



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2023 – 04:27 PM EDT

PDB ID : 4L9Y  
Title : Crystal Structure of Rhodobacter sphaeroides malyI-CoA lyase in complex with magnesium, glyoxylate, and propionyl-CoA  
Authors : Zarzycki, J.; Kerfeld, C.A.  
Deposited on : 2013-06-18  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
buster-report : 1.1.7 (2018)  
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) : 2.35.1

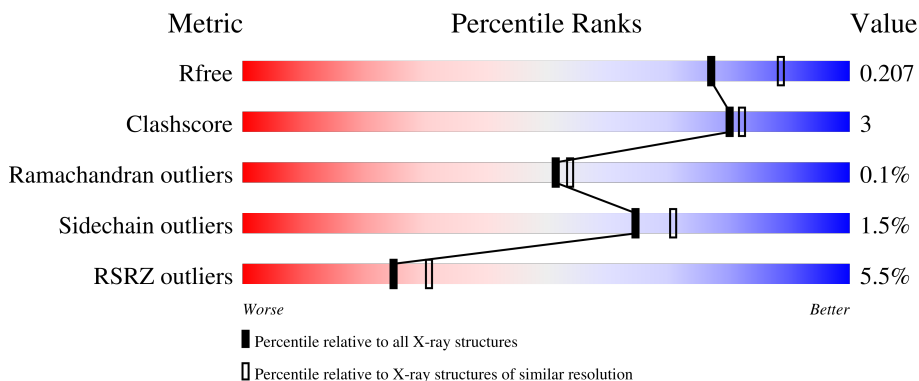
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


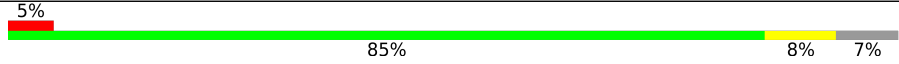
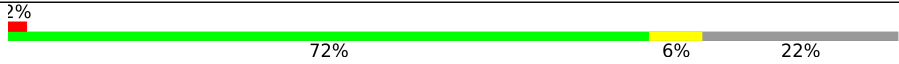
The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



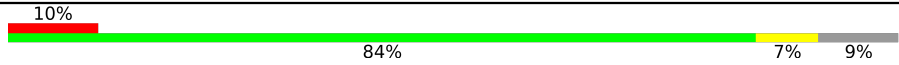
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	339	
1	B	339	
1	C	339	
1	D	339	
1	E	339	

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Mol	Chain	Length	Quality of chain
1	F	339	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '10%', a large green segment labeled '84%', a yellow segment labeled '7%', and a grey segment on the far right labeled '9%'.</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14807 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 Malyl-CoA lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2382	1496	425	449	12	0	0	0
1	B	264	2012	1269	358	375	10	0	0	0
1	C	316	2396	1505	427	452	12	0	0	0
1	D	265	2018	1272	359	377	10	0	0	0
1	E	265	2018	1272	359	377	10	0	0	0
1	F	309	2340	1472	416	441	11	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q3J5L6
A	-19	GLY	-	expression tag	UNP Q3J5L6
A	-18	HIS	-	expression tag	UNP Q3J5L6
A	-17	HIS	-	expression tag	UNP Q3J5L6
A	-16	HIS	-	expression tag	UNP Q3J5L6
A	-15	HIS	-	expression tag	UNP Q3J5L6
A	-14	HIS	-	expression tag	UNP Q3J5L6
A	-13	HIS	-	expression tag	UNP Q3J5L6
A	-12	HIS	-	expression tag	UNP Q3J5L6
A	-11	HIS	-	expression tag	UNP Q3J5L6
A	-10	HIS	-	expression tag	UNP Q3J5L6
A	-9	HIS	-	expression tag	UNP Q3J5L6
A	-8	SER	-	expression tag	UNP Q3J5L6
A	-7	SER	-	expression tag	UNP Q3J5L6
A	-6	GLY	-	expression tag	UNP Q3J5L6
A	-5	HIS	-	expression tag	UNP Q3J5L6
A	-4	ILE	-	expression tag	UNP Q3J5L6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP Q3J5L6
A	-2	GLY	-	expression tag	UNP Q3J5L6
A	-1	ARG	-	expression tag	UNP Q3J5L6
A	0	HIS	-	expression tag	UNP Q3J5L6
B	-20	MET	-	expression tag	UNP Q3J5L6
B	-19	GLY	-	expression tag	UNP Q3J5L6
B	-18	HIS	-	expression tag	UNP Q3J5L6
B	-17	HIS	-	expression tag	UNP Q3J5L6
B	-16	HIS	-	expression tag	UNP Q3J5L6
B	-15	HIS	-	expression tag	UNP Q3J5L6
B	-14	HIS	-	expression tag	UNP Q3J5L6
B	-13	HIS	-	expression tag	UNP Q3J5L6
B	-12	HIS	-	expression tag	UNP Q3J5L6
B	-11	HIS	-	expression tag	UNP Q3J5L6
B	-10	HIS	-	expression tag	UNP Q3J5L6
B	-9	HIS	-	expression tag	UNP Q3J5L6
B	-8	SER	-	expression tag	UNP Q3J5L6
B	-7	SER	-	expression tag	UNP Q3J5L6
B	-6	GLY	-	expression tag	UNP Q3J5L6
B	-5	HIS	-	expression tag	UNP Q3J5L6
B	-4	ILE	-	expression tag	UNP Q3J5L6
B	-3	GLU	-	expression tag	UNP Q3J5L6
B	-2	GLY	-	expression tag	UNP Q3J5L6
B	-1	ARG	-	expression tag	UNP Q3J5L6
B	0	HIS	-	expression tag	UNP Q3J5L6
C	-20	MET	-	expression tag	UNP Q3J5L6
C	-19	GLY	-	expression tag	UNP Q3J5L6
C	-18	HIS	-	expression tag	UNP Q3J5L6
C	-17	HIS	-	expression tag	UNP Q3J5L6
C	-16	HIS	-	expression tag	UNP Q3J5L6
C	-15	HIS	-	expression tag	UNP Q3J5L6
C	-14	HIS	-	expression tag	UNP Q3J5L6
C	-13	HIS	-	expression tag	UNP Q3J5L6
C	-12	HIS	-	expression tag	UNP Q3J5L6
C	-11	HIS	-	expression tag	UNP Q3J5L6
C	-10	HIS	-	expression tag	UNP Q3J5L6
C	-9	HIS	-	expression tag	UNP Q3J5L6
C	-8	SER	-	expression tag	UNP Q3J5L6
C	-7	SER	-	expression tag	UNP Q3J5L6
C	-6	GLY	-	expression tag	UNP Q3J5L6
C	-5	HIS	-	expression tag	UNP Q3J5L6
C	-4	ILE	-	expression tag	UNP Q3J5L6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLU	-	expression tag	UNP Q3J5L6
C	-2	GLY	-	expression tag	UNP Q3J5L6
C	-1	ARG	-	expression tag	UNP Q3J5L6
C	0	HIS	-	expression tag	UNP Q3J5L6
D	-20	MET	-	expression tag	UNP Q3J5L6
D	-19	GLY	-	expression tag	UNP Q3J5L6
D	-18	HIS	-	expression tag	UNP Q3J5L6
D	-17	HIS	-	expression tag	UNP Q3J5L6
D	-16	HIS	-	expression tag	UNP Q3J5L6
D	-15	HIS	-	expression tag	UNP Q3J5L6
D	-14	HIS	-	expression tag	UNP Q3J5L6
D	-13	HIS	-	expression tag	UNP Q3J5L6
D	-12	HIS	-	expression tag	UNP Q3J5L6
D	-11	HIS	-	expression tag	UNP Q3J5L6
D	-10	HIS	-	expression tag	UNP Q3J5L6
D	-9	HIS	-	expression tag	UNP Q3J5L6
D	-8	SER	-	expression tag	UNP Q3J5L6
D	-7	SER	-	expression tag	UNP Q3J5L6
D	-6	GLY	-	expression tag	UNP Q3J5L6
D	-5	HIS	-	expression tag	UNP Q3J5L6
D	-4	ILE	-	expression tag	UNP Q3J5L6
D	-3	GLU	-	expression tag	UNP Q3J5L6
D	-2	GLY	-	expression tag	UNP Q3J5L6
D	-1	ARG	-	expression tag	UNP Q3J5L6
D	0	HIS	-	expression tag	UNP Q3J5L6
E	-20	MET	-	expression tag	UNP Q3J5L6
E	-19	GLY	-	expression tag	UNP Q3J5L6
E	-18	HIS	-	expression tag	UNP Q3J5L6
E	-17	HIS	-	expression tag	UNP Q3J5L6
E	-16	HIS	-	expression tag	UNP Q3J5L6
E	-15	HIS	-	expression tag	UNP Q3J5L6
E	-14	HIS	-	expression tag	UNP Q3J5L6
E	-13	HIS	-	expression tag	UNP Q3J5L6
E	-12	HIS	-	expression tag	UNP Q3J5L6
E	-11	HIS	-	expression tag	UNP Q3J5L6
E	-10	HIS	-	expression tag	UNP Q3J5L6
E	-9	HIS	-	expression tag	UNP Q3J5L6
E	-8	SER	-	expression tag	UNP Q3J5L6
E	-7	SER	-	expression tag	UNP Q3J5L6
E	-6	GLY	-	expression tag	UNP Q3J5L6
E	-5	HIS	-	expression tag	UNP Q3J5L6
E	-4	ILE	-	expression tag	UNP Q3J5L6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLU	-	expression tag	UNP Q3J5L6
E	-2	GLY	-	expression tag	UNP Q3J5L6
E	-1	ARG	-	expression tag	UNP Q3J5L6
E	0	HIS	-	expression tag	UNP Q3J5L6
F	-20	MET	-	expression tag	UNP Q3J5L6
F	-19	GLY	-	expression tag	UNP Q3J5L6
F	-18	HIS	-	expression tag	UNP Q3J5L6
F	-17	HIS	-	expression tag	UNP Q3J5L6
F	-16	HIS	-	expression tag	UNP Q3J5L6
F	-15	HIS	-	expression tag	UNP Q3J5L6
F	-14	HIS	-	expression tag	UNP Q3J5L6
F	-13	HIS	-	expression tag	UNP Q3J5L6
F	-12	HIS	-	expression tag	UNP Q3J5L6
F	-11	HIS	-	expression tag	UNP Q3J5L6
F	-10	HIS	-	expression tag	UNP Q3J5L6
F	-9	HIS	-	expression tag	UNP Q3J5L6
F	-8	SER	-	expression tag	UNP Q3J5L6
F	-7	SER	-	expression tag	UNP Q3J5L6
F	-6	GLY	-	expression tag	UNP Q3J5L6
F	-5	HIS	-	expression tag	UNP Q3J5L6
F	-4	ILE	-	expression tag	UNP Q3J5L6
F	-3	GLU	-	expression tag	UNP Q3J5L6
F	-2	GLY	-	expression tag	UNP Q3J5L6
F	-1	ARG	-	expression tag	UNP Q3J5L6
F	0	HIS	-	expression tag	UNP Q3J5L6

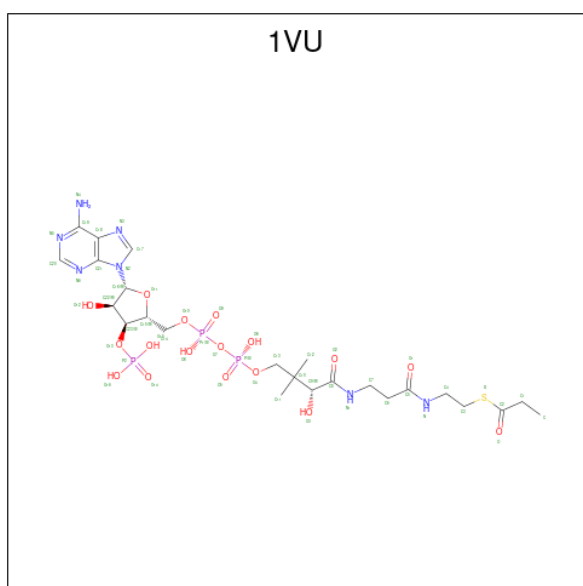
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

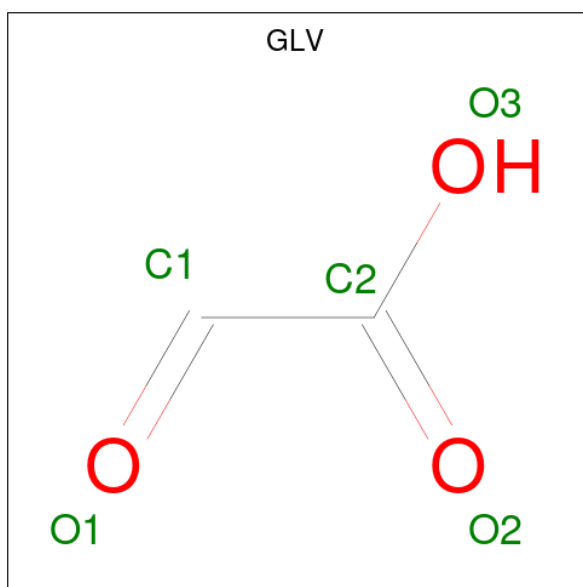
- Molecule 4 is propionyl Coenzyme A (three-letter code: 1VU) (formula: C<sub>24</sub>H<sub>40</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
4	B	1	52	24	7	17	3	1	0	0

- Molecule 5 is GLYOXYLIC ACID (three-letter code: GLV) (formula: C<sub>2</sub>H<sub>2</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 5 2 3	0	0
5	D	1	Total C O 5 2 3	0	0

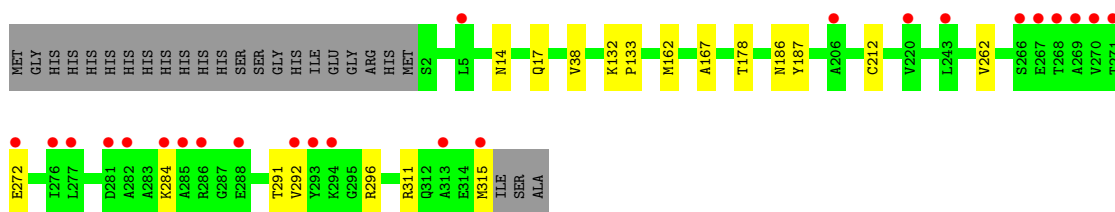
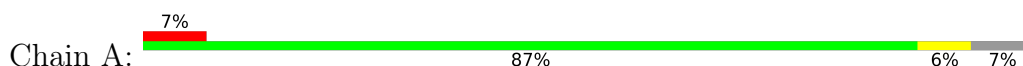
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	210	Total O 210 210	0	0
6	B	244	Total O 244 244	0	0
6	C	308	Total O 308 308	0	0
6	D	261	Total O 261 261	0	0
6	E	260	Total O 260 260	0	0
6	F	286	Total O 286 286	0	0

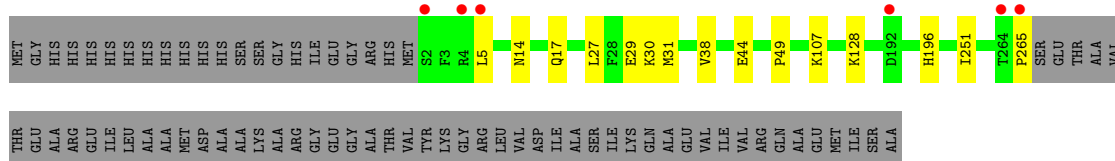
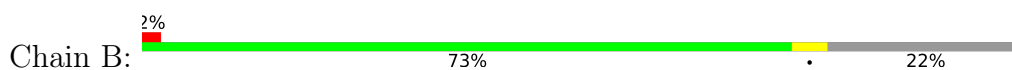
### 3 Residue-property plots [i](#)

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.

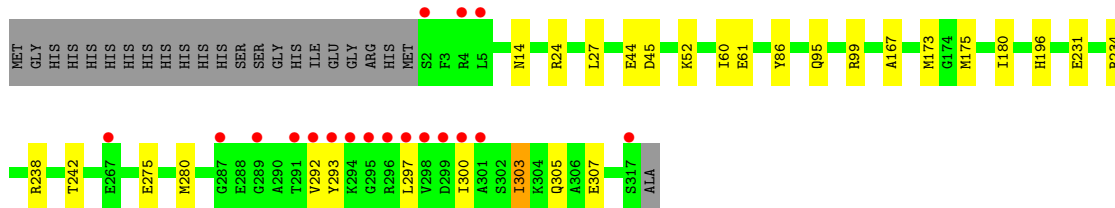
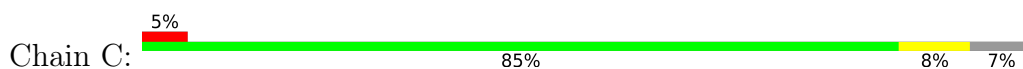
- Molecule 1: Malyl-CoA lyase



- Molecule 1: Malyl-CoA lyase

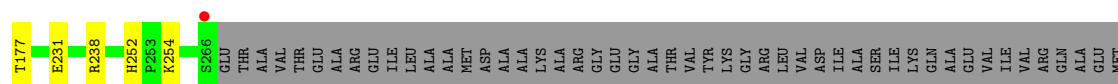


- Molecule 1: Malyl-CoA lyase



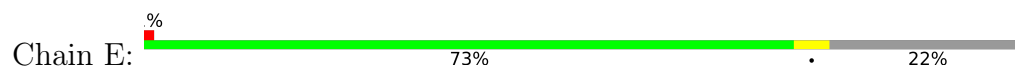
- Molecule 1: Malyl-CoA lyase





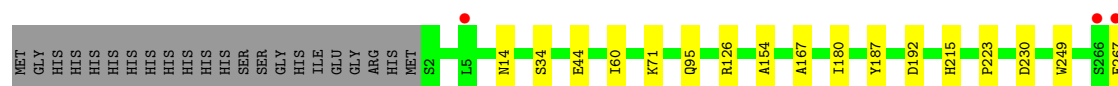
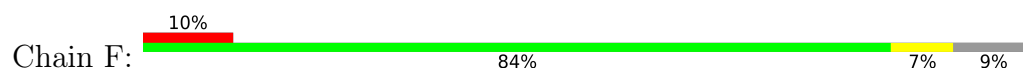
ILE  
SER  
ALA

- Molecule 1: Malyl-CoA lyase



THR  
ALA  
VAL  
THR  
GLU  
ALA  
ARG  
GLU  
ILE  
LEU  
ALA  
MET  
ASP  
SER  
GLY  
HIS  
MET  
THR  
VAL  
TYR  
LYS  
GLY  
ARG  
LEU  
VAL  
ASP  
ILE  
ALA  
SER  
ILE  
LYS  
GLN  
ALA  
GLU  
VAL  
ILE  
VAL  
ARG  
GLN  
ALA  
GLU  
MET  
ILE  
SER  
ALA

- Molecule 1: Malyl-CoA lyase



T268  
A269  
V270  
T271  
E272  
R274  
E275  
L276  
L277  
A278  
A279  
W280  
D281  
A282  
A283  
K284  
A285  
R286  
G287  
A290  
T291  
V292  
Y293  
L297  
V298  
A301  
S302  
I303  
K304  
Q305  
A306  
E307  
V308  
I309  
V310  
ARG  
GLN  
ALA  
GLU  
MET  
ILE  
SER  
ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.21Å 144.00Å 94.22Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	38.79 – 2.10 38.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.79-2.10) 99.5 (38.79-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1303	Depositor
R, $R_{free}$	0.177 , 0.207 0.177 , 0.207	Depositor DCC
$R_{free}$ test set	1995 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtrriage
Anisotropy	0.580	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: MG, CL, GLV, 1VU

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	0.21	0/2431	0.40	0/3300
1	B	0.22	0/2060	0.41	0/2801
1	C	0.22	0/2445	0.40	0/3319
1	D	0.22	0/2066	0.42	0/2809
1	E	0.23	0/2066	0.42	0/2809
1	F	0.22	0/2389	0.41	0/3245
All	All	0.22	0/13457	0.41	0/18283

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2382	0	2350	12	0
1	B	2012	0	1966	11	0
1	C	2396	0	2366	17	0
1	D	2018	0	1971	13	0
1	E	2018	0	1971	13	0
1	F	2340	0	2309	13	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	1	0
3	C	1	0	0	0	0
3	E	1	0	0	1	0
3	F	1	0	0	0	0
4	B	52	0	38	1	0
5	B	5	0	1	0	0
5	D	5	0	1	0	0
6	A	210	0	0	3	0
6	B	244	0	0	2	0
6	C	308	0	0	4	0
6	D	261	0	0	4	0
6	E	260	0	0	4	1
6	F	286	0	0	3	1
All	All	14807	0	12973	70	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 3.

The worst 5 of 70 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:A:178:THR:O	6:A:700:HOH:O	1.91	0.86
1:A:262:VAL:O	6:A:618:HOH:O	1.93	0.83
1:C:61:GLU:OE1	6:C:786:HOH:O	2.00	0.79
1:D:26:ALA:O	6:D:630:HOH:O	2.04	0.76
1:E:4:ARG:NH1	6:E:742:HOH:O	2.20	0.74

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)
6:E:568:HOH:O	6:F:534:HOH:O[2_556]	2.02	0.18

## 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	312/339 (92%)	306 (98%)	6 (2%)	0	100	100
1	B	262/339 (77%)	256 (98%)	6 (2%)	0	100	100
1	C	314/339 (93%)	306 (98%)	8 (2%)	0	100	100
1	D	263/339 (78%)	257 (98%)	6 (2%)	0	100	100
1	E	263/339 (78%)	256 (97%)	6 (2%)	1 (0%)	34	32
1	F	307/339 (91%)	299 (97%)	7 (2%)	1 (0%)	41	41
All	All	1721/2034 (85%)	1680 (98%)	39 (2%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	5	LEU
1	F	192	ASP

### 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	239/260 (92%)	237 (99%)	2 (1%)	81	86
1	B	203/260 (78%)	201 (99%)	2 (1%)	76	82
1	C	241/260 (93%)	234 (97%)	7 (3%)	42	46
1	D	204/260 (78%)	201 (98%)	3 (2%)	65	71
1	E	204/260 (78%)	201 (98%)	3 (2%)	65	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	235/260 (90%)	232 (99%)	3 (1%)	69	75
All	All	1326/1560 (85%)	1306 (98%)	20 (2%)	65	71

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	ARG
1	F	14	ASN
1	F	272	GLU
1	F	44	GLU
1	C	292	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	196	HIS
1	F	194	GLN
1	C	196	HIS
1	B	196	HIS
1	D	196	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 10 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	1VU	B	401	-	46,54,54	1.36	5 (10%)	56,80,80	1.70	10 (17%)
5	GLV	B	402	2	4,4,4	1.28	0	3,4,4	1.36	0
5	GLV	D	401	2	4,4,4	1.29	0	3,4,4	1.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1VU	B	401	-	-	9/49/69/69	0/3/3/3
5	GLV	B	402	2	-	0/0/2/2	-
5	GLV	D	401	2	-	0/0/2/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	1VU	C2-S	-4.10	1.66	1.76
4	B	401	1VU	P1-O8	-2.45	1.43	1.55
4	B	401	1VU	C21-N6	-2.16	1.32	1.35
4	B	401	1VU	P2-O14	-2.13	1.43	1.50
4	B	401	1VU	P-O5	-2.09	1.43	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	1VU	C1-C2-S	7.69	123.14	113.63
4	B	401	1VU	N6-C20-N5	-3.65	122.97	128.68
4	B	401	1VU	O-C2-C1	-3.49	118.28	123.71
4	B	401	1VU	O-C2-S	-3.11	118.58	122.61
4	B	401	1VU	C21-C18-N3	-2.65	106.64	109.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

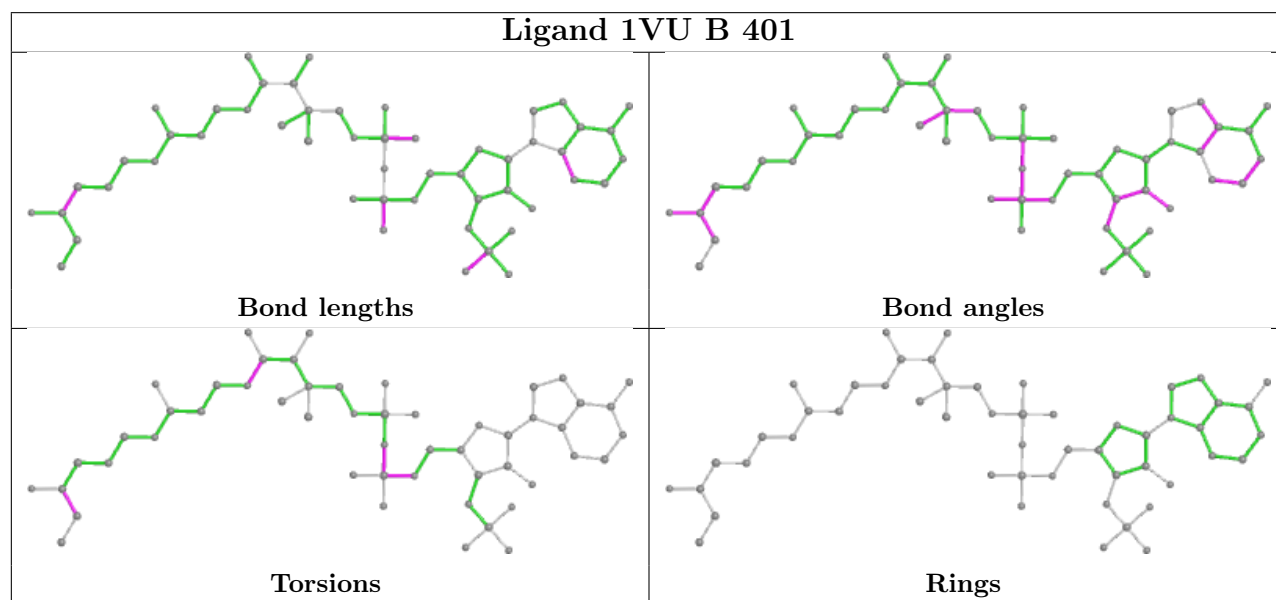
Mol	Chain	Res	Type	Atoms
4	B	401	1VU	C14-O10-P1-O8
4	B	401	1VU	C14-O10-P1-O9
4	B	401	1VU	C14-O10-P1-O7
4	B	401	1VU	C-C1-C2-S
4	B	401	1VU	C-C1-C2-O

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	1VU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

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 [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	314/339 (92%)	0.27	24 (7%) 13 18	12, 26, 52, 62	0
1	B	264/339 (77%)	-0.17	6 (2%) 60 65	11, 21, 36, 43	0
1	C	316/339 (93%)	0.01	18 (5%) 23 29	9, 19, 52, 77	0
1	D	265/339 (78%)	-0.10	8 (3%) 50 56	8, 17, 34, 52	0
1	E	265/339 (78%)	-0.34	5 (1%) 66 71	8, 17, 31, 53	0
1	F	309/339 (91%)	0.06	34 (11%) 5 7	8, 17, 57, 65	0
All	All	1733/2034 (85%)	-0.03	95 (5%) 25 31	8, 19, 49, 77	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	287	GLY	7.2
1	B	5	LEU	6.2
1	F	278	ALA	5.9
1	C	297	LEU	5.9
1	C	301	ALA	5.8

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

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

### 6.3 Carbohydrates [i](#)

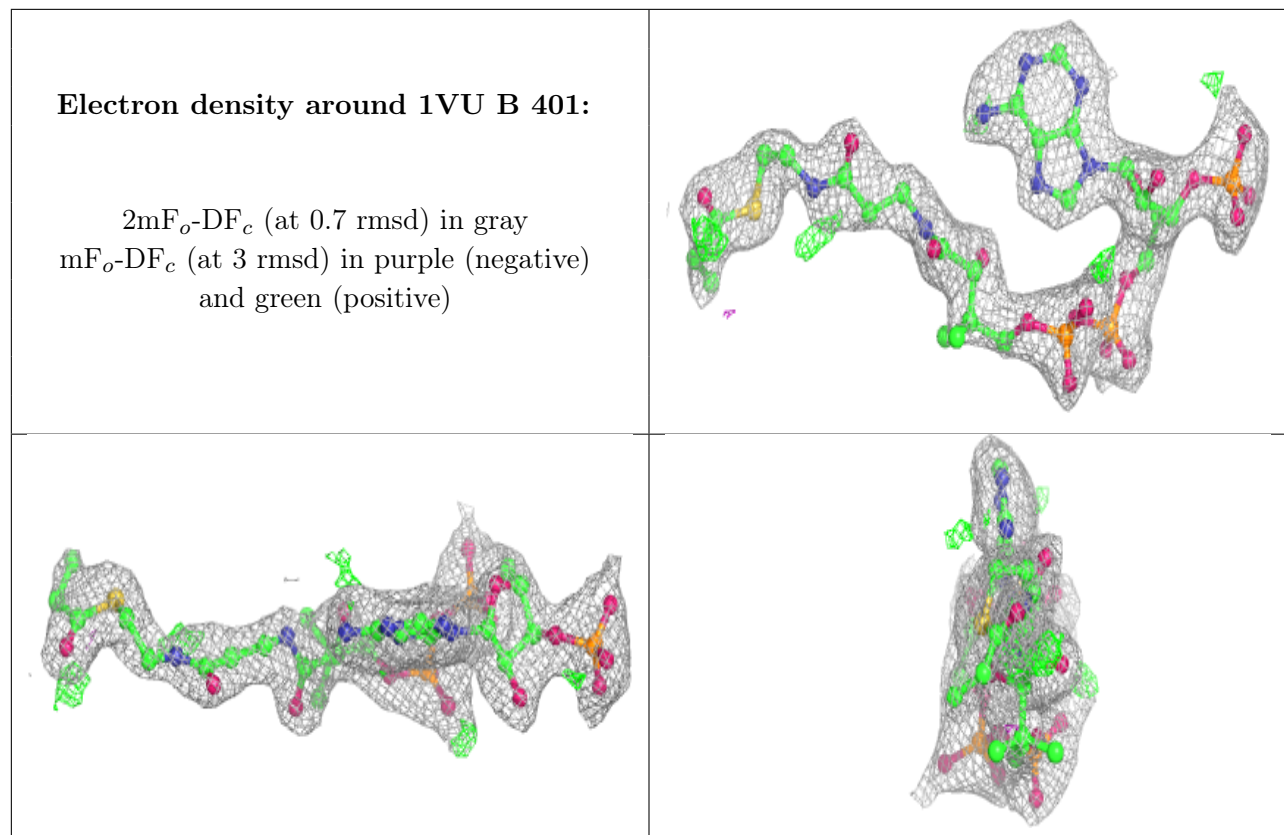
There are no monosaccharides in this entry.

## 6.4 Ligands

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
4	1VU	B	401	52/52	0.89	0.14	26,36,44,48	52
2	MG	E	401	1/1	0.91	0.05	26,26,26,26	0
2	MG	A	401	1/1	0.92	0.05	26,26,26,26	0
2	MG	F	401	1/1	0.93	0.07	22,22,22,22	0
5	GLV	B	402	5/5	0.93	0.18	22,23,24,25	5
2	MG	D	402	1/1	0.95	0.18	20,20,20,20	0
5	GLV	D	401	5/5	0.95	0.21	14,16,19,20	5
2	MG	B	403	1/1	0.97	0.11	26,26,26,26	0
2	MG	C	401	1/1	0.98	0.03	21,21,21,21	0
3	CL	A	402	1/1	0.98	0.09	27,27,27,27	0
3	CL	E	402	1/1	0.98	0.04	21,21,21,21	0
3	CL	F	402	1/1	0.99	0.03	17,17,17,17	0
3	CL	C	402	1/1	0.99	0.03	21,21,21,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.