



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:32 PM GMT

PDB ID : 1KRP  
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 : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

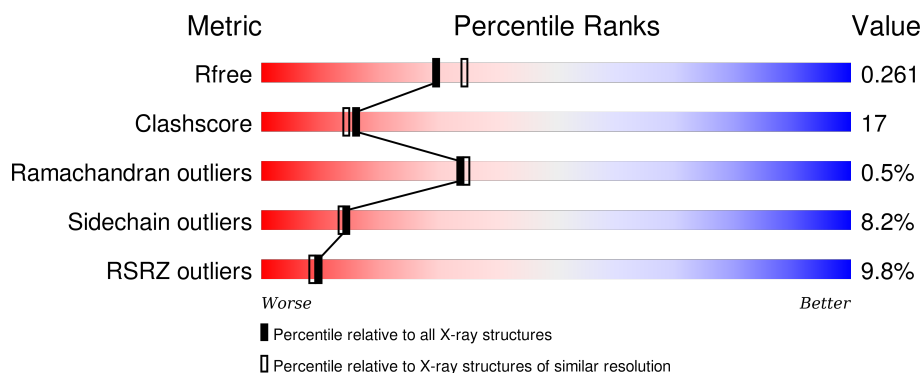
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	3	<div> <div></div> <div>100%</div> </div>
2	A	605	<div> <div>10%</div> <div>62%</div> <div>34%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5086 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(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	B	1	Total	Zn	0	0
			1	1		
3	A	3	Total	Zn	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	262	Total	O	0	0
			262	262		
4	B	6	Total	O	0	0
			6	6		

### 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.

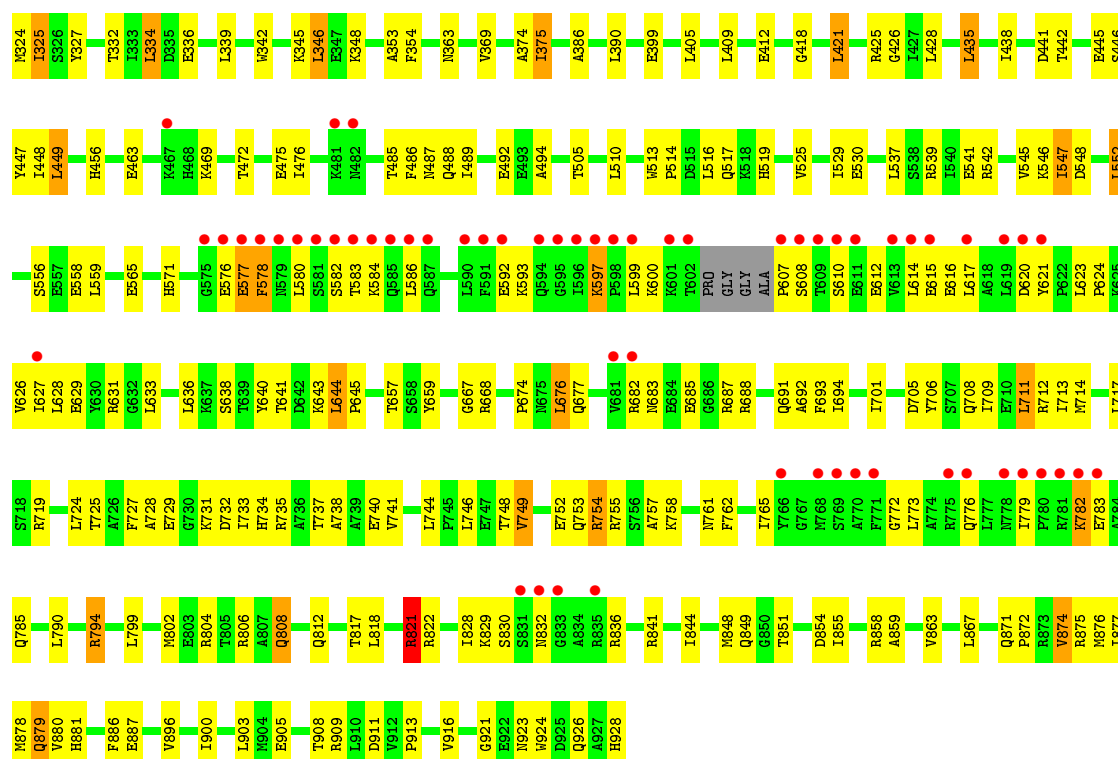
- Molecule 1: DNA (5'-D(P\*TP\*TP\*PST)-3')

Chain B:  100%

T1001  
T1002  
T1003

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

Chain A:  10% 62% 34%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.60 Å   101.60 Å   85.20 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.4 (20.00-2.20) 87.8 (19.93-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 2.21 Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.190 , 0.255 0.203 , 0.261	Depositor DCC
$R_{free}$ test set	3917 reflections (10.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 61.2	EDS
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 41114 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, 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	2.86	3/44 (6.8%)	3.59	9/64 (14.1%)
2	A	0.51	0/4839	0.76	3/6547 (0.0%)
All	All	0.58	3/4883 (0.1%)	0.83	12/6611 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1001	DT	OP3-P	9.38	1.72	1.61
1	B	1001	DT	C5-C7	8.84	1.55	1.50
1	B	1002	DT	C5-C7	5.72	1.53	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1001	DT	C6-C5-C7	-10.58	116.55	122.90
1	B	1002	DT	C6-C5-C7	-8.18	117.99	122.90
1	B	1001	DT	C4'-C3'-C2'	-8.09	95.82	103.10
1	B	1001	DT	C4-C5-C7	7.57	123.54	119.00
1	B	1001	DT	O4'-C1'-N1	7.27	113.09	108.00
1	B	1001	DT	P-O3'-C3'	7.05	128.16	119.70
1	B	1001	DT	P-O5'-C5'	6.38	131.11	120.90
2	A	597	LYS	N-CA-C	6.30	128.00	111.00
2	A	821	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	A	607	PRO	N-CA-CB	5.76	110.21	103.30
1	B	1002	DT	N1-C2-O2	-5.31	118.85	123.10
1	B	1001	DT	O4'-C1'-C2'	-5.01	101.89	105.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	61	0	37	1	0
2	A	4753	0	4753	161	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
4	A	262	0	0	14	0
4	B	6	0	0	0	0
All	All	5086	0	4790	162	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 17.

All (162) 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	1.45	0.97
2:A:615:GLU:HB3	2:A:628:LEU:HD21	1.57	0.84
2:A:711:LEU:HD13	2:A:765:ILE:HD11	1.61	0.80
2:A:485:THR:H	2:A:488:GLN:HE21	1.29	0.80
2:A:855:ILE:HG23	2:A:908:THR:HG21	1.66	0.77
2:A:435:LEU:HD13	2:A:438:ILE:HG12	1.69	0.75
2:A:363:ASN:HD22	2:A:542:ARG:HH11	1.32	0.75
2:A:363:ASN:ND2	2:A:542:ARG:HH11	1.87	0.73
2:A:545:VAL:HG23	2:A:877:ILE:HD12	1.70	0.72
2:A:808:GLN:O	2:A:812:GLN:HG2	1.91	0.70
2:A:600:LYS:CB	2:A:614:LEU:HG	2.22	0.69
2:A:802:MET:O	2:A:806:ARG:HG3	1.91	0.69
2:A:336:GLU:HG3	4:A:216:HOH:O	1.91	0.69
2:A:712:ARG:HD3	2:A:913:PRO:O	1.94	0.68
2:A:674:PRO:HG2	2:A:676:LEU:HD13	1.74	0.68
2:A:677:GLN:HE21	2:A:881:HIS:H	1.41	0.68
2:A:858:ARG:HB2	2:A:908:THR:HG23	1.76	0.67
2:A:668:ARG:HE	2:A:849:GLN:HG3	1.59	0.67
2:A:610:SER:HA	2:A:776:GLN:HE22	1.60	0.67
2:A:735:ARG:HG2	2:A:754:ARG:HG3	1.80	0.64
2:A:717:LEU:HD21	2:A:818:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:677:GLN:NE2	2:A:881:HIS:H	1.96	0.62
2:A:872:PRO:HG2	2:A:874:VAL:HG13	1.80	0.62
2:A:731:LYS:HD2	2:A:746:LEU:HD22	1.82	0.62
2:A:828:ILE:HG23	2:A:829:LYS:HE2	1.82	0.62
2:A:782:LYS:HA	2:A:785:GLN:HB3	1.82	0.62
2:A:421:LEU:HD23	2:A:438:ILE:HG23	1.82	0.60
2:A:548:ASP:HB2	2:A:694:ILE:HD13	1.84	0.60
2:A:399:GLU:HB3	4:A:260:HOH:O	2.03	0.59
2:A:880:VAL:HG11	2:A:924:TRP:CZ2	2.38	0.58
2:A:418:GLY:HA3	2:A:421:LEU:HD13	1.86	0.58
2:A:677:GLN:HG2	2:A:880:VAL:HG23	1.85	0.57
2:A:633:LEU:CD2	2:A:685:GLU:HG3	2.34	0.57
2:A:896:VAL:O	2:A:900:ILE:HG12	2.03	0.57
2:A:612:GLU:HB3	2:A:615:GLU:HG2	1.87	0.57
2:A:463:GLU:OE2	2:A:469:LYS:HE2	2.05	0.57
2:A:863:VAL:HA	2:A:903:LEU:HD13	1.86	0.56
2:A:472:THR:HG23	2:A:475:GLU:H	1.69	0.56
1:B:1003:PST:SP	1:B:1003:PST:H71	2.45	0.55
2:A:624:PRO:HA	2:A:627:ILE:HD12	1.89	0.55
2:A:711:LEU:HD22	2:A:762:PHE:CE1	2.42	0.54
2:A:519:HIS:HD2	4:A:266:HOH:O	1.91	0.54
2:A:353:ALA:HB3	2:A:374:ALA:HB3	1.90	0.54
2:A:772:GLY:O	2:A:776:GLN:HG2	2.08	0.54
2:A:446:SER:OG	2:A:456:HIS:CD2	2.61	0.54
2:A:674:PRO:HG2	2:A:676:LEU:CD1	2.39	0.53
2:A:732:ASP:OD2	2:A:735:ARG:HG3	2.09	0.53
2:A:412:GLU:HG2	4:A:270:HOH:O	2.09	0.52
2:A:924:TRP:O	2:A:928:HIS:HB2	2.09	0.52
2:A:623:LEU:O	2:A:626:VAL:HG22	2.10	0.52
2:A:876:MET:HG3	2:A:886:PHE:CE2	2.45	0.52
2:A:734:HIS:CD2	2:A:758:LYS:HA	2.45	0.52
2:A:582:SER:HB3	2:A:586:LEU:HD12	1.92	0.52
2:A:556:SER:HB2	2:A:641:THR:HG22	1.91	0.51
2:A:448:ILE:HD11	2:A:530:GLU:HG3	1.93	0.51
2:A:519:HIS:CD2	4:A:266:HOH:O	2.64	0.51
2:A:486:PHE:CE2	2:A:494:ALA:HB1	2.45	0.51
2:A:830:SER:HB3	2:A:836:ARG:HB2	1.93	0.51
2:A:487:ASN:H	2:A:487:ASN:HD22	1.57	0.51
2:A:348:LYS:HG3	4:A:196:HOH:O	2.10	0.51
2:A:752:GLU:HA	2:A:755:ARG:NH2	2.26	0.51
2:A:327:TYR:CD1	2:A:492:GLU:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:513:TRP:O	2:A:517:GLN:HG3	2.12	0.50
2:A:556:SER:HA	2:A:641:THR:HG21	1.94	0.49
2:A:556:SER:HB2	2:A:641:THR:CG2	2.42	0.49
2:A:485:THR:H	2:A:488:GLN:NE2	2.06	0.49
2:A:725:THR:O	2:A:729:GLU:HG2	2.13	0.49
2:A:547:ILE:HD11	2:A:693:PHE:CZ	2.48	0.48
2:A:545:VAL:HG21	2:A:693:PHE:HD2	1.78	0.48
2:A:677:GLN:HE21	2:A:881:HIS:N	2.08	0.48
2:A:734:HIS:CD2	2:A:761:ASN:HD22	2.30	0.48
2:A:706:TYR:HB3	2:A:709:ILE:HB	1.96	0.48
2:A:782:LYS:HD2	2:A:782:LYS:N	2.29	0.48
2:A:719:ARG:CZ	2:A:804:ARG:HH12	2.26	0.48
2:A:737:THR:O	2:A:741:VAL:HG23	2.14	0.48
2:A:808:GLN:OE1	2:A:812:GLN:NE2	2.46	0.48
2:A:717:LEU:HD21	2:A:818:LEU:CD1	2.42	0.48
2:A:746:LEU:O	2:A:749:VAL:HG12	2.14	0.48
2:A:446:SER:OG	2:A:456:HIS:HD2	1.96	0.48
2:A:547:ILE:HA	2:A:692:ALA:O	2.14	0.48
2:A:556:SER:CA	2:A:641:THR:HG21	2.42	0.48
2:A:485:THR:OG1	2:A:487:ASN:ND2	2.46	0.48
2:A:485:THR:N	2:A:488:GLN:HE21	2.04	0.47
2:A:705:ASP:O	2:A:916:VAL:HA	2.13	0.47
2:A:342:TRP:O	2:A:346:LEU:HD22	2.14	0.47
2:A:435:LEU:HD13	2:A:438:ILE:CG1	2.43	0.47
2:A:558:GLU:CD	2:A:688:ARG:HH12	2.17	0.47
2:A:727:PHE:CZ	2:A:733:ILE:HG12	2.50	0.47
2:A:519:HIS:CD2	2:A:822:ARG:HH22	2.32	0.46
2:A:539:ARG:HD3	4:A:124:HOH:O	2.15	0.46
2:A:841:ARG:NH1	4:A:167:HOH:O	2.48	0.46
2:A:844:ILE:O	2:A:848:MET:HE2	2.15	0.46
2:A:908:THR:HG22	2:A:909:ARG:H	1.79	0.46
2:A:691:GLN:HA	2:A:923:ASN:OD1	2.14	0.46
2:A:418:GLY:HA2	2:A:505:THR:HG21	1.98	0.46
2:A:683:ASN:O	2:A:687:ARG:HG3	2.16	0.46
2:A:418:GLY:HA3	2:A:421:LEU:CD1	2.46	0.46
2:A:476:ILE:HD12	2:A:489:ILE:HD13	1.99	0.45
2:A:878:MET:HG2	4:A:46:HOH:O	2.17	0.45
2:A:817:THR:OG1	2:A:821:ARG:HB3	2.16	0.45
2:A:921:GLY:HA3	2:A:926:GLN:HB3	1.99	0.45
2:A:571:HIS:CE1	2:A:577:GLU:HG3	2.50	0.45
2:A:513:TRP:HB3	2:A:514:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:905:GLU:HB3	2:A:916:VAL:HG23	1.98	0.45
2:A:828:ILE:CG2	2:A:829:LYS:HE2	2.46	0.45
2:A:706:TYR:OH	2:A:859:ALA:HB2	2.16	0.45
2:A:725:THR:HA	2:A:728:ALA:HB3	1.99	0.45
2:A:638:SER:O	2:A:643:LYS:HG2	2.16	0.45
2:A:559:LEU:HD23	2:A:559:LEU:HA	1.88	0.45
2:A:701:ILE:HG21	2:A:924:TRP:HA	1.98	0.44
2:A:332:THR:HG22	2:A:334:LEU:HD13	1.98	0.44
2:A:565:GLU:HG2	4:A:131:HOH:O	2.17	0.44
2:A:711:LEU:HB2	4:A:34:HOH:O	2.15	0.44
2:A:744:LEU:HD12	2:A:748:THR:OG1	2.18	0.44
2:A:363:ASN:ND2	2:A:542:ARG:NH1	2.62	0.44
2:A:738:ALA:HB2	2:A:757:ALA:HB2	1.98	0.44
2:A:472:THR:HG22	2:A:475:GLU:CG	2.48	0.44
2:A:552:LEU:O	2:A:641:THR:HG23	2.17	0.44
2:A:580:LEU:N	2:A:580:LEU:HD22	2.33	0.44
2:A:909:ARG:HB3	2:A:911:ASP:OD1	2.18	0.43
2:A:645:PRO:HG2	4:A:217:HOH:O	2.17	0.43
2:A:874:VAL:HA	2:A:887:GLU:O	2.18	0.43
2:A:854:ASP:O	2:A:858:ARG:HG3	2.19	0.43
2:A:682:ARG:HH12	2:A:758:LYS:NZ	2.17	0.43
2:A:447:TYR:OH	2:A:667:GLY:HA2	2.19	0.43
2:A:713:ILE:HD13	2:A:851:THR:HB	2.01	0.43
2:A:593:LYS:HG3	2:A:593:LYS:O	2.19	0.43
2:A:487:ASN:ND2	2:A:487:ASN:H	2.16	0.42
2:A:727:PHE:CE1	2:A:733:ILE:HG12	2.54	0.42
2:A:324:MET:HE3	2:A:324:MET:HB3	1.62	0.42
2:A:449:LEU:HD13	2:A:516:LEU:HD23	2.02	0.42
2:A:537:LEU:HD23	2:A:537:LEU:HA	1.85	0.42
2:A:354:PHE:CZ	2:A:428:LEU:HD11	2.55	0.42
2:A:640:TYR:O	2:A:644:LEU:HB2	2.20	0.42
2:A:363:ASN:HD21	2:A:426:GLY:HA3	1.84	0.42
2:A:546:LYS:HB3	2:A:694:ILE:O	2.19	0.42
2:A:448:ILE:HD11	2:A:530:GLU:CG	2.50	0.42
2:A:908:THR:HG22	2:A:909:ARG:N	2.35	0.42
2:A:418:GLY:O	2:A:441:ASP:HA	2.20	0.42
2:A:578:PHE:N	2:A:578:PHE:CD1	2.88	0.41
2:A:657:THR:HG23	2:A:659:TYR:CE2	2.56	0.41
2:A:342:TRP:CZ3	2:A:375:ILE:HD11	2.55	0.41
2:A:806:ARG:HD3	2:A:844:ILE:HD11	2.01	0.41
2:A:830:SER:C	2:A:832:ASN:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:608:SER:O	2:A:612:GLU:HG2	2.20	0.41
2:A:449:LEU:HD12	2:A:449:LEU:HA	1.87	0.41
2:A:734:HIS:HD2	2:A:758:LYS:HA	1.86	0.41
2:A:324:MET:HB3	2:A:325:ILE:H	1.66	0.41
2:A:525:VAL:O	2:A:529:ILE:HB	2.20	0.41
2:A:627:ILE:O	2:A:631:ARG:HG3	2.21	0.41
2:A:879:GLN:NE2	4:A:130:HOH:O	2.54	0.41
2:A:369:VAL:HA	2:A:386:ALA:HB3	2.02	0.41
2:A:682:ARG:HH12	2:A:758:LYS:HZ3	1.68	0.41
2:A:537:LEU:O	2:A:541:GLU:HG3	2.21	0.41
2:A:708:GLN:HE21	2:A:708:GLN:HB3	1.67	0.41
2:A:779:ILE:HD12	2:A:783:GLU:HG3	2.02	0.41
2:A:442:THR:HA	2:A:445:GLU:HB2	2.03	0.40
2:A:875:ARG:HD3	4:A:226:HOH:O	2.21	0.40
2:A:749:VAL:HG23	2:A:753:GLN:HB2	2.03	0.40
2:A:617:LEU:O	2:A:621:TYR:N	2.54	0.40
2:A:714:MET:HB2	2:A:848:MET:SD	2.61	0.40
2:A:345:LYS:HE3	2:A:375:ILE:CD1	2.52	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%)	562 (94%)	32 (5%)	3 (0%)	34 35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	599	LEU
2	A	576	GLU
2	A	597	LYS

### 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%)	459 (92%)	41 (8%)	14	13

All (41) 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	425	ARG
2	A	435	LEU
2	A	449	LEU
2	A	510	LEU
2	A	547	ILE
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	636	LEU
2	A	644	LEU
2	A	676	LEU
2	A	711	LEU
2	A	724	LEU
2	A	749	VAL
2	A	754	ARG

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Mol	Chain	Res	Type
2	A	773	LEU
2	A	782	LYS
2	A	790	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	734	HIS
2	A	776	GLN
2	A	845	ASN
2	A	879	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	PST	B	1003	1,3	12,21,22	1.88	2 (16%)	16,30,33	4.00	2 (12%)

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	1,3	-	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	1003	PST	C6-N1	3.56	1.40	1.35
1	B	1003	PST	C4-N3	4.45	1.41	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1003	PST	C5-C4-N3	-9.19	114.90	125.14
1	B	1003	PST	C4-N3-C2	12.46	126.02	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1003	PST	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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

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	2/3 (66%)	-0.60	0	100 100	37, 37, 37, 61	0
2	A	601/605 (99%)	0.25	59 (9%)	10 8	19, 37, 99, 100	0
All	All	603/608 (99%)	0.25	59 (9%)	10 8	19, 37, 99, 100	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	583	THR	15.4
2	A	607	PRO	12.0
2	A	609	THR	11.8
2	A	610	SER	11.4
2	A	582	SER	10.6
2	A	608	SER	9.8
2	A	611	GLU	8.0
2	A	602	THR	7.8
2	A	598	PRO	7.3
2	A	619	LEU	6.3
2	A	581	SER	5.9
2	A	601	LYS	5.9
2	A	597	LYS	5.7
2	A	576	GLU	5.6
2	A	781	ARG	5.4
2	A	580	LEU	5.3
2	A	682	ARG	5.2
2	A	594	GLN	5.0
2	A	776	GLN	4.9
2	A	586	LEU	4.7
2	A	775	ARG	4.6
2	A	782	LYS	4.6
2	A	577	GLU	4.6
2	A	833	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
2	A	579	ASN	4.4
2	A	620	ASP	4.3
2	A	835	ARG	4.3
2	A	766	TYR	4.0
2	A	596	ILE	4.0
2	A	584	LYS	3.7
2	A	831	SER	3.6
2	A	590	LEU	3.5
2	A	681	VAL	3.5
2	A	779	ILE	3.4
2	A	481	LYS	3.4
2	A	621	TYR	3.3
2	A	768	MET	3.3
2	A	575	GLY	3.2
2	A	771	PHE	3.1
2	A	592	GLU	2.9
2	A	599	LEU	2.8
2	A	832	ASN	2.8
2	A	780	PRO	2.8
2	A	482	ASN	2.7
2	A	769	SER	2.6
2	A	591	PHE	2.6
2	A	587	GLN	2.6
2	A	613	VAL	2.4
2	A	615	GLU	2.4
2	A	617	LEU	2.3
2	A	585	GLN	2.2
2	A	778	ASN	2.2
2	A	614	LEU	2.2
2	A	627	ILE	2.1
2	A	770	ALA	2.1
2	A	578	PHE	2.1
2	A	595	GLY	2.1
2	A	783	GLU	2.1
2	A	467	LYS	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PST	B	1003	20/21	0.98	0.08	-	23,29,35,39	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<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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	1	1/1	0.98	0.05	-2.98	61,61,61,61	0
3	ZN	B	2	1/1	0.99	0.04	-3.19	45,45,45,45	0
3	ZN	A	3	1/1	0.82	0.06	-	87,87,87,87	0
3	ZN	A	320	1/1	0.77	0.10	-	100,100,100,100	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.