



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 30, 2021 – 12:09 PM EST

PDB ID : 7TAV  
Title : Crystal Structure of the PBP2\_YvgL\_like protein Lmo1041 from *Listeria monocytogene*  
Authors : Kim, Y.; Maltseva, M.; Grimshaw, S.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2021-12-21  
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The 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	:	2.25
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)	:	2.25

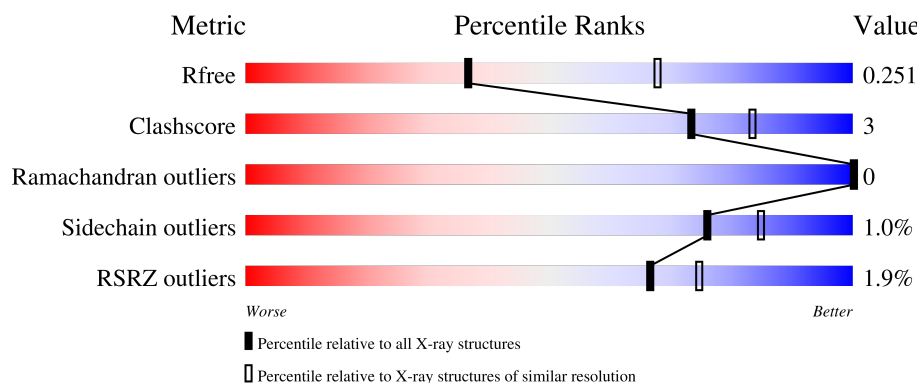
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	233	<div> <div>0%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	B	233	<div> <div>3%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	C	233	<div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	D	233	<div> <div>2%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	E	233	<div> <div>2%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	233	<div><div></div><div>3%</div><div>86%</div><div>11%</div><div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10464 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 Molybdate ABC transporter substrate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1725	1090	284	350	1			
1	B	229	Total	C	N	O	S	0	1	0
			1767	1115	292	359	1			
1	C	224	Total	C	N	O	S	0	0	0
			1717	1085	284	347	1			
1	D	224	Total	C	N	O	S	0	0	0
			1717	1085	284	347	1			
1	E	223	Total	C	N	O	S	0	0	0
			1709	1081	282	345	1			
1	F	226	Total	C	N	O	S	0	0	0
			1732	1094	286	351	1			

There are 18 discrepancies between the modelled and reference sequences:

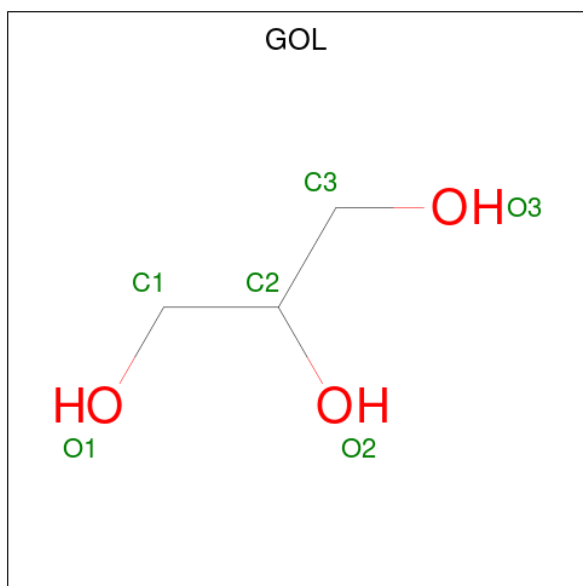
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A5D5LL32
A	-1	ASN	-	expression tag	UNP A0A5D5LL32
A	0	ALA	-	expression tag	UNP A0A5D5LL32
B	-2	SER	-	expression tag	UNP A0A5D5LL32
B	-1	ASN	-	expression tag	UNP A0A5D5LL32
B	0	ALA	-	expression tag	UNP A0A5D5LL32
C	-2	SER	-	expression tag	UNP A0A5D5LL32
C	-1	ASN	-	expression tag	UNP A0A5D5LL32
C	0	ALA	-	expression tag	UNP A0A5D5LL32
D	-2	SER	-	expression tag	UNP A0A5D5LL32
D	-1	ASN	-	expression tag	UNP A0A5D5LL32
D	0	ALA	-	expression tag	UNP A0A5D5LL32
E	-2	SER	-	expression tag	UNP A0A5D5LL32
E	-1	ASN	-	expression tag	UNP A0A5D5LL32
E	0	ALA	-	expression tag	UNP A0A5D5LL32
F	-2	SER	-	expression tag	UNP A0A5D5LL32
F	-1	ASN	-	expression tag	UNP A0A5D5LL32

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP A0A5D5LL32

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	B	1	Total	Ca	0	0
			1	1		
3	C	4	Total	Ca	0	0
			4	4		
3	D	2	Total	Ca	0	0
			2	2		
3	E	4	Total	Ca	0	0
			4	4		
3	F	3	Total	Ca	0	0
			3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O	0	0
			12	12		
6	C	9	Total	O	0	0
			9	9		

*Continued on next page...*

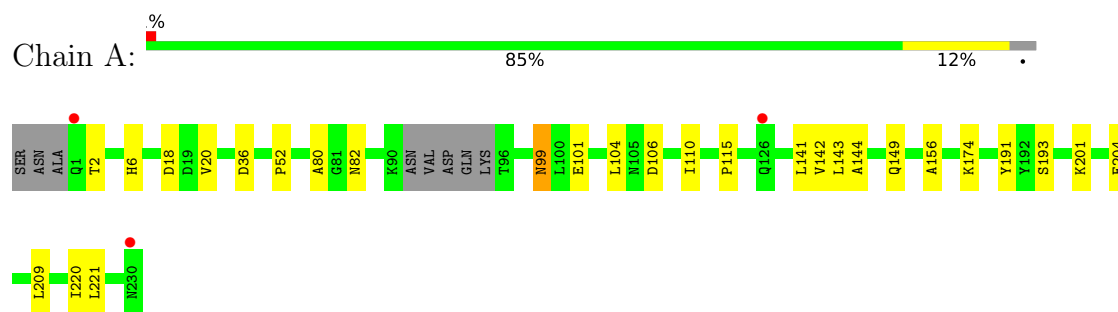
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	3	Total	O	0	0
			3	3		
6	E	4	Total	O	0	0
			4	4		
6	F	8	Total	O	0	0
			8	8		

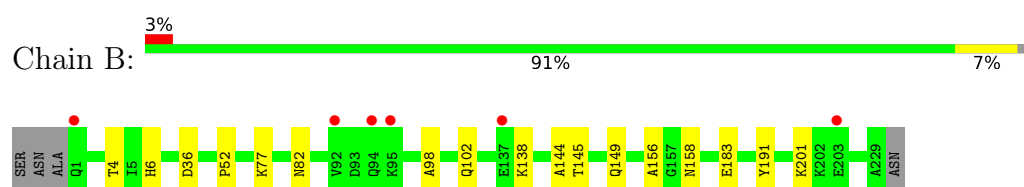
### 3 Residue-property plots [i](#)

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.

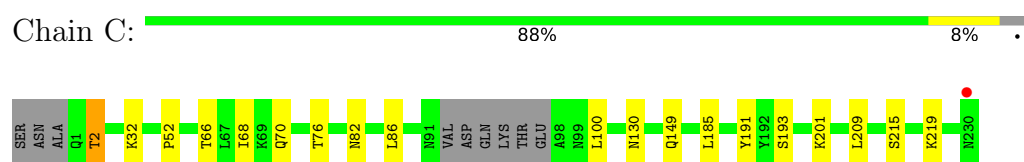
- Molecule 1: Molybdate ABC transporter substrate-binding protein



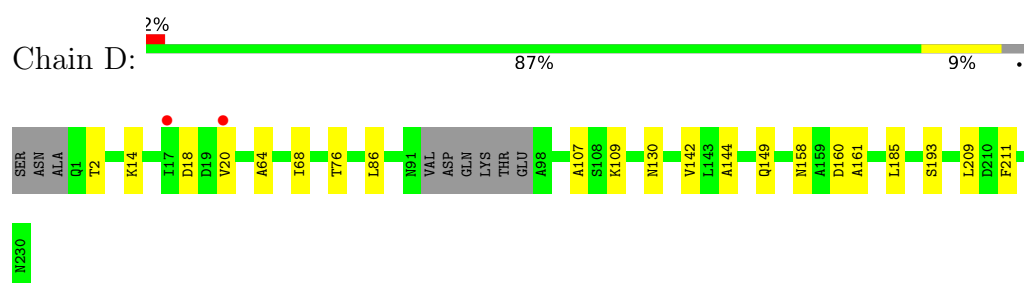
- Molecule 1: Molybdate ABC transporter substrate-binding protein



- Molecule 1: Molybdate ABC transporter substrate-binding protein

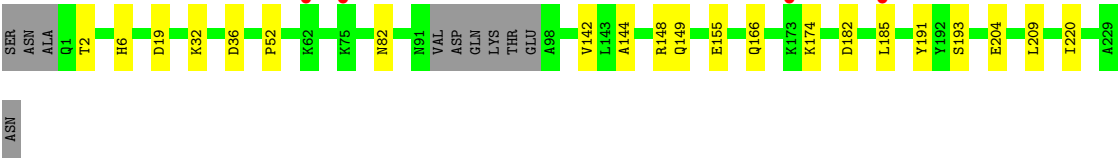
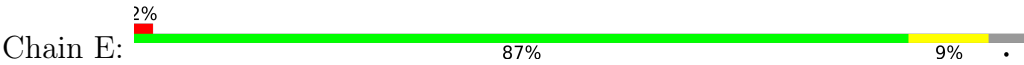


- Molecule 1: Molybdate ABC transporter substrate-binding protein

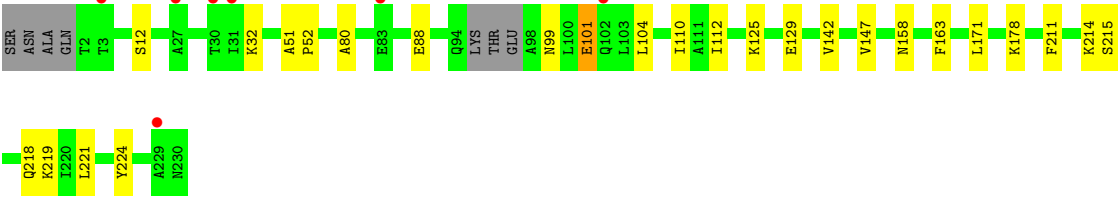
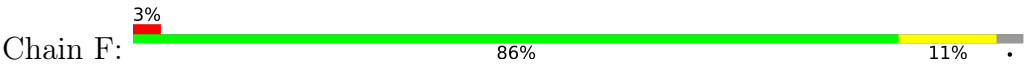


- Molecule 1: Molybdate ABC transporter substrate-binding protein





• Molecule 1: Molybdate ABC transporter substrate-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.72Å 113.72Å 114.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.22 – 2.75 49.24 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (37.22-2.75) 98.9 (49.24-2.75)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.213 , 0.251 0.212 , 0.251	Depositor DCC
$R_{free}$ test set	2227 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l 0.036 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL, CA, 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	0.25	0/1747	0.42	0/2357
1	B	0.24	0/1790	0.42	0/2416
1	C	0.24	0/1739	0.41	0/2346
1	D	0.24	0/1739	0.42	0/2346
1	E	0.24	0/1731	0.41	0/2335
1	F	0.24	0/1754	0.41	0/2367
All	All	0.24	0/10500	0.42	0/14167

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

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	1725	0	1744	16	0
1	B	1767	0	1786	12	0
1	C	1717	0	1737	11	0
1	D	1717	0	1737	14	0
1	E	1709	0	1731	13	0
1	F	1732	0	1747	15	0
2	A	6	0	8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	6	0	8	0	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
3	E	4	0	0	0	0
3	F	3	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	B	1	0	0	1	0
6	A	12	0	0	0	0
6	C	9	0	0	0	0
6	D	3	0	0	0	0
6	E	4	0	0	0	0
6	F	8	0	0	0	0
All	All	10464	0	10498	70	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 (70) 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:52:PRO:HB2	1:F:158:ASN:HB3	1.79	0.65
1:C:201:LYS:NZ	1:D:158:ASN:OD1	2.30	0.62
1:D:193:SER:HB2	1:D:209:LEU:HD22	1.81	0.62
1:C:193:SER:HB2	1:C:209:LEU:HD22	1.82	0.60
1:D:144:ALA:HB1	1:D:149:GLN:HB3	1.83	0.59
1:E:193:SER:HB2	1:E:209:LEU:HD22	1.88	0.56
1:E:144:ALA:HB1	1:E:149:GLN:HB3	1.90	0.54
1:E:182:ASP:HB3	1:E:185:LEU:HG	1.89	0.53
1:C:130:ASN:ND2	1:C:185:LEU:O	2.38	0.53
1:E:204:GLU:OE1	1:E:204:GLU:N	2.41	0.53
1:D:109:LYS:HD3	1:D:142:VAL:HG21	1.91	0.53
1:A:201:LYS:NZ	1:B:156:ALA:O	2.42	0.53
1:F:125:LYS:NZ	1:F:129:GLU:OE2	2.42	0.52
1:B:145:THR:HG23	5:B:303:CL:CL	2.46	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ALA:O	1:B:201:LYS:NZ	2.41	0.52
1:B:144:ALA:HB1	1:B:149:GLN:HB3	1.90	0.51
1:F:80:ALA:HB2	1:F:221:LEU:HD13	1.92	0.51
1:C:52:PRO:HB2	1:D:158:ASN:HB3	1.91	0.51
1:A:80:ALA:HB2	1:A:221:LEU:HD13	1.93	0.51
1:A:104:LEU:HD22	1:A:110:ILE:HD13	1.93	0.51
1:A:144:ALA:HB1	1:A:149:GLN:HB3	1.93	0.50
1:D:20:VAL:HG13	1:D:211:PHE:HE2	1.77	0.50
1:A:6:HIS:NE2	1:A:36:ASP:OD1	2.45	0.49
1:F:104:LEU:HD22	1:F:110:ILE:HD13	1.94	0.49
1:A:193:SER:HB2	1:A:209:LEU:HD22	1.93	0.49
1:C:52:PRO:HD3	1:D:142:VAL:HG11	1.95	0.49
1:D:14:LYS:NZ	1:D:18:ASP:OD2	2.45	0.48
1:E:52:PRO:HD3	1:F:142:VAL:HG11	1.95	0.48
1:A:82:ASN:HB2	1:A:191:TYR:HE1	1.79	0.48
1:C:68:ILE:HD11	1:C:76:THR:HB	1.94	0.48
1:D:130:ASN:ND2	1:D:185:LEU:O	2.47	0.48
1:F:215:SER:HA	1:F:218:GLN:HB2	1.96	0.47
1:A:142:VAL:HG11	1:B:52:PRO:HD3	1.96	0.47
1:C:215:SER:O	1:C:219:LYS:HG2	2.14	0.47
1:F:88:GLU:HG3	1:F:178:LYS:HG3	1.95	0.47
1:E:155:GLU:HB3	1:E:174:LYS:HE3	1.95	0.47
1:D:86:LEU:HD11	1:D:161:ALA:HB1	1.97	0.47
1:A:110:ILE:HB	1:A:141:LEU:HD23	1.96	0.46
1:B:6:HIS:NE2	1:B:36:ASP:OD2	2.48	0.46
1:D:160:ASP:N	1:D:160:ASP:OD1	2.46	0.46
1:E:142:VAL:HG11	1:F:52:PRO:HD3	1.98	0.46
1:A:174:LYS:NZ	1:B:4:THR:OG1	2.49	0.45
1:E:82:ASN:HB2	1:E:191:TYR:HE1	1.81	0.45
1:F:211:PHE:HA	1:F:214:LYS:HD2	1.99	0.44
1:E:6:HIS:NE2	1:E:36:ASP:OD2	2.50	0.44
1:F:12:SER:HB3	1:F:147:VAL:HG11	2.00	0.44
1:A:115:PRO:HD3	1:A:143:LEU:HD22	2.00	0.44
1:B:82:ASN:HB2	1:B:191:TYR:HE1	1.83	0.44
1:D:64:ALA:O	1:D:68:ILE:HG12	2.17	0.44
1:C:82:ASN:HB2	1:C:191:TYR:HE1	1.84	0.43
1:A:52:PRO:HB2	1:B:158:ASN:HB3	2.00	0.42
1:E:2:THR:HG21	1:E:32:LYS:HG2	2.01	0.42
1:A:204:GLU:OE1	1:A:204:GLU:N	2.44	0.41
1:E:19:ASP:HB2	1:E:220:ILE:HG21	2.02	0.41
1:D:76:THR:HA	1:D:193:SER:O	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:LYS:HD3	1:F:32:LYS:HA	1.81	0.41
1:F:51:ALA:HA	1:F:52:PRO:HD3	1.96	0.41
1:A:20:VAL:HG22	1:A:220:ILE:HD12	2.01	0.41
1:B:138:LYS:HB3	1:B:138:LYS:HE2	1.83	0.41
1:A:99:ASN:ND2	1:A:101:GLU:H	2.17	0.41
1:B:98:ALA:HB1	1:B:102:GLN:HB3	2.03	0.41
1:C:66:THR:O	1:C:70:GLN:NE2	2.53	0.41
1:D:107:ALA:HB1	1:D:160:ASP:HB2	2.03	0.41
1:E:148:ARG:HD3	1:E:148:ARG:HA	1.91	0.41
1:C:2:THR:HG21	1:C:32:LYS:HG2	2.02	0.40
1:F:171:LEU:HD21	1:F:224:TYR:HD1	1.85	0.40
1:F:99:ASN:HD21	1:F:101:GLU:HB2	1.85	0.40
1:B:77:LYS:HA	1:B:77:LYS:HD2	1.81	0.40
1:C:86:LEU:HD22	1:C:100:LEU:HD12	2.03	0.40
1:F:112:ILE:HG22	1:F:163:PHE:HB2	2.04	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	221/233 (95%)	217 (98%)	4 (2%)	0	100	100
1	B	228/233 (98%)	224 (98%)	4 (2%)	0	100	100
1	C	220/233 (94%)	215 (98%)	5 (2%)	0	100	100
1	D	220/233 (94%)	217 (99%)	3 (1%)	0	100	100
1	E	219/233 (94%)	217 (99%)	2 (1%)	0	100	100
1	F	222/233 (95%)	218 (98%)	4 (2%)	0	100	100
All	All	1330/1398 (95%)	1308 (98%)	22 (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	185/192 (96%)	181 (98%)	4 (2%)	52	70
1	B	190/192 (99%)	189 (100%)	1 (0%)	88	92
1	C	184/192 (96%)	182 (99%)	2 (1%)	73	84
1	D	184/192 (96%)	183 (100%)	1 (0%)	88	92
1	E	183/192 (95%)	182 (100%)	1 (0%)	88	92
1	F	186/192 (97%)	184 (99%)	2 (1%)	73	84
All	All	1112/1152 (96%)	1101 (99%)	11 (1%)	76	85

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

Mol	Chain	Res	Type
1	A	2	THR
1	A	18	ASP
1	A	99	ASN
1	A	106	ASP
1	B	183	GLU
1	C	2	THR
1	C	149	GLN
1	D	2	THR
1	E	166	GLN
1	F	101	GLU
1	F	219	LYS

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

### 5.3.3 RNA

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 19 are monoatomic - leaving 8 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	SO4	B	302	-	4,4,4	0.18	0	6,6,6	0.05	0
4	SO4	C	305	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	F	305	-	4,4,4	0.16	0	6,6,6	0.07	0
2	GOL	A	301	-	5,5,5	0.89	0	5,5,5	1.02	0
2	GOL	F	301	-	5,5,5	0.92	0	5,5,5	0.96	0
4	SO4	E	305	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	A	306	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	D	303	-	4,4,4	0.15	0	6,6,6	0.05	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	301	-	-	0/4/4/4	-
2	GOL	F	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	GOL	C1-C2-C3-O3
2	F	301	GOL	O2-C2-C3-O3
2	F	301	GOL	O1-C1-C2-C3
2	F	301	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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	225/233 (96%)	0.21	3 (1%) 77 84	45, 54, 67, 87	0
1	B	229/233 (98%)	0.25	6 (2%) 56 65	43, 54, 68, 117	0
1	C	224/233 (96%)	0.19	1 (0%) 92 95	43, 56, 69, 86	0
1	D	224/233 (96%)	0.28	5 (2%) 62 70	47, 59, 72, 87	0
1	E	223/233 (95%)	0.24	4 (1%) 68 76	48, 58, 71, 79	0
1	F	226/233 (96%)	0.36	7 (3%) 49 58	44, 57, 70, 103	0
All	All	1351/1398 (96%)	0.26	26 (1%) 66 75	43, 57, 70, 117	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	VAL	4.1
1	F	3	THR	3.9
1	F	27	ALA	3.2
1	A	1	GLN	2.9
1	B	1	GLN	2.8
1	F	31	ILE	2.6
1	B	94	GLN	2.5
1	B	95	LYS	2.5
1	D	215	SER	2.4
1	E	62	LYS	2.4
1	E	173	LYS	2.3
1	C	230	ASN	2.3
1	E	185	LEU	2.3
1	D	17	ILE	2.3
1	D	220	ILE	2.2
1	D	20	VAL	2.2
1	F	83	GLU	2.2
1	A	230	ASN	2.2
1	F	229	ALA	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	126	GLN	2.2
1	D	221	LEU	2.2
1	B	137	GLU	2.1
1	B	203	GLU	2.1
1	E	75	LYS	2.1
1	F	30	THR	2.1
1	F	102	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	A	305	1/1	0.82	0.10	76,76,76,76	0
3	CA	D	301	1/1	0.83	0.20	62,62,62,62	0
2	GOL	A	301	6/6	0.85	0.22	61,61,61,61	0
2	GOL	F	301	6/6	0.85	0.15	70,70,70,70	0
3	CA	C	303	1/1	0.87	0.11	74,74,74,74	0
3	CA	E	302	1/1	0.88	0.18	78,78,78,78	0
3	CA	F	302	1/1	0.90	0.12	63,63,63,63	0
3	CA	A	304	1/1	0.91	0.05	74,74,74,74	0
3	CA	F	303	1/1	0.92	0.25	61,61,61,61	0
3	CA	E	301	1/1	0.94	0.16	60,60,60,60	0
3	CA	C	304	1/1	0.94	0.06	72,72,72,72	0
3	CA	A	302	1/1	0.94	0.18	61,61,61,61	0
3	CA	D	302	1/1	0.94	0.27	64,64,64,64	0
3	CA	B	301	1/1	0.95	0.23	57,57,57,57	0
3	CA	F	304	1/1	0.95	0.06	70,70,70,70	0
5	CL	B	303	1/1	0.95	0.11	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	C	301	1/1	0.96	0.19	62,62,62,62	0
3	CA	C	302	1/1	0.96	0.21	58,58,58,58	0
3	CA	A	303	1/1	0.96	0.18	56,56,56,56	0
3	CA	E	303	1/1	0.97	0.18	74,74,74,74	0
3	CA	E	304	1/1	0.98	0.26	52,52,52,52	0
4	SO4	B	302	5/5	0.99	0.44	17,23,26,89	0
4	SO4	C	305	5/5	0.99	0.32	26,27,31,32	0
4	SO4	A	306	5/5	0.99	0.33	23,25,29,31	0
4	SO4	E	305	5/5	1.00	0.33	25,33,34,34	0
4	SO4	F	305	5/5	1.00	0.34	20,21,24,39	0
4	SO4	D	303	5/5	1.00	0.28	26,27,33,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.