



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2026 – 10:35 AM JST

PDB ID : 21FT / pdb\_000021ft  
Title : GABA aminotransferase from Arabidopsis thaliana  
Authors : Okoda, N.; Okuda, S.; Tsutsumi, K.; Sano, K.; Kobata, K.; Nagata, K.  
Deposited on : 2025-12-12  
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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
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

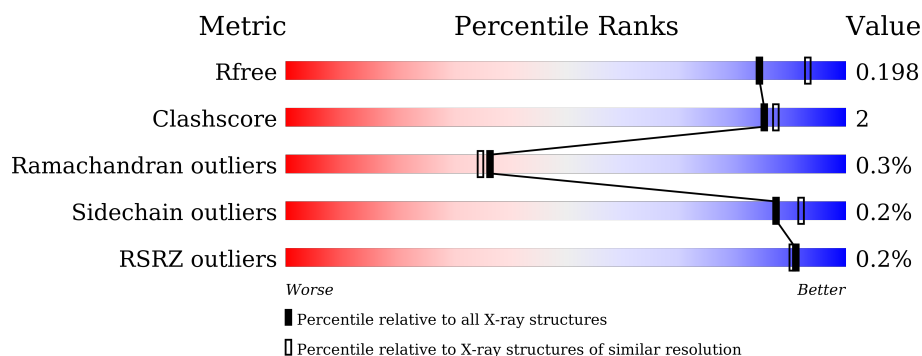
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	474	<div> <div>92%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> <div>• •</div> </div>
1	B	474	<div> <div>91%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> <div>5% •</div> </div>
1	C	474	<div> <div>88%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> <div>8% •</div> </div>
1	D	474	<div> <div>91%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> <div>5% •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15246 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 Gamma-aminobutyrate transaminase POP2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	P	S	0	1	0
			3513	2268	575	653	1	16			
1	B	456	Total	C	N	O	P	S	0	1	0
			3531	2280	579	655	1	16			
1	C	455	Total	C	N	O	P	S	0	2	0
			3525	2276	577	655	1	16			
1	D	455	Total	C	N	O	P	S	0	1	0
			3527	2278	578	654	1	16			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	PHE	conflict	UNP Q94CE5
A	8	ASP	GLU	conflict	UNP Q94CE5
A	470	HIS	-	expression tag	UNP Q94CE5
A	471	HIS	-	expression tag	UNP Q94CE5
A	472	HIS	-	expression tag	UNP Q94CE5
A	473	HIS	-	expression tag	UNP Q94CE5
A	474	HIS	-	expression tag	UNP Q94CE5
B	1	MET	PHE	conflict	UNP Q94CE5
B	8	ASP	GLU	conflict	UNP Q94CE5
B	470	HIS	-	expression tag	UNP Q94CE5
B	471	HIS	-	expression tag	UNP Q94CE5
B	472	HIS	-	expression tag	UNP Q94CE5
B	473	HIS	-	expression tag	UNP Q94CE5
B	474	HIS	-	expression tag	UNP Q94CE5
C	1	MET	PHE	conflict	UNP Q94CE5
C	8	ASP	GLU	conflict	UNP Q94CE5
C	470	HIS	-	expression tag	UNP Q94CE5
C	471	HIS	-	expression tag	UNP Q94CE5
C	472	HIS	-	expression tag	UNP Q94CE5
C	473	HIS	-	expression tag	UNP Q94CE5
C	474	HIS	-	expression tag	UNP Q94CE5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	PHE	conflict	UNP Q94CE5
D	8	ASP	GLU	conflict	UNP Q94CE5
D	470	HIS	-	expression tag	UNP Q94CE5
D	471	HIS	-	expression tag	UNP Q94CE5
D	472	HIS	-	expression tag	UNP Q94CE5
D	473	HIS	-	expression tag	UNP Q94CE5
D	474	HIS	-	expression tag	UNP Q94CE5

- Molecule 2 is water.

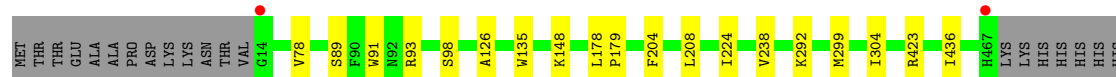
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	308	Total 308	O 308	0	0
2	B	317	Total 317	O 317	0	0
2	C	276	Total 276	O 276	0	0
2	D	249	Total 249	O 249	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

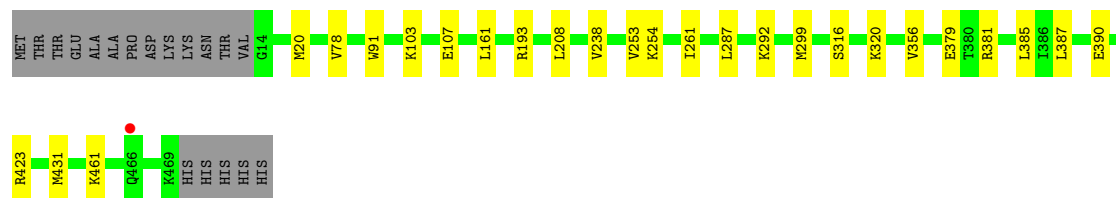
- Molecule 1: Gamma-aminobutyrate transaminase POP2, mitochondrial

Chain A: 




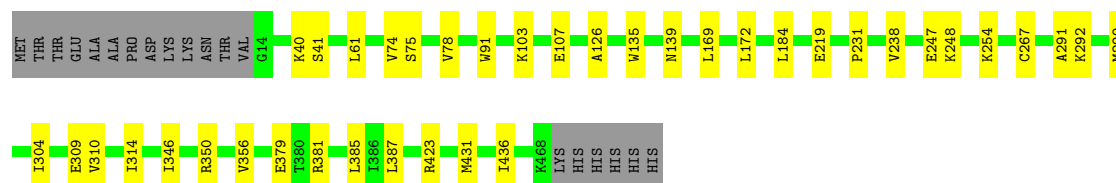
- Molecule 1: Gamma-aminobutyrate transaminase POP2, mitochondrial

Chain B: 



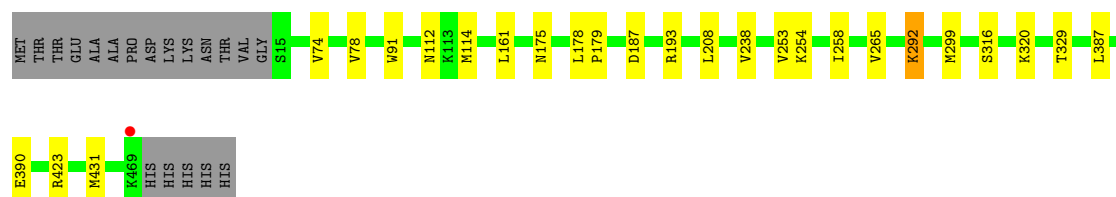
- Molecule 1: Gamma-aminobutyrate transaminase POP2, mitochondrial

Chain C: 



- Molecule 1: Gamma-aminobutyrate transaminase POP2, mitochondrial

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.18Å 78.27Å 93.22Å 96.76° 88.88° 106.11°	Depositor
Resolution (Å)	41.58 – 2.00 41.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (41.58-2.00) 97.0 (41.58-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.50 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.21_5207: ???	Depositor
R, $R_{free}$	0.153 , 0.198 0.153 , 0.198	Depositor DCC
$R_{free}$ test set	5330 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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: 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	0.31	0/3584	0.50	0/4863
1	B	0.31	0/3602	0.51	0/4885
1	C	0.30	0/3599	0.49	0/4882
1	D	0.29	0/3598	0.48	0/4880
All	All	0.30	0/14383	0.49	0/19510

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	3513	0	3489	13	0
1	B	3531	0	3515	17	0
1	C	3525	0	3507	29	0
1	D	3527	0	3512	19	0
2	A	308	0	0	0	0
2	B	317	0	0	0	0
2	C	276	0	0	1	0
2	D	249	0	0	0	0
All	All	15246	0	14023	61	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 2.

All (61) 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:C:78:VAL:HG12	1:D:78:VAL:HG22	1.73	0.70
1:A:78:VAL:HG22	1:B:78:VAL:HG22	1.74	0.70
1:C:346:ILE:HG23	1:C:350:ARG:HD2	1.87	0.56
1:A:98:SER:OG	1:B:20:MET:SD	2.65	0.55
1:C:387:LEU:HD22	1:C:431:MET:HE3	1.90	0.53
1:C:75:SER:HA	1:C:78:VAL:HG22	1.90	0.52
1:D:112:ASN:HB3	1:D:114:MET:HE3	1.92	0.52
1:A:126:ALA:O	1:A:304:ILE:HD11	2.10	0.51
1:B:316:SER:O	1:B:320:LYS:HG2	2.11	0.51
1:C:40:LYS:HD2	1:C:41:SER:H	1.77	0.50
1:D:74:VAL:O	1:D:78:VAL:HG23	2.12	0.49
1:B:387:LEU:HD22	1:B:431:MET:HE3	1.95	0.49
1:A:423:ARG:HD3	1:B:91:TRP:CZ2	2.48	0.48
1:A:91:TRP:CZ2	1:B:423:ARG:HD3	2.48	0.48
1:C:139:ASN:HB3	1:D:175:ASN:ND2	2.29	0.47
1:C:247:GLU:CD	1:C:247:GLU:N	2.72	0.47
1:C:310:VAL:O	1:C:314:ILE:HD13	2.15	0.47
1:B:254:LYS:NZ	1:C:309:GLU:OE2	2.46	0.47
1:D:187:ASP:HB2	1:D:208:LEU:HD22	1.96	0.47
1:D:265:VAL:CG1	1:D:292:LLP:HG2	2.44	0.47
1:C:74:VAL:O	1:C:78:VAL:HG13	2.14	0.47
1:D:316:SER:O	1:D:320:LYS:HG2	2.14	0.47
1:B:261:ILE:HG12	1:B:287:LEU:HB2	1.97	0.46
1:D:265:VAL:HG12	1:D:292:LLP:HG2	1.97	0.46
1:D:193:ARG:NH2	1:D:390:GLU:OE2	2.44	0.45
1:C:169:LEU:HB2	1:C:172:LEU:HD12	1.99	0.45
1:C:356:VAL:HG13	1:C:385:LEU:HG	1.99	0.45
1:C:40:LYS:HD2	1:C:41:SER:N	2.32	0.45
1:C:184:LEU:HD13	1:C:219:GLU:HG3	1.98	0.45
1:A:148:LYS:HB2	1:A:224:ILE:HD13	1.99	0.44
1:C:231:PRO:HD2	1:C:267[A]:CYS:SG	2.58	0.44
1:A:204:PHE:CE2	1:A:208:LEU:HD11	2.53	0.43
1:D:387:LEU:HD22	1:D:431:MET:HE3	1.99	0.43
1:C:379:GLU:OE1	1:C:381:ARG:HD3	2.18	0.43
1:C:385:LEU:HD23	1:C:385:LEU:HA	1.86	0.43
1:C:126:ALA:O	1:C:304:ILE:HD11	2.18	0.43
1:D:178:LEU:HB3	1:D:179:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:LYS:HB3	1:D:254:LYS:HE2	1.74	0.42
1:C:103:LYS:O	1:C:107:GLU:HG3	2.20	0.42
1:A:135:TRP:CZ3	1:B:161:LEU:HD11	2.54	0.42
1:B:461:LYS:HA	1:B:461:LYS:HD2	1.82	0.42
1:A:423:ARG:HD3	1:B:91:TRP:CH2	2.55	0.42
1:C:91:TRP:CH2	1:D:423:ARG:HD3	2.54	0.42
1:D:253:VAL:HG13	1:D:258:ILE:HB	2.01	0.42
1:A:178:LEU:HB3	1:A:179:PRO:HA	2.02	0.42
1:B:193:ARG:NH2	1:B:390:GLU:OE2	2.47	0.42
1:C:299:MET:HE1	1:D:299:MET:SD	2.60	0.42
1:A:299:MET:HE1	1:B:299:MET:SD	2.60	0.41
1:B:379:GLU:OE1	1:B:381:ARG:HD3	2.20	0.41
1:C:436:ILE:H	1:C:436:ILE:HG13	1.68	0.41
1:C:61:LEU:HD23	1:D:329:THR:HA	2.03	0.41
1:C:91:TRP:CZ2	1:D:423:ARG:HD3	2.56	0.41
1:B:356:VAL:HG13	1:B:385:LEU:HG	2.02	0.41
1:C:254:LYS:HE2	1:C:254:LYS:HB2	1.86	0.41
1:B:103:LYS:O	1:B:107:GLU:HG3	2.20	0.41
1:C:248:LYS:NZ	2:C:518:HOH:O	2.51	0.41
1:A:89:SER:HA	1:A:93:ARG:O	2.21	0.41
1:C:423:ARG:HD3	1:D:91:TRP:CZ2	2.56	0.41
1:C:184:LEU:CD1	1:C:219:GLU:HG3	2.51	0.40
1:A:91:TRP:CH2	1:B:423:ARG:HD3	2.56	0.40
1:C:135:TRP:CZ3	1:D:161:LEU:HD11	2.56	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	452/474 (95%)	437 (97%)	14 (3%)	1 (0%)	43 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	454/474 (96%)	440 (97%)	13 (3%)	1 (0%)	43	42
1	C	454/474 (96%)	439 (97%)	13 (3%)	2 (0%)	30	27
1	D	453/474 (96%)	440 (97%)	12 (3%)	1 (0%)	43	42
All	All	1813/1896 (96%)	1756 (97%)	52 (3%)	5 (0%)	36	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	291	ALA
1	B	238	VAL
1	C	238	VAL
1	D	238	VAL
1	A	238	VAL

### 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	372/389 (96%)	371 (100%)	1 (0%)	86	91
1	B	374/389 (96%)	372 (100%)	2 (0%)	81	87
1	C	374/389 (96%)	374 (100%)	0	100	100
1	D	374/389 (96%)	374 (100%)	0	100	100
All	All	1494/1556 (96%)	1491 (100%)	3 (0%)	87	92

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

Mol	Chain	Res	Type
1	A	436	ILE
1	B	208	LEU
1	B	253	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	B	80	GLN
1	B	112	ASN
1	B	282	ASN
1	B	394	ASN
1	C	82	ASN
1	C	175	ASN
1	D	175	ASN
1	D	398	ASN

### 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	292	1	23,24,25	1.17	1 (4%)	25,32,34	1.54	4 (16%)
1	LLP	B	292	1	23,24,25	1.12	1 (4%)	25,32,34	1.44	4 (16%)
1	LLP	D	292	1	23,24,25	1.14	1 (4%)	25,32,34	1.50	6 (24%)
1	LLP	C	292	1	23,24,25	1.07	1 (4%)	25,32,34	1.42	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	A	292	1	-	5/16/17/19	0/1/1/1
1	LLP	B	292	1	-	5/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	D	292	1	-	6/16/17/19	0/1/1/1
1	LLP	C	292	1	-	3/16/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	LLP	P-OP4	4.19	1.73	1.60
1	C	292	LLP	P-OP4	4.01	1.73	1.60
1	D	292	LLP	P-OP4	3.98	1.73	1.60
1	B	292	LLP	P-OP4	3.85	1.72	1.60

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	LLP	CE-NZ-C4'	4.03	131.28	118.90
1	B	292	LLP	CE-NZ-C4'	3.63	130.04	118.90
1	C	292	LLP	CE-NZ-C4'	3.47	129.56	118.90
1	A	292	LLP	OP4-P-OP1	-3.04	97.95	106.47
1	C	292	LLP	C4-C4'-NZ	-2.96	110.72	124.31
1	B	292	LLP	C4-C4'-NZ	-2.90	110.99	124.31
1	A	292	LLP	C4-C4'-NZ	-2.84	111.27	124.31
1	B	292	LLP	OP4-C5'-C5	2.80	114.69	109.35
1	D	292	LLP	CG-CD-CE	2.68	122.90	113.57
1	C	292	LLP	OP2-P-OP4	-2.65	99.68	106.73
1	D	292	LLP	CD-CE-NZ	2.64	117.41	110.93
1	D	292	LLP	OP4-C5'-C5	2.63	114.37	109.35
1	C	292	LLP	OP3-P-OP2	2.60	117.56	107.64
1	D	292	LLP	OP4-P-OP1	-2.41	99.73	106.47
1	D	292	LLP	CE-NZ-C4'	2.19	125.61	118.90
1	B	292	LLP	OP4-P-OP1	-2.15	100.45	106.47
1	D	292	LLP	C4-C4'-NZ	-2.11	114.64	124.31
1	A	292	LLP	C5-C4-C4'	2.02	124.89	121.56

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	292	LLP	O-C-CA-CB
1	B	292	LLP	O-C-CA-CB
1	C	292	LLP	O-C-CA-CB
1	D	292	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	D	292	LLP	CG-CD-CE-NZ
1	D	292	LLP	CA-CB-CG-CD
1	A	292	LLP	C3-C4-C4'-NZ
1	B	292	LLP	C3-C4-C4'-NZ
1	D	292	LLP	C3-C4-C4'-NZ
1	B	292	LLP	CG-CD-CE-NZ
1	A	292	LLP	CD-CE-NZ-C4'
1	B	292	LLP	CD-CE-NZ-C4'
1	D	292	LLP	C5-C4-C4'-NZ
1	C	292	LLP	C3-C4-C4'-NZ
1	C	292	LLP	CD-CE-NZ-C4'
1	D	292	LLP	CD-CE-NZ-C4'
1	A	292	LLP	CG-CD-CE-NZ
1	A	292	LLP	C5-C4-C4'-NZ
1	B	292	LLP	C5-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	292	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	453/474 (95%)	-0.20	2 (0%) 88 88	12, 19, 32, 71	1 (0%)
1	B	455/474 (95%)	-0.20	1 (0%) 91 90	12, 19, 29, 50	1 (0%)
1	C	454/474 (95%)	-0.12	0 100 100	12, 21, 30, 57	2 (0%)
1	D	454/474 (95%)	-0.08	1 (0%) 91 90	13, 22, 37, 63	1 (0%)
All	All	1816/1896 (95%)	-0.15	4 (0%) 91 90	12, 20, 33, 71	5 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	GLY	2.3
1	B	466	GLN	2.1
1	A	467	HIS	2.1
1	D	469	LYS	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. 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	B	292	24/25	0.94	0.08	12,18,23,26	0
1	LLP	C	292	24/25	0.94	0.08	13,17,20,24	0
1	LLP	D	292	24/25	0.94	0.08	17,23,29,31	0
1	LLP	A	292	24/25	0.96	0.07	12,16,19,23	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.