



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2019 – 10:12 PM EDT

PDB ID : 5NSF  
Title : Structure of AzuAla  
Authors : Martins, B.M.  
Deposited on : 2017-04-26  
Resolution : 2.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	2.4
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

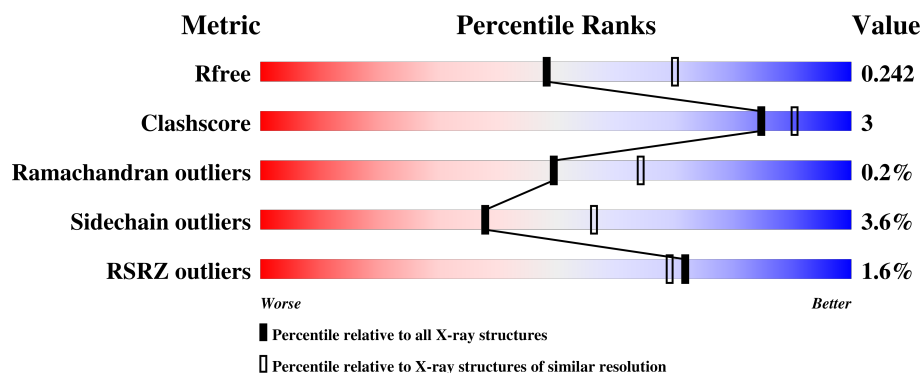
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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))
$R_{free}$	111664	4090 (2.44-2.40)
Clashscore	122126	4587 (2.44-2.40)
Ramachandran outliers	120053	4522 (2.44-2.40)
Sidechain outliers	120020	4523 (2.44-2.40)
RSRZ outliers	108989	3987 (2.44-2.40)

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	318	 88% 8% .
1	B	318	 87% 8% . .
1	C	318	 88% 8% .
1	D	318	 87% 8% . .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20326 atoms, of which 10199 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 Tyrosine-tRNA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	306	Total	C	H	N	O	S	0	2	0
			5004	1572	2541	422	456	13			
1	A	305	Total	C	H	N	O	S	0	2	0
			4985	1567	2530	421	455	12			
1	C	306	Total	C	H	N	O	S	0	2	0
			4995	1570	2535	422	456	12			
1	D	305	Total	C	H	N	O	S	0	1	0
			4966	1562	2519	418	455	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP Q57834
B	-10	ARG	-	expression tag	UNP Q57834
B	-9	GLY	-	expression tag	UNP Q57834
B	-8	SER	-	expression tag	UNP Q57834
B	-7	HIS	-	expression tag	UNP Q57834
B	-6	HIS	-	expression tag	UNP Q57834
B	-5	HIS	-	expression tag	UNP Q57834
B	-4	HIS	-	expression tag	UNP Q57834
B	-3	HIS	-	expression tag	UNP Q57834
B	-2	HIS	-	expression tag	UNP Q57834
B	-1	GLY	-	expression tag	UNP Q57834
B	0	SER	-	expression tag	UNP Q57834
B	32	GLY	TYR	conflict	UNP Q57834
B	65	TRP	LEU	conflict	UNP Q57834
B	70	GLY	HIS	conflict	UNP Q57834
B	108	HIS	PHE	conflict	UNP Q57834
B	109	ASN	GLN	conflict	UNP Q57834
B	158	ALA	ASP	conflict	UNP Q57834
B	162	ASN	LEU	conflict	UNP Q57834
B	286	ARG	ASP	conflict	UNP Q57834
A	-11	MET	-	initiating methionine	UNP Q57834

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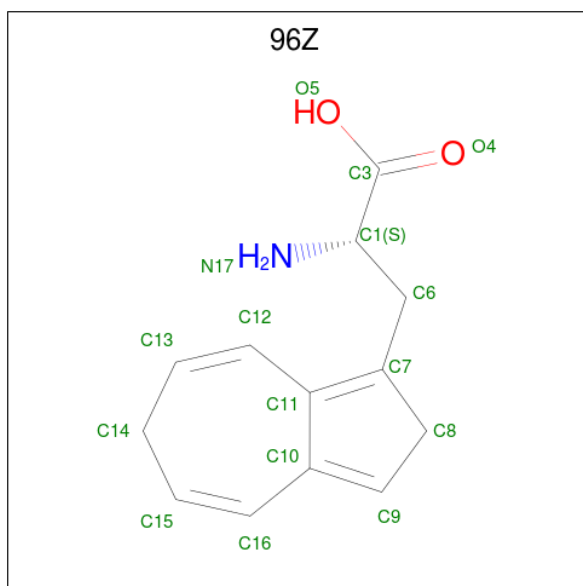
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	ARG	-	expression tag	UNP Q57834
A	-9	GLY	-	expression tag	UNP Q57834
A	-8	SER	-	expression tag	UNP Q57834
A	-7	HIS	-	expression tag	UNP Q57834
A	-6	HIS	-	expression tag	UNP Q57834
A	-5	HIS	-	expression tag	UNP Q57834
A	-4	HIS	-	expression tag	UNP Q57834
A	-3	HIS	-	expression tag	UNP Q57834
A	-2	HIS	-	expression tag	UNP Q57834
A	-1	GLY	-	expression tag	UNP Q57834
A	0	SER	-	expression tag	UNP Q57834
A	32	GLY	TYR	conflict	UNP Q57834
A	65	TRP	LEU	conflict	UNP Q57834
A	70	GLY	HIS	conflict	UNP Q57834
A	108	HIS	PHE	conflict	UNP Q57834
A	109	ASN	GLN	conflict	UNP Q57834
A	158	ALA	ASP	conflict	UNP Q57834
A	162	ASN	LEU	conflict	UNP Q57834
A	286	ARG	ASP	conflict	UNP Q57834
C	-11	MET	-	initiating methionine	UNP Q57834
C	-10	ARG	-	expression tag	UNP Q57834
C	-9	GLY	-	expression tag	UNP Q57834
C	-8	SER	-	expression tag	UNP Q57834
C	-7	HIS	-	expression tag	UNP Q57834
C	-6	HIS	-	expression tag	UNP Q57834
C	-5	HIS	-	expression tag	UNP Q57834
C	-4	HIS	-	expression tag	UNP Q57834
C	-3	HIS	-	expression tag	UNP Q57834
C	-2	HIS	-	expression tag	UNP Q57834
C	-1	GLY	-	expression tag	UNP Q57834
C	0	SER	-	expression tag	UNP Q57834
C	32	GLY	TYR	conflict	UNP Q57834
C	65	TRP	LEU	conflict	UNP Q57834
C	70	GLY	HIS	conflict	UNP Q57834
C	108	HIS	PHE	conflict	UNP Q57834
C	109	ASN	GLN	conflict	UNP Q57834
C	158	ALA	ASP	conflict	UNP Q57834
C	162	ASN	LEU	conflict	UNP Q57834
C	286	ARG	ASP	conflict	UNP Q57834
D	-11	MET	-	initiating methionine	UNP Q57834
D	-10	ARG	-	expression tag	UNP Q57834
D	-9	GLY	-	expression tag	UNP Q57834

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	SER	-	expression tag	UNP Q57834
D	-7	HIS	-	expression tag	UNP Q57834
D	-6	HIS	-	expression tag	UNP Q57834
D	-5	HIS	-	expression tag	UNP Q57834
D	-4	HIS	-	expression tag	UNP Q57834
D	-3	HIS	-	expression tag	UNP Q57834
D	-2	HIS	-	expression tag	UNP Q57834
D	-1	GLY	-	expression tag	UNP Q57834
D	0	SER	-	expression tag	UNP Q57834
D	32	GLY	TYR	conflict	UNP Q57834
D	65	TRP	LEU	conflict	UNP Q57834
D	70	GLY	HIS	conflict	UNP Q57834
D	108	HIS	PHE	conflict	UNP Q57834
D	109	ASN	GLN	conflict	UNP Q57834
D	158	ALA	ASP	conflict	UNP Q57834
D	162	ASN	LEU	conflict	UNP Q57834
D	286	ARG	ASP	conflict	UNP Q57834

- Molecule 2 is (2 {S})-2-azanyl-3-(2,6-dihydroazulen-1-yl)propanoic acid (three-letter code: 96Z) (formula: C<sub>13</sub>H<sub>15</sub>NO<sub>2</sub>).



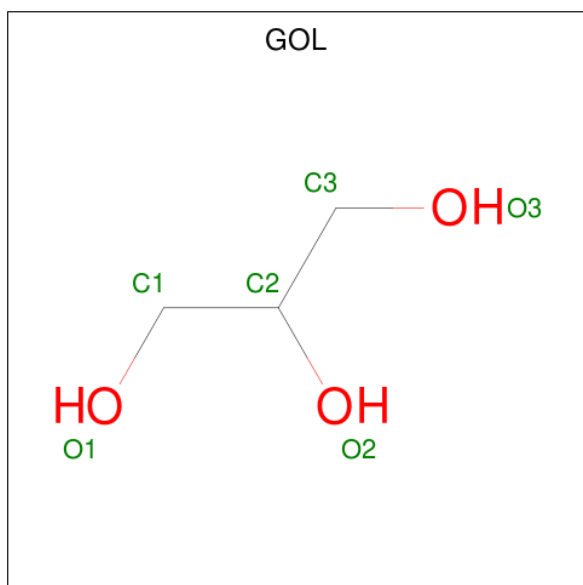
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			28	13	12	1	2		
2	A	1	Total	C	H	N	O	0	0
			28	13	12	1	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	0	0
			28	13	12	1	2		
2	D	1	Total	C	H	N	O	0	0
			28	13	12	1	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

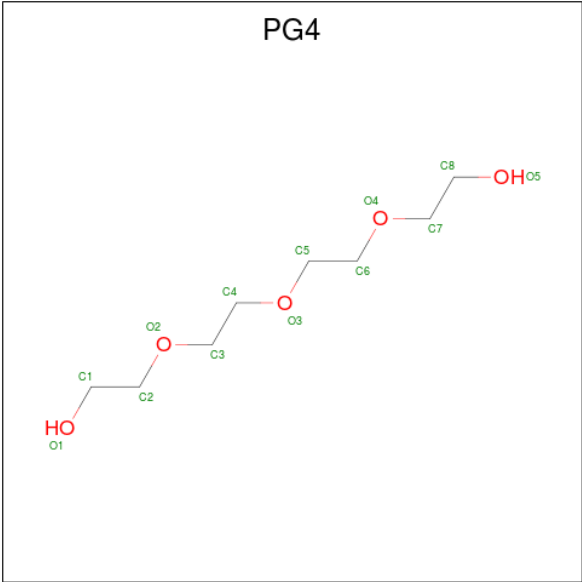


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	2	Total	Ca	0	0
			2	2		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			18	5	10	3		

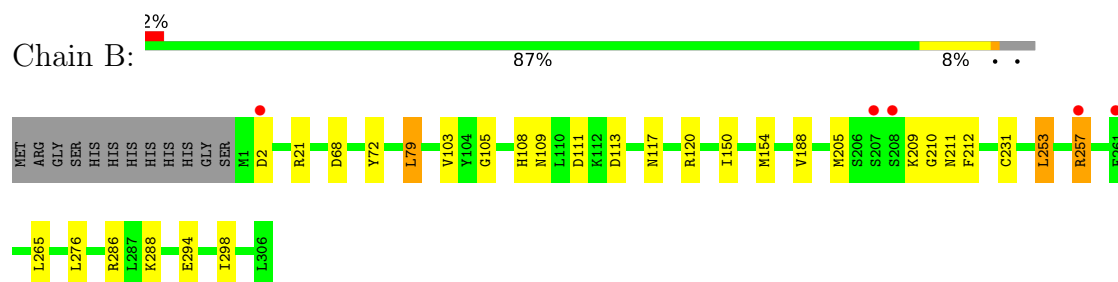
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	61	Total	O	0	0
			61	61		
6	A	55	Total	O	0	0
			55	55		
6	C	67	Total	O	0	0
			67	67		
6	D	32	Total	O	0	0
			32	32		

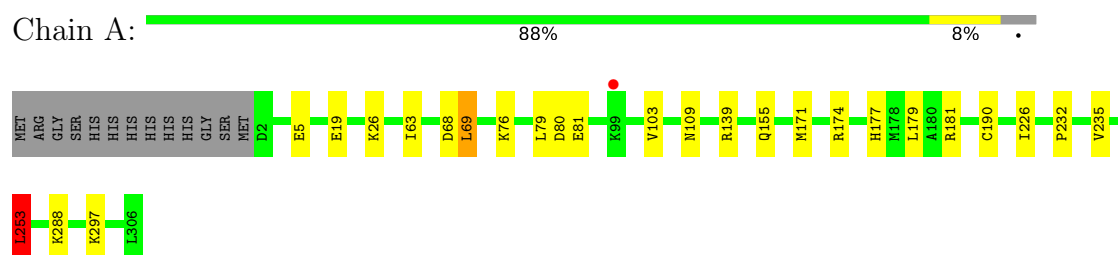
### 3 Residue-property plots [i](#)

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.

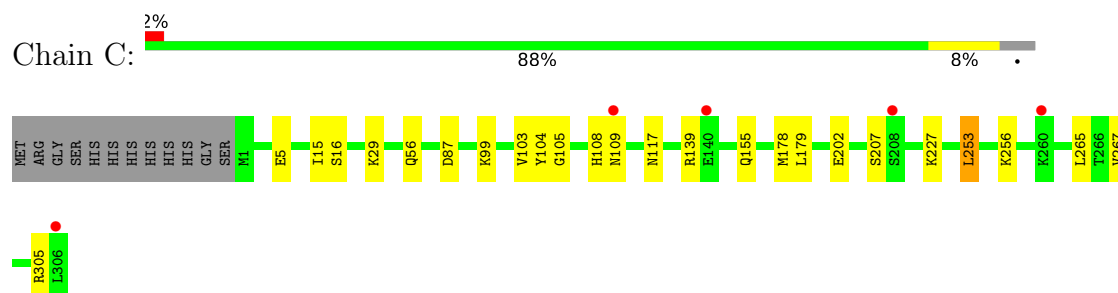
#### • Molecule 1: Tyrosine-tRNA ligase



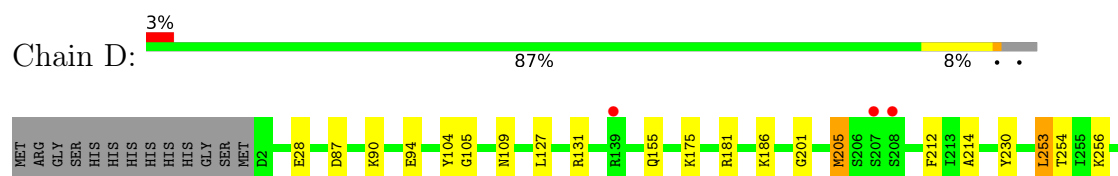
#### • Molecule 1: Tyrosine-tRNA ligase



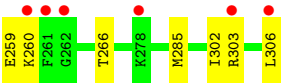
#### • Molecule 1: Tyrosine-tRNA ligase



#### • Molecule 1: Tyrosine-tRNA ligase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.14Å 70.63Å 77.62Å 85.70° 89.75° 83.42°	Depositor
Resolution (Å)	46.27 – 2.43 46.27 – 2.43	Depositor EDS
% Data completeness (in resolution range)	93.4 (46.27-2.43) 93.5 (46.27-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.64 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.10.1-2155_1168: ???)	Depositor
R, $R_{free}$	0.182 , 0.240 0.185 , 0.242	Depositor DCC
$R_{free}$ test set	2089 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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: GOL, CA, PG4, 96Z

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	0/2502	0.50	1/3357 (0.0%)
1	B	0.30	0/2510	0.50	2/3367 (0.1%)
1	C	0.26	0/2507	0.46	0/3364
1	D	0.39	1/2491 (0.0%)	0.53	0/3343
All	All	0.31	1/10010 (0.0%)	0.50	3/13431 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	205	MET	CA-CB	5.02	1.65	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	253	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	253	LEU	CA-CB-CG	5.20	127.26	115.30

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	2455	2530	2533	11	1
1	B	2463	2541	2545	19	0
1	C	2460	2535	2538	9	0
1	D	2447	2519	2520	12	1
2	A	16	12	0	0	0
2	B	16	12	0	0	0
2	C	16	12	0	1	0
2	D	16	12	0	1	0
3	A	6	8	8	0	0
3	B	6	8	8	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	8	10	9	1	0
6	A	55	0	0	0	0
6	B	61	0	0	1	0
6	C	67	0	0	3	0
6	D	32	0	0	2	0
All	All	10127	10199	10161	51	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 3.

The worst 5 of 51 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:186:LYS:NZ	6:D:501:HOH:O	2.00	0.93
1:D:90:LYS:NZ	1:D:94:GLU:OE2	2.16	0.79
1:C:87:ASP:OD1	1:C:104:TYR:OH	2.08	0.71
1:C:155:GLN:OE1	2:C:401:96Z:N17	2.28	0.67
1:A:19:GLU:OE2	1:A:181:ARG:NH2	2.34	0.61

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)
1:A:5:GLU:OE2	1:D:254:THR:OG1[1_556]	2.17	0.03

## 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	305/318 (96%)	302 (99%)	3 (1%)	0	100	100
1	B	306/318 (96%)	302 (99%)	3 (1%)	1 (0%)	43	57
1	C	306/318 (96%)	304 (99%)	2 (1%)	0	100	100
1	D	304/318 (96%)	298 (98%)	5 (2%)	1 (0%)	43	57
All	All	1221/1272 (96%)	1206 (99%)	13 (1%)	2 (0%)	49	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	210	GLY
1	D	259	GLU

### 5.3.2 Protein sidechains [i](#)

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	266/275 (97%)	256 (96%)	10 (4%)	36	54
1	B	267/275 (97%)	261 (98%)	6 (2%)	55	73
1	C	266/275 (97%)	254 (96%)	12 (4%)	30	46
1	D	265/275 (96%)	255 (96%)	10 (4%)	36	54
All	All	1064/1100 (97%)	1026 (96%)	38 (4%)	38	56

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	117	ASN
1	C	202	GLU
1	D	285	MET
1	C	178	MET
1	C	207	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

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	96Z	A	401	-	12,17,17	1.87	4 (33%)	6,23,23	1.47	1 (16%)
3	GOL	A	402	-	5,5,5	0.37	0	5,5,5	0.19	0
5	PG4	A	405	-	7,7,12	0.51	0	6,6,11	0.17	0
2	96Z	B	401	-	12,17,17	1.87	4 (33%)	6,23,23	1.61	1 (16%)
3	GOL	B	402	-	5,5,5	0.37	0	5,5,5	0.16	0
2	96Z	C	401	-	12,17,17	1.87	4 (33%)	6,23,23	1.48	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	96Z	D	401	-	12,17,17	1.87	4 (33%)	6,23,23	1.67	2 (33%)

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	96Z	A	401	-	-	0/4/29/29	0/2/2/2
3	GOL	A	402	-	-	0/4/4/4	-
5	PG4	A	405	-	-	1/5/5/10	-
2	96Z	B	401	-	-	0/4/29/29	0/2/2/2
3	GOL	B	402	-	-	3/4/4/4	-
2	96Z	C	401	-	-	0/4/29/29	0/2/2/2
2	96Z	D	401	-	-	0/4/29/29	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	96Z	C9-C10	4.17	1.39	1.34
2	A	401	96Z	C9-C10	4.16	1.39	1.34
2	B	401	96Z	C9-C10	4.14	1.39	1.34
2	C	401	96Z	C9-C10	4.13	1.39	1.34
2	D	401	96Z	C12-C11	2.66	1.49	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	96Z	C16-C10-C9	-2.82	121.11	126.24
2	D	401	96Z	C16-C10-C9	-2.79	121.16	126.24
2	C	401	96Z	C16-C10-C9	-2.71	121.31	126.24
2	A	401	96Z	C16-C10-C9	-2.60	121.52	126.24
2	D	401	96Z	C1-C6-C7	-2.20	110.23	114.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	GOL	O1-C1-C2-O2
3	B	402	GOL	O1-C1-C2-C3
5	A	405	PG4	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
3	B	402	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	PG4	1	0
2	C	401	96Z	1	0
2	D	401	96Z	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 [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	305/318 (95%)	-0.14	1 (0%) 93 93	20, 38, 65, 89	0
1	B	306/318 (96%)	-0.11	5 (1%) 72 69	21, 39, 67, 148	0
1	C	306/318 (96%)	-0.12	5 (1%) 72 69	24, 38, 66, 96	0
1	D	305/318 (95%)	0.13	9 (2%) 50 47	25, 47, 81, 109	0
All	All	1222/1272 (96%)	-0.06	20 (1%) 72 69	20, 40, 72, 148	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	306	LEU	4.6
1	D	261	PHE	4.5
1	C	208	SER	4.3
1	B	208	SER	3.2
1	D	139	ARG	3.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 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. 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	402	6/6	0.81	0.15	60,73,87,91	0
4	CA	A	404	1/1	0.84	0.10	78,78,78,78	0
5	PG4	A	405	8/13	0.86	0.37	27,37,62,62	0
2	96Z	D	401	16/16	0.91	0.15	32,44,55,59	0
4	CA	B	403	1/1	0.91	0.11	94,94,94,94	0
2	96Z	A	401	16/16	0.92	0.18	23,38,48,53	0
4	CA	A	403	1/1	0.92	0.14	54,54,54,54	0
3	GOL	B	402	6/6	0.92	0.28	55,66,77,79	0
2	96Z	B	401	16/16	0.93	0.14	24,36,46,56	0
2	96Z	C	401	16/16	0.94	0.14	24,39,51,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.