



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:25 PM GMT

PDB ID : 3TW9  
Title : Crystal structure of gluconate dehydratase (TARGET EFI-501679) from Salmonella enterica subsp. enterica serovar Enteritidis str. P125109  
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2011-09-21  
Resolution : 1.70 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

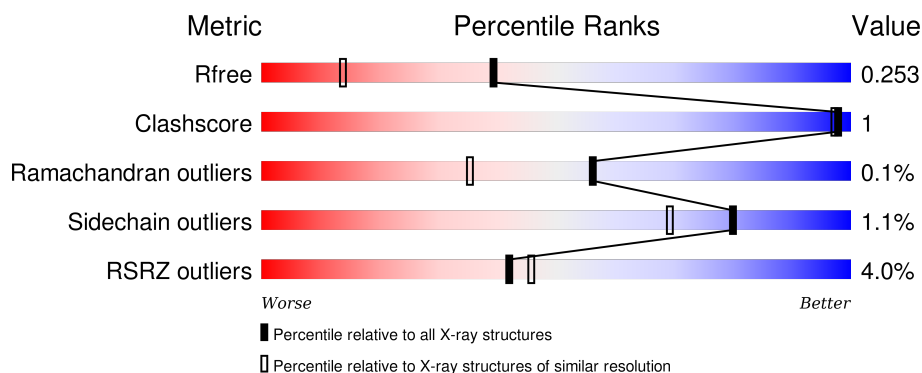
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	442	<div> <div>3%</div> <div>86%</div> <div>11%</div> </div>
1	B	442	<div> <div>5%</div> <div>89%</div> <div>7%</div> </div>
1	C	442	<div> <div>2%</div> <div>87%</div> <div>11%</div> </div>
1	D	442	<div> <div>5%</div> <div>89%</div> <div>8%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13901 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 Putative dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	7	0
			3110	1981	531	577	21			
1	B	410	Total	C	N	O	S	0	9	0
			3244	2070	552	601	21			
1	C	395	Total	C	N	O	S	0	7	0
			3115	1986	527	581	21			
1	D	408	Total	C	N	O	S	0	9	0
			3226	2056	550	599	21			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP B5R541
A	-21	HIS	-	EXPRESSION TAG	UNP B5R541
A	-20	HIS	-	EXPRESSION TAG	UNP B5R541
A	-19	HIS	-	EXPRESSION TAG	UNP B5R541
A	-18	HIS	-	EXPRESSION TAG	UNP B5R541
A	-17	HIS	-	EXPRESSION TAG	UNP B5R541
A	-16	HIS	-	EXPRESSION TAG	UNP B5R541
A	-15	SER	-	EXPRESSION TAG	UNP B5R541
A	-14	SER	-	EXPRESSION TAG	UNP B5R541
A	-13	GLY	-	EXPRESSION TAG	UNP B5R541
A	-12	VAL	-	EXPRESSION TAG	UNP B5R541
A	-11	ASP	-	EXPRESSION TAG	UNP B5R541
A	-10	LEU	-	EXPRESSION TAG	UNP B5R541
A	-9	GLY	-	EXPRESSION TAG	UNP B5R541
A	-8	THR	-	EXPRESSION TAG	UNP B5R541
A	-7	GLU	-	EXPRESSION TAG	UNP B5R541
A	-6	ASN	-	EXPRESSION TAG	UNP B5R541
A	-5	LEU	-	EXPRESSION TAG	UNP B5R541
A	-4	TYR	-	EXPRESSION TAG	UNP B5R541
A	-3	PHE	-	EXPRESSION TAG	UNP B5R541
A	-2	GLN	-	EXPRESSION TAG	UNP B5R541

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP B5R541
A	0	MET	-	EXPRESSION TAG	UNP B5R541
B	-22	MET	-	EXPRESSION TAG	UNP B5R541
B	-21	HIS	-	EXPRESSION TAG	UNP B5R541
B	-20	HIS	-	EXPRESSION TAG	UNP B5R541
B	-19	HIS	-	EXPRESSION TAG	UNP B5R541
B	-18	HIS	-	EXPRESSION TAG	UNP B5R541
B	-17	HIS	-	EXPRESSION TAG	UNP B5R541
B	-16	HIS	-	EXPRESSION TAG	UNP B5R541
B	-15	SER	-	EXPRESSION TAG	UNP B5R541
B	-14	SER	-	EXPRESSION TAG	UNP B5R541
B	-13	GLY	-	EXPRESSION TAG	UNP B5R541
B	-12	VAL	-	EXPRESSION TAG	UNP B5R541
B	-11	ASP	-	EXPRESSION TAG	UNP B5R541
B	-10	LEU	-	EXPRESSION TAG	UNP B5R541
B	-9	GLY	-	EXPRESSION TAG	UNP B5R541
B	-8	THR	-	EXPRESSION TAG	UNP B5R541
B	-7	GLU	-	EXPRESSION TAG	UNP B5R541
B	-6	ASN	-	EXPRESSION TAG	UNP B5R541
B	-5	LEU	-	EXPRESSION TAG	UNP B5R541
B	-4	TYR	-	EXPRESSION TAG	UNP B5R541
B	-3	PHE	-	EXPRESSION TAG	UNP B5R541
B	-2	GLN	-	EXPRESSION TAG	UNP B5R541
B	-1	SER	-	EXPRESSION TAG	UNP B5R541
B	0	MET	-	EXPRESSION TAG	UNP B5R541
C	-22	MET	-	EXPRESSION TAG	UNP B5R541
C	-21	HIS	-	EXPRESSION TAG	UNP B5R541
C	-20	HIS	-	EXPRESSION TAG	UNP B5R541
C	-19	HIS	-	EXPRESSION TAG	UNP B5R541
C	-18	HIS	-	EXPRESSION TAG	UNP B5R541
C	-17	HIS	-	EXPRESSION TAG	UNP B5R541
C	-16	HIS	-	EXPRESSION TAG	UNP B5R541
C	-15	SER	-	EXPRESSION TAG	UNP B5R541
C	-14	SER	-	EXPRESSION TAG	UNP B5R541
C	-13	GLY	-	EXPRESSION TAG	UNP B5R541
C	-12	VAL	-	EXPRESSION TAG	UNP B5R541
C	-11	ASP	-	EXPRESSION TAG	UNP B5R541
C	-10	LEU	-	EXPRESSION TAG	UNP B5R541
C	-9	GLY	-	EXPRESSION TAG	UNP B5R541
C	-8	THR	-	EXPRESSION TAG	UNP B5R541
C	-7	GLU	-	EXPRESSION TAG	UNP B5R541
C	-6	ASN	-	EXPRESSION TAG	UNP B5R541

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	LEU	-	EXPRESSION TAG	UNP B5R541
C	-4	TYR	-	EXPRESSION TAG	UNP B5R541
C	-3	PHE	-	EXPRESSION TAG	UNP B5R541
C	-2	GLN	-	EXPRESSION TAG	UNP B5R541
C	-1	SER	-	EXPRESSION TAG	UNP B5R541
C	0	MET	-	EXPRESSION TAG	UNP B5R541
D	-22	MET	-	EXPRESSION TAG	UNP B5R541
D	-21	HIS	-	EXPRESSION TAG	UNP B5R541
D	-20	HIS	-	EXPRESSION TAG	UNP B5R541
D	-19	HIS	-	EXPRESSION TAG	UNP B5R541
D	-18	HIS	-	EXPRESSION TAG	UNP B5R541
D	-17	HIS	-	EXPRESSION TAG	UNP B5R541
D	-16	HIS	-	EXPRESSION TAG	UNP B5R541
D	-15	SER	-	EXPRESSION TAG	UNP B5R541
D	-14	SER	-	EXPRESSION TAG	UNP B5R541
D	-13	GLY	-	EXPRESSION TAG	UNP B5R541
D	-12	VAL	-	EXPRESSION TAG	UNP B5R541
D	-11	ASP	-	EXPRESSION TAG	UNP B5R541
D	-10	LEU	-	EXPRESSION TAG	UNP B5R541
D	-9	GLY	-	EXPRESSION TAG	UNP B5R541
D	-8	THR	-	EXPRESSION TAG	UNP B5R541
D	-7	GLU	-	EXPRESSION TAG	UNP B5R541
D	-6	ASN	-	EXPRESSION TAG	UNP B5R541
D	-5	LEU	-	EXPRESSION TAG	UNP B5R541
D	-4	TYR	-	EXPRESSION TAG	UNP B5R541
D	-3	PHE	-	EXPRESSION TAG	UNP B5R541
D	-2	GLN	-	EXPRESSION TAG	UNP B5R541
D	-1	SER	-	EXPRESSION TAG	UNP B5R541
D	0	MET	-	EXPRESSION TAG	UNP B5R541

- 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	B	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		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	3	Total	Cl	0	0
			3	3		
3	D	2	Total	Cl	0	0
			2	2		
3	C	4	Total	Cl	0	0
			4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	298	Total	O	0	0
			298	298		

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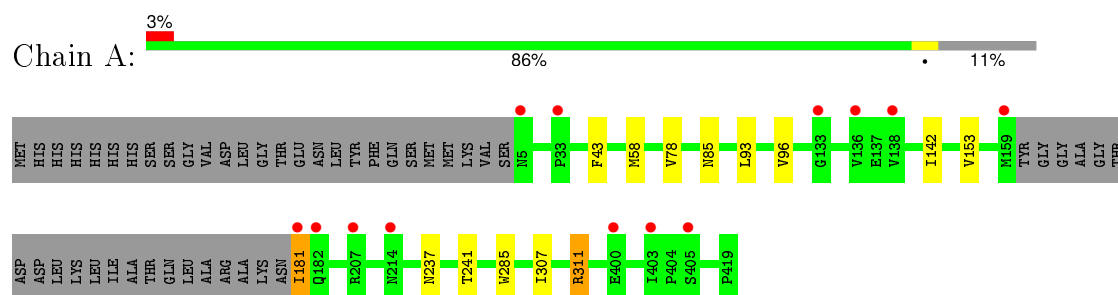
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	279	Total 279	O 279	0	0
4	C	297	Total 297	O 297	0	0
4	D	297	Total 297	O 297	0	0

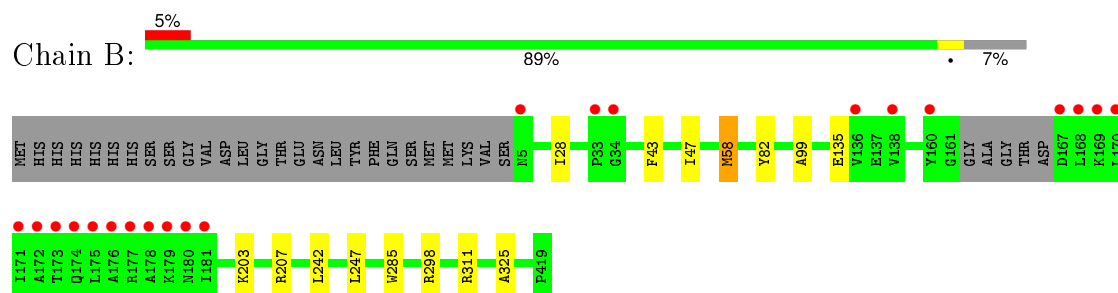
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

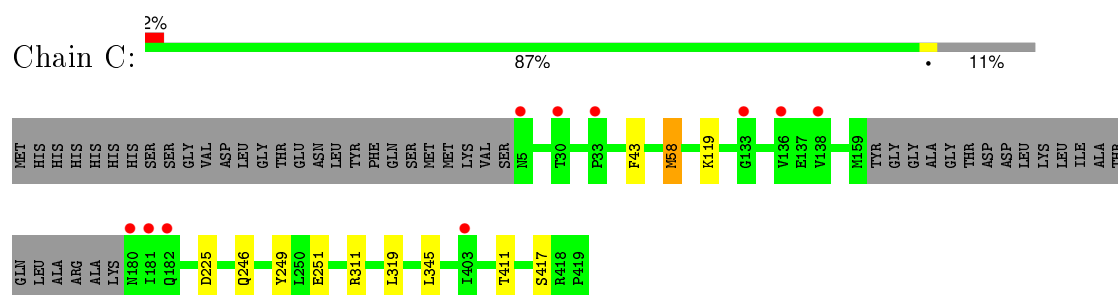
#### • Molecule 1: Putative dehydratase



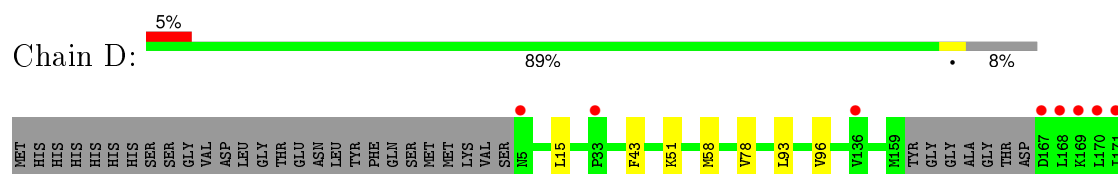
#### • Molecule 1: Putative dehydratase

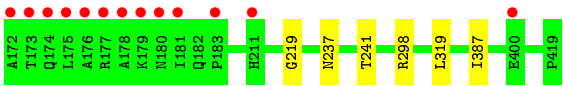


#### • Molecule 1: Putative dehydratase



#### • Molecule 1: Putative dehydratase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.53Å 177.53Å 110.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 45.25 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.70) 99.9 (45.25-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.211 , 0.252 0.213 , 0.253	Depositor DCC
$R_{free}$ test set	5795 reflections (3.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	38 of 209185 reflections (0.018%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13901	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4295e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, 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	0.61	0/3208	0.72	0/4358
1	B	0.60	0/3349	0.71	0/4546
1	C	0.62	0/3213	0.71	0/4366
1	D	0.60	0/3330	0.71	1/4523 (0.0%)
All	All	0.61	0/13100	0.71	1/17793 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	298	ARG	NE-CZ-NH2	-5.83	117.38	120.30

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	3110	0	3088	9	0
1	B	3244	0	3245	9	0
1	C	3115	0	3089	7	0
1	D	3226	0	3218	6	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
4	A	298	0	0	1	0
4	B	279	0	0	0	0
4	C	297	0	0	0	0
4	D	297	0	0	0	0
All	All	13901	0	12672	27	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 1.

All (27) 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:B:58[B]:MET:HA	1:B:58[B]:MET:CE	2.28	0.64
1:D:58[B]:MET:HE2	1:D:96:VAL:HG21	1.82	0.60
1:A:285:TRP:HH2	1:C:319[A]:LEU:HD13	1.67	0.58
1:B:203[B]:LYS:HG2	1:C:246[B]:GLN:OE1	2.04	0.57
1:B:58[B]:MET:HA	1:B:58[B]:MET:HE2	1.94	0.49
1:D:78:VAL:HG23	1:D:93:LEU:HD11	1.94	0.49
1:A:181:ILE:HD13	1:D:219:GLY:HA2	1.95	0.48
1:A:58[B]:MET:HE2	1:A:96:VAL:HG21	1.97	0.47
1:B:58[B]:MET:HA	1:B:58[B]:MET:HE3	1.97	0.46
1:A:78:VAL:HG23	1:A:93:LEU:HD11	1.96	0.46
1:C:58[A]:MET:HE2	1:C:58[A]:MET:HB3	1.61	0.46
1:C:411:THR:HG23	1:C:417[B]:SER:OG	2.16	0.44
1:A:58[B]:MET:HB3	1:A:58[B]:MET:HE2	1.85	0.44
1:A:307:ILE:O	1:A:311[B]:ARG:HB2	2.18	0.44
1:B:28:ILE:HD12	1:B:99:ALA:HB3	2.00	0.43
1:B:285:TRP:HH2	1:D:319[B]:LEU:HD13	1.83	0.43
1:C:58[A]:MET:HA	1:C:58[A]:MET:HE3	2.01	0.43
1:C:225:ASP:HA	1:C:251:GLU:HB3	2.01	0.43
1:A:142:ILE:HG12	1:A:153[B]:VAL:HG11	2.01	0.42
1:D:15:LEU:HD11	1:D:51:LYS:HD2	2.01	0.42
1:D:237:ASN:O	1:D:241:THR:HG23	2.19	0.41
1:A:85:ASN:ND2	4:A:1042:HOH:O	2.53	0.41
1:B:298:ARG:HA	1:B:325:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203[B]:LYS:HE2	1:B:203[B]:LYS:HB2	1.81	0.40
1:C:119:LYS:HG2	1:C:345:LEU:HG	2.03	0.40
1:B:242:LEU:HD13	1:B:247[A]:LEU:HD11	2.03	0.40
1:A:237:ASN:O	1:A:241:THR:HG23	2.22	0.40

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	397/442 (90%)	388 (98%)	9 (2%)	0	100	100
1	B	415/442 (94%)	407 (98%)	7 (2%)	1 (0%)	52	32
1	C	398/442 (90%)	389 (98%)	9 (2%)	0	100	100
1	D	413/442 (93%)	405 (98%)	8 (2%)	0	100	100
All	All	1623/1768 (92%)	1589 (98%)	33 (2%)	1 (0%)	56	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	TYR

### 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	338/370 (91%)	334 (99%)	4 (1%)	78	65
1	B	352/370 (95%)	345 (98%)	7 (2%)	63	44
1	C	339/370 (92%)	334 (98%)	5 (2%)	72	56
1	D	350/370 (95%)	348 (99%)	2 (1%)	90	85
All	All	1379/1480 (93%)	1361 (99%)	18 (1%)	80	62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	PHE
1	A	181	ILE
1	A	311[A]	ARG
1	A	311[B]	ARG
1	B	43	PHE
1	B	47	ILE
1	B	58[A]	MET
1	B	58[B]	MET
1	B	135	GLU
1	B	207	ARG
1	B	311	ARG
1	C	43	PHE
1	C	58[A]	MET
1	C	58[B]	MET
1	C	249	TYR
1	C	311	ARG
1	D	43	PHE
1	D	387	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	B	85	ASN
1	B	180	ASN
1	B	258	ASN
1	C	85	ASN
1	C	91	ASN
1	C	180	ASN
1	C	374	HIS
1	D	174	GLN

### 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 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	A	420	-	5,5,5	0.60	0	5,5,5	0.32	0
2	GOL	B	420	-	5,5,5	0.56	0	5,5,5	0.28	0
2	GOL	C	420	-	5,5,5	0.49	0	5,5,5	0.25	0
2	GOL	D	420	-	5,5,5	0.59	0	5,5,5	0.43	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	A	420	-	-	0/4/4/4	0/0/0/0
2	GOL	B	420	-	-	0/4/4/4	0/0/0/0
2	GOL	C	420	-	-	0/4/4/4	0/0/0/0
2	GOL	D	420	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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 ⓘ

### 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	394/442 (89%)	0.09	13 (3%) 50 54	16, 25, 45, 74	0
1	B	410/442 (92%)	0.40	21 (5%) 32 34	17, 27, 53, 94	0
1	C	395/442 (89%)	0.10	10 (2%) 61 65	15, 25, 44, 79	0
1	D	408/442 (92%)	0.39	21 (5%) 32 34	17, 26, 53, 95	0
All	All	1607/1768 (90%)	0.25	65 (4%) 42 46	15, 26, 50, 95	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	LEU	12.3
1	D	171	ILE	11.8
1	D	170	LEU	11.4
1	B	173	THR	10.2
1	D	175	LEU	10.1
1	B	171	ILE	9.0
1	D	172	ALA	8.8
1	D	178	ALA	8.6
1	B	176	ALA	8.4
1	D	174	GLN	8.2
1	D	167	ASP	8.2
1	B	160	TYR	8.1
1	B	175	LEU	7.5
1	D	169	LYS	7.2
1	B	169	LYS	7.2
1	B	178	ALA	7.1
1	B	177	ARG	7.0
1	D	173	THR	6.0
1	B	167	ASP	5.8
1	D	177	ARG	5.8
1	D	176	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	172	ALA	5.7
1	B	180	ASN	5.6
1	B	174	GLN	5.5
1	D	180	ASN	5.1
1	D	168	LEU	5.0
1	B	168	LEU	4.8
1	C	180	ASN	4.8
1	C	136	VAL	4.5
1	B	33	PRO	4.4
1	D	33	PRO	4.3
1	A	136	VAL	4.2
1	A	182	GLN	4.2
1	C	138	VAL	4.1
1	A	181	ILE	3.8
1	D	179	LYS	3.6
1	B	179	LYS	3.6
1	D	136	VAL	3.5
1	A	5	ASN	3.4
1	B	136	VAL	3.3
1	C	181	ILE	3.2
1	D	5	ASN	3.2
1	D	181	ILE	3.1
1	B	181	ILE	3.1
1	C	30	THR	3.0
1	A	159	MET	2.9
1	B	5	ASN	2.9
1	A	138	VAL	2.8
1	A	133	GLY	2.7
1	C	182	GLN	2.7
1	D	400	GLU	2.6
1	D	211	HIS	2.4
1	C	403	ILE	2.4
1	B	34	GLY	2.4
1	B	138	VAL	2.3
1	C	33	PRO	2.3
1	A	403	ILE	2.2
1	A	405[A]	SER	2.2
1	A	207	ARG	2.2
1	C	5	ASN	2.2
1	D	183	PRO	2.1
1	C	133	GLY	2.1
1	A	33	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	400	GLU	2.0
1	A	214	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 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
3	CL	B	422	1/1	0.85	0.10	1.10	42,42,42,42	0
3	CL	A	423	1/1	0.92	0.09	0.05	43,43,43,43	0
2	GOL	C	420	6/6	0.94	0.09	-0.03	22,25,25,27	0
2	GOL	B	420	6/6	0.96	0.09	-0.38	24,26,27,36	0
3	CL	C	424	1/1	0.98	0.11	-0.39	45,45,45,45	0
2	GOL	D	420	6/6	0.95	0.08	-0.40	21,24,26,28	0
3	CL	A	421	1/1	0.98	0.07	-1.24	23,23,23,23	0
3	CL	C	423	1/1	0.97	0.05	-1.32	45,45,45,45	0
2	GOL	A	420	6/6	0.96	0.07	-1.88	19,24,27,30	0
3	CL	D	421	1/1	0.97	0.06	-	34,34,34,34	0
3	CL	B	421	1/1	0.97	0.05	-	31,31,31,31	0
3	CL	C	421	1/1	0.99	0.06	-	21,21,21,21	1
3	CL	A	422	1/1	0.97	0.07	-	34,34,34,34	0
3	CL	C	422	1/1	0.95	0.06	-	31,31,31,31	0
3	CL	D	422	1/1	0.95	0.23	-	32,32,32,32	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.