



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:14 PM GMT

PDB ID : 4HN3  
Title : The crystal structure of a sex pheromone precursor (lmo1757) from *Listeria monocytogenes* EGD-e  
Authors : Tan, K.; Makowska-Grzyska, M.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2012-10-18  
Resolution : 2.05 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

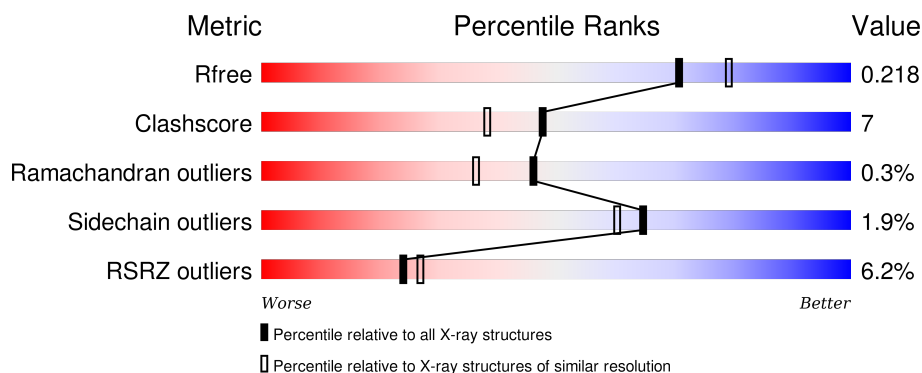
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	350	<div> <div>4%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
1	B	350	<div> <div>5%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
1	C	350	<div> <div>5%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	D	350	<div> <div>8%</div> <div>77%</div> <div>17%</div> <div>6%</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
2	GOL	B	401	-	-	X	X
2	GOL	B	405	-	-	X	X
2	GOL	C	401	-	-	-	X
2	GOL	C	403	-	-	-	X
2	GOL	D	402	-	-	-	X
3	PEG	A	403	-	-	X	X
3	PEG	A	405	-	-	X	X
3	PEG	B	406	-	-	-	X
3	PEG	B	407	-	-	X	-
3	PEG	D	405	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11113 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 Lmo1757 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	Se	0	3	0
			2622	1650	441	527	4			
1	B	334	Total	C	N	O	Se	0	1	0
			2619	1646	443	526	4			
1	C	328	Total	C	N	O	Se	0	1	0
			2582	1623	433	522	4			
1	D	330	Total	C	N	O	Se	0	2	0
			2600	1636	436	524	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	-	EXPRESSION TAG	UNP Q8Y6D1
A	23	ASN	-	EXPRESSION TAG	UNP Q8Y6D1
A	24	ALA	-	EXPRESSION TAG	UNP Q8Y6D1
B	22	SER	-	EXPRESSION TAG	UNP Q8Y6D1
B	23	ASN	-	EXPRESSION TAG	UNP Q8Y6D1
B	24	ALA	-	EXPRESSION TAG	UNP Q8Y6D1
C	22	SER	-	EXPRESSION TAG	UNP Q8Y6D1
C	23	ASN	-	EXPRESSION TAG	UNP Q8Y6D1
C	24	ALA	-	EXPRESSION TAG	UNP Q8Y6D1
D	22	SER	-	EXPRESSION TAG	UNP Q8Y6D1
D	23	ASN	-	EXPRESSION TAG	UNP Q8Y6D1
D	24	ALA	-	EXPRESSION TAG	UNP Q8Y6D1

- 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	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	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	C	1	Total	C	O	0	0
			6	3	3		
2	C	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		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

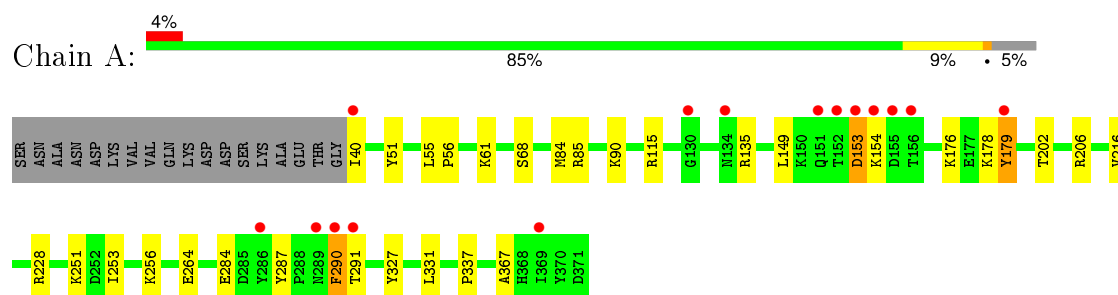
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	195	Total	O	0	0
			195	195		
5	B	116	Total	O	0	0
			116	116		
5	C	156	Total	O	0	0
			156	156		
5	D	78	Total	O	0	0
			78	78		

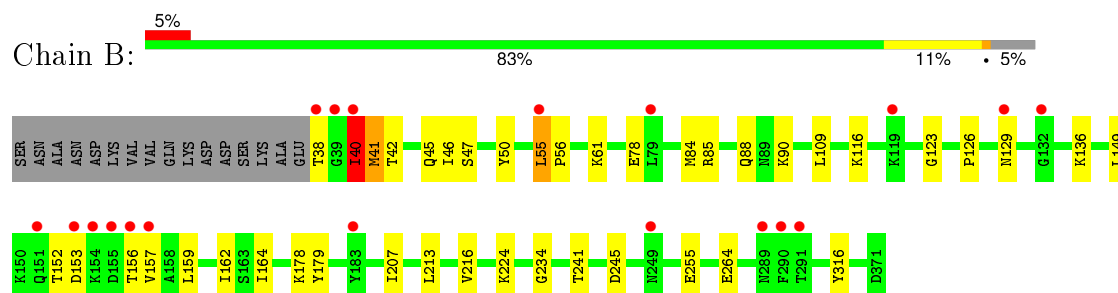
### 3 Residue-property plots [i](#)

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.

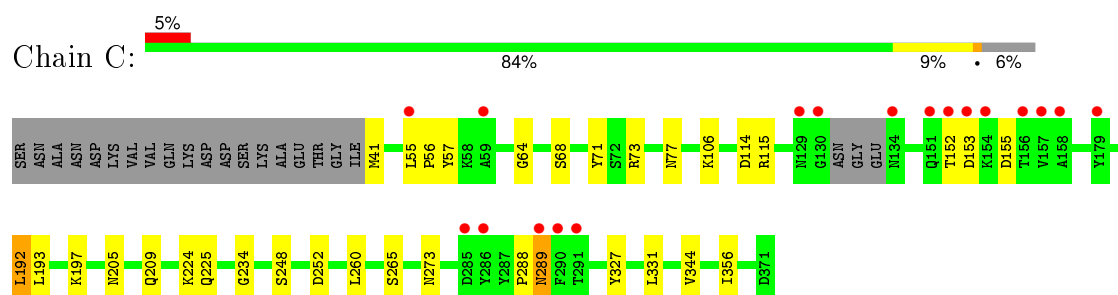
#### • Molecule 1: Lmo1757 protein



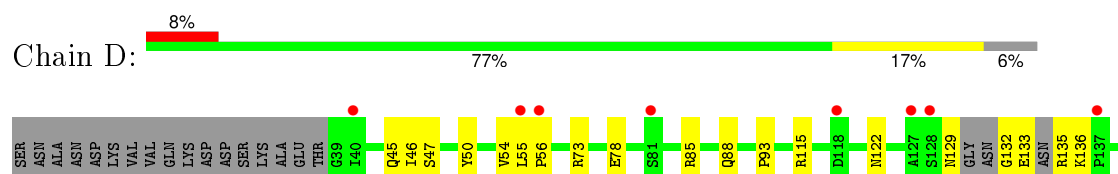
#### • Molecule 1: Lmo1757 protein



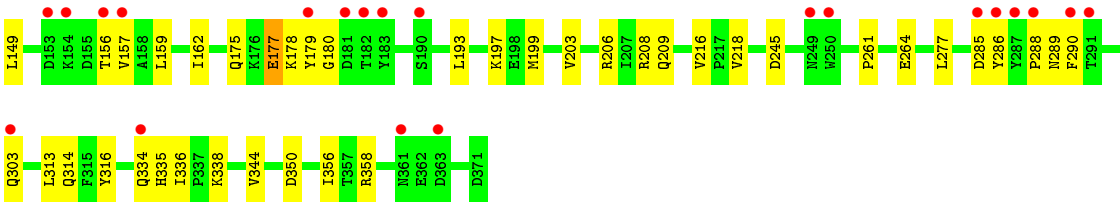
#### • Molecule 1: Lmo1757 protein



#### • Molecule 1: Lmo1757 protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.09Å 99.32Å 104.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.01 – 2.05 36.01 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.01-2.05) 99.2 (36.01-2.05)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.181 , 0.221 0.182 , 0.218	Depositor DCC
$R_{free}$ test set	4879 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.9	EDS
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 97657 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.48% 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, 0.375 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, PEG, BME

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	0.40	0/2677	0.52	0/3625
1	B	0.36	0/2668	0.50	0/3613
1	C	0.37	0/2631	0.51	1/3565 (0.0%)
1	D	0.32	0/2650	0.49	0/3585
All	All	0.36	0/10626	0.51	1/14388 (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	C	192	LEU	CA-CB-CG	6.19	129.54	115.30

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	2622	0	2540	38	0
1	B	2619	0	2525	46	0
1	C	2582	0	2479	30	0
1	D	2600	0	2511	45	0
2	A	12	0	16	4	0
2	B	30	0	40	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	32	1	0
2	D	12	0	16	2	0
3	A	21	0	30	16	0
3	B	14	0	20	8	0
3	C	7	0	10	3	0
3	D	21	0	30	5	0
4	A	4	0	6	0	0
5	A	195	0	0	5	0
5	B	116	0	0	2	0
5	C	156	0	0	1	0
5	D	78	0	0	1	0
All	All	11113	0	10255	154	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 7.

All (154) 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:85:ARG:HE	2:B:401:GOL:H12	1.33	0.93
1:B:178:LYS:NZ	2:B:405:GOL:H12	1.92	0.84
1:C:77:ASN:HD21	3:C:405:PEG:H12	1.42	0.84
1:A:206:ARG:HH21	3:A:405:PEG:H42	1.39	0.83
1:B:178:LYS:NZ	3:B:407:PEG:H31	1.94	0.82
1:A:85:ARG:HE	3:A:403:PEG:H11	1.44	0.81
1:B:264:GLU:HG2	5:B:561:HOH:O	1.82	0.78
1:B:85:ARG:HE	2:B:401:GOL:C1	1.99	0.76
1:D:47:SER:HB3	1:D:50:TYR:CD2	2.21	0.75
1:A:202:THR:HG23	3:A:405:PEG:H41	1.68	0.75
1:D:316:TYR:CE1	3:D:404:PEG:H31	2.22	0.74
2:A:401:GOL:H11	1:B:316:TYR:CE1	2.23	0.73
1:B:178:LYS:NZ	3:B:407:PEG:H12	2.03	0.73
1:D:334:GLN:HB2	1:D:335:HIS:HD2	1.53	0.72
1:D:85:ARG:HD2	2:D:401:GOL:H11	1.70	0.71
1:B:90:LYS:HE3	1:B:241:THR:HG21	1.72	0.70
1:D:115:ARG:NH1	1:D:136:LYS:O	2.25	0.69
1:B:178:LYS:HZ3	3:B:407:PEG:H31	1.56	0.68
1:A:206:ARG:NH2	3:A:405:PEG:H22	2.09	0.68
1:C:56:PRO:HG2	5:C:649:HOH:O	1.93	0.68
1:D:133:GLU:HA	1:D:135:ARG:N	2.10	0.67
1:B:85:ARG:NE	2:B:401:GOL:H12	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:HH21	3:A:405:PEG:H22	1.60	0.67
1:B:41:MSE:HG2	1:B:42:THR:O	1.95	0.66
1:B:40:ILE:HD12	1:B:40:ILE:H	1.59	0.66
1:B:178:LYS:HZ2	2:B:405:GOL:H12	1.60	0.66
1:A:85:ARG:NE	3:A:403:PEG:H11	2.10	0.66
1:B:55:LEU:HA	1:B:56:PRO:C	2.16	0.66
1:B:41:MSE:SE	5:B:586:HOH:O	2.64	0.65
1:C:41:MSE:N	1:C:55:LEU:H	1.94	0.65
1:C:55:LEU:HB3	1:D:286:TYR:HE2	1.62	0.65
1:D:129:ASN:HD21	1:D:136:LYS:H	1.45	0.64
1:A:206:ARG:NH2	3:A:405:PEG:H42	2.11	0.64
1:A:135:ARG:NH2	2:A:402:GOL:H32	2.13	0.64
1:A:85:ARG:HE	3:A:403:PEG:C1	2.09	0.63
1:D:54:VAL:HG21	1:D:149:LEU:HD22	1.81	0.62
1:B:153:ASP:OD1	1:B:156:THR:HG22	1.99	0.62
1:B:40:ILE:HD13	1:B:55:LEU:HD12	1.82	0.61
1:D:303:GLN:HB2	3:D:405:PEG:H22	1.81	0.61
1:D:156:THR:HA	3:D:403:PEG:H22	1.81	0.61
1:B:255:GLU:OE2	2:B:401:GOL:H11	2.00	0.61
2:B:405:GOL:H31	1:C:68:SER:O	2.00	0.61
1:A:264:GLU:OE1	5:A:646:HOH:O	2.16	0.61
1:B:178:LYS:HZ1	3:B:407:PEG:H31	1.66	0.60
1:D:149:LEU:HB3	1:D:157:VAL:HG22	1.83	0.59
1:B:152:THR:OG1	1:B:156:THR:HG23	2.02	0.59
1:D:129:ASN:HD21	1:D:136:LYS:N	2.01	0.58
1:B:126:PRO:HB2	1:B:136:LYS:HE3	1.85	0.58
1:B:159:LEU:HD23	1:B:216:VAL:HG11	1.86	0.58
1:B:38:THR:CB	1:B:156:THR:HA	2.33	0.58
1:A:178:LYS:O	1:A:179:TYR:HB2	2.03	0.58
1:D:129:ASN:ND2	1:D:136:LYS:H	2.03	0.56
1:B:153:ASP:CG	1:B:156:THR:HG22	2.25	0.56
1:A:206:ARG:HE	3:A:405:PEG:H42	1.69	0.56
1:B:40:ILE:CD1	1:B:40:ILE:H	2.18	0.56
1:D:199:MSE:O	1:D:203:VAL:HG23	2.06	0.55
1:B:178:LYS:CE	2:B:405:GOL:H12	2.36	0.55
1:C:55:LEU:HA	1:C:57:TYR:N	2.21	0.55
1:B:129:ASN:OD1	1:B:136:LYS:HG3	2.07	0.55
3:B:407:PEG:H11	1:C:71:TYR:CE1	2.42	0.55
1:A:256:LYS:NZ	1:A:264:GLU:OE2	2.30	0.55
1:D:122:ASN:O	1:D:206:ARG:NH1	2.38	0.54
3:A:403:PEG:O1	3:A:403:PEG:H32	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:HE	3:A:405:PEG:C4	2.22	0.53
1:A:51:TYR:H	1:A:84:MSE:HE2	1.74	0.53
1:A:135:ARG:HH21	2:A:402:GOL:H32	1.73	0.53
1:C:115:ARG:HH21	2:C:402:GOL:H2	1.75	0.51
1:B:40:ILE:HD13	1:B:55:LEU:CD1	2.40	0.51
1:A:216:VAL:HG13	5:A:610:HOH:O	2.10	0.51
1:C:77:ASN:ND2	3:C:405:PEG:H12	2.21	0.51
1:C:41:MSE:N	1:C:55:LEU:HB2	2.26	0.51
2:B:404:GOL:H12	1:C:106:LYS:NZ	2.26	0.51
1:B:90:LYS:NZ	2:B:402:GOL:O3	2.41	0.50
1:D:132:GLY:N	5:D:565:HOH:O	2.43	0.50
1:A:115:ARG:HH21	2:A:402:GOL:H2	1.75	0.50
1:D:334:GLN:CB	1:D:335:HIS:HD2	2.22	0.49
1:A:337:PRO:HG2	5:A:630:HOH:O	2.11	0.49
1:B:84:MSE:O	1:B:88:GLN:HG3	2.12	0.49
1:A:55:LEU:HA	1:A:56:PRO:C	2.33	0.49
2:B:404:GOL:H12	1:C:106:LYS:HZ3	1.78	0.49
1:C:260:LEU:N	1:C:260:LEU:HD12	2.27	0.49
1:C:55:LEU:HB3	1:D:286:TYR:CE2	2.44	0.49
1:C:73[A]:ARG:NH2	3:C:405:PEG:O1	2.46	0.49
1:B:116:LYS:HE2	1:B:123:GLY:O	2.13	0.49
1:D:178:LYS:HE2	1:D:179:TYR:CZ	2.47	0.49
1:D:175:GLN:NE2	1:D:180:GLY:O	2.41	0.49
1:A:228:ARG:HH12	3:A:404:PEG:C1	2.25	0.48
1:D:129:ASN:HD22	1:D:136:LYS:HG3	1.79	0.48
1:D:336:ILE:HG22	1:D:358:ARG:NH2	2.29	0.48
1:D:344:VAL:HB	1:D:356:ILE:HB	1.94	0.48
1:D:55:LEU:HA	1:D:56:PRO:C	2.33	0.48
1:D:193:LEU:O	1:D:197:LYS:HG3	2.14	0.48
1:A:153:ASP:CG	1:A:154:LYS:N	2.67	0.47
1:C:152:THR:O	1:C:153:ASP:HB3	2.15	0.47
3:B:407:PEG:H11	1:C:71:TYR:CD1	2.50	0.46
1:D:336:ILE:HG22	1:D:358:ARG:HH22	1.81	0.46
1:D:45:GLN:O	1:D:46:ILE:HB	2.14	0.46
1:D:149:LEU:HD12	1:D:149:LEU:N	2.30	0.46
1:C:55:LEU:HA	1:C:56:PRO:C	2.36	0.46
1:B:38:THR:CB	1:B:157:VAL:H	2.29	0.46
1:A:149:LEU:HD12	1:A:149:LEU:N	2.31	0.46
1:A:367:ALA:HB3	1:B:46:ILE:HG12	1.98	0.46
1:A:178:LYS:O	1:A:179:TYR:CB	2.63	0.46
1:B:85:ARG:HB3	2:B:401:GOL:H32	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:TYR:OH	3:B:407:PEG:H21	2.15	0.46
1:B:162:ILE:HD11	1:B:207:ILE:HD13	1.98	0.46
1:A:253:ILE:HG23	3:A:403:PEG:H31	1.97	0.46
1:A:251:LYS:HB2	1:A:251:LYS:HE2	1.73	0.45
1:B:207:ILE:HG23	1:B:213:LEU:HD13	1.98	0.45
1:D:159:LEU:HD23	1:D:216:VAL:HG21	1.99	0.45
1:D:129:ASN:ND2	1:D:136:LYS:HG3	2.31	0.45
1:C:153:ASP:C	1:C:155:ASP:H	2.20	0.45
1:A:327:TYR:CE2	1:A:331:LEU:HD11	2.52	0.45
1:B:149:LEU:N	1:B:149:LEU:HD12	2.31	0.45
1:C:192:LEU:HD11	1:C:224:LYS:HG3	1.98	0.45
1:D:193:LEU:HG	1:D:197:LYS:HE3	1.98	0.44
1:C:288:PRO:O	1:C:289:ASN:CB	2.64	0.44
1:A:287:TYR:HB3	1:A:290:PHE:CE2	2.53	0.44
1:A:85:ARG:CD	3:A:403:PEG:H11	2.47	0.44
1:C:327:TYR:CE2	1:C:331:LEU:HD11	2.52	0.44
1:B:45:GLN:NE2	1:B:50:TYR:O	2.47	0.44
1:B:178:LYS:O	1:B:179:TYR:HB2	2.17	0.44
1:D:290:PHE:CE1	1:D:313:LEU:HD22	2.51	0.44
1:C:56:PRO:HA	1:D:286:TYR:CE2	2.53	0.44
1:C:344:VAL:HB	1:C:356:ILE:HB	1.99	0.43
1:C:193:LEU:HD11	1:C:197:LYS:HE3	2.01	0.43
1:C:265:SER:OG	1:C:273:ASN:OD1	2.34	0.43
1:D:288:PRO:O	1:D:289:ASN:CB	2.67	0.43
1:A:90:LYS:HA	1:A:90:LYS:HD3	1.83	0.43
1:D:129:ASN:HD21	1:D:135:ARG:HA	1.83	0.43
1:A:264:GLU:HB2	5:A:556:HOH:O	2.18	0.43
1:A:176:LYS:N	5:A:609:HOH:O	2.43	0.43
1:A:206:ARG:NE	3:A:405:PEG:H42	2.34	0.43
1:B:116:LYS:HE3	1:B:116:LYS:HB2	1.87	0.43
1:A:228:ARG:HH12	3:A:404:PEG:H11	1.83	0.43
1:D:85:ARG:CD	2:D:401:GOL:H11	2.45	0.43
1:C:224:LYS:O	1:C:234:GLY:HA3	2.19	0.43
1:A:68:SER:OG	1:D:177:GLU:HG3	2.19	0.42
1:C:73[B]:ARG:NH1	1:D:350:ASP:OD1	2.52	0.42
1:D:162:ILE:CG2	1:D:218:VAL:HG22	2.48	0.42
1:D:88:GLN:HG2	1:D:93:PRO:HD3	2.01	0.42
1:C:64:GLY:HA3	3:D:404:PEG:H12	2.01	0.42
1:D:261:PRO:HB3	1:D:277:LEU:HD13	2.01	0.42
1:B:224:LYS:O	1:B:234:GLY:HA3	2.20	0.41
1:D:149:LEU:HD23	1:D:157:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLU:HG2	1:A:291:THR:HG22	2.02	0.41
1:C:205:ASN:O	1:C:209:GLN:HG2	2.21	0.41
1:D:157:VAL:HG12	3:D:403:PEG:H21	2.03	0.41
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.83	0.41
1:B:162:ILE:HD12	1:B:164:ILE:HD11	2.03	0.41
1:D:208:ARG:HA	1:D:208:ARG:HD3	1.93	0.41
1:A:61:LYS:HD3	1:A:61:LYS:HA	1.91	0.41
1:B:178:LYS:HZ3	3:B:407:PEG:H12	1.83	0.40
1:B:61:LYS:HA	1:B:61:LYS:HD3	1.88	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	333/350 (95%)	327 (98%)	6 (2%)	0	100	100
1	B	333/350 (95%)	325 (98%)	7 (2%)	1 (0%)	46	36
1	C	325/350 (93%)	317 (98%)	6 (2%)	2 (1%)	30	18
1	D	326/350 (93%)	317 (97%)	8 (2%)	1 (0%)	46	36
All	All	1317/1400 (94%)	1286 (98%)	27 (2%)	4 (0%)	46	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	ILE
1	C	248	SER
1	C	289	ASN
1	D	285	ASP



### 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	280/295 (95%)	276 (99%)	4 (1%)	74	72
1	B	277/295 (94%)	271 (98%)	6 (2%)	60	53
1	C	274/295 (93%)	271 (99%)	3 (1%)	80	79
1	D	277/295 (94%)	268 (97%)	9 (3%)	46	38
All	All	1108/1180 (94%)	1086 (98%)	22 (2%)	65	58

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	153	ASP
1	A	179	TYR
1	A	290	PHE
1	B	40	ILE
1	B	41	MSE
1	B	47	SER
1	B	55	LEU
1	B	78	GLU
1	B	245	ASP
1	C	114	ASP
1	C	225	GLN
1	C	252	ASP
1	D	73[A]	ARG
1	D	73[B]	ARG
1	D	78	GLU
1	D	177	GLU
1	D	209	GLN
1	D	245	ASP
1	D	264	GLU
1	D	314	GLN
1	D	338	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	129	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

23 ligands 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	$\# Z  > 2$
2	GOL	A	401	-	5,5,5	0.38	0	5,5,5	0.24	0
2	GOL	A	402	-	5,5,5	0.34	0	5,5,5	0.23	0
3	PEG	A	403	-	6,6,6	0.57	0	5,5,5	0.76	0
3	PEG	A	404	-	6,6,6	0.62	0	5,5,5	0.74	0
3	PEG	A	405	-	6,6,6	0.61	0	5,5,5	0.83	0
4	BME	A	406	-	3,3,3	0.26	0	2,2,2	0.22	0
2	GOL	B	401	-	5,5,5	0.37	0	5,5,5	0.30	0
2	GOL	B	402	-	5,5,5	0.33	0	5,5,5	0.27	0
2	GOL	B	403	-	5,5,5	0.36	0	5,5,5	0.26	0
2	GOL	B	404	-	5,5,5	0.34	0	5,5,5	0.22	0
2	GOL	B	405	-	5,5,5	0.40	0	5,5,5	0.35	0
3	PEG	B	406	-	6,6,6	0.61	0	5,5,5	0.83	0
3	PEG	B	407	-	6,6,6	0.59	0	5,5,5	0.78	0
2	GOL	C	401	-	5,5,5	0.31	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	C	402	-	5,5,5	0.31	0	5,5,5	0.20	0
2	GOL	C	403	-	5,5,5	0.37	0	5,5,5	0.20	0
2	GOL	C	404	-	5,5,5	0.38	0	5,5,5	0.11	0
3	PEG	C	405	-	6,6,6	0.62	0	5,5,5	0.76	0
2	GOL	D	401	-	5,5,5	0.33	0	5,5,5	0.23	0
2	GOL	D	402	-	5,5,5	0.34	0	5,5,5	0.26	0
3	PEG	D	403	-	6,6,6	0.62	0	5,5,5	0.81	0
3	PEG	D	404	-	6,6,6	0.65	0	5,5,5	0.81	0
3	PEG	D	405	-	6,6,6	0.58	0	5,5,5	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
3	PEG	A	403	-	-	0/4/4/4	0/0/0/0
3	PEG	A	404	-	-	0/4/4/4	0/0/0/0
3	PEG	A	405	-	-	0/4/4/4	0/0/0/0
4	BME	A	406	-	-	0/1/1/1	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402	-	-	0/4/4/4	0/0/0/0
2	GOL	B	403	-	-	0/4/4/4	0/0/0/0
2	GOL	B	404	-	-	0/4/4/4	0/0/0/0
2	GOL	B	405	-	-	0/4/4/4	0/0/0/0
3	PEG	B	406	-	-	0/4/4/4	0/0/0/0
3	PEG	B	407	-	-	0/4/4/4	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	C	402	-	-	0/4/4/4	0/0/0/0
2	GOL	C	403	-	-	0/4/4/4	0/0/0/0
2	GOL	C	404	-	-	0/4/4/4	0/0/0/0
3	PEG	C	405	-	-	0/4/4/4	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0
2	GOL	D	402	-	-	0/4/4/4	0/0/0/0
3	PEG	D	403	-	-	0/4/4/4	0/0/0/0
3	PEG	D	404	-	-	0/4/4/4	0/0/0/0
3	PEG	D	405	-	-	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.

16 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	1	0
2	A	402	GOL	3	0
3	A	403	PEG	6	0
3	A	404	PEG	2	0
3	A	405	PEG	8	0
2	B	401	GOL	5	0
2	B	402	GOL	1	0
2	B	404	GOL	2	0
2	B	405	GOL	4	0
3	B	407	PEG	8	0
2	C	402	GOL	1	0
3	C	405	PEG	3	0
2	D	401	GOL	2	0
3	D	403	PEG	2	0
3	D	404	PEG	2	0
3	D	405	PEG	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	328/350 (93%)	0.08	15 (4%) 36 41	23, 36, 74, 108	0
1	B	330/350 (94%)	0.32	19 (5%) 26 30	25, 45, 81, 116	0
1	C	324/350 (92%)	0.11	18 (5%) 28 32	24, 40, 76, 132	0
1	D	326/350 (93%)	0.44	29 (8%) 12 13	28, 52, 86, 117	0
All	All	1308/1400 (93%)	0.24	81 (6%) 24 27	23, 42, 81, 132	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	40	ILE	6.2
1	D	40	ILE	5.9
1	D	286	TYR	5.5
1	D	127	ALA	5.5
1	A	291	THR	5.2
1	A	290	PHE	5.1
1	C	153	ASP	5.0
1	D	291	THR	5.0
1	D	183	TYR	5.0
1	B	153	ASP	4.9
1	B	290	PHE	4.8
1	D	153	ASP	4.5
1	D	287	TYR	4.4
1	D	55	LEU	4.4
1	B	156	THR	4.3
1	B	39	GLY	4.3
1	A	286	TYR	4.3
1	C	152	THR	4.1
1	D	179	TYR	4.1
1	A	151	GLN	4.1
1	A	179	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	55	LEU	4.0
1	C	286	TYR	3.8
1	C	157	VAL	3.7
1	A	40	ILE	3.7
1	C	154	LYS	3.6
1	A	153	ASP	3.5
1	B	291	THR	3.4
1	A	152	THR	3.3
1	D	182	THR	3.2
1	C	55	LEU	3.2
1	D	290	PHE	3.2
1	C	130	GLY	3.2
1	D	137	PRO	3.1
1	B	38	THR	3.1
1	C	156	THR	3.1
1	D	118	ASP	3.1
1	D	285	ASP	3.1
1	D	128	SER	3.0
1	D	181	ASP	3.0
1	B	132	GLY	3.0
1	A	154	LYS	3.0
1	B	151	GLN	3.0
1	B	157	VAL	2.9
1	B	154	LYS	2.9
1	C	290	PHE	2.8
1	D	363	ASP	2.8
1	C	129	ASN	2.8
1	D	334	GLN	2.8
1	B	183	TYR	2.7
1	A	155	ASP	2.7
1	D	190	SER	2.7
1	C	291	THR	2.7
1	C	151	GLN	2.6
1	C	59	ALA	2.6
1	A	289	ASN	2.5
1	D	361	ASN	2.5
1	A	156	THR	2.5
1	A	130	GLY	2.5
1	A	369	ILE	2.5
1	C	134	ASN	2.4
1	D	154	LYS	2.4
1	B	119	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	134	ASN	2.3
1	C	285	ASP	2.3
1	B	155	ASP	2.3
1	C	289	ASN	2.3
1	B	79	LEU	2.3
1	D	288	PRO	2.2
1	D	156	THR	2.2
1	C	179	TYR	2.2
1	B	249	ASN	2.1
1	D	56	PRO	2.1
1	D	250	TRP	2.1
1	D	157	VAL	2.1
1	B	289	ASN	2.1
1	C	158	ALA	2.1
1	D	249	ASN	2.1
1	D	303	GLN	2.1
1	D	81[A]	SER	2.0
1	B	129	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	PEG	A	405	7/7	0.80	0.26	12.20	43,57,74,74	0
2	GOL	C	401	6/6	0.76	0.24	8.16	63,72,75,76	0
3	PEG	A	403	7/7	0.83	0.26	7.02	48,57,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	D	402	6/6	0.66	0.24	4.62	76,79,88,93	0
2	GOL	B	401	6/6	0.92	0.23	2.74	58,67,71,72	0
2	GOL	C	403	6/6	0.79	0.18	2.50	74,76,81,83	0
3	PEG	D	405	7/7	0.71	0.27	2.31	70,79,81,82	0
2	GOL	B	405	6/6	0.86	0.20	2.27	53,57,67,70	0
3	PEG	B	406	7/7	0.85	0.19	2.08	62,63,65,65	0
2	GOL	D	401	6/6	0.86	0.24	1.66	58,67,69,74	0
3	PEG	C	405	7/7	0.80	0.26	1.51	83,86,92,92	0
2	GOL	A	401	6/6	0.85	0.23	1.33	57,58,68,69	0
3	PEG	D	404	7/7	0.90	0.17	1.18	54,58,72,75	0
2	GOL	A	402	6/6	0.82	0.16	0.65	72,73,76,77	0
2	GOL	B	402	6/6	0.86	0.13	-0.20	86,90,95,97	0
4	BME	A	406	4/4	0.92	0.10	-0.35	51,55,61,84	0
2	GOL	C	402	6/6	0.87	0.12	-0.39	69,74,75,78	0
2	GOL	B	404	6/6	0.85	0.13	-0.76	84,87,89,89	0
3	PEG	D	403	7/7	0.76	0.20	-	70,82,88,92	0
3	PEG	A	404	7/7	0.91	0.18	-	80,85,87,87	0
3	PEG	B	407	7/7	0.67	0.24	-	66,83,86,88	0
2	GOL	C	404	6/6	0.78	0.24	-	63,74,83,84	0
2	GOL	B	403	6/6	0.83	0.24	-	81,83,85,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.