



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:44 pm BST

PDB ID : 3VP6  
Title : Structural characterization of Glutamic Acid Decarboxylase; insights into the mechanism of autoinactivation  
Authors : Langendorf, C.G.; Tuck, K.L.; Key, T.L.G.; Rosado, C.J.; Wong, A.S.M.; Fenalti, G.; Buckle, A.M.; Law, R.H.P.; Whisstock, J.C.  
Deposited on : 2012-02-27  
Resolution : 2.10 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

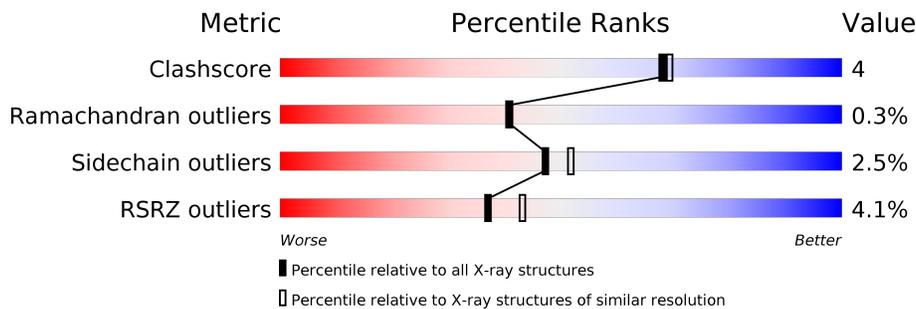
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	511	
1	B	511	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7917 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.

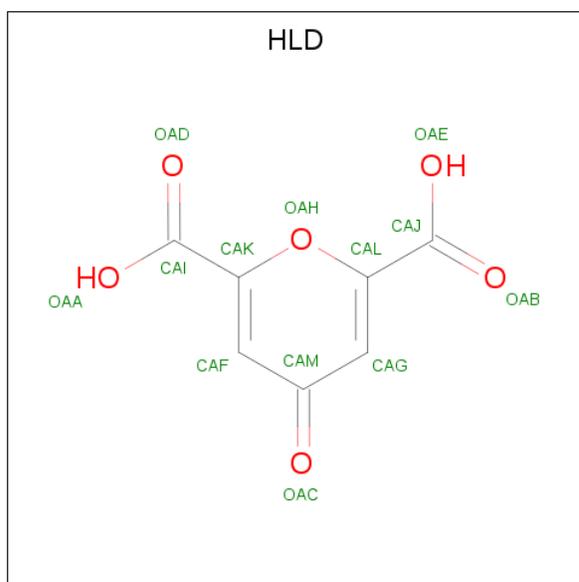
- Molecule 1 is a protein called Glutamate decarboxylase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	500	3841	2478	640	697	1	25	0	0	0
1	B	491	3772	2422	634	691	1	24	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

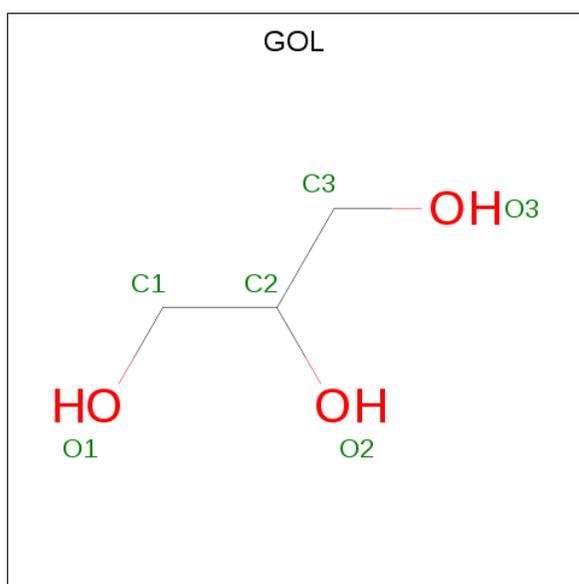
Chain	Residue	Modelled	Actual	Comment	Reference
A	431	HIS	CYS	CONFLICT	UNP Q99259
A	433	SER	GLY	CONFLICT	UNP Q99259
A	438	GLN	PRO	CONFLICT	UNP Q99259
A	441	HIS	GLN	CONFLICT	UNP Q99259
A	595	HIS	-	EXPRESSION TAG	UNP Q99259
A	596	HIS	-	EXPRESSION TAG	UNP Q99259
A	597	HIS	-	EXPRESSION TAG	UNP Q99259
A	598	HIS	-	EXPRESSION TAG	UNP Q99259
A	599	HIS	-	EXPRESSION TAG	UNP Q99259
A	600	HIS	-	EXPRESSION TAG	UNP Q99259
B	431	HIS	CYS	CONFLICT	UNP Q99259
B	433	SER	GLY	CONFLICT	UNP Q99259
B	438	GLN	PRO	CONFLICT	UNP Q99259
B	441	HIS	GLN	CONFLICT	UNP Q99259
B	595	HIS	-	EXPRESSION TAG	UNP Q99259
B	596	HIS	-	EXPRESSION TAG	UNP Q99259
B	597	HIS	-	EXPRESSION TAG	UNP Q99259
B	598	HIS	-	EXPRESSION TAG	UNP Q99259
B	599	HIS	-	EXPRESSION TAG	UNP Q99259
B	600	HIS	-	EXPRESSION TAG	UNP Q99259

- Molecule 2 is 4-oxo-4H-pyran-2,6-dicarboxylic acid (three-letter code: HLD) (formula:  $C_7H_4O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

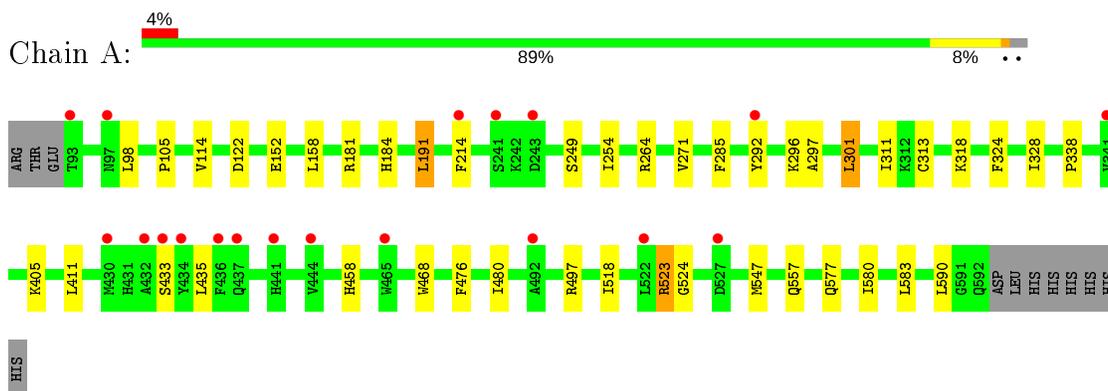
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	132	Total 132	O 132	0	0
4	B	134	Total 134	O 134	0	0

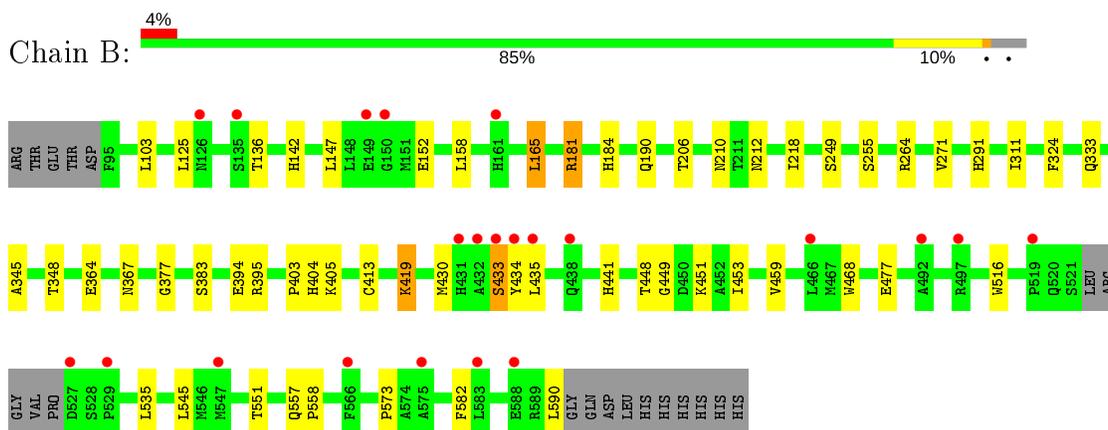
### 3 Residue-property plots [i](#)

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: Glutamate decarboxylase 1



- Molecule 1: Glutamate decarboxylase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.01Å 64.08Å 102.65Å 90.00° 108.14° 90.00°	Depositor
Resolution (Å)	24.25 – 2.10 23.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.25-2.10) 99.9 (23.82-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.10Å)	Xtrriage
Refinement program	BUSTER-TNT 'BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.197 , 0.234 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	3148 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtrriage
Anisotropy	0.325	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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, LLP, HLD

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	0.49	0/3908	0.66	0/5298
1	B	0.51	0/3835	0.67	1/5197 (0.0%)
All	All	0.50	0/7743	0.67	1/10495 (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	B	433	SER	C-N-CA	6.00	136.69	121.70

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	3841	0	3671	29	0
1	B	3772	0	3585	36	0
2	A	13	0	2	2	0
2	B	13	0	2	3	0
3	B	12	0	16	1	0
4	A	132	0	0	3	0
4	B	134	0	0	0	0
All	All	7917	0	7276	56	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 4.

All (56) 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:404:HIS:HD2	1:B:413:CYS:H	1.26	0.82
1:A:191:LEU:HD23	1:A:405:LLP:HE3	1.69	0.73
1:B:404:HIS:CD2	1:B:413:CYS:H	2.08	0.72
1:A:254:ILE:HG12	4:A:1196:HOH:O	1.91	0.70
1:A:292:TYR:HD2	4:A:1214:HOH:O	1.81	0.62
1:B:142:HIS:HB2	1:B:147:LEU:HD21	1.81	0.62
1:B:249:SER:HG	1:B:255:SER:HG	1.43	0.59
1:A:296:LYS:NZ	1:B:449:GLY:O	2.35	0.58
1:B:433:SER:HB2	1:B:435:LEU:HG	1.85	0.57
1:B:190:GLN:HB3	2:B:1001:HLD:OAB	2.05	0.57
1:A:468:TRP:HB3	1:B:158:LEU:HD22	1.89	0.54
1:B:311:ILE:HD12	1:B:324:PHE:HA	1.90	0.53
1:B:291:HIS:HD2	1:B:348:THR:HG21	1.74	0.53
1:B:212:ASN:HB3	1:B:218:ILE:HD11	1.91	0.53
1:A:114:VAL:HG13	1:B:125:LEU:HD13	1.91	0.52
1:B:405:LLP:H4'1	2:B:1001:HLD:OAC	2.10	0.52
1:A:433:SER:HB2	1:B:558:PRO:HD2	1.92	0.52
1:A:285:PHE:CE1	1:A:338:PRO:HB3	2.44	0.51
1:B:551:THR:HB	1:B:582:PHE:HZ	1.75	0.51
1:B:403:PRO:HD2	1:B:413:CYS:O	2.12	0.50
1:A:324:PHE:CZ	1:A:328:ILE:HD11	2.47	0.49
1:A:285:PHE:HE1	1:A:338:PRO:HB3	1.77	0.49
1:A:191:LEU:HB3	1:A:405:LLP:HD3	1.94	0.49
1:A:577:GLN:HA	1:A:580:ILE:HD12	1.94	0.49
1:A:296:LYS:HG3	1:B:430:MET:HG2	1.94	0.49
1:A:181:ARG:HB3	1:A:184:HIS:HB2	1.95	0.48
1:A:158:LEU:HD22	1:B:468:TRP:HB3	1.96	0.48
1:B:383:SER:HA	1:B:477:GLU:HG3	1.96	0.48
1:A:297:ALA:O	1:A:301:LEU:HB2	2.13	0.47
1:B:405:LLP:H4'1	2:B:1001:HLD:CAM	2.45	0.47
1:A:523:ARG:HA	1:A:524:GLY:HA2	1.60	0.47
1:B:367:ASN:HB3	3:B:1003:GOL:H31	1.97	0.46
1:B:206:THR:HG23	1:B:459:VAL:HB	1.98	0.46
1:B:345:ALA:O	1:B:377:GLY:HA3	2.16	0.46
1:A:547:MET:HG3	1:B:441:HIS:CD2	2.50	0.46
1:B:433:SER:HB3	1:B:434:TYR:CA	2.46	0.46
1:A:405:LLP:H4'1	2:A:1001:HLD:CAM	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:PHE:O	1:A:480:ILE:HG12	2.16	0.45
1:B:545:LEU:HD13	1:B:590:LEU:HD12	1.98	0.45
1:A:254:ILE:HD11	1:B:453:ILE:HG23	1.99	0.45
1:B:103:LEU:HD21	1:B:165:LEU:HD21	1.98	0.44
1:B:264:ARG:HD2	1:B:271:VAL:HG11	1.99	0.44
1:A:311:ILE:HD12	1:A:324:PHE:HA	1.99	0.44
1:A:458:HIS:CE1	4:A:1111:HOH:O	2.70	0.44
1:A:518:ILE:HG22	1:A:523:ARG:HG2	2.00	0.43
1:A:313:CYS:HA	1:A:318:LYS:O	2.18	0.42
1:B:394:GLU:O	1:B:419:LYS:NZ	2.52	0.42
1:B:364:GLU:CD	1:B:395:ARG:HH21	2.22	0.42
1:A:324:PHE:CE2	1:A:328:ILE:HD11	2.55	0.41
1:A:264:ARG:HD2	1:A:271:VAL:HG11	2.01	0.41
1:A:105:PRO:HG2	1:B:573:PRO:HB2	2.03	0.41
1:A:405:LLP:H4'1	2:A:1001:HLD:CAG	2.51	0.41
1:B:448:THR:HG22	1:B:451:LYS:HD3	2.03	0.41
1:B:516:TRP:HB3	1:B:535:LEU:HD11	2.01	0.41
1:B:433:SER:HB3	1:B:434:TYR:C	2.41	0.40
1:B:181:ARG:HB3	1:B:184:HIS:HB2	2.03	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	497/511 (97%)	473 (95%)	23 (5%)	1 (0%)	47 49
1	B	486/511 (95%)	468 (96%)	16 (3%)	2 (0%)	34 32
All	All	983/1022 (96%)	941 (96%)	39 (4%)	3 (0%)	41 41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	152	GLU
1	A	152	GLU
1	B	210	ASN

### 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	379/438 (86%)	366 (97%)	13 (3%)	37	39
1	B	372/438 (85%)	366 (98%)	6 (2%)	62	69
All	All	751/876 (86%)	732 (98%)	19 (2%)	47	52

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LEU
1	A	122	ASP
1	A	191	LEU
1	A	214	PHE
1	A	249	SER
1	A	301	LEU
1	A	411	LEU
1	A	435	LEU
1	A	497	ARG
1	A	523	ARG
1	A	557	GLN
1	A	583	LEU
1	A	590	LEU
1	B	136	THR
1	B	165	LEU
1	B	181	ARG
1	B	333	GLN
1	B	419	LYS
1	B	557	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	559	GLN
1	B	333	GLN
1	B	404	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	A	405	1	23,24,25	2.16	6 (26%)	25,32,34	1.89	7 (28%)
1	LLP	B	405	1	23,23,25	1.81	4 (17%)	29,31,34	1.53	7 (24%)

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	405	1	-	6/16/17/19	0/1/1/1
1	LLP	B	405	1	-	6/15/15/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	LLP	C4'-NZ	6.24	1.48	1.27
1	A	405	LLP	C4'-NZ	5.70	1.46	1.27
1	A	405	LLP	C3-C2	5.08	1.46	1.40
1	A	405	LLP	CB-CA	4.13	1.59	1.53
1	A	405	LLP	C4-C4'	3.04	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	LLP	C4-C3	2.91	1.45	1.40
1	B	405	LLP	C4-C4'	2.79	1.51	1.46
1	B	405	LLP	CB-CA	2.74	1.57	1.53
1	A	405	LLP	P-OP4	-2.60	1.51	1.60
1	A	405	LLP	C6-C5	2.48	1.42	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	LLP	CD-CE-NZ	3.74	120.10	110.93
1	B	405	LLP	CB-CA-N	3.62	118.31	108.52
1	B	405	LLP	OP4-P-OP1	3.24	115.56	106.47
1	A	405	LLP	CE-NZ-C4'	-3.23	108.97	118.90
1	A	405	LLP	C4-C4'-NZ	-2.98	110.62	124.31
1	A	405	LLP	CG-CD-CE	2.94	123.79	113.57
1	B	405	LLP	C6-N1-C2	2.82	124.40	119.17
1	B	405	LLP	CE-NZ-C4'	-2.39	111.56	118.90
1	A	405	LLP	C2'-C2-N1	2.35	122.25	117.67
1	A	405	LLP	OP3-P-OP4	2.32	112.89	106.73
1	A	405	LLP	C6-N1-C2	2.25	123.33	119.17
1	B	405	LLP	C4-C4'-NZ	-2.22	114.12	124.31
1	B	405	LLP	C-CA-CB	2.11	118.12	111.96
1	B	405	LLP	C3-C2-N1	-2.10	118.06	120.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	405	LLP	C4-C4'-NZ-CE
1	A	405	LLP	C4-C4'-NZ-CE
1	A	405	LLP	C3-C4-C4'-NZ
1	B	405	LLP	C3-C4-C4'-NZ
1	B	405	LLP	CA-CB-CG-CD
1	A	405	LLP	CA-CB-CG-CD
1	A	405	LLP	CE-CD-CG-CB
1	B	405	LLP	CE-CD-CG-CB
1	A	405	LLP	CD-CE-NZ-C4'
1	B	405	LLP	CG-CD-CE-NZ
1	A	405	LLP	N-CA-CB-CG
1	B	405	LLP	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	405	LLP	4	0
1	B	405	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	HLD	A	1001	-	7,13,13	1.30	0	4,18,18	1.07	1 (25%)
2	HLD	B	1001	-	7,13,13	1.48	0	4,18,18	1.07	0
3	GOL	B	1002	-	5,5,5	0.14	0	5,5,5	0.16	0
3	GOL	B	1003	-	5,5,5	0.12	0	5,5,5	0.28	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	HLD	A	1001	-	-	0/0/8/8	0/1/1/1
2	HLD	B	1001	-	-	0/0/8/8	0/1/1/1
3	GOL	B	1002	-	-	0/4/4/4	-
3	GOL	B	1003	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	1001	HLD	CAG-CAM-CAF	2.09	120.63	117.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1003	GOL	C1-C2-C3-O3
3	B	1003	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	HLD	2	0
2	B	1001	HLD	3	0
3	B	1003	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

### 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	499/511 (97%)	0.20	19 (3%) 40 46	21, 36, 58, 81	0
1	B	490/511 (95%)	0.18	22 (4%) 33 38	16, 33, 66, 91	0
All	All	989/1022 (96%)	0.19	41 (4%) 37 43	16, 35, 60, 91	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	434	TYR	5.2
1	B	433	SER	5.0
1	B	529	PRO	3.9
1	A	434	TYR	3.8
1	A	441	HIS	3.7
1	B	150	GLY	3.7
1	B	435	LEU	3.3
1	B	432	ALA	3.3
1	B	126	ASN	3.2
1	A	527	ASP	3.1
1	A	430	MET	3.1
1	B	527	ASP	3.0
1	A	433	SER	3.0
1	A	241	SER	2.9
1	A	492	ALA	2.9
1	B	519	PRO	2.8
1	A	432	ALA	2.8
1	B	431	HIS	2.8
1	A	243	ASP	2.7
1	B	566	PHE	2.7
1	A	444	VAL	2.6
1	B	492	ALA	2.6
1	A	292	TYR	2.5
1	A	97	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	93	THR	2.4
1	B	149	GLU	2.4
1	A	465	TRP	2.4
1	B	583	LEU	2.4
1	B	438	GLN	2.4
1	A	436	PHE	2.3
1	B	547	MET	2.3
1	B	161	HIS	2.3
1	A	437	GLN	2.2
1	B	588	GLU	2.2
1	B	497	ARG	2.2
1	A	214	PHE	2.2
1	B	135	SER	2.1
1	B	575	ALA	2.1
1	A	522	LEU	2.1
1	B	466	LEU	2.0
1	A	341	VAL	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(Å <sup>2</sup> )	Q<0.9
1	LLP	A	405	24/25	0.94	0.11	26,30,34,40	0
1	LLP	B	405	23/25	0.95	0.11	24,31,34,36	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HLD	B	1001	13/13	0.88	0.17	50,51,59,60	0
3	GOL	B	1002	6/6	0.91	0.15	32,34,38,41	0
3	GOL	B	1003	6/6	0.92	0.15	33,38,42,43	0
2	HLD	A	1001	13/13	0.93	0.18	35,39,42,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.