



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2017 – 05:39 PM EDT

PDB ID : 5TOQ  
Title : High resolution crystal structure of AAT  
Authors : Mueser, T.C.; Dajnowicz, S.; Kovalevsky, A.  
Deposited on : 2016-10-18  
Resolution : 1.20 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029077

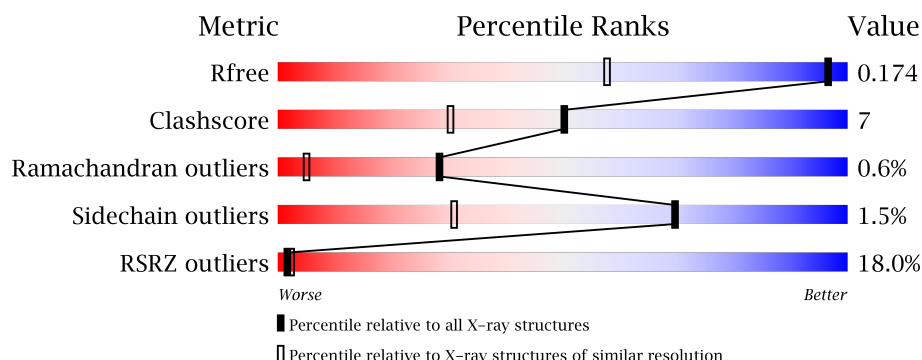
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.20 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))
$R_{free}$	100719	1131 (1.24-1.16)
Clashscore	112137	1201 (1.24-1.16)
Ramachandran outliers	110173	1148 (1.24-1.16)
Sidechain outliers	110143	1147 (1.24-1.16)
RSRZ outliers	101464	1132 (1.24-1.16)

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  $\geq 3$ , 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	414	<div> <div>11%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	B	414	<div> <div>24%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7391 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 Aspartate aminotransferase, cytoplasmic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	P	S	0	8	0
			3360	2134	589	623	1	13			
1	B	392	Total	C	N	O	P	S	0	6	0
			3162	2008	554	585	1	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P00503
A	63	ASN	ASP	conflict	UNP P00503
A	288	GLN	GLU	conflict	UNP P00503
A	376	GLN	GLU	conflict	UNP P00503
B	-1	GLY	-	expression tag	UNP P00503
B	63	ASN	ASP	conflict	UNP P00503
B	288	GLN	GLU	conflict	UNP P00503
B	376	GLN	GLU	conflict	UNP P00503

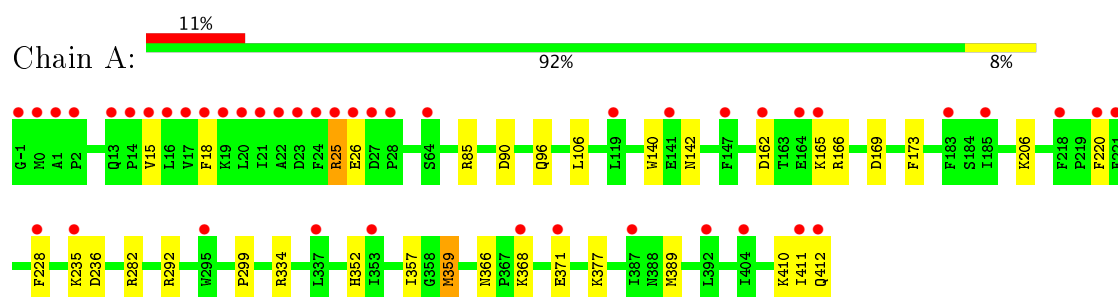
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	505	Total	O	0	0
			505	505		
2	B	364	Total	O	0	0
			364	364		

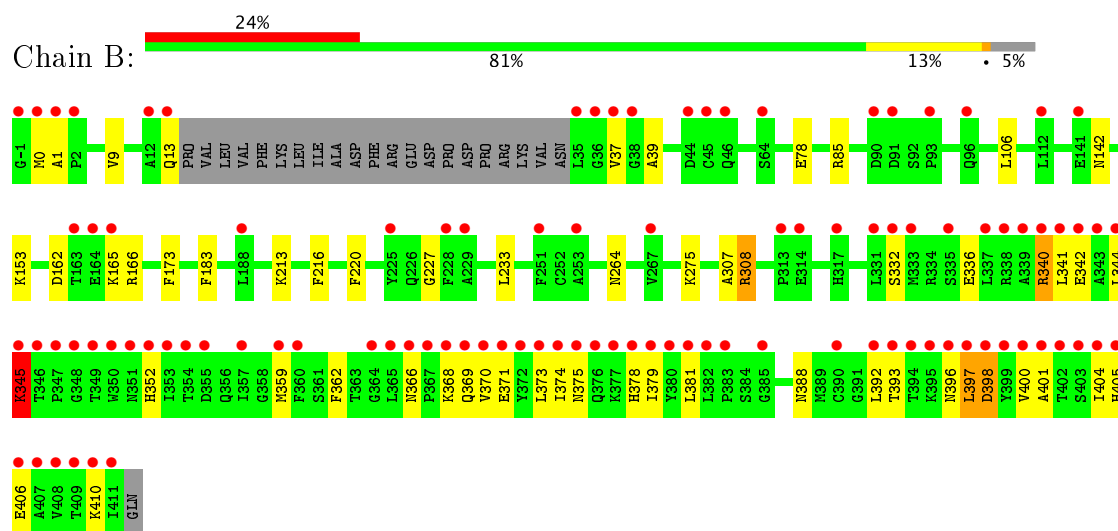
### 3 Residue-property plots

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



- Molecule 1: Aspartate aminotransferase, cytoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.40 Å 124.03 Å 129.26 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 1.20 29.83 – 1.19	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.83-1.20) 98.9 (29.83-1.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 1.19 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.157 , 0.174 0.158 , 0.174	Depositor DCC
$R_{free}$ test set	13875 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.6	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 61.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7391	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

### 5.1 Standard geometry

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	0.32	0/3419	0.59	1/4642 (0.0%)
1	B	0.32	0/3215	0.59	1/4362 (0.0%)
All	All	0.32	0/6634	0.59	2/9004 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	359	MET	CG-SD-CE	12.05	119.48	100.20
1	B	397	LEU	CA-CB-CG	6.37	129.95	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	398	ASP	Peptide

### 5.2 Too-close contacts

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	3360	0	3288	32	0
1	B	3162	0	3093	56	0
2	A	505	0	0	9	1
2	B	364	0	0	7	1
All	All	7391	0	6381	85	1

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 7.

All (85) 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:B:340:ARG:NH1	1:B:401:ALA:HB1	1.57	1.17
1:A:235:LYS:NZ	2:A:501:HOH:O	1.95	0.99
1:B:340:ARG:NH1	1:B:401:ALA:CB	2.27	0.97
1:B:340:ARG:NH2	1:B:401:ALA:O	2.07	0.85
1:A:334:ARG:HA	1:A:389:MET:HE2	1.65	0.79
1:A:368:LYS:NZ	1:A:371:GLU:OE1	2.15	0.79
1:A:142[B]:ASN:ND2	2:A:502:HOH:O	2.23	0.72
1:B:340:ARG:NH2	1:B:401:ALA:C	2.43	0.72
1:A:366:ASN:HD21	1:A:412:GLN:HG3	1.53	0.72
1:B:371:GLU:HA	1:B:374:ILE:HB	1.72	0.71
1:B:340:ARG:HH12	1:B:341:LEU:HD23	1.58	0.68
1:B:142:ASN:ND2	2:B:505:HOH:O	2.28	0.66
1:A:235:LYS:C	1:A:235:LYS:HD3	2.15	0.66
1:A:162:ASP:OD1	1:A:165:LYS:NZ	2.28	0.64
1:A:166:ARG:NH2	2:A:506:HOH:O	2.29	0.63
1:B:227:GLY:HA3	1:B:233:LEU:HD22	1.82	0.62
1:A:357:ILE:HG21	2:A:501:HOH:O	1.97	0.62
1:B:340:ARG:HH12	1:B:401:ALA:HB1	1.60	0.60
1:B:368:LYS:HG3	1:B:371:GLU:CG	2.32	0.59
1:A:366:ASN:ND2	1:A:412:GLN:HG3	2.18	0.59
1:B:13:GLN:O	2:B:502:HOH:O	2.17	0.58
1:B:344:LEU:HB3	1:B:405:HIS:CE1	2.39	0.58
1:B:37:VAL:HG22	1:B:39:ALA:H	1.68	0.58
1:A:140:TRP:CZ3	1:A:142[B]:ASN:HB3	2.40	0.57
1:B:374:ILE:O	1:B:378:HIS:ND1	2.37	0.57
1:B:379:ILE:CD1	1:B:400:VAL:HA	2.35	0.56
1:B:340:ARG:CZ	1:B:401:ALA:CB	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LYS:HG3	1:B:371:GLU:HG3	1.87	0.56
1:A:25:ARG:NH1	1:A:26:GLU:HG3	2.21	0.56
1:B:340:ARG:HH12	1:B:341:LEU:CD2	2.18	0.56
1:A:377:LYS:NZ	2:A:503:HOH:O	2.24	0.54
1:B:368:LYS:HG3	1:B:371:GLU:HB2	1.88	0.54
1:A:140:TRP:CH2	1:A:142[B]:ASN:HB3	2.43	0.54
1:A:292:ARG:NH1	2:B:505:HOH:O	2.41	0.54
1:A:411:ILE:O	1:A:412:GLN:HB2	2.08	0.53
1:B:340:ARG:CZ	1:B:401:ALA:C	2.77	0.53
1:A:15:VAL:HG13	1:A:18:PHE:HB3	1.91	0.52
1:B:340:ARG:HH11	1:B:401:ALA:HB1	1.64	0.52
1:A:162:ASP:HB2	1:A:169:ASP:HB2	1.91	0.52
1:B:406:GLU:HB3	1:B:410:LYS:HD2	1.91	0.52
1:B:406:GLU:OE1	1:B:406:GLU:N	2.42	0.52
1:B:393:THR:N	1:B:396:ASN:OD1	2.40	0.51
1:B:370:VAL:O	1:B:373:LEU:HB2	2.11	0.50
1:A:206:LYS:NZ	2:A:511:HOH:O	2.42	0.49
1:B:359:MET:HG2	1:B:388:ASN:OD1	2.12	0.49
1:A:166:ARG:HD3	1:A:352:HIS:CE1	2.47	0.49
1:A:228:PHE:CZ	1:A:359:MET:CE	2.97	0.48
1:A:410:LYS:HA	1:A:410:LYS:HE2	1.96	0.48
1:B:379:ILE:HD11	1:B:400:VAL:HA	1.94	0.48
1:A:25:ARG:HH12	1:A:26:GLU:HG3	1.78	0.48
1:B:332:SER:O	1:B:336:GLU:HG2	2.14	0.48
1:B:153:LYS:NZ	2:B:510:HOH:O	2.47	0.47
1:B:370:VAL:HG13	1:B:371:GLU:HG2	1.96	0.47
1:B:401:ALA:HA	1:B:404:ILE:HD12	1.96	0.47
1:B:340:ARG:O	1:B:344:LEU:HD12	2.14	0.47
1:A:235:LYS:HD3	1:A:236:ASP:N	2.30	0.47
1:A:106:LEU:HD11	1:B:106:LEU:HD11	1.96	0.47
1:A:85:ARG:NH1	2:A:510:HOH:O	2.39	0.46
1:B:342:GLU:HA	1:B:345:LYS:HD2	1.97	0.46
1:A:228:PHE:CZ	1:A:359:MET:HE1	2.51	0.46
1:B:78:GLU:OE2	1:B:308:ARG:NH1	2.48	0.46
1:A:282[B]:ARG:HD2	1:B:9:VAL:O	2.16	0.45
1:B:275:LYS:NZ	2:B:501:HOH:O	2.16	0.45
1:B:368:LYS:HG3	1:B:371:GLU:CB	2.47	0.45
1:B:366:ASN:OD1	1:B:369:GLN:N	2.49	0.45
1:B:162:ASP:CG	1:B:165:LYS:HG2	2.38	0.44
1:B:78:GLU:HG2	1:B:307:ALA:HB1	2.00	0.44
1:B:371:GLU:O	1:B:375:ASN:N	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ARG:NH2	1:A:26:GLU:OE1	2.51	0.43
1:A:357:ILE:HD13	2:A:501:HOH:O	2.19	0.43
1:B:213:LYS:HE3	2:B:635:HOH:O	2.19	0.43
1:B:340:ARG:NH1	1:B:401:ALA:HB3	2.26	0.42
1:B:340:ARG:HH11	1:B:401:ALA:CB	2.22	0.42
1:B:166:ARG:HD3	1:B:352:HIS:CE1	2.55	0.42
1:B:183:PHE:HA	1:B:216:PHE:O	2.20	0.42
1:B:368:LYS:CG	1:B:371:GLU:HB2	2.50	0.42
1:A:96:GLN:HG2	2:A:529:HOH:O	2.19	0.42
1:B:345:LYS:HD2	1:B:345:LYS:HA	1.90	0.41
1:B:370:VAL:O	1:B:373:LEU:N	2.54	0.41
1:B:370:VAL:HG23	1:B:381:LEU:CD2	2.50	0.41
1:B:392:LEU:HD21	1:B:400:VAL:HG11	2.03	0.41
1:A:299:PRO:HA	1:B:264:ASN:O	2.21	0.41
1:B:85:ARG:HG3	2:B:676:HOH:O	2.21	0.40
1:B:379:ILE:HD13	1:B:400:VAL:HA	2.03	0.40
1:B:227:GLY:HA3	1:B:233:LEU:HD13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:681:HOH:O	2:B:619:HOH:O[3_554]	2.19	0.01

## 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	419/414 (101%)	412 (98%)	7 (2%)	0	100	100
1	B	393/414 (95%)	375 (95%)	13 (3%)	5 (1%)	14	1
All	All	812/828 (98%)	787 (97%)	20 (2%)	5 (1%)	28	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	0	MET
1	B	398	ASP
1	B	1	ALA
1	B	345	LYS
1	B	397	LEU

### 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	360/352 (102%)	356 (99%)	4 (1%)	78	42
1	B	337/352 (96%)	331 (98%)	6 (2%)	64	23
All	All	697/704 (99%)	687 (99%)	10 (1%)	70	33

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	90	ASP
1	A	173	PHE
1	A	220	PHE
1	B	173	PHE
1	B	220	PHE
1	B	308	ARG
1	B	340	ARG
1	B	345	LYS
1	B	362	PHE

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

Mol	Chain	Res	Type
1	B	46	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	258	1	24,24,25	2.48	5 (20%)	28,32,34	1.45	4 (14%)
1	LLP	B	258	1	24,24,25	2.51	5 (20%)	28,32,34	1.38	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	258	1	-	0/15/17/19	0/1/1/1
1	LLP	B	258	1	-	0/15/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	258	LLP	C4-C5	-3.52	1.37	1.42
1	A	258	LLP	C4-C5	-3.22	1.37	1.42
1	B	258	LLP	C6-N1	2.01	1.38	1.34
1	A	258	LLP	C6-N1	2.06	1.38	1.34
1	A	258	LLP	C2'-C2	2.80	1.55	1.50
1	B	258	LLP	C2'-C2	2.91	1.55	1.50
1	A	258	LLP	C4'-NZ	5.65	1.43	1.27
1	B	258	LLP	C4'-NZ	5.78	1.44	1.27
1	B	258	LLP	C4-C4'	8.60	1.62	1.46
1	A	258	LLP	C4-C4'	8.61	1.62	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LLP	C4-C4'-NZ	-3.53	107.50	124.66
1	A	258	LLP	C4-C4'-NZ	-3.47	107.81	124.66
1	A	258	LLP	C5-C6-N1	-3.04	118.73	123.87
1	A	258	LLP	C5'-C5-C6	-2.63	114.80	119.33
1	B	258	LLP	C5-C6-N1	-2.60	119.48	123.87
1	B	258	LLP	C5'-C5-C6	-2.27	115.43	119.33
1	A	258	LLP	OP4-C5'-C5	2.06	113.46	109.32
1	B	258	LLP	OP4-C5'-C5	2.78	114.90	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

### 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	413/414 (99%)	0.87	44 (10%) 7 7	7, 12, 28, 53	0
1	B	391/414 (94%)	1.93	101 (25%) 1 1	8, 16, 50, 64	6 (1%)
All	All	804/828 (97%)	1.39	145 (18%) 2 2	7, 13, 42, 64	6 (0%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	19.9
1	B	397	LEU	17.5
1	B	411	ILE	15.8
1	B	0	MET	15.7
1	B	372	TYR	13.2
1	B	370	VAL	12.6
1	B	401	ALA	12.5
1	B	402	THR	12.4
1	B	368	LYS	12.1
1	B	398	ASP	11.9
1	A	18	PHE	11.4
1	B	343	ALA	10.5
1	B	375	ASN	10.4
1	B	409	THR	10.1
1	B	345	LYS	9.9
1	A	15	VAL	9.6
1	B	374	ILE	9.5
1	B	344	LEU	9.4
1	A	16	LEU	8.9
1	B	379	ILE	8.4
1	B	380	TYR	8.2
1	B	346	THR	7.7
1	B	347	PRO	7.6
1	B	378	HIS	7.5

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Mol	Chain	Res	Type	RSRZ
1	B	-1	GLY	7.4
1	B	400	VAL	7.2
1	B	399	TYR	7.2
1	B	406	GLU	7.1
1	B	404	ILE	7.1
1	B	365	LEU	7.1
1	A	-1	GLY	6.9
1	B	339	ALA	6.9
1	B	373	LEU	6.8
1	B	341	LEU	6.7
1	A	412	GLN	6.5
1	B	340	ARG	6.5
1	B	367	PRO	6.4
1	B	371	GLU	6.4
1	B	350	TRP	6.4
1	B	348	GLY	6.2
1	A	26	GLU	6.1
1	B	377	LYS	6.0
1	A	17	VAL	6.0
1	B	376	GLN	6.0
1	A	25	ARG	5.8
1	B	13	GLN	5.8
1	B	349	THR	5.8
1	B	408	VAL	5.7
1	B	410	LYS	5.7
1	B	37	VAL	5.5
1	B	91	ASP	5.5
1	A	13	GLN	5.5
1	B	405	HIS	5.4
1	B	395	LYS	5.3
1	B	382	LEU	5.2
1	B	353	ILE	5.1
1	B	383	PRO	4.9
1	B	366	ASN	4.8
1	B	396	ASN	4.7
1	B	44	ASP	4.7
1	A	14	PRO	4.7
1	B	385	GLY	4.7
1	B	351	ASN	4.6
1	B	403	SER	4.6
1	A	21	ILE	4.5
1	B	141	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	23	ASP	4.2
1	B	335	SER	4.2
1	B	331	LEU	4.1
1	B	96	GLN	4.1
1	B	407	ALA	4.0
1	B	359	MET	4.0
1	A	1	ALA	3.6
1	A	28	PRO	3.6
1	B	381	LEU	3.5
1	B	357	ILE	3.5
1	B	93	PRO	3.5
1	B	364	GLY	3.5
1	B	342	GLU	3.5
1	B	392	LEU	3.5
1	B	354	THR	3.4
1	B	393	THR	3.4
1	A	22	ALA	3.3
1	A	19	LYS	3.3
1	A	0	MET	3.2
1	B	164	GLU	3.2
1	B	337	LEU	3.1
1	B	369	GLN	3.0
1	B	112	LEU	3.0
1	B	90	ASP	3.0
1	B	338	ARG	3.0
1	A	165	LYS	3.0
1	A	2	PRO	2.9
1	B	360	PHE	2.9
1	B	394	THR	2.9
1	B	38	GLY	2.9
1	B	313	PRO	2.9
1	B	12	ALA	2.9
1	B	332	SER	2.9
1	B	228	PHE	2.8
1	A	220	PHE	2.8
1	B	352	HIS	2.7
1	B	314	GLU	2.7
1	B	35	LEU	2.7
1	B	355	ASP	2.7
1	B	229	ALA	2.7
1	B	165	LYS	2.7
1	A	368	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	141	GLU	2.6
1	B	188	LEU	2.6
1	B	2	PRO	2.6
1	A	27	ASP	2.5
1	B	333[A]	MET	2.5
1	B	163	THR	2.5
1	A	185	ILE	2.5
1	A	162	ASP	2.5
1	B	251	PHE	2.5
1	B	317	HIS	2.5
1	A	387	ILE	2.4
1	A	404	ILE	2.4
1	A	337	LEU	2.4
1	A	164	GLU	2.4
1	A	235	LYS	2.4
1	B	36	GLY	2.4
1	A	147	PHE	2.4
1	B	267	VAL	2.3
1	A	228	PHE	2.3
1	A	353	ILE	2.3
1	B	45	CYS	2.3
1	A	20	LEU	2.2
1	B	253	ALA	2.2
1	A	119	LEU	2.2
1	A	392	LEU	2.2
1	B	225	TYR	2.2
1	B	46	GLN	2.1
1	A	411	ILE	2.1
1	A	371	GLU	2.1
1	A	24	PHE	2.1
1	A	218	PHE	2.1
1	A	64	SER	2.1
1	A	183	PHE	2.1
1	B	64	SER	2.1
1	B	390	CYS	2.1
1	A	295	TRP	2.0
1	A	221	PHE	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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	A	258	24/25	0.98	0.11	-	6,10,14,17	0
1	LLP	B	258	24/25	0.97	0.12	-	8,12,17,19	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.