



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:48 PM UTC

PDB ID : 2KFZ / pdb_00002kfz
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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
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

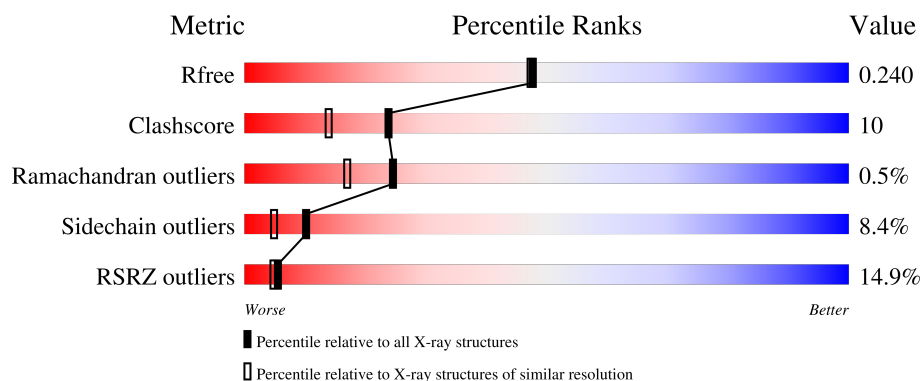
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (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 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	14% 14% 29% 14% 43%
2	A	605	15% 72% 23% ..

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 mutation	UNP P00582

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: 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	B	6	Total	O	0	0
			6	6		

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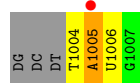
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	307	Total 307	O 307	0	0

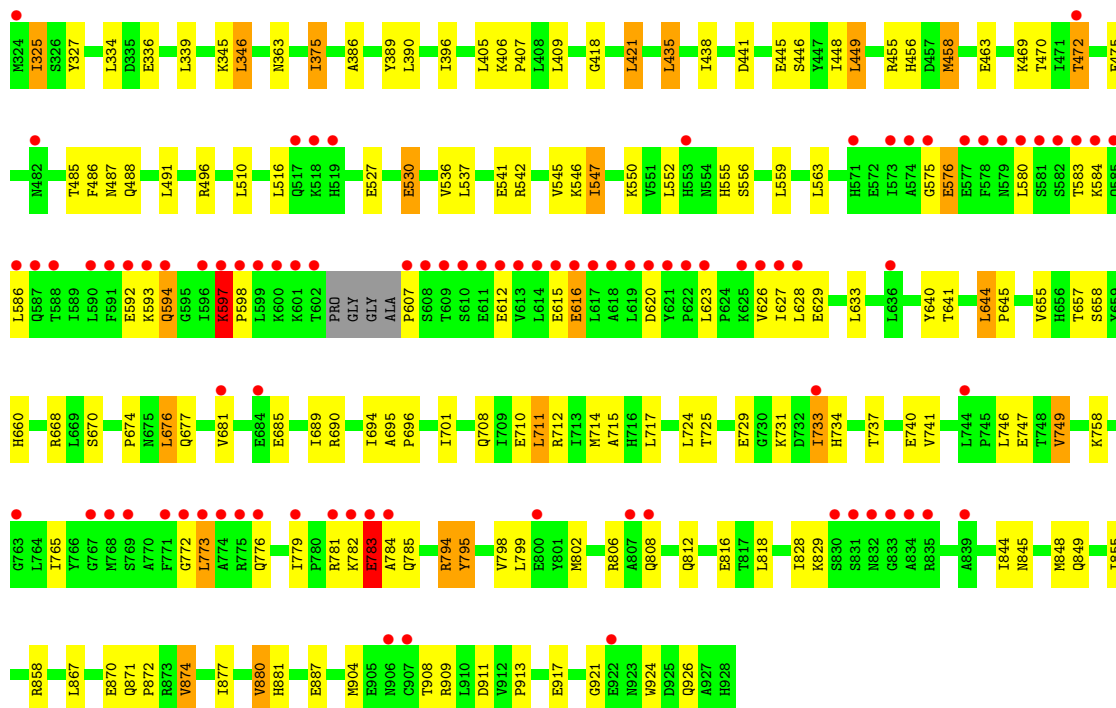
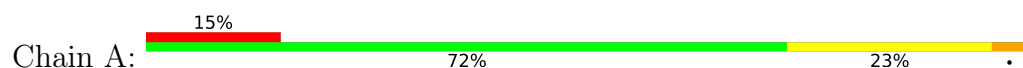
3 Residue-property plots

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



- Molecule 2: KLENOW FRAGMENT OF DNA POLYMERASE I



4 Data and refinement statistics

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 20.00 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.03) 92.6 (20.00-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ 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	5741 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: US1, ZN, MG

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	1.44	0/48	2.75	7/71 (9.9%)
2	A	0.47	0/4839	0.99	20/6547 (0.3%)
All	All	0.49	0/4887	1.03	27/6618 (0.4%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	783	GLU	N-CA-C	-10.19	100.98	113.41
1	B	1004	DT	O3'-P-O5'	-9.19	90.22	104.00
1	B	1005	DA	C3'-C2'-C1'	8.65	114.58	101.60
2	A	597	LYS	N-CA-C	8.20	127.93	109.81
1	B	1005	DA	P-O5'-C5'	7.36	131.04	120.00
1	B	1005	DA	N9-C1'-C2'	-7.19	102.72	113.50
2	A	616	GLU	N-CA-C	-6.65	103.28	111.40
2	A	607	PRO	N-CA-CB	6.53	110.18	103.00
2	A	527	GLU	N-CA-C	6.41	118.34	111.36
2	A	486	PHE	N-CA-C	6.23	118.87	111.33
2	A	689	ILE	N-CA-C	-6.17	104.49	110.42
2	A	795	TYR	CA-C-N	6.03	125.74	119.05
2	A	795	TYR	C-N-CA	6.03	125.74	119.05
2	A	386	ALA	N-CA-C	5.75	118.24	110.88
2	A	694	ILE	N-CA-C	5.74	118.10	109.20
2	A	904	MET	N-CA-C	5.72	117.59	111.36
1	B	1005	DA	O4'-C1'-C2'	-5.71	97.83	106.40
2	A	845	ASN	N-CA-C	5.66	117.31	111.03
2	A	887	GLU	N-CA-C	-5.57	99.33	108.41
1	B	1005	DA	C5'-C4'-C3'	-5.55	106.57	114.90
2	A	530	GLU	N-CA-C	5.54	117.12	111.14
2	A	458	MET	N-CA-C	5.49	117.26	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1005	DA	O4'-C1'-N9	5.47	116.60	108.40
2	A	325	ILE	N-CA-C	-5.45	98.01	109.34
2	A	784	ALA	N-CA-C	-5.43	105.02	111.69
2	A	396	ILE	N-CA-C	-5.10	102.28	109.63
2	A	445	GLU	N-CA-C	-5.09	105.64	111.14

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	96	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	97	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 (97) 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:612:GLU:HB3	2:A:615:GLU:HG2	1.73	0.69
2:A:681:VAL:HA	2:A:690:ARG:HH21	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:712:ARG:HD3	2:A:913:PRO:O	1.95	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
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:H2'	1:B:1005:DA:N3	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:674:PRO:HG2	2:A:676:LEU:HD13	1.90	0.53
2:A:677:GLN:HE21	2:A:881:HIS:N	2.05	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:668:ARG:HE	2:A:849:GLN:HG3	1.73	0.52
2:A:746:LEU:O	2:A:749:VAL:HG12	2.09	0.52
2:A:798:VAL:O	2:A:802:MET:HG3	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:781:ARG:C	2:A:783:GLU:H	2.21	0.48
2:A:363:ASN:ND2	2:A:542:ARG:HH11	2.10	0.48
2:A:802:MET:HE2	2:A:844:ILE:HD13	1.96	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:547:ILE:HD12	2:A:655:VAL:HG21	1.96	0.47
2:A:597:LYS:CG	2:A:598:PRO:HD3	2.45	0.47
2:A:681:VAL:HA	2:A:690:ARG:NH2	2.27	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:710:GLU:H	2:A:710:GLU:CD	2.24	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
2:A:782:LYS:N	2:A:782:LYS:HD2	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:487:ASN:HD22	2:A:487:ASN:H	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:327:TYR:CE1	2:A:496:ARG:HD2	2.55	0.42
2:A:458:MET:HE3	2:A:470:THR:HG21	2.01	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:406:LYS:HB3	2:A:407:PRO:HD3	2.03	0.41
2:A:593:LYS:O	2:A:594:GLN:HB3	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:657:THR:HB	2:A:674:PRO:HD2	2.03	0.41
2:A:711:LEU:CD1	2:A:765:ILE:HD11	2.51	0.41
2:A:487:ASN:H	2:A:487:ASN:ND2	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 [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%)	559 (94%)	35 (6%)	3 (0%)	24 17

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 [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%)	458 (92%)	42 (8%)	10 5

All (42) 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	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	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	733	ILE
2	A	747	GLU
2	A	749	VAL
2	A	773	LEU
2	A	783	GLU
2	A	794	ARG
2	A	799	LEU
2	A	816	GLU
2	A	867	LEU
2	A	870	GLU

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Mol	Chain	Res	Type
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 (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	519	HIS
2	A	528	ASN
2	A	543	ASN
2	A	571	HIS
2	A	677	GLN
2	A	708	GLN
2	A	734	HIS
2	A	871	GLN
2	A	899	GLN
2	A	901	HIS
2	A	906	ASN
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	16,20,21	0.89	1 (6%)	19,28,31	3.26	6 (31%)

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	-	2/7/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1006	US1	C4-N3	2.24	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1006	US1	O4'-C1'-N1	12.56	130.15	107.86
1	B	1006	US1	O4-C4-N3	2.75	123.27	119.27
1	B	1006	US1	C4'-O4'-C1'	-2.74	103.01	109.51
1	B	1006	US1	C1'-N1-C6	-2.49	116.63	121.53
1	B	1006	US1	C2'-C1'-N1	2.12	119.12	113.81
1	B	1006	US1	O4-C4-C5	-2.05	121.63	125.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1006	US1	O4'-C1'-N1-C6
1	B	1006	US1	O4'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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%)	1.72	1 (33%) 1 1	52, 52, 83, 97	0
2	A	601/605 (99%)	0.66	89 (14%) 5 5	16, 34, 96, 100	0
All	All	604/612 (98%)	0.67	90 (14%) 5 5	16, 35, 97, 100	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	583	THR	8.1
2	A	607	PRO	8.1
2	A	598	PRO	7.3
2	A	581	SER	7.1
2	A	601	LYS	6.9
2	A	582	SER	6.9
2	A	610	SER	6.7
2	A	613	VAL	6.4
2	A	609	THR	6.3
2	A	580	LEU	6.0
2	A	596	ILE	5.6
2	A	619	LEU	5.5
2	A	575	GLY	5.4
2	A	830	SER	5.1
2	A	608	SER	4.9
2	A	808	GLN	4.9
2	A	602	THR	4.9
2	A	584	LYS	4.8
2	A	611	GLU	4.6
2	A	574	ALA	4.5
2	A	599	LEU	4.4
2	A	831	SER	4.2
2	A	588	THR	4.1
2	A	600	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
2	A	617	LEU	4.1
2	A	614	LEU	3.9
2	A	585	GLN	3.9
2	A	684	GLU	3.8
2	A	621	TYR	3.8
2	A	626	VAL	3.8
2	A	779	ILE	3.7
2	A	571	HIS	3.6
2	A	612	GLU	3.6
2	A	771	PHE	3.6
2	A	628	LEU	3.5
2	A	591	PHE	3.4
2	A	833	GLY	3.4
2	A	573	ILE	3.4
2	A	618	ALA	3.4
2	A	681	VAL	3.3
2	A	774	ALA	3.3
2	A	784	ALA	3.2
2	A	832	ASN	3.2
2	A	553	HIS	3.2
2	A	768	MET	3.2
1	B	1005	DA	3.2
2	A	616	GLU	3.1
2	A	782	LYS	3.0
2	A	615	GLU	3.0
2	A	783	GLU	2.9
2	A	763	GLY	2.9
2	A	593	LYS	2.9
2	A	577	GLU	2.8
2	A	781	ARG	2.8
2	A	517	GLN	2.8
2	A	776	GLN	2.7
2	A	769	SER	2.7
2	A	586	LEU	2.6
2	A	594	GLN	2.6
2	A	622	PRO	2.6
2	A	636	LEU	2.6
2	A	733	ILE	2.6
2	A	578	PHE	2.5
2	A	587	GLN	2.5
2	A	620	ASP	2.5
2	A	744	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	482	ASN	2.5
2	A	324	MET	2.4
2	A	597	LYS	2.4
2	A	627	ILE	2.4
2	A	835	ARG	2.4
2	A	922	GLU	2.3
2	A	579	ASN	2.3
2	A	518	LYS	2.3
2	A	625	LYS	2.3
2	A	773	LEU	2.3
2	A	775	ARG	2.2
2	A	592	GLU	2.2
2	A	834	ALA	2.2
2	A	839	ALA	2.2
2	A	772	GLY	2.1
2	A	906	ASN	2.1
2	A	472	THR	2.1
2	A	807	ALA	2.1
2	A	623	LEU	2.1
2	A	519	HIS	2.1
2	A	800	GLU	2.0
2	A	590	LEU	2.0
2	A	907	CYS	2.0
2	A	767	GLY	2.0

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. 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
1	US1	B	1006	19/20	0.93	0.12	54,59,71,72	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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
3	ZN	A	2	1/1	0.86	0.21	100,100,100,100	0
3	ZN	A	320	1/1	0.88	0.18	100,100,100,100	0
4	MG	A	321	1/1	0.93	0.17	63,63,63,63	0
3	ZN	A	3	1/1	0.98	0.05	70,70,70,70	0
3	ZN	A	1	1/1	0.99	0.04	39,39,39,39	0

6.5 Other polymers

There are no such residues in this entry.