



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 06:35 PM BST

PDB ID : 4WHX  
Title : X-ray Crystal Structure of an Amino Acid Aminotransferase from Burkholderia pseudomallei Bound to the Co-factor Pyridoxal Phosphate  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID); Fairman, J.W.; Dranow, D.M.; Taylor, B.M.; Lorimer, D.; Edwards, T.E.  
Deposited on : 2014-09-23  
Resolution : 2.05 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 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	:	2.14.4.dev1
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)	:	2.14.4.dev1

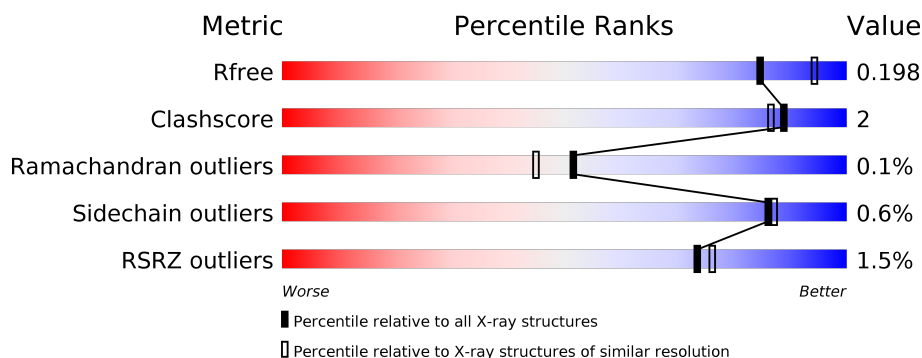
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 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	311	<div> <div>93%</div> <div>5%</div> </div>
1	B	311	<div> <div>%</div> <div>94%</div> </div>
1	C	311	<div> <div>3%</div> <div>94%</div> <div>5%</div> </div>
1	D	311	<div> <div>2%</div> <div>89%</div> <div>9%</div> </div>
1	E	311	<div> <div>2%</div> <div>94%</div> </div>
1	F	311	<div> <div>%</div> <div>94%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15184 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 Branched-chain-amino-acid transaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	P	S	0	1	0
			2372	1497	411	456	1	7			
1	B	306	Total	C	N	O	P	S	0	2	0
			2383	1504	412	459	1	7			
1	C	306	Total	C	N	O	P	S	0	1	0
			2369	1496	412	453	1	7			
1	D	306	Total	C	N	O	P	S	0	1	0
			2361	1489	409	455	1	7			
1	E	306	Total	C	N	O	P	S	0	0	0
			2348	1479	408	453	1	7			
1	F	306	Total	C	N	O	P	S	0	1	0
			2381	1503	413	457	1	7			

There are 24 discrepancies between the modelled and reference sequences:

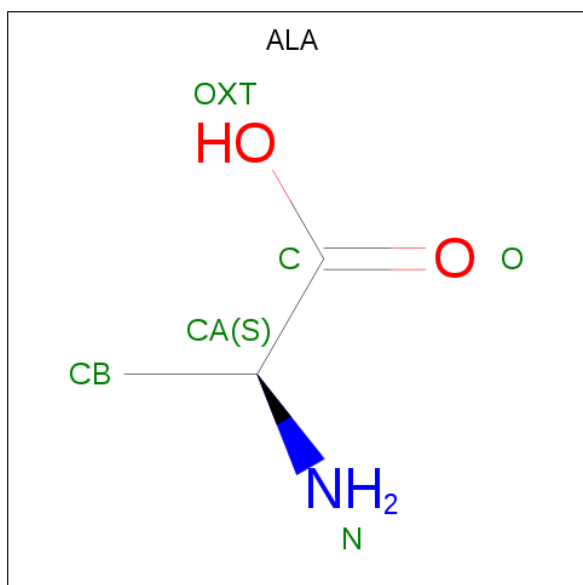
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP B7CIR9
A	-2	PRO	-	expression tag	UNP B7CIR9
A	-1	GLY	-	expression tag	UNP B7CIR9
A	0	SER	-	expression tag	UNP B7CIR9
B	-3	GLY	-	expression tag	UNP B7CIR9
B	-2	PRO	-	expression tag	UNP B7CIR9
B	-1	GLY	-	expression tag	UNP B7CIR9
B	0	SER	-	expression tag	UNP B7CIR9
C	-3	GLY	-	expression tag	UNP B7CIR9
C	-2	PRO	-	expression tag	UNP B7CIR9
C	-1	GLY	-	expression tag	UNP B7CIR9
C	0	SER	-	expression tag	UNP B7CIR9
D	-3	GLY	-	expression tag	UNP B7CIR9
D	-2	PRO	-	expression tag	UNP B7CIR9
D	-1	GLY	-	expression tag	UNP B7CIR9
D	0	SER	-	expression tag	UNP B7CIR9
E	-3	GLY	-	expression tag	UNP B7CIR9

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	PRO	-	expression tag	UNP B7CIR9
E	-1	GLY	-	expression tag	UNP B7CIR9
E	0	SER	-	expression tag	UNP B7CIR9
F	-3	GLY	-	expression tag	UNP B7CIR9
F	-2	PRO	-	expression tag	UNP B7CIR9
F	-1	GLY	-	expression tag	UNP B7CIR9
F	0	SER	-	expression tag	UNP B7CIR9

- Molecule 2 is ALANINE (three-letter code: ALA) (formula:  $C_3H_7NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			6	3	1	2		
2	C	1	Total	C	N	O	0	0
			6	3	1	2		
2	D	1	Total	C	N	O	0	0
			6	3	1	2		
2	E	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	167	Total	O	0	0
			167	167		
4	C	140	Total	O	0	0
			140	140		
4	D	117	Total	O	0	0
			117	117		
4	E	144	Total	O	0	0
			144	144		
4	F	177	Total	O	0	0
			177	177		

### 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.

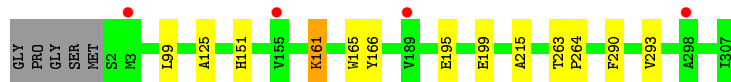
- Molecule 1: Branched-chain-amino-acid transaminase

Chain A: 



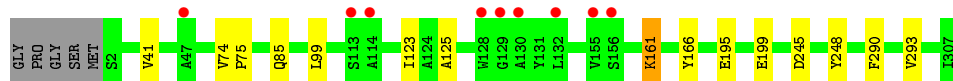
- Molecule 1: Branched-chain-amino-acid transaminase

Chain B: 




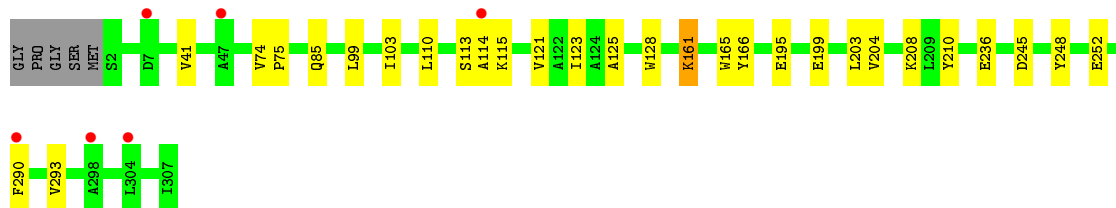
- Molecule 1: Branched-chain-amino-acid transaminase

Chain C: 



- Molecule 1: Branched-chain-amino-acid transaminase

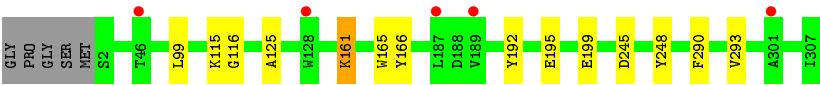
Chain D: 



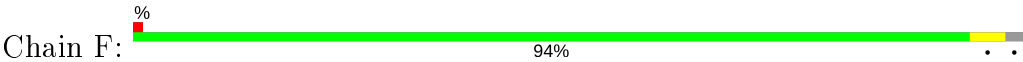
- Molecule 1: Branched-chain-amino-acid transaminase

Chain E: 





● Molecule 1: Branched-chain-amino-acid transaminase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.14Å 230.35Å 77.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.25 – 2.05 48.33 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.0 (42.25-2.05) 98.0 (48.33-2.05)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1769)	Depositor
R, $R_{free}$	0.162 , 0.198 0.164 , 0.198	Depositor DCC
$R_{free}$ test set	5630 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.37% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, EDO

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	0.29	0/2397	0.48	0/3252
1	B	0.28	0/2411	0.48	0/3269
1	C	0.27	0/2394	0.47	0/3247
1	D	0.26	0/2386	0.47	0/3240
1	E	0.28	0/2370	0.46	0/3220
1	F	0.29	0/2406	0.47	0/3261
All	All	0.28	0/14364	0.47	0/19489

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	2372	0	2284	9	0
1	B	2383	0	2304	8	0
1	C	2369	0	2281	9	0
1	D	2361	0	2261	14	0
1	E	2348	0	2235	8	0
1	F	2381	0	2309	9	0
2	A	6	0	4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	0	4	0	0
2	D	6	0	4	1	0
2	E	6	0	4	0	0
3	A	4	0	6	0	0
3	E	4	0	6	0	0
4	A	193	0	0	0	0
4	B	167	0	0	0	0
4	C	140	0	0	0	0
4	D	117	0	0	0	0
4	E	144	0	0	0	0
4	F	177	0	0	0	0
All	All	15184	0	13702	53	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 (53) 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:E:161:LLP:O3	1:E:166:TYR:OH	1.93	0.86
1:B:161:LLP:O3	1:B:166:TYR:OH	1.94	0.84
1:F:161:LLP:O3	1:F:166:TYR:OH	2.00	0.80
1:D:113:SER:O	1:D:115:LYS:N	2.15	0.79
1:A:161:LLP:O3	1:A:166:TYR:OH	2.03	0.76
1:D:161:LLP:O3	1:D:166:TYR:OH	2.02	0.76
1:D:195:GLU:HB2	1:D:199:GLU:O	2.01	0.60
1:D:103:ILE:HG12	1:D:121:VAL:HG22	1.84	0.59
1:D:99:LEU:HD23	1:D:125:ALA:HB2	1.86	0.57
1:C:161:LLP:O3	1:C:166:TYR:OH	2.10	0.57
1:E:195:GLU:HB2	1:E:199:GLU:O	2.05	0.56
1:E:161:LLP:O3	1:E:161:LLP:NZ	2.38	0.56
1:C:85:GLN:HG3	1:C:123:ILE:HD13	1.89	0.54
1:A:195:GLU:HB2	1:A:199:GLU:O	2.08	0.54
1:A:144:LYS:NZ	1:F:175:GLU:OE2	2.33	0.53
1:F:290:PHE:HA	1:F:293:VAL:HG22	1.91	0.53
1:C:195:GLU:HB2	1:C:199:GLU:O	2.09	0.52
1:B:99:LEU:HD23	1:B:125:ALA:HB2	1.91	0.52
1:F:161:LLP:NZ	1:F:161:LLP:O3	2.43	0.51
1:B:161:LLP:O3	1:B:161:LLP:NZ	2.45	0.50
1:E:290:PHE:HA	1:E:293:VAL:HG22	1.95	0.49
1:D:85:GLN:HG3	1:D:123:ILE:HD13	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:LEU:HD23	1:E:125:ALA:HB2	1.95	0.48
1:F:103:ILE:HG12	1:F:121:VAL:HG22	1.96	0.47
1:C:161:LLP:O3	1:C:161:LLP:NZ	2.47	0.47
1:A:161:LLP:O3	1:A:161:LLP:NZ	2.47	0.47
1:C:99:LEU:HD23	1:C:125:ALA:HB2	1.96	0.47
1:A:142:ARG:NE	1:A:267:GLU:OE1	2.47	0.47
1:F:245:ASP:HA	1:F:248:TYR:CD2	2.50	0.46
1:C:74:VAL:HA	1:C:75:PRO:HD3	1.79	0.46
1:D:245:ASP:HA	1:D:248:TYR:CD2	2.51	0.46
1:C:290:PHE:HA	1:C:293:VAL:HG22	1.99	0.45
1:C:245:ASP:HA	1:C:248:TYR:CD2	2.52	0.45
1:B:215:ALA:HB1	1:F:192:TYR:OH	2.17	0.44
1:E:115:LYS:HA	1:E:116:GLY:HA2	1.55	0.44
1:D:208:LYS:NZ	1:D:236:GLU:OE1	2.41	0.44
1:D:290:PHE:HA	1:D:293:VAL:HG22	2.00	0.43
1:D:204:VAL:HB	1:D:252:GLU:HB2	2.00	0.43
1:A:159:ARG:NH1	1:A:214:LEU:O	2.52	0.43
1:A:74:VAL:HA	1:A:75:PRO:HD3	1.83	0.42
1:B:290:PHE:HA	1:B:293:VAL:HG22	2.02	0.42
1:D:74:VAL:HA	1:D:75:PRO:HD3	1.85	0.42
1:A:155:VAL:HG11	1:B:151:HIS:HA	2.01	0.42
1:C:41:VAL:HB	1:C:99:LEU:HB2	2.02	0.42
1:D:203:LEU:HG	1:D:210:TYR:HB2	2.02	0.42
1:E:192:TYR:OH	1:F:215:ALA:HB1	2.20	0.41
1:D:41:VAL:HB	1:D:99:LEU:HB2	2.02	0.41
1:F:134:GLU:OE1	1:F:287:SER:OG	2.38	0.41
1:E:245:ASP:HA	1:E:248:TYR:CD2	2.56	0.41
1:B:195:GLU:HB2	1:B:199:GLU:O	2.20	0.41
1:D:161:LLP:HE2	2:D:401:ALA:HB1	2.03	0.41
1:B:263:THR:HA	1:B:264:PRO:HD3	1.95	0.41
1:A:41:VAL:HB	1:A:99:LEU:HB2	2.04	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	304/311 (98%)	295 (97%)	9 (3%)	0	100	100
1	B	305/311 (98%)	297 (97%)	8 (3%)	0	100	100
1	C	304/311 (98%)	294 (97%)	10 (3%)	0	100	100
1	D	304/311 (98%)	295 (97%)	8 (3%)	1 (0%)	41	31
1	E	303/311 (97%)	296 (98%)	7 (2%)	0	100	100
1	F	304/311 (98%)	293 (96%)	11 (4%)	0	100	100
All	All	1824/1866 (98%)	1770 (97%)	53 (3%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	114	ALA

### 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	237/249 (95%)	234 (99%)	3 (1%)	69	67
1	B	240/249 (96%)	239 (100%)	1 (0%)	91	91
1	C	235/249 (94%)	235 (100%)	0	100	100
1	D	235/249 (94%)	232 (99%)	3 (1%)	69	67
1	E	232/249 (93%)	231 (100%)	1 (0%)	91	91
1	F	240/249 (96%)	239 (100%)	1 (0%)	91	91
All	All	1419/1494 (95%)	1410 (99%)	9 (1%)	86	87

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

Mol	Chain	Res	Type
1	A	128	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	165	TRP
1	A	283	GLU
1	B	165	TRP
1	D	110	LEU
1	D	128	TRP
1	D	165	TRP
1	E	165	TRP
1	F	165	TRP

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

Mol	Chain	Res	Type
1	C	174	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	D	161	1	23,24,25	2.51	5 (21%)	25,32,34	1.47	4 (16%)
1	LLP	F	161	1	23,24,25	2.53	5 (21%)	25,32,34	1.40	4 (16%)
1	LLP	B	161	1	23,24,25	2.40	5 (21%)	25,32,34	1.47	5 (20%)
1	LLP	A	161	1	23,24,25	2.48	5 (21%)	25,32,34	1.42	4 (16%)
1	LLP	C	161	1	23,24,25	2.47	5 (21%)	25,32,34	1.42	3 (12%)
1	LLP	E	161	1	23,24,25	2.55	5 (21%)	25,32,34	1.44	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	D	161	1	-	4/16/17/19	0/1/1/1
1	LLP	F	161	1	-	0/16/17/19	0/1/1/1
1	LLP	B	161	1	-	2/16/17/19	0/1/1/1
1	LLP	A	161	1	-	2/16/17/19	0/1/1/1
1	LLP	C	161	1	-	2/16/17/19	0/1/1/1
1	LLP	E	161	1	-	2/16/17/19	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	161	LLP	C3-C2	7.36	1.48	1.40
1	F	161	LLP	C3-C2	7.18	1.48	1.40
1	C	161	LLP	C3-C2	7.17	1.48	1.40
1	D	161	LLP	C3-C2	7.07	1.48	1.40
1	A	161	LLP	C3-C2	7.03	1.47	1.40
1	B	161	LLP	C3-C2	6.77	1.47	1.40
1	D	161	LLP	C4'-NZ	5.51	1.45	1.27
1	E	161	LLP	C4'-NZ	5.50	1.45	1.27
1	D	161	LLP	C4-C5	5.42	1.48	1.42
1	C	161	LLP	C4'-NZ	5.41	1.45	1.27
1	F	161	LLP	C4-C5	5.41	1.48	1.42
1	B	161	LLP	C4'-NZ	5.38	1.45	1.27
1	F	161	LLP	C4'-NZ	5.38	1.45	1.27
1	A	161	LLP	C4'-NZ	5.34	1.45	1.27
1	E	161	LLP	C4-C5	5.22	1.48	1.42
1	A	161	LLP	C4-C5	5.20	1.48	1.42
1	F	161	LLP	C4-C3	4.96	1.48	1.40
1	C	161	LLP	C4-C5	4.94	1.48	1.42
1	B	161	LLP	C4-C5	4.85	1.48	1.42
1	A	161	LLP	C4-C3	4.65	1.47	1.40
1	C	161	LLP	C4-C3	4.64	1.47	1.40
1	E	161	LLP	C4-C3	4.55	1.47	1.40
1	B	161	LLP	C4-C3	4.47	1.47	1.40
1	D	161	LLP	C4-C3	4.46	1.47	1.40
1	E	161	LLP	C4-C4'	2.97	1.52	1.46
1	D	161	LLP	C4-C4'	2.59	1.51	1.46
1	F	161	LLP	C4-C4'	2.56	1.51	1.46
1	A	161	LLP	C4-C4'	2.55	1.51	1.46
1	C	161	LLP	C4-C4'	2.50	1.51	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	LLP	C4-C4'	2.44	1.51	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	LLP	C4-C4'-NZ	-3.59	107.84	124.31
1	C	161	LLP	C4-C4'-NZ	-3.51	108.19	124.31
1	D	161	LLP	C4-C4'-NZ	-3.37	108.84	124.31
1	F	161	LLP	C4-C4'-NZ	-3.33	109.02	124.31
1	A	161	LLP	C4-C4'-NZ	-3.25	109.37	124.31
1	D	161	LLP	C4-C3-C2	-3.20	118.21	120.19
1	C	161	LLP	C4-C3-C2	-3.17	118.23	120.19
1	E	161	LLP	C4-C4'-NZ	-3.12	109.98	124.31
1	A	161	LLP	C4-C3-C2	-3.06	118.30	120.19
1	E	161	LLP	C3-C4-C5	-2.94	116.01	118.26
1	F	161	LLP	C4-C3-C2	-2.88	118.41	120.19
1	F	161	LLP	C6-N1-C2	2.82	124.38	119.17
1	B	161	LLP	C4-C3-C2	-2.60	118.58	120.19
1	B	161	LLP	C6-N1-C2	2.42	123.64	119.17
1	E	161	LLP	C4-C3-C2	-2.34	118.74	120.19
1	C	161	LLP	C6-N1-C2	2.32	123.47	119.17
1	B	161	LLP	C3-C4-C5	-2.26	116.53	118.26
1	F	161	LLP	C3-C4-C5	-2.24	116.54	118.26
1	A	161	LLP	C3-C4-C5	-2.24	116.54	118.26
1	D	161	LLP	C6-N1-C2	2.20	123.25	119.17
1	B	161	LLP	C2'-C2-N1	2.18	121.92	117.67
1	D	161	LLP	OP3-P-OP2	2.15	115.84	107.64
1	E	161	LLP	C6-N1-C2	2.11	123.07	119.17
1	A	161	LLP	C2'-C2-C3	-2.07	118.33	120.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	161	LLP	N-CA-CB-CG
1	D	161	LLP	C-CA-CB-CG
1	B	161	LLP	C-CA-CB-CG
1	A	161	LLP	N-CA-CB-CG
1	A	161	LLP	C-CA-CB-CG
1	C	161	LLP	C-CA-CB-CG
1	E	161	LLP	C-CA-CB-CG
1	D	161	LLP	CD-CE-NZ-C4'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	B	161	LLP	N-CA-CB-CG
1	C	161	LLP	N-CA-CB-CG
1	E	161	LLP	N-CA-CB-CG
1	D	161	LLP	C3-C4-C4'-NZ

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	161	LLP	2	0
1	F	161	LLP	2	0
1	B	161	LLP	2	0
1	A	161	LLP	2	0
1	C	161	LLP	2	0
1	E	161	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	ALA	C	401	-	2,5,5	0.46	0	2,6,6	0.39	0
2	ALA	A	401	-	2,5,5	0.49	0	2,6,6	0.22	0
3	EDO	A	402	-	3,3,3	0.44	0	2,2,2	0.39	0
2	ALA	E	401	-	2,5,5	0.41	0	2,6,6	0.37	0
3	EDO	E	402	-	3,3,3	0.49	0	2,2,2	0.30	0
2	ALA	D	401	-	2,5,5	0.47	0	2,6,6	0.48	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
2	ALA	C	401	-	-	0/0/4/4	-
2	ALA	A	401	-	-	0/0/4/4	-
3	EDO	A	402	-	-	0/1/1/1	-
2	ALA	E	401	-	-	0/0/4/4	-
3	EDO	E	402	-	-	0/1/1/1	-
2	ALA	D	401	-	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	ALA	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, 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	305/311 (98%)	-0.24	1 (0%)	94 94	21, 30, 48, 74	0
1	B	305/311 (98%)	-0.12	4 (1%)	77 79	20, 31, 50, 61	0
1	C	305/311 (98%)	0.01	9 (2%)	50 54	20, 34, 59, 74	0
1	D	305/311 (98%)	0.05	6 (1%)	65 69	21, 40, 63, 78	0
1	E	305/311 (98%)	0.07	5 (1%)	72 74	21, 37, 58, 74	0
1	F	305/311 (98%)	-0.08	3 (0%)	82 84	20, 29, 45, 66	0
All	All	1830/1866 (98%)	-0.05	28 (1%)	73 76	20, 33, 56, 78	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	114	ALA	4.3
1	E	128	TRP	3.9
1	D	47	ALA	3.5
1	D	298	ALA	3.4
1	C	128	TRP	3.3
1	F	153	VAL	3.1
1	D	7	ASP	3.1
1	C	47	ALA	2.9
1	E	189	VAL	2.8
1	E	301	ALA	2.8
1	C	155	VAL	2.7
1	D	114	ALA	2.6
1	D	290	PHE	2.6
1	B	298	ALA	2.5
1	A	114	ALA	2.5
1	C	113	SER	2.4
1	C	132	LEU	2.3
1	D	304	LEU	2.2
1	B	155	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	3	MET	2.2
1	F	189	VAL	2.2
1	C	130	ALA	2.1
1	B	189	VAL	2.1
1	C	129	GLY	2.1
1	E	46	THR	2.1
1	C	156	SER	2.1
1	F	3	MET	2.1
1	E	187	LEU	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	D	161	24/25	0.97	0.10	29,36,38,40	0
1	LLP	B	161	24/25	0.97	0.11	22,25,28,30	0
1	LLP	E	161	24/25	0.97	0.10	30,33,36,37	0
1	LLP	A	161	24/25	0.98	0.11	26,30,34,37	0
1	LLP	C	161	24/25	0.98	0.10	25,28,30,32	0
1	LLP	F	161	24/25	0.98	0.12	24,28,31,32	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ALA	C	401	6/6	0.75	0.24	53,54,55,56	0
2	ALA	A	401	6/6	0.76	0.23	49,49,50,60	0
2	ALA	E	401	6/6	0.82	0.21	61,63,63,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ALA	D	401	6/6	0.83	0.21	63,63,64,64	0
3	EDO	E	402	4/4	0.90	0.21	43,44,44,45	0
3	EDO	A	402	4/4	0.94	0.19	50,50,50,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.