



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 10:46 AM EST

PDB ID : 4PFM  
Title : SHEWANELLA BENTHICA DHDPS WITH LYSINE AND PYRUVATE  
Authors : Wubben, J.M.; Paxman, J.J.; Dogovski, C.; Panjikar, S.; Perugini, M.A.  
Deposited on : unknown  
Resolution : 2.33 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

<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-20030345  
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-20030345

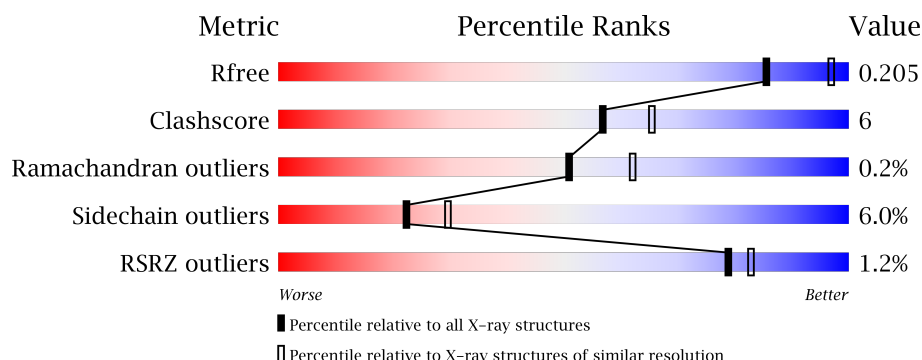
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

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 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	295	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>87%</span> <span>10%</span> </div> </div>
1	B	295	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>85%</span> <span>13%</span> </div> </div>

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
2	LYS	A	301	-	-	-	X
2	LYS	B	301	-	-	-	X
3	GOL	A	303	-	-	-	X
3	GOL	B	303	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4774 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.

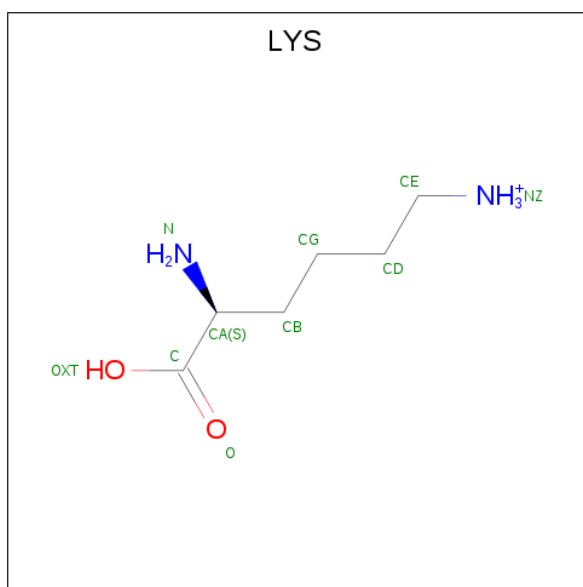
- Molecule 1 is a protein called 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	2	0
			2202	1395	368	429	10			
1	B	295	Total	C	N	O	S	0	2	0
			2200	1393	367	430	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	ALA	conflict	UNP A9DKW4
A	97	VAL	LEU	conflict	UNP A9DKW4
A	98	ALA	VAL	conflict	UNP A9DKW4
A	120	THR	LYS	conflict	UNP A9DKW4
A	167	VAL	LEU	conflict	UNP A9DKW4
A	168	ALA	ASP	conflict	UNP A9DKW4
A	175	ASP	GLU	conflict	UNP A9DKW4
A	209	ILE	LEU	conflict	UNP A9DKW4
B	68	SER	ALA	conflict	UNP A9DKW4
B	97	VAL	LEU	conflict	UNP A9DKW4
B	98	ALA	VAL	conflict	UNP A9DKW4
B	120	THR	LYS	conflict	UNP A9DKW4
B	167	VAL	LEU	conflict	UNP A9DKW4
B	168	ALA	ASP	conflict	UNP A9DKW4
B	175	ASP	GLU	conflict	UNP A9DKW4
B	209	ILE	LEU	conflict	UNP A9DKW4

- Molecule 2 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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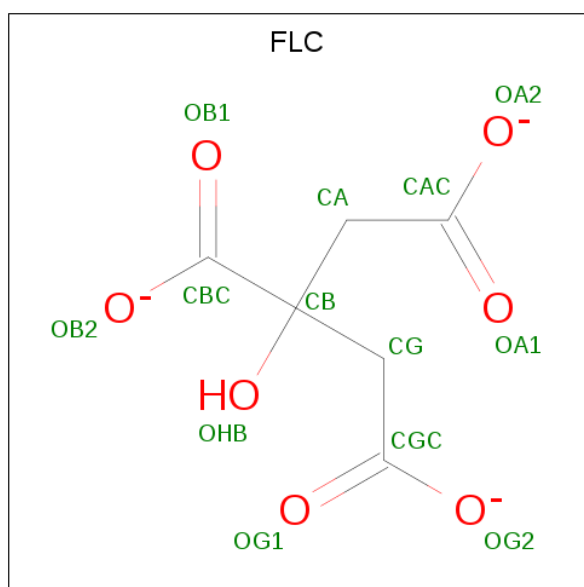
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	6	7		

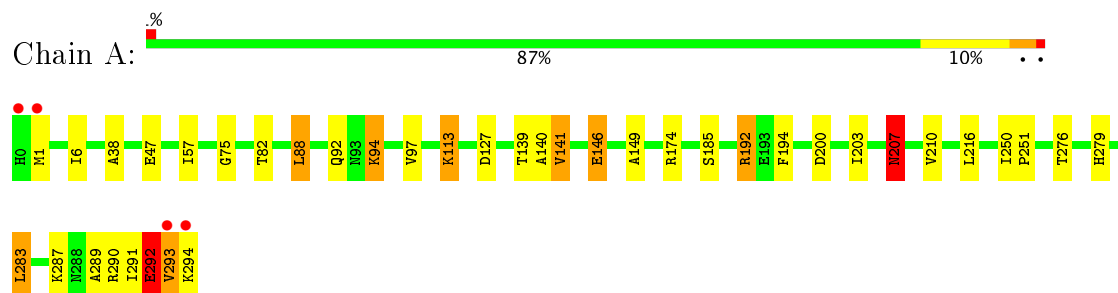
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total	O	0	0
			156	156		
6	B	159	Total	O	0	0
			159	159		

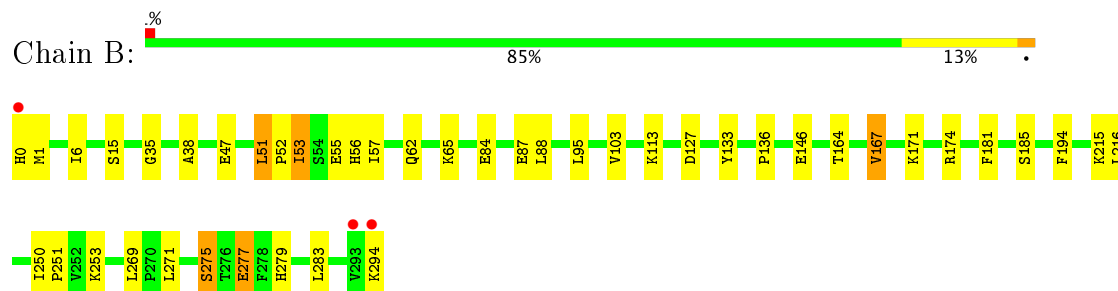
### 3 Residue-property plots [i](#)

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: 4-hydroxy-tetrahydronicotinate synthase



- Molecule 1: 4-hydroxy-tetrahydronicotinate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.27Å 83.93Å 143.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.96 – 2.33 44.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.96-2.33) 99.5 (44.00-2.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.162 , 0.206 0.161 , 0.205	Depositor DCC
$R_{free}$ test set	1963 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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, FLC, KPI, NA

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	1.07	4/2222 (0.2%)	0.95	2/3025 (0.1%)
1	B	1.01	1/2220 (0.0%)	0.91	2/3023 (0.1%)
All	All	1.04	5/4442 (0.1%)	0.93	4/6048 (0.1%)

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	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	GLU	CG-CD	6.26	1.61	1.51
1	B	146	GLU	CG-CD	6.07	1.61	1.51
1	A	141	VAL	CB-CG1	-5.65	1.41	1.52
1	A	207	ASN	CB-CG	-5.05	1.39	1.51
1	A	292	GLU	CG-CD	5.02	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	LEU	CA-CB-CG	6.86	131.09	115.30
1	B	51	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	200	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	B	167	VAL	CG1-CB-CG2	5.81	120.20	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ILE	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	2202	0	2235	27	0
1	B	2200	0	2228	24	0
2	A	20	0	24	3	0
2	B	10	0	12	2	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	13	0	5	1	0
6	A	156	0	0	1	0
6	B	159	0	0	4	0
All	All	4774	0	4520	51	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 6.

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:A:146[A]:GLU:N	1:A:146[A]:GLU:OE1	1.86	1.05
1:A:293:VAL:HG11	6:A:535:HOH:O	1.60	1.01
2:B:301:LYS:O	2:B:301:LYS:HD2	1.84	0.77
1:B:84:GLU:HB2	2:B:301:LYS:HA	1.71	0.72
1:A:94:LYS:H	1:A:94:LYS:HD2	1.57	0.68

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/295 (100%)	285 (97%)	8 (3%)	1 (0%)	44	54
1	B	294/295 (100%)	288 (98%)	6 (2%)	0	100	100
All	All	588/590 (100%)	573 (97%)	14 (2%)	1 (0%)	51	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	VAL

### 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	233/231 (101%)	218 (94%)	15 (6%)	20	26
1	B	233/231 (101%)	220 (94%)	13 (6%)	25	33
All	All	466/462 (101%)	438 (94%)	28 (6%)	22	30

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	B	0	HIS
1	B	277	GLU
1	A	283	LEU
1	A	292	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	207	ASN
1	B	56	HIS
1	B	62	GLN
1	B	150	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	KPI	A	161	1	11,13,14	1.39	2 (18%)	7,15,17	1.65	2 (28%)
1	KPI	B	161	1	11,13,14	1.24	1 (9%)	7,15,17	1.36	1 (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	KPI	A	161	1	-	0/8/14/16	0/0/0/0
1	KPI	B	161	1	-	0/8/14/16	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	KPI	CX2-CX1	-2.95	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	KPI	CX2-CX1	-2.82	1.47	1.52
1	A	161	KPI	C1-CX1	2.59	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	KPI	CD-CE-NZ	-2.86	106.22	110.71
1	A	161	KPI	CE-NZ-CX1	2.54	128.91	122.00
1	B	161	KPI	CE-NZ-CX1	3.17	130.62	122.00

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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	LYS	A	301	-	4,9,9	0.90	0	3,10,10	0.64	0
2	LYS	A	302	-	4,9,9	0.73	0	3,10,10	0.37	0
3	GOL	A	303	-	5,5,5	0.46	0	5,5,5	0.29	0
2	LYS	B	301	-	4,9,9	1.15	1 (25%)	3,10,10	0.77	0
5	FLC	B	302	-	3,12,12	0.81	0	3,17,17	2.68	2 (66%)
3	GOL	B	303	-	5,5,5	0.39	0	5,5,5	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	LYS	A	301	-	-	0/5/9/9	0/0/0/0
2	LYS	A	302	-	-	0/5/9/9	0/0/0/0
3	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	LYS	B	301	-	-	0/5/9/9	0/0/0/0
5	FLC	B	302	-	-	0/6/16/16	0/0/0/0
3	GOL	B	303	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	LYS	CD-CE	2.06	1.61	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	302	FLC	CB-CA-CAC	2.62	119.05	114.95
5	B	302	FLC	CB-CG-CGC	3.66	120.67	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	LYS	3	0
2	B	301	LYS	2	0
5	B	302	FLC	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	294/295 (99%)	-0.21	4 (1%) 75 80	34, 44, 61, 97	0
1	B	294/295 (99%)	-0.11	3 (1%) 82 86	32, 44, 61, 105	0
All	All	588/590 (99%)	-0.16	7 (1%) 79 83	32, 44, 61, 105	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	HIS	6.9
1	B	294	LYS	4.2
1	A	294	LYS	3.9
1	B	293	VAL	3.1
1	A	0	HIS	3.1

### 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	KPI	B	161	14/15	0.96	0.21	-	36,37,50,50	0
1	KPI	A	161	14/15	0.95	0.12	-	33,37,47,47	0

### 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. 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
3	GOL	B	303	6/6	0.71	0.97	43.81	58,60,61,61	6
3	GOL	A	303	6/6	0.82	0.32	6.49	84,91,93,94	0
2	LYS	B	301	10/10	0.86	0.20	3.78	58,60,61,61	0
2	LYS	A	301	10/10	0.97	0.19	3.39	33,41,44,45	0
2	LYS	A	302	10/10	0.95	0.19	0.85	35,42,45,45	0
4	NA	B	304	1/1	0.94	0.12	-0.50	63,63,63,63	0
4	NA	A	304	1/1	0.90	0.11	-1.03	60,60,60,60	0
5	FLC	B	302	13/13	0.49	0.38	-	136,139,139,139	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.