



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 11:51 AM EDT

PDB ID : 4HES  
Title : Structure of a Beta-Lactamase Class A-like Protein from *Veillonella parvula*.  
Authors : Cuff, M.E.; Li, H.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2012-10-04  
Resolution : 1.90 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

<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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

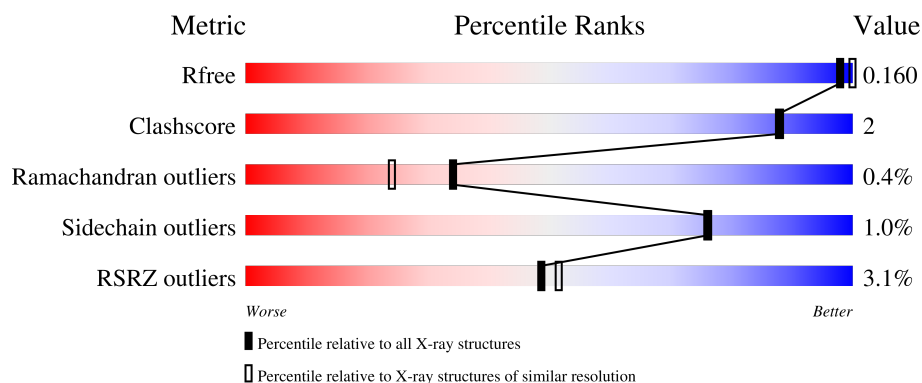
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	275	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	B	275	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	C	275	<div> <div>4%</div> <div> <div></div> <div>94%</div> <div>•••</div> </div> </div>
1	D	275	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>••</div> </div> </div>
1	E	275	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>6% •</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12560 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 Beta-lactamase class A-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	Se	0	6	0
			2229	1398	393	421	3	14			
1	B	275	Total	C	N	O	S	Se	0	9	0
			2254	1414	396	427	3	14			
1	C	268	Total	C	N	O	S	Se	0	3	0
			2142	1347	374	406	3	12			
1	D	268	Total	C	N	O	S	Se	0	4	0
			2160	1359	378	408	3	12			
1	E	268	Total	C	N	O	S	Se	0	4	0
			2158	1354	382	407	3	12			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP D1BLB4
A	-1	ASN	-	EXPRESSION TAG	UNP D1BLB4
A	0	ALA	-	EXPRESSION TAG	UNP D1BLB4
B	-2	SER	-	EXPRESSION TAG	UNP D1BLB4
B	-1	ASN	-	EXPRESSION TAG	UNP D1BLB4
B	0	ALA	-	EXPRESSION TAG	UNP D1BLB4
C	-2	SER	-	EXPRESSION TAG	UNP D1BLB4
C	-1	ASN	-	EXPRESSION TAG	UNP D1BLB4
C	0	ALA	-	EXPRESSION TAG	UNP D1BLB4
D	-2	SER	-	EXPRESSION TAG	UNP D1BLB4
D	-1	ASN	-	EXPRESSION TAG	UNP D1BLB4
D	0	ALA	-	EXPRESSION TAG	UNP D1BLB4
E	-2	SER	-	EXPRESSION TAG	UNP D1BLB4
E	-1	ASN	-	EXPRESSION TAG	UNP D1BLB4
E	0	ALA	-	EXPRESSION TAG	UNP D1BLB4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

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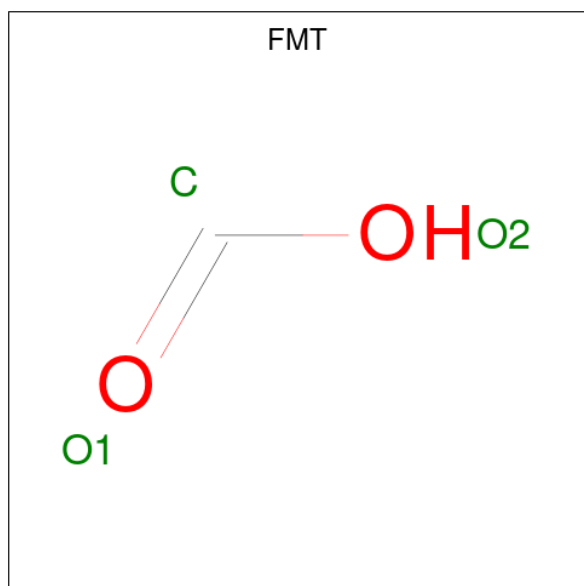
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		

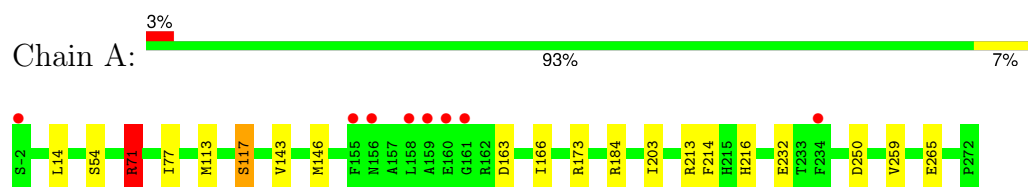
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	316	Total	O	0	0
			316	316		
5	B	337	Total	O	0	0
			337	337		
5	C	255	Total	O	0	0
			255	255		
5	D	299	Total	O	0	0
			299	299		
5	E	290	Total	O	0	0
			290	290		

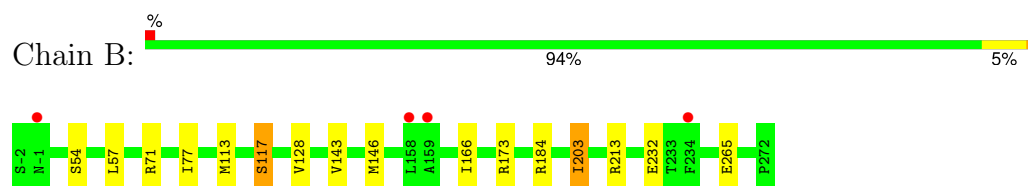
### 3 Residue-property plots [i](#)

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.

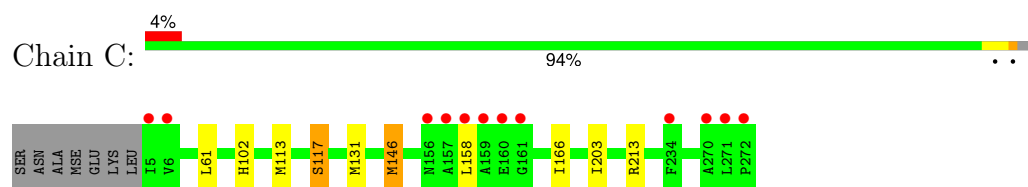
- Molecule 1: Beta-lactamase class A-like protein



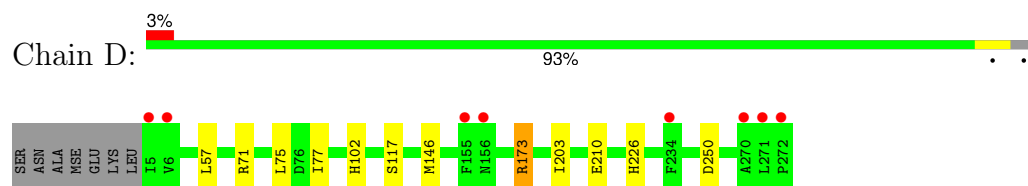
- Molecule 1: Beta-lactamase class A-like protein



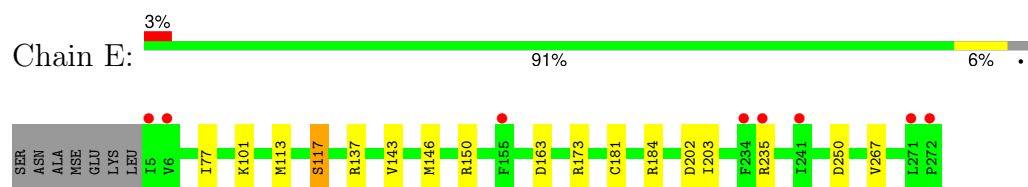
- Molecule 1: Beta-lactamase class A-like protein



- Molecule 1: Beta-lactamase class A-like protein



- Molecule 1: Beta-lactamase class A-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.40Å 163.11Å 113.01Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	33.49 – 1.90 33.49 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (33.49-1.90) 98.0 (33.49-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.137 , 0.160 0.138 , 0.160	Depositor DCC
$R_{free}$ test set	8184 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12560	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 3.38% 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: FMT, NA, 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	0.72	1/2252 (0.0%)	0.86	5/3010 (0.2%)
1	B	0.69	1/2277 (0.0%)	0.82	2/3045 (0.1%)
1	C	0.67	0/2166	0.85	4/2903 (0.1%)
1	D	0.67	0/2185	0.83	4/2927 (0.1%)
1	E	0.68	0/2182	0.85	4/2922 (0.1%)
All	All	0.69	2/11062 (0.0%)	0.84	19/14807 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	GLU	CD-OE1	5.21	1.31	1.25
1	B	232	GLU	CD-OE1	5.12	1.31	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASP	CB-CG-OD1	7.47	125.02	118.30
1	C	131	MSE	CG-SE-CE	-7.33	82.78	98.90
1	C	146	MSE	CG-SE-CE	-7.23	83.00	98.90
1	A	213	ARG	NE-CZ-NH2	6.97	123.78	120.30
1	C	213	ARG	NE-CZ-NH2	5.85	123.23	120.30
1	E	250	ASP	CB-CG-OD1	5.79	123.51	118.30
1	E	163	ASP	CB-CG-OD1	5.68	123.42	118.30
1	D	71	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	213	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	213	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	E	202	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	71	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	D	146	MSE	CG-SE-CE	5.17	110.27	98.90
1	D	173	ARG	NE-CZ-NH2	-5.13	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	202	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	250	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	213	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	A	71	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	163	ASP	CB-CG-OD1	5.05	122.84	118.30

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	2229	0	2209	13	0
1	B	2254	0	2229	11	0
1	C	2142	0	2104	6	0
1	D	2160	0	2126	5	0
1	E	2158	0	2125	8	0
2	A	12	0	16	0	0
2	B	18	0	24	0	0
2	C	12	0	16	0	0
2	D	24	0	32	2	0
2	E	36	0	48	1	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	3	0	1	1	0
4	B	3	0	2	1	0
4	C	3	0	1	1	0
4	D	3	0	2	1	0
4	E	3	0	2	0	0
5	A	316	0	0	2	0
5	B	337	0	0	4	0
5	C	255	0	0	1	0
5	D	299	0	0	1	0
5	E	290	0	0	3	0
All	All	12560	0	10937	45	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 2.

All (45) 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:146[A]:MSE:HG2	1:A:166[A]:ILE:HG13	1.71	0.73
1:B:184[B]:ARG:HG2	5:B:592:HOH:O	1.93	0.68
1:B:203[B]:ILE:HD11	5:B:608:HOH:O	1.97	0.64
1:A:146[A]:MSE:HE3	1:A:166[A]:ILE:HD12	1.81	0.61
1:B:57:LEU:HD12	1:B:166:ILE:CD1	2.30	0.61
1:A:146[A]:MSE:HE3	1:A:166[A]:ILE:CD1	2.31	0.61
1:A:146[B]:MSE:O	1:A:146[B]:MSE:HG3	2.02	0.60
1:B:54:SER:HB2	1:B:166:ILE:HG23	1.83	0.60
1:A:54:SER:HB2	1:A:166[B]:ILE:HG23	1.84	0.58
1:A:71:ARG:CZ	1:A:184[A]:ARG:HH21	2.18	0.57
1:C:61:LEU:HB2	1:C:146:MSE:HE1	1.86	0.57
5:C:560:HOH:O	1:D:210[A]:GLU:HG3	2.06	0.54
1:B:265:GLU:HG3	5:B:557:HOH:O	2.09	0.52
1:A:143:VAL:O	1:A:146[B]:MSE:HG2	2.09	0.52
1:D:102:HIS:HA	2:D:304:GOL:H12	1.93	0.51
1:C:102:HIS:HA	2:D:304:GOL:H2	1.94	0.50
1:C:146:MSE:HG2	1:C:166:ILE:HG13	1.93	0.50
1:A:71:ARG:NH1	1:A:184[A]:ARG:HH21	2.09	0.50
1:A:265:GLU:HG3	5:A:568:HOH:O	2.12	0.48
1:D:173:ARG:HD3	5:D:562:HOH:O	2.13	0.48
1:B:54:SER:CB	1:B:166:ILE:HG23	2.44	0.48
1:E:113:MSE:O	1:E:117:SER:HA	2.14	0.47
1:E:137:ARG:HH22	2:E:306:GOL:H2	1.79	0.47
1:A:14:LEU:HD22	1:A:259:VAL:HG13	1.97	0.47
1:B:146[B]:MSE:HG3	1:B:146[B]:MSE:O	2.14	0.47
1:E:181:CYS:HA	1:E:184[A]:ARG:HG3	1.97	0.47
1:B:113:MSE:O	1:B:117:SER:HA	2.15	0.46
1:B:173:ARG:HD3	5:B:509:HOH:O	2.15	0.46
1:E:235:ARG:HD2	1:E:267:VAL:O	2.16	0.46
1:C:146:MSE:HE3	1:C:146:MSE:HB3	1.71	0.46
1:E:101:LYS:HE2	5:E:661:HOH:O	2.16	0.46
1:E:150:ARG:CZ	5:E:519:HOH:O	2.65	0.45
1:B:143:VAL:O	1:B:146[B]:MSE:HG2	2.15	0.45
1:E:173:ARG:HD3	5:E:564:HOH:O	2.16	0.45
4:A:304:FMT:O1	4:B:304:FMT:O2	2.29	0.44
1:C:146:MSE:HB2	1:C:146:MSE:HE2	1.83	0.44
1:D:57:LEU:HD11	1:D:226:HIS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:MSE:O	1:C:117:SER:HA	2.18	0.43
1:D:75:LEU:C	1:D:75:LEU:HD12	2.40	0.42
1:E:143:VAL:O	1:E:146:MSE:HG2	2.19	0.42
4:C:303:FMT:O1	4:D:305:FMT:O2	2.33	0.42
1:B:128[A]:VAL:O	1:B:128[A]:VAL:HG12	2.20	0.42
1:A:214:PHE:CD2	1:A:216:HIS:CG	3.08	0.41
1:A:173:ARG:HD3	5:A:652:HOH:O	2.20	0.41
1:A:113:MSE:O	1:A:117:SER:HA	2.20	0.41

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	279/275 (102%)	273 (98%)	5 (2%)	1 (0%)	34	24
1	B	282/275 (102%)	274 (97%)	6 (2%)	2 (1%)	22	12
1	C	269/275 (98%)	263 (98%)	5 (2%)	1 (0%)	34	24
1	D	270/275 (98%)	266 (98%)	3 (1%)	1 (0%)	34	24
1	E	270/275 (98%)	264 (98%)	5 (2%)	1 (0%)	34	24
All	All	1370/1375 (100%)	1340 (98%)	24 (2%)	6 (0%)	34	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	203	ILE
1	E	203	ILE
1	A	203	ILE
1	C	203	ILE
1	B	203[A]	ILE
1	B	203[B]	ILE

### 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	241/223 (108%)	238 (99%)	3 (1%)	71	70
1	B	244/223 (109%)	242 (99%)	2 (1%)	81	82
1	C	230/223 (103%)	228 (99%)	2 (1%)	78	79
1	D	233/223 (104%)	231 (99%)	2 (1%)	78	79
1	E	232/223 (104%)	230 (99%)	2 (1%)	78	79
All	All	1180/1115 (106%)	1169 (99%)	11 (1%)	76	79

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	A	77	ILE
1	A	117	SER
1	B	77	ILE
1	B	117	SER
1	C	117	SER
1	C	158	LEU
1	D	77	ILE
1	D	117	SER
1	E	77	ILE
1	E	117	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 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	$\# Z  > 2$
2	GOL	E	305	-	5,5,5	0.38	0	5,5,5	0.41	0
2	GOL	D	302	-	5,5,5	0.49	0	5,5,5	0.79	0
2	GOL	A	302	-	5,5,5	1.06	0	5,5,5	2.09	2 (40%)
2	GOL	B	302	-	5,5,5	0.68	0	5,5,5	0.45	0
2	GOL	E	302	-	5,5,5	0.64	0	5,5,5	0.48	0
2	GOL	B	301	-	5,5,5	0.33	0	5,5,5	0.32	0
2	GOL	A	301	-	5,5,5	0.63	0	5,5,5	0.56	0
2	GOL	E	306	-	5,5,5	0.46	0	5,5,5	0.89	0
4	FMT	A	304	3	2,2,2	1.49	0	1,1,1	0.35	0
2	GOL	E	301	-	5,5,5	0.47	0	5,5,5	0.52	0
2	GOL	C	302	-	5,5,5	0.39	0	5,5,5	0.71	0
2	GOL	D	301	-	5,5,5	0.33	0	5,5,5	0.48	0
4	FMT	D	305	3	2,2,2	1.45	0	1,1,1	0.21	0
4	FMT	B	304	3	2,2,2	1.35	0	1,1,1	0.50	0
2	GOL	D	304	-	5,5,5	0.30	0	5,5,5	0.97	0
2	GOL	D	303	-	5,5,5	0.65	0	5,5,5	0.61	0
2	GOL	E	304	-	5,5,5	0.31	0	5,5,5	0.48	0
4	FMT	E	308	3	2,2,2	1.43	0	1,1,1	0.34	0
4	FMT	C	303	3	2,2,2	1.21	0	1,1,1	0.41	0
2	GOL	C	301	-	5,5,5	0.38	0	5,5,5	0.64	0
2	GOL	E	303	-	5,5,5	0.64	0	5,5,5	0.34	0
2	GOL	B	303	-	5,5,5	0.76	0	5,5,5	0.55	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
2	GOL	E	301	-	-	2/4/4/4	-
2	GOL	C	302	-	-	2/4/4/4	-
2	GOL	D	303	-	-	0/4/4/4	-
2	GOL	E	304	-	-	0/4/4/4	-
2	GOL	E	305	-	-	0/4/4/4	-
2	GOL	D	301	-	-	2/4/4/4	-
2	GOL	A	301	-	-	2/4/4/4	-
2	GOL	D	302	-	-	0/4/4/4	-
2	GOL	C	301	-	-	0/4/4/4	-
2	GOL	A	302	-	-	3/4/4/4	-
2	GOL	B	302	-	-	0/4/4/4	-
2	GOL	B	303	-	-	0/4/4/4	-
2	GOL	E	302	-	-	0/4/4/4	-
2	GOL	E	303	-	-	3/4/4/4	-
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	D	304	-	-	0/4/4/4	-
2	GOL	E	306	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	GOL	O2-C2-C1	-3.48	94.77	109.18
2	A	302	GOL	O2-C2-C3	2.48	119.46	109.18

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	C1-C2-C3-O3
2	A	302	GOL	O1-C1-C2-O2
2	B	301	GOL	C1-C2-C3-O3
2	C	302	GOL	O1-C1-C2-O2
2	C	302	GOL	O1-C1-C2-C3
2	E	301	GOL	C1-C2-C3-O3
2	E	303	GOL	O1-C1-C2-C3
2	A	302	GOL	O1-C1-C2-C3
2	E	306	GOL	O1-C1-C2-C3
2	A	302	GOL	O2-C2-C3-O3
2	E	303	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	301	GOL	O2-C2-C3-O3
2	E	301	GOL	O2-C2-C3-O3
2	A	301	GOL	O2-C2-C3-O3
2	E	303	GOL	O2-C2-C3-O3
2	E	306	GOL	O1-C1-C2-O2
2	D	301	GOL	C1-C2-C3-O3
2	D	301	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	306	GOL	1	0
4	A	304	FMT	1	0
4	D	305	FMT	1	0
4	B	304	FMT	1	0
2	D	304	GOL	2	0
4	C	303	FMT	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	262/275 (95%)	-0.21	8 (3%) 49 51	12, 18, 34, 66	0
1	B	262/275 (95%)	-0.28	4 (1%) 73 76	12, 17, 36, 58	0
1	C	256/275 (93%)	-0.03	12 (4%) 31 34	12, 21, 47, 76	0
1	D	256/275 (93%)	-0.15	8 (3%) 49 51	12, 19, 38, 75	0
1	E	256/275 (93%)	-0.13	8 (3%) 49 51	12, 18, 36, 68	0
All	All	1292/1375 (93%)	-0.16	40 (3%) 49 51	12, 19, 38, 76	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	PHE	5.7
1	E	272	PRO	5.5
1	D	272	PRO	5.1
1	C	272	PRO	4.8
1	E	234	PHE	4.5
1	C	158	LEU	4.5
1	C	5	ILE	4.5
1	A	159	ALA	4.4
1	E	5	ILE	4.3
1	C	234	PHE	4.3
1	D	6	VAL	4.3
1	C	159	ALA	4.2
1	D	234	PHE	3.8
1	B	234	PHE	3.7
1	D	5	ILE	3.5
1	C	161	GLY	3.4
1	C	6	VAL	3.4
1	A	158	LEU	3.3
1	C	157	ALA	3.1
1	C	270	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	271	LEU	2.9
1	B	158	LEU	2.9
1	B	159	ALA	2.7
1	E	6	VAL	2.7
1	B	-1	ASN	2.6
1	A	-2	SER	2.6
1	A	155	PHE	2.6
1	A	234	PHE	2.6
1	A	160	GLU	2.5
1	C	156	ASN	2.5
1	A	161	GLY	2.4
1	E	235	ARG	2.4
1	C	271	LEU	2.3
1	D	270	ALA	2.3
1	A	156	ASN	2.3
1	E	271	LEU	2.2
1	E	155	PHE	2.2
1	E	241	ILE	2.1
1	C	160	GLU	2.1
1	D	156	ASN	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 monosaccharides 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
2	GOL	E	305	6/6	0.63	0.30	63,68,75,79	0
2	GOL	E	303	6/6	0.73	0.27	35,53,57,60	0
2	GOL	E	304	6/6	0.77	0.34	43,57,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	301	6/6	0.77	0.37	49,55,55,55	0
2	GOL	C	302	6/6	0.83	0.26	41,49,51,58	0
2	GOL	A	302	6/6	0.83	0.26	30,38,39,39	0
2	GOL	B	301	6/6	0.84	0.25	54,57,59,60	0
2	GOL	D	301	6/6	0.84	0.21	42,43,48,48	0
2	GOL	D	304	6/6	0.84	0.26	36,39,45,55	0
2	GOL	E	306	6/6	0.88	0.15	38,46,51,54	0
2	GOL	C	301	6/6	0.90	0.17	48,51,56,56	0
2	GOL	E	301	6/6	0.91	0.15	42,48,49,50	0
4	FMT	B	304	3/3	0.91	0.15	26,26,26,31	0
4	FMT	D	305	3/3	0.91	0.12	28,28,32,39	0
2	GOL	E	302	6/6	0.94	0.16	21,25,25,26	0
4	FMT	E	308	3/3	0.94	0.10	26,26,27,31	0
2	GOL	D	303	6/6	0.95	0.12	21,25,26,27	0
4	FMT	C	303	3/3	0.95	0.10	28,28,28,34	0
3	NA	A	303	1/1	0.95	0.18	28,28,28,28	0
4	FMT	A	304	3/3	0.95	0.11	21,21,24,29	0
2	GOL	D	302	6/6	0.96	0.15	21,24,25,26	0
2	GOL	B	303	6/6	0.96	0.13	20,24,25,25	0
2	GOL	B	302	6/6	0.96	0.15	20,23,25,25	0
3	NA	E	307	1/1	0.97	0.16	29,29,29,29	1
3	NA	D	306	1/1	0.99	0.16	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.