



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:04 am GMT

PDB ID : 1PIE  
Title : Crystal Structure of Lactococcus lactis Galactokinase Complexed with Galactose  
Authors : Thoden, J.B.; Holden, H.M.  
Deposited on : 2003-05-30  
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

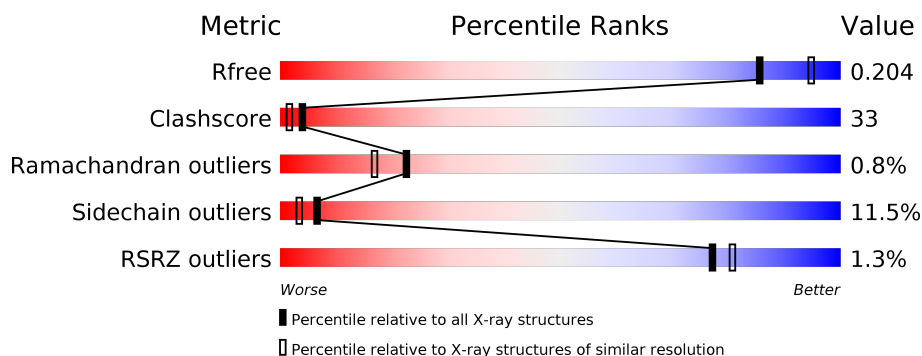
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	419	<div> <div></div> <div> <div></div> <div>35%</div> <div>45%</div> <div>11%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3166 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.

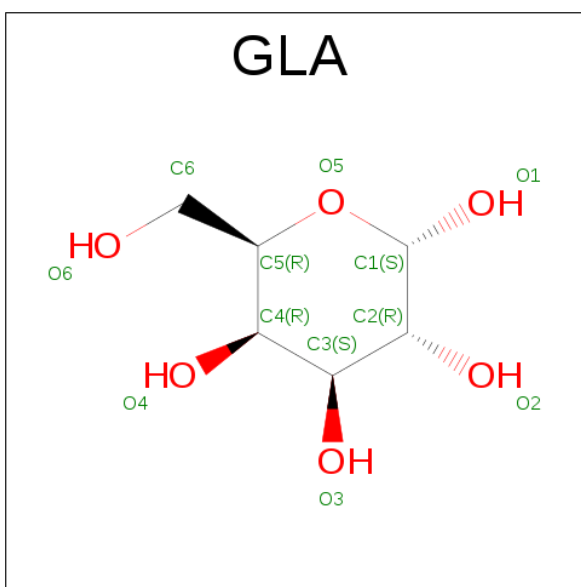
- Molecule 1 is a protein called Galactokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	1	0
			2985	1893	496	588	8			

There are 22 discrepancies between the modelled and reference sequences:

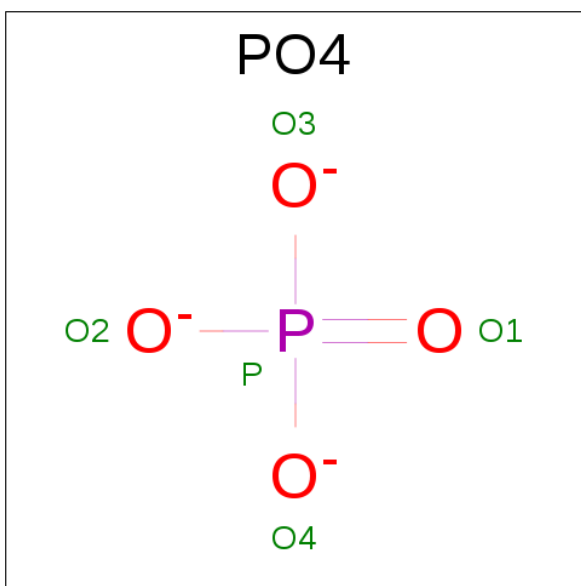
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP Q9R7D7
A	-18	GLY	-	CLONING ARTIFACT	UNP Q9R7D7
A	-17	SER	-	CLONING ARTIFACT	UNP Q9R7D7
A	-16	SER	-	CLONING ARTIFACT	UNP Q9R7D7
A	-15	HIS	-	CLONING ARTIFACT	UNP Q9R7D7
A	-14	HIS	-	CLONING ARTIFACT	UNP Q9R7D7
A	-13	HIS	-	CLONING ARTIFACT	UNP Q9R7D7
A	-12	HIS	-	CLONING ARTIFACT	UNP Q9R7D7
A	-11	HIS	-	CLONING ARTIFACT	UNP Q9R7D7
A	-10	HIS	-	CLONING ARTIFACT	UNP Q9R7D7
A	-9	SER	-	CLONING ARTIFACT	UNP Q9R7D7
A	-8	SER	-	CLONING ARTIFACT	UNP Q9R7D7
A	-7	GLY	-	CLONING ARTIFACT	UNP Q9R7D7
A	-6	LEU	-	CLONING ARTIFACT	UNP Q9R7D7
A	-5	VAL	-	CLONING ARTIFACT	UNP Q9R7D7
A	-4	PRO	-	CLONING ARTIFACT	UNP Q9R7D7
A	-3	ARG	-	CLONING ARTIFACT	UNP Q9R7D7
A	-2	GLY	-	CLONING ARTIFACT	UNP Q9R7D7
A	-1	SER	-	CLONING ARTIFACT	UNP Q9R7D7
A	0	HIS	-	CLONING ARTIFACT	UNP Q9R7D7
A	197	GLU	LEU	CLONING ARTIFACT	UNP Q9R7D7
A	367	ARG	GLU	CLONING ARTIFACT	UNP Q9R7D7

- Molecule 2 is SUGAR (D-GALACTOSE) (three-letter code: GLA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

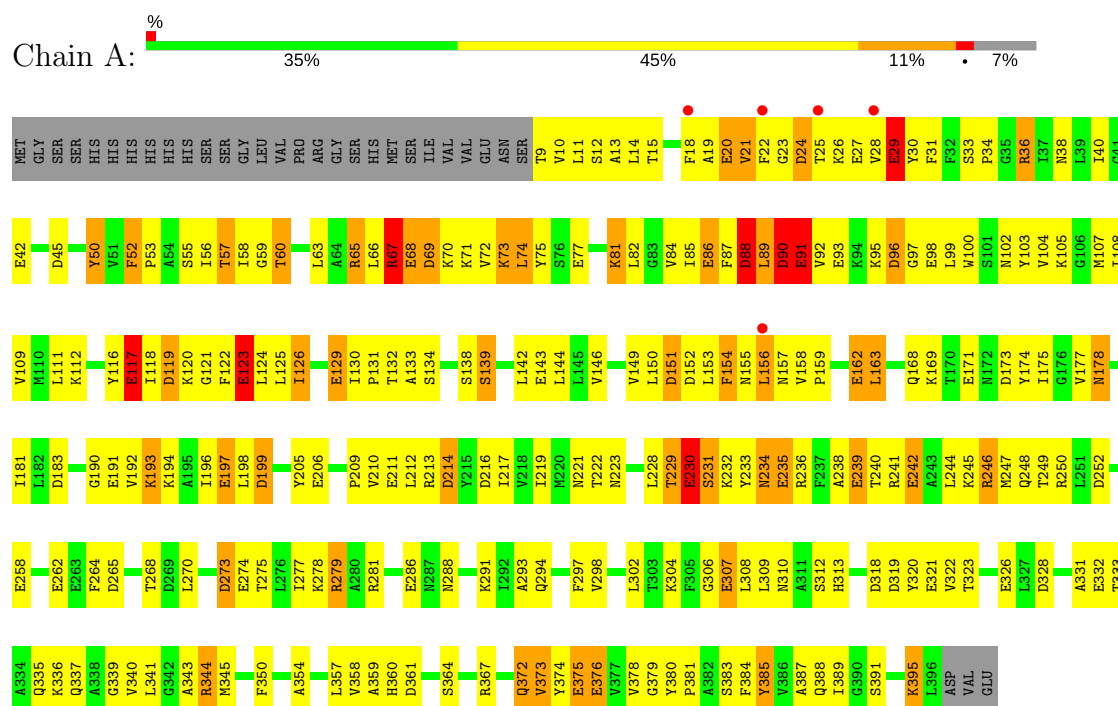
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	164	Total 164	O 164	0	0

### 3 Residue-property plots

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: Galactokinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.40Å 143.40Å 143.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 45.35 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.10) 98.7 (45.35-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 1.84Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.199 , 0.266 0.201 , 0.204	Depositor DCC
$R_{free}$ test set	2897 reflections (11.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 163.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: GLA, PO4

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	1.14	32/3036 (1.1%)	1.60	53/4103 (1.3%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	GLU	CD-OE2	9.18	1.35	1.25
1	A	29	GLU	CD-OE2	7.80	1.34	1.25
1	A	68	GLU	CD-OE2	7.78	1.34	1.25
1	A	230	GLU	CD-OE2	7.68	1.34	1.25
1	A	262	GLU	CD-OE2	7.68	1.34	1.25
1	A	375	GLU	CD-OE2	7.57	1.33	1.25
1	A	86	GLU	CD-OE2	7.29	1.33	1.25
1	A	286	GLU	CD-OE2	7.25	1.33	1.25
1	A	211	GLU	CD-OE2	7.16	1.33	1.25
1	A	129	GLU	CD-OE2	6.93	1.33	1.25
1	A	376	GLU	CD-OE2	6.65	1.32	1.25
1	A	93	GLU	CD-OE2	6.56	1.32	1.25
1	A	307	GLU	CD-OE2	6.46	1.32	1.25
1	A	42	GLU	CD-OE2	6.42	1.32	1.25
1	A	162	GLU	CD-OE2	6.33	1.32	1.25
1	A	191	GLU	CD-OE2	6.27	1.32	1.25
1	A	326	GLU	CD-OE2	6.21	1.32	1.25
1	A	235	GLU	CD-OE2	6.04	1.32	1.25
1	A	77	GLU	CD-OE2	6.04	1.32	1.25
1	A	332	GLU	CD-OE2	6.02	1.32	1.25
1	A	321	GLU	CD-OE2	5.99	1.32	1.25
1	A	258	GLU	CD-OE2	5.98	1.32	1.25
1	A	98	GLU	CD-OE2	5.98	1.32	1.25
1	A	206	GLU	CD-OE2	5.97	1.32	1.25
1	A	91	GLU	CD-OE2	5.95	1.32	1.25
1	A	239	GLU	CD-OE2	5.88	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	GLU	CD-OE2	5.77	1.32	1.25
1	A	123	GLU	CD-OE2	5.77	1.31	1.25
1	A	27	GLU	CD-OE2	5.72	1.31	1.25
1	A	143	GLU	CD-OE2	5.64	1.31	1.25
1	A	117	GLU	CD-OE2	5.26	1.31	1.25
1	A	242	GLU	CD-OE2	5.16	1.31	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ASP	CB-CG-OD1	10.62	127.86	118.30
1	A	241	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	A	214	ASP	CB-CG-OD2	-10.06	109.25	118.30
1	A	214	ASP	CB-CG-OD1	9.29	126.66	118.30
1	A	183	ASP	CB-CG-OD1	9.05	126.45	118.30
1	A	265	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	A	246	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	A	361	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	A	45	ASP	CB-CG-OD2	-8.64	110.52	118.30
1	A	216	ASP	CB-CG-OD1	8.48	125.94	118.30
1	A	199	ASP	CB-CG-OD1	8.38	125.84	118.30
1	A	252	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	216	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	A	246	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	183	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	A	273	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	A	199	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	88	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	A	67	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	A	328	ASP	CB-CG-OD1	7.24	124.82	118.30
1	A	318	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	90	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	A	69	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	A	96	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	252	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	45	ASP	CB-CG-OD1	6.44	124.09	118.30
1	A	240	THR	CA-CB-CG2	-6.32	103.56	112.40
1	A	119	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	154	PHE	CB-CG-CD2	-6.19	116.47	120.80
1	A	36	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	328	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	A	152	ASP	CB-CG-OD2	-6.04	112.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	90	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	318	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	265	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	273	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	67	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	268	THR	CA-CB-CG2	-5.46	104.75	112.40
1	A	69	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	60	THR	CA-CB-CG2	-5.41	104.82	112.40
1	A	152	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	281	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	373	VAL	CA-CB-CG2	-5.22	103.06	110.90
1	A	241	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	88	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	344	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	178	ASN	CA-CB-CG	-5.17	102.04	113.40
1	A	234	ASN	CB-CA-C	5.14	120.69	110.40
1	A	88	ASP	N-CA-CB	5.13	119.83	110.60
1	A	151	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	279	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	119	ASP	CB-CG-OD2	-5.00	113.80	118.30

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	2985	0	2953	198	0
2	A	12	0	12	0	0
3	A	5	0	0	0	0
4	A	164	0	0	4	0
All	All	3166	0	2965	198	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 33.

All (198) 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:28:VAL:HG22	1:A:65:ARG:HG2	1.26	1.07
1:A:59:GLY:HA2	1:A:130:ILE:HD11	1.41	1.02
1:A:67:ARG:HH11	1:A:67:ARG:HG2	1.33	0.91
1:A:28:VAL:CG2	1:A:65:ARG:HG2	2.01	0.89
1:A:380:TYR:HB2	1:A:381:PRO:CD	2.04	0.87
1:A:31:PHE:CD2	1:A:395:LYS:HA	2.10	0.86
1:A:116:TYR:HB3	1:A:156:LEU:HD22	1.58	0.85
1:A:372:GLN:O	1:A:376:GLU:HG3	1.79	0.83
1:A:380:TYR:HB2	1:A:381:PRO:HD3	1.62	0.81
1:A:72:VAL:CG1	1:A:74:LEU:HD21	2.13	0.79
1:A:92:VAL:HA	1:A:105:LYS:HG2	1.65	0.78
1:A:116:TYR:HB3	1:A:156:LEU:CD2	2.13	0.78
1:A:133:ALA:HB2	1:A:228:LEU:HD21	1.66	0.77
1:A:175:ILE:HG22	1:A:177:VAL:HG23	1.65	0.76
1:A:235:GLU:O	1:A:238:ALA:HB3	1.85	0.76
1:A:11:LEU:N	1:A:11:LEU:HD23	2.01	0.75
1:A:236:ARG:HD3	1:A:239:GLU:OE1	1.86	0.75
1:A:151:ASP:HA	1:A:156:LEU:HD12	1.67	0.74
1:A:72:VAL:HG12	1:A:74:LEU:HD21	1.70	0.74
1:A:112:LYS:HA	1:A:116:TYR:O	1.87	0.73
1:A:19:ALA:O	1:A:23:GLY:N	2.20	0.73
1:A:375:GLU:HA	1:A:380:TYR:O	1.88	0.73
1:A:14:LEU:HB3	1:A:63:LEU:HD11	1.72	0.72
1:A:367:ARG:HD3	1:A:384:PHE:HB2	1.72	0.70
1:A:129:GLU:O	1:A:131:PRO:HD3	1.91	0.70
1:A:21:VAL:HG21	1:A:75:TYR:CD2	2.27	0.70
1:A:100:TRP:CH2	1:A:126:ILE:HD13	2.27	0.69
1:A:155[B]:ASN:ND2	4:A:432:HOH:O	2.25	0.69
1:A:31:PHE:CE2	1:A:395:LYS:HB3	2.28	0.68
1:A:157:ASN:O	1:A:159:PRO:HD3	1.93	0.68
1:A:193:LYS:HE2	1:A:209:PRO:HB2	1.76	0.68
1:A:72:VAL:O	1:A:86:GLU:HA	1.94	0.67
1:A:273:ASP:O	1:A:277:ILE:HG13	1.94	0.67
1:A:28:VAL:HG22	1:A:65:ARG:CG	2.15	0.66
1:A:24:ASP:OD1	1:A:25:THR:N	2.28	0.66
1:A:67:ARG:HB2	1:A:121:GLY:C	2.16	0.66
1:A:53:PRO:HD2	1:A:196:ILE:O	1.96	0.66
1:A:231:SER:O	1:A:235:GLU:HG3	1.96	0.66
1:A:19:ALA:HA	1:A:24:ASP:O	1.96	0.65
1:A:178:ASN:HB2	1:A:234:ASN:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:O	1:A:335:GLN:HG3	1.97	0.64
1:A:288:ASN:O	1:A:291:LYS:HB2	1.98	0.64
1:A:367:ARG:HD3	1:A:384:PHE:CB	2.28	0.64
1:A:104:VAL:O	1:A:108:ILE:HG13	1.99	0.63
1:A:88:ASP:O	1:A:90:ASP:N	2.31	0.62
1:A:56:ILE:HD12	1:A:58:ILE:HD12	1.81	0.62
1:A:133:ALA:CB	1:A:228:LEU:HD21	2.30	0.62
1:A:142:LEU:O	1:A:146:VAL:HG23	2.01	0.61
1:A:193:LYS:NZ	1:A:209:PRO:HB3	2.16	0.60
1:A:67:ARG:HH11	1:A:67:ARG:CG	2.11	0.60
1:A:322:VAL:HG12	1:A:350:PHE:CZ	2.37	0.60
1:A:169:LYS:NZ	1:A:173:ASP:OD2	2.29	0.59
1:A:87:PHE:HB2	1:A:91:GLU:OE1	2.01	0.59
1:A:19:ALA:HB2	1:A:25:THR:HG23	1.82	0.59
1:A:168:GLN:NE2	1:A:181:ILE:HG13	2.16	0.59
1:A:250:ARG:HB2	1:A:270:LEU:HD11	1.84	0.58
1:A:95:LYS:HG2	1:A:174:TYR:CE2	2.39	0.58
1:A:34:PRO:HA	1:A:59:GLY:HA3	1.84	0.58
1:A:210:VAL:HG21	1:A:389:ILE:HD13	1.85	0.57
1:A:66:LEU:HD21	1:A:154:PHE:CZ	2.40	0.57
1:A:339:GLY:O	1:A:359:ALA:N	2.32	0.57
1:A:67:ARG:NH1	1:A:67:ARG:HG2	2.10	0.57
1:A:229:THR:O	1:A:230:GLU:HB2	2.05	0.56
1:A:88:ASP:N	1:A:91:GLU:OE2	2.30	0.56
1:A:24:ASP:CG	1:A:25:THR:H	2.10	0.56
1:A:28:VAL:C	1:A:29:GLU:HG2	2.25	0.55
1:A:59:GLY:HA2	1:A:130:ILE:CD1	2.24	0.55
1:A:38:ASN:HA	1:A:53:PRO:HA	1.88	0.55
1:A:81:LYS:HB2	4:A:418:HOH:O	2.07	0.55
1:A:132:THR:CG2	1:A:228:LEU:HD11	2.37	0.55
1:A:21:VAL:HG12	1:A:22:PHE:CD1	2.42	0.55
1:A:221:ASN:HB3	1:A:383:SER:HB2	1.89	0.55
1:A:58:ILE:HG22	1:A:130:ILE:HG13	1.89	0.54
1:A:88:ASP:C	1:A:90:ASP:H	2.10	0.54
1:A:130:ILE:HD12	4:A:481:HOH:O	2.07	0.54
1:A:222:THR:O	1:A:223:ASN:HB2	2.07	0.54
1:A:19:ALA:HB1	1:A:23:GLY:O	2.08	0.54
1:A:322:VAL:HG12	1:A:350:PHE:CE2	2.43	0.53
1:A:323:THR:HG22	1:A:345:MET:SD	2.48	0.53
1:A:232:LYS:HB3	1:A:350:PHE:CE2	2.44	0.53
1:A:11:LEU:O	1:A:12:SER:C	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASP:O	1:A:97:GLY:C	2.47	0.53
1:A:345:MET:HA	1:A:354:ALA:HA	1.90	0.53
1:A:70:LYS:HE2	1:A:119:ASP:O	2.09	0.53
1:A:67:ARG:HB2	1:A:122:PHE:N	2.24	0.52
1:A:375:GLU:O	1:A:376:GLU:C	2.44	0.52
1:A:67:ARG:NH1	1:A:67:ARG:CG	2.71	0.51
1:A:71:LYS:O	1:A:121:GLY:HA3	2.10	0.51
1:A:322:VAL:O	1:A:350:PHE:N	2.38	0.51
1:A:105:LYS:O	1:A:109:VAL:HG23	2.11	0.51
1:A:103:TYR:CE2	1:A:175:ILE:HG13	2.46	0.50
1:A:119:ASP:N	1:A:119:ASP:OD2	2.32	0.50
1:A:18:PHE:CZ	1:A:22:PHE:HD2	2.30	0.50
1:A:378:VAL:HG12	1:A:380:TYR:CD2	2.46	0.50
1:A:11:LEU:O	1:A:15:THR:OG1	2.30	0.50
1:A:193:LYS:HZ3	1:A:209:PRO:HB3	1.76	0.50
1:A:235:GLU:O	1:A:239:GLU:HG3	2.12	0.49
1:A:74:LEU:HB2	1:A:100:TRP:CZ2	2.47	0.49
1:A:229:THR:HG22	1:A:230:GLU:N	2.27	0.49
1:A:146:VAL:HG12	1:A:150:LEU:CD1	2.42	0.49
1:A:374:TYR:O	1:A:375:GLU:C	2.49	0.49
1:A:9:THR:O	1:A:12:SER:N	2.46	0.49
1:A:52:PHE:N	1:A:53:PRO:HD3	2.27	0.49
1:A:168:GLN:HE21	1:A:181:ILE:HG13	1.78	0.49
1:A:107:MET:O	1:A:111:LEU:HB2	2.12	0.49
1:A:192:VAL:HG23	4:A:490:HOH:O	2.12	0.49
1:A:275:THR:O	1:A:279:ARG:HG2	2.13	0.49
1:A:117:GLU:OE2	1:A:118:ILE:N	2.47	0.48
1:A:31:PHE:HE2	1:A:395:LYS:HB3	1.76	0.48
1:A:293:ALA:HA	1:A:308:LEU:HD12	1.96	0.48
1:A:162:GLU:O	1:A:163:LEU:C	2.51	0.48
1:A:302:LEU:HB3	1:A:341:LEU:HD13	1.95	0.48
1:A:50:TYR:CZ	1:A:199:ASP:HB2	2.48	0.48
1:A:219:ILE:N	1:A:385:TYR:O	2.39	0.48
1:A:55:SER:OG	1:A:190:GLY:HA3	2.14	0.48
1:A:339:GLY:O	1:A:358:VAL:HA	2.14	0.48
1:A:304:LYS:HA	1:A:307:GLU:OE1	2.13	0.47
1:A:312:SER:HB3	1:A:344:ARG:HD3	1.96	0.47
1:A:250:ARG:HB2	1:A:270:LEU:CD1	2.43	0.47
1:A:24:ASP:CG	1:A:25:THR:N	2.67	0.47
1:A:378:VAL:HG12	1:A:380:TYR:CE2	2.50	0.47
1:A:14:LEU:HB3	1:A:63:LEU:CD1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HG	1:A:153:LEU:HB3	1.96	0.47
1:A:9:THR:O	1:A:10:VAL:C	2.51	0.47
1:A:11:LEU:O	1:A:15:THR:N	2.31	0.46
1:A:125:LEU:HD23	1:A:125:LEU:C	2.36	0.46
1:A:57:THR:OG1	1:A:388:GLN:HB3	2.15	0.46
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.59	0.46
1:A:193:LYS:NZ	1:A:209:PRO:CB	2.78	0.46
1:A:212:LEU:O	1:A:213:ARG:HB2	2.15	0.46
1:A:193:LYS:CE	1:A:209:PRO:HB2	2.46	0.46
1:A:171:GLU:HA	1:A:171:GLU:OE1	2.16	0.46
1:A:118:ILE:HG23	1:A:154:PHE:CE1	2.50	0.46
1:A:84:VAL:CG1	1:A:85:ILE:N	2.78	0.46
1:A:333:THR:O	1:A:336:LYS:HB2	2.16	0.46
1:A:50:TYR:CE2	1:A:199:ASP:HB2	2.51	0.45
1:A:19:ALA:O	1:A:20:GLU:C	2.53	0.45
1:A:132:THR:HG22	1:A:228:LEU:HD11	1.99	0.45
1:A:9:THR:HG22	1:A:10:VAL:N	2.31	0.45
1:A:111:LEU:HD12	1:A:150:LEU:HD12	2.00	0.44
1:A:306:GLY:O	1:A:309:LEU:HB2	2.17	0.44
1:A:21:VAL:HG21	1:A:75:TYR:CE2	2.52	0.44
1:A:28:VAL:CG1	1:A:29:GLU:N	2.81	0.44
1:A:149:VAL:O	1:A:150:LEU:C	2.55	0.44
1:A:337:GLN:HB2	1:A:340:VAL:HG21	1.98	0.44
1:A:40:ILE:HG22	1:A:52:PHE:HB3	2.00	0.44
1:A:103:TYR:CE2	1:A:139:SER:HB3	2.52	0.44
1:A:217:ILE:HB	1:A:387:ALA:HB3	2.00	0.43
1:A:88:ASP:C	1:A:90:ASP:N	2.70	0.43
1:A:34:PRO:HG3	1:A:391:SER:O	2.18	0.43
1:A:99:LEU:O	1:A:102:ASN:HB2	2.18	0.43
1:A:197:GLU:O	1:A:205:TYR:HA	2.18	0.43
1:A:193:LYS:HE2	1:A:209:PRO:CB	2.47	0.43
1:A:72:VAL:HG12	1:A:74:LEU:CD2	2.45	0.43
1:A:340:VAL:HG22	1:A:358:VAL:HG22	2.00	0.43
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.55	0.43
1:A:310:ASN:OD1	1:A:343:ALA:N	2.47	0.43
1:A:158:VAL:HG11	1:A:163:LEU:HD23	2.01	0.43
1:A:313:HIS:HB2	1:A:344:ARG:CB	2.49	0.43
1:A:33:SER:O	1:A:60:THR:N	2.35	0.43
1:A:380:TYR:CB	1:A:381:PRO:CD	2.84	0.43
1:A:247:MET:HE1	1:A:264:PHE:CD1	2.54	0.43
1:A:169:LYS:O	1:A:173:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:TYR:O	1:A:236:ARG:HB2	2.19	0.42
1:A:249:THR:C	1:A:250:ARG:HD3	2.39	0.42
1:A:30:TYR:CD2	1:A:63:LEU:CD2	3.02	0.42
1:A:82:LEU:N	1:A:82:LEU:HD23	2.34	0.42
1:A:131:PRO:O	1:A:134:SER:OG	2.29	0.42
1:A:132:THR:CG2	1:A:228:LEU:CD1	2.98	0.42
1:A:146:VAL:O	1:A:150:LEU:HG	2.18	0.42
1:A:374:TYR:CE1	1:A:378:VAL:HG21	2.54	0.42
1:A:193:LYS:O	1:A:210:VAL:N	2.33	0.42
1:A:302:LEU:HB3	1:A:341:LEU:CD1	2.50	0.42
1:A:10:VAL:O	1:A:13:ALA:HB3	2.20	0.42
1:A:357:LEU:HA	1:A:357:LEU:HD23	1.59	0.41
1:A:378:VAL:CG1	1:A:380:TYR:CE2	3.02	0.41
1:A:24:ASP:OD1	1:A:26:LYS:N	2.54	0.41
1:A:57:THR:HG21	1:A:388:GLN:HE21	1.85	0.41
1:A:65:ARG:NH1	1:A:123:GLU:OE1	2.54	0.41
1:A:242:GLU:O	1:A:246:ARG:HG3	2.19	0.41
1:A:67:ARG:HG2	1:A:69:ASP:OD1	2.20	0.41
1:A:73:LYS:HG3	1:A:86:GLU:HB3	2.01	0.41
1:A:375:GLU:O	1:A:379:GLY:N	2.49	0.41
1:A:236:ARG:HD3	1:A:236:ARG:HA	1.83	0.41
1:A:244:LEU:O	1:A:248:GLN:HG3	2.20	0.41
1:A:372:GLN:O	1:A:373:VAL:C	2.57	0.41
1:A:50:TYR:HA	1:A:198:LEU:O	2.20	0.41
1:A:71:LYS:O	1:A:121:GLY:CA	2.69	0.41
1:A:159:PRO:O	1:A:163:LEU:HB2	2.21	0.41
1:A:212:LEU:HD21	1:A:297:PHE:HE1	1.85	0.41
1:A:278:LYS:HB3	1:A:319:ASP:O	2.21	0.40
1:A:214:ASP:O	1:A:360:HIS:HB2	2.20	0.40
1:A:56:ILE:H	1:A:56:ILE:HG12	1.73	0.40
1:A:74:LEU:HA	1:A:124:LEU:O	2.21	0.40
1:A:92:VAL:O	1:A:105:LYS:HB3	2.21	0.40
1:A:73:LYS:O	1:A:74:LEU:HD23	2.22	0.40
1:A:236:ARG:HA	1:A:239:GLU:OE1	2.21	0.40
1:A:151:ASP:CA	1:A:156:LEU:HD12	2.45	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	387/419 (92%)	357 (92%)	27 (7%)	3 (1%)	22	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	20	GLU
1	A	230	GLU

### 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	315/348 (90%)	279 (89%)	36 (11%)	7	3

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	24	ASP
1	A	29	GLU
1	A	36	ARG
1	A	52	PHE
1	A	57	THR
1	A	65	ARG
1	A	67	ARG

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Mol	Chain	Res	Type
1	A	68	GLU
1	A	73	LYS
1	A	74	LEU
1	A	81	LYS
1	A	88	ASP
1	A	90	ASP
1	A	91	GLU
1	A	117	GLU
1	A	120	LYS
1	A	123	GLU
1	A	126	ILE
1	A	138	SER
1	A	139	SER
1	A	144	LEU
1	A	156	LEU
1	A	163	LEU
1	A	193	LYS
1	A	194	LYS
1	A	229	THR
1	A	231	SER
1	A	245	LYS
1	A	294	GLN
1	A	298	VAL
1	A	320	TYR
1	A	364	SER
1	A	372	GLN
1	A	385	TYR
1	A	395	LYS

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

Mol	Chain	Res	Type
1	A	165	GLN
1	A	168	GLN
1	A	172	ASN
1	A	294	GLN
1	A	388	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	GLA	A	400	-	12,12,12	0.58	0	17,17,17	1.34	2 (11%)
3	PO4	A	401	-	4,4,4	1.38	0	6,6,6	1.32	1 (16%)

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	GLA	A	400	-	-	0/2/22/22	0/1/1/1
3	PO4	A	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GLA	C4-C3-C2	-2.51	106.41	110.84
3	A	401	PO4	O4-P-O3	2.10	115.61	107.90
2	A	400	GLA	O4-C4-C5	2.20	114.83	109.28

There are no chirality outliers.

There are no torsion outliers.

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 [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	388/419 (92%)	-0.54	5 (1%) 77 81	25, 45, 86, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	PHE	4.2
1	A	156	LEU	3.6
1	A	25	THR	2.9
1	A	22	PHE	2.8
1	A	28	VAL	2.1

### 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	PO4	A	401	5/5	0.90	0.14	1.84	44,44,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLA	A	400	12/12	0.97	0.07	-0.33	20,28,39,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.