



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:52 pm BST

PDB ID : 3RR1  
Title : Crystal structure of enolase PRK14017 (target EFI-500653) from *Ralstonia pickettii* 12J  
Authors : Patskovsky, Y.; Hillerich, B.; Seidel, R.D.; Zencheck, W.D.; Toro, R.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2011-04-28  
Resolution : 1.95 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

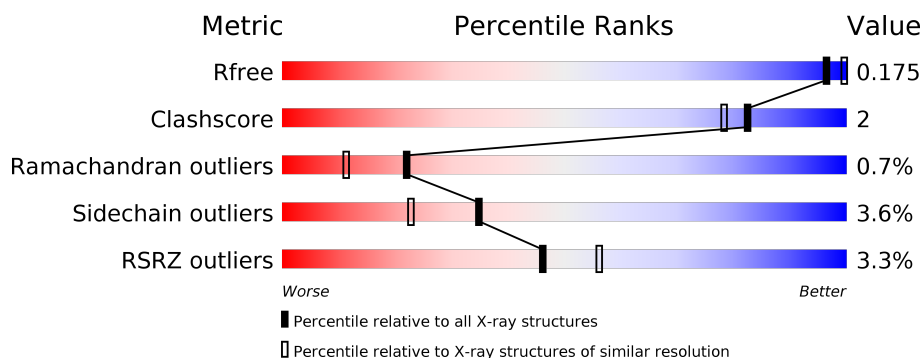
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	405	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>8%</div> </div> </div>
1	B	405	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6119 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 Putative D-galactonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	8	0
			2913	1868	506	524	15			
1	B	376	Total	C	N	O	S	0	10	0
			2940	1881	514	531	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP B2UCA8
A	1	VAL	-	EXPRESSION TAG	UNP B2UCA8
A	383	ALA	-	EXPRESSION TAG	UNP B2UCA8
A	384	GLU	-	EXPRESSION TAG	UNP B2UCA8
A	385	ASN	-	EXPRESSION TAG	UNP B2UCA8
A	386	LEU	-	EXPRESSION TAG	UNP B2UCA8
A	387	TYR	-	EXPRESSION TAG	UNP B2UCA8
A	388	PHE	-	EXPRESSION TAG	UNP B2UCA8
A	389	GLN	-	EXPRESSION TAG	UNP B2UCA8
A	390	SER	-	EXPRESSION TAG	UNP B2UCA8
A	391	HIS	-	EXPRESSION TAG	UNP B2UCA8
A	392	HIS	-	EXPRESSION TAG	UNP B2UCA8
A	393	HIS	-	EXPRESSION TAG	UNP B2UCA8
A	394	HIS	-	EXPRESSION TAG	UNP B2UCA8
A	395	HIS	-	EXPRESSION TAG	UNP B2UCA8
A	396	HIS	-	EXPRESSION TAG	UNP B2UCA8
A	397	TRP	-	EXPRESSION TAG	UNP B2UCA8
A	398	SER	-	EXPRESSION TAG	UNP B2UCA8
A	399	HIS	-	EXPRESSION TAG	UNP B2UCA8
A	400	PRO	-	EXPRESSION TAG	UNP B2UCA8
A	401	GLN	-	EXPRESSION TAG	UNP B2UCA8
A	402	PHE	-	EXPRESSION TAG	UNP B2UCA8
A	403	GLU	-	EXPRESSION TAG	UNP B2UCA8
A	404	LYS	-	EXPRESSION TAG	UNP B2UCA8
B	0	MET	-	EXPRESSION TAG	UNP B2UCA8

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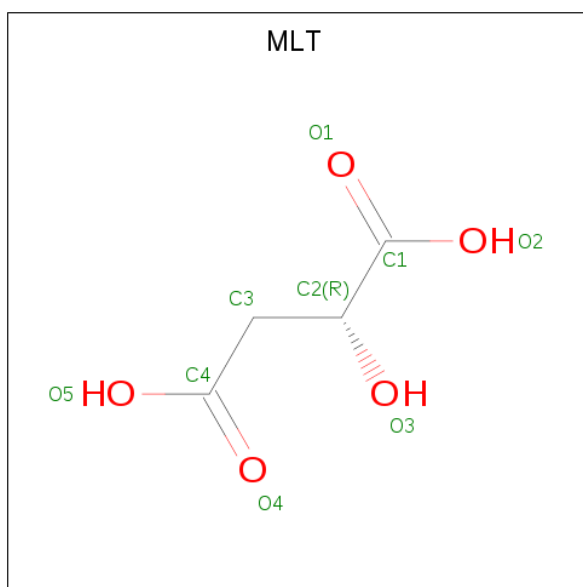
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	VAL	-	EXPRESSION TAG	UNP B2UCA8
B	383	ALA	-	EXPRESSION TAG	UNP B2UCA8
B	384	GLU	-	EXPRESSION TAG	UNP B2UCA8
B	385	ASN	-	EXPRESSION TAG	UNP B2UCA8
B	386	LEU	-	EXPRESSION TAG	UNP B2UCA8
B	387	TYR	-	EXPRESSION TAG	UNP B2UCA8
B	388	PHE	-	EXPRESSION TAG	UNP B2UCA8
B	389	GLN	-	EXPRESSION TAG	UNP B2UCA8
B	390	SER	-	EXPRESSION TAG	UNP B2UCA8
B	391	HIS	-	EXPRESSION TAG	UNP B2UCA8
B	392	HIS	-	EXPRESSION TAG	UNP B2UCA8
B	393	HIS	-	EXPRESSION TAG	UNP B2UCA8
B	394	HIS	-	EXPRESSION TAG	UNP B2UCA8
B	395	HIS	-	EXPRESSION TAG	UNP B2UCA8
B	396	HIS	-	EXPRESSION TAG	UNP B2UCA8
B	397	TRP	-	EXPRESSION TAG	UNP B2UCA8
B	398	SER	-	EXPRESSION TAG	UNP B2UCA8
B	399	HIS	-	EXPRESSION TAG	UNP B2UCA8
B	400	PRO	-	EXPRESSION TAG	UNP B2UCA8
B	401	GLN	-	EXPRESSION TAG	UNP B2UCA8
B	402	PHE	-	EXPRESSION TAG	UNP B2UCA8
B	403	GLU	-	EXPRESSION TAG	UNP B2UCA8
B	404	LYS	-	EXPRESSION TAG	UNP B2UCA8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			9	4	5		

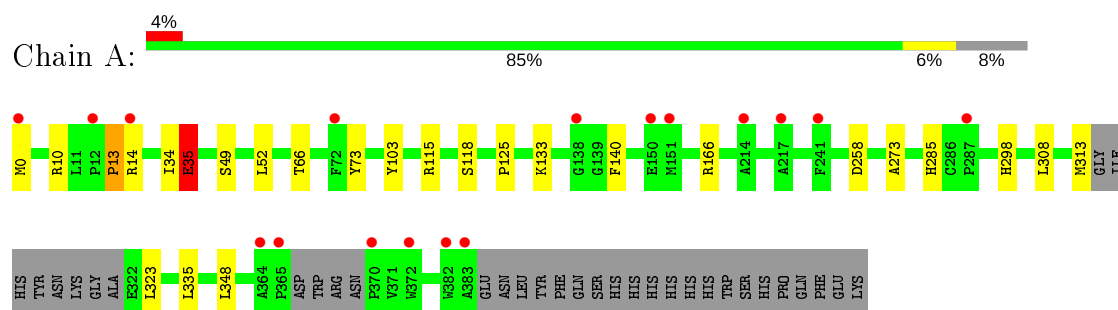
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	147	Total	O	0	0
			147	147		

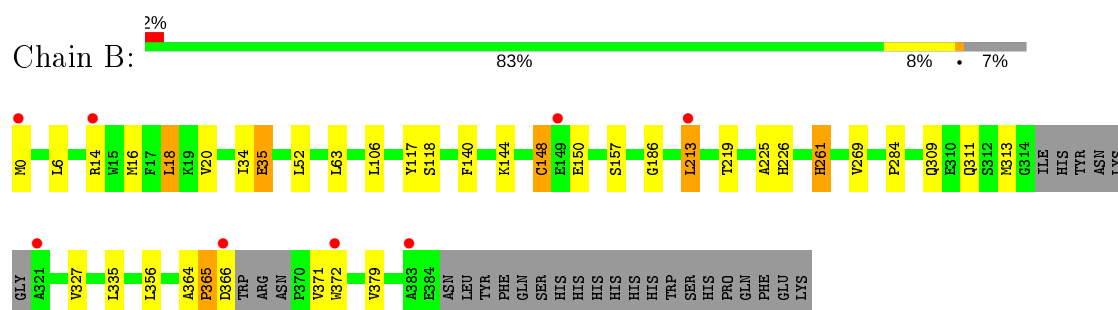
### 3 Residue-property plots [i](#)

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: Putative D-galactonate dehydratase



- Molecule 1: Putative D-galactonate dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.01Å 118.01Å 114.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 47.93 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-1.95) 94.3 (47.93-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.136 , 0.174 0.136 , 0.175	Depositor DCC
$R_{free}$ test set	1676 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.095 for l,-k,h 0.094 for -l,-k,-h 0.090 for -h,-l,-k 0.090 for -h,l,k 0.390 for -k,-h,-l	Xtriage
Reported twinning fraction	0.420 for H, K, L 0.580 for K, H, -L	Depositor
Outliers	0 of 53953 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: MLT, CL

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	0.49	0/3000	0.62	0/4071
1	B	0.54	1/3038 (0.0%)	0.64	1/4122 (0.0%)
All	All	0.51	1/6038 (0.0%)	0.63	1/8193 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	CYS	CB-SG	-5.36	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	LEU	CA-CB-CG	6.80	130.94	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	2913	0	2907	15	0
1	B	2940	0	2939	15	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	4	1	0
4	A	108	0	0	2	0
4	B	147	0	0	0	0
All	All	6119	0	5850	29	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 (29) 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:313:MET:HG2	1:A:323:LEU:HD21	1.60	0.82
1:B:34:ILE:O	1:B:35:GLU:C	2.37	0.63
1:A:298:HIS:HE1	1:A:348:LEU:O	1.89	0.56
2:A:405:CL:CL	2:B:405:CL:CL	2.99	0.55
1:A:140:PHE:HZ	1:A:335:LEU:HD13	1.74	0.53
1:A:258:ASP:OD2	1:A:285:HIS:HD2	1.91	0.53
1:B:117:TYR:HE1	1:B:144:LYS:HB2	1.75	0.51
1:B:117:TYR:CE1	1:B:144:LYS:HB2	2.47	0.49
1:A:66:THR:OG1	1:B:379:VAL:HG11	2.12	0.49
1:B:140:PHE:HZ	1:B:335:LEU:HD13	1.78	0.48
1:A:34:ILE:O	1:A:35:GLU:C	2.53	0.46
1:A:13:PRO:HB2	1:A:14:ARG:H	1.61	0.45
1:A:125:PRO:HG3	1:A:166:ARG:HG3	1.98	0.45
1:A:49:SER:HA	1:A:52:LEU:HD12	1.99	0.45
1:A:115:ARG:HG2	1:A:308:LEU:HD23	1.99	0.44
1:A:73:TYR:CE2	1:B:261:HIS:HE1	2.35	0.44
1:A:285:HIS:ND1	4:A:504:HOH:O	2.36	0.44
1:B:16:MET:HB2	1:B:34:ILE:HD13	2.00	0.44
1:A:103:TYR:H	1:A:298:HIS:CD2	2.36	0.43
1:B:52:LEU:HD23	1:B:63:LEU:HD22	2.02	0.42
1:B:106:LEU:HD13	1:B:269[A]:VAL:HG11	2.01	0.42
1:B:225:ALA:HA	3:B:406:MLT:O5	2.19	0.42
1:A:273:ALA:HB2	4:A:479:HOH:O	2.20	0.41
1:B:186:GLY:HA3	1:B:213:LEU:HD12	2.01	0.41
1:A:10[B]:ARG:NH1	1:A:10[B]:ARG:HB2	2.36	0.41
1:B:284:PRO:HB2	1:B:309:GLN:HE22	1.86	0.41
1:B:35:GLU:HG3	1:B:35:GLU:H	1.65	0.41
1:B:364:ALA:HA	1:B:365:PRO:HD3	1.94	0.41
1:B:6:LEU:HG	1:B:20:VAL:HG22	2.03	0.40

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	374/405 (92%)	354 (95%)	18 (5%)	2 (0%)	29	17
1	B	380/405 (94%)	368 (97%)	9 (2%)	3 (1%)	19	9
All	All	754/810 (93%)	722 (96%)	27 (4%)	5 (1%)	22	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	35	GLU
1	B	150	GLU
1	B	35	GLU
1	B	365	PRO

### 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	297/323 (92%)	293 (99%)	4 (1%)	69	65
1	B	300/323 (93%)	282 (94%)	18 (6%)	19	8
All	All	597/646 (92%)	575 (96%)	22 (4%)	35	22

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	35	GLU
1	A	118	SER
1	A	133	LYS
1	B	0	MET
1	B	14	ARG
1	B	18	LEU
1	B	118	SER
1	B	148	CYS
1	B	157	SER
1	B	213	LEU
1	B	219	THR
1	B	226[A]	HIS
1	B	226[B]	HIS
1	B	261	HIS
1	B	311	GLN
1	B	313	MET
1	B	327	VAL
1	B	356	LEU
1	B	366	ASP
1	B	371	VAL
1	B	372	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	HIS
1	A	298	HIS
1	A	309	GLN
1	B	261	HIS
1	B	285	HIS
1	B	309	GLN

### 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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z  > 2$
3	MLT	B	406	-	2,8,8	1.02	0	3,10,10	3.57	1 (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
3	MLT	B	406	-	-	2/2/8/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	406	MLT	C3-C2-C1	-6.16	103.25	111.10

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	406	MLT	C1-C2-C3-C4
3	B	406	MLT	O3-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	406	MLT	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	372/405 (91%)	0.19	17 (4%) 32 42	24, 45, 75, 106	0
1	B	376/405 (92%)	0.02	8 (2%) 63 72	24, 39, 70, 115	0
All	All	748/810 (92%)	0.10	25 (3%) 46 56	24, 42, 73, 115	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	TRP	4.5
1	A	151	MET	3.8
1	A	364	ALA	3.7
1	B	149	GLU	3.6
1	B	366	ASP	3.5
1	A	150	GLU	3.3
1	B	383	ALA	3.1
1	A	0	MET	3.0
1	B	213	LEU	2.9
1	A	214	ALA	2.7
1	A	382	TRP	2.7
1	A	138	GLY	2.6
1	A	12	PRO	2.6
1	A	241	PHE	2.6
1	B	0	MET	2.6
1	B	321	ALA	2.3
1	A	370	PRO	2.1
1	A	287	PRO	2.1
1	A	217	ALA	2.1
1	A	14	ARG	2.1
1	A	365	PRO	2.1
1	B	14	ARG	2.1
1	A	383	ALA	2.1
1	B	372	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	72	PHE	2.0

## 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(Å <sup>2</sup> )	Q<0.9
3	MLT	B	406	9/9	0.89	0.20	45,60,67,69	0
2	CL	B	405	1/1	0.98	0.07	43,43,43,43	0
2	CL	A	405	1/1	0.99	0.08	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.