



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2ATL
Title : Unmodified Insertion Ternary Complex
Authors : Rechko, O.; Malinina, L.; Cheng, Y.; Kuryavyi, V.; Broyde, S.; Geacintov, N.E.; Patel, D.J.
Deposited on : 2005-08-25
Resolution : 2.80 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 ⓘ symbol.

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

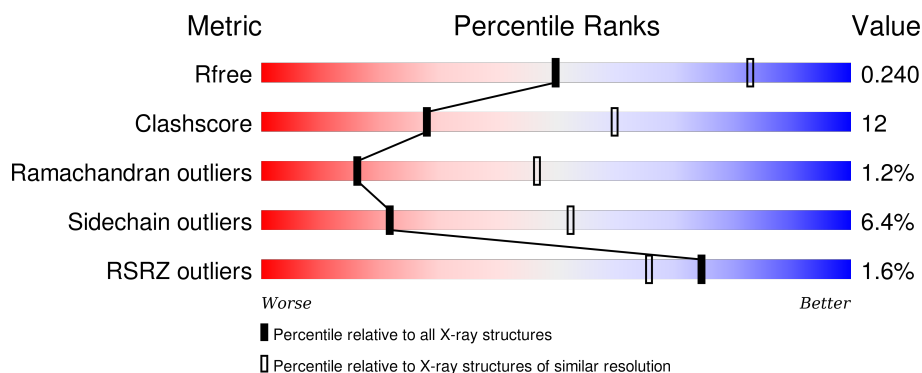
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 $\leq 5\%$. 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	D	13	
1	H	13	
2	E	19	
2	J	19	
3	A	360	

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Mol	Chain	Length	Quality of chain
3	B	360	<div><div></div><div>2%</div><div>64%</div><div>28%</div><div>5%</div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6946 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called 5'-D(*GP*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*A P*(DDG))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	13	Total	C	N	O	P	0	0	0
			272	130	53	77	12			
1	H	13	Total	C	N	O	P	0	0	0
			272	130	53	77	12			

- Molecule 2 is a DNA chain called 5'-D(*CP*T*AP*AP*CP*GP*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	P	0	0	0
			337	162	63	96	16			
2	J	19	Total	C	N	O	P	0	0	0
			376	181	68	109	18			

- Molecule 3 is a protein called Dpo4 polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	341	Total	C	N	O	S	0	0	0
			2739	1757	472	504	6			
3	B	341	Total	C	N	O	S	0	0	0
			2739	1757	472	504	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	CLONING ARTIFACT	UNP Q97W02
A	-6	SER	-	CLONING ARTIFACT	UNP Q97W02
A	-5	HIS	-	CLONING ARTIFACT	UNP Q97W02
A	-4	MET	-	CLONING ARTIFACT	UNP Q97W02
A	-3	GLY	-	CLONING ARTIFACT	UNP Q97W02
A	-2	GLY	-	CLONING ARTIFACT	UNP Q97W02

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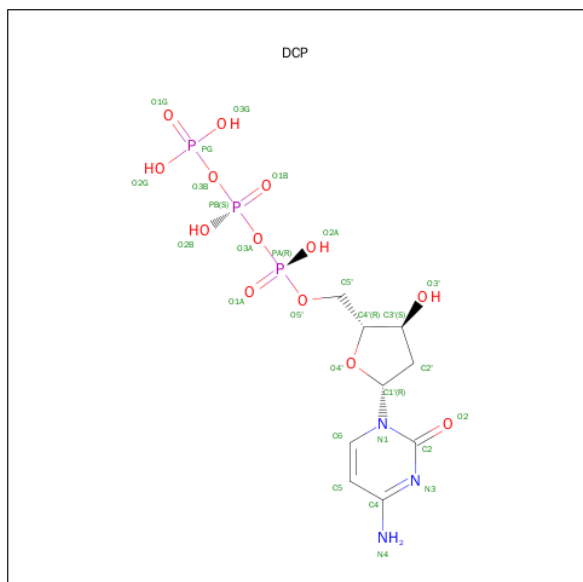
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q97W02
A	0	GLY	-	CLONING ARTIFACT	UNP Q97W02
A	1	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	-7	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	-6	SER	-	CLONING ARTIFACT	UNP Q97W02
B	-5	HIS	-	CLONING ARTIFACT	UNP Q97W02
B	-4	MET	-	CLONING ARTIFACT	UNP Q97W02
B	-3	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	-2	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	-1	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	0	GLY	-	CLONING ARTIFACT	UNP Q97W02
B	1001	GLY	-	CLONING ARTIFACT	UNP Q97W02

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Ca 1 1	0	0
4	B	3	Total Ca 3 3	0	0
4	A	3	Total Ca 3 3	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	52	Total	O	0	0
			52	52		
6	B	57	Total	O	0	0
			57	57		
6	D	13	Total	O	0	0
			13	13		
6	E	12	Total	O	0	0
			12	12		
6	H	10	Total	O	0	0
			10	10		
6	J	3	Total	O	0	0
			3	3		

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: 5'-D(*GP*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*(DDG))-3'

Chain D: 



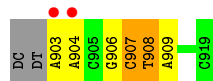
- Molecule 1: 5'-D(*GP*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*(DDG))-3'

Chain H: 



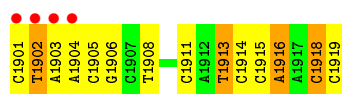
- Molecule 2: 5'-D(*CP*T*AP*AP*CP*GP*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'

Chain E: 



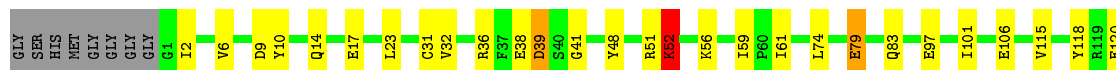
- Molecule 2: 5'-D(*CP*T*AP*AP*CP*GP*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'

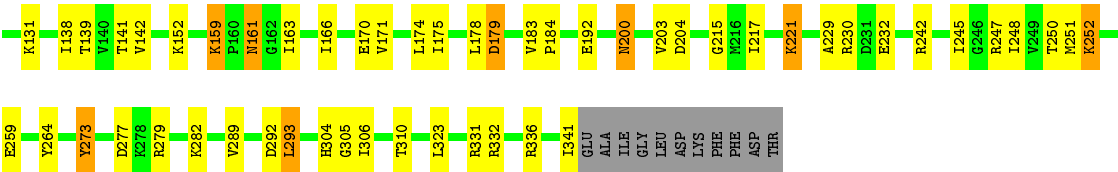
Chain J: 



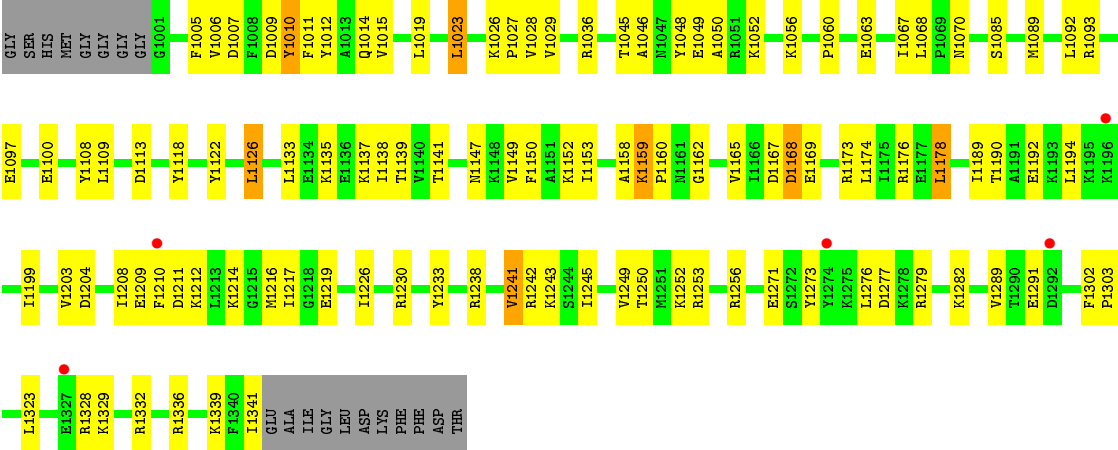
- Molecule 3: Dpo4 polymerase IV

Chain A: 





• Molecule 3: Dpo4 polymerase IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.58Å 101.76Å 112.29Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-2.80) 95.7 (19.87-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.224 , 0.279 0.250 , 0.240	Depositor DCC
R_{free} test set	1396 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27792 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6946	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, DDG, DCP

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	D	0.84	0/282	1.44	1/436 (0.2%)
1	H	0.86	0/282	1.58	6/436 (1.4%)
2	E	0.86	0/377	1.56	5/577 (0.9%)
2	J	0.87	0/420	1.73	11/643 (1.7%)
3	A	0.48	0/2778	0.58	0/3731
3	B	0.45	0/2778	0.58	0/3731
All	All	0.57	0/6917	0.91	23/9554 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1918	DC	O4'-C1'-N1	10.70	115.49	108.00
2	J	1905	DC	P-O3'-C3'	10.27	132.03	119.70
2	E	906	DG	O4'-C1'-N9	-8.92	101.76	108.00
2	E	907	DC	C1'-O4'-C4'	-8.91	101.19	110.10
2	J	1914	DC	O4'-C1'-N1	8.80	114.16	108.00
2	J	1901	DC	P-O3'-C3'	7.63	128.86	119.70
2	E	903	DA	P-O3'-C3'	6.81	127.87	119.70
2	J	1915	DC	O4'-C1'-N1	6.66	112.66	108.00
2	E	908	DT	O4'-C1'-N1	-6.62	103.37	108.00
2	J	1904	DA	O4'-C1'-N9	6.46	112.52	108.00
1	H	1808	DT	O4'-C1'-N1	6.30	112.41	108.00
1	H	1806	DG	O4'-C4'-C3'	-6.12	102.05	104.50
2	J	1908	DT	O4'-C1'-N1	-6.06	103.76	108.00
1	H	1804	DT	O4'-C1'-N1	6.02	112.21	108.00
2	J	1902	DT	P-O3'-C3'	6.02	126.92	119.70
2	E	904	DA	P-O3'-C3'	5.80	126.66	119.70
2	J	1913	DT	O4'-C1'-N1	5.79	112.06	108.00
1	D	803	DT	O4'-C4'-C3'	-5.78	102.19	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1906	DG	O4'-C1'-N9	-5.72	103.99	108.00
1	H	1802	DG	C4'-C3'-C2'	-5.54	98.11	103.10
1	H	1808	DT	P-O3'-C3'	5.47	126.26	119.70
2	J	1916	DA	P-O3'-C3'	5.36	126.13	119.70
1	H	1802	DG	P-O3'-C3'	5.19	125.92	119.70

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	D	272	0	149	4	0
1	H	272	0	149	10	0
2	E	337	0	191	3	0
2	J	376	0	214	8	0
3	A	2739	0	2883	57	0
3	B	2739	0	2880	79	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	D	1	0	0	0	0
4	H	1	0	0	0	0
5	A	28	0	12	3	0
5	B	28	0	12	4	0
6	A	52	0	0	6	0
6	B	57	0	0	6	0
6	D	13	0	0	0	0
6	E	12	0	0	0	0
6	H	10	0	0	1	0
6	J	3	0	0	1	0
All	All	6946	0	6490	156	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 12.

All (156) 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)
3:A:14:GLN:HE22	3:A:139:THR:N	1.66	0.92
3:A:14:GLN:NE2	3:A:139:THR:H	1.70	0.89
3:B:1250:THR:HA	3:B:1332:ARG:HG2	1.60	0.83
3:B:1027:PRO:HG3	3:B:1068:LEU:HD22	1.59	0.82
3:B:1241:VAL:HB	6:B:32:HOH:O	1.80	0.80
3:A:14:GLN:HE22	3:A:139:THR:H	0.84	0.79
3:B:1273:TYR:HA	3:B:1276:LEU:HD12	1.64	0.77
3:B:1014:GLN:NE2	3:B:1138:ILE:HA	2.02	0.74
3:B:1149:VAL:HG23	3:B:1233:TYR:CE2	2.22	0.74
1:H:1804:DT:H3	2:J:1916:DA:H61	1.36	0.74
3:B:1014:GLN:HE22	3:B:1139:THR:H	1.35	0.73
6:H:1504:HOH:O	3:B:1152:LYS:HE3	1.89	0.72
3:B:1208:ILE:HG12	3:B:1209:GLU:H	1.56	0.70
3:B:1141:THR:OG1	3:B:1159:LYS:O	2.09	0.69
3:A:10:TYR:CD2	3:A:48:TYR:CE1	2.81	0.68
3:A:230:ARG:O	3:A:232:GLU:HG3	1.94	0.68
2:J:1902:DT:H2''	2:J:1903:DA:OP2	1.94	0.67
3:A:250:THR:HA	3:A:332:ARG:HG2	1.77	0.67
3:B:1005:PHE:CD1	3:B:1108:TYR:CE1	2.84	0.66
3:A:10:TYR:HD2	3:A:48:TYR:CE1	2.14	0.66
3:A:79:GLU:H	3:A:79:GLU:CD	1.98	0.65
3:A:289:VAL:HB	3:A:332:ARG:HB2	1.80	0.64
3:A:10:TYR:HD2	3:A:48:TYR:HE1	1.45	0.63
3:B:1014:GLN:HE22	3:B:1138:ILE:HA	1.62	0.63
3:B:1026:LYS:HB2	3:B:1027:PRO:HD2	1.78	0.63
3:B:1147:ASN:HD21	3:B:1150:PHE:HD2	1.47	0.63
3:B:1135:LYS:HB3	6:B:121:HOH:O	1.99	0.62
3:A:10:TYR:HA	5:A:414:DCP:O2B	1.98	0.62
3:B:1097:GLU:HB2	6:B:5:HOH:O	1.99	0.62
3:B:1194:LEU:HD21	3:B:1217:ILE:HD13	1.81	0.62
1:H:1803:DT:H5''	1:H:1804:DT:H72	1.80	0.62
3:B:1133:LEU:HD12	3:B:1137:LYS:HA	1.81	0.61
3:B:1250:THR:OG1	3:B:1332:ARG:HD3	2.00	0.61
1:H:1802:DG:H2'	1:H:1803:DT:C6	2.37	0.60
3:B:1199:ILE:HG23	3:B:1204:ASP:HB2	1.84	0.60
3:A:10:TYR:CD2	3:A:48:TYR:HE1	2.19	0.59
3:B:1015:VAL:O	3:B:1019:LEU:HD13	2.02	0.59
3:B:1214:LYS:HE2	3:B:1219:GLU:HG3	1.85	0.59
3:B:1014:GLN:HE22	3:B:1139:THR:N	2.00	0.58
3:A:217:ILE:HD12	3:A:221:LYS:HB3	1.86	0.58
3:B:1149:VAL:O	3:B:1153:ILE:HG13	2.03	0.58
3:A:38:GLU:O	3:A:39:ASP:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1289:VAL:HB	3:B:1332:ARG:HB2	1.87	0.56
3:B:1122:TYR:HE2	3:B:1126:LEU:HD12	1.71	0.56
3:B:1168:ASP:N	3:B:1168:ASP:OD2	2.38	0.55
3:A:10:TYR:HA	5:A:414:DCP:PB	2.47	0.55
3:B:1176:ARG:HA	3:B:1203:VAL:HB	1.89	0.54
3:A:273:TYR:HE1	6:A:509:HOH:O	1.89	0.54
3:B:1122:TYR:CE2	3:B:1126:LEU:HD12	2.42	0.54
2:E:909:DA:P	3:A:336:ARG:HH22	2.30	0.54
3:A:273:TYR:OH	3:A:306:ILE:O	2.24	0.54
3:B:1010:TYR:HA	5:B:1414:DCP:PB	2.48	0.53
3:A:14:GLN:NE2	3:A:138:ILE:HA	2.24	0.53
3:B:1067:ILE:HG22	3:B:1068:LEU:HG	1.89	0.53
3:B:1006:VAL:HG21	3:B:1092:LEU:HD22	1.91	0.52
3:B:1208:ILE:HG12	3:B:1209:GLU:N	2.24	0.51
3:B:1147:ASN:ND2	3:B:1150:PHE:HD2	2.07	0.51
3:B:1256:ARG:NH2	3:B:1323:LEU:O	2.43	0.51
3:B:1048:TYR:O	3:B:1052:LYS:N	2.44	0.51
3:A:174:LEU:HD22	3:A:178:LEU:HB2	1.92	0.51
3:B:1085:SER:O	3:B:1089:MET:HG2	2.10	0.51
3:B:1210:PHE:CE2	3:B:1214:LYS:HD2	2.46	0.50
3:A:166:ILE:HG23	3:A:170:GLU:HB3	1.94	0.50
3:B:1048:TYR:O	3:B:1052:LYS:HG3	2.12	0.50
2:E:907:DC:OP2	3:A:250:THR:OG1	2.23	0.50
1:D:804:DT:H2''	1:D:805:DG:C8	2.47	0.50
1:H:1808:DT:H1'	1:H:1809:DG:H5'	1.92	0.49
1:H:1808:DT:H2''	1:H:1809:DG:OP2	2.12	0.49
3:A:159:LYS:O	3:A:161:ASN:N	2.46	0.49
3:B:1137:LYS:HG2	6:B:57:HOH:O	2.11	0.49
3:B:1242:ARG:HD2	3:B:1245:ILE:HD13	1.94	0.49
3:A:251:MET:HG2	3:A:264:TYR:CG	2.48	0.48
3:B:1011:PHE:HB2	6:B:1501:HOH:O	2.13	0.48
3:B:1049:GLU:CD	3:B:1049:GLU:H	2.17	0.48
3:B:1158:ALA:HB1	3:B:1162:GLY:HA3	1.95	0.48
3:A:142:VAL:O	3:A:163:ILE:HA	2.14	0.48
3:B:1118:TYR:HB3	3:B:1165:VAL:HG11	1.95	0.48
3:A:304:HIS:HD2	3:A:305:GLY:O	1.97	0.48
1:D:802:DG:H1'	1:D:803:DT:H5'	1.95	0.47
3:B:1005:PHE:CE2	3:B:1007:ASP:HB2	2.50	0.47
3:A:251:MET:HA	3:A:264:TYR:CE1	2.49	0.47
3:A:10:TYR:CD2	3:A:48:TYR:CD1	3.03	0.47
3:B:1012:TYR:HB2	3:B:1045:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:141:THR:OG1	3:A:159:LYS:O	2.16	0.47
1:H:1806:DG:H2''	1:H:1807:DA:C8	2.50	0.47
3:A:166:ILE:HG22	3:A:171:VAL:HG23	1.97	0.46
3:A:10:TYR:H	5:A:414:DCP:PG	2.38	0.46
3:A:152:LYS:HE2	6:A:502:HOH:O	2.15	0.46
1:D:801:DG:H2''	1:D:802:DG:C8	2.51	0.46
3:A:9:ASP:O	3:A:10:TYR:C	2.54	0.46
3:B:1011:PHE:O	3:B:1015:VAL:HG23	2.16	0.46
3:A:32:VAL:O	3:A:41:GLY:HA3	2.16	0.46
3:B:1009:ASP:O	3:B:1010:TYR:C	2.54	0.46
1:D:803:DT:H1'	1:D:804:DT:H5'	1.98	0.46
3:A:259:GLU:HA	3:A:259:GLU:OE1	2.15	0.45
3:B:1243:LYS:HG3	6:B:32:HOH:O	2.16	0.45
3:B:1005:PHE:HD1	3:B:1108:TYR:CE1	2.30	0.45
2:J:1903:DA:OP2	2:J:1903:DA:H2'	2.17	0.45
3:A:101:ILE:HD12	3:A:101:ILE:N	2.31	0.45
3:B:1212:LYS:O	3:B:1216:MET:HG2	2.17	0.45
2:J:1918:DC:H2''	2:J:1919:DC:OP2	2.17	0.45
3:B:1291:GLU:OE1	3:B:1329:LYS:HG3	2.17	0.45
5:B:1414:DCP:O5'	5:B:1414:DCP:H6	2.17	0.45
2:J:1913:DT:H2''	6:J:111:HOH:O	2.17	0.45
3:B:1226:ILE:O	3:B:1230:ARG:HB2	2.16	0.45
3:B:1010:TYR:HA	5:B:1414:DCP:O3B	2.17	0.44
2:J:1903:DA:N1	3:B:1036:ARG:NH1	2.64	0.44
3:B:1159:LYS:CB	3:B:1160:PRO:HD3	2.47	0.44
3:A:293:LEU:HD23	3:A:332:ARG:NH1	2.32	0.44
3:B:1005:PHE:HD1	3:B:1108:TYR:CD1	2.36	0.44
3:B:1149:VAL:HG23	3:B:1233:TYR:CZ	2.52	0.44
3:A:48:TYR:HB3	3:A:52:LYS:NZ	2.32	0.44
3:A:251:MET:HG2	3:A:264:TYR:CD2	2.53	0.44
3:B:1189:ILE:HA	3:B:1189:ILE:HD13	1.87	0.44
1:H:1804:DT:C4	1:H:1805:DG:O6	2.71	0.43
3:A:175:ILE:HG12	3:A:229:ALA:HA	2.00	0.43
3:B:1291:GLU:HB2	3:B:1329:LYS:HB2	2.00	0.43
3:B:1174:LEU:HD22	3:B:1178:LEU:HB2	1.99	0.43
3:B:1174:LEU:HA	3:B:1174:LEU:HD23	1.82	0.43
1:H:1805:DG:H2''	1:H:1806:DG:N7	2.33	0.43
1:H:1810:DG:H1'	1:H:1811:DT:H5'	2.01	0.43
3:B:1282:LYS:HB2	3:B:1339:LYS:O	2.18	0.43
3:A:36:ARG:HD3	3:A:252:LYS:O	2.19	0.43
3:A:282:LYS:HE3	3:A:341:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1023:LEU:HB3	3:B:1028:VAL:HG21	2.00	0.43
2:E:908:DT:OP1	3:A:247:ARG:HD2	2.18	0.43
3:B:1049:GLU:HA	3:B:1052:LYS:HG3	2.01	0.43
3:A:56:LYS:O	3:A:59:ILE:HG12	2.19	0.43
3:B:1027:PRO:HB3	3:B:1050:ALA:HA	2.00	0.42
3:A:331:ARG:HD2	6:A:550:HOH:O	2.20	0.42
3:A:215:GLY:HA2	6:A:511:HOH:O	2.19	0.42
1:H:1802:DG:C5	1:H:1803:DT:C4	3.07	0.42
3:B:1192:GLU:C	3:B:1194:LEU:H	2.23	0.42
3:B:1029:VAL:HG13	3:B:1046:ALA:HB2	2.02	0.42
3:B:1060:PRO:HB2	3:B:1063:GLU:HG2	2.02	0.42
3:A:115:VAL:HB	3:A:120:GLU:HB2	2.01	0.42
3:B:1190:THR:O	3:B:1194:LEU:HG	2.19	0.42
3:A:310:THR:HG21	6:A:508:HOH:O	2.19	0.42
3:A:31:CYS:HB3	3:A:61:ILE:HD11	2.01	0.42
2:J:1911:DC:OP2	3:B:1243:LYS:HE3	2.20	0.41
2:J:1902:DT:C2'	2:J:1903:DA:OP2	2.66	0.41
3:B:1089:MET:O	3:B:1093:ARG:HG3	2.20	0.41
3:A:2:ILE:HG23	3:A:118:TYR:HE1	1.84	0.41
3:A:245:ILE:HG13	3:A:279:ARG:HH21	1.86	0.41
3:A:6:VAL:O	3:A:106:GLU:HA	2.20	0.41
3:B:1100:GLU:HB3	3:B:1108:TYR:HB2	2.01	0.41
3:B:1256:ARG:NH1	3:B:1328:ARG:O	2.49	0.41
3:A:74:LEU:HB3	6:A:534:HOH:O	2.20	0.41
3:B:1010:TYR:HA	5:B:1414:DCP:O2B	2.20	0.41
3:B:1092:LEU:HB3	3:B:1109:LEU:HD11	2.03	0.40
3:A:183:VAL:O	3:A:184:PRO:C	2.60	0.40
3:B:1302:PHE:CD2	3:B:1303:PRO:HD2	2.57	0.40
3:A:179:ASP:HA	3:A:200:ASN:O	2.21	0.40
3:A:51:ARG:O	3:A:52:LYS:C	2.59	0.40
3:A:6:VAL:HG22	3:A:142:VAL:HG22	2.03	0.40
3:B:1167:ASP:C	3:B:1169:GLU:N	2.75	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	
3	A	339/360 (94%)	316 (93%)	18 (5%)	5 (2%)	13	40
3	B	339/360 (94%)	305 (90%)	31 (9%)	3 (1%)	21	55
All	All	678/720 (94%)	621 (92%)	49 (7%)	8 (1%)	16	47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	1159	LYS
3	A	52	LYS
3	A	161	ASN
3	B	1279	ARG
3	A	277	ASP
3	A	39	ASP
3	A	159	LYS
3	B	1010	TYR

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	
3	A	299/311 (96%)	279 (93%)	20 (7%)	20	50
3	B	299/311 (96%)	281 (94%)	18 (6%)	24	56
All	All	598/622 (96%)	560 (94%)	38 (6%)	22	52

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

Mol	Chain	Res	Type
3	A	17	GLU
3	A	23	LEU
3	A	52	LYS
3	A	79	GLU

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Mol	Chain	Res	Type
3	A	83	GLN
3	A	97	GLU
3	A	131	LYS
3	A	179	ASP
3	A	192	GLU
3	A	200	ASN
3	A	203	VAL
3	A	204	ASP
3	A	221	LYS
3	A	242	ARG
3	A	248	ILE
3	A	252	LYS
3	A	273	TYR
3	A	292	ASP
3	A	293	LEU
3	A	323	LEU
3	B	1023	LEU
3	B	1056	LYS
3	B	1070	ASN
3	B	1113	ASP
3	B	1126	LEU
3	B	1168	ASP
3	B	1173	ARG
3	B	1178	LEU
3	B	1211	ASP
3	B	1238	ARG
3	B	1241	VAL
3	B	1249	VAL
3	B	1252	LYS
3	B	1253	ARG
3	B	1271	GLU
3	B	1277	ASP
3	B	1336	ARG
3	B	1341	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	14	GLN
3	A	83	GLN
3	A	188	ASN
3	A	304	HIS

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Mol	Chain	Res	Type
3	B	1014	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	DDG	D	813	1,2,4	15,23,24	1.07	1 (6%)	16,33,36	2.91	5 (31%)
1	DDG	H	1813	1,2,4	15,23,24	1.33	2 (13%)	16,33,36	2.97	5 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDG	D	813	1,2,4	-	0/3/18/19	0/3/3/3
1	DDG	H	1813	1,2,4	-	0/3/18/19	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1813	DDG	C2-N1	2.18	1.39	1.35
1	D	813	DDG	C6-N1	3.27	1.39	1.33
1	H	1813	DDG	C6-N1	3.99	1.40	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1813	DDG	C5-C6-N1	-8.47	112.01	123.59
1	D	813	DDG	C5-C6-N1	-8.28	112.27	123.59
1	D	813	DDG	N2-C2-N1	-2.29	113.41	117.20
1	H	1813	DDG	N3-C2-N1	-2.26	124.00	127.44
1	D	813	DDG	C4-C5-N7	2.14	111.44	109.48
1	H	1813	DDG	O4'-C1'-C2'	2.17	109.02	106.67
1	H	1813	DDG	O4'-C4'-C3'	2.19	108.36	104.69
1	D	813	DDG	C3'-C2'-C1'	2.53	105.53	102.71
1	D	813	DDG	C6-N1-C2	6.03	124.31	115.94
1	H	1813	DDG	C6-N1-C2	6.22	124.57	115.94

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\# Z > 2$
5	DCP	A	414	4	21,29,29	0.74	1 (4%)	33,45,45	1.32	5 (15%)
5	DCP	B	1414	4	21,29,29	0.77	0	33,45,45	1.54	6 (18%)

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
5	DCP	A	414	4	-	0/18/34/34	0/2/2/2
5	DCP	B	1414	4	-	0/18/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	414	DCP	PA-O5'	-2.00	1.49	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1414	DCP	PB-O3B-PG	-3.38	121.35	132.67
5	A	414	DCP	PB-O3B-PG	-2.18	125.35	132.67
5	A	414	DCP	C2'-C1'-N1	-2.11	109.02	114.16
5	B	1414	DCP	C2'-C1'-N1	-2.01	109.26	114.16
5	B	1414	DCP	C4'-O4'-C1'	2.11	114.79	109.47
5	A	414	DCP	O4'-C1'-N1	2.50	112.04	107.72
5	B	1414	DCP	O4'-C1'-N1	2.69	112.37	107.72
5	A	414	DCP	O3A-PA-O5'	2.84	110.48	102.94
5	B	1414	DCP	O3A-PA-O5'	2.89	110.60	102.94
5	A	414	DCP	C2-N3-C4	3.68	120.81	115.61
5	B	1414	DCP	C2-N3-C4	3.94	121.17	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	414	DCP	3	0
5	B	1414	DCP	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	D	12/13 (92%)	-0.76	0 100 100	2, 5, 14, 19	0
1	H	12/13 (92%)	0.77	0 100 100	5, 31, 43, 44	0
2	E	17/19 (89%)	-0.12	2 (11%) 6 3	2, 2, 42, 50	0
2	J	19/19 (100%)	1.14	4 (21%) 1 1	2, 21, 50, 54	0
3	A	341/360 (94%)	-0.44	0 100 100	2, 4, 16, 20	0
3	B	341/360 (94%)	0.03	6 (1%) 71 61	2, 10, 18, 20	0
All	All	742/784 (94%)	-0.16	12 (1%) 74 66	2, 7, 19, 54	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	903	DA	4.6
2	J	1902	DT	4.3
2	J	1901	DC	3.7
2	J	1904	DA	3.6
2	E	904	DA	3.1
3	B	1327	GLU	3.0
3	B	1196	LYS	3.0
2	J	1903	DA	3.0
3	B	1210	PHE	2.4
3	B	1048	TYR	2.3
3	B	1274	TYR	2.3
3	B	1292	ASP	2.2

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. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	DDG	D	813	21/22	0.97	0.14	-	2,2,2,2	0
1	DDG	H	1813	21/22	0.95	0.18	-	2,2,2,2	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	DCP	B	1414	28/28	0.91	0.23	0.51	2,2,16,16	0
5	DCP	A	414	28/28	0.96	0.14	-0.88	2,2,17,18	0
4	CA	B	1415	1/1	0.93	0.12	-1.08	2,2,2,2	0
4	CA	A	417	1/1	0.92	0.08	-1.54	7,7,7,7	0
4	CA	A	416	1/1	0.98	0.10	-1.89	2,2,2,2	0
4	CA	A	415	1/1	0.96	0.09	-2.46	2,2,2,2	0
4	CA	B	1417	1/1	0.93	0.06	-5.93	17,17,17,17	0
4	CA	B	1416	1/1	0.87	0.15	-	3,3,3,3	0
4	CA	H	1418	1/1	0.77	0.46	-	99,99,99,99	0
4	CA	D	418	1/1	0.94	0.13	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.