



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:02 am BST

PDB ID : 4Q0C  
Title : 3.1 Å resolution crystal structure of the B. pertussis BvgS periplasmic domain  
Authors : Dupre, E.; Herrou, J.; Lensink, M.F.; Wintjens, R.; Lebedev, A.; Crosson, S.;  
Villeret, V.; Loch, C.; Antoine, R.; Jacob-Dubuisson, F.  
Deposited on : 2014-04-01  
Resolution : 3.10 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  
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

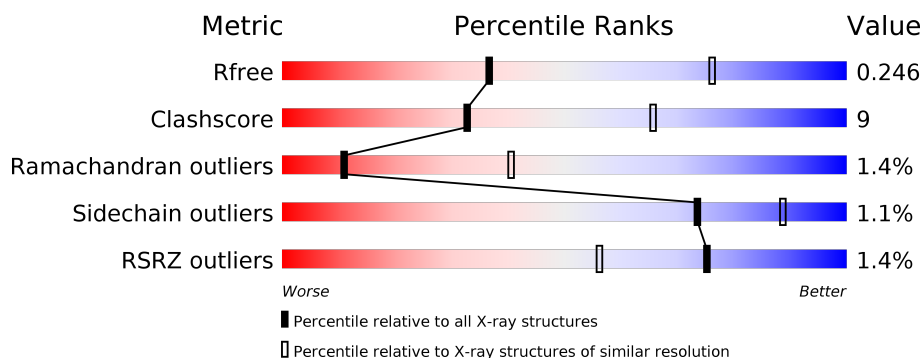
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	584	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>12%</div> </div> </div>
1	B	584	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>12%</div> </div> </div>
1	C	584	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>12%</div> </div> </div>
1	D	584	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>18%</div> <div>12%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15649 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 Virulence sensor protein BvgS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3895	2469	683	734	9			
1	B	513	Total	C	N	O	S	0	0	0
			3913	2485	683	736	9			
1	C	513	Total	C	N	O	S	0	0	0
			3919	2488	684	738	9			
1	D	513	Total	C	N	O	S	0	0	0
			3922	2493	682	738	9			

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	INITIATING METHIONINE	UNP P16575
A	-31	GLN	-	EXPRESSION TAG	UNP P16575
A	-30	TYR	-	EXPRESSION TAG	UNP P16575
A	-29	LYS	-	EXPRESSION TAG	UNP P16575
A	-28	LEU	-	EXPRESSION TAG	UNP P16575
A	-27	ALA	-	EXPRESSION TAG	UNP P16575
A	-26	LEU	-	EXPRESSION TAG	UNP P16575
A	-25	ASN	-	EXPRESSION TAG	UNP P16575
A	-24	GLY	-	EXPRESSION TAG	UNP P16575
A	-23	LYS	-	EXPRESSION TAG	UNP P16575
A	-22	THR	-	EXPRESSION TAG	UNP P16575
A	-21	LEU	-	EXPRESSION TAG	UNP P16575
A	-20	LYS	-	EXPRESSION TAG	UNP P16575
A	-19	GLY	-	EXPRESSION TAG	UNP P16575
A	-18	GLU	-	EXPRESSION TAG	UNP P16575
A	-17	THR	-	EXPRESSION TAG	UNP P16575
A	-16	THR	-	EXPRESSION TAG	UNP P16575
A	-15	THR	-	EXPRESSION TAG	UNP P16575
A	-14	GLU	-	EXPRESSION TAG	UNP P16575
A	-13	ALA	-	EXPRESSION TAG	UNP P16575
A	-12	VAL	-	EXPRESSION TAG	UNP P16575

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	ASP	-	EXPRESSION TAG	UNP P16575
A	-10	ALA	-	EXPRESSION TAG	UNP P16575
A	-9	ALA	-	EXPRESSION TAG	UNP P16575
A	-8	THR	-	EXPRESSION TAG	UNP P16575
A	-7	ALA	-	EXPRESSION TAG	UNP P16575
A	-6	GLU	-	EXPRESSION TAG	UNP P16575
A	-5	LYS	-	EXPRESSION TAG	UNP P16575
A	-4	VAL	-	EXPRESSION TAG	UNP P16575
A	-3	PHE	-	EXPRESSION TAG	UNP P16575
A	-2	LYS	-	EXPRESSION TAG	UNP P16575
A	-1	GLN	-	EXPRESSION TAG	UNP P16575
A	0	TYR	-	EXPRESSION TAG	UNP P16575
A	1	ALA	-	EXPRESSION TAG	UNP P16575
A	2	ASN	-	EXPRESSION TAG	UNP P16575
A	3	ASP	-	EXPRESSION TAG	UNP P16575
A	4	ASN	-	EXPRESSION TAG	UNP P16575
A	5	GLY	-	EXPRESSION TAG	UNP P16575
A	6	VAL	-	EXPRESSION TAG	UNP P16575
A	7	ASP	-	EXPRESSION TAG	UNP P16575
A	8	GLY	-	EXPRESSION TAG	UNP P16575
A	9	GLU	-	EXPRESSION TAG	UNP P16575
A	10	TRP	-	EXPRESSION TAG	UNP P16575
A	11	THR	-	EXPRESSION TAG	UNP P16575
A	12	TYR	-	EXPRESSION TAG	UNP P16575
A	13	ASP	-	EXPRESSION TAG	UNP P16575
A	14	ASP	-	EXPRESSION TAG	UNP P16575
A	15	ALA	-	EXPRESSION TAG	UNP P16575
A	16	THR	-	EXPRESSION TAG	UNP P16575
A	17	LYS	-	EXPRESSION TAG	UNP P16575
A	18	THR	-	EXPRESSION TAG	UNP P16575
A	19	PHE	-	EXPRESSION TAG	UNP P16575
A	20	THR	-	EXPRESSION TAG	UNP P16575
A	21	VAL	-	EXPRESSION TAG	UNP P16575
A	22	THR	-	EXPRESSION TAG	UNP P16575
A	23	GLU	-	EXPRESSION TAG	UNP P16575
A	24	LEU	-	EXPRESSION TAG	UNP P16575
A	25	VAL	-	EXPRESSION TAG	UNP P16575
A	26	PRO	-	EXPRESSION TAG	UNP P16575
A	27	ARG	-	EXPRESSION TAG	UNP P16575
A	28	GLY	-	EXPRESSION TAG	UNP P16575
A	29	SER	-	EXPRESSION TAG	UNP P16575
A	545	GLU	-	EXPRESSION TAG	UNP P16575

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Chain	Residue	Modelled	Actual	Comment	Reference
A	546	HIS	-	EXPRESSION TAG	UNP P16575
A	547	HIS	-	EXPRESSION TAG	UNP P16575
A	548	HIS	-	EXPRESSION TAG	UNP P16575
A	549	HIS	-	EXPRESSION TAG	UNP P16575
A	550	HIS	-	EXPRESSION TAG	UNP P16575
A	551	HIS	-	EXPRESSION TAG	UNP P16575
B	-32	MET	-	INITIATING METHIONINE	UNP P16575
B	-31	GLN	-	EXPRESSION TAG	UNP P16575
B	-30	TYR	-	EXPRESSION TAG	UNP P16575
B	-29	LYS	-	EXPRESSION TAG	UNP P16575
B	-28	LEU	-	EXPRESSION TAG	UNP P16575
B	-27	ALA	-	EXPRESSION TAG	UNP P16575
B	-26	LEU	-	EXPRESSION TAG	UNP P16575
B	-25	ASN	-	EXPRESSION TAG	UNP P16575
B	-24	GLY	-	EXPRESSION TAG	UNP P16575
B	-23	LYS	-	EXPRESSION TAG	UNP P16575
B	-22	THR	-	EXPRESSION TAG	UNP P16575
B	-21	LEU	-	EXPRESSION TAG	UNP P16575
B	-20	LYS	-	EXPRESSION TAG	UNP P16575
B	-19	GLY	-	EXPRESSION TAG	UNP P16575
B	-18	GLU	-	EXPRESSION TAG	UNP P16575
B	-17	THR	-	EXPRESSION TAG	UNP P16575
B	-16	THR	-	EXPRESSION TAG	UNP P16575
B	-15	THR	-	EXPRESSION TAG	UNP P16575
B	-14	GLU	-	EXPRESSION TAG	UNP P16575
B	-13	ALA	-	EXPRESSION TAG	UNP P16575
B	-12	VAL	-	EXPRESSION TAG	UNP P16575
B	-11	ASP	-	EXPRESSION TAG	UNP P16575
B	-10	ALA	-	EXPRESSION TAG	UNP P16575
B	-9	ALA	-	EXPRESSION TAG	UNP P16575
B	-8	THR	-	EXPRESSION TAG	UNP P16575
B	-7	ALA	-	EXPRESSION TAG	UNP P16575
B	-6	GLU	-	EXPRESSION TAG	UNP P16575
B	-5	LYS	-	EXPRESSION TAG	UNP P16575
B	-4	VAL	-	EXPRESSION TAG	UNP P16575
B	-3	PHE	-	EXPRESSION TAG	UNP P16575
B	-2	LYS	-	EXPRESSION TAG	UNP P16575
B	-1	GLN	-	EXPRESSION TAG	UNP P16575
B	0	TYR	-	EXPRESSION TAG	UNP P16575
B	1	ALA	-	EXPRESSION TAG	UNP P16575
B	2	ASN	-	EXPRESSION TAG	UNP P16575
B	3	ASP	-	EXPRESSION TAG	UNP P16575

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	ASN	-	EXPRESSION TAG	UNP P16575
B	5	GLY	-	EXPRESSION TAG	UNP P16575
B	6	VAL	-	EXPRESSION TAG	UNP P16575
B	7	ASP	-	EXPRESSION TAG	UNP P16575
B	8	GLY	-	EXPRESSION TAG	UNP P16575
B	9	GLU	-	EXPRESSION TAG	UNP P16575
B	10	TRP	-	EXPRESSION TAG	UNP P16575
B	11	THR	-	EXPRESSION TAG	UNP P16575
B	12	TYR	-	EXPRESSION TAG	UNP P16575
B	13	ASP	-	EXPRESSION TAG	UNP P16575
B	14	ASP	-	EXPRESSION TAG	UNP P16575
B	15	ALA	-	EXPRESSION TAG	UNP P16575
B	16	THR	-	EXPRESSION TAG	UNP P16575
B	17	LYS	-	EXPRESSION TAG	UNP P16575
B	18	THR	-	EXPRESSION TAG	UNP P16575
B	19	PHE	-	EXPRESSION TAG	UNP P16575
B	20	THR	-	EXPRESSION TAG	UNP P16575
B	21	VAL	-	EXPRESSION TAG	UNP P16575
B	22	THR	-	EXPRESSION TAG	UNP P16575
B	23	GLU	-	EXPRESSION TAG	UNP P16575
B	24	LEU	-	EXPRESSION TAG	UNP P16575
B	25	VAL	-	EXPRESSION TAG	UNP P16575
B	26	PRO	-	EXPRESSION TAG	UNP P16575
B	27	ARG	-	EXPRESSION TAG	UNP P16575
B	28	GLY	-	EXPRESSION TAG	UNP P16575
B	29	SER	-	EXPRESSION TAG	UNP P16575
B	545	GLU	-	EXPRESSION TAG	UNP P16575
B	546	HIS	-	EXPRESSION TAG	UNP P16575
B	547	HIS	-	EXPRESSION TAG	UNP P16575
B	548	HIS	-	EXPRESSION TAG	UNP P16575
B	549	HIS	-	EXPRESSION TAG	UNP P16575
B	550	HIS	-	EXPRESSION TAG	UNP P16575
B	551	HIS	-	EXPRESSION TAG	UNP P16575
C	-32	MET	-	INITIATING METHIONINE	UNP P16575
C	-31	GLN	-	EXPRESSION TAG	UNP P16575
C	-30	TYR	-	EXPRESSION TAG	UNP P16575
C	-29	LYS	-	EXPRESSION TAG	UNP P16575
C	-28	LEU	-	EXPRESSION TAG	UNP P16575
C	-27	ALA	-	EXPRESSION TAG	UNP P16575
C	-26	LEU	-	EXPRESSION TAG	UNP P16575
C	-25	ASN	-	EXPRESSION TAG	UNP P16575
C	-24	GLY	-	EXPRESSION TAG	UNP P16575

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-23	LYS	-	EXPRESSION TAG	UNP P16575
C	-22	THR	-	EXPRESSION TAG	UNP P16575
C	-21	LEU	-	EXPRESSION TAG	UNP P16575
C	-20	LYS	-	EXPRESSION TAG	UNP P16575
C	-19	GLY	-	EXPRESSION TAG	UNP P16575
C	-18	GLU	-	EXPRESSION TAG	UNP P16575
C	-17	THR	-	EXPRESSION TAG	UNP P16575
C	-16	THR	-	EXPRESSION TAG	UNP P16575
C	-15	THR	-	EXPRESSION TAG	UNP P16575
C	-14	GLU	-	EXPRESSION TAG	UNP P16575
C	-13	ALA	-	EXPRESSION TAG	UNP P16575
C	-12	VAL	-	EXPRESSION TAG	UNP P16575
C	-11	ASP	-	EXPRESSION TAG	UNP P16575
C	-10	ALA	-	EXPRESSION TAG	UNP P16575
C	-9	ALA	-	EXPRESSION TAG	UNP P16575
C	-8	THR	-	EXPRESSION TAG	UNP P16575
C	-7	ALA	-	EXPRESSION TAG	UNP P16575
C	-6	GLU	-	EXPRESSION TAG	UNP P16575
C	-5	LYS	-	EXPRESSION TAG	UNP P16575
C	-4	VAL	-	EXPRESSION TAG	UNP P16575
C	-3	PHE	-	EXPRESSION TAG	UNP P16575
C	-2	LYS	-	EXPRESSION TAG	UNP P16575
C	-1	GLN	-	EXPRESSION TAG	UNP P16575
C	0	TYR	-	EXPRESSION TAG	UNP P16575
C	1	ALA	-	EXPRESSION TAG	UNP P16575
C	2	ASN	-	EXPRESSION TAG	UNP P16575
C	3	ASP	-	EXPRESSION TAG	UNP P16575
C	4	ASN	-	EXPRESSION TAG	UNP P16575
C	5	GLY	-	EXPRESSION TAG	UNP P16575
C	6	VAL	-	EXPRESSION TAG	UNP P16575
C	7	ASP	-	EXPRESSION TAG	UNP P16575
C	8	GLY	-	EXPRESSION TAG	UNP P16575
C	9	GLU	-	EXPRESSION TAG	UNP P16575
C	10	TRP	-	EXPRESSION TAG	UNP P16575
C	11	THR	-	EXPRESSION TAG	UNP P16575
C	12	TYR	-	EXPRESSION TAG	UNP P16575
C	13	ASP	-	EXPRESSION TAG	UNP P16575
C	14	ASP	-	EXPRESSION TAG	UNP P16575
C	15	ALA	-	EXPRESSION TAG	UNP P16575
C	16	THR	-	EXPRESSION TAG	UNP P16575
C	17	LYS	-	EXPRESSION TAG	UNP P16575
C	18	THR	-	EXPRESSION TAG	UNP P16575

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Chain	Residue	Modelled	Actual	Comment	Reference
C	19	PHE	-	EXPRESSION TAG	UNP P16575
C	20	THR	-	EXPRESSION TAG	UNP P16575
C	21	VAL	-	EXPRESSION TAG	UNP P16575
C	22	THR	-	EXPRESSION TAG	UNP P16575
C	23	GLU	-	EXPRESSION TAG	UNP P16575
C	24	LEU	-	EXPRESSION TAG	UNP P16575
C	25	VAL	-	EXPRESSION TAG	UNP P16575
C	26	PRO	-	EXPRESSION TAG	UNP P16575
C	27	ARG	-	EXPRESSION TAG	UNP P16575
C	28	GLY	-	EXPRESSION TAG	UNP P16575
C	29	SER	-	EXPRESSION TAG	UNP P16575
C	545	GLU	-	EXPRESSION TAG	UNP P16575
C	546	HIS	-	EXPRESSION TAG	UNP P16575
C	547	HIS	-	EXPRESSION TAG	UNP P16575
C	548	HIS	-	EXPRESSION TAG	UNP P16575
C	549	HIS	-	EXPRESSION TAG	UNP P16575
C	550	HIS	-	EXPRESSION TAG	UNP P16575
C	551	HIS	-	EXPRESSION TAG	UNP P16575
D	-32	MET	-	INITIATING METHIONINE	UNP P16575
D	-31	GLN	-	EXPRESSION TAG	UNP P16575
D	-30	TYR	-	EXPRESSION TAG	UNP P16575
D	-29	LYS	-	EXPRESSION TAG	UNP P16575
D	-28	LEU	-	EXPRESSION TAG	UNP P16575
D	-27	ALA	-	EXPRESSION TAG	UNP P16575
D	-26	LEU	-	EXPRESSION TAG	UNP P16575
D	-25	ASN	-	EXPRESSION TAG	UNP P16575
D	-24	GLY	-	EXPRESSION TAG	UNP P16575
D	-23	LYS	-	EXPRESSION TAG	UNP P16575
D	-22	THR	-	EXPRESSION TAG	UNP P16575
D	-21	LEU	-	EXPRESSION TAG	UNP P16575
D	-20	LYS	-	EXPRESSION TAG	UNP P16575
D	-19	GLY	-	EXPRESSION TAG	UNP P16575
D	-18	GLU	-	EXPRESSION TAG	UNP P16575
D	-17	THR	-	EXPRESSION TAG	UNP P16575
D	-16	THR	-	EXPRESSION TAG	UNP P16575
D	-15	THR	-	EXPRESSION TAG	UNP P16575
D	-14	GLU	-	EXPRESSION TAG	UNP P16575
D	-13	ALA	-	EXPRESSION TAG	UNP P16575
D	-12	VAL	-	EXPRESSION TAG	UNP P16575
D	-11	ASP	-	EXPRESSION TAG	UNP P16575
D	-10	ALA	-	EXPRESSION TAG	UNP P16575
D	-9	ALA	-	EXPRESSION TAG	UNP P16575

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	THR	-	EXPRESSION TAG	UNP P16575
D	-7	ALA	-	EXPRESSION TAG	UNP P16575
D	-6	GLU	-	EXPRESSION TAG	UNP P16575
D	-5	LYS	-	EXPRESSION TAG	UNP P16575
D	-4	VAL	-	EXPRESSION TAG	UNP P16575
D	-3	PHE	-	EXPRESSION TAG	UNP P16575
D	-2	LYS	-	EXPRESSION TAG	UNP P16575
D	-1	GLN	-	EXPRESSION TAG	UNP P16575
D	0	TYR	-	EXPRESSION TAG	UNP P16575
D	1	ALA	-	EXPRESSION TAG	UNP P16575
D	2	ASN	-	EXPRESSION TAG	UNP P16575
D	3	ASP	-	EXPRESSION TAG	UNP P16575
D	4	ASN	-	EXPRESSION TAG	UNP P16575
D	5	GLY	-	EXPRESSION TAG	UNP P16575
D	6	VAL	-	EXPRESSION TAG	UNP P16575
D	7	ASP	-	EXPRESSION TAG	UNP P16575
D	8	GLY	-	EXPRESSION TAG	UNP P16575
D	9	GLU	-	EXPRESSION TAG	UNP P16575
D	10	TRP	-	EXPRESSION TAG	UNP P16575
D	11	THR	-	EXPRESSION TAG	UNP P16575
D	12	TYR	-	EXPRESSION TAG	UNP P16575
D	13	ASP	-	EXPRESSION TAG	UNP P16575
D	14	ASP	-	EXPRESSION TAG	UNP P16575
D	15	ALA	-	EXPRESSION TAG	UNP P16575
D	16	THR	-	EXPRESSION TAG	UNP P16575
D	17	LYS	-	EXPRESSION TAG	UNP P16575
D	18	THR	-	EXPRESSION TAG	UNP P16575
D	19	PHE	-	EXPRESSION TAG	UNP P16575
D	20	THR	-	EXPRESSION TAG	UNP P16575
D	21	VAL	-	EXPRESSION TAG	UNP P16575
D	22	THR	-	EXPRESSION TAG	UNP P16575
D	23	GLU	-	EXPRESSION TAG	UNP P16575
D	24	LEU	-	EXPRESSION TAG	UNP P16575
D	25	VAL	-	EXPRESSION TAG	UNP P16575
D	26	PRO	-	EXPRESSION TAG	UNP P16575
D	27	ARG	-	EXPRESSION TAG	UNP P16575
D	28	GLY	-	EXPRESSION TAG	UNP P16575
D	29	SER	-	EXPRESSION TAG	UNP P16575
D	545	GLU	-	EXPRESSION TAG	UNP P16575
D	546	HIS	-	EXPRESSION TAG	UNP P16575
D	547	HIS	-	EXPRESSION TAG	UNP P16575
D	548	HIS	-	EXPRESSION TAG	UNP P16575

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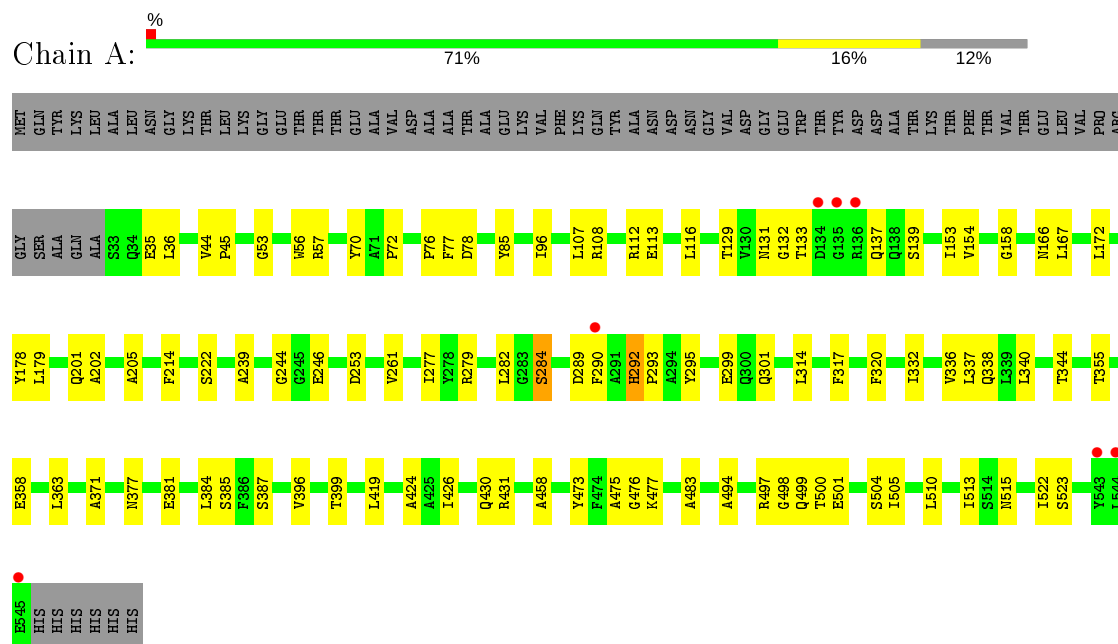
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Chain	Residue	Modelled	Actual	Comment	Reference
D	549	HIS	-	EXPRESSION TAG	UNP P16575
D	550	HIS	-	EXPRESSION TAG	UNP P16575
D	551	HIS	-	EXPRESSION TAG	UNP P16575

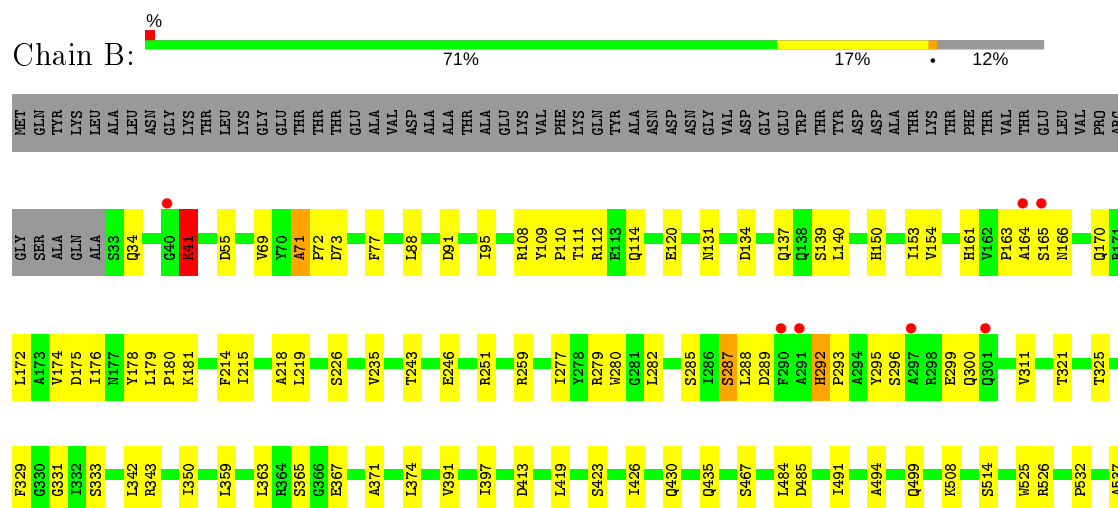
### 3 Residue-property plots

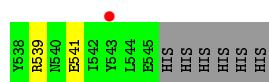
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Virulence sensor protein BvgS



#### • Molecule 1: Virulence sensor protein BvgS

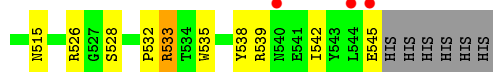
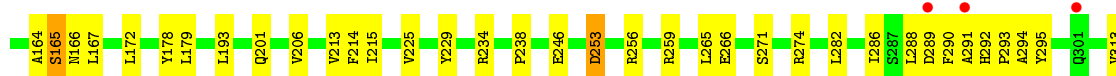




• Molecule 1: Virulence sensor protein BvgS



• Molecule 1: Virulence sensor protein BvgS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.45Å 285.82Å 128.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.10 19.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.99-3.10) 99.4 (19.99-3.10)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.09Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.181 , 0.245 0.184 , 0.246	Depositor DCC
$R_{free}$ test set	2000 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.6	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	15649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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	0.50	0/3978	0.72	1/5433 (0.0%)
1	B	0.50	0/3995	0.70	0/5455
1	C	0.51	0/4002	0.71	0/5463
1	D	0.50	0/4006	0.70	1/5469 (0.0%)
All	All	0.51	0/15981	0.71	2/21820 (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	B	0	1
1	C	0	2
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASP	CB-CG-OD1	5.37	123.14	118.30
1	D	132	GLY	N-CA-C	-5.21	100.07	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	289	ASP	Peptide
1	C	292	HIS	Peptide
1	C	70	TYR	Peptide
1	D	135	GLY	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	3895	0	3818	63	0
1	B	3913	0	3867	69	0
1	C	3919	0	3861	80	0
1	D	3922	0	3878	82	0
All	All	15649	0	15424	270	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 9.

All (270) 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:D:158:GLY:HA2	1:D:328:GLN:HE22	1.42	0.84
1:D:76:PRO:HG3	1:D:282:LEU:HD11	1.60	0.84
1:B:172:LEU:HD11	1:B:215:ILE:HG12	1.61	0.83
1:C:165:SER:N	1:C:166:ASN:HA	2.01	0.76
1:B:296:SER:O	1:B:300:GLN:HG2	1.87	0.75
1:C:172:LEU:HD11	1:C:215:ILE:HG12	1.69	0.73
1:B:120:GLU:HA	1:B:251:ARG:HD2	1.70	0.72
1:B:71:ALA:HB3	1:B:72:PRO:HD3	1.72	0.71
1:C:296:SER:HB3	1:C:299:GLU:H	1.54	0.71
1:D:388:ARG:HD3	1:D:511:TYR:CE1	2.25	0.71
1:C:325:THR:HG23	1:D:533:ARG:HD3	1.75	0.69
1:B:69:VAL:HG23	1:B:108:ARG:HG3	1.74	0.69
1:D:58:TRP:CD2	1:D:256:ARG:HD3	2.29	0.67
1:C:154:VAL:HB	1:C:214:PHE:HB3	1.77	0.67
1:D:164:ALA:O	1:D:166:ASN:N	2.21	0.66
1:A:317:PHE:CD2	1:A:320:PHE:HB2	2.31	0.65
1:D:69:VAL:HG23	1:D:108:ARG:HG3	1.78	0.65
1:A:515:ASN:HD22	1:B:280:TRP:HE3	1.43	0.65
1:C:72:PRO:O	1:C:73:ASP:HB2	1.96	0.65
1:D:135:GLY:HA2	1:D:137:GLN:H	1.62	0.64
1:C:396:VAL:HG12	1:C:483:ALA:HA	1.79	0.64
1:A:317:PHE:HD2	1:A:320:PHE:HB2	1.62	0.63
1:D:165:SER:O	1:D:165:SER:OG	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:PRO:HG3	1:C:282:LEU:HD11	1.81	0.63
1:C:416:THR:HG22	1:C:437:LYS:HD3	1.80	0.63
1:A:53:GLY:O	1:A:57:ARG:HG3	1.99	0.63
1:D:72:PRO:O	1:D:73:ASP:HB2	1.98	0.62
1:B:293:PRO:HB2	1:B:295:TYR:CZ	2.35	0.62
1:C:363:LEU:HD11	1:C:371:ALA:HB2	1.81	0.62
1:A:53:GLY:HA2	1:A:56:TRP:HB2	1.81	0.62
1:C:222:SER:HB2	1:C:284:SER:OG	2.00	0.62
1:C:71:ALA:HB1	1:C:72:PRO:HD3	1.80	0.62
1:C:71:ALA:HB1	1:C:72:PRO:CD	2.29	0.62
1:D:371:ALA:HB3	1:D:494:ALA:HB3	1.83	0.61
1:C:70:TYR:HD1	1:C:71:ALA:HB3	1.66	0.61
1:C:531:ASP:OD2	1:C:534:THR:OG1	2.17	0.61
1:D:396:VAL:HG12	1:D:483:ALA:HA	1.82	0.60
1:A:510:LEU:HD23	1:A:513:ILE:HD12	1.83	0.60
1:B:285:SER:HA	1:B:288:LEU:HD13	1.84	0.60
1:A:289:ASP:N	1:A:290:PHE:HA	2.17	0.59
1:C:111:THR:H	1:C:114:GLN:HG3	1.67	0.59
1:B:296:SER:HB3	1:B:299:GLU:H	1.67	0.58
1:C:311:VAL:HB	1:C:350:ILE:HD13	1.85	0.58
1:C:477:LYS:HG3	1:D:539:ARG:NH2	2.19	0.58
1:C:449:LEU:HD22	1:D:538:TYR:CZ	2.39	0.57
1:A:167:LEU:HD23	1:A:172:LEU:HD22	1.87	0.57
1:D:172:LEU:HD11	1:D:215:ILE:HG13	1.85	0.57
1:C:201:GLN:OE1	1:D:485:ASP:HA	2.05	0.57
1:C:324:ARG:HD2	1:C:328:GLN:HB3	1.87	0.57
1:B:329:PHE:CD2	1:B:350:ILE:HG13	2.40	0.57
1:C:285:SER:HA	1:C:288:LEU:HD12	1.86	0.56
1:B:71:ALA:HB2	1:B:110:PRO:O	2.05	0.56
1:D:484:LEU:HD13	1:D:486:LEU:HD12	1.86	0.56
1:A:475:ALA:O	1:B:539:ARG:NH2	2.38	0.56
1:D:419:LEU:HD22	1:D:426:ILE:HG12	1.88	0.56
1:B:154:VAL:HG22	1:B:235:VAL:HG22	1.88	0.56
1:A:317:PHE:HE2	1:A:320:PHE:CD2	2.24	0.56
1:B:299:GLU:OE2	1:B:508:LYS:NZ	2.39	0.56
1:C:158:GLY:HA2	1:C:328:GLN:NE2	2.21	0.55
1:C:96:ILE:HA	1:C:264:VAL:HG11	1.87	0.55
1:B:537:ALA:O	1:B:541:GLU:HG2	2.06	0.55
1:D:137:GLN:HG2	1:D:139:SER:HB3	1.89	0.55
1:A:131:ASN:OD1	1:A:133:THR:HG22	2.05	0.55
1:B:77:PHE:CE1	1:B:246:GLU:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ALA:HB3	1:B:494:ALA:HB3	1.89	0.55
1:A:154:VAL:HB	1:A:214:PHE:HB3	1.88	0.54
1:C:163:PRO:HG2	1:C:170:GLN:HE21	1.72	0.54
1:D:111:THR:OG1	1:D:114:GLN:HG3	2.07	0.54
1:B:34:GLN:O	1:B:108:ARG:N	2.31	0.54
1:C:69:VAL:HG13	1:C:108:ARG:HG3	1.90	0.54
1:C:165:SER:HB2	1:C:168:ALA:H	1.72	0.54
1:D:234:ARG:HD2	1:D:338:GLN:OE1	2.08	0.54
1:B:71:ALA:HB2	1:B:111:THR:HA	1.88	0.54
1:C:231:ASN:HD21	1:D:528:SER:HA	1.73	0.54
1:B:137:GLN:C	1:B:139:SER:H	2.12	0.53
1:C:51:LEU:HB2	1:C:56:TRP:CE2	2.43	0.53
1:D:158:GLY:CA	1:D:328:GLN:HE22	2.17	0.53
1:A:132:GLY:HA3	1:A:244:GLY:H	1.73	0.53
1:B:55:ASP:OD1	1:B:259:ARG:NH1	2.41	0.53
1:D:71:ALA:HB3	1:D:72:PRO:HD3	1.90	0.53
1:A:337:LEU:HD23	1:A:340:LEU:HD12	1.89	0.53
1:D:157:ILE:HG23	1:D:328:GLN:HE21	1.72	0.53
1:D:416:THR:HA	1:D:437:LYS:O	2.09	0.53
1:B:311:VAL:HB	1:B:350:ILE:HD13	1.89	0.53
1:C:64:VAL:HG11	1:C:105:LYS:HD3	1.90	0.53
1:A:419:LEU:HD22	1:A:426:ILE:HG12	1.90	0.53
1:B:287:SER:HB3	1:B:343:ARG:NH1	2.24	0.52
1:C:219:LEU:HD22	1:C:282:LEU:HD13	1.91	0.52
1:C:473:TYR:O	1:D:539:ARG:HD2	2.09	0.52
1:A:158:GLY:C	1:C:367:GLU:HG2	2.29	0.52
1:A:295:TYR:CE1	1:A:505:ILE:HG23	2.45	0.52
1:C:280:TRP:HE3	1:D:515:ASN:HD22	1.58	0.52
1:C:329:PHE:CD2	1:C:350:ILE:HG13	2.45	0.52
1:A:153:ILE:HG13	1:A:239:ALA:HB2	1.92	0.52
1:A:292:HIS:H	1:A:293:PRO:CD	2.23	0.52
1:D:77:PHE:CE1	1:D:246:GLU:HG3	2.44	0.52
1:A:76:PRO:HG3	1:A:282:LEU:HD11	1.91	0.51
1:B:41:LYS:HE3	1:B:279:ARG:HD2	1.92	0.51
1:B:277:ILE:HG23	1:B:282:LEU:HB2	1.92	0.51
1:D:164:ALA:C	1:D:166:ASN:H	2.13	0.51
1:B:164:ALA:C	1:B:166:ASN:H	2.14	0.51
1:B:154:VAL:HB	1:B:214:PHE:HB3	1.93	0.51
1:D:238:PRO:HD3	1:D:290:PHE:CD2	2.46	0.51
1:A:396:VAL:HG12	1:A:483:ALA:HA	1.92	0.50
1:D:426:ILE:O	1:D:430:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD13	1:B:280:TRP:CD1	2.47	0.50
1:A:201:GLN:NE2	1:B:485:ASP:HA	2.27	0.49
1:A:476:GLY:O	1:A:477:LYS:HD3	2.12	0.49
1:B:77:PHE:CZ	1:B:246:GLU:HG3	2.47	0.49
1:B:426:ILE:O	1:B:430:GLN:HG2	2.13	0.49
1:A:201:GLN:HE22	1:B:485:ASP:HA	1.78	0.49
1:C:460:VAL:HG22	1:C:484:LEU:HD11	1.94	0.49
1:C:206:VAL:HG21	1:C:214:PHE:HB2	1.93	0.49
1:D:33:SER:HB3	1:D:109:TYR:CE1	2.49	0.48
1:B:91:ASP:O	1:B:95:ILE:HG13	2.14	0.48
1:C:111:THR:N	1:C:114:GLN:HG3	2.28	0.48
1:B:131:ASN:HD22	1:B:243:THR:HB	1.78	0.48
1:C:285:SER:O	1:C:288:LEU:HB2	2.12	0.48
1:D:172:LEU:HB3	1:D:193:LEU:HD23	1.95	0.48
1:B:419:LEU:HD22	1:B:426:ILE:HG12	1.95	0.47
1:B:467:SER:HB3	1:B:526:ARG:HE	1.78	0.47
1:C:137:GLN:C	1:C:139:SER:H	2.16	0.47
1:C:149:ASP:OD1	1:C:217:ASP:HB2	2.14	0.47
1:C:154:VAL:HG22	1:C:235:VAL:HG22	1.96	0.47
1:C:473:TYR:CE1	1:D:532:PRO:HA	2.48	0.47
1:A:279:ARG:HG3	1:B:514:SER:HB2	1.96	0.47
1:A:317:PHE:CE2	1:A:320:PHE:CD2	3.02	0.47
1:A:70:TYR:HD1	1:A:72:PRO:HD2	1.79	0.47
1:D:105:LYS:HB3	1:D:105:LYS:HE2	1.72	0.47
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.78	0.47
1:A:96:ILE:HD13	1:A:261:VAL:HG13	1.97	0.47
1:B:423:SER:HB3	1:B:426:ILE:HG13	1.97	0.47
1:C:250:VAL:HG12	1:C:254:ASN:HB3	1.97	0.47
1:D:178:TYR:CD1	1:D:179:LEU:HG	2.50	0.47
1:B:331:GLY:HA2	1:B:525:TRP:CE2	2.50	0.47
1:B:91:ASP:OD2	1:B:279:ARG:NH2	2.46	0.47
1:D:397:ILE:HG23	1:D:484:LEU:HD21	1.96	0.47
1:B:109:TYR:HA	1:B:110:PRO:HD3	1.80	0.46
1:D:100:LEU:O	1:D:102:MET:HG2	2.15	0.46
1:D:391:VAL:HB	1:D:491:ILE:HB	1.96	0.46
1:A:295:TYR:OH	1:A:344:THR:HG22	2.15	0.46
1:A:371:ALA:HB3	1:A:494:ALA:HB3	1.97	0.46
1:D:167:LEU:HD21	1:D:213:VAL:HG11	1.97	0.46
1:D:58:TRP:CE2	1:D:256:ARG:HD3	2.51	0.46
1:A:377:ASN:O	1:A:381:GLU:HG3	2.16	0.46
1:B:391:VAL:HB	1:B:491:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LYS:HG2	1:B:539:ARG:HH21	1.81	0.46
1:A:78:ASP:OD1	1:A:85:TYR:OH	2.27	0.46
1:D:206:VAL:HG21	1:D:214:PHE:HB2	1.96	0.46
1:B:287:SER:HB3	1:B:343:ARG:HH12	1.81	0.46
1:C:41:LYS:HG3	1:C:43:ALA:H	1.81	0.46
1:A:35:GLU:HA	1:A:107:LEU:HA	1.98	0.46
1:A:112:ARG:HB3	1:A:113:GLU:OE2	2.15	0.45
1:B:174:VAL:HG12	1:B:175:ASP:O	2.16	0.45
1:C:201:GLN:HE21	1:C:201:GLN:HB3	1.59	0.45
1:C:404:ASP:O	1:C:415:ARG:NH2	2.40	0.45
1:C:77:PHE:CE1	1:C:246:GLU:HG3	2.51	0.45
1:D:253:ASP:OD1	1:D:253:ASP:N	2.49	0.45
1:C:225:VAL:HA	1:C:229:TYR:HB2	1.97	0.45
1:A:77:PHE:CE1	1:A:246:GLU:HG3	2.51	0.45
1:C:271:SER:HB2	1:D:271:SER:OG	2.17	0.45
1:B:359:LEU:HD22	1:B:374:LEU:HD21	1.98	0.45
1:B:467:SER:HB3	1:B:526:ARG:NE	2.31	0.45
1:C:88:LEU:HD22	1:C:92:TYR:HE2	1.81	0.44
1:A:222:SER:HB2	1:A:284:SER:HB2	1.99	0.44
1:A:363:LEU:HD23	1:A:384:LEU:HD21	2.00	0.44
1:A:385:SER:HB2	1:A:497:ARG:HA	1.97	0.44
1:D:39:VAL:CG2	1:D:84:ARG:HB3	2.47	0.44
1:D:340:LEU:HD21	1:D:510:LEU:HD23	1.98	0.44
1:A:431:ARG:HH11	1:A:431:ARG:HB3	1.82	0.44
1:D:70:TYR:CE1	1:D:112:ARG:HG3	2.51	0.44
1:C:477:LYS:CD	1:D:542:ILE:HG21	2.47	0.44
1:A:137:GLN:C	1:A:139:SER:H	2.21	0.44
1:A:202:ALA:O	1:A:205:ALA:HB3	2.17	0.44
1:B:178:TYR:CD1	1:B:179:LEU:HG	2.53	0.44
1:B:153:ILE:HG12	1:B:215:ILE:CD1	2.47	0.44
1:C:485:ASP:HA	1:D:201:GLN:NE2	2.32	0.44
1:B:277:ILE:HA	1:B:277:ILE:HD13	1.82	0.44
1:C:41:LYS:HD2	1:C:42:ALA:H	1.83	0.44
1:D:377:ASN:CG	1:D:424:ALA:HB2	2.38	0.44
1:D:484:LEU:HB3	1:D:486:LEU:HG	1.99	0.44
1:A:314:LEU:HD12	1:A:317:PHE:CD1	2.53	0.43
1:A:332:ILE:HD13	1:A:522:ILE:HG12	2.00	0.43
1:C:449:LEU:HD21	1:D:535:TRP:HZ3	1.82	0.43
1:D:265:LEU:HA	1:D:265:LEU:HD23	1.73	0.43
1:B:363:LEU:HD12	1:B:363:LEU:HA	1.70	0.43
1:D:137:GLN:HG2	1:D:139:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:ARG:O	1:D:259:ARG:HB3	2.19	0.43
1:C:388:ARG:NH1	1:D:86:GLU:OE2	2.50	0.43
1:B:163:PRO:HG2	1:B:170:GLN:HE21	1.84	0.43
1:C:116:LEU:O	1:C:119:LEU:HB3	2.18	0.43
1:C:325:THR:CG2	1:D:533:ARG:HD3	2.44	0.43
1:C:175:ASP:HB3	1:C:178:TYR:HB2	2.00	0.43
1:A:399:THR:HG22	1:A:458:ALA:HB2	2.01	0.43
1:B:292:HIS:H	1:B:293:PRO:CD	2.31	0.43
1:D:324:ARG:HD2	1:D:328:GLN:HB3	1.99	0.43
1:C:167:LEU:HD23	1:C:172:LEU:HD22	2.00	0.43
1:D:58:TRP:CE3	1:D:256:ARG:HD3	2.53	0.43
1:B:73:ASP:HB2	1:B:108:ARG:NH2	2.34	0.43
1:A:430:GLN:H	1:A:430:GLN:HG2	1.69	0.43
1:D:467:SER:HB3	1:D:526:ARG:NE	2.34	0.43
1:D:467:SER:HB3	1:D:526:ARG:NH2	2.33	0.43
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.72	0.42
1:C:321:THR:HG22	1:C:333:SER:HB2	2.00	0.42
1:C:397:ILE:HG23	1:C:484:LEU:HD21	2.01	0.42
1:D:274:ARG:HG2	1:D:286:ILE:HD12	2.00	0.42
1:A:426:ILE:O	1:A:430:GLN:HG2	2.19	0.42
1:C:135:GLY:HA2	1:C:137:GLN:HB2	2.00	0.42
1:C:166:ASN:HB3	1:C:188:TYR:HE1	1.84	0.42
1:C:311:VAL:HB	1:C:350:ILE:CD1	2.49	0.42
1:C:371:ALA:HB3	1:C:494:ALA:HB3	2.01	0.42
1:D:154:VAL:HB	1:D:214:PHE:HB3	2.01	0.42
1:D:238:PRO:HD3	1:D:290:PHE:CG	2.54	0.42
1:B:172:LEU:HD11	1:B:215:ILE:CG1	2.42	0.42
1:B:365:SER:OG	1:B:367:GLU:HG3	2.19	0.42
1:C:295:TYR:HB2	1:C:300:GLN:HG3	2.01	0.42
1:C:62:LYS:O	1:C:64:VAL:N	2.43	0.42
1:D:131:ASN:HB3	1:D:132:GLY:H	1.59	0.42
1:A:355:THR:OG1	1:A:358:GLU:HB2	2.18	0.42
1:A:377:ASN:CG	1:A:424:ALA:HB2	2.40	0.42
1:A:473:TYR:CE1	1:B:532:PRO:HA	2.55	0.42
1:C:167:LEU:HD22	1:C:188:TYR:CE1	2.55	0.42
1:D:158:GLY:HA2	1:D:328:GLN:NE2	2.22	0.42
1:D:292:HIS:N	1:D:293:PRO:CD	2.82	0.42
1:C:485:ASP:HA	1:D:201:GLN:HE22	1.85	0.42
1:D:413:ASP:HA	1:D:435:GLN:HB3	2.01	0.42
1:C:178:TYR:CD1	1:C:179:LEU:HG	2.55	0.42
1:C:69:VAL:O	1:C:108:ARG:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:VAL:HA	1:D:229:TYR:HB2	2.02	0.42
1:D:62:LYS:HD3	1:D:102:MET:HE1	2.02	0.42
1:A:332:ILE:O	1:A:336:VAL:HG23	2.20	0.41
1:B:111:THR:HB	1:B:114:GLN:HG3	2.02	0.41
1:C:51:LEU:HB2	1:C:56:TRP:NE1	2.35	0.41
1:C:70:TYR:CD1	1:C:71:ALA:HB3	2.50	0.41
1:D:292:HIS:N	1:D:293:PRO:HD3	2.35	0.41
1:A:431:ARG:NH1	1:A:431:ARG:HB3	2.35	0.41
1:B:176:ILE:HD11	1:B:181:LYS:HE2	2.03	0.41
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.83	0.41
1:D:78:ASP:OD1	1:D:85:TYR:OH	2.34	0.41
1:A:36:LEU:HD11	1:A:108:ARG:HD2	2.02	0.41
1:B:179:LEU:HA	1:B:180:PRO:HD3	1.86	0.41
1:B:397:ILE:HG23	1:B:484:LEU:HD21	2.01	0.41
1:A:299:GLU:OE2	1:A:504:SER:OG	2.23	0.41
1:B:134:ASP:O	1:B:140:LEU:HD22	2.20	0.41
1:D:326:ASP:HB2	1:D:328:GLN:CB	2.51	0.41
1:D:377:ASN:O	1:D:381:GLU:HG3	2.21	0.41
1:A:336:VAL:O	1:A:340:LEU:HG	2.20	0.41
1:A:498:GLY:O	1:A:500:THR:HG23	2.21	0.41
1:D:484:LEU:HD13	1:D:486:LEU:CD1	2.50	0.41
1:A:113:GLU:HA	1:A:116:LEU:HB2	2.02	0.41
1:A:277:ILE:HA	1:A:277:ILE:HD13	1.80	0.41
1:C:202:ALA:O	1:C:205:ALA:HB3	2.21	0.41
1:B:112:ARG:HH21	1:B:134:ASP:HB3	1.86	0.41
1:C:536:TYR:CE1	1:D:539:ARG:HD3	2.56	0.41
1:D:313:VAL:HG12	1:D:372:GLY:HA3	2.01	0.41
1:D:152:VAL:HG11	1:D:288:LEU:HD23	2.03	0.41
1:A:137:GLN:O	1:A:139:SER:N	2.53	0.40
1:A:178:TYR:CD1	1:A:179:LEU:HG	2.56	0.40
1:A:501:GLU:O	1:A:505:ILE:HG13	2.21	0.40
1:D:144:VAL:HG21	1:D:266:GLU:HG3	2.02	0.40
1:B:150:HIS:O	1:B:218:ALA:HB2	2.22	0.40
1:B:413:ASP:HA	1:B:435:GLN:HB2	2.02	0.40
1:C:44:VAL:HG11	1:C:98:HIS:HB3	2.03	0.40
1:C:153:ILE:HG12	1:C:215:ILE:CD1	2.50	0.40
1:B:435:GLN:H	1:B:435:GLN:HG2	1.61	0.40
1:C:179:LEU:HD12	1:C:184:LEU:HD21	2.03	0.40
1:D:295:TYR:CE1	1:D:505:ILE:HG23	2.57	0.40
1:B:321:THR:HG22	1:B:333:SER:HB2	2.02	0.40
1:B:342:LEU:HA	1:B:342:LEU:HD12	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ALA:CB	1:C:72:PRO:CD	2.98	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	511/584 (88%)	486 (95%)	22 (4%)	3 (1%)	25	59
1	B	511/584 (88%)	483 (94%)	22 (4%)	6 (1%)	13	44
1	C	511/584 (88%)	477 (93%)	26 (5%)	8 (2%)	9	37
1	D	511/584 (88%)	484 (95%)	16 (3%)	11 (2%)	6	29
All	All	2044/2336 (88%)	1930 (94%)	86 (4%)	28 (1%)	11	40

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	LYS
1	B	71	ALA
1	B	161	HIS
1	C	41	LYS
1	C	71	ALA
1	C	161	HIS
1	C	292	HIS
1	D	71	ALA
1	D	165	SER
1	D	291	ALA
1	D	294	ALA
1	A	166	ASN
1	B	165	SER
1	C	296	SER

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Mol	Chain	Res	Type
1	C	164	ALA
1	D	136	ARG
1	D	161	HIS
1	A	292	HIS
1	B	292	HIS
1	B	499	GLN
1	D	131	ASN
1	D	132	GLY
1	A	499	GLN
1	C	52	ASP
1	C	529	ASP
1	D	289	ASP
1	D	499	GLN
1	D	73	ASP

### 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	397/472 (84%)	391 (98%)	6 (2%)	65	85
1	B	402/472 (85%)	398 (99%)	4 (1%)	76	90
1	C	403/472 (85%)	400 (99%)	3 (1%)	84	93
1	D	405/472 (86%)	400 (99%)	5 (1%)	71	88
All	All	1607/1888 (85%)	1589 (99%)	18 (1%)	73	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	284	SER
1	A	301	GLN
1	A	338	GLN
1	A	387	SER
1	A	523	SER
1	B	41	LYS

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Mol	Chain	Res	Type
1	B	226	SER
1	B	287	SER
1	B	325	THR
1	C	160	ARG
1	C	271	SER
1	C	526	ARG
1	D	72	PRO
1	D	253	ASP
1	D	445	SER
1	D	533	ARG
1	D	545	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	435	GLN
1	B	123	GLN
1	B	170	GLN
1	C	170	GLN
1	C	231	ASN
1	C	240	HIS
1	D	201	GLN
1	D	328	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 [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 ⓘ

### 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	513/584 (87%)	-0.59	7 (1%) 75 56	10, 29, 70, 241	0
1	B	513/584 (87%)	-0.54	8 (1%) 72 51	11, 34, 74, 202	0
1	C	513/584 (87%)	-0.47	7 (1%) 75 56	8, 32, 79, 156	0
1	D	513/584 (87%)	-0.48	6 (1%) 79 61	15, 36, 81, 168	0
All	All	2052/2336 (87%)	-0.52	28 (1%) 75 56	8, 33, 78, 241	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	545	GLU	6.4
1	A	135	GLY	5.8
1	B	40	GLY	4.9
1	C	544	LEU	4.3
1	A	290	PHE	4.0
1	D	544	LEU	4.0
1	D	545	GLU	3.7
1	A	543	TYR	2.8
1	A	136	ARG	2.7
1	B	291	ALA	2.7
1	C	165	SER	2.7
1	A	134	ASP	2.7
1	B	164	ALA	2.6
1	A	545	GLU	2.5
1	C	292	HIS	2.5
1	C	42	ALA	2.4
1	A	544	LEU	2.3
1	B	301	GLN	2.2
1	C	164	ALA	2.1
1	B	290	PHE	2.1
1	D	291	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	165	SER	2.1
1	B	297	ALA	2.1
1	D	289	ASP	2.1
1	B	543	TYR	2.0
1	C	290	PHE	2.0
1	D	301	GLN	2.0
1	D	540	ASN	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.