



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2016 – 09:36 PM EDT

PDB ID : 5K2M  
Title : Bifunctional LysX/ArgX from *Thermococcus kodakarensis* with LysW-gamma-AAA  
Authors : Yoshida, A.; Tomita, T.; Nishiyama, M.  
Deposited on : 2016-05-19  
Resolution : 2.18 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

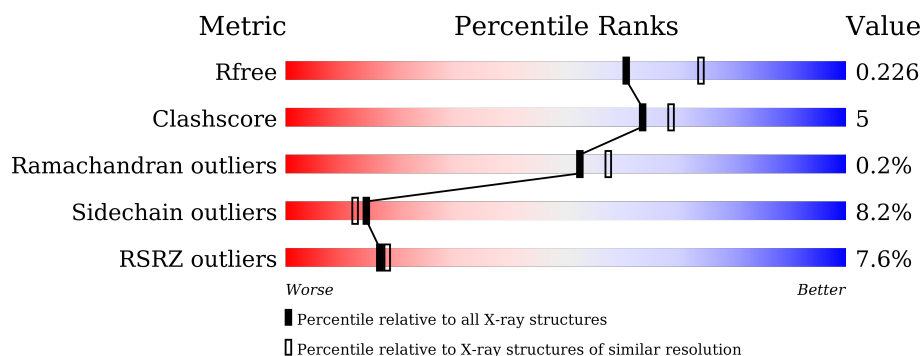
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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))
$R_{free}$	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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. 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	273	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	273	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
1	C	273	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>.</div> </div> </div>
1	D	273	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>
1	G	273	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>.</div> </div> </div>
1	H	273	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	I	273	
1	J	273	
2	E	53	
2	F	53	
2	K	53	
2	L	53	
2	M	53	
2	N	53	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	G	302	-	-	-	X
5	MG	G	303	-	-	-	X
6	SO4	C	302	-	-	-	X
7	UN1	I	303	-	-	-	X
7	UN1	K	101	-	-	-	X
7	UN1	L	101	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19516 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 RimK-related lysine biosynthesis protein.

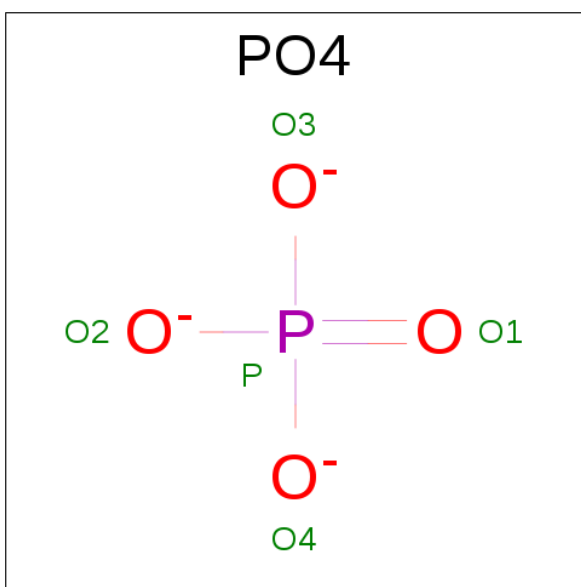
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2153	1380	367	399	7			
1	B	273	Total	C	N	O	S	0	0	0
			2153	1380	367	399	7			
1	C	273	Total	C	N	O	S	0	0	0
			2141	1374	361	399	7			
1	D	270	Total	C	N	O	S	0	0	0
			2110	1354	354	395	7			
1	G	273	Total	C	N	O	S	0	0	0
			2153	1380	367	399	7			
1	H	272	Total	C	N	O	S	0	0	0
			2141	1373	365	396	7			
1	I	273	Total	C	N	O	S	0	0	0
			2143	1374	363	399	7			
1	J	273	Total	C	N	O	S	0	0	0
			2153	1380	367	399	7			

- Molecule 2 is a protein called Probable lysine biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	52	Total	C	N	O	S	0	0	0
			396	248	56	88	4			
2	F	53	Total	C	N	O	S	0	0	0
			400	251	57	87	5			
2	K	11	Total	C	N	O		0	0	0
			85	54	12	19				
2	L	30	Total	C	N	O		0	0	0
			217	137	34	46				
2	M	9	Total	C	N	O		0	0	0
			68	43	10	15				
2	N	33	Total	C	N	O		0	0	0
			247	160	36	51				

- # ADP

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).

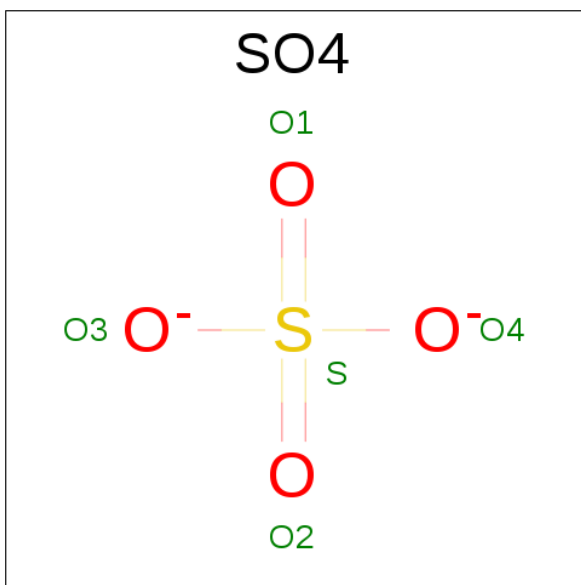


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

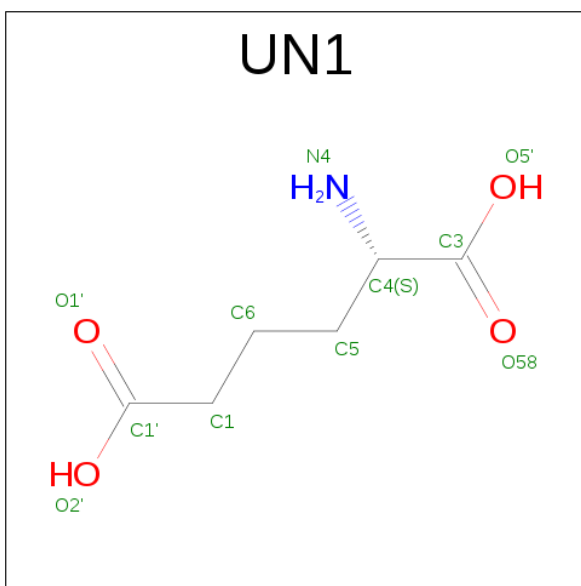
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Mg	0	0
			2	2		
5	G	1	Total	Mg	0	0
			1	1		
5	B	2	Total	Mg	0	0
			2	2		
5	A	2	Total	Mg	0	0
			2	2		
5	J	2	Total	Mg	0	0
			2	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-AMINOHEXANEDIOIC ACID (three-letter code: UN1) (formula:  $C_6H_{11}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			11	6	1	4		
7	F	1	Total	C	N	O	0	0
			11	6	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	I	1	Total	C	N	O	0	0
			11	6	1	4		
7	K	1	Total	C	N	O	0	0
			11	6	1	4		
7	L	1	Total	C	N	O	0	0
			11	6	1	4		
7	N	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	1	Total	Zn	0	0
			1	1		
8	E	1	Total	Zn	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	98	Total	O	0	0
			98	98		
9	B	112	Total	O	0	0
			112	112		
9	C	59	Total	O	0	0
			59	59		
9	D	75	Total	O	0	0
			75	75		
9	E	12	Total	O	0	0
			12	12		
9	F	8	Total	O	0	0
			8	8		
9	G	52	Total	O	0	0
			52	52		
9	H	88	Total	O	0	0
			88	88		
9	I	38	Total	O	0	0
			38	38		
9	J	74	Total	O	0	0
			74	74		
9	K	1	Total	O	0	0
			1	1		

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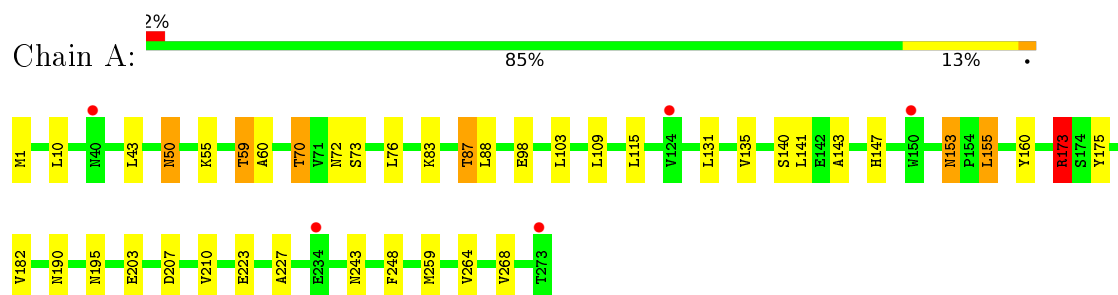
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	5	Total	O	0	0
			5	5		
9	N	6	Total	O	0	0
			6	6		

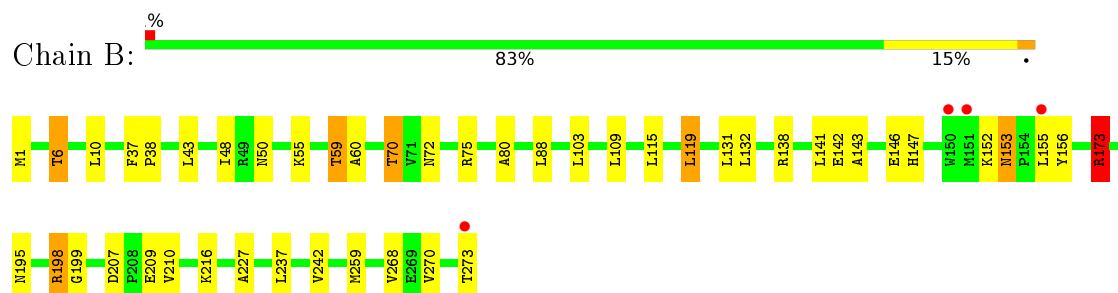
### 3 Residue-property plots [i](#)

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.

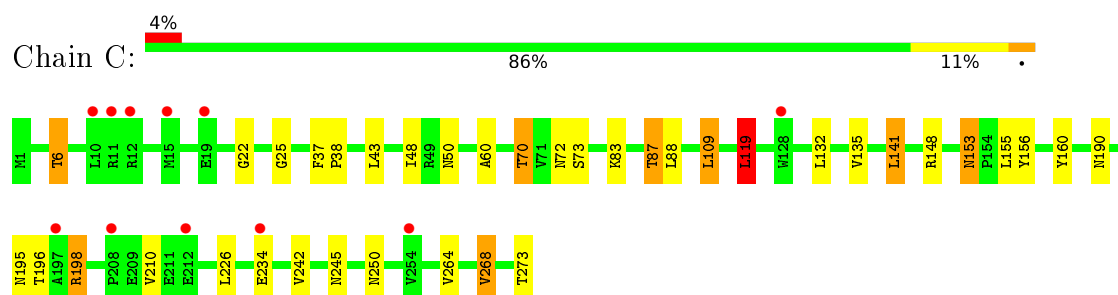
- Molecule 1: RimK-related lysine biosynthesis protein



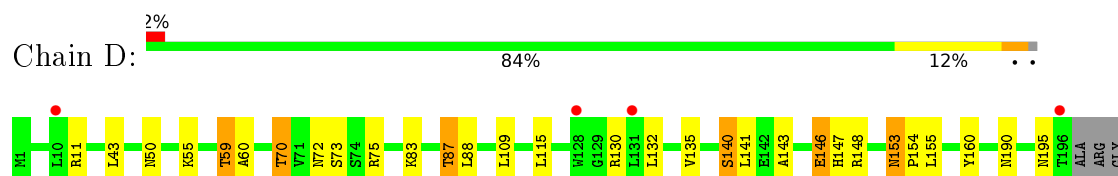
- Molecule 1: RimK-related lysine biosynthesis protein

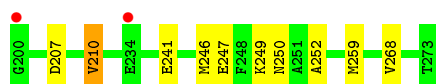


- Molecule 1: RimK-related lysine biosynthesis protein

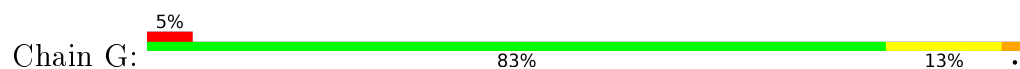


- Molecule 1: RimK-related lysine biosynthesis protein

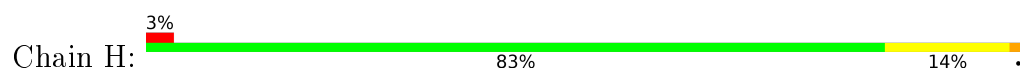




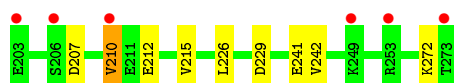
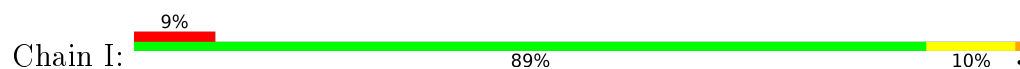
- Molecule 1: RimK-related lysine biosynthesis protein



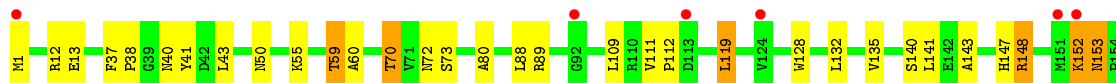
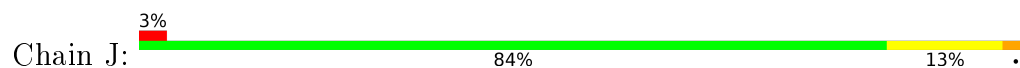
- Molecule 1: RimK-related lysine biosynthesis protein



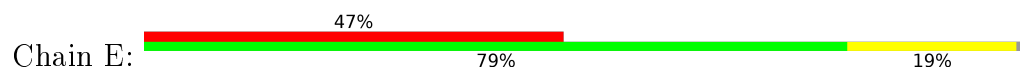
- Molecule 1: RimK-related lysine biosynthesis protein

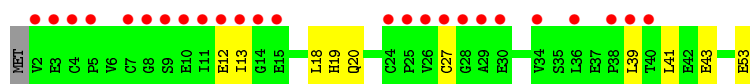


- Molecule 1: RimK-related lysine biosynthesis protein

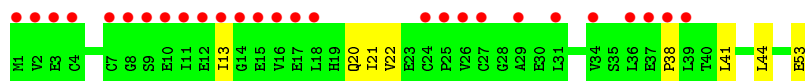
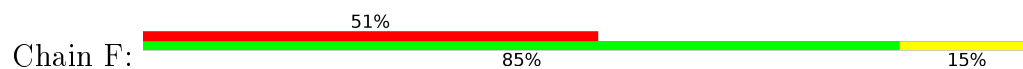


- Molecule 2: Probable lysine biosynthesis protein

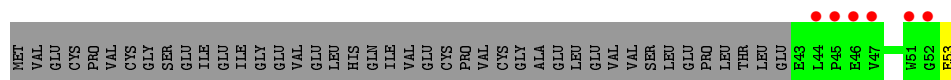




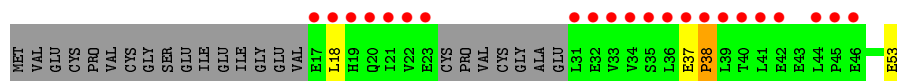
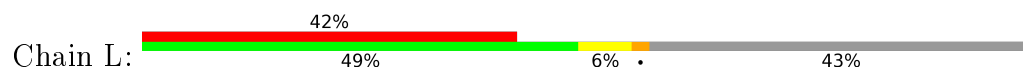
- Molecule 2: Probable lysine biosynthesis protein



- Molecule 2: Probable lysine biosynthesis protein



- Molecule 2: Probable lysine biosynthesis protein



- Molecule 2: Probable lysine biosynthesis protein



- Molecule 2: Probable lysine biosynthesis protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.15Å 135.10Å 136.98Å 90.00° 97.49° 90.00°	Depositor
Resolution (Å)	50.00 – 2.18 42.74 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.18) 99.2 (42.74-2.18)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.18Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.180 , 0.220 0.190 , 0.226	Depositor DCC
$R_{free}$ test set	7126 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: UN1, ZN, ADP, PO4, MG, 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	0.43	0/2202	0.67	2/2978 (0.1%)
1	B	0.42	0/2202	0.67	3/2978 (0.1%)
1	C	0.38	0/2190	0.61	1/2964 (0.0%)
1	D	0.41	0/2156	0.61	0/2916
1	G	0.43	0/2202	0.63	2/2978 (0.1%)
1	H	0.43	0/2190	0.66	1/2964 (0.0%)
1	I	0.36	0/2192	0.58	1/2967 (0.0%)
1	J	0.38	0/2202	0.63	1/2978 (0.0%)
2	E	0.39	0/402	0.52	0/548
2	F	0.37	0/406	0.54	0/553
2	K	0.46	0/87	0.56	0/117
2	L	0.39	0/220	0.52	0/299
2	M	0.51	0/70	0.59	0/96
2	N	0.39	0/250	0.51	0/341
All	All	0.41	0/18971	0.63	11/25677 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	119	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	173	ARG	NE-CZ-NH2	-5.87	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	LEU	CA-CB-CG	5.74	128.49	115.30
1	A	173	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	J	119	LEU	CA-CB-CG	5.47	127.89	115.30
1	G	43	LEU	CA-CB-CG	5.42	127.77	115.30
1	I	119	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	173	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	198	ARG	N-CA-C	5.11	124.79	111.00
1	B	119	LEU	CA-CB-CG	5.07	126.97	115.30
1	G	119	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	37	GLU	Peptide

## 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	2153	0	2140	27	0
1	B	2153	0	2140	31	0
1	C	2141	0	2118	23	0
1	D	2110	0	2083	22	0
1	G	2153	0	2140	29	0
1	H	2141	0	2122	27	0
1	I	2143	0	2118	16	0
1	J	2153	0	2140	24	0
2	E	396	0	367	7	0
2	F	400	0	376	5	0
2	K	85	0	65	2	0
2	L	217	0	174	3	0
2	M	68	0	48	2	0
2	N	247	0	227	1	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	27	0	12	0	0
3	G	27	0	12	0	0
3	H	27	0	12	1	0
3	I	27	0	12	1	0
3	J	27	0	12	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	G	5	0	0	0	0
4	I	5	0	0	0	0
4	J	5	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
5	J	2	0	0	0	0
6	C	5	0	0	0	0
6	H	5	0	0	0	0
7	E	11	0	7	0	0
7	F	11	0	7	0	0
7	I	11	0	9	0	0
7	K	11	0	7	0	0
7	L	11	0	7	0	0
7	N	11	0	7	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	A	98	0	0	0	0
9	B	112	0	0	1	0
9	C	59	0	0	0	0
9	D	75	0	0	0	0
9	E	12	0	0	0	0
9	F	8	0	0	0	0
9	G	52	0	0	0	0
9	H	88	0	0	0	0
9	I	38	0	0	1	0
9	J	74	0	0	0	0
9	K	1	0	0	0	0
9	L	5	0	0	0	0
9	N	6	0	0	0	0
All	All	19516	0	18398	194	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.



All (194) 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:H:173:ARG:NH2	2:L:53:GLU:OE1	2.01	0.92
1:A:55:LYS:O	1:A:59:THR:HG23	1.70	0.90
1:B:55:LYS:O	1:B:59:THR:HG23	1.74	0.88
1:B:173:ARG:NH2	2:F:53:GLU:OE1	2.07	0.87
1:A:173:ARG:NH2	2:E:53:GLU:OE1	2.12	0.83
1:H:83:LYS:O	1:H:87:THR:HG23	1.79	0.81
1:G:173:ARG:NH2	2:K:53:GLU:OE1	2.17	0.78
1:H:87:THR:HG21	1:H:160:TYR:OH	1.85	0.76
1:H:70:THR:HG22	1:H:72:ASN:O	1.85	0.75
1:J:152:LYS:HD2	1:J:153:ASN:N	2.00	0.75
1:C:83:LYS:O	1:C:87:THR:HG23	1.87	0.75
1:D:60:ALA:HB1	1:D:70:THR:HG21	1.69	0.74
1:H:148:ARG:HE	1:J:147:HIS:HE1	1.36	0.74
1:G:83:LYS:O	1:G:87:THR:HG23	1.89	0.73
1:D:83:LYS:O	1:D:87:THR:HG23	1.89	0.72
1:H:226:LEU:HD22	1:H:242:VAL:CG1	2.21	0.70
1:G:55:LYS:O	1:G:59:THR:HG23	1.93	0.69
1:B:60:ALA:HB1	1:B:70:THR:HG21	1.75	0.69
1:A:60:ALA:HB1	1:A:70:THR:HG21	1.74	0.69
1:B:147:HIS:HE1	1:D:148:ARG:HE	1.41	0.69
1:G:6:THR:CG2	1:G:50:ASN:HD21	2.07	0.68
1:C:22:GLY:HA2	1:C:25:GLY:O	1.94	0.68
1:I:229:ASP:OD2	9:I:401:HOH:O	2.12	0.67
1:G:6:THR:CG2	1:G:50:ASN:ND2	2.59	0.66
2:E:13:ILE:HD11	2:E:41:LEU:HD11	1.78	0.66
1:B:70:THR:HG22	1:B:72:ASN:O	1.96	0.65
3:H:301:ADP:O3B	3:H:301:ADP:O2A	2.15	0.65
1:G:87:THR:HG21	1:G:160:TYR:OH	1.97	0.65
1:I:52:SER:OG	2:M:50:ASP:OD2	2.09	0.64
1:D:153:ASN:HD22	1:D:154:PRO:HD2	1.63	0.64
2:F:13:ILE:HD11	2:F:41:LEU:HD11	1.79	0.63
1:C:226:LEU:HD22	1:C:242:VAL:CG1	2.29	0.63
1:A:83:LYS:O	1:A:87:THR:HG23	1.98	0.62
1:H:55:LYS:O	1:H:59:THR:HG23	1.98	0.62
1:A:103:LEU:HG	1:B:59:THR:HG22	1.81	0.62
1:C:6:THR:HG22	1:C:48:ILE:HA	1.79	0.62
1:A:173:ARG:NE	1:A:227:ALA:HB1	2.14	0.62
1:C:87:THR:HG21	1:C:160:TYR:OH	2.00	0.62
2:E:13:ILE:HD12	2:E:39:LEU:HD11	1.82	0.62
1:B:6:THR:HG23	1:B:50:ASN:ND2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:THR:HG21	1:D:160:TYR:OH	2.01	0.61
1:J:55:LYS:O	1:J:59:THR:HG23	2.00	0.61
1:H:60:ALA:HB1	1:H:70:THR:HG21	1.81	0.61
1:G:153:ASN:HD22	1:G:153:ASN:C	2.03	0.61
1:C:6:THR:HG23	1:C:50:ASN:ND2	2.17	0.60
1:A:50:ASN:HD22	1:A:50:ASN:H	1.50	0.60
1:G:226:LEU:HD22	1:G:242:VAL:HG13	1.84	0.60
1:B:147:HIS:CE1	1:D:148:ARG:HE	2.20	0.60
1:A:87:THR:HG21	1:A:160:TYR:OH	2.02	0.59
1:B:6:THR:CG2	1:B:50:ASN:HD21	2.16	0.59
1:B:147:HIS:HE1	1:D:148:ARG:NE	2.00	0.58
2:F:13:ILE:HG21	2:F:22:VAL:HG11	1.84	0.58
1:D:55:LYS:O	1:D:59:THR:HG23	2.04	0.57
1:G:55:LYS:O	1:G:59:THR:CG2	2.52	0.57
1:I:128:TRP:N	1:I:129:GLY:HA2	2.19	0.57
1:H:226:LEU:HD22	1:H:242:VAL:HG12	1.87	0.57
1:B:6:THR:HG23	1:B:50:ASN:HD21	1.69	0.56
1:J:60:ALA:HB1	1:J:70:THR:HG21	1.87	0.56
1:B:70:THR:CG2	1:B:72:ASN:O	2.52	0.56
1:C:60:ALA:HB1	1:C:70:THR:HG21	1.86	0.56
1:G:60:ALA:HB1	1:G:70:THR:HG21	1.88	0.56
1:H:55:LYS:O	1:H:59:THR:CG2	2.54	0.56
1:H:70:THR:CG2	1:H:72:ASN:O	2.54	0.56
1:H:148:ARG:HE	1:J:147:HIS:CE1	2.22	0.56
1:J:55:LYS:O	1:J:59:THR:CG2	2.54	0.56
1:A:147:HIS:HE1	1:C:148:ARG:HE	1.53	0.55
1:H:50:ASN:H	1:H:50:ASN:HD22	1.53	0.55
1:D:70:THR:CG2	1:D:72:ASN:O	2.55	0.55
1:D:55:LYS:O	1:D:59:THR:CG2	2.54	0.54
1:H:148:ARG:NE	1:J:147:HIS:HE1	2.04	0.54
1:G:70:THR:CG2	1:G:72:ASN:O	2.56	0.54
1:H:60:ALA:CB	1:H:70:THR:HG21	2.38	0.54
1:A:59:THR:HG22	1:B:103:LEU:HG	1.90	0.54
1:I:127:SER:C	1:I:129:GLY:HA2	2.29	0.53
1:D:60:ALA:CB	1:D:70:THR:HG21	2.36	0.53
1:G:173:ARG:NE	1:G:227:ALA:HB1	2.23	0.52
1:I:127:SER:O	1:I:128:TRP:HB2	2.09	0.52
1:A:70:THR:CG2	1:A:72:ASN:O	2.57	0.51
1:B:138:ARG:NH1	1:B:142:GLU:OE1	2.43	0.51
1:B:6:THR:CG2	1:B:50:ASN:ND2	2.73	0.51
1:C:70:THR:CG2	1:C:72:ASN:O	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:ASN:HB3	1:H:156:TYR:CD2	2.46	0.51
1:G:80:ALA:HB1	1:G:242:VAL:HG12	1.90	0.51
1:H:207:ASP:HB3	1:H:210:VAL:HG13	1.92	0.51
1:D:207:ASP:HB3	1:D:210:VAL:HG13	1.91	0.51
1:H:119:LEU:HD22	1:H:135:VAL:HB	1.92	0.51
1:G:119:LEU:CD2	1:G:135:VAL:HB	2.40	0.51
1:B:131:LEU:HA	1:D:146:GLU:OE1	2.11	0.50
1:A:60:ALA:CB	1:A:70:THR:HG21	2.40	0.50
1:B:60:ALA:CB	1:B:70:THR:HG21	2.41	0.50
1:C:153:ASN:HB3	1:C:156:TYR:CD2	2.47	0.50
1:J:70:THR:HG22	1:J:73:SER:HA	1.93	0.50
1:C:50:ASN:O	1:C:245:ASN:ND2	2.45	0.50
2:E:18:LEU:HG	2:E:19:HIS:CD2	2.47	0.50
1:I:226:LEU:HD22	1:I:242:VAL:CG1	2.42	0.50
1:I:119:LEU:HD22	1:I:135:VAL:HB	1.94	0.50
1:A:10:LEU:HB2	2:E:20:GLN:HA	1.94	0.49
1:A:264:VAL:O	1:A:268:VAL:HG13	2.12	0.49
1:B:173:ARG:NE	1:B:227:ALA:HB1	2.28	0.49
1:G:148:ARG:HE	1:I:147:HIS:HE1	1.59	0.49
1:C:195:ASN:HD21	3:C:301:ADP:C5'	2.26	0.49
1:D:50:ASN:H	1:D:50:ASN:HD22	1.59	0.49
1:H:248:PHE:HB2	1:H:259:MET:HG3	1.94	0.49
1:B:10:LEU:HB2	2:F:20:GLN:HA	1.95	0.48
1:H:129:GLY:O	1:H:198:ARG:NH1	2.46	0.48
1:J:70:THR:CG2	1:J:72:ASN:O	2.61	0.48
1:A:70:THR:HG22	1:A:73:SER:HA	1.95	0.48
1:C:109:LEU:HD12	1:C:141:LEU:HD13	1.94	0.48
1:D:70:THR:HG22	1:D:72:ASN:O	2.12	0.48
1:D:11:ARG:NH1	2:E:43:GLU:OE1	2.46	0.48
1:G:6:THR:HG21	1:G:50:ASN:HD21	1.78	0.48
1:G:6:THR:HG23	1:G:50:ASN:ND2	2.27	0.48
1:I:195:ASN:HD21	3:I:301:ADP:C5'	2.27	0.48
1:G:82:ASP:OD2	1:G:124:VAL:CG1	2.62	0.47
1:G:227:ALA:HB3	1:G:243:ASN:HB2	1.97	0.47
1:C:6:THR:CG2	1:C:50:ASN:ND2	2.77	0.47
1:A:143:ALA:O	1:A:147:HIS:HD2	1.98	0.47
1:B:209:GLU:HG2	1:B:237:LEU:HD12	1.96	0.47
1:D:70:THR:HG22	1:D:73:SER:HA	1.96	0.47
1:A:248:PHE:HB2	1:A:259:MET:HG3	1.96	0.47
1:G:70:THR:HG22	1:G:73:SER:HA	1.95	0.47
1:H:48:ILE:HG13	1:H:70:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:80:ALA:HB1	1:J:242:VAL:HG13	1.97	0.47
1:C:195:ASN:HB2	1:C:198:ARG:HB2	1.97	0.47
1:A:153:ASN:ND2	1:A:155:LEU:HB2	2.31	0.46
1:A:153:ASN:C	1:A:153:ASN:HD22	2.19	0.46
1:B:6:THR:HG22	1:B:48:ILE:HA	1.98	0.46
1:A:175:TYR:HB2	1:A:182:VAL:HG22	1.98	0.46
1:C:119:LEU:HD22	1:C:135:VAL:HB	1.98	0.46
1:I:212:GLU:O	1:I:215:VAL:HG12	2.16	0.46
1:B:138:ARG:NE	9:B:405:HOH:O	2.48	0.46
1:B:146:GLU:HB3	1:D:130:ARG:O	2.17	0.45
1:D:135:VAL:HG13	1:D:140:SER:HB2	1.97	0.45
1:G:6:THR:HG23	1:G:50:ASN:HD21	1.81	0.45
1:I:153:ASN:HB3	1:I:156:TYR:CD2	2.51	0.45
1:J:143:ALA:O	1:J:147:HIS:HD2	1.99	0.45
1:A:207:ASP:HB3	1:A:210:VAL:HG13	1.99	0.45
1:C:37:PHE:HA	1:C:38:PRO:C	2.37	0.45
1:H:45:VAL:HB	1:H:271:ALA:HB2	1.99	0.45
1:B:37:PHE:HA	1:B:38:PRO:C	2.38	0.44
1:C:60:ALA:CB	1:C:70:THR:HG21	2.48	0.44
1:J:264:VAL:O	1:J:268:VAL:HG13	2.17	0.44
1:G:207:ASP:HB3	1:G:210:VAL:HG13	1.99	0.44
1:I:82:ASP:OD2	1:I:124:VAL:HG13	2.17	0.44
1:J:135:VAL:HG13	1:J:140:SER:HB2	1.99	0.44
1:G:243:ASN:HB3	2:K:53:GLU:O	2.18	0.44
1:A:195:ASN:HD21	3:A:301:ADP:C5'	2.30	0.43
1:G:80:ALA:HB1	1:G:242:VAL:CG1	2.48	0.43
1:C:226:LEU:HD22	1:C:242:VAL:HG12	1.98	0.43
1:J:37:PHE:HA	1:J:38:PRO:C	2.39	0.43
1:C:70:THR:HG22	1:C:73:SER:HA	2.00	0.43
1:A:70:THR:HG23	1:A:72:ASN:O	2.18	0.43
1:G:250:ASN:HD22	1:G:253:ARG:HH21	1.65	0.43
1:J:60:ALA:CB	1:J:70:THR:HG21	2.48	0.43
1:B:207:ASP:HB3	1:B:210:VAL:HG13	2.00	0.43
1:A:243:ASN:HB3	2:E:53:GLU:OXT	2.18	0.43
1:G:37:PHE:HA	1:G:38:PRO:C	2.39	0.43
1:B:143:ALA:O	1:B:147:HIS:HD2	2.01	0.42
1:B:153:ASN:HB3	1:B:156:TYR:CD2	2.55	0.42
1:B:198:ARG:N	1:B:199:GLY:HA2	2.34	0.42
1:C:6:THR:CG2	1:C:50:ASN:HD21	2.32	0.42
1:H:204:PRO:HD3	1:H:254:VAL:HG13	2.00	0.42
1:J:41:TYR:HB3	1:J:43:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:50:ASN:HD22	1:J:50:ASN:H	1.67	0.42
2:L:37:GLU:CB	2:L:38:PRO:HD3	2.49	0.42
1:B:80:ALA:HB1	1:B:242:VAL:HG23	2.02	0.42
1:A:76:LEU:HD22	1:A:223:GLU:HG3	2.02	0.41
1:I:226:LEU:HD13	1:I:242:VAL:HG11	2.01	0.41
1:B:48:ILE:HG13	1:B:70:THR:HG23	2.03	0.41
1:J:207:ASP:HB3	1:J:210:VAL:HG13	2.01	0.41
2:F:21:ILE:CD1	2:F:44:LEU:HD21	2.50	0.41
1:I:207:ASP:HB3	1:I:210:VAL:HG13	2.01	0.41
1:C:196:THR:HG21	1:C:250:ASN:ND2	2.35	0.41
1:B:195:ASN:HD22	1:B:195:ASN:H	1.67	0.41
1:H:111:VAL:N	1:H:112:PRO:CD	2.83	0.41
1:I:152:LYS:HB3	1:J:152:LYS:HE3	2.02	0.41
2:M:48:GLU:C	2:M:50:ASP:H	2.24	0.41
1:D:252:ALA:HB2	1:D:259:MET:HG3	2.03	0.41
1:A:50:ASN:H	1:A:50:ASN:ND2	2.17	0.41
1:J:153:ASN:HB3	1:J:156:TYR:CD2	2.55	0.41
1:J:250:ASN:HD22	1:J:253:ARG:HH21	1.69	0.41
1:D:143:ALA:O	1:D:147:HIS:HD2	2.03	0.41
1:H:226:LEU:HD13	1:H:242:VAL:HG11	2.03	0.41
1:A:135:VAL:HG13	1:A:140:SER:HB2	2.03	0.41
1:G:271:ALA:C	1:G:273:THR:H	2.24	0.41
1:J:148:ARG:CG	1:J:148:ARG:HH11	2.34	0.41
1:D:83:LYS:CE	1:D:241:GLU:OE1	2.70	0.40
1:J:128:TRP:CE2	2:N:52:GLY:HA2	2.56	0.40
1:G:119:LEU:HD23	1:G:119:LEU:C	2.41	0.40
1:G:190:ASN:C	1:G:190:ASN:HD22	2.25	0.40
1:H:245:ASN:O	2:L:53:GLU:HA	2.21	0.40
1:J:111:VAL:N	1:J:112:PRO:CD	2.84	0.40
1:C:264:VAL:O	1:C:268:VAL:HG13	2.22	0.40
1:H:152:LYS:HG2	1:I:152:LYS:HG2	2.04	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	271/273 (99%)	269 (99%)	2 (1%)	0	100	100
1	B	271/273 (99%)	266 (98%)	5 (2%)	0	100	100
1	C	271/273 (99%)	268 (99%)	3 (1%)	0	100	100
1	D	266/273 (97%)	262 (98%)	3 (1%)	1 (0%)	39	40
1	G	271/273 (99%)	265 (98%)	6 (2%)	0	100	100
1	H	270/273 (99%)	268 (99%)	2 (1%)	0	100	100
1	I	271/273 (99%)	265 (98%)	6 (2%)	0	100	100
1	J	271/273 (99%)	266 (98%)	5 (2%)	0	100	100
2	E	50/53 (94%)	46 (92%)	4 (8%)	0	100	100
2	F	51/53 (96%)	49 (96%)	1 (2%)	1 (2%)	9	5
2	K	9/53 (17%)	8 (89%)	1 (11%)	0	100	100
2	L	26/53 (49%)	22 (85%)	3 (12%)	1 (4%)	4	1
2	M	7/53 (13%)	6 (86%)	1 (14%)	0	100	100
2	N	29/53 (55%)	26 (90%)	2 (7%)	1 (3%)	5	2
All	All	2334/2502 (93%)	2286 (98%)	44 (2%)	4 (0%)	52	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	246	MET
2	L	38	PRO
2	N	38	PRO
2	F	38	PRO

### 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	224/224 (100%)	207 (92%)	17 (8%)	16	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	224/224 (100%)	203 (91%)	21 (9%)	11	9
1	C	222/224 (99%)	205 (92%)	17 (8%)	16	14
1	D	219/224 (98%)	198 (90%)	21 (10%)	10	8
1	G	224/224 (100%)	201 (90%)	23 (10%)	9	7
1	H	222/224 (99%)	202 (91%)	20 (9%)	12	10
1	I	222/224 (99%)	208 (94%)	14 (6%)	22	22
1	J	224/224 (100%)	203 (91%)	21 (9%)	11	9
2	E	47/48 (98%)	45 (96%)	2 (4%)	35	40
2	F	47/48 (98%)	47 (100%)	0	100	100
2	K	8/48 (17%)	8 (100%)	0	100	100
2	L	20/48 (42%)	19 (95%)	1 (5%)	30	33
2	M	6/48 (12%)	6 (100%)	0	100	100
2	N	26/48 (54%)	25 (96%)	1 (4%)	40	46
All	All	1935/2080 (93%)	1777 (92%)	158 (8%)	14	12

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	43	LEU
1	A	50	ASN
1	A	59	THR
1	A	70	THR
1	A	87	THR
1	A	88	LEU
1	A	98	GLU
1	A	109	LEU
1	A	115	LEU
1	A	131	LEU
1	A	141	LEU
1	A	153	ASN
1	A	155	LEU
1	A	173	ARG
1	A	190	ASN
1	A	203	GLU
1	B	1	MET
1	B	6	THR

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Mol	Chain	Res	Type
1	B	43	LEU
1	B	59	THR
1	B	70	THR
1	B	75	ARG
1	B	88	LEU
1	B	109	LEU
1	B	115	LEU
1	B	119	LEU
1	B	132	LEU
1	B	141	LEU
1	B	152	LYS
1	B	153	ASN
1	B	155	LEU
1	B	173	ARG
1	B	216	LYS
1	B	259	MET
1	B	268	VAL
1	B	270	VAL
1	B	273	THR
1	C	6	THR
1	C	43	LEU
1	C	70	THR
1	C	87	THR
1	C	88	LEU
1	C	109	LEU
1	C	119	LEU
1	C	132	LEU
1	C	141	LEU
1	C	153	ASN
1	C	155	LEU
1	C	190	ASN
1	C	198	ARG
1	C	210	VAL
1	C	234	GLU
1	C	268	VAL
1	C	273	THR
1	D	43	LEU
1	D	59	THR
1	D	70	THR
1	D	75	ARG
1	D	87	THR
1	D	88	LEU

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Mol	Chain	Res	Type
1	D	109	LEU
1	D	115	LEU
1	D	132	LEU
1	D	140	SER
1	D	141	LEU
1	D	146	GLU
1	D	153	ASN
1	D	155	LEU
1	D	190	ASN
1	D	195	ASN
1	D	210	VAL
1	D	247	GLU
1	D	249	LYS
1	D	250	ASN
1	D	268	VAL
2	E	12	GLU
2	E	27	CYS
1	G	1	MET
1	G	6	THR
1	G	23	GLU
1	G	43	LEU
1	G	59	THR
1	G	70	THR
1	G	75	ARG
1	G	87	THR
1	G	88	LEU
1	G	109	LEU
1	G	119	LEU
1	G	124	VAL
1	G	132	LEU
1	G	140	SER
1	G	141	LEU
1	G	146	GLU
1	G	153	ASN
1	G	155	LEU
1	G	173	ARG
1	G	174	SER
1	G	190	ASN
1	G	216	LYS
1	G	229	ASP
1	H	12	ARG
1	H	18	LYS

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Mol	Chain	Res	Type
1	H	43	LEU
1	H	50	ASN
1	H	59	THR
1	H	70	THR
1	H	87	THR
1	H	88	LEU
1	H	93	LYS
1	H	109	LEU
1	H	115	LEU
1	H	119	LEU
1	H	124	VAL
1	H	131	LEU
1	H	132	LEU
1	H	141	LEU
1	H	153	ASN
1	H	174	SER
1	H	209	GLU
1	H	210	VAL
1	I	26	GLU
1	I	40	ASN
1	I	88	LEU
1	I	109	LEU
1	I	119	LEU
1	I	132	LEU
1	I	141	LEU
1	I	148	ARG
1	I	153	ASN
1	I	155	LEU
1	I	198	ARG
1	I	210	VAL
1	I	241	GLU
1	I	272	LYS
1	J	1	MET
1	J	12	ARG
1	J	13	GLU
1	J	40	ASN
1	J	59	THR
1	J	70	THR
1	J	88	LEU
1	J	89	ARG
1	J	109	LEU
1	J	119	LEU

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Mol	Chain	Res	Type
1	J	132	LEU
1	J	141	LEU
1	J	148	ARG
1	J	152	LYS
1	J	153	ASN
1	J	155	LEU
1	J	210	VAL
1	J	241	GLU
1	J	242	VAL
1	J	270	VAL
1	J	273	THR
2	L	18	LEU
2	N	44	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	147	HIS
1	A	153	ASN
1	A	190	ASN
1	A	195	ASN
1	B	40	ASN
1	B	50	ASN
1	B	147	HIS
1	B	153	ASN
1	B	195	ASN
1	C	50	ASN
1	C	147	HIS
1	C	153	ASN
1	C	195	ASN
1	C	250	ASN
1	D	50	ASN
1	D	147	HIS
1	D	153	ASN
2	F	19	HIS
1	G	50	ASN
1	G	53	HIS
1	G	147	HIS
1	G	153	ASN
1	G	190	ASN
1	G	195	ASN

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Mol	Chain	Res	Type
1	G	243	ASN
1	G	250	ASN
1	H	50	ASN
1	H	53	HIS
1	H	147	HIS
1	H	153	ASN
1	I	50	ASN
1	I	147	HIS
1	I	153	ASN
1	I	195	ASN
1	J	50	ASN
1	J	53	HIS
1	J	147	HIS
1	J	153	ASN
1	J	195	ASN
1	J	245	ASN
1	J	250	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 11 are monoatomic - leaving 21 for Mogul analysis.

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
3	ADP	A	301	5	24,29,29	0.94	1 (4%)	23,45,45	1.78	4 (17%)
4	PO4	A	302	5	4,4,4	0.73	0	6,6,6	0.23	0
3	ADP	B	301	5	24,29,29	1.03	1 (4%)	23,45,45	1.80	4 (17%)
4	PO4	B	302	5	4,4,4	0.59	0	6,6,6	0.23	0
3	ADP	C	301	-	24,29,29	0.93	1 (4%)	23,45,45	1.73	3 (13%)
6	SO4	C	302	-	4,4,4	0.38	0	6,6,6	0.18	0
3	ADP	D	301	-	24,29,29	0.94	1 (4%)	23,45,45	1.85	3 (13%)
7	UN1	E	101	2	4,10,10	0.29	0	3,12,12	0.20	0
7	UN1	F	101	2	4,10,10	0.31	0	3,12,12	0.13	0
3	ADP	G	301	5	24,29,29	0.96	1 (4%)	23,45,45	1.65	2 (8%)
4	PO4	G	302	5	4,4,4	0.55	0	6,6,6	0.23	0
3	ADP	H	301	5	24,29,29	0.91	1 (4%)	23,45,45	1.86	3 (13%)
6	SO4	H	302	5	4,4,4	0.53	0	6,6,6	0.29	0
3	ADP	I	301	-	24,29,29	0.96	1 (4%)	23,45,45	1.84	3 (13%)
4	PO4	I	302	-	4,4,4	0.58	0	6,6,6	0.24	0
7	UN1	I	303	-	4,10,10	0.37	0	3,12,12	0.34	0
3	ADP	J	301	5	24,29,29	0.93	1 (4%)	23,45,45	1.70	4 (17%)
4	PO4	J	302	5	4,4,4	0.54	0	6,6,6	0.26	0
7	UN1	K	101	2	4,10,10	0.19	0	3,12,12	0.55	0
7	UN1	L	101	2	4,10,10	0.28	0	3,12,12	0.22	0
7	UN1	N	101	2	4,10,10	0.37	0	3,12,12	0.15	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	ADP	A	301	5	-	0/12/32/32	0/3/3/3
4	PO4	A	302	5	-	0/0/0/0	0/0/0/0
3	ADP	B	301	5	-	0/12/32/32	0/3/3/3
4	PO4	B	302	5	-	0/0/0/0	0/0/0/0
3	ADP	C	301	-	-	0/12/32/32	0/3/3/3
6	SO4	C	302	-	-	0/0/0/0	0/0/0/0
3	ADP	D	301	-	-	0/12/32/32	0/3/3/3
7	UN1	E	101	2	-	0/4/10/10	0/0/0/0
7	UN1	F	101	2	-	0/4/10/10	0/0/0/0
3	ADP	G	301	5	-	0/12/32/32	0/3/3/3
4	PO4	G	302	5	-	0/0/0/0	0/0/0/0
3	ADP	H	301	5	-	0/12/32/32	0/3/3/3
6	SO4	H	302	5	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	I	301	-	-	0/12/32/32	0/3/3/3
4	PO4	I	302	-	-	0/0/0/0	0/0/0/0
7	UN1	I	303	-	-	0/4/10/10	0/0/0/0
3	ADP	J	301	5	-	0/12/32/32	0/3/3/3
4	PO4	J	302	5	-	0/0/0/0	0/0/0/0
7	UN1	K	101	2	-	0/4/10/10	0/0/0/0
7	UN1	L	101	2	-	0/4/10/10	0/0/0/0
7	UN1	N	101	2	-	0/4/10/10	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	ADP	C5-C4	2.47	1.46	1.40
3	J	301	ADP	C5-C4	2.69	1.46	1.40
3	D	301	ADP	C5-C4	2.73	1.46	1.40
3	G	301	ADP	C5-C4	2.75	1.46	1.40
3	C	301	ADP	C5-C4	2.80	1.46	1.40
3	I	301	ADP	C5-C4	3.04	1.47	1.40
3	A	301	ADP	C5-C4	3.08	1.47	1.40
3	B	301	ADP	C5-C4	3.38	1.48	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	301	ADP	N3-C2-N1	-7.33	123.12	128.87
3	H	301	ADP	N3-C2-N1	-7.20	123.21	128.87
3	D	301	ADP	N3-C2-N1	-7.00	123.37	128.87
3	B	301	ADP	N3-C2-N1	-6.99	123.38	128.87
3	A	301	ADP	N3-C2-N1	-6.91	123.44	128.87
3	J	301	ADP	N3-C2-N1	-6.55	123.73	128.87
3	G	301	ADP	N3-C2-N1	-6.34	123.89	128.87
3	C	301	ADP	N3-C2-N1	-6.29	123.93	128.87
3	C	301	ADP	C1'-N9-C4	-2.15	124.41	126.81
3	A	301	ADP	C1'-N9-C4	-2.07	124.49	126.81
3	J	301	ADP	C1'-N9-C4	-2.00	124.57	126.81
3	I	301	ADP	C2-N1-C6	2.00	122.34	118.77
3	J	301	ADP	O3B-PB-O1B	2.03	117.27	110.63
3	D	301	ADP	N6-C6-N1	2.04	121.93	118.52
3	J	301	ADP	N6-C6-N1	2.07	121.99	118.52
3	B	301	ADP	O3B-PB-O2B	2.10	115.16	107.44
3	D	301	ADP	O3B-PB-O2B	2.15	115.33	107.44
3	A	301	ADP	N6-C6-N1	2.19	122.20	118.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	ADP	N6-C6-N1	2.20	122.21	118.52
3	B	301	ADP	C2-N1-C6	2.21	122.72	118.77
3	H	301	ADP	O2B-PB-O1B	2.22	117.89	110.63
3	A	301	ADP	C2-N1-C6	2.23	122.75	118.77
3	H	301	ADP	N6-C6-N1	2.42	122.58	118.52
3	G	301	ADP	N6-C6-N1	2.47	122.66	118.52
3	I	301	ADP	N6-C6-N1	2.66	122.97	118.52
3	B	301	ADP	N6-C6-N1	2.66	122.98	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	ADP	1	0
3	C	301	ADP	1	0
3	H	301	ADP	1	0
3	I	301	ADP	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, 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	273/273 (100%)	0.14	5 (1%) 71 72	34, 45, 62, 82	0
1	B	273/273 (100%)	0.21	4 (1%) 76 77	36, 45, 62, 88	0
1	C	273/273 (100%)	0.40	11 (4%) 42 44	39, 54, 78, 91	0
1	D	270/273 (98%)	0.08	6 (2%) 65 66	35, 47, 69, 87	0
1	G	273/273 (100%)	0.32	14 (5%) 32 34	36, 50, 70, 94	0
1	H	272/273 (99%)	0.20	8 (2%) 55 57	36, 44, 60, 74	0
1	I	273/273 (100%)	0.58	24 (8%) 12 13	41, 59, 82, 94	0
1	J	273/273 (100%)	0.25	9 (3%) 50 52	40, 50, 67, 89	0
2	E	52/53 (98%)	2.32	25 (48%) 0 0	45, 70, 95, 99	0
2	F	53/53 (100%)	2.22	27 (50%) 0 0	45, 75, 93, 98	0
2	K	11/53 (20%)	2.02	6 (54%) 0 0	71, 82, 98, 99	0
2	L	30/53 (56%)	3.74	22 (73%) 0 0	58, 99, 121, 133	0
2	M	9/53 (16%)	2.03	4 (44%) 0 0	68, 77, 91, 96	0
2	N	33/53 (62%)	1.91	14 (42%) 0 0	52, 79, 94, 100	0
All	All	2368/2502 (94%)	0.44	179 (7%) 17 18	34, 50, 80, 133	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	18	LEU	10.1
2	L	40	THR	9.8
2	L	31	LEU	8.5
2	L	39	LEU	8.4
2	L	37	GLU	7.6
2	N	37	GLU	7.4
2	F	7	CYS	7.2
2	L	38	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
2	F	24	CYS	6.4
2	F	13	ILE	6.4
2	E	13	ILE	6.2
2	F	10	GLU	6.1
2	E	28	GLY	5.9
2	E	27	CYS	5.8
2	F	37	GLU	5.7
1	J	273	THR	5.6
2	E	11	ILE	5.6
1	C	128	TRP	5.5
1	I	206	SER	5.5
2	L	36	LEU	5.4
2	M	44	LEU	5.3
2	N	29	ALA	5.3
2	L	35	SER	5.2
2	E	24	CYS	5.1
2	L	41	LEU	5.1
2	F	1	MET	5.0
2	E	26	VAL	5.0
2	E	10	GLU	4.9
1	B	273	THR	4.8
2	E	15	GLU	4.4
1	I	203	GLU	4.3
2	L	20	GLN	4.3
2	N	16	VAL	4.2
1	D	200	GLY	4.2
2	E	7	CYS	4.2
1	I	201	LYS	4.1
2	N	44	LEU	4.1
1	C	12	ARG	4.1
2	E	39	LEU	4.0
2	E	14	GLY	4.0
2	F	36	LEU	4.0
2	L	21	ILE	4.0
2	E	12	GLU	3.9
2	F	2	VAL	3.9
2	F	25	PRO	3.9
2	E	2	VAL	3.9
2	L	22	VAL	3.8
2	N	38	PRO	3.8
2	L	34	VAL	3.8
2	F	27	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	L	46	GLU	3.7
2	E	5	PRO	3.7
2	K	52	GLY	3.7
1	J	92	GLY	3.7
1	B	150	TRP	3.7
1	I	200	GLY	3.7
2	N	36	LEU	3.6
2	F	26	VAL	3.6
2	E	30	GLU	3.6
1	G	199	GLY	3.5
2	N	42	GLU	3.5
1	D	128	TRP	3.4
2	E	29	ALA	3.4
1	I	196	THR	3.4
1	C	234	GLU	3.4
2	F	38	PRO	3.4
1	I	186	TYR	3.4
2	E	25	PRO	3.4
1	A	234	GLU	3.3
2	N	40	THR	3.3
1	G	12	ARG	3.3
1	I	190	ASN	3.2
2	E	36	LEU	3.2
2	M	45	PRO	3.2
2	L	42	GLU	3.2
1	G	200	GLY	3.2
2	E	8	GLY	3.1
2	L	44	LEU	3.1
2	L	19	HIS	3.1
2	L	23	GLU	3.1
2	F	15	GLU	3.1
2	K	44	LEU	3.1
1	I	198	ARG	3.1
1	G	10	LEU	3.1
2	N	41	LEU	3.1
2	F	11	ILE	3.1
1	C	10	LEU	3.0
1	C	208	PRO	3.0
1	I	273	THR	3.0
2	E	9	SER	3.0
2	F	8	GLY	2.9
1	I	41	TYR	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	188	TYR	2.9
1	C	15	MET	2.9
2	E	3	GLU	2.9
1	G	155	LEU	2.9
1	I	202	ALA	2.9
1	G	196	THR	2.8
2	K	46	GLU	2.8
1	D	196	THR	2.8
2	L	32	GLU	2.8
2	F	9	SER	2.8
2	F	3	GLU	2.7
1	I	40	ASN	2.7
2	K	45	PRO	2.7
2	K	51	TRP	2.7
1	C	197	ALA	2.7
2	N	34	VAL	2.7
1	I	191	HIS	2.7
2	F	29	ALA	2.7
1	G	15	MET	2.7
1	J	124	VAL	2.7
1	H	152	LYS	2.7
1	C	254	VAL	2.6
2	F	4	CYS	2.6
1	A	124	VAL	2.6
1	I	128	TRP	2.6
1	J	234	GLU	2.6
2	L	33	VAL	2.5
1	H	156	TYR	2.5
1	J	151	MET	2.5
1	C	19	GLU	2.5
1	A	150	TRP	2.5
1	H	131	LEU	2.5
1	H	155	LEU	2.5
2	E	38	PRO	2.5
2	N	18	LEU	2.4
1	I	15	MET	2.4
1	C	212	GLU	2.4
2	N	20	GLN	2.4
1	G	128	TRP	2.4
1	J	152	LYS	2.4
2	N	39	LEU	2.4
2	F	39	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	45	PRO	2.4
2	E	4	CYS	2.3
2	M	48	GLU	2.3
2	M	47	VAL	2.3
1	I	151	MET	2.3
2	F	17	GLU	2.3
2	L	17	GLU	2.3
2	E	40	THR	2.3
2	F	12	GLU	2.3
1	B	151	MET	2.3
1	I	42	ASP	2.3
1	A	40	ASN	2.3
1	G	151	MET	2.3
1	H	151	MET	2.3
1	I	249	LYS	2.3
1	J	113	ASP	2.3
2	F	14	GLY	2.3
2	F	31	LEU	2.2
1	G	234	GLU	2.2
1	I	199	GLY	2.2
1	I	210	VAL	2.2
2	F	16	VAL	2.2
1	A	273	THR	2.2
1	D	10	LEU	2.2
1	H	197	ALA	2.2
1	I	10	LEU	2.2
1	J	1	MET	2.2
1	D	234	GLU	2.1
2	E	34	VAL	2.1
2	F	18	LEU	2.1
1	H	12	ARG	2.1
1	H	124	VAL	2.1
2	F	34	VAL	2.1
1	G	201	LYS	2.1
1	G	124	VAL	2.1
1	G	197	ALA	2.1
1	D	131	LEU	2.0
2	K	47	VAL	2.0
1	I	125	PHE	2.0
1	I	253	ARG	2.0
2	N	30	GLU	2.0
1	B	155	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	11	ARG	2.0
1	G	130	ARG	2.0
1	J	272	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	UN1	L	101	11/11	0.83	0.30	4.70	38,40,41,43	0
7	UN1	K	101	11/11	0.79	0.39	3.69	50,52,59,60	0
6	SO4	C	302	5/5	0.79	0.35	2.74	109,110,112,113	0
5	MG	G	303	1/1	0.86	0.19	2.69	58,58,58,58	0
7	UN1	I	303	11/11	0.78	0.35	2.64	60,65,68,70	0
4	PO4	G	302	5/5	0.96	0.24	2.46	59,62,62,64	0
7	UN1	E	101	11/11	0.96	0.17	1.69	41,44,45,45	0
5	MG	H	304	1/1	0.94	0.21	1.44	64,64,64,64	0
4	PO4	I	302	5/5	0.95	0.22	1.28	59,61,63,64	0
7	UN1	N	101	11/11	0.97	0.14	0.58	36,38,40,40	0
6	SO4	H	302	5/5	0.97	0.15	0.44	57,58,59,60	0
3	ADP	D	301	27/27	0.93	0.14	-0.11	33,36,63,71	0
7	UN1	F	101	11/11	0.93	0.11	-0.27	37,41,43,44	0
3	ADP	H	301	27/27	0.95	0.12	-0.53	29,33,55,56	0
3	ADP	C	301	27/27	0.95	0.12	-0.66	29,38,69,72	0
3	ADP	B	301	27/27	0.98	0.10	-0.89	29,33,39,43	0
3	ADP	I	301	27/27	0.97	0.13	-1.05	37,40,51,53	0
4	PO4	A	302	5/5	0.99	0.09	-1.08	39,40,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	J	301	27/27	0.98	0.10	-1.08	31,33,41,45	0
3	ADP	A	301	27/27	0.98	0.09	-1.20	28,31,38,39	0
3	ADP	G	301	27/27	0.96	0.10	-1.26	33,36,57,62	0
8	ZN	F	102	1/1	0.98	0.15	-1.63	54,54,54,54	0
4	PO4	J	302	5/5	0.99	0.10	-1.70	41,41,42,43	0
4	PO4	B	302	5/5	0.99	0.07	-1.87	36,37,39,41	0
8	ZN	E	102	1/1	0.98	0.14	-2.12	57,57,57,57	0
5	MG	H	303	1/1	0.86	0.09	-2.37	52,52,52,52	0
5	MG	B	304	1/1	0.96	0.04	-2.57	45,45,45,45	0
5	MG	A	304	1/1	0.99	0.07	-2.65	42,42,42,42	0
5	MG	A	303	1/1	0.96	0.07	-2.69	37,37,37,37	0
5	MG	B	303	1/1	0.98	0.06	-2.81	42,42,42,42	0
5	MG	J	303	1/1	0.95	0.06	-3.26	42,42,42,42	0
5	MG	J	304	1/1	0.95	0.05	-3.89	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.