



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:08 AM UTC

PDB ID : 1J4A / pdb_00001j4a
Title : INSIGHTS INTO DOMAIN CLOSURE, SUBSTRATE SPECIFICITY AND CATALYSIS OF D-LACTATE DEHYDROGENASE FROM LACTOBACILLUS BULGARICUS
Authors : Razeto, A.; Kochhar, S.; Hottinger, H.; Dauter, M.; Wilson, K.S.; Lamzin, V.S.
Deposited on : 2001-08-18
Resolution : 1.90 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

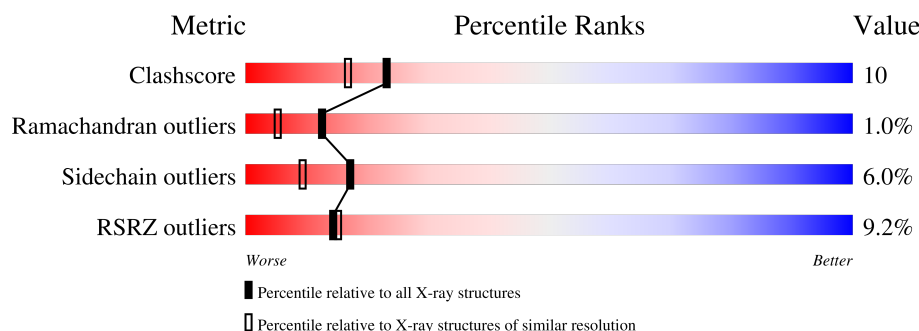
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	333	7% 81% 16% ..
1	B	333	4% 79% 19% ..
1	C	333	21% 64% 23% 8% 5% .
1	D	333	4% 78% 19% .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1402	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11428 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 D-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	39	8	0
			2632	1677	441	504	10			
1	B	331	Total	C	N	O	S	11	5	0
			2616	1665	440	501	10			
1	C	331	Total	C	N	O	S	416	2	0
			2603	1655	438	500	10			
1	D	332	Total	C	N	O	S	30	5	0
			2622	1668	440	504	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ILE	THR	SEE REMARK 999	UNP P26297
A	117	ARG	ALA	SEE REMARK 999	UNP P26297
A	152	VAL	ILE	SEE REMARK 999	UNP P26297
A	297	LYS	HIS	engineered mutation	UNP P26297
B	59	ILE	THR	SEE REMARK 999	UNP P26297
B	117	ARG	ALA	SEE REMARK 999	UNP P26297
B	152	VAL	ILE	SEE REMARK 999	UNP P26297
B	297	LYS	HIS	engineered mutation	UNP P26297
C	59	ILE	THR	SEE REMARK 999	UNP P26297
C	117	ARG	ALA	SEE REMARK 999	UNP P26297
C	152	VAL	ILE	SEE REMARK 999	UNP P26297
C	297	LYS	HIS	engineered mutation	UNP P26297
D	59	ILE	THR	SEE REMARK 999	UNP P26297
D	117	ARG	ALA	SEE REMARK 999	UNP P26297
D	152	VAL	ILE	SEE REMARK 999	UNP P26297
D	297	LYS	HIS	engineered mutation	UNP P26297

- 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	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	B	1	Total	O	S	0	0
			5	4	1		
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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	239	Total	O	0	0
			239	239		

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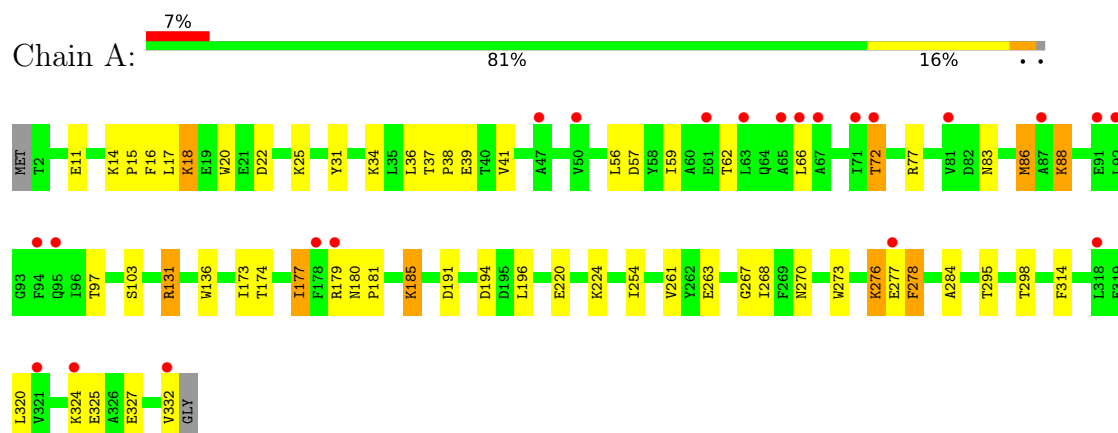
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	265	Total 265	O 265	0	0
3	C	160	Total 160	O 160	0	0
3	D	236	Total 236	O 236	0	0

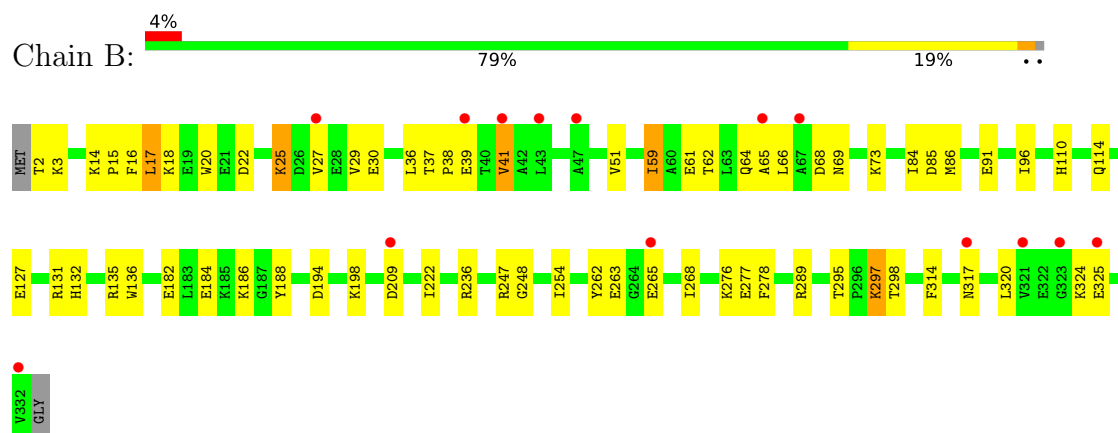
3 Residue-property plots [i](#)

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.

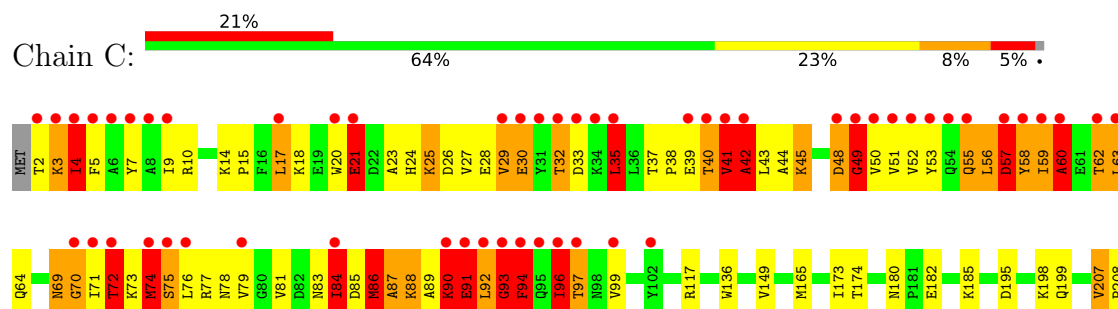
• Molecule 1: D-LACTATE DEHYDROGENASE



• Molecule 1: D-LACTATE DEHYDROGENASE

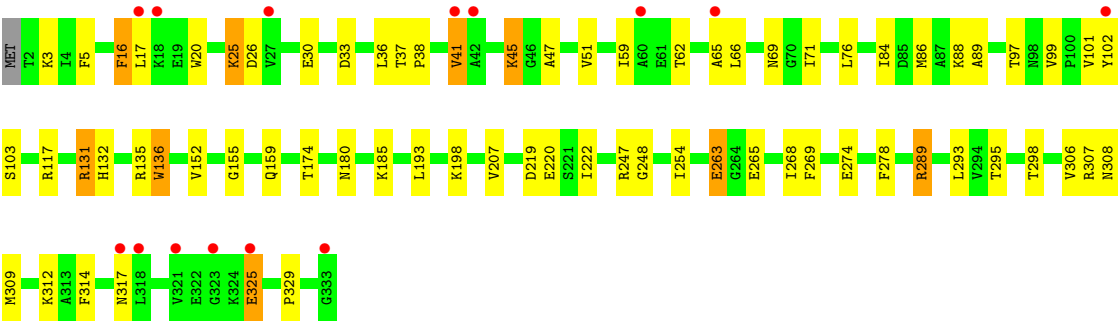
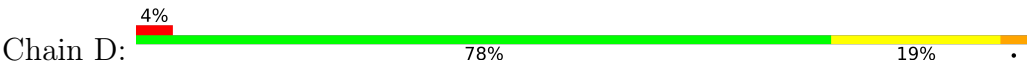


• Molecule 1: D-LACTATE DEHYDROGENASE





● Molecule 1: D-LACTATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	94.30Å 188.00Å 193.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.00 – 1.90 19.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.00-1.90) 98.2 (19.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.259 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11428	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: 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	0.61	2/2713 (0.1%)	1.24	14/3677 (0.4%)
1	B	0.56	0/2684	1.23	7/3639 (0.2%)
1	C	2.43	61/2658 (2.3%)	2.27	100/3604 (2.8%)
1	D	0.61	2/2690 (0.1%)	1.32	18/3649 (0.5%)
All	All	1.32	65/10745 (0.6%)	1.58	139/14569 (1.0%)

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	C	0	21
1	D	0	1
All	All	0	22

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	ALA	CA-C	-42.63	0.93	1.52
1	C	74	MET	N-CA	36.21	1.89	1.46
1	C	58	TYR	C-N	-32.98	0.88	1.33
1	C	96	ILE	CA-CB	-31.16	1.10	1.54
1	C	27	VAL	CA-CB	-29.70	1.25	1.54
1	C	90	LYS	CA-C	27.07	1.89	1.52
1	C	96	ILE	C-N	26.30	1.69	1.33
1	C	73	LYS	C-N	26.15	1.66	1.33
1	C	25	LYS	CA-C	-22.44	1.22	1.52
1	C	55	GLN	CA-CB	19.27	1.84	1.53
1	C	72	THR	C-N	18.26	1.59	1.33
1	C	318	LEU	CA-CB	-17.92	1.25	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	LYS	CA-C	17.90	1.77	1.52
1	C	97	THR	CA-C	15.87	1.71	1.52
1	C	26	ASP	C-N	15.65	1.51	1.33
1	C	58	TYR	CA-C	15.15	1.70	1.53
1	C	38	PRO	CA-C	13.30	1.71	1.52
1	D	45	LYS	CG-CD	13.22	1.92	1.52
1	C	73	LYS	N-CA	13.16	1.62	1.46
1	C	39	GLU	N-CA	12.93	1.62	1.46
1	C	93	GLY	N-CA	-12.81	1.26	1.45
1	C	42	ALA	N-CA	-12.40	1.30	1.46
1	C	92	LEU	C-O	-12.03	1.07	1.24
1	C	26	ASP	N-CA	11.85	1.62	1.46
1	C	74	MET	CA-C	-11.44	1.38	1.52
1	C	89	ALA	N-CA	11.32	1.60	1.46
1	C	73	LYS	CA-CB	11.28	1.69	1.53
1	C	58	TYR	CA-CB	-11.25	1.36	1.53
1	C	21	GLU	C-N	-10.83	1.19	1.33
1	C	26	ASP	CA-CB	-10.45	1.36	1.54
1	C	60	ALA	CA-CB	9.82	1.70	1.53
1	C	38	PRO	C-N	9.21	1.46	1.33
1	C	97	THR	N-CA	8.89	1.56	1.45
1	C	57	ASP	N-CA	8.76	1.57	1.46
1	C	332	VAL	CB-CG1	-8.74	1.23	1.52
1	C	91	GLU	CA-CB	-8.64	1.39	1.53
1	C	30	GLU	CD-OE1	8.40	1.41	1.25
1	C	48	ASP	N-CA	8.29	1.56	1.46
1	C	38	PRO	N-CA	8.12	1.57	1.47
1	C	297	LYS	CD-CE	-7.75	1.29	1.52
1	C	35	LEU	C-N	7.70	1.42	1.33
1	C	70	GLY	CA-C	-7.57	1.40	1.51
1	C	45	LYS	N-CA	7.36	1.55	1.46
1	C	25	LYS	C-N	7.29	1.46	1.33
1	C	40	THR	CA-CB	7.28	1.65	1.53
1	C	185	LYS	CG-CD	7.09	1.73	1.52
1	C	325	GLU	N-CA	7.05	1.54	1.46
1	C	236	ARG	CZ-NH2	7.00	1.42	1.33
1	C	88	LYS	C-N	-6.88	1.24	1.33
1	C	7	TYR	CB-CG	-6.58	1.37	1.51
1	C	90	LYS	N-CA	6.45	1.54	1.46
1	C	86	MET	C-N	6.37	1.42	1.33
1	C	44	ALA	C-N	6.36	1.42	1.33
1	C	39	GLU	CA-CB	6.12	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	57	ASP	CA-CB	-5.99	1.43	1.53
1	C	84	ILE	N-CA	5.85	1.53	1.46
1	C	63	LEU	N-CA	-5.68	1.39	1.46
1	C	71	ILE	CA-CB	-5.46	1.47	1.53
1	A	325	GLU	CG-CD	5.24	1.65	1.52
1	C	69	ASN	N-CA	5.24	1.52	1.46
1	C	84	ILE	CA-CB	-5.17	1.47	1.53
1	C	49	GLY	CA-C	-5.09	1.44	1.51
1	A	220	GLU	CG-CD	-5.04	1.39	1.52
1	D	268	ILE	CG1-CD1	-5.04	1.32	1.51
1	C	25	LYS	N-CA	5.01	1.52	1.46

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	GLN	O-C-N	-56.40	53.99	122.24
1	C	60	ALA	N-CA-C	29.95	148.95	113.01
1	C	74	MET	CA-C-O	-27.05	92.37	121.31
1	D	325	GLU	CA-CB-CG	-21.68	70.75	114.10
1	C	58	TYR	CA-C-N	21.13	160.00	121.97
1	C	58	TYR	C-N-CA	21.13	160.00	121.97
1	C	86	MET	O-C-N	-20.71	95.04	122.59
1	C	26	ASP	CA-CB-CG	18.08	130.68	112.60
1	C	324	LYS	CA-C-N	-15.67	101.15	122.30
1	C	324	LYS	C-N-CA	-15.67	101.15	122.30
1	C	96	ILE	O-C-N	-15.09	106.95	123.10
1	C	58	TYR	O-C-N	-13.30	102.46	122.67
1	C	58	TYR	N-CA-C	-12.92	94.37	110.65
1	C	90	LYS	CA-C-O	-12.63	105.45	119.97
1	C	92	LEU	CA-C-N	12.57	146.05	121.41
1	C	92	LEU	C-N-CA	12.57	146.05	121.41
1	C	48	ASP	N-CA-CB	-12.50	90.36	110.98
1	C	58	TYR	N-CA-CB	12.12	124.29	110.35
1	C	48	ASP	CA-CB-CG	12.01	124.61	112.60
1	C	332	VAL	CA-CB-CG1	11.74	130.36	110.40
1	C	48	ASP	N-CA-C	11.58	129.27	112.94
1	C	25	LYS	CA-C-N	-11.57	101.94	122.42
1	C	25	LYS	C-N-CA	-11.57	101.94	122.42
1	C	62	THR	CA-C-N	-11.50	105.50	120.44
1	C	62	THR	C-N-CA	-11.50	105.50	120.44
1	C	7	TYR	CA-CB-CG	10.80	133.35	113.90
1	C	73	LYS	O-C-N	-10.34	109.93	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29	VAL	CA-C-O	10.29	130.40	120.31
1	D	45	LYS	CB-CG-CD	-10.07	88.15	111.30
1	C	297	LYS	CG-CD-CE	9.53	133.21	111.30
1	C	84	ILE	CA-CB-CG2	9.48	126.62	110.50
1	C	41	VAL	CA-C-N	9.46	139.62	121.54
1	C	41	VAL	C-N-CA	9.46	139.62	121.54
1	C	60	ALA	CB-CA-C	-9.10	91.61	110.17
1	C	318	LEU	N-CA-CB	8.99	123.55	110.06
1	C	35	LEU	O-C-N	-8.70	111.02	122.59
1	C	56	LEU	O-C-N	8.58	134.15	122.48
1	C	69	ASN	CA-CB-CG	-8.50	104.10	112.60
1	C	74	MET	CB-CA-C	-8.45	94.51	111.91
1	C	58	TYR	CB-CA-C	-8.36	100.29	111.74
1	C	2	THR	N-CA-CB	-8.35	97.31	111.50
1	C	73	LYS	CA-C-N	8.27	135.83	122.10
1	C	73	LYS	C-N-CA	8.27	135.83	122.10
1	C	265	GLU	CG-CD-OE2	-8.26	99.40	118.40
1	C	89	ALA	N-CA-CB	-8.23	97.95	110.13
1	C	92	LEU	CA-C-O	7.96	129.55	119.12
1	C	21	GLU	O-C-N	-7.87	112.13	122.59
1	D	131	ARG	CD-NE-CZ	7.75	135.25	124.40
1	C	42	ALA	N-CA-C	-7.74	94.32	110.80
1	C	96	ILE	CB-CA-C	7.70	122.36	110.50
1	C	38	PRO	N-CA-C	7.60	128.13	112.47
1	C	38	PRO	O-C-N	-7.60	112.38	122.64
1	A	77	ARG	CD-NE-CZ	7.45	134.82	124.40
1	C	236	ARG	CD-NE-CZ	7.32	134.65	124.40
1	C	91	GLU	N-CA-CB	7.27	120.87	109.82
1	C	27	VAL	N-CA-CB	7.18	125.78	110.64
1	C	42	ALA	O-C-N	7.00	131.89	122.59
1	D	71	ILE	N-CA-C	6.85	117.74	107.80
1	A	41	VAL	CA-CB-CG2	6.73	121.84	110.40
1	C	91	GLU	CB-CA-C	6.67	121.52	110.92
1	C	55	GLN	N-CA-CB	-6.61	100.62	110.61
1	C	81	VAL	CB-CA-C	-6.58	100.49	111.29
1	C	325	GLU	CA-CB-CG	-6.55	101.00	114.10
1	C	59	ILE	CG1-CB-CG2	-6.51	91.16	110.70
1	C	91	GLU	O-C-N	-6.48	115.14	122.08
1	C	79	VAL	O-C-N	6.47	130.66	122.57
1	C	92	LEU	O-C-N	-6.45	112.85	122.39
1	D	16	PHE	CA-CB-CG	-6.30	107.50	113.80
1	C	90	LYS	CB-CA-C	-6.29	98.60	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	ARG	CA-C-N	6.11	125.73	119.56
1	D	289	ARG	C-N-CA	6.11	125.73	119.56
1	C	87	ALA	O-C-N	6.07	130.66	122.59
1	C	58	TYR	CA-CB-CG	-6.01	103.08	113.90
1	A	16	PHE	CA-CB-CG	-6.00	107.80	113.80
1	A	86	MET	CG-SD-CE	5.94	113.96	100.90
1	C	43	LEU	N-CA-C	-5.90	104.19	111.33
1	A	18	LYS	CD-CE-NZ	5.88	130.71	111.90
1	A	325	GLU	CB-CG-CD	-5.79	102.75	112.60
1	D	99	VAL	CA-C-N	5.77	125.30	119.19
1	D	99	VAL	C-N-CA	5.77	125.30	119.19
1	B	247	ARG	CA-C-N	5.75	126.36	119.98
1	B	247	ARG	C-N-CA	5.75	126.36	119.98
1	C	42	ALA	N-CA-CB	5.70	120.11	110.49
1	D	278	PHE	CA-C-N	5.66	125.27	119.56
1	D	278	PHE	C-N-CA	5.66	125.27	119.56
1	C	89	ALA	CA-C-N	5.64	128.88	120.31
1	C	89	ALA	C-N-CA	5.64	128.88	120.31
1	C	55	GLN	CB-CA-C	5.62	119.67	110.17
1	C	96	ILE	N-CA-CB	5.61	120.63	111.44
1	C	264	GLY	CA-C-O	5.60	124.55	118.95
1	C	24	HIS	CA-CB-CG	-5.60	108.20	113.80
1	D	269	PHE	CA-CB-CG	5.56	119.36	113.80
1	C	89	ALA	N-CA-C	-5.56	104.62	111.40
1	C	84	ILE	CA-CB-CG1	5.54	119.83	110.40
1	C	91	GLU	CA-C-O	5.54	127.17	121.07
1	A	131	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	B	289	ARG	CA-C-N	5.50	125.11	119.56
1	B	289	ARG	C-N-CA	5.50	125.11	119.56
1	C	3	LYS	N-CA-CB	5.49	119.38	110.77
1	A	180	ASN	CA-C-N	5.48	125.13	119.05
1	A	180	ASN	C-N-CA	5.48	125.13	119.05
1	C	86	MET	CA-C-N	5.47	132.00	121.54
1	C	86	MET	C-N-CA	5.47	132.00	121.54
1	A	278	PHE	CA-C-N	5.47	125.30	119.28
1	A	278	PHE	C-N-CA	5.47	125.30	119.28
1	D	207	VAL	CA-C-N	5.46	125.37	119.85
1	D	207	VAL	C-N-CA	5.46	125.37	119.85
1	C	99	VAL	CA-C-N	5.44	124.96	119.19
1	C	99	VAL	C-N-CA	5.44	124.96	119.19
1	C	185	LYS	CB-CG-CD	-5.44	98.79	111.30
1	D	180	ASN	CA-C-N	5.40	124.59	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	180	ASN	C-N-CA	5.40	124.59	118.97
1	C	43	LEU	O-C-N	5.38	127.83	122.12
1	C	93	GLY	O-C-N	-5.36	115.73	122.70
1	C	60	ALA	N-CA-CB	-5.33	101.06	110.39
1	A	131	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	C	89	ALA	O-C-N	5.25	128.53	122.17
1	B	16	PHE	CA-CB-CG	-5.25	108.55	113.80
1	C	23	ALA	N-CA-C	-5.24	105.18	112.30
1	D	263	GLU	CB-CA-C	5.21	120.79	110.17
1	A	179	ARG	N-CA-C	5.20	117.10	108.20
1	C	24	HIS	CB-CA-C	5.15	120.68	110.42
1	C	93	GLY	CA-C-O	-5.12	111.67	120.57
1	C	328	THR	CA-C-N	5.11	125.01	119.85
1	C	328	THR	C-N-CA	5.11	125.01	119.85
1	C	207	VAL	CA-C-N	5.09	125.00	119.85
1	C	207	VAL	C-N-CA	5.09	125.00	119.85
1	A	191	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	278	PHE	CA-C-N	5.06	125.51	120.04
1	B	278	PHE	C-N-CA	5.06	125.51	120.04
1	C	4	ILE	CG1-CB-CG2	-5.04	95.57	110.70
1	C	180	ASN	CA-C-N	5.04	124.65	119.05
1	C	180	ASN	C-N-CA	5.04	124.65	119.05
1	C	289	ARG	CA-C-N	5.03	124.64	119.56
1	C	289	ARG	C-N-CA	5.03	124.64	119.56
1	C	290	PRO	N-CA-CB	5.03	108.33	103.51
1	C	23	ALA	CA-C-O	5.02	125.60	119.78
1	C	236	ARG	NH1-CZ-NH2	-5.01	112.78	119.30
1	D	198	LYS	CB-CG-CD	5.00	122.81	111.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	21	GLU	Mainchain
1	C	265	GLU	Sidechain
1	C	3	LYS	Mainchain
1	C	30	GLU	Sidechain
1	C	35	LEU	Mainchain
1	C	41	VAL	Mainchain
1	C	49	GLY	Mainchain
1	C	55	GLN	Mainchain
1	C	58	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	C	60	ALA	Peptide,Mainchain
1	C	70	GLY	Mainchain
1	C	74	MET	Mainchain
1	C	86	MET	Mainchain
1	C	90	LYS	Peptide,Mainchain
1	C	91	GLU	Peptide
1	C	92	LEU	Peptide
1	C	93	GLY	Mainchain
1	C	94	PHE	Sidechain
1	C	97	THR	Mainchain
1	D	152	VAL	Mainchain

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	2632	0	2632	39	0
1	B	2616	0	2612	70	0
1	C	2603	0	2588	42	0
1	D	2622	0	2609	59	0
2	A	20	0	0	2	0
2	B	20	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
3	A	239	0	0	5	0
3	B	265	0	0	8	1
3	C	160	0	0	2	0
3	D	236	0	0	4	1
All	All	11428	0	10441	205	2

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 10.

All (205) 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:51:VAL:HG22	1:D:317:ASN:ND2	1.43	1.33
1:D:51:VAL:CG2	1:D:317:ASN:ND2	1.92	1.31
1:B:51:VAL:HG22	1:B:317:ASN:ND2	1.52	1.24
1:D:248:GLY:HA3	1:D:254:ILE:HD12	1.30	1.08
1:B:262:TYR:O	1:B:265:GLU:HG2	1.56	1.06
1:D:41:VAL:HG11	1:D:65:ALA:HB1	1.43	1.00
1:D:51:VAL:HG22	1:D:317:ASN:HD21	0.96	0.99
1:B:51:VAL:CG2	1:B:317:ASN:ND2	2.27	0.96
1:D:25:LYS:HD2	1:D:25:LYS:H	1.31	0.95
1:D:51:VAL:CG2	1:D:317:ASN:HD22	1.64	0.93
1:B:84:ILE:CG2	1:B:86:MET:HE3	1.97	0.93
1:D:59:ILE:HG13	1:D:62:THR:H	1.35	0.91
1:B:84:ILE:HG21	1:B:86:MET:HE3	1.50	0.90
1:B:51:VAL:HG22	1:B:317:ASN:HD22	1.37	0.89
1:D:51:VAL:HG23	1:D:317:ASN:ND2	1.84	0.89
1:B:51:VAL:CG2	1:B:317:ASN:HD22	1.85	0.88
1:A:36:LEU:HD21	1:A:66:LEU:HD11	1.55	0.87
1:B:51:VAL:HG22	1:B:317:ASN:HD21	1.32	0.86
1:B:17:LEU:HD11	1:B:29:VAL:HG11	1.57	0.86
1:D:25:LYS:H	1:D:25:LYS:CD	1.81	0.84
1:B:248:GLY:HA3	1:B:254:ILE:HD12	1.58	0.84
1:C:41:VAL:HG23	1:C:42:ALA:H	1.43	0.84
1:A:181:PRO:O	1:A:185:LYS:HE3	1.78	0.83
1:B:186:LYS:HE2	1:B:188:TYR:HE2	1.45	0.82
1:B:41:VAL:HG22	1:B:66:LEU:HD23	1.60	0.81
1:D:155:GLY:O	1:D:159[A]:GLN:HG3	1.82	0.79
1:D:84:ILE:CG2	1:D:86:MET:HE3	2.13	0.78
1:B:127:GLU:HG3	3:B:2644:HOH:O	1.83	0.78
1:D:25:LYS:HD2	1:D:25:LYS:N	1.96	0.77
1:A:88:LYS:HB2	1:A:88:LYS:NZ	1.99	0.77
1:B:86:MET:HA	1:B:86:MET:HE2	1.67	0.77
1:D:248:GLY:CA	1:D:254:ILE:HD12	2.14	0.77
1:B:36:LEU:HD11	1:B:41:VAL:HG23	1.68	0.76
1:B:37:THR:HB	1:B:38:PRO:HD2	1.67	0.75
1:D:36:LEU:HD21	1:D:66:LEU:HD11	1.68	0.74
1:B:194:ASP:O	1:B:198[A]:LYS:HG3	1.86	0.74
1:D:41:VAL:HG12	3:D:4631:HOH:O	1.87	0.73
1:D:84:ILE:HG21	1:D:86:MET:HE3	1.71	0.73
1:B:186:LYS:HE2	1:B:188:TYR:CE2	2.23	0.72
1:D:248:GLY:HA3	1:D:254:ILE:CD1	2.16	0.72
1:A:263[B]:GLU:HG2	3:A:1445:HOH:O	1.88	0.72
1:A:136:TRP:HB3	1:B:298[B]:THR:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLU:OE2	1:B:297:LYS:NZ	2.24	0.69
1:D:41:VAL:HG21	1:D:66:LEU:N	2.08	0.69
2:A:1402:SO4:O3	3:A:1470:HOH:O	2.10	0.69
1:A:59:ILE:HG13	1:A:62:THR:H	1.57	0.69
1:A:37:THR:HB	1:A:38:PRO:CD	2.24	0.67
1:B:41:VAL:HG22	1:B:66:LEU:CD2	2.25	0.66
1:B:84:ILE:HG22	1:B:86:MET:HE3	1.76	0.66
1:B:209:ASP:OD2	1:B:209:ASP:O	2.15	0.64
1:C:17:LEU:HD11	1:C:314:PHE:CZ	2.32	0.64
1:C:52:VAL:HG23	1:C:76:LEU:HD23	1.80	0.64
1:D:37:THR:HB	1:D:38:PRO:CD	2.28	0.64
1:A:17:LEU:HD21	1:A:314:PHE:CZ	2.33	0.63
1:A:88:LYS:HB2	1:A:88:LYS:HZ3	1.64	0.63
1:B:276:LYS:NZ	3:B:2659:HOH:O	2.28	0.63
1:C:298:THR:HG22	1:D:136:TRP:HB3	1.80	0.62
1:B:25:LYS:H	1:B:25:LYS:HD3	1.63	0.62
1:C:4:ILE:HA	1:C:49:GLY:O	2.00	0.62
1:C:195:ASP:O	1:C:199:GLN:HG2	1.98	0.62
1:B:25:LYS:HD3	1:B:25:LYS:N	2.15	0.62
1:B:22:ASP:O	1:B:25:LYS:HD2	1.98	0.62
1:A:11:GLU:HA	1:A:14:LYS:HD2	1.81	0.61
1:B:25:LYS:H	1:B:25:LYS:CD	2.14	0.61
1:A:59:ILE:CG1	1:A:62:THR:H	2.14	0.61
1:B:73:LYS:HD3	1:B:320:LEU:HB3	1.82	0.61
1:D:41:VAL:HG11	1:D:65:ALA:CB	2.27	0.60
1:C:20:TRP:CE2	1:C:314:PHE:HB3	2.36	0.60
1:A:57:ASP:OD1	1:A:83:ASN:HB2	2.01	0.60
1:C:222:ILE:HG23	1:C:254:ILE:HD11	1.83	0.60
1:D:59:ILE:CD1	3:D:4623:HOH:O	2.49	0.59
1:B:37:THR:HB	1:B:38:PRO:CD	2.30	0.59
1:C:53:TYR:CE1	1:C:78:ASN:HB3	2.37	0.59
1:D:59:ILE:HG13	1:D:62:THR:N	2.13	0.59
1:D:84:ILE:HG21	1:D:86:MET:CE	2.31	0.59
1:C:117:ARG:HB3	3:C:3424:HOH:O	2.02	0.59
1:D:289:ARG:NH2	3:D:4513:HOH:O	2.36	0.59
1:B:248:GLY:HA3	1:B:254:ILE:CD1	2.32	0.59
1:D:37:THR:HB	1:D:38:PRO:HD2	1.84	0.59
1:A:173:ILE:HG13	1:A:196[A]:LEU:CD1	2.34	0.58
1:A:276[A]:LYS:NZ	1:A:276[A]:LYS:HB3	2.19	0.58
1:A:332:VAL:O	1:A:332:VAL:HG13	2.03	0.58
1:A:34:LYS:HE3	3:A:1615:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298[A]:THR:HG22	1:B:136:TRP:HB3	1.86	0.58
1:C:60:ALA:HA	1:C:63:LEU:H	1.69	0.58
1:B:86:MET:HE1	1:B:96:ILE:HD12	1.86	0.57
1:C:14:LYS:HB2	1:C:15:PRO:HD3	1.87	0.56
1:A:37:THR:HB	1:A:38:PRO:HD2	1.88	0.56
1:A:88:LYS:HB2	1:A:88:LYS:HZ2	1.70	0.56
1:D:84:ILE:CG2	1:D:86:MET:CE	2.84	0.55
1:B:41:VAL:HG11	1:B:65:ALA:O	2.07	0.55
1:C:41:VAL:HG23	1:C:42:ALA:N	2.19	0.55
1:B:85:ASP:OD1	3:B:2548:HOH:O	2.18	0.54
1:B:61:GLU:HB2	3:B:2563:HOH:O	2.06	0.54
1:B:59:ILE:CG1	1:B:62:THR:H	2.20	0.54
1:C:149:VAL:HG11	1:C:165[B]:MET:HG3	1.90	0.54
1:C:220:GLU:O	1:C:224:LYS:HG3	2.08	0.54
1:B:41:VAL:HG11	1:B:65:ALA:C	2.33	0.54
1:C:4:ILE:HG12	1:C:317:ASN:OD1	2.07	0.53
1:D:59:ILE:HD13	3:D:4623:HOH:O	2.08	0.53
1:C:173:ILE:CD1	1:C:199:GLN:HG3	2.38	0.53
1:D:86:MET:HE2	1:D:86:MET:HA	1.92	0.52
1:D:41:VAL:CG2	1:D:66:LEU:HD23	2.39	0.52
1:B:3:LYS:NZ	3:B:2654:HOH:O	2.28	0.52
1:C:305:ALA:O	1:C:309:MET:HG3	2.09	0.52
1:A:97:THR:HG23	1:A:320:LEU:HD11	1.92	0.52
1:D:41:VAL:HG22	1:D:66:LEU:HD23	1.90	0.52
1:D:41:VAL:HG13	1:D:69:ASN:ND2	2.25	0.51
1:C:268:ILE:HD12	1:C:279:PRO:HG2	1.92	0.51
1:C:5:PHE:O	1:C:50:VAL:HA	2.10	0.51
1:D:41:VAL:HG22	1:D:66:LEU:HA	1.92	0.51
1:B:41:VAL:HG11	1:B:65:ALA:HB1	1.92	0.51
1:B:277:GLU:OE2	3:B:2502:HOH:O	2.18	0.50
1:B:25:LYS:N	1:B:25:LYS:CD	2.74	0.50
1:B:297:LYS:NZ	1:B:297:LYS:HB2	2.26	0.50
1:D:26:ASP:OD2	1:D:26:ASP:N	2.45	0.49
1:B:59:ILE:HG13	1:B:62:THR:H	1.77	0.49
1:A:276[A]:LYS:HB3	1:A:276[A]:LYS:HZ2	1.76	0.48
1:A:194:ASP:OD2	1:A:224:LYS:NZ	2.46	0.48
1:D:20:TRP:CE2	1:D:314:PHE:HB3	2.48	0.48
1:B:30:GLU:HG3	3:B:2654:HOH:O	2.13	0.48
1:D:222:ILE:HD13	1:D:254:ILE:HD11	1.96	0.48
1:D:131:ARG:O	1:D:132:HIS:HB2	2.13	0.48
1:A:177:ILE:HG13	3:A:1509:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LYS:HB2	1:B:25:LYS:HE2	1.68	0.47
1:B:41:VAL:CG1	1:B:69:ASN:ND2	2.77	0.47
1:D:295:THR:HB	1:D:298[A]:THR:HG22	1.95	0.47
1:A:20:TRP:CE2	1:A:314:PHE:HB3	2.50	0.47
1:B:209:ASP:HB2	1:B:236:ARG:HG3	1.97	0.47
1:C:72:THR:HG23	1:C:94:PHE:HA	1.96	0.47
1:D:308:ASN:O	1:D:312:LYS:HG3	2.15	0.47
1:B:295:THR:HB	1:B:298[A]:THR:CG2	2.46	0.46
1:C:59:ILE:O	1:C:62:THR:HB	2.15	0.46
1:A:270:ASN:HA	1:B:135:ARG:HA	1.97	0.46
1:C:195:ASP:HB3	3:C:3560:HOH:O	2.15	0.46
1:D:306:VAL:HA	1:D:309:MET:HE3	1.98	0.46
1:B:20:TRP:CE2	1:B:314:PHE:HB3	2.50	0.46
1:A:261:VAL:HB	2:A:1402:SO4:O3	2.14	0.46
1:C:9:ILE:HD12	1:C:17:LEU:HD22	1.97	0.46
1:B:131:ARG:O	1:B:132:HIS:HB2	2.14	0.46
1:D:102:TYR:CD2	1:D:103:SER:N	2.84	0.46
1:B:41:VAL:CG2	1:B:66:LEU:HG	2.46	0.46
1:B:222:ILE:HG21	1:B:254:ILE:HD11	1.97	0.46
1:C:207:VAL:HB	1:C:208:PRO:HD2	1.97	0.46
1:B:248:GLY:CA	1:B:254:ILE:HD12	2.37	0.45
1:A:88:LYS:NZ	1:A:88:LYS:CB	2.66	0.45
1:D:33:ASP:OD2	1:D:33:ASP:N	2.34	0.45
1:A:72:THR:HG23	1:A:72:THR:O	2.16	0.45
1:C:136:TRP:HB3	1:D:298[B]:THR:HG22	1.98	0.45
1:A:267:GLY:O	1:A:268:ILE:HD13	2.16	0.45
1:B:295:THR:HB	1:B:298[A]:THR:HG22	1.98	0.45
1:C:53:TYR:HB2	1:C:77:ARG:CZ	2.47	0.45
1:C:306:VAL:O	1:C:310:VAL:HG23	2.17	0.45
1:B:25:LYS:H	1:B:25:LYS:CE	2.29	0.44
1:D:155:GLY:O	1:D:159[B]:GLN:HG3	2.15	0.44
1:C:76:LEU:HD22	1:C:78:ASN:OD1	2.17	0.44
1:A:131:ARG:HD3	3:A:1573:HOH:O	2.17	0.44
1:A:295:THR:HB	1:A:298[B]:THR:HG22	2.00	0.44
1:B:262:TYR:HB3	1:B:265:GLU:HB3	2.00	0.44
1:B:297:LYS:NZ	1:B:297:LYS:CB	2.81	0.44
1:C:10:ARG:HH12	1:C:53:TYR:HE2	1.66	0.44
1:C:96:ILE:O	1:C:330:VAL:N	2.51	0.44
1:B:2:THR:HG22	1:B:27:VAL:HG13	2.00	0.43
1:A:39:GLU:OE1	1:A:39:GLU:N	2.51	0.43
1:B:262:TYR:O	1:B:265:GLU:CG	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:VAL:HG22	1:C:75:SER:HB3	2.01	0.43
1:D:219:ASP:CG	1:D:247:ARG:HH21	2.27	0.43
1:C:270:ASN:HA	1:D:135:ARG:HA	2.00	0.43
1:A:173:ILE:HG13	1:A:196[A]:LEU:HD12	2.01	0.43
1:B:22:ASP:O	1:B:25:LYS:CD	2.66	0.43
1:B:59:ILE:HG12	1:B:62:THR:H	1.83	0.43
1:C:17:LEU:HD11	1:C:314:PHE:CE1	2.53	0.43
1:D:37:THR:CB	1:D:38:PRO:CD	2.91	0.43
1:D:88:LYS:HD3	1:D:88:LYS:HA	1.87	0.43
1:C:90:LYS:O	1:C:91:GLU:C	2.62	0.42
1:B:110:HIS:O	1:B:114:GLN:HG2	2.20	0.42
1:C:84:ILE:HD13	1:C:84:ILE:HG21	1.75	0.42
1:D:5:PHE:CE1	1:D:30[B]:GLU:HG2	2.54	0.42
1:D:117:ARG:CZ	1:D:293[B]:LEU:HD21	2.49	0.42
1:D:16:PHE:CE2	1:D:307:ARG:HB2	2.53	0.42
1:C:210:VAL:HB	1:C:211:PRO:HD2	2.01	0.42
1:B:64:GLN:NE2	1:B:68:ASP:OD2	2.53	0.42
1:C:17:LEU:HD12	1:C:17:LEU:HA	1.83	0.42
1:A:14:LYS:O	1:A:18:LYS:HG3	2.20	0.42
1:A:14:LYS:HE2	1:A:31:TYR:OH	2.19	0.42
1:D:97:THR:HG22	1:D:329:PRO:HA	2.01	0.42
1:D:295:THR:HB	1:D:298[A]:THR:CG2	2.49	0.42
1:B:236:ARG:HD3	3:B:2629:HOH:O	2.18	0.42
1:C:40:THR:O	1:C:41:VAL:C	2.63	0.42
1:A:22:ASP:O	1:A:25:LYS:HE3	2.20	0.41
1:A:278:PHE:CD2	1:A:284:ALA:HB2	2.55	0.41
1:B:37:THR:CB	1:B:38:PRO:CD	2.95	0.41
1:D:41:VAL:CG2	1:D:66:LEU:HA	2.50	0.41
1:D:193:LEU:HD23	1:D:193:LEU:HA	1.94	0.41
1:C:17:LEU:HD13	1:C:310:VAL:CG1	2.51	0.41
1:A:273:TRP:C	1:A:276[A]:LYS:HG3	2.46	0.41
1:C:14:LYS:N	1:C:15:PRO:CD	2.84	0.41
1:C:32:THR:OG1	1:C:33:ASP:N	2.54	0.41
1:D:88:LYS:O	1:D:89:ALA:C	2.63	0.41
1:B:297:LYS:HB2	1:B:297:LYS:HZ2	1.85	0.41
1:D:51:VAL:HG21	1:D:317:ASN:HD22	1.69	0.41
1:D:3:LYS:HB3	1:D:47:ALA:HA	2.03	0.40
1:B:14:LYS:N	1:B:15:PRO:CD	2.84	0.40
1:B:41:VAL:CG1	1:B:69:ASN:HD22	2.33	0.40
1:A:14:LYS:N	1:A:15:PRO:CD	2.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2531:HOH:O	3:B:2531:HOH:O[3_555]	1.36	0.84
3:D:4513:HOH:O	3:D:4513:HOH:O[3_655]	2.01	0.19

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	337/333 (101%)	324 (96%)	12 (4%)	1 (0%)	36	29
1	B	334/333 (100%)	324 (97%)	10 (3%)	0	100	100
1	C	329/333 (99%)	287 (87%)	30 (9%)	12 (4%)	2	0
1	D	335/333 (101%)	324 (97%)	11 (3%)	0	100	100
All	All	1335/1332 (100%)	1259 (94%)	63 (5%)	13 (1%)	12	5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	25	LYS
1	C	35	LEU
1	C	41	VAL
1	C	42	ALA
1	C	45	LYS
1	C	86	MET
1	C	87	ALA
1	C	93	GLY
1	C	21	GLU
1	C	57	ASP
1	C	85	ASP
1	C	83	ASN
1	A	103	SER

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	285/278 (102%)	272 (95%)	13 (5%)	24	16
1	B	282/278 (101%)	268 (95%)	14 (5%)	22	14
1	C	279/278 (100%)	253 (91%)	26 (9%)	8	3
1	D	282/278 (101%)	268 (95%)	14 (5%)	22	14
All	All	1128/1112 (101%)	1061 (94%)	67 (6%)	17	10

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	72	THR
1	A	86	MET
1	A	88	LYS
1	A	174	THR
1	A	177	ILE
1	A	185	LYS
1	A	254	ILE
1	A	276[A]	LYS
1	A	276[B]	LYS
1	A	277	GLU
1	A	324	LYS
1	A	327	GLU
1	B	17	LEU
1	B	18	LYS
1	B	25	LYS
1	B	39	GLU
1	B	41	VAL
1	B	59	ILE
1	B	91	GLU
1	B	182	GLU
1	B	184	GLU
1	B	263	GLU
1	B	268	ILE

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Mol	Chain	Res	Type
1	B	297	LYS
1	B	324	LYS
1	B	325	GLU
1	C	4	ILE
1	C	17	LEU
1	C	18	LYS
1	C	28	GLU
1	C	29	VAL
1	C	32	THR
1	C	37	THR
1	C	48	ASP
1	C	56	LEU
1	C	57	ASP
1	C	64	GLN
1	C	69	ASN
1	C	72	THR
1	C	74	MET
1	C	75	SER
1	C	84	ILE
1	C	88	LYS
1	C	91	GLU
1	C	94	PHE
1	C	96	ILE
1	C	174	THR
1	C	182	GLU
1	C	198	LYS
1	C	253	LYS
1	C	322	GLU
1	C	324	LYS
1	D	17	LEU
1	D	25	LYS
1	D	41	VAL
1	D	45	LYS
1	D	76	LEU
1	D	101	VAL
1	D	136	TRP
1	D	174	THR
1	D	185	LYS
1	D	220	GLU
1	D	263	GLU
1	D	265	GLU
1	D	274	GLU

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Mol	Chain	Res	Type
1	D	325	GLU

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	317	ASN
1	B	55	GLN
1	B	159	GLN
1	B	317	ASN
1	C	199	GLN
1	C	227	GLN
1	D	317	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 [i](#)

11 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	D	4400	-	4,4,4	0.65	0	6,6,6	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	2401	-	4,4,4	0.58	0	6,6,6	0.30	0
2	SO4	B	2400	-	4,4,4	0.72	0	6,6,6	0.35	0
2	SO4	C	3400	-	4,4,4	0.57	0	6,6,6	0.44	0
2	SO4	A	1403	-	4,4,4	0.73	0	6,6,6	0.23	0
2	SO4	A	1401	-	4,4,4	0.59	0	6,6,6	0.29	0
2	SO4	B	2403	-	4,4,4	0.72	0	6,6,6	0.30	0
2	SO4	A	1402	-	4,4,4	0.63	0	6,6,6	0.10	0
2	SO4	D	4401	-	4,4,4	0.63	0	6,6,6	0.27	0
2	SO4	B	2402	-	4,4,4	0.72	0	6,6,6	0.27	0
2	SO4	A	1400	-	4,4,4	0.69	0	6,6,6	0.55	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1402	SO4	2	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	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	48:ASP	C	49:GLY	N	2.02
1	C	96:ILE	C	97:THR	N	1.69
1	C	73:LYS	C	74:MET	N	1.66
1	C	21:GLU	C	22:ASP	N	1.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	58:TYR	C	59:ILE	N	0.88

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	331/333 (99%)	0.30	22 (6%) 24 26	10, 26, 46, 54	21 (6%)
1	B	331/333 (99%)	0.17	14 (4%) 40 43	10, 25, 41, 55	10 (3%)
1	C	298/333 (89%)	1.02	69 (23%) 2 2	9, 28, 67, 85	48 (16%)
1	D	332/333 (99%)	0.30	14 (4%) 40 43	10, 28, 44, 55	15 (4%)
All	All	1292/1332 (96%)	0.43	119 (9%) 14 15	9, 27, 49, 85	94 (7%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	60	ALA	9.8
1	C	58	TYR	8.1
1	C	84	ILE	7.6
1	C	96	ILE	7.5
1	D	317	ASN	6.6
1	C	41	VAL	6.1
1	C	29	VAL	5.8
1	C	63	LEU	5.8
1	C	94	PHE	5.7
1	C	332	VAL	5.6
1	C	2	THR	5.6
1	C	42	ALA	5.4
1	B	317	ASN	5.3
1	C	92	LEU	5.3
1	C	39	GLU	5.2
1	C	72	THR	5.2
1	C	4	ILE	4.9
1	C	97	THR	4.8
1	C	311	VAL	4.6
1	C	5	PHE	4.5
1	C	318	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	321	VAL	4.4
1	C	93	GLY	4.3
1	A	332	VAL	4.3
1	C	76	LEU	4.3
1	C	59	ILE	4.3
1	C	55	GLN	4.3
1	C	57	ASP	4.2
1	A	178	PHE	4.1
1	D	102	TYR	4.1
1	B	41	VAL	4.1
1	C	17	LEU	4.0
1	C	48	ASP	4.0
1	C	35	LEU	4.0
1	C	7	TYR	4.0
1	D	333	GLY	3.9
1	C	6	ALA	3.9
1	C	323	GLY	3.7
1	C	314	PHE	3.7
1	C	95	GLN	3.7
1	C	71	ILE	3.6
1	C	50	VAL	3.6
1	C	20	TRP	3.6
1	C	40	THR	3.6
1	C	30	GLU	3.5
1	C	62	THR	3.4
1	D	42	ALA	3.2
1	D	17	LEU	3.2
1	C	54	GLN	3.2
1	C	52	VAL	3.1
1	C	320	LEU	3.1
1	C	53	TYR	3.1
1	A	87	ALA	3.0
1	C	9	ILE	3.0
1	C	74	MET	3.0
1	A	72	THR	3.0
1	C	326	ALA	3.0
1	C	31	TYR	3.0
1	C	91	GLU	3.0
1	D	321	VAL	2.9
1	C	102	TYR	2.9
1	C	90	LYS	2.9
1	C	32	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	49	GLY	2.9
1	A	67	ALA	2.8
1	A	94	PHE	2.8
1	C	325	GLU	2.8
1	B	39	GLU	2.8
1	B	209	ASP	2.8
1	C	70	GLY	2.8
1	A	50	VAL	2.8
1	C	51	VAL	2.8
1	C	79	VAL	2.8
1	C	324	LYS	2.7
1	A	321	VAL	2.7
1	C	99	VAL	2.6
1	B	265	GLU	2.6
1	C	3	LYS	2.6
1	B	67	ALA	2.6
1	C	319	GLU	2.5
1	A	324	LYS	2.5
1	B	43	LEU	2.5
1	C	21	GLU	2.5
1	C	313	ALA	2.5
1	C	34	LYS	2.5
1	D	318	LEU	2.4
1	A	71	ILE	2.4
1	B	321	VAL	2.4
1	D	41	VAL	2.4
1	A	63	LEU	2.4
1	C	75	SER	2.4
1	D	65	ALA	2.4
1	C	33	ASP	2.4
1	A	61[A]	GLU	2.4
1	C	329	PRO	2.4
1	D	323	GLY	2.4
1	A	318	LEU	2.3
1	C	322	GLU	2.3
1	B	325	GLU	2.3
1	A	65	ALA	2.3
1	A	81	VAL	2.2
1	A	277	GLU	2.2
1	A	92	LEU	2.2
1	B	47	ALA	2.2
1	B	65	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	315	ASP	2.2
1	A	66	LEU	2.2
1	A	95	GLN	2.1
1	A	179	ARG	2.1
1	D	18	LYS	2.1
1	A	91	GLU	2.1
1	A	47	ALA	2.1
1	D	60	ALA	2.1
1	C	8	ALA	2.1
1	D	325	GLU	2.0
1	B	332	VAL	2.0
1	B	323	GLY	2.0
1	B	27	VAL	2.0
1	D	27	VAL	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($\text{\AA}^2$)	Q<0.9
2	SO4	B	2403	5/5	0.71	0.29	43,43,45,45	5
2	SO4	B	2402	5/5	0.80	0.18	54,59,59,60	0
2	SO4	A	1403	5/5	0.82	0.19	40,40,42,43	5
2	SO4	A	1402	5/5	0.91	0.21	49,52,53,54	0
2	SO4	A	1401	5/5	0.93	0.11	46,46,48,49	0
2	SO4	D	4401	5/5	0.93	0.18	40,41,46,48	0
2	SO4	B	2400	5/5	0.95	0.11	36,38,41,42	0
2	SO4	D	4400	5/5	0.96	0.08	35,38,41,43	0
2	SO4	B	2401	5/5	0.96	0.10	32,33,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1400	5/5	0.97	0.09	29,29,34,35	0
2	SO4	C	3400	5/5	0.97	0.08	34,37,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.