



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:19 PM GMT

PDB ID : 1J4A  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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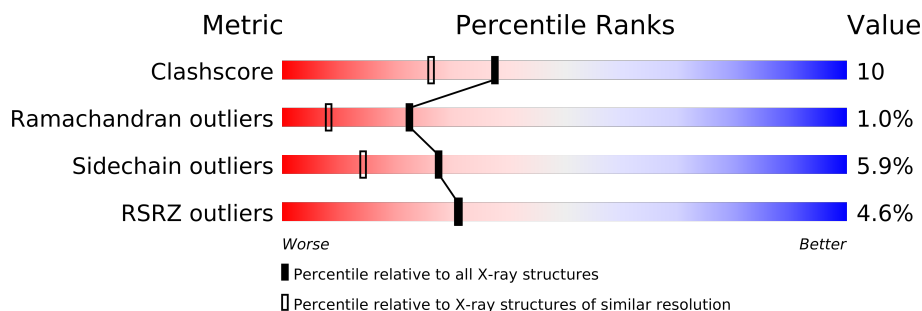
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	333	
1	B	333	
1	C	333	
1	D	333	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	1402	-	X
2	SO4	B	2400	-	X
2	SO4	B	2402	-	X
2	SO4	B	2403	-	X
2	SO4	D	4401	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11428 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

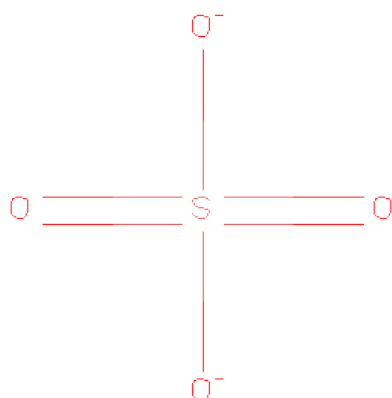
- Molecule 1 is a protein called D-LACTATE DEHYDROGENASE.

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	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	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	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	UNP P26297

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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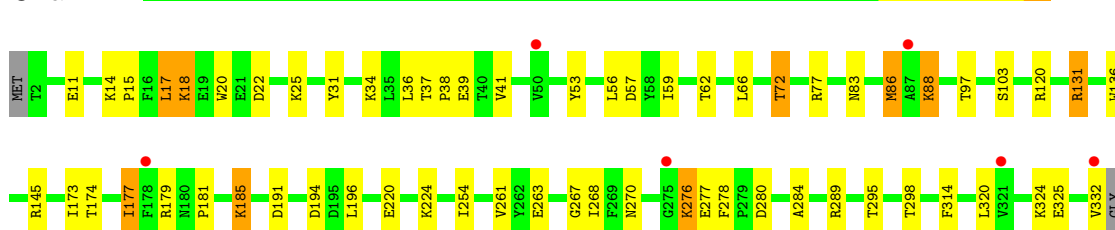
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	265	Total 265	O 265	0	0
3	C	160	Total 160	O 160	0	0
3	D	236	Total 236	O 236	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

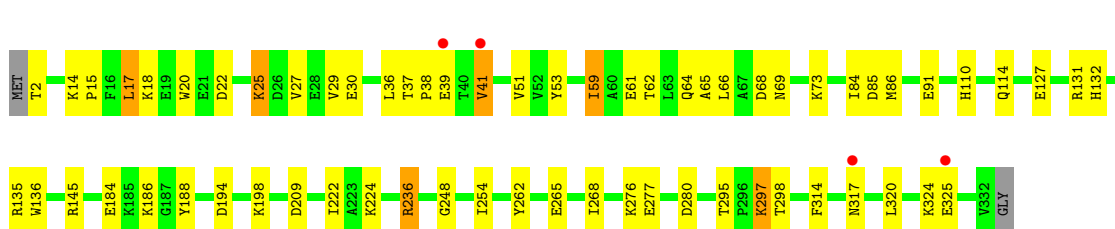
#### • Molecule 1: D-LACTATE DEHYDROGENASE

Chain A:



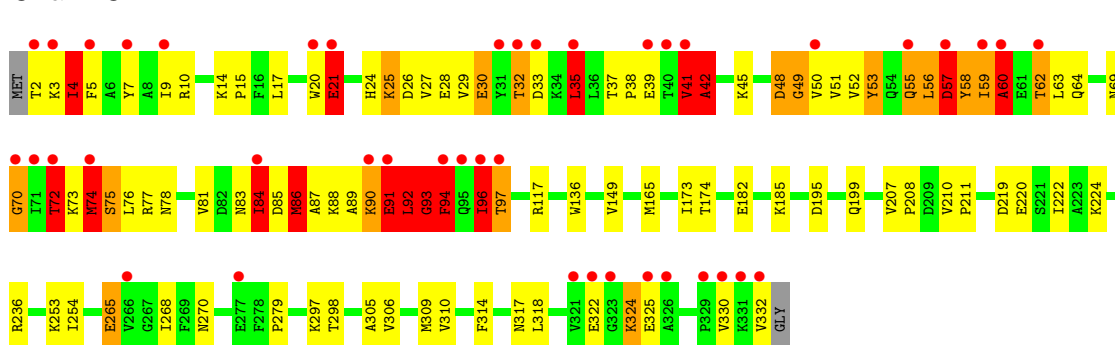
#### • Molecule 1: D-LACTATE DEHYDROGENASE

Chain B:



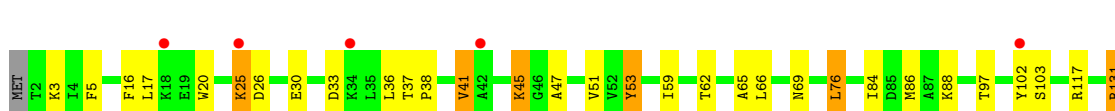
#### • Molecule 1: D-LACTATE DEHYDROGENASE

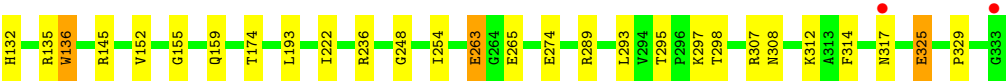
Chain C:



#### • Molecule 1: D-LACTATE DEHYDROGENASE

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.30Å 188.00Å 193.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.00 – 1.90 18.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.00-1.90) 98.3 (18.99-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.204 , 0.259 0.202 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 132346 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.



## 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.57	3/2713 (0.1%)	1.02	12/3677 (0.3%)
1	B	0.44	0/2684	0.94	3/3639 (0.1%)
1	C	1.58	45/2658 (1.7%)	1.73	78/3604 (2.2%)
1	D	0.52	2/2690 (0.1%)	1.04	11/3649 (0.3%)
All	All	0.90	50/10745 (0.5%)	1.22	104/14569 (0.7%)

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 (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	ALA	CA-C	-22.73	0.93	1.52
1	C	74	MET	N-CA	21.63	1.89	1.46
1	C	58	TYR	C-N	-19.68	0.88	1.34
1	C	96	ILE	CA-CB	-19.24	1.10	1.54
1	C	96	ILE	C-N	15.49	1.69	1.34
1	C	30	GLU	CD-OE1	14.24	1.41	1.25
1	C	73	LYS	C-N	14.15	1.66	1.34
1	C	27	VAL	CA-CB	-14.08	1.25	1.54
1	C	90	LYS	CA-C	13.97	1.89	1.52
1	C	55	GLN	CA-CB	13.92	1.84	1.53
1	C	332	VAL	CB-CG1	-13.88	1.23	1.52
1	C	93	GLY	N-CA	-12.84	1.26	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	318	LEU	CA-CB	-12.47	1.25	1.53
1	D	45	LYS	CG-CD	11.66	1.92	1.52
1	C	25	LYS	CA-C	-11.63	1.22	1.52
1	C	72	THR	C-N	11.20	1.59	1.34
1	C	7	TYR	CB-CG	-9.66	1.37	1.51
1	C	73	LYS	CA-C	9.26	1.77	1.52
1	C	38	PRO	CA-C	9.22	1.71	1.52
1	C	297	LYS	CD-CE	-8.82	1.29	1.51
1	A	325	GLU	CG-CD	8.81	1.65	1.51
1	C	60	ALA	CA-CB	8.78	1.70	1.52
1	A	220	GLU	CG-CD	-8.33	1.39	1.51
1	C	39	GLU	N-CA	8.26	1.62	1.46
1	C	92	LEU	C-O	-8.19	1.07	1.23
1	C	73	LYS	N-CA	8.15	1.62	1.46
1	C	42	ALA	N-CA	-8.08	1.30	1.46
1	C	58	TYR	CA-CB	-8.03	1.36	1.53
1	C	26	ASP	N-CA	7.88	1.62	1.46
1	C	26	ASP	CA-CB	-7.86	1.36	1.53
1	C	26	ASP	C-N	7.71	1.51	1.34
1	C	236	ARG	CZ-NH2	7.30	1.42	1.33
1	C	97	THR	CA-C	7.13	1.71	1.52
1	C	70	GLY	CA-C	-7.10	1.40	1.51
1	C	89	ALA	N-CA	7.00	1.60	1.46
1	C	73	LYS	CA-CB	7.00	1.69	1.53
1	D	325	GLU	CB-CG	6.71	1.65	1.52
1	A	41	VAL	CB-CG2	-6.60	1.39	1.52
1	C	58	TYR	CA-C	6.58	1.70	1.52
1	C	21	GLU	C-N	-6.42	1.19	1.34
1	C	91	GLU	CA-CB	-6.42	1.39	1.53
1	C	185	LYS	CG-CD	6.25	1.73	1.52
1	C	38	PRO	N-CA	6.16	1.57	1.47
1	C	57	ASP	N-CA	5.57	1.57	1.46
1	C	74	MET	CA-C	-5.46	1.38	1.52
1	C	38	PRO	C-N	5.45	1.46	1.34
1	C	48	ASP	CB-CG	-5.36	1.40	1.51
1	C	26	ASP	CB-CG	5.27	1.62	1.51
1	C	25	LYS	C-N	5.25	1.46	1.34
1	C	97	THR	N-CA	5.04	1.56	1.46

All (104) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	GLN	O-C-N	-42.94	53.99	122.70
1	D	325	GLU	CA-CB-CG	-19.39	70.75	113.40
1	C	86	MET	O-C-N	-17.29	95.04	122.70
1	C	58	TYR	C-N-CA	15.32	160.00	121.70
1	C	60	ALA	N-CA-C	14.06	148.95	111.00
1	C	74	MET	CA-C-O	-13.21	92.37	120.10
1	C	332	VAL	CA-CB-CG1	12.97	130.36	110.90
1	C	58	TYR	O-C-N	-12.65	102.46	122.70
1	C	60	ALA	CB-CA-C	-12.33	91.61	110.10
1	C	236	ARG	NE-CZ-NH1	12.31	126.46	120.30
1	C	92	LEU	C-N-CA	11.31	146.05	122.30
1	C	48	ASP	N-CA-CB	-11.24	90.36	110.60
1	C	7	TYR	CA-CB-CG	10.50	133.35	113.40
1	C	7	TYR	CB-CG-CD2	-10.33	114.80	121.00
1	A	179	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	C	96	ILE	O-C-N	-9.84	106.95	122.70
1	C	265	GLU	CG-CD-OE2	-9.45	99.40	118.30
1	C	94	PHE	CB-CG-CD2	-9.44	114.19	120.80
1	C	59	ILE	CG1-CB-CG2	-9.20	91.16	111.40
1	D	45	LYS	CB-CG-CD	-9.02	88.15	111.60
1	C	58	TYR	CA-C-N	8.96	136.91	117.20
1	C	30	GLU	OE1-CD-OE2	-8.84	112.69	123.30
1	C	89	ALA	N-CA-CB	-8.68	97.95	110.10
1	A	86	MET	CG-SD-CE	8.60	113.96	100.20
1	D	131	ARG	CD-NE-CZ	8.32	135.25	123.60
1	A	18	LYS	CD-CE-NZ	8.27	130.71	111.70
1	C	324	LYS	C-N-CA	-8.22	101.15	121.70
1	A	77	ARG	CD-NE-CZ	8.02	134.82	123.60
1	C	96	ILE	CA-C-N	-7.99	99.62	117.20
1	C	73	LYS	O-C-N	-7.98	109.93	122.70
1	C	74	MET	CB-CA-C	-7.95	94.51	110.40
1	A	120	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	D	131	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	C	25	LYS	C-N-CA	-7.90	101.94	121.70
1	C	236	ARG	CD-NE-CZ	7.89	134.65	123.60
1	C	84	ILE	CA-CB-CG2	7.86	126.62	110.90
1	C	26	ASP	CA-CB-CG	7.86	130.68	113.40
1	A	131	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	C	58	TYR	N-CA-CB	7.61	124.29	110.60
1	C	26	ASP	CB-CG-OD2	7.50	125.05	118.30
1	C	35	LEU	O-C-N	-7.30	111.02	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	VAL	CA-CB-CG2	7.29	121.84	110.90
1	B	280	ASP	CB-CG-OD1	7.24	124.81	118.30
1	C	73	LYS	CA-C-N	7.21	133.06	117.20
1	C	4	ILE	CG1-CB-CG2	-7.20	95.57	111.40
1	C	41	VAL	C-N-CA	7.17	139.62	121.70
1	C	56	LEU	O-C-N	7.16	134.15	122.70
1	C	42	ALA	N-CA-CB	7.15	120.11	110.10
1	A	289	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	C	297	LYS	CG-CD-CE	7.10	133.21	111.90
1	C	219	ASP	CB-CG-OD1	7.04	124.64	118.30
1	C	86	MET	CA-C-N	6.99	132.58	117.20
1	C	90	LYS	CA-C-O	-6.98	105.45	120.10
1	C	265	GLU	OE1-CD-OE2	6.86	131.53	123.30
1	C	2	THR	N-CA-CB	-6.84	97.31	110.30
1	C	48	ASP	N-CA-C	6.77	129.27	111.00
1	A	191	ASP	CB-CG-OD1	6.64	124.28	118.30
1	C	21	GLU	O-C-N	-6.61	112.13	122.70
1	C	318	LEU	N-CA-CB	6.58	123.55	110.40
1	D	131	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	C	27	VAL	N-CA-CB	6.49	125.78	111.50
1	C	62	THR	C-N-CA	-6.48	105.50	121.70
1	C	90	LYS	CA-C-N	-6.47	102.97	117.20
1	C	60	ALA	N-CA-CB	-6.46	101.06	110.10
1	C	38	PRO	O-C-N	-6.45	112.38	122.70
1	D	297	LYS	CD-CE-NZ	6.41	126.44	111.70
1	A	131	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	C	42	ALA	N-CA-C	-6.18	94.32	111.00
1	C	38	PRO	N-CA-C	6.17	128.13	112.10
1	C	58	TYR	N-CA-C	-6.16	94.37	111.00
1	C	86	MET	CG-SD-CE	6.11	109.98	100.20
1	A	280	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	92	LEU	O-C-N	-6.09	112.85	123.20
1	C	58	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	C	236	ARG	NH1-CZ-NH2	-6.02	112.78	119.40
1	C	7	TYR	CB-CG-CD1	6.01	124.61	121.00
1	D	236	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	D	53	TYR	CB-CG-CD1	6.00	124.60	121.00
1	C	48	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	90	LYS	CB-CA-C	-5.90	98.60	110.40
1	D	76	LEU	CA-CB-CG	5.89	128.84	115.30
1	C	74	MET	CG-SD-CE	5.88	109.61	100.20
1	B	236	ARG	NE-CZ-NH1	5.80	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	ALA	O-C-N	5.75	131.89	122.70
1	C	81	VAL	CB-CA-C	-5.74	100.49	111.40
1	C	91	GLU	N-CA-CB	5.71	120.87	110.60
1	C	332	VAL	CG1-CB-CG2	5.70	120.03	110.90
1	C	297	LYS	CD-CE-NZ	5.68	124.77	111.70
1	B	145	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	73	LYS	C-N-CA	5.65	135.83	121.70
1	C	325	GLU	CA-CB-CG	-5.64	101.00	113.40
1	C	91	GLU	CB-CA-C	5.56	121.52	110.40
1	C	55	GLN	N-CA-CB	-5.54	100.62	110.60
1	C	58	TYR	CA-CB-CG	-5.43	103.08	113.40
1	A	289	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	96	ILE	CB-CA-C	5.38	122.36	111.60
1	C	27	VAL	CA-CB-CG2	5.30	118.86	110.90
1	D	263	GLU	CB-CA-C	5.19	120.79	110.40
1	D	53	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	C	24	HIS	CB-CA-C	5.14	120.68	110.40
1	C	48	ASP	CA-CB-CG	5.10	124.61	113.40
1	C	55	GLN	CA-C-N	-5.10	105.99	117.20
1	C	58	TYR	CB-CA-C	-5.05	100.29	110.40
1	C	81	VAL	CA-CB-CG2	5.03	118.45	110.90

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
1	C	60	ALA	Mainchain,Peptide
1	C	70	GLY	Mainchain
1	C	74	MET	Mainchain
1	C	86	MET	Mainchain
1	C	90	LYS	Mainchain,Peptide
1	C	91	GLU	Peptide
1	C	92	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	C	93	GLY	Mainchain
1	C	94	PHE	Sidechain
1	C	97	THR	Mainchain
1	D	152	VAL	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2632	0	2632	37	0
1	B	2616	0	2612	72	0
1	C	2603	0	2586	40	0
1	D	2622	0	2609	56	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	7	1
3	C	160	0	0	2	0
3	D	236	0	0	4	1
All	All	11428	0	10439	200	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (200) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:51:VAL:CG2	1:B:317:ASN:ND2	2.27	0.96
1:D:25:LYS:H	1:D:25:LYS:HD2	1.31	0.95
1:D:51:VAL:CG2	1:D:317:ASN:HD22	1.64	0.93
1:D:59:ILE:HG13	1:D:62:THR:H	1.35	0.91
1:D:51:VAL:HG23	1:D:317:ASN:ND2	1.84	0.89
1:B:51:VAL:HG22	1:B:317:ASN:HD22	1.37	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:CD	1:D:25:LYS:H	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: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:NZ	1:A:88:LYS:HB2	1.99	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: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
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:B:84:ILE:HG21	1:B:86:MET:HE3	1.76	0.68
1:A:37:THR:HB	1:A:38:PRO:CD	2.24	0.67
1:B:276:LYS:NZ	3:B:2659:HOH:O	2.28	0.67
1:B:41:VAL:HG22	1:B:66:LEU:CD2	2.25	0.66
1:D:84:ILE:HG22	1:D:86:MET:HE2	1.79	0.65
1:D:84:ILE:CG2	1:D:86:MET:HE2	2.26	0.64
1:B:209:ASP:O	1:B:209:ASP:OD2	2.15	0.64
1:C:17:LEU:HD11	1:C:314:PHE:CZ	2.32	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:HZ3	1:A:88:LYS:HB2	1.64	0.63
1:C:298:THR:HG22	1:D:136:TRP:HB3	1.80	0.62
1:B:25:LYS:HD3	1:B:25:LYS:H	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:B:25:LYS:CD	1:B:25:LYS:H	2.14	0.61
1:A:11:GLU:HA	1:A:14:LYS:HD2	1.81	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:D:84:ILE:HG21	1:D:86:MET:CE	2.31	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:D:59:ILE:HG13	1:D:62:THR:N	2.13	0.59
1:B:37:THR:HB	1:B:38:PRO:CD	2.30	0.59
1:B:86:MET:HE2	1:B:86:MET:HA	1.82	0.59
1:C:53:TYR:CE1	1:C:78:ASN:HB3	2.37	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:332:VAL:HG13	1:A:332:VAL:O	2.03	0.58
1:A:276[A]:LYS:NZ	1:A:276[A]:LYS:HB3	2.19	0.58
1:C:60:ALA:HA	1:C:63:LEU:H	1.69	0.58
1:A:34:LYS:HE3	3:A:1615:HOH:O	2.04	0.58
1:A:298[A]:THR:HG22	1:B:136:TRP:HB3	1.86	0.58
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:D:84:ILE:CG2	1:D:86:MET:CE	2.84	0.56
1:B:84:ILE:HG22	1:B:86:MET:HE2	1.86	0.56
1:A:88:LYS:HZ2	1:A:88:LYS:HB2	1.70	0.56
1:B:84:ILE:HG21	1:B:86:MET:CE	2.37	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:220:GLU:O	1:C:224:LYS:HG3	2.08	0.54
1:C:149:VAL:HG11	1:C:165[B]:MET:HG3	1.90	0.54
1:D:59:ILE:HD13	3:D:4623:HOH:O	2.08	0.53
1:C:4:ILE:HG12	1:C:317:ASN:OD1	2.07	0.53
1:C:173:ILE:CD1	1:C:199:GLN:HG3	2.38	0.53
1:D:41:VAL:CG2	1:D:66:LEU:HD23	2.39	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:D:84:ILE:HG21	1:D:86:MET:HE3	1.91	0.51
1:B:277:GLU:OE2	3:B:2502:HOH:O	2.18	0.50
1:B:25:LYS:CD	1:B:25:LYS:N	2.74	0.50
1:B:297:LYS:NZ	1:B:297:LYS:HB2	2.26	0.50
1:D:26:ASP:N	1:D:26:ASP:OD2	2.45	0.49
1:B:41:VAL:HG11	1:B:65:ALA:C	2.33	0.49
1:B:84:ILE:CG2	1:B:86:MET:HE2	2.43	0.49
1:B:84:ILE:CG2	1:B:86:MET:CE	2.91	0.49
1:B:59:ILE:HG13	1:B:62:THR:H	1.77	0.49
1:D:20:TRP:CE2	1:D:314:PHE:HB3	2.48	0.48
1:D:222:ILE:HD13	1:D:254:ILE:HD11	1.96	0.48
1:B:30:GLU:HG3	3:B:2654:HOH:O	2.13	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
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:A:194:ASP:OD2	1:A:224:LYS:NZ	2.46	0.47
1:D:295:THR:HB	1:D:298[A]:THR:HG22	1.95	0.47
1:B:209:ASP:HB2	1:B:236:ARG:HG3	1.97	0.47
1:A:20:TRP:CE2	1:A:314:PHE:HB3	2.50	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:C:195:ASP:HB3	3:C:3560:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:270:ASN:HA	1:B:135:ARG:HA	1.97	0.46
1:B:86:MET:CE	1:B:86:MET:HA	2.45	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:222:ILE:HG21	1:B:254:ILE:HD11	1.97	0.46
1:B:41:VAL:CG2	1:B:66:LEU:HG	2.46	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:CB	1:A:88:LYS:NZ	2.66	0.45
1:D:33:ASP:N	1:D:33:ASP:OD2	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:B:295:THR:HB	1:B:298[A]:THR:HG22	1.98	0.45
1:C:306:VAL:O	1:C:310:VAL:HG23	2.17	0.45
1:C:53:TYR:HB2	1:C:77:ARG:CZ	2.47	0.45
1:A:267:GLY:O	1:A:268:ILE:HD13	2.16	0.45
1:D:155:GLY:O	1:D:159[B]:GLN:HG3	2.15	0.44
1:B:25:LYS:CE	1:B:25:LYS:H	2.29	0.44
1:C:76:LEU:HD22	1:C:78:ASN:OD1	2.17	0.44
1:A:295:THR:HB	1:A:298[B]:THR:HG22	2.00	0.44
1:A:131:ARG:HD3	3:A:1573:HOH:O	2.17	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:B:262:TYR:O	1:B:265:GLU:CG	2.46	0.43
1:B:297:LYS:HZ2	1:B:297:LYS:HB2	1.82	0.43
1:A:39:GLU:N	1:A:39:GLU:OE1	2.51	0.43
1:C:51:VAL:HG22	1:C:75:SER:HB3	2.01	0.43
1:C:270:ASN:HA	1:D:135:ARG:HA	2.00	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:B:22:ASP:O	1:B:25:LYS:CD	2.66	0.43
1:A:173:ILE:HG13	1:A:196[A]:LEU:HD12	2.01	0.43
1:B:59:ILE:HG12	1:B:62:THR:H	1.83	0.43
1:D:88:LYS:HD3	1:D:88:LYS:HA	1.87	0.43
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:17:LEU:HA	1:C:17:LEU:HD12	1.83	0.42
1:B:64:GLN:NE2	1:B:68:ASP:OD2	2.53	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:295:THR:HB	1:D:298[A]:THR:CG2	2.49	0.42
1:D:97:THR:HG22	1:D:329:PRO:HA	2.01	0.42
1:B:236:ARG:HD3	3:B:2629:HOH:O	2.18	0.42
1:D:41:VAL:CG2	1:D:66:LEU:HA	2.50	0.41
1:B:37:THR:CB	1:B:38:PRO:CD	2.95	0.41
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: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: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: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:41:VAL:CG1	1:B:69:ASN:HD22	2.33	0.40
1:B:198[B]:LYS:HZ1	1:B:224:LYS:HD3	1.87	0.40
1:B:14:LYS:N	1:B:15:PRO:CD	2.84	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 symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	337/333 (101%)	324 (96%)	12 (4%)	1 (0%)	50	37
1	B	334/333 (100%)	324 (97%)	10 (3%)	0	100	100
1	C	329/333 (99%)	287 (87%)	30 (9%)	12 (4%)	5	0
1	D	335/333 (101%)	324 (97%)	11 (3%)	0	100	100
All	All	1335/1332 (100%)	1259 (94%)	63 (5%)	13 (1%)	22	8

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%)	270 (95%)	15 (5%)	32	18
1	B	282/278 (101%)	269 (95%)	13 (5%)	37	23
1	C	279/278 (100%)	254 (91%)	25 (9%)	14	5
1	D	282/278 (101%)	269 (95%)	13 (5%)	37	23
All	All	1128/1112 (101%)	1062 (94%)	66 (6%)	28	14

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	53	TYR
1	A	56	LEU
1	A	72	THR
1	A	86	MET
1	A	88	LYS
1	A	145	ARG
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	B	17	LEU
1	B	18	LYS
1	B	25	LYS
1	B	39	GLU
1	B	41	VAL
1	B	53	TYR
1	B	59	ILE
1	B	91	GLU
1	B	184	GLU
1	B	268	ILE
1	B	297	LYS
1	B	324	LYS
1	B	325	GLU
1	C	4	ILE
1	C	28	GLU
1	C	29	VAL
1	C	32	THR
1	C	37	THR
1	C	48	ASP
1	C	53	TYR
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

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Mol	Chain	Res	Type
1	C	88	LYS
1	C	91	GLU
1	C	92	LEU
1	C	94	PHE
1	C	96	ILE
1	C	174	THR
1	C	182	GLU
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	53	TYR
1	D	76	LEU
1	D	136	TRP
1	D	145	ARG
1	D	174	THR
1	D	263	GLU
1	D	265	GLU
1	D	274	GLU
1	D	325	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	GLN
1	B	317	ASN
1	C	199	GLN
1	D	317	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	1400	-	4,4,4	0.92	0	6,6,6	0.51	0
2	SO4	A	1401	-	4,4,4	0.96	0	6,6,6	0.27	0
2	SO4	A	1402	-	4,4,4	0.91	0	6,6,6	0.13	0
2	SO4	A	1403	-	4,4,4	1.03	0	6,6,6	0.22	0
2	SO4	B	2400	-	4,4,4	0.93	0	6,6,6	0.37	0
2	SO4	B	2401	-	4,4,4	0.91	0	6,6,6	0.27	0
2	SO4	B	2402	-	4,4,4	1.01	0	6,6,6	0.28	0
2	SO4	B	2403	-	4,4,4	1.00	0	6,6,6	0.18	0
2	SO4	C	3400	-	4,4,4	0.84	0	6,6,6	0.37	0
2	SO4	D	4400	-	4,4,4	0.86	0	6,6,6	0.32	0
2	SO4	D	4401	-	4,4,4	0.90	0	6,6,6	0.37	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	SO4	A	1400	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1402	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1403	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2400	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2402	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2403	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3400	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	4400	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4401	-	-	0/0/0/0	0/0/0/0

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	331/333 (99%)	0.05	6 (1%) 65 67	13, 27, 47, 54	14 (4%)
1	B	331/333 (99%)	-0.03	4 (1%) 75 78	12, 25, 42, 55	5 (1%)
1	C	298/333 (89%)	0.57	42 (14%) 3 3	18, 29, 74, 87	46 (15%)
1	D	332/333 (99%)	0.03	7 (2%) 60 62	17, 28, 45, 55	10 (3%)
All	All	1292/1332 (96%)	0.14	59 (4%) 31 31	12, 28, 56, 87	75 (5%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	84	ILE	6.8
1	C	94	PHE	6.8
1	C	62	THR	6.3
1	C	41	VAL	6.3
1	C	2	THR	5.6
1	C	323	GLY	5.4
1	C	71	ILE	5.4
1	C	59	ILE	5.0
1	C	72	THR	4.7
1	D	317	ASN	4.7
1	C	325	GLU	4.4
1	C	91	GLU	4.3
1	C	60	ALA	4.1
1	C	5	PHE	3.9
1	C	332	VAL	3.9
1	C	35	LEU	3.7
1	C	331	LYS	3.7
1	C	321	VAL	3.5
1	A	332	VAL	3.5
1	B	317	ASN	3.5
1	B	325	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	55	GLN	3.4
1	C	50	VAL	3.2
1	A	87	ALA	3.2
1	C	3	LYS	3.2
1	A	275	GLY	3.1
1	A	178	PHE	3.0
1	C	322	GLU	3.0
1	C	39	GLU	3.0
1	C	7	TYR	2.9
1	C	330	VAL	2.9
1	C	97	THR	2.9
1	C	21	GLU	2.8
1	C	90	LYS	2.8
1	B	41	VAL	2.8
1	C	326	ALA	2.7
1	C	9	ILE	2.7
1	B	39	GLU	2.6
1	C	57	ASP	2.6
1	C	96	ILE	2.6
1	D	102	TYR	2.6
1	D	25	LYS	2.5
1	C	74	MET	2.5
1	C	20	TRP	2.4
1	C	70	GLY	2.4
1	C	277	GLU	2.3
1	C	40	THR	2.3
1	C	95	GLN	2.3
1	D	333	GLY	2.3
1	A	321	VAL	2.3
1	C	31	TYR	2.2
1	D	34	LYS	2.2
1	C	33	ASP	2.2
1	C	266	VAL	2.2
1	D	42	ALA	2.2
1	C	329	PRO	2.2
1	C	32	THR	2.1
1	A	50	VAL	2.0
1	D	18	LYS	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	2402	5/5	0.31	15.29	54,59,59,60	0
2	SO4	B	2403	5/5	0.36	11.76	43,43,45,45	5
2	SO4	A	1402	5/5	0.30	10.05	49,52,53,54	0
2	SO4	B	2400	5/5	0.15	2.62	36,38,41,42	0
2	SO4	D	4401	5/5	0.22	2.62	40,41,46,48	0
2	SO4	A	1403	5/5	0.16	1.57	40,40,42,43	5
2	SO4	D	4400	5/5	0.10	0.61	35,38,41,43	0
2	SO4	A	1400	5/5	0.09	0.52	29,29,34,35	0
2	SO4	A	1401	5/5	0.14	0.47	46,46,48,49	0
2	SO4	B	2401	5/5	0.10	0.41	32,33,37,37	0
2	SO4	C	3400	5/5	0.09	-0.53	34,37,39,41	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.