



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:56 AM UTC

PDB ID : 2KZZ / pdb_00002kzz
Title : KLENOW FRAGMENT WITH NORMAL SUBSTRATE AND ZINC ONLY
Authors : Brautigam, C.A.; Sun, S.; Piccirilli, J.A.; Steitz, T.A.
Deposited on : 1998-07-07
Resolution : 2.25 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

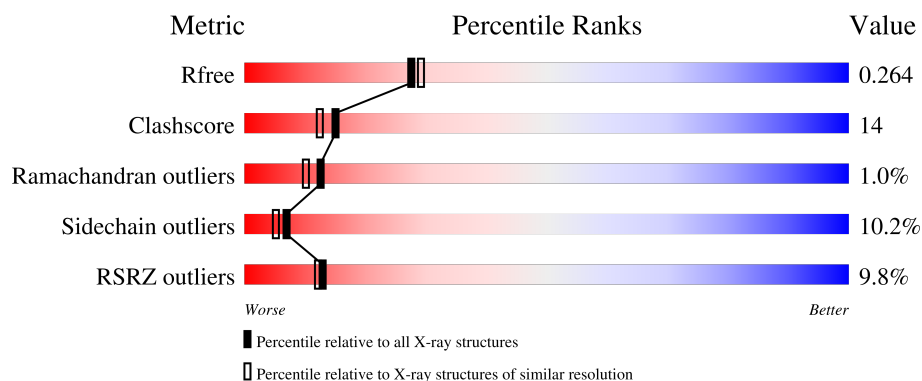
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 ≥ 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	7	
2	A	605	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5001 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*T*AP*CP*G)-3').

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

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

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

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 ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is water.

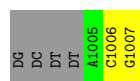
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	A	202	Total	O	0	0
			202	202		

3 Residue-property plots

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.

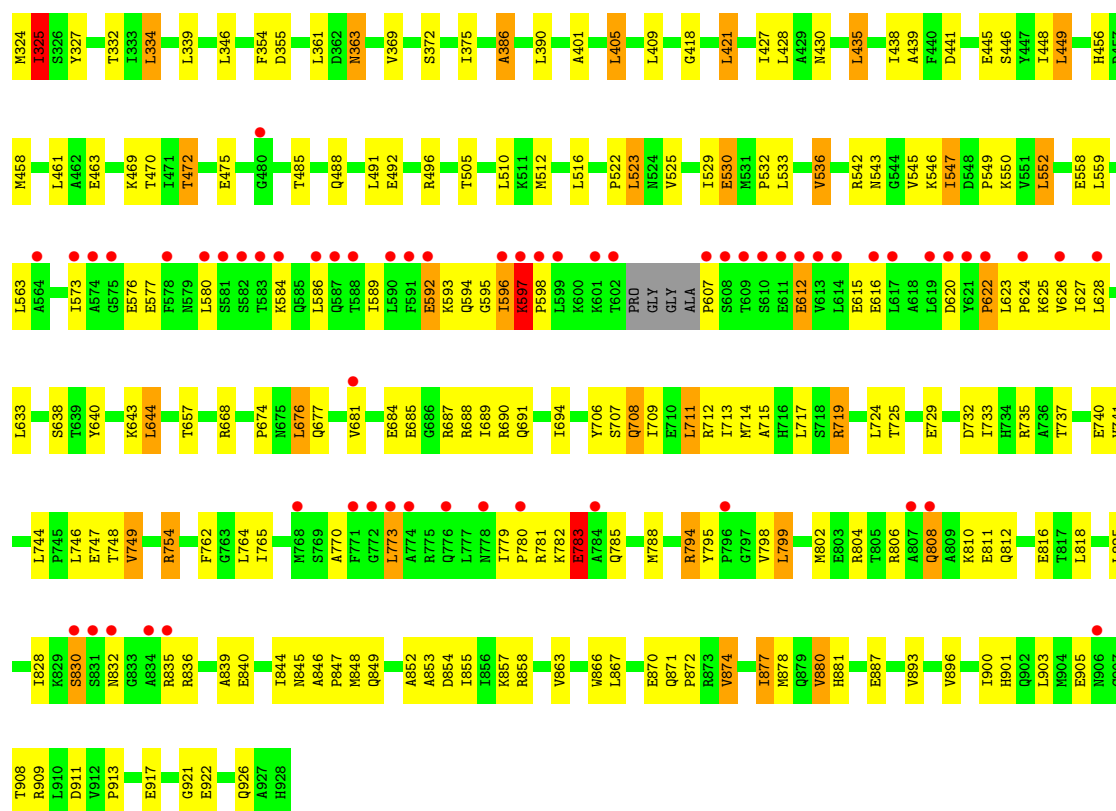
- Molecule 1: DNA (5'-D(*GP*CP*TP*T*AP*CP*G)-3')

Chain B: 



- Molecule 2: PROTEIN (DNA POLYMERASE I)

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	101.70Å 101.70Å 85.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	84.4 (20.00-2.25) 80.6 (20.00-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.26Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.202 , 0.251 0.217 , 0.264	Depositor DCC
R_{free} test set	2491 reflections (7.13%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5001	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.31	1/46 (2.2%)	2.00	2/70 (2.9%)
2	A	0.59	0/4839	1.07	22/6547 (0.3%)
All	All	0.60	1/4885 (0.0%)	1.09	24/6617 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1006	DC	O3'-P	-5.55	1.52	1.61

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1006	DC	P-O3'-C3'	9.06	133.79	120.20
2	A	597	LYS	N-CA-C	8.95	129.58	109.81
2	A	783	GLU	N-CA-C	-8.95	100.01	112.45
2	A	439	ALA	N-CA-C	7.45	120.48	111.40
2	A	795	TYR	CA-C-N	7.26	126.89	119.19
2	A	795	TYR	C-N-CA	7.26	126.89	119.19
2	A	694	ILE	N-CA-C	7.21	120.37	109.20
2	A	887	GLU	N-CA-C	-6.93	96.98	108.34
2	A	363	ASN	N-CA-C	6.88	118.43	111.07
2	A	386	ALA	N-CA-C	6.78	119.56	110.88
2	A	689	ILE	N-CA-C	-6.71	103.97	110.42
2	A	607	PRO	N-CA-CB	6.53	110.18	103.00
1	B	1006	DC	P-O5'-C5'	6.06	129.10	120.00
2	A	877	ILE	N-CA-C	6.05	121.93	109.34
2	A	893	VAL	N-CA-C	6.00	121.81	109.34
2	A	530	GLU	N-CA-C	5.87	117.35	111.07
2	A	830	SER	N-CA-C	5.78	123.12	110.80
2	A	595	GLY	N-CA-C	-5.59	102.44	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	852	ALA	N-CA-C	-5.11	105.62	111.14
2	A	832	ASN	N-CA-C	-5.10	101.96	110.17
2	A	445	GLU	N-CA-C	-5.07	105.65	111.07
2	A	596	ILE	N-CA-C	5.06	115.26	107.77
2	A	845	ASN	N-CA-C	5.04	116.63	111.03
2	A	512	MET	N-CA-C	5.04	117.89	111.69

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	1	0
2	A	4753	0	4753	131	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	202	0	0	6	0
4	B	1	0	0	0	0
All	All	5001	0	4776	131	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 14.

All (131) 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)
2:A:717:LEU:HD21	2:A:818:LEU:HD11	1.27	1.12
2:A:472:THR:HG22	2:A:475:GLU:HG3	1.47	0.96
2:A:681:VAL:HA	2:A:690:ARG:HH21	1.37	0.89
2:A:740:GLU:HB3	2:A:794:ARG:HG2	1.57	0.86
2:A:855:ILE:HG23	2:A:908:THR:HG21	1.59	0.84
2:A:545:VAL:HG23	2:A:877:ILE:HD12	1.59	0.83
2:A:677:GLN:HE21	2:A:881:HIS:H	1.29	0.76
2:A:677:GLN:NE2	2:A:881:HIS:H	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:681:VAL:HA	2:A:690:ARG:NH2	2.03	0.74
2:A:324:MET:HA	2:A:324:MET:HE3	1.72	0.71
2:A:485:THR:H	2:A:488:GLN:HE21	1.36	0.71
2:A:921:GLY:HA3	2:A:926:GLN:HB3	1.74	0.69
2:A:717:LEU:HD21	2:A:818:LEU:CD1	2.16	0.69
2:A:808:GLN:O	2:A:812:GLN:HG2	1.94	0.68
2:A:448:ILE:HD11	2:A:530:GLU:HG3	1.76	0.68
2:A:746:LEU:O	2:A:749:VAL:HG12	1.93	0.67
2:A:863:VAL:HA	2:A:903:LEU:HD13	1.78	0.66
2:A:715:ALA:HB1	2:A:724:LEU:HD12	1.79	0.64
2:A:492:GLU:O	2:A:496:ARG:HG3	1.99	0.63
2:A:712:ARG:HD3	2:A:913:PRO:O	1.99	0.63
2:A:779:ILE:HD12	2:A:783:GLU:HG3	1.81	0.62
2:A:458:MET:HE3	2:A:470:THR:HG21	1.80	0.62
2:A:908:THR:HG22	2:A:909:ARG:H	1.64	0.62
2:A:324:MET:O	2:A:325:ILE:HG13	2.01	0.60
2:A:677:GLN:HG2	2:A:880:VAL:HG23	1.82	0.60
2:A:674:PRO:HG2	2:A:676:LEU:HD13	1.83	0.60
2:A:706:TYR:HB3	2:A:709:ILE:HB	1.84	0.59
2:A:782:LYS:HA	2:A:785:GLN:HB3	1.83	0.59
2:A:922:GLU:HB2	2:A:926:GLN:HE22	1.68	0.59
2:A:586:LEU:HD22	2:A:627:ILE:HD13	1.84	0.59
2:A:435:LEU:HD13	2:A:438:ILE:HG12	1.85	0.58
2:A:677:GLN:HE21	2:A:881:HIS:N	1.99	0.57
2:A:922:GLU:HB2	2:A:926:GLN:NE2	2.20	0.57
2:A:798:VAL:O	2:A:802:MET:HG3	2.04	0.56
2:A:878:MET:HG2	4:A:50:HOH:O	2.05	0.56
2:A:725:THR:O	2:A:729:GLU:HG2	2.06	0.56
2:A:354:PHE:HZ	2:A:428:LEU:HD11	1.71	0.56
2:A:638:SER:O	2:A:643:LYS:HG2	2.04	0.56
2:A:446:SER:OG	2:A:456:HIS:HD2	1.88	0.56
2:A:909:ARG:HB3	2:A:911:ASP:OD1	2.05	0.56
2:A:802:MET:HE2	2:A:844:ILE:HD13	1.86	0.55
2:A:363:ASN:HD22	2:A:542:ARG:HH11	1.53	0.55
2:A:418:GLY:O	2:A:441:ASP:HA	2.07	0.55
2:A:640:TYR:O	2:A:644:LEU:HB2	2.07	0.55
2:A:589:ILE:O	2:A:593:LYS:HG2	2.07	0.54
2:A:573:ILE:HG21	2:A:623:LEU:HB2	1.89	0.54
2:A:363:ASN:ND2	2:A:542:ARG:HH11	2.06	0.54
2:A:472:THR:HG22	2:A:475:GLU:CG	2.31	0.53
2:A:668:ARG:HG3	2:A:853:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:597:LYS:HG3	2:A:598:PRO:HD3	1.90	0.52
2:A:773:LEU:HD22	2:A:773:LEU:O	2.09	0.52
2:A:523:LEU:HD12	4:A:102:HOH:O	2.10	0.52
2:A:737:THR:O	2:A:741:VAL:HG23	2.09	0.52
2:A:802:MET:O	2:A:806:ARG:HG3	2.09	0.52
2:A:580:LEU:HD12	2:A:627:ILE:HG12	1.92	0.52
2:A:782:LYS:N	2:A:782:LYS:HD2	2.24	0.52
2:A:355:ASP:HB3	2:A:372:SER:OG	2.11	0.51
2:A:744:LEU:HD12	2:A:748:THR:OG1	2.10	0.51
2:A:418:GLY:HA3	2:A:421:LEU:HD13	1.93	0.50
2:A:657:THR:HG22	4:A:56:HOH:O	2.11	0.50
2:A:332:THR:HG22	2:A:334:LEU:HD13	1.91	0.50
2:A:449:LEU:HD13	2:A:516:LEU:HG	1.93	0.50
2:A:612:GLU:HB3	2:A:615:GLU:HG2	1.93	0.50
2:A:908:THR:HG22	2:A:909:ARG:N	2.27	0.49
2:A:707:SER:C	2:A:708:GLN:HG2	2.37	0.49
2:A:684:GLU:O	2:A:687:ARG:HB2	2.13	0.49
2:A:779:ILE:HB	2:A:783:GLU:HG2	1.95	0.49
2:A:872:PRO:HG2	2:A:874:VAL:HG13	1.93	0.48
2:A:657:THR:HB	2:A:674:PRO:HD2	1.95	0.48
2:A:668:ARG:HE	2:A:849:GLN:HG3	1.79	0.48
2:A:770:ALA:HA	2:A:788:MET:SD	2.54	0.47
2:A:427:ILE:O	2:A:430:ASN:HB2	2.14	0.47
2:A:633:LEU:CD2	2:A:685:GLU:HG3	2.45	0.47
2:A:418:GLY:HA2	2:A:505:THR:HG21	1.96	0.47
2:A:735:ARG:HB3	2:A:749:VAL:HG11	1.96	0.47
2:A:846:ALA:HB3	2:A:847:PRO:HD3	1.97	0.46
2:A:324:MET:HG3	2:A:325:ILE:H	1.79	0.46
2:A:633:LEU:HD21	2:A:685:GLU:HG3	1.97	0.46
2:A:765:ILE:HA	2:A:848:MET:HE1	1.96	0.46
2:A:615:GLU:HB3	2:A:628:LEU:HD21	1.96	0.46
2:A:623:LEU:O	2:A:626:VAL:HG22	2.16	0.46
2:A:327:TYR:CD1	2:A:492:GLU:HB3	2.51	0.46
2:A:677:GLN:HG3	4:A:23:HOH:O	2.16	0.46
2:A:781:ARG:C	2:A:783:GLU:H	2.24	0.46
2:A:354:PHE:CZ	2:A:428:LEU:HD11	2.50	0.46
2:A:559:LEU:O	2:A:563:LEU:HG	2.17	0.45
2:A:717:LEU:CD2	2:A:818:LEU:HD11	2.20	0.45
2:A:713:ILE:HG21	2:A:848:MET:HA	1.98	0.45
2:A:808:GLN:OE1	2:A:812:GLN:NE2	2.50	0.45
2:A:558:GLU:CD	2:A:688:ARG:HH12	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:901:HIS:NE2	2:A:905:GLU:OE2	2.50	0.44
2:A:327:TYR:CE1	2:A:496:ARG:HD2	2.52	0.44
2:A:401:ALA:O	2:A:405:LEU:HB2	2.17	0.44
2:A:463:GLU:OE2	2:A:469:LYS:HE2	2.17	0.44
2:A:687:ARG:O	2:A:691:GLN:HG3	2.17	0.44
2:A:719:ARG:CZ	2:A:804:ARG:HH12	2.31	0.44
2:A:853:ALA:O	2:A:857:LYS:HG3	2.17	0.44
2:A:592:GLU:HG2	2:A:592:GLU:O	2.18	0.44
2:A:711:LEU:HD22	2:A:762:PHE:CE1	2.52	0.44
2:A:836:ARG:O	2:A:840:GLU:HG3	2.18	0.43
2:A:799:LEU:HD23	2:A:799:LEU:HA	1.79	0.43
2:A:844:ILE:O	2:A:848:MET:HE2	2.18	0.43
2:A:732:ASP:OD2	2:A:754:ARG:NH1	2.52	0.43
2:A:552:LEU:HD12	2:A:552:LEU:HA	1.77	0.43
2:A:713:ILE:HD11	2:A:855:ILE:HD12	2.01	0.43
2:A:764:LEU:HD13	2:A:798:VAL:HG11	2.00	0.43
2:A:369:VAL:HA	2:A:386:ALA:HB3	2.02	0.42
2:A:858:ARG:HB2	2:A:908:THR:HG23	2.01	0.42
2:A:525:VAL:O	2:A:529:ILE:HB	2.20	0.42
2:A:780:PRO:O	2:A:783:GLU:HB3	2.19	0.42
2:A:714:MET:HB2	2:A:848:MET:SD	2.59	0.42
2:A:446:SER:OG	2:A:461:LEU:HD21	2.20	0.42
2:A:623:LEU:N	2:A:624:PRO:HD2	2.35	0.42
2:A:896:VAL:O	2:A:900:ILE:HG12	2.20	0.42
2:A:854:ASP:O	2:A:858:ARG:HG3	2.20	0.42
2:A:708:GLN:HE21	2:A:708:GLN:HB3	1.57	0.42
2:A:533:LEU:HD12	2:A:536:VAL:HG21	2.02	0.42
2:A:668:ARG:HB2	4:A:80:HOH:O	2.19	0.41
2:A:825:LEU:HD22	2:A:839:ALA:O	2.19	0.41
2:A:324:MET:CG	2:A:325:ILE:H	2.30	0.41
2:A:547:ILE:O	2:A:549:PRO:HD3	2.21	0.41
2:A:668:ARG:CG	2:A:853:ALA:HB2	2.50	0.41
2:A:729:GLU:HG2	2:A:729:GLU:H	1.77	0.41
2:A:740:GLU:HB3	2:A:794:ARG:CG	2.40	0.41
2:A:597:LYS:CG	2:A:598:PRO:HD3	2.50	0.41
2:A:421:LEU:HD12	2:A:421:LEU:HA	1.92	0.40
2:A:532:PRO:HB3	4:A:185:HOH:O	2.21	0.40
2:A:866:TRP:HE1	2:A:870:GLU:CD	2.29	0.40
2:A:622:PRO:O	2:A:625:LYS:HB3	2.21	0.40
2:A:810:LYS:HA	2:A:828:ILE:HG12	2.03	0.40
1:B:1007:DG:N3	2:A:361:LEU:HG	2.37	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%)	548 (92%)	43 (7%)	6 (1%)	12 10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	325	ILE
2	A	576	GLU
2	A	597	LYS
2	A	830	SER
2	A	594	GLN
2	A	622	PRO

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%)	449 (90%)	51 (10%)	7 5

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	325	ILE
2	A	334	LEU

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Mol	Chain	Res	Type
2	A	339	LEU
2	A	346	LEU
2	A	375	ILE
2	A	390	LEU
2	A	405	LEU
2	A	409	LEU
2	A	421	LEU
2	A	435	LEU
2	A	449	LEU
2	A	472	THR
2	A	491	LEU
2	A	510	LEU
2	A	522	PRO
2	A	523	LEU
2	A	536	VAL
2	A	543	ASN
2	A	546	LYS
2	A	547	ILE
2	A	550	LYS
2	A	552	LEU
2	A	577	GLU
2	A	584	LYS
2	A	592	GLU
2	A	596	ILE
2	A	612	GLU
2	A	616	GLU
2	A	620	ASP
2	A	644	LEU
2	A	676	LEU
2	A	708	GLN
2	A	711	LEU
2	A	719	ARG
2	A	733	ILE
2	A	747	GLU
2	A	749	VAL
2	A	754	ARG
2	A	773	LEU
2	A	783	GLU
2	A	794	ARG
2	A	799	LEU
2	A	808	GLN
2	A	811	GLU

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Mol	Chain	Res	Type
2	A	816	GLU
2	A	835	ARG
2	A	867	LEU
2	A	871	GLN
2	A	874	VAL
2	A	880	VAL
2	A	917	GLU

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	519	HIS
2	A	528	ASN
2	A	543	ASN
2	A	571	HIS
2	A	677	GLN
2	A	708	GLN
2	A	716	HIS
2	A	734	HIS
2	A	785	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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

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, 95th 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 ²)	Q<0.9
1	B	3/7 (42%)	-0.03	0 100 100	38, 38, 41, 43	0
2	A	601/605 (99%)	0.42	59 (9%) 13 12	16, 37, 94, 100	0
All	All	604/612 (98%)	0.42	59 (9%) 13 12	16, 38, 94, 100	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	581	SER	6.8
2	A	598	PRO	5.9
2	A	613	VAL	5.6
2	A	602	THR	5.4
2	A	608	SER	5.4
2	A	610	SER	4.9
2	A	621	TYR	4.9
2	A	607	PRO	4.7
2	A	582	SER	4.2
2	A	599	LEU	4.2
2	A	601	LYS	3.9
2	A	564	ALA	3.9
2	A	480	GLY	3.8
2	A	583	THR	3.7
2	A	830	SER	3.7
2	A	580	LEU	3.6
2	A	774	ALA	3.4
2	A	619	LEU	3.4
2	A	626	VAL	3.3
2	A	588	THR	3.3
2	A	832	ASN	3.3
2	A	776	GLN	3.2
2	A	574	ALA	3.2
2	A	768	MET	3.0

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Mol	Chain	Res	Type	RSRZ
2	A	617	LEU	2.9
2	A	587	GLN	2.9
2	A	778	ASN	2.9
2	A	681	VAL	2.8
2	A	616	GLU	2.8
2	A	609	THR	2.7
2	A	573	ILE	2.7
2	A	614	LEU	2.7
2	A	771	PHE	2.7
2	A	906	ASN	2.7
2	A	591	PHE	2.6
2	A	808	GLN	2.6
2	A	772	GLY	2.6
2	A	584	LYS	2.5
2	A	796	PRO	2.5
2	A	831	SER	2.5
2	A	597	LYS	2.5
2	A	807	ALA	2.4
2	A	575	GLY	2.4
2	A	578	PHE	2.4
2	A	835	ARG	2.4
2	A	784	ALA	2.3
2	A	773	LEU	2.3
2	A	590	LEU	2.3
2	A	628	LEU	2.3
2	A	586	LEU	2.2
2	A	596	ILE	2.2
2	A	611	GLU	2.2
2	A	612	GLU	2.2
2	A	592	GLU	2.2
2	A	834	ALA	2.2
2	A	780	PRO	2.1
2	A	622	PRO	2.1
2	A	624	PRO	2.1
2	A	620	ASP	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 [i](#)

There are no oligosaccharides 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, 95th 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	ZN	A	3	1/1	0.82	0.23	100,100,100,100	0
3	ZN	B	2	1/1	0.94	0.11	77,77,77,77	0
3	ZN	A	1	1/1	0.98	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.