Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:21 AM GMT

PDB ID	:	2KFZ
Title	:	KLENOW FRAGMENT WITH BRIDGING-SULFUR SUBSTRATE AND ZINC ONLY
Authors	:	Brautigam, C.A.; Sun, S.; Piccirilli, J.A.; Steitz, T.A.
Deposited on	:	1998-07-02
Resolution	:	2.03 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:

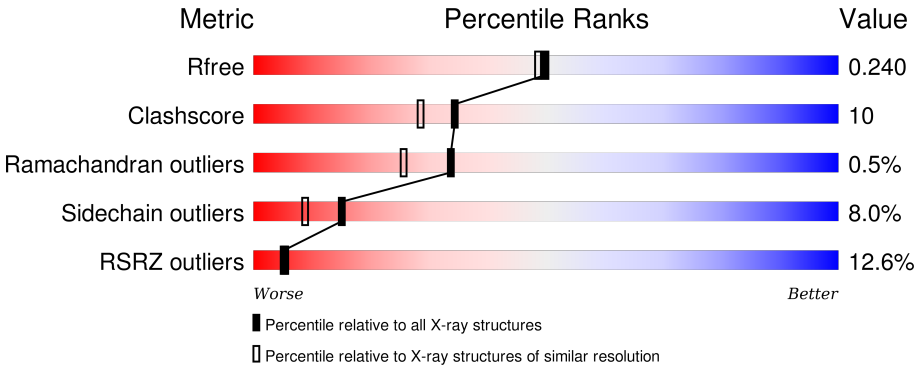
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.03 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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% 29% 14% 14% 43%
2	A	605	12% 74% 22% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5134 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 5'-D(*GP*CP*TP*TP*AP*(US1)P*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	4	Total	C	N	O	P	S	0	0	1
			63	29	12	18	3	1			

- Molecule 2 is a protein called KLENOW FRAGMENT OF 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	A	4	Total	Zn	0	0
			4	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	307	Total	O	0	0
			307	307		

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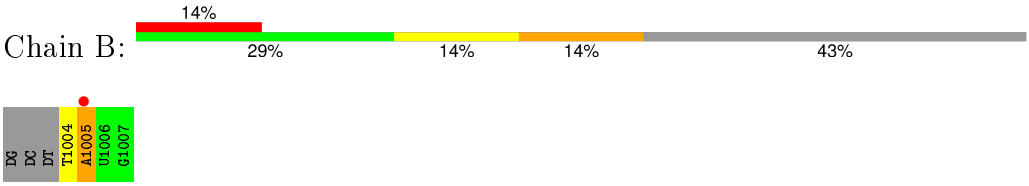
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	6	Total O 6 6	0	0

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.

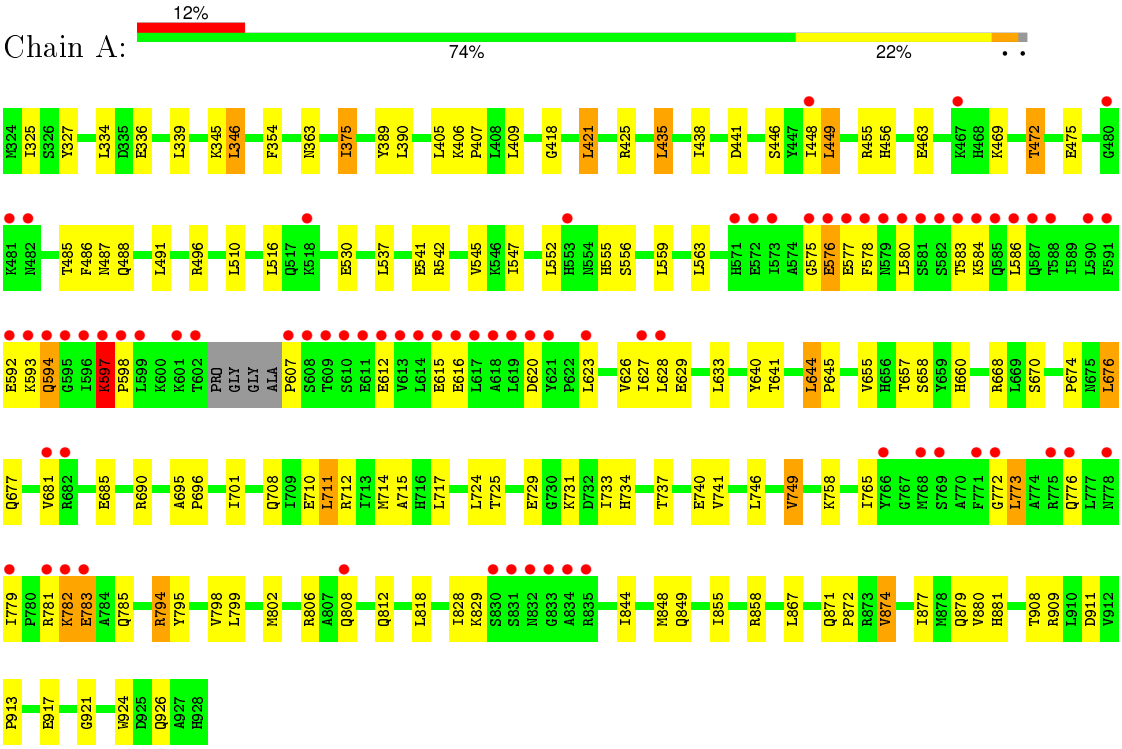
- Molecule 1: 5'-D(*GP*CP*TP*TP*AP*(US1)P*G)-3'

Chain B:



- Molecule 2: KLENOW FRAGMENT OF 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	102.90Å 102.90Å 86.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.03 19.92 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.03) 92.8 (19.92-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.02Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.215 , 0.255 0.233 , 0.240	Depositor DCC
R_{free} test set	5419 reflections (10.04%)	DCC
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 74.5	EDS
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 57410 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5134	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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, MG, US1

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	2.34	2/48 (4.2%)	3.73	9/71 (12.7%)
2	A	0.36	0/4839	0.65	2/6547 (0.0%)
All	All	0.43	2/4887 (0.0%)	0.76	11/6618 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1005	DA	O4'-C1'	5.46	1.48	1.42
1	B	1005	DA	C2'-C1'	5.29	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1005	DA	O4'-C1'-N9	12.29	116.60	108.00
1	B	1005	DA	O4'-C1'-C2'	-10.09	97.83	105.90
1	B	1005	DA	C3'-C2'-C1'	10.07	114.58	102.50
1	B	1005	DA	N9-C4-C5	8.74	109.30	105.80
1	B	1005	DA	O4'-C4'-C3'	7.65	110.59	106.00
1	B	1004	DT	O3'-P-O5'	-7.25	90.22	104.00
1	B	1005	DA	P-O5'-C5'	6.34	131.04	120.90
2	A	597	LYS	N-CA-C	6.27	127.93	111.00
2	A	607	PRO	N-CA-CB	5.73	110.18	103.30
1	B	1005	DA	N3-C4-N9	-5.69	122.85	127.40
1	B	1005	DA	N9-C1'-C2'	-5.20	102.72	112.60

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	63	0	32	6	0
2	A	4753	0	4752	95	0
3	A	4	0	0	0	0
4	A	1	0	0	0	0
5	A	307	0	0	7	0
5	B	6	0	0	0	0
All	All	5134	0	4784	96	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 (96) 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	1.62	0.81
2:A:855:ILE:HG23	2:A:908:THR:HG21	1.66	0.77
2:A:677:GLN:HE21	2:A:881:HIS:H	1.34	0.75
2:A:782:LYS:HA	2:A:785:GLN:HB3	1.74	0.70
2:A:681:VAL:HA	2:A:690:ARG:HH21	1.57	0.69
2:A:612:GLU:HB3	2:A:615:GLU:HG2	1.73	0.69
2:A:485:THR:H	2:A:488:GLN:HE21	1.41	0.69
2:A:808:GLN:O	2:A:812:GLN:HG2	1.94	0.68
2:A:472:THR:HG22	2:A:475:GLU:HG3	1.76	0.67
2:A:712:ARG:HD3	2:A:913:PRO:O	1.95	0.67
1:B:1005:DA:P	2:A:455:ARG:HH21	2.20	0.65
2:A:545:VAL:HG23	2:A:877:ILE:HD12	1.79	0.65
2:A:677:GLN:NE2	2:A:881:HIS:H	1.95	0.64
2:A:448:ILE:HD11	2:A:530:GLU:HG3	1.79	0.64
2:A:802:MET:O	2:A:806:ARG:HG3	1.99	0.62
2:A:435:LEU:HD13	2:A:438:ILE:HG12	1.81	0.61
2:A:677:GLN:HG2	2:A:880:VAL:HG23	1.82	0.61
2:A:711:LEU:HD13	2:A:765:ILE:HD11	1.82	0.60
2:A:740:GLU:HG2	5:A:276:HOH:O	2.00	0.60
2:A:725:THR:O	2:A:729:GLU:HG2	2.01	0.60
2:A:779:ILE:HD12	2:A:783:GLU:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:363:ASN:HD22	2:A:542:ARG:HH11	1.51	0.59
2:A:717:LEU:HD21	2:A:818:LEU:HD11	1.84	0.58
2:A:657:THR:HG22	5:A:149:HOH:O	2.02	0.58
2:A:772:GLY:O	2:A:776:GLN:HG2	2.02	0.58
2:A:336:GLU:HG3	5:A:144:HOH:O	2.05	0.57
2:A:872:PRO:HG2	2:A:874:VAL:HG13	1.88	0.56
1:B:1005:DA:N3	1:B:1005:DA:H2'	2.19	0.56
2:A:858:ARG:HB2	2:A:908:THR:HG23	1.88	0.55
2:A:921:GLY:HA3	2:A:926:GLN:HB3	1.87	0.55
2:A:677:GLN:HE21	2:A:881:HIS:N	2.05	0.53
2:A:674:PRO:HG2	2:A:676:LEU:HD13	1.90	0.53
2:A:828:ILE:HG23	2:A:829:LYS:HE2	1.89	0.53
2:A:449:LEU:HD13	2:A:516:LEU:HG	1.90	0.53
2:A:597:LYS:HG3	2:A:598:PRO:HD3	1.90	0.53
2:A:446:SER:OG	2:A:456:HIS:HD2	1.90	0.53
2:A:640:TYR:O	2:A:644:LEU:HB2	2.09	0.53
2:A:696:PRO:HB2	5:A:143:HOH:O	2.08	0.52
2:A:798:VAL:O	2:A:802:MET:HG3	2.08	0.52
2:A:746:LEU:O	2:A:749:VAL:HG12	2.09	0.52
2:A:668:ARG:HE	2:A:849:GLN:HG3	1.73	0.52
2:A:556:SER:HB2	2:A:641:THR:HG22	1.91	0.52
2:A:737:THR:O	2:A:741:VAL:HG23	2.11	0.51
2:A:472:THR:HG22	2:A:475:GLU:CG	2.40	0.51
2:A:418:GLY:HA3	2:A:421:LEU:HD13	1.93	0.51
2:A:586:LEU:HD22	2:A:627:ILE:HD13	1.93	0.50
2:A:418:GLY:HA3	2:A:421:LEU:CD1	2.42	0.50
2:A:828:ILE:CG2	2:A:829:LYS:HE2	2.42	0.49
2:A:421:LEU:HD23	2:A:438:ILE:HG23	1.93	0.49
2:A:346:LEU:CD1	2:A:375:ILE:HG23	2.43	0.48
2:A:363:ASN:ND2	2:A:542:ARG:HH11	2.10	0.48
1:B:1005:DA:N6	2:A:658:SER:HB3	2.28	0.47
1:B:1005:DA:OP2	2:A:455:ARG:NH2	2.47	0.47
2:A:681:VAL:HA	2:A:690:ARG:NH2	2.27	0.47
2:A:597:LYS:CG	2:A:598:PRO:HD3	2.45	0.47
2:A:547:ILE:HD12	2:A:655:VAL:HG21	1.96	0.47
2:A:909:ARG:HB3	2:A:911:ASP:OD1	2.15	0.47
2:A:389:TYR:OH	2:A:491:LEU:HD13	2.15	0.46
2:A:733:ILE:HG13	5:A:92:HOH:O	2.15	0.46
2:A:463:GLU:OE2	2:A:469:LYS:HE2	2.14	0.46
2:A:908:THR:HG22	2:A:909:ARG:H	1.79	0.46
2:A:615:GLU:HB3	2:A:628:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:782:LYS:HD2	2:A:782:LYS:N	2.31	0.45
2:A:717:LEU:HD21	2:A:818:LEU:CD1	2.46	0.45
2:A:580:LEU:HD12	2:A:627:ILE:HG12	1.99	0.45
2:A:734:HIS:CD2	2:A:758:LYS:HA	2.52	0.45
2:A:645:PRO:HG2	5:A:145:HOH:O	2.17	0.44
2:A:537:LEU:O	2:A:541:GLU:HG3	2.18	0.44
2:A:623:LEU:O	2:A:626:VAL:HG22	2.18	0.43
2:A:345:LYS:HD2	5:A:267:HOH:O	2.19	0.43
2:A:633:LEU:CD2	2:A:685:GLU:HG3	2.48	0.43
2:A:781:ARG:C	2:A:783:GLU:H	2.21	0.43
2:A:487:ASN:H	2:A:487:ASN:HD22	1.67	0.43
2:A:715:ALA:HB1	2:A:724:LEU:HD12	2.01	0.43
1:B:1005:DA:P	2:A:455:ARG:NH2	2.90	0.43
1:B:1005:DA:N7	2:A:660:HIS:CE1	2.87	0.42
2:A:773:LEU:HD22	2:A:773:LEU:O	2.19	0.42
2:A:844:ILE:O	2:A:848:MET:HE2	2.19	0.42
2:A:327:TYR:CE1	2:A:496:ARG:HD2	2.55	0.42
2:A:660:HIS:HB2	2:A:670:SER:OG	2.19	0.42
2:A:731:LYS:HD2	2:A:746:LEU:HD22	2.02	0.42
2:A:695:ALA:HB2	2:A:701:ILE:HG12	2.01	0.41
2:A:418:GLY:O	2:A:441:ASP:HA	2.21	0.41
2:A:701:ILE:HG21	2:A:924:TRP:HA	2.02	0.41
2:A:593:LYS:O	2:A:594:GLN:HB3	2.19	0.41
2:A:710:GLU:H	2:A:710:GLU:CD	2.24	0.41
2:A:406:LYS:HB3	2:A:407:PRO:HD3	2.03	0.41
2:A:740:GLU:HG3	2:A:795:TYR:OH	2.21	0.41
2:A:559:LEU:O	2:A:563:LEU:HG	2.21	0.41
2:A:575:GLY:O	2:A:576:GLU:HG2	2.21	0.41
2:A:711:LEU:CD1	2:A:765:ILE:HD11	2.51	0.41
2:A:657:THR:HB	2:A:674:PRO:HD2	2.03	0.41
2:A:487:ASN:ND2	2:A:487:ASN:H	2.18	0.40
2:A:555:HIS:O	2:A:559:LEU:HG	2.21	0.40
2:A:446:SER:OG	2:A:456:HIS:CD2	2.73	0.40
2:A:714:MET:HB2	2:A:848:MET:SD	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	559 (94%)	35 (6%)	3 (0%)	34 26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	576	GLU
2	A	597	LYS
2	A	594	GLN

5.3.2 Protein sidechains

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 9

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

Mol	Chain	Res	Type
2	A	325	ILE
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

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Mol	Chain	Res	Type
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	486	PHE
2	A	510	LEU
2	A	552	LEU
2	A	577	GLU
2	A	578	PHE
2	A	583	THR
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	711	LEU
2	A	749	VAL
2	A	773	LEU
2	A	782	LYS
2	A	783	GLU
2	A	794	ARG
2	A	799	LEU
2	A	867	LEU
2	A	871	GLN
2	A	874	VAL
2	A	879	GLN
2	A	917	GLU

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

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Mol	Chain	Res	Type
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	926	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	US1	B	1006	1	9,20,21	1.99	2 (22%)	12,28,31	5.35	5 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	US1	B	1006	1	-	0/3/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1006	US1	C6-N1	2.03	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1006	US1	C4-N3	5.03	1.42	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1006	US1	C5-C4-N3	-3.13	115.10	123.12
1	B	1006	US1	C4'-O4'-C1'	-2.55	103.01	109.47
1	B	1006	US1	C2'-C1'-N1	2.04	119.12	114.16
1	B	1006	US1	C4-N3-C2	12.00	126.03	114.14
1	B	1006	US1	O4'-C1'-N1	12.96	130.15	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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

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%)	1.23	1 (33%)	0	1	52, 52, 83, 97	0
2	A	601/605 (99%)	0.75	75 (12%)	5	5	16, 34, 96, 100	0
All	All	604/612 (98%)	0.75	76 (12%)	5	5	16, 35, 97, 100	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	607	PRO	18.4
2	A	583	THR	18.1
2	A	610	SER	15.4
2	A	609	THR	12.1
2	A	608	SER	11.7
2	A	582	SER	11.5
2	A	602	THR	11.4
2	A	581	SER	10.2
2	A	598	PRO	9.2
2	A	619	LEU	9.2
2	A	601	LYS	8.2
2	A	611	GLU	7.9
2	A	596	ILE	7.7
2	A	597	LYS	7.0
2	A	594	GLN	6.9
2	A	620	ASP	6.5
2	A	781	ARG	6.2
2	A	775	ARG	6.0
2	A	621	TYR	5.7
2	A	771	PHE	5.7
2	A	599	LEU	5.6
2	A	575	GLY	5.6
2	A	682	ARG	5.6
2	A	591	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
2	A	779	ILE	5.1
2	A	831	SER	5.1
2	A	584	LYS	4.8
2	A	587	GLN	4.7
2	A	616	GLU	4.7
2	A	577	GLU	4.6
2	A	830	SER	4.6
2	A	580	LEU	4.3
2	A	576	GLU	4.2
2	A	613	VAL	4.2
2	A	681	VAL	4.1
2	A	835	ARG	4.1
2	A	592	GLU	4.1
2	A	615	GLU	3.9
2	A	614	LEU	3.8
2	A	833	GLY	3.7
2	A	590	LEU	3.7
2	A	768	MET	3.6
2	A	782	LYS	3.6
2	A	617	LEU	3.5
2	A	586	LEU	3.5
2	A	783	GLU	3.4
2	A	778	ASN	3.4
2	A	628	LEU	3.4
2	A	482	ASN	3.3
2	A	766	TYR	3.2
2	A	612	GLU	3.2
2	A	585	GLN	3.2
2	A	618	ALA	3.2
2	A	518	LYS	3.1
2	A	808	GLN	3.1
2	A	623	LEU	3.0
2	A	481	LYS	3.0
2	A	579	ASN	2.9
2	A	588	THR	2.8
2	A	578	PHE	2.8
2	A	834	ALA	2.8
2	A	776	GLN	2.7
2	A	832	ASN	2.7
2	A	553	HIS	2.6
2	A	595	GLY	2.6
2	A	571	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1005	DA	2.5
2	A	772	GLY	2.5
2	A	480	GLY	2.5
2	A	573	ILE	2.4
2	A	448	ILE	2.3
2	A	627	ILE	2.3
2	A	572	GLU	2.3
2	A	467	LYS	2.2
2	A	593	LYS	2.2
2	A	769	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	US1	B	1006	19/20	0.94	0.12	-	54,59,71,72	0

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	A	2	1/1	0.66	0.14	1.55	100,100,100,100	0
3	ZN	A	1	1/1	0.99	0.05	-2.91	39,39,39,39	0
4	MG	A	321	1/1	0.94	0.10	-6.71	63,63,63,63	0
3	ZN	A	320	1/1	0.90	0.18	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	A	3	1/1	0.96	0.05	-	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.