



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:21 PM GMT

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 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

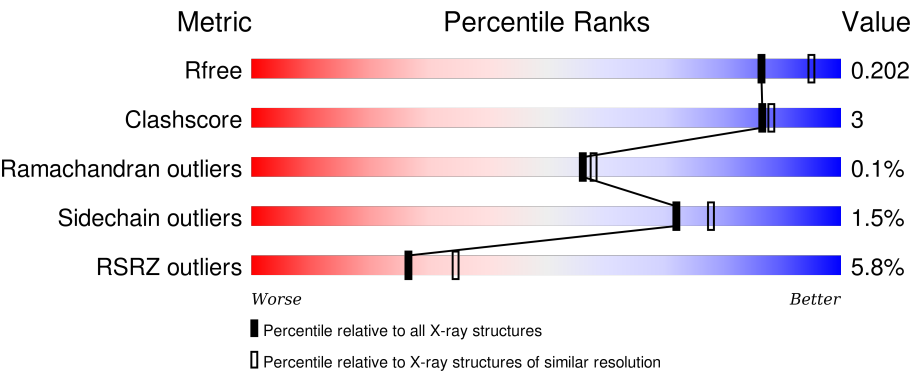
# 1 Overall quality at a glance i

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 <sub>free</sub>	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 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	339	<div><div>7%</div><div>87%6%7%</div></div>
1	B	339	<div><div>2%</div><div>73%•22%</div></div>
1	C	339	<div><div>6%</div><div>85%8%7%</div></div>
1	D	339	<div><div>3%</div><div>72%6%22%</div></div>
1	E	339	<div><div>•</div><div>73%•22%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	339	

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
5	GLV	B	402	-	-	-	X

## 2 Entry composition

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

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

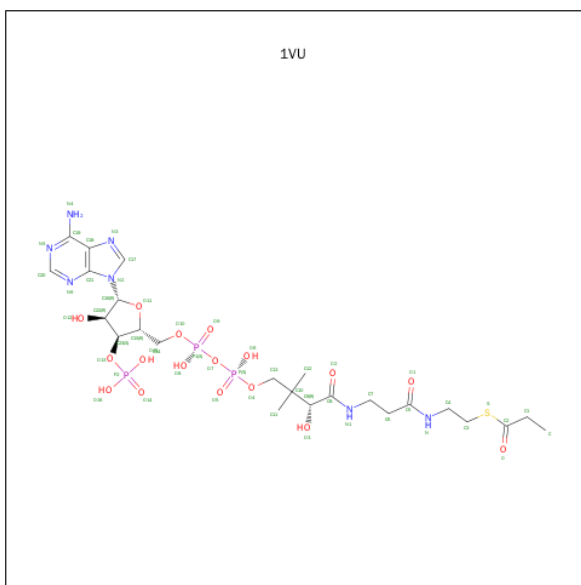
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	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	A	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	F	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

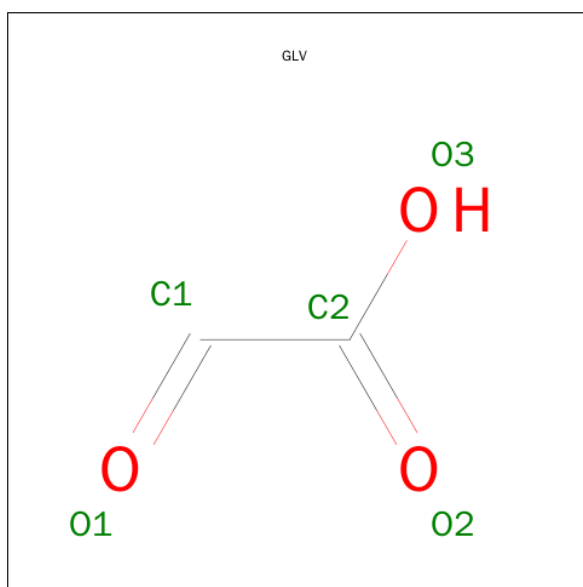
- Molecule 4 is PROPIONYL COENZYME A (three-letter code: 1VU) (formula:  $C_{24}H_{40}N_7O_{17}P_3S$ ).



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

- Molecule 5 is GLYOXYLIC ACID (three-letter code: GLV) (formula:  $C_2H_2O_3$ ).





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

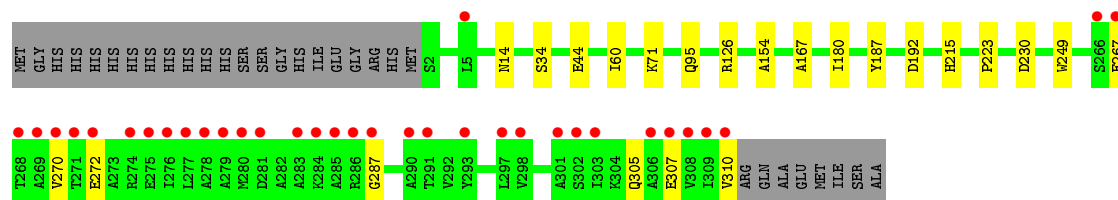
- Molecule 6 is water.

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



- Molecule 1: Malyl-CoA lyase





## 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)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1303)	Depositor
R, $R_{free}$	0.177 , 0.207 0.175 , 0.202	Depositor DCC
$R_{free}$ test set	1995 reflections (1.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.5	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 113573 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 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: 1VU, MG, GLV, CL

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.

All (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
1:E:32:ALA:O	6:E:619:HOH:O	2.08	0.70
1:E:230:ASP:OD2	6:E:684:HOH:O	2.13	0.67
1:B:265:PRO:O	6:B:681:HOH:O	2.12	0.67
1:D:2:SER:O	6:D:675:HOH:O	2.12	0.67
1:F:230:ASP:OD2	6:F:707:HOH:O	2.16	0.61
1:E:94:GLU:HG2	1:E:128:LYS:HE3	1.85	0.59
1:D:231:GLU:OE1	6:D:600:HOH:O	2.17	0.58
1:F:167:ALA:HB2	1:F:180:ILE:HG23	1.87	0.56
1:E:30:LYS:NZ	6:E:756:HOH:O	2.39	0.56
1:F:34:SER:O	1:F:71:LYS:NZ	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:GLU:OE2	1:C:234:ARG:NH1	2.40	0.54
1:E:167:ALA:HB2	1:E:180:ILE:HG23	1.89	0.54
1:A:17:GLN:HG2	1:A:38:VAL:HB	1.91	0.53
1:B:44:GLU:OE2	1:B:107:LYS:NZ	2.37	0.52
1:C:167:ALA:HB2	1:C:180:ILE:HG23	1.92	0.52
1:A:272:GLU:OE2	1:A:296:ARG:NH1	2.44	0.51
1:F:307:GLU:HA	1:F:310:VAL:HG22	1.94	0.50
1:F:223:PRO:HD3	1:F:249:TRP:CE3	2.47	0.49
1:F:126:ARG:HG3	6:F:667:HOH:O	2.11	0.49
1:D:175:MET:HB3	1:D:177:THR:HG23	1.95	0.48
1:F:287:GLY:HA2	6:F:719:HOH:O	2.14	0.47
1:F:270:VAL:HG23	1:F:310:VAL:HG12	1.95	0.47
1:B:30:LYS:NZ	4:B:401:1VU:O12	2.39	0.47
1:F:60:ILE:HD13	1:F:95:GLN:HB2	1.95	0.47
1:C:52:LYS:HB3	6:C:581:HOH:O	2.16	0.46
1:E:5:LEU:HB3	1:E:6:GLN:H	1.55	0.46
1:F:267:GLU:HA	1:F:270:VAL:HG12	1.97	0.46
1:C:280:MET:SD	1:C:303:ILE:HD12	2.55	0.46
1:B:196:HIS:CD2	1:C:196:HIS:HD2	2.35	0.45
1:B:29:GLU:HB2	6:B:614:HOH:O	2.15	0.45
1:C:45:ASP:OD2	6:C:503:HOH:O	2.21	0.44
1:D:252:HIS:ND1	1:D:254:LYS:HG2	2.33	0.44
1:D:17:GLN:HG2	1:D:38:VAL:HB	2.00	0.44
1:D:93:LEU:HD11	1:D:134:LEU:HD22	2.01	0.43
1:E:128:LYS:HA	1:E:128:LYS:HD3	1.88	0.43
1:A:132:LYS:HA	1:A:133:PRO:HD2	1.91	0.43
1:D:125:GLU:HG2	1:D:130:ARG:HD3	2.01	0.43
1:A:284:LYS:HZ3	1:B:49:PRO:HD2	1.82	0.43
1:D:177:THR:O	6:D:591:HOH:O	2.20	0.42
1:A:167:ALA:HB3	3:A:402:CL:CL	2.56	0.42
1:C:275:GLU:OE1	1:C:293:TYR:OH	2.25	0.42
1:D:238:ARG:HB3	1:E:186:ASN:HB3	2.00	0.42
1:B:27:LEU:O	1:B:31:MET:HG3	2.19	0.42
1:A:162:MET:HB3	1:A:212:CYS:SG	2.60	0.42
1:E:242:THR:HG21	1:F:187:TYR:HB2	2.01	0.41
1:E:167:ALA:HB3	3:E:402:CL:CL	2.57	0.41
1:C:86:TYR:CZ	1:D:124:ILE:HG12	2.55	0.41
1:F:154:ALA:HB2	1:F:215:HIS:CE1	2.56	0.41
1:C:305:GLN:OE1	6:C:772:HOH:O	2.22	0.41
1:C:60:ILE:HD13	1:C:95:GLN:HB2	2.03	0.41
1:B:17:GLN:HG2	1:B:38:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ALA:O	1:E:71:LYS:HE2	2.21	0.41
1:E:252:HIS:ND1	1:E:254:LYS:HG2	2.35	0.41
1:A:186:ASN:HB3	1:C:238:ARG:HB3	2.03	0.41
1:A:291:THR:OG1	1:A:292:VAL:N	2.54	0.41
1:D:60:ILE:HD13	1:D:95:GLN:HB2	2.03	0.41
1:C:24:ARG:CZ	1:C:27:LEU:HD11	2.51	0.41
1:B:251:ILE:H	1:B:251:ILE:HG13	1.77	0.41
1:A:311:ARG:O	6:A:696:HOH:O	2.22	0.41
1:A:187:TYR:HB2	1:C:242:THR:HG21	2.02	0.41
1:B:196:HIS:HD2	1:C:196:HIS:HD2	1.68	0.40
1:C:173:MET:HB2	1:C:175:MET:HG3	2.03	0.40
1:D:171:ALA:HB2	1:F:305:GLN:HG3	2.03	0.40
1:B:128:LYS:HA	1:B:128:LYS:HD3	1.92	0.40
1:C:99:ARG:HD2	1:C:99:ARG:HA	1.88	0.40

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

### 5.3.1 Protein backbone

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%)	39	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	307/339 (91%)	299 (97%)	7 (2%)	1 (0%)	46	45
All	All	1721/2034 (85%)	1680 (98%)	39 (2%)	2 (0%)	56	58

All (2) Ramachandran outliers are listed below:

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

### 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	239/260 (92%)	237 (99%)	2 (1%)	86	91
1	B	203/260 (78%)	201 (99%)	2 (1%)	82	87
1	C	241/260 (93%)	234 (97%)	7 (3%)	50	53
1	D	204/260 (78%)	201 (98%)	3 (2%)	72	78
1	E	204/260 (78%)	201 (98%)	3 (2%)	72	78
1	F	235/260 (90%)	232 (99%)	3 (1%)	76	82
All	All	1326/1560 (85%)	1306 (98%)	20 (2%)	72	78

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	315	MET
1	B	5	LEU
1	B	14	ASN
1	C	14	ASN
1	C	44	GLU
1	C	292	VAL
1	C	297	LEU
1	C	300	ILE

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Mol	Chain	Res	Type
1	C	303	ILE
1	C	307	GLU
1	D	5	LEU
1	D	14	ASN
1	D	44	GLU
1	E	4	ARG
1	E	5	LEU
1	E	14	ASN
1	F	14	ASN
1	F	44	GLU
1	F	272	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	B	54	GLN
1	B	184	GLN
1	B	196	HIS
1	C	196	HIS
1	D	196	HIS
1	F	194	GLN
1	F	196	HIS

### 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 ⓘ

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	-	44,54,54	1.42	5 (11%)	55,80,80	2.39	11 (20%)
5	GLV	B	402	2	1,4,4	0.30	0	0,4,4	0.00	-
5	GLV	D	401	2	1,4,4	0.29	0	0,4,4	0.00	-

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	-	-	1/48/69/69	0/3/3/3
5	GLV	B	402	2	-	0/0/2/2	0/0/0/0
5	GLV	D	401	2	-	0/0/2/2	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	1VU	C2-S	-4.88	1.66	1.76
4	B	401	1VU	P1-O8	-2.61	1.43	1.54
4	B	401	1VU	P2-O14	-2.28	1.43	1.51
4	B	401	1VU	P-O5	-2.10	1.43	1.51
4	B	401	1VU	O-C2	-2.02	1.17	1.21

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	1VU	N6-C20-N5	-7.74	122.97	128.89
4	B	401	1VU	O-C2-C1	-5.54	118.28	123.70
4	B	401	1VU	O-C2-S	-5.36	118.58	122.83
4	B	401	1VU	C21-C18-N3	-3.09	106.64	109.48
4	B	401	1VU	P1-O7-P	-2.73	125.05	132.73
4	B	401	1VU	O12-C22-C23	-2.42	104.17	111.16
4	B	401	1VU	C16-N2-C21	-2.21	123.60	126.94
4	B	401	1VU	O13-C23-C22	-2.15	103.14	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	1VU	O10-P1-O9	2.24	118.29	109.62
4	B	401	1VU	C11-C10-C13	2.36	111.57	108.50
4	B	401	1VU	C1-C2-S	10.88	123.14	113.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	1VU	O-C2-C1-C

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

## 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 ⓘ

### 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	314/339 (92%)	0.33	25 (7%) 15 21	12, 26, 52, 62	0
1	B	264/339 (77%)	-0.13	6 (2%) 64 70	11, 21, 36, 43	0
1	C	316/339 (93%)	0.06	22 (6%) 19 26	9, 19, 52, 77	0
1	D	265/339 (78%)	-0.05	9 (3%) 49 58	8, 17, 34, 52	0
1	E	265/339 (78%)	-0.30	5 (1%) 70 75	8, 17, 31, 53	0
1	F	309/339 (91%)	0.12	34 (11%) 7 10	8, 17, 57, 65	0
All	All	1733/2034 (85%)	0.02	101 (5%) 26 34	8, 19, 49, 77	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	287	GLY	7.4
1	B	5	LEU	6.5
1	F	278	ALA	6.2
1	C	297	LEU	6.2
1	C	301	ALA	6.1
1	C	291	THR	5.9
1	C	295	GLY	5.8
1	E	5	LEU	5.7
1	F	268	THR	5.5
1	F	276	ILE	5.3
1	F	303	ILE	5.1
1	C	5	LEU	5.1
1	F	284	LYS	5.0
1	F	281	ASP	4.9
1	A	5	LEU	4.9
1	F	266	SER	4.8
1	F	271	THR	4.6
1	A	267	GLU	4.5
1	F	277	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	298	VAL	4.4
1	A	285	ALA	4.3
1	A	268	THR	4.2
1	C	296	ARG	4.1
1	C	293	TYR	4.0
1	C	292	VAL	4.0
1	A	266	SER	4.0
1	A	313	ALA	4.0
1	F	279	ALA	3.8
1	C	287	GLY	3.8
1	D	5	LEU	3.7
1	F	269	ALA	3.7
1	F	274	ARG	3.6
1	F	285	ALA	3.6
1	A	293	TYR	3.6
1	F	310	VAL	3.6
1	C	294	LYS	3.6
1	F	5	LEU	3.5
1	F	286	ARG	3.4
1	C	4	ARG	3.4
1	F	298	VAL	3.4
1	C	299	ASP	3.4
1	F	270	VAL	3.4
1	F	275	GLU	3.4
1	C	317	SER	3.3
1	A	269	ALA	3.3
1	A	288	GLU	3.2
1	C	289	GLY	3.2
1	D	131	THR	3.1
1	D	70	ARG	3.1
1	A	284	LYS	3.1
1	B	2	SER	3.1
1	F	307	GLU	3.1
1	F	267	GLU	3.0
1	F	280	MET	3.0
1	F	291	THR	3.0
1	F	306	ALA	3.0
1	B	4	ARG	3.0
1	F	302	SER	3.0
1	D	266	SER	3.0
1	A	272	GLU	2.9
1	C	2	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	315	MET	2.8
1	E	266	SER	2.8
1	A	271	THR	2.8
1	C	267	GLU	2.7
1	F	272	GLU	2.7
1	F	293	TYR	2.7
1	A	243	LEU	2.6
1	B	265	PRO	2.6
1	F	308	VAL	2.6
1	A	206	ALA	2.6
1	A	281	ASP	2.6
1	F	301	ALA	2.5
1	E	4	ARG	2.5
1	A	270	VAL	2.5
1	F	290	ALA	2.5
1	C	300	ILE	2.4
1	A	282	ALA	2.4
1	F	309	ILE	2.4
1	A	277	LEU	2.4
1	A	220	VAL	2.4
1	B	192	ASP	2.3
1	F	297	LEU	2.3
1	F	283	ALA	2.3
1	D	2	SER	2.3
1	A	276	ILE	2.3
1	D	132	LYS	2.2
1	B	264	THR	2.2
1	D	4	ARG	2.2
1	A	292	VAL	2.2
1	E	50	ASP	2.2
1	D	140	ILE	2.2
1	E	192	ASP	2.1
1	A	131	THR	2.1
1	A	286	ARG	2.1
1	C	316	ILE	2.1
1	C	311	ARG	2.1
1	C	312	GLN	2.1
1	A	294	LYS	2.1
1	C	192	ASP	2.0
1	D	98	ASP	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
5	GLV	B	402	5/5	0.93	0.18	2.60	22,23,24,25	5
5	GLV	D	401	5/5	0.95	0.21	1.34	14,16,19,20	5
2	MG	D	402	1/1	0.95	0.18	0.55	20,20,20,20	0
4	1VU	B	401	52/52	0.89	0.14	0.19	26,36,44,48	52
3	CL	A	402	1/1	0.99	0.09	-0.83	27,27,27,27	0
2	MG	B	403	1/1	0.97	0.11	-0.96	26,26,26,26	0
2	MG	F	401	1/1	0.93	0.07	-1.40	22,22,22,22	0
3	CL	F	402	1/1	0.99	0.03	-3.09	17,17,17,17	0
3	CL	C	402	1/1	0.99	0.03	-3.72	21,21,21,21	0
3	CL	E	402	1/1	0.98	0.04	-4.31	21,21,21,21	0
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	C	401	1/1	0.98	0.03	-	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.