



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 05:47 AM EDT

PDB ID : 3DBY  
Title : Crystal structure of uncharacterized protein from *Bacillus cereus* G9241 (CSAP Target)  
Authors : Ramagopal, U.A.; Bonanno, J.B.; Ozyurt, S.; Freeman, J.; Wasserman, S.; Hu, S.; Groshong, C.; Rodgers, L.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-06-02  
Resolution : 2.10 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

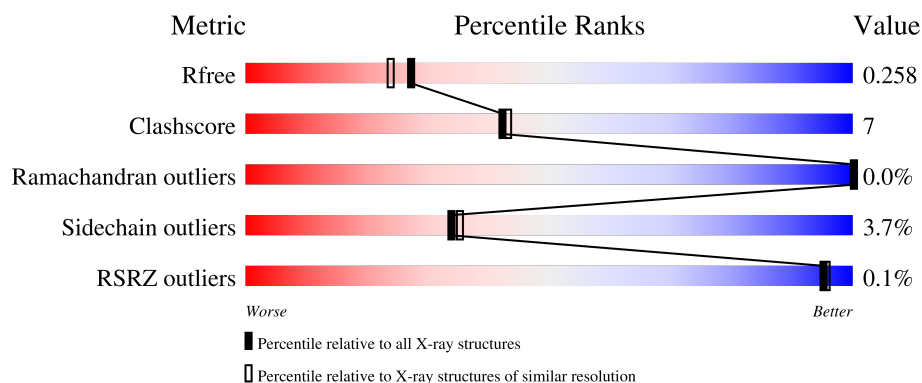
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	269	 83% 11% . .
1	B	269	 86% 11% ...
1	C	269	 85% 13% ..
1	D	269	 85% 13% ..

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Mol	Chain	Length	Quality of chain
1	E	269	 84% 10% . .
1	F	269	 85% 13% ..
1	G	269	 77% 16% . .
1	H	269	 85% 12% ..
1	I	269	 73% 22% . .
1	J	269	 83% 13% ..
1	K	269	 80% 14% . .
1	L	269	 81% 14% . .
1	M	269	 80% 16% .
1	N	269	 81% 13% . .
1	O	269	 74% 20% . .
1	P	269	 82% 14% . .
1	Q	269	 87% 10% ..
1	R	269	 87% 11% ..
1	S	269	 80% 15% . .
1	T	269	 88% 11% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	R	308	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 45580 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 uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	3	0
			2130	1382	347	393	8			
1	B	266	Total	C	N	O	S	0	4	0
			2217	1435	374	399	9			
1	C	267	Total	C	N	O	S	0	2	0
			2215	1433	373	401	8			
1	D	266	Total	C	N	O	S	0	5	0
			2226	1441	376	400	9			
1	E	257	Total	C	N	O	S	0	4	0
			2139	1387	348	396	8			
1	F	267	Total	C	N	O	S	0	4	0
			2228	1443	377	399	9			
1	G	257	Total	C	N	O	S	0	1	0
			2113	1372	349	384	8			
1	H	265	Total	C	N	O	S	0	4	0
			2219	1434	376	400	9			
1	I	257	Total	C	N	O	S	0	1	0
			2114	1373	346	386	9			
1	J	266	Total	C	N	O	S	0	5	0
			2230	1441	376	405	8			
1	K	257	Total	C	N	O	S	0	2	0
			2121	1377	346	390	8			
1	L	260	Total	C	N	O	S	0	2	0
			2146	1392	356	389	9			
1	M	259	Total	C	N	O	S	0	1	0
			2127	1380	351	388	8			
1	N	259	Total	C	N	O	S	0	0	0
			2124	1377	351	388	8			
1	O	257	Total	C	N	O	S	0	2	0
			2123	1378	347	389	9			
1	P	266	Total	C	N	O	S	0	2	0
			2207	1427	372	400	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	266	Total	C	N	O	S	0	6	0
			2227	1441	372	405	9			
1	R	265	Total	C	N	O	S	0	4	0
			2216	1434	373	400	9			
1	S	257	Total	C	N	O	S	0	3	0
			2130	1382	347	392	9			
1	T	267	Total	C	N	O	S	0	1	0
			2207	1428	371	399	9			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q4MWP8
A	2	LEU	-	expression tag	UNP Q4MWP8
A	261	GLU	-	expression tag	UNP Q4MWP8
A	262	GLY	-	expression tag	UNP Q4MWP8
A	263	HIS	-	expression tag	UNP Q4MWP8
A	264	HIS	-	expression tag	UNP Q4MWP8
A	265	HIS	-	expression tag	UNP Q4MWP8
A	266	HIS	-	expression tag	UNP Q4MWP8
A	267	HIS	-	expression tag	UNP Q4MWP8
A	268	HIS	-	expression tag	UNP Q4MWP8
B	1	SER	-	expression tag	UNP Q4MWP8
B	2	LEU	-	expression tag	UNP Q4MWP8
B	261	GLU	-	expression tag	UNP Q4MWP8
B	262	GLY	-	expression tag	UNP Q4MWP8
B	263	HIS	-	expression tag	UNP Q4MWP8
B	264	HIS	-	expression tag	UNP Q4MWP8
B	265	HIS	-	expression tag	UNP Q4MWP8
B	266	HIS	-	expression tag	UNP Q4MWP8
B	267	HIS	-	expression tag	UNP Q4MWP8
B	268	HIS	-	expression tag	UNP Q4MWP8
C	1	SER	-	expression tag	UNP Q4MWP8
C	2	LEU	-	expression tag	UNP Q4MWP8
C	261	GLU	-	expression tag	UNP Q4MWP8
C	262	GLY	-	expression tag	UNP Q4MWP8
C	263	HIS	-	expression tag	UNP Q4MWP8
C	264	HIS	-	expression tag	UNP Q4MWP8
C	265	HIS	-	expression tag	UNP Q4MWP8
C	266	HIS	-	expression tag	UNP Q4MWP8
C	267	HIS	-	expression tag	UNP Q4MWP8
C	268	HIS	-	expression tag	UNP Q4MWP8
D	1	SER	-	expression tag	UNP Q4MWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	LEU	-	expression tag	UNP Q4MWP8
D	261	GLU	-	expression tag	UNP Q4MWP8
D	262	GLY	-	expression tag	UNP Q4MWP8
D	263	HIS	-	expression tag	UNP Q4MWP8
D	264	HIS	-	expression tag	UNP Q4MWP8
D	265	HIS	-	expression tag	UNP Q4MWP8
D	266	HIS	-	expression tag	UNP Q4MWP8
D	267	HIS	-	expression tag	UNP Q4MWP8
D	268	HIS	-	expression tag	UNP Q4MWP8
E	1	SER	-	expression tag	UNP Q4MWP8
E	2	LEU	-	expression tag	UNP Q4MWP8
E	261	GLU	-	expression tag	UNP Q4MWP8
E	262	GLY	-	expression tag	UNP Q4MWP8
E	263	HIS	-	expression tag	UNP Q4MWP8
E	264	HIS	-	expression tag	UNP Q4MWP8
E	265	HIS	-	expression tag	UNP Q4MWP8
E	266	HIS	-	expression tag	UNP Q4MWP8
E	267	HIS	-	expression tag	UNP Q4MWP8
E	268	HIS	-	expression tag	UNP Q4MWP8
F	1	SER	-	expression tag	UNP Q4MWP8
F	2	LEU	-	expression tag	UNP Q4MWP8
F	261	GLU	-	expression tag	UNP Q4MWP8
F	262	GLY	-	expression tag	UNP Q4MWP8
F	263	HIS	-	expression tag	UNP Q4MWP8
F	264	HIS	-	expression tag	UNP Q4MWP8
F	265	HIS	-	expression tag	UNP Q4MWP8
F	266	HIS	-	expression tag	UNP Q4MWP8
F	267	HIS	-	expression tag	UNP Q4MWP8
F	268	HIS	-	expression tag	UNP Q4MWP8
G	1	SER	-	expression tag	UNP Q4MWP8
G	2	LEU	-	expression tag	UNP Q4MWP8
G	261	GLU	-	expression tag	UNP Q4MWP8
G	262	GLY	-	expression tag	UNP Q4MWP8
G	263	HIS	-	expression tag	UNP Q4MWP8
G	264	HIS	-	expression tag	UNP Q4MWP8
G	265	HIS	-	expression tag	UNP Q4MWP8
G	266	HIS	-	expression tag	UNP Q4MWP8
G	267	HIS	-	expression tag	UNP Q4MWP8
G	268	HIS	-	expression tag	UNP Q4MWP8
H	1	SER	-	expression tag	UNP Q4MWP8
H	2	LEU	-	expression tag	UNP Q4MWP8
H	261	GLU	-	expression tag	UNP Q4MWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	262	GLY	-	expression tag	UNP Q4MWP8
H	263	HIS	-	expression tag	UNP Q4MWP8
H	264	HIS	-	expression tag	UNP Q4MWP8
H	265	HIS	-	expression tag	UNP Q4MWP8
H	266	HIS	-	expression tag	UNP Q4MWP8
H	267	HIS	-	expression tag	UNP Q4MWP8
H	268	HIS	-	expression tag	UNP Q4MWP8
I	1	SER	-	expression tag	UNP Q4MWP8
I	2	LEU	-	expression tag	UNP Q4MWP8
I	261	GLU	-	expression tag	UNP Q4MWP8
I	262	GLY	-	expression tag	UNP Q4MWP8
I	263	HIS	-	expression tag	UNP Q4MWP8
I	264	HIS	-	expression tag	UNP Q4MWP8
I	265	HIS	-	expression tag	UNP Q4MWP8
I	266	HIS	-	expression tag	UNP Q4MWP8
I	267	HIS	-	expression tag	UNP Q4MWP8
I	268	HIS	-	expression tag	UNP Q4MWP8
J	1	SER	-	expression tag	UNP Q4MWP8
J	2	LEU	-	expression tag	UNP Q4MWP8
J	261	GLU	-	expression tag	UNP Q4MWP8
J	262	GLY	-	expression tag	UNP Q4MWP8
J	263	HIS	-	expression tag	UNP Q4MWP8
J	264	HIS	-	expression tag	UNP Q4MWP8
J	265	HIS	-	expression tag	UNP Q4MWP8
J	266	HIS	-	expression tag	UNP Q4MWP8
J	267	HIS	-	expression tag	UNP Q4MWP8
J	268	HIS	-	expression tag	UNP Q4MWP8
K	1	SER	-	expression tag	UNP Q4MWP8
K	2	LEU	-	expression tag	UNP Q4MWP8
K	261	GLU	-	expression tag	UNP Q4MWP8
K	262	GLY	-	expression tag	UNP Q4MWP8
K	263	HIS	-	expression tag	UNP Q4MWP8
K	264	HIS	-	expression tag	UNP Q4MWP8
K	265	HIS	-	expression tag	UNP Q4MWP8
K	266	HIS	-	expression tag	UNP Q4MWP8
K	267	HIS	-	expression tag	UNP Q4MWP8
K	268	HIS	-	expression tag	UNP Q4MWP8
L	1	SER	-	expression tag	UNP Q4MWP8
L	2	LEU	-	expression tag	UNP Q4MWP8
L	261	GLU	-	expression tag	UNP Q4MWP8
L	262	GLY	-	expression tag	UNP Q4MWP8
L	263	HIS	-	expression tag	UNP Q4MWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	264	HIS	-	expression tag	UNP Q4MWP8
L	265	HIS	-	expression tag	UNP Q4MWP8
L	266	HIS	-	expression tag	UNP Q4MWP8
L	267	HIS	-	expression tag	UNP Q4MWP8
L	268	HIS	-	expression tag	UNP Q4MWP8
M	1	SER	-	expression tag	UNP Q4MWP8
M	2	LEU	-	expression tag	UNP Q4MWP8
M	261	GLU	-	expression tag	UNP Q4MWP8
M	262	GLY	-	expression tag	UNP Q4MWP8
M	263	HIS	-	expression tag	UNP Q4MWP8
M	264	HIS	-	expression tag	UNP Q4MWP8
M	265	HIS	-	expression tag	UNP Q4MWP8
M	266	HIS	-	expression tag	UNP Q4MWP8
M	267	HIS	-	expression tag	UNP Q4MWP8
M	268	HIS	-	expression tag	UNP Q4MWP8
N	1	SER	-	expression tag	UNP Q4MWP8
N	2	LEU	-	expression tag	UNP Q4MWP8
N	261	GLU	-	expression tag	UNP Q4MWP8
N	262	GLY	-	expression tag	UNP Q4MWP8
N	263	HIS	-	expression tag	UNP Q4MWP8
N	264	HIS	-	expression tag	UNP Q4MWP8
N	265	HIS	-	expression tag	UNP Q4MWP8
N	266	HIS	-	expression tag	UNP Q4MWP8
N	267	HIS	-	expression tag	UNP Q4MWP8
N	268	HIS	-	expression tag	UNP Q4MWP8
O	1	SER	-	expression tag	UNP Q4MWP8
O	2	LEU	-	expression tag	UNP Q4MWP8
O	261	GLU	-	expression tag	UNP Q4MWP8
O	262	GLY	-	expression tag	UNP Q4MWP8
O	263	HIS	-	expression tag	UNP Q4MWP8
O	264	HIS	-	expression tag	UNP Q4MWP8
O	265	HIS	-	expression tag	UNP Q4MWP8
O	266	HIS	-	expression tag	UNP Q4MWP8
O	267	HIS	-	expression tag	UNP Q4MWP8
O	268	HIS	-	expression tag	UNP Q4MWP8
P	1	SER	-	expression tag	UNP Q4MWP8
P	2	LEU	-	expression tag	UNP Q4MWP8
P	261	GLU	-	expression tag	UNP Q4MWP8
P	262	GLY	-	expression tag	UNP Q4MWP8
P	263	HIS	-	expression tag	UNP Q4MWP8
P	264	HIS	-	expression tag	UNP Q4MWP8
P	265	HIS	-	expression tag	UNP Q4MWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
P	266	HIS	-	expression tag	UNP Q4MWP8
P	267	HIS	-	expression tag	UNP Q4MWP8
P	268	HIS	-	expression tag	UNP Q4MWP8
Q	1	SER	-	expression tag	UNP Q4MWP8
Q	2	LEU	-	expression tag	UNP Q4MWP8
Q	261	GLU	-	expression tag	UNP Q4MWP8
Q	262	GLY	-	expression tag	UNP Q4MWP8
Q	263	HIS	-	expression tag	UNP Q4MWP8
Q	264	HIS	-	expression tag	UNP Q4MWP8
Q	265	HIS	-	expression tag	UNP Q4MWP8
Q	266	HIS	-	expression tag	UNP Q4MWP8
Q	267	HIS	-	expression tag	UNP Q4MWP8
Q	268	HIS	-	expression tag	UNP Q4MWP8
R	1	SER	-	expression tag	UNP Q4MWP8
R	2	LEU	-	expression tag	UNP Q4MWP8
R	261	GLU	-	expression tag	UNP Q4MWP8
R	262	GLY	-	expression tag	UNP Q4MWP8
R	263	HIS	-	expression tag	UNP Q4MWP8
R	264	HIS	-	expression tag	UNP Q4MWP8
R	265	HIS	-	expression tag	UNP Q4MWP8
R	266	HIS	-	expression tag	UNP Q4MWP8
R	267	HIS	-	expression tag	UNP Q4MWP8
R	268	HIS	-	expression tag	UNP Q4MWP8
S	1	SER	-	expression tag	UNP Q4MWP8
S	2	LEU	-	expression tag	UNP Q4MWP8
S	261	GLU	-	expression tag	UNP Q4MWP8
S	262	GLY	-	expression tag	UNP Q4MWP8
S	263	HIS	-	expression tag	UNP Q4MWP8
S	264	HIS	-	expression tag	UNP Q4MWP8
S	265	HIS	-	expression tag	UNP Q4MWP8
S	266	HIS	-	expression tag	UNP Q4MWP8
S	267	HIS	-	expression tag	UNP Q4MWP8
S	268	HIS	-	expression tag	UNP Q4MWP8
T	1	SER	-	expression tag	UNP Q4MWP8
T	2	LEU	-	expression tag	UNP Q4MWP8
T	261	GLU	-	expression tag	UNP Q4MWP8
T	262	GLY	-	expression tag	UNP Q4MWP8
T	263	HIS	-	expression tag	UNP Q4MWP8
T	264	HIS	-	expression tag	UNP Q4MWP8
T	265	HIS	-	expression tag	UNP Q4MWP8
T	266	HIS	-	expression tag	UNP Q4MWP8
T	267	HIS	-	expression tag	UNP Q4MWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
T	268	HIS	-	expression tag	UNP Q4MWP8

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

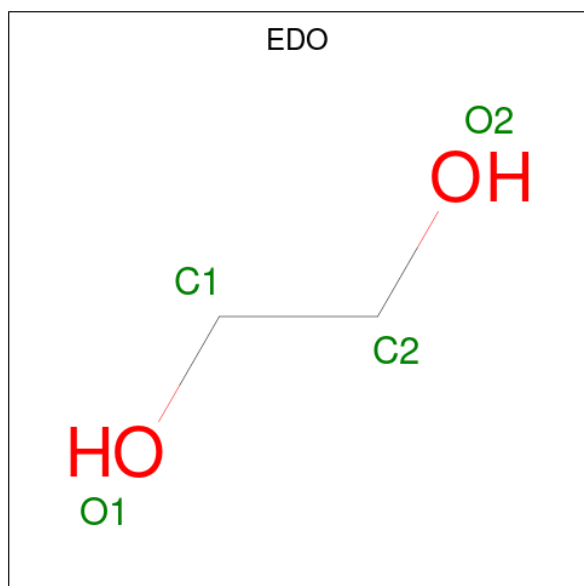
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Fe 2	0	0
2	B	2	Total 2	Fe 2	0	0
2	C	2	Total 2	Fe 2	0	0
2	D	2	Total 2	Fe 2	0	0
2	E	2	Total 2	Fe 2	0	0
2	F	2	Total 2	Fe 2	0	0
2	G	2	Total 2	Fe 2	0	0
2	H	2	Total 2	Fe 2	0	0
2	I	2	Total 2	Fe 2	0	0
2	J	2	Total 2	Fe 2	0	0
2	K	2	Total 2	Fe 2	0	0
2	L	2	Total 2	Fe 2	0	0
2	M	2	Total 2	Fe 2	0	0
2	N	2	Total 2	Fe 2	0	0
2	O	2	Total 2	Fe 2	0	0
2	P	2	Total 2	Fe 2	0	0
2	Q	2	Total 2	Fe 2	0	0
2	R	2	Total 2	Fe 2	0	0
2	S	2	Total 2	Fe 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	T	2	Total	Fe	0	0
			2	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	R	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		
4	B	152	Total	O	0	0
			152	152		
4	C	139	Total	O	0	0
			139	139		
4	D	132	Total	O	0	0
			132	132		
4	E	117	Total	O	0	0
			117	117		
4	F	147	Total	O	0	0
			147	147		

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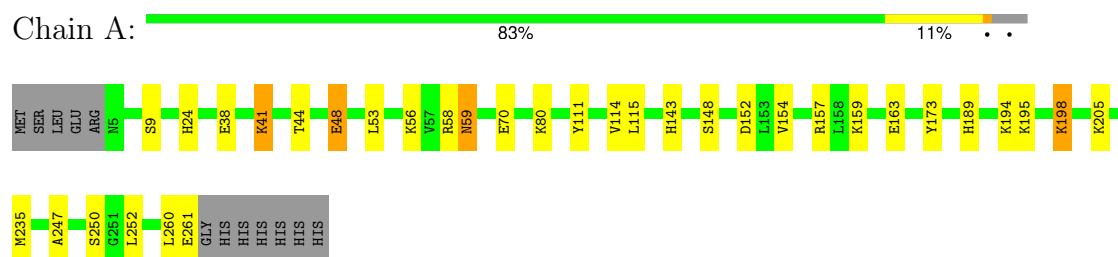
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	82	Total 82	O 82	0	0
4	H	117	Total 117	O 117	0	0
4	I	41	Total 41	O 41	0	0
4	J	93	Total 93	O 93	0	0
4	K	73	Total 73	O 73	0	0
4	L	109	Total 109	O 109	0	0
4	M	59	Total 59	O 59	0	0
4	N	110	Total 110	O 110	0	0
4	O	41	Total 41	O 41	0	0
4	P	84	Total 84	O 84	0	0
4	Q	123	Total 123	O 123	0	0
4	R	128	Total 128	O 128	0	0
4	S	84	Total 84	O 84	0	0
4	T	132	Total 132	O 132	0	0

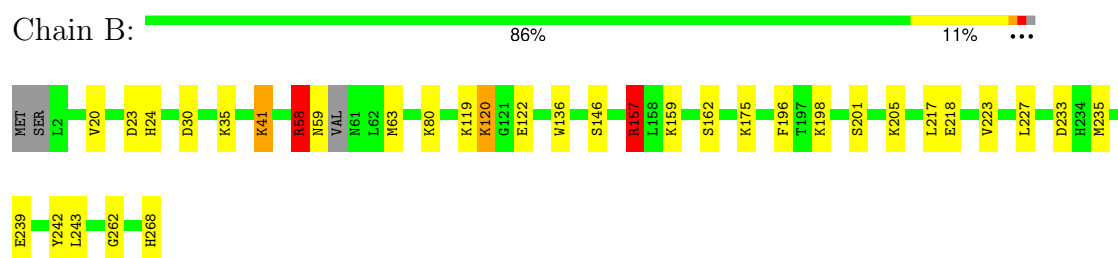
### 3 Residue-property plots [i](#)

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.

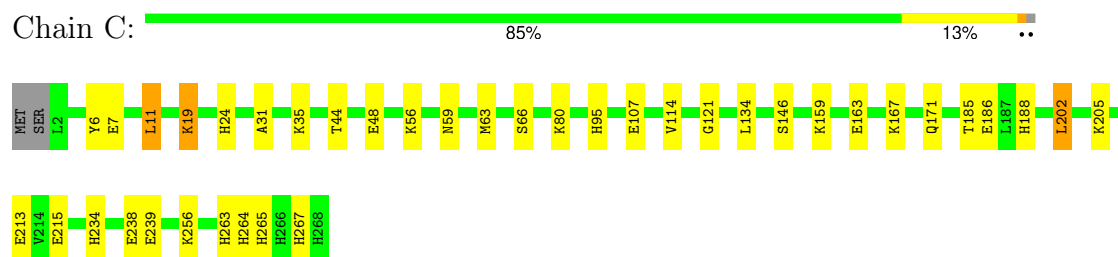
- Molecule 1: uncharacterized protein



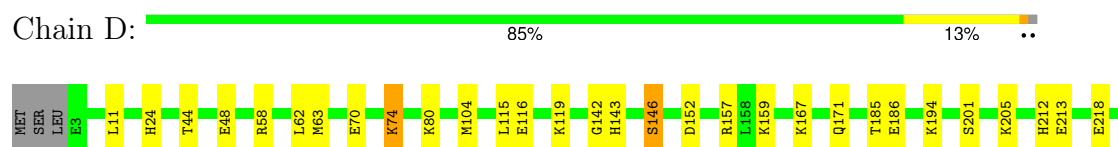
- Molecule 1: uncharacterized protein



- Molecule 1: uncharacterized protein



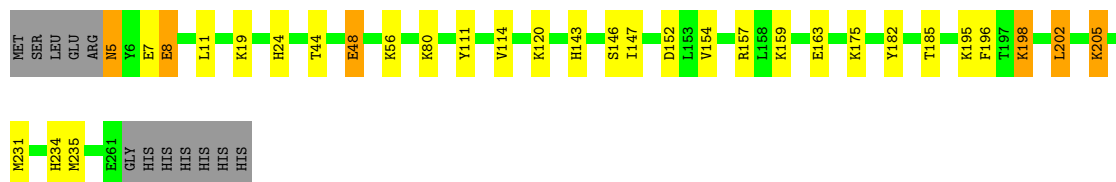
- Molecule 1: uncharacterized protein





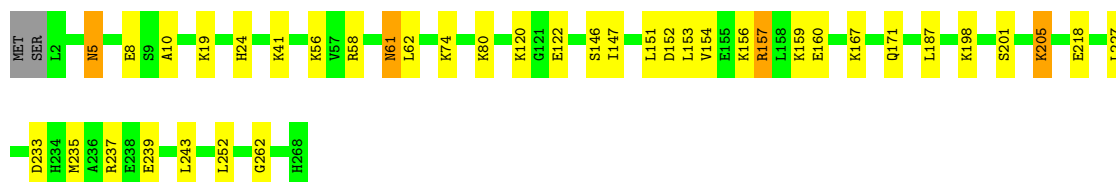
- Molecule 1: uncharacterized protein

Chain E: 84% 10% . .



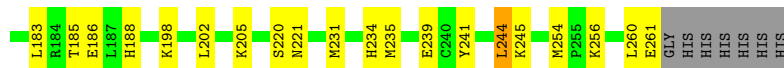
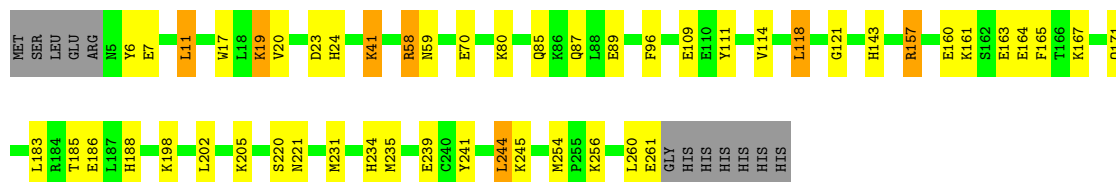
- Molecule 1: uncharacterized protein

Chain F: 85% 13% . .



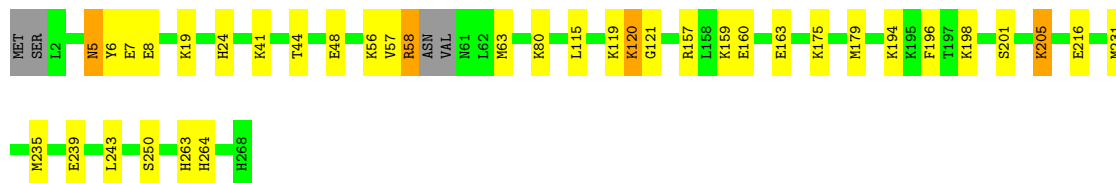
- Molecule 1: uncharacterized protein

Chain G: 77% 16% . .



- Molecule 1: uncharacterized protein

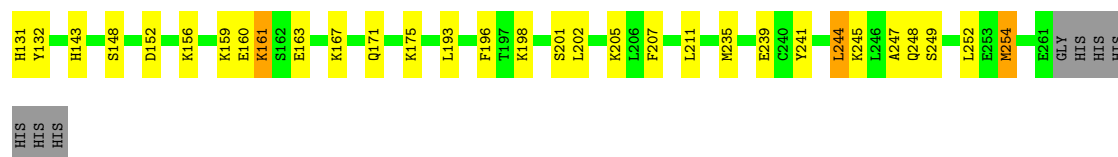
Chain H: 85% 12% . .



- Molecule 1: uncharacterized protein

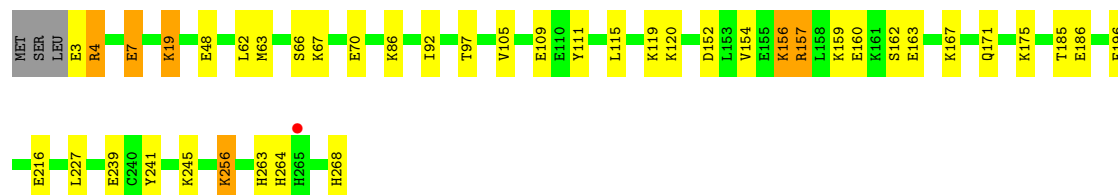
Chain I: 73% 22% . .





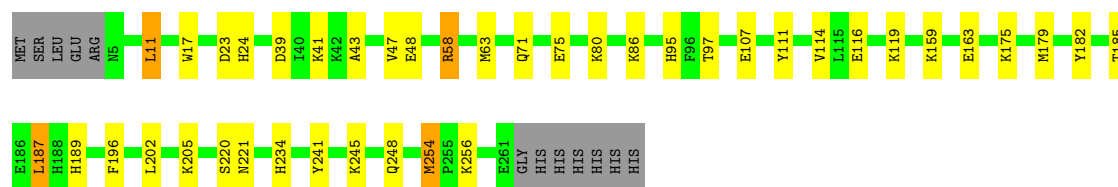
- Molecule 1: uncharacterized protein

Chain J: 83% 13% ..



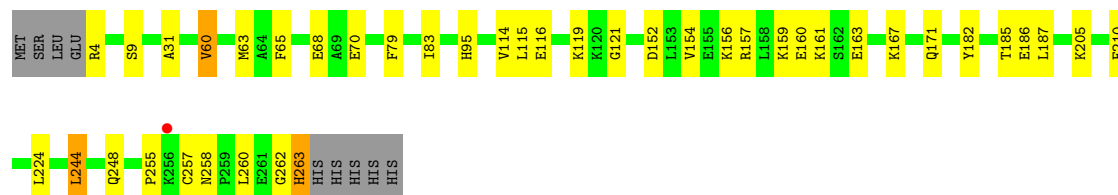
- Molecule 1: uncharacterized protein

Chain K: 80% 14% ..



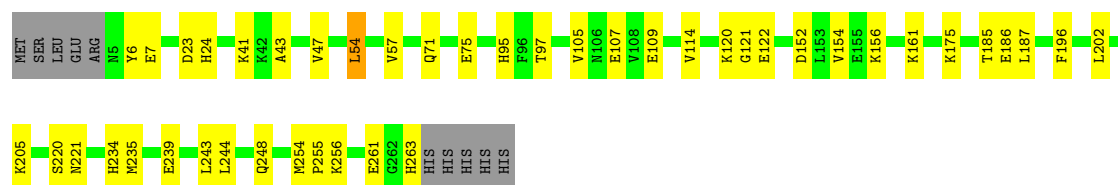
- Molecule 1: uncharacterized protein

Chain L: 81% 14% ..



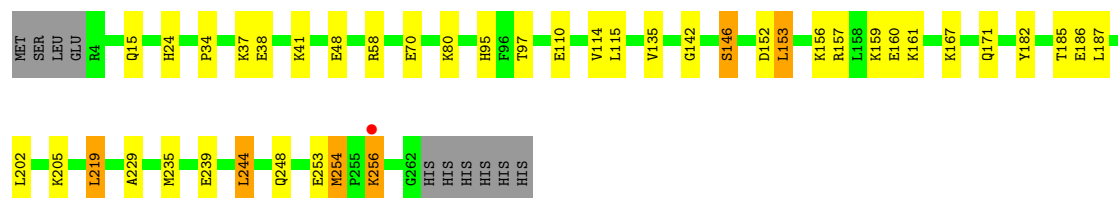
- Molecule 1: uncharacterized protein

Chain M: 80% 16% .



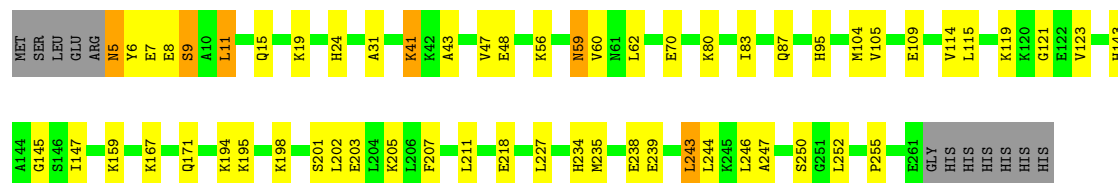
- Molecule 1: uncharacterized protein

Chain N: 81% 13% ..



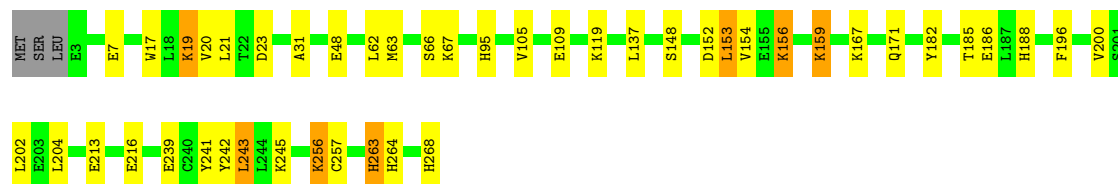
- Molecule 1: uncharacterized protein

Chain O: 74% 20%



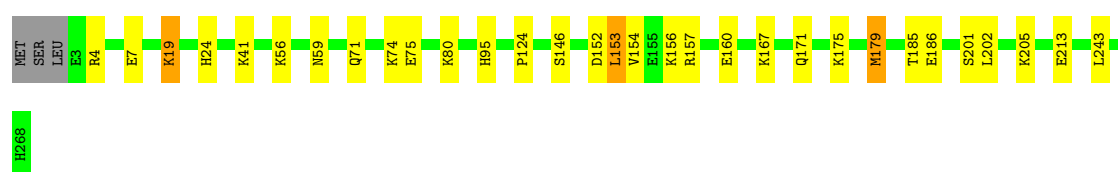
- Molecule 1: uncharacterized protein

Chain P: 82% 14%



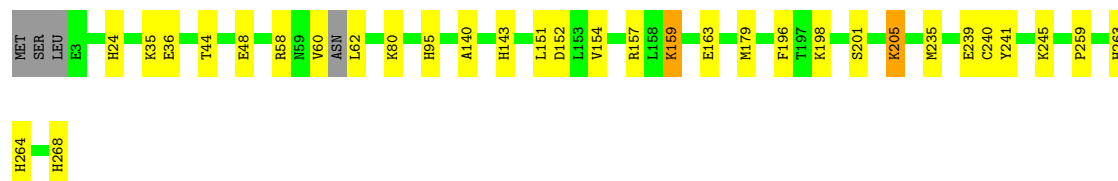
- Molecule 1: uncharacterized protein

Chain Q: 87% 10%



- Molecule 1: uncharacterized protein

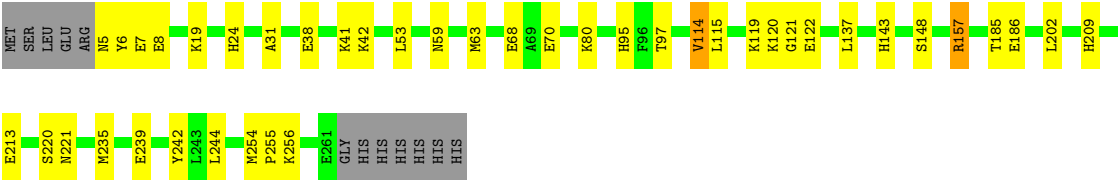
Chain R: 87% 11%



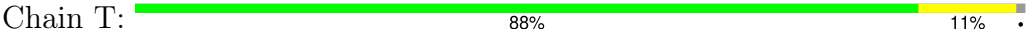
- Molecule 1: uncharacterized protein

Chain S: 80% 15%





• Molecule 1: uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.81Å 167.81Å 582.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 49.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.10) 96.6 (49.69-2.10)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.198 , 0.258 0.199 , 0.258	Depositor DCC
$R_{free}$ test set	17434 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 19.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.470 for -h-k,k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	45580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6188e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.81	1/2186 (0.0%)	0.75	1/2947 (0.0%)
1	B	0.88	0/2286	0.82	2/3078 (0.1%)
1	C	0.81	0/2278	0.75	1/3070 (0.0%)
1	D	0.87	0/2298	0.76	3/3094 (0.1%)
1	E	0.82	0/2195	0.77	3/2959 (0.1%)
1	F	0.86	0/2297	0.80	2/3093 (0.1%)
1	G	0.72	0/2166	0.74	0/2920
1	H	0.80	0/2278	0.77	1/3066 (0.0%)
1	I	0.65	0/2167	0.66	0/2921
1	J	0.75	0/2299	0.75	0/3097
1	K	0.70	0/2177	0.72	1/2935 (0.0%)
1	L	0.78	0/2204	0.74	2/2970 (0.1%)
1	M	0.73	0/2182	0.70	0/2943
1	N	0.75	0/2174	0.76	3/2930 (0.1%)
1	O	0.65	0/2176	0.70	0/2933
1	P	0.73	0/2270	0.74	1/3059 (0.0%)
1	Q	0.82	0/2302	0.80	4/3101 (0.1%)
1	R	0.84	0/2278	0.75	1/3066 (0.0%)
1	S	0.74	0/2183	0.72	1/2943 (0.0%)
1	T	0.82	0/2266	0.78	2/3053 (0.1%)
All	All	0.78	1/44662 (0.0%)	0.75	28/60178 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	TYR	CD1-CE1	5.18	1.47	1.39

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	LEU	CA-CB-CG	9.43	136.99	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	ARG	NE-CZ-NH1	-7.67	116.47	120.30
1	Q	157	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	B	157	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	T	157	ARG	NE-CZ-NH1	-7.00	116.80	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	2130	0	2118	30	0
1	B	2217	0	2194	25	0
1	C	2215	0	2189	22	0
1	D	2226	0	2213	26	0
1	E	2139	0	2123	27	0
1	F	2228	0	2218	33	0
1	G	2113	0	2110	48	0
1	H	2219	0	2191	39	0
1	I	2114	0	2110	40	0
1	J	2230	0	2202	35	0
1	K	2121	0	2113	29	0
1	L	2146	0	2140	36	0
1	M	2127	0	2109	23	0
1	N	2124	0	2117	37	0
1	O	2123	0	2115	35	0
1	P	2207	0	2178	32	0
1	Q	2227	0	2204	18	0
1	R	2216	0	2191	35	0
1	S	2130	0	2113	27	0
1	T	2207	0	2185	18	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
3	B	4	0	6	2	0
3	R	4	0	6	4	0
4	A	110	0	0	1	0
4	B	152	0	0	3	0
4	C	139	0	0	3	0
4	D	132	0	0	2	0
4	E	117	0	0	2	0
4	F	147	0	0	3	0
4	G	82	0	0	5	0
4	H	117	0	0	5	0
4	I	41	0	0	1	0
4	J	93	0	0	2	0
4	K	73	0	0	0	0
4	L	109	0	0	6	0
4	M	59	0	0	0	0
4	N	110	0	0	1	0
4	O	41	0	0	1	0
4	P	84	0	0	1	0
4	Q	123	0	0	2	0
4	R	128	0	0	1	0
4	S	84	0	0	3	0
4	T	132	0	0	3	0
All	All	45580	0	43145	595	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 7.

The worst 5 of 595 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:J:159:LYS:HE2	1:J:163:GLU:OE1	1.33	1.24
1:D:58[B]:ARG:HH11	1:D:58[B]:ARG:HB2	1.00	1.12
1:K:58:ARG:HG3	1:K:58:ARG:HH21	1.01	1.12
1:F:157:ARG:HB3	1:F:157:ARG:NH2	1.65	1.11
1:G:41:LYS:HE3	1:G:41:LYS:HA	1.30	1.10

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	258/269 (96%)	256 (99%)	2 (1%)	0	100	100
1	B	266/269 (99%)	263 (99%)	2 (1%)	1 (0%)	34	32
1	C	267/269 (99%)	263 (98%)	4 (2%)	0	100	100
1	D	269/269 (100%)	266 (99%)	3 (1%)	0	100	100
1	E	259/269 (96%)	259 (100%)	0	0	100	100
1	F	269/269 (100%)	268 (100%)	1 (0%)	0	100	100
1	G	256/269 (95%)	250 (98%)	6 (2%)	0	100	100
1	H	265/269 (98%)	262 (99%)	3 (1%)	0	100	100
1	I	256/269 (95%)	253 (99%)	3 (1%)	0	100	100
1	J	269/269 (100%)	267 (99%)	2 (1%)	0	100	100
1	K	257/269 (96%)	254 (99%)	3 (1%)	0	100	100
1	L	260/269 (97%)	258 (99%)	2 (1%)	0	100	100
1	M	258/269 (96%)	256 (99%)	2 (1%)	0	100	100
1	N	257/269 (96%)	253 (98%)	4 (2%)	0	100	100
1	O	257/269 (96%)	254 (99%)	3 (1%)	0	100	100
1	P	266/269 (99%)	260 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	270/269 (100%)	265 (98%)	5 (2%)	0	100	100
1	R	265/269 (98%)	263 (99%)	2 (1%)	0	100	100
1	S	258/269 (96%)	254 (98%)	4 (2%)	0	100	100
1	T	266/269 (99%)	264 (99%)	2 (1%)	0	100	100
All	All	5248/5380 (98%)	5188 (99%)	59 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	58	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	232/240 (97%)	225 (97%)	7 (3%)	41	44
1	B	241/240 (100%)	234 (97%)	7 (3%)	42	46
1	C	240/240 (100%)	231 (96%)	9 (4%)	33	34
1	D	242/240 (101%)	236 (98%)	6 (2%)	47	52
1	E	233/240 (97%)	225 (97%)	8 (3%)	37	39
1	F	242/240 (101%)	235 (97%)	7 (3%)	42	46
1	G	229/240 (95%)	214 (93%)	15 (7%)	16	14
1	H	240/240 (100%)	231 (96%)	9 (4%)	33	34
1	I	230/240 (96%)	219 (95%)	11 (5%)	25	24
1	J	242/240 (101%)	229 (95%)	13 (5%)	22	20
1	K	231/240 (96%)	221 (96%)	10 (4%)	29	29
1	L	233/240 (97%)	228 (98%)	5 (2%)	53	59
1	M	230/240 (96%)	220 (96%)	10 (4%)	29	29
1	N	230/240 (96%)	216 (94%)	14 (6%)	18	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	231/240 (96%)	217 (94%)	14 (6%)	18	16
1	P	239/240 (100%)	230 (96%)	9 (4%)	33	34
1	Q	243/240 (101%)	236 (97%)	7 (3%)	42	46
1	R	240/240 (100%)	236 (98%)	4 (2%)	60	67
1	S	231/240 (96%)	224 (97%)	7 (3%)	41	44
1	T	239/240 (100%)	234 (98%)	5 (2%)	53	59
All	All	4718/4800 (98%)	4541 (96%)	177 (4%)	34	34

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	261	GLU
1	O	243	LEU
1	N	48	GLU
1	N	256	LYS
1	P	188	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	71	GLN
1	O	55	ASN
1	S	209	HIS
1	L	95	HIS
1	N	15	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 monosaccharides in this entry.



## 5.6 Ligand geometry

Of 42 ligands modelled in this entry, 40 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
3	EDO	R	308	-	3,3,3	0.40	0	2,2,2	0.57	0
3	EDO	B	308	-	3,3,3	0.52	0	2,2,2	0.25	0

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
3	EDO	R	308	-	-	0/1/1/1	-
3	EDO	B	308	-	-	0/1/1/1	-

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.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	308	EDO	4	0
3	B	308	EDO	2	0

## 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	257/269 (95%)	-0.68	0 100 100	12, 20, 38, 50	0
1	B	266/269 (98%)	-0.75	0 100 100	9, 16, 28, 45	0
1	C	267/269 (99%)	-0.73	0 100 100	12, 18, 33, 46	0
1	D	266/269 (98%)	-0.73	0 100 100	11, 18, 30, 40	0
1	E	257/269 (95%)	-0.65	0 100 100	11, 20, 38, 49	0
1	F	267/269 (99%)	-0.71	0 100 100	9, 16, 29, 38	0
1	G	257/269 (95%)	-0.55	0 100 100	15, 24, 43, 52	0
1	H	265/269 (98%)	-0.69	0 100 100	12, 20, 31, 39	0
1	I	257/269 (95%)	-0.50	0 100 100	20, 30, 49, 56	0
1	J	266/269 (98%)	-0.58	1 (0%) 92 93	17, 25, 35, 47	0
1	K	257/269 (95%)	-0.58	0 100 100	16, 25, 42, 53	0
1	L	260/269 (96%)	-0.67	1 (0%) 92 93	16, 22, 36, 51	0
1	M	259/269 (96%)	-0.63	0 100 100	16, 25, 41, 55	0
1	N	259/269 (96%)	-0.68	1 (0%) 92 93	16, 22, 35, 46	0
1	O	257/269 (95%)	-0.45	0 100 100	20, 29, 50, 58	0
1	P	266/269 (98%)	-0.60	0 100 100	16, 25, 35, 44	0
1	Q	266/269 (98%)	-0.72	0 100 100	12, 18, 34, 45	0
1	R	265/269 (98%)	-0.72	0 100 100	11, 18, 29, 45	0
1	S	257/269 (95%)	-0.59	0 100 100	16, 24, 42, 52	0
1	T	267/269 (99%)	-0.73	0 100 100	12, 20, 32, 43	0
All	All	5238/5380 (97%)	-0.65	3 (0%) 95 96	9, 22, 39, 58	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	256	LYS	2.9
1	J	265	HIS	2.4
1	N	256	LYS	2.3

## 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 monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	308	4/4	0.82	0.15	30,34,35,36	0
3	EDO	R	308	4/4	0.94	0.08	27,28,29,30	0
2	FE	M	307	1/1	0.97	0.03	46,46,46,46	0
2	FE	D	306	1/1	0.98	0.04	35,35,35,35	0
2	FE	N	307	1/1	0.98	0.04	48,48,48,48	0
2	FE	O	307	1/1	0.98	0.02	53,53,53,53	0
2	FE	P	306	1/1	0.98	0.04	45,45,45,45	0
2	FE	R	306	1/1	0.98	0.03	36,36,36,36	0
2	FE	G	307	1/1	0.98	0.03	42,42,42,42	0
2	FE	M	306	1/1	0.98	0.04	48,48,48,48	0
2	FE	F	307	1/1	0.99	0.03	29,29,29,29	0
2	FE	A	307	1/1	0.99	0.05	43,43,43,43	0
2	FE	H	306	1/1	0.99	0.03	34,34,34,34	0
2	FE	H	307	1/1	0.99	0.03	35,35,35,35	0
2	FE	I	306	1/1	0.99	0.02	54,54,54,54	0
2	FE	I	307	1/1	0.99	0.03	54,54,54,54	0
2	FE	J	306	1/1	0.99	0.03	43,43,43,43	0
2	FE	J	307	1/1	0.99	0.03	44,44,44,44	0
2	FE	K	306	1/1	0.99	0.05	48,48,48,48	0
2	FE	L	306	1/1	0.99	0.05	39,39,39,39	0
2	FE	L	307	1/1	0.99	0.04	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE	B	306	1/1	0.99	0.03	35,35,35,35	0
2	FE	B	307	1/1	0.99	0.03	32,32,32,32	0
2	FE	N	306	1/1	0.99	0.03	38,38,38,38	0
2	FE	C	306	1/1	0.99	0.04	36,36,36,36	0
2	FE	O	306	1/1	0.99	0.04	51,51,51,51	0
2	FE	A	306	1/1	0.99	0.03	38,38,38,38	0
2	FE	D	307	1/1	0.99	0.04	37,37,37,37	0
2	FE	P	307	1/1	0.99	0.04	45,45,45,45	0
2	FE	Q	306	1/1	0.99	0.03	40,40,40,40	0
2	FE	Q	307	1/1	0.99	0.03	32,32,32,32	0
2	FE	E	306	1/1	0.99	0.03	36,36,36,36	0
2	FE	T	306	1/1	0.99	0.04	36,36,36,36	0
2	FE	T	307	1/1	0.99	0.03	37,37,37,37	0
2	FE	E	307	1/1	0.99	0.05	42,42,42,42	0
2	FE	F	306	1/1	0.99	0.04	34,34,34,34	0
2	FE	S	306	1/1	1.00	0.04	39,39,39,39	0
2	FE	S	307	1/1	1.00	0.04	46,46,46,46	0
2	FE	G	306	1/1	1.00	0.03	39,39,39,39	0
2	FE	K	307	1/1	1.00	0.04	49,49,49,49	0
2	FE	C	307	1/1	1.00	0.02	31,31,31,31	0
2	FE	R	307	1/1	1.00	0.04	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.