



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 01:48 PM EDT

PDB ID : 2KZM  
Title : KLENOW FRAGMENT WITH NORMAL SUBSTRATE AND ZINC AND MANGANESE  
Authors : Brautigam, C.A.; Sun, S.; Piccirilli, J.A.; Steitz, T.A.  
Deposited on : 1998-07-03  
Resolution : 2.60 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.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

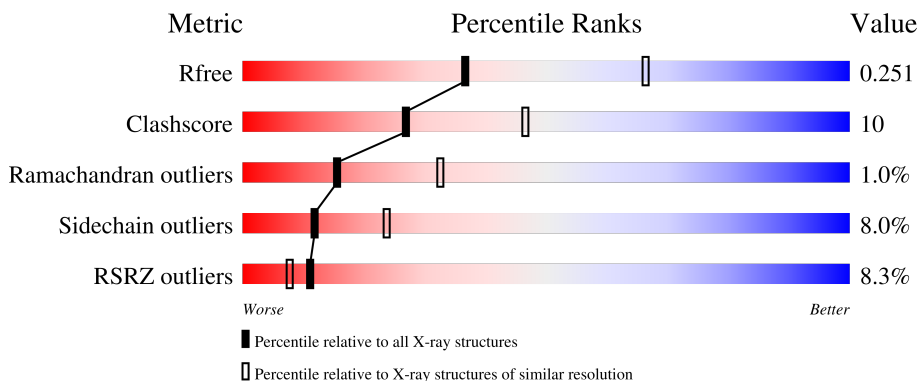
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of 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	8	
2	A	605	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4895 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 DNA (5'-D(\*GP\*CP\*TP\*TP\*A\*CP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	3	42	19	8	13	2	0	0	1

- Molecule 2 is a protein called PROTEIN (DNA POLYMERASE I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	601	4753	3008	830	899	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	MET	VAL	engineered mutation	UNP P00582

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	B	1	1	1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	2	2	2	0	0

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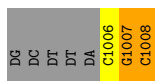
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	96	Total	O	0	0
			96	96		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

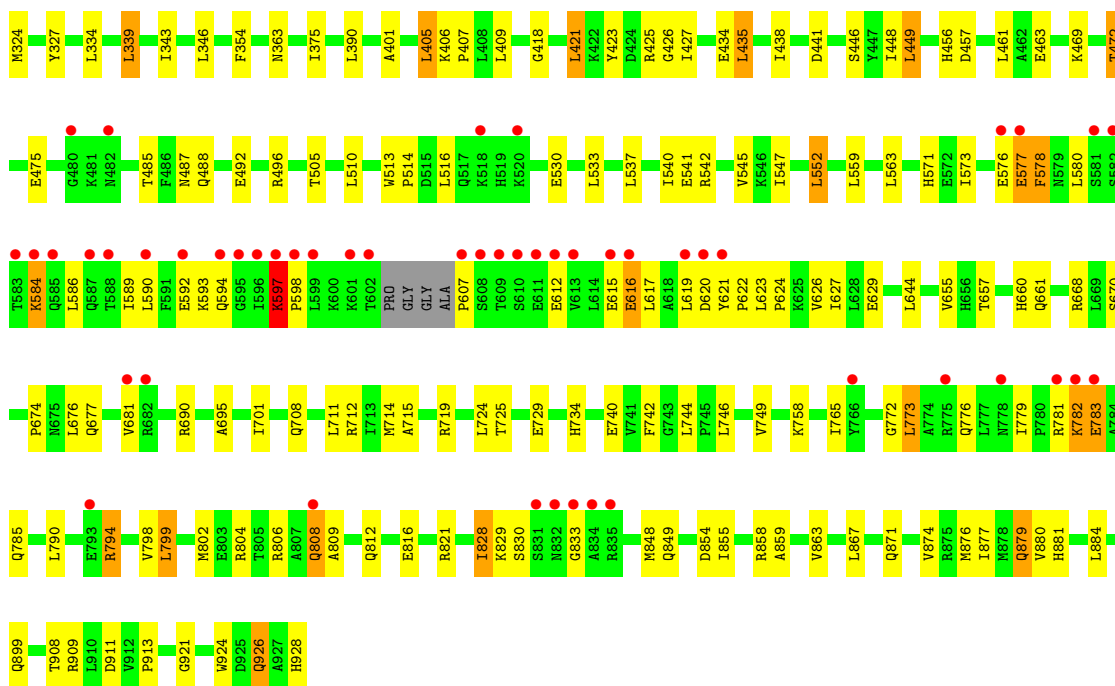
- Molecule 1: DNA (5'-D(\*GP\*CP\*TP\*TP\*A\*CP\*GP\*C)-3')

Chain B: 



- Molecule 2: PROTEIN (DNA POLYMERASE I)

Chain A: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.60Å 102.60Å 86.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-2.60) 85.9 (19.96-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 2.59Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.195 , 0.243 0.205 , 0.251	Depositor DCC
$R_{free}$ test set	2016 reflections (8.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtrriage
Anisotropy	0.176	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 70.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: ZN, MN

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	7.47	11/46 (23.9%)	5.29	24/70 (34.3%)
2	A	0.40	0/4839	0.66	2/6547 (0.0%)
All	All	0.83	11/4885 (0.2%)	0.85	26/6617 (0.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1006	DC	O3'-P	-31.66	1.23	1.61
1	B	1007	DG	C2'-C1'	28.17	1.80	1.52
1	B	1007	DG	N7-C5	-10.11	1.33	1.39
1	B	1007	DG	O4'-C1'	-9.86	1.30	1.42
1	B	1007	DG	P-O5'	9.61	1.69	1.59
1	B	1007	DG	C5-C6	-9.35	1.33	1.42
1	B	1007	DG	N1-C2	8.94	1.45	1.37
1	B	1007	DG	N9-C4	-8.07	1.31	1.38
1	B	1008	DC	N3-C4	-5.84	1.29	1.33
1	B	1007	DG	C2-N2	5.51	1.40	1.34
1	B	1007	DG	O3'-P	-5.22	1.54	1.61

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1007	DG	O4'-C1'-N9	16.51	119.56	108.00
1	B	1006	DC	O3'-P-O5'	-12.04	81.12	104.00
1	B	1008	DC	N3-C2-O2	-11.43	113.90	121.90
1	B	1007	DG	C6-C5-N7	-11.28	123.63	130.40
1	B	1007	DG	O4'-C4'-C3'	10.39	112.23	106.00
1	B	1007	DG	O4'-C1'-C2'	-9.37	98.40	105.90
1	B	1008	DC	N1-C2-N3	9.34	125.74	119.20
1	B	1008	DC	C6-N1-C2	-9.11	116.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1007	DG	N1-C6-O6	8.33	124.90	119.90
1	B	1007	DG	C2-N3-C4	-8.24	107.78	111.90
1	B	1007	DG	P-O3'-C3'	7.53	128.74	119.70
1	B	1007	DG	N3-C4-C5	7.31	132.25	128.60
2	A	597	LYS	N-CA-C	7.26	130.61	111.00
1	B	1007	DG	C1'-O4'-C4'	7.07	117.17	110.10
1	B	1007	DG	C4-C5-C6	6.81	122.89	118.80
1	B	1007	DG	C4-C5-N7	6.69	113.47	110.80
1	B	1007	DG	C4'-C3'-C2'	-6.55	97.21	103.10
1	B	1007	DG	C8-N9-C1'	6.47	135.41	127.00
1	B	1007	DG	C5-C6-N1	-6.43	108.28	111.50
1	B	1008	DC	C4'-C3'-C2'	-6.40	97.34	103.10
1	B	1007	DG	C4-N9-C1'	-6.35	118.25	126.50
1	B	1006	DC	OP1-P-O3'	6.28	119.02	105.20
2	A	607	PRO	N-CA-CB	5.70	110.14	103.30
1	B	1007	DG	C5-N7-C8	-5.60	101.50	104.30
1	B	1008	DC	C4-C5-C6	5.54	120.17	117.40
1	B	1008	DC	C2-N3-C4	-5.42	117.19	119.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	42	0	23	4	0
2	A	4753	0	4753	94	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	96	0	0	1	0
5	B	2	0	0	1	0
All	All	4895	0	4776	98	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 10.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:DG:C1'	1:B:1007:DG:C2'	1.80	1.54
2:A:855:ILE:HG23	2:A:908:THR:HG21	1.66	0.76
2:A:472:THR:HG22	2:A:475:GLU:HG3	1.68	0.75
2:A:740:GLU:HB3	2:A:794:ARG:HG2	1.67	0.75
2:A:677:GLN:HE21	2:A:881:HIS:H	1.33	0.73
2:A:485:THR:H	2:A:488:GLN:HE21	1.35	0.72
2:A:921:GLY:HA3	2:A:926:GLN:HB3	1.72	0.71
2:A:681:VAL:HA	2:A:690:ARG:HH21	1.56	0.70
1:B:1007:DG:N7	5:B:102:HOH:O	2.24	0.70
1:B:1008:DC:H5	5:A:101:HOH:O	1.75	0.69
2:A:363:ASN:HD22	2:A:542:ARG:HH11	1.39	0.68
2:A:677:GLN:HG2	2:A:880:VAL:HG23	1.76	0.67
2:A:677:GLN:NE2	2:A:881:HIS:H	1.93	0.67
2:A:363:ASN:ND2	2:A:542:ARG:HH11	1.93	0.66
2:A:435:LEU:HD13	2:A:438:ILE:HG12	1.78	0.66
2:A:448:ILE:HD11	2:A:530:GLU:HG3	1.77	0.66
2:A:772:GLY:O	2:A:776:GLN:HG2	1.95	0.65
1:B:1007:DG:C2'	1:B:1007:DG:N9	2.58	0.64
2:A:808:GLN:O	2:A:812:GLN:HG2	1.97	0.64
2:A:712:ARG:HD3	2:A:913:PRO:O	1.99	0.63
2:A:714:MET:HB2	2:A:848:MET:SD	2.40	0.61
2:A:802:MET:O	2:A:806:ARG:HG3	2.01	0.61
2:A:623:LEU:O	2:A:626:VAL:HG22	2.01	0.60
2:A:782:LYS:HA	2:A:785:GLN:HB3	1.85	0.58
2:A:586:LEU:HD22	2:A:627:ILE:HD13	1.85	0.57
2:A:798:VAL:O	2:A:802:MET:HG3	2.04	0.57
2:A:513:TRP:HB3	2:A:514:PRO:HD3	1.86	0.56
2:A:418:GLY:HA3	2:A:421:LEU:HD13	1.88	0.56
2:A:449:LEU:HD13	2:A:516:LEU:HG	1.88	0.54
2:A:657:THR:HB	2:A:674:PRO:HD2	1.90	0.54
2:A:472:THR:HG22	2:A:475:GLU:CG	2.36	0.53
2:A:537:LEU:O	2:A:541:GLU:HG3	2.09	0.53
2:A:715:ALA:HB1	2:A:724:LEU:HD12	1.91	0.52
2:A:324:MET:HA	2:A:324:MET:CE	2.41	0.51
2:A:545:VAL:HG23	2:A:877:ILE:HD12	1.94	0.50
2:A:746:LEU:O	2:A:749:VAL:HG12	2.11	0.50
2:A:858:ARG:HB2	2:A:908:THR:HG23	1.93	0.50
2:A:571:HIS:CE1	2:A:577:GLU:HG3	2.47	0.50
2:A:668:ARG:HE	2:A:849:GLN:HG3	1.77	0.49
2:A:423:TYR:O	2:A:427:ILE:HG12	2.13	0.49
2:A:446:SER:OG	2:A:456:HIS:HD2	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:597:LYS:HG3	2:A:598:PRO:HD3	1.93	0.49
2:A:711:LEU:HD13	2:A:765:ILE:HD11	1.95	0.49
2:A:418:GLY:HA3	2:A:421:LEU:CD1	2.43	0.49
2:A:828:ILE:HG23	2:A:829:LYS:HE2	1.95	0.48
2:A:463:GLU:OE2	2:A:469:LYS:HE2	2.13	0.48
2:A:617:LEU:O	2:A:621:TYR:HB2	2.13	0.48
2:A:677:GLN:HE21	2:A:881:HIS:N	2.07	0.48
2:A:854:ASP:O	2:A:858:ARG:HG3	2.12	0.48
2:A:725:THR:O	2:A:729:GLU:HG2	2.13	0.48
2:A:418:GLY:O	2:A:441:ASP:HA	2.13	0.48
2:A:779:ILE:HD12	2:A:783:GLU:HG3	1.96	0.48
2:A:612:GLU:HB3	2:A:615:GLU:HG2	1.95	0.48
2:A:740:GLU:HB3	2:A:794:ARG:CG	2.41	0.47
2:A:809:ALA:HB1	2:A:828:ILE:HD13	1.97	0.47
2:A:559:LEU:O	2:A:563:LEU:HG	2.15	0.47
2:A:660:HIS:HB2	2:A:670:SER:OG	2.14	0.47
2:A:573:ILE:HG21	2:A:623:LEU:HB2	1.97	0.47
2:A:327:TYR:CD1	2:A:492:GLU:HB3	2.50	0.47
2:A:418:GLY:HA2	2:A:505:THR:HG21	1.97	0.47
2:A:547:ILE:HD12	2:A:655:VAL:HG21	1.97	0.47
2:A:808:GLN:OE1	2:A:812:GLN:NE2	2.48	0.47
2:A:623:LEU:N	2:A:624:PRO:HD2	2.31	0.46
2:A:339:LEU:HD22	2:A:343:ILE:HG13	1.97	0.46
2:A:734:HIS:CD2	2:A:758:LYS:HA	2.50	0.46
2:A:681:VAL:HA	2:A:690:ARG:NH2	2.27	0.46
2:A:859:ALA:O	2:A:863:VAL:HG23	2.16	0.45
2:A:401:ALA:O	2:A:405:LEU:HB2	2.16	0.45
2:A:879:GLN:HG2	2:A:884:LEU:HD23	1.97	0.45
2:A:589:ILE:O	2:A:593:LYS:HG2	2.16	0.44
2:A:540:ILE:HD11	2:A:876:MET:SD	2.58	0.44
2:A:781:ARG:C	2:A:783:GLU:H	2.22	0.43
2:A:899:GLN:NE2	2:A:899:GLN:HA	2.34	0.43
2:A:571:HIS:HD2	2:A:578:PHE:CE1	2.37	0.42
2:A:406:LYS:HB3	2:A:407:PRO:HD3	2.00	0.42
2:A:492:GLU:O	2:A:496:ARG:HG3	2.19	0.42
2:A:719:ARG:CZ	2:A:804:ARG:HH12	2.32	0.42
2:A:590:LEU:HD23	2:A:623:LEU:HD23	2.01	0.42
2:A:773:LEU:HD22	2:A:773:LEU:O	2.19	0.42
2:A:584:LYS:HD2	2:A:584:LYS:HA	1.85	0.41
2:A:909:ARG:HB3	2:A:911:ASP:OD1	2.19	0.41
2:A:580:LEU:HD22	2:A:580:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:552:LEU:HD12	2:A:552:LEU:HA	1.95	0.41
2:A:449:LEU:HD12	2:A:449:LEU:HA	1.86	0.41
2:A:487:ASN:HD22	2:A:487:ASN:H	1.69	0.41
2:A:674:PRO:HG2	2:A:676:LEU:CD1	2.51	0.41
2:A:487:ASN:H	2:A:487:ASN:ND2	2.18	0.41
2:A:597:LYS:CG	2:A:598:PRO:HD3	2.51	0.41
2:A:457:ASP:O	2:A:461:LEU:HG	2.20	0.41
2:A:782:LYS:N	2:A:782:LYS:HD2	2.36	0.41
2:A:799:LEU:HD23	2:A:799:LEU:HA	1.85	0.41
2:A:533:LEU:HD23	2:A:661:GLN:NE2	2.36	0.40
2:A:924:TRP:O	2:A:928:HIS:HB2	2.21	0.40
2:A:363:ASN:HD21	2:A:426:GLY:HA3	1.86	0.40
2:A:742:PHE:HB2	2:A:744:LEU:HD21	2.03	0.40
2:A:485:THR:OG1	2:A:487:ASN:ND2	2.54	0.40
2:A:616:GLU:O	2:A:619:LEU:HD23	2.21	0.40
2:A:695:ALA:HB2	2:A:701:ILE:HG12	2.03	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
2	A	597/605 (99%)	555 (93%)	36 (6%)	6 (1%)	15 32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	597	LYS
2	A	576	GLU
2	A	830	SER
2	A	594	GLN
2	A	622	PRO

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Mol	Chain	Res	Type
2	A	833	GLY

### 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
2	A	500/510 (98%)	460 (92%)	40 (8%)	12 24

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	334	LEU
2	A	339	LEU
2	A	346	LEU
2	A	354	PHE
2	A	375	ILE
2	A	390	LEU
2	A	405	LEU
2	A	409	LEU
2	A	421	LEU
2	A	425	ARG
2	A	434	GLU
2	A	435	LEU
2	A	449	LEU
2	A	472	THR
2	A	510	LEU
2	A	552	LEU
2	A	577	GLU
2	A	578	PHE
2	A	584	LYS
2	A	592	GLU
2	A	616	GLU
2	A	620	ASP
2	A	629	GLU
2	A	644	LEU
2	A	708	GLN

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Mol	Chain	Res	Type
2	A	773	LEU
2	A	782	LYS
2	A	783	GLU
2	A	790	LEU
2	A	794	ARG
2	A	799	LEU
2	A	808	GLN
2	A	816	GLU
2	A	821	ARG
2	A	828	ILE
2	A	867	LEU
2	A	871	GLN
2	A	874	VAL
2	A	879	GLN
2	A	926	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	363	ASN
2	A	456	HIS
2	A	487	ASN
2	A	488	GLN
2	A	543	ASN
2	A	571	HIS
2	A	677	GLN
2	A	708	GLN
2	A	734	HIS
2	A	776	GLN
2	A	845	ASN
2	A	899	GLN
2	A	906	ASN
2	A	926	GLN

### 5.3.3 RNA

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1006:DC	O3'	1007:DG	P	1.23

## 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	3/8 (37%)	-0.82	0 <b>100</b> <b>100</b>	28, 28, 51, 53	0
2	A	601/605 (99%)	-0.01	50 (8%) <b>11</b> <b>8</b>	14, 36, 97, 100	0
All	All	604/613 (98%)	-0.02	50 (8%) <b>11</b> <b>8</b>	14, 36, 97, 100	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	607	PRO	11.7
2	A	583	THR	11.1
2	A	608	SER	10.5
2	A	602	THR	9.0
2	A	582	SER	8.3
2	A	610	SER	7.9
2	A	598	PRO	6.9
2	A	581	SER	6.8
2	A	609	THR	6.8
2	A	576	GLU	6.1
2	A	619	LEU	5.9
2	A	620	ASP	5.5
2	A	594	GLN	5.5
2	A	597	LYS	5.1
2	A	611	GLU	4.9
2	A	596	ILE	4.9
2	A	577	GLU	4.8
2	A	781	ARG	4.4
2	A	588	THR	4.4
2	A	682	ARG	4.3
2	A	621	TYR	4.3
2	A	585	GLN	3.7
2	A	584	LYS	3.6
2	A	775	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
2	A	681	VAL	3.5
2	A	778	ASN	3.4
2	A	590	LEU	3.4
2	A	615	GLU	3.4
2	A	616	GLU	3.2
2	A	833	GLY	3.2
2	A	587	GLN	3.1
2	A	834	ALA	3.0
2	A	599	LEU	3.0
2	A	482	ASN	3.0
2	A	835	ARG	2.9
2	A	601	LYS	2.8
2	A	592	GLU	2.7
2	A	518	LYS	2.6
2	A	782	LYS	2.6
2	A	831	SER	2.5
2	A	832	ASN	2.4
2	A	766	TYR	2.3
2	A	808	GLN	2.3
2	A	613	VAL	2.2
2	A	595	GLY	2.1
2	A	793	GLU	2.1
2	A	520	LYS	2.1
2	A	480	GLY	2.1
2	A	612	GLU	2.1
2	A	783	GLU	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 monosaccharides 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
3	MN	B	2	1/1	0.94	0.08	69,69,69,69	0
4	ZN	A	1	1/1	1.00	0.08	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.