



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2021 – 02:09 PM JST

PDB ID : 7CWY  
Title : Crystal structure of a tyrosine decarboxylase from *Enterococcus faecalis* in complex with the cofactor PLP  
Authors : Yu, X.; Gong, M.; Huang, J.; Liu, W.; Chen, C.; Guo, R.  
Deposited on : 2020-09-01  
Resolution : 2.59 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.

---

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 : 2.23.1  
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) : 2.23.1

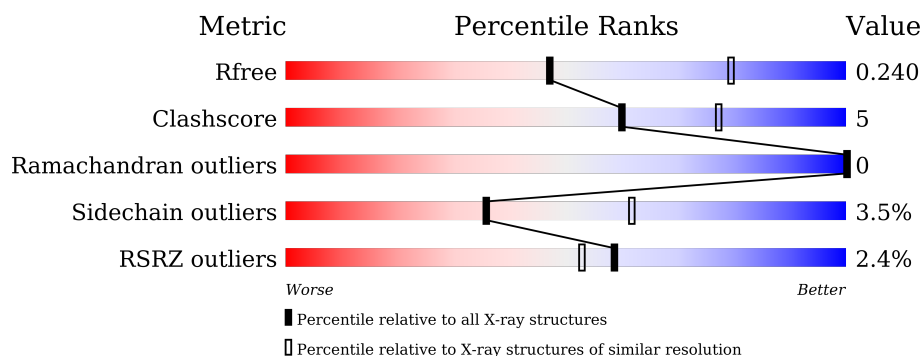
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	620	<div> <div> <div>0%</div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	620	<div> <div>4%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	C	620	<div> <div>3%</div> <div>80%</div> <div>15%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14452 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 Decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	P	S	0	0	0
			4799	3062	793	922	1	21			
1	B	603	Total	C	N	O	P	S	0	0	0
			4800	3065	793	920	1	21			
1	C	593	Total	C	N	O	P	S	0	0	0
			4695	2997	775	901	1	21			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	LYS	GLU	conflict	UNP Q8KXD2
B	62	LYS	GLU	conflict	UNP Q8KXD2
C	62	LYS	GLU	conflict	UNP Q8KXD2

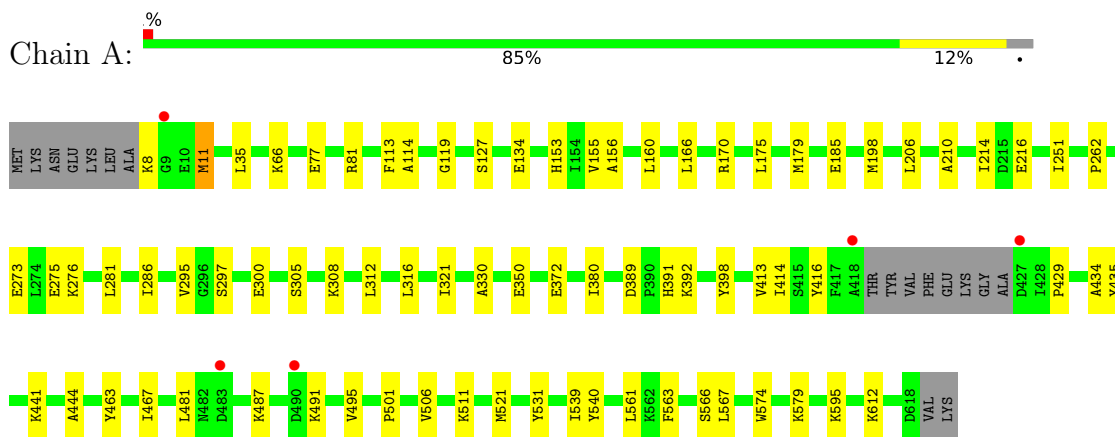
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	83	Total	O	0	0
			83	83		
2	B	41	Total	O	0	0
			41	41		
2	C	34	Total	O	0	0
			34	34		

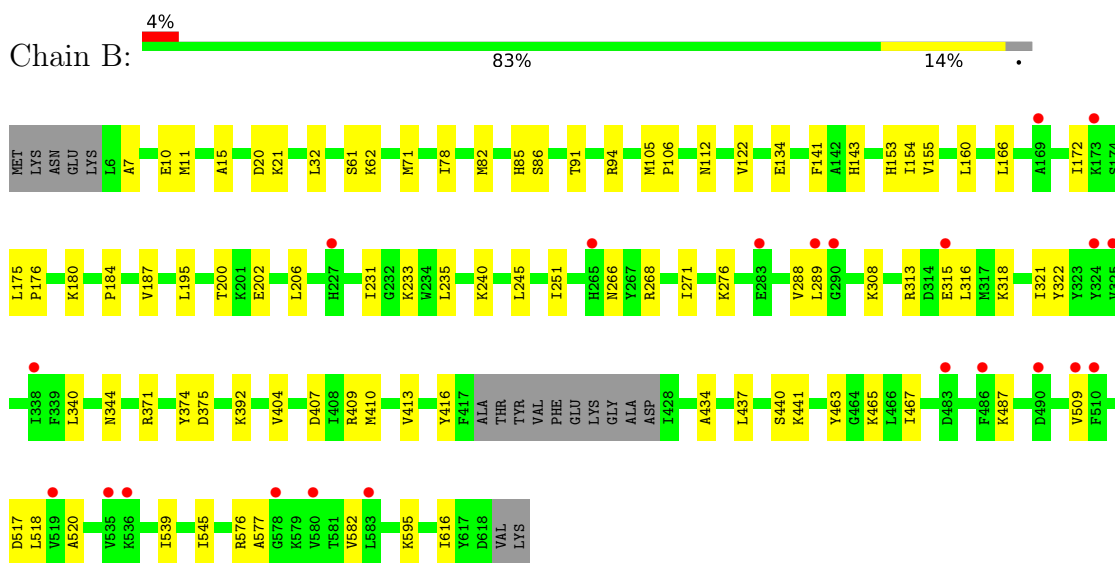
### 3 Residue-property plots [i](#)

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.

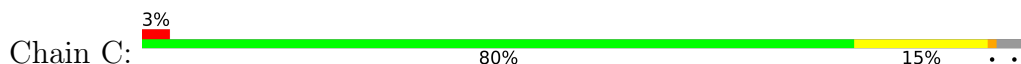
- Molecule 1: Decarboxylase

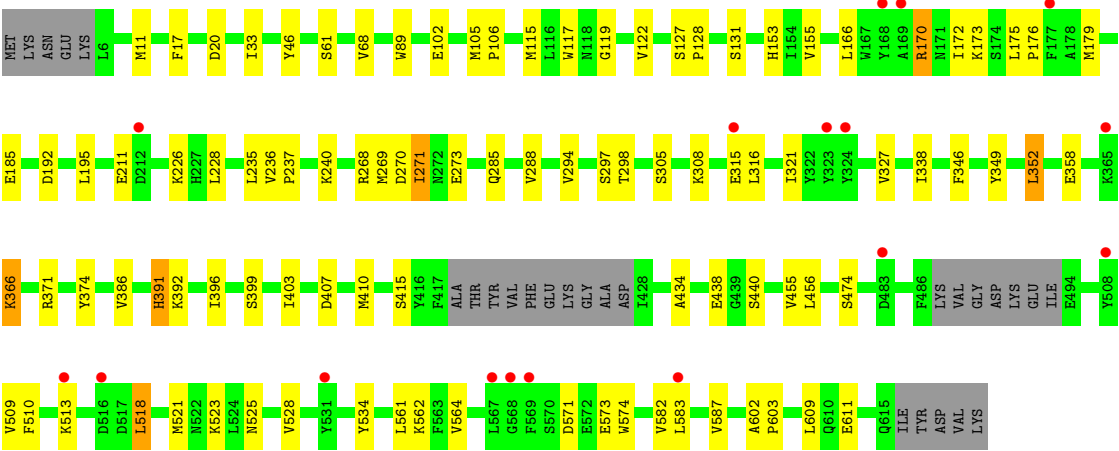


- Molecule 1: Decarboxylase



- Molecule 1: Decarboxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.53Å 132.53Å 390.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.95 – 2.59 24.95 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.95-2.59) 99.2 (24.95-2.59)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.60Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.196 , 0.248 0.207 , 0.240	Depositor DCC
$R_{free}$ test set	3173 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: 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	0.46	0/4892	0.65	0/6638
1	B	0.44	0/4893	0.62	0/6639
1	C	0.54	0/4786	0.74	0/6497
All	All	0.48	0/14571	0.67	0/19774

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

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	4799	0	4599	40	0
1	B	4800	0	4608	54	0
1	C	4695	0	4478	42	0
2	A	83	0	0	4	0
2	B	41	0	0	1	0
2	C	34	0	0	0	0
All	All	14452	0	13685	129	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 5.

All (129) 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:172:ILE:HG21	1:B:200:THR:HG23	1.73	0.71
1:B:316:LEU:HB3	1:B:321:ILE:HB	1.77	0.66
1:B:7:ALA:HB3	1:B:10:GLU:HB2	1.77	0.66
1:A:175:LEU:O	1:A:179:MET:HG3	1.96	0.65
1:B:160:LEU:HD21	1:C:438:GLU:HA	1.79	0.65
1:C:561:LEU:HA	1:C:564:VAL:HG22	1.79	0.63
1:B:134:GLU:OE2	1:B:441:LYS:NZ	2.31	0.62
1:B:517:ASP:OD1	1:B:576:ARG:NH2	2.33	0.62
1:B:240:LYS:HE3	1:B:245:LEU:HD21	1.83	0.61
1:C:407:ASP:HB3	1:C:410:MET:HG3	1.83	0.60
1:A:511:LYS:HB2	1:A:521:MET:SD	2.42	0.60
1:A:595:LYS:NZ	2:A:703:HOH:O	2.35	0.59
1:B:160:LEU:HD12	1:B:437:LEU:HD22	1.85	0.59
1:C:509:VAL:HG13	1:C:582:VAL:HG23	1.86	0.58
1:C:525:ASN:HA	1:C:528:VAL:HG22	1.86	0.57
1:B:410:MET:O	1:B:413:VAL:HG22	2.05	0.56
1:B:85:HIS:HB3	1:C:128:PRO:HB2	1.87	0.55
1:A:153:HIS:CE1	1:A:155:VAL:HG22	2.42	0.55
1:B:487:LYS:HD2	1:B:487:LYS:N	2.21	0.55
1:A:275:GLU:HG3	1:A:312:LEU:HD11	1.88	0.54
1:A:216:GLU:N	2:A:705:HOH:O	2.41	0.54
1:A:77:GLU:OE1	1:A:81:ARG:HD2	2.08	0.54
1:A:416:TYR:O	1:A:434:ALA:HB1	2.08	0.53
1:B:463:TYR:O	1:B:467:ILE:HG12	2.09	0.52
1:B:180:LYS:O	1:B:184:PRO:HG3	2.10	0.52
1:C:17:PHE:HD1	1:C:102:GLU:HG2	1.74	0.52
1:A:262:PRO:HD2	1:A:273:GLU:HB3	1.92	0.52
1:B:517:ASP:HB3	1:B:520:ALA:HB3	1.91	0.52
1:A:316:LEU:HB3	1:A:321:ILE:HB	1.92	0.51
1:B:371:ARG:NH2	2:B:704:HOH:O	2.42	0.51
1:B:235:LEU:HD13	1:B:288:VAL:HG13	1.92	0.51
1:A:297:SER:OG	1:A:300:GLU:HG2	2.11	0.50
1:C:153:HIS:CE1	1:C:155:VAL:HG22	2.46	0.50
1:A:156:ALA:HB3	1:A:160:LEU:HD12	1.94	0.50
1:B:509:VAL:HG12	1:B:582:VAL:HA	1.93	0.50
1:B:271:ILE:HG13	1:B:308:LYS:HD2	1.94	0.49
1:A:305:SER:HB3	1:A:308:LYS:HD3	1.95	0.49
1:B:78:ILE:O	1:B:82:MET:HG2	2.13	0.49
1:B:266:ASN:HB3	1:B:268:ARG:HE	1.77	0.49
1:B:371:ARG:HA	1:B:374:TYR:HB3	1.93	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ARG:HD3	1:A:251:ILE:HG13	1.95	0.48
1:B:160:LEU:CD2	1:C:438:GLU:HA	2.42	0.48
1:C:20:ASP:N	1:C:20:ASP:OD1	2.46	0.48
1:A:134:GLU:OE2	1:A:441:LYS:HE2	2.13	0.48
1:A:501:PRO:HG3	1:A:506:VAL:HG22	1.95	0.48
1:C:371:ARG:HA	1:C:374:TYR:HB3	1.96	0.48
1:B:141:PHE:HB3	1:B:404:VAL:HG22	1.94	0.47
1:C:192:ASP:HA	1:C:195:LEU:HD12	1.97	0.47
1:A:330:ALA:O	1:A:389:ASP:HB2	2.15	0.47
1:B:371:ARG:O	1:B:375:ASP:N	2.40	0.47
1:A:281:LEU:HD22	1:A:286:ILE:HB	1.97	0.46
1:B:407:ASP:OD1	1:B:409:ARG:HG3	2.15	0.46
1:B:441:LYS:HB3	1:B:441:LYS:HE2	1.63	0.46
1:C:122:VAL:HB	1:C:440:SER:HA	1.96	0.46
1:A:413:VAL:HG23	1:A:414:ILE:HG23	1.98	0.46
1:C:528:VAL:HG21	1:C:583:LEU:HD11	1.97	0.46
1:B:86:SER:HB3	1:C:117:TRP:CD1	2.51	0.45
1:B:11:MET:O	1:B:465:LYS:NZ	2.38	0.45
1:B:134:GLU:HG3	1:B:154:ILE:HD12	1.97	0.45
1:B:154:ILE:HB	1:B:441:LYS:HZ3	1.81	0.45
1:B:32:LEU:HD11	1:B:112:ASN:ND2	2.31	0.45
1:B:233:LYS:O	1:B:289:LEU:N	2.49	0.45
1:A:11:MET:HE2	1:A:11:MET:HB2	1.55	0.45
1:B:340:LEU:HD13	1:B:344:ASN:OD1	2.16	0.45
1:C:11:MET:HE3	1:C:455:VAL:O	2.17	0.45
1:B:15:ALA:HB1	1:C:68:VAL:HG23	1.98	0.44
1:C:170:ARG:HE	1:C:170:ARG:HB3	1.46	0.44
1:A:276:LYS:HD2	2:A:724:HOH:O	2.17	0.44
1:C:518:LEU:HB2	1:C:573:GLU:HG3	2.00	0.44
1:A:170:ARG:NH1	1:A:251:ILE:O	2.51	0.44
1:A:295:VAL:HG21	1:A:380:ILE:HD11	2.00	0.44
1:B:276:LYS:HE3	1:B:276:LYS:HB2	1.64	0.44
1:C:17:PHE:CD1	1:C:102:GLU:HG2	2.53	0.43
1:B:153:HIS:CE1	1:B:155:VAL:HG22	2.53	0.43
1:B:166:LEU:HG	1:B:251:ILE:HG21	2.00	0.43
1:C:316:LEU:HB3	1:C:321:ILE:HB	2.01	0.43
1:C:327:VAL:HB	1:C:386:VAL:HG13	2.01	0.43
1:A:561:LEU:HD13	1:A:574:TRP:CD1	2.53	0.43
1:B:416:TYR:O	1:B:434:ALA:HB1	2.19	0.43
1:B:122:VAL:HB	1:B:440:SER:HA	2.01	0.42
1:B:315:GLU:HA	1:B:318:LYS:HE2	1.99	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:ALA:HB3	1:C:603:PRO:HD3	2.01	0.42
1:A:166:LEU:HG	1:A:251:ILE:HG21	2.01	0.42
1:B:187:VAL:HB	1:B:195:LEU:HD21	2.00	0.42
1:C:11:MET:HE3	1:C:456:LEU:HD23	2.01	0.42
1:C:175:LEU:O	1:C:179:MET:HG3	2.18	0.42
1:C:391:HIS:HA	1:C:396:ILE:O	2.20	0.42
1:C:415:SER:HA	1:C:434:ALA:O	2.20	0.42
1:C:474:SER:HA	1:C:587:VAL:HG21	2.01	0.42
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.88	0.42
1:C:271:ILE:H	1:C:271:ILE:HG12	1.56	0.42
1:A:198:MET:HE1	1:A:206:LEU:HD12	2.01	0.42
1:A:210:ALA:O	1:A:214:ILE:HG13	2.20	0.42
1:C:237:PRO:HG2	1:C:294:VAL:HG23	2.00	0.42
1:B:313:ARG:NH1	1:B:322:TYR:OH	2.51	0.42
1:A:540:TYR:O	2:A:701:HOH:O	2.21	0.42
1:B:91:THR:HG21	1:B:94:ARG:HB2	2.00	0.42
1:A:35:LEU:HB3	1:A:113:PHE:CD1	2.55	0.42
1:B:143:HIS:HB3	1:B:344:ASN:ND2	2.35	0.42
1:B:21:LYS:HE3	1:C:46:TYR:O	2.19	0.41
1:C:510:PHE:HZ	1:C:609:LEU:HD13	1.84	0.41
1:B:105:MET:N	1:B:106:PRO:HD2	2.35	0.41
1:C:352:LEU:HD12	1:C:352:LEU:HA	1.84	0.41
1:B:20:ASP:OD1	1:B:20:ASP:N	2.53	0.41
1:B:202:GLU:O	1:B:206:LEU:HG	2.20	0.41
1:C:366:LYS:HE3	1:C:366:LYS:HB2	1.83	0.41
1:A:119:GLY:HA3	1:A:127:SER:HB2	2.01	0.41
1:A:539:ILE:HD12	1:A:539:ILE:HA	1.92	0.41
1:C:349:TYR:O	1:C:352:LEU:HB2	2.19	0.41
1:A:481:LEU:HD22	1:A:495:VAL:HG11	2.01	0.41
1:B:176:PRO:HB2	1:B:195:LEU:HB3	2.01	0.41
1:B:539:ILE:HD11	1:B:545:ILE:HG12	2.03	0.41
1:B:32:LEU:HD11	1:B:112:ASN:HD22	1.85	0.41
1:C:105:MET:N	1:C:106:PRO:HD2	2.36	0.41
1:A:429:PRO:HB3	1:A:435:TYR:CE2	2.56	0.41
1:A:531:TYR:HB3	1:A:612:LYS:HG2	2.02	0.41
1:B:518:LEU:HD23	1:B:577:ALA:HB3	2.02	0.41
1:C:119:GLY:HA3	1:C:127:SER:HB2	2.03	0.41
1:C:518:LEU:HD23	1:C:574:TRP:HA	2.02	0.41
1:A:114:ALA:HB3	1:A:444:ALA:HA	2.03	0.40
1:A:350:GLU:H	1:A:350:GLU:HG2	1.66	0.40
1:A:563:PHE:CZ	1:A:567:LEU:HD11	2.56	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ASP:HB3	1:C:273:GLU:HB2	2.02	0.40
1:A:391:HIS:CD2	1:A:398:TYR:CE1	3.09	0.40
1:A:463:TYR:O	1:A:467:ILE:HG12	2.21	0.40
1:A:563:PHE:O	1:A:566:SER:OG	2.31	0.40
1:B:71:MET:SD	1:C:106:PRO:HD3	2.61	0.40
1:C:33:ILE:HD13	1:C:33:ILE:HA	1.93	0.40
1:C:235:LEU:HD13	1:C:288:VAL:HG13	2.04	0.40

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	598/620 (96%)	576 (96%)	22 (4%)	0	100	100
1	B	598/620 (96%)	575 (96%)	23 (4%)	0	100	100
1	C	586/620 (94%)	560 (96%)	26 (4%)	0	100	100
All	All	1782/1860 (96%)	1711 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	505/524 (96%)	497 (98%)	8 (2%)	62	82
1	B	505/524 (96%)	500 (99%)	5 (1%)	76	90
1	C	491/524 (94%)	451 (92%)	40 (8%)	11	23
All	All	1501/1572 (96%)	1448 (96%)	53 (4%)	36	62

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	11	MET
1	A	66	LYS
1	A	185	GLU
1	A	372	GLU
1	A	487	LYS
1	A	491	LYS
1	A	579	LYS
1	B	61	SER
1	B	62	LYS
1	B	231	ILE
1	B	595	LYS
1	B	616	ILE
1	C	61	SER
1	C	89	TRP
1	C	115	MET
1	C	131	SER
1	C	166	LEU
1	C	170	ARG
1	C	172	ILE
1	C	173	LYS
1	C	176	PRO
1	C	185	GLU
1	C	211	GLU
1	C	226	LYS
1	C	228	LEU
1	C	236	VAL
1	C	240	LYS
1	C	268	ARG
1	C	269	MET
1	C	271	ILE
1	C	285	GLN
1	C	297	SER
1	C	298	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	305	SER
1	C	308	LYS
1	C	315	GLU
1	C	338	ILE
1	C	346	PHE
1	C	352	LEU
1	C	358	GLU
1	C	366	LYS
1	C	391	HIS
1	C	399	SER
1	C	403	ILE
1	C	513	LYS
1	C	518	LEU
1	C	521	MET
1	C	523	LYS
1	C	534	TYR
1	C	562	LYS
1	C	571	ASP
1	C	611	GLU

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

Mol	Chain	Res	Type
1	A	565	ASN
1	C	100	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	392	1	23,24,25	0.65	0	25,32,34	0.74	1 (4%)
1	LLP	A	392	1	23,24,25	0.64	0	25,32,34	0.69	1 (4%)
1	LLP	C	392	1	23,24,25	0.60	0	25,32,34	0.75	1 (4%)

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	392	1	-	5/16/17/19	0/1/1/1
1	LLP	A	392	1	-	4/16/17/19	0/1/1/1
1	LLP	C	392	1	-	6/16/17/19	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	392	LLP	OP4-C5'-C5	2.74	114.56	109.35
1	C	392	LLP	OP4-C5'-C5	2.64	114.38	109.35
1	A	392	LLP	OP4-C5'-C5	2.20	113.54	109.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	392	LLP	C3-C4-C4'-NZ
1	A	392	LLP	C4-C4'-NZ-CE
1	A	392	LLP	O-C-CA-CB
1	B	392	LLP	C4-C4'-NZ-CE
1	B	392	LLP	O-C-CA-CB
1	C	392	LLP	C4-C4'-NZ-CE
1	C	392	LLP	O-C-CA-CB
1	C	392	LLP	CG-CD-CE-NZ
1	A	392	LLP	CG-CD-CE-NZ
1	B	392	LLP	CG-CD-CE-NZ
1	B	392	LLP	C-CA-CB-CG
1	C	392	LLP	CD-CE-NZ-C4'
1	B	392	LLP	C3-C4-C4'-NZ
1	C	392	LLP	C3-C4-C4'-NZ

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	C	392	LLP	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 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	602/620 (97%)	-0.18	5 (0%) 86 84	27, 45, 69, 86	0
1	B	602/620 (97%)	0.07	22 (3%) 41 34	29, 56, 76, 91	0
1	C	592/620 (95%)	0.14	17 (2%) 51 45	30, 54, 87, 100	0
All	All	1796/1860 (96%)	0.01	44 (2%) 59 53	27, 51, 79, 100	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	ALA	6.9
1	B	283	GLU	4.7
1	C	583	LEU	4.2
1	B	535	VAL	4.1
1	C	568	GLY	4.1
1	C	567	LEU	3.7
1	B	290	GLY	3.5
1	B	583	LEU	3.3
1	B	169	ALA	3.1
1	C	365	LYS	3.0
1	C	169	ALA	3.0
1	C	569	PHE	3.0
1	C	531	TYR	2.9
1	B	173	LYS	2.9
1	A	427	ASP	2.9
1	B	289	LEU	2.7
1	B	509	VAL	2.7
1	C	168	TYR	2.6
1	A	9	GLY	2.6
1	C	315	GLU	2.6
1	B	578	GLY	2.6
1	B	483	ASP	2.6
1	B	490	ASP	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	324	TYR	2.6
1	C	483	ASP	2.6
1	C	508	TYR	2.5
1	C	324	TYR	2.4
1	C	323	TYR	2.3
1	C	177	PHE	2.3
1	A	483	ASP	2.2
1	B	325	VAL	2.2
1	B	315	GLU	2.2
1	B	519	VAL	2.2
1	C	513	LYS	2.2
1	C	212	ASP	2.2
1	B	486	PHE	2.2
1	A	490	ASP	2.1
1	B	227	HIS	2.1
1	B	580	VAL	2.1
1	B	338	ILE	2.1
1	B	536	LYS	2.1
1	C	516	ASP	2.1
1	B	265	HIS	2.0
1	B	510	PHE	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
1	LLP	B	392	24/25	0.95	0.16	39,43,50,52	0
1	LLP	C	392	24/25	0.96	0.13	35,45,51,52	0
1	LLP	A	392	24/25	0.97	0.11	32,36,43,46	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.