



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:40 AM UTC

PDB ID : 1PIE / pdb_00001pie
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

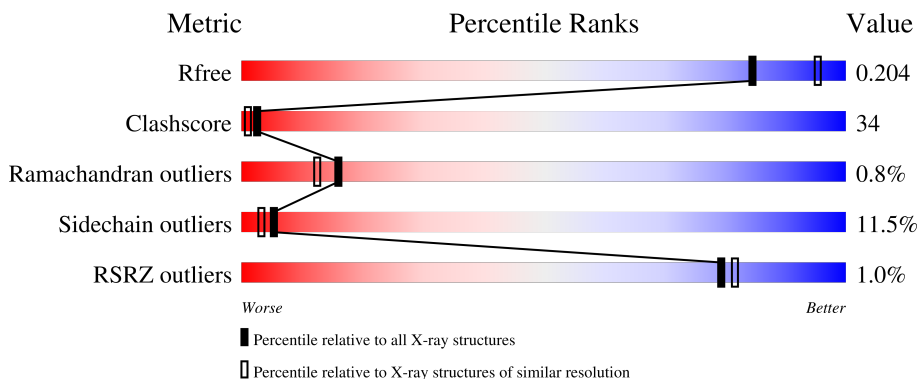
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	419	36% 46% 10% 7%

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.

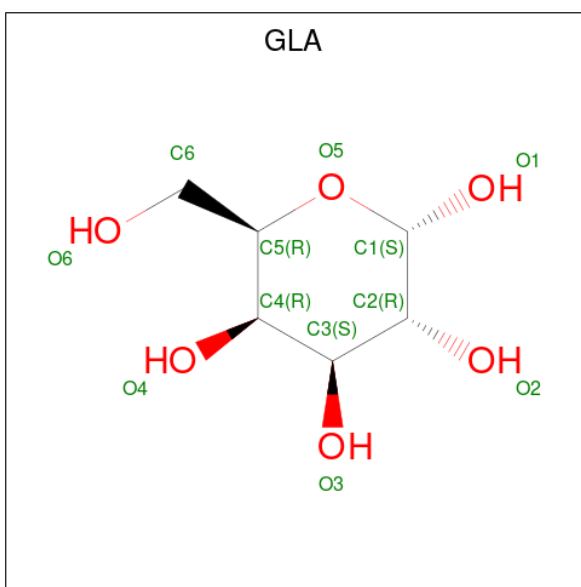
- Molecule 1 is a protein called Galactokinase.

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 alpha-D-galactopyranose (CCD ID: GLA) (formula: C₆H₁₂O₆).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

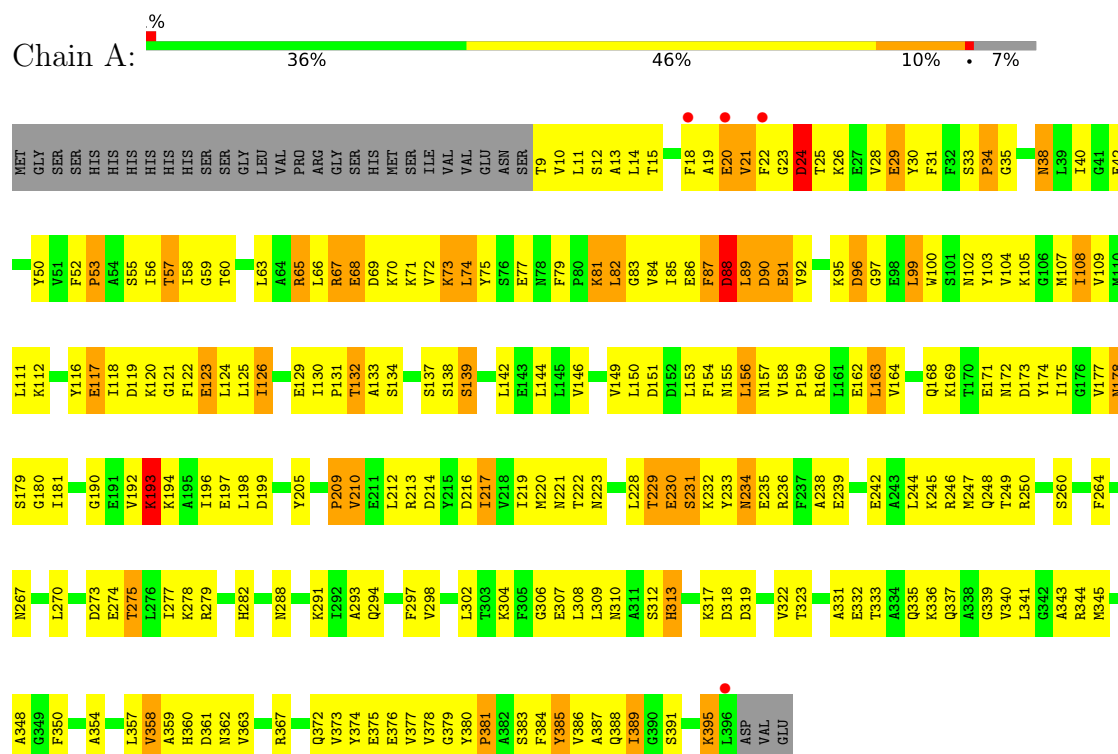
- Molecule 4 is water.

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, 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: Galactokinase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	143.40Å 143.40Å 143.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.10) 99.3 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	4234 reflections (10.22%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 200.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3166	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PO4, GLA

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	1.28	3/3036 (0.1%)	1.84	49/4103 (1.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	PRO	C-N	-5.57	1.28	1.33
1	A	274	GLU	CD-OE2	5.47	1.35	1.25
1	A	210	VAL	N-CA	-5.12	1.41	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ASN	CA-CB-CG	-10.56	102.04	112.60
1	A	377	VAL	N-CA-C	8.09	118.86	110.36
1	A	82	LEU	N-CA-C	-8.05	103.60	113.50
1	A	79	PHE	CA-CB-CG	7.96	121.76	113.80
1	A	313	HIS	CA-CB-CG	-7.47	106.33	113.80
1	A	260	SER	N-CA-C	-7.44	100.51	110.55
1	A	96	ASP	CA-CB-CG	-6.92	105.68	112.60
1	A	282	HIS	CA-CB-CG	-6.64	107.16	113.80
1	A	117	GLU	N-CA-C	6.63	119.63	108.02
1	A	363	VAL	N-CA-C	6.47	116.64	110.42
1	A	180	GLY	N-CA-C	-6.15	104.32	112.81
1	A	318	ASP	N-CA-C	6.10	120.82	112.04
1	A	87	PHE	CA-C-N	-6.09	112.13	122.67
1	A	87	PHE	C-N-CA	-6.09	112.13	122.67
1	A	88	ASP	N-CA-CB	6.05	119.83	110.46
1	A	361	ASP	N-CA-CB	5.96	119.51	110.28
1	A	348	ALA	N-CA-C	5.93	118.23	111.11
1	A	137	SER	N-CA-C	5.83	119.89	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	PRO	CB-CA-C	-5.79	102.00	111.56
1	A	389	ILE	CB-CA-C	5.71	117.77	111.08
1	A	267	ASN	N-CA-C	5.71	119.23	112.72
1	A	209	PRO	CB-CA-C	-5.68	103.66	111.21
1	A	99	LEU	CA-C-N	5.56	128.29	120.28
1	A	99	LEU	C-N-CA	5.56	128.29	120.28
1	A	217	ILE	CA-C-N	-5.56	115.93	122.93
1	A	217	ILE	C-N-CA	-5.56	115.93	122.93
1	A	34	PRO	CA-C-N	5.53	128.44	122.69
1	A	34	PRO	C-N-CA	5.53	128.44	122.69
1	A	179	SER	N-CA-C	5.50	115.64	107.88
1	A	361	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	358	VAL	N-CA-C	5.44	116.57	108.46
1	A	234	ASN	CB-CA-C	5.44	120.69	110.63
1	A	24	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	362	ASN	CA-C-O	5.30	125.69	119.28
1	A	38	ASN	CB-CA-C	-5.29	101.51	110.19
1	A	79	PHE	CB-CA-C	5.29	119.88	111.15
1	A	53	PRO	CB-CA-C	-5.26	102.88	111.56
1	A	172	ASN	CA-CB-CG	5.25	117.84	112.60
1	A	132	THR	CA-C-N	-5.23	114.41	123.25
1	A	132	THR	C-N-CA	-5.23	114.41	123.25
1	A	193	LYS	CB-CA-C	5.17	119.70	111.48
1	A	83	GLY	N-CA-C	-5.12	102.50	112.02
1	A	68	GLU	N-CA-C	-5.12	105.16	111.40
1	A	172	ASN	CB-CA-C	-5.08	103.07	110.95
1	A	35	GLY	N-CA-C	-5.08	105.80	112.81
1	A	217	ILE	N-CA-CB	5.08	117.76	111.41
1	A	332	GLU	CA-C-N	-5.04	113.13	120.29
1	A	332	GLU	C-N-CA	-5.04	113.13	120.29
1	A	216	ASP	CA-CB-CG	5.01	117.61	112.60

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	204	0
2	A	12	0	12	0	0
3	A	5	0	0	0	0
4	A	164	0	0	5	0
All	All	3166	0	2965	204	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 34.

All (204) 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:HG2	1:A:67:ARG:HH11	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:HD23	1:A:11:LEU:N	2.01	0.75
1:A:236:ARG:HD3	1:A:239:GLU:OE1	1.86	0.75
1:A:72:VAL:HG12	1:A:74:LEU:HD21	1.70	0.74
1:A:151:ASP:HA	1:A:156:LEU:HD12	1.67	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:67:ARG:HB2	1:A:121:GLY:C	2.16	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:24:ASP:CG	1:A:25:THR:H	2.10	0.60
1:A:28:VAL:C	1:A:29:GLU:HG2	2.25	0.60
1:A:67:ARG:HH11	1:A:67:ARG:CG	2.11	0.60
1:A:193:LYS:NZ	1:A:209:PRO:HB3	2.16	0.60
1:A:322:VAL:HG12	1:A:350:PHE:CZ	2.37	0.60
1:A:88:ASP:C	1:A:90:ASP:H	2.10	0.59
1:A:87:PHE:HB2	1:A:91:GLU:OE1	2.01	0.59
1:A:169:LYS:NZ	1:A:173:ASP:OD2	2.29	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:11:LEU:O	1:A:12:SER:C	2.43	0.58
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:96:ASP:O	1:A:97:GLY:C	2.47	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:HG2	1:A:67:ARG:NH1	2.10	0.57
1:A:247:MET:HE1	1:A:264:PHE:CD1	2.40	0.56
1:A:88:ASP:N	1:A:91:GLU:OE2	2.30	0.56
1:A:229:THR:O	1:A:230:GLU:HB2	2.05	0.56
1:A:375:GLU:O	1:A:376:GLU:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:21:VAL:HG12	1:A:22:PHE:CD1	2.42	0.55
1:A:132:THR:CG2	1:A:228:LEU:HD11	2.37	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:130:ILE:HD12	4:A:481:HOH:O	2.07	0.54
1:A:374:TYR:O	1:A:375:GLU:C	2.49	0.54
1:A:19:ALA:HB1	1:A:23:GLY:O	2.08	0.54
1:A:232:LYS:HB3	1:A:350:PHE:CE2	2.44	0.53
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:222:THR:O	1:A:223:ASN:HB2	2.07	0.53
1:A:162:GLU:O	1:A:163:LEU:C	2.51	0.53
1:A:70:LYS:HE2	1:A:119:ASP:O	2.09	0.53
1:A:345:MET:HA	1:A:354:ALA:HA	1.90	0.53
1:A:24:ASP:CG	1:A:25:THR:N	2.67	0.52
1:A:67:ARG:HB2	1:A:122:PHE:N	2.24	0.52
1:A:67:ARG:CG	1:A:67:ARG:NH1	2.71	0.51
1:A:9:THR:O	1:A:10:VAL:C	2.51	0.51
1:A:193:LYS:HZ1	1:A:209:PRO:HB3	1.75	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:OD2	1:A:119:ASP:N	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:125:LEU:C	1:A:125:LEU:HD23	2.36	0.50
1:A:11:LEU:O	1:A:15:THR:OG1	2.30	0.50
1:A:19:ALA:O	1:A:20:GLU:C	2.53	0.49
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:146:VAL:HG12	1:A:150:LEU:CD1	2.42	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:149:VAL:O	1:A:150:LEU:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:THR:O	1:A:279:ARG:HG2	2.13	0.49
1:A:31:PHE:HE2	1:A:395:LYS:HB3	1.76	0.48
1:A:117:GLU:OE2	1:A:118:ILE:N	2.47	0.48
1:A:229:THR:HG22	1:A:230:GLU:N	2.27	0.48
1:A:293:ALA:HA	1:A:308:LEU:HD12	1.96	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:249:THR:C	1:A:250:ARG:HD3	2.39	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
1:A:66:LEU:HG	1:A:153:LEU:HB3	1.96	0.47
1:A:11:LEU:O	1:A:15:THR:N	2.31	0.46
1:A:57:THR:OG1	1:A:388:GLN:HB3	2.15	0.46
1:A:89:LEU:HA	1:A:89:LEU:HD23	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:88:ASP:C	1:A:90:ASP:N	2.70	0.46
1:A:171:GLU:HA	1:A:171:GLU:OE1	2.16	0.46
1:A:84:VAL:CG1	1:A:85:ILE:N	2.78	0.46
1:A:118:ILE:HG23	1:A:154:PHE:CE1	2.50	0.46
1:A:333:THR:O	1:A:336:LYS:HB2	2.16	0.46
1:A:372:GLN:O	1:A:373:VAL:C	2.57	0.46
1:A:50:TYR:CE2	1:A:199:ASP:HB2	2.51	0.45
1:A:132:THR:HG22	1:A:228:LEU:HD11	1.99	0.45
1:A:317:LYS:NZ	4:A:463:HOH:O	2.49	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:40:ILE:HG22	1:A:52:PHE:HB3	2.00	0.44
1:A:337:GLN:HB2	1:A:340:VAL:HG21	1.98	0.44
1:A:103:TYR:CE2	1:A:139:SER:HB3	2.52	0.44
1:A:373:VAL:O	1:A:374:TYR:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:HB	1:A:387:ALA:HB3	2.00	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:72:VAL:HG12	1:A:74:LEU:CD2	2.45	0.43
1:A:193:LYS:HE2	1:A:209:PRO:CB	2.47	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:220:MET:HE3	1:A:354:ALA:HB3	2.01	0.43
1:A:169:LYS:O	1:A:173:ASP:HB2	2.19	0.42
1:A:233:TYR:O	1:A:236:ARG:HB2	2.19	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:159:PRO:O	1:A:160:ARG:C	2.63	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:247:MET:HE1	1:A:264:PHE:HD1	1.83	0.42
1:A:10:VAL:O	1:A:13:ALA:HB3	2.20	0.42
1:A:357:LEU:HD23	1:A:357:LEU:HA	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: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:242:GLU:O	1:A:246:ARG:HG3	2.19	0.41
1:A:375:GLU:O	1:A:379:GLY:N	2.49	0.41
1:A:81:LYS:C	1:A:82:LEU:HD23	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:214:ASP:O	1:A:360:HIS:HB2	2.20	0.40
1:A:73:LYS:O	1:A:74:LEU:HD23	2.22	0.40
1:A:92:VAL:O	1:A:105:LYS:HB3	2.21	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%)	16 12

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%)	5 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	42	GLU
1	A	57	THR
1	A	65	ARG
1	A	67	ARG
1	A	68	GLU
1	A	73	LYS
1	A	74	LEU
1	A	77	GLU
1	A	81	LYS
1	A	88	ASP
1	A	90	ASP
1	A	91	GLU
1	A	108	ILE
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	164	VAL
1	A	193	LYS
1	A	194	LYS
1	A	229	THR
1	A	231	SER
1	A	245	LYS
1	A	275	THR
1	A	294	GLN
1	A	298	VAL
1	A	385	TYR
1	A	386	VAL
1	A	395	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	168	GLN
1	A	294	GLN
1	A	388	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	PO4	A	401	-	4,4,4	1.66	1 (25%)	6,6,6	1.57	1 (16%)
2	GLA	A	400	-	12,12,12	0.55	0	17,17,17	1.31	2 (11%)

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	-	-	1/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PO4	P-O2	-2.40	1.47	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GLA	C4-C3-C2	-2.52	106.41	110.83
3	A	401	PO4	O4-P-O3	2.47	115.61	107.91
2	A	400	GLA	O4-C4-C5	2.24	114.83	109.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	GLA	O5-C5-C6-O6

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, 95th 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	388/419 (92%)	-0.27	4 (1%) 79 81	25, 45, 86, 100	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	PHE	2.3
1	A	20	GLU	2.3
1	A	22	PHE	2.1
1	A	396	LEU	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
3	PO4	A	401	5/5	0.86	0.18	44,44,80,80	0
2	GLA	A	400	12/12	0.98	0.04	20,28,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.