



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:37 AM UTC

PDB ID : 8TC7 / pdb\_00008tc7  
Title : Human asparaginyl-tRNA synthetase, apo form  
Authors : Dogovski, C.; Metcalfe, R.D.; Xie, S.C.; Morton, C.J.; Tilley, L.; Griffin, M.D.W.  
Deposited on : 2023-06-30  
Resolution : 1.90 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.

The types of validation reports are described at

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

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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

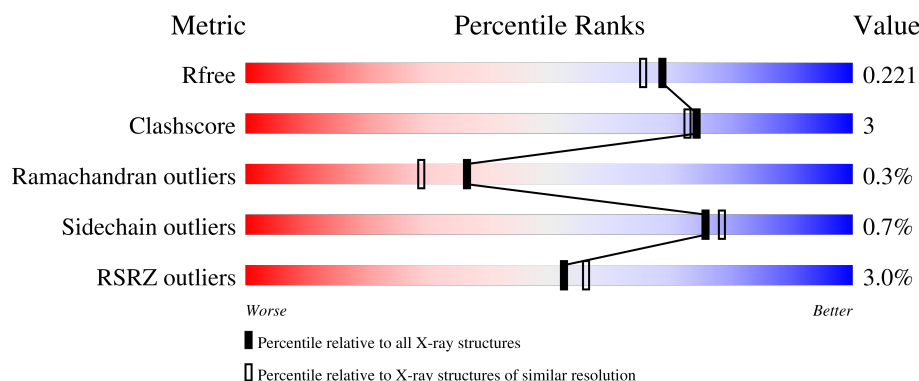
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

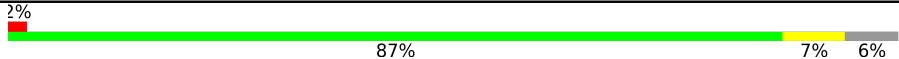



The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 of 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	453	
1	B	453	
1	C	453	
1	D	453	

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	B	609	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15123 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 Asparagine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	2	0
			3471	2215	593	637	26			
1	B	429	Total	C	N	O	S	0	2	0
			3488	2224	597	641	26			
1	C	428	Total	C	N	O	S	0	0	0
			3464	2210	590	638	26			
1	D	428	Total	C	N	O	S	0	0	0
			3461	2207	591	637	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLY	-	expression tag	UNP O43776
A	97	MET	-	expression tag	UNP O43776
B	96	GLY	-	expression tag	UNP O43776
B	97	MET	-	expression tag	UNP O43776
C	96	GLY	-	expression tag	UNP O43776
C	97	MET	-	expression tag	UNP O43776
D	96	GLY	-	expression tag	UNP O43776
D	97	MET	-	expression tag	UNP O43776

- Molecule 2 is GLYCEROL (CCD ID: 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		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	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		
2	B	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 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

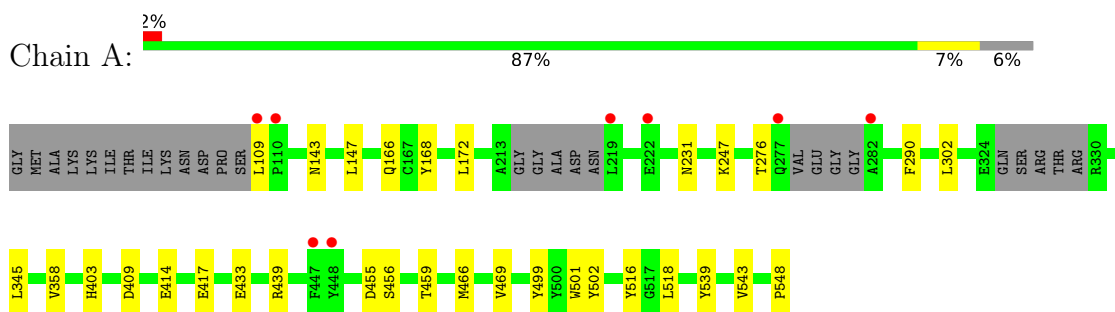
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	288	Total O 288 288	0	0
4	B	329	Total O 329 329	0	0
4	C	229	Total O 229 229	0	0
4	D	259	Total O 259 259	0	0

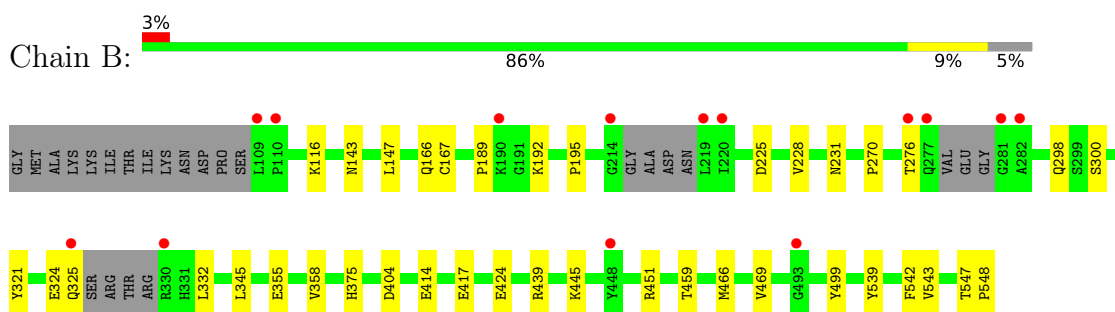
### 3 Residue-property plots [i](#)

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.

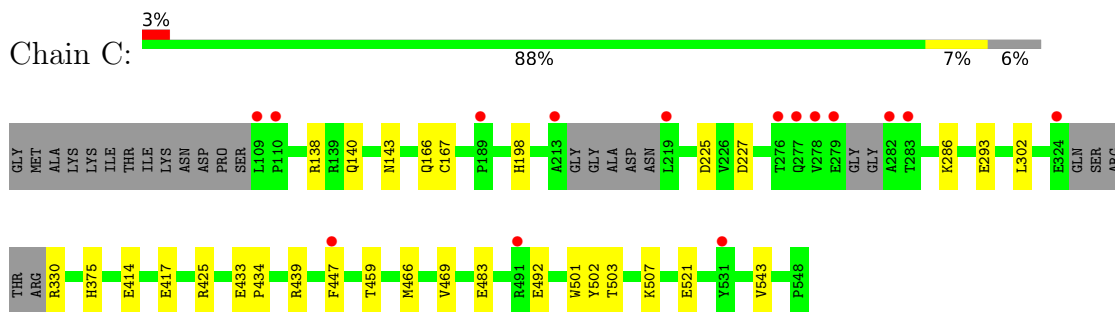
- Molecule 1: Asparagine-tRNA ligase, cytoplasmic



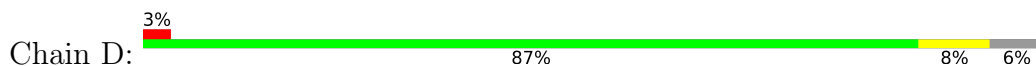
- Molecule 1: Asparagine-tRNA ligase, cytoplasmic

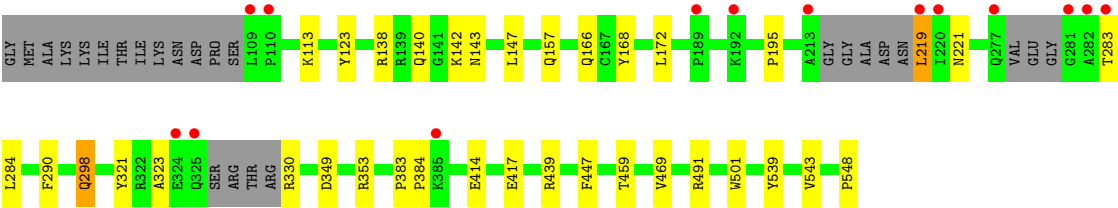


- Molecule 1: Asparagine-tRNA ligase, cytoplasmic



- Molecule 1: Asparagine-tRNA ligase, cytoplasmic







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.49Å 127.19Å 163.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.58 – 1.90 46.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.58-1.90) 99.8 (46.58-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.180 , 0.217 0.186 , 0.221	Depositor DCC
$R_{free}$ test set	9081 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7501e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CL, 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	0.55	0/3555	0.67	0/4810
1	B	0.56	0/3572	0.68	0/4832
1	C	0.49	0/3547	0.63	0/4800
1	D	0.53	0/3544	0.64	1/4795 (0.0%)
All	All	0.54	0/14218	0.65	1/19237 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	298	GLN	CA-CB-CG	-5.55	103.00	114.10

There are no chirality outliers.

There are no planarity outliers.

### 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	3471	0	3399	23	0
1	B	3488	0	3413	26	0
1	C	3464	0	3394	19	0
1	D	3461	0	3390	19	1
2	A	42	0	54	5	1
2	B	54	0	70	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	18	0	23	1	0
2	D	18	0	24	1	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
4	A	288	0	0	7	0
4	B	329	0	0	12	0
4	C	229	0	0	7	0
4	D	259	0	0	1	0
All	All	15123	0	13767	85	1

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 3.

The worst 5 of 85 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)
3:B:610:CL:CL	4:B:968:HOH:O	2.32	0.84
1:B:167:CYS:SG	4:B:1012:HOH:O	2.39	0.81
1:C:483:GLU:OE2	4:C:701:HOH:O	2.00	0.77
1:B:375:HIS:ND1	4:B:705:HOH:O	2.18	0.75
1:B:231:ASN:HB3	2:B:603:GOL:H32	1.70	0.72

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:LYS:NZ	2:A:607:GOL:O1[2_455]	2.13	0.07

## 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	420/453 (93%)	410 (98%)	9 (2%)	1 (0%)	43	36
1	B	423/453 (93%)	414 (98%)	7 (2%)	2 (0%)	24	16
1	C	420/453 (93%)	414 (99%)	5 (1%)	1 (0%)	43	36
1	D	420/453 (93%)	410 (98%)	9 (2%)	1 (0%)	43	36
All	All	1683/1812 (93%)	1648 (98%)	30 (2%)	5 (0%)	36	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	324	GLU
1	A	469	VAL
1	C	469	VAL
1	D	469	VAL
1	B	469	VAL

### 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	380/398 (96%)	377 (99%)	3 (1%)	73	75
1	B	381/398 (96%)	377 (99%)	4 (1%)	68	70
1	C	380/398 (96%)	379 (100%)	1 (0%)	86	88
1	D	379/398 (95%)	376 (99%)	3 (1%)	73	75
All	All	1520/1592 (96%)	1509 (99%)	11 (1%)	76	78

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	198	HIS
1	D	147	LEU
1	D	330	ARG
1	D	219	LEU
1	B	325	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	143	ASN
1	D	166	GLN
1	D	532	HIS
1	A	375	HIS
1	A	229	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](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	GOL	A	603	-	5,5,5	1.44	1 (20%)	5,5,5	0.89	0
2	GOL	B	606	-	5,5,5	1.69	1 (20%)	5,5,5	1.00	0
2	GOL	B	601	-	5,5,5	1.07	0	5,5,5	1.68	2 (40%)
2	GOL	D	601	-	5,5,5	0.86	0	5,5,5	1.68	2 (40%)
2	GOL	A	606	-	5,5,5	2.61	2 (40%)	5,5,5	1.21	0
2	GOL	B	603	-	5,5,5	1.19	0	5,5,5	1.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	605	-	5,5,5	1.04	0	5,5,5	1.07	0
2	GOL	B	602	-	5,5,5	1.19	1 (20%)	5,5,5	1.56	1 (20%)
2	GOL	B	605	-	5,5,5	1.02	0	5,5,5	1.05	1 (20%)
2	GOL	A	602	-	5,5,5	1.45	1 (20%)	5,5,5	0.90	0
2	GOL	A	607	-	5,5,5	1.11	1 (20%)	5,5,5	1.32	1 (20%)
2	GOL	B	609	-	5,5,5	1.33	1 (20%)	5,5,5	1.13	1 (20%)
2	GOL	C	601	-	5,5,5	1.02	0	5,5,5	0.84	0
2	GOL	B	604	-	5,5,5	1.34	1 (20%)	5,5,5	1.09	0
2	GOL	A	601	-	5,5,5	0.67	0	5,5,5	1.48	1 (20%)
2	GOL	D	603	-	5,5,5	1.24	0	5,5,5	0.83	0
2	GOL	C	603	-	5,5,5	1.85	2 (40%)	5,5,5	2.15	2 (40%)
2	GOL	B	608	-	5,5,5	1.21	0	5,5,5	0.81	0
2	GOL	D	602	-	5,5,5	1.34	1 (20%)	5,5,5	1.40	1 (20%)
2	GOL	C	602	-	5,5,5	0.83	0	5,5,5	1.10	0
2	GOL	A	604	-	5,5,5	0.75	0	5,5,5	1.20	0
2	GOL	B	607	-	5,5,5	0.65	0	5,5,5	1.17	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	603	-	-	2/4/4/4	-
2	GOL	B	606	-	-	3/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	D	601	-	-	0/4/4/4	-
2	GOL	A	606	-	-	2/4/4/4	-
2	GOL	B	603	-	-	2/4/4/4	-
2	GOL	A	605	-	-	0/4/4/4	-
2	GOL	B	602	-	-	0/4/4/4	-
2	GOL	B	605	-	-	2/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	A	607	-	-	0/4/4/4	-
2	GOL	B	609	-	-	4/4/4/4	-
2	GOL	C	601	-	-	0/4/4/4	-
2	GOL	B	604	-	-	1/4/4/4	-
2	GOL	A	601	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	603	-	-	0/4/4/4	-
2	GOL	C	603	-	-	0/4/4/4	-
2	GOL	B	608	-	-	2/4/4/4	-
2	GOL	D	602	-	-	2/4/4/4	-
2	GOL	C	602	-	-	0/4/4/4	-
2	GOL	A	604	-	-	0/4/4/4	-
2	GOL	B	607	-	-	1/4/4/4	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	GOL	O3-C3	4.45	1.61	1.42
2	A	606	GOL	C3-C2	3.42	1.64	1.51
2	B	606	GOL	C1-C2	3.38	1.64	1.51
2	C	603	GOL	O3-C3	-2.81	1.30	1.42
2	A	602	GOL	O2-C2	-2.77	1.35	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	GOL	C3-C2-C1	-3.99	97.15	111.80
2	B	602	GOL	C3-C2-C1	-2.69	101.93	111.80
2	D	602	GOL	C3-C2-C1	-2.58	102.33	111.80
2	B	601	GOL	O1-C1-C2	-2.42	99.47	110.38
2	A	601	GOL	O2-C2-C3	2.40	119.14	109.18

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-O2
2	A	603	GOL	C1-C2-C3-O3
2	B	601	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-C3
2	B	605	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	603	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	GOL	1	0
2	B	605	GOL	1	0
2	A	602	GOL	2	0
2	A	607	GOL	1	1
2	A	601	GOL	1	0
2	D	603	GOL	1	0
2	C	603	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	426/453 (94%)	-0.11	8 (1%) 66 70	18, 38, 72, 105	2 (0%)
1	B	429/453 (94%)	-0.16	14 (3%) 49 52	20, 37, 77, 118	2 (0%)
1	C	428/453 (94%)	-0.04	15 (3%) 47 50	24, 43, 89, 117	0
1	D	428/453 (94%)	-0.05	14 (3%) 49 52	25, 41, 89, 128	0
All	All	1711/1812 (94%)	-0.09	51 (2%) 52 56	18, 39, 81, 128	4 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	6.0
1	B	219	LEU	5.8
1	C	278	VAL	4.9
1	D	189	PRO	4.3
1	D	282	ALA	4.2

### 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, 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( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	606	6/6	0.66	0.17	60,67,73,74	0
2	GOL	B	603	6/6	0.80	0.15	63,68,74,78	0
2	GOL	A	607	6/6	0.83	0.13	65,67,71,73	0
2	GOL	C	603	6/6	0.83	0.15	38,41,45,54	0
2	GOL	A	606	6/6	0.85	0.15	36,37,46,52	0
2	GOL	D	601	6/6	0.85	0.13	43,54,57,62	0
2	GOL	B	604	6/6	0.86	0.12	50,58,62,73	0
2	GOL	A	605	6/6	0.86	0.17	47,65,67,81	0
2	GOL	B	609	6/6	0.87	0.13	35,44,50,60	0
2	GOL	C	601	6/6	0.87	0.11	48,53,54,74	0
2	GOL	B	601	6/6	0.89	0.11	44,52,58,60	0
3	CL	C	604	1/1	0.89	0.10	83,83,83,83	0
2	GOL	B	607	6/6	0.90	0.11	47,54,58,73	0
2	GOL	A	604	6/6	0.90	0.10	47,49,61,64	0
2	GOL	B	605	6/6	0.91	0.12	59,65,66,74	0
2	GOL	B	608	6/6	0.91	0.11	40,61,65,72	0
2	GOL	D	602	6/6	0.91	0.10	41,51,61,67	0
2	GOL	C	602	6/6	0.91	0.10	47,51,55,57	0
2	GOL	A	601	6/6	0.92	0.09	35,42,44,48	0
2	GOL	D	603	6/6	0.93	0.09	35,44,51,52	0
3	CL	B	610	1/1	0.93	0.10	70,70,70,70	0
2	GOL	B	602	6/6	0.93	0.08	36,40,45,45	0
2	GOL	A	603	6/6	0.94	0.08	43,49,52,53	0
2	GOL	A	602	6/6	0.94	0.10	45,48,61,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.