



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2018 – 06:03 pm GMT

PDB ID : 1V00  
Title : Erythrina cristagalli lectin  
Authors : Turton, K.; Natesh, R.; Thiyagarajan, N.; Chaddock, J.A.; Acharya, K.R.  
Deposited on : 2004-03-21  
Resolution : 1.70 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

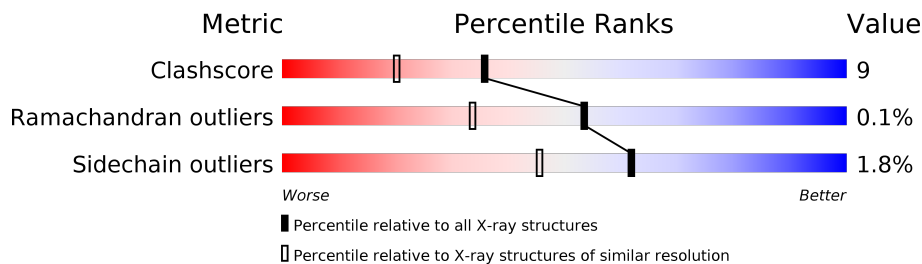
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	122078	4165 (1.70-1.70)
Ramachandran outliers	120005	4098 (1.70-1.70)
Sidechain outliers	119972	4098 (1.70-1.70)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	242	
1	B	242	
1	C	242	
1	D	242	

## 2 Entry composition [i](#)

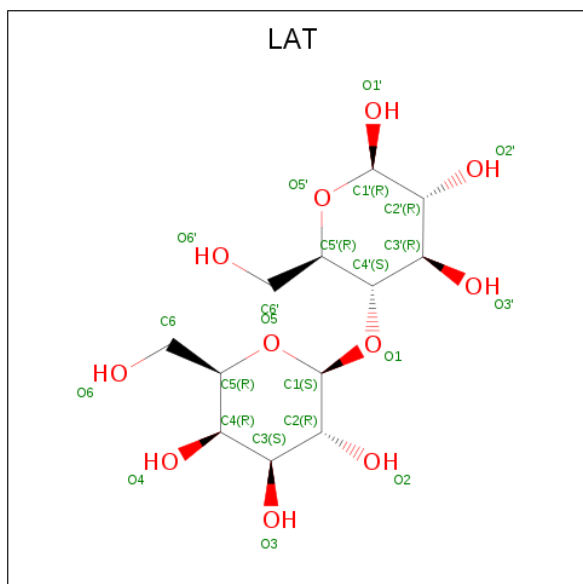
There are 5 unique types of molecules in this entry. The entry contains 8656 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LECTIN (ECL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	1
			1856	1189	302	362	3			
1	B	240	Total	C	N	O	S	0	0	0
			1862	1193	302	364	3			
1	C	241	Total	C	N	O	S	0	0	1
			1863	1193	303	364	3			
1	D	240	Total	C	N	O	S	0	0	1
			1856	1189	302	362	3			

- Molecule 2 is BETA-LACTOSE (three-letter code: LAT) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

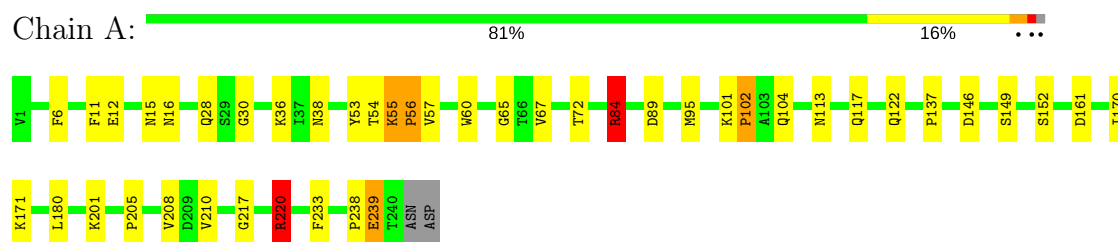
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	296	Total	O	0	0
			296	296		
5	B	223	Total	O	0	0
			223	223		
5	C	330	Total	O	0	0
			330	330		
5	D	270	Total	O	0	0
			270	270		

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

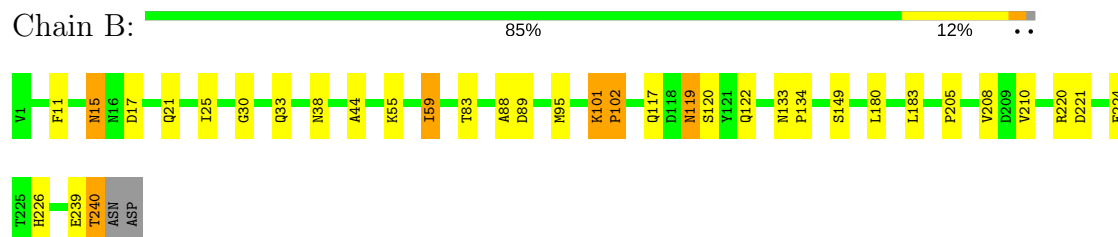
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

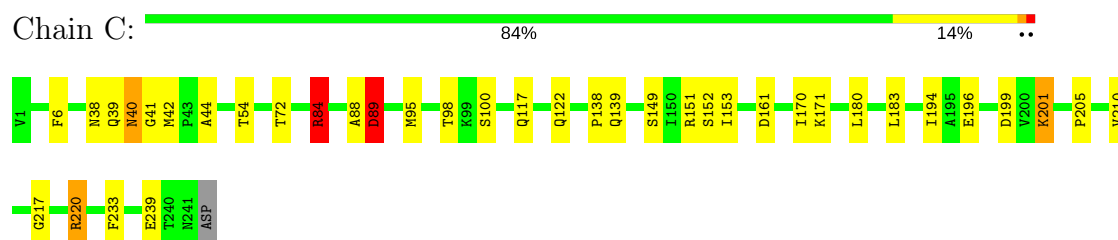
#### • Molecule 1: LECTIN (ECL)



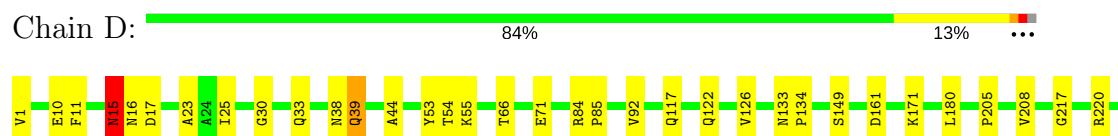
#### • Molecule 1: LECTIN (ECL)



#### • Molecule 1: LECTIN (ECL)



#### • Molecule 1: LECTIN (ECL)





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.90Å 167.23Å 55.13Å 90.00° 97.08° 90.00°	Depositor
Resolution (Å)	21.12 – 1.70	Depositor
% Data completeness (in resolution range)	99.8 (21.12-1.70)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.172 , 0.195	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LAT, CA, MN

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	1.42	15/1907 (0.8%)	1.65	21/2609 (0.8%)
1	B	0.63	3/1913 (0.2%)	0.75	5/2617 (0.2%)
1	C	0.77	7/1913 (0.4%)	1.03	8/2617 (0.3%)
1	D	1.23	9/1906 (0.5%)	1.03	17/2607 (0.7%)
All	All	1.06	34/7639 (0.4%)	1.17	51/10450 (0.5%)

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	1	1
1	C	0	1
1	D	1	2
All	All	2	4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	ARG	NE-CZ	-33.65	0.89	1.33
1	D	239	GLU	C-O	30.20	1.80	1.23
1	D	239	GLU	CD-OE1	29.40	1.57	1.25
1	A	220	ARG	CZ-NH2	22.23	1.61	1.33
1	C	89	ASP	CG-OD2	21.99	1.75	1.25
1	D	239	GLU	CG-CD	-18.67	1.24	1.51
1	A	220	ARG	CZ-NH1	18.48	1.57	1.33
1	A	56	PRO	N-CD	-18.07	1.22	1.47
1	B	102	PRO	N-CD	-18.07	1.22	1.47
1	A	102	PRO	N-CD	-18.04	1.22	1.47
1	A	220	ARG	NE-CZ	-16.77	1.11	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	GLU	CD-OE1	15.50	1.42	1.25
1	D	239	GLU	CB-CG	-12.80	1.27	1.52
1	C	84	ARG	NE-CZ	-12.30	1.17	1.33
1	A	239	GLU	CD-OE2	11.83	1.38	1.25
1	D	238	PRO	CA-C	10.01	1.72	1.52
1	D	239	GLU	CA-CB	8.87	1.73	1.53
1	A	84	ARG	CG-CD	8.46	1.73	1.51
1	D	239	GLU	N-CA	7.97	1.62	1.46
1	C	89	ASP	CG-OD1	7.92	1.43	1.25
1	C	84	ARG	CZ-NH2	7.76	1.43	1.33
1	D	10	GLU	CB-CG	7.46	1.66	1.52
1	B	101	LYS	C-N	-7.41	1.20	1.34
1	B	55	LYS	CD-CE	6.89	1.68	1.51
1	A	239	GLU	CA-C	-6.88	1.35	1.52
1	A	102	PRO	CB-CG	6.69	1.83	1.50
1	A	239	GLU	CB-CG	6.36	1.64	1.52
1	C	152	SER	C-N	-6.10	1.20	1.34
1	C	84	ARG	CZ-NH1	5.93	1.40	1.33
1	D	239	GLU	CA-C	5.72	1.67	1.52
1	A	238	PRO	C-N	-5.66	1.21	1.34
1	A	84	ARG	CZ-NH2	-5.58	1.25	1.33
1	A	220	ARG	CD-NE	-5.28	1.37	1.46
1	C	151	ARG	C-N	-5.08	1.22	1.34

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	NE-CZ-NH2	32.66	136.63	120.30
1	A	220	ARG	NE-CZ-NH1	31.26	135.93	120.30
1	A	84	ARG	NH1-CZ-NH2	-28.43	88.12	119.40
1	A	220	ARG	NE-CZ-NH2	-27.85	106.37	120.30
1	C	84	ARG	CD-NE-CZ	26.40	160.56	123.60
1	A	84	ARG	NE-CZ-NH1	23.11	131.86	120.30
1	D	239	GLU	CA-CB-CG	19.28	155.82	113.40
1	A	239	GLU	OE1-CD-OE2	-18.93	100.58	123.30
1	D	239	GLU	CA-C-O	18.69	159.35	120.10
1	C	84	ARG	NE-CZ-NH2	-16.09	112.25	120.30
1	A	220	ARG	CD-NE-CZ	15.44	145.22	123.60
1	C	84	ARG	NE-CZ-NH1	13.99	127.29	120.30
1	A	239	GLU	CA-C-O	-11.52	95.92	120.10
1	A	239	GLU	CB-CG-CD	11.20	144.44	114.20
1	A	239	GLU	CB-CA-C	10.90	132.21	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	239	GLU	OE1-CD-OE2	-10.69	110.47	123.30
1	A	239	GLU	O-C-N	10.01	138.71	122.70
1	A	102	PRO	N-CD-CG	9.60	117.60	103.20
1	C	152	SER	O-C-N	-8.94	108.40	122.70
1	A	239	GLU	CG-CD-OE1	8.74	135.79	118.30
1	D	238	PRO	C-N-CA	8.73	143.52	121.70
1	D	239	GLU	N-CA-C	8.55	134.10	111.00
1	D	15	ASN	N-CA-CB	8.49	125.88	110.60
1	B	102	PRO	N-CD-CG	8.39	115.79	103.20
1	A	239	GLU	CA-CB-CG	-7.83	96.17	113.40
1	D	239	GLU	CB-CA-C	7.66	125.72	110.40
1	D	208	VAL	CB-CA-C	-7.11	97.89	111.40
1	C	89	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	B	83	THR	CA-CB-CG2	-6.63	103.12	112.40
1	D	208	VAL	CA-CB-CG1	-6.58	101.03	110.90
1	D	10	GLU	CG-CD-OE1	-6.57	105.16	118.30
1	D	161	ASP	CB-CA-C	6.51	123.43	110.40
1	D	238	PRO	CA-C-N	-6.44	103.04	117.20
1	D	10	GLU	CG-CD-OE2	6.36	131.01	118.30
1	A	239	GLU	N-CA-CB	6.08	121.54	110.60
1	D	239	GLU	CG-CD-OE1	6.07	130.44	118.30
1	D	239	GLU	N-CA-CB	-5.89	99.99	110.60
1	B	239	GLU	CA-C-N	-5.81	104.41	117.20
1	B	239	GLU	O-C-N	5.67	131.77	122.70
1	A	56	PRO	N-CD-CG	5.53	111.49	103.20
1	C	239	GLU	N-CA-C	-5.53	96.08	111.00
1	C	217	GLY	N-CA-C	5.52	126.89	113.10
1	A	217	GLY	N-CA-C	5.49	126.84	113.10
1	D	217	GLY	N-CA-C	5.47	126.78	113.10
1	A	238	PRO	C-N-CA	5.36	135.09	121.70
1	D	15	ASN	CB-CG-ND2	-5.21	104.19	116.70
1	C	89	ASP	CA-CB-CG	5.14	124.71	113.40
1	A	161	ASP	N-CA-C	-5.12	97.16	111.00
1	B	59	ILE	O-C-N	-5.04	114.63	122.70
1	A	137	PRO	N-CA-C	-5.03	99.02	112.10
1	A	55	LYS	C-N-CD	-5.02	109.55	120.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	239	GLU	CA
1	D	239	GLU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	ARG	Sidechain
1	C	84	ARG	Sidechain
1	D	15	ASN	Sidechain
1	D	238	PRO	Mainchain

## 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	1856	0	1792	42	0
1	B	1862	0	1800	27	0
1	C	1863	0	1797	35	0
1	D	1856	0	1793	27	0
2	A	23	0	21	0	0
2	B	23	0	22	0	0
2	C	23	0	22	1	0
2	D	23	0	22	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	296	0	0	16	1
5	B	223	0	0	1	0
5	C	330	0	0	6	1
5	D	270	0	0	2	0
All	All	8656	0	7269	129	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

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:A:102:PRO:CG	1:A:102:PRO:CB	1.83	1.39
1:A:180:LEU:HB2	5:A:2251:HOH:O	1.23	1.36
1:A:180:LEU:HD21	5:A:2230:HOH:O	1.29	1.29
1:C:89:ASP:OD2	1:C:89:ASP:CG	1.75	1.24
1:D:239:GLU:O	1:D:239:GLU:C	1.80	1.19
1:A:146:ASP:OD1	1:A:152:SER:OG	1.70	1.06
1:A:53:TYR:CE2	1:A:55:LYS:HB2	2.04	0.93
1:D:15:ASN:OD1	1:D:17:ASP:N	2.06	0.88
1:B:15:ASN:C	1:B:15:ASN:OD1	2.14	0.86
1:C:220:ARG:NH1	5:C:2305:HOH:O	2.16	0.78
1:A:65:GLY:O	1:A:201:LYS:NZ	2.15	0.78
5:A:2251:HOH:O	1:C:180:LEU:HD22	1.83	0.78
1:A:171:LYS:CE	5:A:2230:HOH:O	2.36	0.73
1:D:39:GLN:CD	1:D:39:GLN:H	1.93	0.72
1:B:15:ASN:OD1	1:B:17:ASP:N	2.23	0.71
1:D:66:THR:HG21	1:D:239:GLU:HB2	1.74	0.70
5:A:2251:HOH:O	1:C:180:LEU:CD2	2.40	0.69
1:A:101:LYS:HB3	1:A:102:PRO:HD2	1.75	0.69
1:A:171:LYS:HE2	5:A:2230:HOH:O	1.92	0.67
1:A:12:GLU:HG3	1:A:15:ASN:HB2	1.78	0.66
1:C:199:ASP:OD1	1:C:201:LYS:HG2	1.96	0.65
1:B:117:GLN:HA	1:B:149:SER:HB2	1.77	0.65
1:C:117:GLN:HA	1:C:149:SER:HB2	1.78	0.65
1:C:40:ASN:ND2	1:C:42:MET:H	1.95	0.64
1:A:180:LEU:HD22	1:C:180:LEU:HD13	1.80	0.63
5:A:2250:HOH:O	1:C:171:LYS:CE	2.47	0.62
1:B:11:PHE:O	1:B:30:GLY:HA2	2.00	0.62
1:B:15:ASN:O	1:B:15:ASN:OD1	2.18	0.61
1:A:84:ARG:HD3	5:A:2144:HOH:O	2.00	0.60
1:A:117:GLN:HA	1:A:149:SER:HB2	1.83	0.60
1:D:66:THR:CG2	1:D:239:GLU:HG2	2.32	0.59
1:B:95:MET:HG2	1:B:210:VAL:HG12	1.84	0.59
1:D:38:ASN:HB3	1:D:39:GLN:NE2	2.17	0.59
1:D:15:ASN:C	1:D:15:ASN:OD1	2.42	0.58
1:C:201:LYS:HB3	1:C:201:LYS:HZ3	1.69	0.58
1:B:59:ILE:HG12	1:B:208:VAL:HG22	1.86	0.58
1:A:53:TYR:HE2	1:A:55:LYS:HB2	1.64	0.57
1:B:180:LEU:HD21	5:D:2224:HOH:O	2.03	0.57
1:B:220:ARG:HG2	1:B:221:ASP:OD1	2.05	0.56
1:D:122:GLN:HB3	1:D:205:PRO:HD3	1.88	0.56
1:A:101:LYS:HB3	1:A:102:PRO:CD	2.35	0.56
1:B:240:THR:CG2	5:B:2220:HOH:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LYS:HD2	5:C:2289:HOH:O	2.06	0.55
1:D:11:PHE:O	1:D:30:GLY:HA2	2.08	0.54
1:A:84:ARG:NE	5:A:2144:HOH:O	2.34	0.54
5:A:2250:HOH:O	1:C:171:LYS:HE2	2.08	0.54
1:D:15:ASN:OD1	1:D:16:ASN:N	2.42	0.53
1:D:66:THR:HG21	1:D:239:GLU:HG2	1.91	0.53
1:D:25:ILE:HD11	1:D:33:GLN:NE2	2.23	0.53
1:B:119:ASN:N	1:B:119:ASN:HD22	2.06	0.52
1:A:180:LEU:CD2	5:A:2230:HOH:O	2.12	0.52
1:A:84:ARG:CD	5:A:2144:HOH:O	2.56	0.52
1:C:54:THR:O	1:C:54:THR:HG22	2.07	0.52
1:C:84:ARG:NH2	5:C:2177:HOH:O	2.18	0.52
1:C:180:LEU:HD12	1:C:194:ILE:O	2.09	0.52
1:A:53:TYR:OH	5:A:2105:HOH:O	2.14	0.51
1:C:138:PRO:HG2	1:C:139:GLN:NE2	2.25	0.51
1:C:88:ALA:CB	1:C:89:ASP:HA	2.36	0.51
1:A:84:ARG:NH1	5:A:2145:HOH:O	2.44	0.50
1:A:101:LYS:CB	1:A:102:PRO:CD	2.87	0.50
1:C:40:ASN:HD22	1:C:41:GLY:N	2.09	0.50
1:C:95:MET:HG2	1:C:210:VAL:HG12	1.94	0.50
1:C:88:ALA:HB1	1:C:89:ASP:HA	1.93	0.50
1:C:153:ILE:HD12	1:C:196:GLU:HG2	1.93	0.49
1:A:16:ASN:O	1:A:54:THR:HG21	2.13	0.49
1:D:84:ARG:HG2	1:D:84:ARG:HH11	1.78	0.48
1:B:180:LEU:C	1:B:180:LEU:HD12	2.34	0.48
1:A:11:PHE:O	1:A:30:GLY:HA2	2.13	0.48
1:B:38:ASN:ND2	1:B:44:ALA:HB2	2.29	0.48
1:B:122:GLN:HB3	1:B:205:PRO:HD3	1.96	0.48
1:C:122:GLN:HB3	1:C:205:PRO:HD3	1.96	0.48
1:C:38:ASN:ND2	1:C:44:ALA:HB2	2.29	0.48
1:B:21:GLN:HB3	1:B:102:PRO:HG3	1.96	0.47
1:B:38:ASN:HD21	1:B:44:ALA:HB2	1.79	0.47
1:A:36:LYS:HE3	1:A:38:ASN:HD22	1.79	0.47
1:A:180:LEU:HD22	1:C:180:LEU:CD1	2.45	0.47
1:A:220:ARG:NH2	5:A:2270:HOH:O	0.62	0.46
1:A:60:TRP:CE3	1:A:201:LYS:HG3	2.51	0.46
1:D:133:ASN:HB3	1:D:134:PRO:CD	2.45	0.46
1:D:16:ASN:O	1:D:54:THR:HG21	2.14	0.46
1:D:53:TYR:CE2	1:D:55:LYS:HB2	2.50	0.46
1:D:117:GLN:HG2	1:D:149:SER:CB	2.45	0.46
1:A:72:THR:HG22	1:A:170:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HA	1:A:102:PRO:HD3	1.53	0.46
1:B:119:ASN:HD22	1:B:120:SER:N	2.13	0.46
1:A:122:GLN:HB3	1:A:205:PRO:HD3	1.98	0.46
1:D:92:VAL:HG23	1:D:126:VAL:O	2.16	0.45
1:A:60:TRP:CE3	1:A:201:LYS:CG	2.99	0.45
1:D:38:ASN:ND2	1:D:44:ALA:HB2	2.31	0.45
1:A:53:TYR:CD2	1:A:55:LYS:HB2	2.49	0.45
1:C:89:ASP:OD2	2:C:1240:LAT:O3	2.21	0.45
1:A:57:VAL:N	1:A:208:VAL:O	2.43	0.45
1:D:117:GLN:HG2	1:D:149:SER:OG	2.17	0.45
1:D:220:ARG:HD3	5:D:2250:HOH:O	2.17	0.45
1:B:119:ASN:HD22	1:B:120:SER:H	1.63	0.44
1:B:101:LYS:HB3	1:B:102:PRO:HD2	1.99	0.44
1:C:98:THR:HB	5:C:2298:HOH:O	2.18	0.44
1:D:71:GLU:OE1	1:D:171:LYS:HD3	2.17	0.44
1:D:180:LEU:C	1:D:180:LEU:HD12	2.38	0.44
1:B:224:GLU:HG3	1:B:226:HIS:CE1	2.54	0.43
1:C:6:PHE:CE2	1:C:233:PHE:HB3	2.53	0.43
1:A:36:LYS:HE3	1:A:38:ASN:ND2	2.34	0.43
1:A:67:VAL:CG2	1:A:201:LYS:HE2	2.48	0.43
1:B:133:ASN:HB3	1:B:134:PRO:CD	2.49	0.43
1:C:72:THR:HG22	1:C:170:ILE:HB	2.01	0.43
1:B:183:LEU:HD23	1:B:183:LEU:C	2.39	0.43
1:B:25:ILE:HD11	1:B:33:GLN:NE2	2.34	0.42
1:C:39:GLN:HG3	5:C:2094:HOH:O	2.19	0.42
1:A:95:MET:HG2	1:A:210:VAL:HG12	2.00	0.42
1:D:133:ASN:HB3	1:D:134:PRO:HD2	2.02	0.42
1:C:88:ALA:HA	1:C:89:ASP:HA	1.66	0.42
1:D:84:ARG:HA	1:D:85:PRO:C	2.40	0.42
1:A:6:PHE:CE2	1:A:233:PHE:HB3	2.54	0.42
1:A:146:ASP:HB3	1:A:149:SER:O	2.21	0.41
1:A:28:GLN:NE2	5:A:2052:HOH:O	2.54	0.41
1:C:40:ASN:HD22	1:C:40:ASN:C	2.23	0.41
1:B:59:ILE:CG1	1:B:208:VAL:HG22	2.51	0.41
1:D:117:GLN:HA	1:D:149:SER:HB2	2.03	0.41
1:A:180:LEU:C	1:A:180:LEU:HD12	2.40	0.41
1:B:88:ALA:HB1	1:B:89:ASP:CG	2.42	0.41
1:C:183:LEU:C	1:C:183:LEU:HD23	2.42	0.41
1:A:104:GLN:HG3	1:A:113:ASN:HA	2.04	0.40
1:C:88:ALA:HB1	1:C:89:ASP:CG	2.42	0.40
1:D:23:ALA:O	1:D:25:ILE:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HA	1:A:56:PRO:HD3	1.35	0.40
1:B:119:ASN:N	1:B:119:ASN:ND2	2.69	0.40
1:C:100:SER:HB3	5:C:2182:HOH:O	2.20	0.40
1:B:117:GLN:HG3	1:B:149:SER:HB2	2.02	0.40
1:C:88:ALA:HB1	1:C:89:ASP:CA	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2060:HOH:O	5:C:2161:HOH:O[1_655]	0.22	1.98

## 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	238/242 (98%)	233 (98%)	4 (2%)	1 (0%)	36	19
1	B	238/242 (98%)	231 (97%)	7 (3%)	0	100	100
1	C	238/242 (98%)	231 (97%)	7 (3%)	0	100	100
1	D	237/242 (98%)	232 (98%)	5 (2%)	0	100	100
All	All	951/968 (98%)	927 (98%)	23 (2%)	1 (0%)	53	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLU

### 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	205/208 (99%)	202 (98%)	3 (2%)	67	53
1	B	206/208 (99%)	203 (98%)	3 (2%)	67	53
1	C	206/208 (99%)	200 (97%)	6 (3%)	45	25
1	D	205/208 (99%)	202 (98%)	3 (2%)	67	53
All	All	822/832 (99%)	807 (98%)	15 (2%)	62	45

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	89	ASP
1	A	220	ARG
1	B	15	ASN
1	B	119	ASN
1	B	240	THR
1	C	40	ASN
1	C	84	ARG
1	C	89	ASP
1	C	161	ASP
1	C	201	LYS
1	C	220	ARG
1	D	1	VAL
1	D	39	GLN
1	D	239	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	38	ASN
1	A	80	GLN
1	A	122	GLN

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Mol	Chain	Res	Type
1	B	33	GLN
1	B	38	ASN
1	B	39	GLN
1	B	80	GLN
1	B	117	GLN
1	B	119	ASN
1	B	156	GLN
1	C	33	GLN
1	C	38	ASN
1	C	40	ASN
1	C	80	GLN
1	C	117	GLN
1	C	119	ASN
1	D	33	GLN
1	D	38	ASN
1	D	39	GLN
1	D	80	GLN
1	D	119	ASN
1	D	122	GLN
1	D	156	GLN
1	D	202	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LAT	A	1240	-	24,24,24	0.99	1 (4%)	35,35,35	0.89	1 (2%)
2	LAT	B	1240	-	24,24,24	1.40	3 (12%)	35,35,35	0.87	1 (2%)
2	LAT	C	1240	-	24,24,24	0.71	0	35,35,35	0.76	0
2	LAT	D	1240	-	24,24,24	0.72	0	35,35,35	0.75	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	LAT	A	1240	-	-	0/8/48/48	0/2/2/2
2	LAT	B	1240	-	-	0/8/48/48	0/2/2/2
2	LAT	C	1240	-	-	0/8/48/48	0/2/2/2
2	LAT	D	1240	-	-	0/8/48/48	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1240	LAT	O6'-C6'	-3.24	1.28	1.42
2	B	1240	LAT	C4-C3	2.03	1.57	1.52
2	B	1240	LAT	C1-C2	2.37	1.59	1.52
2	B	1240	LAT	C3-C2	3.92	1.62	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1240	LAT	C4-C3-C2	-3.03	105.51	110.83
2	A	1240	LAT	O6'-C6'-C5'	2.69	120.68	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1240	LAT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	B	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	239:GLU	C	240:THR	N	3.11
1	C	240:THR	C	241:ASN	N	2.69
1	B	101:LYS	C	102:PRO	N	1.20
1	C	152:SER	C	153:ILE	N	1.20

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.