



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2016 – 11:23 AM GMT

PDB ID : 4YFB  
Title : Structure of N-acylhomoserine lactone acylase MacQ in complex with phenylacetic acid  
Authors : Yasutake, Y.; Kusada, H.; Kimura, N.  
Deposited on : 2015-02-25  
Resolution : 1.75 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  
<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

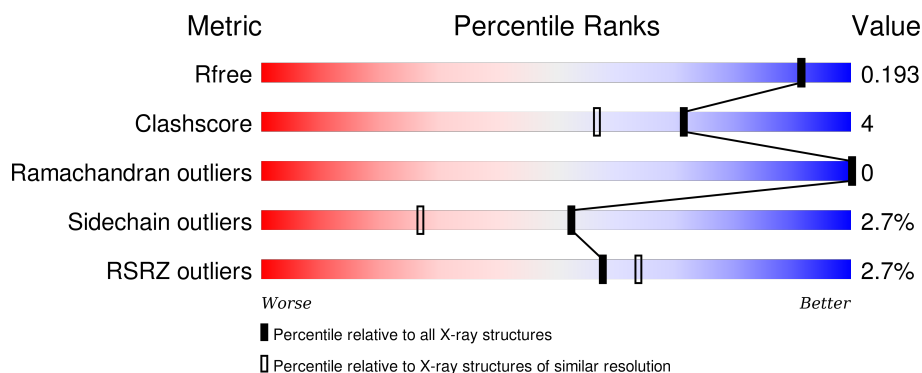
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	178	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>84%</span> <span>10% • 6%</span> </div> </div>
1	D	178	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>84%</span> <span>9% • 6%</span> </div> </div>
1	G	178	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 87%; height: 10px; background-color: green;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>87%</span> <span>8% • •</span> </div> </div>
1	J	178	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>84%</span> <span>9% • 6%</span> </div> </div>
2	B	27	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 33%; height: 10px; background-color: red;"></div> <div style="width: 41%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> <div style="width: 44%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>33%</span> <span>41%</span> <span>15%</span> <span>44%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	E	27	
2	H	27	
2	K	27	
3	C	581	
3	F	581	
3	I	581	
3	L	581	

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
4	PAC	C	601[A]	-	-	X	X
4	PAC	C	601[B]	-	-	X	X
4	PAC	F	601[A]	-	-	-	X
4	PAC	F	601[B]	-	-	X	X
4	PAC	I	601[A]	-	-	X	X
4	PAC	I	601[B]	-	-	X	X
4	PAC	L	601[A]	-	-	X	X
4	PAC	L	601[B]	-	-	X	X
5	GOL	C	602	-	-	-	X
5	GOL	F	602	-	-	-	X
5	GOL	I	602	-	-	-	X
5	GOL	L	602	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25587 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 Protein related to penicillin acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	1	0
			1301	809	244	242	6			
1	D	168	Total	C	N	O	S	0	2	0
			1307	813	244	244	6			
1	G	171	Total	C	N	O	S	0	0	0
			1311	813	247	245	6			
1	J	167	Total	C	N	O	S	0	0	0
			1289	802	243	238	6			

- Molecule 2 is a protein called Protein related to penicillin acylase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	0	0	0
			110	68	22	20			
2	E	14	Total	C	N	O	0	0	0
			106	66	21	19			
2	H	15	Total	C	N	O	0	0	0
			110	68	22	20			
2	K	16	Total	C	N	O	0	0	0
			119	73	23	23			

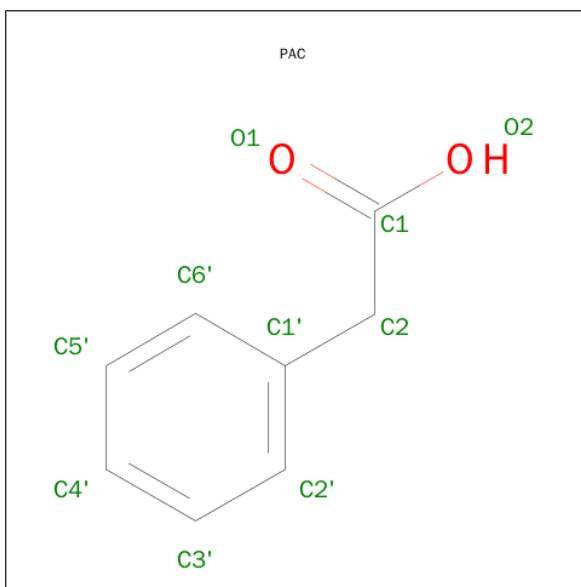
- Molecule 3 is a protein called Protein related to penicillin acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	575	Total	C	N	O	S	0	2	0
			4362	2748	763	832	19			
3	F	575	Total	C	N	O	S	0	2	0
			4362	2748	763	832	19			
3	I	575	Total	C	N	O	S	0	0	0
			4353	2739	763	832	19			
3	L	574	Total	C	N	O	S	0	1	0
			4352	2740	763	830	19			

There are 32 discrepancies between the modelled and reference sequences:

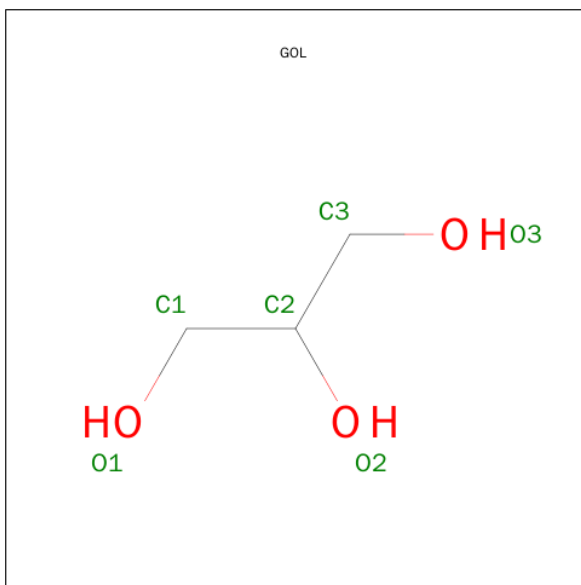
Chain	Residue	Modelled	Actual	Comment	Reference
C	574	LEU	-	expression tag	UNP A0A0A1VBK6
C	575	GLU	-	expression tag	UNP A0A0A1VBK6
C	576	HIS	-	expression tag	UNP A0A0A1VBK6
C	577	HIS	-	expression tag	UNP A0A0A1VBK6
C	578	HIS	-	expression tag	UNP A0A0A1VBK6
C	579	HIS	-	expression tag	UNP A0A0A1VBK6
C	580	HIS	-	expression tag	UNP A0A0A1VBK6
C	581	HIS	-	expression tag	UNP A0A0A1VBK6
F	574	LEU	-	expression tag	UNP A0A0A1VBK6
F	575	GLU	-	expression tag	UNP A0A0A1VBK6
F	576	HIS	-	expression tag	UNP A0A0A1VBK6
F	577	HIS	-	expression tag	UNP A0A0A1VBK6
F	578	HIS	-	expression tag	UNP A0A0A1VBK6
F	579	HIS	-	expression tag	UNP A0A0A1VBK6
F	580	HIS	-	expression tag	UNP A0A0A1VBK6
F	581	HIS	-	expression tag	UNP A0A0A1VBK6
I	574	LEU	-	expression tag	UNP A0A0A1VBK6
I	575	GLU	-	expression tag	UNP A0A0A1VBK6
I	576	HIS	-	expression tag	UNP A0A0A1VBK6
I	577	HIS	-	expression tag	UNP A0A0A1VBK6
I	578	HIS	-	expression tag	UNP A0A0A1VBK6
I	579	HIS	-	expression tag	UNP A0A0A1VBK6
I	580	HIS	-	expression tag	UNP A0A0A1VBK6
I	581	HIS	-	expression tag	UNP A0A0A1VBK6
L	574	LEU	-	expression tag	UNP A0A0A1VBK6
L	575	GLU	-	expression tag	UNP A0A0A1VBK6
L	576	HIS	-	expression tag	UNP A0A0A1VBK6
L	577	HIS	-	expression tag	UNP A0A0A1VBK6
L	578	HIS	-	expression tag	UNP A0A0A1VBK6
L	579	HIS	-	expression tag	UNP A0A0A1VBK6
L	580	HIS	-	expression tag	UNP A0A0A1VBK6
L	581	HIS	-	expression tag	UNP A0A0A1VBK6

- Molecule 4 is 2-PHENYLACETIC ACID (three-letter code: PAC) (formula:  $C_8H_8O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	1
			20	16	4		
4	F	1	Total	C	O	0	1
			20	16	4		
4	I	1	Total	C	O	0	1
			20	16	4		
4	L	1	Total	C	O	0	1
			20	16	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	L	1	Total C O 6 3 3	0	0

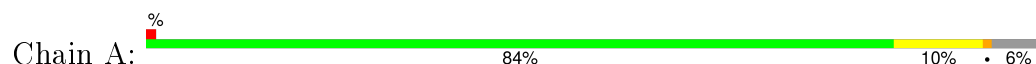
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	148	Total O 148 148	0	0
6	B	3	Total O 3 3	0	0
6	C	506	Total O 506 506	0	0
6	D	137	Total O 137 137	0	0
6	E	3	Total O 3 3	0	0
6	F	449	Total O 449 449	0	0
6	G	127	Total O 127 127	0	0
6	H	9	Total O 9 9	0	0
6	I	404	Total O 404 404	0	0
6	J	140	Total O 140 140	0	0
6	K	7	Total O 7 7	0	0
6	L	468	Total O 468 468	0	0

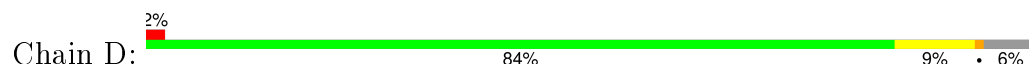
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

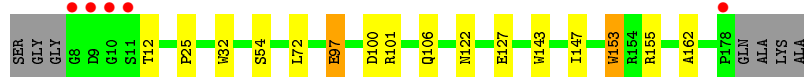
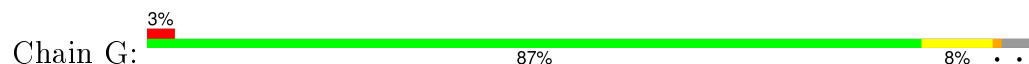
- Molecule 1: Protein related to penicillin acylase



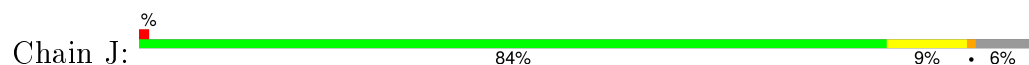
- Molecule 1: Protein related to penicillin acylase



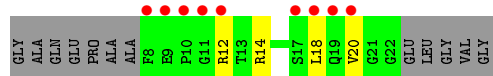
- Molecule 1: Protein related to penicillin acylase



- Molecule 1: Protein related to penicillin acylase

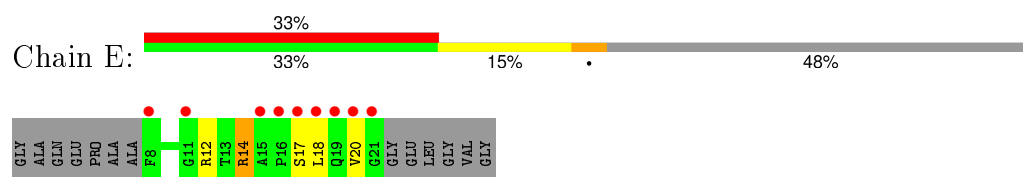


- Molecule 2: Protein related to penicillin acylase

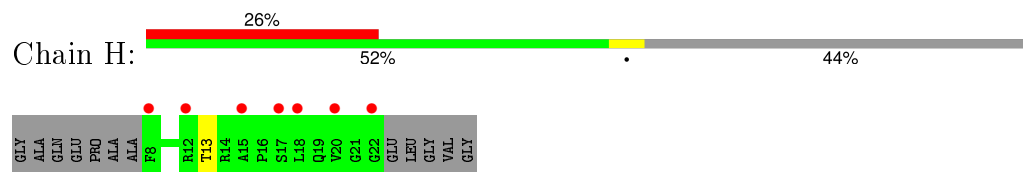


- Molecule 2: Protein related to penicillin acylase

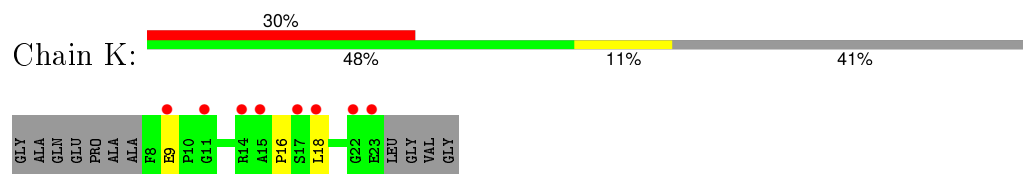




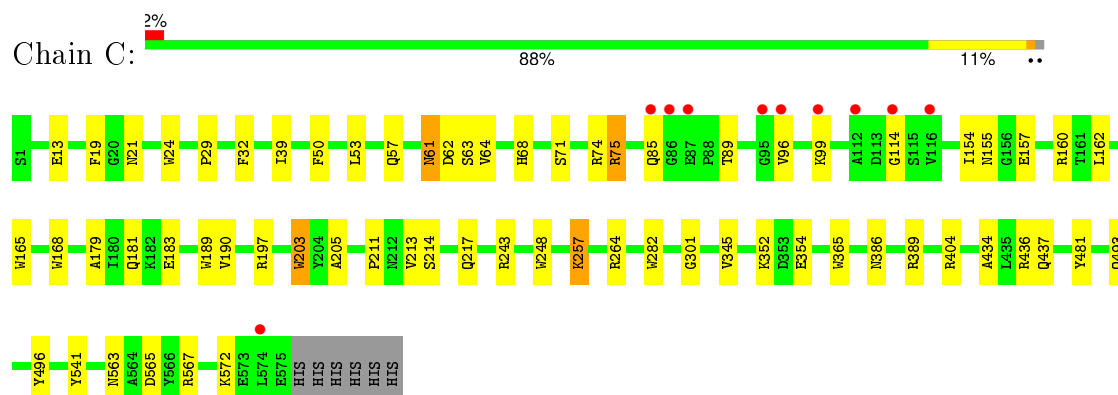
- Molecule 2: Protein related to penicillin acylase



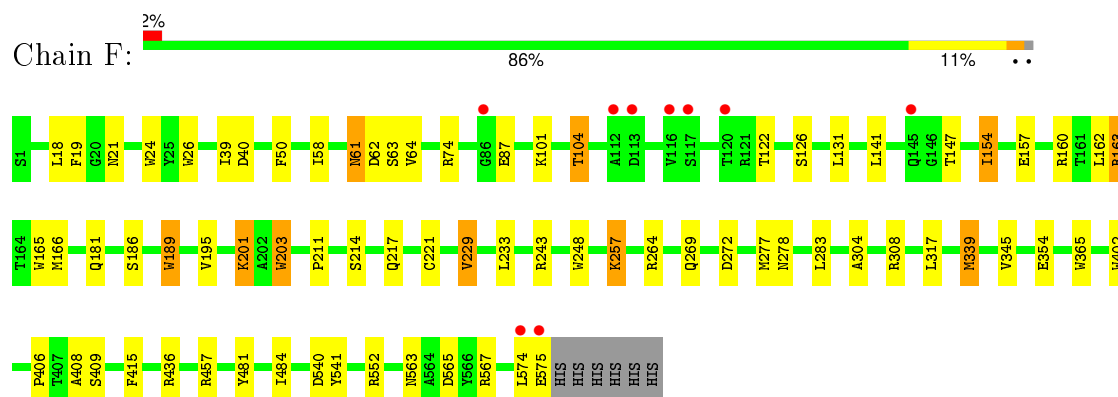
- Molecule 2: Protein related to penicillin acylase



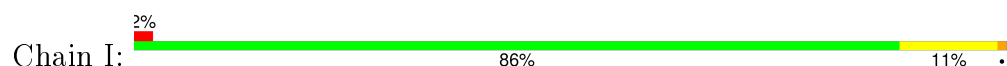
- Molecule 3: Protein related to penicillin acylase

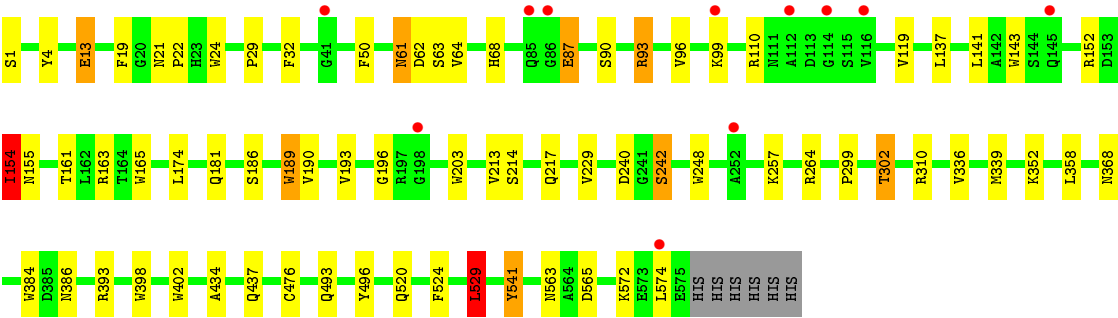


- Molecule 3: Protein related to penicillin acylase

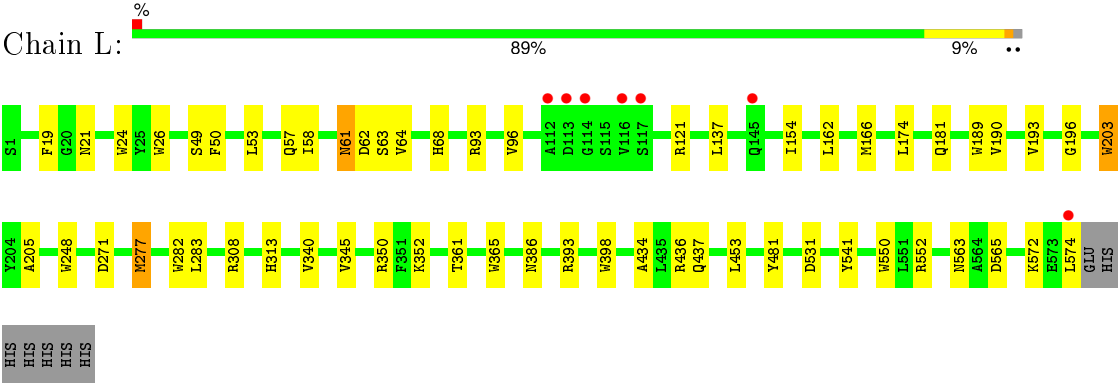


- Molecule 3: Protein related to penicillin acylase





● Molecule 3: Protein related to penicillin acylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.47Å 139.03Å 122.00Å 90.00° 111.06° 90.00°	Depositor
Resolution (Å)	25.14 – 1.75 25.14 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.14-1.75) 99.9 (25.14-1.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.29 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.161 , 0.193 0.160 , 0.193	Depositor DCC
$R_{free}$ test set	16060 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 319403 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	25587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.74% 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: GOL, PAC

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	1.09	1/1335 (0.1%)	0.98	1/1808 (0.1%)
1	D	1.09	2/1344 (0.1%)	1.03	6/1820 (0.3%)
1	G	1.03	4/1342 (0.3%)	0.92	1/1817 (0.1%)
1	J	1.13	3/1320 (0.2%)	1.07	5/1788 (0.3%)
2	B	0.82	0/112	0.97	0/150
2	E	0.98	0/108	0.85	0/145
2	H	1.01	0/112	0.83	0/150
2	K	0.83	0/121	0.91	0/162
3	C	1.10	8/4482 (0.2%)	1.05	13/6115 (0.2%)
3	F	1.14	11/4482 (0.2%)	1.08	19/6115 (0.3%)
3	I	1.06	9/4467 (0.2%)	0.97	14/6094 (0.2%)
3	L	1.12	9/4466 (0.2%)	1.03	13/6093 (0.2%)
All	All	1.10	47/23691 (0.2%)	1.02	72/32257 (0.2%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	TRP	CD2-CE2	7.74	1.50	1.41
3	L	398	TRP	CD2-CE2	7.68	1.50	1.41
3	L	282	TRP	CD2-CE2	7.67	1.50	1.41
3	F	24	TRP	CD2-CE2	7.50	1.50	1.41
3	F	26	TRP	CD2-CE2	7.43	1.50	1.41
3	F	203	TRP	CD2-CE2	7.03	1.49	1.41
3	L	203	TRP	CD2-CE2	6.92	1.49	1.41
3	F	165	TRP	CD2-CE2	6.79	1.49	1.41
3	L	550	TRP	CD2-CE2	6.62	1.49	1.41
1	G	32	TRP	CD2-CE2	6.59	1.49	1.41
3	I	165	TRP	CD2-CE2	6.57	1.49	1.41
1	G	153	TRP	CD2-CE2	6.36	1.49	1.41
3	F	402	TRP	CD2-CE2	6.32	1.49	1.41
3	L	24	TRP	CD2-CE2	6.30	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	248	TRP	CD2-CE2	6.17	1.48	1.41
1	G	143	TRP	CD2-CE2	6.14	1.48	1.41
3	F	126	SER	CB-OG	6.12	1.50	1.42
3	I	402	TRP	CD2-CE2	6.08	1.48	1.41
3	I	143	TRP	CD2-CE2	6.03	1.48	1.41
3	C	165	TRP	CD2-CE2	5.92	1.48	1.41
3	I	4	TYR	CG-CD2	5.82	1.46	1.39
3	C	354	GLU	CD-OE2	-5.67	1.19	1.25
3	F	186	SER	CB-OG	5.64	1.49	1.42
3	I	24	TRP	CD2-CE2	5.62	1.48	1.41
1	D	32	TRP	CD2-CE2	5.56	1.48	1.41
3	C	168	TRP	CD2-CE2	5.54	1.48	1.41
3	I	189	TRP	CD2-CE2	5.48	1.48	1.41
3	L	248	TRP	CD2-CE2	5.45	1.47	1.41
3	C	203	TRP	CD2-CE2	5.43	1.47	1.41
3	F	40	ASP	CB-CG	5.39	1.63	1.51
3	L	26	TRP	CD2-CE2	5.38	1.47	1.41
3	C	365	TRP	CD2-CE2	5.34	1.47	1.41
1	J	76	SER	CB-OG	5.34	1.49	1.42
3	F	189	TRP	CD2-CE2	5.34	1.47	1.41
3	F	365	TRP	CD2-CE2	5.34	1.47	1.41
3	I	398	TRP	CD2-CE2	5.25	1.47	1.41
3	C	189	TRP	CD2-CE2	5.23	1.47	1.41
1	J	153	TRP	CD2-CE2	5.22	1.47	1.41
3	F	354	GLU	CD-OE2	-5.17	1.20	1.25
3	L	365	TRP	CD2-CE2	5.16	1.47	1.41
1	J	58	TYR	CG-CD2	5.15	1.45	1.39
3	L	282	TRP	CG-CD1	5.14	1.44	1.36
1	G	127	GLU	CD-OE2	5.10	1.31	1.25
3	C	282	TRP	CD2-CE2	5.09	1.47	1.41
3	C	24	TRP	CD2-CE2	5.06	1.47	1.41
3	I	384	TRP	CD2-CE2	5.01	1.47	1.41
1	D	41	TYR	CE1-CZ	5.00	1.45	1.38

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	339	MET	CG-SD-CE	-13.16	79.15	100.20
3	C	404	ARG	NE-CZ-NH2	9.07	124.84	120.30
3	I	264	ARG	NE-CZ-NH2	8.91	124.75	120.30
3	F	567	ARG	NE-CZ-NH2	8.66	124.63	120.30
3	C	62	ASP	CB-CG-OD1	8.46	125.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	404	ARG	NE-CZ-NH1	-8.21	116.20	120.30
1	J	82	ARG	NE-CZ-NH2	8.19	124.39	120.30
1	J	154	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	J	123	ARG	NE-CZ-NH2	-7.66	116.47	120.30
3	I	264	ARG	NE-CZ-NH1	-7.43	116.59	120.30
3	F	264	ARG	NE-CZ-NH2	-7.41	116.59	120.30
3	F	163	ARG	NE-CZ-NH2	-7.37	116.62	120.30
3	L	271	ASP	CB-CG-OD1	-7.29	111.74	118.30
3	L	62	ASP	CB-CG-OD1	7.24	124.81	118.30
3	I	393	ARG	NE-CZ-NH2	-7.13	116.73	120.30
3	C	436	ARG	NE-CZ-NH1	-7.11	116.75	120.30
3	F	272	ASP	CB-CG-OD1	7.07	124.66	118.30
3	F	436	ARG	NE-CZ-NH1	-6.91	116.85	120.30
3	L	393	ARG	NE-CZ-NH2	-6.82	116.89	120.30
3	F	540	ASP	CB-CG-OD1	6.73	124.35	118.30
1	D	154	ARG	NE-CZ-NH2	-6.67	116.97	120.30
3	F	243	ARG	NE-CZ-NH1	-6.54	117.03	120.30
3	C	75	ARG	NE-CZ-NH1	6.45	123.53	120.30
3	L	121	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	J	19	ARG	NE-CZ-NH1	-6.44	117.08	120.30
3	L	308	ARG	NE-CZ-NH2	-6.34	117.13	120.30
3	F	552	ARG	NE-CZ-NH2	6.27	123.44	120.30
3	I	62	ASP	CB-CG-OD1	6.26	123.94	118.30
3	L	436	ARG	NE-CZ-NH1	-6.23	117.18	120.30
3	F	160	ARG	NE-CZ-NH2	6.21	123.40	120.30
3	L	93	ARG	NE-CZ-NH2	-6.19	117.20	120.30
3	L	350	ARG	NE-CZ-NH2	-6.04	117.28	120.30
3	C	567	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	D	28	LYS	CD-CE-NZ	-5.96	97.99	111.70
3	F	540	ASP	CB-CG-OD2	-5.92	112.97	118.30
3	C	264	ARG	NE-CZ-NH2	-5.92	117.34	120.30
3	L	436	ARG	NE-CZ-NH2	5.89	123.24	120.30
3	I	154	ILE	CG1-CB-CG2	5.88	124.35	111.40
3	C	243	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	I	529	LEU	CB-CG-CD2	5.79	120.85	111.00
1	G	100	ASP	CB-CG-OD1	5.76	123.48	118.30
3	I	163	ARG	NE-CZ-NH2	-5.74	117.43	120.30
3	C	75	ARG	NE-CZ-NH2	-5.66	117.47	120.30
3	F	163	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	82	ARG	NE-CZ-NH1	-5.63	117.48	120.30
3	F	457	ARG	NE-CZ-NH1	-5.55	117.53	120.30
3	I	493	GLN	CA-CB-CG	-5.52	101.25	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	393	ARG	NE-CZ-NH1	5.52	123.06	120.30
3	F	317	LEU	CB-CG-CD1	5.50	120.35	111.00
3	F	40	ASP	CB-CG-OD1	5.48	123.23	118.30
3	F	201	LYS	CD-CE-NZ	-5.46	99.15	111.70
1	D	126	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	J	82	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	D	87	ASP	CB-CG-OD1	5.33	123.09	118.30
3	I	93	ARG	NE-CZ-NH1	5.30	122.95	120.30
3	L	453	LEU	CB-CG-CD1	-5.27	102.05	111.00
3	C	389	ARG	NE-CZ-NH2	-5.26	117.67	120.30
3	L	277	MET	CG-SD-CE	5.26	108.61	100.20
3	L	531	ASP	CB-CG-OD1	5.24	123.01	118.30
3	C	197	ARG	NE-CZ-NH2	5.23	122.92	120.30
3	I	110	ARG	NE-CZ-NH1	-5.22	117.69	120.30
3	I	93	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	I	310	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	C	160	ARG	NE-CZ-NH1	-5.19	117.70	120.30
3	F	457	ARG	NE-CZ-NH2	5.19	122.90	120.30
3	F	339	MET	CB-CG-SD	-5.19	96.83	112.40
1	D	155	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	C	436	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	D	82	ARG	NE-CZ-NH2	5.09	122.84	120.30
3	I	152	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	F	62	ASP	CB-CG-OD1	5.04	122.84	118.30
3	L	552	ARG	NE-CZ-NH1	-5.03	117.79	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	1301	0	1239	12	0
1	D	1307	0	1245	9	0
1	G	1311	0	1243	8	0
1	J	1289	0	1228	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	110	0	108	4	0
2	E	106	0	105	7	0
2	H	110	0	108	1	0
2	K	119	0	114	1	0
3	C	4362	0	4181	44	0
3	F	4362	0	4181	41	0
3	I	4353	0	4161	46	0
3	L	4352	0	4165	36	0
4	C	20	0	14	11	0
4	F	20	0	14	7	0
4	I	20	0	14	11	0
4	L	20	0	14	10	0
5	C	6	0	8	1	0
5	F	6	0	8	1	0
5	I	6	0	8	2	0
5	L	6	0	8	0	0
6	A	148	0	0	0	0
6	B	3	0	0	0	0
6	C	506	0	0	2	0
6	D	137	0	0	0	0
6	E	3	0	0	1	0
6	F	449	0	0	3	0
6	G	127	0	0	0	0
6	H	9	0	0	0	0
6	I	404	0	0	5	0
6	J	140	0	0	2	0
6	K	7	0	0	0	0
6	L	468	0	0	1	0
All	All	25587	0	22166	196	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 4.

All (196) 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)
4:I:601[A]:PAC:C2'	4:I:601[A]:PAC:O2	1.83	1.20
4:L:601[A]:PAC:H2'	4:L:601[A]:PAC:O2	1.36	1.15
4:C:601[A]:PAC:C6'	4:C:601[A]:PAC:O2	1.80	1.13
4:C:601[A]:PAC:H6'	4:C:601[A]:PAC:O2	1.26	1.02
3:F:50:PHE:CE1	4:F:601[A]:PAC:H3'	1.95	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:17:SER:HB2	6:E:102:HOH:O	1.62	0.97
4:I:601[A]:PAC:H2'	4:I:601[A]:PAC:O2	1.16	0.96
1:J:122:ASN:HD21	1:J:147:ILE:H	1.14	0.96
1:J:12:THR:HG21	3:L:574:LEU:HD23	1.50	0.94
4:L:601[A]:PAC:C2'	4:L:601[A]:PAC:O2	2.10	0.93
3:I:190:VAL:HG11	4:I:601[B]:PAC:H2'	1.52	0.91
1:D:122:ASN:HD21	1:D:147:ILE:H	1.22	0.87
1:G:122:ASN:HD21	1:G:147:ILE:H	1.18	0.86
3:I:50:PHE:CZ	4:I:601[A]:PAC:H5'	2.12	0.84
3:I:50:PHE:CE1	4:I:601[A]:PAC:H5'	2.13	0.83
1:A:122:ASN:HD21	1:A:147:ILE:H	1.22	0.82
3:F:50:PHE:HE1	4:F:601[A]:PAC:H3'	1.45	0.81
3:L:50:PHE:CE1	4:L:601[A]:PAC:H5'	2.16	0.80
3:I:13:GLU:HG2	6:I:1016:HOH:O	1.78	0.80
3:L:50:PHE:H	3:L:57:GLN:HE22	1.28	0.80
3:C:61:ASN:HD22	3:C:63:SER:H	1.28	0.78
3:C:68:HIS:HB2	4:C:601[A]:PAC:H5'	1.66	0.77
1:J:12:THR:CG2	3:L:574:LEU:HD23	2.14	0.77
3:L:50:PHE:H	3:L:57:GLN:NE2	1.82	0.77
3:F:189:TRP:CH2	4:F:601[B]:PAC:H2'	2.20	0.76
6:C:895:HOH:O	3:I:302:THR:HG21	1.86	0.75
3:I:61:ASN:HD22	3:I:63:SER:H	1.35	0.74
3:C:257:LYS:N	3:C:257:LYS:HD2	2.01	0.74
3:L:58:ILE:HD11	4:L:601[B]:PAC:H2'	1.68	0.73
5:F:602:GOL:H31	6:F:794:HOH:O	1.88	0.73
3:C:50:PHE:CZ	4:C:601[A]:PAC:H3'	2.23	0.72
3:F:61:ASN:HD22	3:F:63:SER:H	1.37	0.72
3:L:61:ASN:HD22	3:L:63:SER:H	1.39	0.70
3:I:240:ASP:OD1	3:I:242:SER:HB2	1.94	0.67
3:I:61:ASN:ND2	3:I:63:SER:H	1.93	0.66
3:C:61:ASN:ND2	3:C:63:SER:H	1.93	0.66
1:A:101:ARG:NH1	3:C:157:GLU:OE2	2.27	0.65
3:F:61:ASN:ND2	3:F:63:SER:H	1.95	0.64
3:I:214:SER:H	3:I:217:GLN:HE21	1.44	0.64
1:A:176:GLN:HG3	2:E:12:ARG:NH1	2.13	0.64
3:F:189:TRP:HH2	4:F:601[B]:PAC:H2'	1.64	0.62
3:F:214:SER:H	3:F:217:GLN:HE21	1.48	0.62
3:I:19:PHE:CZ	3:I:21:ASN:HB2	2.35	0.61
1:G:97:GLU:OE1	1:G:101:ARG:HD2	2.00	0.61
3:L:53:LEU:HD12	3:L:57:GLN:NE2	2.16	0.61
3:L:563:ASN:ND2	3:L:565:ASP:H	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:LEU:HG	3:L:166:MET:SD	2.40	0.60
3:I:190:VAL:HG11	4:I:601[B]:PAC:C2'	2.26	0.60
3:I:32:PHE:HZ	4:I:601[B]:PAC:H6'	1.66	0.60
3:L:61:ASN:ND2	3:L:63:SER:H	2.00	0.60
3:I:336:VAL:HA	3:I:339:MET:HG2	1.84	0.59
3:F:181:GLN:NE2	3:F:203:TRP:HE1	2.00	0.59
3:L:189:TRP:CH2	4:L:601[B]:PAC:H6'	2.38	0.59
3:L:19:PHE:CZ	3:L:21:ASN:HB2	2.39	0.58
3:I:61:ASN:ND2	3:I:64:VAL:H	2.01	0.58
3:F:201:LYS:HD2	3:F:269:GLN:HB3	1.85	0.58
3:F:50:PHE:CZ	4:F:601[A]:PAC:H3'	2.39	0.58
3:L:181:GLN:NE2	3:L:203:TRP:HE1	2.01	0.57
3:F:61:ASN:C	3:F:61:ASN:HD22	2.06	0.57
3:C:114:GLY:HA3	3:F:406:PRO:HB3	1.87	0.57
3:C:301:GLY:O	3:I:302:THR:HB	2.05	0.56
3:I:352:LYS:NZ	3:I:386:ASN:HD21	2.03	0.56
1:A:110:LEU:HD13	3:C:162:LEU:HD23	1.88	0.56
3:C:190:VAL:HG11	4:C:601[B]:PAC:H6'	1.86	0.56
3:F:18:LEU:HB2	3:F:195[B]:VAL:HG22	1.86	0.56
1:G:12:THR:HG22	3:I:574:LEU:HD23	1.87	0.56
3:C:352:LYS:NZ	3:C:386:ASN:HD21	2.03	0.55
3:I:190:VAL:CG1	4:I:601[B]:PAC:H2'	2.31	0.55
2:B:18:LEU:HB3	3:C:74:ARG:HH12	1.72	0.55
3:C:214:SER:H	3:C:217:GLN:HE21	1.54	0.55
3:I:368:ASN:ND2	6:I:1034:HOH:O	2.37	0.55
3:F:563:ASN:ND2	3:F:565:ASP:H	2.06	0.54
3:C:181:GLN:NE2	3:C:203:TRP:HE1	2.06	0.54
3:I:87:GLU:HG2	3:I:90:SER:HB2	1.89	0.54
3:I:154:ILE:HD12	3:I:155:ASN:N	2.23	0.54
1:J:176:GLN:NE2	6:J:317:HOH:O	2.41	0.54
3:F:229:VAL:HG13	3:F:233:LEU:HD12	1.90	0.53
3:F:19:PHE:CZ	3:F:21:ASN:HB2	2.43	0.53
3:L:361:THR:HG23	6:L:1093:HOH:O	2.09	0.53
3:C:563:ASN:ND2	3:C:565:ASP:H	2.08	0.52
3:C:32:PHE:CZ	4:C:601[B]:PAC:H2'	2.44	0.52
2:B:18:LEU:CB	3:C:74:ARG:HH12	2.23	0.52
3:F:181:GLN:HE22	3:F:203:TRP:HE1	1.57	0.51
3:C:213:VAL:HA	3:C:217:GLN:NE2	2.26	0.51
3:L:352:LYS:NZ	3:L:386:ASN:HD21	2.08	0.51
3:L:181:GLN:HE22	3:L:203:TRP:HE1	1.58	0.50
3:F:257:LYS:H	3:F:257:LYS:HD3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ARG:NH1	3:F:157:GLU:OE2	2.32	0.50
3:C:50:PHE:HZ	4:C:601[A]:PAC:H3'	1.76	0.50
3:C:154[A]:ILE:HG23	3:C:248:TRP:CZ3	2.46	0.50
3:F:104:THR:HB	3:F:122:THR:OG1	2.12	0.49
1:G:122:ASN:ND2	1:G:147:ILE:H	1.99	0.49
1:A:106:GLN:HG3	1:A:153:TRP:CH2	2.48	0.49
1:D:122:ASN:ND2	1:D:147:ILE:H	2.01	0.49
3:L:345:VAL:HG22	3:L:481:TYR:CZ	2.48	0.48
3:C:75:ARG:O	3:C:154[A]:ILE:HG13	2.13	0.48
3:C:13:GLU:O	6:C:701:HOH:O	2.20	0.48
3:I:434:ALA:HA	3:I:437:GLN:HE21	1.78	0.48
3:I:13:GLU:CG	6:I:1016:HOH:O	2.47	0.48
3:C:179:ALA:O	3:C:183:GLU:HG3	2.13	0.48
3:I:32:PHE:CZ	4:I:601[B]:PAC:H6'	2.46	0.48
3:I:181:GLN:NE2	3:I:203:TRP:HE1	2.11	0.48
3:I:174:LEU:HB2	3:I:196:GLY:HA3	1.96	0.48
3:I:563:ASN:ND2	3:I:565:ASP:H	2.12	0.48
2:E:18:LEU:HD13	3:F:74:ARG:HH12	1.79	0.48
3:L:50:PHE:CE1	4:L:601[A]:PAC:C5'	2.95	0.47
1:J:106:GLN:HG3	1:J:153:TRP:CH2	2.50	0.47
3:L:434:ALA:HA	3:L:437:GLN:HE21	1.78	0.47
3:F:154[A]:ILE:HG23	3:F:248:TRP:HZ3	1.80	0.47
3:I:68:HIS:HB2	4:I:601[A]:PAC:H3'	1.97	0.47
3:F:339:MET:HE3	6:F:824:HOH:O	2.14	0.47
1:J:156:ILE:HD13	3:L:162:LEU:HD22	1.95	0.47
3:I:61:ASN:C	3:I:61:ASN:HD22	2.19	0.47
3:F:154[A]:ILE:HG13	3:F:211:PRO:HG3	1.97	0.47
3:I:193:VAL:HA	3:I:203:TRP:O	2.15	0.46
3:L:49:SER:HA	3:L:57:GLN:HE21	1.78	0.46
3:C:19:PHE:CZ	3:C:21:ASN:HB2	2.51	0.46
3:L:189:TRP:HH2	4:L:601[B]:PAC:H6'	1.80	0.46
3:C:53:LEU:HD12	3:C:57:GLN:OE1	2.16	0.46
3:L:61:ASN:ND2	3:L:64:VAL:H	2.13	0.46
3:I:213:VAL:HA	3:I:217:GLN:NE2	2.32	0.45
1:A:176:GLN:HE21	2:E:12:ARG:HH11	1.63	0.45
3:F:189:TRP:CH2	4:F:601[B]:PAC:C2'	2.96	0.45
3:F:345:VAL:HG22	3:F:481:TYR:CZ	2.52	0.45
1:D:110:LEU:HG	3:F:166:MET:SD	2.56	0.45
3:C:434:ALA:HA	3:C:437:GLN:HE21	1.81	0.45
3:C:496:TYR:CZ	5:C:602:GOL:H11	2.52	0.45
3:C:68:HIS:HB2	4:C:601[A]:PAC:C5'	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:58:ILE:HD11	4:F:601[B]:PAC:H6'	1.99	0.45
3:L:68:HIS:HD2	4:L:601[B]:PAC:H3'	1.83	0.44
3:C:61:ASN:C	3:C:61:ASN:HD22	2.21	0.44
1:D:60:GLY:HA2	1:D:87:ASP:HA	2.00	0.44
1:J:122:ASN:ND2	1:J:147:ILE:H	1.97	0.44
3:C:32:PHE:CE1	4:C:601[B]:PAC:H2'	2.53	0.44
2:B:12:ARG:NH1	1:D:174:ASN:OD1	2.51	0.44
3:F:61:ASN:ND2	3:F:64:VAL:H	2.15	0.44
3:L:61:ASN:HD22	3:L:61:ASN:C	2.21	0.44
3:I:213:VAL:HA	3:I:217:GLN:HE22	1.82	0.44
1:D:35:ALA:HB2	3:F:39:ILE:HG12	2.00	0.44
3:L:190:VAL:HG11	4:L:601[A]:PAC:C2'	2.48	0.44
3:I:339:MET:HE3	6:I:754:HOH:O	2.16	0.44
3:C:181:GLN:HE22	3:C:203:TRP:HE1	1.65	0.43
3:L:58:ILE:HD11	4:L:601[B]:PAC:C2'	2.45	0.43
1:J:12:THR:HG21	3:L:574:LEU:CD2	2.35	0.43
3:C:50:PHE:CE1	4:C:601[A]:PAC:H3'	2.53	0.43
3:C:61:ASN:ND2	3:C:64[B]:VAL:H	2.16	0.43
3:C:154[A]:ILE:HG12	3:C:211:PRO:HD3	1.99	0.43
1:A:35:ALA:HB2	3:C:39:ILE:HG12	2.00	0.43
3:I:476:CYS:SG	5:I:602:GOL:H32	2.59	0.43
1:G:54:SER:HB3	3:I:29:PRO:HB3	1.99	0.43
3:F:304:ALA:HA	3:F:415:PHE:CD1	2.53	0.43
3:F:217:GLN:O	3:F:221:CYS:HB2	2.18	0.43
1:G:162:ALA:HB3	3:I:189:TRP:CE2	2.54	0.43
3:F:574:LEU:O	3:F:575:GLU:HB2	2.18	0.43
3:L:174:LEU:HB2	3:L:196:GLY:HA3	2.01	0.43
3:L:203:TRP:CZ2	3:L:205:ALA:HB2	2.54	0.43
3:F:154[A]:ILE:HG23	3:F:248:TRP:CZ3	2.54	0.43
1:D:123:ARG:HD2	1:D:123:ARG:HH11	1.68	0.43
1:A:54:SER:HB3	3:C:29:PRO:HB3	2.01	0.42
3:C:203:TRP:CZ2	3:C:205:ALA:HB2	2.55	0.42
3:L:53:LEU:HD12	3:L:57:GLN:HE22	1.83	0.42
1:A:177:PRO:HG3	3:C:89:THR:CG2	2.49	0.42
3:C:61:ASN:ND2	3:C:64[A]:VAL:H	2.17	0.42
2:K:16:PRO:HD3	3:L:137:LEU:HD13	2.01	0.42
3:I:524:PHE:HA	3:I:541:TYR:CE1	2.54	0.42
2:E:18:LEU:HB3	3:F:74:ARG:HH12	1.84	0.42
3:L:193:VAL:HA	3:L:203:TRP:O	2.20	0.41
3:F:257:LYS:HD3	6:F:1079:HOH:O	2.20	0.41
3:F:101:LYS:HE3	3:F:101:LYS:HB3	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:O	1:A:160:ASN:HB2	2.20	0.41
3:L:283:LEU:O	3:L:313:HIS:CE1	2.73	0.41
3:I:520:GLN:HG2	6:I:703:HOH:O	2.20	0.41
3:F:308:ARG:HD3	3:F:484:ILE:HD11	2.03	0.41
1:J:122:ASN:ND2	1:J:146:PRO:HA	2.34	0.41
3:I:496:TYR:CG	5:I:602:GOL:H2	2.54	0.41
3:C:345:VAL:HG22	3:C:481:TYR:CZ	2.56	0.41
1:G:25:PRO:HD3	3:I:529:LEU:HD11	2.02	0.41
3:I:161:THR:HG22	3:I:186:SER:O	2.21	0.41
3:C:50:PHE:HE1	4:C:601[B]:PAC:H2'	1.86	0.41
3:I:1:SER:OG	4:I:601[A]:PAC:O1	2.34	0.41
1:A:176:GLN:HE21	2:E:12:ARG:NH1	2.18	0.41
3:F:257:LYS:N	3:F:257:LYS:HD3	2.35	0.41
3:I:1:SER:HB3	3:I:22:PRO:HA	2.02	0.41
3:C:213:VAL:HA	3:C:217:GLN:HE22	1.86	0.41
3:C:154[A]:ILE:HD12	3:C:155:ASN:N	2.35	0.41
2:H:13:THR:HA	3:I:137:LEU:O	2.21	0.41
1:J:97:GLU:HB2	6:J:297:HOH:O	2.21	0.41
3:F:408:ALA:O	3:F:409:SER:HB2	2.21	0.41
3:I:181:GLN:HE22	3:I:203:TRP:HE1	1.69	0.40
3:I:299:PRO:HB3	3:I:302:THR:HG23	2.03	0.40
2:B:18:LEU:HB3	3:C:74:ARG:NH1	2.34	0.40
1:G:106:GLN:HG3	1:G:153:TRP:CH2	2.56	0.40
1:A:82:ARG:NH2	2:E:14:ARG:HD3	2.37	0.40
3:L:19:PHE:CE1	3:L:340:VAL:HG21	2.56	0.40
1:D:19:ARG:HH21	1:D:19:ARG:HD3	1.78	0.40
3:F:277:MET:O	3:F:278:ASN:HB2	2.21	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	167/178 (94%)	160 (96%)	7 (4%)	0	100	100
1	D	168/178 (94%)	162 (96%)	6 (4%)	0	100	100
1	G	169/178 (95%)	163 (96%)	6 (4%)	0	100	100
1	J	165/178 (93%)	160 (97%)	5 (3%)	0	100	100
2	B	13/27 (48%)	13 (100%)	0	0	100	100
2	E	12/27 (44%)	10 (83%)	2 (17%)	0	100	100
2	H	13/27 (48%)	13 (100%)	0	0	100	100
2	K	14/27 (52%)	14 (100%)	0	0	100	100
3	C	575/581 (99%)	554 (96%)	21 (4%)	0	100	100
3	F	575/581 (99%)	555 (96%)	20 (4%)	0	100	100
3	I	573/581 (99%)	551 (96%)	22 (4%)	0	100	100
3	L	573/581 (99%)	554 (97%)	19 (3%)	0	100	100
All	All	3017/3144 (96%)	2909 (96%)	108 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	127/130 (98%)	122 (96%)	5 (4%)	39	14
1	D	128/130 (98%)	126 (98%)	2 (2%)	70	52
1	G	127/130 (98%)	124 (98%)	3 (2%)	57	31
1	J	125/130 (96%)	122 (98%)	3 (2%)	57	31
2	B	11/17 (65%)	9 (82%)	2 (18%)	2	0
2	E	11/17 (65%)	9 (82%)	2 (18%)	2	0
2	H	11/17 (65%)	11 (100%)	0	100	100
2	K	12/17 (71%)	10 (83%)	2 (17%)	3	0
3	C	448/452 (99%)	439 (98%)	9 (2%)	63	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	448/452 (99%)	434 (97%)	14 (3%)	47	21
3	I	446/452 (99%)	429 (96%)	17 (4%)	40	15
3	L	446/452 (99%)	439 (98%)	7 (2%)	70	52
All	All	2340/2396 (98%)	2274 (97%)	66 (3%)	52	25

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	39	PHE
1	A	72	LEU
1	A	97	GLU
1	A	155	ARG
2	B	14	ARG
2	B	20	VAL
3	C	61	ASN
3	C	71	SER
3	C	85	GLN
3	C	96	VAL
3	C	99	LYS
3	C	257	LYS
3	C	493	GLN
3	C	541	TYR
3	C	572	LYS
1	D	72	LEU
1	D	155	ARG
2	E	14	ARG
2	E	20	VAL
3	F	61	ASN
3	F	87	GLU
3	F	104	THR
3	F	131	LEU
3	F	141	LEU
3	F	147	THR
3	F	154[A]	ILE
3	F	154[B]	ILE
3	F	162	LEU
3	F	163	ARG
3	F	229	VAL
3	F	257	LYS
3	F	283	LEU

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Mol	Chain	Res	Type
3	F	541	TYR
1	G	72	LEU
1	G	97	GLU
1	G	155	ARG
3	I	13	GLU
3	I	61	ASN
3	I	87	GLU
3	I	93	ARG
3	I	96	VAL
3	I	99	LYS
3	I	119	VAL
3	I	141	LEU
3	I	154	ILE
3	I	229	VAL
3	I	242	SER
3	I	257	LYS
3	I	302	THR
3	I	358	LEU
3	I	529	LEU
3	I	541	TYR
3	I	572	LYS
1	J	72	LEU
1	J	97	GLU
1	J	155	ARG
2	K	9	GLU
2	K	18	LEU
3	L	61	ASN
3	L	96	VAL
3	L	154[A]	ILE
3	L	154[B]	ILE
3	L	277	MET
3	L	541	TYR
3	L	572	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	176	GLN
3	C	61	ASN
3	C	85	GLN
3	C	145	GLN

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Mol	Chain	Res	Type
3	C	181	GLN
3	C	217	GLN
3	C	368	ASN
3	C	376	GLN
3	C	386	ASN
3	C	437	GLN
3	C	493	GLN
3	C	563	ASN
1	D	122	ASN
3	F	61	ASN
3	F	181	GLN
3	F	217	GLN
3	F	368	ASN
3	F	386	ASN
3	F	437	GLN
3	F	563	ASN
1	G	122	ASN
3	I	61	ASN
3	I	85	GLN
3	I	181	GLN
3	I	217	GLN
3	I	368	ASN
3	I	386	ASN
3	I	437	GLN
3	I	563	ASN
1	J	122	ASN
3	L	57	GLN
3	L	61	ASN
3	L	145	GLN
3	L	181	GLN
3	L	217	GLN
3	L	368	ASN
3	L	386	ASN
3	L	437	GLN
3	L	563	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands 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$
4	PAC	C	601[A]	-	7,10,10	1.06	1 (14%)	9,12,12	2.92	5 (55%)
4	PAC	C	601[B]	-	7,10,10	0.94	0	9,12,12	3.03	3 (33%)
5	GOL	C	602	-	5,5,5	1.34	1 (20%)	5,5,5	1.96	2 (40%)
4	PAC	F	601[A]	-	7,10,10	0.63	0	9,12,12	2.26	1 (11%)
4	PAC	F	601[B]	-	7,10,10	1.27	1 (14%)	9,12,12	3.30	6 (66%)
5	GOL	F	602	-	5,5,5	1.74	1 (20%)	5,5,5	0.69	0
4	PAC	I	601[A]	-	7,10,10	0.60	0	9,12,12	2.25	3 (33%)
4	PAC	I	601[B]	-	7,10,10	1.50	2 (28%)	9,12,12	3.45	4 (44%)
5	GOL	I	602	-	5,5,5	1.25	1 (20%)	5,5,5	0.86	0
4	PAC	L	601[A]	-	7,10,10	0.59	0	9,12,12	1.84	4 (44%)
4	PAC	L	601[B]	-	7,10,10	1.21	1 (14%)	9,12,12	3.48	6 (66%)
5	GOL	L	602	-	5,5,5	0.72	0	5,5,5	1.52	1 (20%)

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
4	PAC	C	601[A]	-	-	0/2/4/4	0/1/1/1
4	PAC	C	601[B]	-	-	0/2/4/4	0/1/1/1
5	GOL	C	602	-	-	0/4/4/4	0/0/0/0
4	PAC	F	601[A]	-	-	0/2/4/4	0/1/1/1
4	PAC	F	601[B]	-	-	0/2/4/4	0/1/1/1
5	GOL	F	602	-	-	0/4/4/4	0/0/0/0
4	PAC	I	601[A]	-	-	0/2/4/4	0/1/1/1
4	PAC	I	601[B]	-	-	0/2/4/4	0/1/1/1
5	GOL	I	602	-	-	0/4/4/4	0/0/0/0
4	PAC	L	601[A]	-	-	0/2/4/4	0/1/1/1
4	PAC	L	601[B]	-	-	0/2/4/4	0/1/1/1
5	GOL	L	602	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601[A]	PAC	C2-C1'	-2.26	1.44	1.52
4	I	601[B]	PAC	C5'-C6'	2.14	1.43	1.38
4	F	601[B]	PAC	C2-C1'	2.23	1.59	1.52
5	I	602	GOL	O2-C2	2.37	1.50	1.43
4	L	601[B]	PAC	C2-C1'	2.40	1.60	1.52
4	I	601[B]	PAC	C2-C1'	2.53	1.60	1.52
5	C	602	GOL	O2-C2	2.81	1.51	1.43
5	F	602	GOL	O2-C2	3.21	1.52	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601[A]	PAC	C1-C2-C1'	-6.71	97.56	112.72
4	F	601[A]	PAC	C1-C2-C1'	-5.58	100.11	112.72
4	I	601[A]	PAC	C1-C2-C1'	-4.90	101.65	112.72
4	I	601[B]	PAC	C6'-C1'-C2'	-3.48	112.41	118.15
5	C	602	GOL	C3-C2-C1	-3.29	97.19	111.06
4	F	601[B]	PAC	C6'-C1'-C2'	-3.26	112.77	118.15
4	F	601[B]	PAC	C5'-C4'-C3'	-3.14	114.52	119.88
4	L	601[B]	PAC	C6'-C1'-C2'	-2.99	113.21	118.15
4	L	601[A]	PAC	C5'-C4'-C3'	-2.93	114.89	119.88
4	C	601[A]	PAC	C5'-C6'-C1'	-2.87	116.30	120.65
4	C	601[B]	PAC	C6'-C1'-C2'	-2.73	113.65	118.15
5	L	602	GOL	C3-C2-C1	-2.53	100.38	111.06
4	I	601[A]	PAC	C5'-C4'-C3'	-2.51	115.61	119.88
4	C	601[A]	PAC	C3'-C2'-C1'	-2.48	116.89	120.65
4	L	601[A]	PAC	C6'-C1'-C2'	-2.46	114.10	118.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	601[B]	PAC	C5'-C4'-C3'	-2.10	116.31	119.88
4	C	601[A]	PAC	C2-C1'-C6'	-2.06	114.78	120.93
4	L	601[A]	PAC	C1-C2-C1'	-2.05	108.09	112.72
4	L	601[B]	PAC	C2-C1'-C2'	2.01	126.94	120.93
4	I	601[B]	PAC	C4'-C5'-C6'	2.04	123.04	120.20
4	L	601[A]	PAC	C4'-C5'-C6'	2.17	123.22	120.20
4	F	601[B]	PAC	C2-C1'-C6'	2.18	127.47	120.93
4	L	601[B]	PAC	C4'-C3'-C2'	2.39	123.52	120.20
5	C	602	GOL	O2-C2-C3	2.44	120.18	108.47
4	C	601[B]	PAC	C5'-C6'-C1'	2.84	124.96	120.65
4	F	601[B]	PAC	C4'-C5'-C6'	2.91	124.25	120.20
4	I	601[A]	PAC	C4'-C5'-C6'	3.04	124.43	120.20
4	C	601[A]	PAC	C6'-C1'-C2'	3.11	123.29	118.15
4	L	601[B]	PAC	C5'-C6'-C1'	3.66	126.20	120.65
4	F	601[B]	PAC	C3'-C2'-C1'	3.69	126.25	120.65
4	I	601[B]	PAC	C3'-C2'-C1'	4.22	127.05	120.65
4	F	601[B]	PAC	C1-C2-C1'	6.99	128.50	112.72
4	C	601[B]	PAC	C1-C2-C1'	7.62	129.93	112.72
4	I	601[B]	PAC	C1-C2-C1'	8.00	130.78	112.72
4	L	601[B]	PAC	C1-C2-C1'	8.28	131.42	112.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601[A]	PAC	7	0
4	C	601[B]	PAC	4	0
5	C	602	GOL	1	0
4	F	601[A]	PAC	3	0
4	F	601[B]	PAC	4	0
5	F	602	GOL	1	0
4	I	601[A]	PAC	6	0
4	I	601[B]	PAC	5	0
5	I	602	GOL	2	0
4	L	601[A]	PAC	5	0
4	L	601[B]	PAC	5	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	168/178 (94%)	-0.41	2 (1%) 81 86	11, 18, 29, 44	0
1	D	168/178 (94%)	-0.41	3 (1%) 71 78	11, 18, 31, 47	0
1	G	171/178 (96%)	-0.33	5 (2%) 55 61	14, 20, 35, 54	0
1	J	167/178 (93%)	-0.49	1 (0%) 90 92	12, 17, 28, 46	0
2	B	15/27 (55%)	3.05	9 (60%) 0 0	44, 56, 61, 63	0
2	E	14/27 (51%)	2.92	9 (64%) 0 0	42, 54, 58, 60	0
2	H	15/27 (55%)	1.97	7 (46%) 0 0	31, 36, 46, 47	0
2	K	16/27 (59%)	2.20	8 (50%) 0 0	32, 43, 55, 56	0
3	C	575/581 (98%)	-0.33	10 (1%) 73 80	10, 17, 36, 58	0
3	F	575/581 (98%)	-0.29	9 (1%) 74 81	9, 18, 36, 56	0
3	I	575/581 (98%)	-0.21	11 (1%) 70 76	12, 21, 37, 54	0
3	L	574/581 (98%)	-0.35	7 (1%) 81 86	10, 18, 32, 48	0
All	All	3033/3144 (96%)	-0.27	81 (2%) 58 64	9, 19, 38, 63	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	18	LEU	7.1
3	C	86	GLY	6.7
3	L	574	LEU	6.7
3	I	112	ALA	6.4
3	F	112	ALA	5.7
3	L	112	ALA	5.6
2	B	8	PHE	5.4
1	G	8	GLY	5.2
2	B	17	SER	5.1
3	F	574	LEU	5.1
2	K	23	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
3	F	86	GLY	4.6
2	E	17	SER	4.6
3	C	574	LEU	4.5
3	C	112	ALA	4.5
2	B	11	GLY	4.4
3	C	85	GLN	4.4
2	K	17	SER	4.3
2	B	10	PRO	4.3
3	F	116	VAL	4.3
2	E	16	PRO	4.2
2	B	12	ARG	4.1
1	D	11	SER	4.1
2	B	18	LEU	4.0
3	I	85	GLN	3.9
2	E	20	VAL	3.9
1	A	11	SER	3.8
2	E	8	PHE	3.8
3	I	574	LEU	3.8
1	J	12	THR	3.7
2	E	19	GLN	3.5
2	H	18	LEU	3.4
1	G	9	ASP	3.3
2	H	17	SER	3.3
3	C	116	VAL	3.3
2	B	19	GLN	3.2
2	H	22	GLY	3.2
2	B	20	VAL	3.2
2	B	9	GLU	3.1
3	I	198	GLY	3.1
2	E	11	GLY	3.0
1	D	178	PRO	3.0
3	C	114	GLY	2.9
3	F	575	GLU	2.9
2	E	15	ALA	2.8
2	H	8	PHE	2.8
3	I	114	GLY	2.8
3	F	117	SER	2.8
3	L	117	SER	2.7
3	I	252	ALA	2.7
2	K	18	LEU	2.7
2	K	11	GLY	2.6
3	I	99	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	15	ALA	2.6
1	A	12	THR	2.6
2	K	9	GLU	2.6
3	I	116	VAL	2.6
3	I	145	GLN	2.5
3	C	87	GLU	2.5
3	C	99	LYS	2.5
2	H	20	VAL	2.4
3	L	116	VAL	2.4
3	C	96	VAL	2.3
3	L	113	ASP	2.3
2	K	22	GLY	2.3
3	C	95	GLY	2.3
1	G	178	PRO	2.3
3	L	114	GLY	2.3
3	I	86	GLY	2.3
3	L	145	GLN	2.2
3	I	41	GLY	2.2
2	K	14	ARG	2.2
2	H	12	ARG	2.2
2	K	15	ALA	2.2
3	F	113	ASP	2.2
1	G	11	SER	2.1
3	F	145	GLN	2.1
3	F	120	THR	2.1
1	D	104	ALA	2.1
1	G	10	GLY	2.0
2	E	21	GLY	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](#)

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(Å <sup>2</sup> )	Q<0.9
4	PAC	F	601[A]	10/10	0.91	0.18	7.59	14,18,21,22	10
4	PAC	F	601[B]	10/10	0.91	0.18	6.91	19,23,27,28	10
4	PAC	C	601[B]	10/10	0.92	0.18	6.30	17,19,20,20	10
4	PAC	I	601[A]	10/10	0.90	0.19	6.28	18,20,21,21	10
4	PAC	C	601[A]	10/10	0.92	0.18	6.23	13,18,19,20	10
4	PAC	I	601[B]	10/10	0.90	0.19	6.10	15,22,25,26	10
5	GOL	F	602	6/6	0.87	0.17	5.17	14,25,33,42	0
4	PAC	L	601[A]	10/10	0.91	0.15	4.04	16,22,25,26	10
5	GOL	L	602	6/6	0.94	0.14	3.94	16,26,27,29	0
4	PAC	L	601[B]	10/10	0.91	0.15	3.90	17,22,25,28	10
5	GOL	I	602	6/6	0.90	0.14	3.88	16,26,29,30	0
5	GOL	C	602	6/6	0.89	0.14	2.45	15,28,30,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.