



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 09:12 PM UTC

PDB ID : 9LKG / pdb_00009lkg
Title : Ornithine decarboxylase from *Lactocaseibacillus rhamnosus*
Authors : Kim, D.S.; Park, J.H.; Adiko, N.N.; Seo, H.T.
Deposited on : 2025-01-16
Resolution : 2.09 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

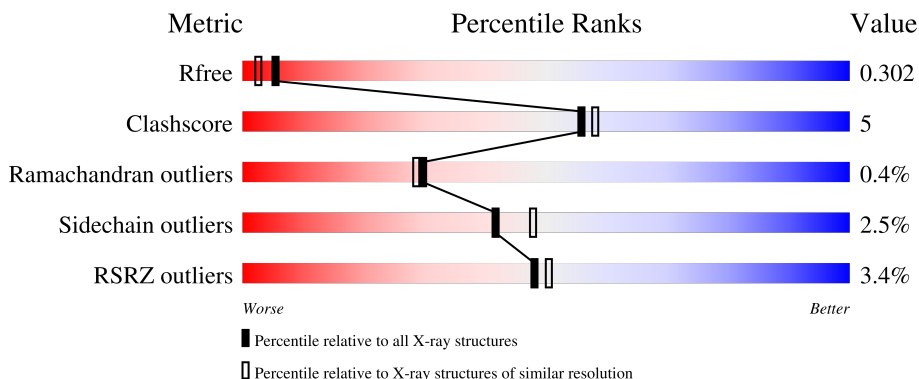
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	693	 3% 87% 12%
1	B	693	 4% 87% 11% .
1	C	693	 3% 86% 14%
1	D	693	 3% 87% 12% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 22182 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 Ornithine decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	C	693	5324	3410	912	993	1	8	15	0	0
1	A	693	5324	3410	912	993	1	8	15	0	0
1	B	692	5324	3408	912	995	1	8	15	0	0
1	D	692	5324	3408	912	995	1	8	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	ASP	ASN	conflict	UNP A0AAN4BJQ6
C	66	TYR	HIS	conflict	UNP A0AAN4BJQ6
C	102	GLU	GLY	conflict	UNP A0AAN4BJQ6
C	455	VAL	ALA	conflict	UNP A0AAN4BJQ6
C	620	ASP	GLU	conflict	UNP A0AAN4BJQ6
C	654	GLU	PRO	conflict	UNP A0AAN4BJQ6
A	17	ASP	ASN	conflict	UNP A0AAN4BJQ6
A	66	TYR	HIS	conflict	UNP A0AAN4BJQ6
A	102	GLU	GLY	conflict	UNP A0AAN4BJQ6
A	455	VAL	ALA	conflict	UNP A0AAN4BJQ6
A	620	ASP	GLU	conflict	UNP A0AAN4BJQ6
A	654	GLU	PRO	conflict	UNP A0AAN4BJQ6
B	17	ASP	ASN	conflict	UNP A0AAN4BJQ6
B	66	TYR	HIS	conflict	UNP A0AAN4BJQ6
B	102	GLU	GLY	conflict	UNP A0AAN4BJQ6
B	455	VAL	ALA	conflict	UNP A0AAN4BJQ6
B	620	ASP	GLU	conflict	UNP A0AAN4BJQ6
B	654	GLU	PRO	conflict	UNP A0AAN4BJQ6
D	17	ASP	ASN	conflict	UNP A0AAN4BJQ6
D	66	TYR	HIS	conflict	UNP A0AAN4BJQ6
D	102	GLU	GLY	conflict	UNP A0AAN4BJQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	455	VAL	ALA	conflict	UNP A0AAN4BJQ6
D	620	ASP	GLU	conflict	UNP A0AAN4BJQ6
D	654	GLU	PRO	conflict	UNP A0AAN4BJQ6

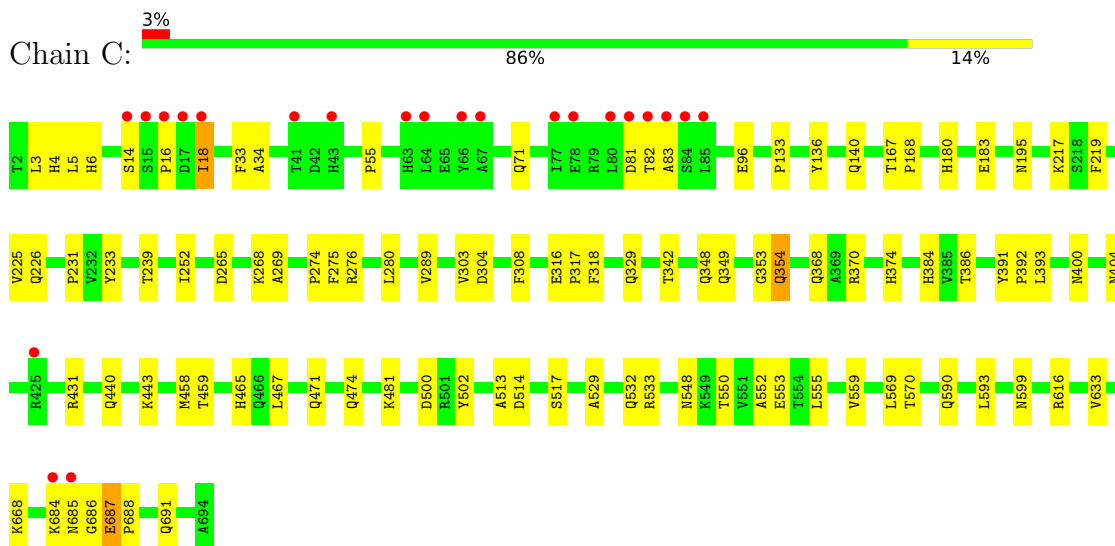
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	218	Total O 218 218	0	0
2	A	220	Total O 220 220	0	0
2	B	232	Total O 232 232	0	0
2	D	216	Total O 216 216	0	0

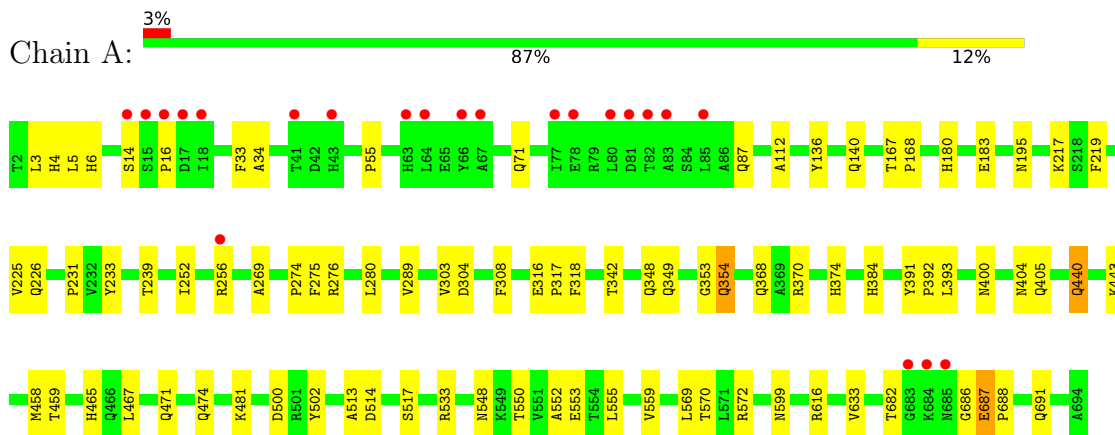
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

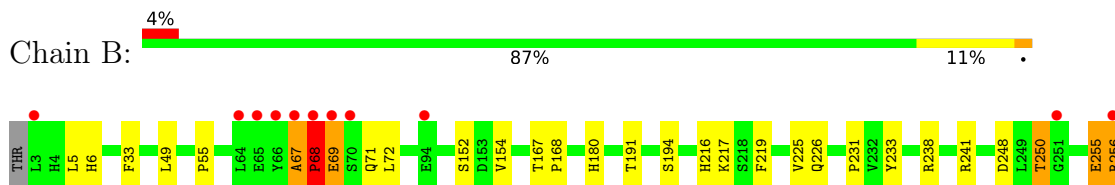
- Molecule 1: Ornithine decarboxylase

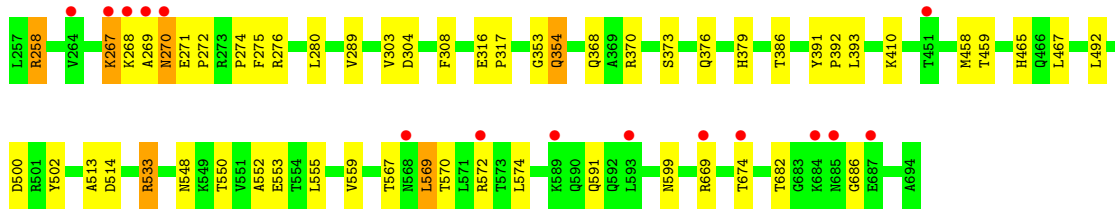


- Molecule 1: Ornithine decarboxylase

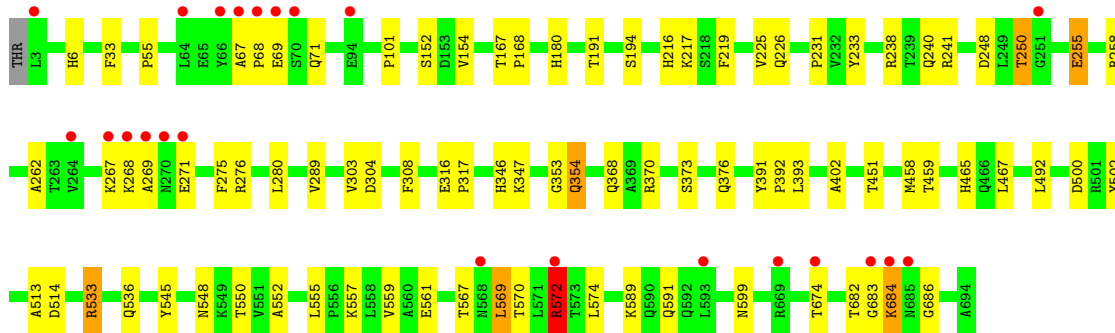
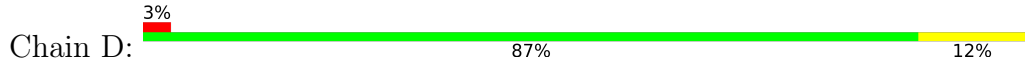


- Molecule 1: Ornithine decarboxylase





● Molecule 1: Ornithine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.78Å 80.61Å 121.82Å 86.75° 80.61° 70.83°	Depositor
Resolution (Å)	47.25 – 2.09 47.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.25-2.09) 96.5 (47.25-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.278 , 0.301 0.281 , 0.302	Depositor DCC
R_{free} test set	7220 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtrriage
Anisotropy	0.181	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22182	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 93.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1645e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.57	2/5437 (0.0%)	0.85	3/7435 (0.0%)
1	B	0.56	2/5436 (0.0%)	0.87	4/7433 (0.1%)
1	C	0.57	1/5437 (0.0%)	0.85	3/7435 (0.0%)
1	D	0.56	1/5436 (0.0%)	0.85	3/7433 (0.0%)
All	All	0.56	6/21746 (0.0%)	0.85	13/29736 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	6
1	C	0	3
1	D	0	2
All	All	0	15

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	HIS	CE1-NE2	5.52	1.38	1.32
1	D	216	HIS	CE1-NE2	5.50	1.38	1.32
1	A	4	HIS	CE1-NE2	5.17	1.37	1.32
1	C	384	HIS	CE1-NE2	5.11	1.37	1.32
1	A	384	HIS	CE1-NE2	5.10	1.37	1.32
1	B	379	HIS	CE1-NE2	5.01	1.37	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	ASN	N-CA-C	-12.03	98.97	112.57
1	D	231	PRO	N-CA-C	6.87	125.22	111.69
1	B	231	PRO	N-CA-C	6.76	125.01	111.69
1	D	68	PRO	N-CA-CB	6.68	110.27	103.25
1	A	231	PRO	N-CA-C	6.47	125.80	112.47
1	C	231	PRO	N-CA-C	6.46	125.77	112.47
1	B	68	PRO	N-CA-CB	5.79	109.33	103.25
1	C	16	PRO	N-CA-CB	5.66	108.72	103.46
1	A	16	PRO	N-CA-CB	5.46	108.54	103.46
1	D	69	GLU	N-CA-C	-5.30	104.17	111.81
1	C	231	PRO	CB-CA-C	-5.18	103.01	111.56
1	B	267	LYS	N-CA-C	-5.09	105.86	111.71
1	A	231	PRO	CB-CA-C	-5.03	103.27	111.56

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	ARG	Sidechain
1	A	533	ARG	Sidechain
1	A	572	ARG	Sidechain
1	A	616	ARG	Sidechain
1	B	241	ARG	Sidechain
1	B	256	ARG	Sidechain
1	B	258	ARG	Sidechain
1	B	533	ARG	Sidechain
1	B	572	ARG	Sidechain
1	B	669	ARG	Sidechain
1	C	431	ARG	Sidechain
1	C	533	ARG	Sidechain
1	C	616	ARG	Sidechain
1	D	241	ARG	Sidechain
1	D	572	ARG	Sidechain

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	5324	0	5219	44	0
1	B	5324	0	5231	50	0
1	C	5324	0	5219	58	0
1	D	5324	0	5231	47	0
2	A	220	0	0	4	0
2	B	232	0	0	4	0
2	C	218	0	0	4	0
2	D	216	0	0	1	0
All	All	22182	0	20900	196	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 (196) 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:262:ALA:HB2	1:D:269:ALA:HB2	1.46	0.96
1:A:465:HIS:HD2	1:A:467:LEU:H	1.16	0.94
1:C:465:HIS:HD2	1:C:467:LEU:H	1.16	0.93
1:D:262:ALA:HB2	1:D:269:ALA:CB	1.99	0.93
1:B:465:HIS:HD2	1:B:467:LEU:H	1.15	0.91
1:D:465:HIS:HD2	1:D:467:LEU:H	1.15	0.91
1:B:268:LYS:C	1:B:270:ASN:H	1.83	0.86
1:B:67:ALA:O	1:B:68:PRO:CB	2.26	0.82
1:B:682:THR:CG2	1:B:686:GLY:HA2	2.15	0.76
1:B:233:TYR:H	1:B:599:ASN:HD21	1.32	0.75
1:D:233:TYR:H	1:D:599:ASN:HD21	1.33	0.75
1:B:682:THR:HG23	1:B:686:GLY:HA2	1.69	0.74
1:C:233:TYR:H	1:C:599:ASN:HD21	1.33	0.73
1:C:4:HIS:HD2	1:C:96:GLU:OE2	1.71	0.73
1:A:233:TYR:H	1:A:599:ASN:HD21	1.33	0.72
1:D:346:HIS:HE1	1:D:347:LLP:OP1	1.72	0.72
1:D:262:ALA:CB	1:D:269:ALA:HB2	2.18	0.71
1:A:471:GLN:H	1:A:474:GLN:HE21	1.38	0.70
1:C:471:GLN:H	1:C:474:GLN:HE21	1.39	0.69
1:D:238:ARG:HE	1:D:591:GLN:NE2	1.91	0.68
1:B:268:LYS:C	1:B:270:ASN:N	2.51	0.68
1:B:238:ARG:HE	1:B:591:GLN:NE2	1.92	0.68
1:D:258:ARG:NH1	1:D:269:ALA:O	2.29	0.65
1:D:240:GLN:HG3	1:D:589:LYS:HE3	1.79	0.65
1:B:268:LYS:HA	1:B:271:GLU:HG3	1.79	0.64
1:D:545:TYR:CZ	1:D:572:ARG:HG3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:ARG:NH1	1:D:536:GLN:OE1	2.23	0.63
1:A:374:HIS:HE1	2:A:790:HOH:O	1.83	0.62
1:C:440:GLN:HA	1:C:443:LYS:HD2	1.82	0.62
1:B:459:THR:O	1:B:465:HIS:HE1	1.81	0.62
1:D:459:THR:O	1:D:465:HIS:HE1	1.81	0.62
1:A:459:THR:O	1:A:465:HIS:HE1	1.83	0.62
1:C:459:THR:O	1:C:465:HIS:HE1	1.83	0.61
1:B:271:GLU:N	2:B:701:HOH:O	2.33	0.61
1:A:502:TYR:HA	1:A:555:LEU:HD21	1.83	0.60
1:D:682:THR:CG2	1:D:686:GLY:HA2	2.31	0.60
1:C:374:HIS:HE1	2:C:815:HOH:O	1.85	0.60
1:C:502:TYR:HA	1:C:555:LEU:HD21	1.84	0.60
1:C:687:GLU:HG2	1:C:688:PRO:HD2	1.83	0.59
1:B:68:PRO:O	1:B:69:GLU:O	2.20	0.59
1:C:368:GLN:NE2	1:C:370:ARG:HE	2.00	0.59
1:D:373:SER:H	1:D:376:GLN:NE2	1.99	0.59
1:B:373:SER:H	1:B:376:GLN:NE2	2.00	0.59
1:A:368:GLN:NE2	1:A:370:ARG:HE	2.00	0.59
1:C:348:GLN:HE22	1:C:481:LYS:HZ2	1.50	0.58
1:A:348:GLN:HE22	1:A:481:LYS:HZ2	1.50	0.58
1:A:687:GLU:HG2	1:A:688:PRO:HD2	1.84	0.58
1:B:238:ARG:HE	1:B:591:GLN:HE21	1.49	0.58
1:D:238:ARG:HE	1:D:591:GLN:HE21	1.49	0.58
1:B:368:GLN:NE2	1:B:370:ARG:HE	2.01	0.58
1:D:368:GLN:NE2	1:D:370:ARG:HE	2.01	0.58
1:D:373:SER:H	1:D:376:GLN:HE21	1.52	0.58
1:B:373:SER:H	1:B:376:GLN:HE21	1.52	0.58
1:B:502:TYR:HA	1:B:555:LEU:HD21	1.86	0.57
1:B:465:HIS:CD2	1:B:467:LEU:H	2.08	0.57
1:D:465:HIS:CD2	1:D:467:LEU:H	2.08	0.56
1:D:502:TYR:HA	1:D:555:LEU:HD21	1.86	0.56
1:A:471:GLN:H	1:A:474:GLN:NE2	2.02	0.56
1:D:682:THR:HG23	1:D:686:GLY:HA2	1.88	0.56
1:C:471:GLN:H	1:C:474:GLN:NE2	2.03	0.56
1:B:353:GLY:O	1:B:354:GLN:HB2	2.05	0.55
1:D:353:GLY:O	1:D:354:GLN:HB2	2.05	0.55
1:C:684:LYS:C	1:C:686:GLY:H	2.15	0.55
1:B:269:ALA:HA	1:B:274:PRO:HG3	1.89	0.55
1:A:465:HIS:CD2	1:A:467:LEU:H	2.08	0.54
1:C:316:GLU:N	1:C:317:PRO:CD	2.70	0.54
1:C:465:HIS:CD2	1:C:467:LEU:H	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLU:N	1:A:317:PRO:CD	2.70	0.54
1:A:349:GLN:NE2	1:A:400:ASN:HD21	2.05	0.53
1:D:262:ALA:CA	1:D:269:ALA:HB2	2.39	0.53
1:C:349:GLN:NE2	1:C:400:ASN:HD21	2.06	0.53
1:C:353:GLY:O	1:C:354:GLN:HB2	2.06	0.53
1:B:258:ARG:NH2	1:B:272:PRO:O	2.42	0.52
1:D:316:GLU:N	1:D:317:PRO:CD	2.72	0.52
1:A:353:GLY:O	1:A:354:GLN:HB2	2.07	0.52
1:B:167:THR:N	1:B:168:PRO:CD	2.73	0.52
1:D:167:THR:N	1:D:168:PRO:CD	2.73	0.52
1:A:348:GLN:NE2	1:A:481:LYS:NZ	2.58	0.52
1:C:348:GLN:NE2	1:C:481:LYS:NZ	2.58	0.52
1:B:316:GLU:N	1:B:317:PRO:CD	2.73	0.52
1:C:81:ASP:O	1:C:82:THR:C	2.54	0.51
1:C:239:THR:HG22	1:C:467:LEU:HG	1.93	0.51
1:A:239:THR:HG22	1:A:467:LEU:HG	1.93	0.51
1:C:348:GLN:HE22	1:C:481:LYS:NZ	2.09	0.50
1:A:348:GLN:HE22	1:A:481:LYS:NZ	2.09	0.50
1:D:683:GLY:O	1:D:684:LYS:C	2.55	0.50
1:C:225:VAL:HG12	1:C:226:GLN:HE21	1.75	0.50
1:A:225:VAL:HG12	1:A:226:GLN:HE21	1.76	0.50
1:B:49:LEU:HB3	1:B:72:LEU:HD11	1.94	0.50
1:B:268:LYS:O	1:B:269:ALA:HB3	2.10	0.50
1:D:368:GLN:HE22	1:D:370:ARG:HH21	1.60	0.50
1:A:167:THR:N	1:A:168:PRO:CD	2.75	0.50
1:B:368:GLN:HE22	1:B:370:ARG:HH21	1.60	0.50
1:C:167:THR:N	1:C:168:PRO:CD	2.75	0.49
1:A:440:GLN:HG3	1:A:443:LYS:HD2	1.93	0.49
1:C:354:GLN:HG2	1:B:386:THR:HG21	1.94	0.49
1:B:248:ASP:OD1	1:B:250:THR:OG1	2.23	0.49
1:D:248:ASP:OD1	1:D:250:THR:OG1	2.23	0.48
1:A:682:THR:CG2	1:A:686:GLY:HA2	2.43	0.48
1:B:458:MET:HE2	1:B:465:HIS:HB2	1.95	0.48
1:C:684:LYS:C	1:C:686:GLY:N	2.71	0.48
1:D:458:MET:HE2	1:D:465:HIS:HB2	1.95	0.48
1:D:552:ALA:HA	1:D:559:VAL:HG21	1.94	0.48
1:B:552:ALA:HA	1:B:559:VAL:HG21	1.94	0.48
1:B:55:PRO:HA	1:B:71:GLN:O	2.14	0.47
1:D:180:HIS:HD2	2:D:717:HOH:O	1.97	0.47
1:B:270:ASN:C	2:B:701:HOH:O	2.58	0.47
1:D:275:PHE:HB2	1:D:303:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:PHE:HB2	1:C:303:VAL:HG12	1.97	0.47
1:B:275:PHE:HB2	1:B:303:VAL:HG12	1.97	0.47
1:A:252:ILE:HD11	2:A:860:HOH:O	2.15	0.47
1:A:275:PHE:HB2	1:A:303:VAL:HG12	1.97	0.47
1:C:458:MET:HE2	1:C:465:HIS:HB2	1.97	0.46
1:B:180:HIS:HD2	2:B:720:HOH:O	1.97	0.46
1:A:458:MET:HE2	1:A:465:HIS:HB2	1.97	0.46
1:D:572:ARG:HG2	1:D:572:ARG:HH11	1.80	0.46
1:D:225:VAL:HG12	1:D:226:GLN:HE21	1.79	0.46
1:C:552:ALA:HA	1:C:559:VAL:HG21	1.97	0.46
1:C:136:TYR:O	1:C:140:GLN:HG2	2.16	0.46
1:B:225:VAL:HG12	1:B:226:GLN:HE21	1.80	0.46
1:C:252:ILE:HD11	2:C:870:HOH:O	2.16	0.45
1:B:500:ASP:HB2	1:B:513:ALA:HB2	1.98	0.45
1:D:6:HIS:O	1:D:33:PHE:HA	2.17	0.45
1:D:569:LEU:HD23	1:D:574:LEU:HB2	1.98	0.45
1:B:6:HIS:O	1:B:33:PHE:HA	2.17	0.45
1:C:593:LEU:C	1:C:593:LEU:HD23	2.41	0.45
1:A:552:ALA:HA	1:A:559:VAL:HG21	1.98	0.45
1:D:500:ASP:HB2	1:D:513:ALA:HB2	1.98	0.45
1:C:329:GLN:NE2	2:C:709:HOH:O	2.50	0.45
1:B:269:ALA:C	1:B:271:GLU:H	2.25	0.45
1:B:569:LEU:HD23	1:B:574:LEU:HB2	1.98	0.45
1:A:269:ALA:HA	1:A:274:PRO:HB3	1.99	0.45
1:C:269:ALA:HA	1:C:274:PRO:HB3	1.99	0.45
1:A:136:TYR:O	1:A:140:GLN:HG2	2.17	0.45
1:C:180:HIS:HD2	2:C:773:HOH:O	1.99	0.44
1:C:550:THR:HA	1:C:570:THR:HA	1.99	0.44
1:A:6:HIS:O	1:A:33:PHE:HA	2.17	0.44
1:C:6:HIS:O	1:C:33:PHE:HA	2.17	0.44
1:C:276:ARG:O	1:C:304:ASP:HB2	2.18	0.44
1:A:276:ARG:O	1:A:304:ASP:HB2	2.18	0.44
1:D:255:GLU:CD	1:D:255:GLU:H	2.26	0.44
1:C:18:ILE:HD12	1:C:18:ILE:HA	1.78	0.44
1:C:55:PRO:HA	1:C:71:GLN:O	2.17	0.44
1:C:368:GLN:HE22	1:C:370:ARG:HH21	1.66	0.44
1:A:55:PRO:HA	1:A:71:GLN:O	2.17	0.44
1:A:550:THR:HA	1:A:570:THR:HA	1.99	0.43
1:A:112:ALA:O	2:A:701:HOH:O	2.21	0.43
1:A:368:GLN:HE22	1:A:370:ARG:HH21	1.66	0.43
1:B:255:GLU:CD	1:B:255:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:PRO:HA	1:D:71:GLN:O	2.19	0.43
1:D:391:TYR:N	1:D:392:PRO:CD	2.82	0.42
1:A:195:ASN:HD22	1:A:342:THR:HG21	1.85	0.42
1:A:550:THR:OG1	1:A:553:GLU:HG2	2.19	0.42
1:C:5:LEU:HB2	1:C:34:ALA:HB2	2.00	0.42
1:C:440:GLN:OE1	1:C:443:LYS:HE3	2.19	0.42
1:C:500:ASP:HB2	1:C:513:ALA:HB2	2.00	0.42
1:A:500:ASP:HB2	1:A:513:ALA:HB2	2.00	0.42
1:A:633:VAL:HG22	1:A:691:GLN:O	2.20	0.42
1:C:195:ASN:HD22	1:C:342:THR:HG21	1.85	0.42
1:C:391:TYR:N	1:C:392:PRO:CD	2.81	0.42
1:A:391:TYR:N	1:A:392:PRO:CD	2.82	0.42
1:B:391:TYR:N	1:B:392:PRO:CD	2.83	0.42
1:C:550:THR:OG1	1:C:553:GLU:HG2	2.20	0.42
1:A:5:LEU:HB2	1:A:34:ALA:HB2	2.00	0.42
1:C:514:ASP:HB2	1:C:517:SER:OG	2.20	0.42
1:D:191:THR:HA	1:D:194:SER:HB2	2.01	0.42
1:C:386:THR:HG21	1:B:354:GLN:HG2	2.00	0.42
1:B:276:ARG:O	1:B:304:ASP:HB2	2.20	0.42
1:D:276:ARG:O	1:D:304:ASP:HB2	2.20	0.42
1:C:633:VAL:HG22	1:C:691:GLN:O	2.20	0.41
1:B:191:THR:HA	1:B:194:SER:HB2	2.01	0.41
1:D:280:LEU:O	1:D:308:PHE:HA	2.20	0.41
1:C:81:ASP:C	1:C:83:ALA:N	2.76	0.41
1:C:318:PHE:CZ	1:C:404:ASN:HB3	2.55	0.41
1:A:318:PHE:CZ	1:A:404:ASN:HB3	2.56	0.41
1:A:514:ASP:HB2	1:A:517:SER:OG	2.21	0.41
1:C:233:TYR:N	1:C:599:ASN:HD21	2.11	0.41
1:B:550:THR:HA	1:B:570:THR:HA	2.02	0.41
1:C:593:LEU:HD23	1:C:593:LEU:O	2.20	0.41
1:C:133:PRO:HB3	1:B:5:LEU:HD11	2.03	0.41
1:C:183:GLU:OE2	1:C:374:HIS:HD2	2.04	0.41
1:C:529:ALA:HA	1:C:532:GLN:HE21	1.85	0.41
1:B:280:LEU:O	1:B:308:PHE:HA	2.20	0.41
1:B:410:LYS:HE3	2:B:810:HOH:O	2.19	0.41
1:A:183:GLU:OE2	1:A:374:HIS:HD2	2.04	0.41
1:B:152:SER:OG	1:B:154:VAL:HG12	2.21	0.41
1:D:101:PRO:HG3	1:D:402:ALA:HB2	2.03	0.41
1:D:550:THR:HA	1:D:570:THR:HA	2.02	0.41
1:D:557:LYS:O	1:D:561:GLU:HG3	2.21	0.41
1:D:152:SER:OG	1:D:154:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:LYS:HA	1:D:271:GLU:HG3	2.02	0.41
1:A:180:HIS:HD2	2:A:771:HOH:O	2.03	0.40
1:C:280:LEU:O	1:C:308:PHE:HA	2.21	0.40
1:A:280:LEU:O	1:A:308:PHE:HA	2.21	0.40
1:B:550:THR:OG1	1:B:553:GLU:HG2	2.21	0.40
1:C:265:ASP:OD2	1:C:268:LYS:HE2	2.21	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	690/693 (100%)	674 (98%)	15 (2%)	1 (0%)	48	50
1	B	689/693 (99%)	669 (97%)	16 (2%)	4 (1%)	21	18
1	C	690/693 (100%)	673 (98%)	15 (2%)	2 (0%)	36	36
1	D	689/693 (99%)	667 (97%)	19 (3%)	3 (0%)	30	28
All	All	2758/2772 (100%)	2683 (97%)	65 (2%)	10 (0%)	30	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	ALA
1	B	68	PRO
1	D	67	ALA
1	B	69	GLU
1	B	354	GLN
1	D	354	GLN
1	C	354	GLN
1	A	354	GLN
1	D	684	LYS

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Mol	Chain	Res	Type
1	C	685	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	544/555 (98%)	532 (98%)	12 (2%)	45	53
1	B	547/555 (99%)	532 (97%)	15 (3%)	39	45
1	C	544/555 (98%)	532 (98%)	12 (2%)	45	53
1	D	547/555 (99%)	531 (97%)	16 (3%)	37	42
All	All	2182/2220 (98%)	2127 (98%)	55 (2%)	42	48

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	LEU
1	C	14	SER
1	C	18	ILE
1	C	217	LYS
1	C	219	PHE
1	C	289	VAL
1	C	393	LEU
1	C	548	ASN
1	C	569	LEU
1	C	590	GLN
1	C	668	LYS
1	C	687	GLU
1	A	3	LEU
1	A	14	SER
1	A	87	GLN
1	A	217	LYS
1	A	219	PHE
1	A	289	VAL
1	A	393	LEU
1	A	405	GLN

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Mol	Chain	Res	Type
1	A	440	GLN
1	A	548	ASN
1	A	569	LEU
1	A	687	GLU
1	B	217	LYS
1	B	219	PHE
1	B	250	THR
1	B	255	GLU
1	B	256	ARG
1	B	267	LYS
1	B	289	VAL
1	B	393	LEU
1	B	492	LEU
1	B	514	ASP
1	B	533	ARG
1	B	548	ASN
1	B	567	THR
1	B	569	LEU
1	B	674	THR
1	D	217	LYS
1	D	219	PHE
1	D	250	THR
1	D	255	GLU
1	D	267	LYS
1	D	289	VAL
1	D	393	LEU
1	D	451	THR
1	D	492	LEU
1	D	514	ASP
1	D	533	ARG
1	D	548	ASN
1	D	567	THR
1	D	569	LEU
1	D	572	ARG
1	D	674	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4	HIS
1	C	28	HIS
1	C	48	GLN

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Mol	Chain	Res	Type
1	C	139	HIS
1	C	180	HIS
1	C	195	ASN
1	C	215	ASN
1	C	226	GLN
1	C	329	GLN
1	C	348	GLN
1	C	349	GLN
1	C	357	GLN
1	C	368	GLN
1	C	374	HIS
1	C	405	GLN
1	C	465	HIS
1	C	474	GLN
1	C	532	GLN
1	C	584	GLN
1	C	590	GLN
1	C	599	ASN
1	C	600	ASN
1	C	678	GLN
1	A	6	HIS
1	A	28	HIS
1	A	48	GLN
1	A	124	HIS
1	A	139	HIS
1	A	180	HIS
1	A	189	ASN
1	A	195	ASN
1	A	215	ASN
1	A	226	GLN
1	A	294	GLN
1	A	346	HIS
1	A	348	GLN
1	A	349	GLN
1	A	354	GLN
1	A	368	GLN
1	A	374	HIS
1	A	405	GLN
1	A	465	HIS
1	A	474	GLN
1	A	584	GLN
1	A	590	GLN

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Mol	Chain	Res	Type
1	A	599	ASN
1	A	600	ASN
1	A	678	GLN
1	B	6	HIS
1	B	139	HIS
1	B	195	ASN
1	B	215	ASN
1	B	226	GLN
1	B	368	GLN
1	B	376	GLN
1	B	465	HIS
1	B	532	GLN
1	B	540	GLN
1	B	548	ASN
1	B	584	GLN
1	B	591	GLN
1	B	599	ASN
1	B	600	ASN
1	D	6	HIS
1	D	124	HIS
1	D	139	HIS
1	D	189	ASN
1	D	195	ASN
1	D	215	ASN
1	D	226	GLN
1	D	329	GLN
1	D	346	HIS
1	D	354	GLN
1	D	368	GLN
1	D	376	GLN
1	D	379	HIS
1	D	465	HIS
1	D	532	GLN
1	D	540	GLN
1	D	584	GLN
1	D	591	GLN
1	D	599	ASN
1	D	600	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	D	347	1	23,24,25	0.49	0	25,32,34	0.69	0
1	LLP	A	347	1	23,24,25	0.46	0	25,32,34	0.58	0
1	LLP	B	347	1	23,24,25	0.47	0	25,32,34	0.65	0
1	LLP	C	347	1	23,24,25	0.47	0	25,32,34	0.64	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
1	LLP	D	347	1	-	2/16/17/19	0/1/1/1
1	LLP	A	347	1	-	5/16/17/19	0/1/1/1
1	LLP	B	347	1	-	8/16/17/19	0/1/1/1
1	LLP	C	347	1	-	4/16/17/19	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	347	LLP	C4-C4'-NZ-CE
1	A	347	LLP	C4-C4'-NZ-CE
1	B	347	LLP	C4-C4'-NZ-CE
1	B	347	LLP	C5'-OP4-P-OP1
1	B	347	LLP	C5'-OP4-P-OP2
1	D	347	LLP	C4-C4'-NZ-CE
1	C	347	LLP	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	A	347	LLP	CG-CD-CE-NZ
1	A	347	LLP	C3-C4-C4'-NZ
1	B	347	LLP	C4-C5-C5'-OP4
1	C	347	LLP	CD-CE-NZ-C4'
1	A	347	LLP	CD-CE-NZ-C4'
1	C	347	LLP	C3-C4-C4'-NZ
1	B	347	LLP	C3-C4-C4'-NZ
1	D	347	LLP	C3-C4-C4'-NZ
1	B	347	LLP	C6-C5-C5'-OP4
1	B	347	LLP	C5'-OP4-P-OP3
1	A	347	LLP	C5-C4-C4'-NZ
1	B	347	LLP	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	347	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
1	A	692/693 (99%)	0.11	22 (3%) 50 53	14, 25, 44, 71	0
1	B	691/693 (99%)	0.09	26 (3%) 44 46	14, 25, 42, 65	0
1	C	692/693 (99%)	0.11	22 (3%) 50 53	14, 25, 45, 67	0
1	D	691/693 (99%)	0.08	23 (3%) 49 51	14, 25, 42, 64	0
All	All	2766/2772 (99%)	0.10	93 (3%) 48 50	14, 25, 44, 71	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	PRO	13.3
1	B	270	ASN	11.1
1	B	68	PRO	9.6
1	D	269	ALA	8.3
1	B	269	ALA	6.9
1	D	69	GLU	6.0
1	C	83	ALA	5.9
1	B	268	LYS	5.9
1	B	69	GLU	5.7
1	C	684	LYS	5.7
1	C	77	ILE	5.6
1	B	685	ASN	5.6
1	A	77	ILE	5.4
1	B	66	TYR	5.4
1	A	83	ALA	5.3
1	A	685	ASN	5.3
1	D	270	ASN	5.2
1	D	3	LEU	5.1
1	C	685	ASN	5.1
1	A	63	HIS	4.9
1	D	685	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	16	PRO	4.7
1	B	67	ALA	4.6
1	D	268	LYS	4.6
1	D	67	ALA	4.5
1	D	66	TYR	4.5
1	C	63	HIS	4.4
1	C	16	PRO	4.3
1	C	80	LEU	4.3
1	C	17	ASP	4.3
1	A	80	LEU	4.3
1	D	684	LYS	4.2
1	A	17	ASP	4.0
1	C	64	LEU	3.6
1	A	256	ARG	3.6
1	A	64	LEU	3.5
1	C	81	ASP	3.4
1	A	81	ASP	3.4
1	C	15	SER	3.4
1	A	82	THR	3.4
1	A	15	SER	3.3
1	C	78	GLU	3.3
1	D	572	ARG	3.2
1	C	82	THR	3.2
1	B	568	ASN	3.2
1	B	3	LEU	3.2
1	B	64	LEU	3.1
1	D	568	ASN	3.1
1	C	14	SER	3.1
1	B	94	GLU	3.0
1	B	251	GLY	3.0
1	A	78	GLU	3.0
1	D	674	THR	3.0
1	D	64	LEU	3.0
1	A	684	LYS	2.9
1	A	14	SER	2.9
1	B	572	ARG	2.8
1	D	251	GLY	2.8
1	C	41	THR	2.8
1	B	669	ARG	2.7
1	C	85	LEU	2.7
1	A	41	THR	2.7
1	C	84	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	674	THR	2.7
1	D	94	GLU	2.6
1	B	267	LYS	2.6
1	C	43	HIS	2.5
1	D	267	LYS	2.5
1	A	43	HIS	2.5
1	A	85	LEU	2.5
1	A	683	GLY	2.5
1	B	687	GLU	2.5
1	D	271	GLU	2.4
1	C	425	ARG	2.4
1	B	451	THR	2.4
1	B	65	GLU	2.3
1	C	66	TYR	2.3
1	D	683	GLY	2.3
1	D	593	LEU	2.3
1	A	66	TYR	2.3
1	B	589	LYS	2.2
1	A	18	ILE	2.2
1	C	67	ALA	2.2
1	D	669	ARG	2.2
1	B	593	LEU	2.2
1	D	70	SER	2.2
1	B	684	LYS	2.2
1	B	264	VAL	2.1
1	D	264	VAL	2.1
1	B	256	ARG	2.1
1	A	67	ALA	2.1
1	C	18	ILE	2.1
1	B	70	SER	2.1

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, 95th 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 ²)	Q<0.9
1	LLP	C	347	24/25	0.92	0.08	16,20,20,20	15
1	LLP	A	347	24/25	0.92	0.08	16,20,20,20	15
1	LLP	D	347	24/25	0.92	0.12	16,21,24,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LLP	B	347	24/25	0.95	0.06	16,20,20,20	15

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.