



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:04 AM UTC

PDB ID : 4YFB / pdb\_00004yfb  
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 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)

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<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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

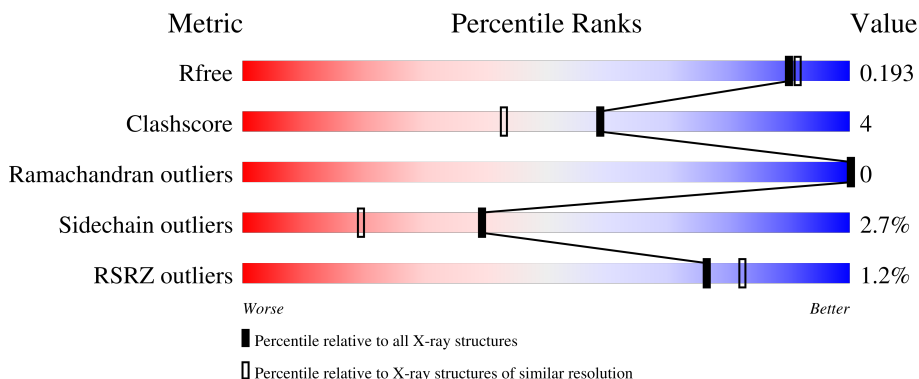
# 1 Overall quality at a glance

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))
$R_{free}$	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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	178	 81% 13% 6%
1	D	178	 86% 8% 6%
1	G	178	 89% 7% . .
1	J	178	 84% 9% . 6%
2	B	27	 37% 41% 15% 44%

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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	-
4	PAC	F	601[B]	-	X	X	-
4	PAC	I	601[A]	-	-	X	-
4	PAC	I	601[B]	-	X	X	-
4	PAC	L	601[A]	-	-	X	-
4	PAC	L	601[B]	-	X	X	-

## 2 Entry composition [i](#)

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

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

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

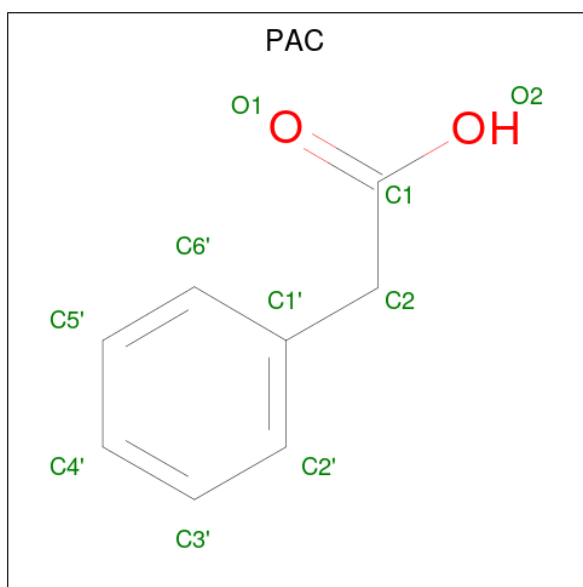
- Molecule 3 is a protein called Protein related to penicillin acylase.

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

There are 32 discrepancies between the modelled and reference sequences:

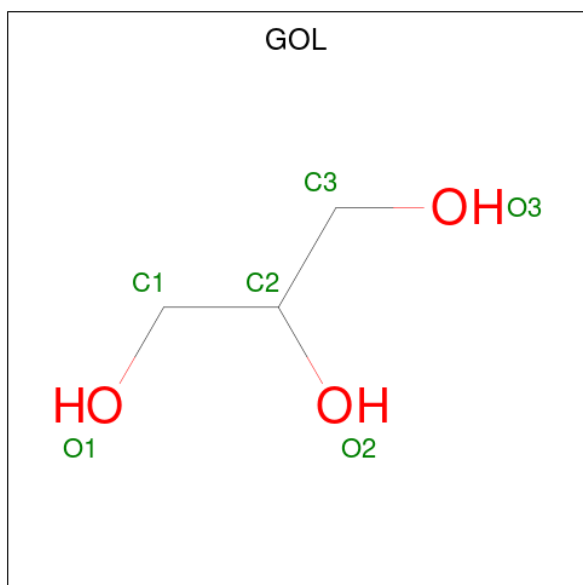
Chain	Residue	Modelled	Actual	Comment	Reference
C	574	LEU	-	expression tag	UNP A0A0A1VBK6
C	575	GLU	-	expression tag	UNP A0A0A1VBK6
C	576	HIS	-	expression tag	UNP A0A0A1VBK6
C	577	HIS	-	expression tag	UNP A0A0A1VBK6
C	578	HIS	-	expression tag	UNP A0A0A1VBK6
C	579	HIS	-	expression tag	UNP A0A0A1VBK6
C	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 (CCD ID: 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 (CCD ID: 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

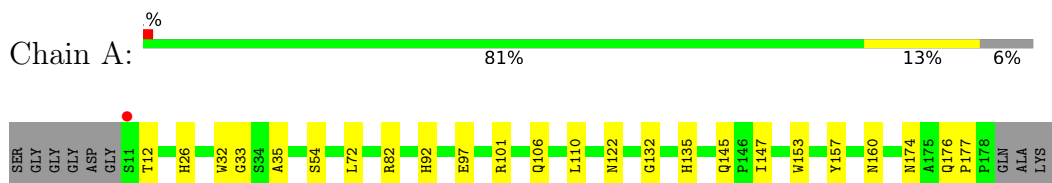
- Molecule 6 is water.

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

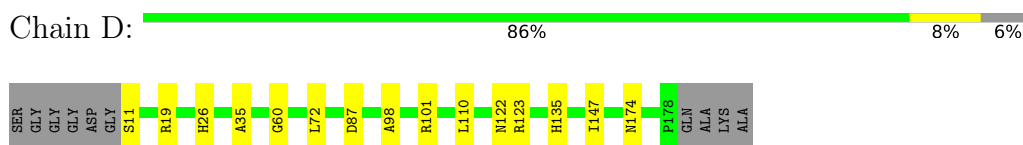
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

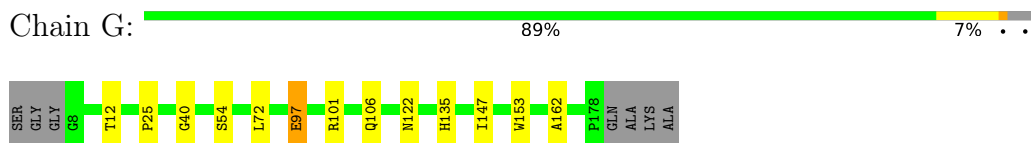
- Molecule 1: Protein related to penicillin acylase



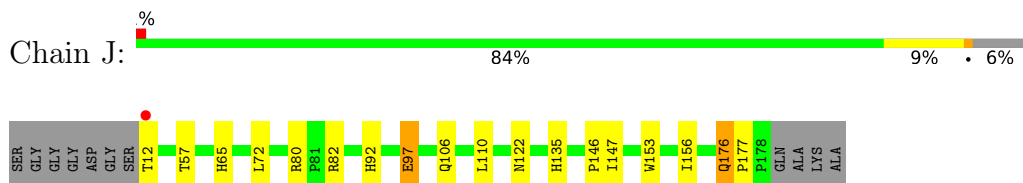
- Molecule 1: Protein related to penicillin acylase



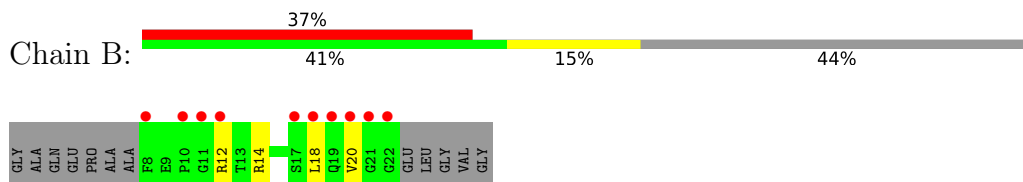
- Molecule 1: Protein related to penicillin acylase



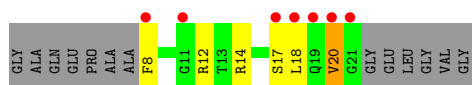
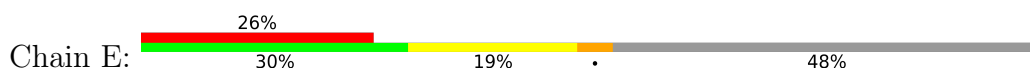
- Molecule 1: Protein related to penicillin acylase



- Molecule 2: Protein related to penicillin acylase



- Molecule 2: Protein related to penicillin acylase



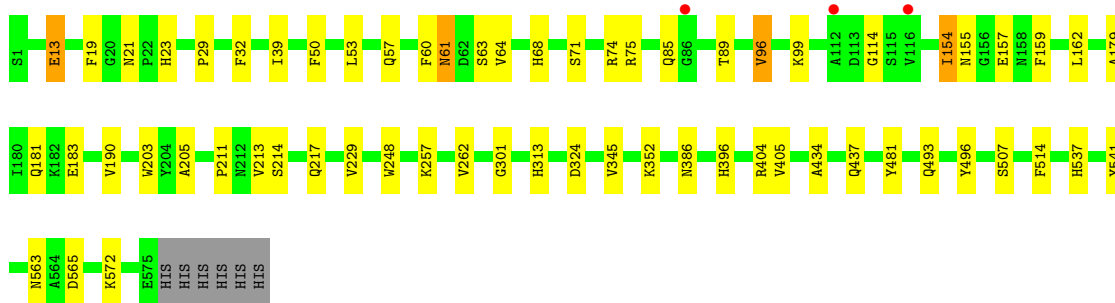
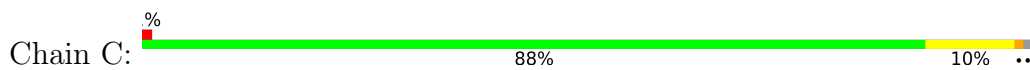
• Molecule 2: Protein related to penicillin acylase



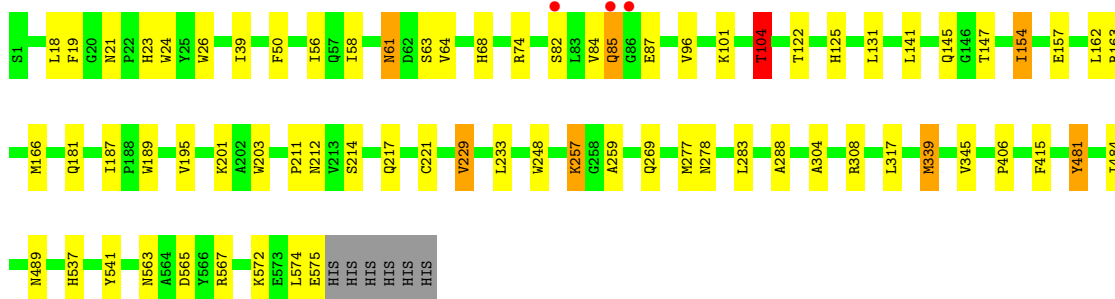
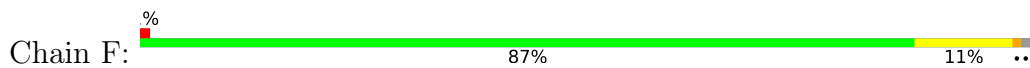
• Molecule 2: Protein related to penicillin acylase



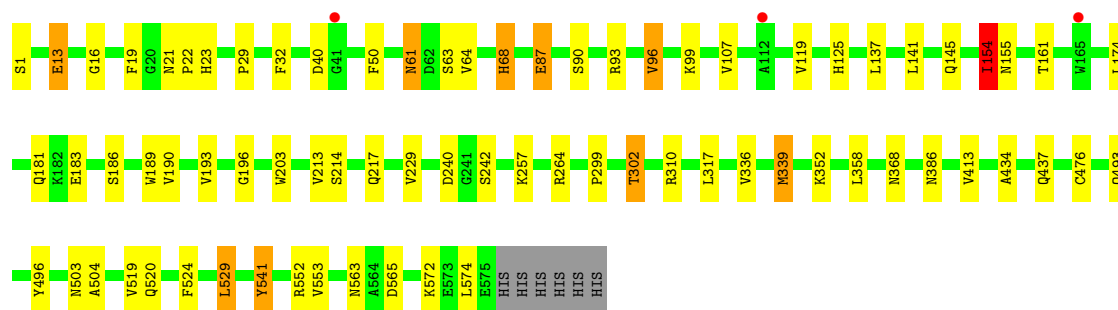
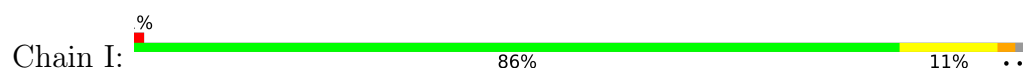
• Molecule 3: Protein related to penicillin acylase



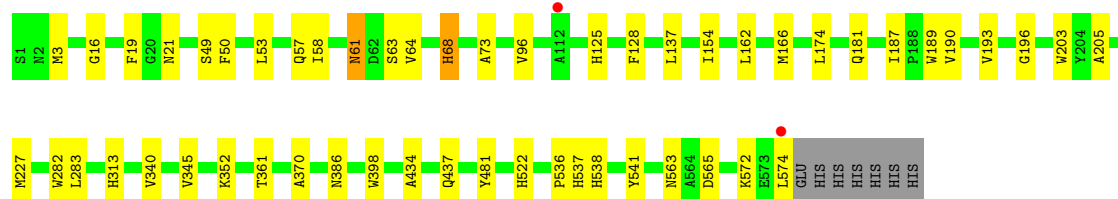
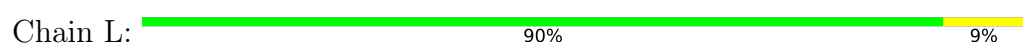
• Molecule 3: Protein related to penicillin acylase



• 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) 99.8 (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)	Xtrriage
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 (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	25587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.35	6/1335 (0.4%)	1.14	3/1808 (0.2%)
1	D	1.32	2/1344 (0.1%)	1.16	1/1820 (0.1%)
1	G	1.26	2/1342 (0.1%)	1.09	0/1817
1	J	1.37	6/1320 (0.5%)	1.22	3/1788 (0.2%)
2	B	1.14	0/112	1.17	0/150
2	E	1.45	1/108 (0.9%)	1.24	0/145
2	H	1.51	2/112 (1.8%)	1.10	0/150
2	K	1.08	0/121	1.17	0/162
3	C	1.35	7/4482 (0.2%)	1.19	10/6115 (0.2%)
3	F	1.37	14/4482 (0.3%)	1.20	6/6115 (0.1%)
3	I	1.29	10/4467 (0.2%)	1.16	14/6094 (0.2%)
3	L	1.35	12/4466 (0.3%)	1.16	1/6093 (0.0%)
All	All	1.33	62/23691 (0.3%)	1.17	38/32257 (0.1%)

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	339	MET	SD-CE	-7.96	1.59	1.79
3	F	68	HIS	CG-CD2	7.50	1.44	1.35
2	E	20	VAL	CA-C	7.25	1.61	1.52
1	A	135	HIS	ND1-CE1	6.81	1.39	1.32
3	L	16	GLY	N-CA	6.69	1.53	1.45

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	339	MET	CG-SD-CE	-9.89	79.15	100.90
1	D	98	ALA	N-CA-C	-7.21	103.50	111.36
3	I	96	VAL	CA-C-N	6.72	127.09	119.83
3	I	96	VAL	C-N-CA	6.72	127.09	119.83
3	F	104	THR	CB-CA-C	6.44	120.62	110.19

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
2	B	110	0	108	4	0
2	E	106	0	105	8	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	42	0
3	I	4353	0	4161	46	0
3	L	4352	0	4165	38	0
4	C	20	0	14	11	0
4	F	20	0	14	7	0
4	I	20	0	14	10	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	200	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.

The worst 5 of 200 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:O2	4:L:601[A]:PAC:H2'	1.36	1.15
4:C:601[A]:PAC:O2	4:C:601[A]:PAC:C6'	1.80	1.13
4:C:601[A]:PAC:O2	4:C:601[A]:PAC:H6'	1.26	1.02
3:F:50:PHE:CE1	4:F:601[A]:PAC:H3'	1.95	1.02

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/130 (98%)	124 (98%)	3 (2%)	43	23
1	D	128/130 (98%)	126 (98%)	2 (2%)	55	38
1	G	127/130 (98%)	125 (98%)	2 (2%)	55	38
1	J	125/130 (96%)	123 (98%)	2 (2%)	55	38
2	B	11/17 (65%)	9 (82%)	2 (18%)	2	0
2	E	11/17 (65%)	10 (91%)	1 (9%)	9	1
2	H	11/17 (65%)	11 (100%)	0	100	100
2	K	12/17 (71%)	10 (83%)	2 (17%)	2	0
3	C	448/452 (99%)	437 (98%)	11 (2%)	42	22
3	F	448/452 (99%)	430 (96%)	18 (4%)	28	9
3	I	446/452 (99%)	428 (96%)	18 (4%)	28	9
3	L	446/452 (99%)	440 (99%)	6 (1%)	61	46
All	All	2340/2396 (98%)	2273 (97%)	67 (3%)	39	17

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	72	LEU
2	K	9	GLU
3	L	541	TYR
3	F	141	LEU
3	F	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	61	ASN

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Mol	Chain	Res	Type
3	I	448	GLN
3	I	85	GLN
3	I	368	ASN
3	L	57	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	F	601[B]	-	10,10,10	2.08	2 (20%)	12,12,12	3.20	8 (66%)
5	GOL	C	602	-	5,5,5	1.37	1 (20%)	5,5,5	2.26	2 (40%)
4	PAC	C	601[B]	-	10,10,10	1.53	1 (10%)	12,12,12	2.78	7 (58%)
4	PAC	I	601[A]	-	10,10,10	0.96	0	12,12,12	2.14	4 (33%)
4	PAC	C	601[A]	-	10,10,10	1.58	1 (10%)	12,12,12	2.77	6 (50%)
4	PAC	F	601[A]	-	10,10,10	1.02	1 (10%)	12,12,12	2.04	2 (16%)
5	GOL	L	602	-	5,5,5	0.74	0	5,5,5	1.76	1 (20%)
4	PAC	L	601[B]	-	10,10,10	2.08	3 (30%)	12,12,12	3.12	7 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	F	602	-	5,5,5	1.80	1 (20%)	5,5,5	0.72	0
4	PAC	L	601[A]	-	10,10,10	1.14	1 (10%)	12,12,12	1.88	3 (25%)
5	GOL	I	602	-	5,5,5	1.29	1 (20%)	5,5,5	0.93	0
4	PAC	I	601[B]	-	10,10,10	2.25	3 (30%)	12,12,12	3.10	8 (66%)

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

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	601[B]	PAC	C2-C1'	5.73	1.60	1.51
4	L	601[B]	PAC	C2-C1'	5.46	1.60	1.51
4	F	601[B]	PAC	C2-C1'	5.10	1.59	1.51
4	C	601[A]	PAC	C2-C1'	-4.60	1.44	1.51
4	C	601[B]	PAC	C2-C1'	3.96	1.58	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	601[B]	PAC	C1'-C2-C1	6.22	131.42	113.71
4	I	601[B]	PAC	C1'-C2-C1	6.00	130.78	113.71
4	C	601[B]	PAC	C1'-C2-C1	5.70	129.93	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601[A]	PAC	C1'-C2-C1	-5.68	97.56	113.71
4	F	601[B]	PAC	C1'-C2-C1	5.20	128.50	113.71

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	602	GOL	C1-C2-C3-O3
4	F	601[A]	PAC	C6'-C1'-C2-C1
4	F	601[A]	PAC	C2'-C1'-C2-C1
4	L	601[A]	PAC	C2'-C1'-C2-C1
4	L	601[A]	PAC	C6'-C1'-C2-C1

There are no ring outliers.

11 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	601[B]	PAC	4	0
5	C	602	GOL	1	0
4	C	601[B]	PAC	4	0
4	I	601[A]	PAC	5	0
4	C	601[A]	PAC	7	0
4	F	601[A]	PAC	3	0
4	L	601[B]	PAC	5	0
5	F	602	GOL	1	0
4	L	601[A]	PAC	5	0
5	I	602	GOL	2	0
4	I	601[B]	PAC	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.63	1 (0%) 85 89	11, 18, 29, 44	1 (0%)
1	D	168/178 (94%)	-0.56	0 100 100	10, 18, 31, 47	2 (1%)
1	G	171/178 (96%)	-0.43	0 100 100	14, 20, 35, 54	0
1	J	167/178 (93%)	-0.59	1 (0%) 85 89	12, 17, 28, 46	0
2	B	15/27 (55%)	2.53	10 (66%) 0 0	44, 56, 61, 63	0
2	E	14/27 (51%)	2.43	7 (50%) 0 0	42, 54, 58, 60	0
2	H	15/27 (55%)	1.17	3 (20%) 3 3	31, 36, 46, 47	0
2	K	16/27 (59%)	1.32	2 (12%) 8 9	32, 43, 55, 56	0
3	C	575/581 (98%)	-0.50	3 (0%) 87 90	9, 17, 36, 58	2 (0%)
3	F	575/581 (98%)	-0.46	3 (0%) 87 90	8, 18, 36, 56	2 (0%)
3	I	575/581 (98%)	-0.34	3 (0%) 87 90	12, 21, 37, 54	0
3	L	574/581 (98%)	-0.54	2 (0%) 90 92	7, 18, 32, 48	1 (0%)
All	All	3033/3144 (96%)	-0.43	35 (1%) 76 82	7, 19, 38, 63	8 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	20	VAL	6.5
2	E	20	VAL	5.5
3	F	86	GLY	4.2
3	L	574	LEU	4.1
2	E	21	GLY	4.0

### 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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
5	GOL	F	602	6/6	0.88	0.15	14,25,33,42	0
4	PAC	I	601[B]	10/10	0.89	0.11	15,22,25,26	10
4	PAC	I	601[A]	10/10	0.89	0.11	18,20,21,21	10
4	PAC	L	601[B]	10/10	0.90	0.10	17,22,25,28	10
4	PAC	L	601[A]	10/10	0.90	0.10	16,22,25,26	10
4	PAC	C	601[B]	10/10	0.92	0.11	17,19,20,20	10
4	PAC	F	601[A]	10/10	0.92	0.09	14,18,21,22	10
4	PAC	F	601[B]	10/10	0.92	0.09	19,23,27,28	10
4	PAC	C	601[A]	10/10	0.92	0.11	13,18,19,20	10
5	GOL	C	602	6/6	0.93	0.11	15,28,30,36	0
5	GOL	I	602	6/6	0.93	0.12	16,26,29,30	0
5	GOL	L	602	6/6	0.95	0.11	16,26,27,29	0

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

There are no such residues in this entry.