Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:01 PM GMT

PDB ID	:	3SJJ
Title	:	RB69 DNA Polymerase Triple Mutant (L561A/S565G/Y567A) Ternary Complex with dUpNpp and a Deoxy-terminated Primer in the presence of Mn2+
Authors	:	Wang, M.; Wang, J.; Konigsberg, W.H.
Deposited on	:	2011-06-21
Resolution	:	2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

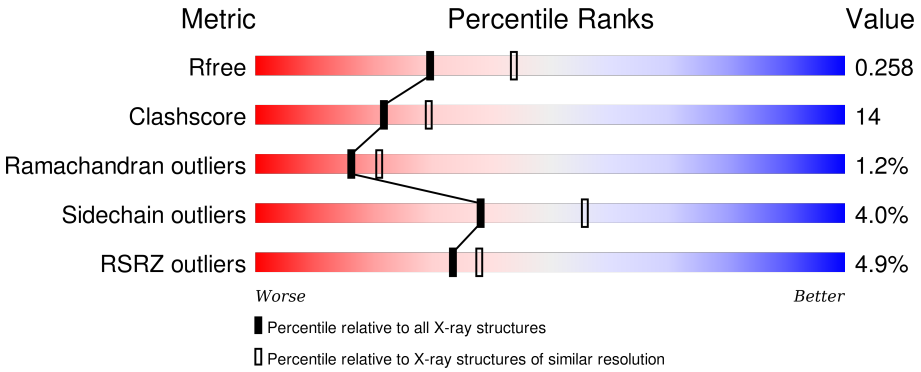
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	903	5% 77% 22%
2	T	18	6% 39% 50% 11%
3	P	13	46% 46% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8152 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 protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	901	Total	C	N	O	S	0	1	0
			7349	4718	1225	1373	33			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	561	ALA	LEU	ENGINEERED MUTATION	UNP Q38087
A	565	GLY	SER	ENGINEERED MUTATION	UNP Q38087
A	567	ALA	TYR	ENGINEERED MUTATION	UNP Q38087
A	902	ALA	ASP	CONFLICT	UNP Q38087

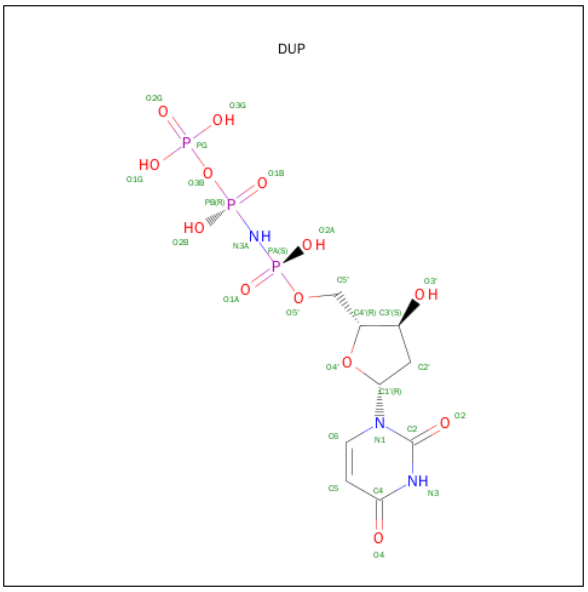
- Molecule 2 is a DNA chain called 5'-D(*TP*CP*AP*AP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	18	Total	C	N	O	P	0	0	0
			367	175	71	104	17			

- Molecule 3 is a DNA chain called 5'-D(*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			

- Molecule 4 is 2'-DEOXYURIDINE 5'-ALPHA,BETA-IMIDO-TRIPHOSPHATE (three-letter code: DUP) (formula: $C_9H_{16}N_3O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	Mn	0	0
			7	7		

- Molecule 6 is water.

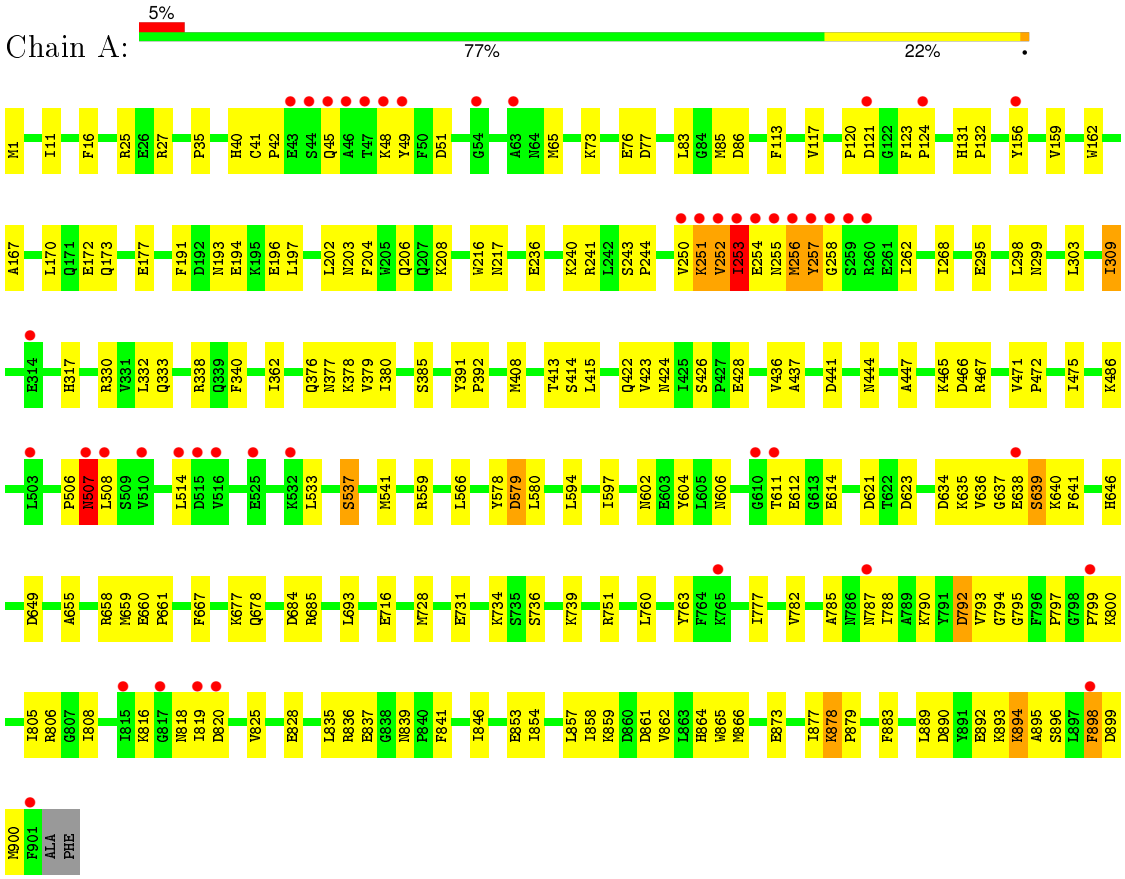
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	0
			121	121		
6	T	12	Total	O	0	0
			12	12		
6	P	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

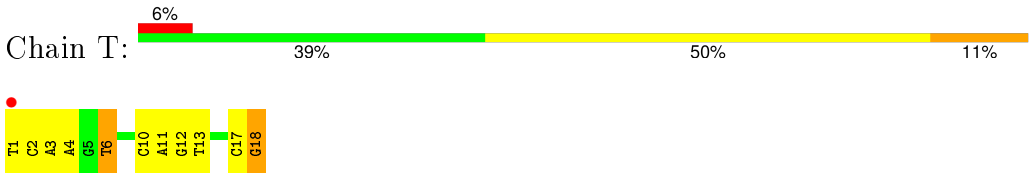
- Molecule 1: DNA polymerase

Chain A:



- Molecule 2: 5'-D(*TP*CP*AP*AP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3'

Chain T:



- Molecule 3: 5'-D(*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*C)-3'

Chain P:


G103
C104
G105
C108
T109
G110
T113
A114
C115

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.56Å 118.22Å 130.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.25 – 2.38 47.23 – 2.38	Depositor EDS
% Data completeness (in resolution range)	91.2 (47.25-2.38) 91.3 (47.23-2.38)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.265 0.199 , 0.258	Depositor DCC
R_{free} test set	2286 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 44752 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8152	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	A	0.41	0/7531	0.53	0/10177
2	T	0.75	0/412	1.45	6/634 (0.9%)
3	P	0.75	0/294	1.42	5/452 (1.1%)
All	All	0.45	0/8237	0.67	11/11263 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	108	DC	O4'-C4'-C3'	-7.44	101.53	104.50
2	T	17	DC	O4'-C1'-N1	7.12	112.98	108.00
3	P	115	DC	O4'-C4'-C3'	-7.00	101.70	104.50
2	T	17	DC	C3'-C2'-C1'	-5.99	95.31	102.50
3	P	115	DC	C1'-O4'-C4'	-5.63	104.47	110.10
2	T	10	DC	P-O3'-C3'	5.58	126.40	119.70
3	P	113	DT	P-O3'-C3'	-5.58	113.01	119.70
3	P	108	DC	C1'-O4'-C4'	-5.44	104.66	110.10
2	T	6	DT	O4'-C1'-N1	5.33	111.73	108.00
2	T	6	DT	C5-C4-O4	-5.28	121.21	124.90
2	T	18	DG	O4'-C1'-C2'	-5.02	101.88	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	A	7349	0	7250	207	1
2	T	367	0	203	11	1
3	P	263	0	148	5	0
4	A	28	0	12	0	0
5	A	7	0	0	0	0
6	A	121	0	0	6	0
6	P	5	0	0	0	0
6	T	12	0	0	1	0
All	All	8152	0	7613	218	1

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 (218) 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)
1:A:898:PHE:CB	1:A:899:ASP:HA	1.54	1.32
1:A:254:GLU:CB	1:A:255:ASN:HA	1.52	1.29
1:A:893:LYS:CA	1:A:894:LYS:HB2	1.63	1.28
1:A:638:GLU:HA	1:A:639:SER:O	1.37	1.20
1:A:639:SER:CB	1:A:640:LYS:HA	1.66	1.20
1:A:254:GLU:HB2	1:A:255:ASN:CA	1.77	1.13
1:A:793:VAL:HB	1:A:794:GLY:CA	1.78	1.12
1:A:639:SER:HB2	1:A:640:LYS:HA	1.29	1.11
1:A:898:PHE:HB3	1:A:899:ASP:HA	1.12	1.09
1:A:506:PRO:HA	1:A:507:ASN:CB	1.82	1.08
1:A:251:LYS:H	1:A:252:VAL:HB	1.19	1.07
1:A:506:PRO:HA	1:A:507:ASN:HB3	1.36	1.06
1:A:825:VAL:HB	1:A:828:GLU:HG3	1.29	1.06
1:A:639:SER:OG	1:A:640:LYS:HB2	1.54	1.05
1:A:639:SER:OG	1:A:640:LYS:CB	2.06	1.03
1:A:638:GLU:HA	1:A:639:SER:C	1.81	1.00
1:A:893:LYS:HA	1:A:894:LYS:HB2	1.05	1.00
1:A:639:SER:CB	1:A:640:LYS:CA	2.41	0.99
1:A:639:SER:OG	1:A:640:LYS:HA	1.61	0.99
1:A:898:PHE:CB	1:A:899:ASP:CA	2.40	0.99
1:A:893:LYS:HA	1:A:894:LYS:CB	1.93	0.98
1:A:251:LYS:N	1:A:252:VAL:HB	1.78	0.98
1:A:898:PHE:HB2	1:A:899:ASP:HA	1.43	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LYS:HE3	1:A:377:ASN:ND2	1.78	0.97
1:A:639:SER:OG	1:A:640:LYS:CA	2.15	0.95
1:A:893:LYS:CB	1:A:894:LYS:HB2	1.97	0.95
1:A:793:VAL:HB	1:A:794:GLY:HA3	1.47	0.94
2:T:2:DC:H2"	2:T:3:DA:OP1	1.67	0.94
1:A:637:GLY:HA2	1:A:638:GLU:HB2	1.46	0.94
1:A:793:VAL:HB	1:A:794:GLY:HA2	1.51	0.93
1:A:11:ILE:HD12	1:A:16:PHE:CD2	2.04	0.92
1:A:893:LYS:CA	1:A:894:LYS:CB	2.48	0.91
1:A:898:PHE:HB3	1:A:899:ASP:CA	1.99	0.91
1:A:638:GLU:CA	1:A:639:SER:C	2.40	0.89
1:A:254:GLU:HB2	1:A:255:ASN:HA	0.88	0.88
1:A:250:VAL:HA	1:A:251:LYS:HB3	1.55	0.87
1:A:309:ILE:O	1:A:309:ILE:HD13	1.78	0.83
1:A:251:LYS:CA	1:A:252:VAL:HB	2.08	0.82
1:A:792:ASP:HB3	1:A:793:VAL:CG1	2.08	0.82
1:A:684:ASP:HB2	6:A:976:HOH:O	1.79	0.82
1:A:254:GLU:CB	1:A:255:ASN:CA	2.41	0.81
1:A:893:LYS:HB2	1:A:894:LYS:CB	2.11	0.80
1:A:252:VAL:HA	1:A:253:ILE:O	1.80	0.80
1:A:250:VAL:HA	1:A:251:LYS:CB	2.12	0.79
1:A:638:GLU:CA	1:A:639:SER:O	2.27	0.79
1:A:254:GLU:HB3	1:A:255:ASN:HA	1.65	0.78
1:A:251:LYS:HG3	1:A:262:ILE:HG23	1.64	0.78
1:A:594:LEU:HD23	1:A:594:LEU:O	1.84	0.77
1:A:793:VAL:CB	1:A:794:GLY:CA	2.56	0.76
1:A:41:CYS:HB2	1:A:42:PRO:CD	2.15	0.75
1:A:638:GLU:H	1:A:640:LYS:N	1.85	0.72
1:A:893:LYS:CB	1:A:894:LYS:CB	2.68	0.72
1:A:792:ASP:HB3	1:A:793:VAL:HG12	1.70	0.71
1:A:173:GLN:HG3	6:A:924:HOH:O	1.90	0.71
1:A:216:TRP:O	1:A:217:ASN:HB2	1.90	0.71
1:A:441:ASP:HA	6:A:991:HOH:O	1.91	0.70
1:A:506:PRO:CA	1:A:507:ASN:CB	2.66	0.70
1:A:893:LYS:HB2	1:A:894:LYS:HB3	1.73	0.70
1:A:594:LEU:HD23	1:A:594:LEU:C	2.13	0.69
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.28	0.69
1:A:120:PRO:HG3	1:A:156:TYR:HE1	1.56	0.69
1:A:825:VAL:HB	1:A:828:GLU:CG	2.17	0.69
1:A:48:LYS:HE3	1:A:377:ASN:HD21	1.59	0.67
1:A:506:PRO:HA	1:A:507:ASN:HB2	1.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ASN:OD1	1:A:857:LEU:HD11	1.95	0.67
1:A:639:SER:HB2	1:A:640:LYS:CA	2.11	0.66
1:A:638:GLU:N	1:A:639:SER:C	2.50	0.65
1:A:250:VAL:CA	1:A:251:LYS:CB	2.75	0.64
1:A:120:PRO:HG3	1:A:156:TYR:CE1	2.32	0.64
1:A:123:PHE:CD1	1:A:124:PRO:HD2	2.33	0.63
2:T:2:DC:OP2	2:T:3:DA:N7	2.30	0.63
1:A:86:ASP:OD1	2:T:1:DT:H5"	1.99	0.63
1:A:506:PRO:CA	1:A:507:ASN:HB3	2.22	0.63
1:A:898:PHE:HB2	1:A:899:ASP:CA	2.18	0.62
1:A:203:ASN:ND2	1:A:241:ARG:HH22	1.97	0.62
1:A:251:LYS:HD2	1:A:252:VAL:O	1.99	0.62
1:A:197:LEU:C	1:A:197:LEU:HD23	2.20	0.62
1:A:251:LYS:HA	1:A:252:VAL:HB	1.82	0.62
2:T:12:DG:H2'	2:T:13:DT:H72	1.81	0.61
1:A:362:ILE:HD12	2:T:3:DA:O3'	2.01	0.60
1:A:578:TYR:O	1:A:579:ASP:HB2	2.00	0.60
1:A:604:TYR:OH	1:A:658:ARG:HB3	2.01	0.60
1:A:792:ASP:OD2	1:A:795:GLY:HA2	2.02	0.60
1:A:76:GLU:HG3	1:A:77:ASP:N	2.14	0.60
1:A:805:ILE:HA	1:A:808:ILE:HD12	1.83	0.60
1:A:25:ARG:HH11	1:A:27:ARG:HH22	1.47	0.60
1:A:792:ASP:OD2	1:A:793:VAL:HA	2.01	0.60
1:A:854:ILE:HG23	1:A:859:LYS:HB2	1.83	0.60
1:A:641:PHE:HB3	1:A:646:HIS:HB3	1.82	0.60
1:A:839:ASN:OD1	1:A:841:PHE:HB2	2.02	0.59
1:A:637:GLY:CA	1:A:638:GLU:HB2	2.25	0.58
1:A:244:PRO:HD3	1:A:268:ILE:HD11	1.86	0.58
1:A:660:GLU:HB3	1:A:661:PRO:HD3	1.86	0.58
1:A:612:GLU:HA	1:A:612:GLU:OE2	2.03	0.57
1:A:792:ASP:HB3	1:A:793:VAL:HG13	1.86	0.57
1:A:898:PHE:HB2	1:A:899:ASP:OD1	2.04	0.57
1:A:203:ASN:HD22	1:A:241:ARG:HH22	1.53	0.57
1:A:252:VAL:HA	1:A:253:ILE:C	2.23	0.56
1:A:638:GLU:N	1:A:640:LYS:N	2.52	0.56
1:A:376:GLN:HE21	1:A:378:LYS:HE3	1.70	0.56
1:A:41:CYS:HB2	1:A:42:PRO:HD3	1.87	0.56
1:A:85:MET:HA	1:A:380:ILE:HD11	1.87	0.56
1:A:255:ASN:O	1:A:256:MET:HB3	2.05	0.56
1:A:471:VAL:HB	1:A:472:PRO:HD3	1.87	0.56
1:A:475:ILE:HD12	1:A:566:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:OE2	1:A:172:GLU:N	2.37	0.56
1:A:638:GLU:H	1:A:639:SER:C	2.09	0.56
1:A:48:LYS:HE3	1:A:377:ASN:HD22	1.66	0.55
1:A:594:LEU:CD2	1:A:594:LEU:C	2.74	0.55
1:A:836:ARG:NH2	1:A:864:HIS:O	2.35	0.55
1:A:655:ALA:HA	1:A:659:MET:HE2	1.88	0.54
1:A:428:GLU:O	1:A:428:GLU:HG2	2.06	0.54
1:A:792:ASP:CB	1:A:793:VAL:HA	2.38	0.54
1:A:508:LEU:HD12	1:A:508:LEU:N	2.21	0.54
1:A:799:PRO:O	1:A:800:LYS:HB2	2.08	0.54
1:A:537:SER:O	1:A:541:MET:HG3	2.08	0.53
1:A:73:LYS:O	1:A:76:GLU:HG2	2.09	0.53
1:A:637:GLY:O	1:A:640:LYS:HB3	2.09	0.52
1:A:408:MET:HE1	1:A:659:MET:HE1	1.92	0.52
1:A:202:LEU:O	1:A:206:GLN:HG2	2.09	0.52
1:A:253:ILE:HG12	1:A:254:GLU:N	2.25	0.52
1:A:658:ARG:O	1:A:661:PRO:HD2	2.10	0.52
1:A:797:PRO:HG2	1:A:806:ARG:NH1	2.25	0.52
1:A:408:MET:CE	1:A:659:MET:HE1	2.40	0.51
1:A:578:TYR:CZ	1:A:580:LEU:HD13	2.45	0.51
3:P:104:DC:H2"	3:P:105:DG:OP2	2.11	0.51
1:A:330:ARG:HH11	1:A:333:GLN:HE22	1.58	0.51
1:A:655:ALA:O	1:A:660:GLU:HB2	2.11	0.51
1:A:252:VAL:CA	1:A:253:ILE:O	2.54	0.50
1:A:132:PRO:HA	1:A:194:GLU:OE1	2.11	0.50
1:A:42:PRO:HD2	1:A:45:GLN:HE21	1.76	0.50
1:A:878:LYS:HB2	1:A:879:PRO:HD3	1.94	0.49
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.91	0.49
2:T:2:DC:C2'	2:T:3:DA:OP1	2.50	0.49
1:A:251:LYS:HA	1:A:252:VAL:O	2.12	0.48
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.94	0.48
1:A:864:HIS:CD2	6:A:1008:HOH:O	2.66	0.48
1:A:422:GLN:HG3	1:A:678:GLN:O	2.14	0.48
1:A:883:PHE:N	1:A:883:PHE:CD1	2.80	0.48
1:A:636:VAL:HG12	1:A:637:GLY:O	2.14	0.48
1:A:436:VAL:HG12	1:A:437:ALA:O	2.13	0.48
1:A:298:LEU:O	1:A:299:ASN:HB2	2.14	0.48
2:T:2:DC:O2	2:T:2:DC:C2'	2.62	0.48
1:A:641:PHE:HA	1:A:646:HIS:ND1	2.29	0.48
1:A:793:VAL:CB	1:A:794:GLY:HA3	2.30	0.47
1:A:854:ILE:HD11	1:A:858:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:HD13	1:A:537:SER:HB3	1.97	0.47
1:A:621:ASP:C	1:A:621:ASP:OD1	2.52	0.47
1:A:254:GLU:HB2	1:A:255:ASN:CB	2.43	0.47
1:A:785:ALA:HB1	1:A:788:ILE:HD11	1.97	0.47
1:A:465:LYS:O	1:A:677:LYS:HE2	2.15	0.47
1:A:777:ILE:CG2	1:A:777:ILE:O	2.64	0.46
1:A:559:ARG:HH11	1:A:559:ARG:HG3	1.80	0.46
1:A:611:THR:OG1	1:A:614:GLU:OE2	2.34	0.46
1:A:862:VAL:O	1:A:866:MET:HG3	2.16	0.46
2:T:11:DA:C2	3:P:110:DG:C2	3.04	0.46
1:A:40:HIS:HE1	1:A:51:ASP:OD2	1.99	0.46
1:A:597:ILE:HD12	1:A:597:ILE:HA	1.66	0.46
3:P:113:DT:H2"	3:P:114:DA:O5'	2.15	0.45
2:T:6:DT:OP1	6:T:112:HOH:O	2.21	0.45
1:A:251:LYS:CD	1:A:252:VAL:O	2.62	0.45
1:A:640:LYS:HG2	1:A:640:LYS:O	2.15	0.45
1:A:191:PHE:HD2	1:A:196:GLU:HG3	1.81	0.45
1:A:338:ARG:HB3	1:A:340:PHE:CZ	2.52	0.45
1:A:634:ASP:C	1:A:636:VAL:H	2.21	0.44
2:T:12:DG:H2'	2:T:13:DT:C7	2.48	0.44
1:A:121:ASP:OD2	1:A:131:HIS:CE1	2.71	0.44
1:A:861:ASP:O	1:A:865:TRP:HD1	2.00	0.44
1:A:256:MET:HA	1:A:258:GLY:HA2	1.98	0.44
1:A:415:LEU:HD22	1:A:623:ASP:HB3	1.99	0.44
1:A:634:ASP:C	1:A:636:VAL:N	2.71	0.43
1:A:408:MET:HE3	1:A:659:MET:CE	2.49	0.43
1:A:117:VAL:HG13	1:A:132:PRO:O	2.18	0.43
1:A:578:TYR:OH	1:A:580:LEU:HD13	2.18	0.43
1:A:890:ASP:HB3	1:A:892:GLU:O	2.18	0.43
1:A:362:ILE:HD12	2:T:4:DA:P	2.58	0.43
1:A:597:ILE:HG12	1:A:667:PHE:CE2	2.54	0.43
1:A:597:ILE:HB	1:A:667:PHE:CZ	2.54	0.43
1:A:736:SER:HA	1:A:782:VAL:HB	2.01	0.43
1:A:251:LYS:HB3	1:A:262:ILE:O	2.18	0.43
1:A:658:ARG:C	1:A:661:PRO:HD2	2.39	0.43
1:A:251:LYS:HA	1:A:252:VAL:CB	2.46	0.42
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.54	0.42
1:A:408:MET:CE	1:A:659:MET:CE	2.97	0.42
1:A:251:LYS:HA	1:A:251:LYS:HD2	1.67	0.42
1:A:794:GLY:HA2	1:A:795:GLY:HA2	1.70	0.42
1:A:295:GLU:HB2	6:A:949:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:VAL:CB	1:A:794:GLY:HA2	2.24	0.42
1:A:444:ASN:HB2	6:A:991:HOH:O	2.20	0.42
1:A:236:GLU:HG2	1:A:240:LYS:HE2	2.01	0.42
1:A:486:LYS:NZ	1:A:716:GLU:OE1	2.31	0.42
1:A:391:TYR:HB2	1:A:392:PRO:HD2	2.01	0.42
1:A:873:GLU:HA	1:A:877:ILE:HB	2.02	0.42
1:A:83:LEU:HB3	1:A:379:VAL:HG12	2.02	0.42
1:A:131:HIS:HD2	1:A:156:TYR:OH	2.02	0.42
1:A:728:MET:HE2	3:P:114:DA:H3'	2.02	0.42
1:A:792:ASP:CB	1:A:793:VAL:HG12	2.45	0.41
1:A:42:PRO:HD2	1:A:45:GLN:NE2	2.35	0.41
1:A:131:HIS:HA	1:A:132:PRO:HD3	1.87	0.41
1:A:25:ARG:HH11	1:A:27:ARG:NH2	2.16	0.41
1:A:159:VAL:HG21	1:A:317:HIS:CG	2.55	0.41
1:A:413:THR:O	1:A:414:SER:C	2.58	0.41
1:A:197:LEU:CD2	1:A:197:LEU:C	2.89	0.41
1:A:170:LEU:HA	1:A:177:GLU:HG3	2.01	0.41
1:A:193:ASN:O	1:A:196:GLU:HG2	2.21	0.41
1:A:896:SER:C	1:A:898:PHE:H	2.23	0.41
1:A:73:LYS:O	1:A:76:GLU:CG	2.68	0.41
3:P:105:DG:H8	3:P:105:DG:OP2	2.04	0.41
1:A:423:VAL:O	1:A:424:ASN:HB3	2.21	0.41
1:A:777:ILE:HD11	1:A:853:GLU:HA	2.02	0.41
1:A:731:GLU:N	1:A:731:GLU:OE1	2.49	0.41
1:A:35:PRO:HG3	1:A:65:MET:HG2	2.03	0.41
1:A:602:ASN:O	1:A:606:ASN:ND2	2.36	0.40
1:A:162:TRP:CZ2	1:A:167:ALA:HB2	2.56	0.40
1:A:751:ARG:CZ	1:A:763:TYR:HB2	2.51	0.40
1:A:257:TYR:HA	1:A:258:GLY:HA2	1.51	0.40
1:A:685:ARG:HD2	1:A:685:ARG:C	2.42	0.40
1:A:660:GLU:CB	1:A:661:PRO:HD3	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:OH	2:T:18:DG:OP2[1_655]	2.18	0.02

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
1	A	900/903 (100%)	840 (93%)	49 (5%)	11 (1%)	16 21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ILE
1	A	639	SER
1	A	894	LYS
1	A	895	ALA
1	A	898	PHE
1	A	507	ASN
1	A	579	ASP
1	A	790	LYS
1	A	252	VAL
1	A	251	LYS
1	A	256	MET

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
1	A	796/796 (100%)	764 (96%)	32 (4%)	38 56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	113	PHE
1	A	243	SER
1	A	253	ILE
1	A	257	TYR
1	A	303	LEU
1	A	309	ILE
1	A	332	LEU
1	A	385	SER
1	A	426	SER
1	A	466	ASP
1	A	467	ARG
1	A	507	ASN
1	A	514	LEU
1	A	537	SER
1	A	635	LYS
1	A	649	ASP
1	A	693	LEU
1	A	734	LYS
1	A	739	LYS
1	A	760	LEU
1	A	787	ASN
1	A	792	ASP
1	A	816	LYS
1	A	819	ILE
1	A	820	ASP
1	A	835	LEU
1	A	837	GLU
1	A	846	ILE
1	A	878	LYS
1	A	889	LEU
1	A	900	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	45	GLN
1	A	131	HIS
1	A	203	ASN
1	A	206	GLN
1	A	333	GLN
1	A	354	GLN

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Mol	Chain	Res	Type
1	A	376	GLN
1	A	377	ASN
1	A	539	ASN
1	A	546	GLN
1	A	564	ASN
1	A	761	GLN
1	A	787	ASN
1	A	823	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
4	DUP	A	904	5	23,29,29	1.88	4 (17%)	32,45,45	2.02	7 (21%)

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
4	DUP	A	904	5	-	0/13/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	DUP	PB-O3B	2.10	1.61	1.59
4	A	904	DUP	PA-O1A	3.84	1.50	1.46
4	A	904	DUP	O4-C4	4.65	1.35	1.24
4	A	904	DUP	PB-O1B	4.80	1.51	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	904	DUP	C2'-C1'-N1	-3.79	104.93	114.16
4	A	904	DUP	O5'-PA-O1A	-2.30	103.80	113.31
4	A	904	DUP	O1A-PA-N3A	-2.22	108.49	111.90
4	A	904	DUP	O4'-C1'-N1	2.83	112.62	107.72
4	A	904	DUP	O2B-PB-O1B	4.06	118.47	110.00
4	A	904	DUP	O2A-PA-O1A	4.97	120.37	110.00
4	A	904	DUP	C4-N3-C2	6.05	120.14	114.14

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^{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	A	901/903 (99%)	0.29	45 (4%) 32 37	29, 49, 86, 134	0
2	T	18/18 (100%)	0.48	1 (5%) 28 32	31, 56, 135, 165	0
3	P	13/13 (100%)	0.65	0 100 100	33, 53, 115, 120	0
All	All	932/934 (99%)	0.30	46 (4%) 33 38	29, 49, 87, 165	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	GLY	10.3
1	A	257	TYR	8.2
2	T	1	DT	7.5
1	A	44	SER	7.1
1	A	252	VAL	6.9
1	A	260	ARG	6.6
1	A	46	ALA	6.4
1	A	253	ILE	6.1
1	A	259	SER	5.3
1	A	819	ILE	4.9
1	A	254	GLU	4.6
1	A	256	MET	4.5
1	A	817	GLY	4.0
1	A	63	ALA	4.0
1	A	610	GLY	3.9
1	A	48	LYS	3.9
1	A	255	ASN	3.9
1	A	515	ASP	3.7
1	A	43	GLU	3.6
1	A	45	GLN	3.5
1	A	516	VAL	3.4
1	A	47	THR	3.4
1	A	799	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	510	VAL	3.1
1	A	507	ASN	3.1
1	A	514	LEU	3.0
1	A	815	ILE	2.9
1	A	898	PHE	2.9
1	A	54	GLY	2.8
1	A	820	ASP	2.7
1	A	525	GLU	2.6
1	A	901	PHE	2.6
1	A	156	TYR	2.5
1	A	314	GLU	2.5
1	A	250	VAL	2.4
1	A	532	LYS	2.3
1	A	251	LYS	2.2
1	A	508	LEU	2.2
1	A	787	ASN	2.2
1	A	611	THR	2.1
1	A	121	ASP	2.1
1	A	765	LYS	2.1
1	A	638	GLU	2.0
1	A	124	PRO	2.0
1	A	503	LEU	2.0
1	A	49	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	MN	A	905	1/1	0.97	0.16	0.08	40,40,40,40	0
5	MN	A	907	1/1	0.90	0.14	-0.78	86,86,86,86	0
4	DUP	A	904	28/28	0.98	0.09	-2.77	10,19,24,26	0
5	MN	A	909	1/1	0.97	0.31	-	87,87,87,87	0
5	MN	A	906	1/1	0.99	0.12	-	39,39,39,39	0
5	MN	A	910	1/1	0.93	0.11	-	81,81,81,81	0
5	MN	A	908	1/1	0.98	0.24	-	76,76,76,76	0
5	MN	A	911	1/1	0.97	0.17	-	90,90,90,90	0

6.5 Other polymers (i)

There are no such residues in this entry.