



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:17 PM BST

PDB ID : 5GJM
Title : Crystal structure of Lysine decarboxylase from Selenomonas ruminantium in C2 space group
Authors : Sagong, H.-Y.; Kim, K.-J.
Deposited on : 2016-07-01
Resolution : 2.91 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.2

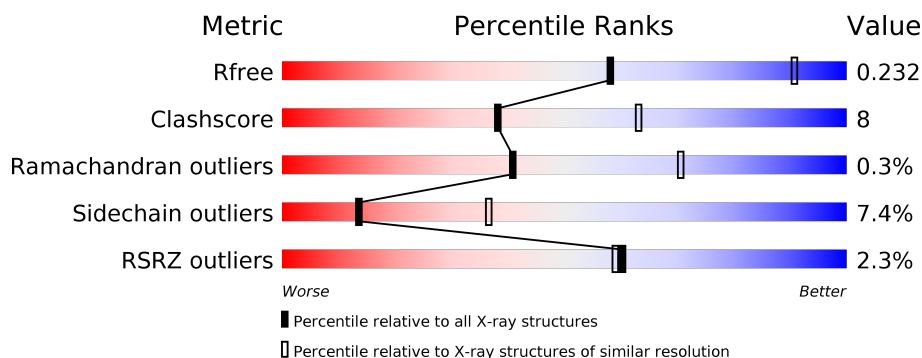
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 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	393	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	393	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 6%</div> </div> </div>

2 Entry composition [i](#)

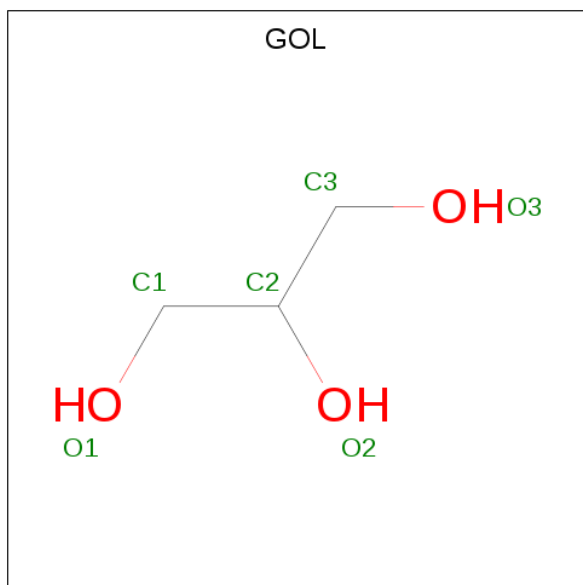
There are 3 unique types of molecules in this entry. The entry contains 5913 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysine/ornithine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2943	1877	495	552	19			
1	B	368	Total	C	N	O	S	0	0	0
			2842	1817	475	530	20			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		

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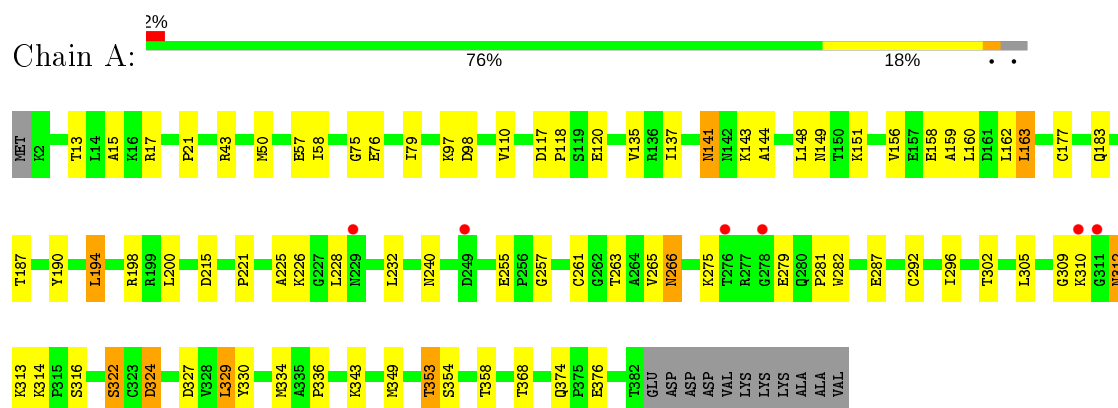
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	55	Total	O	0	0
			55	55		

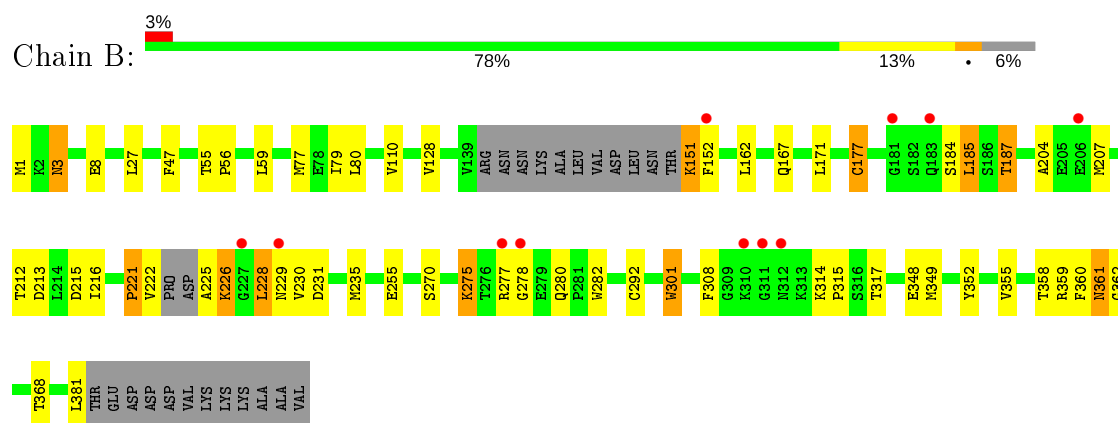
3 Residue-property plots [i](#)

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: Lysine/ornithine decarboxylase



• Molecule 1: Lysine/ornithine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.45Å 70.79Å 88.06Å 90.00° 101.03° 90.00°	Depositor
Resolution (Å)	50.00 – 2.91 24.62 – 2.91	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-2.91) 94.9 (24.62-2.91)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.15 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.177 , 0.234 0.177 , 0.232	Depositor DCC
R_{free} test set	930 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.802	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5913	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.71	0/3009	0.82	0/4076
1	B	0.71	0/2905	0.79	0/3929
All	All	0.71	0/5914	0.80	0/8005

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	ASN	Peptide
1	B	228	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2943	0	2911	48	0
1	B	2842	0	2812	44	0
2	A	6	0	8	3	0
3	A	67	0	0	1	0
3	B	55	0	0	1	0
All	All	5913	0	5731	87	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 8.

All (87) 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:187:THR:HG22	1:B:235:MET:HG3	1.20	1.19
1:B:187:THR:HG22	1:B:235:MET:CG	1.81	1.10
1:B:187:THR:CG2	1:B:235:MET:HG3	1.88	1.02
1:A:322:SER:HB2	1:A:327:ASP:OD2	1.70	0.90
1:B:77:MET:CE	1:B:110:VAL:HG21	2.01	0.90
1:A:275:LYS:HE3	1:B:152:PHE:CE1	2.11	0.86
1:A:329:LEU:O	2:A:401:GOL:O2	1.93	0.84
1:B:185:LEU:HD11	1:B:235:MET:CE	2.07	0.83
1:B:1:MET:O	1:B:226:LYS:HG3	1.85	0.77
1:B:185:LEU:HD11	1:B:235:MET:HE3	1.66	0.76
1:A:313:LYS:HB3	1:A:334:MET:HG3	1.68	0.75
1:A:312:ASN:O	1:A:313:LYS:HG3	1.87	0.74
1:A:75:GLY:O	1:A:79:ILE:HG13	1.88	0.74
1:B:1:MET:O	1:B:226:LYS:CG	2.36	0.73
1:B:280:GLN:NE2	1:B:317:THR:OG1	2.24	0.71
1:B:228:LEU:HG	1:B:229:ASN:H	1.56	0.69
1:B:185:LEU:HD11	1:B:235:MET:HE1	1.75	0.67
1:A:353:THR:HG22	1:A:354:SER:N	2.11	0.66
1:A:353:THR:HG22	1:A:354:SER:H	1.61	0.65
1:A:275:LYS:CE	1:B:152:PHE:CE1	2.80	0.64
1:B:77:MET:HE1	1:B:110:VAL:HG21	1.78	0.64
1:B:187:THR:HG22	1:B:235:MET:HG2	1.75	0.64
1:A:118:PRO:HD3	1:A:162:LEU:HD21	1.79	0.63
1:A:358:THR:HG22	1:B:358:THR:HG22	1.81	0.62
1:A:292:CYS:HB3	1:A:349:MET:HE3	1.81	0.62
1:A:141:ASN:ND2	1:A:143:LYS:HB2	2.15	0.62
1:A:160:LEU:HD13	1:A:200:LEU:HD22	1.82	0.62
1:A:177:CYS:HB3	1:A:215:ASP:HB3	1.83	0.61
1:B:8:GLU:HG3	1:B:308:PHE:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ALA:HB2	1:A:302:THR:HG22	1.84	0.59
1:A:305:LEU:HD22	1:A:330:TYR:CE2	2.38	0.59
1:B:47:PHE:O	1:B:255:GLU:HA	2.03	0.58
1:B:292:CYS:HB3	1:B:349:MET:HE1	1.85	0.58
1:B:177:CYS:HB3	1:B:215:ASP:HB3	1.85	0.57
1:B:79:ILE:HG23	3:B:454:HOH:O	2.04	0.57
1:A:292:CYS:HB3	1:A:349:MET:CE	2.35	0.57
1:A:143:LYS:O	1:A:144:ALA:HB3	2.06	0.56
1:B:1:MET:O	1:B:226:LYS:HG2	2.04	0.56
1:A:265:VAL:C	1:A:266:ASN:HD22	2.09	0.56
1:B:352:TYR:HA	1:B:355:VAL:CG2	2.36	0.55
1:A:57:GLU:OE1	1:A:57:GLU:N	2.32	0.55
1:B:230:VAL:HG22	1:B:231:ASP:N	2.22	0.55
1:B:204:ALA:O	1:B:207:MET:HB3	2.07	0.55
1:B:360:PHE:O	1:B:361:ASN:HB2	2.05	0.55
1:A:13:THR:OG1	1:A:376:GLU:OE2	2.17	0.53
1:A:183:GLN:OE1	1:A:221:PRO:HA	2.08	0.52
1:A:353:THR:CG2	1:A:354:SER:N	2.72	0.52
1:A:17:ARG:HH21	1:A:374:GLN:HE21	1.57	0.52
1:A:137:ILE:HD11	1:A:159:ALA:HB1	1.92	0.52
1:A:158:GLU:O	1:A:158:GLU:HG2	2.09	0.51
1:A:151:LYS:HG3	1:B:282:TRP:HZ3	1.73	0.51
1:A:177:CYS:HA	1:A:215:ASP:O	2.11	0.50
1:A:302:THR:HG23	2:A:401:GOL:H2	1.93	0.50
1:B:77:MET:HE3	1:B:110:VAL:HG21	1.91	0.50
1:B:167:GLN:HA	1:B:171:LEU:O	2.13	0.49
1:B:301:TRP:CZ3	1:B:348:GLU:OE1	2.65	0.49
3:A:537:HOH:O	1:B:278:GLY:HA3	2.12	0.48
1:A:177:CYS:CB	1:A:215:ASP:HB3	2.44	0.48
1:B:212:THR:HG23	1:B:213:ASP:OD1	2.14	0.47
1:A:76:GLU:HG3	1:B:362:GLY:HA3	1.95	0.47
1:A:312:ASN:HB3	1:A:336:PRO:HA	1.95	0.47
1:B:275:LYS:HB2	1:B:282:TRP:HB2	1.96	0.46
1:A:190:TYR:O	1:A:194:LEU:HB2	2.16	0.46
1:B:221:PRO:O	1:B:222:VAL:C	2.55	0.45
1:A:15:ALA:HB1	1:A:343:LYS:HE3	1.99	0.45
1:B:292:CYS:HB3	1:B:349:MET:CE	2.47	0.45
1:A:156:VAL:HG13	1:A:200:LEU:HD11	1.98	0.45
1:A:221:PRO:HB2	1:A:228:LEU:HD11	1.99	0.45
1:A:135:VAL:HB	1:A:163:LEU:HD13	1.99	0.44
1:B:151:LYS:HB3	1:B:152:PHE:H	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HD13	1:A:261:CYS:SG	2.57	0.44
1:B:301:TRP:HZ3	1:B:348:GLU:OE1	2.00	0.44
1:A:43:ARG:H	1:A:240:ASN:HD21	1.66	0.44
1:A:21:PRO:HG3	1:A:287:GLU:HG2	1.99	0.43
1:B:3:ASN:HB3	1:B:225:ALA:HB2	2.00	0.43
1:A:312:ASN:OD1	1:A:313:LYS:N	2.52	0.43
1:A:215:ASP:OD2	1:A:255:GLU:OE2	2.37	0.42
1:A:296:ILE:HG12	2:A:401:GOL:H11	2.01	0.42
1:A:322:SER:HB3	1:A:324:ASP:HB2	2.02	0.42
1:B:55:THR:HA	1:B:56:PRO:HD3	1.84	0.42
1:A:281:PRO:HD2	1:A:316:SER:HA	2.02	0.41
1:B:230:VAL:HG22	1:B:231:ASP:H	1.83	0.41
1:A:309:GLY:C	1:A:310:LYS:HG2	2.41	0.41
1:B:222:VAL:HB	1:B:225:ALA:O	2.21	0.41
1:B:280:GLN:HG3	1:B:315:PRO:O	2.21	0.41
1:B:151:LYS:HA	1:B:151:LYS:HD3	1.82	0.40
1:A:97:LYS:HD2	1:A:120:GLU:OE2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	379/393 (96%)	370 (98%)	8 (2%)	1 (0%)	41	70
1	B	362/393 (92%)	353 (98%)	8 (2%)	1 (0%)	41	70
All	All	741/786 (94%)	723 (98%)	16 (2%)	2 (0%)	41	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	GLY

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Mol	Chain	Res	Type
1	B	221	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/319 (97%)	286 (93%)	23 (7%)	13	36
1	B	297/319 (93%)	275 (93%)	22 (7%)	13	36
All	All	606/638 (95%)	561 (93%)	45 (7%)	13	36

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	MET
1	A	98	ASP
1	A	110	VAL
1	A	117	ASP
1	A	141	ASN
1	A	148	LEU
1	A	149	ASN
1	A	163	LEU
1	A	187	THR
1	A	194	LEU
1	A	198	ARG
1	A	226	LYS
1	A	232	LEU
1	A	263	THR
1	A	266	ASN
1	A	279	GLU
1	A	282	TRP
1	A	314	LYS
1	A	322	SER
1	A	324	ASP
1	A	329	LEU
1	A	353	THR

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Mol	Chain	Res	Type
1	A	368	THR
1	B	3	ASN
1	B	27	LEU
1	B	59	LEU
1	B	80	LEU
1	B	128	VAL
1	B	151	LYS
1	B	162	LEU
1	B	177	CYS
1	B	184	SER
1	B	185	LEU
1	B	187	THR
1	B	216	ILE
1	B	226	LYS
1	B	270	SER
1	B	275	LYS
1	B	277	ARG
1	B	301	TRP
1	B	314	LYS
1	B	359	ARG
1	B	361	ASN
1	B	368	THR
1	B	381	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	149	ASN
1	A	240	ASN
1	A	266	ASN
1	A	374	GLN
1	B	240	ASN
1	B	280	GLN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	401	-	5,5,5	0.77	0	5,5,5	1.51	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	401	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GOL	C3-C2-C1	2.19	120.22	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3
2	A	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	381/393 (96%)	-0.37	6 (1%) 72 71	6, 21, 40, 63	0
1	B	368/393 (93%)	-0.41	11 (2%) 50 46	7, 17, 46, 74	0
All	All	749/786 (95%)	-0.39	17 (2%) 60 59	6, 19, 44, 74	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	GLY	3.9
1	A	276	THR	3.3
1	B	310	LYS	3.0
1	B	181	GLY	2.9
1	B	183	GLN	2.9
1	B	311	GLY	2.8
1	B	152	PHE	2.8
1	A	310	LYS	2.7
1	B	229	ASN	2.7
1	A	249	ASP	2.6
1	B	312	ASN	2.6
1	A	311	GLY	2.5
1	B	278	GLY	2.3
1	B	206	GLU	2.3
1	A	229	ASN	2.3
1	B	227	GLY	2.1
1	B	277	ARG	2.0

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 [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
2	GOL	A	401	6/6	0.87	0.38	35,38,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.