Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 02:58 PM EDT

PDB ID	:	1KFS
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

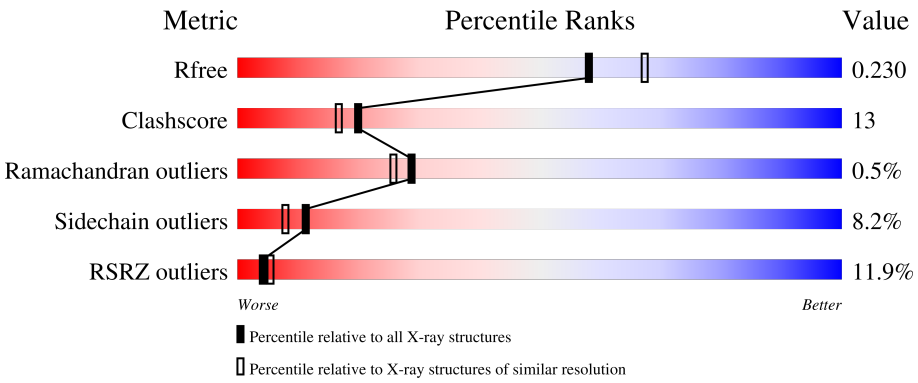
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	14% 29% 57%
2	A	605	12% 70% 25% • •

2 Entry composition (i)

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
			Total	C	H	N	O	P			
1	B	3	63	29	1	13	17	3	0	0	0

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

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

- Molecule 5 is water.

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

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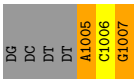
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	309	309	309	0	0

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.

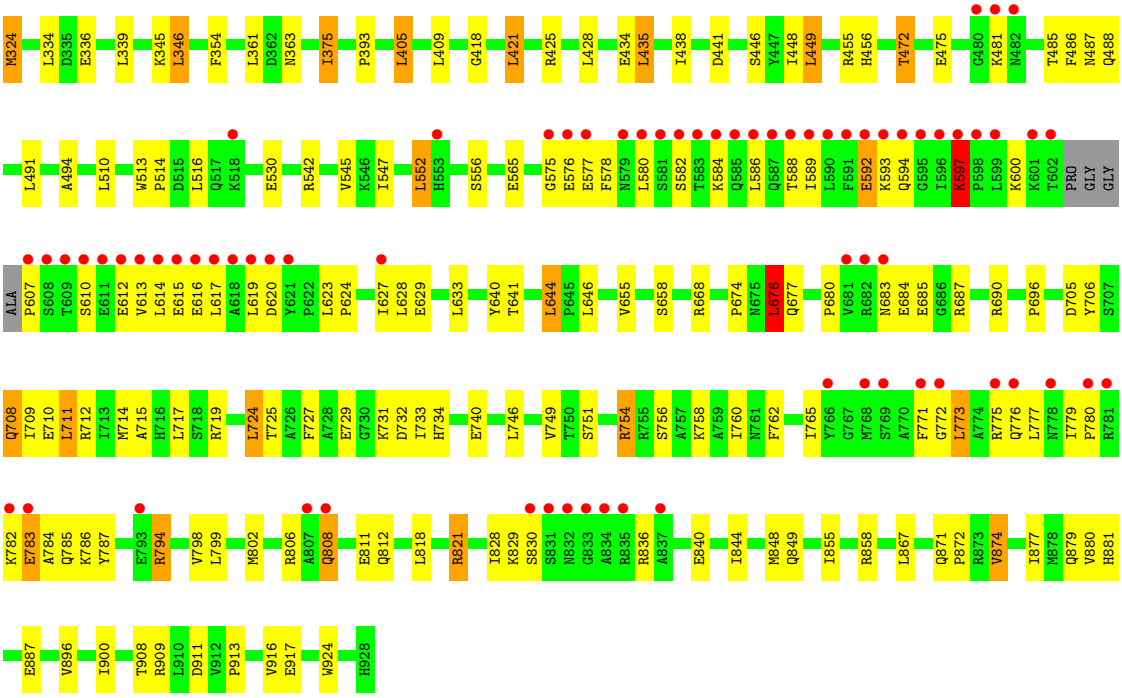
• Molecule 1: DNA (5'-D(*GP*CP*TP*TP*AP*CP*G)-3')

Chain B: 14% 29% 57%



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

Chain A: 12% 70% 25%



4 Data and refinement statistics (i)

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 19.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	86.2 (20.00-2.10) 97.5 (19.95-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	5.50	Depositor
$< I/\sigma(I) >$ [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)	0.41 , 77.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	3.47	7/69 (10.1%)	5.15	25/104 (24.0%)
2	A	0.50	0/4839	0.75	6/6547 (0.1%)
All	All	0.65	7/4908 (0.1%)	0.98	31/6651 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1005	DA	C2'-C1'	15.88	1.68	1.52
1	B	1005	DA	C4'-C3'	-10.87	1.41	1.52
1	B	1007	DG	C2-N3	7.57	1.38	1.32
1	B	1005	DA	C2-N3	-5.58	1.28	1.33
1	B	1007	DG	N9-C4	-5.31	1.33	1.38
1	B	1005	DA	N9-C4	-5.25	1.34	1.37
1	B	1005	DA	O4'-C1'	5.23	1.48	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1005	DA	O4'-C1'-N9	26.65	126.65	108.00
1	B	1005	DA	O4'-C1'-C2'	-18.69	90.95	105.90
1	B	1005	DA	N9-C1'-C2'	-11.71	90.34	112.60
1	B	1007	DG	C5-N7-C8	-9.70	99.45	104.30
1	B	1007	DG	N7-C8-N9	9.51	117.86	113.10
1	B	1005	DA	P-O5'-C5'	9.20	135.62	120.90
1	B	1005	DA	C3'-C2'-C1'	9.18	113.51	102.50
1	B	1007	DG	C8-N9-C4	-8.75	102.90	106.40
1	B	1006	DC	C4'-C3'-C2'	-8.35	95.59	103.10
1	B	1006	DC	P-O3'-C3'	7.99	129.29	119.70
1	B	1005	DA	N3-C4-N9	-7.56	121.35	127.40
1	B	1005	DA	N9-C4-C5	7.26	108.70	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1005	DA	C5-C6-N1	-7.12	114.14	117.70
1	B	1007	DG	C6-C5-N7	-7.05	126.17	130.40
1	B	1005	DA	O5'-C5'-C4'	-6.79	94.02	111.00
1	B	1006	DC	O4'-C4'-C3'	6.77	110.06	106.00
1	B	1007	DG	C4-C5-N7	6.69	113.47	110.80
1	B	1005	DA	C1'-O4'-C4'	6.23	116.33	110.10
2	A	821	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	1005	DA	OP2-P-O3'	6.14	118.71	105.20
1	B	1005	DA	C2-N3-C4	-6.09	107.56	110.60
2	A	597	LYS	N-CA-C	5.93	127.02	111.00
1	B	1007	DG	C4'-C3'-C2'	-5.80	97.88	103.10
2	A	607	PRO	N-CA-CB	5.74	110.19	103.30
1	B	1005	DA	C8-N9-C1'	5.61	137.79	127.70
2	A	676	LEU	CA-CB-CG	5.56	128.08	115.30
1	B	1005	DA	C4'-C3'-O3'	-5.39	96.21	109.70
1	B	1005	DA	C4-N9-C1'	-5.16	117.01	126.30
2	A	405	LEU	CA-CB-CG	5.08	126.98	115.30
1	B	1007	DG	O4'-C4'-C3'	-5.01	102.50	104.50
2	A	887	GLU	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

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	62	1	34	5	0
2	A	4753	0	4753	120	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
All	All	5135	1	4787	121	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 (121) 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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:324:MET:HE2	5:A:247:HOH:O	2.12	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:844:ILE:O	2:A:848:MET:HE2	2.14	0.47
2:A:732:ASP:OD2	2:A:754:ARG:NH1	2.47	0.47
2:A:324:MET:HA	2:A:324:MET:CE	2.45	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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%)	29 26

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%)	459 (92%)	41 (8%)	11 8

All (41) 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	405	LEU
2	A	409	LEU
2	A	421	LEU

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Mol	Chain	Res	Type
2	A	425	ARG
2	A	435	LEU
2	A	449	LEU
2	A	472	THR
2	A	510	LEU
2	A	552	LEU
2	A	578	PHE
2	A	584	LYS
2	A	592	GLU
2	A	597	LYS
2	A	616	GLU
2	A	620	ASP
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
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	821	ARG
2	A	867	LEU
2	A	871	GLN
2	A	874	VAL
2	A	879	GLN
2	A	917	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) 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

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Mol	Chain	Res	Type
2	A	571	HIS
2	A	677	GLN
2	A	708	GLN
2	A	716	HIS
2	A	734	HIS
2	A	776	GLN
2	A	812	GLN
2	A	845	ASN
2	A	879	GLN
2	A	899	GLN
2	A	901	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 monosaccharides 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 (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, 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%)	0.08	0 100 100	29, 29, 38, 60	0
2	A	601/605 (99%)	0.50	72 (11%) 4 5	12, 31, 88, 100	0
All	All	604/612 (98%)	0.50	72 (11%) 4 5	12, 31, 88, 100	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	583	THR	15.7
2	A	607	PRO	13.3
2	A	608	SER	13.2
2	A	610	SER	12.3
2	A	601	LYS	10.1
2	A	609	THR	9.5
2	A	602	THR	9.2
2	A	596	ILE	8.4
2	A	581	SER	8.2
2	A	598	PRO	7.5
2	A	619	LEU	7.1
2	A	582	SER	7.0
2	A	781	ARG	6.5
2	A	597	LYS	6.5
2	A	681	VAL	6.3
2	A	621	TYR	5.9
2	A	599	LEU	5.9
2	A	611	GLU	5.9
2	A	591	PHE	5.8
2	A	594	GLN	5.8
2	A	620	ASP	5.8
2	A	590	LEU	5.8
2	A	682	ARG	5.7
2	A	588	THR	5.6

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Mol	Chain	Res	Type	RSRZ
2	A	616	GLU	5.4
2	A	575	GLY	5.1
2	A	775	ARG	5.0
2	A	577	GLU	4.8
2	A	576	GLU	4.7
2	A	831	SER	4.6
2	A	584	LYS	4.5
2	A	612	GLU	3.9
2	A	771	PHE	3.9
2	A	585	GLN	3.9
2	A	808	GLN	3.9
2	A	587	GLN	3.8
2	A	833	GLY	3.8
2	A	586	LEU	3.8
2	A	832	ASN	3.8
2	A	615	GLU	3.7
2	A	835	ARG	3.7
2	A	776	GLN	3.6
2	A	768	MET	3.4
2	A	592	GLU	3.4
2	A	481	LYS	3.3
2	A	783	GLU	3.3
2	A	830	SER	3.2
2	A	613	VAL	3.2
2	A	782	LYS	3.2
2	A	482	ASN	3.1
2	A	778	ASN	3.1
2	A	593	LYS	3.1
2	A	579	ASN	3.0
2	A	766	TYR	3.0
2	A	769	SER	2.9
2	A	480	GLY	2.9
2	A	772	GLY	2.9
2	A	834	ALA	2.8
2	A	618	ALA	2.7
2	A	589	ILE	2.7
2	A	617	LEU	2.7
2	A	614	LEU	2.4
2	A	780	PRO	2.4
2	A	837	ALA	2.3
2	A	518	LYS	2.3
2	A	595	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	627	ILE	2.2
2	A	793	GLU	2.2
2	A	683	ASN	2.1
2	A	553	HIS	2.1
2	A	580	LEU	2.1
2	A	807	ALA	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 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, 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(Å^2)	Q<0.9
4	ZN	A	320	1/1	0.77	0.08	99,99,99,99	0
4	ZN	A	3	1/1	0.95	0.04	66,66,66,66	0
3	MG	B	2	1/1	0.98	0.06	36,36,36,36	0
4	ZN	A	1	1/1	0.99	0.04	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.