



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 05:45 am BST

PDB ID : 4PEL  
Title : S1C mutant of Penicillin G acylase from *Kluyvera citrophila*  
Authors : Ramasamy, S.; Chand, D.; Varshney, N.K.; Brannigan, J.A.; Wilkinson, A.J.; Suresh, C.G.  
Deposited on : 2014-04-24  
Resolution : 2.80 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 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

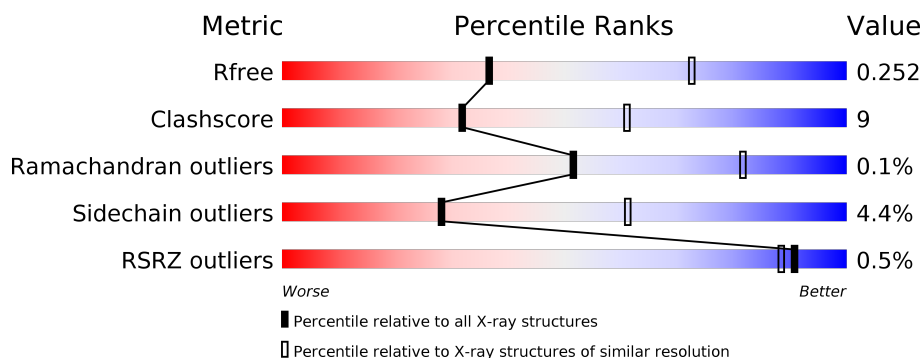
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	222	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	222	<div> <div></div> <div>76%</div> <div>10%</div> <div>•</div> <div>13%</div> </div>
1	E	222	<div> <div></div> <div>75%</div> <div>12%</div> <div></div> <div>13%</div> </div>
1	G	222	<div> <div></div> <div>74%</div> <div>13%</div> <div></div> <div>13%</div> </div>
2	B	565	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>••</div> </div> </div>
2	D	565	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>••</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	565	<div><div></div><div>82%</div><div>15%</div><div>..</div></div>
2	H	565	<div><div></div><div>80%</div><div>17%</div><div>..</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23734 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 Penicillin G acylase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			
1	C	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			
1	E	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			
1	G	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	LEU	VAL	conflict	UNP P07941
A	168	LYS	ASN	conflict	UNP P07941
A	169	GLN	ASP	conflict	UNP P07941
A	170	GLN	GLU	conflict	UNP P07941
A	196	ALA	SER	conflict	UNP P07941
C	162	LEU	VAL	conflict	UNP P07941
C	168	LYS	ASN	conflict	UNP P07941
C	169	GLN	ASP	conflict	UNP P07941
C	170	GLN	GLU	conflict	UNP P07941
C	196	ALA	SER	conflict	UNP P07941
E	162	LEU	VAL	conflict	UNP P07941
E	168	LYS	ASN	conflict	UNP P07941
E	169	GLN	ASP	conflict	UNP P07941
E	170	GLN	GLU	conflict	UNP P07941
E	196	ALA	SER	conflict	UNP P07941
G	162	LEU	VAL	conflict	UNP P07941
G	168	LYS	ASN	conflict	UNP P07941
G	169	GLN	ASP	conflict	UNP P07941
G	170	GLN	GLU	conflict	UNP P07941
G	196	ALA	SER	conflict	UNP P07941

- Molecule 2 is a protein called Penicillin G acylase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			
2	D	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			
2	F	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			
2	H	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	CYS	SER	engineered mutation	UNP P07941
B	123	HIS	ASP	conflict	UNP P07941
B	132	ALA	ARG	conflict	UNP P07941
B	144	ASP	ALA	conflict	UNP P07941
B	211	GLY	-	insertion	UNP P07941
B	212	THR	ASP	conflict	UNP P07941
B	270	THR	ILE	conflict	UNP P07941
B	291	ARG	LEU	conflict	UNP P07941
B	295	ASN	-	insertion	UNP P07941
B	419	GLN	GLU	conflict	UNP P07941
B	526	ILE	LYS	conflict	UNP P07941
B	558	LEU	-	expression tag	UNP P07941
B	559	GLU	-	expression tag	UNP P07941
B	560	HIS	-	expression tag	UNP P07941
B	561	HIS	-	expression tag	UNP P07941
B	562	HIS	-	expression tag	UNP P07941
B	563	HIS	-	expression tag	UNP P07941
B	564	HIS	-	expression tag	UNP P07941
B	565	HIS	-	expression tag	UNP P07941
D	1	CYS	SER	engineered mutation	UNP P07941
D	123	HIS	ASP	conflict	UNP P07941
D	132	ALA	ARG	conflict	UNP P07941
D	144	ASP	ALA	conflict	UNP P07941
D	211	GLY	-	insertion	UNP P07941
D	212	THR	ASP	conflict	UNP P07941
D	270	THR	ILE	conflict	UNP P07941
D	291	ARG	LEU	conflict	UNP P07941
D	295	ASN	-	insertion	UNP P07941
D	419	GLN	GLU	conflict	UNP P07941
D	526	ILE	LYS	conflict	UNP P07941

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	558	LEU	-	expression tag	UNP P07941
D	559	GLU	-	expression tag	UNP P07941
D	560	HIS	-	expression tag	UNP P07941
D	561	HIS	-	expression tag	UNP P07941
D	562	HIS	-	expression tag	UNP P07941
D	563	HIS	-	expression tag	UNP P07941
D	564	HIS	-	expression tag	UNP P07941
D	565	HIS	-	expression tag	UNP P07941
F	1	CYS	SER	engineered mutation	UNP P07941
F	123	HIS	ASP	conflict	UNP P07941
F	132	ALA	ARG	conflict	UNP P07941
F	144	ASP	ALA	conflict	UNP P07941
F	211	GLY	-	insertion	UNP P07941
F	212	THR	ASP	conflict	UNP P07941
F	270	THR	ILE	conflict	UNP P07941
F	291	ARG	LEU	conflict	UNP P07941
F	295	ASN	-	insertion	UNP P07941
F	419	GLN	GLU	conflict	UNP P07941
F	526	ILE	LYS	conflict	UNP P07941
F	558	LEU	-	expression tag	UNP P07941
F	559	GLU	-	expression tag	UNP P07941
F	560	HIS	-	expression tag	UNP P07941
F	561	HIS	-	expression tag	UNP P07941
F	562	HIS	-	expression tag	UNP P07941
F	563	HIS	-	expression tag	UNP P07941
F	564	HIS	-	expression tag	UNP P07941
F	565	HIS	-	expression tag	UNP P07941
H	1	CYS	SER	engineered mutation	UNP P07941
H	123	HIS	ASP	conflict	UNP P07941
H	132	ALA	ARG	conflict	UNP P07941
H	144	ASP	ALA	conflict	UNP P07941
H	211	GLY	-	insertion	UNP P07941
H	212	THR	ASP	conflict	UNP P07941
H	270	THR	ILE	conflict	UNP P07941
H	291	ARG	LEU	conflict	UNP P07941
H	295	ASN	-	insertion	UNP P07941
H	419	GLN	GLU	conflict	UNP P07941
H	526	ILE	LYS	conflict	UNP P07941
H	558	LEU	-	expression tag	UNP P07941
H	559	GLU	-	expression tag	UNP P07941
H	560	HIS	-	expression tag	UNP P07941
H	561	HIS	-	expression tag	UNP P07941

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	562	HIS	-	expression tag	UNP P07941
H	563	HIS	-	expression tag	UNP P07941
H	564	HIS	-	expression tag	UNP P07941
H	565	HIS	-	expression tag	UNP P07941

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0

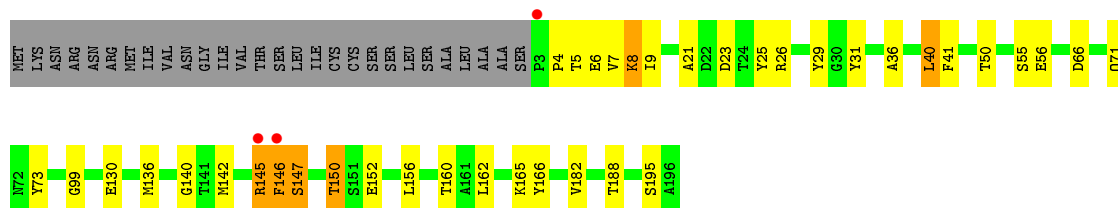
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	9	Total O 9 9	0	0
4	C	1	Total O 1 1	0	0
4	D	3	Total O 3 3	0	0
4	F	7	Total O 7 7	0	0
4	G	1	Total O 1 1	0	0
4	H	11	Total O 11 11	0	0

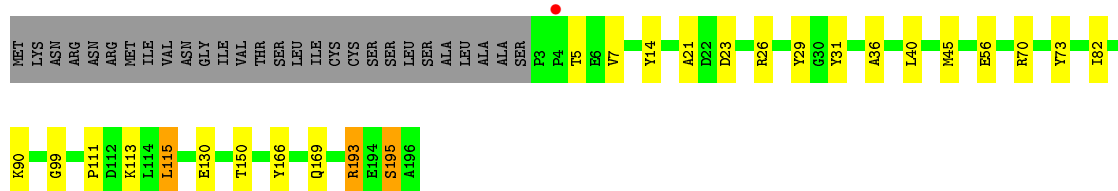
### 3 Residue-property plots

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.

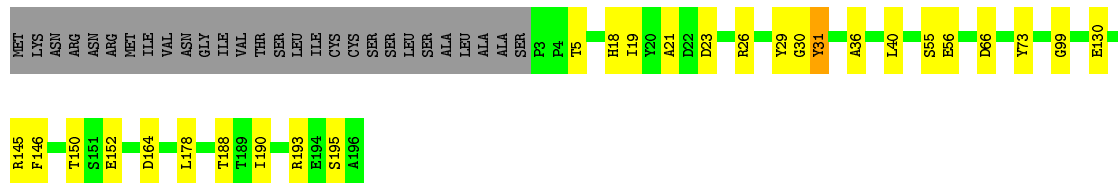
- Molecule 1: Penicillin G acylase subunit alpha



- Molecule 1: Penicillin G acylase subunit alpha



- Molecule 1: Penicillin G acylase subunit alpha



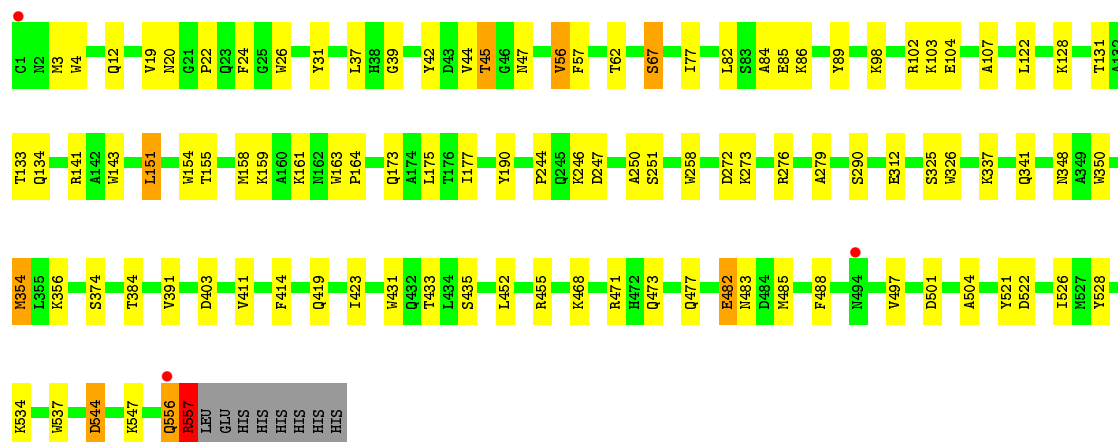
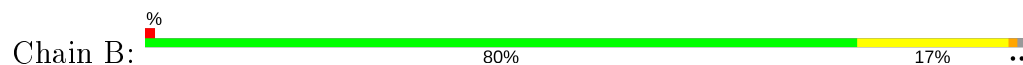
- Molecule 1: Penicillin G acylase subunit alpha



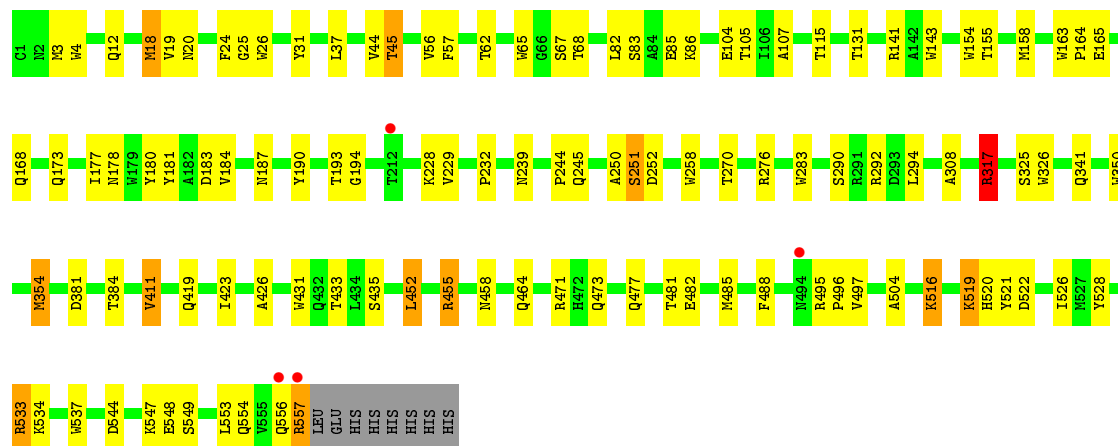
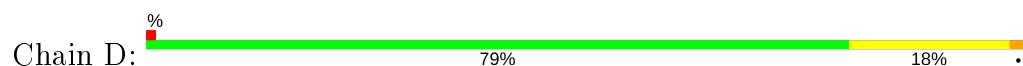




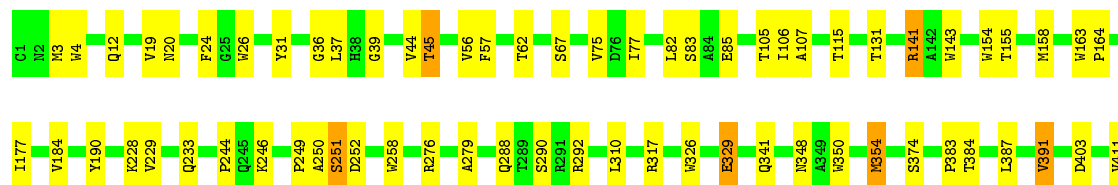
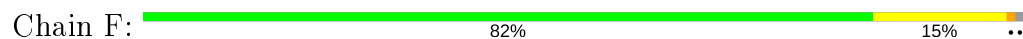
• Molecule 2: Penicillin G acylase subunit beta



• Molecule 2: Penicillin G acylase subunit beta

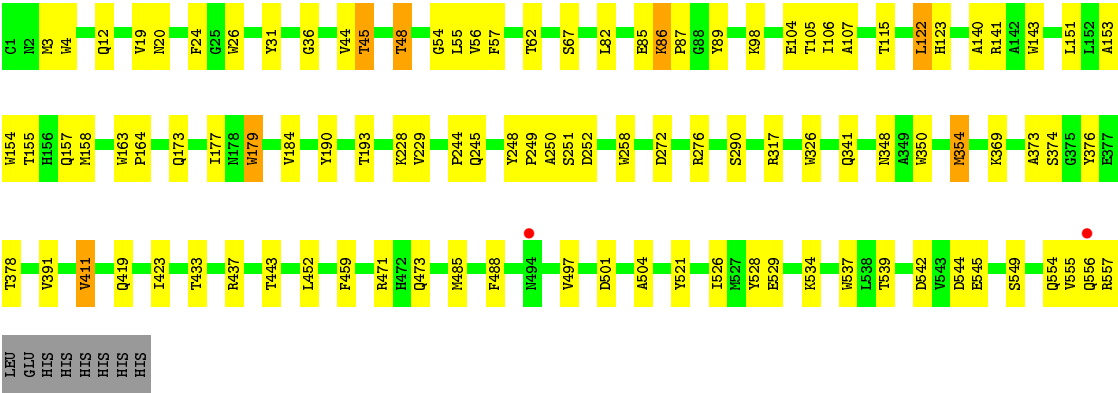
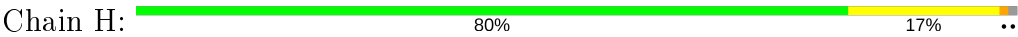


• Molecule 2: Penicillin G acylase subunit beta





● Molecule 2: Penicillin G acylase subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.26 Å 96.26 Å 100.21 Å 69.27° 69.27° 76.77°	Depositor
Resolution (Å)	38.24 – 2.80 38.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.4 (38.24-2.80) 88.4 (38.21-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.214 , 0.251 0.216 , 0.252	Depositor DCC
$R_{free}$ test set	3420 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 24.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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 ⓘ

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

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	0.64	2/1584 (0.1%)	0.76	2/2146 (0.1%)
1	C	0.48	0/1584	0.67	0/2146
1	E	0.51	0/1584	0.72	1/2146 (0.0%)
1	G	0.51	0/1584	0.72	2/2146 (0.1%)
2	B	0.54	1/4507 (0.0%)	0.73	1/6147 (0.0%)
2	D	0.52	0/4507	0.73	5/6147 (0.1%)
2	F	0.52	0/4507	0.70	3/6147 (0.0%)
2	H	0.52	1/4507 (0.0%)	0.72	2/6147 (0.0%)
All	All	0.53	4/24364 (0.0%)	0.72	16/33172 (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	A	0	1
2	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	LYS	C-N	-11.42	1.07	1.34
1	A	9	ILE	C-N	-7.28	1.17	1.34
2	H	179	TRP	CB-CG	-7.16	1.37	1.50
2	B	557	ARG	CA-C	6.31	1.69	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	557	ARG	N-CA-C	9.25	135.97	111.00
1	G	145	ARG	CB-CA-C	-7.47	95.47	110.40
1	A	40	LEU	N-CA-C	-6.83	92.56	111.00
1	E	164	ASP	CB-CA-C	6.69	123.78	110.40
2	D	354	MET	CG-SD-CE	6.52	110.62	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	LYS	Mainchain
2	B	556	GLN	Mainchain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1545	0	1505	36	0
1	C	1545	0	1507	30	0
1	E	1545	0	1507	23	0
1	G	1545	0	1507	52	1
2	B	4379	0	4198	77	1
2	D	4379	0	4198	107	0
2	F	4379	0	4198	62	0
2	H	4379	0	4198	95	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	2	0	0	0	0
4	B	9	0	0	1	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
4	F	7	0	0	0	0
4	G	1	0	0	0	0
4	H	11	0	0	1	0
All	All	23734	0	22818	414	1

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.

The worst 5 of 414 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:G:107:VAL:HG13	1:G:114:LEU:O	1.12	1.28
1:A:145:ARG:HG2	1:A:146:PHE:N	1.55	1.18
1:G:107:VAL:HA	1:G:114:LEU:HB3	1.18	1.17
1:G:107:VAL:CG1	1:G:114:LEU:O	1.93	1.16
1:G:106:LYS:O	1:G:114:LEU:HD12	1.44	1.16

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:LYS:NZ	1:G:108:ASN:O[1_565]	1.90	0.30

## 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	192/222 (86%)	184 (96%)	8 (4%)	0	100	100
1	C	192/222 (86%)	186 (97%)	6 (3%)	0	100	100
1	E	192/222 (86%)	187 (97%)	5 (3%)	0	100	100
1	G	192/222 (86%)	184 (96%)	8 (4%)	0	100	100
2	B	555/565 (98%)	537 (97%)	18 (3%)	0	100	100
2	D	555/565 (98%)	533 (96%)	21 (4%)	1 (0%)	47	78
2	F	555/565 (98%)	538 (97%)	16 (3%)	1 (0%)	47	78
2	H	555/565 (98%)	535 (96%)	19 (3%)	1 (0%)	47	78
All	All	2988/3148 (95%)	2884 (96%)	101 (3%)	3 (0%)	51	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	251	SER
2	D	251	SER
2	F	251	SER

### 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	164/188 (87%)	155 (94%)	9 (6%)	21	52
1	C	164/188 (87%)	156 (95%)	8 (5%)	25	57
1	E	164/188 (87%)	159 (97%)	5 (3%)	41	75
1	G	164/188 (87%)	159 (97%)	5 (3%)	41	75
2	B	449/457 (98%)	425 (95%)	24 (5%)	22	54
2	D	449/457 (98%)	428 (95%)	21 (5%)	26	59
2	F	449/457 (98%)	429 (96%)	20 (4%)	27	60
2	H	449/457 (98%)	432 (96%)	17 (4%)	33	67
All	All	2452/2580 (95%)	2343 (96%)	109 (4%)	28	61

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	290	SER
2	D	557	ARG
2	H	354	MET
2	D	317	ARG
2	D	482	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	274	GLN
2	F	274	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	203	HIS
2	D	245	GLN
2	H	245	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2



All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	9:ILE	C	10:VAL	N	1.17
1	A	8:LYS	C	9:ILE	N	1.07

## 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	194/222 (87%)	-0.46	3 (1%) 73 68	26, 47, 78, 114	0
1	C	194/222 (87%)	-0.39	1 (0%) 91 88	24, 54, 82, 98	0
1	E	194/222 (87%)	-0.58	0 100 100	26, 43, 67, 98	0
1	G	194/222 (87%)	-0.46	1 (0%) 91 88	31, 47, 68, 93	0
2	B	557/565 (98%)	-0.40	3 (0%) 91 88	23, 45, 73, 113	0
2	D	557/565 (98%)	-0.35	4 (0%) 87 84	27, 50, 79, 103	0
2	F	557/565 (98%)	-0.47	0 100 100	25, 44, 67, 93	0
2	H	557/565 (98%)	-0.42	2 (0%) 92 91	24, 45, 68, 101	0
All	All	3004/3148 (95%)	-0.43	14 (0%) 91 88	23, 46, 74, 114	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	556	GLN	4.1
1	G	114	LEU	3.6
1	A	3	PRO	3.4
2	H	556	GLN	2.7
2	B	494	ASN	2.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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. 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	CA	G	601	1/1	0.96	0.06	44,44,44,44	0
3	CA	A	601	1/1	0.98	0.09	30,30,30,30	0
3	CA	C	601	1/1	0.99	0.07	34,34,34,34	0
3	CA	E	601	1/1	0.99	0.10	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.