Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:21 PM GMT

PDB ID	:	1OMI
Title	:	Crystal structure of PrfA,the transcriptional regulator in Listeria monocytogenes
Authors	:	Thirumuruhan, R.; Rajashankar, K.; Fedorov, A.A.; Dodatko, T.; Chance, M.R.; Cossart, P.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2003-02-25
Resolution	:	2.80 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

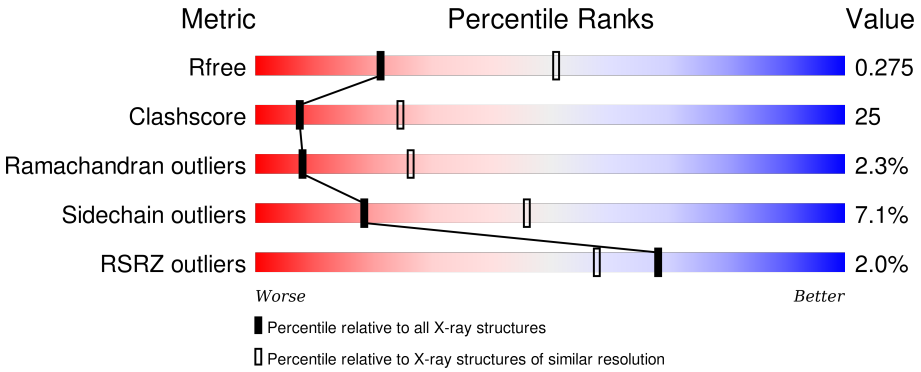
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 >=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 <=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	248	2% 39% 46% 5% 10%
1	B	248	% 52% 35% • 8%

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	A	3001	-	X	-	-
2	GOL	B	3002	-	X	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3700 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 Listeriolysin regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1833	1201	285	340	7			
1	B	227	Total	C	N	O	S	0	0	0
			1855	1215	288	345	7			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	990	GLY	-	CLONING ARTIFACT	UNP P22262
A	991	SER	-	CLONING ARTIFACT	UNP P22262
A	992	HIS	-	CLONING ARTIFACT	UNP P22262
A	993	MET	-	CLONING ARTIFACT	UNP P22262
A	994	ALA	-	CLONING ARTIFACT	UNP P22262
A	995	SER	-	CLONING ARTIFACT	UNP P22262
A	996	MET	-	CLONING ARTIFACT	UNP P22262
A	997	THR	-	CLONING ARTIFACT	UNP P22262
A	998	GLY	-	CLONING ARTIFACT	UNP P22262
A	999	GLY	-	CLONING ARTIFACT	UNP P22262
A	1000	GLN	-	CLONING ARTIFACT	UNP P22262
A	1001	GLN	-	CLONING ARTIFACT	UNP P22262
A	1002	MET	-	CLONING ARTIFACT	UNP P22262
A	1003	GLY	-	CLONING ARTIFACT	UNP P22262
A	1004	ARG	-	CLONING ARTIFACT	UNP P22262
A	1005	GLY	-	CLONING ARTIFACT	UNP P22262
A	1006	SER	-	CLONING ARTIFACT	UNP P22262
B	1990	GLY	-	CLONING ARTIFACT	UNP P22262
B	1991	SER	-	CLONING ARTIFACT	UNP P22262
B	1992	HIS	-	CLONING ARTIFACT	UNP P22262
B	1993	MET	-	CLONING ARTIFACT	UNP P22262
B	1994	ALA	-	CLONING ARTIFACT	UNP P22262
B	1995	SER	-	CLONING ARTIFACT	UNP P22262
B	1996	MET	-	CLONING ARTIFACT	UNP P22262
B	1997	THR	-	CLONING ARTIFACT	UNP P22262

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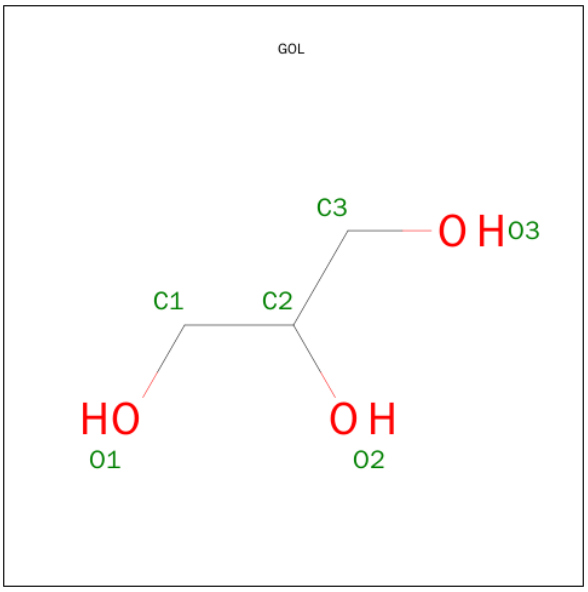
Chain	Residue	Modelled	Actual	Comment	Reference
B	1998	GLY	-	CLONING ARTIFACT	UNP P22262
B	1999	GLY	-	CLONING ARTIFACT	UNP P22262
B	2000	GLN	-	CLONING ARTIFACT	UNP P22262
B	2001	GLN	-	CLONING ARTIFACT	UNP P22262
B	2002	MET	-	CLONING ARTIFACT	UNP P22262
B	2003	GLY	-	CLONING ARTIFACT	UNP P22262
B	2004	ARG	-	CLONING ARTIFACT	UNP P22262
B	2005	GLY	-	CLONING ARTIFACT	UNP P22262
B	2006	SER	-	CLONING ARTIFACT	UNP P22262

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



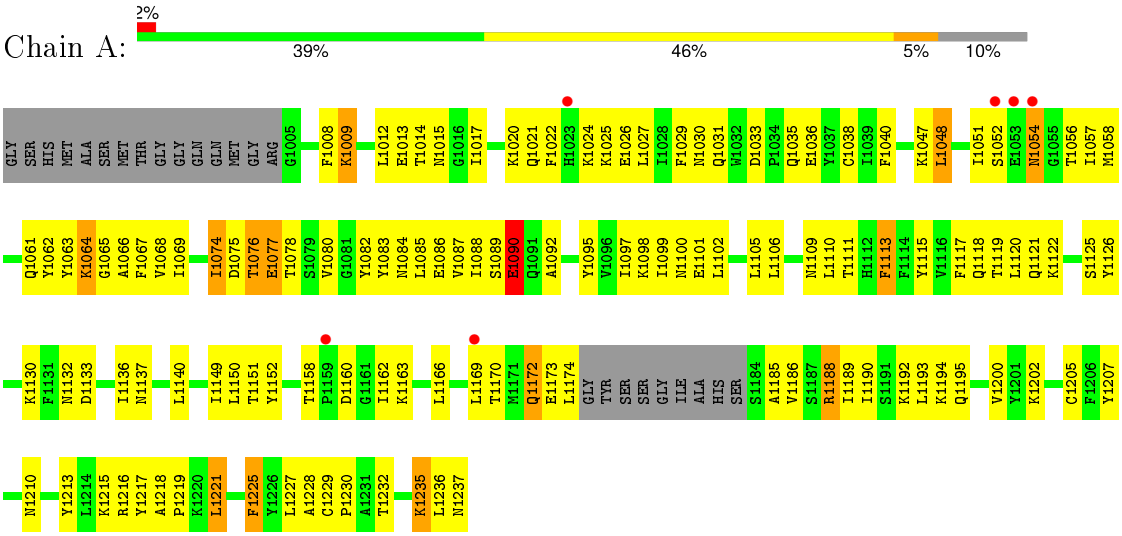
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

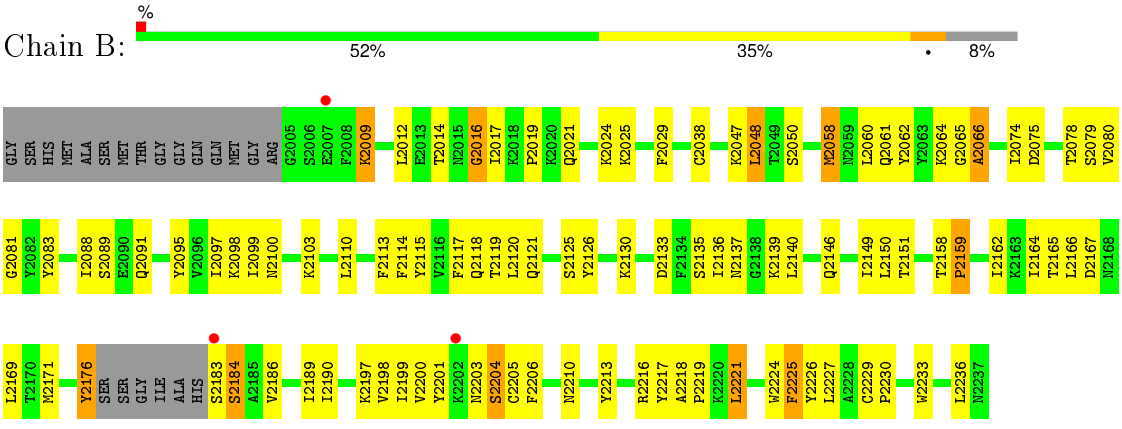
- Molecule 1: Listeriolysin regulatory protein

Chain A:



- Molecule 1: Listeriolysin regulatory protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.43Å 72.09Å 114.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 28.58 – 2.68	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.80) 96.7 (28.58-2.68)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.244 , 0.278 0.243 , 0.275	Depositor DCC
R_{free} test set	699 reflections (4.89%)	DCC
Wilson B-factor (Å^2)	73.8	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.2	EDS
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 16402 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3700	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.39	0/1874	0.62	1/2528 (0.0%)
1	B	0.43	0/1897	0.62	1/2559 (0.0%)
All	All	0.41	0/3771	0.62	2/5087 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1038	CYS	N-CA-C	-5.39	96.44	111.00
1	B	2038	CYS	N-CA-C	-5.36	96.53	111.00

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	1833	0	1844	118	0
1	B	1855	0	1861	93	0
2	A	6	0	5	1	0
2	B	6	0	5	0	0
All	All	3700	0	3715	189	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 25.

All (189) 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:A:1031:GLN:HE21	1:A:1084:ASN:HD21	1.15	0.94
1:A:1012:LEU:HD22	1:A:1017:ILE:CD1	1.98	0.93
1:A:1031:GLN:HE21	1:A:1084:ASN:ND2	1.73	0.86
1:A:1215:LYS:HE3	1:A:1237:ASN:ND2	1.95	0.82
1:A:1012:LEU:HD22	1:A:1017:ILE:HD13	1.64	0.79
1:A:1200:VAL:HG22	1:A:1207:TYR:HB2	1.65	0.79
1:B:2048:LEU:CD2	1:B:2083:TYR:HB3	2.13	0.79
1:B:2064:LYS:NZ	1:B:2064:LYS:HB3	2.00	0.77
1:A:1012:LEU:CD2	1:A:1017:ILE:HD12	2.15	0.77
1:A:1012:LEU:HD22	1:A:1017:ILE:HD12	1.67	0.75
1:A:1110:LEU:HD11	1:B:2110:LEU:HD11	1.67	0.74
1:A:1121:GLN:HE22	1:B:2074:ILE:H	1.36	0.74
1:B:2158:THR:HB	1:B:2159:PRO:CD	2.19	0.73
1:A:1036:GLU:HG3	1:A:1077:GLU:O	1.89	0.72
1:B:2048:LEU:HD21	1:B:2083:TYR:HB3	1.70	0.71
1:A:1030:ASN:O	2:A:3001:GOL:H11	1.91	0.70
1:B:2074:ILE:HD12	1:B:2075:ASP:N	2.07	0.69
1:A:1227:LEU:HD12	1:B:2081:GLY:HA2	1.74	0.69
1:B:2074:ILE:O	1:B:2103:LYS:HE2	1.92	0.69
1:A:1101:GLU:O	1:A:1105:LEU:HG	1.94	0.67
1:A:1048:LEU:HD21	1:A:1083:TYR:CB	2.24	0.67
1:A:1048:LEU:CD2	1:A:1083:TYR:HB3	2.25	0.67
1:A:1031:GLN:NE2	1:A:1084:ASN:HD21	1.89	0.67
1:A:1074:ILE:HG12	1:B:2117:PHE:CD2	2.30	0.66
1:B:2146:GLN:HG2	1:B:2176:TYR:OH	1.95	0.66
1:B:2226:TYR:O	1:B:2230:PRO:HG3	1.96	0.65
1:A:1064:LYS:HG3	1:A:1065:GLY:N	2.11	0.65
1:B:2229:CYS:N	1:B:2230:PRO:HD3	2.12	0.64
1:A:1102:LEU:O	1:A:1106:LEU:HG	1.98	0.64
1:B:2024:LYS:O	1:B:2025:LYS:HB2	1.97	0.64
1:B:2019:PRO:HB3	1:B:2095:TYR:CZ	2.33	0.64
1:B:2047:LYS:HB3	1:B:2088:ILE:HD11	1.80	0.63
1:A:1051:ILE:HD12	1:A:1057:ILE:HD13	1.81	0.63
1:A:1031:GLN:NE2	1:A:1051:ILE:HG12	2.13	0.63
1:B:2048:LEU:HD21	1:B:2083:TYR:CB	2.29	0.63
1:A:1048:LEU:HD22	1:A:1083:TYR:HB3	1.79	0.63
1:B:2064:LYS:HZ2	1:B:2064:LYS:HB3	1.63	0.62
1:B:2158:THR:HB	1:B:2159:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:ASP:HB3	1:B:2118:GLN:NE2	2.15	0.62
1:B:2136:ILE:HG22	1:B:2137:ASN:OD1	1.99	0.62
1:A:1012:LEU:CD2	1:A:1017:ILE:CD1	2.74	0.61
1:A:1061:GLN:HG3	1:A:1062:TYR:N	2.15	0.60
1:A:1109:ASN:OD1	1:A:1111:THR:HB	2.02	0.60
1:A:1031:GLN:HE22	1:A:1051:ILE:HG12	1.65	0.60
1:B:2186:VAL:O	1:B:2190:ILE:HG12	2.02	0.60
1:B:2021:GLN:CG	1:B:2091:GLN:HE21	2.15	0.59
1:A:1026:GLU:C	1:A:1027:LEU:HD22	2.23	0.59
1:B:2017:ILE:O	1:B:2017:ILE:HG22	2.02	0.59
1:B:2099:ILE:HG23	1:B:2100:ASN:N	2.18	0.58
1:A:1024:LYS:O	1:A:1025:LYS:HB2	2.02	0.58
1:A:1024:LYS:HG2	1:A:1089:SER:O	2.02	0.58
1:B:2218:ALA:N	1:B:2219:PRO:HD3	2.16	0.58
1:A:1200:VAL:CG2	1:A:1207:TYR:HB2	2.33	0.58
1:A:1215:LYS:HE3	1:A:1237:ASN:HD22	1.67	0.58
1:A:1189:ILE:O	1:A:1193:LEU:HG	2.04	0.57
1:B:2009:LYS:NZ	1:B:2009:LYS:HB3	2.20	0.57
1:A:1048:LEU:CD2	1:A:1083:TYR:CB	2.81	0.57
1:B:2061:GLN:HG3	1:B:2062:TYR:N	2.20	0.57
1:B:2019:PRO:HD3	1:B:2095:TYR:CE2	2.40	0.57
1:B:2047:LYS:HD3	1:B:2088:ILE:HD11	1.87	0.56
1:B:2048:LEU:HD22	1:B:2083:TYR:HB3	1.88	0.56
1:A:1227:LEU:CD1	1:B:2081:GLY:HA2	2.35	0.56
1:B:2065:GLY:O	1:B:2066:ALA:HB3	2.05	0.56
1:A:1136:ILE:HG22	1:A:1137:ASN:OD1	2.04	0.56
1:A:1099:ILE:HG23	1:A:1100:ASN:N	2.20	0.56
1:A:1218:ALA:N	1:A:1219:PRO:HD3	2.21	0.56
1:B:2198:VAL:HG12	1:B:2199:ILE:HG23	1.88	0.55
1:A:1020:LYS:HD2	1:A:1020:LYS:N	2.22	0.55
1:A:1009:LYS:HB3	1:A:1009:LYS:NZ	2.22	0.55
1:B:2158:THR:CB	1:B:2159:PRO:CD	2.84	0.55
1:A:1192:LYS:O	1:A:1195:GLN:HB3	2.07	0.54
1:A:1149:ILE:HG22	1:A:1225:PHE:CE1	2.43	0.54
1:A:1122:LYS:HE3	1:A:1228:ALA:HB1	1.90	0.54
1:B:2151:THR:HA	1:B:2164:ILE:CD1	2.38	0.53
1:B:2203:ASN:O	1:B:2205:CYS:SG	2.66	0.53
1:A:1210:ASN:ND2	1:A:1213:TYR:HB2	2.24	0.53
1:A:1074:ILE:HD12	1:A:1075:ASP:N	2.24	0.53
1:A:1012:LEU:O	1:A:1017:ILE:HB	2.09	0.53
1:A:1088:ILE:CG2	1:A:1170:THR:HG23	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:LYS:HG3	1:A:1090:GLU:HA	1.90	0.53
1:A:1048:LEU:HD21	1:A:1083:TYR:HB2	1.90	0.52
1:A:1133:ASP:OD2	1:A:1221:LEU:HB2	2.09	0.52
1:A:1074:ILE:HG13	1:B:2121:GLN:HE22	1.74	0.52
1:A:1022:PHE:HA	1:A:1026:GLU:OE2	2.10	0.52
1:A:1008:PHE:O	1:A:1012:LEU:HG	2.09	0.52
1:B:2210:ASN:ND2	1:B:2213:TYR:HB2	2.24	0.52
1:B:2089:SER:OG	1:B:2091:GLN:O	2.27	0.52
1:A:1082:TYR:OH	1:B:2227:LEU:HD21	2.10	0.52
1:A:1069:ILE:HD12	1:A:1085:LEU:HD21	1.92	0.52
1:B:2226:TYR:HD2	1:B:2233:TRP:CE3	2.29	0.51
1:B:2216:ARG:HH11	1:B:2216:ARG:HG3	1.75	0.51
1:B:2009:LYS:HD3	1:B:2095:TYR:OH	2.09	0.51
1:A:1009:LYS:O	1:A:1013:GLU:HG3	2.11	0.51
1:B:2199:ILE:HD12	1:B:2206:PHE:CE1	2.45	0.51
1:B:2047:LYS:HB3	1:B:2088:ILE:CD1	2.41	0.51
1:A:1232:THR:HA	1:A:1235:LYS:HE2	1.93	0.50
1:B:2047:LYS:CG	1:B:2088:ILE:HD11	2.42	0.50
1:B:2133:ASP:OD2	1:B:2221:LEU:HB2	2.12	0.50
1:A:1076:THR:O	1:A:1078:THR:HG23	2.12	0.50
1:A:1216:ARG:HH11	1:A:1216:ARG:HG3	1.76	0.50
1:A:1074:ILE:H	1:B:2121:GLN:HE22	1.60	0.50
1:A:1115:TYR:O	1:A:1119:THR:HG23	2.12	0.50
1:A:1047:LYS:HD3	1:A:1088:ILE:HD11	1.93	0.50
1:B:2064:LYS:HZ3	1:B:2064:LYS:HB3	1.76	0.50
1:A:1009:LYS:HD3	1:A:1095:TYR:OH	2.12	0.50
1:A:1215:LYS:HE3	1:A:1237:ASN:HD21	1.75	0.50
1:A:1080:VAL:HG22	1:B:2125:SER:HB3	1.94	0.49
1:B:2021:GLN:HG3	1:B:2091:GLN:HE21	1.76	0.49
1:B:2229:CYS:N	1:B:2230:PRO:CD	2.75	0.49
1:A:1080:VAL:CG2	1:B:2125:SER:HB3	2.41	0.49
1:A:1058:MET:HE1	1:B:2135:SER:HB3	1.95	0.49
1:B:2115:TYR:O	1:B:2119:THR:HG23	2.13	0.49
1:B:2203:ASN:O	1:B:2204:SER:C	2.51	0.48
1:A:1033:ASP:OD1	1:A:1035:GLN:N	2.40	0.48
1:B:2165:THR:O	1:B:2166:LEU:HG	2.12	0.48
1:A:1185:ALA:O	1:A:1188:ARG:N	2.47	0.48
1:B:2014:THR:C	1:B:2016:GLY:H	2.16	0.47
1:B:2217:TYR:C	1:B:2219:PRO:HD3	2.34	0.47
1:B:2167:ASP:OD2	1:B:2169:LEU:HB2	2.15	0.47
1:B:2074:ILE:O	1:B:2103:LYS:CE	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:SER:C	1:A:1054:ASN:H	2.18	0.47
1:A:1163:LYS:HE2	1:A:1205:CYS:SG	2.55	0.46
1:A:1117:PHE:CD2	1:B:2074:ILE:CG1	2.98	0.46
1:A:1225:PHE:HE2	1:A:1232:THR:HG21	1.81	0.46
1:A:1088:ILE:HG22	1:A:1170:THR:HG23	1.97	0.46
1:B:2047:LYS:CB	1:B:2088:ILE:HD11	2.46	0.46
1:A:1066:ALA:O	1:A:1067:PHE:HB2	2.14	0.46
1:B:2149:ILE:HG22	1:B:2225:PHE:CE1	2.50	0.45
1:A:1117:PHE:HB3	1:B:2074:ILE:HD11	1.98	0.45
1:A:1022:PHE:HB2	1:A:1087:VAL:HG21	1.97	0.45
1:A:1173:GLU:O	1:A:1174:LEU:HD23	2.16	0.45
1:A:1186:VAL:O	1:A:1190:ILE:HG12	2.16	0.45
1:B:2162:ILE:HD13	1:B:2236:LEU:HD13	1.98	0.45
1:A:1126:TYR:CE1	1:A:1130:LYS:HD3	2.52	0.45
1:A:1097:ILE:HG22	1:A:1098:LYS:O	2.16	0.45
1:A:1017:ILE:HD11	1:A:1105:LEU:CD1	2.46	0.45
1:A:1012:LEU:HD23	1:A:1017:ILE:HD12	1.94	0.45
1:A:1151:THR:HG23	1:A:1162:ILE:HG21	1.99	0.45
1:A:1158:THR:C	1:A:1160:ASP:H	2.21	0.45
1:A:1051:ILE:HD12	1:A:1057:ILE:CD1	2.46	0.44
1:B:2021:GLN:CG	1:B:2091:GLN:NE2	2.79	0.44
1:A:1190:ILE:O	1:A:1194:LYS:HG3	2.17	0.44
1:B:2126:TYR:CE1	1:B:2130:LYS:HD3	2.52	0.44
1:A:1149:ILE:HG22	1:A:1225:PHE:HE1	1.83	0.44
1:A:1118:GLN:NE2	1:B:2075:ASP:HB3	2.33	0.43
1:A:1052:SER:C	1:A:1054:ASN:N	2.70	0.43
1:B:2183:SER:OG	1:B:2184:SER:N	2.51	0.43
1:B:2029:PHE:CD1	1:B:2029:PHE:C	2.92	0.43
1:A:1217:TYR:C	1:A:1219:PRO:HD3	2.38	0.43
1:A:1082:TYR:CE2	1:B:2227:LEU:HD11	2.53	0.43
1:A:1012:LEU:HB3	1:A:1017:ILE:HB	2.00	0.43
1:B:2097:ILE:HG22	1:B:2098:LYS:O	2.18	0.43
1:A:1027:LEU:N	1:A:1027:LEU:HD22	2.33	0.43
1:A:1029:PHE:C	1:A:1029:PHE:CD1	2.92	0.43
1:B:2125:SER:HG	1:B:2224:TRP:HE1	1.64	0.42
1:B:2047:LYS:CD	1:B:2088:ILE:HD11	2.49	0.42
1:B:2050:SER:O	1:B:2058:MET:HB2	2.19	0.42
1:B:2197:LYS:HE3	1:B:2197:LYS:HB2	1.83	0.42
1:A:1048:LEU:HB2	1:A:1063:TYR:HE1	1.83	0.42
1:A:1140:LEU:O	1:A:1140:LEU:HD22	2.19	0.42
1:A:1125:SER:HB3	1:B:2080:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:CYS:N	1:A:1230:PRO:HD3	2.34	0.42
1:A:1202:LYS:O	1:A:1207:TYR:HE1	2.02	0.42
1:A:1074:ILE:H	1:A:1074:ILE:HG13	1.46	0.42
1:A:1074:ILE:HD13	1:B:2114:PHE:CD1	2.55	0.42
1:A:1031:GLN:HG2	1:A:1084:ASN:OD1	2.20	0.42
1:A:1169:LEU:O	1:A:1172:GLN:HG3	2.20	0.42
1:A:1074:ILE:HG13	1:B:2121:GLN:NE2	2.35	0.42
1:B:2218:ALA:N	1:B:2219:PRO:CD	2.83	0.42
1:A:1172:GLN:C	1:A:1174:LEU:H	2.23	0.42
1:A:1132:ASN:HB2	1:B:2060:LEU:HD21	2.00	0.42
1:A:1221:LEU:HA	1:A:1221:LEU:HD23	1.90	0.41
1:B:2221:LEU:HD23	1:B:2221:LEU:HA	1.91	0.41
1:B:2139:LYS:HB3	1:B:2189:ILE:CD1	2.50	0.41
1:A:1013:GLU:C	1:A:1015:ASN:H	2.24	0.41
1:B:2099:ILE:CG2	1:B:2100:ASN:N	2.82	0.41
1:A:1027:LEU:CD1	1:A:1086:GLU:HB2	2.50	0.41
1:B:2078:THR:CG2	1:B:2079:SER:N	2.83	0.41
1:B:2140:LEU:HD22	1:B:2140:LEU:O	2.20	0.41
1:A:1225:PHE:CE2	1:A:1232:THR:HG21	2.55	0.41
1:A:1113:PHE:HE2	1:B:2117:PHE:CD1	2.38	0.41
1:A:1017:ILE:HG22	1:A:1095:TYR:HD2	1.85	0.41
1:A:1152:TYR:HD2	1:A:1236:LEU:HD12	1.85	0.41
1:A:1040:PHE:HB3	1:A:1095:TYR:HB2	2.02	0.41
1:B:2200:VAL:HG12	1:B:2201:TYR:N	2.36	0.41
1:B:2048:LEU:HA	1:B:2048:LEU:HD23	1.91	0.40
1:A:1117:PHE:CD2	1:B:2074:ILE:HG13	2.56	0.40
1:A:1099:ILE:CG2	1:A:1100:ASN:N	2.85	0.40
1:B:2166:LEU:O	1:B:2167:ASP:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	220/248 (89%)	196 (89%)	19 (9%)	5 (2%)	8 26
1	B	223/248 (90%)	202 (91%)	16 (7%)	5 (2%)	8 28
All	All	443/496 (89%)	398 (90%)	35 (8%)	10 (2%)	8 26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1077	GLU
1	B	2184	SER
1	B	2204	SER
1	B	2066	ALA
1	A	1092	ALA
1	A	1014	THR
1	A	1090	GLU
1	A	1235	LYS
1	B	2159	PRO
1	B	2016	GLY

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	203/219 (93%)	185 (91%)	18 (9%)	12 34
1	B	205/219 (94%)	194 (95%)	11 (5%)	27 60
All	All	408/438 (93%)	379 (93%)	29 (7%)	18 46

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1009	LYS
1	A	1021	GLN
1	A	1048	LEU
1	A	1054	ASN
1	A	1056	THR
1	A	1064	LYS

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Mol	Chain	Res	Type
1	A	1068	VAL
1	A	1074	ILE
1	A	1076	THR
1	A	1090	GLU
1	A	1113	PHE
1	A	1120	LEU
1	A	1150	LEU
1	A	1166	LEU
1	A	1172	GLN
1	A	1188	ARG
1	A	1221	LEU
1	A	1225	PHE
1	B	2009	LYS
1	B	2012	LEU
1	B	2048	LEU
1	B	2058	MET
1	B	2113	PHE
1	B	2120	LEU
1	B	2150	LEU
1	B	2171	MET
1	B	2176	TYR
1	B	2221	LEU
1	B	2225	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1021	GLN
1	A	1031	GLN
1	A	1035	GLN
1	A	1118	GLN
1	A	1121	GLN
1	A	1172	GLN
1	A	1237	ASN
1	B	2015	ASN
1	B	2021	GLN
1	B	2059	ASN
1	B	2091	GLN
1	B	2118	GLN
1	B	2121	GLN
1	B	2168	ASN
1	B	2172	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	3001	-	5,5,5	4.68	4 (80%)	5,5,5	5.65	3 (60%)
2	GOL	B	3002	-	5,5,5	4.56	5 (100%)	5,5,5	5.58	3 (60%)

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	3001	-	-	0/4/4/4	0/0/0/0
2	GOL	B	3002	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	GOL	C3-C2	-8.02	1.21	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	GOL	C3-C2	-7.71	1.22	1.52
2	A	3001	GOL	C1-C2	-2.71	1.41	1.52
2	B	3002	GOL	C1-C2	-2.53	1.42	1.52
2	B	3002	GOL	O2-C2	-2.02	1.37	1.43
2	A	3001	GOL	O3-C3	3.26	1.56	1.42
2	B	3002	GOL	O3-C3	3.36	1.56	1.42
2	B	3002	GOL	O1-C1	4.75	1.62	1.42
2	A	3001	GOL	O1-C1	4.84	1.63	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3002	GOL	O1-C1-C2	3.30	126.17	110.18
2	A	3001	GOL	O1-C1-C2	3.63	127.77	110.18
2	B	3002	GOL	O2-C2-C3	6.61	138.98	108.65
2	A	3001	GOL	O2-C2-C3	6.64	139.11	108.65
2	B	3002	GOL	O3-C3-C2	10.00	158.70	110.18
2	A	3001	GOL	O3-C3-C2	10.07	159.02	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	224/248 (90%)	0.06	6 (2%)	58	45	41, 82, 112, 136	0
1	B	227/248 (91%)	-0.23	3 (1%)	79	71	38, 69, 109, 125	0
All	All	451/496 (90%)	-0.09	9 (1%)	68	58	38, 75, 112, 136	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2183	SER	3.3
1	A	1052	SER	2.9
1	B	2007	GLU	2.6
1	A	1159	PRO	2.5
1	A	1023	HIS	2.5
1	B	2202	LYS	2.5
1	A	1054	ASN	2.4
1	A	1053	GLU	2.2
1	A	1169	LEU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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^{th} 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^2)	Q<0.9
2	GOL	B	3002	6/6	0.88	0.28	3.39	48,49,52,52	0
2	GOL	A	3001	6/6	0.89	0.14	-1.53	54,55,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.