



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:10 PM GMT

PDB ID : 1NSU  
Title : Crystal structure of galactose mutarotase from *Lactococcus lactis* mutant H96N complexed with galactose  
Authors : Holden, H.M.; Thoden, J.B.  
Deposited on : 2003-01-28  
Resolution : 1.80 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](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.

---

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

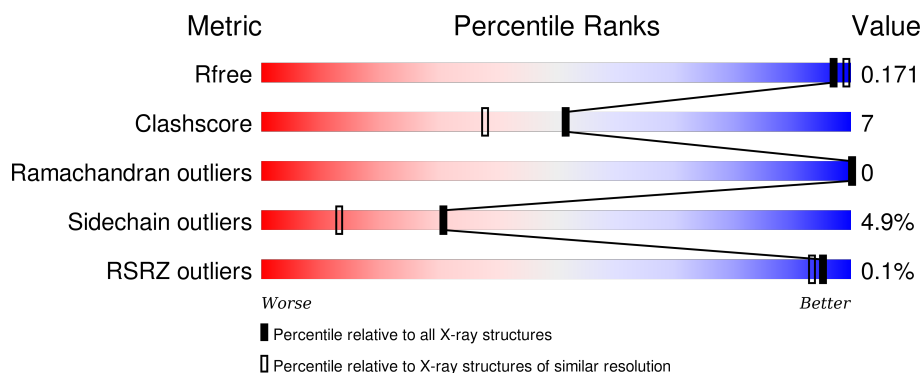
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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  $\geq 3$ , 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	347	 68% 24% 6% •
1	B	347	 74% 22% • •

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
3	NA	A	1401	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5802 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.

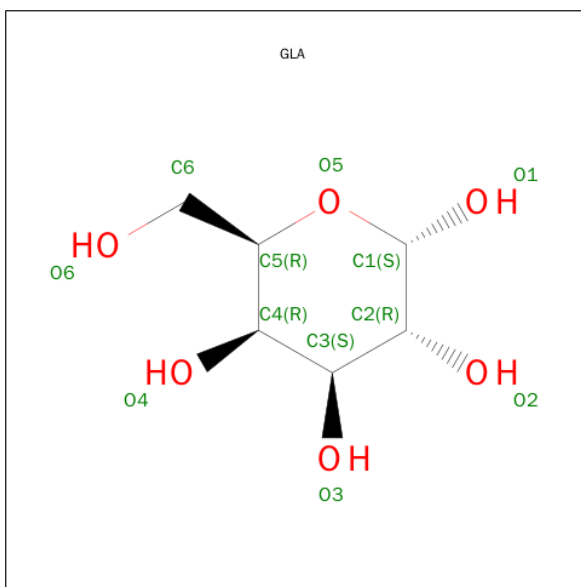
- Molecule 1 is a protein called GALACTOSE MUTAROTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	4	0
			2656	1674	446	533	3			
1	B	346	Total	C	N	O	S	0	0	0
			2715	1709	465	538	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	GLU	CLONING ARTIFACT	UNP Q9ZB17
A	96	ASN	HIS	ENGINEERED	UNP Q9ZB17
A	340	LEU	-	EXPRESSION TAG	UNP Q9ZB17
A	341	GLU	-	EXPRESSION TAG	UNP Q9ZB17
A	342	HIS	-	EXPRESSION TAG	UNP Q9ZB17
A	343	HIS	-	EXPRESSION TAG	UNP Q9ZB17
A	344	HIS	-	EXPRESSION TAG	UNP Q9ZB17
A	345	HIS	-	EXPRESSION TAG	UNP Q9ZB17
A	346	HIS	-	EXPRESSION TAG	UNP Q9ZB17
A	347	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	2	SER	GLU	CLONING ARTIFACT	UNP Q9ZB17
B	96	ASN	HIS	ENGINEERED	UNP Q9ZB17
B	340	LEU	-	EXPRESSION TAG	UNP Q9ZB17
B	341	GLU	-	EXPRESSION TAG	UNP Q9ZB17
B	342	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	343	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	344	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	345	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	346	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	347	HIS	-	EXPRESSION TAG	UNP Q9ZB17

- 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		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

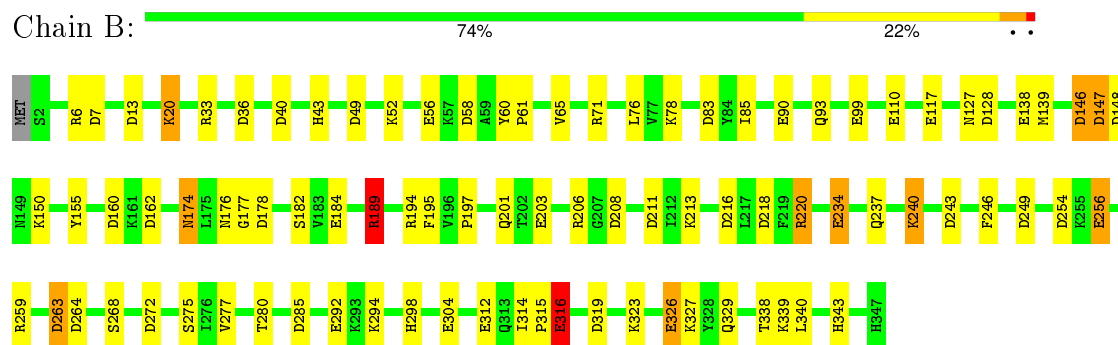
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	184	Total	O	0	0
			184	184		
4	B	222	Total	O	0	0
			222	222		



- Molecule 1: GALACTOSE MUTAROTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.90 Å 76.20 Å 210.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 61.75 – 1.77	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-1.80) 92.1 (61.75-1.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.77 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.173 , 0.236 0.168 , 0.171	Depositor DCC
$R_{free}$ test set	6455 reflections (11.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.910	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 87.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 66093 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5802	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: GLA, NA

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	0.99	19/2723 (0.7%)	1.41	52/3685 (1.4%)
1	B	0.98	12/2772 (0.4%)	1.45	58/3751 (1.5%)
All	All	0.99	31/5495 (0.6%)	1.43	110/7436 (1.5%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	GLU	CD-OE2	6.76	1.33	1.25
1	B	316	GLU	CD-OE2	6.72	1.33	1.25
1	A	100	GLU	CD-OE2	6.67	1.32	1.25
1	B	117	GLU	CD-OE2	6.63	1.32	1.25
1	A	184	GLU	CD-OE2	6.46	1.32	1.25
1	A	256	GLU	CD-OE2	6.41	1.32	1.25
1	A	99	GLU	CD-OE2	6.39	1.32	1.25
1	A	326	GLU	CD-OE2	6.37	1.32	1.25
1	B	99	GLU	CD-OE2	6.26	1.32	1.25
1	B	184	GLU	CD-OE2	6.19	1.32	1.25
1	A	316	GLU	CD-OE2	6.11	1.32	1.25
1	B	256	GLU	CD-OE2	6.09	1.32	1.25
1	B	292	GLU	CD-OE2	5.95	1.32	1.25
1	B	326	GLU	CD-OE2	5.89	1.32	1.25
1	A	90	GLU	CD-OE2	5.74	1.31	1.25
1	A	312	GLU	CD-OE2	5.71	1.31	1.25
1	B	138	GLU	CD-OE2	5.63	1.31	1.25
1	B	234	GLU	CD-OE2	5.61	1.31	1.25
1	A	203	GLU	CD-OE2	5.60	1.31	1.25
1	B	110	GLU	CD-OE2	5.55	1.31	1.25
1	A	156	GLU	CD-OE2	5.51	1.31	1.25
1	B	312	GLU	CD-OE2	5.45	1.31	1.25
1	A	138	GLU	CD-OE2	5.45	1.31	1.25
1	A	304	GLU	CD-OE2	5.41	1.31	1.25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	GLU	CD-OE2	5.31	1.31	1.25
1	A	292[A]	GLU	CD-OE2	5.28	1.31	1.25
1	A	292[B]	GLU	CD-OE2	5.28	1.31	1.25
1	B	203	GLU	CD-OE2	5.13	1.31	1.25
1	A	222	GLU	CD-OE2	5.12	1.31	1.25
1	A	90	GLU	CD-OE1	-5.08	1.20	1.25
1	A	234	GLU	CD-OE2	5.02	1.31	1.25

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ASP	CB-CG-OD1	9.41	126.77	118.30
1	B	146	ASP	CB-CG-OD2	-9.24	109.98	118.30
1	B	249	ASP	CB-CG-OD2	-9.21	110.01	118.30
1	A	249	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	B	263	ASP	CB-CG-OD1	8.41	125.87	118.30
1	A	71	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	178	ASP	CB-CG-OD1	8.28	125.75	118.30
1	B	243	ASP	CB-CG-OD1	8.07	125.57	118.30
1	A	259	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	148	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	272	ASP	CB-CG-OD1	7.91	125.42	118.30
1	B	13	ASP	CB-CG-OD2	-7.87	111.21	118.30
1	A	147	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	B	178	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	B	249	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	74	ASP	CB-CG-OD2	-7.57	111.48	118.30
1	B	49	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	A	194	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	36	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	A	272	ASP	CB-CG-OD2	-7.45	111.59	118.30
1	B	254	ASP	CB-CG-OD1	7.45	125.01	118.30
1	B	220	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	A	146	ASP	CB-CG-OD1	7.36	124.92	118.30
1	B	58	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	264	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	B	243	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	A	7	ASP	CB-CG-OD1	7.26	124.83	118.30
1	B	6	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	208	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	36	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	113	ASP	CB-CG-OD2	-7.17	111.85	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ASP	CB-CG-OD1	7.15	124.73	118.30
1	B	162	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	254	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	330	ALA	N-CA-CB	7.05	119.97	110.10
1	A	272	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	146	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	B	259	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	B	49	ASP	CB-CG-OD1	6.83	124.45	118.30
1	B	272	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	A	7	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	B	83	ASP	CB-CG-OD1	6.82	124.44	118.30
1	B	160	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	36	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	40	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	200	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	178	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	B	259	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	B	160	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	285	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	B	40	ASP	CB-CG-OD2	-6.52	112.44	118.30
1	B	162	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	B	218	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	83	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	B	71	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	319	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	33	ARG	N-CA-CB	-6.39	99.09	110.60
1	A	208	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	162	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	254	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	128	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	194	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	220	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	264	ASP	CB-CG-OD1	6.18	123.86	118.30
1	B	319	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	160	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	147	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	178	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	211	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	206	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	33	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	33	ARG	N-CA-CB	-6.05	99.72	110.60
1	B	147	ASP	CB-CG-OD1	6.00	123.70	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	A	249	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	71	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	148	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	74	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	162	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	229	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	A	218	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	285	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	218	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	40	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	189	ARG	N-CA-CB	5.63	120.73	110.60
1	B	189	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	263	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	58	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	216	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	211	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	216	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	263	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	254	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	200	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	36	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	B	264	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	7	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	319	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	148	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	263	ASP	CB-CG-OD1	5.26	123.03	118.30
1	B	139	MET	CB-CA-C	-5.23	99.93	110.40
1	B	147	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	49	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	40	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	285	ASP	CB-CG-OD1	5.12	122.90	118.30
1	B	128	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	33	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	216	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	174	ASN	N-CA-CB	5.04	119.67	110.60
1	B	194	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	2656	0	2590	48	0
1	B	2715	0	2633	25	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	1	0	0	0	0
4	A	184	0	0	1	0
4	B	222	0	0	2	0
All	All	5802	0	5247	72	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 (72) 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:338:THR:HG22	1:B:339:LYS:HG3	1.46	0.96
1:A:199:LYS:HE2	1:A:204:ILE:HD11	1.60	0.81
1:A:20:LYS:HD2	1:A:147:ASP:OD2	1.89	0.72
1:A:193[A]:SER:HB2	1:A:213:LYS:HE3	1.77	0.66
1:B:338:THR:CG2	1:B:339:LYS:HG3	2.23	0.65
1:A:232:ASN:O	1:A:237:GLN:NE2	2.29	0.65
1:A:294:LYS:HB2	1:A:294:LYS:NZ	2.12	0.65
1:B:263:ASP:H	1:B:343:HIS:HD1	1.45	0.64
1:A:193[B]:SER:HB3	1:A:213:LYS:HE3	1.80	0.63
1:B:189:ARG:NH2	1:B:256:GLU:O	2.30	0.63
1:B:146:ASP:OD2	1:B:150:LYS:NZ	2.32	0.61
1:A:231:SER:OG	1:A:233:MET:HG3	2.00	0.61
1:A:180:SER:HA	1:A:296:VAL:HG13	1.82	0.61
1:A:78:LYS:HE3	1:A:83:ASP:OD1	2.01	0.60
1:A:76:LEU:HD23	1:A:77:VAL:N	2.19	0.57
1:B:316:GLU:HB2	4:B:2534:HOH:O	2.05	0.57
1:A:19:ASN:HB2	1:A:147:ASP:OD1	2.04	0.56
1:A:201:GLN:NE2	1:A:201:GLN:H	2.04	0.56
1:A:201:GLN:CD	1:A:201:GLN:H	2.11	0.54
1:A:156:GLU:HB3	1:A:327:LYS:HZ2	1.73	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193[B]:SER:CB	1:A:213:LYS:HE3	2.38	0.53
1:B:263:ASP:O	4:B:2412:HOH:O	2.19	0.52
1:A:289:LEU:HD23	1:A:294:LYS:HA	1.90	0.52
1:A:216:ASP:OD1	1:A:231:SER:HB2	2.09	0.52
1:A:280:THR:O	1:A:298:HIS:HA	2.11	0.51
1:A:291:HIS:O	1:A:292[B]:GLU:HB2	2.11	0.50
1:B:277:VAL:HB	1:B:304:GLU:HB2	1.91	0.50
1:A:291:HIS:O	1:A:292[A]:GLU:HB2	2.11	0.50
1:A:200:ASP:HB2	1:A:201:GLN:NE2	2.28	0.49
1:B:174:ASN:OD1	1:B:176:ASN:HB2	2.14	0.48
1:A:174:ASN:OD1	1:A:176:ASN:HB2	2.14	0.47
1:B:60:TYR:N	1:B:61:PRO:CD	2.78	0.46
1:A:323:LYS:HB2	1:A:326:GLU:HG3	1.97	0.46
1:A:82:LYS:HD3	1:A:84:TYR:CE1	2.51	0.46
1:A:148:ASP:O	1:A:149:ASN:HB2	2.15	0.46
1:A:255:LYS:NZ	4:A:1424:HOH:O	2.44	0.46
1:A:219:PHE:CD2	1:A:223:LYS:HG2	2.51	0.46
1:A:60:TYR:N	1:A:61:PRO:CD	2.79	0.45
1:A:219:PHE:CE2	1:A:223:LYS:HG2	2.51	0.45
1:B:20:LYS:HE3	1:B:147:ASP:OD2	2.17	0.45
1:A:186:HIS:HD1	1:A:186:HIS:N	2.15	0.45
1:A:227:ASN:HD22	1:A:227:ASN:N	2.15	0.45
1:A:130:THR:HG23	1:B:127:ASN:HB2	1.99	0.44
1:A:213:LYS:HG2	1:A:220:ARG:CZ	2.48	0.44
1:B:340:LEU:HD12	1:B:340:LEU:HA	1.70	0.44
1:B:237:GLN:O	1:B:240:LYS:HE2	2.16	0.44
1:B:90:GLU:O	1:B:93:GLN:HB2	2.18	0.44
1:B:52:LYS:HE2	1:B:56:GLU:OE2	2.17	0.44
1:A:285:ASP:O	1:A:286:LEU:C	2.57	0.43
1:B:256:GLU:HG3	1:B:268:SER:HB3	2.01	0.43
1:B:213:LYS:HD3	1:B:220:ARG:CZ	2.48	0.43
1:B:155:TYR:O	1:B:329:GLN:HA	2.19	0.43
1:A:212:ILE:O	1:A:215:THR:HG23	2.18	0.43
1:B:246:PHE:O	1:B:275:SER:HB2	2.19	0.43
1:A:296:VAL:O	1:A:297:HIS:C	2.57	0.43
1:A:156:GLU:HG2	1:A:329:GLN:HG2	2.01	0.43
1:A:178:ASP:OD1	1:A:293:LYS:HD3	2.18	0.43
1:A:109:TYR:HA	1:A:121:LYS:O	2.20	0.42
1:A:221:GLN:O	1:A:222:GLU:C	2.55	0.42
1:A:232:ASN:C	1:A:237:GLN:HE21	2.22	0.42
1:A:306:GLN:NE2	1:A:309:PRO:HD3	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:HD2	1:A:147:ASP:CG	2.40	0.41
1:A:244:HIS:HA	1:A:245:PRO:HD3	1.84	0.41
1:A:212:ILE:HD12	1:A:217:LEU:O	2.20	0.41
1:A:38:GLN:HB2	1:A:42:LYS:O	2.20	0.41
1:B:197:PRO:HD2	1:B:208:ASP:O	2.21	0.41
1:B:314:ILE:HA	1:B:315:PRO:HD2	1.90	0.41
1:A:297:HIS:O	1:A:298:HIS:HB2	2.21	0.40
1:B:43:HIS:O	1:B:177:GLY:HA2	2.20	0.40
1:B:76:LEU:HD12	1:B:85:ILE:HG12	2.03	0.40
1:A:294:LYS:CB	1:A:294:LYS:NZ	2.82	0.40
1:B:280:THR:O	1:B:298:HIS:HA	2.22	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	341/347 (98%)	317 (93%)	24 (7%)	0	100	100
1	B	344/347 (99%)	326 (95%)	18 (5%)	0	100	100
All	All	685/694 (99%)	643 (94%)	42 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	296/300 (99%)	281 (95%)	15 (5%)	29	12
1	B	299/300 (100%)	285 (95%)	14 (5%)	32	14
All	All	595/600 (99%)	566 (95%)	29 (5%)	31	13

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

Mol	Chain	Res	Type
1	A	20	LYS
1	A	33	ARG
1	A	76	LEU
1	A	78	LYS
1	A	186	HIS
1	A	195	PHE
1	A	199	LYS
1	A	201	GLN
1	A	227	ASN
1	A	234	GLU
1	A	264	ASP
1	A	275	SER
1	A	286	LEU
1	A	294	LYS
1	A	339	LYS
1	B	20	LYS
1	B	65	VAL
1	B	78	LYS
1	B	182	SER
1	B	189	ARG
1	B	195	PHE
1	B	201	GLN
1	B	234	GLU
1	B	240	LYS
1	B	294	LYS
1	B	316	GLU
1	B	323	LYS
1	B	326	GLU
1	B	327	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	201	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	227	ASN
1	B	38	GLN
1	B	224	GLN
1	B	295	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GLA	A	1400	-	12,12,12	1.01	1 (8%)	17,17,17	1.19	2 (11%)
2	GLA	B	2400	-	12,12,12	0.79	0	17,17,17	1.23	1 (5%)

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	1400	-	-	0/2/22/22	0/1/1/1
2	GLA	B	2400	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1400	GLA	O5-C1	2.64	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1400	GLA	C4-C3-C2	-2.05	106.97	110.79
2	A	1400	GLA	O2-C2-C3	-2.03	105.76	110.34
2	B	2400	GLA	C3-C4-C5	-2.03	106.66	110.20

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	339/347 (97%)	-0.76	1 (0%) 94 92	12, 22, 54, 86	0
1	B	346/347 (99%)	-0.87	0 100 100	10, 19, 45, 60	0
All	All	685/694 (98%)	-0.82	1 (0%) 95 93	10, 20, 51, 86	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	3.9

### 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	NA	A	1401	1/1	0.85	0.13	5.45	34,34,34,34	0
2	GLA	B	2400	12/12	0.96	0.08	1.65	19,28,51,63	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLA	A	1400	12/12	0.94	0.08	1.15	21,27,48,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.