



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:49 PM GMT

PDB ID : 4W91  
Title : Crystal structure of a cysteine desulfurase SufS from Brucella suis bound to PLP  
Authors : Seattle Structural Genomics Center for Infectious Disease  
Deposited on : 2014-08-26  
Resolution : 2.45 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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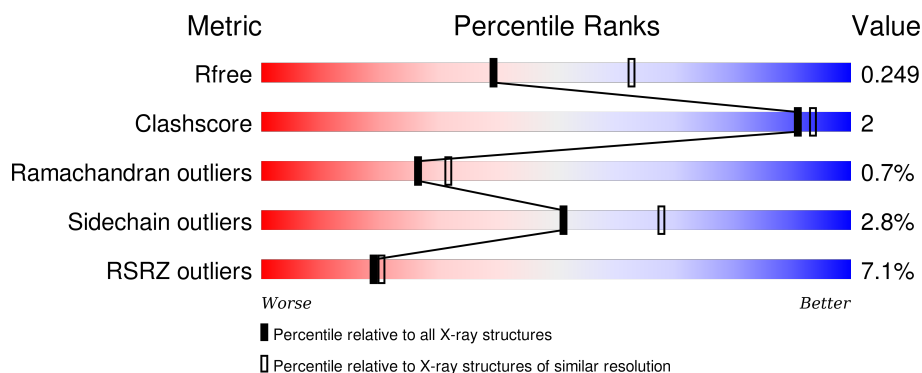
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

**i**

## X-RAY DIFFRACTION

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.



<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	422	<div><div>% 88%</div><div>6% . .</div></div>	
1	B	422	<div><div>% 88%</div><div>6% . .</div></div>	
1	C	422	<div><div>86%</div><div>9% . .</div></div>	
1	D	422	<div><div>87%</div><div>7% . .</div></div>	
1	E	422	<div><div>87%</div><div>8% . .</div></div>	

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Mol	Chain	Length	Quality of chain
1	F	422	<div><div>%</div><div><div></div><div>88%</div><div>6%</div><div></div><div></div></div></div>
1	G	422	<div><div>3%</div><div><div></div><div>87%</div><div>8%</div><div></div><div>5%</div></div></div>
1	H	422	<div><div>5%</div><div><div></div><div>89%</div><div>5%</div><div></div><div>5%</div></div></div>
1	I	422	<div><div>30%</div><div><div></div><div>90%</div><div></div><div></div><div>6%</div></div></div>
1	J	422	<div><div>27%</div><div><div></div><div>81%</div><div></div><div></div><div>16%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30371 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 Aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	P	S	0	2	0
			3117	1974	558	573	1	11			
1	B	405	Total	C	N	O	P	S	0	0	0
			3110	1970	555	574	1	10			
1	C	404	Total	C	N	O	P	S	0	0	0
			3118	1973	558	576	1	10			
1	D	404	Total	C	N	O	P	S	0	1	0
			3131	1982	560	577	1	11			
1	E	404	Total	C	N	O	P	S	0	0	0
			3083	1952	548	572	1	10			
1	F	404	Total	C	N	O	P	S	0	1	0
			3097	1961	552	573	1	10			
1	G	403	Total	C	N	O	P	S	0	0	0
			3041	1931	536	563	1	10			
1	H	400	Total	C	N	O	P	S	0	0	0
			3041	1927	542	560	1	11			
1	I	398	Total	C	N	O	P	S	0	0	0
			2764	1728	501	525	1	9			
1	J	356	Total	C	N	O	P	S	0	0	0
			2508	1575	449	474	1	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP D0BBJ1
A	-6	ALA	-	expression tag	UNP D0BBJ1
A	-5	HIS	-	expression tag	UNP D0BBJ1
A	-4	HIS	-	expression tag	UNP D0BBJ1
A	-3	HIS	-	expression tag	UNP D0BBJ1
A	-2	HIS	-	expression tag	UNP D0BBJ1
A	-1	HIS	-	expression tag	UNP D0BBJ1
A	0	HIS	-	expression tag	UNP D0BBJ1
B	-7	MET	-	initiating methionine	UNP D0BBJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	ALA	-	expression tag	UNP D0BBJ1
B	-5	HIS	-	expression tag	UNP D0BBJ1
B	-4	HIS	-	expression tag	UNP D0BBJ1
B	-3	HIS	-	expression tag	UNP D0BBJ1
B	-2	HIS	-	expression tag	UNP D0BBJ1
B	-1	HIS	-	expression tag	UNP D0BBJ1
B	0	HIS	-	expression tag	UNP D0BBJ1
C	-7	MET	-	initiating methionine	UNP D0BBJ1
C	-6	ALA	-	expression tag	UNP D0BBJ1
C	-5	HIS	-	expression tag	UNP D0BBJ1
C	-4	HIS	-	expression tag	UNP D0BBJ1
C	-3	HIS	-	expression tag	UNP D0BBJ1
C	-2	HIS	-	expression tag	UNP D0BBJ1
C	-1	HIS	-	expression tag	UNP D0BBJ1
C	0	HIS	-	expression tag	UNP D0BBJ1
D	-7	MET	-	initiating methionine	UNP D0BBJ1
D	-6	ALA	-	expression tag	UNP D0BBJ1
D	-5	HIS	-	expression tag	UNP D0BBJ1
D	-4	HIS	-	expression tag	UNP D0BBJ1
D	-3	HIS	-	expression tag	UNP D0BBJ1
D	-2	HIS	-	expression tag	UNP D0BBJ1
D	-1	HIS	-	expression tag	UNP D0BBJ1
D	0	HIS	-	expression tag	UNP D0BBJ1
E	-7	MET	-	initiating methionine	UNP D0BBJ1
E	-6	ALA	-	expression tag	UNP D0BBJ1
E	-5	HIS	-	expression tag	UNP D0BBJ1
E	-4	HIS	-	expression tag	UNP D0BBJ1
E	-3	HIS	-	expression tag	UNP D0BBJ1
E	-2	HIS	-	expression tag	UNP D0BBJ1
E	-1	HIS	-	expression tag	UNP D0BBJ1
E	0	HIS	-	expression tag	UNP D0BBJ1
F	-7	MET	-	initiating methionine	UNP D0BBJ1
F	-6	ALA	-	expression tag	UNP D0BBJ1
F	-5	HIS	-	expression tag	UNP D0BBJ1
F	-4	HIS	-	expression tag	UNP D0BBJ1
F	-3	HIS	-	expression tag	UNP D0BBJ1
F	-2	HIS	-	expression tag	UNP D0BBJ1
F	-1	HIS	-	expression tag	UNP D0BBJ1
F	0	HIS	-	expression tag	UNP D0BBJ1
G	-7	MET	-	initiating methionine	UNP D0BBJ1
G	-6	ALA	-	expression tag	UNP D0BBJ1
G	-5	HIS	-	expression tag	UNP D0BBJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	HIS	-	expression tag	UNP D0BBJ1
G	-3	HIS	-	expression tag	UNP D0BBJ1
G	-2	HIS	-	expression tag	UNP D0BBJ1
G	-1	HIS	-	expression tag	UNP D0BBJ1
G	0	HIS	-	expression tag	UNP D0BBJ1
H	-7	MET	-	initiating methionine	UNP D0BBJ1
H	-6	ALA	-	expression tag	UNP D0BBJ1
H	-5	HIS	-	expression tag	UNP D0BBJ1
H	-4	HIS	-	expression tag	UNP D0BBJ1
H	-3	HIS	-	expression tag	UNP D0BBJ1
H	-2	HIS	-	expression tag	UNP D0BBJ1
H	-1	HIS	-	expression tag	UNP D0BBJ1
H	0	HIS	-	expression tag	UNP D0BBJ1
I	-7	MET	-	initiating methionine	UNP D0BBJ1
I	-6	ALA	-	expression tag	UNP D0BBJ1
I	-5	HIS	-	expression tag	UNP D0BBJ1
I	-4	HIS	-	expression tag	UNP D0BBJ1
I	-3	HIS	-	expression tag	UNP D0BBJ1
I	-2	HIS	-	expression tag	UNP D0BBJ1
I	-1	HIS	-	expression tag	UNP D0BBJ1
I	0	HIS	-	expression tag	UNP D0BBJ1
J	-7	MET	-	initiating methionine	UNP D0BBJ1
J	-6	ALA	-	expression tag	UNP D0BBJ1
J	-5	HIS	-	expression tag	UNP D0BBJ1
J	-4	HIS	-	expression tag	UNP D0BBJ1
J	-3	HIS	-	expression tag	UNP D0BBJ1
J	-2	HIS	-	expression tag	UNP D0BBJ1
J	-1	HIS	-	expression tag	UNP D0BBJ1
J	0	HIS	-	expression tag	UNP D0BBJ1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0

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

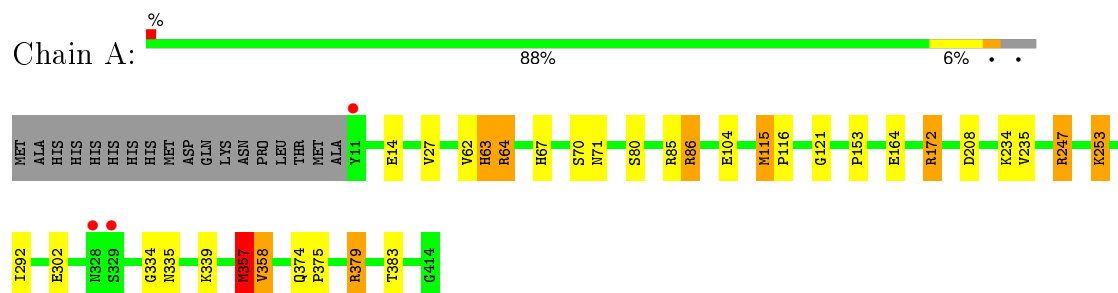
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total 46	O 46	0	0
3	B	52	Total 52	O 52	0	0
3	C	38	Total 38	O 38	0	0
3	D	54	Total 54	O 54	0	0
3	E	41	Total 41	O 41	0	0
3	F	49	Total 49	O 49	0	0
3	G	41	Total 41	O 41	0	0
3	H	28	Total 28	O 28	0	0
3	I	2	Total 2	O 2	0	0
3	J	3	Total 3	O 3	0	0

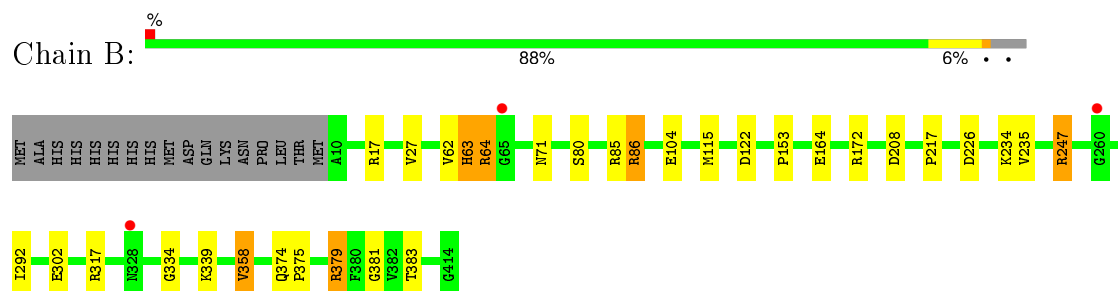
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

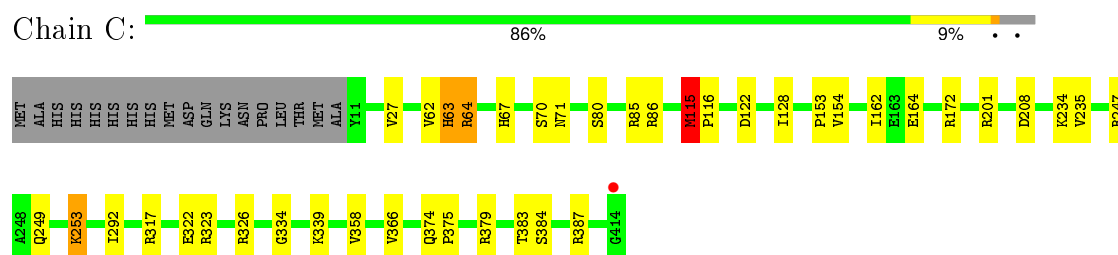
- Molecule 1: Aminotransferase



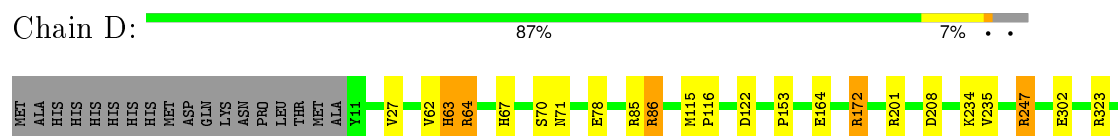
- Molecule 1: Aminotransferase



- Molecule 1: Aminotransferase



- Molecule 1: Aminotransferase

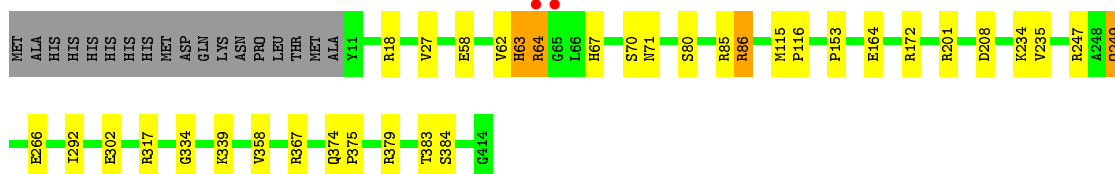






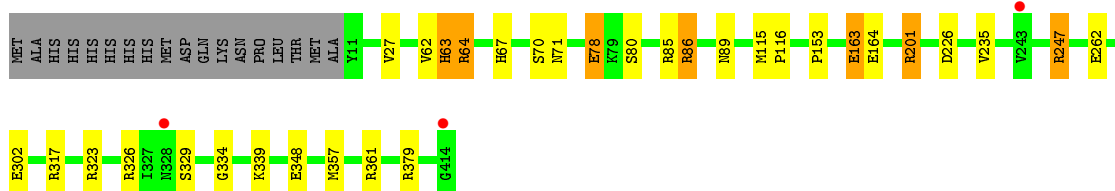
• Molecule 1: Aminotransferase

Chain E: 87% 8% . .



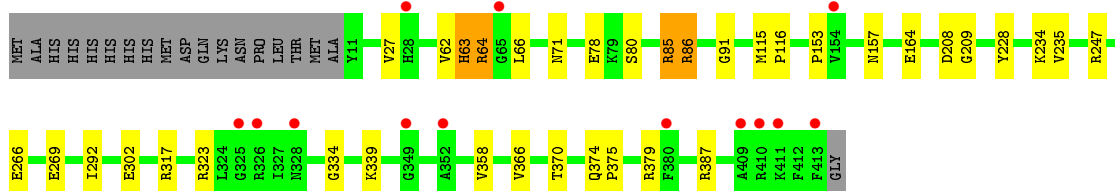
• Molecule 1: Aminotransferase

Chain F: 88% 6% . .



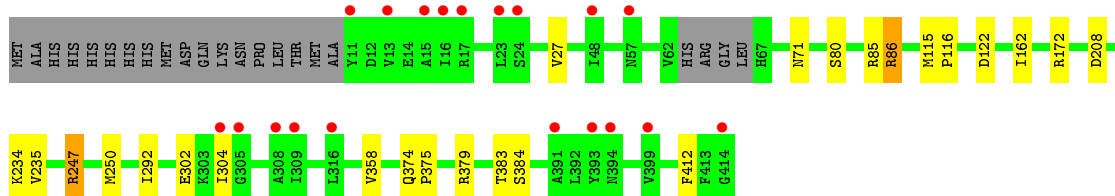
• Molecule 1: Aminotransferase

Chain G: 87% 3% 8% 5%



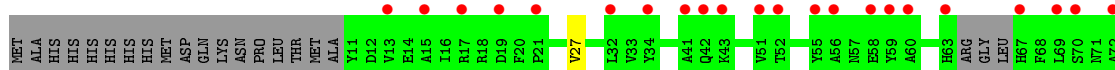
• Molecule 1: Aminotransferase

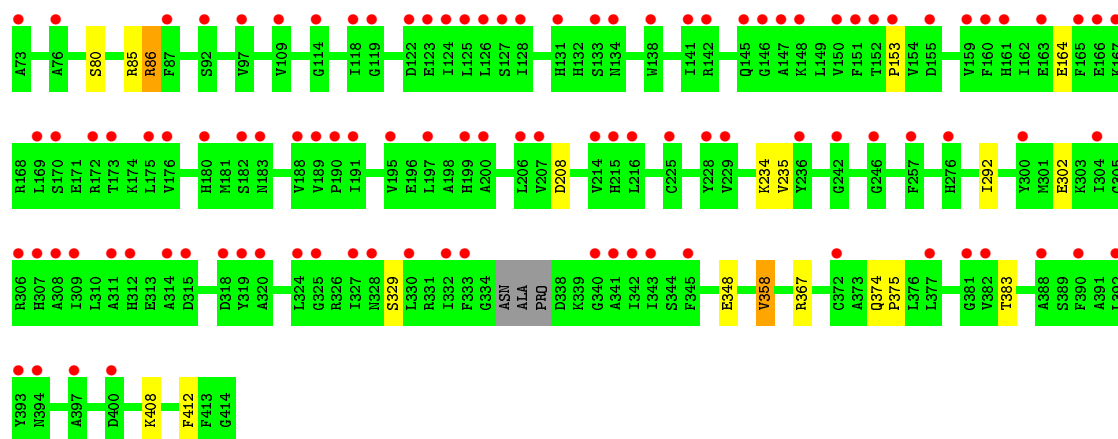
Chain H: 89% 5% 5%



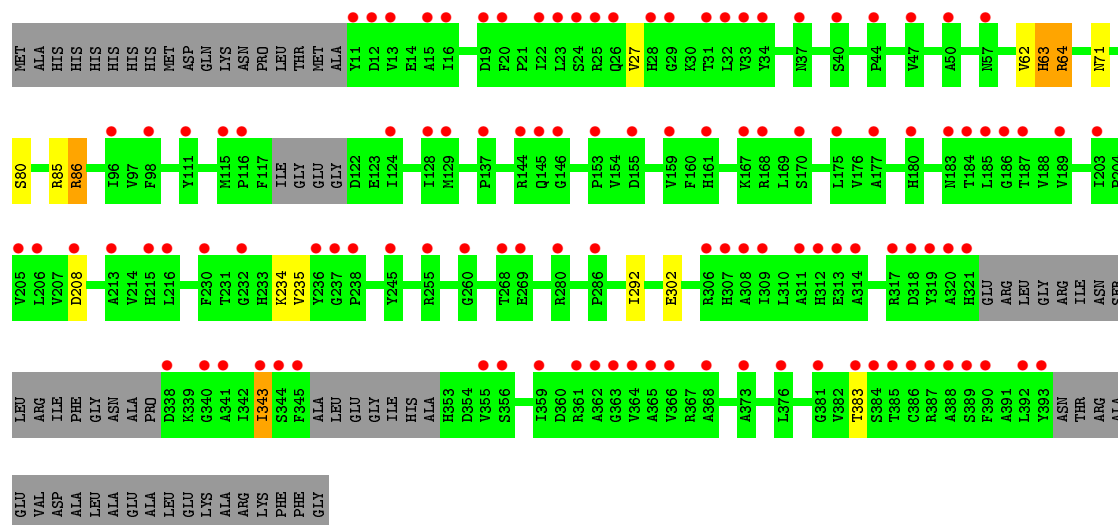
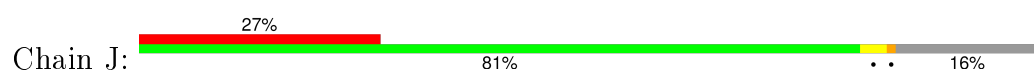
• Molecule 1: Aminotransferase

Chain I: 90% 30% 6%





• Molecule 1: Aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.85Å 121.91Å 133.72Å 111.49° 106.53° 89.81°	Depositor
Resolution (Å)	50.00 – 2.45 48.39 – 2.45	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.45) 84.4 (48.39-2.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.237 , 0.252 0.231 , 0.249	Depositor DCC
$R_{free}$ test set	8955 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	1.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 178357 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: LLP, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.57	0/3168	0.77	7/4301 (0.2%)
1	B	0.58	0/3155	0.70	3/4284 (0.1%)
1	C	0.60	2/3163 (0.1%)	0.75	7/4293 (0.2%)
1	D	0.62	1/3179 (0.0%)	0.73	4/4312 (0.1%)
1	E	0.59	0/3128	0.76	11/4254 (0.3%)
1	F	0.58	1/3146 (0.0%)	0.71	3/4277 (0.1%)
1	G	0.52	1/3084 (0.0%)	0.70	3/4201 (0.1%)
1	H	0.52	0/3084	0.73	5/4194 (0.1%)
1	I	0.48	0/2794	0.66	2/3822 (0.1%)
1	J	0.47	0/2538	0.64	3/3472 (0.1%)
All	All	0.56	5/30439 (0.0%)	0.72	48/41410 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	78	GLU	CD-OE2	5.69	1.31	1.25
1	G	78	GLU	CD-OE2	5.55	1.31	1.25
1	F	80	SER	CA-CB	5.49	1.61	1.52
1	C	384	SER	CA-CB	-5.25	1.45	1.52
1	C	384	SER	CB-OG	-5.04	1.35	1.42

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	C	201	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	A	379	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	D	247	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	A	247	ARG	NE-CZ-NH2	-8.62	115.99	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3117	0	3023	21	0
1	B	3110	0	3014	16	0
1	C	3118	0	3025	16	0
1	D	3131	0	3050	17	0
1	E	3083	0	2952	12	0
1	F	3097	0	2974	15	0
1	G	3041	0	2898	16	0
1	H	3041	0	2919	10	0
1	I	2764	0	2423	9	0
1	J	2508	0	2183	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
3	A	46	0	0	1	0
3	B	52	0	0	1	0
3	C	38	0	0	0	0
3	D	54	0	0	0	0
3	E	41	0	0	0	0
3	F	49	0	0	0	0
3	G	41	0	0	1	0
3	H	28	0	0	2	0
3	I	2	0	0	0	0
3	J	3	0	0	0	0
All	All	30371	0	28461	126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 126 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:F:78:GLU:HA	1:F:78:GLU:OE1	1.67	0.94
1:H:247:ARG:HD3	3:H:621:HOH:O	1.81	0.79
1:C:115:MET:HB3	1:C:116:PRO:HD3	1.75	0.69
1:D:115:MET:HB3	1:D:116:PRO:HD3	1.76	0.68
1:H:115:MET:HB3	1:H:116:PRO:HD3	1.77	0.67

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	403/422 (96%)	390 (97%)	10 (2%)	3 (1%)	26	32
1	B	402/422 (95%)	389 (97%)	10 (2%)	3 (1%)	26	32
1	C	401/422 (95%)	388 (97%)	10 (2%)	3 (1%)	26	32
1	D	402/422 (95%)	388 (96%)	11 (3%)	3 (1%)	26	32
1	E	401/422 (95%)	388 (97%)	10 (2%)	3 (1%)	26	32
1	F	402/422 (95%)	389 (97%)	10 (2%)	3 (1%)	26	32
1	G	400/422 (95%)	387 (97%)	10 (2%)	3 (1%)	24	28
1	H	395/422 (94%)	384 (97%)	10 (2%)	1 (0%)	46	57
1	I	391/422 (93%)	380 (97%)	10 (3%)	1 (0%)	46	57
1	J	347/422 (82%)	335 (96%)	9 (3%)	3 (1%)	21	25
All	All	3944/4220 (94%)	3818 (97%)	100 (2%)	26 (1%)	26	32

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	B	64	ARG
1	C	64	ARG

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Mol	Chain	Res	Type
1	D	64	ARG
1	E	64	ARG

### 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	312/341 (92%)	301 (96%)	11 (4%)	43	60
1	B	311/341 (91%)	303 (97%)	8 (3%)	54	70
1	C	313/341 (92%)	303 (97%)	10 (3%)	46	63
1	D	316/341 (93%)	307 (97%)	9 (3%)	51	68
1	E	305/341 (89%)	295 (97%)	10 (3%)	45	61
1	F	308/341 (90%)	299 (97%)	9 (3%)	50	66
1	G	297/341 (87%)	288 (97%)	9 (3%)	48	65
1	H	300/341 (88%)	293 (98%)	7 (2%)	58	74
1	I	233/341 (68%)	229 (98%)	4 (2%)	68	81
1	J	215/341 (63%)	210 (98%)	5 (2%)	58	74
All	All	2910/3410 (85%)	2828 (97%)	82 (3%)	51	68

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	383	THR
1	E	379	ARG
1	I	358	VAL
1	E	27	VAL
1	E	201	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	335	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 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	LLP	A	234	1	23,24,25	3.50	4 (17%)	28,32,34	1.14	2 (7%)
1	LLP	B	234	1	23,24,25	2.95	5 (21%)	28,32,34	1.39	6 (21%)
1	LLP	C	234	1	23,24,25	3.15	5 (21%)	28,32,34	1.22	3 (10%)
1	LLP	D	234	1	23,24,25	3.43	5 (21%)	28,32,34	1.34	4 (14%)
1	LLP	E	234	1	23,24,25	2.73	6 (26%)	28,32,34	1.29	4 (14%)
1	LLP	F	234	1	23,24,25	3.03	5 (21%)	28,32,34	1.30	4 (14%)
1	LLP	G	234	1	23,24,25	3.50	5 (21%)	28,32,34	1.25	5 (17%)
1	LLP	H	234	1	23,24,25	3.48	5 (21%)	28,32,34	1.27	6 (21%)
1	LLP	I	234	1	23,24,25	3.38	5 (21%)	28,32,34	1.21	4 (14%)
1	LLP	J	234	1	23,24,25	3.27	5 (21%)	28,32,34	1.34	4 (14%)

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	LLP	A	234	1	-	0/15/17/19	0/1/1/1
1	LLP	B	234	1	-	0/15/17/19	0/1/1/1
1	LLP	C	234	1	-	0/15/17/19	0/1/1/1
1	LLP	D	234	1	-	0/15/17/19	0/1/1/1
1	LLP	E	234	1	-	0/15/17/19	0/1/1/1
1	LLP	F	234	1	-	0/15/17/19	0/1/1/1
1	LLP	G	234	1	-	0/15/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	H	234	1	-	0/15/17/19	0/1/1/1
1	LLP	I	234	1	-	0/15/17/19	0/1/1/1
1	LLP	J	234	1	-	0/15/17/19	0/1/1/1

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	234	LLP	CB-CA	-2.27	1.51	1.53
1	E	234	LLP	CB-CA	-2.26	1.51	1.53
1	I	234	LLP	C4-C4'	2.09	1.50	1.46
1	D	234	LLP	C4-C4'	2.10	1.50	1.46
1	C	234	LLP	C4-C4'	2.44	1.50	1.46

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	234	LLP	C3-C4-C5	-2.61	116.15	118.11
1	J	234	LLP	C4-C4'-NZ	-2.45	111.41	125.06
1	H	234	LLP	O-C-CA	-2.43	119.17	125.49
1	B	234	LLP	C3-C4-C5	-2.40	116.31	118.11
1	D	234	LLP	C4-C4'-NZ	-2.40	111.72	125.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	234	LLP	1	0
1	B	234	LLP	1	0
1	C	234	LLP	1	0
1	D	234	LLP	1	0
1	E	234	LLP	1	0
1	G	234	LLP	1	0
1	H	234	LLP	1	0
1	I	234	LLP	1	0
1	J	234	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	403/422 (95%)	-0.01	3 (0%) 89 90	39, 52, 68, 79	0
1	B	404/422 (95%)	0.03	3 (0%) 89 90	39, 50, 65, 80	0
1	C	403/422 (95%)	-0.06	1 (0%) 95 96	43, 54, 65, 71	0
1	D	403/422 (95%)	-0.01	0 100 100	41, 49, 60, 67	0
1	E	403/422 (95%)	-0.05	2 (0%) 91 92	40, 52, 68, 77	0
1	F	403/422 (95%)	0.07	3 (0%) 89 90	41, 55, 72, 82	0
1	G	402/422 (95%)	0.24	13 (3%) 51 54	51, 63, 87, 105	0
1	H	399/422 (94%)	0.34	19 (4%) 34 37	55, 69, 81, 89	0
1	I	397/422 (94%)	1.68	126 (31%) 1 0	66, 89, 125, 143	0
1	J	355/422 (84%)	1.68	113 (31%) 1 0	70, 85, 106, 116	0
All	All	3972/4220 (94%)	0.37	283 (7%) 19 20	39, 58, 98, 143	0

The worst 5 of 283 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	126	LEU	12.0
1	J	203	ILE	7.9
1	I	76	ALA	7.6
1	J	373	ALA	7.4
1	I	304	ILE	7.2

### 6.2 Non-standard residues in protein, DNA, RNA chains

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( $\text{\AA}^2$ )	Q<0.9
1	LLP	H	234	24/25	0.96	0.16	-	54,56,59,61	0
1	LLP	I	234	24/25	0.89	0.22	-	72,75,80,82	0
1	LLP	F	234	24/25	0.98	0.17	-	42,44,46,47	0
1	LLP	J	234	24/25	0.90	0.22	-	75,77,79,80	0
1	LLP	C	234	24/25	0.97	0.15	-	44,46,47,47	0
1	LLP	A	234	24/25	0.97	0.14	-	40,43,44,45	0
1	LLP	G	234	24/25	0.97	0.15	-	54,57,59,59	0
1	LLP	D	234	24/25	0.97	0.17	-	41,41,42,43	0
1	LLP	E	234	24/25	0.98	0.15	-	41,42,44,45	0
1	LLP	B	234	24/25	0.98	0.16	-	38,40,41,41	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ )	Q<0.9
2	CL	I	501	1/1	0.84	0.17	-	79,79,79,79	0
2	CL	C	501	1/1	0.85	0.14	-	86,86,86,86	0
2	CL	B	501	1/1	0.81	0.22	-	69,69,69,69	0
2	CL	E	501	1/1	0.82	0.20	-	72,72,72,72	0
2	CL	D	501	1/1	0.87	0.17	-	52,52,52,52	0
2	CL	H	501	1/1	0.70	0.15	-	71,71,71,71	0
2	CL	A	501	1/1	0.85	0.18	-	69,69,69,69	0

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

There are no such residues in this entry.