



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:32 PM GMT

PDB ID : 1XSL  
Title : Crystal Structure of human DNA polymerase lambda in complex with a one nucleotide DNA gap  
Authors : Garcia-Diaz, M.; Bebenek, K.; Krahn, J.M.; Kunkel, T.A.; Pedersen, L.C.  
Deposited on : 2004-10-19  
Resolution : 2.30 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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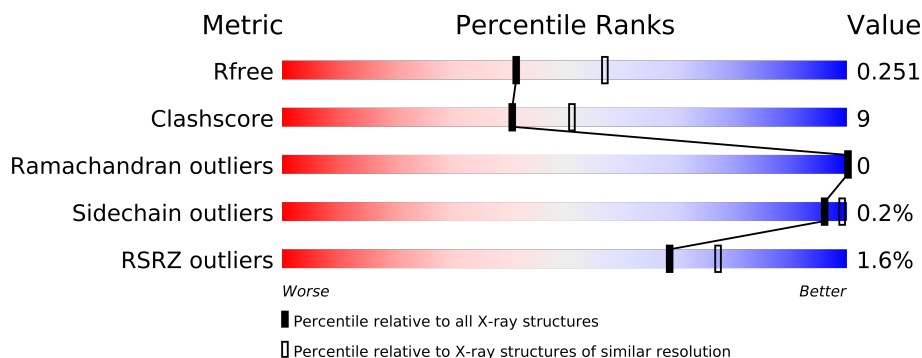
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	B	11	<div><div></div><div></div></div>
1	F	11	<div><div></div><div></div></div>
1	J	11	<div><div></div><div></div></div>
1	N	11	<div><div></div><div></div></div>
2	C	6	<div><div></div><div></div></div>
2	G	6	<div><div></div><div></div></div>
2	K	6	<div><div></div><div></div></div>
2	O	6	<div><div></div><div></div></div>
3	D	4	<div><div></div><div></div></div>
3	H	4	<div><div></div><div></div></div>
3	L	4	<div><div></div><div></div></div>
3	P	4	<div><div></div><div></div></div>
4	A	335	<div><div></div><div></div></div>
4	E	335	<div><div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	I	335	
4	M	335	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	NA	A	961	-	X
5	NA	I	963	-	X
6	MG	F	992	-	X
7	CAC	D	950	X	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12778 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 DNA chain called 5'-D(\*CP\*GP\*GP\*CP\*AP\*GP\*CP\*GP\*CP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	11	Total	C	N	O	P	0	0	0
			222	105	45	62	10			
1	F	11	Total	C	N	O	P	0	0	0
			222	105	45	62	10			
1	J	11	Total	C	N	O	P	0	0	0
			222	105	45	62	10			
1	N	11	Total	C	N	O	P	0	0	0
			222	105	45	62	10			

- Molecule 2 is a DNA chain called 5'-D(\*GP\*TP\*GP\*CP\*GP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			121	58	23	35	5			
2	G	6	Total	C	N	O	P	0	0	0
			121	58	23	35	5			
2	K	6	Total	C	N	O	P	0	0	0
			121	58	23	35	5			
2	O	6	Total	C	N	O	P	0	0	0
			121	58	23	35	5			

- Molecule 3 is a DNA chain called 5'-D(P\*GP\*CP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
3	H	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
3	L	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
3	P	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

- Molecule 4 is a protein called DNA polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	327	Total	C	N	O	S	0	1	0
			2577	1616	474	475	12			
4	E	325	Total	C	N	O	S	0	0	0
			2522	1584	464	462	12			
4	I	326	Total	C	N	O	S	0	1	0
			2532	1591	461	468	12			
4	M	327	Total	C	N	O	S	0	2	0
			2586	1621	475	478	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	INITIATING METHIONINE	UNP Q9UGP5
E	241	MET	-	INITIATING METHIONINE	UNP Q9UGP5
I	241	MET	-	INITIATING METHIONINE	UNP Q9UGP5
M	241	MET	-	INITIATING METHIONINE	UNP Q9UGP5

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Na	0	0
			1	1		
5	E	1	Total	Na	0	0
			1	1		
5	I	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		
5	N	1	Total	Na	0	0
			1	1		
5	M	1	Total	Na	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

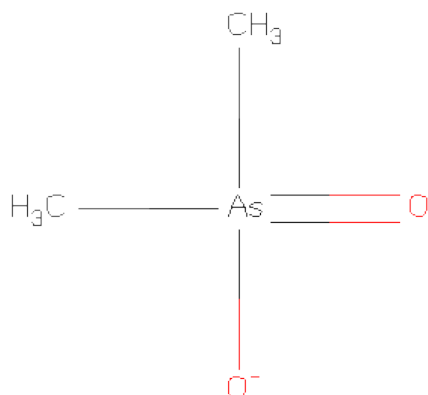
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula:  $\text{C}_2\text{H}_6\text{AsO}_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	205	Total	O	0	0
			205	205		
8	B	30	Total	O	0	0
			30	30		
8	C	13	Total	O	0	0
			13	13		
8	D	8	Total	O	0	0
			8	8		
8	E	104	Total	O	0	0
			104	104		
8	F	15	Total	O	0	0
			15	15		
8	G	11	Total	O	0	0
			11	11		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	15	Total 15	O 15	0	0
8	I	121	Total 121	O 121	0	0
8	J	28	Total 28	O 28	0	0
8	K	13	Total 13	O 13	0	0
8	L	8	Total 8	O 8	0	0
8	M	231	Total 231	O 231	0	0
8	N	24	Total 24	O 24	0	0
8	O	12	Total 12	O 12	0	0
8	P	5	Total 5	O 5	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: 5'-D(\*CP\*GP\*GP\*CP\*AP\*GP\*CP\*GP\*CP\*AP\*C)-3'

Chain B: 



- Molecule 1: 5'-D(\*CP\*GP\*GP\*CP\*AP\*GP\*CP\*GP\*CP\*AP\*C)-3'

Chain F: 



- Molecule 1: 5'-D(\*CP\*GP\*GP\*CP\*AP\*GP\*CP\*GP\*CP\*AP\*C)-3'

Chain J: 



- Molecule 1: 5'-D(\*CP\*GP\*GP\*CP\*AP\*GP\*CP\*GP\*CP\*AP\*C)-3'

Chain N: 



- Molecule 2: 5'-D(\*GP\*TP\*GP\*CP\*GP\*C)-3'

Chain C: 



- Molecule 2: 5'-D(\*GP\*TP\*GP\*CP\*GP\*C)-3'

Chain G: 



- Molecule 2: 5'-D(\*GP\*TP\*GP\*CP\*GP\*C)-3'



Chain K: 



- Molecule 2: 5'-D(\*GP\*TP\*GP\*CP\*GP\*C)-3'

Chain O: 



- Molecule 3: 5'-D(P\*GP\*CP\*CP\*G)-3'

Chain D: 



- Molecule 3: 5'-D(P\*GP\*CP\*CP\*G)-3'

Chain H: 



- Molecule 3: 5'-D(P\*GP\*CP\*CP\*G)-3'

Chain L: 



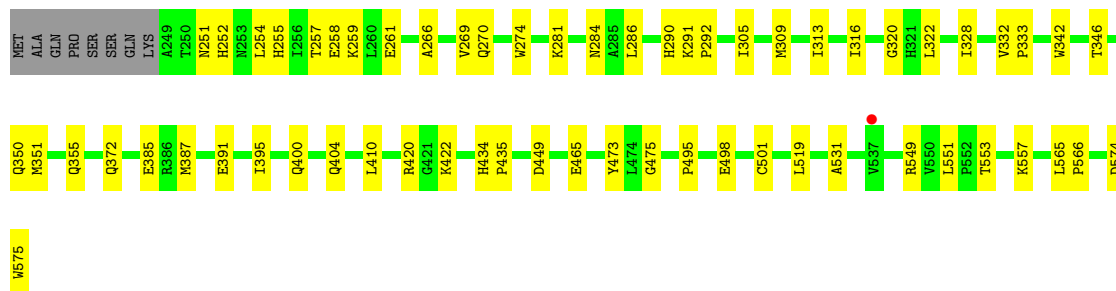
- Molecule 3: 5'-D(P\*GP\*CP\*CP\*G)-3'

Chain P: 



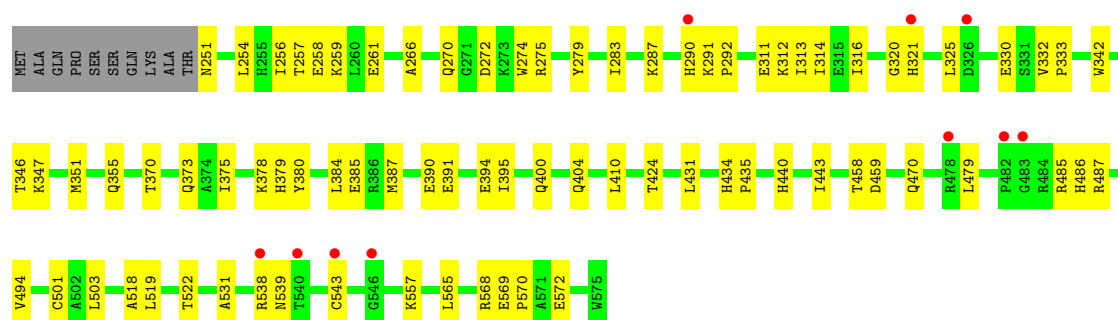
- Molecule 4: DNA polymerase lambda

Chain A: 



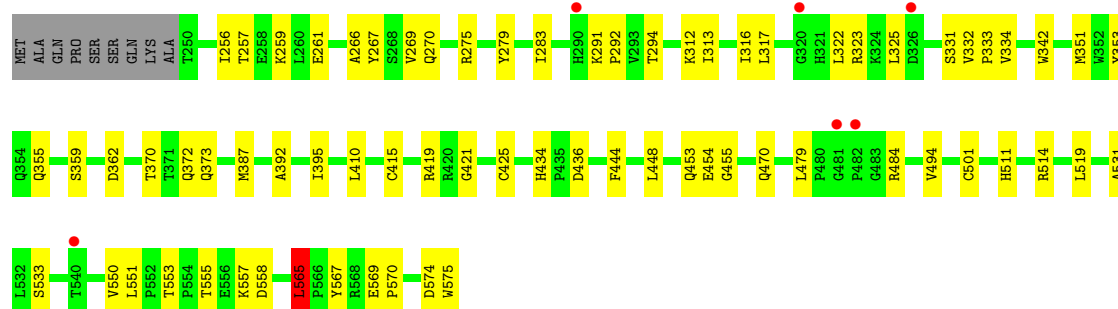
- Molecule 4: DNA polymerase lambda

Chain E: 



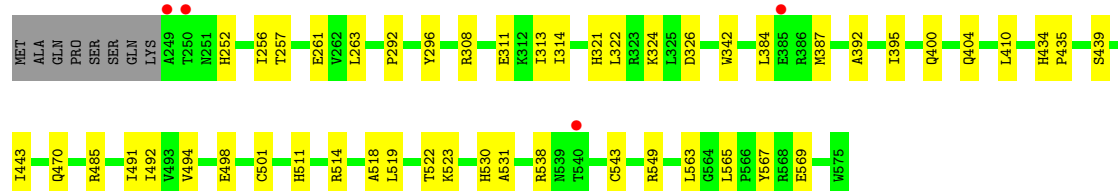
• Molecule 4: DNA polymerase lambda

Chain I:



• Molecule 4: DNA polymerase lambda

Chain M:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.50Å 98.81Å 104.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.47 – 2.30 28.47 – 2.28	Depositor EDS
% Data completeness (in resolution range)	93.2 (28.47-2.30) 92.2 (28.47-2.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.207 , 0.252 0.208 , 0.251	Depositor DCC
$R_{free}$ test set	4166 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 88029 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CAC, NA, MG

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	B	0.39	0/249	0.70	0/382
1	F	0.37	0/249	0.69	0/382
1	J	0.35	0/249	0.65	0/382
1	N	0.40	0/249	0.75	0/382
2	C	0.40	0/135	0.71	0/207
2	G	0.33	0/135	0.63	0/207
2	K	0.34	0/135	0.64	0/207
2	O	0.43	0/135	0.64	0/207
3	D	0.94	1/92 (1.1%)	0.74	0/138
3	H	0.97	1/92 (1.1%)	0.75	0/138
3	L	0.94	1/92 (1.1%)	0.70	0/138
3	P	0.94	1/92 (1.1%)	0.75	0/138
4	A	0.39	0/2631	0.60	0/3551
4	E	0.32	0/2575	0.56	0/3479
4	I	0.38	1/2583 (0.0%)	0.55	0/3491
4	M	0.37	0/2640	0.60	0/3563
All	All	0.40	5/12333 (0.0%)	0.60	0/16992

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
3	H	0	1
3	L	0	1
4	I	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	565	LEU	C-N	8.21	1.49	1.34
3	D	1	DG	OP3-P	-7.29	1.52	1.61
3	P	1	DG	OP3-P	-7.14	1.52	1.61
3	H	1	DG	OP3-P	-7.12	1.52	1.61
3	L	1	DG	OP3-P	-7.07	1.52	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	1	DG	Sidechain
4	I	565	LEU	Mainchain
3	L	1	DG	Sidechain

## 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	B	222	0	123	4	0
1	F	222	0	123	8	0
1	J	222	0	123	5	0
1	N	222	0	123	4	0
2	C	121	0	69	1	0
2	G	121	0	69	3	0
2	K	121	0	69	1	0
2	O	121	0	69	2	0
3	D	83	0	45	0	0
3	H	83	0	45	1	0
3	L	83	0	45	0	0
3	P	83	0	45	0	0
4	A	2577	0	2560	43	0
4	E	2522	0	2490	57	0
4	I	2532	0	2498	54	0
4	M	2586	0	2565	36	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
6	B	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	D	5	0	0	0	0
8	A	205	0	0	2	0
8	B	30	0	0	1	0
8	C	13	0	0	0	0
8	D	8	0	0	0	0
8	E	104	0	0	3	0
8	F	15	0	0	0	0
8	G	11	0	0	0	0
8	H	15	0	0	0	0
8	I	121	0	0	2	0
8	J	28	0	0	2	0
8	K	13	0	0	0	0
8	L	8	0	0	0	0
8	M	231	0	0	1	0
8	N	24	0	0	0	0
8	O	12	0	0	0	0
8	P	5	0	0	0	0
All	All	12778	0	11061	213	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 9.

All (213) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:470:GLN:HG3	4:E:494:VAL:HG12	1.49	0.93
4:M:410:LEU:HD11	4:M:443:ILE:HD13	1.52	0.90
4:M:470:GLN:HG2	4:M:494:VAL:HG12	1.53	0.88
4:I:470:GLN:HG2	4:I:494:VAL:HG12	1.57	0.87
4:E:539:ASN:HD21	4:E:543:CYS:HB2	1.41	0.85
4:E:410:LEU:HD11	4:E:443:ILE:HD13	1.60	0.83
4:A:387:MET:HE1	4:A:395:ILE:HD12	1.61	0.81
4:E:387:MET:HE2	4:E:391:GLU:HB3	1.63	0.80
4:A:519:LEU:HD13	4:A:565:LEU:HD11	1.64	0.79
4:E:539:ASN:ND2	4:E:543:CYS:HB2	1.96	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:291:LYS:HE2	4:E:292:PRO:O	1.85	0.76
4:I:533:SER:HB3	4:I:550:VAL:HA	1.69	0.75
4:A:252:HIS:HB3	4:A:292:PRO:HG3	1.68	0.74
4:I:351:MET:O	4:I:355:GLN:HG3	1.88	0.72
1:F:10:DA:H2''	1:F:11:DC:C5'	2.19	0.72
4:M:519:LEU:CD2	4:M:565:LEU:HD11	2.19	0.72
4:E:256:ILE:HD13	4:E:313:ILE:HG23	1.71	0.72
4:M:387:MET:HE1	4:M:392:ALA:HA	1.71	0.71
1:F:10:DA:H2''	1:F:11:DC:H5''	1.72	0.71
4:I:279:TYR:OH	4:I:312:LYS:HE2	1.90	0.71
4:A:346:THR:O	4:A:350:GLN:HG3	1.91	0.70
4:E:501:CYS:SG	4:E:531:ALA:HA	2.31	0.70
4:E:385:GLU:HG3	4:E:485:ARG:NH1	2.06	0.70
4:E:251:ASN:ND2	4:E:287:LYS:HG2	2.07	0.69
4:M:263:LEU:HD21	4:M:324:LYS:HD2	1.73	0.69
4:I:331:SER:O	4:I:334[A]:VAL:HG22	1.92	0.69
4:E:261:GLU:HG2	4:E:283:ILE:HD13	1.73	0.69
4:A:387:MET:CE	4:A:395:ILE:HD12	2.22	0.68
4:M:321[B]:HIS:NE2	4:M:326:ASP:OD2	2.27	0.68
4:M:519:LEU:HD22	4:M:565:LEU:HD11	1.76	0.68
4:M:387:MET:HE1	4:M:395:ILE:HD12	1.76	0.68
1:F:10:DA:C2'	1:F:11:DC:H5''	2.25	0.67
4:A:290:HIS:CD2	4:A:291:LYS:HG2	2.29	0.66
4:I:569:GLU:HG3	4:I:570:PRO:HD2	1.78	0.66
4:M:523:LYS:HE3	4:M:563:LEU:O	1.97	0.65
4:I:501:CYS:SG	4:I:531:ALA:HA	2.36	0.65
4:I:257:THR:O	4:I:261:GLU:HG3	1.95	0.65
4:A:291:LYS:HE2	4:A:292:PRO:O	1.97	0.65
4:M:387:MET:CE	4:M:395:ILE:HD12	2.28	0.63
4:E:330:GLU:O	4:E:333:PRO:HD2	1.99	0.63
4:E:519:LEU:HD22	4:E:565:LEU:HD11	1.81	0.62
4:I:470:GLN:CG	4:I:494:VAL:HG12	2.26	0.61
1:J:10:DA:H2''	1:J:11:DC:H5'	1.81	0.61
4:A:501:CYS:SG	4:A:531:ALA:HA	2.40	0.61
4:I:519:LEU:HD13	4:I:565:LEU:HD11	1.83	0.60
1:B:1:DC:H2'	1:B:2:DG:C8	2.37	0.60
4:A:286:LEU:HD21	4:A:313:ILE:HD13	1.84	0.60
4:A:259:LYS:HE3	4:A:320:GLY:O	2.02	0.59
4:E:569:GLU:HG3	4:E:570:PRO:HD2	1.84	0.59
4:A:266:ALA:O	4:A:270:GLN:HG3	2.03	0.59
4:I:266:ALA:O	4:I:270:GLN:HG3	2.03	0.59
1:J:10:DA:H2''	1:J:11:DC:C5'	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:I:279:TYR:O	4:I:283:ILE:HG13	2.04	0.58
4:M:470:GLN:CG	4:M:494:VAL:HG12	2.29	0.58
4:M:549:ARG:HG2	4:M:549:ARG:HH11	1.68	0.58
4:E:311:GLU:O	4:E:314:ILE:HG22	2.04	0.58
2:K:5:DG:H4'	4:I:342:TRP:CZ2	2.39	0.58
4:E:316:ILE:HG12	4:E:321:HIS:O	2.04	0.58
8:J:851:HOH:O	4:I:514:ARG:HD3	2.04	0.57
4:M:501:CYS:SG	4:M:531:ALA:HA	2.44	0.57
2:G:1:DG:H2'	2:G:2:DT:H72	1.87	0.57
4:I:470:GLN:HG2	4:I:494:VAL:CG1	2.34	0.57
4:I:370:THR:OG1	4:I:373:GLN:HG3	2.04	0.57
4:E:332:VAL:HB	4:E:333:PRO:HD3	1.87	0.56
4:E:257:THR:O	4:E:261:GLU:HG3	2.05	0.56
4:A:332:VAL:HB	4:A:333:PRO:HD3	1.87	0.56
4:I:261:GLU:HG2	4:I:283:ILE:HD13	1.87	0.56
1:F:10:DA:H1'	1:F:11:DC:H5''	1.87	0.56
4:M:511:HIS:ND1	4:M:514:ARG:NH2	2.53	0.56
4:I:479:LEU:O	4:I:484:ARG:HG3	2.05	0.56
4:M:321[B]:HIS:HD2	4:M:322:LEU:N	2.05	0.55
4:A:400:GLN:O	4:A:404:GLN:HG3	2.05	0.55
4:I:291:LYS:HE2	4:I:292:PRO:O	2.06	0.55
4:E:380:TYR:O	4:E:384:LEU:HD23	2.06	0.55
4:E:470:GLN:CG	4:E:494:VAL:HG12	2.29	0.55
4:E:519:LEU:CD2	4:E:565:LEU:HD11	2.35	0.55
4:A:351:MET:O	4:A:355:GLN:HG3	2.07	0.55
4:A:284:ASN:HB2	4:A:575:TRP:CZ2	2.41	0.55
1:J:6:DG:H2''	1:J:7:DC:OP2	2.05	0.55
4:A:251:ASN:HD21	4:A:254:LEU:HA	1.72	0.55
4:I:511:HIS:ND1	4:I:514:ARG:NH2	2.55	0.55
4:I:387:MET:HE1	4:I:392:ALA:HA	1.89	0.55
4:E:385:GLU:HG3	4:E:485:ARG:HH12	1.70	0.54
1:B:9:DC:H2'	1:B:10:DA:C8	2.42	0.54
4:M:387:MET:HE2	4:M:392:ALA:N	2.22	0.54
4:I:275:ARG:HH11	4:I:275:ARG:HB2	1.73	0.54
1:F:1:DC:H2''	1:F:2:DG:C8	2.42	0.53
4:E:266:ALA:O	4:E:270:GLN:HG3	2.09	0.53
4:E:538:ARG:HA	4:E:543:CYS:O	2.08	0.53
4:M:321[B]:HIS:CD2	4:M:322:LEU:N	2.76	0.53
4:M:485:ARG:HH11	4:M:485:ARG:HG3	1.74	0.53
8:J:494:HOH:O	4:I:372:GLN:HG3	2.09	0.52
2:G:1:DG:H2'	2:G:2:DT:C7	2.40	0.52
2:O:5:DG:H4'	4:M:342:TRP:CZ2	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:I:567:TYR:HE1	4:I:569:GLU:OE2	1.92	0.52
4:E:568:ARG:HG2	4:E:572:GLU:HB2	1.91	0.51
4:E:261:GLU:CG	4:E:283:ILE:HD13	2.40	0.51
4:E:390:GLU:O	4:E:394:GLU:HG3	2.11	0.51
4:E:378:LYS:HE2	4:E:379:HIS:CE1	2.46	0.51
1:J:10:DA:H1'	1:J:11:DC:H5''	1.91	0.51
4:I:275:ARG:NH1	4:I:275:ARG:HB2	2.25	0.51
4:M:470:GLN:HG2	4:M:494:VAL:CG1	2.34	0.50
4:A:269:VAL:O	4:A:346:THR:HG22	2.11	0.50
4:E:320:GLY:HA2	8:E:1060:HOH:O	2.11	0.50
1:N:1:DC:H2''	1:N:2:DG:C8	2.45	0.50
4:I:531:ALA:HB1	8:I:982:HOH:O	2.12	0.50
4:E:259:LYS:HB3	4:E:325:LEU:HD11	1.92	0.50
4:E:370:THR:HG23	4:E:373:GLN:OE1	2.10	0.50
4:M:256:ILE:HD13	4:M:313:ILE:HG23	1.94	0.50
4:A:305:ILE:HG23	4:A:309:MET:HB3	1.91	0.50
4:E:312:LYS:O	4:E:316:ILE:HG13	2.12	0.50
4:E:557:LYS:HG3	8:E:1020:HOH:O	2.12	0.50
4:I:387:MET:HE1	4:I:395:ILE:HD12	1.93	0.50
1:J:1:DC:H2''	1:J:2:DG:C8	2.47	0.49
4:I:259:LYS:HD2	4:I:316:ILE:HD13	1.93	0.49
4:E:290:HIS:CE1	4:E:291:LYS:HG2	2.48	0.49
4:A:519:LEU:CD1	4:A:565:LEU:HD11	2.41	0.49
1:N:6:DG:H2''	1:N:7:DC:OP2	2.11	0.49
4:A:251:ASN:ND2	4:A:254:LEU:HA	2.28	0.48
2:G:5:DG:H4'	4:E:342:TRP:CZ2	2.48	0.48
1:B:7:DC:H2'	1:B:8:DG:C8	2.47	0.48
4:A:557:LYS:HG3	8:A:1091:HOH:O	2.13	0.48
4:E:410:LEU:HD21	4:E:443:ILE:CD1	2.43	0.48
4:E:387:MET:HE1	4:E:395:ILE:HD12	1.96	0.48
1:F:10:DA:C1'	1:F:11:DC:H5''	2.45	0.47
4:A:254:LEU:HG	4:A:258:GLU:OE1	2.14	0.47
4:I:267:TYR:CZ	4:I:275:ARG:HD3	2.49	0.47
4:I:519:LEU:CD1	4:I:565:LEU:HD11	2.44	0.47
4:E:254:LEU:O	4:E:258:GLU:HG3	2.14	0.47
1:F:10:DA:H2''	1:F:11:DC:H5'	1.93	0.47
4:A:255[B]:HIS:HE1	4:A:320:GLY:O	1.98	0.47
4:E:272:ASP:OD2	4:E:275:ARG:NH1	2.47	0.47
4:A:387:MET:HE2	4:A:391:GLU:HB3	1.96	0.47
4:I:359:SER:O	4:I:362:ASP:HB2	2.13	0.47
4:E:351:MET:O	4:E:355:GLN:HG3	2.15	0.47
1:N:9:DC:H2''	1:N:10:DA:C8	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:486:HIS:O	4:E:487:ARG:HD3	2.15	0.47
4:E:400:GLN:O	4:E:404:GLN:HG3	2.13	0.47
4:M:498:GLU:HG2	4:M:530:HIS:O	2.13	0.47
4:M:257:THR:O	4:M:261:GLU:HB2	2.14	0.46
4:A:422:LYS:NZ	4:A:574:ASP:OD1	2.46	0.46
4:I:387:MET:CE	4:I:395:ILE:HD12	2.46	0.46
4:I:415:CYS:HA	4:I:419:ARG:HB2	1.96	0.46
1:N:7:DC:H2"	1:N:8:DG:C8	2.51	0.46
4:E:346:THR:HG23	4:E:347:LYS:N	2.30	0.46
4:E:394:GLU:HB2	4:E:479:LEU:HD11	1.98	0.46
4:I:294:THR:HA	4:I:317:LEU:HD21	1.98	0.46
4:I:551:LEU:O	4:I:553:THR:HG23	2.17	0.45
4:E:440:HIS:HA	4:E:443:ILE:HD12	1.97	0.45
4:A:316:ILE:HD11	4:A:322:LEU:HD22	1.98	0.45
4:E:370:THR:OG1	4:E:373:GLN:HG3	2.16	0.45
2:O:1:DG:C5	4:A:549:ARG:HD3	2.52	0.45
4:I:410:LEU:HD23	4:I:434:HIS:HB2	1.99	0.45
4:E:531:ALA:HB2	8:E:1014:HOH:O	2.17	0.45
4:E:431:LEU:HD23	4:E:503:LEU:HG	1.98	0.45
4:A:420:ARG:HH11	4:A:420:ARG:HG3	1.82	0.44
4:I:454:GLU:HG2	4:I:454:GLU:O	2.18	0.44
4:A:328:ILE:CG2	4:A:332:VAL:HG21	2.47	0.44
4:M:296:TYR:N	4:M:314:ILE:HD11	2.32	0.44
4:M:434:HIS:ND1	4:M:435:PRO:HD2	2.33	0.44
4:I:557:LYS:HD3	4:I:567:TYR:CD2	2.53	0.43
4:A:257:THR:O	4:A:261:GLU:HG3	2.18	0.43
4:I:332:VAL:HB	4:I:333:PRO:HD3	1.99	0.43
4:I:419:ARG:C	4:I:421:GLY:H	2.20	0.43
4:I:444:PHE:CZ	4:I:448:LEU:HD11	2.54	0.43
4:I:453:GLN:C	4:I:455:GLY:H	2.20	0.43
4:E:274:TRP:HA	4:E:274:TRP:CE3	2.54	0.43
4:I:555:THR:O	4:I:558:ASP:HB2	2.18	0.43
4:I:334[A]:VAL:HG21	4:I:353:TYR:CD2	2.53	0.43
4:E:458:THR:HG21	4:E:486:HIS:CD2	2.54	0.43
4:I:574:ASP:O	4:I:575:TRP:HB3	2.19	0.43
4:M:518:ALA:O	4:M:522:THR:HG23	2.19	0.43
4:E:387:MET:O	4:E:424:THR:HA	2.20	0.42
4:E:316:ILE:HA	4:E:321:HIS:O	2.19	0.42
4:M:252:HIS:HB3	4:M:292:PRO:HD3	2.01	0.42
4:I:322:LEU:HB3	4:I:325:LEU:HD12	2.00	0.42
4:E:391:GLU:O	4:E:395:ILE:HG13	2.20	0.42
4:M:567:TYR:HE1	4:M:569:GLU:OE2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:I:256:ILE:HD13	4:I:313:ILE:HG23	2.01	0.42
4:A:291:LYS:HB2	4:A:292:PRO:CD	2.50	0.42
4:I:436:ASP:C	4:I:436:ASP:OD1	2.57	0.42
4:M:400:GLN:O	4:M:404:GLN:HG3	2.19	0.42
4:E:279:TYR:OH	4:E:312:LYS:HE2	2.18	0.42
4:M:519:LEU:CD2	4:M:565:LEU:CD1	2.95	0.42
4:I:267:TYR:CE2	4:I:275:ARG:HD3	2.54	0.42
4:M:308:ARG:O	4:M:311[A]:GLU:HB2	2.19	0.42
4:M:538:ARG:HA	4:M:543:CYS:O	2.20	0.42
8:B:234:HOH:O	4:A:372:GLN:HG3	2.18	0.42
4:I:519:LEU:HD23	4:I:519:LEU:C	2.40	0.42
4:E:434:HIS:HA	4:E:435:PRO:HD3	1.91	0.41
4:A:281:LYS:HA	4:A:575:TRP:CH2	2.55	0.41
4:I:269:VAL:HG21	4:I:332:VAL:HG13	2.01	0.41
4:A:434:HIS:HA	4:A:435:PRO:HD3	1.91	0.41
4:I:387:MET:HG2	4:I:425:CYS:O	2.20	0.41
4:M:434:HIS:CD2	4:M:439:SER:HB2	2.55	0.41
4:I:322:LEU:O	4:I:323:ARG:C	2.57	0.41
4:M:384:LEU:HD23	4:M:384:LEU:HA	1.73	0.41
4:A:410:LEU:HD23	4:A:434:HIS:HB2	2.00	0.41
4:M:531:ALA:HB2	8:M:1052:HOH:O	2.21	0.41
4:A:519:LEU:HD23	4:A:519:LEU:C	2.41	0.41
4:I:557:LYS:HG2	8:I:1070:HOH:O	2.21	0.41
4:M:491:ILE:C	4:M:492:ILE:HG13	2.41	0.41
2:C:5:DG:H4'	4:A:342:TRP:CZ2	2.55	0.41
4:A:274:TRP:HB2	8:A:1143:HOH:O	2.20	0.41
1:F:6:DG:H2''	1:F:7:DC:OP2	2.21	0.41
4:A:565:LEU:HA	4:A:566:PRO:HD3	1.90	0.41
4:E:375:ILE:HD13	4:E:459:ASP:HB3	2.02	0.41
4:A:495:PRO:HG2	4:A:498:GLU:HG3	2.04	0.40
1:B:9:DC:H5'	4:A:465:GLU:HA	2.03	0.40
4:E:518:ALA:O	4:E:522:THR:HG23	2.22	0.40
4:A:551:LEU:O	4:A:553:THR:HG23	2.22	0.40
3:H:3:DC:H2''	3:H:4:DG:C8	2.57	0.40
4:A:473:TYR:CE2	4:A:475:GLY:HA3	2.56	0.40

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	
4	A	326/335 (97%)	313 (96%)	13 (4%)	0	100	100
4	E	323/335 (96%)	309 (96%)	14 (4%)	0	100	100
4	I	325/335 (97%)	307 (94%)	18 (6%)	0	100	100
4	M	327/335 (98%)	319 (98%)	8 (2%)	0	100	100
All	All	1301/1340 (97%)	1248 (96%)	53 (4%)	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	
4	A	273/281 (97%)	271 (99%)	2 (1%)	91	97
4	E	263/281 (94%)	263 (100%)	0	100	100
4	I	264/281 (94%)	264 (100%)	0	100	100
4	M	274/281 (98%)	274 (100%)	0	100	100
All	All	1074/1124 (96%)	1072 (100%)	2 (0%)	96	99

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	385	GLU
4	A	449	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	290	HIS
4	A	486	HIS
4	E	350	GLN
4	E	486	HIS
4	M	255	HIS

### 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 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	$\# Z  > 2$
7	CAC	D	950	-	4,4,4	6.62	3 (75%)	6,6,6	12.90	3 (50%)

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
7	CAC	D	950	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	950	CAC	O2-AS	-9.14	1.58	1.68
7	D	950	CAC	AS-C2	-9.04	1.76	1.90
7	D	950	CAC	AS-C1	3.12	1.95	1.90

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	950	CAC	O2-AS-O1	-31.18	105.81	112.54
7	D	950	CAC	O2-AS-C2	-4.36	105.58	109.15
7	D	950	CAC	C2-AS-C1	2.26	114.59	109.43

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	B	11/11 (100%)	-0.71	0 100 100	25, 31, 41, 44	0
1	F	11/11 (100%)	-0.58	0 100 100	39, 45, 52, 54	0
1	J	11/11 (100%)	-0.49	0 100 100	35, 41, 53, 57	0
1	N	11/11 (100%)	-0.63	0 100 100	25, 30, 41, 47	0
2	C	6/6 (100%)	-0.51	0 100 100	24, 26, 46, 48	0
2	G	6/6 (100%)	-0.57	0 100 100	40, 44, 59, 59	0
2	K	6/6 (100%)	-0.44	0 100 100	36, 36, 51, 53	0
2	O	6/6 (100%)	-0.52	0 100 100	23, 25, 39, 39	0
3	D	4/4 (100%)	-0.74	0 100 100	34, 34, 42, 43	0
3	H	4/4 (100%)	-0.41	0 100 100	44, 51, 52, 53	0
3	L	4/4 (100%)	-0.56	0 100 100	44, 49, 52, 55	0
3	P	4/4 (100%)	-0.59	0 100 100	33, 34, 39, 42	0
4	A	327/335 (97%)	-0.17	1 (0%) 91 96	18, 34, 65, 83	0
4	E	325/335 (97%)	0.02	10 (3%) 47 56	30, 49, 76, 91	0
4	I	326/335 (97%)	-0.07	6 (1%) 65 74	33, 47, 75, 91	0
4	M	327/335 (97%)	-0.25	4 (1%) 75 83	20, 32, 58, 81	1 (0%)
All	All	1389/1424 (97%)	-0.15	21 (1%) 68 78	18, 41, 71, 91	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	249	ALA	5.8
4	E	326	ASP	4.0
4	E	543	CYS	3.3
4	E	483	GLY	3.3
4	E	321	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
4	M	385	GLU	3.2
4	I	540	THR	3.1
4	E	546	GLY	3.1
4	E	290	HIS	3.0
4	E	538	ARG	2.6
4	M	540	THR	2.5
4	I	481	GLY	2.3
4	E	540	THR	2.3
4	E	482	PRO	2.3
4	I	482	PRO	2.2
4	M	250	THR	2.2
4	A	537	VAL	2.2
4	I	320	GLY	2.1
4	E	478	ARG	2.1
4	I	326	ASP	2.1
4	I	290	HIS	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
7	CAC	D	950	5/5	0.50	16.29	121,122,122,122	5
6	MG	F	992	1/1	0.16	4.43	50,50,50,50	0
5	NA	A	961	1/1	0.19	4.00	30,30,30,30	0
5	NA	I	963	1/1	0.17	3.35	53,53,53,53	0
5	NA	E	962	1/1	0.14	0.99	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NA	M	964	1/1	0.11	0.76	29,29,29,29	0
6	MG	H	993	1/1	0.08	-2.14	85,85,85,85	0
6	MG	B	991	1/1	0.07	-2.88	62,62,62,62	0
5	NA	N	966	1/1	0.06	-3.44	53,53,53,53	0
5	NA	J	965	1/1	0.04	-8.23	52,52,52,52	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.