



## Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:58 am BST

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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

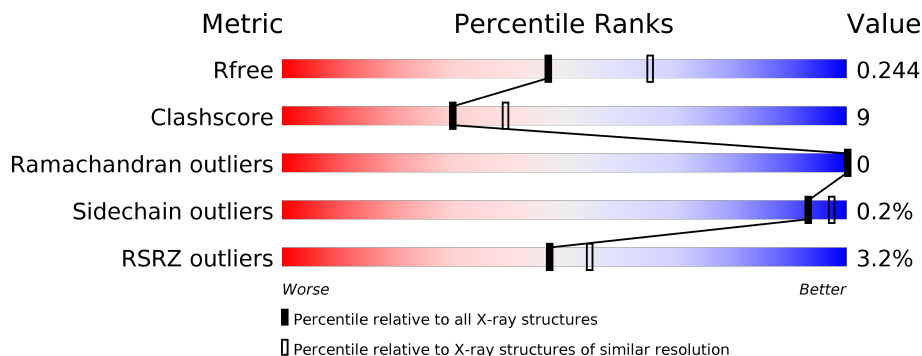
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.






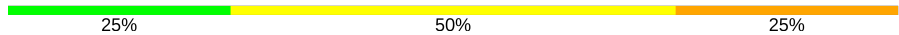






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	11	
1	F	11	
1	J	11	
1	N	11	
2	C	6	
2	G	6	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	K	6	 83% 17%
2	O	6	 67% 33%
3	D	4	 75% 25%
3	H	4	 25% 50% 25%
3	L	4	 75% 25%
3	P	4	 75% 25%
4	A	335	 2% 79% 18% •
4	E	335	 5% 73% 24% •
4	I	335	 4% 76% 21% •
4	M	335	 2% 83% 15% •

## 2 Entry composition [i](#)

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

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

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

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

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

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

- 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			

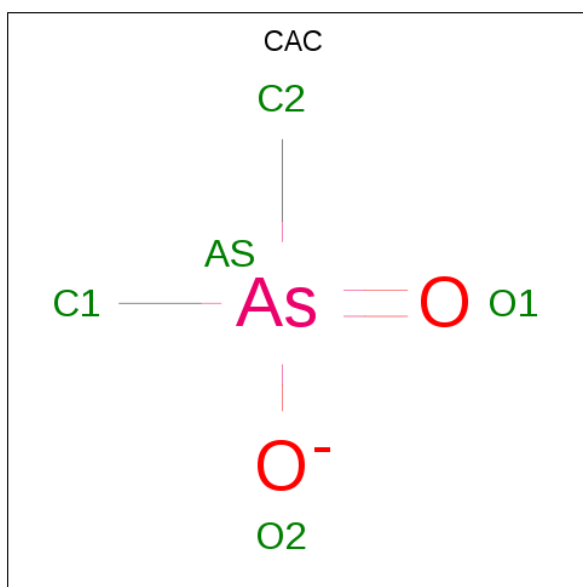
There are 4 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	B	30	30	30	0	0
8	C	13	13	13	0	0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	D	8	Total 8	O 8	0	0
8	F	15	Total 15	O 15	0	0
8	G	11	Total 11	O 11	0	0
8	H	15	Total 15	O 15	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	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
8	A	205	Total 205	O 205	0	0
8	E	104	Total 104	O 104	0	0
8	I	121	Total 121	O 121	0	0
8	M	231	Total 231	O 231	0	0

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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: 

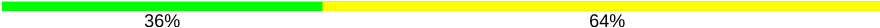


- Molecule 1: 5'-D(\*CP\*GP\*GP\*CP\*AP\*GP\*CP\*GP\*CP\*AP\*C)-3'

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: 83% 17%



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

Chain O: 67% 33%



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

Chain D: 75% 25%



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

Chain H: 25% 50% 25%



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

Chain L: 75% 25%



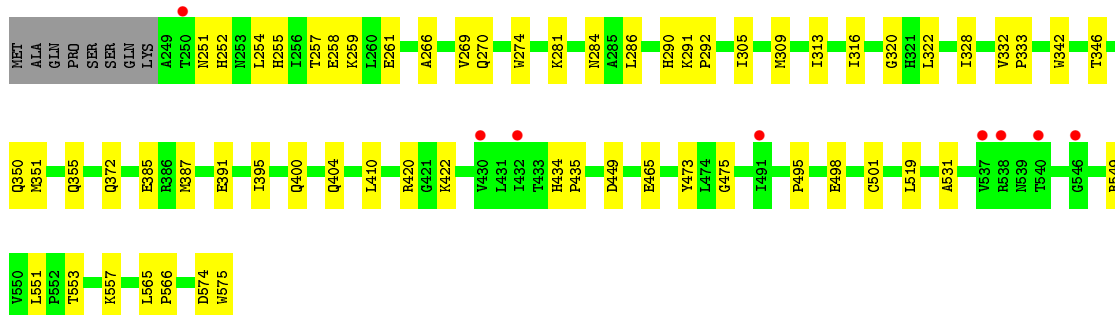
- Molecule 3: 5'-D(P\*GP\*CP\*CP\*G)-3'

Chain P: 75% 25%

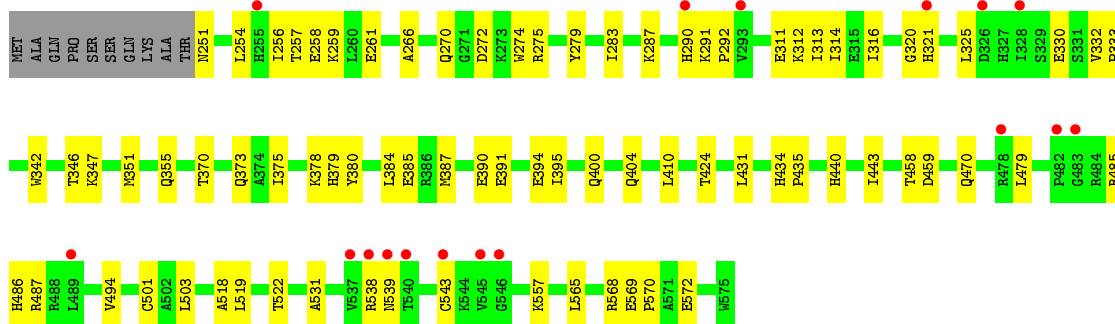


- Molecule 4: DNA polymerase lambda

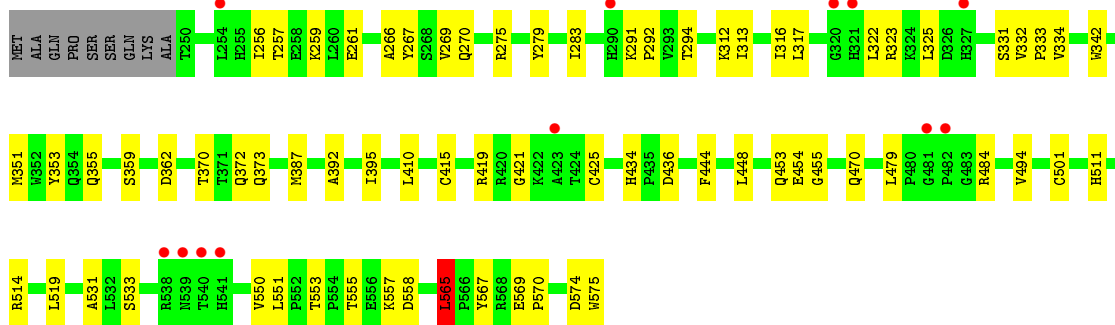
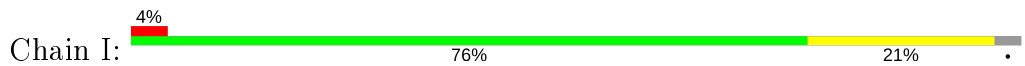
Chain A: 2% 79% 18%



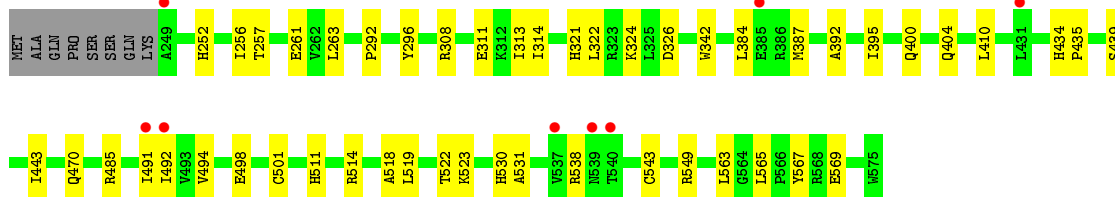
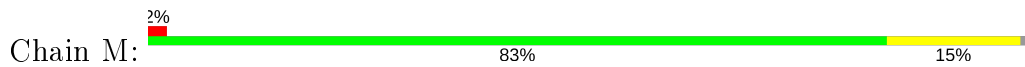
• Molecule 4: DNA polymerase lambda



• Molecule 4: DNA polymerase lambda



• Molecule 4: DNA polymerase lambda



## 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)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.207 , 0.252 0.197 , 0.244	Depositor DCC
$R_{free}$ test set	4378 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtrriage
Anisotropy	0.106	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage'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.

<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 [i](#)

### 5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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	B	1	0	0	0	0
5	F	1	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1	0	0	0	0
6	D	5	0	0	0	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	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

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 9.

All (213) 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)
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

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:539:ASN:ND2	4:E:543:CYS:HB2	1.96	0.79
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:387:MET:HE1	4:M:395:ILE:HD12	1.76	0.68
4:M:519:LEU:HD22	4:M:565:LEU:HD11	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:E:316:ILE:HG12	4:E:321:HIS:O	2.04	0.58
2:K:5:DG:H4'	4:I:342:TRP:CZ2	2.39	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:370:THR:OG1	4:I:373:GLN:HG3	2.04	0.57
4:I:470:GLN:HG2	4:I:494:VAL:CG1	2.34	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:A:400:GLN:O	4:A:404:GLN:HG3	2.05	0.55
4:M:321[B]:HIS:HD2	4:M:322:LEU:N	2.05	0.55
4:E:380:TYR:O	4:E:384:LEU:HD23	2.06	0.55
4:I:291:LYS:HE2	4:I:292:PRO:O	2.06	0.55
4:A:351:MET:O	4:A:355:GLN:HG3	2.07	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:251:ASN:HD21	4:A:254:LEU:HA	1.72	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: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
1:B:9:DC:H2'	1:B:10:DA:C8	2.42	0.54
4:E:385:GLU:HG3	4:E:485:ARG:HH12	1.70	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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:269:VAL:O	4:A:346:THR:HG22	2.11	0.50
4:M:470:GLN:HG2	4:M:494:VAL:CG1	2.34	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:A:305:ILE:HG23	4:A:309:MET:HB3	1.91	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: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
4:I:259:LYS:HD2	4:I:316:ILE:HD13	1.93	0.49
1:J:1:DC:H2''	1:J:2:DG:C8	2.47	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
4:A:557:LYS:HG3	8:A:1091:HOH:O	2.13	0.48
1:B:7:DC:H2'	1:B:8:DG:C8	2.47	0.48
2:G:5:DG:H4'	4:E:342:TRP:CZ2	2.48	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
4:A:254:LEU:HG	4:A:258:GLU:OE1	2.14	0.47
1:F:10:DA:C1'	1:F:11:DC:H5''	2.45	0.47
4:I:267:TYR:CZ	4:I:275:ARG:HD3	2.49	0.47
4:E:254:LEU:O	4:E:258:GLU:HG3	2.14	0.47
4:I:519:LEU:CD1	4:I:565:LEU:HD11	2.44	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:387:MET:HE2	4:A:391:GLU:HB3	1.96	0.47
4:E:351:MET:O	4:E:355:GLN:HG3	2.15	0.47
4:I:359:SER:O	4:I:362:ASP:HB2	2.13	0.47
1:N:9:DC:H2'	1:N:10:DA:C8	2.50	0.47
4:E:400:GLN:O	4:E:404:GLN:HG3	2.13	0.47
4:E:486:HIS:O	4:E:487:ARG:HD3	2.15	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
4:E:346:THR:HG23	4:E:347:LYS:N	2.30	0.46
1:N:7:DC:H2'	1:N:8:DG:C8	2.51	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:431:LEU:HD23	4:E:503:LEU:HG	1.98	0.45
4:E:531:ALA:HB2	8:E:1014:HOH:O	2.17	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: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:557:LYS:HD3	4:I:567:TYR:CD2	2.53	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:E:458:THR:HG21	4:E:486:HIS:CD2	2.54	0.43
4:I:334[A]:VAL:HG21	4:I:353:TYR:CD2	2.53	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:316:ILE:HA	4:E:321:HIS:O	2.19	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:387:MET:O	4:E:424:THR:HA	2.20	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
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: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:519:LEU:CD2	4:M:565:LEU:CD1	2.95	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:A:434:HIS:HA	4:A:435:PRO:HD3	1.91	0.41
4:I:269:VAL:HG21	4:I:332:VAL:HG13	2.01	0.41
4:I:322:LEU:O	4:I:323:ARG:C	2.57	0.41
4:I:387:MET:HG2	4:I:425:CYS:O	2.20	0.41
4:M:384:LEU:HD23	4:M:384:LEU:HA	1.73	0.41
4:M:434:HIS:CD2	4:M:439:SER:HB2	2.55	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:274:TRP:HB2	8:A:1143:HOH:O	2.20	0.41
2:C:5:DG:H4'	4:A:342:TRP:CZ2	2.55	0.41
4:M:491:ILE:C	4:M:492:ILE:HG13	2.41	0.41
4:A:519:LEU:HD23	4:A:519:LEU:C	2.41	0.41
1:F:6:DG:H2''	1:F:7:DC:OP2	2.21	0.41
4:I:557:LYS:HG2	8:I:1070:HOH:O	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
4:A:551:LEU:O	4:A:553:THR:HG23	2.22	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
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 [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	
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 [i](#)

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%)	84	92
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%)	93	97

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 [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 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	$\# Z  > 2$
6	CAC	D	950	-	0,4,4	0.00	-	0,6,6	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.72	0	100 100	25, 31, 41, 44	0
1	F	11/11 (100%)	-0.33	0	100 100	39, 45, 52, 54	0
1	J	11/11 (100%)	-0.33	0	100 100	35, 41, 53, 57	0
1	N	11/11 (100%)	-0.55	0	100 100	25, 30, 41, 47	0
2	C	6/6 (100%)	-0.38	0	100 100	24, 26, 46, 48	0
2	G	6/6 (100%)	-0.43	0	100 100	40, 44, 59, 59	0
2	K	6/6 (100%)	-0.23	0	100 100	36, 36, 51, 53	0
2	O	6/6 (100%)	-0.44	0	100 100	23, 25, 39, 39	0
3	D	4/4 (100%)	-0.71	0	100 100	34, 34, 42, 43	0
3	H	4/4 (100%)	-0.21	0	100 100	44, 51, 52, 53	0
3	L	4/4 (100%)	-0.60	0	100 100	44, 49, 52, 55	0
3	P	4/4 (100%)	-0.57	0	100 100	33, 34, 39, 42	0
4	A	327/335 (97%)	-0.07	8 (2%)	59 66	18, 34, 65, 83	0
4	E	325/335 (97%)	0.24	17 (5%)	27 34	30, 49, 76, 91	0
4	I	326/335 (97%)	0.13	12 (3%)	41 48	33, 47, 75, 91	0
4	M	327/335 (97%)	-0.14	8 (2%)	59 66	20, 32, 58, 81	1 (0%)
All	All	1389/1424 (97%)	0.01	45 (3%)	47 54	18, 41, 71, 91	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	249	ALA	7.0
4	E	326	ASP	4.6
4	I	540	THR	4.4
4	E	290	HIS	4.2
4	E	321	HIS	4.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	E	483	GLY	3.9
4	E	543	CYS	3.8
4	I	541	HIS	3.6
4	M	540	THR	3.1
4	E	546	GLY	2.9
4	E	545	VAL	2.8
4	A	250	THR	2.8
4	M	385	GLU	2.8
4	M	492	ILE	2.8
4	I	320	GLY	2.7
4	I	254	LEU	2.7
4	E	255	HIS	2.7
4	I	481	GLY	2.6
4	I	290	HIS	2.6
4	E	540	THR	2.5
4	A	430	VAL	2.5
4	I	482	PRO	2.5
4	E	538	ARG	2.5
4	A	537	VAL	2.5
4	I	538	ARG	2.5
4	I	539	ASN	2.4
4	A	491	ILE	2.4
4	E	478	ARG	2.4
4	M	539	ASN	2.3
4	I	321	HIS	2.3
4	I	327	HIS	2.3
4	A	538	ARG	2.2
4	E	293	VAL	2.2
4	E	489	LEU	2.2
4	E	537	VAL	2.1
4	E	539	ASN	2.1
4	A	540	THR	2.1
4	M	431	LEU	2.1
4	M	491	ILE	2.1
4	M	537	VAL	2.1
4	E	482	PRO	2.1
4	A	432	ILE	2.1
4	I	423	ALA	2.0
4	A	546	GLY	2.0
4	E	328	ILE	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	B	991	1/1	0.26	0.09	62,62,62,62	0
7	NA	I	963	1/1	0.55	0.16	53,53,53,53	0
7	NA	N	966	1/1	0.85	0.06	53,53,53,53	0
7	NA	J	965	1/1	0.85	0.05	52,52,52,52	0
7	NA	E	962	1/1	0.86	0.18	55,55,55,55	0
5	MG	F	992	1/1	0.88	0.16	50,50,50,50	0
5	MG	H	993	1/1	0.88	0.09	85,85,85,85	0
7	NA	A	961	1/1	0.89	0.23	30,30,30,30	0
6	CAC	D	950	5/5	0.92	0.54	121,122,122,122	5
7	NA	M	964	1/1	0.96	0.12	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.