



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:47 PM UTC

PDB ID : 6J9S / pdb_00006j9s
Title : Penta mutant of Lactobacillus casei lactate dehydrogenase
Authors : Arai, K.; Miyanaga, A.; Uchikoba, H.; Fushinobu, S.; Taguchi, H.
Deposited on : 2019-01-24
Resolution : 2.00 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:

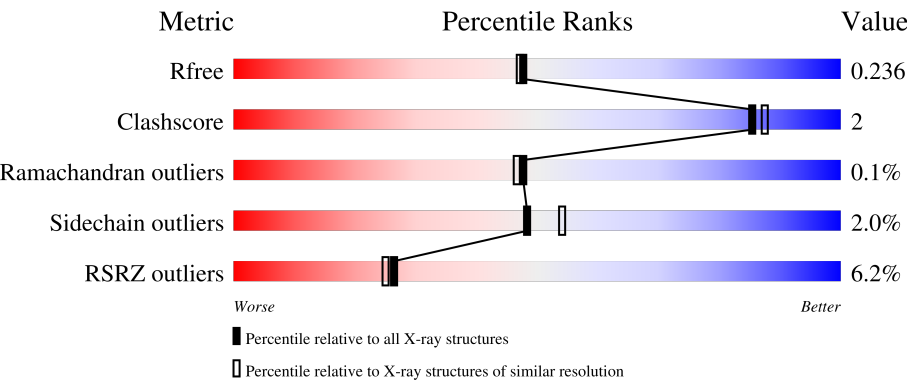
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	9% 83% 6% 10%
1	B	326	5% 88% 8% ...
1	C	326	6% 84% 7% 8%
1	D	326	8% 83% 7% 9%
1	E	326	4% 89% 7% ...

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Mol	Chain	Length	Quality of chain
1	F	326	4% 90% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14730 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	294	Total	C	N	O	S	0	0	0
			2263	1447	375	435	6			
1	B	315	Total	C	N	O	S	0	0	0
			2422	1547	403	466	6			
1	C	299	Total	C	N	O	S	0	0	0
			2302	1472	382	442	6			
1	D	297	Total	C	N	O	S	0	0	0
			2287	1463	379	439	6			
1	E	315	Total	C	N	O	S	0	0	0
			2422	1547	403	466	6			
1	F	315	Total	C	N	O	S	0	0	0
			2422	1547	403	466	6			

There are 30 discrepancies between the modelled and reference sequences:

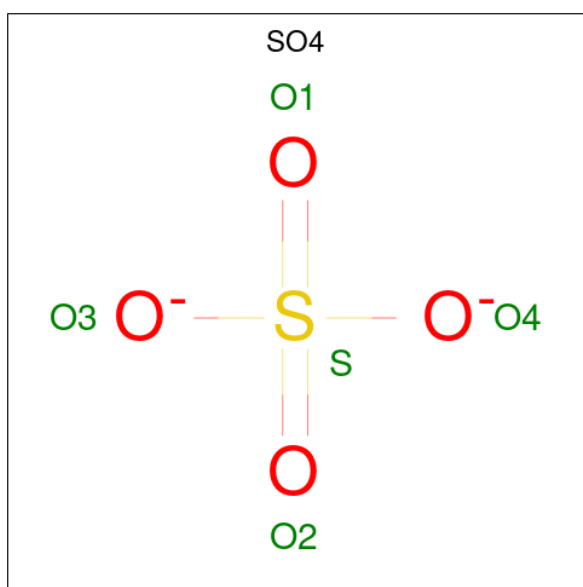
Chain	Residue	Modelled	Actual	Comment	Reference
A	55	GLU	SER	engineered mutation	UNP S6C1Z0
A	56	ASP	ASN	engineered mutation	UNP S6C1Z0
A	164	LYS	GLU	engineered mutation	UNP S6C1Z0
A	223	ASN	ASP	engineered mutation	UNP S6C1Z0
A	224	LYS	ALA	engineered mutation	UNP S6C1Z0
B	55	GLU	SER	engineered mutation	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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is GLYCEROL (CCD ID: 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		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

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

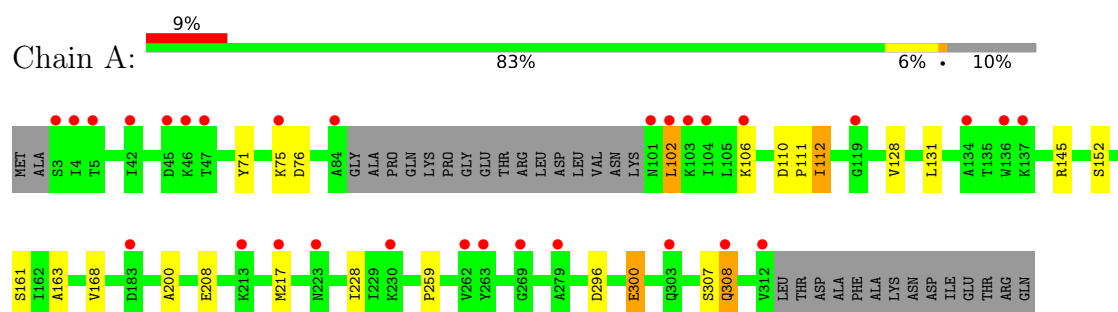
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	111	Total	O	0	0
			111	111		
4	C	69	Total	O	0	0
			69	69		
4	D	82	Total	O	0	0
			82	82		
4	E	117	Total	O	0	0
			117	117		
4	F	79	Total	O	0	0
			79	79		

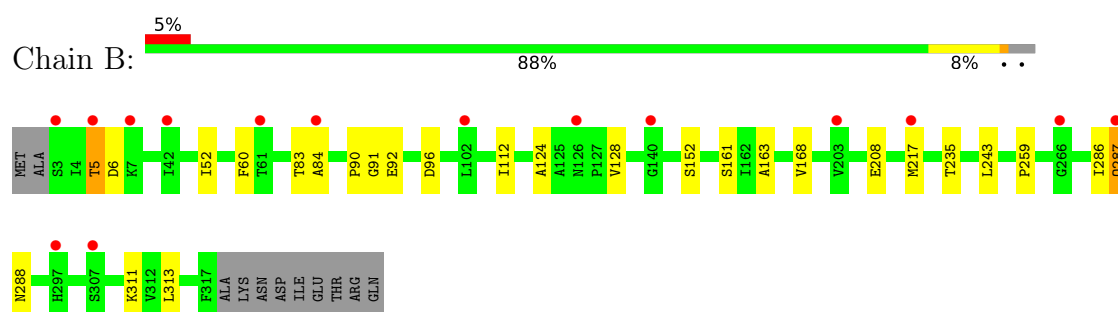
3 Residue-property plots [i](#)

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.

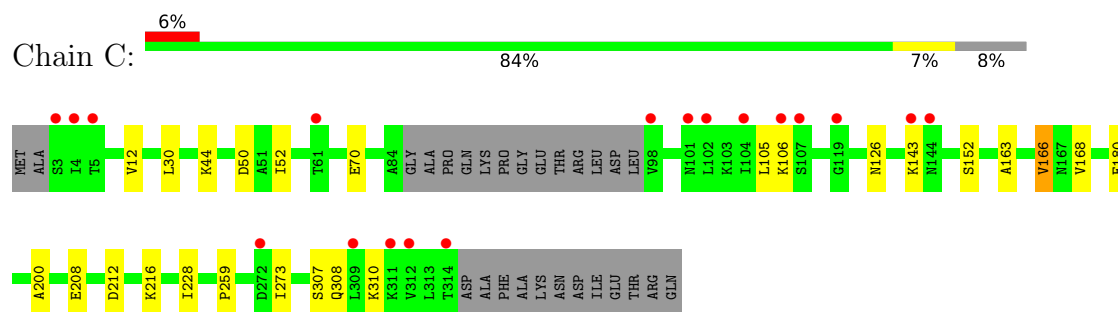
- Molecule 1: L-lactate dehydrogenase



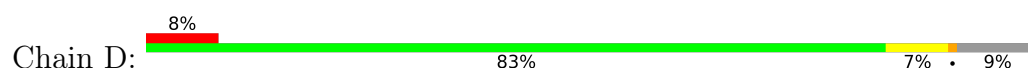
- Molecule 1: L-lactate dehydrogenase

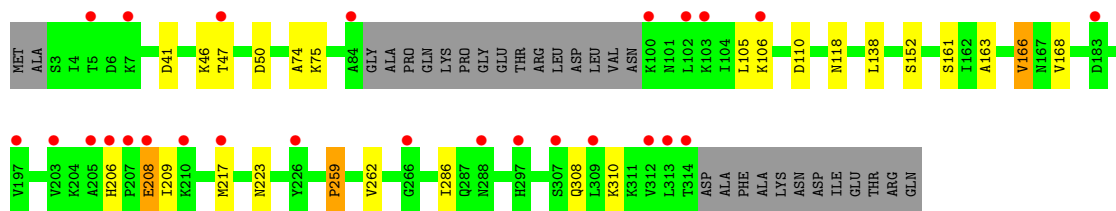


- Molecule 1: L-lactate dehydrogenase

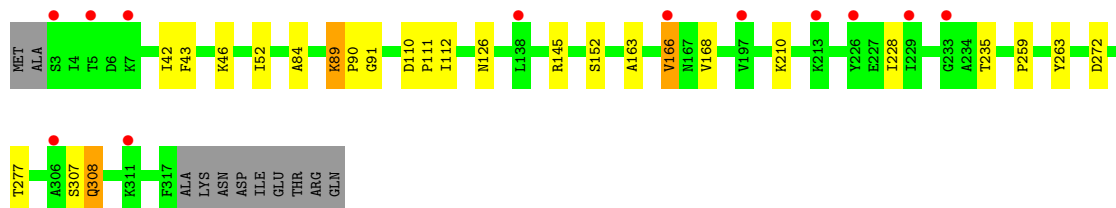
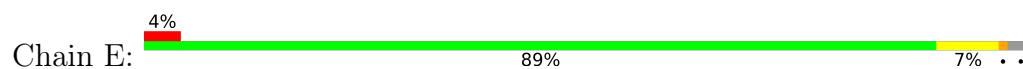


- Molecule 1: L-lactate dehydrogenase

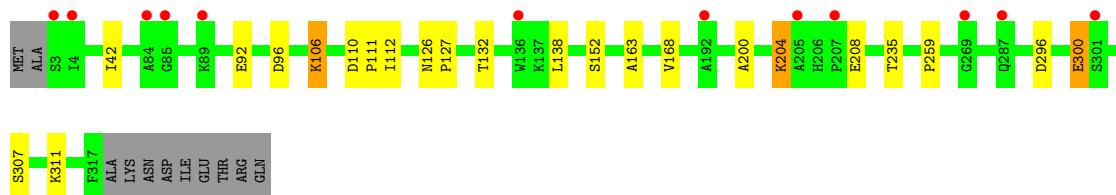
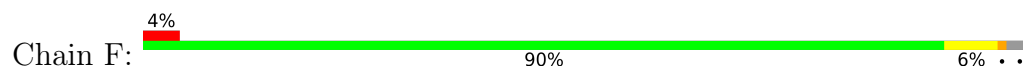




● Molecule 1: L-lactate dehydrogenase



● 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	163.57Å 82.89Å 180.83Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	41.07 – 2.00 41.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (41.07-2.00) 96.9 (41.07-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.209 , 0.234 (Not available) , 0.236	Depositor DCC
R_{free} test set	7948 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14730	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	1.13	1/2303 (0.0%)	1.05	6/3120 (0.2%)
1	B	1.24	4/2466 (0.2%)	1.20	11/3343 (0.3%)
1	C	1.13	5/2342 (0.2%)	1.05	3/3173 (0.1%)
1	D	1.22	3/2327 (0.1%)	1.08	4/3152 (0.1%)
1	E	1.26	2/2466 (0.1%)	1.10	7/3343 (0.2%)
1	F	1.16	0/2466	1.00	3/3343 (0.1%)
All	All	1.19	15/14370 (0.1%)	1.08	34/19474 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	ALA	N-CA	14.36	1.66	1.46
1	D	105	LEU	N-CA	7.68	1.55	1.46
1	C	105	LEU	N-CA	7.55	1.55	1.46
1	E	307	SER	N-CA	6.38	1.53	1.46
1	D	259	PRO	N-CA	-6.00	1.40	1.47
1	C	12	VAL	N-CA	-5.95	1.39	1.46
1	B	60	PHE	C-O	-5.89	1.15	1.24
1	A	200	ALA	N-CA	5.38	1.52	1.46
1	C	70	GLU	N-CA	5.28	1.52	1.45
1	B	5	THR	CA-C	5.28	1.59	1.53
1	B	83	THR	C-N	-5.23	1.26	1.33
1	C	30	LEU	C-O	-5.21	1.18	1.24
1	D	208	GLU	CA-C	5.17	1.59	1.52
1	C	180	GLU	C-O	-5.07	1.17	1.23
1	E	277	THR	CA-C	5.03	1.57	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	THR	CA-C-N	-19.82	90.82	123.33
1	B	83	THR	C-N-CA	-19.82	90.82	123.33
1	B	6	ASP	N-CA-C	-11.63	99.79	114.56
1	D	105	LEU	N-CA-C	11.61	125.04	111.11
1	B	83	THR	O-C-N	-11.04	109.46	122.27
1	C	105	LEU	N-CA-C	10.60	123.83	111.11
1	D	166	VAL	N-CA-CB	-7.77	100.26	112.07
1	C	166	VAL	N-CA-CB	-7.27	101.02	112.07
1	B	5	THR	CB-CA-C	-6.46	102.77	111.88
1	B	128	VAL	N-CA-C	6.42	117.21	110.72
1	E	91	GLY	N-CA-C	-6.35	106.67	114.92
1	E	166	VAL	N-CA-CB	-6.22	101.62	112.08
1	A	308	GLN	N-CA-CB	-6.21	100.99	110.12
1	E	308	GLN	N-CA-CB	-6.16	101.06	110.12
1	B	287	GLN	N-CA-C	-6.08	97.86	110.80
1	E	308	GLN	CG-CD-NE2	6.06	125.49	116.40
1	A	112	ILE	CG1-CB-CG2	-5.96	92.81	110.70
1	A	102	LEU	N-CA-C	5.71	118.72	111.69
1	F	112	ILE	CA-CB-CG1	-5.56	100.95	110.40
1	E	126	ASN	N-CA-C	5.43	117.78	110.29
1	B	288	ASN	N-CA-CB	-5.42	102.37	110.17
1	B	5	THR	N-CA-C	-5.34	103.25	110.68
1	D	208	GLU	CB-CA-C	5.29	121.05	109.99
1	B	112	ILE	CA-CB-CG1	-5.25	101.48	110.40
1	F	42	ILE	CB-CA-C	-5.22	105.09	112.14
1	E	112	ILE	CA-CB-CG1	-5.21	101.54	110.40
1	A	308	GLN	CG-CD-NE2	5.18	124.18	116.40
1	B	91	GLY	N-CA-C	5.18	122.75	115.30
1	C	126	ASN	CB-CA-C	5.16	116.14	108.87
1	A	145	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	A	128	VAL	N-CA-C	5.13	115.85	110.62
1	E	145	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	D	118	ASN	N-CA-CB	-5.09	105.68	111.79
1	F	132	THR	N-CA-C	-5.04	105.70	111.14

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	2263	0	2288	12	0
1	B	2422	0	2451	11	0
1	C	2302	0	2334	9	0
1	D	2287	0	2319	15	0
1	E	2422	0	2451	9	0
1	F	2422	0	2451	11	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	1	0
2	F	10	0	0	1	0
3	B	12	0	16	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	12	0	16	0	0
3	F	6	0	8	0	0
4	A	52	0	0	0	0
4	B	111	0	0	0	0
4	C	69	0	0	1	0
4	D	82	0	0	1	0
4	E	117	0	0	0	0
4	F	79	0	0	0	0
All	All	14730	0	14350	63	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 (63) 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:235:THR:HG21	2:B:401:SO4:O3	1.71	0.89
1:F:235:THR:HG21	2:F:401:SO4:O2	1.77	0.84
1:D:262:VAL:HG12	1:D:286:ILE:CD1	2.10	0.82
1:D:262:VAL:HG12	1:D:286:ILE:HD13	1.71	0.71
1:D:262:VAL:HG12	1:D:286:ILE:HD11	1.77	0.65
1:F:106:LYS:HG2	1:F:138:LEU:HD22	1.79	0.64
1:B:5:THR:O	1:B:5:THR:OG1	2.14	0.63
1:F:106:LYS:HG2	1:F:138:LEU:CD2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:ASP:O	1:F:300:GLU:HG2	2.02	0.60
1:D:262:VAL:CG1	1:D:286:ILE:HD13	2.33	0.58
1:A:296:ASP:O	1:A:300:GLU:HG2	2.02	0.58
1:D:106:LYS:HD3	1:D:138:LEU:HD22	1.85	0.58
1:C:273:ILE:HG21	1:C:310:LYS:HG2	1.85	0.57
1:F:200:ALA:O	1:F:204:LYS:HD3	2.06	0.56
1:B:90:PRO:HG3	1:C:200:ALA:HB2	1.87	0.55
1:E:235:THR:HG21	2:E:401:SO4:O3	2.07	0.54
1:D:106:LYS:HD2	1:D:110:ASP:OD1	2.11	0.50
1:D:161:SER:OG	1:D:217:MET:HG3	2.13	0.49
1:A:75:LYS:CG	1:A:76:ASP:N	2.75	0.49
1:D:310:LYS:HE3	1:D:310:LYS:HB2	1.61	0.48
1:A:71:TYR:CD1	1:A:112:ILE:HD12	2.50	0.46
1:E:42:ILE:HD11	1:E:43:PHE:CE1	2.50	0.46
1:A:102:LEU:HD23	1:A:131:LEU:CD2	2.46	0.46
1:F:296:ASP:O	1:F:300:GLU:CG	2.63	0.46
1:A:75:LYS:HG3	1:A:76:ASP:N	2.29	0.46
1:E:163:ALA:HB1	1:E:168:VAL:O	2.15	0.46
1:C:44:LYS:NZ	4:C:504:HOH:O	2.48	0.46
1:C:152:SER:HA	1:C:259:PRO:HG2	1.98	0.45
1:F:92:GLU:HG2	1:F:96:ASP:HB3	1.99	0.45
1:F:110:ASP:HB2	1:F:111:PRO:HD3	1.99	0.44
1:B:161:SER:OG	1:B:217:MET:HG3	2.16	0.44
1:A:296:ASP:O	1:A:300:GLU:CG	2.65	0.44
1:F:126:ASN:ND2	1:F:127:PRO:HA	2.32	0.44
1:A:161:SER:OG	1:A:217:MET:HG3	2.18	0.44
1:B:152:SER:HA	1:B:259:PRO:HG2	2.00	0.44
1:D:106:LYS:HD3	1:D:138:LEU:CD2	2.48	0.44
1:F:163:ALA:HB1	1:F:168:VAL:O	2.18	0.43
1:D:286:ILE:HD12	4:D:564:HOH:O	2.17	0.43
1:A:71:TYR:CD1	1:A:112:ILE:CD1	3.01	0.43
1:A:163:ALA:HB1	1:A:168:VAL:O	2.19	0.43
1:A:228:ILE:HG12	1:B:52:ILE:HG13	1.99	0.43
1:C:163:ALA:HB1	1:C:168:VAL:O	2.18	0.43
1:D:152:SER:HA	1:D:259:PRO:HG2	2.00	0.42
1:B:286:ILE:HG22	1:B:287:GLN:O	2.18	0.42
1:B:163:ALA:HB1	1:B:168:VAL:O	2.19	0.42
1:E:89:LYS:HB2	1:E:90:PRO:HD2	2.00	0.42
1:B:92:GLU:HG2	1:B:96:ASP:HB3	2.02	0.42
1:C:228:ILE:HG12	1:E:52:ILE:HG13	2.02	0.42
1:B:311:LYS:O	1:B:311:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASP:O	1:C:216:LYS:HG3	2.20	0.41
1:A:152:SER:HA	1:A:259:PRO:HG2	2.02	0.41
1:D:41:ASP:HB3	1:D:47:THR:CG2	2.50	0.41
1:E:263:TYR:CZ	1:E:272:ASP:HA	2.56	0.41
1:D:206:HIS:HB3	1:D:209:ILE:HG12	2.02	0.41
1:C:52:ILE:HG13	1:E:228:ILE:HG12	2.03	0.41
1:F:152:SER:HA	1:F:259:PRO:HG2	2.02	0.41
1:C:273:ILE:CG2	1:C:310:LYS:HG2	2.49	0.40
1:D:74:ALA:O	1:D:75:LYS:C	2.63	0.40
1:E:152:SER:HA	1:E:259:PRO:HG2	2.02	0.40
1:B:124:ALA:HB2	1:B:243:LEU:HD21	2.04	0.40
1:D:163:ALA:HB1	1:D:168:VAL:O	2.21	0.40
1:A:110:ASP:HB2	1:A:111:PRO:HD3	2.04	0.40
1:E:110:ASP:HB2	1:E:111:PRO:HD3	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	290/326 (89%)	282 (97%)	8 (3%)	0	100	100
1	B	313/326 (96%)	303 (97%)	10 (3%)	0	100	100
1	C	295/326 (90%)	288 (98%)	7 (2%)	0	100	100
1	D	293/326 (90%)	285 (97%)	8 (3%)	0	100	100
1	E	313/326 (96%)	305 (97%)	7 (2%)	1 (0%)	36	35
1	F	313/326 (96%)	304 (97%)	9 (3%)	0	100	100
All	All	1817/1956 (93%)	1767 (97%)	49 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	84	ALA

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	244/270 (90%)	239 (98%)	5 (2%)	48	54
1	B	261/270 (97%)	259 (99%)	2 (1%)	73	80
1	C	249/270 (92%)	242 (97%)	7 (3%)	38	41
1	D	247/270 (92%)	241 (98%)	6 (2%)	43	47
1	E	261/270 (97%)	256 (98%)	5 (2%)	50	56
1	F	261/270 (97%)	255 (98%)	6 (2%)	44	49
All	All	1523/1620 (94%)	1492 (98%)	31 (2%)	48	54

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	LYS
1	A	208	GLU
1	A	300	GLU
1	A	307	SER
1	A	308	GLN
1	B	208	GLU
1	B	313	LEU
1	C	50	ASP
1	C	106	LYS
1	C	143	LYS
1	C	166	VAL
1	C	208	GLU
1	C	307	SER
1	C	308	GLN
1	D	46	LYS
1	D	50	ASP
1	D	166	VAL
1	D	208	GLU

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Mol	Chain	Res	Type
1	D	223	ASN
1	D	308	GLN
1	E	46	LYS
1	E	89	LYS
1	E	166	VAL
1	E	210	LYS
1	E	308	GLN
1	F	106	LYS
1	F	204	LYS
1	F	208	GLU
1	F	300	GLU
1	F	307	SER
1	F	311	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	D	118	ASN
1	D	223	ASN
1	F	31	GLN
1	F	126	ASN
1	F	223	ASN
1	F	284	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

19 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	SO4	A	401	-	4,4,4	0.78	0	6,6,6	0.56	0
2	SO4	E	401	-	4,4,4	0.67	0	6,6,6	0.85	0
2	SO4	F	402	-	4,4,4	0.46	0	6,6,6	0.51	0
3	GOL	B	403	-	5,5,5	0.38	0	5,5,5	0.69	0
3	GOL	D	403	-	5,5,5	1.62	0	5,5,5	2.34	2 (40%)
2	SO4	C	402	-	4,4,4	0.51	0	6,6,6	0.98	0
3	GOL	E	403	-	5,5,5	1.56	1 (20%)	5,5,5	1.48	1 (20%)
3	GOL	E	404	-	5,5,5	0.79	0	5,5,5	1.57	2 (40%)
2	SO4	D	402	-	4,4,4	1.35	1 (25%)	6,6,6	1.07	1 (16%)
2	SO4	C	401	-	4,4,4	0.49	0	6,6,6	1.18	0
2	SO4	B	402	-	4,4,4	0.82	0	6,6,6	0.67	0
2	SO4	E	402	-	4,4,4	0.92	0	6,6,6	1.00	0
2	SO4	D	401	-	4,4,4	0.46	0	6,6,6	1.13	0
2	SO4	B	401	-	4,4,4	0.35	0	6,6,6	0.74	0
3	GOL	C	403	-	5,5,5	0.98	0	5,5,5	0.57	0
2	SO4	A	402	-	4,4,4	0.54	0	6,6,6	0.63	0
3	GOL	B	404	-	5,5,5	0.75	0	5,5,5	1.45	1 (20%)
2	SO4	F	401	-	4,4,4	0.70	0	6,6,6	0.68	0
3	GOL	F	403	-	5,5,5	0.64	0	5,5,5	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
3	GOL	F	403	-	-	2/4/4/4	-
3	GOL	D	403	-	-	3/4/4/4	-
3	GOL	E	403	-	-	2/4/4/4	-
3	GOL	C	403	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	B	404	-	-	1/4/4/4	-
3	GOL	E	404	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	403	GOL	O3-C3	2.21	1.51	1.42
2	D	402	SO4	O2-S	2.04	1.56	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	403	GOL	O1-C1-C2	3.55	126.35	110.38
3	D	403	GOL	O3-C3-C2	3.11	124.37	110.38
3	B	404	GOL	O2-C2-C1	2.79	120.72	109.18
3	E	403	GOL	O1-C1-C2	2.71	122.57	110.38
3	E	404	GOL	O1-C1-C2	-2.41	99.53	110.38
3	E	404	GOL	O2-C2-C3	2.09	117.82	109.18
2	D	402	SO4	O3-S-O1	-2.05	98.82	109.56

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	GOL	C1-C2-C3-O3
3	D	403	GOL	O1-C1-C2-O2
3	D	403	GOL	O1-C1-C2-C3
3	E	403	GOL	C1-C2-C3-O3
3	F	403	GOL	C1-C2-C3-O3
3	E	403	GOL	O2-C2-C3-O3
3	D	403	GOL	C1-C2-C3-O3
3	B	404	GOL	O2-C2-C3-O3
3	F	403	GOL	O2-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3
3	E	404	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	SO4	1	0
2	B	401	SO4	1	0
2	F	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	294/326 (90%)	0.72	30 (10%)	12 11	34, 52, 78, 124	0
1	B	315/326 (96%)	0.48	15 (4%)	35 34	31, 46, 67, 87	0
1	C	299/326 (91%)	0.69	18 (6%)	27 26	33, 50, 74, 94	0
1	D	297/326 (91%)	0.57	26 (8%)	15 14	31, 44, 75, 95	0
1	E	315/326 (96%)	0.43	12 (3%)	44 43	32, 42, 63, 88	0
1	F	315/326 (96%)	0.67	12 (3%)	44 43	33, 51, 70, 86	0
All	All	1835/1956 (93%)	0.59	113 (6%)	26 25	31, 47, 72, 124	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	LEU	7.0
1	A	312	VAL	5.8
1	B	5	THR	4.8
1	D	312	VAL	4.4
1	C	314	THR	4.3
1	A	84	ALA	4.2
1	A	183	ASP	4.1
1	D	205	ALA	4.0
1	C	5	THR	3.8
1	D	203	VAL	3.8
1	B	84	ALA	3.7
1	F	269	GLY	3.6
1	D	206	HIS	3.6
1	C	309	LEU	3.5
1	B	217	MET	3.5
1	A	213	LYS	3.5
1	C	102	LEU	3.4
1	B	42	ILE	3.3
1	D	226	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	61	THR	3.2
1	A	4	ILE	3.1
1	C	272	ASP	3.1
1	B	203	VAL	3.1
1	C	143	LYS	3.1
1	F	89	LYS	3.1
1	D	47	THR	3.0
1	D	100	LYS	3.0
1	D	266	GLY	3.0
1	D	297	HIS	3.0
1	A	46	LYS	2.9
1	D	102	LEU	2.9
1	B	297	HIS	2.9
1	E	226	TYR	2.9
1	D	103	LYS	2.9
1	E	233	GLY	2.9
1	A	104	ILE	2.8
1	C	106	LYS	2.8
1	A	3	SER	2.8
1	D	207	PRO	2.8
1	F	4	ILE	2.8
1	C	3	SER	2.8
1	A	101	ASN	2.7
1	C	4	ILE	2.7
1	E	3	SER	2.7
1	A	103	LYS	2.7
1	F	205	ALA	2.7
1	B	126	ASN	2.6
1	A	303	GLN	2.6
1	F	84	ALA	2.6
1	D	183	ASP	2.6
1	D	314	THR	2.6
1	C	101	ASN	2.5
1	E	229	ILE	2.5
1	A	279	ALA	2.5
1	D	313	LEU	2.5
1	B	266	GLY	2.5
1	C	98	VAL	2.5
1	B	307	SER	2.5
1	A	217	MET	2.5
1	E	311	LYS	2.5
1	F	85	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	2.5
1	D	208	GLU	2.4
1	B	102	LEU	2.4
1	C	104	ILE	2.4
1	E	166	VAL	2.4
1	F	136	TRP	2.4
1	D	210	LYS	2.4
1	B	287	GLN	2.4
1	A	75	LYS	2.4
1	C	61	THR	2.4
1	A	230	LYS	2.3
1	E	197	VAL	2.3
1	A	136	TRP	2.3
1	D	84	ALA	2.3
1	E	7	LYS	2.3
1	A	5	THR	2.3
1	A	47	THR	2.3
1	D	5	THR	2.3
1	E	5	THR	2.3
1	A	223	ASN	2.3
1	D	7	LYS	2.3
1	A	106	LYS	2.2
1	D	106	LYS	2.2
1	A	119	GLY	2.2
1	C	107	SER	2.2
1	E	213	LYS	2.2
1	A	262	VAL	2.2
1	A	269	GLY	2.2
1	E	138	LEU	2.2
1	A	308	GLN	2.1
1	C	119	GLY	2.1
1	A	134	ALA	2.1
1	F	3	SER	2.1
1	D	288	ASN	2.1
1	F	287	GLN	2.1
1	D	197	VAL	2.1
1	C	311	LYS	2.1
1	D	307	SER	2.1
1	C	144	ASN	2.1
1	B	3	SER	2.1
1	D	217	MET	2.1
1	C	312	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	301	SER	2.1
1	D	309	LEU	2.0
1	A	45	ASP	2.0
1	F	207	PRO	2.0
1	E	306	ALA	2.0
1	F	192	ALA	2.0
1	A	137	LYS	2.0
1	B	7	LYS	2.0
1	B	140	GLY	2.0
1	A	263	TYR	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
3	GOL	D	403	6/6	0.83	0.19	44,59,62,63	0
2	SO4	E	401	5/5	0.88	0.11	51,55,68,81	0
3	GOL	F	403	6/6	0.88	0.11	47,62,64,66	0
3	GOL	E	403	6/6	0.89	0.14	52,55,57,61	0
3	GOL	C	403	6/6	0.91	0.10	49,60,62,62	0
2	SO4	D	401	5/5	0.91	0.11	49,51,66,70	0
2	SO4	C	401	5/5	0.91	0.10	55,57,69,81	0
3	GOL	B	404	6/6	0.91	0.13	44,50,55,55	0
3	GOL	E	404	6/6	0.93	0.09	44,45,47,49	0
2	SO4	A	401	5/5	0.94	0.08	58,59,72,75	0
3	GOL	B	403	6/6	0.94	0.08	47,51,53,59	0
2	SO4	F	402	5/5	0.95	0.08	52,52,56,62	0
2	SO4	B	402	5/5	0.95	0.11	44,45,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	E	402	5/5	0.95	0.13	44,45,48,49	0
2	SO4	F	401	5/5	0.95	0.09	54,54,63,67	0
2	SO4	D	402	5/5	0.96	0.10	41,42,49,49	0
2	SO4	B	401	5/5	0.96	0.07	48,48,64,70	0
2	SO4	C	402	5/5	0.96	0.09	50,51,54,56	0
2	SO4	A	402	5/5	0.96	0.11	47,48,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.