



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:40 PM UTC

PDB ID : 1KFS / pdb_00001kfs
Title : DNA POLYMERASE I KLENOW FRAGMENT (E.C.2.7.7.7) MUTANT/DNA COMPLEX
Authors : Brautigam, C.A.; Steitz, T.A.
Deposited on : 1997-08-18
Resolution : 2.10 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

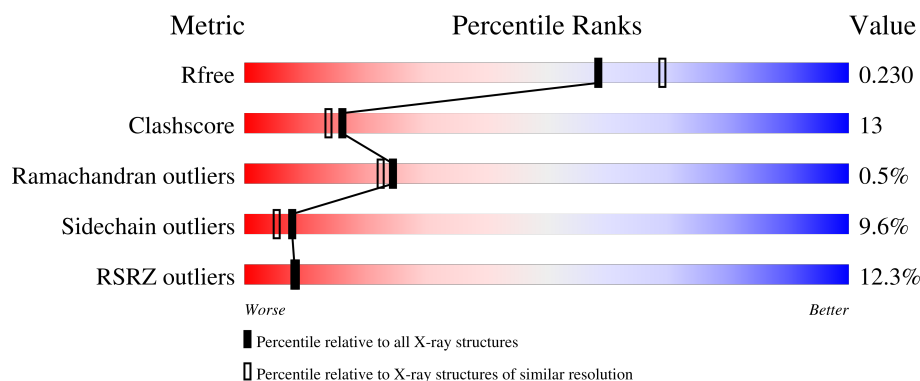
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 5 unique types of molecules in this entry. The entry contains 5136 atoms, of which 1 is hydrogen 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*AP*CP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	3	Total	C	H	N	O	P	0	0	0
			63	29	1	13	17	3			

- Molecule 2 is a protein called PROTEIN (DNA POLYMERASE I KLENOW FRAGMENT (E.C.2.7.7.7)).

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Zn	0	0
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	7	Total	O	0	0
			7	7		

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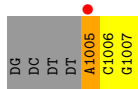
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	309	Total 309	O 309	0	0

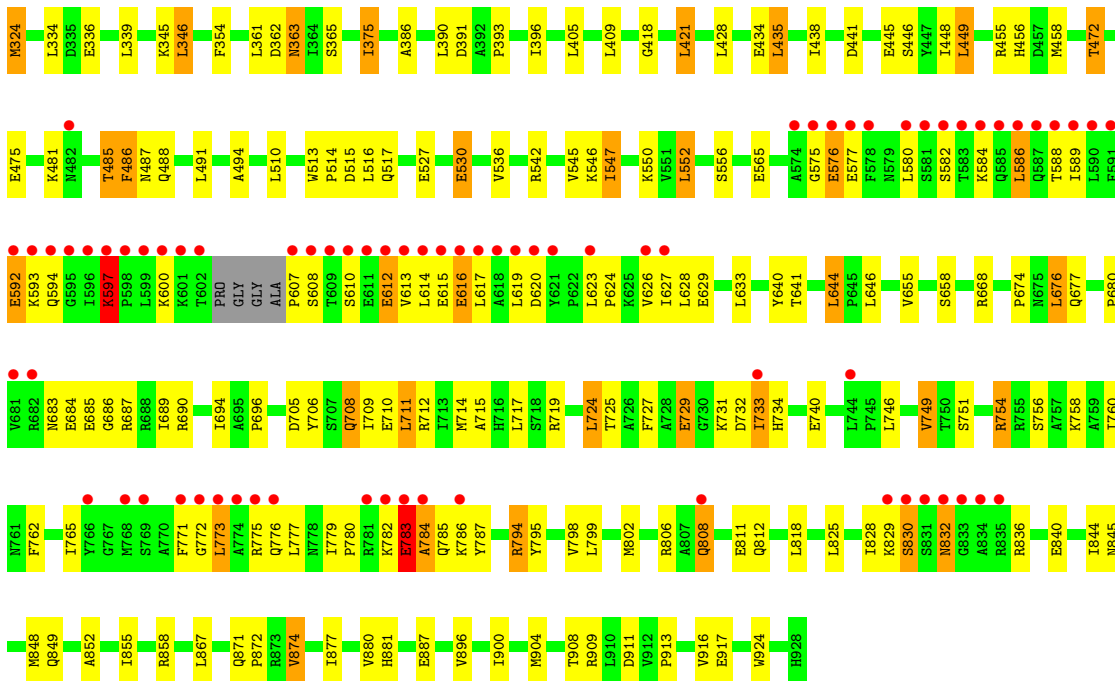
3 Residue-property plots

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*TP*AP*CP*G)-3')



- Molecule 2: PROTEIN (DNA POLYMERASE I KLENOW FRAGMENT (E.C.2.7.7.7))



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 85.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	86.2 (20.00-2.10) 97.4 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	5.50	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.09Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.195 , 0.219 0.214 , 0.230	Depositor DCC
R_{free} test set	6909 reflections (8.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 76.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5136	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: MG, 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	1.73	2/69 (2.9%)	3.65	11/104 (10.6%)
2	A	0.65	0/4839	1.08	29/6547 (0.4%)
All	All	0.68	2/4908 (0.0%)	1.16	40/6651 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1005	DA	C2'-C1'	7.64	1.68	1.52
1	B	1005	DA	C4'-C3'	-5.54	1.41	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1005	DA	N9-C1'-C2'	-15.44	90.34	113.50
1	B	1005	DA	O4'-C1'-N9	12.17	126.65	108.40
1	B	1005	DA	O5'-C5'-C4'	-11.19	94.02	110.80
2	A	783	GLU	N-CA-C	-10.93	99.45	113.12
1	B	1005	DA	P-O5'-C5'	10.41	135.62	120.00
1	B	1005	DA	O4'-C1'-C2'	-10.30	90.95	106.40
1	B	1005	DA	C4'-C3'-O3'	-9.19	96.21	110.00
1	B	1005	DA	C3'-C2'-C1'	7.94	113.51	101.60
2	A	597	LYS	N-CA-C	7.79	127.02	109.81
1	B	1005	DA	C8-N9-C1'	7.16	137.79	127.05
2	A	887	GLU	N-CA-C	-7.00	97.49	108.90
2	A	527	GLU	N-CA-C	6.78	118.75	111.36
2	A	616	GLU	N-CA-C	-6.74	103.54	111.03
1	B	1005	DA	C4-N9-C1'	-6.69	117.01	127.05
2	A	586	LEU	N-CA-C	6.68	118.64	111.36
2	A	607	PRO	N-CA-CB	6.54	110.19	103.00
2	A	795	TYR	CA-C-N	6.33	126.08	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	795	TYR	C-N-CA	6.33	126.08	119.05
2	A	689	ILE	N-CA-C	-6.31	104.36	110.42
2	A	694	ILE	N-CA-C	6.30	118.23	109.29
2	A	486	PHE	N-CA-C	6.26	119.77	111.75
2	A	530	GLU	N-CA-C	6.23	117.87	111.14
2	A	784	ALA	N-CA-C	-6.19	104.61	111.36
1	B	1006	DC	P-O3'-C3'	6.06	129.29	120.20
2	A	832	ASN	N-CA-C	-6.05	100.89	109.96
1	B	1005	DA	C5'-C4'-C3'	-5.95	105.98	114.90
2	A	386	ALA	N-CA-C	5.89	118.41	110.88
2	A	485	THR	N-CA-C	-5.67	102.12	110.52
2	A	608	SER	N-CA-C	5.62	117.10	110.97
2	A	825	LEU	CA-C-N	5.60	125.12	119.19
2	A	825	LEU	C-N-CA	5.60	125.12	119.19
2	A	363	ASN	N-CA-C	5.52	116.97	111.07
2	A	458	MET	N-CA-C	5.45	117.22	111.28
2	A	852	ALA	N-CA-C	-5.37	105.33	111.07
2	A	686	GLY	N-CA-C	-5.31	106.35	112.73
2	A	445	GLU	N-CA-C	-5.24	105.47	111.07
2	A	904	MET	N-CA-C	5.19	117.02	111.36
2	A	845	ASN	N-CA-C	5.17	116.72	111.14
2	A	396	ILE	N-CA-C	-5.13	102.24	109.63
2	A	391	ASP	N-CA-C	5.02	118.71	112.58

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	62	1	34	5	0
2	A	4753	0	4753	125	0
3	B	1	0	0	0	0
4	A	3	0	0	0	0
5	A	309	0	0	9	0
5	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5135	1	4787	126	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 13.

All (126) 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:740:GLU:HB3	2:A:794:ARG:HG2	1.49	0.95
2:A:828:ILE:HG23	2:A:829:LYS:HE2	1.57	0.86
2:A:782:LYS:HA	2:A:785:GLN:HB3	1.65	0.78
2:A:485:THR:H	2:A:488:GLN:HE21	1.30	0.78
2:A:855:ILE:HG23	2:A:908:THR:HG21	1.66	0.77
2:A:677:GLN:HE21	2:A:881:HIS:H	1.32	0.76
2:A:545:VAL:HG23	2:A:877:ILE:HD12	1.66	0.76
2:A:363:ASN:HD22	2:A:542:ARG:HH11	1.36	0.74
2:A:712:ARG:HD3	2:A:913:PRO:O	1.89	0.73
2:A:696:PRO:HB2	5:A:143:HOH:O	1.89	0.72
2:A:612:GLU:HB3	2:A:615:GLU:HG2	1.72	0.71
2:A:600:LYS:CB	2:A:614:LEU:HG	2.20	0.71
2:A:446:SER:OG	2:A:456:HIS:HD2	1.75	0.69
2:A:336:GLU:HG3	5:A:144:HOH:O	1.94	0.65
2:A:418:GLY:HA3	2:A:421:LEU:HD13	1.77	0.65
2:A:711:LEU:HD13	2:A:765:ILE:HD11	1.78	0.64
2:A:435:LEU:HD13	2:A:438:ILE:HG12	1.81	0.62
2:A:772:GLY:O	2:A:776:GLN:HG2	2.01	0.61
2:A:640:TYR:O	2:A:644:LEU:HB2	1.99	0.61
2:A:746:LEU:O	2:A:749:VAL:HG12	2.01	0.60
2:A:324:MET:HA	2:A:324:MET:HE3	1.81	0.60
2:A:782:LYS:HA	2:A:785:GLN:CB	2.29	0.60
2:A:363:ASN:ND2	2:A:542:ARG:HH11	1.98	0.60
2:A:575:GLY:O	2:A:576:GLU:HG2	2.02	0.60
2:A:872:PRO:HG2	2:A:874:VAL:HG13	1.82	0.60
2:A:717:LEU:HD21	2:A:818:LEU:HD11	1.84	0.59
2:A:346:LEU:CD1	2:A:375:ILE:HG23	2.33	0.59
2:A:858:ARG:HB2	2:A:908:THR:HG23	1.85	0.58
2:A:740:GLU:HG2	5:A:277:HOH:O	2.02	0.58
2:A:802:MET:HE2	2:A:844:ILE:HD13	1.85	0.58
2:A:828:ILE:CG2	2:A:829:LYS:HE2	2.32	0.58
2:A:556:SER:HB2	2:A:641:THR:HG22	1.86	0.57
2:A:731:LYS:HD2	2:A:746:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:677:GLN:HE21	2:A:881:HIS:N	2.01	0.56
2:A:586:LEU:HD22	2:A:627:ILE:HD13	1.86	0.56
2:A:836:ARG:O	2:A:840:GLU:HG3	2.06	0.56
2:A:674:PRO:HG2	2:A:676:LEU:HD13	1.88	0.56
2:A:421:LEU:HD23	2:A:438:ILE:HG23	1.87	0.56
2:A:677:GLN:NE2	2:A:881:HIS:H	2.02	0.55
1:B:1005:DA:OP1	2:A:455:ARG:NH2	2.40	0.55
2:A:588:THR:O	2:A:592:GLU:HB3	2.07	0.54
2:A:725:THR:O	2:A:729:GLU:HG2	2.07	0.54
2:A:808:GLN:O	2:A:812:GLN:HG2	2.07	0.54
1:B:1005:DA:P	2:A:455:ARG:HH21	2.31	0.54
2:A:684:GLU:O	2:A:687:ARG:HB2	2.08	0.53
2:A:565:GLU:HG2	5:A:157:HOH:O	2.07	0.53
2:A:802:MET:O	2:A:806:ARG:HG3	2.09	0.53
2:A:547:ILE:HD12	2:A:655:VAL:HG21	1.91	0.52
2:A:586:LEU:HD11	2:A:627:ILE:HG21	1.91	0.52
2:A:324:MET:HE2	5:A:247:HOH:O	2.09	0.52
2:A:779:ILE:HD12	2:A:783:GLU:HG3	1.92	0.52
2:A:610:SER:HA	2:A:776:GLN:HE22	1.76	0.51
2:A:556:SER:HB2	2:A:641:THR:CG2	2.41	0.51
2:A:600:LYS:CB	2:A:613:VAL:HB	2.40	0.51
2:A:668:ARG:HE	2:A:849:GLN:HG3	1.76	0.51
2:A:633:LEU:CD2	2:A:685:GLU:HG3	2.41	0.50
2:A:448:ILE:HD11	2:A:530:GLU:HG3	1.92	0.50
2:A:487:ASN:HD22	2:A:487:ASN:H	1.59	0.50
2:A:734:HIS:CD2	2:A:758:LYS:HA	2.47	0.50
2:A:717:LEU:HD21	2:A:818:LEU:CD1	2.42	0.49
2:A:727:PHE:CE1	2:A:733:ILE:HG12	2.47	0.49
2:A:345:LYS:HD2	5:A:268:HOH:O	2.13	0.48
2:A:393:PRO:HD2	2:A:491:LEU:HD22	1.95	0.48
2:A:487:ASN:H	2:A:487:ASN:ND2	2.11	0.47
2:A:580:LEU:HD22	2:A:580:LEU:N	2.29	0.47
2:A:617:LEU:HB3	2:A:624:PRO:HG3	1.95	0.47
2:A:765:ILE:HA	2:A:848:MET:HE1	1.96	0.47
2:A:732:ASP:OD2	2:A:754:ARG:NH1	2.47	0.47
2:A:586:LEU:CD1	2:A:627:ILE:HG21	2.44	0.46
1:B:1005:DA:N6	2:A:658:SER:HB3	2.31	0.46
2:A:751:SER:HB3	5:A:166:HOH:O	2.16	0.46
2:A:615:GLU:HB3	2:A:628:LEU:HD21	1.96	0.46
2:A:783:GLU:O	2:A:786:LYS:HB3	2.15	0.46
2:A:683:ASN:OD1	2:A:684:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:677:GLN:HB3	5:A:194:HOH:O	2.16	0.46
2:A:677:GLN:HG2	2:A:880:VAL:HG23	1.97	0.46
2:A:547:ILE:HD13	2:A:644:LEU:HG	1.97	0.46
2:A:909:ARG:HB3	2:A:911:ASP:OD1	2.16	0.46
2:A:486:PHE:CE2	2:A:494:ALA:HB1	2.51	0.45
2:A:362:ASP:OD2	2:A:365:SER:OG	2.34	0.45
2:A:418:GLY:O	2:A:441:ASP:HA	2.17	0.45
2:A:756:SER:HA	2:A:777:LEU:HD11	1.99	0.45
2:A:589:ILE:O	2:A:593:LYS:HG2	2.16	0.45
2:A:576:GLU:HG3	2:A:577:GLU:O	2.16	0.45
2:A:614:LEU:HB2	2:A:628:LEU:HD13	1.99	0.45
2:A:711:LEU:HD22	2:A:762:PHE:CE1	2.52	0.45
2:A:324:MET:HA	2:A:324:MET:CE	2.45	0.45
2:A:513:TRP:HB3	2:A:514:PRO:HD3	2.00	0.44
2:A:580:LEU:HD12	2:A:627:ILE:HG12	1.99	0.44
2:A:880:VAL:HG11	2:A:924:TRP:HZ2	1.82	0.44
2:A:472:THR:HG22	2:A:475:GLU:H	1.82	0.44
2:A:481:LYS:HB3	2:A:481:LYS:HE2	1.84	0.44
2:A:346:LEU:HD13	2:A:375:ILE:HG23	2.00	0.44
2:A:418:GLY:HA3	2:A:421:LEU:CD1	2.46	0.44
2:A:472:THR:HG22	2:A:475:GLU:HG3	2.00	0.43
2:A:773:LEU:HD13	2:A:784:ALA:HB1	1.99	0.43
2:A:808:GLN:OE1	2:A:812:GLN:NE2	2.51	0.43
2:A:706:TYR:HB3	2:A:709:ILE:HB	2.00	0.43
2:A:711:LEU:HD23	2:A:733:ILE:HD13	1.98	0.43
2:A:690:ARG:HG2	2:A:924:TRP:CE3	2.53	0.43
1:B:1005:DA:N3	1:B:1005:DA:C2'	2.79	0.43
2:A:880:VAL:HG11	2:A:924:TRP:CZ2	2.54	0.43
2:A:715:ALA:HB1	2:A:724:LEU:HD13	2.00	0.43
2:A:354:PHE:CZ	2:A:428:LEU:HD11	2.54	0.42
2:A:708:GLN:HE21	2:A:708:GLN:HB3	1.61	0.42
2:A:798:VAL:O	2:A:802:MET:HG3	2.19	0.42
2:A:714:MET:HB2	2:A:848:MET:SD	2.59	0.42
2:A:830:SER:C	2:A:832:ASN:H	2.27	0.42
2:A:808:GLN:HA	2:A:811:GLU:HB3	2.01	0.42
2:A:760:ILE:HD11	2:A:787:TYR:HB3	2.01	0.41
2:A:705:ASP:O	2:A:916:VAL:HA	2.19	0.41
2:A:710:GLU:OE1	2:A:765:ILE:HG21	2.20	0.41
2:A:623:LEU:N	2:A:624:PRO:HD2	2.35	0.41
2:A:771:PHE:O	2:A:775:ARG:HG3	2.21	0.41
2:A:896:VAL:O	2:A:900:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:DG:N3	2:A:361:LEU:HG	2.36	0.41
2:A:780:PRO:O	2:A:783:GLU:HB3	2.20	0.41
2:A:434:GLU:HG3	5:A:303:HOH:O	2.20	0.41
2:A:515:ASP:C	2:A:517:GLN:H	2.29	0.41
2:A:619:LEU:N	2:A:619:LEU:HD22	2.36	0.41
2:A:773:LEU:HD22	2:A:773:LEU:O	2.20	0.41
2:A:552:LEU:HD12	2:A:552:LEU:HA	1.96	0.41
2:A:582:SER:HA	2:A:586:LEU:HB2	2.03	0.41
2:A:449:LEU:HD13	2:A:516:LEU:HG	2.02	0.40
2:A:623:LEU:HG	2:A:627:ILE:CD1	2.52	0.40
2:A:449:LEU:HD12	2:A:449:LEU:HA	1.82	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%)	566 (95%)	28 (5%)	3 (0%)	24	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	830	SER
2	A	594	GLN
2	A	597	LYS

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%)	452 (90%)	48 (10%)	8 5

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	324	MET
2	A	334	LEU
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	510	LEU
2	A	536	VAL
2	A	546	LYS
2	A	547	ILE
2	A	550	LYS
2	A	552	LEU
2	A	576	GLU
2	A	584	LYS
2	A	592	GLU
2	A	597	LYS
2	A	612	GLU
2	A	616	GLU
2	A	620	ASP
2	A	626	VAL
2	A	629	GLU
2	A	644	LEU
2	A	646	LEU
2	A	676	LEU
2	A	680	PRO
2	A	708	GLN
2	A	711	LEU
2	A	719	ARG
2	A	724	LEU

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Mol	Chain	Res	Type
2	A	729	GLU
2	A	733	ILE
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	867	LEU
2	A	871	GLN
2	A	874	VAL
2	A	917	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) 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	585	GLN
2	A	677	GLN
2	A	708	GLN
2	A	716	HIS
2	A	734	HIS
2	A	776	GLN
2	A	785	GLN
2	A	812	GLN
2	A	832	ASN
2	A	845	ASN
2	A	899	GLN
2	A	901	HIS
2	A	906	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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](#)

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%)	0.57	1 (33%) 1 1	29, 29, 38, 61	0
2	A	601/605 (99%)	0.45	73 (12%) 8 9	12, 31, 88, 100	0
All	All	604/612 (98%)	0.45	74 (12%) 8 8	12, 31, 88, 100	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	610	SER	8.8
2	A	607	PRO	7.5
2	A	608	SER	7.3
2	A	598	PRO	6.6
2	A	609	THR	6.3
2	A	583	THR	6.2
2	A	602	THR	5.7
2	A	581	SER	5.5
2	A	582	SER	5.0
2	A	601	LYS	4.9
2	A	599	LEU	4.6
2	A	588	THR	4.5
2	A	613	VAL	4.4
2	A	580	LEU	4.3
2	A	619	LEU	4.1
2	A	618	ALA	4.0
2	A	586	LEU	4.0
2	A	590	LEU	3.9
2	A	584	LYS	3.8
2	A	596	ILE	3.8
2	A	621	TYR	3.8
2	A	681	VAL	3.8
2	A	771	PHE	3.7
2	A	626	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	A	575	GLY	3.6
2	A	808	GLN	3.5
2	A	831	SER	3.3
2	A	574	ALA	3.3
2	A	776	GLN	3.3
2	A	591	PHE	3.3
2	A	617	LEU	3.3
2	A	782	LYS	3.3
2	A	597	LYS	3.1
2	A	600	LYS	3.1
2	A	587	GLN	3.1
2	A	585	GLN	3.0
2	A	616	GLU	3.0
2	A	833	GLY	2.9
2	A	614	LEU	2.8
2	A	772	GLY	2.8
2	A	593	LYS	2.8
2	A	595	GLY	2.7
2	A	830	SER	2.7
2	A	769	SER	2.7
2	A	784	ALA	2.6
2	A	627	ILE	2.6
2	A	834	ALA	2.6
2	A	682	ARG	2.6
2	A	774	ALA	2.5
2	A	829	LYS	2.5
2	A	832	ASN	2.5
2	A	611	GLU	2.5
2	A	775	ARG	2.5
2	A	615	GLU	2.4
2	A	781	ARG	2.4
2	A	768	MET	2.4
2	A	612	GLU	2.3
2	A	773	LEU	2.3
2	A	578	PHE	2.3
2	A	623	LEU	2.3
2	A	594	GLN	2.3
2	A	482	ASN	2.2
2	A	766	TYR	2.2
2	A	835	ARG	2.2
2	A	620	ASP	2.2
2	A	576	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	783	GLU	2.1
2	A	744	LEU	2.1
2	A	786	LYS	2.1
2	A	589	ILE	2.1
2	A	733	ILE	2.1
2	A	577	GLU	2.1
2	A	592	GLU	2.1
1	B	1005	DA	2.1

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 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
4	ZN	A	320	1/1	0.89	0.14	99,99,99,99	0
4	ZN	A	3	1/1	0.97	0.06	66,66,66,66	0
3	MG	B	2	1/1	0.98	0.04	36,36,36,36	0
4	ZN	A	1	1/1	0.99	0.03	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.