



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:24 AM UTC

PDB ID : 2R2D / pdb\_00002r2d  
Title : Structure of a quorum-quenching lactonase (AiiB) from *Agrobacterium tumefaciens*  
Authors : Liu, D.; Thomas, P.W.; Momb, J.; Hoang, Q.; Petsko, G.A.; Ringe, D.; Fast, W.  
Deposited on : 2007-08-24  
Resolution : 1.75 Å(reported)

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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 : 4-5-2 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

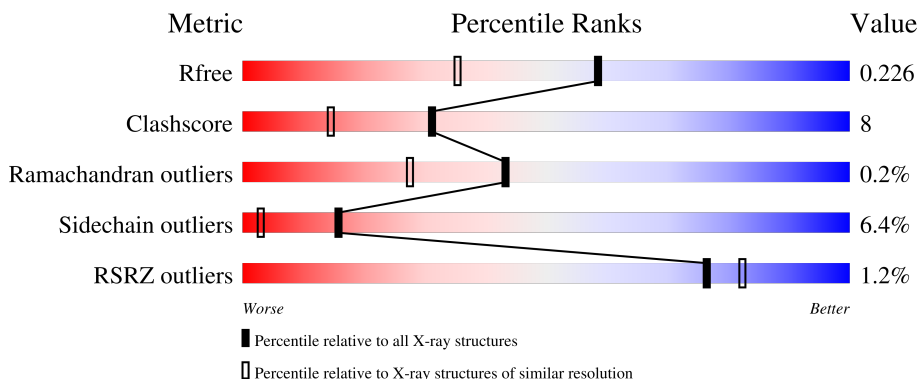
# 1 Overall quality at a glance

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.



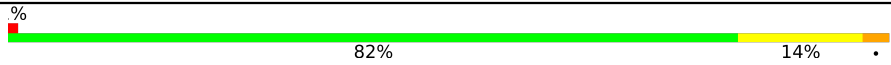
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	276	 88% 11% .
1	B	276	 84% 13% .
1	C	276	 87% 12% .
1	D	276	 83% 13% .
1	E	276	 79% 18% . .

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Mol	Chain	Length	Quality of chain
1	F	276	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a green segment on the left labeled '82%' and a yellow segment on the right labeled '14%'. A small red square is at the beginning of the bar, and a small black dot is at the end. A '%' symbol is positioned above the bar.</p>

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	GOL	B	282	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15215 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.

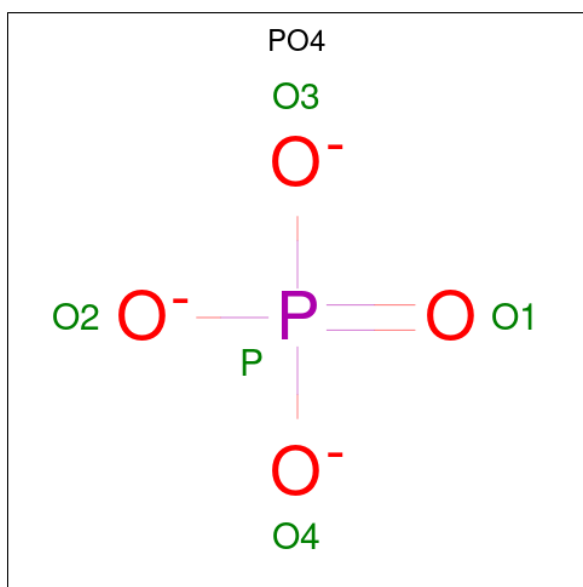
- Molecule 1 is a protein called Zn-dependent hydrolases.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	17	0
			2278	1433	408	428	9			
1	B	276	Total	C	N	O	S	0	17	0
			2264	1430	404	421	9			
1	C	276	Total	C	N	O	S	0	18	0
			2271	1427	404	431	9			
1	D	276	Total	C	N	O	S	0	14	0
			2244	1409	400	426	9			
1	E	276	Total	C	N	O	S	0	23	0
			2311	1454	407	440	10			
1	F	276	Total	C	N	O	S	0	6	0
			2200	1383	392	416	9			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

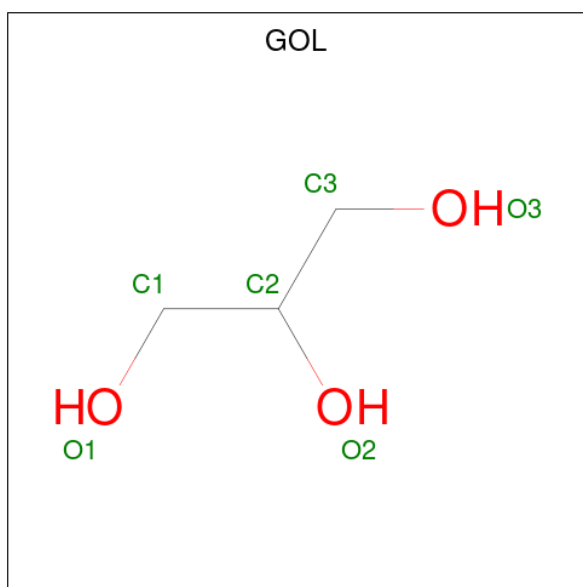
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 10 8 2	0	1
3	D	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	301	Total O 301 301	0	0
5	B	277	Total O 277 277	0	0

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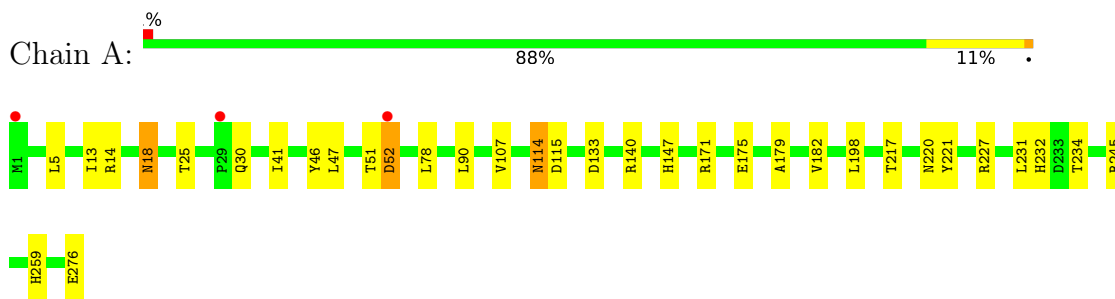
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	C	303	Total 305	O 305	0	2
5	D	201	Total 201	O 201	0	0
5	E	239	Total 239	O 239	0	0
5	F	200	Total 202	O 202	0	2

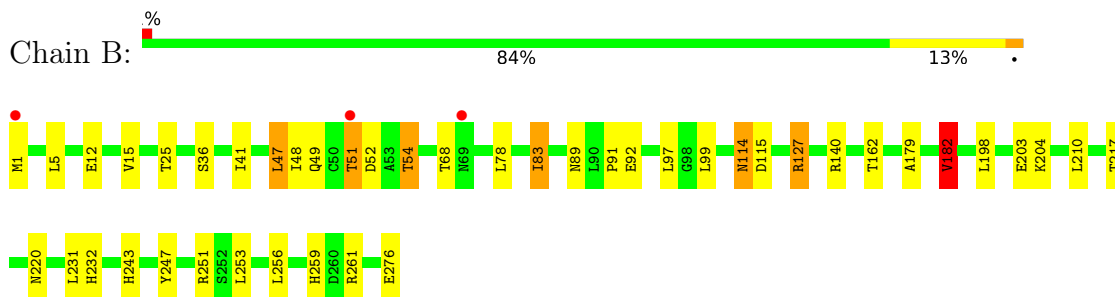
### 3 Residue-property plots [i](#)

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.

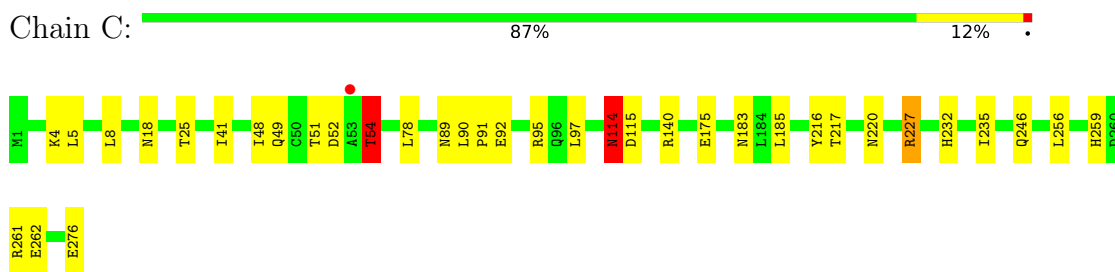
- Molecule 1: Zn-dependent hydrolases



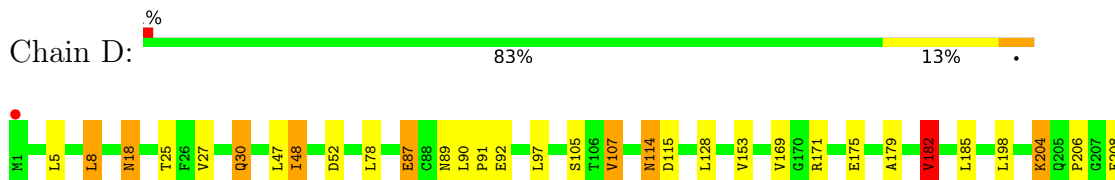
- Molecule 1: Zn-dependent hydrolases



- Molecule 1: Zn-dependent hydrolases

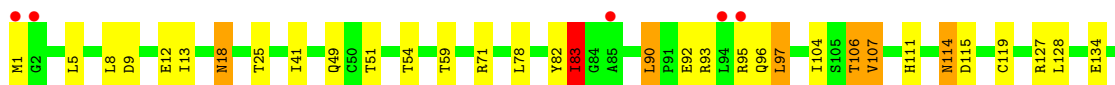
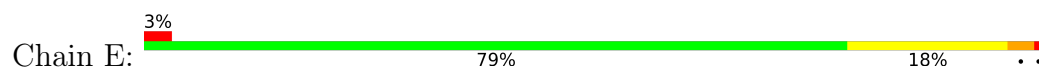


- Molecule 1: Zn-dependent hydrolases

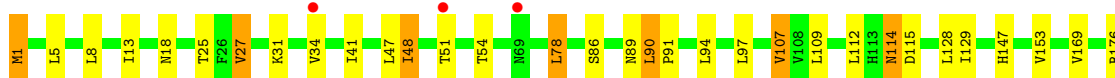
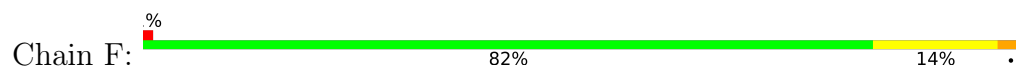




- Molecule 1: Zn-dependent hydrolases



- Molecule 1: Zn-dependent hydrolases



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.15Å 158.03Å 80.44Å 90.00° 104.48° 90.00°	Depositor
Resolution (Å)	18.10 – 1.75 18.10 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.5 (18.10-1.75) 96.5 (18.10-1.75)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.159 , 0.213 (Not available) , 0.226	Depositor DCC
$R_{free}$ test set	9324 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 61.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.012 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	15215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: ZN, PO4, 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	0.83	0/2362	0.86	0/3207
1	B	0.78	1/2360 (0.0%)	0.87	1/3204 (0.0%)
1	C	0.81	0/2359	0.85	1/3204 (0.0%)
1	D	0.74	0/2321	0.92	1/3153 (0.0%)
1	E	0.79	0/2397	0.92	2/3255 (0.1%)
1	F	0.75	0/2272	0.90	1/3087 (0.0%)
All	All	0.79	1/14071 (0.0%)	0.89	6/19110 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	VAL	CA-CB	5.07	1.60	1.55

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	182	VAL	CB-CA-C	6.54	120.06	110.77
1	D	182	VAL	CB-CA-C	5.76	118.29	111.32
1	E	270	SER	N-CA-C	5.68	118.38	111.78
1	E	83	ILE	CB-CA-C	5.56	117.05	110.93
1	B	182	VAL	CB-CA-C	5.18	116.89	110.73

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	2278	0	2246	24	1
1	B	2264	0	2250	46	0
1	C	2271	0	2224	35	0
1	D	2244	0	2197	26	0
1	E	2311	0	2268	64	2
1	F	2200	0	2146	30	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	15	0	0	1	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
3	F	5	0	0	0	0
4	A	18	0	24	3	0
4	B	12	0	16	10	0
4	C	12	0	16	2	0
4	D	6	0	8	0	0
4	E	6	0	8	0	0
4	F	6	0	8	1	0
5	A	301	0	0	8	0
5	B	277	0	0	10	0
5	C	305	0	0	3	0
5	D	201	0	0	3	1
5	E	239	0	0	7	0
5	F	202	0	0	5	0
All	All	15215	0	13411	222	2

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 8.

The worst 5 of 222 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:E:93[A]:ARG:NH1	1:E:269[A]:LYS:HD2	1.46	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261[B]:ARG:CZ	1:C:262[B]:GLU:OE2	1.86	1.23
1:E:267[A]:LEU:O	1:E:268[A]:ILE:HG13	1.35	1.21
1:C:261[B]:ARG:NH2	1:C:262[B]:GLU:OE2	1.74	1.20
1:E:93[A]:ARG:HH11	1:E:269[A]:LYS:CD	1.57	1.18

All (2) 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)
1:E:97:LEU:O	5:D:446:HOH:O[1_556]	2.13	0.07
1:A:231:LEU:O	1:E:227[A]:ARG:NH2[1_455]	2.18	0.02

## 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	292/276 (106%)	281 (96%)	11 (4%)	0	100	100
1	B	291/276 (105%)	277 (95%)	14 (5%)	0	100	100
1	C	292/276 (106%)	282 (97%)	9 (3%)	1 (0%)	36	21
1	D	288/276 (104%)	275 (96%)	11 (4%)	2 (1%)	18	7
1	E	296/276 (107%)	280 (95%)	14 (5%)	2 (1%)	18	7
1	F	281/276 (102%)	269 (96%)	12 (4%)	0	100	100
All	All	1740/1656 (105%)	1664 (96%)	71 (4%)	5 (0%)	43	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	269[A]	LYS
1	E	269[B]	LYS
1	D	204[A]	LYS

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Mol	Chain	Res	Type
1	D	204[B]	LYS
1	C	114	ASN

### 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	249/232 (107%)	237 (95%)	12 (5%)	23 6
1	B	249/232 (107%)	236 (95%)	13 (5%)	21 5
1	C	250/232 (108%)	241 (96%)	9 (4%)	31 11
1	D	246/232 (106%)	223 (91%)	23 (9%)	8 1
1	E	253/232 (109%)	228 (90%)	25 (10%)	7 1
1	F	239/232 (103%)	221 (92%)	18 (8%)	12 2
All	All	1486/1392 (107%)	1386 (93%)	100 (7%)	16 3

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1[A]	MET
1	E	162[B]	THR
1	F	268	ILE
1	E	18	ASN
1	E	106	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	49	GLN
1	F	89	ASN
1	F	220	ASN
1	C	114	ASN
1	C	89	ASN

### 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](#)

Of 32 ligands modelled in this entry, 12 are monoatomic - leaving 20 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	GOL	F	280	-	5,5,5	0.45	0	5,5,5	0.59	0
3	PO4	A	279	2	4,4,4	0.98	0	6,6,6	0.67	0
4	GOL	D	280	-	5,5,5	0.50	0	5,5,5	0.78	0
4	GOL	C	282	-	5,5,5	0.28	0	5,5,5	0.47	0
4	GOL	C	281	-	5,5,5	0.29	0	5,5,5	0.89	0
3	PO4	E	279	2	4,4,4	0.89	0	6,6,6	0.91	0
3	PO4	C	280[B]	-	4,4,4	1.10	0	6,6,6	0.48	0
3	PO4	F	279	2	4,4,4	0.73	0	6,6,6	0.60	0
4	GOL	B	282	-	5,5,5	0.41	0	5,5,5	0.91	0
3	PO4	D	279	2	4,4,4	0.68	0	6,6,6	0.42	0
4	GOL	E	281	-	5,5,5	0.45	0	5,5,5	0.73	0
3	PO4	E	280	-	4,4,4	0.96	0	6,6,6	0.49	0
4	GOL	A	282	-	5,5,5	0.45	0	5,5,5	0.48	0
4	GOL	A	281	-	5,5,5	0.47	0	5,5,5	0.63	0
3	PO4	C	280[A]	-	4,4,4	0.99	0	6,6,6	0.66	0
4	GOL	A	280	-	5,5,5	0.44	0	5,5,5	0.89	0
3	PO4	C	279	2	4,4,4	1.17	0	6,6,6	0.62	0
3	PO4	B	279	2	4,4,4	1.03	0	6,6,6	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	B	280	-	4,4,4	0.96	0	6,6,6	0.62	0
4	GOL	B	281	-	5,5,5	0.40	0	5,5,5	0.75	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	GOL	F	280	-	-	2/4/4/4	-
4	GOL	E	281	-	-	3/4/4/4	-
4	GOL	D	280	-	-	3/4/4/4	-
4	GOL	A	282	-	-	2/4/4/4	-
4	GOL	B	282	-	-	2/4/4/4	-
4	GOL	C	282	-	-	2/4/4/4	-
4	GOL	A	281	-	-	2/4/4/4	-
4	GOL	B	281	-	-	2/4/4/4	-
4	GOL	C	281	-	-	0/4/4/4	-
4	GOL	A	280	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	280	GOL	C1-C2-C3-O3
4	A	282	GOL	C1-C2-C3-O3
4	A	282	GOL	O2-C2-C3-O3
4	C	282	GOL	O1-C1-C2-C3
4	D	280	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	280	GOL	1	0
4	C	282	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	281	GOL	1	0
4	B	282	GOL	10	0
4	A	282	GOL	1	0
3	C	280[A]	PO4	1	0
4	A	280	GOL	2	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	276/276 (100%)	-0.42	3 (1%) 78 83	11, 28, 42, 56	17 (6%)
1	B	276/276 (100%)	-0.29	3 (1%) 78 83	15, 31, 44, 63	17 (6%)
1	C	276/276 (100%)	-0.39	1 (0%) 88 91	14, 28, 40, 53	18 (6%)
1	D	276/276 (100%)	-0.01	2 (0%) 84 88	16, 34, 54, 65	14 (5%)
1	E	276/276 (100%)	0.08	8 (2%) 53 60	15, 35, 51, 58	23 (8%)
1	F	276/276 (100%)	0.01	3 (1%) 78 83	19, 38, 50, 69	6 (2%)
All	All	1656/1656 (100%)	-0.17	20 (1%) 76 82	11, 32, 48, 69	95 (5%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34[A]	VAL	5.5
1	E	267[A]	LEU	5.3
1	E	2[A]	GLY	4.5
1	E	85	ALA	3.2
1	E	274	PHE	3.0

### 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
4	GOL	A	281	6/6	0.74	0.13	47,55,56,57	0
4	GOL	B	281	6/6	0.81	0.13	51,53,55,55	0
3	PO4	E	280	5/5	0.83	0.14	47,48,49,50	5
4	GOL	A	282	6/6	0.84	0.08	52,52,53,53	0
4	GOL	B	282	6/6	0.85	0.10	43,50,53,57	0
4	GOL	D	280	6/6	0.89	0.08	46,47,49,51	0
4	GOL	F	280	6/6	0.90	0.09	51,53,53,55	0
4	GOL	E	281	6/6	0.91	0.09	49,51,52,52	0
4	GOL	C	281	6/6	0.91	0.10	40,43,44,50	0
4	GOL	C	282	6/6	0.92	0.07	46,53,54,56	0
3	PO4	B	280	5/5	0.92	0.13	46,48,49,49	5
4	GOL	A	280	6/6	0.93	0.07	40,42,43,43	0
3	PO4	C	280[B]	5/5	0.96	0.11	43,44,46,46	5
3	PO4	C	280[A]	5/5	0.96	0.11	42,44,44,44	5
3	PO4	B	279	5/5	0.99	0.04	26,26,28,29	0
3	PO4	F	279	5/5	0.99	0.03	30,31,35,35	0
3	PO4	D	279	5/5	0.99	0.03	29,29,30,31	0
3	PO4	E	279	5/5	0.99	0.04	32,33,35,36	0
2	ZN	C	277	1/1	1.00	0.01	24,24,24,24	0
2	ZN	C	278	1/1	1.00	0.02	23,23,23,23	0
2	ZN	D	277	1/1	1.00	0.01	30,30,30,30	0
2	ZN	D	278	1/1	1.00	0.02	28,28,28,28	0
2	ZN	E	277	1/1	1.00	0.02	32,32,32,32	0
2	ZN	E	278	1/1	1.00	0.02	29,29,29,29	0
2	ZN	F	277	1/1	1.00	0.01	33,33,33,33	0
2	ZN	F	278	1/1	1.00	0.01	32,32,32,32	0
3	PO4	A	279	5/5	1.00	0.03	22,23,25,28	0
2	ZN	A	277	1/1	1.00	0.02	24,24,24,24	0
2	ZN	A	278	1/1	1.00	0.02	23,23,23,23	0
3	PO4	C	279	5/5	1.00	0.03	21,23,25,25	0
2	ZN	B	277	1/1	1.00	0.02	27,27,27,27	0
2	ZN	B	278	1/1	1.00	0.04	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.