



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:34 PM GMT

PDB ID : 1KSP  
Title : DNA polymerase I Klenow fragment (E.C.2.7.7.7) mutant/DNA complex  
Authors : Brautigam, C.A.; Steitz, T.A.  
Deposited on : 1997-08-19  
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

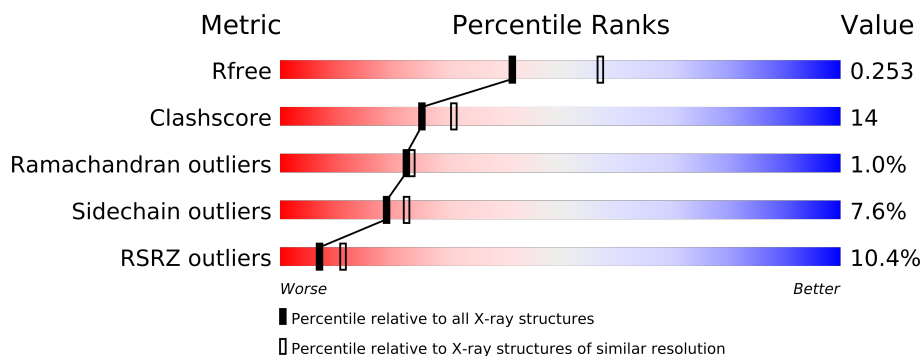
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	3	<div><div></div><div></div></div>
2	A	605	<div><div></div><div></div></div>

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ZN	A	320	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5026 atoms, of which 0 are hydrogen and 0 are deuterium.

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(P\*TP\*TP\*PST)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	3	Total	C	N	O	P	S	0	0	0
			61	30	6	21	3	1			

- 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	UNP P00582

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	4	Total	O	0	0
			4	4		

### 3 Residue-property plots

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.

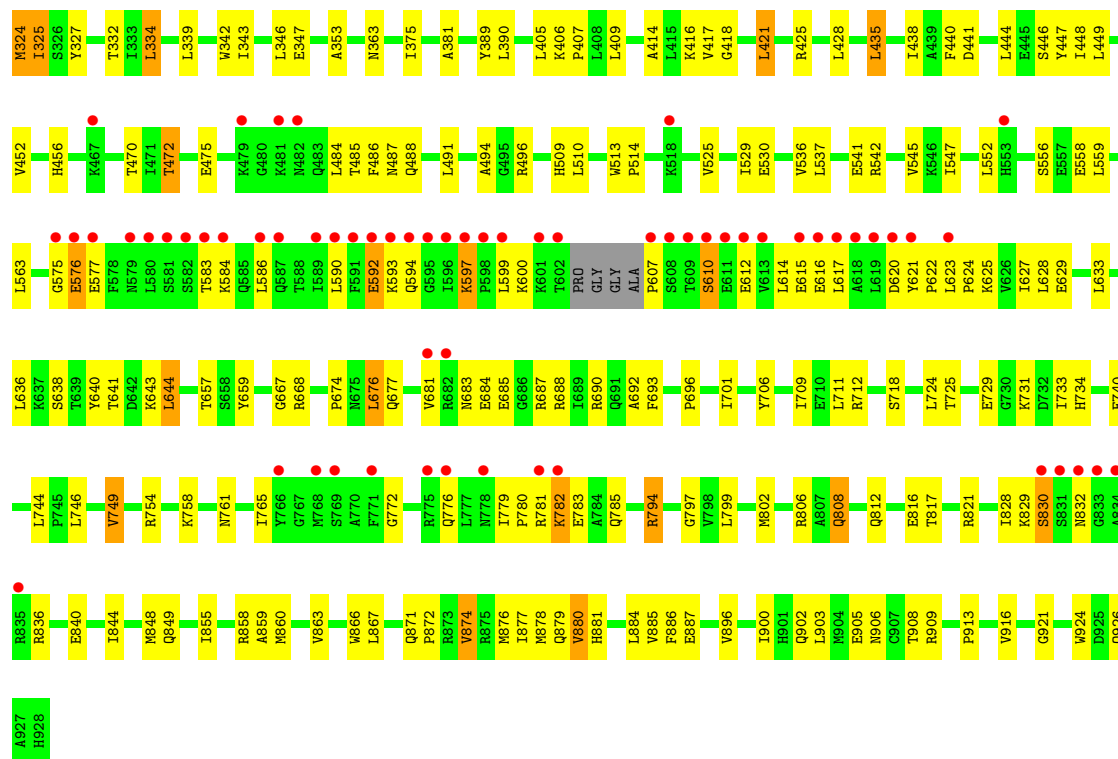
- Molecule 1: DNA (5'-D(P\*TP\*TP\*PST)-3')

Chain B: 



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

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.56Å 101.56Å 85.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.30) 91.1 (19.92-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.30Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.193 , 0.241 0.209 , 0.253	Depositor DCC
$R_{free}$ test set	3541 reflections (11.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 39.8	EDS
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 37149 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	3.50	4/44 (9.1%)	4.83	16/64 (25.0%)
2	A	0.41	1/4839 (0.0%)	0.68	4/6547 (0.1%)
All	All	0.52	5/4883 (0.1%)	0.82	20/6611 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1001	DT	C2'-C1'	-11.61	1.40	1.52
1	B	1002	DT	C5-C7	10.45	1.56	1.50
1	B	1001	DT	C5-C7	6.52	1.53	1.50
2	A	592	GLU	C-N	5.79	1.47	1.34
1	B	1001	DT	O4'-C1'	-5.29	1.35	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1001	DT	O4'-C1'-N1	17.32	120.13	108.00
1	B	1001	DT	C4'-C3'-C2'	-11.95	92.34	103.10
1	B	1001	DT	O4'-C4'-C3'	-9.94	100.04	106.00
1	B	1001	DT	N3-C2-O2	-9.23	116.76	122.30
1	B	1001	DT	OP1-P-OP2	7.86	131.39	119.60
1	B	1001	DT	C5-C4-O4	7.46	130.12	124.90
1	B	1001	DT	N1-C1'-C2'	-7.22	98.89	112.60
1	B	1001	DT	O5'-P-OP1	-6.96	99.44	105.70
2	A	325	ILE	N-CA-C	-6.96	92.21	111.00
1	B	1001	DT	C6-C5-C7	-6.79	118.83	122.90
1	B	1001	DT	N1-C2-O2	6.70	128.46	123.10
1	B	1001	DT	C5'-C4'-O4'	-6.53	96.89	109.30
1	B	1001	DT	C3'-C2'-C1'	6.51	110.31	102.50
1	B	1001	DT	N3-C4-O4	-6.49	116.00	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1001	DT	C5'-C4'-C3'	6.22	125.29	114.10
2	A	607	PRO	N-CA-CB	6.05	110.56	103.30
1	B	1002	DT	C6-C5-C7	-5.78	119.43	122.90
2	A	597	LYS	N-CA-C	5.75	126.53	111.00
1	B	1001	DT	C5-C6-N1	-5.41	120.45	123.70
2	A	324	MET	O-C-N	5.07	130.81	122.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	61	0	37	0	0
2	A	4753	0	4753	132	0
3	A	2	0	0	0	0
4	A	206	0	0	6	0
4	B	4	0	0	0	0
All	All	5026	0	4790	132	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (132) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:740:GLU:HB3	2:A:794:ARG:HG2	1.53	0.90
2:A:485:THR:H	2:A:488:GLN:HE21	1.20	0.88
2:A:677:GLN:HE21	2:A:881:HIS:H	1.27	0.83
2:A:855:ILE:HG23	2:A:908:THR:HG21	1.67	0.77
2:A:472:THR:HG22	2:A:475:GLU:HG3	1.71	0.72
2:A:575:GLY:O	2:A:576:GLU:HG2	1.93	0.68
2:A:485:THR:H	2:A:488:GLN:NE2	1.91	0.68
2:A:731:LYS:HD2	2:A:746:LEU:HD22	1.77	0.67
2:A:586:LEU:HD11	2:A:627:ILE:HG21	1.79	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:363:ASN:HD22	2:A:542:ARG:HH11	1.44	0.64
2:A:610:SER:HA	2:A:776:GLN:HE22	1.61	0.64
2:A:908:THR:HG22	2:A:909:ARG:H	1.64	0.63
2:A:872:PRO:HG2	2:A:874:VAL:HG13	1.79	0.62
2:A:418:GLY:HA3	2:A:421:LEU:HD13	1.81	0.62
2:A:612:GLU:HB3	2:A:615:GLU:HG2	1.82	0.62
2:A:921:GLY:HA3	2:A:926:GLN:HB3	1.80	0.62
2:A:668:ARG:HE	2:A:849:GLN:HG3	1.65	0.61
2:A:677:GLN:HE21	2:A:881:HIS:N	1.98	0.61
2:A:681:VAL:HA	2:A:690:ARG:HH21	1.66	0.60
2:A:446:SER:OG	2:A:456:HIS:HD2	1.85	0.60
2:A:363:ASN:ND2	2:A:542:ARG:HH11	2.00	0.60
2:A:485:THR:N	2:A:488:GLN:HE21	1.95	0.59
2:A:808:GLN:O	2:A:812:GLN:HG2	2.02	0.59
2:A:332:THR:HG22	2:A:334:LEU:HD13	1.84	0.59
2:A:779:ILE:HD12	2:A:783:GLU:HG3	1.85	0.59
2:A:725:THR:O	2:A:729:GLU:HG2	2.03	0.59
2:A:674:PRO:HG2	2:A:676:LEU:HD13	1.86	0.58
2:A:677:GLN:NE2	2:A:881:HIS:H	1.98	0.57
2:A:545:VAL:HG23	2:A:877:ILE:HD12	1.86	0.56
2:A:772:GLY:O	2:A:776:GLN:HG2	2.05	0.56
2:A:802:MET:O	2:A:806:ARG:HG3	2.06	0.56
2:A:858:ARG:HB2	2:A:908:THR:HG23	1.89	0.55
2:A:472:THR:HG22	2:A:475:GLU:CG	2.37	0.54
2:A:706:TYR:HB3	2:A:709:ILE:HB	1.90	0.54
2:A:905:GLU:HB3	2:A:916:VAL:HG23	1.89	0.54
2:A:435:LEU:HD13	2:A:438:ILE:HG12	1.90	0.53
2:A:556:SER:HA	2:A:641:THR:HG21	1.88	0.53
2:A:418:GLY:HA3	2:A:421:LEU:CD1	2.38	0.53
2:A:559:LEU:O	2:A:563:LEU:HG	2.08	0.53
2:A:447:TYR:OH	2:A:667:GLY:HA2	2.07	0.53
2:A:816:GLU:HA	2:A:821:ARG:O	2.09	0.53
2:A:712:ARG:HD3	2:A:913:PRO:O	2.08	0.53
2:A:638:SER:O	2:A:643:LYS:HG2	2.09	0.53
2:A:711:LEU:HD13	2:A:765:ILE:HD11	1.92	0.52
2:A:677:GLN:HG2	2:A:880:VAL:HG23	1.90	0.52
2:A:733:ILE:HG13	4:A:39:HOH:O	2.09	0.52
2:A:696:PRO:HB2	4:A:194:HOH:O	2.09	0.52
2:A:817:THR:OG1	2:A:821:ARG:HB3	2.09	0.51
2:A:701:ILE:HG21	2:A:924:TRP:HA	1.92	0.51
2:A:633:LEU:CD2	2:A:685:GLU:HG3	2.40	0.51
2:A:874:VAL:HA	2:A:887:GLU:O	2.11	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:878:MET:HB2	2:A:885:VAL:HB	1.92	0.50
2:A:674:PRO:HG2	2:A:676:LEU:CD1	2.40	0.50
2:A:593:LYS:NZ	2:A:623:LEU:HD22	2.27	0.50
2:A:844:ILE:O	2:A:848:MET:HE2	2.12	0.50
2:A:780:PRO:O	2:A:783:GLU:HB3	2.11	0.49
2:A:830:SER:HB3	2:A:836:ARG:HB2	1.95	0.49
2:A:629:GLU:O	2:A:633:LEU:HG	2.13	0.48
2:A:600:LYS:CB	2:A:614:LEU:HG	2.44	0.48
2:A:782:LYS:HA	2:A:785:GLN:HB3	1.96	0.48
2:A:406:LYS:HB3	2:A:407:PRO:HD3	1.95	0.48
2:A:617:LEU:HB2	2:A:624:PRO:HG3	1.96	0.48
2:A:640:TYR:O	2:A:644:LEU:HB2	2.13	0.48
2:A:417:VAL:HA	2:A:440:PHE:O	2.14	0.47
2:A:590:LEU:HA	2:A:593:LYS:HE2	1.96	0.47
2:A:513:TRP:HB3	2:A:514:PRO:HD3	1.95	0.47
2:A:343:ILE:O	2:A:347:GLU:HG3	2.15	0.47
2:A:448:ILE:HD11	2:A:530:GLU:HG3	1.97	0.47
2:A:828:ILE:CG2	2:A:829:LYS:HE2	2.45	0.47
2:A:327:TYR:CE1	2:A:496:ARG:HD2	2.50	0.47
2:A:683:ASN:OD1	2:A:684:GLU:N	2.48	0.46
2:A:863:VAL:HA	2:A:903:LEU:HD13	1.97	0.46
2:A:879:GLN:HG2	2:A:884:LEU:CD2	2.46	0.46
2:A:615:GLU:HB3	2:A:628:LEU:HD21	1.97	0.46
2:A:556:SER:CA	2:A:641:THR:HG21	2.46	0.46
2:A:590:LEU:O	2:A:593:LYS:HG2	2.16	0.45
2:A:324:MET:HE3	2:A:496:ARG:NH2	2.32	0.45
2:A:876:MET:HG3	2:A:886:PHE:CE2	2.51	0.45
2:A:537:LEU:O	2:A:541:GLU:HG3	2.17	0.45
2:A:623:LEU:HG	2:A:627:ILE:HD11	1.99	0.45
2:A:614:LEU:O	2:A:624:PRO:HB2	2.17	0.45
2:A:860:MET:SD	2:A:879:GLN:HG3	2.56	0.45
2:A:545:VAL:HG21	2:A:693:PHE:HD2	1.81	0.45
2:A:525:VAL:O	2:A:529:ILE:HB	2.16	0.44
2:A:486:PHE:CE2	2:A:494:ALA:HB1	2.52	0.44
2:A:593:LYS:HZ3	2:A:623:LEU:HD22	1.82	0.44
2:A:733:ILE:HD12	2:A:734:HIS:N	2.31	0.44
2:A:389:TYR:OH	2:A:491:LEU:HD13	2.17	0.44
2:A:902:GLN:O	2:A:906:ASN:HB2	2.17	0.44
2:A:740:GLU:HG2	4:A:219:HOH:O	2.17	0.44
2:A:734:HIS:CD2	2:A:758:LYS:HA	2.52	0.44
2:A:487:ASN:H	2:A:487:ASN:HD22	1.66	0.44
2:A:711:LEU:HD23	2:A:733:ILE:HD13	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:830:SER:C	2:A:832:ASN:H	2.20	0.44
2:A:896:VAL:O	2:A:900:ILE:HG12	2.17	0.44
2:A:830:SER:OG	2:A:832:ASN:HB3	2.18	0.44
2:A:622:PRO:O	2:A:625:LYS:HB3	2.18	0.44
2:A:746:LEU:O	2:A:749:VAL:HG13	2.18	0.43
2:A:781:ARG:O	2:A:782:LYS:HB2	2.18	0.43
2:A:593:LYS:NZ	2:A:623:LEU:CD2	2.81	0.43
2:A:836:ARG:O	2:A:840:GLU:HG3	2.17	0.43
2:A:866:TRP:HH2	2:A:896:VAL:HG13	1.83	0.43
2:A:657:THR:HG22	4:A:49:HOH:O	2.17	0.43
2:A:828:ILE:HG23	2:A:829:LYS:HE2	2.00	0.43
2:A:734:HIS:CD2	2:A:761:ASN:HD22	2.37	0.42
2:A:353:ALA:HA	2:A:417:VAL:O	2.19	0.42
2:A:879:GLN:NE2	4:A:91:HOH:O	2.49	0.42
2:A:558:GLU:CD	2:A:688:ARG:HH12	2.22	0.42
2:A:687:ARG:HG2	2:A:690:ARG:HH12	1.84	0.42
2:A:657:THR:HG23	2:A:659:TYR:CE2	2.54	0.42
2:A:782:LYS:N	2:A:782:LYS:HD2	2.34	0.42
2:A:859:ALA:O	2:A:863:VAL:HG23	2.19	0.42
2:A:324:MET:CE	2:A:496:ARG:NH2	2.82	0.42
2:A:633:LEU:HD22	2:A:685:GLU:HG3	2.01	0.42
2:A:428:LEU:HD12	2:A:435:LEU:HG	2.01	0.42
2:A:808:GLN:OE1	2:A:812:GLN:NE2	2.54	0.41
2:A:908:THR:HG22	2:A:909:ARG:N	2.32	0.41
2:A:414:ALA:O	2:A:416:LYS:HD2	2.20	0.41
2:A:879:GLN:HG2	2:A:884:LEU:HD23	2.01	0.41
2:A:418:GLY:O	2:A:441:ASP:HA	2.21	0.41
2:A:472:THR:O	2:A:475:GLU:HB2	2.21	0.41
2:A:718:SER:HB2	2:A:797:GLY:C	2.41	0.41
2:A:452:VAL:HG22	4:A:19:HOH:O	2.21	0.41
2:A:617:LEU:HB3	2:A:621:TYR:HB2	2.02	0.41
2:A:547:ILE:HA	2:A:692:ALA:O	2.20	0.41
2:A:342:TRP:CZ2	2:A:381:ALA:HB2	2.56	0.41
2:A:444:LEU:HD13	2:A:530:GLU:HB3	2.03	0.40
2:A:484:LEU:HA	2:A:488:GLN:NE2	2.37	0.40
2:A:417:VAL:HG11	2:A:509:HIS:HB2	2.03	0.40
2:A:547:ILE:HD13	2:A:644:LEU:HG	2.03	0.40
2:A:902:GLN:HA	2:A:906:ASN:HD22	1.86	0.40
2:A:617:LEU:O	2:A:621:TYR:N	2.53	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%)	557 (93%)	34 (6%)	6 (1%)	22	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	830	SER
2	A	594	GLN
2	A	597	LYS
2	A	599	LEU
2	A	576	GLU
2	A	610	SER

### 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%)	462 (92%)	38 (8%)	19	22

All (38) 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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	421	LEU
2	A	425	ARG
2	A	435	LEU
2	A	449	LEU
2	A	470	THR
2	A	472	THR
2	A	510	LEU
2	A	536	VAL
2	A	552	LEU
2	A	577	GLU
2	A	583	THR
2	A	584	LYS
2	A	592	GLU
2	A	616	GLU
2	A	620	ASP
2	A	636	LEU
2	A	644	LEU
2	A	676	LEU
2	A	724	LEU
2	A	744	LEU
2	A	749	VAL
2	A	754	ARG
2	A	782	LYS
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	880	VAL

Some 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	543	ASN
2	A	571	HIS
2	A	677	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	708	GLN
2	A	716	HIS
2	A	734	HIS
2	A	776	GLN
2	A	845	ASN
2	A	879	GLN
2	A	899	GLN
2	A	906	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	PST	B	1003	1	18,21,22	1.14	1 (5%)	22,30,33	1.55	1 (4%)

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	PST	B	1003	1	-	0/4/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1003	PST	C6-N1	2.38	1.40	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1003	PST	C6-N1-C2	-6.21	120.64	122.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	3/3 (100%)	0.07	0 100 100	27, 27, 34, 57	0
2	A	601/605 (99%)	0.59	62 (10%) 7 11	14, 32, 93, 100	0
All	All	604/608 (99%)	0.59	62 (10%) 7 11	14, 33, 93, 100	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	583	THR	17.2
2	A	607	PRO	15.4
2	A	610	SER	12.7
2	A	608	SER	12.4
2	A	609	THR	11.9
2	A	602	THR	11.3
2	A	582	SER	9.5
2	A	598	PRO	9.4
2	A	611	GLU	9.0
2	A	594	GLN	8.0
2	A	601	LYS	7.3
2	A	771	PHE	7.2
2	A	619	LEU	7.1
2	A	621	TYR	6.4
2	A	682	ARG	6.0
2	A	587	GLN	5.9
2	A	596	ILE	5.7
2	A	597	LYS	5.5
2	A	620	ASP	5.5
2	A	576	GLU	5.4
2	A	834	ALA	5.3
2	A	831	SER	5.3
2	A	775	ARG	5.2
2	A	768	MET	5.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	A	577	GLU	5.1
2	A	580	LEU	5.1
2	A	584	LYS	4.9
2	A	575	GLY	4.8
2	A	590	LEU	4.8
2	A	776	GLN	4.7
2	A	681	VAL	4.7
2	A	595	GLY	4.5
2	A	481	LYS	4.4
2	A	781	ARG	4.3
2	A	766	TYR	4.3
2	A	833	GLY	4.0
2	A	592	GLU	3.9
2	A	586	LEU	3.8
2	A	591	PHE	3.8
2	A	830	SER	3.7
2	A	782	LYS	3.5
2	A	835	ARG	3.3
2	A	581	SER	3.2
2	A	617	LEU	3.2
2	A	482	ASN	3.1
2	A	832	ASN	3.1
2	A	467	LYS	3.0
2	A	579	ASN	3.0
2	A	613	VAL	3.0
2	A	599	LEU	3.0
2	A	593	LYS	2.8
2	A	618	ALA	2.8
2	A	615	GLU	2.6
2	A	616	GLU	2.5
2	A	778	ASN	2.3
2	A	553	HIS	2.2
2	A	769	SER	2.1
2	A	623	LEU	2.1
2	A	479	LYS	2.1
2	A	518	LYS	2.1
2	A	612	GLU	2.0
2	A	589	ILE	2.0



## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	PST	B	1003	20/21	0.09	-1.24	18,26,33,34	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	A	320	1/1	0.24	2.31	100,100,100,100	0
3	ZN	A	3	1/1	0.04	-2.77	74,74,74,74	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.