

# wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 05:02 pm GMT

PDB ID : 6YAB

Title: Crystal structure of PnrA from S. pneumoniae in complex with uridine

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Deposited on : 2020-03-12

Resolution : 2.30 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

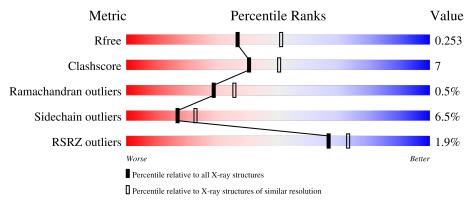
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$		
$R_{free}$	130704	5042 (2.30-2.30)		
Clashscore	141614	5643 (2.30-2.30)		
Ramachandran outliers	138981	5575 (2.30-2.30)		
Sidechain outliers	138945	5575 (2.30-2.30)		
RSRZ outliers	127900	4938 (2.30-2.30)		

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 >=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 <=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	BBB	331	83%	14%	•
1	CCC	331	80%	18%	
2	AAA	329	83%	15%	•
3	DDD	330	86%	11%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NI	DDD	401	-	-	X	-
7	ACT	BBB	404	-	-	X	-



# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10272 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 Lipoprotein.

$\mathbf{Mol}$	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	CCC	331	Total 2483	C 1552	N 424	O 506	S	0	1	0	
			2400	1002	424	500	1				
1	BBB	330	Total	$\mathbf{C}$	N	Ο	S	0	1 0	0	
1	מממ	330	2477	1549	423	504	1		1	U	

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	3	SER	-	expression tag	UNP A0A0H2UPF3
CCC	4	SER	-	expression tag	UNP A0A0H2UPF3
CCC	5	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	6	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	7	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	8	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	9	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	10	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	11	MET	-	expression tag	UNP A0A0H2UPF3
CCC	12	SER	-	expression tag	UNP A0A0H2UPF3
CCC	13	GLY	-	expression tag	UNP A0A0H2UPF3
CCC	14	GLU	-	expression tag	UNP A0A0H2UPF3
CCC	15	ASN	-	expression tag	UNP A0A0H2UPF3
CCC	16	LEU	-	expression tag	UNP A0A0H2UPF3
CCC	17	TYR	-	expression tag	UNP A0A0H2UPF3
CCC	18	PHE	-	expression tag	UNP A0A0H2UPF3
CCC	19	GLN	-	expression tag	UNP A0A0H2UPF3
CCC	20	GLY	-	expression tag	UNP A0A0H2UPF3
CCC	21	ALA	-	expression tag	UNP A0A0H2UPF3
CCC	22	SER	-	expression tag	UNP A0A0H2UPF3
BBB	3	SER	-	expression tag	UNP A0A0H2UPF3
BBB	4	SER	-	expression tag	UNP A0A0H2UPF3
BBB	5	HIS	-	expression tag	UNP A0A0H2UPF3
BBB	6	HIS	-	expression tag	UNP A0A0H2UPF3
BBB	7	HIS	-	expression tag	UNP A0A0H2UPF3

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	8	HIS	-	expression tag	UNP A0A0H2UPF3
BBB	9	HIS	-	expression tag	UNP A0A0H2UPF3
BBB	10	HIS	-	expression tag	UNP A0A0H2UPF3
BBB	11	MET	_	expression tag	UNP A0A0H2UPF3
BBB	12	SER	-	expression tag	UNP A0A0H2UPF3
BBB	13	GLY	-	expression tag	UNP A0A0H2UPF3
BBB	14	GLU	-	expression tag	UNP A0A0H2UPF3
BBB	15	ASN	-	expression tag	UNP A0A0H2UPF3
BBB	16	LEU	-	expression tag	UNP A0A0H2UPF3
BBB	17	TYR	-	expression tag	UNP A0A0H2UPF3
BBB	18	PHE	-	expression tag	UNP A0A0H2UPF3
BBB	19	GLN	-	expression tag	UNP A0A0H2UPF3
BBB	20	GLY	-	expression tag	UNP A0A0H2UPF3
BBB	21	ALA	-	expression tag	UNP A0A0H2UPF3
BBB	22	SER	-	expression tag	UNP A0A0H2UPF3

• Molecule 2 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	AAA	329	Total	C	N	0	S	0	0	0
			2466	1543	421	501	1	_	_	

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	5	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	6	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	7	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	8	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	9	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	10	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	11	MET	-	expression tag	UNP A0A0H2UPF3
AAA	12	SER	-	expression tag	UNP A0A0H2UPF3
AAA	13	GLY	-	expression tag	UNP A0A0H2UPF3
AAA	14	GLU	-	expression tag	UNP A0A0H2UPF3
AAA	15	ASN	-	expression tag	UNP A0A0H2UPF3
AAA	16	LEU	-	expression tag	UNP A0A0H2UPF3
AAA	17	TYR	-	expression tag	UNP A0A0H2UPF3
AAA	18	PHE	-	expression tag	UNP A0A0H2UPF3
AAA	19	GLN	-	expression tag	UNP A0A0H2UPF3
AAA	20	GLY	-	expression tag	UNP A0A0H2UPF3
AAA	21	ALA	-	expression tag	UNP A0A0H2UPF3

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	22	SER	-	expression tag	UNP A0A0H2UPF3

• Molecule 3 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	DDD	329	Total 2463	C 1540	N 420	O 502	S 1	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

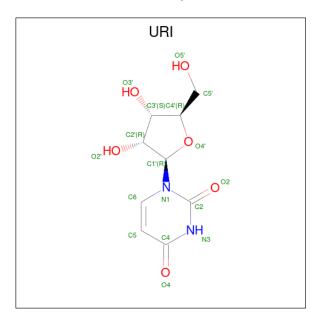
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	3	SER	-	expression tag	UNP A0A0H2UPF3
DDD	4	SER	-	expression tag	UNP A0A0H2UPF3
DDD	5	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	6	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	7	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	8	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	9	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	10	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	11	MET	-	expression tag	UNP A0A0H2UPF3
DDD	12	SER	-	expression tag	UNP A0A0H2UPF3
DDD	13	GLY	-	expression tag	UNP A0A0H2UPF3
DDD	14	GLU	-	expression tag	UNP A0A0H2UPF3
DDD	15	ASN	-	expression tag	UNP A0A0H2UPF3
DDD	16	LEU	-	expression tag	UNP A0A0H2UPF3
DDD	17	TYR	-	expression tag	UNP A0A0H2UPF3
DDD	18	PHE	-	expression tag	UNP A0A0H2UPF3
DDD	19	GLN	-	expression tag	UNP A0A0H2UPF3
DDD	20	GLY	-	expression tag	UNP A0A0H2UPF3
DDD	21	ALA	-	expression tag	UNP A0A0H2UPF3
DDD	22	SER	-	expression tag	UNP A0A0H2UPF3

• Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	CCC	2	Total Ni 2 2	0	0
4	BBB	3	Total Ni 3 3	0	0
4	DDD	4	Total Ni 4 4	0	0

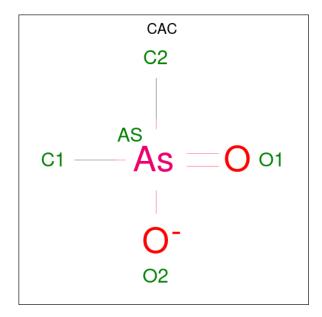


 $\bullet$  Molecule 5 is URIDINE (three-letter code: URI) (formula:  $\mathrm{C_9H_{12}N_2O_6}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	CCC	1	Total C N O 17 9 2 6	0	0
5	AAA	1	Total C N O 17 9 2 6	0	0
5	BBB	1	Total C N O 17 9 2 6	0	0
5	DDD	1	Total C N O 17 9 2 6	0	0

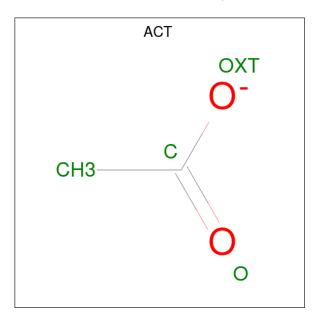
 $\bullet$  Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula:  $\mathrm{C_2H_6AsO_2}).$ 





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	CCC	1	Total 5	As 1	C 2	O 2	0	0

 $\bullet$  Molecule 7 is ACETATE ION (three-letter code: ACT) (formula:  $\mathrm{C_2H_3O_2}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	BBB	1	Total C O 4 2 2	0	0
7	BBB	1	Total C O 4 2 2	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	CCC	102	Total O 102 102	0	0
8	AAA	84	Total O 84 84	0	0
8	BBB	87	Total O 87 87	0	0
8	DDD	20	Total O 20 20	0	0

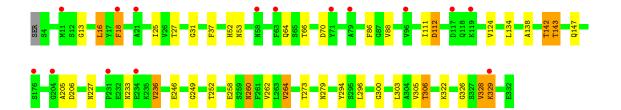


## 3 Residue-property plots (i)

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: Lipoprotein Chain CCC: • Molecule 1: Lipoprotein Chain BBB: 83% • Molecule 2: Lipoprotein Chain AAA: 83% 15% • Molecule 3: Lipoprotein Chain DDD: 86% 11%







# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 2 2 21	Depositor	
Cell constants	78.02Å 304.31Å 128.50Å	Donogitor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	49.09 - 2.30	Depositor	
resolution (A)	49.09 - 2.30	EDS	
% Data completeness	100.0 (49.09-2.30)	Depositor	
(in resolution range)	99.9 (49.09-2.30)	EDS	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	3.61 (at 2.29Å)	Xtriage	
Refinement program	REFMAC 5.8.0258	Depositor	
P.P.	0.210 , $0.250$	Depositor	
$R, R_{free}$	0.214 , $0.253$	DCC	
$R_{free}$ test set	3438 reflections $(5.04%)$	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage	
Anisotropy	0.072	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.31, 32.3	EDS	
L-test for twinning <sup>2</sup>	$ < L > = 0.48, < L^2> = 0.31$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
$F_o, F_c$ correlation	0.95	EDS	
Total number of atoms	10272	wwPDB-VP	
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 14.14% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



 $<sup>^1 {\</sup>rm Intensities}$  estimated from amplitudes.

# 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: NI, ACT, CAC, URI

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		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	BBB	0.69	0/2522	0.79	0/3406	
1	CCC	0.71	0/2528	0.80	0/3414	
2	AAA	0.71	0/2508	0.81	1/3387~(0.0%)	
3	DDD	0.69	0/2505	0.79	1/3384~(0.0%)	
All	All	0.70	0/10063	0.80	$2/13591 \ (0.0\%)$	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	DDD	18	PHE	CB-CA-C	5.05	120.51	110.40
2	AAA	333	LYS	CA-C-O	-5.03	109.54	120.10

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	BBB	2477	0	2396	33	1
1	CCC	2483	0	2401	45	1
2	AAA	2466	0	2385	35	2
3	DDD	2463	0	2377	33	0
4	BBB	3	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CCC	2	0	0	0	1
4	DDD	4	0	0	0	2
5	AAA	17	0	12	0	0
5	BBB	17	0	12	0	0
5	CCC	17	0	12	0	0
5	DDD	17	0	12	0	0
6	CCC	5	0	0	1	0
7	BBB	8	0	6	3	0
8	AAA	84	0	0	5	0
8	BBB	87	0	0	5	0
8	CCC	102	0	0	4	1
8	DDD	20	0	0	0	1
All	All	10272	0	9613	141	5

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.

The worst 5 of 141 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({f A})$	overlap (Å)
3:DDD:322:LYS:HB3	3:DDD:328:VAL:HG22	1.40	1.03
3:DDD:322:LYS:HB3	3:DDD:328:VAL:CG2	1.94	0.95
2:AAA:11:MET:CG	8:AAA:565:HOH:O	2.28	0.81
2:AAA:227:ASN:HD21	2:AAA:236:VAL:H	1.30	0.80
2:AAA:252:THR:HG22	2:AAA:258:GLU:HG3	1.63	0.79

All (5) 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	$egin{aligned} & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$	Clash overlap (Å)
2:AAA:8:HIS:NE2	4:DDD:401:NI:NI[4 556]	1.35	$\frac{\text{overlap }(\mathbf{A})}{0.85}$
1:BBB:282:GLU:OE2	4:CCC:402:NI:NI[6 445]		
	1	1.51	0.69
2:AAA:8:HIS:CE1	4:DDD:401:NI:NI[4_556]	1.56	0.64
1:CCC:282:GLU:OE2	4:BBB:402:NI:NI[6_444]	1.68	0.52
8:CCC:550:HOH:O	8:DDD:517:HOH:O[3_455]	2.18	0.02



### 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	Perce	entiles
1	BBB	329/331~(99%)	316 (96%)	11 (3%)	2 (1%)	25	31
1	CCC	330/331 (100%)	315 (96%)	14 (4%)	1 (0%)	41	50
2	AAA	327/329~(99%)	309 (94%)	16 (5%)	2 (1%)	25	31
3	DDD	327/330 (99%)	311 (95%)	14 (4%)	2 (1%)	25	31
All	All	1313/1321 (99%)	1251 (95%)	55 (4%)	7 (0%)	29	35

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AAA	306	THR
1	BBB	306	THR
3	DDD	306	THR
1	BBB	112	ASP
1	CCC	112	ASP

#### 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	BBB	$255/255 \; (100\%)$	234 (92%)	21 (8%)	11 14		
1	CCC	$256/255 \; (100\%)$	238 (93%)	18 (7%)	15 19		
2	AAA	253/253 (100%)	238 (94%)	15 (6%)	19 27		
3	DDD	253/254 (100%)	241 (95%)	12 (5%)	26 37		
All	All	1017/1017 (100%)	951 (94%)	66 (6%)	17 23		



5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	DDD	53	ASN
3	DDD	143	THR
3	DDD	329	LYS
2	AAA	142	THR
2	AAA	102	GLU

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

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 9 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	Mol Type Chei		in Res	Link	Bond lengths			Bond angles		
MIOI	Mol Type Chain	Chain	res	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CAC	CCC	404	-	0,4,4	-	-	0,6,6	-	-
5	URI	DDD	402	-	18,18,18	0.30	0	26,26,26	0.51	0
7	ACT	BBB	404	-	3,3,3	0.91	0	3,3,3	0.97	0
7	ACT	BBB	405	-	3,3,3	1.04	0	3,3,3	0.75	0
5	URI	CCC	403	-	18,18,18	0.22	0	26,26,26	0.52	0



Mal Trees		e Chain Res		Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dec	Link	Bo	ond leng	ths	В	ond ang	les
Mol   Type	Chain K	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2													
5	URI	BBB	403	-	18,18,18	0.38	0	26,26,26	0.43	0												
5	URI	AAA	401	-	18,18,18	0.30	0	26,26,26	0.54	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
5	URI	CCC	403	-	-	0/6/22/22	0/2/2/2
5	URI	AAA	401	-	-	0/6/22/22	0/2/2/2
5	URI	DDD	402	-	-	0/6/22/22	0/2/2/2
5	URI	BBB	403	-	-	0/6/22/22	0/2/2/2

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	CCC	404	CAC	1	0
7	BBB	404	ACT	2	0
7	BBB	405	ACT	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,  $95^{th}$  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>	# RSRZ > 2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	BBB	330/331 (99%)	-0.01	3 (0%) 84	1 88	29, 49, 89, 107	0
1	CCC	331/331 (100%)	-0.13	2 (0%) 89	92	27, 46, 81, 106	0
2	AAA	329/329 (100%)	-0.03	5 (1%) 73	3 79	27, 50, 81, 137	0
3	DDD	329/330 (99%)	0.36	15 (4%) 3	2 39	47, 73, 109, 122	0
All	All	1319/1321 (99%)	0.05	25 (1%) 6	6 73	27, 54, 97, 137	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AAA	16	LEU	4.1
1	BBB	204	GLY	3.8
3	DDD	63	PHE	3.4
3	DDD	117	ASP	2.8
2	AAA	7	HIS	2.7

#### 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 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,  $95^{th}$  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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
6	CAC	CCC	404	5/5	0.82	0.14	144,147,154,166	0
7	ACT	BBB	405	4/4	0.84	0.18	77,78,80,87	0
7	ACT	BBB	404	4/4	0.87	0.15	65,70,71,77	0
4	NI	BBB	401	1/1	0.90	0.09	82,82,82,82	0
4	NI	DDD	404	1/1	0.94	0.06	78,78,78,78	0
4	NI	DDD	403	1/1	0.95	0.21	59,59,59,59	0
5	URI	DDD	402	17/17	0.96	0.11	46,50,54,56	0
4	NI	DDD	401	1/1	0.97	0.08	59,59,59,59	0
4	NI	BBB	402	1/1	0.98	0.15	30,30,30,30	0
5	URI	CCC	403	17/17	0.98	0.10	30,33,38,38	0
5	URI	AAA	401	17/17	0.98	0.10	29,35,39,40	0
5	URI	BBB	403	17/17	0.98	0.12	33,36,39,42	0
4	NI	DDD	405	1/1	0.99	0.07	44,44,44,44	0
4	NI	CCC	402	1/1	0.99	0.14	31,31,31,31	0
4	NI	BBB	406	1/1	1.00	0.08	97,97,97,97	0
4	NI	CCC	401	1/1	1.00	0.11	34,34,34,34	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

