



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:22 am GMT

PDB ID : 3TWB  
Title : Crystal structure of gluconate dehydratase (TARGET EFI-501679) from Salmonella enterica subsp. enterica serovar Enteritidis str. P125109 complexed with magnesium and gluconic acid  
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 : 1.76 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

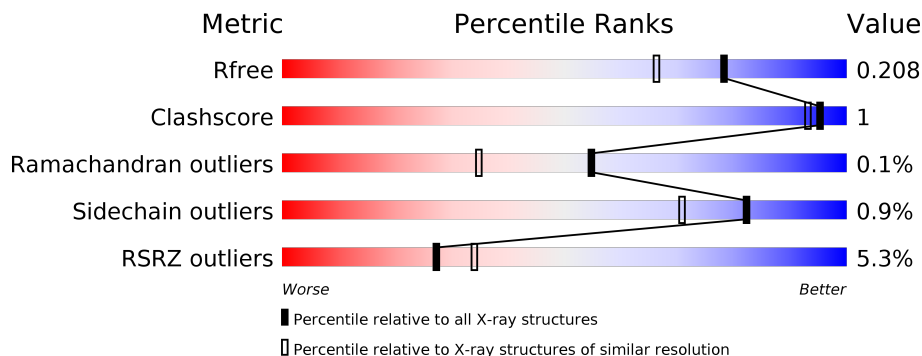
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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))
$R_{free}$	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (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 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>4%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>
1	B	442	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
1	C	442	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
1	D	442	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>6%</div> </div> </div>
1	E	442	<div> <div>12%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>

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
3	GOL	A	421	-	-	-	X
3	GOL	B	421	-	-	-	X
3	GOL	C	421	-	-	-	X
3	GOL	C	423	-	-	-	X
3	GOL	D	423	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18525 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	415	Total	C	N	O	S	0	5	0
			3248	2064	555	609	20			
1	B	416	Total	C	N	O	S	0	10	0
			3278	2085	558	614	21			
1	C	417	Total	C	N	O	S	0	13	0
			3302	2103	563	616	20			
1	D	416	Total	C	N	O	S	0	15	0
			3314	2113	568	612	21			
1	E	415	Total	C	N	O	S	0	4	0
			3252	2066	560	606	20			

There are 115 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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	EXPRESSION TAG	UNP B5R541
A	-2	GLN	-	EXPRESSION TAG	UNP B5R541
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLU	-	EXPRESSION TAG	UNP B5R541
C	-6	ASN	-	EXPRESSION TAG	UNP B5R541
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
E	-22	MET	-	EXPRESSION TAG	UNP B5R541
E	-21	HIS	-	EXPRESSION TAG	UNP B5R541
E	-20	HIS	-	EXPRESSION TAG	UNP B5R541
E	-19	HIS	-	EXPRESSION TAG	UNP B5R541
E	-18	HIS	-	EXPRESSION TAG	UNP B5R541
E	-17	HIS	-	EXPRESSION TAG	UNP B5R541
E	-16	HIS	-	EXPRESSION TAG	UNP B5R541
E	-15	SER	-	EXPRESSION TAG	UNP B5R541
E	-14	SER	-	EXPRESSION TAG	UNP B5R541
E	-13	GLY	-	EXPRESSION TAG	UNP B5R541
E	-12	VAL	-	EXPRESSION TAG	UNP B5R541

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	ASP	-	EXPRESSION TAG	UNP B5R541
E	-10	LEU	-	EXPRESSION TAG	UNP B5R541
E	-9	GLY	-	EXPRESSION TAG	UNP B5R541
E	-8	THR	-	EXPRESSION TAG	UNP B5R541
E	-7	GLU	-	EXPRESSION TAG	UNP B5R541
E	-6	ASN	-	EXPRESSION TAG	UNP B5R541
E	-5	LEU	-	EXPRESSION TAG	UNP B5R541
E	-4	TYR	-	EXPRESSION TAG	UNP B5R541
E	-3	PHE	-	EXPRESSION TAG	UNP B5R541
E	-2	GLN	-	EXPRESSION TAG	UNP B5R541
E	-1	SER	-	EXPRESSION TAG	UNP B5R541
E	0	MET	-	EXPRESSION TAG	UNP B5R541

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

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

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



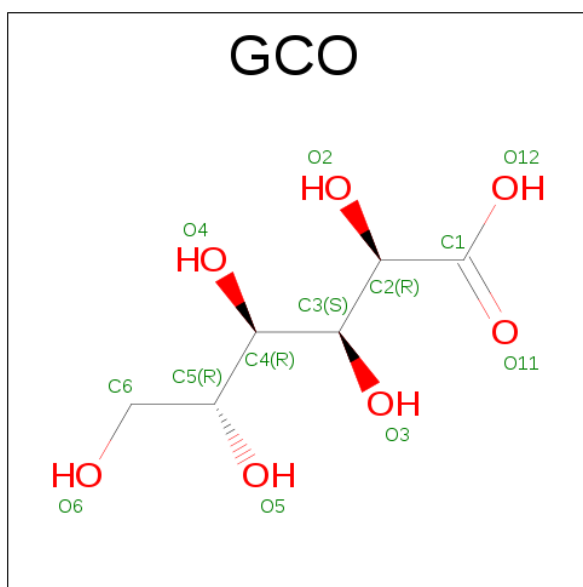
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is SUGAR (GLUCONIC ACID) (three-letter code: GCO) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>7</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		
5	B	1	Total	C	O	0	0
			13	6	7		
5	C	1	Total	C	O	0	0
			13	6	7		
5	D	1	Total	C	O	0	0
			13	6	7		
5	E	1	Total	C	O	0	0
			13	6	7		

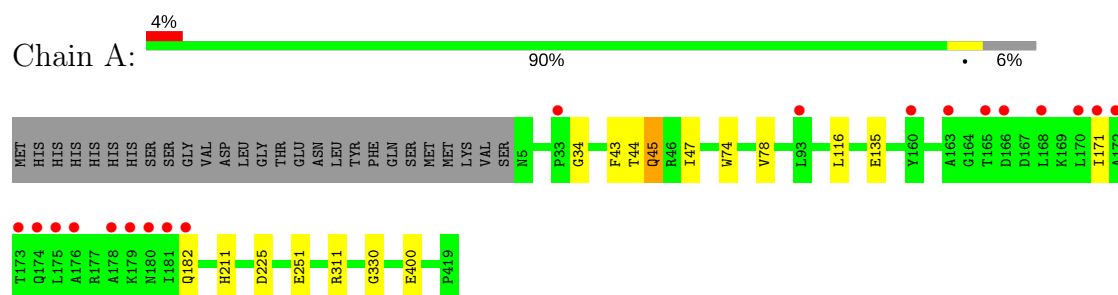
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	466	Total	O	0	0
			466	466		
6	B	388	Total	O	0	0
			388	388		
6	C	465	Total	O	0	0
			465	465		
6	D	447	Total	O	0	0
			447	447		
6	E	250	Total	O	0	0
			250	250		

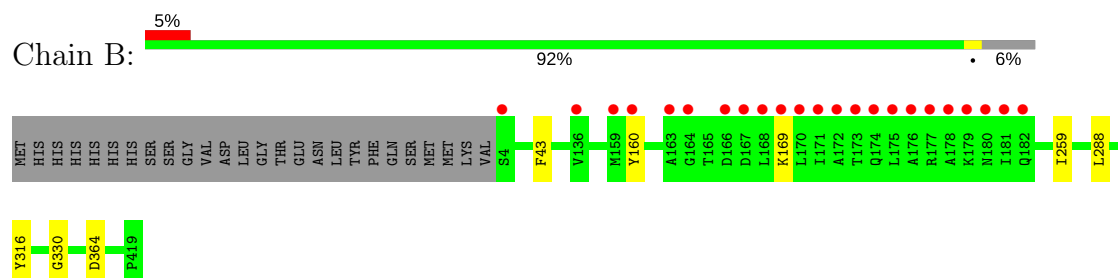
### 3 Residue-property plots [i](#)

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

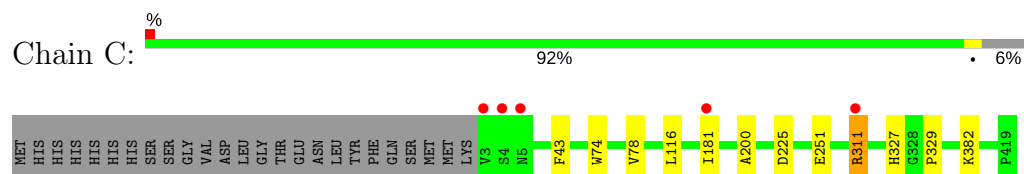
- Molecule 1: Putative dehydratase



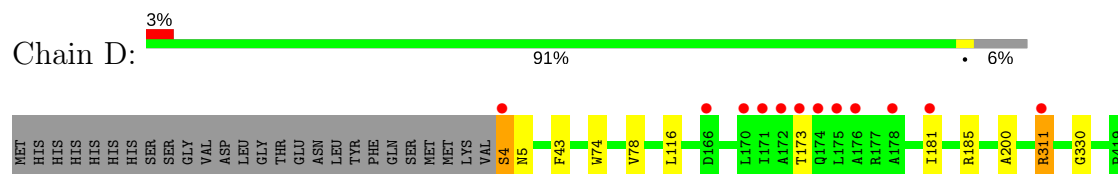
- Molecule 1: Putative dehydratase



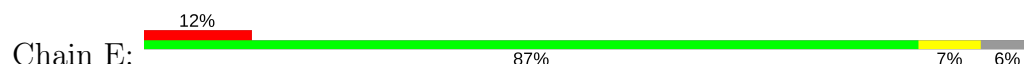
- Molecule 1: Putative dehydratase

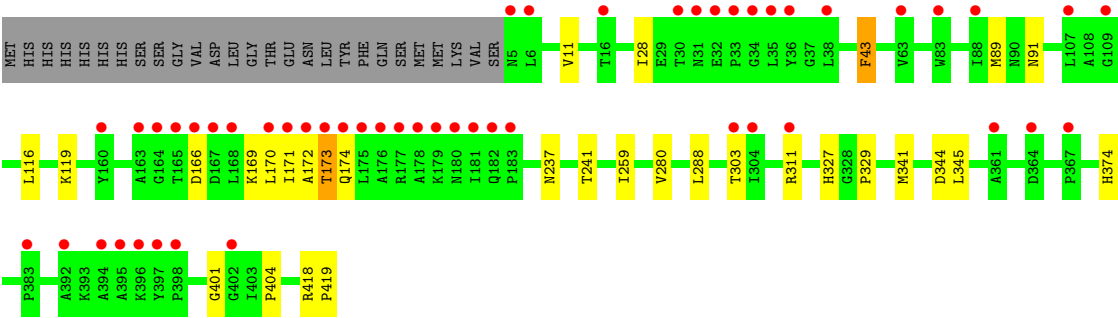


- Molecule 1: Putative dehydratase



- Molecule 1: Putative dehydratase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.73Å 144.73Å 447.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.76 49.88 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-1.76) 99.8 (49.88-1.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.170 , 0.206 0.171 , 0.208	Depositor DCC
$R_{free}$ test set	6988 reflections (3.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18525	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: GOL, MG, GCO, 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	0.67	1/3342 (0.0%)	0.71	0/4542
1	B	0.64	0/3388	0.69	0/4604
1	C	0.65	0/3421	0.71	0/4648
1	D	0.66	0/3439	0.71	2/4666 (0.0%)
1	E	0.55	0/3343	0.67	0/4540
All	All	0.64	1/16933 (0.0%)	0.70	2/23000 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	GLU	CG-CD	-5.59	1.43	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311[A]	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	D	311[B]	ARG	NE-CZ-NH1	-5.24	117.68	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	3248	0	3218	9	0
1	B	3278	0	3252	4	1
1	C	3302	0	3303	6	0
1	D	3314	0	3334	5	0
1	E	3252	0	3227	21	0
2	A	1	0	0	0	0
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
3	A	12	0	16	2	0
3	B	6	0	8	1	0
3	C	12	0	16	0	0
3	D	12	0	16	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	1	0
5	A	13	0	10	0	0
5	B	13	0	11	1	0
5	C	13	0	10	1	0
5	D	13	0	10	0	0
5	E	13	0	11	1	0
6	A	466	0	0	0	1
6	B	388	0	0	1	0
6	C	465	0	0	1	0
6	D	447	0	0	1	0
6	E	250	0	0	3	0
All	All	18525	0	16442	45	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 1.

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:E:89:MET:HG2	4:E:421:CL:CL	2.21	0.77
1:E:171:ILE:HG22	6:E:1611:HOH:O	1.85	0.75
1:E:170:LEU:O	1:E:170:LEU:HD12	1.91	0.70
1:E:169:LYS:NZ	1:E:401:GLY:O	2.28	0.66
1:E:170:LEU:C	1:E:170:LEU:HD12	2.18	0.63
1:B:160:TYR:HH	5:B:422:GCO:HO3	1.48	0.61
1:C:382:LYS:NZ	6:C:778:HOH:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLY:H	3:A:424:GOL:H2	1.67	0.57
1:A:116:LEU:HD22	1:A:311:ARG:HD3	1.88	0.54
1:C:327:HIS:NE2	5:C:424:GCO:H2	2.23	0.53
1:E:166:ASP:O	1:E:174:GLN:NE2	2.41	0.53
1:D:4:SER:HA	6:D:1845:HOH:O	2.09	0.52
1:B:330:GLY:HA2	3:B:421:GOL:H11	1.92	0.50
1:C:116:LEU:O	1:C:311[A]:ARG:NH1	2.44	0.50
1:E:11:VAL:HG22	1:E:28:ILE:HG12	1.93	0.50
1:E:169:LYS:HG2	6:E:443:HOH:O	2.12	0.50
1:A:44:THR:HA	1:A:47:ILE:HD13	1.93	0.49
1:C:74:TRP:CH2	1:C:78[B]:VAL:HG21	2.47	0.49
1:E:116:LEU:HD22	1:E:311[A]:ARG:HD3	1.95	0.47
1:B:259:ILE:HB	1:B:288:LEU:HD21	1.96	0.47
1:A:45:GLN:HE21	1:A:45:GLN:H	1.63	0.47
1:D:74:TRP:CH2	1:D:78[B]:VAL:HG21	2.49	0.47
1:E:171:ILE:O	1:E:172:ALA:HB3	2.15	0.46
1:E:171:ILE:HG13	1:E:171:ILE:O	2.15	0.46
1:C:181:ILE:HG23	1:C:200:ALA:HB1	1.99	0.45
1:A:74:TRP:CH2	1:A:78[B]:VAL:HG21	2.52	0.44
1:E:119:LYS:HG2	1:E:345:LEU:HG	1.99	0.44
1:E:237:ASN:O	1:E:241:THR:HG23	2.17	0.44
1:E:341:MET:HA	1:E:344:ASP:HB2	2.00	0.43
1:B:169:LYS:HA	6:B:465:HOH:O	2.18	0.43
1:E:327:HIS:NE2	5:E:422:GCO:H2	2.34	0.43
1:A:45:GLN:H	1:A:45:GLN:NE2	2.17	0.43
1:E:259:ILE:HB	1:E:288:LEU:HD21	2.00	0.42
1:D:181:ILE:HG23	1:D:200:ALA:HB1	2.02	0.42
1:E:418:ARG:HA	1:E:419:PRO:HD3	1.94	0.42
1:D:116:LEU:HD22	1:D:311[B]:ARG:HE	1.85	0.42
1:E:280:VAL:HG12	1:E:303:THR:HG22	2.01	0.41
1:A:330:GLY:HA2	3:A:421:GOL:H32	2.01	0.41
1:A:135:GLU:HB3	1:A:211:HIS:CD2	2.55	0.41
1:A:225:ASP:HA	1:A:251:GLU:HB3	2.02	0.41
1:C:225:ASP:HA	1:C:251:GLU:HB3	2.02	0.41
1:E:171:ILE:HG23	1:E:173:THR:H	1.85	0.41
1:E:404:PRO:HD3	6:E:488:HOH:O	2.20	0.41
1:E:43:PHE:HB2	1:E:91:ASN:ND2	2.35	0.41
1:D:330:GLY:HA2	3:D:421:GOL:H32	2.04	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)
1:B:316:TYR:OH	6:A:498:HOH:O[4_555]	2.16	0.04

## 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	418/442 (95%)	406 (97%)	12 (3%)	0	100	100
1	B	424/442 (96%)	416 (98%)	8 (2%)	0	100	100
1	C	428/442 (97%)	419 (98%)	8 (2%)	1 (0%)	51	31
1	D	429/442 (97%)	420 (98%)	9 (2%)	0	100	100
1	E	417/442 (94%)	401 (96%)	15 (4%)	1 (0%)	51	31
All	All	2116/2210 (96%)	2062 (97%)	52 (2%)	2 (0%)	55	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	329	PRO
1	E	329	PRO

### 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	350/370 (95%)	346 (99%)	4 (1%)	78	64
1	B	355/370 (96%)	353 (99%)	2 (1%)	89	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	360/370 (97%)	357 (99%)	3 (1%)	85	75
1	D	361/370 (98%)	355 (98%)	6 (2%)	66	47
1	E	349/370 (94%)	346 (99%)	3 (1%)	82	71
All	All	1775/1850 (96%)	1757 (99%)	18 (1%)	82	67

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

Mol	Chain	Res	Type
1	A	43	PHE
1	A	45	GLN
1	A	171	ILE
1	A	182	GLN
1	B	43	PHE
1	B	364	ASP
1	C	43	PHE
1	C	311[A]	ARG
1	C	311[B]	ARG
1	D	4	SER
1	D	5	ASN
1	D	43	PHE
1	D	173	THR
1	D	185[A]	ARG
1	D	185[B]	ARG
1	E	43	PHE
1	E	173	THR
1	E	374	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	182	GLN
1	C	10	ASN
1	E	75	GLN
1	E	174	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\# Z  > 2$
3	GOL	A	421	-	5,5,5	0.55	0	5,5,5	0.60	0
5	GCO	A	423	2	9,12,12	1.07	1 (11%)	12,16,16	1.81	3 (25%)
3	GOL	A	424	-	5,5,5	0.42	0	5,5,5	0.65	0
3	GOL	B	421	-	5,5,5	0.46	0	5,5,5	0.76	0
5	GCO	B	422	2	9,12,12	1.08	1 (11%)	12,16,16	1.82	3 (25%)
3	GOL	C	421	-	5,5,5	0.57	0	5,5,5	0.47	0
3	GOL	C	423	-	5,5,5	0.30	0	5,5,5	0.36	0
5	GCO	C	424	2	9,12,12	1.17	2 (22%)	12,16,16	0.94	0
3	GOL	D	421	-	5,5,5	0.38	0	5,5,5	0.51	0
5	GCO	D	422	2	9,12,12	1.21	0	12,16,16	1.69	2 (16%)
3	GOL	D	423	-	5,5,5	0.45	0	5,5,5	0.21	0
5	GCO	E	422	2	9,12,12	0.92	0	12,16,16	1.00	1 (8%)

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
3	GOL	A	421	-	-	0/4/4/4	0/0/0/0
5	GCO	A	423	2	-	0/14/18/18	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	424	-	-	0/4/4/4	0/0/0/0
3	GOL	B	421	-	-	0/4/4/4	0/0/0/0
5	GCO	B	422	2	-	0/14/18/18	0/0/0/0
3	GOL	C	421	-	-	0/4/4/4	0/0/0/0
3	GOL	C	423	-	-	0/4/4/4	0/0/0/0
5	GCO	C	424	2	-	0/14/18/18	0/0/0/0
3	GOL	D	421	-	-	0/4/4/4	0/0/0/0
5	GCO	D	422	2	-	0/14/18/18	0/0/0/0
3	GOL	D	423	-	-	0/4/4/4	0/0/0/0
5	GCO	E	422	2	-	0/14/18/18	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	422	GCO	O4-C4	-2.38	1.37	1.43
5	A	423	GCO	O4-C4	-2.34	1.37	1.43
5	C	424	GCO	O5-C5	-2.32	1.38	1.43
5	C	424	GCO	O4-C4	-2.29	1.37	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	422	GCO	C4-C3-C2	-2.31	109.45	113.58
5	A	423	GCO	C4-C3-C2	-2.29	109.47	113.58
5	E	422	GCO	O4-C4-C3	2.12	114.54	109.46
5	D	422	GCO	O2-C2-C1	2.41	117.00	111.13
5	A	423	GCO	O2-C2-C1	2.60	117.45	111.13
5	B	422	GCO	O2-C2-C1	2.61	117.48	111.13
5	A	423	GCO	O2-C2-C3	2.86	113.86	107.52
5	B	422	GCO	O2-C2-C3	2.86	113.86	107.52
5	D	422	GCO	O2-C2-C3	4.15	116.72	107.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	421	GOL	1	0
3	A	424	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	421	GOL	1	0
5	B	422	GCO	1	0
5	C	424	GCO	1	0
3	D	421	GOL	1	0
5	E	422	GCO	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	415/442 (93%)	-0.19	19 (4%) 33 39	9, 16, 38, 74	0
1	B	416/442 (94%)	-0.06	23 (5%) 26 32	10, 18, 50, 91	0
1	C	417/442 (94%)	-0.49	5 (1%) 79 85	10, 14, 26, 70	0
1	D	416/442 (94%)	-0.26	12 (2%) 52 59	10, 16, 33, 75	0
1	E	415/442 (93%)	0.70	51 (12%) 5 6	15, 32, 62, 106	0
All	All	2079/2210 (94%)	-0.06	110 (5%) 27 34	9, 17, 47, 106	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	ILE	11.0
1	E	173	THR	9.0
1	B	181	ILE	8.0
1	B	172	ALA	7.2
1	E	181	ILE	6.6
1	D	171	ILE	6.2
1	E	168	LEU	6.2
1	E	171	ILE	6.1
1	E	172	ALA	6.0
1	A	181	ILE	5.7
1	B	175	LEU	5.6
1	B	180	ASN	5.6
1	A	173	THR	5.5
1	B	173	THR	5.5
1	E	33	PRO	5.4
1	B	176	ALA	5.3
1	E	175	LEU	5.2
1	D	4	SER	5.2
1	A	171	ILE	5.2
1	A	176	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	4	SER	5.0
1	E	179	LYS	4.7
1	A	174	GLN	4.7
1	E	163	ALA	4.6
1	B	179	LYS	4.6
1	E	174	GLN	4.6
1	E	392	ALA	4.5
1	B	174	GLN	4.5
1	E	6	LEU	4.4
1	B	166	ASP	4.4
1	B	163	ALA	4.3
1	A	168	LEU	4.2
1	D	175	LEU	4.2
1	D	173	THR	4.0
1	D	181	ILE	4.0
1	A	178	ALA	3.9
1	B	168	LEU	3.9
1	E	36	TYR	3.9
1	E	176	ALA	3.9
1	E	180	ASN	3.7
1	E	396	LYS	3.7
1	E	107	LEU	3.7
1	E	170	LEU	3.6
1	E	177	ARG	3.5
1	B	182	GLN	3.4
1	B	159	MET	3.4
1	B	178	ALA	3.4
1	D	172	ALA	3.4
1	A	175	LEU	3.3
1	E	397	TYR	3.3
1	C	3	VAL	3.3
1	E	398	PRO	3.3
1	E	182	GLN	3.3
1	B	169	LYS	3.2
1	E	166	ASP	3.2
1	B	136	VAL	3.2
1	E	35	LEU	3.2
1	E	361	ALA	3.1
1	E	63	VAL	3.1
1	E	364	ASP	3.1
1	E	165	THR	3.1
1	E	5	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	33	PRO	3.0
1	B	170	LEU	2.9
1	E	31	ASN	2.9
1	E	30	THR	2.9
1	D	174[A]	GLN	2.8
1	B	4	SER	2.8
1	D	166	ASP	2.8
1	B	167	ASP	2.8
1	A	182	GLN	2.7
1	C	181	ILE	2.7
1	B	160	TYR	2.7
1	D	176	ALA	2.7
1	D	311[A]	ARG	2.7
1	E	395	ALA	2.7
1	E	178	ALA	2.6
1	E	16	THR	2.6
1	E	394	ALA	2.6
1	D	170	LEU	2.6
1	E	304	ILE	2.6
1	E	88	ILE	2.5
1	B	177[A]	ARG	2.5
1	E	311[A]	ARG	2.5
1	A	160	TYR	2.5
1	A	163	ALA	2.5
1	A	179	LYS	2.5
1	E	383	PRO	2.4
1	A	180	ASN	2.4
1	C	5	ASN	2.4
1	A	172	ALA	2.4
1	D	178	ALA	2.4
1	A	166	ASP	2.4
1	E	38	LEU	2.4
1	B	164	GLY	2.4
1	E	183	PRO	2.2
1	E	83	TRP	2.2
1	E	34	GLY	2.2
1	A	165	THR	2.2
1	C	311[A]	ARG	2.2
1	E	32	GLU	2.2
1	E	164	GLY	2.2
1	E	402	GLY	2.2
1	A	170	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	109	GLY	2.1
1	A	93	LEU	2.1
1	E	367	PRO	2.1
1	E	167	ASP	2.1
1	E	303	THR	2.0
1	E	160	TYR	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	GOL	B	421	6/6	0.92	0.12	4.63	24,27,35,43	0
3	GOL	C	423	6/6	0.95	0.23	4.36	24,34,43,49	0
3	GOL	C	421	6/6	0.96	0.09	4.11	14,15,16,18	0
3	GOL	D	423	6/6	0.95	0.23	3.38	25,32,37,37	0
3	GOL	A	421	6/6	0.95	0.09	2.99	16,20,22,23	0
3	GOL	A	424	6/6	0.92	0.23	1.93	27,47,50,55	0
5	GCO	C	424	13/13	0.95	0.09	1.88	11,16,34,48	0
5	GCO	B	422	13/13	0.87	0.16	1.17	16,23,52,57	0
3	GOL	D	421	6/6	0.97	0.07	1.00	18,21,24,25	0
5	GCO	D	422	13/13	0.94	0.11	0.96	15,22,49,56	0
5	GCO	A	423	13/13	0.94	0.12	0.80	14,20,44,46	0
5	GCO	E	422	13/13	0.91	0.12	-0.04	25,35,58,69	0
2	MG	A	420	1/1	1.00	0.04	-1.02	14,14,14,14	0
2	MG	C	420	1/1	1.00	0.04	-1.16	12,12,12,12	0
2	MG	B	420	1/1	1.00	0.02	-1.53	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	E	420	1/1	0.99	0.04	-1.93	24,24,24,24	0
2	MG	D	420	1/1	1.00	0.03	-1.94	14,14,14,14	0
4	CL	C	422	1/1	0.97	0.06	-2.66	19,19,19,19	0
4	CL	A	422	1/1	0.98	0.09	-3.34	19,19,19,19	0
4	CL	E	421	1/1	0.90	0.15	-	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.