Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 02:02 PM EDT

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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

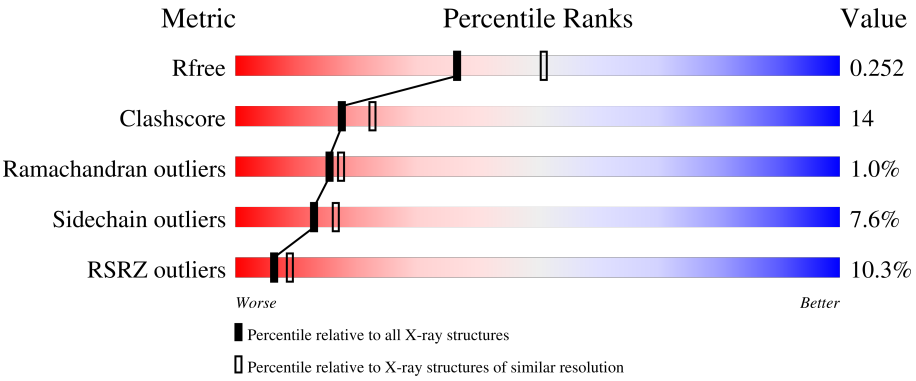
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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 <=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	100%
2	A	605	10% 66% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5026 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 mutation	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.

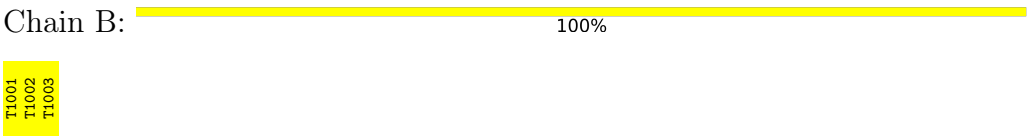
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	O	0	0
			4	4		
4	A	206	Total	O	0	0
			206	206		

3 Residue-property plots (i)

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.

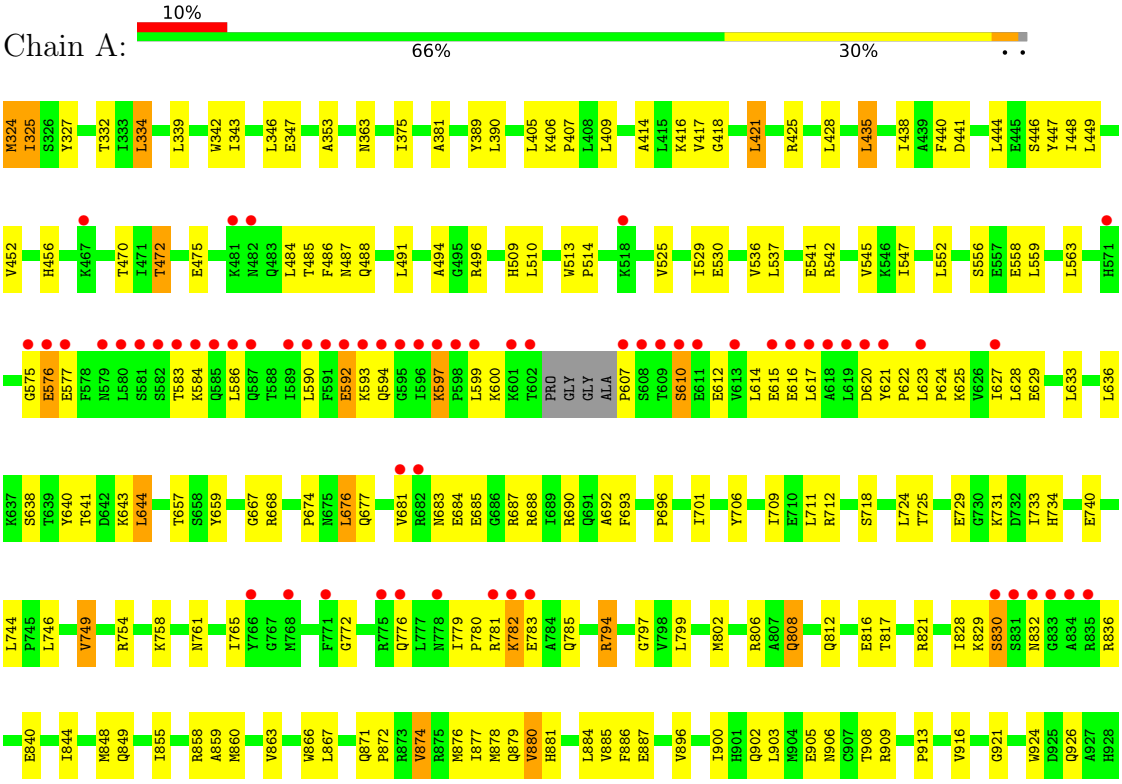
• Molecule 1: DNA (5'-D(P*TP*TP*PST)-3')

Chain B:



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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.20 (at 2.30Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.193 , 0.241 0.212 , 0.252	Depositor DCC
R_{free} test set	3760 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5026	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: PST, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 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	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

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 14.

All (132) 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	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:363:ASN:HD22	2:A:542:ARG:HH11	1.44	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:638:SER:O	2:A:643:LYS:HG2	2.09	0.53
2:A:712:ARG:HD3	2:A:913:PRO:O	2.08	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:701:ILE:HG21	2:A:924:TRP:HA	1.92	0.51
2:A:817:THR:OG1	2:A:821:ARG:HB3	2.09	0.51
2:A:633:LEU:CD2	2:A:685:GLU:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:874:VAL:HA	2:A:887:GLU:O	2.11	0.50
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: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:513:TRP:HB3	2:A:514:PRO:HD3	1.95	0.47
2:A:590:LEU:HA	2:A:593:LYS:HE2	1.96	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:556:SER:CA	2:A:641:THR:HG21	2.46	0.46
2:A:615:GLU:HB3	2:A:628:LEU:HD21	1.97	0.46
2:A:324:MET:HE3	2:A:496:ARG:NH2	2.32	0.45
2:A:590:LEU:O	2:A:593:LYS:HG2	2.16	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:486:PHE:CE2	2:A:494:ALA:HB1	2.52	0.44
2:A:525:VAL:O	2:A:529:ILE:HB	2.16	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:487:ASN:HD22	2:A:487:ASN:H	1.66	0.44
2:A:734:HIS:CD2	2:A:758:LYS:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:740:GLU:HG2	4:A:219:HOH:O	2.17	0.44
2:A:711:LEU:HD23	2:A:733:ILE:HD13	2.00	0.44
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:622:PRO:O	2:A:625:LYS:HB3	2.18	0.44
2:A:830:SER:OG	2:A:832:ASN: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:353:ALA:HA	2:A:417:VAL:O	2.19	0.42
2:A:558:GLU:CD	2:A:688:ARG:HH12	2.22	0.42
2:A:734:HIS:CD2	2:A:761:ASN:HD22	2.37	0.42
2:A:879:GLN:NE2	4:A:91:HOH:O	2.49	0.42
2:A:657:THR:HG23	2:A:659:TYR:CE2	2.54	0.42
2:A:687:ARG:HG2	2:A:690:ARG:HH12	1.84	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:414:ALA:O	2:A:416:LYS:HD2	2.20	0.41
2:A:908:THR:HG22	2:A:909:ARG:N	2.32	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:452:VAL:HG22	4:A:19:HOH:O	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:342:TRP:CZ2	2:A:381:ALA:HB2	2.56	0.41
2:A:547:ILE:HA	2:A:692:ALA:O	2.20	0.41
2:A:617:LEU:HB3	2:A:621:TYR:HB2	2.02	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 (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%)	557 (93%)	34 (6%)	6 (1%)	15 17

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 (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%)	462 (92%)	38 (8%)	13 16

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	325	ILE
2	A	334	LEU

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Mol	Chain	Res	Type
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	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

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

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Mol	Chain	Res	Type
2	A	487	ASN
2	A	488	GLN
2	A	519	HIS
2	A	543	ASN
2	A	571	HIS
2	A	677	GLN
2	A	708	GLN
2	A	716	HIS
2	A	734	HIS
2	A	776	GLN
2	A	845	ASN
2	A	879	GLN
2	A	899	GLN
2	A	906	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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	15,21,22	1.37	1 (6%)	16,30,33	3.18	1 (6%)

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	C4-N3	2.94	1.38	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1003	PST	C4-N3-C2	12.31	125.54	115.14

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

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 (i)

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	2/3 (66%)	-0.48	0 100 100	34, 34, 34, 57	0
2	A	601/605 (99%)	0.51	62 (10%) 6 9	14, 32, 93, 100	0
All	All	603/608 (99%)	0.50	62 (10%) 6 9	14, 32, 93, 100	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	607	PRO	15.0
2	A	583	THR	14.3
2	A	609	THR	14.1
2	A	610	SER	13.6
2	A	608	SER	13.6
2	A	582	SER	11.1
2	A	602	THR	10.7
2	A	598	PRO	8.9
2	A	601	LYS	8.7
2	A	611	GLU	7.7
2	A	594	GLN	7.5
2	A	621	TYR	6.3
2	A	771	PHE	6.3
2	A	619	LEU	6.0
2	A	576	GLU	5.8
2	A	587	GLN	5.7
2	A	834	ALA	5.5
2	A	620	ASP	5.3
2	A	775	ARG	5.3
2	A	682	ARG	5.3
2	A	586	LEU	5.1
2	A	581	SER	5.0
2	A	590	LEU	4.9
2	A	580	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
2	A	831	SER	4.8
2	A	776	GLN	4.8
2	A	577	GLU	4.8
2	A	781	ARG	4.6
2	A	597	LYS	4.5
2	A	768	MET	4.5
2	A	584	LYS	4.3
2	A	575	GLY	4.3
2	A	596	ILE	4.2
2	A	481	LYS	4.1
2	A	830	SER	3.9
2	A	595	GLY	3.9
2	A	782	LYS	3.9
2	A	766	TYR	3.9
2	A	599	LEU	3.8
2	A	592	GLU	3.6
2	A	482	ASN	3.5
2	A	579	ASN	3.4
2	A	832	ASN	3.4
2	A	681	VAL	3.4
2	A	835	ARG	3.4
2	A	833	GLY	3.3
2	A	467	LYS	3.0
2	A	617	LEU	2.9
2	A	618	ALA	2.8
2	A	591	PHE	2.7
2	A	615	GLU	2.7
2	A	593	LYS	2.5
2	A	623	LEU	2.5
2	A	613	VAL	2.5
2	A	616	GLU	2.5
2	A	627	ILE	2.3
2	A	778	ASN	2.2
2	A	585	GLN	2.2
2	A	783	GLU	2.1
2	A	589	ILE	2.1
2	A	518	LYS	2.0
2	A	571	HIS	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, 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	B-factors(Å^2)	Q<0.9
1	PST	B	1003	20/21	0.97	0.09	18,26,33,34	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	ZN	A	3	1/1	0.84	0.05	74,74,74,74	0
3	ZN	A	320	1/1	0.96	0.26	100,100,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.