



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:53 pm BST

PDB ID : 5ELN  
Title : Crystal Structure of Lysyl-tRNA Synthetase from *Cryptosporidium parvum* complexed with L-lysine  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2015-11-04  
Resolution : 1.90 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

<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

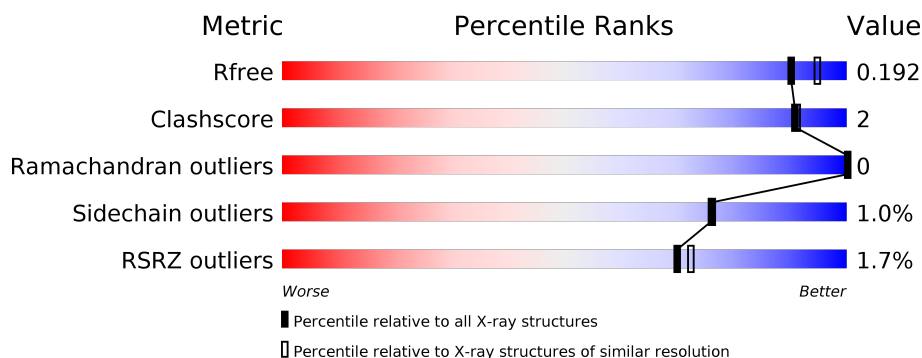
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	535	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 88%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>88%</span> <span>5%</span> <span>6%</span> </div> </div>
1	B	535	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 89%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>3%</span> <span>89%</span> <span>•</span> <span>6%</span> </div> </div>
1	C	535	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 88%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>88%</span> <span>5%</span> <span>7%</span> </div> </div>
1	D	535	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>89%</span> <span>•</span> <span>7%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18253 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-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	12	0
			4090	2627	677	758	28			
1	B	501	Total	C	N	O	S	0	14	0
			4062	2617	671	746	28			
1	C	497	Total	C	N	O	S	0	14	0
			4066	2617	673	747	29			
1	D	496	Total	C	N	O	S	0	6	0
			3996	2561	664	743	28			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP Q5CR27
A	26	ALA	-	expression tag	UNP Q5CR27
A	27	HIS	-	expression tag	UNP Q5CR27
A	28	HIS	-	expression tag	UNP Q5CR27
A	29	HIS	-	expression tag	UNP Q5CR27
A	30	HIS	-	expression tag	UNP Q5CR27
A	31	HIS	-	expression tag	UNP Q5CR27
A	32	HIS	-	expression tag	UNP Q5CR27
A	33	MET	-	expression tag	UNP Q5CR27
A	34	GLY	-	expression tag	UNP Q5CR27
A	35	THR	-	expression tag	UNP Q5CR27
A	36	LEU	-	expression tag	UNP Q5CR27
A	37	GLU	-	expression tag	UNP Q5CR27
A	38	ALA	-	expression tag	UNP Q5CR27
A	39	GLN	-	expression tag	UNP Q5CR27
A	40	THR	-	expression tag	UNP Q5CR27
A	41	GLN	-	expression tag	UNP Q5CR27
A	42	GLY	-	expression tag	UNP Q5CR27
A	43	PRO	-	expression tag	UNP Q5CR27
A	44	GLY	-	expression tag	UNP Q5CR27
A	45	SER	-	expression tag	UNP Q5CR27

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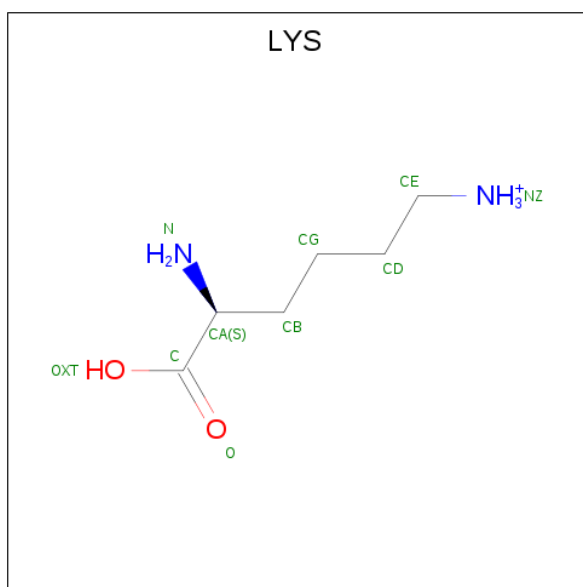
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	MET	-	initiating methionine	UNP Q5CR27
B	26	ALA	-	expression tag	UNP Q5CR27
B	27	HIS	-	expression tag	UNP Q5CR27
B	28	HIS	-	expression tag	UNP Q5CR27
B	29	HIS	-	expression tag	UNP Q5CR27
B	30	HIS	-	expression tag	UNP Q5CR27
B	31	HIS	-	expression tag	UNP Q5CR27
B	32	HIS	-	expression tag	UNP Q5CR27
B	33	MET	-	expression tag	UNP Q5CR27
B	34	GLY	-	expression tag	UNP Q5CR27
B	35	THR	-	expression tag	UNP Q5CR27
B	36	LEU	-	expression tag	UNP Q5CR27
B	37	GLU	-	expression tag	UNP Q5CR27
B	38	ALA	-	expression tag	UNP Q5CR27
B	39	GLN	-	expression tag	UNP Q5CR27
B	40	THR	-	expression tag	UNP Q5CR27
B	41	GLN	-	expression tag	UNP Q5CR27
B	42	GLY	-	expression tag	UNP Q5CR27
B	43	PRO	-	expression tag	UNP Q5CR27
B	44	GLY	-	expression tag	UNP Q5CR27
B	45	SER	-	expression tag	UNP Q5CR27
C	25	MET	-	initiating methionine	UNP Q5CR27
C	26	ALA	-	expression tag	UNP Q5CR27
C	27	HIS	-	expression tag	UNP Q5CR27
C	28	HIS	-	expression tag	UNP Q5CR27
C	29	HIS	-	expression tag	UNP Q5CR27
C	30	HIS	-	expression tag	UNP Q5CR27
C	31	HIS	-	expression tag	UNP Q5CR27
C	32	HIS	-	expression tag	UNP Q5CR27
C	33	MET	-	expression tag	UNP Q5CR27
C	34	GLY	-	expression tag	UNP Q5CR27
C	35	THR	-	expression tag	UNP Q5CR27
C	36	LEU	-	expression tag	UNP Q5CR27
C	37	GLU	-	expression tag	UNP Q5CR27
C	38	ALA	-	expression tag	UNP Q5CR27
C	39	GLN	-	expression tag	UNP Q5CR27
C	40	THR	-	expression tag	UNP Q5CR27
C	41	GLN	-	expression tag	UNP Q5CR27
C	42	GLY	-	expression tag	UNP Q5CR27
C	43	PRO	-	expression tag	UNP Q5CR27
C	44	GLY	-	expression tag	UNP Q5CR27
C	45	SER	-	expression tag	UNP Q5CR27

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Chain	Residue	Modelled	Actual	Comment	Reference
D	25	MET	-	initiating methionine	UNP Q5CR27
D	26	ALA	-	expression tag	UNP Q5CR27
D	27	HIS	-	expression tag	UNP Q5CR27
D	28	HIS	-	expression tag	UNP Q5CR27
D	29	HIS	-	expression tag	UNP Q5CR27
D	30	HIS	-	expression tag	UNP Q5CR27
D	31	HIS	-	expression tag	UNP Q5CR27
D	32	HIS	-	expression tag	UNP Q5CR27
D	33	MET	-	expression tag	UNP Q5CR27
D	34	GLY	-	expression tag	UNP Q5CR27
D	35	THR	-	expression tag	UNP Q5CR27
D	36	LEU	-	expression tag	UNP Q5CR27
D	37	GLU	-	expression tag	UNP Q5CR27
D	38	ALA	-	expression tag	UNP Q5CR27
D	39	GLN	-	expression tag	UNP Q5CR27
D	40	THR	-	expression tag	UNP Q5CR27
D	41	GLN	-	expression tag	UNP Q5CR27
D	42	GLY	-	expression tag	UNP Q5CR27
D	43	PRO	-	expression tag	UNP Q5CR27
D	44	GLY	-	expression tag	UNP Q5CR27
D	45	SER	-	expression tag	UNP Q5CR27

- Molecule 2 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	6	2	2		
2	C	1	Total	C	N	O	0	0
			10	6	2	2		
2	D	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

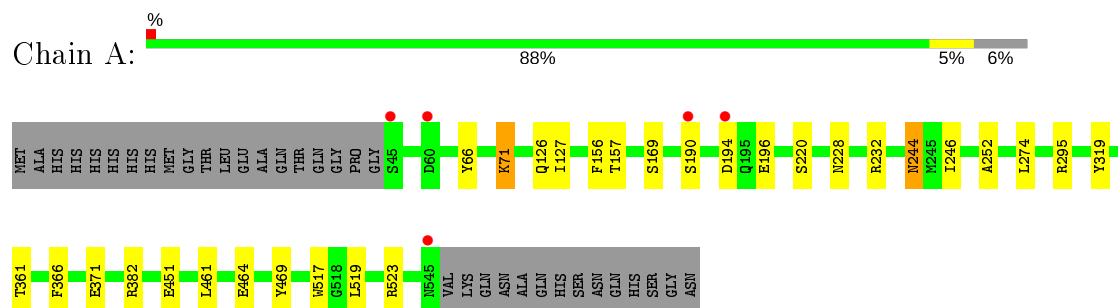
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	458	Total	O	0	3
			461	461		
5	B	441	Total	O	0	5
			446	446		
5	C	540	Total	O	0	3
			543	543		
5	D	503	Total	O	0	4
			507	507		

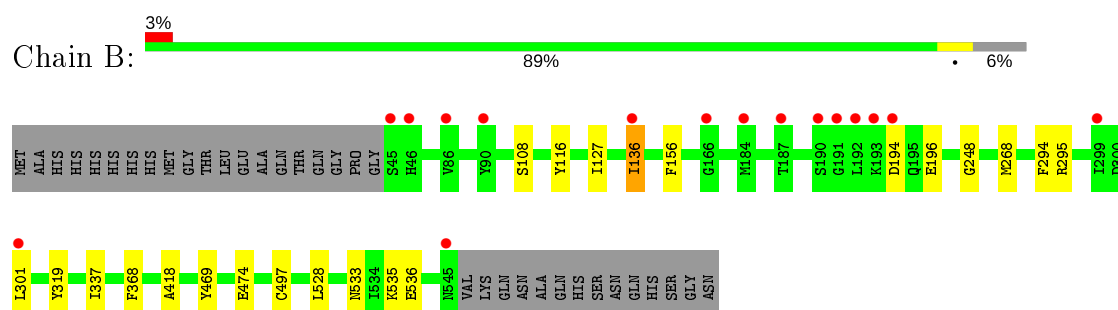
### 3 Residue-property plots [i](#)

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.

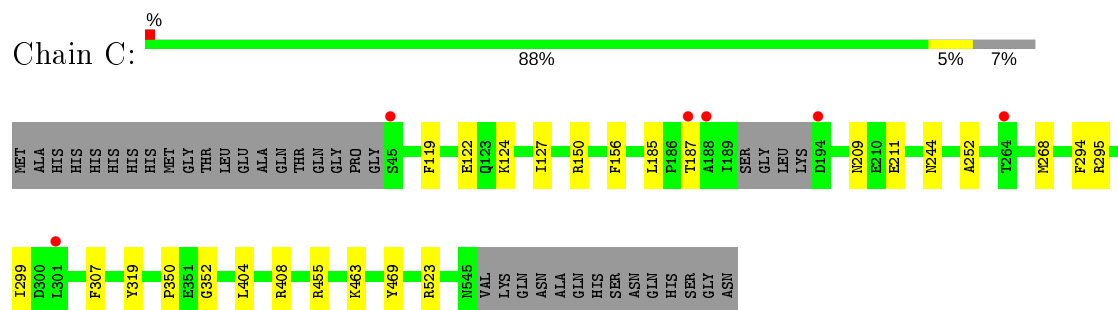
#### • Molecule 1: Lysine-tRNA ligase



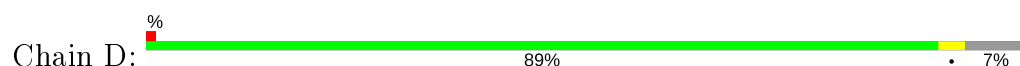
#### • Molecule 1: Lysine-tRNA ligase



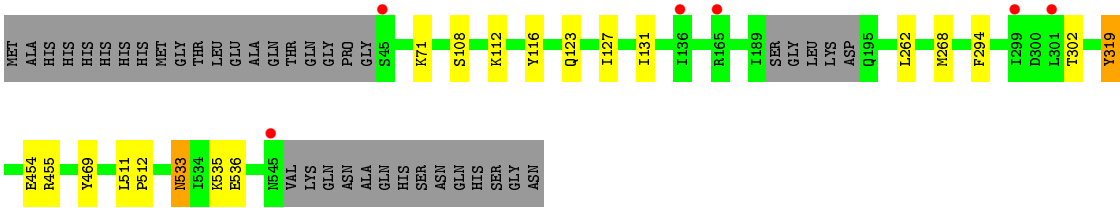
#### • Molecule 1: Lysine-tRNA ligase



#### • Molecule 1: Lysine-tRNA ligase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.92Å 119.45Å 143.63Å 90.00° 90.31° 90.00°	Depositor
Resolution (Å)	19.98 – 1.90 19.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.98-1.90) 99.7 (19.98-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 1.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.154 , 0.192 0.154 , 0.192	Depositor DCC
$R_{free}$ test set	9618 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.106 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18253	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 3.58% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO

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	0.41	0/4216	0.55	0/5689
1	B	0.39	0/4200	0.55	0/5678
1	C	0.44	0/4203	0.58	0/5672
1	D	0.42	0/4106	0.57	0/5545
All	All	0.41	0/16725	0.56	0/22584

There are no bond length outliers.

There are no bond angle outliers.

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	4090	0	4064	16	0
1	B	4062	0	4013	14	0
1	C	4066	0	4051	14	0
1	D	3996	0	3905	13	0
2	A	10	0	12	0	0
2	B	10	0	12	0	0
2	C	10	0	12	0	0
2	D	10	0	12	0	0
3	A	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	18	0	0
3	C	8	0	12	0	0
3	D	4	0	6	0	0
4	C	6	0	8	0	0
5	A	461	0	0	3	0
5	B	446	0	0	0	0
5	C	543	0	0	1	0
5	D	507	0	0	3	0
All	All	18253	0	16143	55	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 2.

All (55) 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:112:LYS:HD2	1:D:131:ILE:HG21	1.64	0.79
1:B:136:ILE:H	1:B:136:ILE:HD13	1.47	0.79
1:D:533[A]:ASN:HD22	1:D:536:GLU:HG2	1.49	0.78
1:C:150:ARG:NH2	1:C:185:LEU:O	2.21	0.72
1:A:361:THR:OG1	5:A:801:HOH:O	2.08	0.71
1:D:533[A]:ASN:HD21	1:D:535:LYS:HB2	1.61	0.66
1:B:301:LEU:O	1:B:533[B]:ASN:ND2	2.38	0.57
1:C:295[A]:ARG:HD2	1:C:307:PHE:CE1	2.41	0.55
1:C:463:LYS:HG2	1:C:523[A]:ARG:CZ	2.37	0.55
1:B:116:TYR:HB2	1:B:127:ILE:HB	1.90	0.52
1:B:533[B]:ASN:HD21	1:B:535:LYS:HG3	1.73	0.52
1:C:295[A]:ARG:HD2	1:C:307:PHE:HE1	1.74	0.51
1:C:124:LYS:HG2	5:C:1152:HOH:O	2.11	0.51
1:B:136:ILE:H	1:B:136:ILE:CD1	2.20	0.50
1:D:533[A]:ASN:ND2	1:D:536:GLU:HG2	2.22	0.50
1:C:127:ILE:HG21	1:C:156:PHE:CD1	2.47	0.50
1:A:244:ASN:HB2	1:A:246:ILE:O	2.12	0.49
1:A:382:ARG:HD2	1:A:451:GLU:OE2	2.12	0.49
1:C:350:PRO:C	1:C:352:GLY:H	2.15	0.49
1:B:337[B]:ILE:HD12	1:B:528:LEU:HD13	1.95	0.49
1:C:252:ALA:HB1	1:C:295[A]:ARG:HG2	1.95	0.49
1:A:366:PHE:HB3	1:A:371:GLU:HG3	1.95	0.49
1:B:194:ASP:OD2	1:B:196:GLU:HB2	2.12	0.49
1:D:268:MET:HE1	1:D:294:PHE:CD1	2.49	0.47
1:A:66:TYR:CE2	1:B:474:GLU:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:MET:HE1	1:C:294:PHE:CD1	2.50	0.47
1:B:533[A]:ASN:OD1	1:B:536:GLU:HG2	2.15	0.47
1:A:126:GLN:O	1:A:169:SER:HA	2.14	0.46
1:D:302:THR:HB	5:D:1168:HOH:O	2.16	0.46
1:C:299:ILE:HD12	1:D:262:LEU:HD11	1.98	0.46
1:A:228:ASN:O	1:A:232:ARG:HG2	2.15	0.46
1:A:71[A]:LYS:HE2	1:A:71[A]:LYS:HA	1.97	0.46
1:A:127:ILE:HG21	1:A:156:PHE:CD1	2.51	0.45
1:D:71:LYS:NZ	5:D:817:HOH:O	2.49	0.44
1:A:194:ASP:OD1	1:A:196:GLU:HB2	2.17	0.44
1:A:157[B]:THR:HG23	5:A:881:HOH:O	2.18	0.43
1:A:517:TRP:CH2	1:A:519:LEU:HB2	2.54	0.43
1:B:268:MET:HE1	1:B:294:PHE:CD1	2.53	0.43
1:D:116:TYR:HB2	1:D:127:ILE:HB	1.99	0.43
1:D:123:GLN:NE2	5:D:803:HOH:O	2.29	0.43
1:D:319:TYR:CD1	1:D:454:GLU:HB3	2.53	0.43
1:A:190:SER:HB2	5:A:1146:HOH:O	2.19	0.42
1:B:301:LEU:O	1:B:533[A]:ASN:HB2	2.19	0.42
1:C:209:ASN:HD21	1:C:211:GLU:HB2	1.84	0.42
1:D:511:LEU:HD12	1:D:512:PRO:HD2	2.00	0.42
1:C:455:ARG:HA	1:C:469:TYR:HB3	2.02	0.42
1:A:252:ALA:HB2	1:A:295:ARG:NH1	2.35	0.41
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.91	0.41
1:A:464:GLU:HB3	1:A:523[B]:ARG:HH11	1.85	0.41
1:B:368:PHE:CZ	1:B:418:ALA:HB2	2.56	0.41
1:C:404:LEU:HD13	1:C:408:ARG:CZ	2.50	0.41
1:B:127:ILE:HG21	1:B:156:PHE:CD1	2.55	0.41
1:B:248:GLY:HA2	1:B:497:CYS:SG	2.61	0.41
1:C:119:PHE:CZ	1:C:122:GLU:HA	2.55	0.41
1:D:455:ARG:HA	1:D:469:TYR:HB3	2.04	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	511/535 (96%)	500 (98%)	11 (2%)	0	100	100
1	B	513/535 (96%)	504 (98%)	9 (2%)	0	100	100
1	C	507/535 (95%)	496 (98%)	11 (2%)	0	100	100
1	D	498/535 (93%)	484 (97%)	14 (3%)	0	100	100
All	All	2029/2140 (95%)	1984 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	450/471 (96%)	443 (98%)	7 (2%)	62	60
1	B	440/471 (93%)	434 (99%)	6 (1%)	67	65
1	C	447/471 (95%)	444 (99%)	3 (1%)	84	84
1	D	432/471 (92%)	428 (99%)	4 (1%)	78	79
All	All	1769/1884 (94%)	1749 (99%)	20 (1%)	76	73

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71[A]	LYS
1	A	71[B]	LYS
1	A	220	SER
1	A	244	ASN
1	A	274	LEU
1	A	319	TYR
1	A	469	TYR
1	B	108	SER
1	B	136	ILE
1	B	295[A]	ARG

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Mol	Chain	Res	Type
1	B	295[B]	ARG
1	B	319	TYR
1	B	469	TYR
1	C	187	THR
1	C	244	ASN
1	C	319	TYR
1	D	108	SER
1	D	319	TYR
1	D	533[A]	ASN
1	D	533[B]	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	265	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

14 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
3	EDO	B	604	-	3,3,3	0.53	0	2,2,2	0.37	0
4	GOL	C	604	-	5,5,5	0.33	0	5,5,5	0.62	0
3	EDO	C	603	-	3,3,3	0.57	0	2,2,2	0.20	0
3	EDO	A	604	-	3,3,3	0.44	0	2,2,2	0.45	0
3	EDO	B	603	-	3,3,3	0.44	0	2,2,2	0.40	0
3	EDO	D	602	-	3,3,3	0.60	0	2,2,2	0.32	0
3	EDO	C	602	-	3,3,3	0.57	0	2,2,2	0.19	0
3	EDO	A	602	-	3,3,3	0.58	0	2,2,2	0.08	0
3	EDO	B	602	-	3,3,3	0.50	0	2,2,2	0.10	0
3	EDO	A	603	-	3,3,3	0.46	0	2,2,2	0.55	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
3	EDO	B	604	-	-	0/1/1/1	-
4	GOL	C	604	-	-	2/4/4/4	-
3	EDO	C	603	-	-	1/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	D	602	-	-	0/1/1/1	-
3	EDO	C	602	-	-	0/1/1/1	-
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	B	602	-	-	0/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	604	GOL	O1-C1-C2-C3
4	C	604	GOL	O1-C1-C2-O2
3	C	603	EDO	O1-C1-C2-O2
3	A	602	EDO	O1-C1-C2-O2

There are no ring outliers.



No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	501/535 (93%)	-0.38	5 (0%) 82 84	13, 23, 44, 76	0
1	B	501/535 (93%)	-0.23	16 (3%) 47 50	13, 25, 54, 69	0
1	C	497/535 (92%)	-0.51	6 (1%) 79 81	10, 20, 42, 62	0
1	D	496/535 (92%)	-0.39	6 (1%) 79 81	11, 22, 45, 79	0
All	All	1995/2140 (93%)	-0.38	33 (1%) 70 72	10, 22, 47, 79	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	LEU	4.0
1	C	187	THR	3.6
1	B	46	HIS	3.4
1	D	136	ILE	3.3
1	B	301	LEU	3.3
1	C	194	ASP	3.2
1	B	193	LYS	3.0
1	B	45	SER	3.0
1	D	301	LEU	2.9
1	B	191	GLY	2.9
1	A	45	SER	2.9
1	B	299	ILE	2.9
1	A	545	ASN	2.8
1	B	545	ASN	2.8
1	D	299	ILE	2.6
1	C	45	SER	2.6
1	D	45	SER	2.6
1	D	545	ASN	2.6
1	A	190	SER	2.4
1	B	184	MET	2.4
1	A	194	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	194	ASP	2.3
1	B	190	SER	2.3
1	B	90	TYR	2.3
1	B	166	GLY	2.3
1	B	86	VAL	2.2
1	B	136	ILE	2.2
1	B	187	THR	2.2
1	D	165	ARG	2.2
1	C	188	ALA	2.1
1	C	301	LEU	2.1
1	C	264	THR	2.0
1	A	60	ASP	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
4	GOL	C	604	6/6	0.83	0.15	40,42,48,50	0
3	EDO	C	603	4/4	0.84	0.22	39,43,44,50	0
3	EDO	A	603	4/4	0.92	0.16	32,33,38,40	0
3	EDO	A	604	4/4	0.95	0.09	25,26,30,32	0
2	LYS	B	601	10/10	0.96	0.08	14,16,19,24	0
3	EDO	B	604	4/4	0.96	0.12	27,34,36,36	0
3	EDO	D	602	4/4	0.97	0.12	16,21,23,25	0
2	LYS	D	601	10/10	0.97	0.08	10,13,17,17	0
3	EDO	C	602	4/4	0.97	0.07	21,25,26,28	0
3	EDO	A	602	4/4	0.97	0.11	20,23,32,32	0
3	EDO	B	602	4/4	0.97	0.14	23,26,32,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	603	4/4	0.97	0.07	19,20,29,30	0
2	LYS	A	601	10/10	0.98	0.08	12,14,19,23	0
2	LYS	C	601	10/10	0.98	0.07	9,12,18,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.