



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 04:08 am BST

PDB ID : 2ZJG  
Title : Crystal structural of mouse kynurenine aminotransferase III  
Authors : Han, Q.; Cai, T.; Tagle, D.A.; Robinson, H.; Li, J.  
Deposited on : 2008-03-07  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

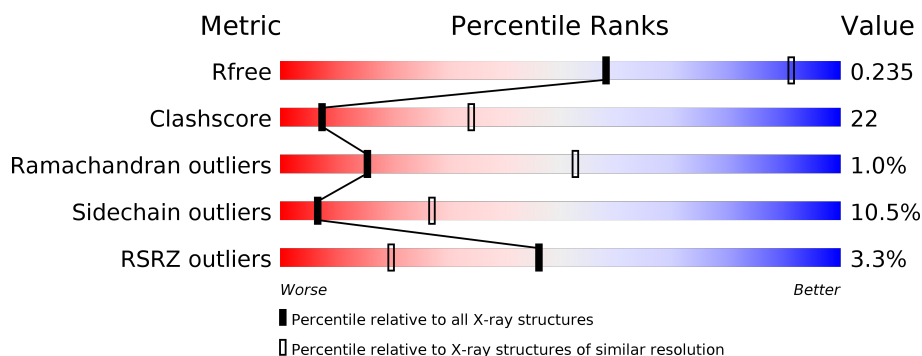
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	410	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>6%</div> </div> </div>
1	B	410	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>30%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	500	-	-	X	-
2	GOL	A	501	-	-	X	-
2	GOL	B	503	-	X	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6694 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 Kynurenine-oxoglutarate transaminase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	P	S	0	0	0
			3268	2108	537	604	1	18			
1	B	410	Total	C	N	O	P	S	0	0	0
			3268	2108	537	604	1	18			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

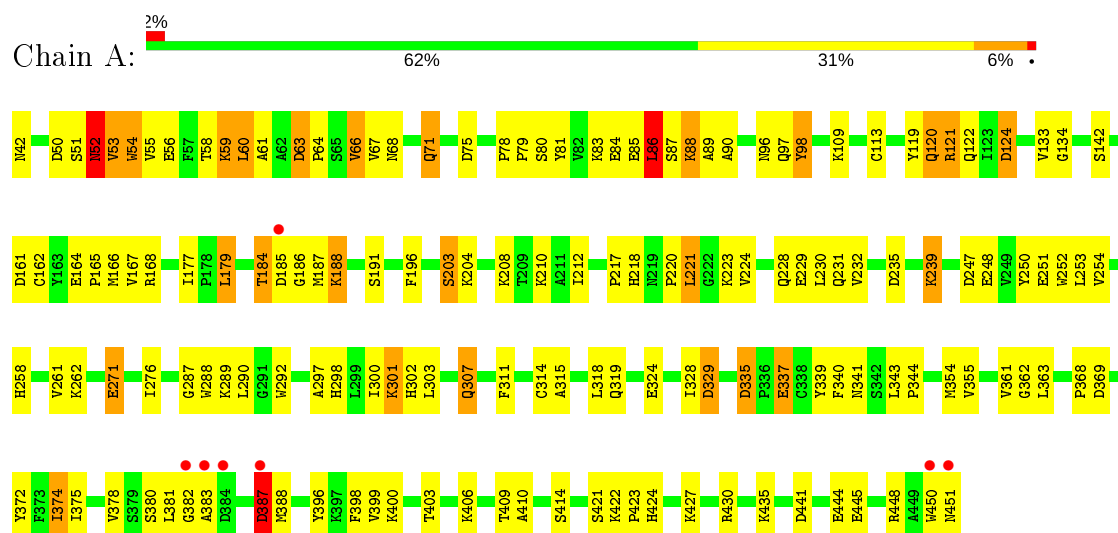
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	60	Total	O	0	0
			60	60		

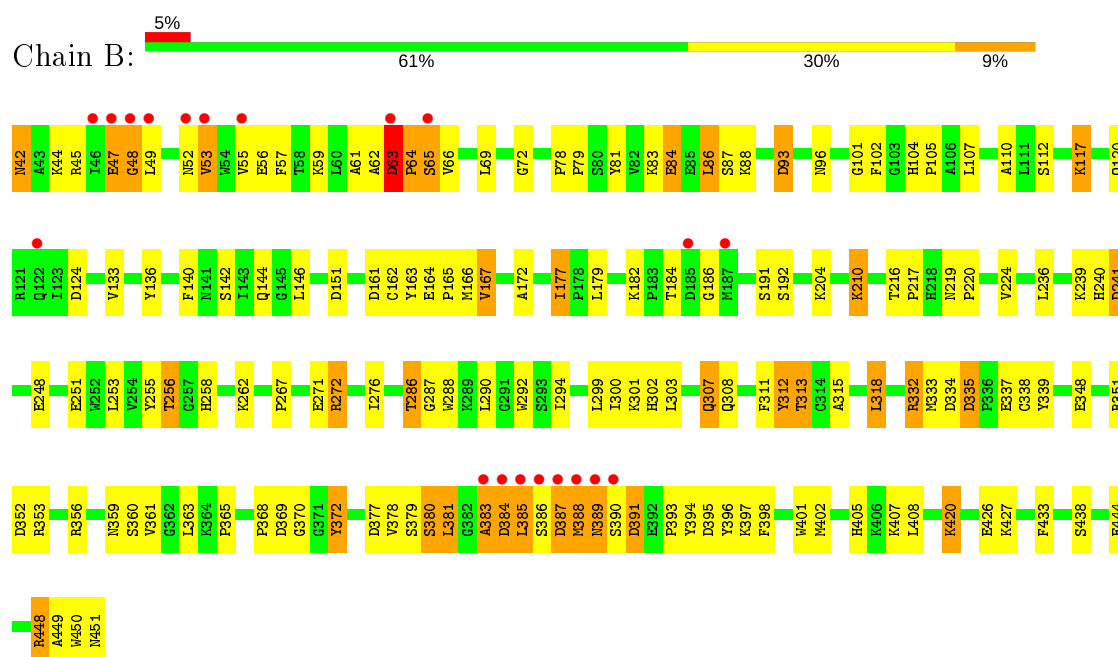
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Kynurenine-oxoglutarate transaminase 3



- Molecule 1: Kynurenine-oxoglutarate transaminase 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.09 Å 91.09 Å 233.05 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 3.00 29.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.58-3.00) 97.3 (29.58-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 3.00 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.222 , 0.233 0.223 , 0.235	Depositor DCC
$R_{free}$ test set	999 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6694	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, 0.333 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: GOL, LLP

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	1.15	3/3331 (0.1%)	0.97	7/4525 (0.2%)
1	B	1.13	2/3331 (0.1%)	0.98	9/4525 (0.2%)
All	All	1.14	5/6662 (0.1%)	0.98	16/9050 (0.2%)

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	1	5
1	B	1	9
All	All	2	14

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	PHE	CE2-CZ	5.31	1.47	1.37
1	A	314	CYS	CB-SG	-5.29	1.73	1.81
1	A	251	GLU	CG-CD	5.19	1.59	1.51
1	B	110	ALA	CA-CB	-5.17	1.41	1.52
1	A	98	TYR	CD2-CE2	5.06	1.47	1.39

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	GLY	N-CA-C	-5.72	98.80	113.10
1	B	335	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	356	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	377	ASP	CB-CG-OD2	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ASP	CB-CG-OD2	5.36	123.12	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	256	THR	CB
1	B	286	THR	CB

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	GLY	Peptide
1	A	289	LYS	Peptide
1	A	362	GLY	Peptide
1	A	388	MET	Peptide
1	A	52	ASN	Peptide

## 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	3268	0	3235	154	0
1	B	3268	0	3235	169	0
2	A	24	0	32	9	0
2	B	30	0	40	3	0
3	A	44	0	0	0	0
3	B	60	0	0	8	0
All	All	6694	0	6542	292	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 22.

The worst 5 of 292 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:387:ASP:OD1	1:B:388:MET:HG3	1.12	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:VAL:HG13	1:B:407:LYS:O	1.43	1.19
1:A:88:LYS:HB3	1:A:88:LYS:NZ	1.55	1.12
1:B:334:ASP:HB3	3:B:524:HOH:O	1.48	1.12
1:B:448:ARG:HH11	1:B:448:ARG:HG3	0.97	1.10

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	407/410 (99%)	371 (91%)	32 (8%)	4 (1%)	15	53
1	B	407/410 (99%)	369 (91%)	34 (8%)	4 (1%)	15	53
All	All	814/820 (99%)	740 (91%)	66 (8%)	8 (1%)	15	53

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	PRO
1	B	65	SER
1	B	312	TYR
1	A	86	LEU
1	A	203	SER

### 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	357/357 (100%)	315 (88%)	42 (12%)	5	22
1	B	357/357 (100%)	324 (91%)	33 (9%)	9	34
All	All	714/714 (100%)	639 (90%)	75 (10%)	7	27

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	TYR
1	A	451	ASN
1	B	385	LEU
1	A	374	ILE
1	A	427	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	451	ASN
1	B	42	ASN
1	B	240	HIS
1	A	341	ASN
1	A	405	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	LLP	B	281	1	23,24,25	2.06	9 (39%)	25,32,34	2.13	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	A	281	1	23,24,25	1.94	4 (17%)	25,32,34	1.82	7 (28%)

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
1	LLP	B	281	1	-	8/16/17/19	0/1/1/1
1	LLP	A	281	1	-	8/16/17/19	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	LLP	O3-C3	-5.74	1.23	1.37
1	B	281	LLP	O3-C3	-4.13	1.27	1.37
1	A	281	LLP	C3-C2	-3.26	1.37	1.40
1	B	281	LLP	P-OP3	-3.20	1.42	1.54
1	B	281	LLP	CE-NZ	3.19	1.53	1.46

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	LLP	OP4-C5'-C5	4.93	118.75	109.35
1	B	281	LLP	C4-C4'-NZ	-4.86	101.99	124.31
1	B	281	LLP	C4-C3-C2	-4.78	117.23	120.19
1	A	281	LLP	OP4-C5'-C5	4.08	117.13	109.35
1	A	281	LLP	C3-C4-C5	3.55	120.98	118.26

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	281	LLP	C5'-OP4-P-OP1
1	B	281	LLP	C5'-OP4-P-OP2
1	B	281	LLP	C5'-OP4-P-OP3
1	A	281	LLP	C5'-OP4-P-OP2
1	A	281	LLP	C5'-OP4-P-OP3

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GOL	A	500	-	5,5,5	0.87	0	5,5,5	2.46	4 (80%)
2	GOL	B	502	-	5,5,5	0.46	0	5,5,5	0.50	0
2	GOL	B	501	-	5,5,5	0.59	0	5,5,5	0.51	0
2	GOL	A	501	-	5,5,5	0.36	0	5,5,5	1.06	0
2	GOL	A	502	-	5,5,5	0.52	0	5,5,5	0.25	0
2	GOL	B	500	-	5,5,5	0.53	0	5,5,5	0.85	0
2	GOL	B	504	-	5,5,5	0.39	0	5,5,5	0.31	0
2	GOL	B	503	-	5,5,5	0.68	0	5,5,5	2.08	4 (80%)
2	GOL	A	503	-	5,5,5	0.48	0	5,5,5	0.69	0

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	500	-	-	0/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	B	501	-	-	3/4/4/4	-
2	GOL	A	501	-	-	1/4/4/4	-
2	GOL	A	502	-	-	2/4/4/4	-
2	GOL	B	500	-	-	2/4/4/4	-
2	GOL	B	504	-	-	2/4/4/4	-
2	GOL	B	503	-	-	2/4/4/4	-
2	GOL	A	503	-	-	1/4/4/4	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	GOL	C3-C2-C1	-3.30	98.87	111.70
2	A	500	GOL	O3-C3-C2	-2.80	96.78	110.20
2	A	500	GOL	O2-C2-C1	-2.71	97.21	109.12
2	B	503	GOL	C3-C2-C1	-2.43	102.26	111.70
2	B	503	GOL	O2-C2-C3	2.28	119.18	109.12

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	GOL	O1-C1-C2-C3
2	A	502	GOL	O1-C1-C2-O2
2	A	502	GOL	O1-C1-C2-C3
2	B	500	GOL	O1-C1-C2-C3
2	B	504	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	GOL	5	0
2	B	502	GOL	2	0
2	B	501	GOL	1	0
2	A	501	GOL	5	0
2	A	502	GOL	1	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 [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	409/410 (99%)	-0.24	7 (1%) 70 41	12, 25, 56, 76	0
1	B	409/410 (99%)	-0.16	20 (4%) 29 11	13, 28, 66, 80	0
All	All	818/820 (99%)	-0.20	27 (3%) 46 20	12, 26, 58, 80	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	387	ASP	5.1
1	B	386	SER	4.9
1	B	389	ASN	4.3
1	B	384	ASP	4.0
1	B	385	LEU	3.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	A	281	24/25	0.96	0.23	17,24,31,32	0
1	LLP	B	281	24/25	0.97	0.22	19,23,29,31	0

### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	B	504	6/6	0.48	0.31	88,90,90,91	0
2	GOL	A	503	6/6	0.55	0.36	75,75,77,77	0
2	GOL	B	500	6/6	0.59	0.27	57,66,67,69	0
2	GOL	B	502	6/6	0.75	0.40	49,55,57,58	0
2	GOL	B	501	6/6	0.81	0.27	55,57,58,59	0
2	GOL	A	502	6/6	0.85	0.27	37,48,53,54	0
2	GOL	A	501	6/6	0.87	0.25	43,48,49,51	0
2	GOL	B	503	6/6	0.96	0.29	38,40,46,52	0
2	GOL	A	500	6/6	0.96	0.19	17,20,23,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.