



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:45 PM GMT

PDB ID : 4PU4  
Title : Shewanella oneidensis MR-1 Toxin Antitoxin System HipA, HipB and its operator DNA complex (space group P21)  
Authors : Wen, Y.; Behiels, E.; Felix, J.; Elegheert, J.; Vergauwen, B.; Devreese, B.; Savvides, S.  
Deposited on : 2014-03-12  
Resolution : 3.79 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

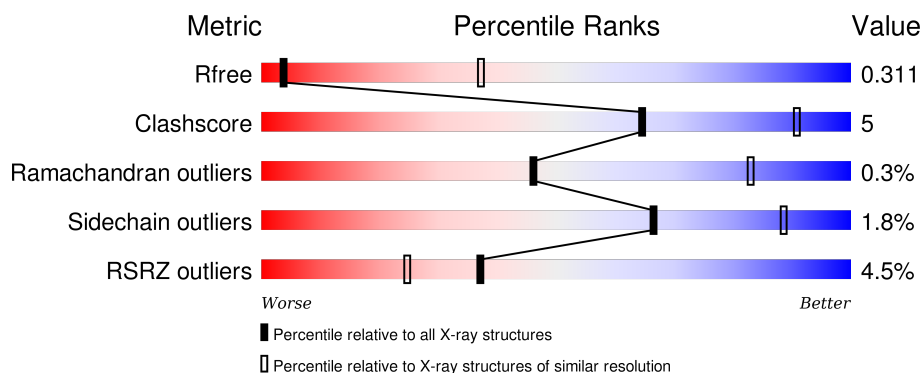
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.79 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))
$R_{free}$	91344	1273 (4.06-3.50)
Clashscore	102246	1412 (4.06-3.50)
Ramachandran outliers	100387	1351 (4.06-3.50)
Sidechain outliers	100360	1347 (4.06-3.50)
RSRZ outliers	91569	1281 (4.06-3.50)

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	454	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>
1	B	454	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>8%</div> </div> </div>
2	C	118	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>9%</div> <div>42%</div> </div> </div>
2	D	118	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>10%</div> <div>34%</div> </div> </div>
3	Q	26	<div> <div></div> <div> <div></div> <div>77%</div> <div>15%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	P	26	 A horizontal bar chart showing the quality of chain 4. The bar is divided into three segments: a green segment representing 69%, a yellow segment representing 23%, and a grey segment representing 8%. The percentages are labeled below the corresponding segments.

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17122 atoms, of which 8359 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	420	Total	C	H	N	O	P	S	0	0	0
			6655	2133	3322	566	616	1	17			
1	B	419	Total	C	H	N	O	P	S	0	0	0
			6637	2128	3311	565	615	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	78	Total	C	H	N	O	S	0	0	0
			1209	371	619	100	116	3			
2	C	68	Total	C	H	N	O	S	0	0	0
			1067	325	556	87	96	3			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	EXPRESSION TAG	UNP Q8EIX4
D	-18	GLY	-	EXPRESSION TAG	UNP Q8EIX4
D	-17	SER	-	EXPRESSION TAG	UNP Q8EIX4
D	-16	SER	-	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	HIS	-	EXPRESSION TAG	UNP Q8EIX4
D	-9	SER	-	EXPRESSION TAG	UNP Q8EIX4
D	-8	SER	-	EXPRESSION TAG	UNP Q8EIX4

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	VAL	-	EXPRESSION TAG	UNP Q8EIX4
C	-4	PRO	-	EXPRESSION TAG	UNP Q8EIX4
C	-3	ARG	-	EXPRESSION TAG	UNP Q8EIX4
C	-2	GLY	-	EXPRESSION TAG	UNP Q8EIX4
C	-1	SER	-	EXPRESSION TAG	UNP Q8EIX4
C	0	HIS	-	EXPRESSION TAG	UNP Q8EIX4
C	1	MET	-	EXPRESSION TAG	UNP Q8EIX4
C	2	MET	-	EXPRESSION TAG	UNP Q8EIX4
C	3	ASN	-	EXPRESSION TAG	UNP Q8EIX4
C	4	GLY	-	EXPRESSION TAG	UNP Q8EIX4
C	5	THR	-	EXPRESSION TAG	UNP Q8EIX4
C	6	ASP	-	EXPRESSION TAG	UNP Q8EIX4
C	7	ILE	-	EXPRESSION TAG	UNP Q8EIX4
C	8	LYS	-	EXPRESSION TAG	UNP Q8EIX4
C	9	ALA	-	EXPRESSION TAG	UNP Q8EIX4
C	10	LYS	-	EXPRESSION TAG	UNP Q8EIX4
C	11	VAL	-	EXPRESSION TAG	UNP Q8EIX4
C	12	TYR	-	EXPRESSION TAG	UNP Q8EIX4
C	13	GLU	-	EXPRESSION TAG	UNP Q8EIX4
C	14	ASP	-	EXPRESSION TAG	UNP Q8EIX4
C	15	THR	-	EXPRESSION TAG	UNP Q8EIX4
C	16	LEU	-	EXPRESSION TAG	UNP Q8EIX4
C	17	LEU	-	EXPRESSION TAG	UNP Q8EIX4
C	18	GLU	-	EXPRESSION TAG	UNP Q8EIX4
C	19	THR	-	EXPRESSION TAG	UNP Q8EIX4
C	20	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
			795	246	279	101	144	25			

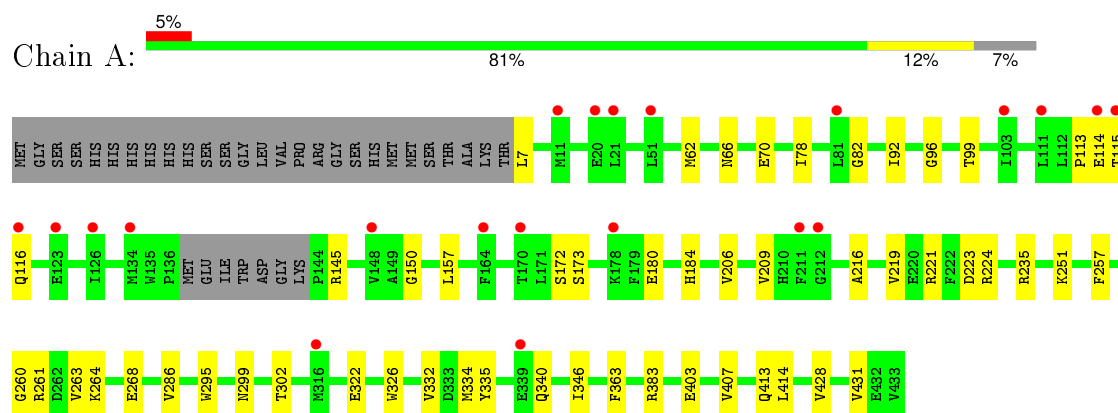
- Molecule 4 is a DNA chain called Operator DNA.

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			

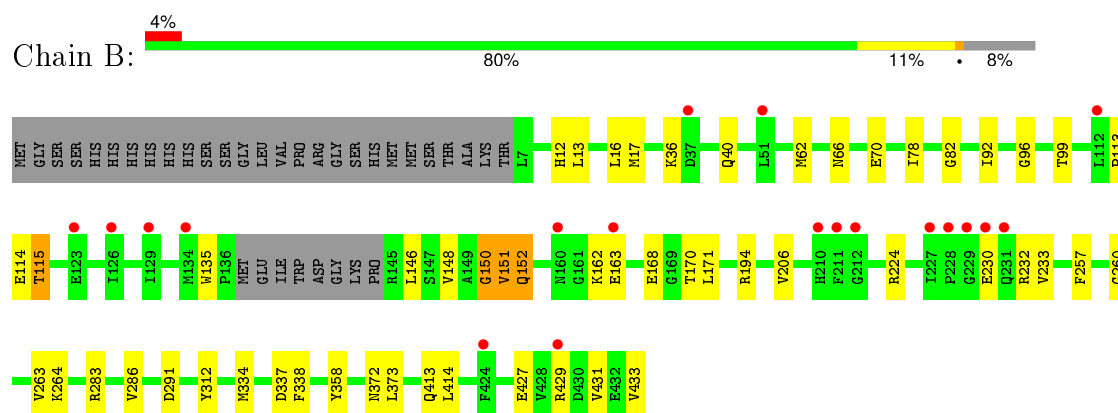
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

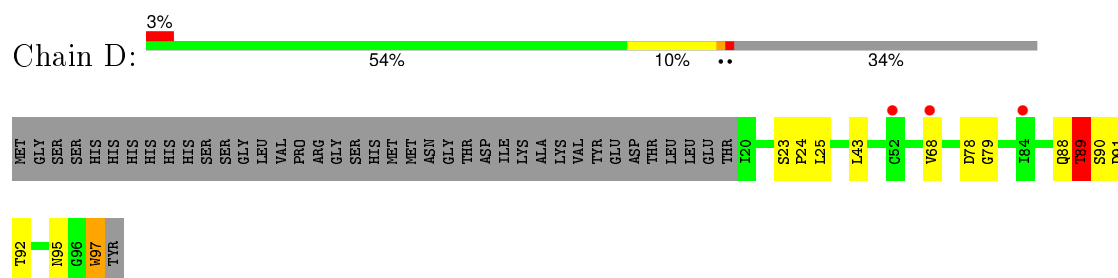
- Molecule 1: Toxin-antitoxin system toxin HipA family



- Molecule 1: Toxin-antitoxin system toxin HipA family

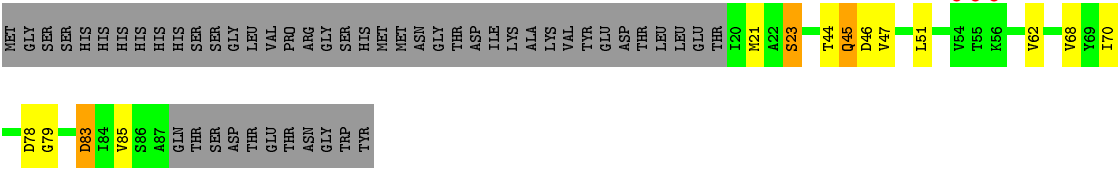


- Molecule 2: Toxin-antitoxin system antidote transcriptional repressor Xre family

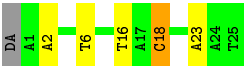
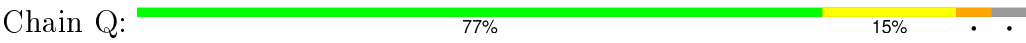


- Molecule 2: Toxin-antitoxin system antidote transcriptional repressor Xre family

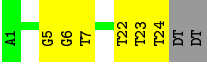




● Molecule 3: Operator DNA



● Molecule 4: Operator DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.24Å 57.33Å 171.38Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	47.57 – 3.79 47.57 – 3.79	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.57-3.79) 97.0 (47.57-3.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1287)	Depositor
R, $R_{free}$	0.236 , 0.306 0.236 , 0.311	Depositor DCC
$R_{free}$ test set	692 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.1	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 68.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 13858 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	17122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.27	0/3396	0.44	0/4598
1	B	0.29	0/3388	0.48	2/4587 (0.0%)
2	C	0.27	0/513	0.47	0/689
2	D	0.31	0/594	0.53	0/801
3	Q	0.54	0/581	1.23	3/894 (0.3%)
4	P	0.58	0/543	1.43	6/835 (0.7%)
All	All	0.33	0/9015	0.66	11/12404 (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
2	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	24	DT	O4'-C4'-C3'	-7.61	101.43	106.00
4	P	23	DT	O4'-C1'-N1	7.00	112.90	108.00
3	Q	6	DT	O4'-C4'-C3'	-6.98	101.71	104.50
4	P	6	DG	O4'-C1'-N9	6.58	112.60	108.00
1	B	150	GLY	N-CA-C	-6.29	97.38	113.10
3	Q	18	DC	O4'-C4'-C3'	-5.77	102.19	104.50
3	Q	6	DT	C1'-O4'-C4'	-5.40	104.70	110.10
4	P	22	DT	O4'-C1'-N1	5.22	111.66	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	GLY	C-N-CA	5.18	134.66	121.70
4	P	22	DT	O4'-C1'-C2'	-5.08	101.84	105.90
4	P	6	DG	O4'-C1'-C2'	-5.08	101.84	105.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	23	SER	Peptide
2	D	89	THR	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	3333	3322	3311	35	0
1	B	3326	3311	3303	36	0
2	C	511	556	556	12	0
2	D	590	619	619	10	0
3	Q	516	279	279	5	0
4	P	487	272	273	2	0
All	All	8763	8359	8341	85	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 5.

All (85) 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:B:334:MET:SD	1:B:413:GLN:NE2	2.42	0.93
2:C:45:GLN:OE1	2:C:46:ASP:N	2.22	0.73
1:A:114:GLU:N	1:A:115:THR:HA	2.06	0.71
1:A:332:VAL:O	1:A:340:GLN:NE2	2.24	0.70
1:B:99:THR:O	1:B:224:ARG:NH2	2.24	0.70
1:B:114:GLU:N	1:B:115:THR:HA	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:THR:O	1:A:224:ARG:NH2	2.25	0.69
1:A:257:PHE:HB2	1:A:263:VAL:HG11	1.75	0.68
1:B:427:GLU:O	1:B:431:VAL:HG23	1.93	0.68
1:B:70:GLU:OE1	1:B:70:GLU:N	2.28	0.67
1:B:232:ARG:NH1	1:B:233:VAL:O	2.28	0.67
1:A:70:GLU:N	1:A:70:GLU:OE2	2.28	0.67
1:B:194:ARG:NH2	1:B:206:VAL:O	2.28	0.67
1:B:283:ARG:NH1	2:D:91:ASP:OD1	2.25	0.65
1:A:221:ARG:NH2	1:A:223:ASP:OD2	2.31	0.63
3:Q:23:DA:N7	4:P:5:DG:N2	2.49	0.61
1:A:334:MET:SD	1:A:413:GLN:NE2	2.74	0.61
1:B:150:GLY:HA2	1:B:151:VAL:HG12	1.82	0.61
2:C:83:ASP:N	2:C:83:ASP:OD1	2.34	0.60
1:A:145:ARG:NH2	1:A:150:GLY:O	2.35	0.59
1:B:372:ASN:OD1	1:B:429:ARG:NH1	2.37	0.57
1:A:260:GLY:O	1:A:264:LYS:N	2.38	0.56
1:A:157:LEU:N	1:A:173:SER:OG	2.39	0.55
1:A:286:VAL:HG23	2:D:79:GLY:O	2.07	0.55
1:B:13:LEU:N	1:B:16:LEU:O	2.40	0.55
1:A:383:ARG:NH2	3:Q:2:DA:OP2	2.41	0.54
1:B:113:PRO:N	1:B:114:GLU:HA	2.23	0.53
1:A:180:GLU:OE2	1:A:184:HIS:N	2.38	0.53
2:D:25:LEU:HD13	2:C:85:VAL:HA	1.91	0.51
1:A:322:GLU:OE1	1:A:322:GLU:N	2.44	0.51
1:B:260:GLY:O	1:B:264:LYS:N	2.44	0.51
1:B:291:ASP:OD2	1:B:312:TYR:OH	2.19	0.51
1:A:172:SER:OG	1:A:235:ARG:NH2	2.45	0.50
1:A:428:VAL:O	1:A:431:VAL:HG22	2.11	0.50
1:B:358:TYR:OH	1:B:433:VAL:HG13	2.12	0.50
1:B:62:MET:O	1:B:66:ASN:ND2	2.45	0.49
1:A:335:TYR:O	1:A:340:GLN:NE2	2.45	0.49
1:B:286:VAL:HG23	2:C:79:GLY:O	2.12	0.49
1:A:286:VAL:HG12	2:D:43:LEU:HD11	1.95	0.49
1:B:257:PHE:HB2	1:B:263:VAL:HG11	1.94	0.49
1:B:230:GLU:N	1:B:230:GLU:OE1	2.45	0.49
2:C:62:VAL:HG22	2:C:68:VAL:HG21	1.94	0.48
1:B:151:VAL:HG22	1:B:152:GLN:H	1.79	0.48
1:A:113:PRO:N	1:A:114:GLU:HA	2.28	0.48
1:A:206:VAL:HG12	1:A:219:VAL:HG13	1.97	0.47
2:D:89:THR:HB	2:D:90:SER:C	2.34	0.47
1:B:151:VAL:HG13	1:B:152:GLN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:SER:CB	2:D:24:PRO:CD	2.93	0.47
1:B:286:VAL:HG13	2:C:51:LEU:CD2	2.44	0.47
1:B:113:PRO:CG	1:B:114:GLU:HA	2.45	0.46
1:A:403:GLU:O	1:A:407:VAL:HG23	2.15	0.46
1:A:78:ILE:O	1:A:82:GLY:N	2.48	0.46
1:B:36:LYS:CD	1:B:36:LYS:N	2.79	0.46
1:A:299:ASN:HA	1:A:302:THR:HG22	1.98	0.45
1:B:162:LYS:HG3	1:B:163:GLU:H	1.81	0.45
1:A:62:MET:O	1:A:66:ASN:ND2	2.48	0.45
3:Q:18:DC:N4	4:P:7:DT:O4	2.50	0.44
1:A:346:ILE:HG23	1:A:363:PHE:HB2	2.00	0.44
1:B:115:THR:OG1	1:B:168:GLU:O	2.30	0.44
2:D:97:TRP:N	2:D:97:TRP:CD1	2.86	0.43
1:B:170:THR:HG23	1:B:171:LEU:HD12	2.00	0.43
2:D:78:ASP:OD1	2:D:79:GLY:N	2.51	0.43
1:A:295:TRP:HA	1:A:326:TRP:CH2	2.53	0.43
1:A:92:ILE:O	1:A:96:GLY:N	2.51	0.43
1:A:115:THR:OG1	1:A:116:GLN:N	2.51	0.43
1:A:251:LYS:NZ	1:A:268:GLU:O	2.43	0.43
1:B:151:VAL:HG13	1:B:152:GLN:H	1.84	0.43
2:D:68:VAL:H	2:C:70:ILE:HG22	1.84	0.43
1:B:12:HIS:HA	1:B:17:MET:HA	2.01	0.42
1:A:263:VAL:O	1:A:263:VAL:HG12	2.19	0.42
1:A:261:ARG:CZ	1:A:261:ARG:HB3	2.49	0.42
1:B:92:ILE:O	1:B:96:GLY:N	2.53	0.42
1:B:373:LEU:CD1	2:C:51:LEU:CD1	2.98	0.42
1:A:209:VAL:HG23	1:A:216:ALA:HB3	2.01	0.41
1:B:78:ILE:O	1:B:82:GLY:N	2.53	0.41
2:D:92:THR:O	2:D:95:ASN:N	2.53	0.41
1:B:171:LEU:HG	1:B:233:VAL:HG23	2.02	0.41
1:A:383:ARG:NE	3:Q:2:DA:OP1	2.48	0.41
2:C:44:THR:OG1	2:C:47:VAL:HG12	2.20	0.41
1:B:373:LEU:HD13	2:C:51:LEU:CD1	2.51	0.41
3:Q:16:DT:OP2	2:C:68:VAL:HG12	2.21	0.40
1:A:261:ARG:HA	1:A:264:LYS:CG	2.51	0.40
1:B:286:VAL:HG13	2:C:51:LEU:HD22	2.03	0.40
1:A:257:PHE:HB2	1:A:263:VAL:CG1	2.49	0.40
1:B:148:VAL:HG11	1:B:338:PHE:HB3	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	415/454 (91%)	407 (98%)	8 (2%)	0	100	100
1	B	414/454 (91%)	404 (98%)	8 (2%)	2 (0%)	34	77
2	C	66/118 (56%)	63 (96%)	2 (3%)	1 (2%)	13	58
2	D	76/118 (64%)	73 (96%)	3 (4%)	0	100	100
All	All	971/1144 (85%)	947 (98%)	21 (2%)	3 (0%)	46	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	VAL
1	B	152	GLN
2	C	23	SER

### 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	357/386 (92%)	355 (99%)	2 (1%)	90	96
1	B	356/386 (92%)	350 (98%)	6 (2%)	68	89
2	C	57/101 (56%)	53 (93%)	4 (7%)	19	60
2	D	66/101 (65%)	63 (96%)	3 (4%)	34	73
All	All	836/974 (86%)	821 (98%)	15 (2%)	66	88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	414	LEU
1	B	40	GLN
1	B	115	THR
1	B	135	TRP
1	B	146	LEU
1	B	337	ASP
1	B	414	LEU
2	D	88	GLN
2	D	89	THR
2	D	97	TRP
2	C	21	MET
2	C	45	GLN
2	C	78	ASP
2	C	83	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	GLN
1	B	66	ASN
1	B	175	HIS
1	B	413	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	SEP	A	147	1	8,9,10	1.52	1 (12%)	8,12,14	1.29	1 (12%)
1	SEP	B	147	1	8,9,10	1.53	1 (12%)	8,12,14	1.54	1 (12%)

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	-	0/6/8/10	0/0/0/0
1	SEP	B	147	1	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	SEP	P-O1P	3.09	1.61	1.51
1	B	147	SEP	P-O1P	3.16	1.61	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	SEP	OG-CB-CA	2.66	110.55	108.27
1	B	147	SEP	OG-CB-CA	3.02	110.85	108.27

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](#)

There are no ligands in this entry.

## 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

### 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	419/454 (92%)	0.42	21 (5%) 32 21	35, 78, 145, 172	0
1	B	418/454 (92%)	0.33	19 (4%) 37 25	26, 67, 129, 181	0
2	C	68/118 (57%)	0.32	3 (4%) 38 25	30, 54, 86, 95	0
2	D	78/118 (66%)	0.27	3 (3%) 44 30	27, 56, 122, 127	0
3	Q	25/26 (96%)	-0.14	0 100 100	65, 106, 137, 141	0
4	P	24/26 (92%)	-0.16	0 100 100	66, 109, 126, 138	0
All	All	1032/1196 (86%)	0.34	46 (4%) 37 25	26, 70, 136, 181	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	GLY	5.8
1	B	126	ILE	4.5
1	A	170	THR	3.8
1	B	231	GLN	3.7
1	A	123	GLU	3.7
1	A	20	GLU	3.5
1	B	230	GLU	3.5
1	B	112	LEU	3.4
1	B	134	MET	3.4
1	A	114	GLU	3.3
1	A	212	GLY	3.2
1	A	116	GLN	3.1
1	A	211	PHE	3.0
1	A	81	LEU	3.0
1	B	228	PRO	2.9
1	A	164	PHE	2.9
1	B	123	GLU	2.9
1	A	178	LYS	2.9
1	A	115	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	210	HIS	2.8
1	A	126	ILE	2.7
1	B	429	ARG	2.6
1	B	227	ILE	2.5
1	A	11	MET	2.5
2	D	68	VAL	2.5
1	A	111	LEU	2.4
1	A	316	MET	2.4
1	B	163	GLU	2.4
1	B	37	ASP	2.4
1	B	160	ASN	2.3
1	A	21	LEU	2.3
2	D	52	CYS	2.3
1	A	134	MET	2.2
1	B	129	ILE	2.2
1	A	148	VAL	2.2
1	B	51	LEU	2.2
2	C	54	VAL	2.2
1	B	212	GLY	2.1
1	A	339	GLU	2.1
2	D	84	ILE	2.1
1	B	211	PHE	2.1
1	B	424	PHE	2.0
1	A	51	LEU	2.0
2	C	55	THR	2.0
2	C	56	LYS	2.0
1	A	103	ILE	2.0

## 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	SEP	B	147	10/11	0.87	0.20	-	38,84,102,102	0
1	SEP	A	147	10/11	0.73	0.39	-	136,149,174,181	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.