Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:39 AM GMT

PDB ID	:	2KZZ
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
http://wwpdb.org/validation/2016/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:

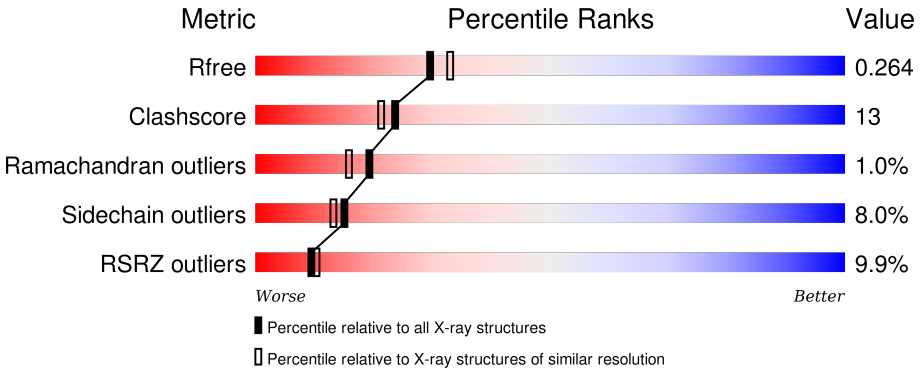
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.25 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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% 14% 14% 57%
2	A	605	10% 68% 27%

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	UNP P00582

- Molecule 3 is ZINC ION (three-letter code: 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.

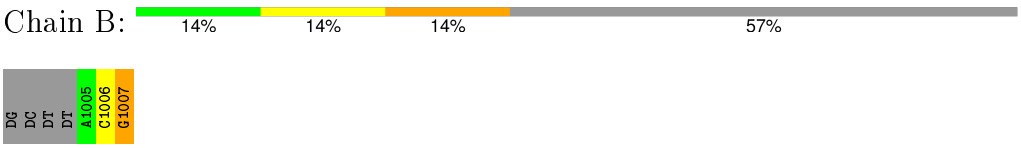
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	202	Total	O	0	0
			202	202		
4	B	1	Total	O	0	0
			1	1		

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 errors 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.

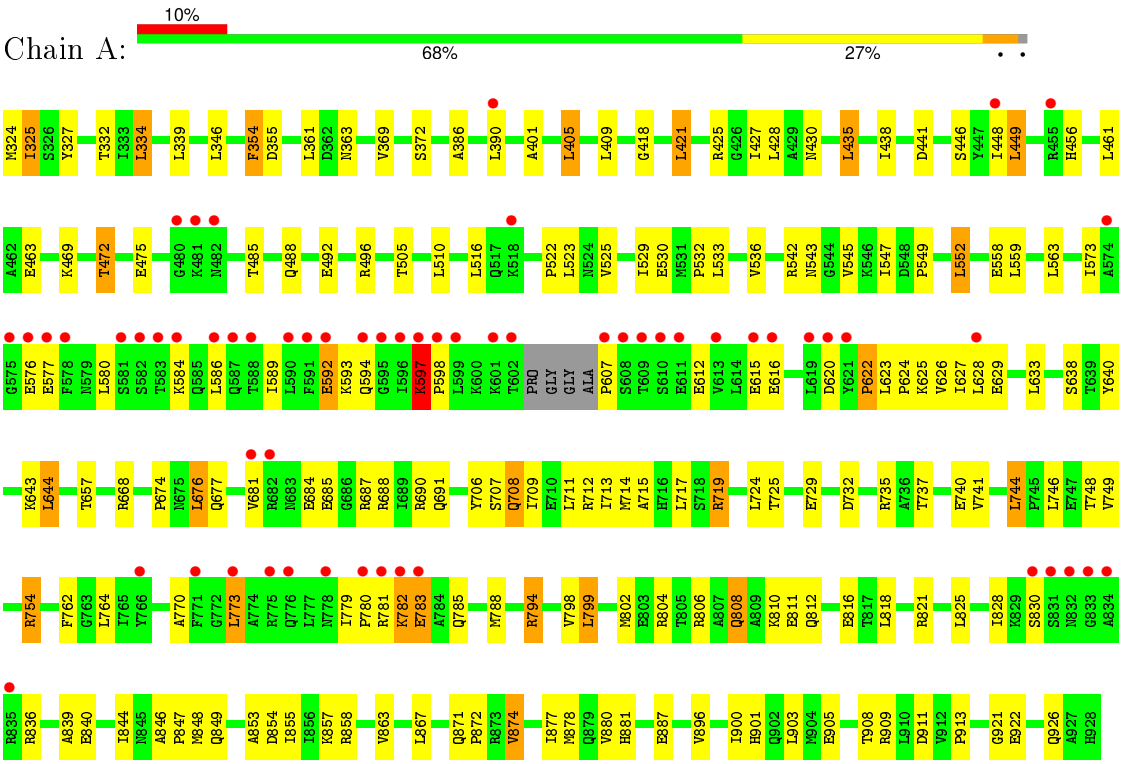
- Molecule 1: DNA (5'-D(*GP*CP*TP*T*AP*CP*G)-3')

Chain B:



- Molecule 2: PROTEIN (DNA POLYMERASE I)

Chain A:



4 Data and refinement statistics (i)

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 19.95 – 2.25	Depositor EDS
% Data completeness (in resolution range)	84.4 (20.00-2.25) 80.7 (19.95-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [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	2376 reflections (7.13%)	DCC
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 62.1	EDS
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 34952 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	2.57	4/46 (8.7%)	3.31	10/70 (14.3%)
2	A	0.46	0/4839	0.73	3/6547 (0.0%)
All	All	0.52	4/4885 (0.1%)	0.80	13/6617 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1006	DC	O3'-P	-6.93	1.52	1.61
1	B	1006	DC	N1-C6	6.35	1.41	1.37
1	B	1007	DG	N9-C4	-5.29	1.33	1.38
1	B	1006	DC	P-O5'	5.12	1.64	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1006	DC	P-O3'-C3'	11.74	133.79	119.70
1	B	1007	DG	C5-N7-C8	-7.91	100.34	104.30
1	B	1007	DG	C8-N9-C4	-7.37	103.45	106.40
1	B	1007	DG	C4'-C3'-C2'	-7.34	96.49	103.10
2	A	597	LYS	N-CA-C	6.88	129.58	111.00
1	B	1007	DG	N7-C8-N9	6.87	116.54	113.10
1	B	1006	DC	C4'-C3'-C2'	-6.70	97.07	103.10
1	B	1007	DG	O4'-C4'-C3'	-6.02	102.09	104.50
2	A	607	PRO	N-CA-CB	5.74	110.18	103.30
1	B	1007	DG	N9-C4-C5	5.62	107.65	105.40
1	B	1006	DC	C2-N3-C4	5.47	122.63	119.90
2	A	887	GLU	N-CA-C	-5.19	96.98	111.00
1	B	1006	DC	P-O5'-C5'	5.12	129.10	120.90

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	42	0	23	1	0
2	A	4753	0	4753	126	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	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: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
2:A:681:VAL:HA	2:A:690:ARG:NH2	2.03	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:878:MET:HG2	4:A:50:HOH:O	2.05	0.56
2:A:798:VAL:O	2:A:802:MET:HG3	2.04	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: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
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:802:MET:O	2:A:806:ARG:HG3	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:580:LEU:HD12	2:A:627:ILE:HG12	1.92	0.52
2:A:782:LYS:HD2	2:A:782:LYS:N	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:657:THR:HG22	4:A:56:HOH:O	2.11	0.50
2:A:418:GLY:HA3	2:A:421:LEU:HD13	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:779:ILE:HB	2:A:783:GLU:HG2	1.95	0.49
2:A:684:GLU:O	2:A:687:ARG:HB2	2.13	0.49
2:A:844:ILE:O	2:A:848:MET:HE2	2.13	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:735:ARG:HB3	2:A:749:VAL:HG11	1.96	0.47
2:A:418:GLY:HA2	2:A:505:THR:HG21	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: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:677:GLN:HG3	4:A:23:HOH:O	2.16	0.46
2:A:327:TYR:CD1	2:A:492:GLU:HB3	2.51	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: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:853:ALA:O	2:A:857:LYS:HG3	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:463:GLU:OE2	2:A:469:LYS:HE2	2.17	0.44
2:A:707:SER:C	2:A:708:GLN:HG2	2.37	0.44
2:A:711:LEU:HD22	2:A:762:PHE:CE1	2.52	0.44
2:A:592:GLU:HG2	2:A:592:GLU:O	2.18	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:732:ASP:OD2	2:A:754:ARG:NH1	2.52	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:552:LEU:HD12	2:A:552:LEU:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:858:ARG:HB2	2:A:908:THR:HG23	2.01	0.42
2:A:369:VAL:HA	2:A:386:ALA:HB3	2.02	0.42
2:A:780:PRO:O	2:A:783:GLU:HB3	2.19	0.42
2:A:525:VAL:O	2:A:529:ILE:HB	2.20	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:HB3	2:A:708:GLN:HE21	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:740:GLU:HB3	2:A:794:ARG:CG	2.40	0.41
2:A:729:GLU:HG2	2:A:729:GLU:H	1.77	0.41
2:A:668:ARG:CG	2:A:853:ALA:HB2	2.50	0.41
2:A:547:ILE:O	2:A:549:PRO:HD3	2.21	0.41
2:A:597:LYS:CG	2:A:598:PRO:HD3	2.50	0.41
2:A:781:ARG:C	2:A:783:GLU:H	2.24	0.40
2:A:421:LEU:HA	2:A:421:LEU:HD12	1.92	0.40
2:A:532:PRO:HB3	4:A:185:HOH:O	2.21	0.40
2:A:558:GLU:CD	2:A:688:ARG:HH12	2.25	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%)	19 16

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%)	460 (92%)	40 (8%)	15 13

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	390	LEU
2	A	405	LEU
2	A	409	LEU
2	A	421	LEU
2	A	425	ARG
2	A	435	LEU
2	A	449	LEU
2	A	472	THR
2	A	510	LEU
2	A	522	PRO
2	A	543	ASN

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Mol	Chain	Res	Type
2	A	552	LEU
2	A	577	GLU
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	676	LEU
2	A	708	GLN
2	A	719	ARG
2	A	744	LEU
2	A	754	ARG
2	A	773	LEU
2	A	782	LYS
2	A	783	GLU
2	A	794	ARG
2	A	799	LEU
2	A	808	GLN
2	A	811	GLU
2	A	816	GLU
2	A	821	ARG
2	A	867	LEU
2	A	871	GLN
2	A	874	VAL

Some 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	543	ASN
2	A	571	HIS
2	A	677	GLN
2	A	708	GLN
2	A	716	HIS
2	A	734	HIS
2	A	812	GLN
2	A	845	ASN

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Mol	Chain	Res	Type
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 carbohydrates 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, 95^{th} 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%)	-0.51	0 100 100	38, 38, 41, 43	0
2	A	601/605 (99%)	0.28	60 (9%) 9 10	16, 37, 94, 100	0
All	All	604/612 (98%)	0.28	60 (9%) 9 10	16, 38, 94, 100	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	610	SER	10.8
2	A	608	SER	9.7
2	A	583	THR	8.4
2	A	594	GLN	8.3
2	A	607	PRO	8.1
2	A	609	THR	7.6
2	A	602	THR	7.4
2	A	601	LYS	7.2
2	A	598	PRO	7.1
2	A	619	LEU	6.5
2	A	587	GLN	6.2
2	A	596	ILE	6.1
2	A	621	TYR	5.6
2	A	620	ASP	5.6
2	A	597	LYS	5.6
2	A	588	THR	5.3
2	A	613	VAL	5.2
2	A	682	ARG	5.1
2	A	782	LYS	4.7
2	A	681	VAL	4.6
2	A	576	GLU	4.6
2	A	835	ARG	4.5
2	A	590	LEU	4.3
2	A	595	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
2	A	781	ARG	4.3
2	A	832	ASN	4.3
2	A	771	PHE	4.1
2	A	599	LEU	4.0
2	A	611	GLU	3.9
2	A	831	SER	3.8
2	A	775	ARG	3.8
2	A	581	SER	3.8
2	A	833	GLY	3.6
2	A	834	ALA	3.3
2	A	616	GLU	3.2
2	A	584	LYS	3.2
2	A	582	SER	3.2
2	A	778	ASN	3.1
2	A	518	LYS	3.0
2	A	577	GLU	3.0
2	A	592	GLU	3.0
2	A	830	SER	2.9
2	A	574	ALA	2.9
2	A	776	GLN	2.9
2	A	615	GLU	2.8
2	A	482	ASN	2.8
2	A	481	LYS	2.7
2	A	780	PRO	2.7
2	A	591	PHE	2.6
2	A	783	GLU	2.6
2	A	578	PHE	2.6
2	A	586	LEU	2.5
2	A	480	GLY	2.5
2	A	628	LEU	2.4
2	A	390	LEU	2.3
2	A	455	ARG	2.3
2	A	448	ILE	2.2
2	A	773	LEU	2.1
2	A	766	TYR	2.1
2	A	575	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	B	2	1/1	0.85	0.06	-3.01	77,77,77,77	0
3	ZN	A	1	1/1	0.99	0.05	-3.99	26,26,26,26	0
3	ZN	A	3	1/1	0.72	0.19	-	100,100,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.