



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:48 PM GMT

PDB ID : 4LCA  
Title : Crystal structure of probable sugar kinase protein from Rhizobium Etli CFN 42 complexed with thymidine  
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Lafluer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)  
Deposited on : 2013-06-21  
Resolution : 1.50 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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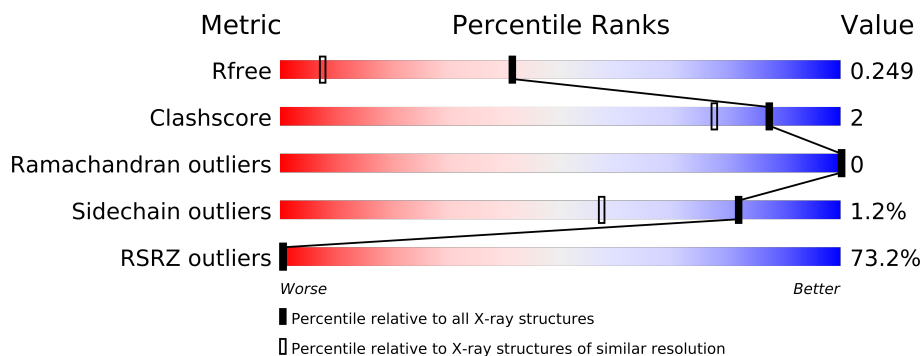
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.50 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))
$R_{free}$	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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	352	
1	B	352	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	THM	B	402[A]	-	X
3	THM	B	402[B]	-	X
3	THM	B	405	-	X
4	DMS	B	404	-	X
5	K	B	406	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5997 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 Probable sugar kinase protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	Se	0	11	0
			2565	1607	450	490	8	10			
1	B	330	Total	C	N	O	S	Se	0	10	0
			2557	1599	445	495	8	10			

There are 44 discrepancies between the modelled and reference sequences:

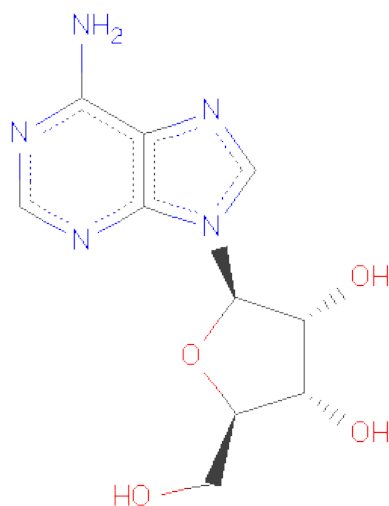
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MSE	-	EXPRESSION TAG	UNP Q2KDX6
A	-22	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-21	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-20	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-19	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-18	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-17	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-16	SER	-	EXPRESSION TAG	UNP Q2KDX6
A	-15	SER	-	EXPRESSION TAG	UNP Q2KDX6
A	-14	GLY	-	EXPRESSION TAG	UNP Q2KDX6
A	-13	VAL	-	EXPRESSION TAG	UNP Q2KDX6
A	-12	ASP	-	EXPRESSION TAG	UNP Q2KDX6
A	-11	LEU	-	EXPRESSION TAG	UNP Q2KDX6
A	-10	GLY	-	EXPRESSION TAG	UNP Q2KDX6
A	-9	THR	-	EXPRESSION TAG	UNP Q2KDX6
A	-8	GLU	-	EXPRESSION TAG	UNP Q2KDX6
A	-7	ASN	-	EXPRESSION TAG	UNP Q2KDX6
A	-6	LEU	-	EXPRESSION TAG	UNP Q2KDX6
A	-5	TYR	-	EXPRESSION TAG	UNP Q2KDX6
A	-4	PHE	-	EXPRESSION TAG	UNP Q2KDX6
A	-3	GLN	-	EXPRESSION TAG	UNP Q2KDX6
A	-2	SER	-	EXPRESSION TAG	UNP Q2KDX6
B	-23	MSE	-	EXPRESSION TAG	UNP Q2KDX6
B	-22	HIS	-	EXPRESSION TAG	UNP Q2KDX6
B	-21	HIS	-	EXPRESSION TAG	UNP Q2KDX6

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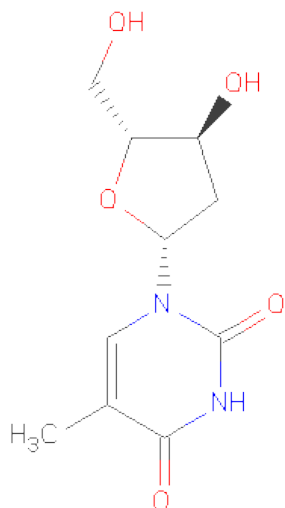
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	EXPRESSION TAG	UNP Q2KDX6
B	-19	HIS	-	EXPRESSION TAG	UNP Q2KDX6
B	-18	HIS	-	EXPRESSION TAG	UNP Q2KDX6
B	-17	HIS	-	EXPRESSION TAG	UNP Q2KDX6
B	-16	SER	-	EXPRESSION TAG	UNP Q2KDX6
B	-15	SER	-	EXPRESSION TAG	UNP Q2KDX6
B	-14	GLY	-	EXPRESSION TAG	UNP Q2KDX6
B	-13	VAL	-	EXPRESSION TAG	UNP Q2KDX6
B	-12	ASP	-	EXPRESSION TAG	UNP Q2KDX6
B	-11	LEU	-	EXPRESSION TAG	UNP Q2KDX6
B	-10	GLY	-	EXPRESSION TAG	UNP Q2KDX6
B	-9	THR	-	EXPRESSION TAG	UNP Q2KDX6
B	-8	GLU	-	EXPRESSION TAG	UNP Q2KDX6
B	-7	ASN	-	EXPRESSION TAG	UNP Q2KDX6
B	-6	LEU	-	EXPRESSION TAG	UNP Q2KDX6
B	-5	TYR	-	EXPRESSION TAG	UNP Q2KDX6
B	-4	PHE	-	EXPRESSION TAG	UNP Q2KDX6
B	-3	GLN	-	EXPRESSION TAG	UNP Q2KDX6
B	-2	SER	-	EXPRESSION TAG	UNP Q2KDX6

- Molecule 2 is ADENOSINE (three-letter code: ADN) (formula:  $C_{10}H_{13}N_5O_4$ ).



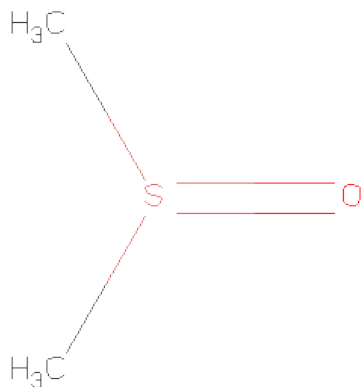
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is THYMIDINE (three-letter code: THM) (formula:  $C_{10}H_{14}N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	17	1
			34	20	4	10		
3	B	1	Total	C	N	O	16	1
			34	20	4	10		
3	B	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	A	1	Total K 1 1	0	0

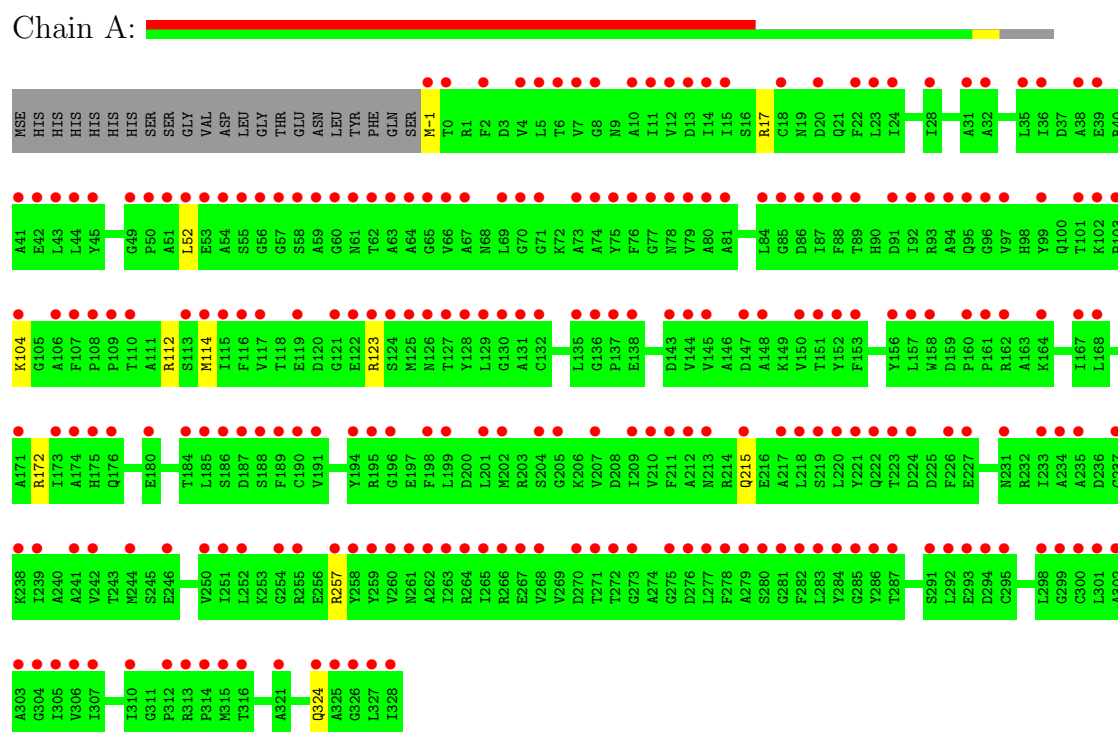
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	331	Total O 331 331	0	0
6	B	401	Total O 403 403	0	2

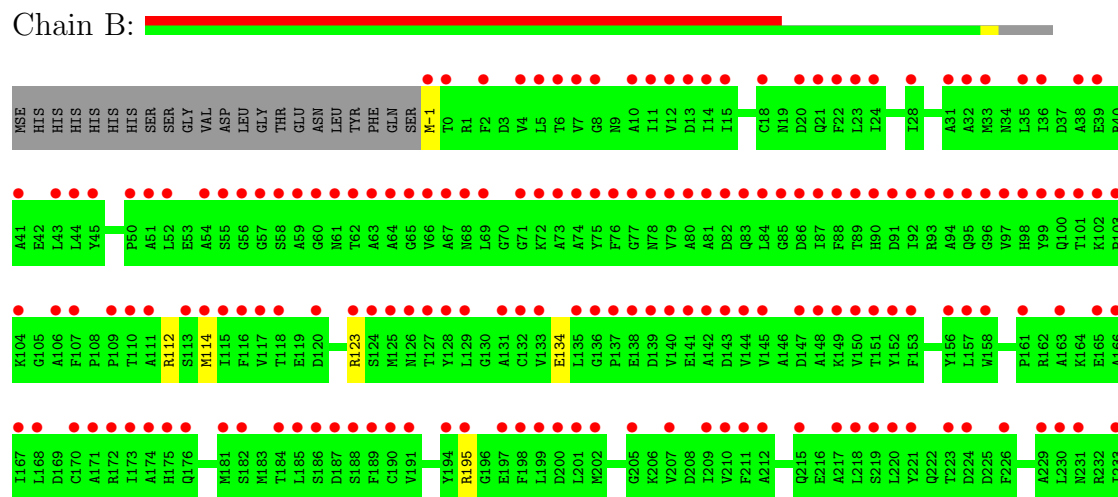
### 3 Residue-property plots

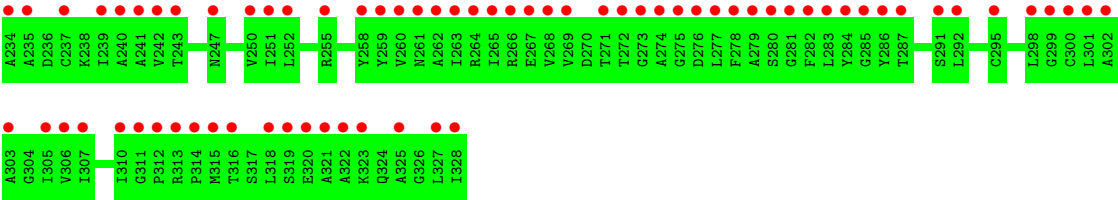
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: Probable sugar kinase protein



- Molecule 1: Probable sugar kinase protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.52Å 80.78Å 82.66Å 90.00° 98.09° 90.00°	Depositor
Resolution (Å)	40.18 – 1.50 40.18 – 1.49	Depositor EDS
% Data completeness (in resolution range)	95.2 (40.18-1.50) 94.6 (40.18-1.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.200 , 0.248 0.201 , 0.249	Depositor DCC
$R_{free}$ test set	5180 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 100.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 104081 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	5997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.38 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5659e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, K, DMS, THM

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	0.44	0/2625	0.64	1/3531 (0.0%)
1	B	0.51	0/2614	0.69	1/3517 (0.0%)
All	All	0.48	0/5239	0.67	2/7048 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	MSE	CA-CB-CG	-5.85	103.36	113.30
1	A	114	MSE	CA-CB-CG	-5.69	103.63	113.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2565	0	0	8	0
1	B	2557	0	0	5	0
2	A	19	0	0	0	0
2	B	19	0	0	0	0
3	A	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	51	0	0	1	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	331	0	0	7	0
6	B	403	0	0	3	0
All	All	5997	0	0	13	0

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 2.

All (13) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:195[B]:ARG:NH1	1:B:195[B]:ARG:CG	2.41	0.84
1:A:257[B]:ARG:NH1	1:A:257[B]:ARG:CG	2.54	0.71
1:B:-1:MSE:N	6:B:667:HOH:O	2.34	0.60
1:A:172:ARG:NH2	6:A:811:HOH:O	2.34	0.60
1:A:-1:MSE:N	6:A:735:HOH:O	2.38	0.56
1:A:-1:MSE:N	6:A:675:HOH:O	2.40	0.53
1:B:195[B]:ARG:CZ	6:B:815:HOH:O	2.60	0.49
1:A:104:LYS:NZ	6:A:783:HOH:O	2.46	0.48
1:A:215:GLN:CG	6:A:802:HOH:O	2.61	0.48
1:B:-1:MSE:N	6:B:814:HOH:O	2.51	0.44
1:B:134:GLU:OE2	3:B:405:THM:O5'	2.37	0.42
1:A:257[B]:ARG:NH1	6:A:652:HOH:O	2.53	0.42
1:A:17:ARG:NH1	6:A:768:HOH:O	2.51	0.42

There are no symmetry-related clashes.

## 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	339/352 (96%)	335 (99%)	4 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	338/352 (96%)	333 (98%)	5 (2%)	0	100	100
All	All	677/704 (96%)	668 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	268/266 (101%)	262 (98%)	6 (2%)	64	28
1	B	267/266 (100%)	265 (99%)	2 (1%)	91	76
All	All	535/532 (101%)	527 (98%)	8 (2%)	82	47

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52[A]	LEU
1	A	52[B]	LEU
1	A	112	ARG
1	A	123[A]	ARG
1	A	123[B]	ARG
1	A	324	GLN
1	B	112	ARG
1	B	123	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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$
2	ADN	A	401	-	21,21,21	1.38	3 (14%)	31,31,31	2.30	7 (22%)
3	THM	A	402[A]	-	18,18,18	2.11	5 (27%)	21,26,26	7.04	7 (33%)
3	THM	A	402[B]	-	18,18,18	1.06	2 (11%)	21,26,26	2.62	5 (23%)
4	DMS	A	403	-	3,3,3	0.48	0	3,3,3	0.77	0
4	DMS	A	404	-	3,3,3	0.51	0	3,3,3	0.51	0
2	ADN	B	401	-	21,21,21	1.23	2 (9%)	31,31,31	2.93	8 (25%)
3	THM	B	402[A]	-	18,18,18	1.36	2 (11%)	21,26,26	4.00	7 (33%)
3	THM	B	402[B]	-	18,18,18	1.23	3 (16%)	21,26,26	2.41	5 (23%)
4	DMS	B	403	-	3,3,3	0.51	0	3,3,3	0.42	0
4	DMS	B	404	-	3,3,3	0.58	0	3,3,3	0.50	0
3	THM	B	405	-	18,18,18	1.24	2 (11%)	21,26,26	1.77	3 (14%)

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	ADN	A	401	-	-	0/6/22/22	0/1/3/3
3	THM	A	402[A]	-	-	0/3/18/18	0/2/2/2
3	THM	A	402[B]	-	-	0/3/18/18	0/2/2/2
4	DMS	A	403	-	-	0/0/0/0	0/0/0/0
4	DMS	A	404	-	-	0/0/0/0	0/0/0/0
2	ADN	B	401	-	-	0/6/22/22	0/1/3/3
3	THM	B	402[A]	-	-	0/3/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	THM	B	402[B]	-	-	0/3/18/18	0/2/2/2
4	DMS	B	403	-	-	0/0/0/0	0/0/0/0
4	DMS	B	404	-	-	0/0/0/0	0/0/0/0
3	THM	B	405	-	-	0/3/18/18	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[A]	THM	C4-N3	-6.12	1.27	1.37
3	B	405	THM	C2-N1	3.64	1.42	1.38
2	B	401	ADN	C5-C4	3.54	1.48	1.40
3	A	402[A]	THM	C2-N3	-3.34	1.30	1.37
3	B	402[B]	THM	C2-N1	3.28	1.42	1.38
3	A	402[A]	THM	C2-N1	3.28	1.42	1.38
3	B	402[A]	THM	C4-N3	-3.21	1.31	1.37
2	A	401	ADN	C5-C4	3.17	1.47	1.40
3	A	402[A]	THM	C4-C5	3.03	1.49	1.42
3	B	405	THM	C4-C5	2.96	1.49	1.42
3	B	402[A]	THM	C2-N1	2.86	1.41	1.38
3	B	402[B]	THM	C4-C5	2.71	1.48	1.42
2	A	401	ADN	C4-N9	-2.65	1.33	1.37
3	A	402[B]	THM	C2-N1	2.53	1.41	1.38
3	A	402[B]	THM	C4-C5	2.33	1.47	1.42
2	A	401	ADN	O4'-C1'	2.30	1.44	1.41
3	A	402[A]	THM	O2-C2	-2.23	1.18	1.23
3	B	402[B]	THM	C4-N3	-2.12	1.33	1.37
2	B	401	ADN	C2'-C1'	-2.06	1.50	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[A]	THM	C6-N1-C2	-25.85	115.07	122.41
3	A	402[A]	THM	N3-C2-N1	16.85	130.03	115.97
3	B	402[A]	THM	C6-N1-C2	-13.60	118.54	122.41
2	B	401	ADN	N3-C2-N1	-9.87	120.45	128.71
2	B	401	ADN	C4'-O4'-C1'	-8.81	100.19	109.75
3	A	402[B]	THM	C6-N1-C2	-7.88	120.17	122.41
3	B	402[B]	THM	N3-C2-N1	7.34	122.10	115.97
2	A	401	ADN	C4'-O4'-C1'	-7.13	102.00	109.75
3	B	402[A]	THM	N3-C2-N1	7.06	121.86	115.97
3	A	402[B]	THM	N3-C2-N1	6.94	121.76	115.97
3	B	402[A]	THM	C5M-C5-C4	-6.93	113.97	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ADN	N3-C2-N1	-6.74	123.08	128.71
3	B	402[B]	THM	C6-N1-C2	-6.25	120.63	122.41
3	B	405	THM	N3-C2-N1	5.69	120.72	115.97
2	B	401	ADN	C2-N1-C6	5.56	128.81	118.77
3	A	402[A]	THM	O4'-C1'-N1	4.80	116.71	107.68
3	A	402[A]	THM	C5-C6-N1	-4.62	117.09	121.59
2	A	401	ADN	N3-C4-N9	4.35	133.29	125.43
2	B	401	ADN	N3-C4-N9	4.30	133.19	125.43
3	B	402[A]	THM	O4'-C1'-N1	4.19	115.55	107.68
3	B	405	THM	C6-N1-C2	-4.03	121.26	122.41
3	A	402[A]	THM	C4-N3-C2	-3.72	117.75	125.39
2	B	401	ADN	N6-C6-N1	3.46	126.15	119.36
3	B	402[A]	THM	C5M-C5-C6	3.42	125.87	118.59
3	A	402[A]	THM	C6-C5-C4	3.42	123.40	115.11
3	A	402[B]	THM	O4'-C1'-N1	3.25	113.79	107.68
3	B	402[A]	THM	C5-C6-N1	-2.86	118.80	121.59
3	B	402[B]	THM	C5-C6-N1	-2.83	118.84	121.59
3	A	402[A]	THM	C5M-C5-C4	-2.74	118.24	121.04
2	A	401	ADN	C2-N1-C6	2.64	123.54	118.77
2	B	401	ADN	C1'-N9-C4	-2.62	122.11	126.64
2	A	401	ADN	C1'-N9-C4	-2.59	122.15	126.64
3	A	402[B]	THM	C2'-C1'-N1	-2.56	107.43	114.08
2	A	401	ADN	N6-C6-N1	2.54	124.36	119.36
3	B	402[B]	THM	C4-N3-C2	-2.53	120.21	125.39
3	B	405	THM	C4-N3-C2	-2.37	120.53	125.39
3	A	402[B]	THM	C4-N3-C2	-2.33	120.62	125.39
2	B	401	ADN	C5-C4-N9	-2.24	103.93	107.16
2	B	401	ADN	C8-N9-C4	2.18	108.56	106.90
2	A	401	ADN	C5-C4-N3	-2.14	121.04	125.70
3	B	402[A]	THM	C6-C5-C4	2.07	120.14	115.11
3	B	402[B]	THM	C2'-C1'-N1	-2.06	108.75	114.08

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	330/352 (93%)	2.86	237 (71%) 0 0	15, 21, 34, 53	0
1	B	330/352 (93%)	2.93	248 (75%) 0 0	12, 18, 32, 67	0
All	All	660/704 (93%)	2.90	485 (73%) 0 0	12, 20, 33, 67	0

All (485) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	ARG	10.4
1	A	263	ILE	9.6
1	A	328	ILE	8.4
1	B	263	ILE	7.9
1	B	266	ARG	7.4
1	A	266	ARG	6.9
1	A	267	GLU	6.7
1	B	75	TYR	6.7
1	A	259	TYR	6.6
1	B	153	PHE	6.1
1	B	76	PHE	5.9
1	A	15	ILE	5.8
1	B	259	TYR	5.8
1	B	199	LEU	5.8
1	B	97	VAL	5.7
1	A	52[A]	LEU	5.7
1	A	97	VAL	5.6
1	A	76	PHE	5.5
1	B	226	PHE	5.5
1	A	4	VAL	5.5
1	A	158	TRP	5.5
1	B	5	LEU	5.4
1	B	173	ILE	5.4
1	A	255	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	260[A]	VAL	5.3
1	A	115	ILE	5.2
1	B	92	ILE	5.2
1	A	64	ALA	5.2
1	A	107	PHE	5.2
1	B	328	ILE	5.2
1	B	207[A]	VAL	5.2
1	A	239	ILE	5.2
1	A	135	LEU	5.2
1	A	5	LEU	5.1
1	B	84	LEU	5.1
1	B	66	VAL	5.1
1	A	14	ILE	5.0
1	A	79	VAL	5.0
1	A	11	ILE	5.0
1	B	158	TRP	5.0
1	B	211	PHE	5.0
1	B	170	CYS	4.9
1	A	221	TYR	4.9
1	A	201	LEU	4.9
1	A	301	LEU	4.9
1	A	300	CYS	4.9
1	B	107	PHE	4.9
1	B	307	ILE	4.9
1	B	18	CYS	4.9
1	B	176	GLN	4.9
1	B	79	VAL	4.8
1	B	15	ILE	4.8
1	B	99	TYR	4.8
1	B	115	ILE	4.7
1	B	239	ILE	4.7
1	B	300	CYS	4.7
1	A	87	ILE	4.7
1	B	35	LEU	4.7
1	B	52	LEU	4.7
1	A	128	TYR	4.7
1	B	59	ALA	4.6
1	B	267	GLU	4.6
1	A	283	LEU	4.6
1	A	88	PHE	4.6
1	B	156	TYR	4.6
1	B	2	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	84	LEU	4.5
1	A	92	ILE	4.5
1	A	265	ILE	4.4
1	B	11	ILE	4.4
1	B	210[A]	VAL	4.4
1	B	220	LEU	4.4
1	A	2	PHE	4.4
1	B	12	VAL	4.4
1	B	190	CYS	4.4
1	A	194	TYR	4.4
1	B	198	PHE	4.4
1	B	278	PHE	4.4
1	B	283	LEU	4.4
1	B	14	ILE	4.4
1	A	190	CYS	4.3
1	A	237[A]	CYS	4.3
1	A	75	TYR	4.3
1	A	218	LEU	4.3
1	B	218	LEU	4.3
1	B	279	ALA	4.3
1	A	153	PHE	4.3
1	B	4	VAL	4.3
1	B	191	VAL	4.3
1	B	237[A]	CYS	4.3
1	A	325	ALA	4.3
1	B	64	ALA	4.3
1	B	116	PHE	4.3
1	B	209	ILE	4.2
1	B	301	LEU	4.2
1	B	67	ALA	4.2
1	B	303	ALA	4.2
1	B	201	LEU	4.2
1	A	191	VAL	4.2
1	A	327	LEU	4.1
1	A	31	ALA	4.1
1	B	54	ALA	4.1
1	A	210[A]	VAL	4.1
1	B	242	VAL	4.1
1	A	58[A]	SER	4.1
1	A	6	THR	4.1
1	B	265	ILE	4.1
1	A	41	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	63	ALA	4.0
1	B	51	ALA	4.0
1	B	312	PRO	4.0
1	B	77	GLY	4.0
1	B	85	GLY	4.0
1	A	24	ILE	4.0
1	B	135	LEU	4.0
1	A	57	GLY	4.0
1	B	194	TYR	4.0
1	B	205	GLY	4.0
1	A	66	VAL	4.0
1	B	7	VAL	4.0
1	A	131	ALA	4.0
1	B	172[A]	ARG	4.0
1	A	116	PHE	3.9
1	A	43	LEU	3.9
1	B	277	LEU	3.9
1	B	6	THR	3.9
1	B	268	VAL	3.9
1	A	54	ALA	3.9
1	B	73	ALA	3.9
1	A	36	ILE	3.9
1	B	269	VAL	3.9
1	A	282	PHE	3.9
1	B	185	LEU	3.9
1	A	156	TYR	3.9
1	B	195[A]	ARG	3.9
1	A	7	VAL	3.8
1	A	279	ALA	3.8
1	B	31	ALA	3.8
1	A	136	GLY	3.8
1	A	205	GLY	3.8
1	A	291	SER	3.8
1	B	24	ILE	3.8
1	A	217	ALA	3.8
1	B	63	ALA	3.8
1	B	74	ALA	3.8
1	B	60	GLY	3.8
1	A	35	LEU	3.8
1	A	199	LEU	3.8
1	A	292	LEU	3.8
1	A	45	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	152	TYR	3.8
1	B	0	THR	3.8
1	A	94	ALA	3.8
1	A	211	PHE	3.8
1	A	56	GLY	3.8
1	A	152	TYR	3.8
1	A	69	LEU	3.7
1	A	277	LEU	3.7
1	B	128	TYR	3.7
1	B	212	ALA	3.7
1	A	51	ALA	3.7
1	A	28	ILE	3.7
1	B	144	VAL	3.7
1	A	49	GLY	3.7
1	A	38	ALA	3.7
1	B	174	ALA	3.7
1	B	252	LEU	3.7
1	A	162[A]	ARG	3.7
1	B	57	GLY	3.7
1	A	303	ALA	3.6
1	B	262	ALA	3.6
1	B	305	ILE	3.6
1	B	58[A]	SER	3.6
1	A	12	VAL	3.6
1	A	150	VAL	3.6
1	B	132	CYS	3.6
1	A	167	ILE	3.6
1	A	272	THR	3.6
1	B	20	ASP	3.6
1	A	132	CYS	3.6
1	B	131	ALA	3.6
1	B	44	LEU	3.6
1	B	264	ARG	3.6
1	A	268	VAL	3.5
1	B	168	LEU	3.5
1	A	315	MSE	3.5
1	B	140	VAL	3.5
1	A	215	GLN	3.5
1	B	145	VAL	3.5
1	B	325	ALA	3.5
1	A	227	GLU	3.5
1	B	43	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	292	LEU	3.5
1	B	223	THR	3.5
1	A	242	VAL	3.5
1	B	56	GLY	3.5
1	A	278	PHE	3.5
1	A	80	ALA	3.4
1	B	87	ILE	3.4
1	B	273	GLY	3.4
1	B	298	LEU	3.4
1	B	117	VAL	3.4
1	B	260	VAL	3.4
1	B	221	TYR	3.4
1	B	281	GLY	3.4
1	A	220	LEU	3.4
1	B	302	ALA	3.4
1	B	284	TYR	3.4
1	A	60	GLY	3.4
1	A	109	PRO	3.4
1	A	186	SER	3.4
1	A	189	PHE	3.4
1	B	62	THR	3.4
1	A	195[A]	ARG	3.4
1	B	88	PHE	3.4
1	A	103	PRO	3.4
1	B	157	LEU	3.4
1	B	327	LEU	3.4
1	A	198	PHE	3.3
1	A	157	LEU	3.3
1	A	73	ALA	3.3
1	A	173	ILE	3.3
1	A	99	TYR	3.3
1	B	258	TYR	3.3
1	B	215	GLN	3.3
1	B	189	PHE	3.3
1	B	282	PHE	3.3
1	A	23	LEU	3.3
1	A	307	ILE	3.3
1	A	42	GLU	3.3
1	B	291	SER	3.3
1	A	59	ALA	3.3
1	A	127	THR	3.2
1	B	202	MSE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	32	ALA	3.2
1	B	229	ALA	3.2
1	B	321	ALA	3.2
1	A	71	GLY	3.2
1	B	318	LEU	3.2
1	A	74	ALA	3.2
1	B	224	ASP	3.2
1	A	89	THR	3.2
1	A	44	LEU	3.2
1	A	102	LYS	3.2
1	A	67	ALA	3.2
1	B	32	ALA	3.2
1	A	85	GLY	3.2
1	A	284	TYR	3.1
1	B	310	ILE	3.1
1	A	77	GLY	3.1
1	A	280	SER	3.1
1	B	219[A]	SER	3.1
1	A	310	ILE	3.1
1	A	326	GLY	3.1
1	B	69	LEU	3.1
1	B	80	ALA	3.1
1	B	230	LEU	3.1
1	A	22	PHE	3.1
1	A	234	ALA	3.1
1	A	219[A]	SER	3.1
1	B	323	LYS	3.1
1	A	207[A]	VAL	3.1
1	B	150	VAL	3.1
1	B	231	ASN	3.1
1	B	217	ALA	3.1
1	A	312	PRO	3.1
1	A	286	TYR	3.0
1	B	313	ARG	3.0
1	B	41	ALA	3.0
1	B	163	ALA	3.0
1	A	246	GLU	3.0
1	A	184	THR	3.0
1	A	223	THR	3.0
1	A	262	ALA	3.0
1	B	50	PRO	3.0
1	B	81	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	226	PHE	3.0
1	B	280	SER	3.0
1	B	167	ILE	3.0
1	B	250	VAL	2.9
1	A	0	THR	2.9
1	A	168	LEU	2.9
1	B	100[A]	GLN	2.9
1	A	10	ALA	2.9
1	A	96	GLY	2.9
1	B	247	ASN	2.9
1	B	71	GLY	2.9
1	B	96	GLY	2.9
1	B	295	CYS	2.9
1	B	98	HIS	2.9
1	B	61	ASN	2.9
1	B	78	ASN	2.9
1	B	142	ALA	2.9
1	B	171	ALA	2.9
1	B	306	VAL	2.9
1	A	295	CYS	2.9
1	A	251	ILE	2.9
1	B	28	ILE	2.9
1	A	62	THR	2.9
1	A	151	THR	2.9
1	B	151	THR	2.9
1	B	286	TYR	2.9
1	A	306	VAL	2.9
1	B	272	THR	2.8
1	B	311	GLY	2.8
1	A	294	ASP	2.8
1	A	241	ALA	2.8
1	B	241	ALA	2.8
1	A	65	GLY	2.8
1	A	143	ASP	2.8
1	B	10	ALA	2.8
1	B	240	ALA	2.8
1	B	251	ILE	2.8
1	B	186	SER	2.8
1	B	299	GLY	2.8
1	A	-1	MSE	2.8
1	A	114	MSE	2.8
1	B	36	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	243	THR	2.8
1	B	261	ASN	2.8
1	A	176	GLN	2.8
1	A	145	VAL	2.8
1	A	130	GLY	2.8
1	A	18	CYS	2.8
1	B	94	ALA	2.7
1	A	281	GLY	2.7
1	A	202	MSE	2.7
1	A	70	GLY	2.7
1	A	305	ILE	2.7
1	B	137	PRO	2.7
1	A	252	LEU	2.7
1	B	127	THR	2.7
1	A	110	THR	2.7
1	B	200	ASP	2.7
1	A	273	GLY	2.7
1	A	123[A]	ARG	2.7
1	B	255	ARG	2.7
1	B	314	PRO	2.7
1	A	129	LEU	2.6
1	A	298	LEU	2.6
1	A	314	PRO	2.6
1	B	103	PRO	2.6
1	A	235	ALA	2.6
1	A	124	SER	2.6
1	A	233	ILE	2.6
1	B	101	THR	2.6
1	B	45	TYR	2.6
1	B	148	ALA	2.6
1	B	143[A]	ASP	2.6
1	A	8	GLY	2.6
1	B	65	GLY	2.6
1	A	117	VAL	2.6
1	B	104	LYS	2.6
1	A	122	GLU	2.6
1	A	148	ALA	2.6
1	B	271	THR	2.6
1	A	185	LEU	2.6
1	A	20	ASP	2.6
1	A	50	PRO	2.6
1	A	55	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	102	LYS	2.6
1	B	320	GLU	2.5
1	A	224	ASP	2.5
1	A	113	SER	2.5
1	B	276	ASP	2.5
1	B	21	GLN	2.5
1	A	174	ALA	2.5
1	B	124	SER	2.5
1	B	161	PRO	2.5
1	A	196	GLY	2.5
1	B	233	ILE	2.5
1	B	184	THR	2.5
1	A	39	GLU	2.5
1	B	275	GLY	2.5
1	B	8	GLY	2.4
1	B	82	ASP	2.4
1	A	61	ASN	2.4
1	A	108	PRO	2.4
1	A	238	LYS	2.4
1	B	319	SER	2.4
1	A	257[A]	ARG	2.4
1	A	101	THR	2.4
1	A	147	ASP	2.4
1	A	212	ALA	2.4
1	A	121	GLY	2.4
1	A	138	GLU	2.4
1	A	313	ARG	2.4
1	B	120	ASP	2.4
1	A	78	ASN	2.4
1	A	119	GLU	2.4
1	A	144	VAL	2.4
1	A	180	GLU	2.4
1	B	125	MSE	2.4
1	B	13	ASP	2.3
1	B	90	HIS	2.3
1	B	175	HIS	2.3
1	A	271	THR	2.3
1	B	91	ASP	2.3
1	B	22	PHE	2.3
1	B	55	SER	2.3
1	A	137	PRO	2.3
1	B	114	MSE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	81	ALA	2.3
1	A	285	GLY	2.3
1	A	126	ASN	2.3
1	A	261	ASN	2.3
1	B	315	MSE	2.3
1	A	302	ALA	2.3
1	B	129	LEU	2.3
1	A	187	ASP	2.3
1	A	324	GLN	2.3
1	A	175	HIS	2.3
1	A	171	ALA	2.3
1	A	321	ALA	2.3
1	B	106	ALA	2.3
1	B	235	ALA	2.3
1	A	93	ARG	2.3
1	A	204	SER	2.3
1	B	138	GLU	2.3
1	A	316	THR	2.3
1	A	13	ASP	2.2
1	A	53	GLU	2.2
1	B	95	GLN	2.2
1	B	109	PRO	2.2
1	A	299	GLY	2.2
1	A	91	ASP	2.2
1	A	270	ASP	2.2
1	B	39	GLU	2.2
1	B	111	ALA	2.2
1	A	104	LYS	2.2
1	A	209	ILE	2.2
1	B	86	ASP	2.2
1	B	118	THR	2.2
1	B	287	THR	2.2
1	B	23	LEU	2.2
1	A	275	GLY	2.2
1	A	293	GLU	2.2
1	A	304	GLY	2.2
1	A	125	MSE	2.2
1	B	89	THR	2.2
1	A	250	VAL	2.2
1	B	322	ALA	2.2
1	B	197	GLU	2.2
1	A	95	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	161	PRO	2.2
1	A	276	ASP	2.1
1	B	93	ARG	2.1
1	A	244	MSE	2.1
1	B	113	SER	2.1
1	B	68	ASN	2.1
1	B	126	ASN	2.1
1	B	83	GLN	2.1
1	B	136	GLY	2.1
1	B	-1	MSE	2.1
1	A	213	ASN	2.1
1	B	110	THR	2.1
1	A	86	ASP	2.1
1	B	38	ALA	2.1
1	B	274	ALA	2.1
1	B	181	MSE	2.1
1	A	287	THR	2.1
1	B	316	THR	2.1
1	A	106	ALA	2.1
1	A	254	GLY	2.1
1	A	231	ASN	2.1
1	A	258	TYR	2.1
1	B	188	SER	2.1
1	B	285	GLY	2.1
1	B	72	LYS	2.1
1	A	160	PRO	2.1
1	B	234	ALA	2.1
1	B	123	ARG	2.1
1	B	139	ASP	2.0
1	B	147	ASP	2.0
1	B	133	VAL	2.0
1	A	164	LYS	2.0
1	B	149	LYS	2.0
1	B	166	ALA	2.0
1	B	182	SER	2.0
1	B	165	GLU	2.0
1	B	187	ASP	2.0
1	B	33	MSE	2.0
1	B	141	GLU	2.0
1	A	188	SER	2.0
1	A	222	GLN	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
5	K	B	406	1/1	0.35	4.52	44,44,44,44	0
4	DMS	B	404	4/4	0.27	3.01	31,43,43,44	0
3	THM	B	402[B]	17/17	0.34	2.62	27,39,47,47	17
3	THM	B	402[A]	17/17	0.34	2.53	27,38,45,46	17
3	THM	B	405	17/17	0.31	2.02	24,29,35,40	17
4	DMS	A	404	4/4	0.33	1.69	37,39,42,45	0
3	THM	A	402[A]	17/17	0.30	1.37	25,33,36,36	17
3	THM	A	402[B]	17/17	0.30	1.32	25,34,38,39	17
2	ADN	B	401	19/19	0.23	-0.45	11,14,15,16	0
4	DMS	B	403	4/4	0.18	-0.91	24,24,28,29	0
2	ADN	A	401	19/19	0.20	-1.23	13,15,17,18	0
4	DMS	A	403	4/4	0.18	-1.33	23,24,26,28	0
5	K	A	405	1/1	0.15	-1.90	45,45,45,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.