



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 08:36 AM UTC

PDB ID : 2QLR / pdb\_00002qlr  
Title : Crystal structure of human kynurenine aminotransferase II  
Authors : Han, Q.; Robinson, R.; Li, J.  
Deposited on : 2007-07-13  
Resolution : 2.30 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

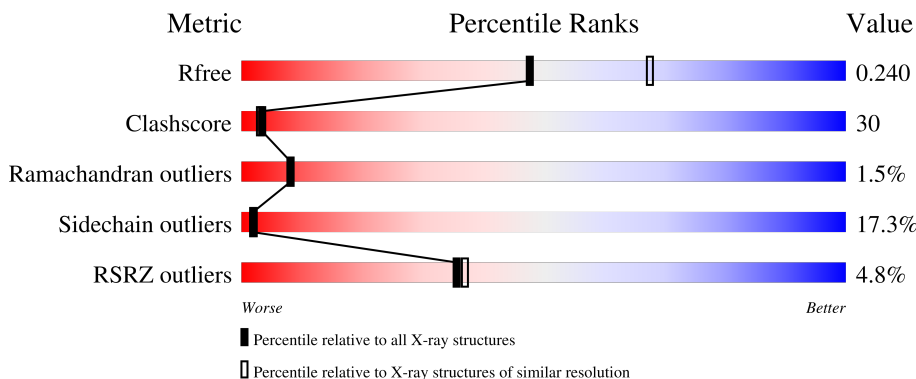
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	425	 5% (poor fit), 48% (0 outliers), 36% (1 outlier), 10% (2 outliers), 6% (3+ outliers)
1	B	425	 4% (poor fit), 44% (0 outliers), 39% (1 outlier), 15% (2 outliers), 0% (3+ outliers)
1	C	425	 4% (poor fit), 45% (0 outliers), 40% (1 outlier), 12% (2 outliers), 0% (3+ outliers)
1	D	425	 5% (poor fit), 42% (0 outliers), 40% (1 outlier), 15% (2 outliers), 0% (3+ outliers)

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	D	427	-	-	X	-
2	GOL	D	428	-	-	X	-
2	GOL	D	429	-	X	X	-

## 2 Entry composition [i](#)

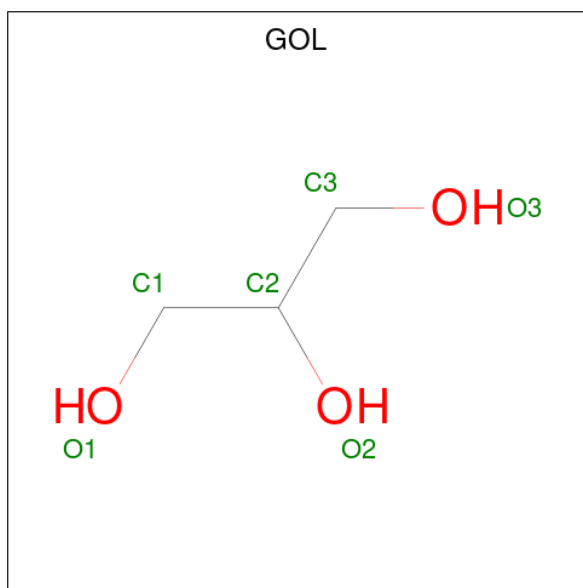
There are 3 unique types of molecules in this entry. The entry contains 14176 atoms, of which 0 are hydrogens and 0 are deuteriums.

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/alpha-aminoadipate aminotransferase mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	425	Total 3347	C 2147	N 560	O 621	P 1	S 18	0	0	0
1	B	425	Total 3348	C 2147	N 560	O 622	P 1	S 18	0	0	0
1	C	425	Total 3347	C 2147	N 560	O 621	P 1	S 18	0	0	0
1	D	425	Total 3348	C 2147	N 560	O 622	P 1	S 18	0	0	0

- 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
			Total	C	O		
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0

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

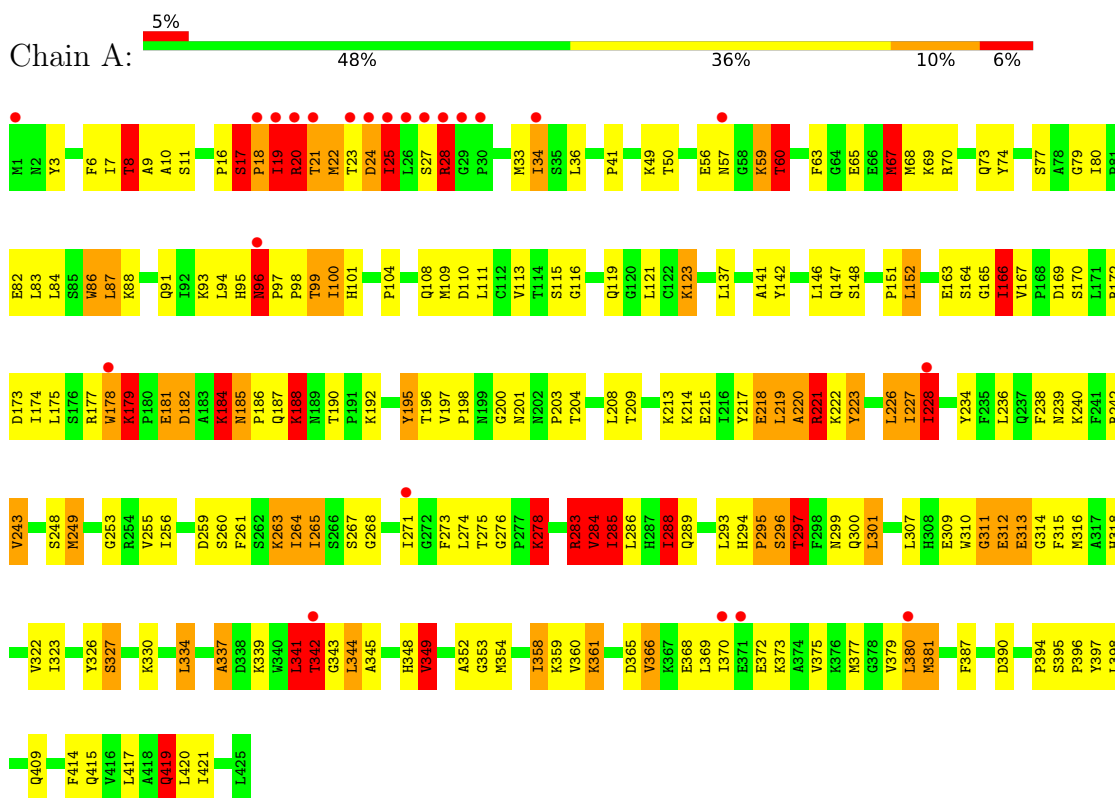
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total 166	O 166	0	0
3	B	199	Total 199	O 199	0	0
3	C	166	Total 166	O 166	0	0
3	D	183	Total 183	O 183	0	0

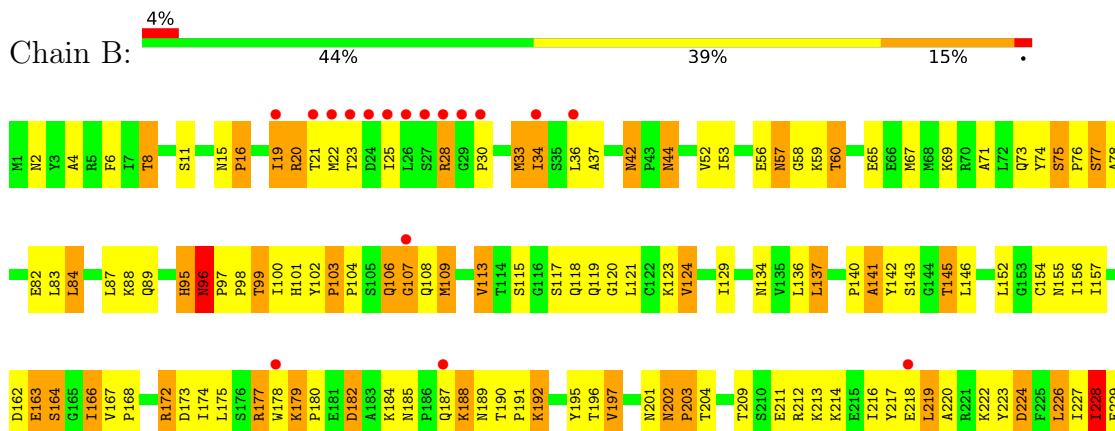
### 3 Residue-property plots [i](#)

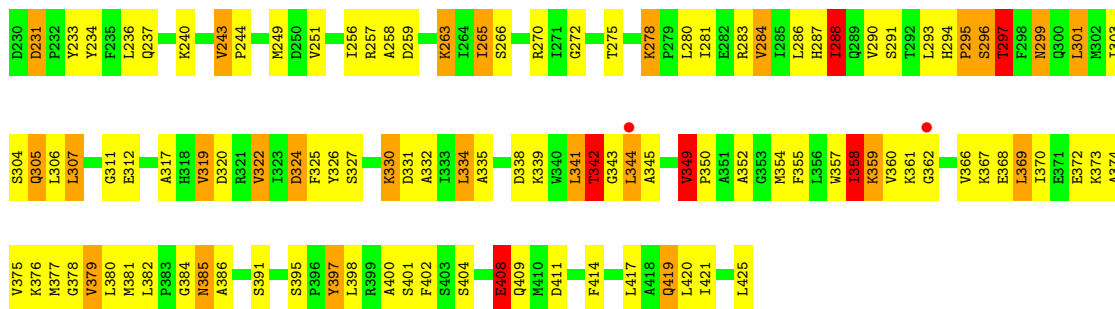
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

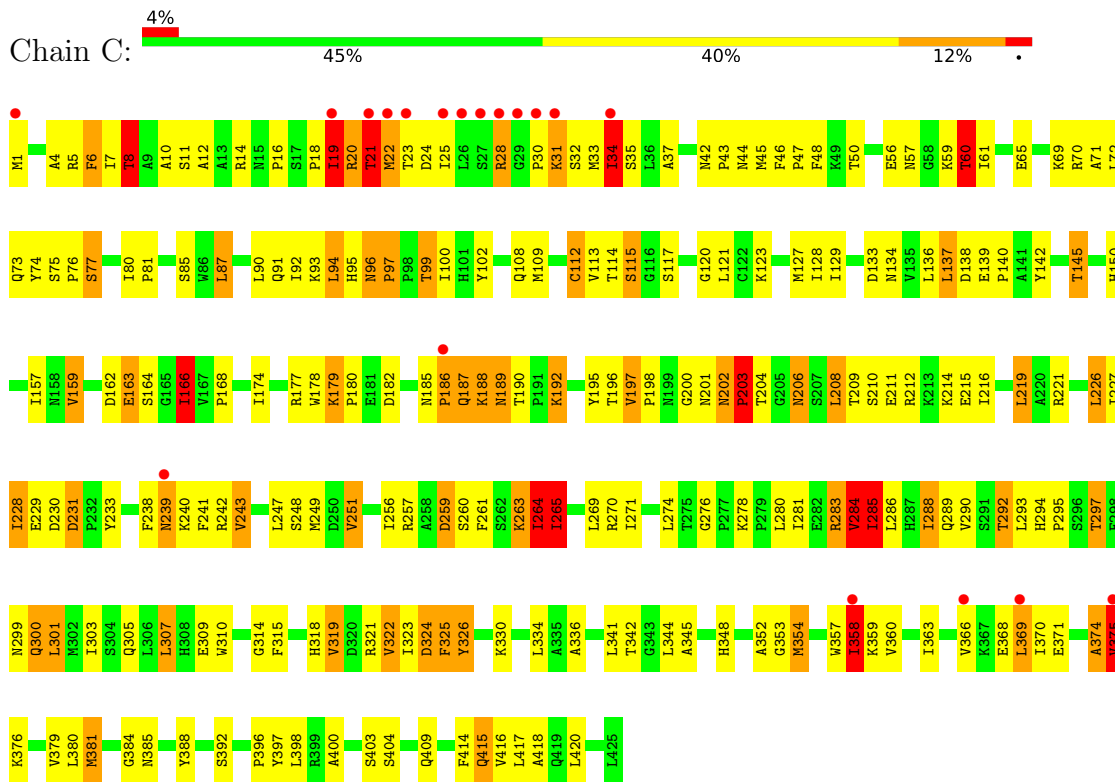


- Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

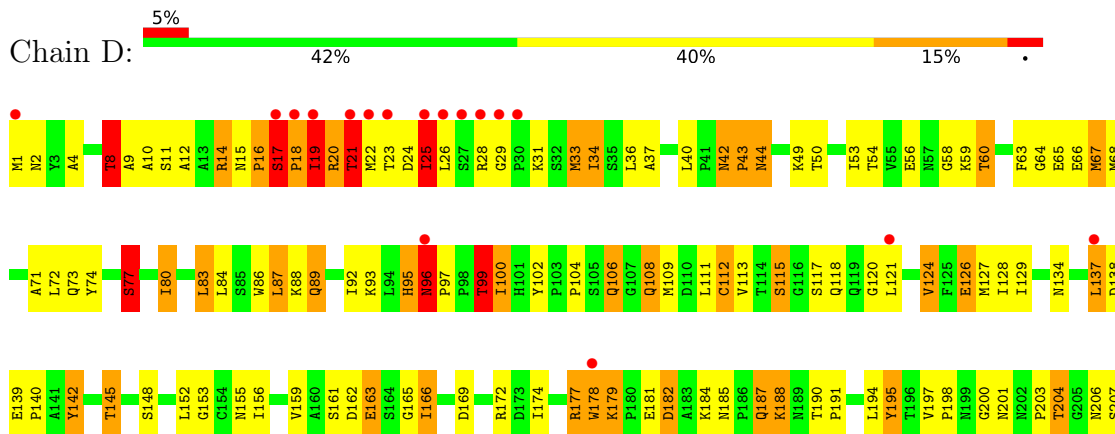


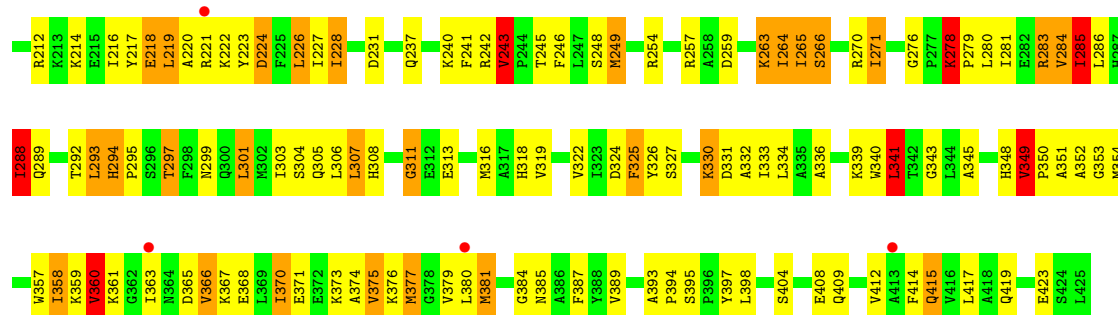


• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial



• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.50Å 70.97Å 121.13Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	30.11 – 2.30 30.11 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.11-2.30) 96.3 (30.11-2.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.242 , 0.256 0.226 , 0.240	Depositor DCC
$R_{free}$ test set	3883 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.56$ , $\langle L^2 \rangle = 0.40$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.65 % 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 5.4387e-05. 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: 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	1.59	29/3404 (0.9%)	1.62	66/4620 (1.4%)
1	B	1.65	36/3405 (1.1%)	1.60	68/4620 (1.5%)
1	C	1.63	30/3404 (0.9%)	1.62	51/4620 (1.1%)
1	D	1.67	42/3405 (1.2%)	1.63	70/4620 (1.5%)
All	All	1.63	137/13618 (1.0%)	1.62	255/18480 (1.4%)

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	5
1	B	0	4
1	C	0	5
1	D	1	4
All	All	1	18

The worst 5 of 137 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ILE	CA-CB	9.93	1.66	1.54
1	D	12	ALA	CA-CB	9.89	1.69	1.53
1	D	288	ILE	CA-CB	9.69	1.66	1.54
1	D	96	ASN	CA-CB	9.29	1.60	1.52
1	C	34	ILE	CA-CB	8.73	1.64	1.54

The worst 5 of 255 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	ILE	N-CA-C	11.58	121.28	111.90
1	D	227	ILE	CA-C-N	-10.88	108.97	123.12
1	D	227	ILE	C-N-CA	-10.88	108.97	123.12
1	D	128	ILE	N-CA-C	10.76	120.61	111.90
1	C	22	MET	N-CA-C	-9.93	100.45	111.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	188	LYS	CA

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	SER	Peptide
1	A	188	LYS	Peptide
1	A	19	ILE	Peptide
1	A	341	LEU	Peptide
1	A	342	THR	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	3347	0	3357	214	0
1	B	3348	0	3356	213	0
1	C	3347	0	3357	212	0
1	D	3348	0	3357	212	0
2	A	12	0	16	1	0
2	B	6	0	8	0	0
2	C	30	0	40	7	0
2	D	24	0	32	24	0
3	A	166	0	0	24	0
3	B	199	0	0	27	0
3	C	166	0	0	17	0
3	D	183	0	0	34	0
All	All	14176	0	13523	809	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 30.

The worst 5 of 809 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:D:137:LEU:C	1:D:137:LEU:HD23	1.61	1.25
1:D:60:THR:HG22	3:D:555:HOH:O	1.38	1.22
1:D:182:ASP:HB2	3:D:568:HOH:O	1.40	1.22
1:C:166:ILE:HD11	1:C:216:ILE:CD1	1.71	1.18
1:C:166:ILE:HD11	1:C:216:ILE:HD11	1.24	1.16

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	422/425 (99%)	381 (90%)	33 (8%)	8 (2%)	6 5
1	B	422/425 (99%)	391 (93%)	26 (6%)	5 (1%)	10 12
1	C	422/425 (99%)	393 (93%)	24 (6%)	5 (1%)	10 12
1	D	422/425 (99%)	381 (90%)	33 (8%)	8 (2%)	6 5
All	All	1688/1700 (99%)	1546 (92%)	116 (7%)	26 (2%)	8 8

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	28	ARG
1	B	203	PRO
1	C	203	PRO
1	D	19	ILE

### 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	369/369 (100%)	310 (84%)	59 (16%)	2	2
1	B	369/369 (100%)	308 (84%)	61 (16%)	2	2
1	C	369/369 (100%)	304 (82%)	65 (18%)	2	2
1	D	369/369 (100%)	299 (81%)	70 (19%)	1	1
All	All	1476/1476 (100%)	1221 (83%)	255 (17%)	2	2

5 of 255 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	376	LYS
1	D	221	ARG
1	C	159	VAL
1	D	218	GLU
1	D	327	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	57	ASN
1	D	385	ASN
1	D	106	GLN
1	D	239	ASN
1	B	118	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](#)

4 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	A	263	1	23,24,25	1.70	5 (21%)	25,32,34	1.85	7 (28%)
1	LLP	C	263	1	23,24,25	2.04	7 (30%)	25,32,34	1.96	7 (28%)
1	LLP	D	263	1	23,24,25	1.84	5 (21%)	25,32,34	2.04	9 (36%)
1	LLP	B	263	1	23,24,25	2.26	7 (30%)	25,32,34	1.81	9 (36%)

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	A	263	1	-	3/16/17/19	0/1/1/1
1	LLP	C	263	1	-	5/16/17/19	0/1/1/1
1	LLP	D	263	1	-	5/16/17/19	0/1/1/1
1	LLP	B	263	1	-	6/16/17/19	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	LLP	O3-C3	-6.25	1.22	1.36
1	B	263	LLP	CE-NZ	5.28	1.58	1.46
1	D	263	LLP	O3-C3	-4.73	1.26	1.36
1	A	263	LLP	O3-C3	-4.73	1.26	1.36
1	B	263	LLP	C4-C4'	4.33	1.55	1.46

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	LLP	OP2-P-OP4	-4.55	94.80	106.67
1	C	263	LLP	CE-NZ-C4'	-4.49	104.33	118.72
1	D	263	LLP	C5'-C5-C6	-4.34	112.29	119.36
1	D	263	LLP	CD-CE-NZ	4.12	121.74	110.83
1	D	263	LLP	C4-C4'-NZ	-4.02	105.48	124.04

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	263	LLP	N-CA-CB-CG
1	B	263	LLP	C-CA-CB-CG
1	C	263	LLP	C5-C4-C4'-NZ
1	C	263	LLP	CG-CD-CE-NZ
1	C	263	LLP	C4-C4'-NZ-CE

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	263	LLP	5	0
1	C	263	LLP	1	0
1	D	263	LLP	1	0
1	B	263	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	D	426	-	5,5,5	0.75	0	5,5,5	1.05	0
2	GOL	C	429	-	5,5,5	0.54	0	5,5,5	0.54	0
2	GOL	D	427	-	5,5,5	0.40	0	5,5,5	0.58	0
2	GOL	C	427	-	5,5,5	0.58	0	5,5,5	1.13	0
2	GOL	C	426	-	5,5,5	0.54	0	5,5,5	0.67	0
2	GOL	C	428	-	5,5,5	0.57	0	5,5,5	1.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	C	430	-	5,5,5	0.65	0	5,5,5	0.85	0
2	GOL	D	429	-	5,5,5	1.15	0	5,5,5	2.32	3 (60%)
2	GOL	A	426	-	5,5,5	0.32	0	5,5,5	0.95	0
2	GOL	D	428	-	5,5,5	0.96	0	5,5,5	1.72	1 (20%)
2	GOL	A	427	-	5,5,5	0.39	0	5,5,5	0.60	0
2	GOL	B	426	-	5,5,5	0.53	0	5,5,5	1.06	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 Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	426	-	-	4/4/4/4	-
2	GOL	C	429	-	-	2/4/4/4	-
2	GOL	D	427	-	-	2/4/4/4	-
2	GOL	C	427	-	-	2/4/4/4	-
2	GOL	C	426	-	-	2/4/4/4	-
2	GOL	C	428	-	-	4/4/4/4	-
2	GOL	C	430	-	-	4/4/4/4	-
2	GOL	D	429	-	-	3/4/4/4	-
2	GOL	A	426	-	-	2/4/4/4	-
2	GOL	D	428	-	-	3/4/4/4	-
2	GOL	A	427	-	-	4/4/4/4	-
2	GOL	B	426	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	429	GOL	O1-C1-C2	3.49	126.09	110.38
2	D	429	GOL	O2-C2-C3	-3.00	96.75	109.18
2	D	428	GOL	O3-C3-C2	2.57	121.97	110.38
2	D	429	GOL	O3-C3-C2	2.38	121.10	110.38

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	426	GOL	O2-C2-C3-O3
2	C	426	GOL	C1-C2-C3-O3
2	C	426	GOL	O2-C2-C3-O3
2	C	427	GOL	C1-C2-C3-O3
2	C	428	GOL	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	427	GOL	4	0
2	C	427	GOL	2	0
2	C	428	GOL	2	0
2	C	430	GOL	3	0
2	D	429	GOL	11	0
2	A	426	GOL	1	0
2	D	428	GOL	9	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	424/425 (99%)	0.38	23 (5%) 31 33	24, 36, 54, 78	0
1	B	424/425 (99%)	0.33	19 (4%) 38 40	23, 34, 51, 92	0
1	C	424/425 (99%)	0.32	19 (4%) 38 40	23, 35, 52, 77	0
1	D	424/425 (99%)	0.36	21 (4%) 34 35	23, 35, 52, 84	0
All	All	1696/1700 (99%)	0.35	82 (4%) 35 37	23, 35, 53, 92	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	ILE	6.4
1	C	29	GLY	6.3
1	A	25	ILE	5.4
1	B	25	ILE	5.1
1	B	26	LEU	4.7

### 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	C	263	24/25	0.95	0.07	27,30,34,37	0
1	LLP	D	263	24/25	0.95	0.09	23,32,35,35	0
1	LLP	A	263	24/25	0.96	0.07	23,33,36,36	0
1	LLP	B	263	24/25	0.96	0.07	23,30,33,34	0

### 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(Å <sup>2</sup> )	Q<0.9
2	GOL	C	430	6/6	0.64	0.18	48,53,56,57	0
2	GOL	C	429	6/6	0.66	0.16	63,66,68,69	0
2	GOL	D	427	6/6	0.68	0.17	55,56,59,62	0
2	GOL	A	426	6/6	0.69	0.19	68,70,71,72	0
2	GOL	C	426	6/6	0.76	0.16	59,64,65,65	0
2	GOL	D	429	6/6	0.76	0.33	23,30,40,43	0
2	GOL	D	428	6/6	0.77	0.22	46,51,52,53	0
2	GOL	B	426	6/6	0.79	0.15	63,64,66,66	0
2	GOL	C	428	6/6	0.80	0.17	54,56,58,60	0
2	GOL	D	426	6/6	0.81	0.14	44,52,55,59	0
2	GOL	C	427	6/6	0.85	0.13	34,47,53,54	0
2	GOL	A	427	6/6	0.88	0.10	58,61,62,63	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.