



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:32 am BST

PDB ID : 3PNZ  
Title : Crystal structure of the lactonase Lmo2620 from *Listeria monocytogenes*  
Authors : Fedorov, A.A.; Fedorov, E.V.; Xiang, D.F.; Raushel, F.M.; Almo, S.C.  
Deposited on : 2010-11-20  
Resolution : 1.60 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

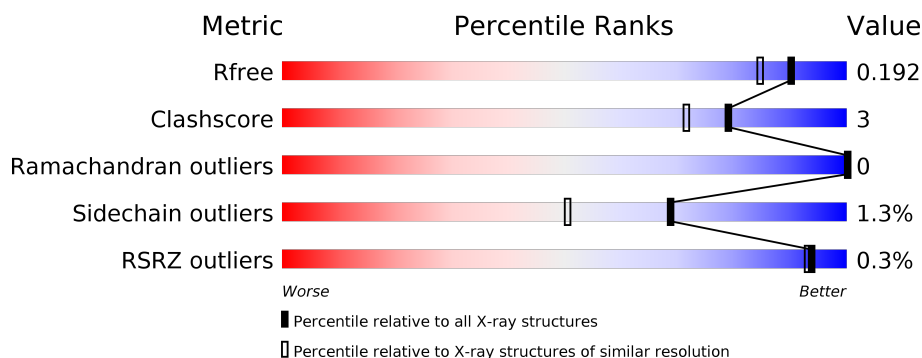
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 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	330	<div> <div style="width: 93%;"></div> <div style="width: 6%;"></div> <div style="width: 1%;"></div> </div> <div>93% 6% .</div>
1	B	330	<div> <div style="width: 91%;"></div> <div style="width: 8%;"></div> <div style="width: 1%;"></div> </div> <div>91% 8% .</div>
1	C	330	<div> <div style="width: 93%;"></div> <div style="width: 6%;"></div> <div style="width: 1%;"></div> </div> <div>93% 6% .</div>
1	D	330	<div> <div style="width: 92%;"></div> <div style="width: 8%;"></div> <div style="width: 1%;"></div> </div> <div>92% 8% .</div>
1	E	330	<div> <div style="width: 92%;"></div> <div style="width: 7%;"></div> <div style="width: 1%;"></div> </div> <div>92% 7% .</div>
1	F	330	<div> <div style="width: 91%;"></div> <div style="width: 8%;"></div> <div style="width: 1%;"></div> </div> <div>91% 8% .</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
2	GOL	B	333	-	-	X	-
2	GOL	E	333	-	-	X	-

## 2 Entry composition [i](#)

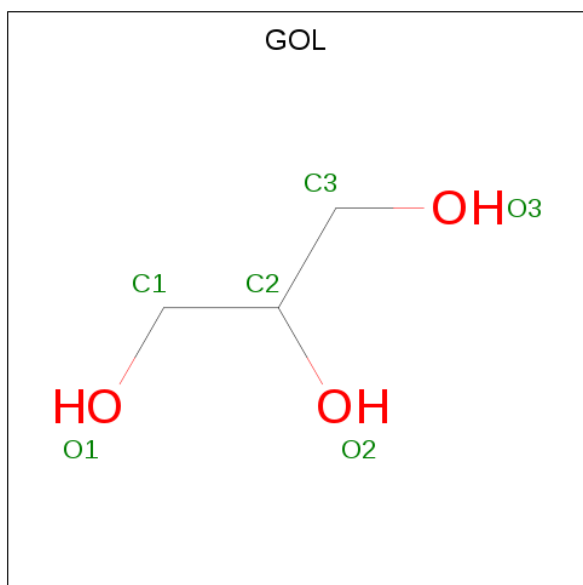
There are 5 unique types of molecules in this entry. The entry contains 17578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphotriesterase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	1	0
			2648	1701	435	505	7			
1	B	329	Total	C	N	O	S	0	0	0
			2640	1696	434	504	6			
1	C	328	Total	C	N	O	S	0	0	0
			2630	1690	432	502	6			
1	D	328	Total	C	N	O	S	0	3	0
			2656	1706	438	506	6			
1	E	328	Total	C	N	O	S	0	0	0
			2630	1690	432	502	6			
1	F	328	Total	C	N	O	S	0	1	0
			2638	1694	434	504	6			

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

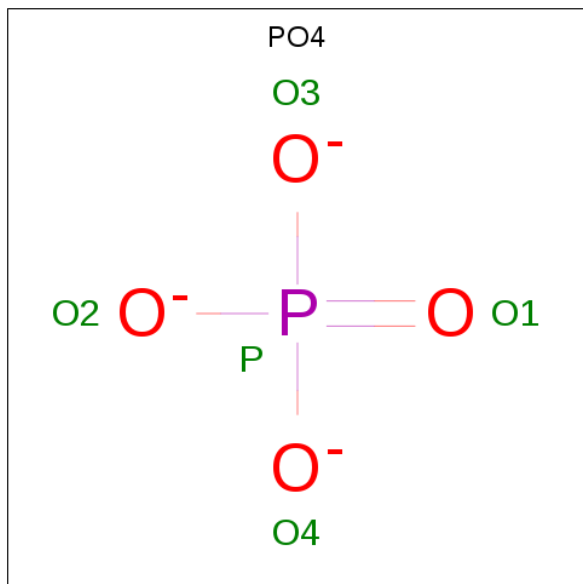


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	P 1	0	0
4	A	1	Total 5	O 4	P 1	0	0
4	A	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	222	Total	O	0	0
			222	222		
5	B	217	Total	O	0	0
			217	217		
5	C	283	Total	O	0	0
			283	283		
5	D	242	Total	O	0	0
			242	242		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	276	Total	O	0	0
			276	276		
5	F	253	Total	O	0	0
			253	253		



### 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: Phosphotriesterase family protein



- Molecule 1: Phosphotriesterase family protein



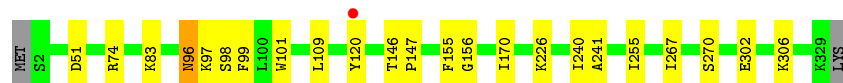
- Molecule 1: Phosphotriesterase family protein



- Molecule 1: Phosphotriesterase family protein



- Molecule 1: Phosphotriesterase family protein



- Molecule 1: Phosphotriesterase family protein

Chain F: 

91%

8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.72Å 62.93Å 152.74Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	39.58 – 1.60 39.58 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.0 (39.58-1.60) 93.9 (39.58-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.178 , 0.198 0.172 , 0.192	Depositor DCC
$R_{free}$ test set	18173 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.460 for -l,k,h 0.013 for h,-k,-l 0.013 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17578	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 3.13% 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, ZN, PO4, KCX

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	0.32	0/2700	0.50	0/3650
1	B	0.32	0/2692	0.50	0/3640
1	C	0.37	0/2682	0.54	0/3629
1	D	0.35	0/2708	0.53	0/3663
1	E	0.37	0/2682	0.53	0/3629
1	F	0.36	0/2690	0.53	0/3640
All	All	0.35	0/16154	0.52	0/21851

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2648	0	2580	13	0
1	B	2640	0	2572	16	0
1	C	2630	0	2559	13	0
1	D	2656	0	2589	12	0
1	E	2630	0	2559	18	0
1	F	2638	0	2564	16	0
2	A	12	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	18	0	24	4	0
2	C	36	0	48	3	0
2	D	18	0	24	0	0
2	E	24	0	32	6	0
2	F	18	0	24	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
4	C	20	0	0	1	0
4	D	15	0	0	1	0
4	E	25	0	0	1	0
4	F	15	0	0	1	0
5	A	222	0	0	1	0
5	B	217	0	0	1	0
5	C	283	0	0	2	0
5	D	242	0	0	0	0
5	E	276	0	0	0	0
5	F	253	0	0	1	0
All	All	17578	0	15591	87	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 3.

All (87) 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)
2:B:333:GOL:H31	5:B:978:HOH:O	1.84	0.78
1:D:106[A]:LYS:HD2	1:D:109:LEU:HG	1.78	0.66
1:C:226:LYS:HZ1	2:C:335:GOL:H31	1.64	0.62
1:A:323:ALA:O	1:A:327:THR:HG23	2.01	0.60
1:A:96:ASN:C	1:A:96:ASN:HD22	2.02	0.60
1:E:96:ASN:HD22	1:E:96:ASN:C	2.03	0.60
1:B:323:ALA:O	1:B:327:THR:HG23	2.01	0.59
1:A:298:ARG:HG3	1:F:223:TYR:CE2	2.38	0.59
1:B:230:LYS:NZ	2:B:333:GOL:H12	2.19	0.57
1:B:298:ARG:HG3	1:D:223:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:LYS:HE2	2:E:333:GOL:H2	1.88	0.56
1:E:241:ALA:HB3	2:E:331:GOL:H31	1.89	0.55
1:E:226:LYS:CE	2:E:333:GOL:H2	2.39	0.53
1:C:96:ASN:HB3	1:C:100:LEU:HD12	1.91	0.53
5:A:384:HOH:O	1:E:83:LYS:HD3	2.07	0.53
1:E:74:ARG:HE	2:E:332:GOL:C1	2.23	0.51
1:A:113:ILE:HG23	1:A:122:TRP:CD1	2.47	0.50
1:F:97:LYS:HD2	1:F:99:PHE:CE2	2.47	0.50
1:C:241:ALA:HB3	2:C:332:GOL:H31	1.94	0.49
1:B:4:ILE:HD12	1:B:13:PRO:HA	1.95	0.49
1:E:155:PHE:CD1	1:E:170:ILE:HG12	2.48	0.49
1:B:230:LYS:HZ2	2:B:333:GOL:H12	1.78	0.48
1:B:105:ILE:HD13	1:B:113:ILE:HD11	1.95	0.48
1:D:255:ILE:HG23	1:D:267:ILE:HD13	1.94	0.47
1:C:97:LYS:HZ3	4:C:339:PO4:P	2.37	0.47
1:F:255:ILE:HG23	1:F:267:ILE:HD13	1.97	0.47
1:F:97:LYS:HZ3	4:F:336:PO4:P	2.38	0.47
2:A:332:GOL:H2	1:E:147:PRO:HG3	1.98	0.46
1:C:97:LYS:HA	5:C:1263:HOH:O	2.14	0.46
1:D:113:ILE:HG23	1:D:122:TRP:CE2	2.51	0.46
1:E:96:ASN:O	1:E:156:GLY:HA3	2.16	0.46
1:E:255:ILE:HG23	1:E:267:ILE:HD13	1.98	0.46
1:A:4:ILE:HD12	1:A:13:PRO:HA	1.97	0.46
1:A:255:ILE:HG23	1:A:267:ILE:HD13	1.98	0.45
1:F:321:ASN:HB2	1:F:322:PRO:HD3	1.98	0.45
1:E:96:ASN:ND2	1:E:96:ASN:C	2.70	0.45
1:D:155:PHE:CD1	1:D:170:ILE:HG12	2.51	0.45
1:D:4:ILE:HD12	1:D:13:PRO:HA	1.99	0.45
1:B:226:LYS:HB3	2:B:333:GOL:O3	2.17	0.45
1:C:255:ILE:HG23	1:C:267:ILE:HD13	1.98	0.45
1:F:98:SER:HA	1:F:101:TRP:CD2	2.52	0.44
1:A:96:ASN:ND2	1:A:96:ASN:C	2.68	0.44
1:E:240:ILE:O	1:E:241:ALA:HB3	2.17	0.44
1:F:146:THR:HB	1:F:147:PRO:HD2	2.00	0.43
1:B:56:ALA:HB2	1:B:87:ILE:HD11	2.01	0.43
1:A:209:GLU:HG3	2:A:332:GOL:H32	1.99	0.43
1:D:226:LYS:HE2	1:D:230:LYS:HE3	2.00	0.43
1:F:161:MET:HE2	1:F:161:MET:HB2	1.69	0.43
1:C:155:PHE:CD1	1:C:170:ILE:HG12	2.54	0.43
1:D:96:ASN:HB3	1:D:100:LEU:HD12	2.01	0.43
1:E:302:GLU:HG2	1:E:306:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ALA:HB2	1:A:87:ILE:HD11	2.01	0.42
1:B:214:GLY:HA2	1:B:236:SER:HB3	2.00	0.42
1:F:96:ASN:CG	1:F:97:LYS:H	2.20	0.42
1:E:98:SER:HA	1:E:101:TRP:CD2	2.54	0.42
1:C:188:THR:OG1	1:C:191:GLY:HA2	2.19	0.42
1:F:315:LYS:HD3	5:F:528:HOH:O	2.19	0.42
1:A:70:ASP:HA	1:A:119:TYR:CZ	2.55	0.42
1:C:98:SER:HA	1:C:101:TRP:CD2	2.55	0.42
1:B:70:ASP:HA	1:B:119:TYR:CZ	2.54	0.42
1:C:226:LYS:HZ1	2:C:335:GOL:C1	2.32	0.42
1:D:98:SER:HA	1:D:101:TRP:CD2	2.54	0.42
1:A:238:ASP:HA	1:A:270:SER:O	2.20	0.42
1:D:142:GLY:HA3	1:D:146:THR:O	2.20	0.42
1:F:4:ILE:HD13	1:F:16:LEU:HD22	2.02	0.42
1:B:104:LYS:HE3	1:B:117:GLU:OE2	2.20	0.41
1:B:321:ASN:HB2	1:B:322:PRO:HD3	2.01	0.41
1:E:226:LYS:NZ	2:E:333:GOL:H2	2.35	0.41
1:C:301:ASP:O	1:C:305:GLU:HG3	2.21	0.41
1:D:97:LYS:HZ3	4:D:336:PO4:P	2.44	0.41
1:D:214:GLY:HA2	1:D:236:SER:HB3	2.02	0.41
1:F:8:TYR:CG	2:F:331:GOL:H12	2.55	0.41
1:B:110:LYS:N	1:B:111:PRO:CD	2.84	0.41
1:E:97:LYS:HZ3	4:E:337:PO4:P	2.43	0.41
1:C:296:VAL:HB	1:C:297:PRO:HD3	2.03	0.41
1:F:106:LYS:HD2	1:F:109:LEU:HG	2.03	0.41
1:F:110:LYS:N	1:F:111:PRO:CD	2.84	0.41
1:A:296:VAL:HB	1:A:297:PRO:HD3	2.03	0.40
1:B:101:TRP:HA	1:B:119:TYR:HB2	2.03	0.40
1:E:146:THR:HB	1:E:147:PRO:HD2	2.02	0.40
1:A:98:SER:HA	1:A:101:TRP:CD2	2.56	0.40
1:B:96:ASN:O	1:B:156:GLY:HA3	2.21	0.40
1:C:305:GLU:HG3	5:C:1373:HOH:O	2.20	0.40
1:F:154:KCX:HA	1:F:185:HIS:O	2.21	0.40
1:B:255:ILE:HG23	1:B:267:ILE:HD13	2.04	0.40
1:E:226:LYS:HZ3	2:E:333:GOL:H2	1.86	0.40
1:F:16:LEU:HD11	1:F:62:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/330 (99%)	319 (98%)	8 (2%)	0	100	100
1	B	326/330 (99%)	317 (97%)	9 (3%)	0	100	100
1	C	325/330 (98%)	317 (98%)	8 (2%)	0	100	100
1	D	328/330 (99%)	320 (98%)	8 (2%)	0	100	100
1	E	325/330 (98%)	317 (98%)	8 (2%)	0	100	100
1	F	326/330 (99%)	318 (98%)	8 (2%)	0	100	100
All	All	1957/1980 (99%)	1908 (98%)	49 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	277/277 (100%)	274 (99%)	3 (1%)	73	57
1	B	276/277 (100%)	274 (99%)	2 (1%)	84	73
1	C	275/277 (99%)	271 (98%)	4 (2%)	65	44
1	D	278/277 (100%)	275 (99%)	3 (1%)	73	57
1	E	275/277 (99%)	269 (98%)	6 (2%)	52	27
1	F	276/277 (100%)	273 (99%)	3 (1%)	73	57
All	All	1657/1662 (100%)	1636 (99%)	21 (1%)	69	50



All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASP
1	A	96	ASN
1	A	270	SER
1	B	51	ASP
1	B	270	SER
1	C	51	ASP
1	C	99	PHE
1	C	120	TYR
1	C	270	SER
1	D	51	ASP
1	D	120	TYR
1	D	270	SER
1	E	51	ASP
1	E	96	ASN
1	E	99	PHE
1	E	109	LEU
1	E	120	TYR
1	E	270	SER
1	F	51	ASP
1	F	120	TYR
1	F	270	SER

Some 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 ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	KCX	D	154	1,3	7,11,12	0.66	0	4,12,14	1.53	1 (25%)
1	KCX	C	154	1,3	7,11,12	0.65	0	4,12,14	0.83	0
1	KCX	F	154	1,3	7,11,12	0.69	0	4,12,14	1.38	1 (25%)
1	KCX	E	154	1,3	7,11,12	0.62	0	4,12,14	1.19	1 (25%)
1	KCX	B	154	1,3	7,11,12	0.57	0	4,12,14	0.51	0
1	KCX	A	154	1,3	7,11,12	0.68	0	4,12,14	0.78	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
1	KCX	D	154	1,3	-	0/7/10/12	-
1	KCX	C	154	1,3	-	1/7/10/12	-
1	KCX	F	154	1,3	-	0/7/10/12	-
1	KCX	E	154	1,3	-	1/7/10/12	-
1	KCX	B	154	1,3	-	0/7/10/12	-
1	KCX	A	154	1,3	-	0/7/10/12	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	KCX	CE-NZ-CX	-2.79	118.23	122.95
1	F	154	KCX	CE-NZ-CX	-2.41	118.86	122.95
1	E	154	KCX	CE-NZ-CX	-2.03	119.50	122.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	154	KCX	O-C-CA-CB
1	E	154	KCX	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	154	KCX	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 54 ligands modelled in this entry, 12 are monoatomic - leaving 42 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	PO4	E	340	-	4,4,4	0.89	0	6,6,6	0.52	0
2	GOL	C	333	-	5,5,5	0.35	0	5,5,5	0.25	0
4	PO4	B	338	-	4,4,4	0.83	0	6,6,6	0.49	0
2	GOL	E	333	-	5,5,5	0.40	0	5,5,5	0.30	0
2	GOL	D	331	-	5,5,5	0.33	0	5,5,5	0.32	0
2	GOL	F	331	-	5,5,5	0.37	0	5,5,5	0.41	0
4	PO4	F	336	3	4,4,4	1.05	0	6,6,6	0.47	0
2	GOL	A	331	-	5,5,5	0.34	0	5,5,5	0.32	0
2	GOL	C	331	-	5,5,5	0.33	0	5,5,5	0.34	0
2	GOL	B	333	-	5,5,5	0.43	0	5,5,5	0.46	0
2	GOL	D	333	-	5,5,5	0.31	0	5,5,5	0.42	0
2	GOL	C	334	-	5,5,5	0.33	0	5,5,5	0.30	0
4	PO4	E	338	-	4,4,4	0.92	0	6,6,6	0.39	0
2	GOL	B	331	-	5,5,5	0.52	0	5,5,5	0.65	0
4	PO4	A	335	3	4,4,4	1.06	0	6,6,6	0.57	0
2	GOL	B	332	-	5,5,5	0.34	0	5,5,5	0.34	0
4	PO4	C	339	3	4,4,4	1.08	0	6,6,6	0.55	0
2	GOL	F	332	-	5,5,5	0.41	0	5,5,5	0.38	0
2	GOL	D	332	-	5,5,5	0.42	0	5,5,5	0.49	0
4	PO4	E	339	-	4,4,4	0.94	0	6,6,6	0.43	0
4	PO4	E	337	3	4,4,4	1.05	0	6,6,6	0.61	0
4	PO4	E	341	-	4,4,4	0.86	0	6,6,6	0.48	0
4	PO4	C	340	-	4,4,4	0.86	0	6,6,6	0.41	0
4	PO4	C	341	-	4,4,4	0.82	0	6,6,6	0.55	0
2	GOL	E	334	-	5,5,5	0.32	0	5,5,5	0.49	0
4	PO4	A	336	-	4,4,4	0.82	0	6,6,6	0.44	0
4	PO4	D	337	-	4,4,4	0.89	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	B	337	-	4,4,4	0.84	0	6,6,6	0.38	0
2	GOL	C	332	-	5,5,5	0.35	0	5,5,5	0.33	0
4	PO4	B	336	3	4,4,4	1.08	0	6,6,6	0.62	0
2	GOL	E	332	-	5,5,5	0.35	0	5,5,5	0.43	0
4	PO4	F	338	-	4,4,4	0.88	0	6,6,6	0.47	0
2	GOL	C	335	-	5,5,5	0.37	0	5,5,5	0.37	0
4	PO4	D	338	-	4,4,4	0.96	0	6,6,6	0.38	0
4	PO4	F	337	-	4,4,4	0.85	0	6,6,6	0.30	0
4	PO4	C	342	-	4,4,4	0.89	0	6,6,6	0.49	0
4	PO4	D	336	3	4,4,4	1.04	0	6,6,6	0.50	0
2	GOL	A	332	-	5,5,5	0.38	0	5,5,5	0.36	0
2	GOL	C	336	-	5,5,5	0.34	0	5,5,5	0.46	0
2	GOL	E	331	-	5,5,5	0.37	0	5,5,5	0.32	0
4	PO4	A	337	-	4,4,4	0.93	0	6,6,6	0.41	0
2	GOL	F	333	-	5,5,5	0.37	0	5,5,5	0.17	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	334	-	-	2/4/4/4	-
2	GOL	C	333	-	-	0/4/4/4	-
2	GOL	C	334	-	-	4/4/4/4	-
2	GOL	B	331	-	-	2/4/4/4	-
2	GOL	E	333	-	-	2/4/4/4	-
2	GOL	D	331	-	-	0/4/4/4	-
2	GOL	B	332	-	-	4/4/4/4	-
2	GOL	F	331	-	-	2/4/4/4	-
2	GOL	C	332	-	-	1/4/4/4	-
2	GOL	F	332	-	-	0/4/4/4	-
2	GOL	A	332	-	-	4/4/4/4	-
2	GOL	D	332	-	-	2/4/4/4	-
2	GOL	C	336	-	-	2/4/4/4	-
2	GOL	A	331	-	-	4/4/4/4	-
2	GOL	E	332	-	-	1/4/4/4	-
2	GOL	C	331	-	-	1/4/4/4	-
2	GOL	B	333	-	-	3/4/4/4	-
2	GOL	E	331	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	335	-	-	3/4/4/4	-
2	GOL	F	333	-	-	3/4/4/4	-
2	GOL	D	333	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	333	GOL	O1-C1-C2-C3
2	F	331	GOL	O1-C1-C2-C3
2	A	331	GOL	O1-C1-C2-O2
2	A	331	GOL	O1-C1-C2-C3
2	C	334	GOL	C1-C2-C3-O3
2	B	332	GOL	C1-C2-C3-O3
2	E	334	GOL	O1-C1-C2-O2
2	E	334	GOL	O1-C1-C2-C3
2	C	335	GOL	C1-C2-C3-O3
2	C	336	GOL	O1-C1-C2-C3
2	F	331	GOL	O1-C1-C2-O2
2	C	331	GOL	C1-C2-C3-O3
2	B	333	GOL	C1-C2-C3-O3
2	D	333	GOL	C1-C2-C3-O3
2	C	334	GOL	O1-C1-C2-C3
2	B	331	GOL	O1-C1-C2-C3
2	E	332	GOL	C1-C2-C3-O3
2	A	332	GOL	O1-C1-C2-C3
2	A	332	GOL	C1-C2-C3-O3
2	F	333	GOL	O1-C1-C2-C3
2	E	333	GOL	O1-C1-C2-O2
2	C	334	GOL	O1-C1-C2-O2
2	B	331	GOL	O1-C1-C2-O2
2	A	332	GOL	O2-C2-C3-O3
2	C	336	GOL	O1-C1-C2-O2
2	C	334	GOL	O2-C2-C3-O3
2	B	332	GOL	O2-C2-C3-O3
2	C	335	GOL	O2-C2-C3-O3
2	A	332	GOL	O1-C1-C2-O2
2	D	333	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	331	GOL	O2-C2-C3-O3
2	F	333	GOL	O1-C1-C2-O2
2	F	333	GOL	C1-C2-C3-O3
2	B	333	GOL	O1-C1-C2-C3
2	D	332	GOL	C1-C2-C3-O3
2	B	332	GOL	O1-C1-C2-C3
2	C	332	GOL	C1-C2-C3-O3
2	B	333	GOL	O2-C2-C3-O3
2	B	332	GOL	O1-C1-C2-O2
2	A	331	GOL	C1-C2-C3-O3
2	C	335	GOL	O1-C1-C2-C3
2	D	332	GOL	O2-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	333	GOL	4	0
2	F	331	GOL	1	0
4	F	336	PO4	1	0
2	B	333	GOL	4	0
4	C	339	PO4	1	0
4	E	337	PO4	1	0
2	C	332	GOL	1	0
2	E	332	GOL	1	0
2	C	335	GOL	2	0
4	D	336	PO4	1	0
2	A	332	GOL	2	0
2	E	331	GOL	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 [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	328/330 (99%)	-0.43	2 (0%) 89 89	15, 23, 35, 46	0
1	B	328/330 (99%)	-0.47	1 (0%) 94 93	15, 23, 36, 46	0
1	C	327/330 (99%)	-0.50	1 (0%) 94 93	13, 19, 28, 36	0
1	D	327/330 (99%)	-0.46	1 (0%) 94 93	13, 19, 31, 41	0
1	E	327/330 (99%)	-0.50	1 (0%) 94 93	13, 19, 28, 37	0
1	F	327/330 (99%)	-0.45	0 100 100	14, 19, 31, 41	0
All	All	1964/1980 (99%)	-0.47	6 (0%) 94 93	13, 20, 32, 46	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	PRO	2.9
1	A	36	ASP	2.4
1	E	120	TYR	2.3
1	B	36	ASP	2.3
1	C	120	TYR	2.3
1	D	120	TYR	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	F	154	12/13	0.91	0.09	14,18,25,25	3
1	KCX	C	154	12/13	0.95	0.08	11,14,20,20	3
1	KCX	D	154	12/13	0.95	0.08	13,17,24,25	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KCX	E	154	12/13	0.95	0.08	12,14,20,21	3
1	KCX	B	154	12/13	0.97	0.07	17,18,24,27	3
1	KCX	A	154	12/13	0.97	0.07	15,18,25,25	2

## 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. 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( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	333	6/6	0.80	0.22	39,39,42,46	0
2	GOL	C	335	6/6	0.81	0.20	38,41,44,52	0
2	GOL	F	333	6/6	0.82	0.17	36,37,39,41	0
2	GOL	C	336	6/6	0.85	0.23	44,49,51,53	0
2	GOL	E	333	6/6	0.87	0.15	40,41,43,50	0
3	ZN	D	335	1/1	0.87	0.11	26,26,26,26	1
2	GOL	E	334	6/6	0.87	0.27	30,39,40,41	0
3	ZN	F	335	1/1	0.88	0.10	24,24,24,24	1
4	PO4	C	339	5/5	0.89	0.16	23,23,25,29	5
4	PO4	E	341	5/5	0.89	0.23	52,57,68,71	0
2	GOL	B	332	6/6	0.89	0.18	39,40,42,43	0
4	PO4	E	337	5/5	0.89	0.16	23,24,25,29	5
2	GOL	B	333	6/6	0.90	0.24	33,34,41,42	0
2	GOL	A	332	6/6	0.90	0.19	25,31,34,35	0
2	GOL	C	332	6/6	0.90	0.19	28,29,31,31	0
2	GOL	D	333	6/6	0.90	0.18	28,30,39,42	0
2	GOL	A	331	6/6	0.91	0.21	39,41,43,45	0
2	GOL	E	332	6/6	0.91	0.11	30,32,42,45	0
4	PO4	D	336	5/5	0.92	0.14	24,26,30,31	4
2	GOL	D	332	6/6	0.92	0.23	26,26,28,30	0
2	GOL	B	331	6/6	0.93	0.22	27,32,36,37	0
4	PO4	A	337	5/5	0.93	0.19	42,53,56,62	0
2	GOL	F	332	6/6	0.93	0.19	25,27,28,37	0
4	PO4	B	336	5/5	0.93	0.13	27,27,29,29	4
2	GOL	E	331	6/6	0.93	0.19	30,30,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	F	331	6/6	0.93	0.14	32,35,37,39	0
4	PO4	B	338	5/5	0.94	0.19	45,49,53,54	0
4	PO4	D	338	5/5	0.94	0.15	42,51,53,53	0
4	PO4	E	340	5/5	0.94	0.24	39,43,50,53	0
4	PO4	C	341	5/5	0.94	0.10	38,46,52,53	0
4	PO4	C	342	5/5	0.95	0.22	41,43,52,52	0
4	PO4	F	336	5/5	0.95	0.14	25,26,29,29	4
4	PO4	E	339	5/5	0.95	0.12	36,45,53,54	0
2	GOL	C	334	6/6	0.95	0.12	36,37,42,47	0
4	PO4	F	338	5/5	0.95	0.18	41,48,52,53	0
2	GOL	D	331	6/6	0.96	0.08	23,24,26,29	0
4	PO4	A	335	5/5	0.96	0.11	25,27,28,29	4
3	ZN	B	335	1/1	0.97	0.07	24,24,24,24	1
2	GOL	C	331	6/6	0.97	0.08	23,24,28,29	0
3	ZN	A	334	1/1	0.97	0.10	25,25,25,25	1
3	ZN	A	333	1/1	0.98	0.09	26,26,26,26	1
3	ZN	C	338	1/1	0.98	0.08	25,25,25,25	1
4	PO4	D	337	5/5	0.99	0.06	22,23,24,24	0
4	PO4	E	338	5/5	0.99	0.06	21,21,25,25	0
4	PO4	C	340	5/5	0.99	0.05	21,22,25,25	0
4	PO4	F	337	5/5	0.99	0.06	23,23,24,26	0
3	ZN	E	335	1/1	0.99	0.10	21,21,21,21	1
3	ZN	E	336	1/1	0.99	0.09	25,25,25,25	1
4	PO4	B	337	5/5	0.99	0.06	26,28,29,33	0
3	ZN	C	337	1/1	0.99	0.07	22,22,22,22	1
3	ZN	F	334	1/1	0.99	0.09	23,23,23,23	1
3	ZN	D	334	1/1	0.99	0.09	24,24,24,24	1
3	ZN	B	334	1/1	0.99	0.07	28,28,28,28	1
4	PO4	A	336	5/5	0.99	0.06	26,28,29,31	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.