



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:53 PM UTC

PDB ID : 6J9U / pdb_00006j9u
Title : Complex structure of Lactobacillus casei lactate dehydrogenase penta mutant with pyruvate
Authors : Arai, K.; Miyanaga, A.; Uchikoba, H.; Fushinobu, S.; Taguchi, H.
Deposited on : 2019-01-24
Resolution : 2.79 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)
Xtriage (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

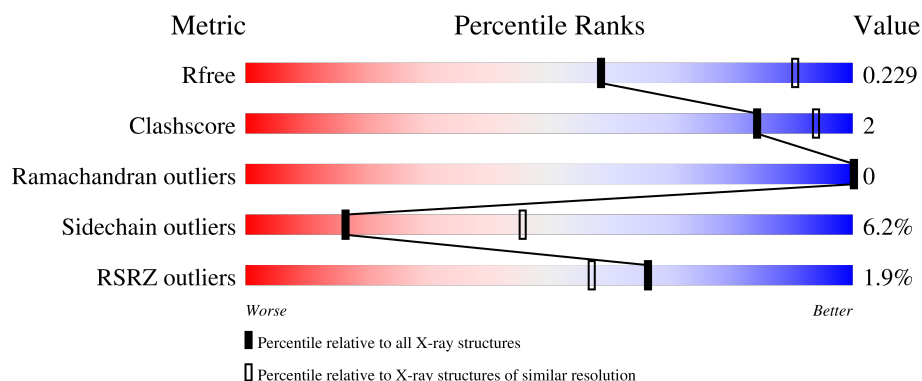
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	326	4% 83% 10% 6%
1	B	326	2% 86% 10% .
1	C	326	% 83% 12% ..
1	D	326	2% 84% 12% .
1	E	326	% 87% 10% ..

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Mol	Chain	Length	Quality of chain
1	F	326	% 86% 10% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PYR	A	401	-	X	-	-
2	PYR	C	401	-	X	-	-
2	PYR	D	401	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14596 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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2354	1505	392	451	6			
1	B	315	Total	C	N	O	S	0	0	0
			2422	1547	403	466	6			
1	C	315	Total	C	N	O	S	0	0	0
			2422	1547	403	466	6			
1	D	315	Total	C	N	O	S	0	0	0
			2422	1547	403	466	6			
1	E	315	Total	C	N	O	S	0	0	0
			2421	1547	403	465	6			
1	F	316	Total	C	N	O	S	0	0	0
			2427	1550	404	467	6			

There are 30 discrepancies between the modelled and reference sequences:

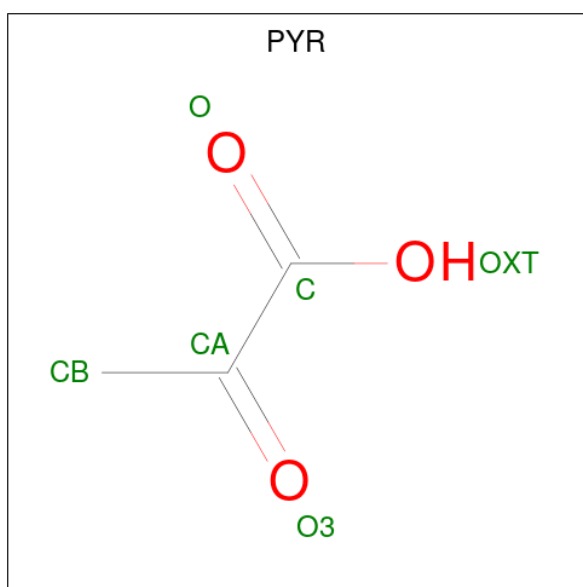
Chain	Residue	Modelled	Actual	Comment	Reference
A	55	GLU	SER	engineered mutation	UNP S6C1Z0
A	56	ASP	ASN	engineered mutation	UNP S6C1Z0
A	164	LYS	GLU	engineered mutation	UNP S6C1Z0
A	223	ASN	ASP	engineered mutation	UNP S6C1Z0
A	224	LYS	ALA	engineered mutation	UNP S6C1Z0
B	55	GLU	SER	engineered mutation	UNP S6C1Z0
B	56	ASP	ASN	engineered mutation	UNP S6C1Z0
B	164	LYS	GLU	engineered mutation	UNP S6C1Z0
B	223	ASN	ASP	engineered mutation	UNP S6C1Z0
B	224	LYS	ALA	engineered mutation	UNP S6C1Z0
C	55	GLU	SER	engineered mutation	UNP S6C1Z0
C	56	ASP	ASN	engineered mutation	UNP S6C1Z0
C	164	LYS	GLU	engineered mutation	UNP S6C1Z0
C	223	ASN	ASP	engineered mutation	UNP S6C1Z0
C	224	LYS	ALA	engineered mutation	UNP S6C1Z0
D	55	GLU	SER	engineered mutation	UNP S6C1Z0
D	56	ASP	ASN	engineered mutation	UNP S6C1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	164	LYS	GLU	engineered mutation	UNP S6C1Z0
D	223	ASN	ASP	engineered mutation	UNP S6C1Z0
D	224	LYS	ALA	engineered mutation	UNP S6C1Z0
E	55	GLU	SER	engineered mutation	UNP S6C1Z0
E	56	ASP	ASN	engineered mutation	UNP S6C1Z0
E	164	LYS	GLU	engineered mutation	UNP S6C1Z0
E	223	ASN	ASP	engineered mutation	UNP S6C1Z0
E	224	LYS	ALA	engineered mutation	UNP S6C1Z0
F	55	GLU	SER	engineered mutation	UNP S6C1Z0
F	56	ASP	ASN	engineered mutation	UNP S6C1Z0
F	164	LYS	GLU	engineered mutation	UNP S6C1Z0
F	223	ASN	ASP	engineered mutation	UNP S6C1Z0
F	224	LYS	ALA	engineered mutation	UNP S6C1Z0

- Molecule 2 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	4	Total	O	0	0
			4	4		
4	C	11	Total	O	0	0
			11	11		

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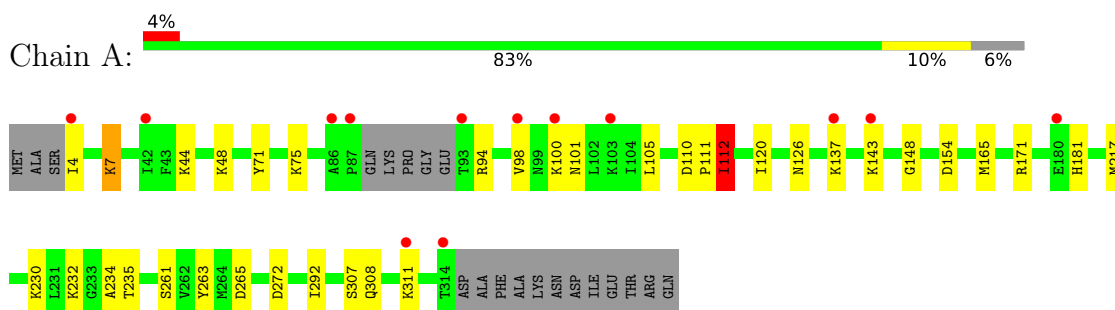
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	20	Total 20	O 20	0	0
4	E	13	Total 13	O 13	0	0
4	F	14	Total 14	O 14	0	0

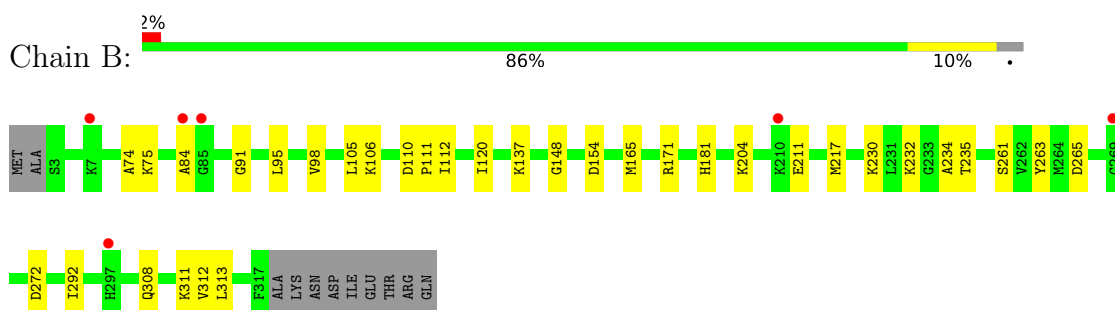
3 Residue-property plots [i](#)

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.

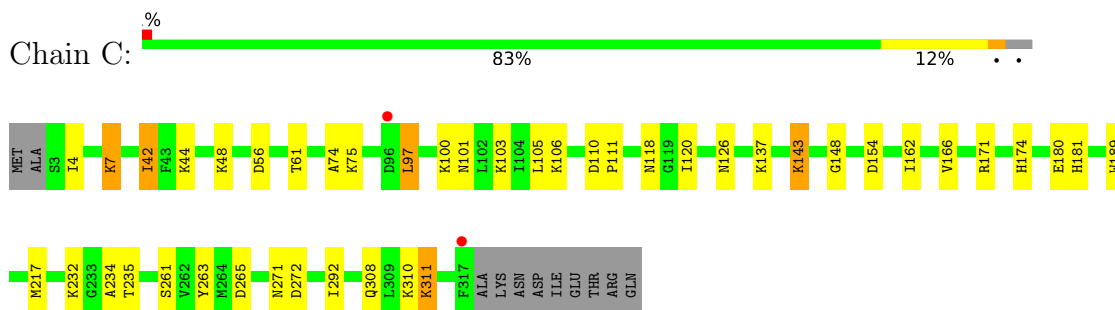
- Molecule 1: L-lactate dehydrogenase



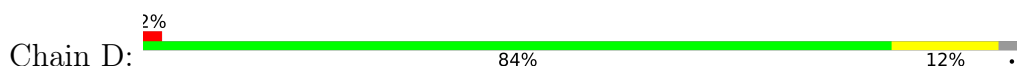
- Molecule 1: L-lactate dehydrogenase

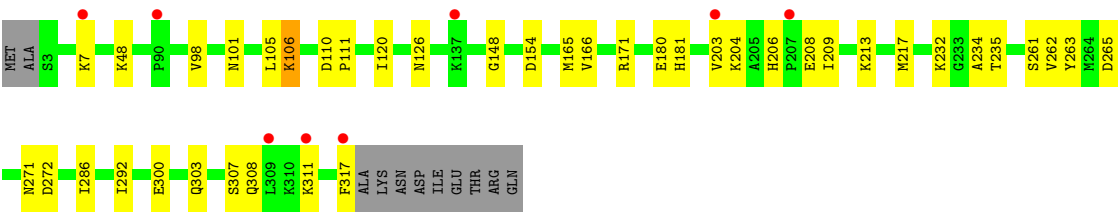


- Molecule 1: L-lactate dehydrogenase

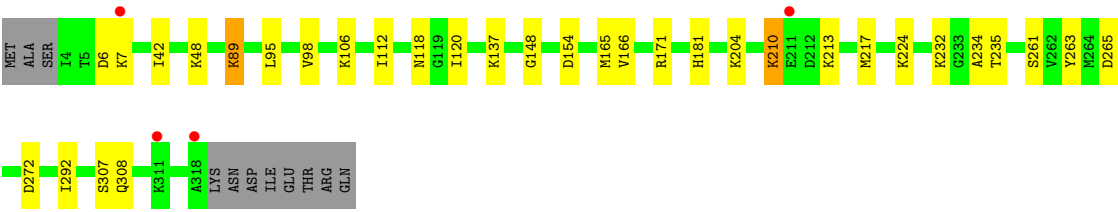
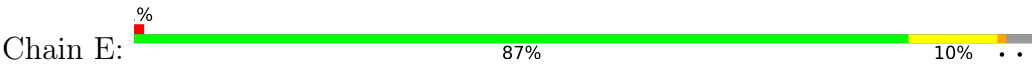


- Molecule 1: L-lactate dehydrogenase

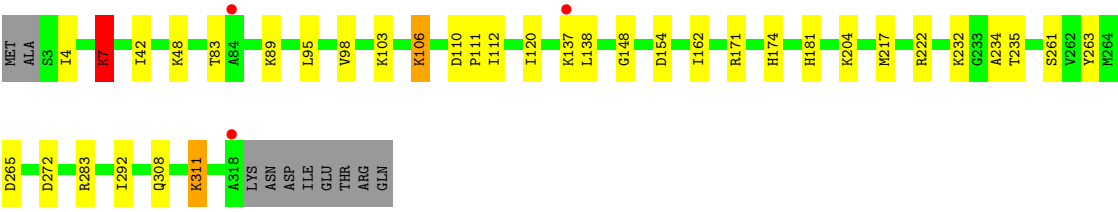
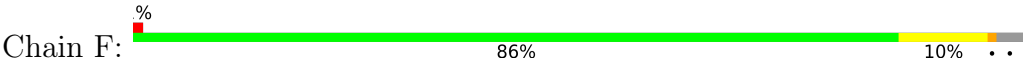




● Molecule 1: L-lactate dehydrogenase



● Molecule 1: L-lactate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.32Å 82.80Å 180.15Å 90.00° 91.52° 90.00°	Depositor
Resolution (Å)	46.90 – 2.79 46.90 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.90-2.79) 97.0 (46.90-2.79)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.227 0.197 , 0.229	Depositor DCC
R_{free} test set	2998 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14596	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, PYR

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	0.86	0/2395	0.95	6/3246 (0.2%)
1	B	0.88	1/2466 (0.0%)	0.95	2/3343 (0.1%)
1	C	0.89	2/2466 (0.1%)	0.98	7/3343 (0.2%)
1	D	0.94	0/2466	1.03	5/3343 (0.1%)
1	E	0.94	0/2465	0.97	4/3342 (0.1%)
1	F	0.83	0/2471	0.96	9/3350 (0.3%)
All	All	0.89	3/14729 (0.0%)	0.97	33/19967 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	LEU	C-O	-5.42	1.17	1.24
1	C	310	LYS	CA-C	5.31	1.59	1.52
1	C	61	THR	C-O	-5.10	1.19	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	ILE	CB-CA-C	-8.81	100.50	112.04
1	E	7	LYS	CB-CG-CD	7.33	128.16	111.30
1	D	213	LYS	N-CA-C	-7.21	103.43	111.28
1	D	98	VAL	N-CA-C	6.93	117.07	110.42
1	F	83	THR	N-CA-C	6.81	122.69	113.97
1	D	105	LEU	N-CA-C	6.78	119.25	111.11
1	A	98	VAL	N-CA-C	6.66	116.81	110.42
1	A	112	ILE	CG1-CB-CG2	-6.63	90.81	110.70
1	C	97	LEU	N-CA-C	6.50	120.51	112.59
1	A	112	ILE	CA-CB-CG1	6.48	121.41	110.40
1	C	143	LYS	CG-CD-CE	6.46	126.16	111.30
1	C	42	ILE	N-CA-CB	6.30	118.34	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	222	ARG	CG-CD-NE	6.28	125.81	112.00
1	B	84	ALA	N-CA-C	6.22	119.68	108.17
1	A	105	LEU	N-CA-C	6.21	118.56	111.11
1	E	7	LYS	CA-CB-CG	-6.20	101.69	114.10
1	C	311	LYS	CB-CA-C	-6.12	101.28	110.88
1	B	98	VAL	N-CA-C	5.99	116.72	110.62
1	F	83	THR	CA-C-N	-5.90	114.73	123.11
1	F	83	THR	C-N-CA	-5.90	114.73	123.11
1	F	98	VAL	N-CA-C	5.81	116.54	110.62
1	C	105	LEU	N-CA-C	5.75	118.01	111.11
1	F	308	GLN	N-CA-CB	5.66	118.45	110.12
1	D	106	LYS	CA-CB-CG	5.42	124.94	114.10
1	E	98	VAL	N-CA-C	5.42	116.15	110.62
1	F	89	LYS	CA-CB-CG	5.37	124.83	114.10
1	D	271	ASN	N-CA-C	5.29	117.80	108.75
1	C	271	ASN	N-CA-C	5.29	117.79	108.75
1	F	7	LYS	CB-CG-CD	5.18	123.22	111.30
1	A	100	LYS	CA-CB-CG	5.05	124.20	114.10
1	E	89	LYS	N-CA-CB	5.03	115.58	109.74
1	F	222	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	A	308	GLN	N-CA-CB	-5.03	102.73	110.12

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	2354	0	2390	10	0
1	B	2422	0	2451	10	0
1	C	2422	0	2451	16	0
1	D	2422	0	2451	11	0
1	E	2421	0	2451	10	0
1	F	2427	0	2456	13	0
2	A	6	0	0	0	0
2	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	6	0	0	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	E	10	0	0	1	0
3	F	10	0	0	0	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	C	11	0	0	0	0
4	D	20	0	0	0	0
4	E	13	0	0	1	0
4	F	14	0	0	0	0
All	All	14596	0	14650	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (66) 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:165:MET:SD	1:D:217:MET:HE1	2.23	0.79
1:A:165:MET:SD	1:A:217:MET:HE1	2.29	0.73
1:B:165:MET:SD	1:B:217:MET:HE1	2.29	0.72
1:E:165:MET:SD	1:E:217:MET:HE1	2.32	0.70
1:A:4:ILE:O	1:A:7:LYS:HG3	1.98	0.63
1:C:4:ILE:O	1:C:7:LYS:HG3	2.00	0.62
1:A:154:ASP:OD2	1:A:181:HIS:ND1	2.38	0.55
1:F:4:ILE:O	1:F:7:LYS:HG3	2.06	0.55
1:C:162:ILE:HG12	1:C:217:MET:HE1	1.89	0.55
1:F:162:ILE:HG12	1:F:217:MET:HE1	1.89	0.54
1:E:154:ASP:OD2	1:E:181:HIS:ND1	2.40	0.53
1:C:162:ILE:HG12	1:C:217:MET:CE	2.40	0.52
1:B:154:ASP:OD2	1:B:181:HIS:ND1	2.42	0.51
1:D:154:ASP:OD2	1:D:181:HIS:ND1	2.38	0.51
1:F:162:ILE:HG12	1:F:217:MET:CE	2.41	0.51
1:E:6:ASP:OD2	1:F:283:ARG:NH1	2.45	0.50
1:C:154:ASP:OD2	1:C:181:HIS:ND1	2.38	0.50
1:F:154:ASP:OD2	1:F:181:HIS:ND1	2.39	0.50
1:F:232:LYS:HE3	1:F:234:ALA:O	2.13	0.49
1:F:106:LYS:HG2	1:F:138:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LYS:HD3	1:D:7:LYS:HB3	1.94	0.48
1:B:91:GLY:HA3	1:C:189:TRP:CD1	2.48	0.48
1:C:232:LYS:HE3	1:C:234:ALA:O	2.13	0.48
1:E:232:LYS:HE3	1:E:234:ALA:O	2.13	0.48
1:D:232:LYS:HE3	1:D:234:ALA:O	2.14	0.48
1:B:232:LYS:HE3	1:B:234:ALA:O	2.13	0.48
1:E:263:TYR:CZ	1:E:272:ASP:HA	2.49	0.47
1:A:232:LYS:HE3	1:A:234:ALA:O	2.14	0.47
1:D:101:ASN:ND2	1:D:126:ASN:O	2.47	0.47
3:E:401:SO4:O4	4:E:501:HOH:O	2.15	0.47
1:A:263:TYR:CZ	1:A:272:ASP:HA	2.50	0.46
1:A:4:ILE:O	1:A:7:LYS:CG	2.63	0.46
1:B:263:TYR:CZ	1:B:272:ASP:HA	2.49	0.46
1:D:262:VAL:HG12	1:D:286:ILE:CD1	2.47	0.45
1:C:4:ILE:O	1:C:7:LYS:CG	2.65	0.45
1:F:311:LYS:HE3	1:F:311:LYS:HB2	1.60	0.45
1:F:110:ASP:HB2	1:F:111:PRO:HD3	1.99	0.44
1:C:110:ASP:HB2	1:C:111:PRO:HD3	2.00	0.44
1:E:148:GLY:HA3	1:E:261:SER:HB2	2.00	0.44
1:B:148:GLY:HA3	1:B:261:SER:HB2	2.00	0.43
1:F:148:GLY:HA3	1:F:261:SER:HB2	2.00	0.43
1:A:101:ASN:ND2	1:A:126:ASN:O	2.51	0.43
1:E:210:LYS:HE2	1:E:213:LYS:HD3	2.00	0.43
1:B:110:ASP:HB2	1:B:111:PRO:HD3	2.01	0.43
1:C:148:GLY:HA3	1:C:261:SER:HB2	2.00	0.43
1:E:210:LYS:HE2	1:E:213:LYS:CD	2.49	0.43
1:F:263:TYR:CZ	1:F:272:ASP:HA	2.53	0.43
1:C:101:ASN:ND2	1:C:126:ASN:O	2.51	0.42
1:A:71:TYR:CD1	1:A:112:ILE:CD1	3.02	0.42
1:D:148:GLY:HA3	1:D:261:SER:HB2	2.00	0.42
1:A:148:GLY:HA3	1:A:261:SER:HB2	2.00	0.42
1:A:110:ASP:HB2	1:A:111:PRO:HD3	2.01	0.42
1:B:211:GLU:O	1:B:211:GLU:HG3	2.18	0.42
1:C:56:ASP:OD1	1:E:224:LYS:NZ	2.53	0.42
1:D:263:TYR:CZ	1:D:272:ASP:HA	2.55	0.42
1:C:174:HIS:CE1	1:F:174:HIS:CE1	3.08	0.41
3:C:402:SO4:O4	1:F:174:HIS:NE2	2.40	0.41
1:C:74:ALA:O	1:C:75:LYS:C	2.64	0.41
1:D:206:HIS:ND1	1:D:208:GLU:OE2	2.54	0.41
1:C:118:ASN:O	1:C:118:ASN:CG	2.63	0.41
1:C:263:TYR:CZ	1:C:272:ASP:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:HG22	1:D:209:ILE:HG22	2.03	0.41
1:D:110:ASP:HB2	1:D:111:PRO:HD3	2.03	0.41
1:B:74:ALA:O	1:B:75:LYS:C	2.64	0.41
1:E:118:ASN:O	1:E:118:ASN:CG	2.64	0.40
1:B:308:GLN:O	1:B:312:VAL:HG23	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	302/326 (93%)	292 (97%)	10 (3%)	0	100	100
1	B	313/326 (96%)	306 (98%)	7 (2%)	0	100	100
1	C	313/326 (96%)	305 (97%)	8 (3%)	0	100	100
1	D	313/326 (96%)	304 (97%)	9 (3%)	0	100	100
1	E	313/326 (96%)	304 (97%)	9 (3%)	0	100	100
1	F	314/326 (96%)	306 (98%)	8 (2%)	0	100	100
All	All	1868/1956 (96%)	1817 (97%)	51 (3%)	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	254/270 (94%)	238 (94%)	16 (6%)	16	45
1	B	261/270 (97%)	248 (95%)	13 (5%)	22	54
1	C	261/270 (97%)	242 (93%)	19 (7%)	13	38
1	D	261/270 (97%)	245 (94%)	16 (6%)	17	46
1	E	260/270 (96%)	243 (94%)	17 (6%)	15	43
1	F	261/270 (97%)	246 (94%)	15 (6%)	18	49
All	All	1558/1620 (96%)	1462 (94%)	96 (6%)	16	45

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	44	LYS
1	A	48	LYS
1	A	75	LYS
1	A	94	ARG
1	A	112	ILE
1	A	120	ILE
1	A	137	LYS
1	A	143	LYS
1	A	171	ARG
1	A	230	LYS
1	A	235	THR
1	A	265	ASP
1	A	292	ILE
1	A	307	SER
1	A	311	LYS
1	B	95	LEU
1	B	106	LYS
1	B	112	ILE
1	B	120	ILE
1	B	137	LYS
1	B	171	ARG
1	B	204	LYS
1	B	230	LYS
1	B	235	THR
1	B	265	ASP
1	B	292	ILE
1	B	311	LYS
1	B	313	LEU
1	C	7	LYS

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Mol	Chain	Res	Type
1	C	42	ILE
1	C	44	LYS
1	C	48	LYS
1	C	97	LEU
1	C	100	LYS
1	C	103	LYS
1	C	106	LYS
1	C	120	ILE
1	C	137	LYS
1	C	143	LYS
1	C	166	VAL
1	C	171	ARG
1	C	180	GLU
1	C	235	THR
1	C	265	ASP
1	C	292	ILE
1	C	308	GLN
1	C	311	LYS
1	D	48	LYS
1	D	106	LYS
1	D	120	ILE
1	D	166	VAL
1	D	171	ARG
1	D	180	GLU
1	D	204	LYS
1	D	235	THR
1	D	265	ASP
1	D	292	ILE
1	D	300	GLU
1	D	303	GLN
1	D	307	SER
1	D	308	GLN
1	D	311	LYS
1	D	317	PHE
1	E	42	ILE
1	E	48	LYS
1	E	89	LYS
1	E	95	LEU
1	E	106	LYS
1	E	112	ILE
1	E	120	ILE
1	E	137	LYS

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Mol	Chain	Res	Type
1	E	166	VAL
1	E	171	ARG
1	E	204	LYS
1	E	210	LYS
1	E	235	THR
1	E	265	ASP
1	E	292	ILE
1	E	307	SER
1	E	308	GLN
1	F	7	LYS
1	F	42	ILE
1	F	48	LYS
1	F	95	LEU
1	F	103	LYS
1	F	106	LYS
1	F	112	ILE
1	F	120	ILE
1	F	137	LYS
1	F	171	ARG
1	F	204	LYS
1	F	235	THR
1	F	265	ASP
1	F	292	ILE
1	F	311	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	191	HIS
1	C	99	ASN
1	E	174	HIS
1	E	284	ASN
1	E	288	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	PYR	C	401	-	5,5,5	2.46	2 (40%)	3,6,6	2.88	1 (33%)
3	SO4	C	402	-	4,4,4	0.57	0	6,6,6	0.54	0
3	SO4	F	401	-	4,4,4	0.52	0	6,6,6	0.61	0
2	PYR	A	401	-	5,5,5	1.99	3 (60%)	3,6,6	1.84	1 (33%)
3	SO4	B	402	-	4,4,4	0.50	0	6,6,6	0.33	0
3	SO4	E	402	-	4,4,4	0.58	0	6,6,6	0.47	0
3	SO4	B	401	-	4,4,4	0.59	0	6,6,6	0.58	0
3	SO4	A	402	-	4,4,4	0.42	0	6,6,6	0.67	0
2	PYR	D	401	-	5,5,5	2.85	3 (60%)	3,6,6	3.32	2 (66%)
3	SO4	D	402	-	4,4,4	0.65	0	6,6,6	0.52	0
3	SO4	E	401	-	4,4,4	0.62	0	6,6,6	0.45	0
3	SO4	F	402	-	4,4,4	0.53	0	6,6,6	0.32	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	PYR	C	401	-	-	4/4/4/4	-
2	PYR	D	401	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PYR	A	401	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	PYR	CA-C	-4.74	1.38	1.54
2	C	401	PYR	CA-C	-4.25	1.40	1.54
2	D	401	PYR	OXT-C	-3.30	1.21	1.30
2	C	401	PYR	OXT-C	-3.14	1.22	1.30
2	A	401	PYR	CA-C	-3.02	1.44	1.54
2	A	401	PYR	OXT-C	-2.34	1.24	1.30
2	D	401	PYR	CB-CA	2.29	1.54	1.50
2	A	401	PYR	CB-CA	2.02	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PYR	O3-CA-CB	5.20	131.43	119.77
2	C	401	PYR	O3-CA-CB	4.92	130.78	119.77
2	A	401	PYR	O3-CA-CB	3.03	126.55	119.77
2	D	401	PYR	OXT-C-CA	2.11	119.45	113.59

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PYR	OXT-C-CA-CB
2	C	401	PYR	O-C-CA-CB
2	C	401	PYR	OXT-C-CA-CB
2	D	401	PYR	O-C-CA-CB
2	D	401	PYR	OXT-C-CA-CB
2	A	401	PYR	O-C-CA-CB
2	C	401	PYR	OXT-C-CA-O3
2	D	401	PYR	OXT-C-CA-O3
2	C	401	PYR	O-C-CA-O3
2	D	401	PYR	O-C-CA-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	SO4	1	0
3	E	401	SO4	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, 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	306/326 (93%)	0.24	13 (4%) 40 32	29, 53, 81, 101	0
1	B	315/326 (96%)	-0.04	6 (1%) 66 57	28, 44, 65, 83	0
1	C	315/326 (96%)	0.08	2 (0%) 85 80	29, 48, 78, 93	0
1	D	315/326 (96%)	-0.01	8 (2%) 58 48	24, 41, 72, 98	0
1	E	315/326 (96%)	-0.12	4 (1%) 75 66	26, 39, 59, 83	0
1	F	316/326 (96%)	0.02	3 (0%) 81 74	31, 48, 68, 79	0
All	All	1882/1956 (96%)	0.03	36 (1%) 66 57	24, 45, 73, 101	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	ALA	4.0
1	F	84	ALA	3.8
1	D	317	PHE	3.6
1	A	180	GLU	3.5
1	D	90	PRO	3.4
1	E	318	ALA	3.2
1	B	269	GLY	3.0
1	A	87	PRO	3.0
1	A	311	LYS	3.0
1	A	93	THR	3.0
1	B	7	LYS	2.9
1	F	318	ALA	2.9
1	D	207	PRO	2.8
1	E	7	LYS	2.8
1	A	42	ILE	2.8
1	C	96	ASP	2.7
1	A	137	LYS	2.6
1	D	7	LYS	2.6
1	E	211	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	203	VAL	2.5
1	C	317	PHE	2.5
1	A	100	LYS	2.4
1	A	314	THR	2.4
1	B	297	HIS	2.4
1	A	143	LYS	2.4
1	B	85	GLY	2.3
1	D	137	LYS	2.3
1	A	98	VAL	2.3
1	D	311	LYS	2.2
1	A	103	LYS	2.2
1	E	311	LYS	2.2
1	A	4	ILE	2.1
1	A	86	ALA	2.0
1	D	309	LEU	2.0
1	B	210	LYS	2.0
1	F	137	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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
2	PYR	A	401	6/6	0.78	0.14	46,49,54,54	0
2	PYR	C	401	6/6	0.79	0.15	49,50,52,53	0
2	PYR	D	401	6/6	0.86	0.12	29,36,39,41	0
3	SO4	E	402	5/5	0.91	0.11	66,68,76,85	0
3	SO4	C	402	5/5	0.92	0.11	67,72,77,80	0
3	SO4	E	401	5/5	0.93	0.10	63,66,74,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	402	5/5	0.94	0.11	58,59,69,69	0
3	SO4	F	401	5/5	0.94	0.10	63,65,76,79	0
3	SO4	B	402	5/5	0.95	0.08	86,86,87,90	0
3	SO4	B	401	5/5	0.95	0.09	62,70,74,77	0
3	SO4	A	402	5/5	0.96	0.11	67,69,72,79	0
3	SO4	F	402	5/5	0.96	0.08	74,76,80,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.