



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 12, 2025 – 04:14 pm BST

PDB ID : 9R35 / pdb\_00009r35  
Title : Crystal structure of the Pseudomonas putida Xre-RES toxin-antitoxin complex bound to promoter DNA  
Authors : Henriksen, F.O.G.; Brodersen, D.E.  
Deposited on : 2025-05-02  
Resolution : 2.70 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

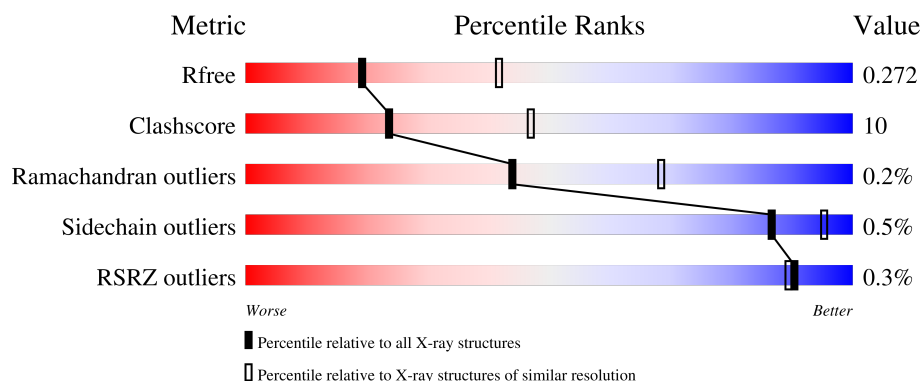
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.





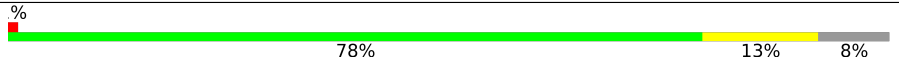
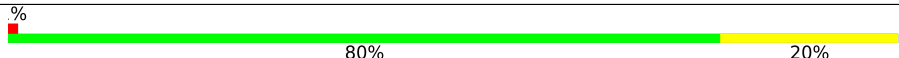
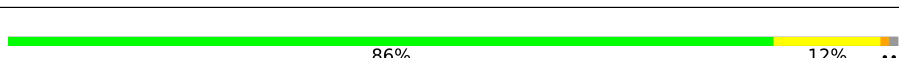
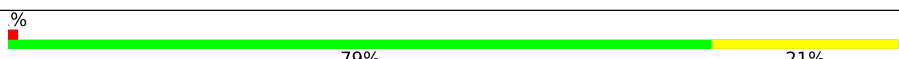
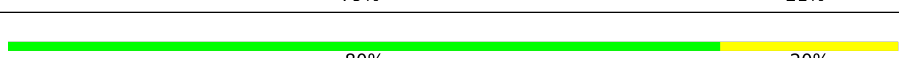
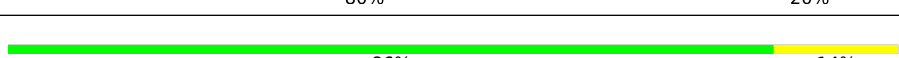
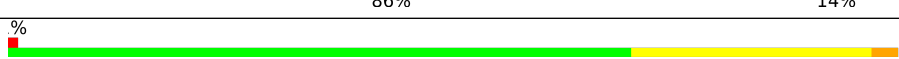

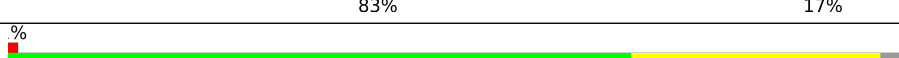







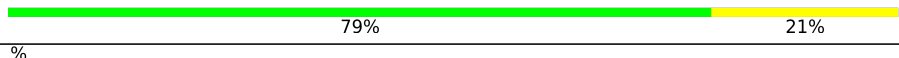
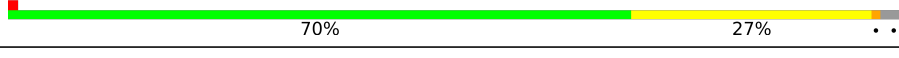
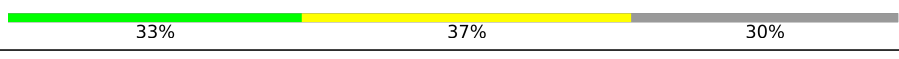
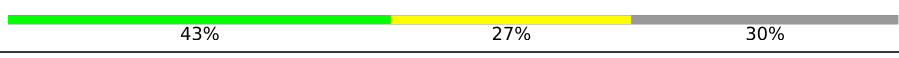
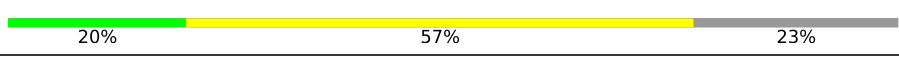
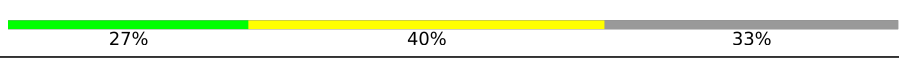
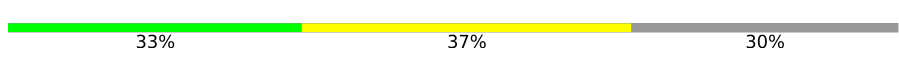
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	158	<div> <div></div> <div>73%</div> <div>18%</div> <div>9%</div> </div>
1	D	158	<div> <div>74%</div> <div>18%</div> <div>8%</div> </div>
1	G	158	<div> <div>77%</div> <div>15%</div> <div>8%</div> </div>
1	J	158	<div> <div>68%</div> <div>23%</div> <div>9%</div> </div>
1	M	158	<div> <div>71%</div> <div>21%</div> <div>8%</div> </div>

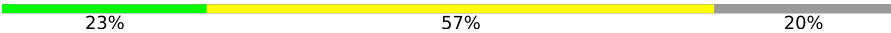
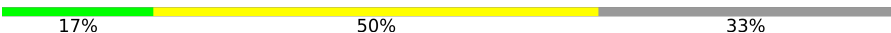
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Mol	Chain	Length	Quality of chain
1	P	158	
1	S	158	
1	V	158	
2	B	149	
2	C	149	
2	E	149	
2	F	149	
2	H	149	
2	I	149	
2	K	149	
2	L	149	
2	N	149	
2	O	149	
2	Q	149	
2	R	149	
2	T	149	
2	U	149	
2	W	149	
2	X	149	
3	a	30	
3	d	30	
3	f	30	
3	h	30	
4	b	30	
4	c	30	

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Mol	Chain	Length	Quality of chain
4	e	30	 23% 57% 20%
4	g	30	 17% 50% 33%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31517 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 Toxin Res.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1116	710	195	207	4			
1	D	145	Total	C	N	O	S	0	0	0
			1128	719	196	209	4			
1	G	145	Total	C	N	O	S	0	0	0
			1128	719	196	209	4			
1	J	144	Total	C	N	O	S	0	0	0
			1116	710	195	207	4			
1	M	145	Total	C	N	O	S	0	0	0
			1128	719	196	209	4			
1	P	145	Total	C	N	O	S	0	0	0
			1128	719	196	209	4			
1	S	145	Total	C	N	O	S	0	0	0
			1128	719	196	209	4			
1	V	145	Total	C	N	O	S	0	0	0
			1128	719	196	209	4			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q88K57
A	-11	GLY	-	expression tag	UNP Q88K57
A	-10	SER	-	expression tag	UNP Q88K57
A	-9	SER	-	expression tag	UNP Q88K57
A	-8	HIS	-	expression tag	UNP Q88K57
A	-7	HIS	-	expression tag	UNP Q88K57
A	-6	HIS	-	expression tag	UNP Q88K57
A	-5	HIS	-	expression tag	UNP Q88K57
A	-4	HIS	-	expression tag	UNP Q88K57
A	-3	HIS	-	expression tag	UNP Q88K57
A	-2	SER	-	expression tag	UNP Q88K57
A	-1	GLN	-	expression tag	UNP Q88K57
A	0	ASP	-	expression tag	UNP Q88K57

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	-	expression tag	UNP Q88K57
D	-12	MET	-	initiating methionine	UNP Q88K57
D	-11	GLY	-	expression tag	UNP Q88K57
D	-10	SER	-	expression tag	UNP Q88K57
D	-9	SER	-	expression tag	UNP Q88K57
D	-8	HIS	-	expression tag	UNP Q88K57
D	-7	HIS	-	expression tag	UNP Q88K57
D	-6	HIS	-	expression tag	UNP Q88K57
D	-5	HIS	-	expression tag	UNP Q88K57
D	-4	HIS	-	expression tag	UNP Q88K57
D	-3	HIS	-	expression tag	UNP Q88K57
D	-2	SER	-	expression tag	UNP Q88K57
D	-1	GLN	-	expression tag	UNP Q88K57
D	0	ASP	-	expression tag	UNP Q88K57
D	1	PRO	-	expression tag	UNP Q88K57
G	-12	MET	-	initiating methionine	UNP Q88K57
G	-11	GLY	-	expression tag	UNP Q88K57
G	-10	SER	-	expression tag	UNP Q88K57
G	-9	SER	-	expression tag	UNP Q88K57
G	-8	HIS	-	expression tag	UNP Q88K57
G	-7	HIS	-	expression tag	UNP Q88K57
G	-6	HIS	-	expression tag	UNP Q88K57
G	-5	HIS	-	expression tag	UNP Q88K57
G	-4	HIS	-	expression tag	UNP Q88K57
G	-3	HIS	-	expression tag	UNP Q88K57
G	-2	SER	-	expression tag	UNP Q88K57
G	-1	GLN	-	expression tag	UNP Q88K57
G	0	ASP	-	expression tag	UNP Q88K57
G	1	PRO	-	expression tag	UNP Q88K57
J	-12	MET	-	initiating methionine	UNP Q88K57
J	-11	GLY	-	expression tag	UNP Q88K57
J	-10	SER	-	expression tag	UNP Q88K57
J	-9	SER	-	expression tag	UNP Q88K57
J	-8	HIS	-	expression tag	UNP Q88K57
J	-7	HIS	-	expression tag	UNP Q88K57
J	-6	HIS	-	expression tag	UNP Q88K57
J	-5	HIS	-	expression tag	UNP Q88K57
J	-4	HIS	-	expression tag	UNP Q88K57
J	-3	HIS	-	expression tag	UNP Q88K57
J	-2	SER	-	expression tag	UNP Q88K57
J	-1	GLN	-	expression tag	UNP Q88K57
J	0	ASP	-	expression tag	UNP Q88K57

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1	PRO	-	expression tag	UNP Q88K57
M	-12	MET	-	initiating methionine	UNP Q88K57
M	-11	GLY	-	expression tag	UNP Q88K57
M	-10	SER	-	expression tag	UNP Q88K57
M	-9	SER	-	expression tag	UNP Q88K57
M	-8	HIS	-	expression tag	UNP Q88K57
M	-7	HIS	-	expression tag	UNP Q88K57
M	-6	HIS	-	expression tag	UNP Q88K57
M	-5	HIS	-	expression tag	UNP Q88K57
M	-4	HIS	-	expression tag	UNP Q88K57
M	-3	HIS	-	expression tag	UNP Q88K57
M	-2	SER	-	expression tag	UNP Q88K57
M	-1	GLN	-	expression tag	UNP Q88K57
M	0	ASP	-	expression tag	UNP Q88K57
M	1	PRO	-	expression tag	UNP Q88K57
P	-12	MET	-	initiating methionine	UNP Q88K57
P	-11	GLY	-	expression tag	UNP Q88K57
P	-10	SER	-	expression tag	UNP Q88K57
P	-9	SER	-	expression tag	UNP Q88K57
P	-8	HIS	-	expression tag	UNP Q88K57
P	-7	HIS	-	expression tag	UNP Q88K57
P	-6	HIS	-	expression tag	UNP Q88K57
P	-5	HIS	-	expression tag	UNP Q88K57
P	-4	HIS	-	expression tag	UNP Q88K57
P	-3	HIS	-	expression tag	UNP Q88K57
P	-2	SER	-	expression tag	UNP Q88K57
P	-1	GLN	-	expression tag	UNP Q88K57
P	0	ASP	-	expression tag	UNP Q88K57
P	1	PRO	-	expression tag	UNP Q88K57
S	-12	MET	-	initiating methionine	UNP Q88K57
S	-11	GLY	-	expression tag	UNP Q88K57
S	-10	SER	-	expression tag	UNP Q88K57
S	-9	SER	-	expression tag	UNP Q88K57
S	-8	HIS	-	expression tag	UNP Q88K57
S	-7	HIS	-	expression tag	UNP Q88K57
S	-6	HIS	-	expression tag	UNP Q88K57
S	-5	HIS	-	expression tag	UNP Q88K57
S	-4	HIS	-	expression tag	UNP Q88K57
S	-3	HIS	-	expression tag	UNP Q88K57
S	-2	SER	-	expression tag	UNP Q88K57
S	-1	GLN	-	expression tag	UNP Q88K57
S	0	ASP	-	expression tag	UNP Q88K57

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Chain	Residue	Modelled	Actual	Comment	Reference
S	1	PRO	-	expression tag	UNP Q88K57
V	-12	MET	-	initiating methionine	UNP Q88K57
V	-11	GLY	-	expression tag	UNP Q88K57
V	-10	SER	-	expression tag	UNP Q88K57
V	-9	SER	-	expression tag	UNP Q88K57
V	-8	HIS	-	expression tag	UNP Q88K57
V	-7	HIS	-	expression tag	UNP Q88K57
V	-6	HIS	-	expression tag	UNP Q88K57
V	-5	HIS	-	expression tag	UNP Q88K57
V	-4	HIS	-	expression tag	UNP Q88K57
V	-3	HIS	-	expression tag	UNP Q88K57
V	-2	SER	-	expression tag	UNP Q88K57
V	-1	GLN	-	expression tag	UNP Q88K57
V	0	ASP	-	expression tag	UNP Q88K57
V	1	PRO	-	expression tag	UNP Q88K57

- Molecule 2 is a protein called XRE anti-toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	C	148	Total	C	N	O	S	0	0	0
			1183	745	210	223	5			
2	E	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	F	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	H	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	I	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	K	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	L	145	Total	C	N	O	S	0	0	0
			1163	732	207	219	5			
2	N	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	O	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	Q	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	R	146	Total	C	N	O	S	0	0	0
			1167	734	208	220	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	U	148	Total	C	N	O	S	0	0	0
			1183	745	210	223	5			
2	W	149	Total	C	N	O	S	0	0	0
			1192	751	211	225	5			
2	X	145	Total	C	N	O	S	0	0	0
			1163	732	207	219	5			

- Molecule 3 is a DNA chain called DNA reverse (30-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	a	21	Total	C	N	O	P	0	0	0
			420	203	67	130	20			
3	d	21	Total	C	N	O	P	0	0	0
			420	203	67	130	20			
3	f	23	Total	C	N	O	P	0	0	0
			461	222	75	142	22			
3	h	20	Total	C	N	O	P	0	0	0
			399	193	62	125	19			

- Molecule 4 is a DNA chain called DNA forward (30-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	b	21	Total	C	N	O	P	0	0	0
			435	206	91	118	20			
4	c	21	Total	C	N	O	P	0	0	0
			435	206	91	118	20			
4	e	24	Total	C	N	O	P	0	0	0
			496	235	101	137	23			
4	g	20	Total	C	N	O	P	0	0	0
			415	196	89	111	19			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	1	Total	O	0	0
			1	1		
5	D	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	5	Total O 5 5	0	0
5	F	6	Total O 6 6	0	0
5	G	3	Total O 3 3	0	0
5	H	2	Total O 2 2	0	0
5	I	3	Total O 3 3	0	0
5	J	3	Total O 3 3	0	0
5	K	3	Total O 3 3	0	0
5	L	3	Total O 3 3	0	0
5	M	4	Total O 4 4	0	0
5	N	2	Total O 2 2	0	0
5	O	1	Total O 1 1	0	0
5	P	1	Total O 1 1	0	0
5	Q	2	Total O 2 2	0	0
5	S	3	Total O 3 3	0	0
5	T	2	Total O 2 2	0	0
5	U	1	Total O 1 1	0	0
5	V	1	Total O 1 1	0	0
5	W	1	Total O 1 1	0	0
5	X	2	Total O 2 2	0	0
5	a	1	Total O 1 1	0	0
5	b	1	Total O 1 1	0	0

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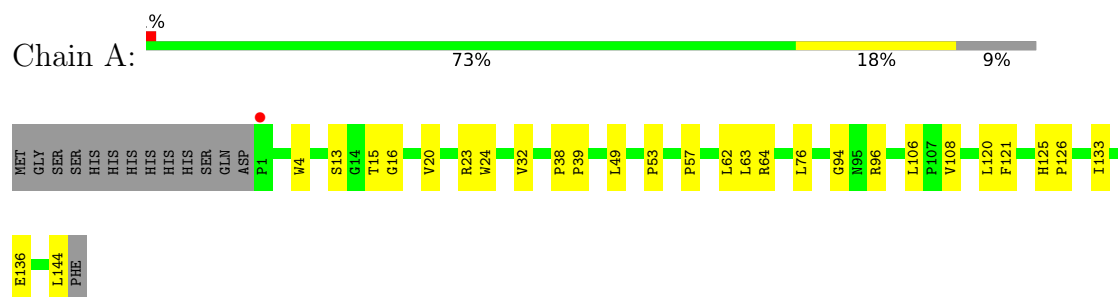
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	e	1	Total 1	O 1	0	0
5	f	2	Total 2	O 2	0	0
5	g	1	Total 1	O 1	0	0
5	h	2	Total 2	O 2	0	0

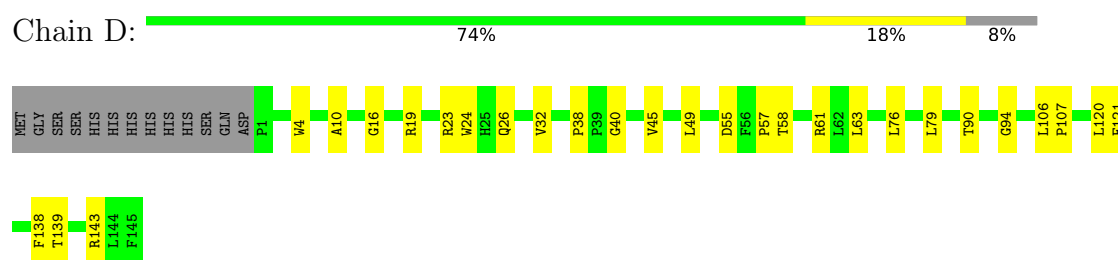
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

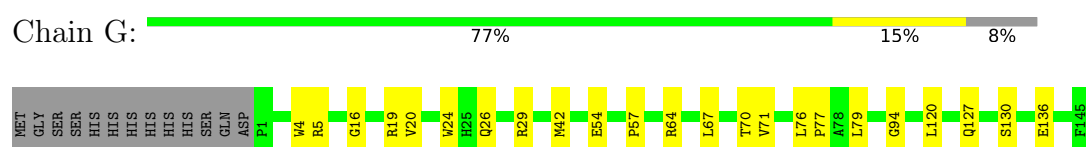
#### • Molecule 1: Toxin Res



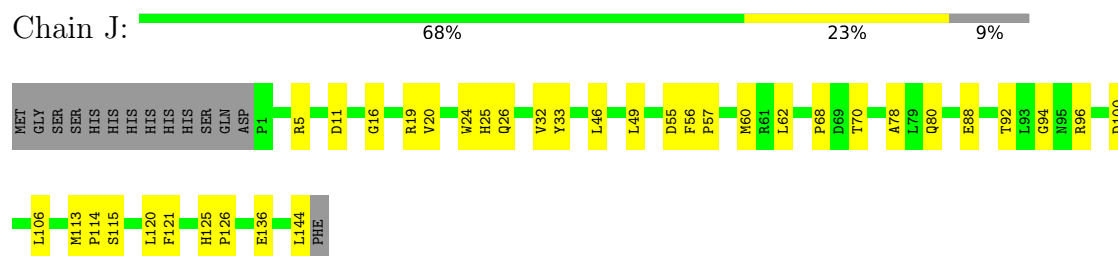
#### • Molecule 1: Toxin Res



#### • Molecule 1: Toxin Res

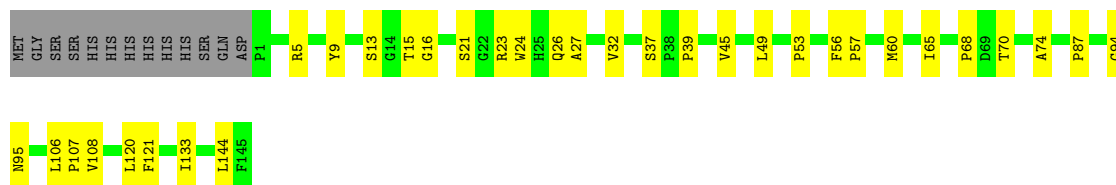


#### • Molecule 1: Toxin Res




#### • Molecule 1: Toxin Res

Chain M:  71% 21% 8%



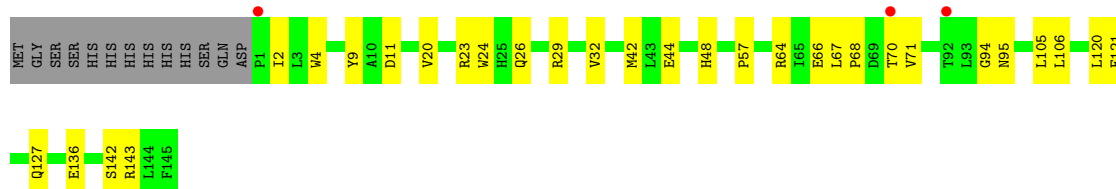
• Molecule 1: Toxin Res

Chain P:  74% 18% 8%




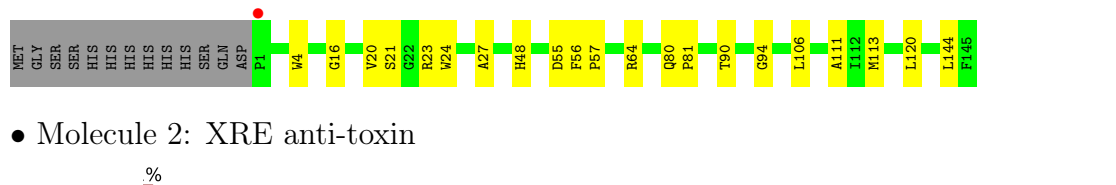
• Molecule 1: Toxin Res

Chain S:  73% 19% 8%




• Molecule 1: Toxin Res

Chain V:  78% 13% 8%




• Molecule 2: XRE anti-toxin

Chain B:  80% 20%

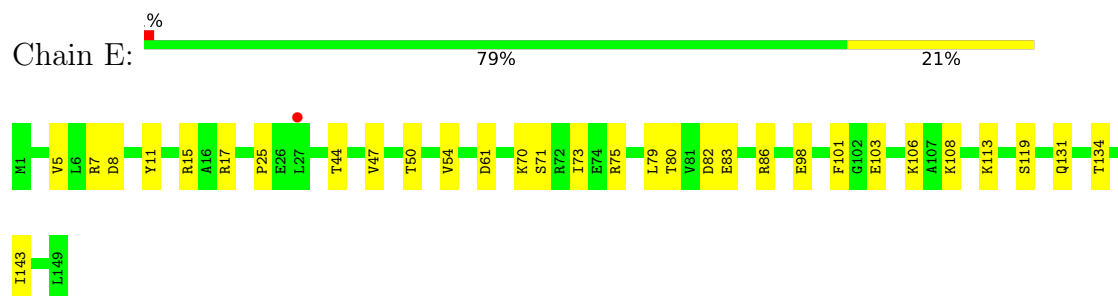


• Molecule 2: XRE anti-toxin

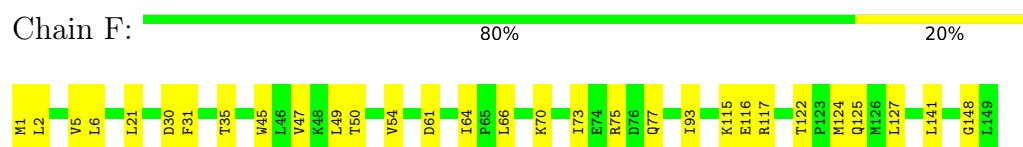
Chain C:  86% 12% ..



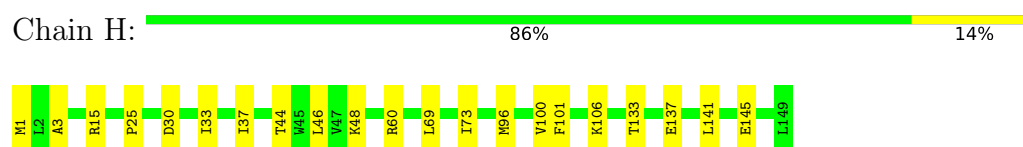
- Molecule 2: XRE anti-toxin



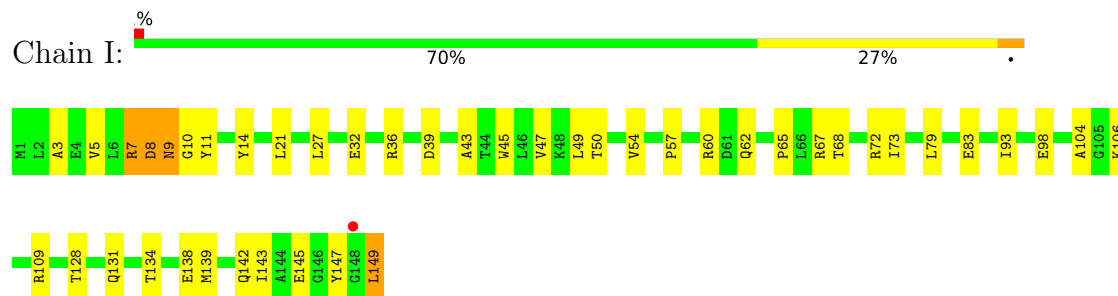
- Molecule 2: XRE anti-toxin



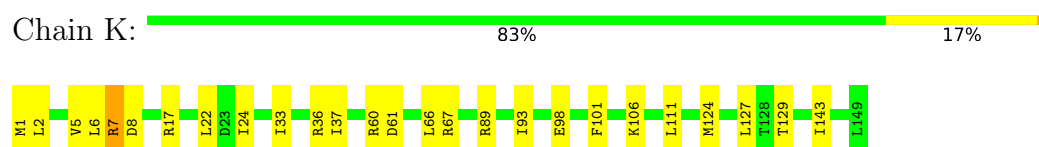
- Molecule 2: XRE anti-toxin



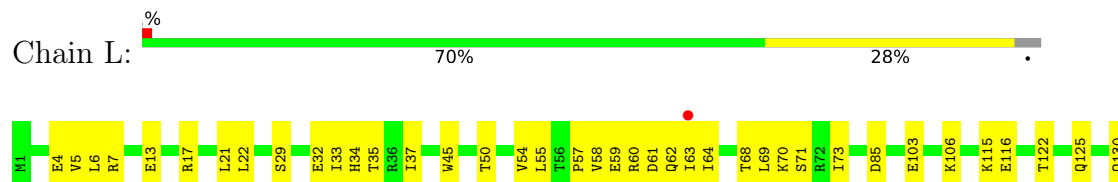
- Molecule 2: XRE anti-toxin

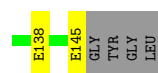


- Molecule 2: XRE anti-toxin



- Molecule 2: XRE anti-toxin





- Molecule 2: XRE anti-toxin

Chain N: 82% 18%



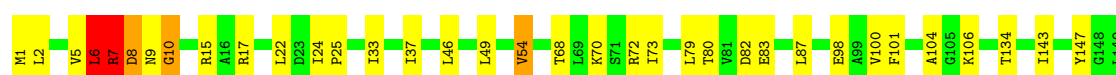
- Molecule 2: XRE anti-toxin

Chain O: 77% 22% .



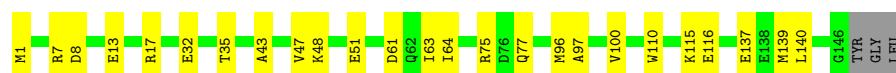
- Molecule 2: XRE anti-toxin

Chain Q: 77% 20% ..



- Molecule 2: XRE anti-toxin

Chain R: 81% 17% .



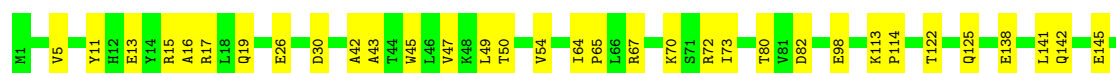
- Molecule 2: XRE anti-toxin

Chain T: 85% 15% .




- Molecule 2: XRE anti-toxin

Chain U: 77% 22% .



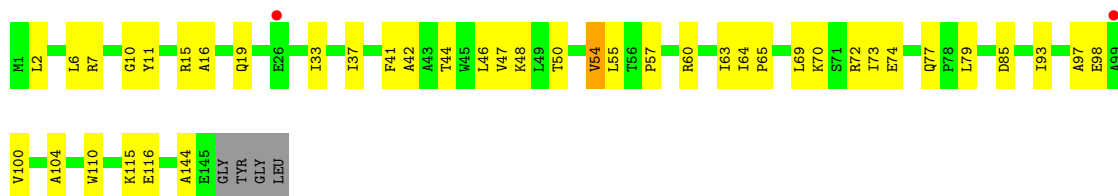
- Molecule 2: XRE anti-toxin

Chain W:  79% 21%



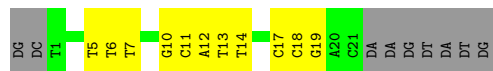
- Molecule 2: XRE anti-toxin

Chain X:  70% 27% ..



- Molecule 3: DNA reverse (30-mer)

Chain a:  33% 37% 30%



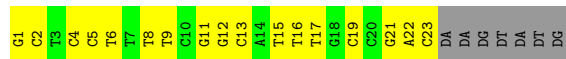
- Molecule 3: DNA reverse (30-mer)

Chain d:  43% 27% 30%

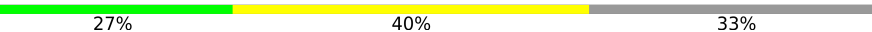


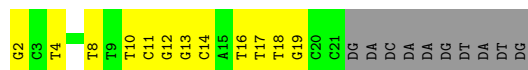
- Molecule 3: DNA reverse (30-mer)

Chain f:  20% 57% 23%



- Molecule 3: DNA reverse (30-mer)

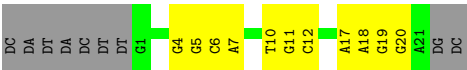
Chain h:  27% 40% 33%



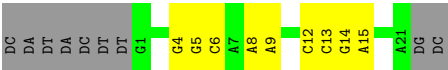
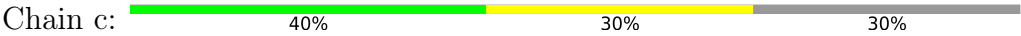
- Molecule 4: DNA forward (30-mer)

Chain b:  33% 37% 30%

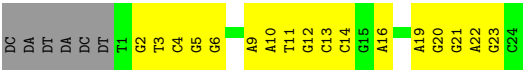




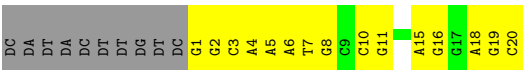
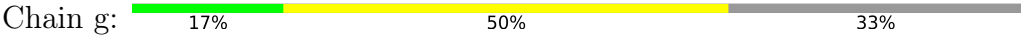
● Molecule 4: DNA forward (30-mer)



● Molecule 4: DNA forward (30-mer)



● Molecule 4: DNA forward (30-mer)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.23Å 185.11Å 170.79Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	26.03 – 2.70 26.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.3 (26.03-2.70) 97.3 (26.03-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.61Å)	Xtriage
Refinement program	PHENIX 2.8.3	Depositor
R, $R_{free}$	0.228 , 0.269 0.245 , 0.272	Depositor DCC
$R_{free}$ test set	2027 reflections (1.35%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.6	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 72.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.430 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	31517	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.78% 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

### 5.1 Standard geometry

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	0.22	0/1147	0.35	0/1572
1	D	0.21	0/1160	0.36	0/1588
1	G	0.22	0/1160	0.36	0/1588
1	J	0.23	0/1147	0.37	0/1572
1	M	0.22	0/1160	0.35	0/1588
1	P	0.21	0/1160	0.36	0/1588
1	S	0.22	0/1160	0.36	0/1588
1	V	0.20	0/1160	0.36	0/1588
2	B	0.19	0/1212	0.34	0/1636
2	C	0.24	0/1203	0.38	0/1625
2	E	0.21	0/1212	0.35	0/1636
2	F	0.23	0/1212	0.39	0/1636
2	H	0.19	0/1212	0.32	0/1636
2	I	0.26	0/1212	0.49	0/1636
2	K	0.22	0/1212	0.42	1/1636 (0.1%)
2	L	0.20	0/1182	0.46	1/1597 (0.1%)
2	N	0.19	0/1212	0.34	0/1636
2	O	0.22	0/1212	0.38	0/1636
2	Q	0.27	0/1212	0.44	1/1636 (0.1%)
2	R	0.21	0/1186	0.40	0/1602
2	T	0.20	0/1212	0.36	0/1636
2	U	0.18	0/1203	0.40	0/1625
2	W	0.19	0/1212	0.35	0/1636
2	X	0.21	0/1182	0.51	1/1597 (0.1%)
3	a	0.24	0/467	0.40	0/718
3	d	0.25	0/467	0.44	0/718
3	f	0.29	0/513	0.57	0/789
3	h	0.22	0/443	0.38	0/681
4	b	0.22	0/491	0.33	0/757
4	c	0.20	0/491	0.36	0/757
4	e	0.25	0/559	0.49	0/862
4	g	0.23	0/469	0.38	0/723
All	All	0.22	0/32442	0.39	4/44719 (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
2	E	0	1
2	I	0	1
2	K	0	1
2	O	0	1
2	Q	0	1
2	R	0	1
All	All	0	6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	L	58	VAL	N-CA-C	-6.16	107.86	113.71
2	Q	54	VAL	N-CA-C	-5.37	107.57	113.43
2	K	8	ASP	N-CA-C	-5.14	106.69	113.12
2	X	54	VAL	N-CA-C	-5.06	108.91	113.71

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	7	ARG	Sidechain
2	I	7	ARG	Sidechain
2	K	7	ARG	Sidechain
2	O	7	ARG	Sidechain
2	Q	7	ARG	Sidechain

## 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	1116	0	1114	17	2
1	D	1128	0	1123	35	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1128	0	1123	22	1
1	J	1116	0	1114	32	2
1	M	1128	0	1123	25	0
1	P	1128	0	1123	22	0
1	S	1128	0	1123	30	0
1	V	1128	0	1123	19	0
2	B	1192	0	1208	22	0
2	C	1183	0	1197	13	0
2	E	1192	0	1208	22	0
2	F	1192	0	1208	35	0
2	H	1192	0	1208	17	0
2	I	1192	0	1208	38	6
2	K	1192	0	1208	25	0
2	L	1163	0	1182	30	7
2	N	1192	0	1208	28	0
2	O	1192	0	1208	20	1
2	Q	1192	0	1208	29	0
2	R	1167	0	1185	13	1
2	T	1192	0	1208	27	0
2	U	1183	0	1197	26	3
2	W	1192	0	1208	27	0
2	X	1163	0	1182	39	3
3	a	420	0	241	14	0
3	d	420	0	241	8	0
3	f	461	0	263	27	0
3	h	399	0	230	22	0
4	b	435	0	235	10	0
4	c	435	0	235	8	0
4	e	496	0	269	27	1
4	g	415	0	223	23	0
5	A	4	0	0	0	0
5	B	1	0	0	0	0
5	D	4	0	0	7	0
5	E	5	0	0	2	0
5	F	6	0	0	5	0
5	G	3	0	0	4	0
5	H	2	0	0	0	0
5	I	3	0	0	5	0
5	J	3	0	0	0	0
5	K	3	0	0	3	0
5	L	3	0	0	0	0
5	M	4	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	2	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	Q	2	0	0	0	0
5	S	3	0	0	5	0
5	T	2	0	0	4	0
5	U	1	0	0	3	0
5	V	1	0	0	1	0
5	W	1	0	0	0	0
5	X	2	0	0	3	0
5	a	1	0	0	0	0
5	b	1	0	0	0	0
5	e	1	0	0	0	0
5	f	2	0	0	1	0
5	g	1	0	0	1	0
5	h	2	0	0	2	0
All	All	31517	0	30134	598	14

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 10.

The worst 5 of 598 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)
5:M:201:HOH:O	2:N:106:LYS:CE	1.89	1.20
5:M:201:HOH:O	2:N:106:LYS:HD3	1.50	1.08
2:K:17:ARG:HD2	5:K:201:HOH:O	1.53	1.07
1:S:29:ARG:HG3	5:S:201:HOH:O	1.52	1.06
2:U:125:GLN:HB3	5:U:201:HOH:O	1.53	1.05

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:145:GLU:OE2	2:L:116:GLU:OE1[2_544]	1.33	0.87
1:D:143:ARG:NH2	2:L:13:GLU:OE2[1_455]	1.42	0.78
2:I:145:GLU:CD	2:L:116:GLU:OE1[2_544]	1.60	0.60
2:I:145:GLU:OE1	2:L:116:GLU:OE1[2_544]	1.69	0.51
2:O:145:GLU:OE2	2:R:116:GLU:OE2[2_555]	1.73	0.47

## 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	142/158 (90%)	142 (100%)	0	0	100	100
1	D	143/158 (90%)	141 (99%)	2 (1%)	0	100	100
1	G	143/158 (90%)	142 (99%)	1 (1%)	0	100	100
1	J	142/158 (90%)	142 (100%)	0	0	100	100
1	M	143/158 (90%)	143 (100%)	0	0	100	100
1	P	143/158 (90%)	143 (100%)	0	0	100	100
1	S	143/158 (90%)	141 (99%)	2 (1%)	0	100	100
1	V	143/158 (90%)	142 (99%)	1 (1%)	0	100	100
2	B	147/149 (99%)	144 (98%)	2 (1%)	1 (1%)	19	42
2	C	146/149 (98%)	142 (97%)	3 (2%)	1 (1%)	19	42
2	E	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
2	F	147/149 (99%)	144 (98%)	3 (2%)	0	100	100
2	H	147/149 (99%)	144 (98%)	3 (2%)	0	100	100
2	I	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
2	K	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
2	L	143/149 (96%)	135 (94%)	8 (6%)	0	100	100
2	N	147/149 (99%)	144 (98%)	3 (2%)	0	100	100
2	O	147/149 (99%)	144 (98%)	2 (1%)	1 (1%)	19	42
2	Q	147/149 (99%)	141 (96%)	2 (1%)	4 (3%)	4	10
2	R	144/149 (97%)	141 (98%)	2 (1%)	1 (1%)	19	42
2	T	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
2	U	146/149 (98%)	143 (98%)	3 (2%)	0	100	100
2	W	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
2	X	143/149 (96%)	132 (92%)	11 (8%)	0	100	100
All	All	3481/3648 (95%)	3412 (98%)	61 (2%)	8 (0%)	44	68

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	ASP
2	Q	8	ASP
2	Q	7	ARG
2	Q	10	GLY
2	C	8	ASP

### 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	123/136 (90%)	123 (100%)	0	100	100
1	D	124/136 (91%)	124 (100%)	0	100	100
1	G	124/136 (91%)	124 (100%)	0	100	100
1	J	123/136 (90%)	123 (100%)	0	100	100
1	M	124/136 (91%)	124 (100%)	0	100	100
1	P	124/136 (91%)	124 (100%)	0	100	100
1	S	124/136 (91%)	124 (100%)	0	100	100
1	V	124/136 (91%)	124 (100%)	0	100	100
2	B	127/127 (100%)	127 (100%)	0	100	100
2	C	126/127 (99%)	124 (98%)	2 (2%)	58	82
2	E	127/127 (100%)	126 (99%)	1 (1%)	79	91
2	F	127/127 (100%)	126 (99%)	1 (1%)	79	91
2	H	127/127 (100%)	127 (100%)	0	100	100
2	I	127/127 (100%)	123 (97%)	4 (3%)	35	64
2	K	127/127 (100%)	126 (99%)	1 (1%)	79	91
2	L	125/127 (98%)	124 (99%)	1 (1%)	79	91
2	N	127/127 (100%)	127 (100%)	0	100	100
2	O	127/127 (100%)	126 (99%)	1 (1%)	79	91
2	Q	127/127 (100%)	125 (98%)	2 (2%)	58	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	125/127 (98%)	125 (100%)	0	100	100
2	T	127/127 (100%)	126 (99%)	1 (1%)	79	91
2	U	126/127 (99%)	126 (100%)	0	100	100
2	W	127/127 (100%)	127 (100%)	0	100	100
2	X	125/127 (98%)	125 (100%)	0	100	100
All	All	3014/3120 (97%)	3000 (100%)	14 (0%)	86	95

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	149	LEU
2	K	7	ARG
2	T	149	LEU
2	Q	6	LEU
2	Q	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	125	GLN
2	T	142	GLN
2	N	142	GLN
2	R	131	GLN
1	V	118	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

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	144/158 (91%)	-0.91	1 (0%) 84 83	56, 73, 100, 137	0
1	D	145/158 (91%)	-0.92	0 100 100	63, 74, 100, 137	0
1	G	145/158 (91%)	-0.82	0 100 100	60, 77, 104, 163	0
1	J	144/158 (91%)	-0.88	0 100 100	62, 74, 109, 146	0
1	M	145/158 (91%)	-0.81	0 100 100	61, 77, 106, 126	0
1	P	145/158 (91%)	-0.84	1 (0%) 84 83	64, 78, 104, 127	1 (0%)
1	S	145/158 (91%)	-0.78	3 (2%) 63 63	62, 79, 106, 190	0
1	V	145/158 (91%)	-0.89	1 (0%) 84 83	62, 78, 113, 172	1 (0%)
2	B	149/149 (100%)	-0.71	1 (0%) 84 83	61, 80, 106, 128	0
2	C	148/149 (99%)	-0.81	0 100 100	53, 76, 100, 127	0
2	E	149/149 (100%)	-0.85	1 (0%) 84 83	63, 84, 122, 145	0
2	F	149/149 (100%)	-0.80	0 100 100	58, 83, 116, 149	0
2	H	149/149 (100%)	-0.88	0 100 100	59, 81, 108, 141	0
2	I	149/149 (100%)	-0.68	1 (0%) 84 83	75, 116, 154, 190	1 (0%)
2	K	149/149 (100%)	-0.89	0 100 100	57, 86, 123, 160	0
2	L	145/149 (97%)	-0.63	1 (0%) 84 83	58, 94, 183, 225	0
2	N	149/149 (100%)	-0.74	0 100 100	63, 84, 108, 153	0
2	O	149/149 (100%)	-0.83	0 100 100	62, 77, 103, 135	0
2	Q	149/149 (100%)	-0.88	0 100 100	66, 85, 133, 186	0
2	R	146/149 (97%)	-0.76	0 100 100	67, 85, 106, 132	0
2	T	149/149 (100%)	-0.82	0 100 100	60, 83, 115, 130	0
2	U	148/149 (99%)	-0.78	0 100 100	82, 117, 157, 174	0
2	W	149/149 (100%)	-0.90	0 100 100	60, 90, 127, 167	0
2	X	145/149 (97%)	-0.61	2 (1%) 73 73	60, 102, 181, 234	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	a	21/30 (70%)	-1.11	0 100 100	110, 134, 163, 164	0
3	d	21/30 (70%)	-1.24	0 100 100	102, 142, 201, 227	0
3	f	23/30 (76%)	-1.01	0 100 100	120, 148, 180, 203	0
3	h	20/30 (66%)	-1.24	0 100 100	104, 144, 181, 185	0
4	b	21/30 (70%)	-1.19	0 100 100	101, 131, 156, 208	0
4	c	21/30 (70%)	-1.12	0 100 100	122, 157, 236, 274	0
4	e	24/30 (80%)	-1.14	0 100 100	120, 160, 187, 191	0
4	g	20/30 (66%)	-1.08	0 100 100	127, 157, 232, 243	0
All	All	3700/3888 (95%)	-0.83	12 (0%) 90 89	53, 85, 148, 274	3 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	148	GLY	3.9
1	S	70	THR	3.3
1	S	1	PRO	3.2
2	E	27	LEU	2.8
1	A	1	PRO	2.8

## 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 oligosaccharides 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.