



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 06:10 pm BST

PDB ID : 4PU3  
Title : Shewanella oneidensis MR-1 Toxin Antitoxin System HipA, HipB and its operator DNA complex (space group P212121)  
Authors : Wen, Y.; Behiels, E.; Felix, J.; Elegheert, J.; Vergauwen, B.; Devreese, B.; Savvides, S.  
Deposited on : 2014-03-12  
Resolution : 3.39 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 : 1.8.5 (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

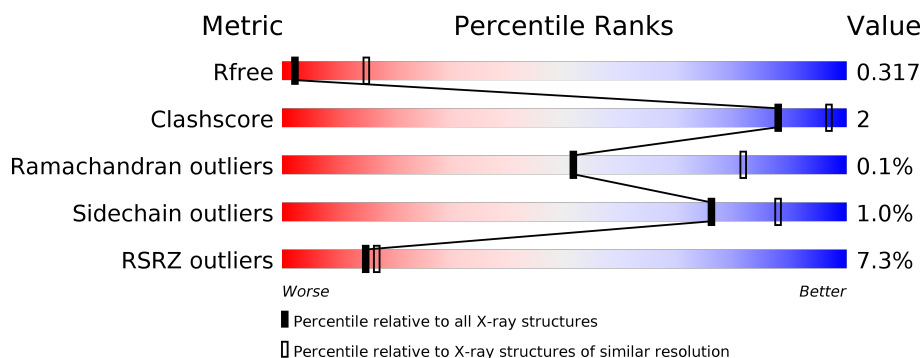
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.39 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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	454	<div> <div>8%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
1	B	454	<div> <div>7%</div> <div>90%</div> <div>•</div> <div>6%</div> </div>
2	C	118	<div> <div>3%</div> <div>54%</div> <div>• •</div> <div>40%</div> </div>
2	D	118	<div> <div>3%</div> <div>58%</div> <div>•</div> <div>40%</div> </div>
3	Q	26	<div> <div>4%</div> <div>85%</div> <div>8%</div> <div>• •</div> </div>
4	P	26	<div> <div>85%</div> <div>8%</div> <div>8%</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
1	SEP	A	147	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17163 atoms, of which 8358 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 Toxin-antitoxin system toxin HipA family.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	426	Total	C	H	N	O	P	S	0	0	0
			6706	2147	3342	572	626	1	18			
1	B	426	Total	C	H	N	O	P	S	0	0	0
			6663	2143	3308	573	621	1	17			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q8EIX3
A	-19	GLY	-	EXPRESSION TAG	UNP Q8EIX3
A	-18	SER	-	EXPRESSION TAG	UNP Q8EIX3
A	-17	SER	-	EXPRESSION TAG	UNP Q8EIX3
A	-16	HIS	-	EXPRESSION TAG	UNP Q8EIX3
A	-15	HIS	-	EXPRESSION TAG	UNP Q8EIX3
A	-14	HIS	-	EXPRESSION TAG	UNP Q8EIX3
A	-13	HIS	-	EXPRESSION TAG	UNP Q8EIX3
A	-12	HIS	-	EXPRESSION TAG	UNP Q8EIX3
A	-11	HIS	-	EXPRESSION TAG	UNP Q8EIX3
A	-10	SER	-	EXPRESSION TAG	UNP Q8EIX3
A	-9	SER	-	EXPRESSION TAG	UNP Q8EIX3
A	-8	GLY	-	EXPRESSION TAG	UNP Q8EIX3
A	-7	LEU	-	EXPRESSION TAG	UNP Q8EIX3
A	-6	VAL	-	EXPRESSION TAG	UNP Q8EIX3
A	-5	PRO	-	EXPRESSION TAG	UNP Q8EIX3
A	-4	ARG	-	EXPRESSION TAG	UNP Q8EIX3
A	-3	GLY	-	EXPRESSION TAG	UNP Q8EIX3
A	-2	SER	-	EXPRESSION TAG	UNP Q8EIX3
A	-1	HIS	-	EXPRESSION TAG	UNP Q8EIX3
A	0	MET	-	EXPRESSION TAG	UNP Q8EIX3
B	-20	MET	-	EXPRESSION TAG	UNP Q8EIX3
B	-19	GLY	-	EXPRESSION TAG	UNP Q8EIX3
B	-18	SER	-	EXPRESSION TAG	UNP Q8EIX3
B	-17	SER	-	EXPRESSION TAG	UNP Q8EIX3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP Q8EIX3
B	-15	HIS	-	EXPRESSION TAG	UNP Q8EIX3
B	-14	HIS	-	EXPRESSION TAG	UNP Q8EIX3
B	-13	HIS	-	EXPRESSION TAG	UNP Q8EIX3
B	-12	HIS	-	EXPRESSION TAG	UNP Q8EIX3
B	-11	HIS	-	EXPRESSION TAG	UNP Q8EIX3
B	-10	SER	-	EXPRESSION TAG	UNP Q8EIX3
B	-9	SER	-	EXPRESSION TAG	UNP Q8EIX3
B	-8	GLY	-	EXPRESSION TAG	UNP Q8EIX3
B	-7	LEU	-	EXPRESSION TAG	UNP Q8EIX3
B	-6	VAL	-	EXPRESSION TAG	UNP Q8EIX3
B	-5	PRO	-	EXPRESSION TAG	UNP Q8EIX3
B	-4	ARG	-	EXPRESSION TAG	UNP Q8EIX3
B	-3	GLY	-	EXPRESSION TAG	UNP Q8EIX3
B	-2	SER	-	EXPRESSION TAG	UNP Q8EIX3
B	-1	HIS	-	EXPRESSION TAG	UNP Q8EIX3
B	0	MET	-	EXPRESSION TAG	UNP Q8EIX3

- Molecule 2 is a protein called Toxin-antitoxin system antidote transcriptional repressor Xre family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	71	Total	C	H	N	O	S	0	0	0
			1118	347	577	91	100	3			
2	C	71	Total	C	H	N	O	S	0	0	0
			1118	347	577	91	100	3			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	EXPRESSION TAG	UNP Q8EIX4
D	-19	GLY	-	EXPRESSION TAG	UNP Q8EIX4
D	-18	SER	-	EXPRESSION TAG	UNP Q8EIX4
D	-17	SER	-	EXPRESSION TAG	UNP Q8EIX4
D	-16	HIS	-	EXPRESSION TAG	UNP Q8EIX4
D	-15	HIS	-	EXPRESSION TAG	UNP Q8EIX4
D	-14	HIS	-	EXPRESSION TAG	UNP Q8EIX4
D	-13	HIS	-	EXPRESSION TAG	UNP Q8EIX4
D	-12	HIS	-	EXPRESSION TAG	UNP Q8EIX4
D	-11	HIS	-	EXPRESSION TAG	UNP Q8EIX4
D	-10	SER	-	EXPRESSION TAG	UNP Q8EIX4
D	-9	SER	-	EXPRESSION TAG	UNP Q8EIX4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	GLY	-	EXPRESSION TAG	UNP Q8EIX4
D	-7	LEU	-	EXPRESSION TAG	UNP Q8EIX4
D	-6	VAL	-	EXPRESSION TAG	UNP Q8EIX4
D	-5	PRO	-	EXPRESSION TAG	UNP Q8EIX4
D	-4	ARG	-	EXPRESSION TAG	UNP Q8EIX4
D	-3	GLY	-	EXPRESSION TAG	UNP Q8EIX4
D	-2	SER	-	EXPRESSION TAG	UNP Q8EIX4
D	-1	HIS	-	EXPRESSION TAG	UNP Q8EIX4
D	0	MET	-	EXPRESSION TAG	UNP Q8EIX4
D	1	MET	-	EXPRESSION TAG	UNP Q8EIX4
D	2	ASN	-	EXPRESSION TAG	UNP Q8EIX4
D	3	GLY	-	EXPRESSION TAG	UNP Q8EIX4
D	4	THR	-	EXPRESSION TAG	UNP Q8EIX4
D	5	ASP	-	EXPRESSION TAG	UNP Q8EIX4
D	6	ILE	-	EXPRESSION TAG	UNP Q8EIX4
D	7	LYS	-	EXPRESSION TAG	UNP Q8EIX4
D	8	ALA	-	EXPRESSION TAG	UNP Q8EIX4
D	9	LYS	-	EXPRESSION TAG	UNP Q8EIX4
D	10	VAL	-	EXPRESSION TAG	UNP Q8EIX4
D	11	TYR	-	EXPRESSION TAG	UNP Q8EIX4
D	12	GLU	-	EXPRESSION TAG	UNP Q8EIX4
D	13	ASP	-	EXPRESSION TAG	UNP Q8EIX4
D	14	THR	-	EXPRESSION TAG	UNP Q8EIX4
D	15	LEU	-	EXPRESSION TAG	UNP Q8EIX4
D	16	LEU	-	EXPRESSION TAG	UNP Q8EIX4
D	17	GLU	-	EXPRESSION TAG	UNP Q8EIX4
D	18	THR	-	EXPRESSION TAG	UNP Q8EIX4
D	19	ILE	-	EXPRESSION TAG	UNP Q8EIX4
C	-20	MET	-	EXPRESSION TAG	UNP Q8EIX4
C	-19	GLY	-	EXPRESSION TAG	UNP Q8EIX4
C	-18	SER	-	EXPRESSION TAG	UNP Q8EIX4
C	-17	SER	-	EXPRESSION TAG	UNP Q8EIX4
C	-16	HIS	-	EXPRESSION TAG	UNP Q8EIX4
C	-15	HIS	-	EXPRESSION TAG	UNP Q8EIX4
C	-14	HIS	-	EXPRESSION TAG	UNP Q8EIX4
C	-13	HIS	-	EXPRESSION TAG	UNP Q8EIX4
C	-12	HIS	-	EXPRESSION TAG	UNP Q8EIX4
C	-11	HIS	-	EXPRESSION TAG	UNP Q8EIX4
C	-10	SER	-	EXPRESSION TAG	UNP Q8EIX4
C	-9	SER	-	EXPRESSION TAG	UNP Q8EIX4
C	-8	GLY	-	EXPRESSION TAG	UNP Q8EIX4
C	-7	LEU	-	EXPRESSION TAG	UNP Q8EIX4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	VAL	-	EXPRESSION TAG	UNP Q8EIX4
C	-5	PRO	-	EXPRESSION TAG	UNP Q8EIX4
C	-4	ARG	-	EXPRESSION TAG	UNP Q8EIX4
C	-3	GLY	-	EXPRESSION TAG	UNP Q8EIX4
C	-2	SER	-	EXPRESSION TAG	UNP Q8EIX4
C	-1	HIS	-	EXPRESSION TAG	UNP Q8EIX4
C	0	MET	-	EXPRESSION TAG	UNP Q8EIX4
C	1	MET	-	EXPRESSION TAG	UNP Q8EIX4
C	2	ASN	-	EXPRESSION TAG	UNP Q8EIX4
C	3	GLY	-	EXPRESSION TAG	UNP Q8EIX4
C	4	THR	-	EXPRESSION TAG	UNP Q8EIX4
C	5	ASP	-	EXPRESSION TAG	UNP Q8EIX4
C	6	ILE	-	EXPRESSION TAG	UNP Q8EIX4
C	7	LYS	-	EXPRESSION TAG	UNP Q8EIX4
C	8	ALA	-	EXPRESSION TAG	UNP Q8EIX4
C	9	LYS	-	EXPRESSION TAG	UNP Q8EIX4
C	10	VAL	-	EXPRESSION TAG	UNP Q8EIX4
C	11	TYR	-	EXPRESSION TAG	UNP Q8EIX4
C	12	GLU	-	EXPRESSION TAG	UNP Q8EIX4
C	13	ASP	-	EXPRESSION TAG	UNP Q8EIX4
C	14	THR	-	EXPRESSION TAG	UNP Q8EIX4
C	15	LEU	-	EXPRESSION TAG	UNP Q8EIX4
C	16	LEU	-	EXPRESSION TAG	UNP Q8EIX4
C	17	GLU	-	EXPRESSION TAG	UNP Q8EIX4
C	18	THR	-	EXPRESSION TAG	UNP Q8EIX4
C	19	ILE	-	EXPRESSION TAG	UNP Q8EIX4

- Molecule 3 is a DNA chain called Operator DNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	Q	25	Total	C	H	N	O	P	0	0	0
			799	247	282	101	144	25			

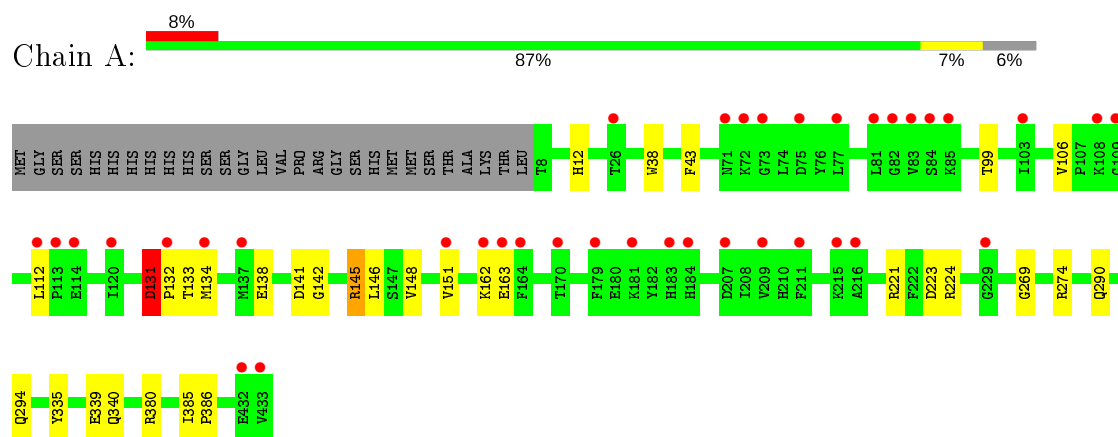
- Molecule 4 is a DNA chain called Operator DNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	P	24	Total	C	H	N	O	P	0	0	0
			759	235	272	79	149	24			

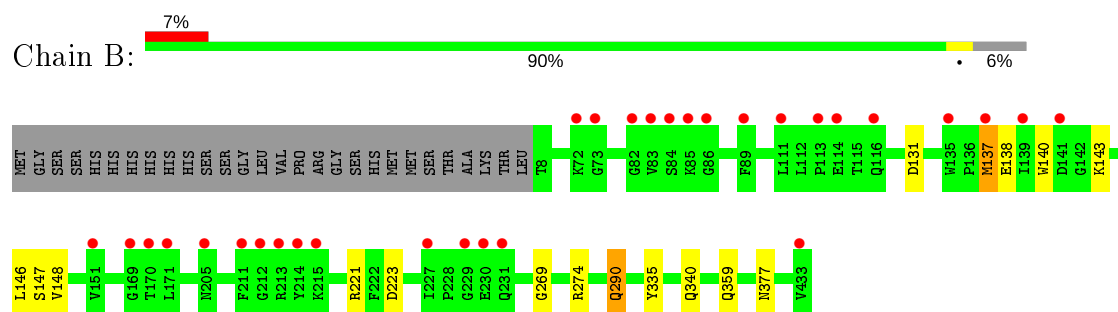
### 3 Residue-property plots [i](#)

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.

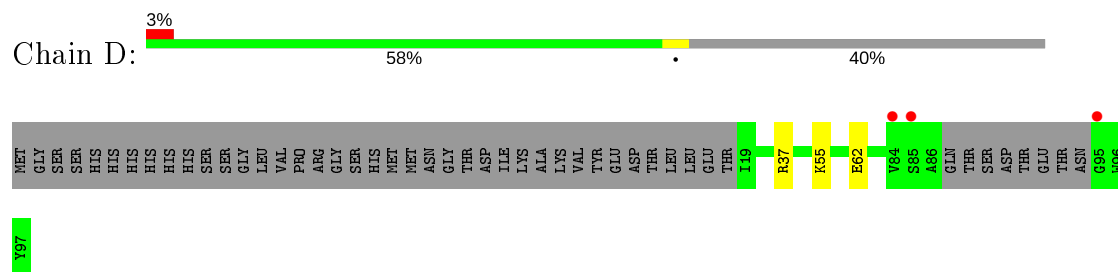
- Molecule 1: Toxin-antitoxin system toxin HipA family



- Molecule 1: Toxin-antitoxin system toxin HipA family



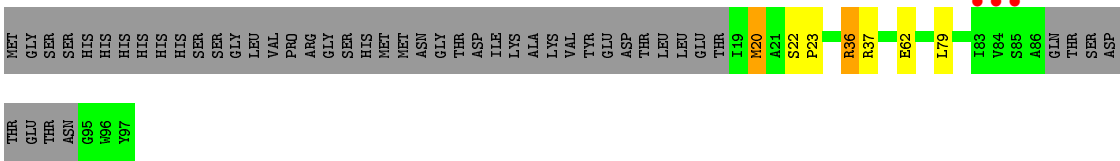
- Molecule 2: Toxin-antitoxin system antidote transcriptional repressor Xre family



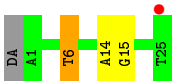
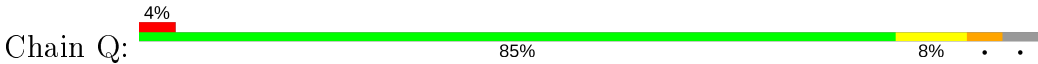
- Molecule 2: Toxin-antitoxin system antidote transcriptional repressor Xre family



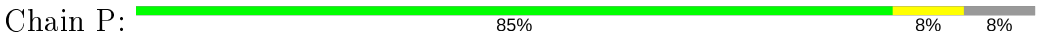




• Molecule 3: Operator DNA



• Molecule 4: Operator DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.82Å 122.45Å 189.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 3.39 49.38 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.38-3.39) 98.9 (49.38-3.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1287)	Depositor
R, $R_{free}$	0.256 , 0.315 0.257 , 0.317	Depositor DCC
$R_{free}$ test set	961 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 28.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17163	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2648e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

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

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	0.23	0/3426	0.42	0/4638
1	B	0.23	0/3420	0.41	0/4635
2	C	0.22	0/545	0.39	0/732
2	D	0.22	0/545	0.40	0/732
3	Q	0.48	0/582	1.14	2/896 (0.2%)
4	P	0.47	0/543	1.27	2/835 (0.2%)
All	All	0.27	0/9061	0.59	4/12468 (0.0%)

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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	6	DG	O4'-C1'-N9	6.22	112.35	108.00
4	P	6	DG	C1'-O4'-C4'	-5.89	104.21	110.10
3	Q	14	DA	O4'-C1'-N9	5.53	111.87	108.00
3	Q	6	DT	O4'-C4'-C3'	-5.25	102.40	104.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	LEU	Peptide
1	A	131	ASP	Peptide
1	B	137	MET	Peptide
1	B	143	LYS	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	3364	3342	3332	16	0
1	B	3355	3308	3298	10	0
2	C	541	577	577	4	0
2	D	541	577	577	2	0
3	Q	517	282	282	2	0
4	P	487	272	273	1	0
All	All	8805	8358	8339	33	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.

The worst 5 of 33 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:294:GLN:OE1	1:A:380:ARG:NH2	2.23	0.72
1:B:146:LEU:CB	1:B:147:SEP:HA	2.24	0.67
2:D:55:LYS:HE2	3:Q:6:DT:H72	1.78	0.65
1:A:335:TYR:O	1:A:340:GLN:NE2	2.31	0.64
2:C:36:ARG:NH1	2:C:79:LEU:O	2.31	0.63

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	423/454 (93%)	413 (98%)	10 (2%)	0	100	100
1	B	423/454 (93%)	413 (98%)	9 (2%)	1 (0%)	47	78
2	C	67/118 (57%)	67 (100%)	0	0	100	100
2	D	67/118 (57%)	67 (100%)	0	0	100	100
All	All	980/1144 (86%)	960 (98%)	19 (2%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	VAL

### 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	359/386 (93%)	355 (99%)	4 (1%)	73	86
1	B	354/386 (92%)	352 (99%)	2 (1%)	86	94
2	C	59/101 (58%)	57 (97%)	2 (3%)	37	65
2	D	59/101 (58%)	59 (100%)	0	100	100
All	All	831/974 (85%)	823 (99%)	8 (1%)	76	88

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
2	C	36	ARG
1	B	290	GLN
1	A	151	VAL
1	B	131	ASP

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 ⓘ

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	SEP	A	147	1	8,9,10	1.56	1 (12%)	8,12,14	1.50	2 (25%)
1	SEP	B	147	1	8,9,10	1.58	1 (12%)	8,12,14	1.49	2 (25%)

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	SEP	A	147	1	-	1/5/8/10	-
1	SEP	B	147	1	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	SEP	P-O1P	3.47	1.61	1.50
1	A	147	SEP	P-O1P	3.42	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	SEP	OG-CB-CA	2.92	110.99	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	147	SEP	P-OG-CB	-2.73	110.77	118.30
1	A	147	SEP	OG-CB-CA	2.56	110.64	108.14
1	B	147	SEP	P-OG-CB	-2.25	112.10	118.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	147	SEP	N-CA-CB-OG
1	B	147	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	147	SEP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	425/454 (93%)	0.52	38 (8%) 9 11	9, 48, 115, 135	0
1	B	425/454 (93%)	0.55	31 (7%) 15 17	6, 34, 110, 150	0
2	C	71/118 (60%)	0.35	3 (4%) 36 35	6, 19, 47, 55	0
2	D	71/118 (60%)	0.32	3 (4%) 36 35	9, 21, 50, 70	0
3	Q	25/26 (96%)	0.31	1 (4%) 38 37	22, 56, 97, 123	0
4	P	24/26 (92%)	0.21	0 100 100	21, 56, 82, 95	0
All	All	1041/1196 (87%)	0.49	76 (7%) 15 17	6, 38, 111, 150	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	THR	7.9
1	B	137	MET	6.7
1	B	169	GLY	5.9
1	B	231	GLN	5.9
1	A	108	LYS	5.4

### 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	SEP	B	147	10/11	0.73	0.38	41,49,64,80	0
1	SEP	A	147	10/11	0.78	0.50	49,64,77,84	0



### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.