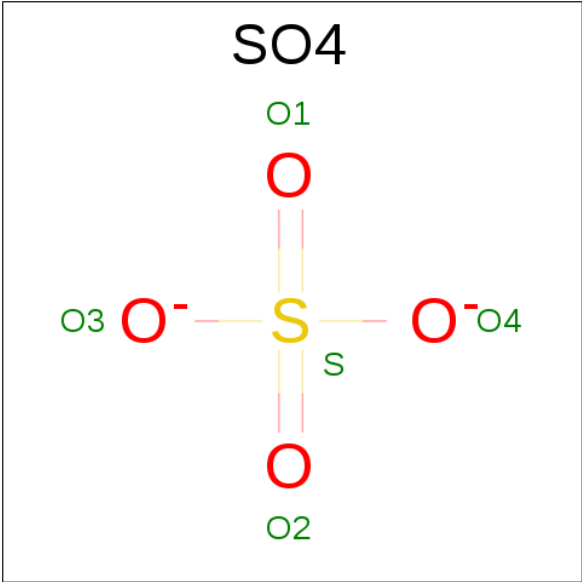
- Molecule 1 is a protein called Aminotransferase TlmJ.

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).



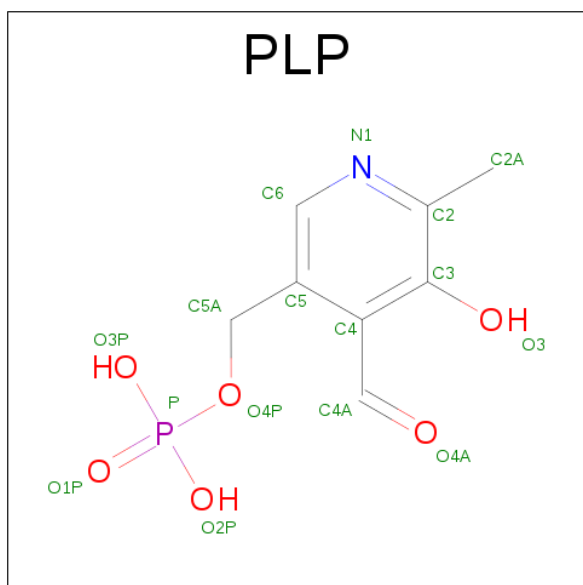
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	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		
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 (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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		

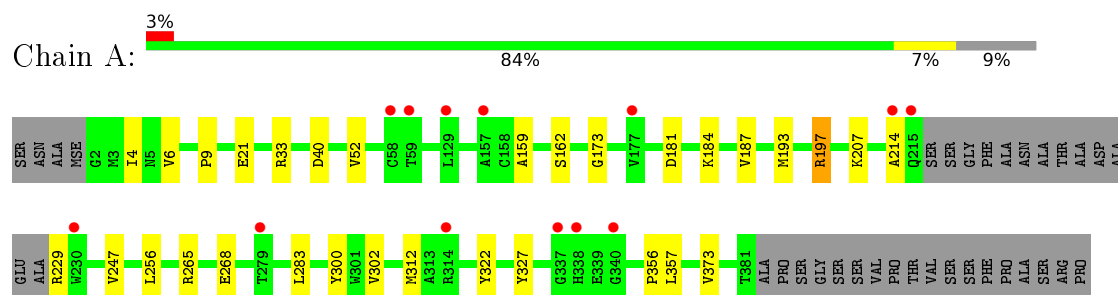
- Molecule 4 is water.

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		

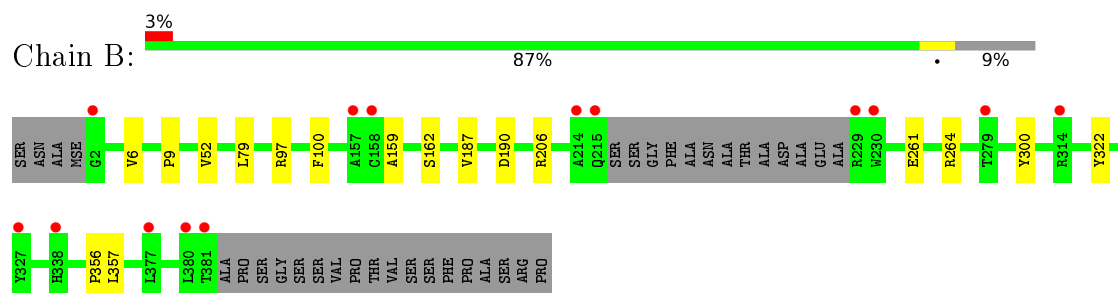
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

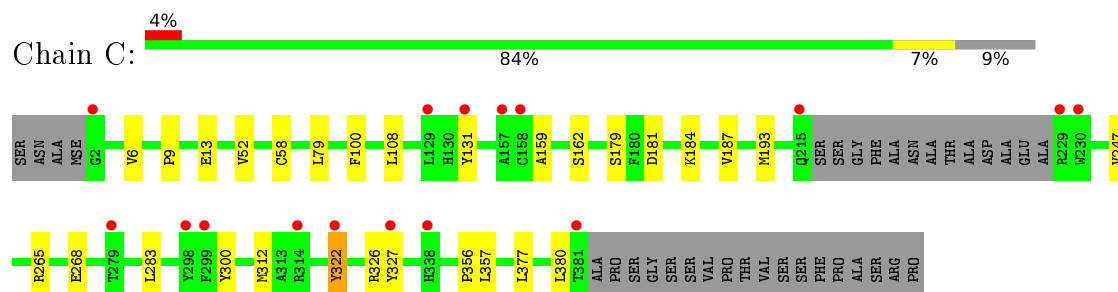
• Molecule 1: Aminotransferase TlmJ



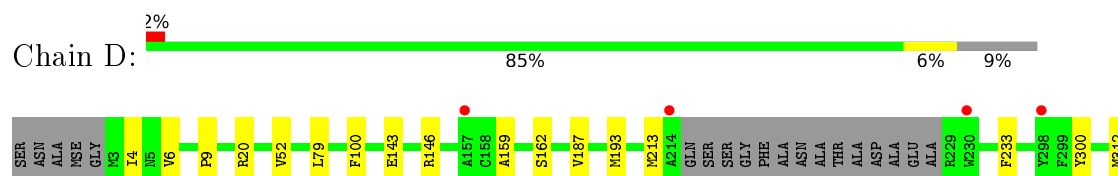
• Molecule 1: Aminotransferase TlmJ

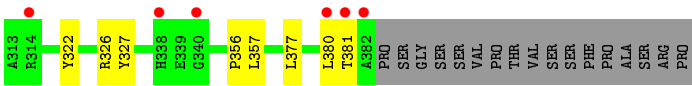


• Molecule 1: Aminotransferase TlmJ



• 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	139.60 Å 198.09 Å 60.56 Å 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 2.18 Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.190 , 0.233 0.186 , 0.231	Depositor DCC
R_{free} test set	4187 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

¹ Intensities estimated from amplitudes.

² 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: LLP, SO4, 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:9:PRO:HB3	1:B:187:VAL:HG21	1.92	0.51
1:B:6:VAL:HG23	1:B:322:TYR:HD2	1.75	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:326:ARG:HA	1:D:327:TYR:HA	1.73	0.45
1:D:6:VAL:HA	1:D:356:PRO:HA	1.99	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:181:ASP:OD2	1:C:184:LLP:HE3	2.18	0.44
1:C:79:LEU:O	1:C:100:PHE:HA	2.17	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:HA	1:D:377:LEU:HD12	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	93	97
1	B	281/301 (93%)	281 (100%)	0	100	100
1	C	283/301 (94%)	282 (100%)	1 (0%)	93	97
1	D	282/301 (94%)	281 (100%)	1 (0%)	93	97
All	All	1126/1204 (94%)	1123 (100%)	3 (0%)	94	98

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

Some 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	A	184	1	22,24,25	2.95	7 (31%)	28,32,34	1.26	4 (14%)
1	LLP	B	184	1	22,24,25	2.93	7 (31%)	28,32,34	1.22	3 (10%)
1	LLP	C	184	1	22,24,25	2.93	9 (40%)	28,32,34	1.24	5 (17%)
1	LLP	D	184	1	22,24,25	2.96	8 (36%)	28,32,34	1.21	4 (14%)

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	A	184	1	-	1/15/17/19	0/1/1/1
1	LLP	B	184	1	-	1/15/17/19	0/1/1/1
1	LLP	C	184	1	-	1/15/17/19	0/1/1/1
1	LLP	D	184	1	-	1/15/17/19	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	LLP	C4-C5	-4.11	1.36	1.42
1	D	184	LLP	C4-C5	-4.08	1.36	1.42
1	B	184	LLP	C4-C5	-3.95	1.36	1.42
1	C	184	LLP	C4-C5	-3.91	1.36	1.42
1	A	184	LLP	C4-C3	-2.38	1.37	1.40
1	D	184	LLP	C4-C3	-2.26	1.38	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	LLP	C4-C3	-2.14	1.38	1.40
1	C	184	LLP	C4-C3	-2.11	1.38	1.40
1	C	184	LLP	P-OP2	-2.04	1.47	1.54
1	D	184	LLP	C5'-C5	2.07	1.56	1.51
1	C	184	LLP	C5'-C5	2.19	1.56	1.51
1	B	184	LLP	C3-C2	2.58	1.42	1.40
1	C	184	LLP	C3-C2	2.84	1.42	1.40
1	B	184	LLP	C6-N1	2.85	1.40	1.34
1	C	184	LLP	C6-N1	2.88	1.40	1.34
1	D	184	LLP	C6-N1	2.94	1.40	1.34
1	D	184	LLP	C2'-C2	2.96	1.56	1.50
1	A	184	LLP	C6-N1	3.00	1.40	1.34
1	A	184	LLP	C2'-C2	3.02	1.56	1.50
1	B	184	LLP	C2'-C2	3.04	1.56	1.50
1	C	184	LLP	C2'-C2	3.09	1.56	1.50
1	D	184	LLP	C3-C2	3.11	1.43	1.40
1	A	184	LLP	C3-C2	3.12	1.43	1.40
1	A	184	LLP	C4'-NZ	5.65	1.44	1.27
1	C	184	LLP	C4'-NZ	5.69	1.44	1.27
1	D	184	LLP	C4'-NZ	5.76	1.44	1.27
1	B	184	LLP	C4'-NZ	5.78	1.44	1.27
1	C	184	LLP	C4-C4'	9.19	1.62	1.46
1	A	184	LLP	C4-C4'	9.20	1.62	1.46
1	B	184	LLP	C4-C4'	9.34	1.62	1.46
1	D	184	LLP	C4-C4'	9.34	1.62	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	LLP	CE-NZ-C4'	-3.18	109.66	119.14
1	D	184	LLP	CE-NZ-C4'	-2.87	110.57	119.14
1	C	184	LLP	CE-NZ-C4'	-2.81	110.77	119.14
1	B	184	LLP	CE-NZ-C4'	-2.78	110.86	119.14
1	A	184	LLP	C4-C4'-NZ	-2.69	110.17	125.14
1	C	184	LLP	C4-C4'-NZ	-2.66	110.35	125.14
1	D	184	LLP	C4-C4'-NZ	-2.64	110.46	125.14
1	B	184	LLP	C4-C4'-NZ	-2.56	110.89	125.14
1	B	184	LLP	C5-C6-N1	-2.36	119.74	123.86
1	A	184	LLP	C5-C6-N1	-2.33	119.79	123.86
1	C	184	LLP	C5-C6-N1	-2.29	119.85	123.86
1	C	184	LLP	O-C-CA	-2.22	119.78	125.72
1	D	184	LLP	C5-C6-N1	-2.17	120.07	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	LLP	O-C-CA	-2.02	120.30	125.72
1	D	184	LLP	O-C-CA	-2.00	120.34	125.72
1	C	184	LLP	C3-C4-C5	2.27	119.91	118.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	184	LLP	C4-C4'-NZ-CE
1	D	184	LLP	C4-C4'-NZ-CE
1	B	184	LLP	C4-C4'-NZ-CE
1	C	184	LLP	C4-C4'-NZ-CE

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	401	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	402	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	404	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	A	405	-	4,4,4	0.26	0	6,6,6	0.06	0
3	PLP	A	406	-	12,12,16	1.28	1 (8%)	15,16,23	1.10	1 (6%)
2	SO4	B	401	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	403	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	404	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	405	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	406	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	407	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	408	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	B	409	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	C	401	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	C	402	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	C	403	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	C	404	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	C	405	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	C	406	-	4,4,4	0.25	0	6,6,6	0.05	0
2	SO4	C	407	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	C	408	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	D	401	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	D	402	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	D	403	-	4,4,4	0.24	0	6,6,6	0.08	0
3	PLP	D	404	-	12,12,16	1.33	2 (16%)	15,16,23	1.14	1 (6%)

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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	A	404	-	-	0/0/0/0	0/0/0/0
2	SO4	A	405	-	-	0/0/0/0	0/0/0/0
3	PLP	A	406	-	-	0/4/4/8	0/1/1/1
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0
2	SO4	B	403	-	-	0/0/0/0	0/0/0/0
2	SO4	B	404	-	-	0/0/0/0	0/0/0/0
2	SO4	B	405	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	406	-	-	0/0/0/0	0/0/0/0
2	SO4	B	407	-	-	0/0/0/0	0/0/0/0
2	SO4	B	408	-	-	0/0/0/0	0/0/0/0
2	SO4	B	409	-	-	0/0/0/0	0/0/0/0
2	SO4	C	401	-	-	0/0/0/0	0/0/0/0
2	SO4	C	402	-	-	0/0/0/0	0/0/0/0
2	SO4	C	403	-	-	0/0/0/0	0/0/0/0
2	SO4	C	404	-	-	0/0/0/0	0/0/0/0
2	SO4	C	405	-	-	0/0/0/0	0/0/0/0
2	SO4	C	406	-	-	0/0/0/0	0/0/0/0
2	SO4	C	407	-	-	0/0/0/0	0/0/0/0
2	SO4	C	408	-	-	0/0/0/0	0/0/0/0
2	SO4	D	401	-	-	0/0/0/0	0/0/0/0
2	SO4	D	402	-	-	0/0/0/0	0/0/0/0
2	SO4	D	403	-	-	0/0/0/0	0/0/0/0
3	PLP	D	404	-	-	0/4/4/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	PLP	C3-C2	-2.36	1.39	1.40
3	A	406	PLP	C2-N1	2.24	1.38	1.33
3	D	404	PLP	C2-N1	2.30	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	-2.77	115.53	119.81
3	A	406	PLP	C3-C4-C4A	-2.63	115.75	119.81

There are no chirality outliers.

There are no torsion outliers.

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

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, 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%)	46 48	24, 33, 58, 76	0
1	B	359/402 (89%)	-0.01	14 (3%)	43 45	21, 30, 54, 82	0
1	C	359/402 (89%)	0.03	16 (4%)	37 39	22, 31, 54, 91	0
1	D	358/402 (89%)	-0.02	10 (2%)	56 58	24, 33, 58, 82	0
All	All	1435/1608 (89%)	0.01	53 (3%)	45 47	21, 32, 56, 91	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	GLY	6.5
1	B	338	HIS	5.2
1	D	338	HIS	4.4
1	A	215	GLN	4.2
1	D	382	ALA	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	A	157	ALA	3.3
1	D	381	THR	3.3
1	C	158	CYS	3.3
1	A	230	TRP	3.2
1	D	230	TRP	3.2
1	C	279	THR	3.1
1	C	215	GLN	3.1
1	B	230	TRP	3.1
1	A	340	GLY	3.0
1	B	380	LEU	3.0
1	B	229	ARG	3.0
1	A	279	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	157	ALA	2.9
1	D	157	ALA	2.9
1	B	158	CYS	2.8
1	A	129	LEU	2.8
1	B	377	LEU	2.8
1	A	177	VAL	2.8
1	B	157	ALA	2.7
1	C	131	TYR	2.7
1	C	2	GLY	2.7
1	B	381	THR	2.6
1	B	214	ALA	2.6
1	B	314	ARG	2.5
1	D	214	ALA	2.5
1	C	129	LEU	2.5
1	C	381	THR	2.4
1	D	340	GLY	2.4
1	D	380	LEU	2.4
1	C	322	TYR	2.4
1	D	298	TYR	2.3
1	C	299	PHE	2.3
1	B	215	GLN	2.3
1	A	337	GLY	2.3
1	C	298	TYR	2.3
1	A	214	ALA	2.3
1	A	314	ARG	2.3
1	A	338	HIS	2.2
1	D	314	ARG	2.2
1	C	229	ARG	2.1
1	A	59	THR	2.1
1	B	327	TYR	2.1
1	C	327	TYR	2.0
1	A	58	CYS	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
1	LLP	A	184	24/25	0.97	0.20	-	20,27,32,35	0
1	LLP	B	184	24/25	0.96	0.21	-	17,24,29,35	0
1	LLP	C	184	24/25	0.98	0.22	-	20,27,35,41	0
1	LLP	D	184	24/25	0.96	0.19	-	24,28,33,36	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	PLP	A	406	12/16	0.76	0.31	8.99	60,63,66,71	0
3	PLP	D	404	12/16	0.85	0.24	6.77	60,70,77,80	0
2	SO4	C	405	5/5	0.77	0.25	6.66	91,94,96,96	0
2	SO4	C	406	5/5	0.81	0.24	4.94	101,103,104,105	5
2	SO4	B	405	5/5	0.86	0.20	3.30	85,86,89,89	0
2	SO4	B	407	5/5	0.78	0.43	2.01	109,109,112,113	5
2	SO4	C	403	5/5	0.93	0.20	1.81	72,76,78,81	0
2	SO4	B	408	5/5	0.86	0.24	0.97	84,89,91,92	5
2	SO4	A	404	5/5	0.89	0.21	0.49	113,114,114,116	0
2	SO4	B	403	5/5	0.94	0.16	0.09	74,78,81,82	0
2	SO4	A	401	5/5	0.95	0.13	-0.57	72,73,75,79	0
2	SO4	D	401	5/5	0.95	0.10	-1.05	84,84,84,85	0
2	SO4	D	403	5/5	0.85	0.21	-	91,93,96,98	0
2	SO4	A	402	5/5	0.91	0.16	-	90,92,94,95	5
2	SO4	B	404	5/5	0.96	0.18	-	80,80,81,84	0
2	SO4	B	401	5/5	0.98	0.18	-	53,62,66,67	0
2	SO4	C	404	5/5	0.93	0.19	-	95,95,96,99	0
2	SO4	C	408	5/5	0.85	0.30	-	104,105,105,106	5
2	SO4	A	403	5/5	0.79	0.26	-	50,59,63,73	5
2	SO4	A	405	5/5	0.85	0.28	-	77,78,84,86	5
2	SO4	B	409	5/5	0.87	0.28	-	74,78,80,81	5
2	SO4	D	402	5/5	0.84	0.32	-	96,97,97,100	5
2	SO4	B	406	5/5	0.79	0.29	-	110,110,110,112	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	402	5/5	0.86	0.21	-	87,91,91,92	0
2	SO4	C	401	5/5	0.94	0.15	-	77,77,79,81	0
2	SO4	C	407	5/5	0.84	0.28	-	83,86,87,91	5
2	SO4	C	402	5/5	0.94	0.24	-	71,72,79,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.