Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:34 AM GMT

PDB ID	:	2ASJ
Title	:	oxoG-modified Preinsertion Binary Complex
Authors	:	Rechkoblit, O.; Malinina, L.; Cheng, Y.; Kuryavyi, V.; Broyde, S.; Geacintov, N.E.; Patel, D.J.
Deposited on	:	2005-08-23
Resolution	:	2.35 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:

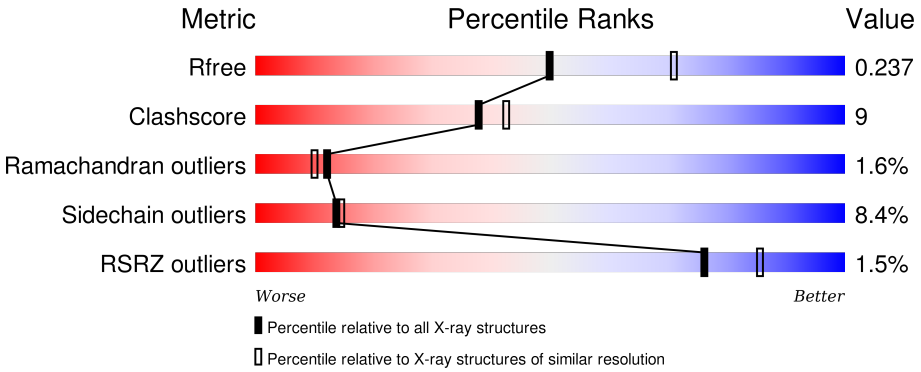
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	D	13	46% 46% 8%
1	H	13	23% 62% 15%
2	E	19	16% 47% 5% 32%
2	J	19	32% 32% 5% 32%
3	A	360	3% 69% 23% • 5%

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Mol	Chain	Length	Quality of chain
3	B	360	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6677 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*AP*(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*TP*AP*AP*CP*(8OG)*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	P	0	0	0
			254	123	45	74	12			
2	J	13	Total	C	N	O	P	0	0	0
			254	123	45	74	12			

- Molecule 3 is a protein called DNA 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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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	B	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0

- Molecule 5 is water.

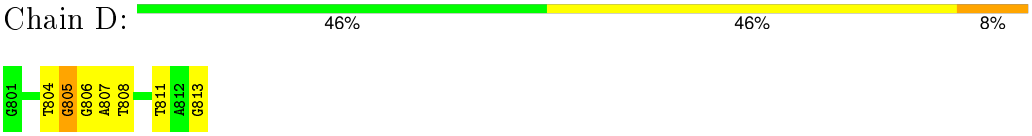
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	45	Total O 45 45	0	0
5	B	61	Total O 61 61	0	0
5	D	11	Total O 11 11	0	0
5	E	9	Total O 9 9	0	0
5	H	10	Total O 10 10	0	0
5	J	8	Total O 8 8	0	0

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:

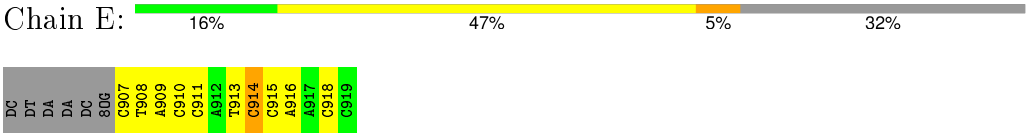


• Molecule 1: 5'-D(*GP*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*(DDG))-3'

Chain H:

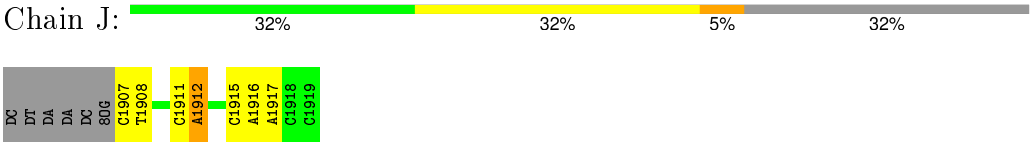
• Molecule 2: 5'-D(*CP*TP*AP*AP*CP*(8OG)*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'

Chain E:



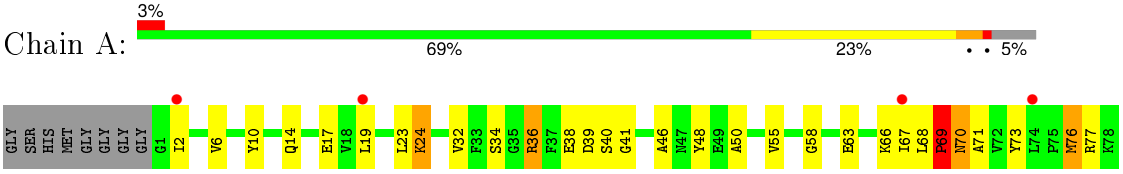
• Molecule 2: 5'-D(*CP*TP*AP*AP*CP*(8OG)*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'

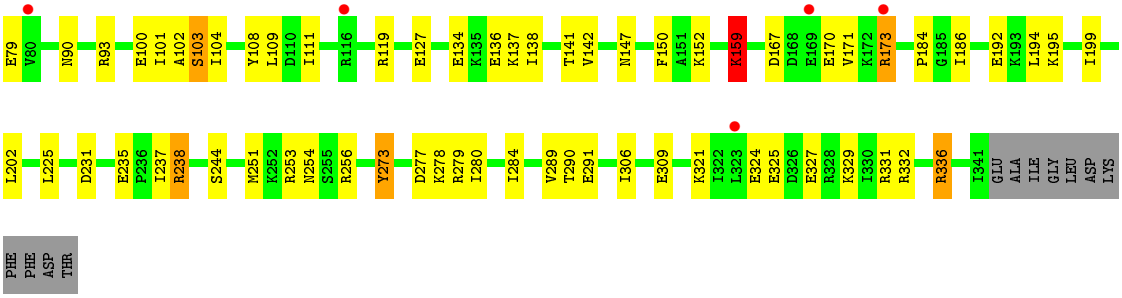
Chain J:



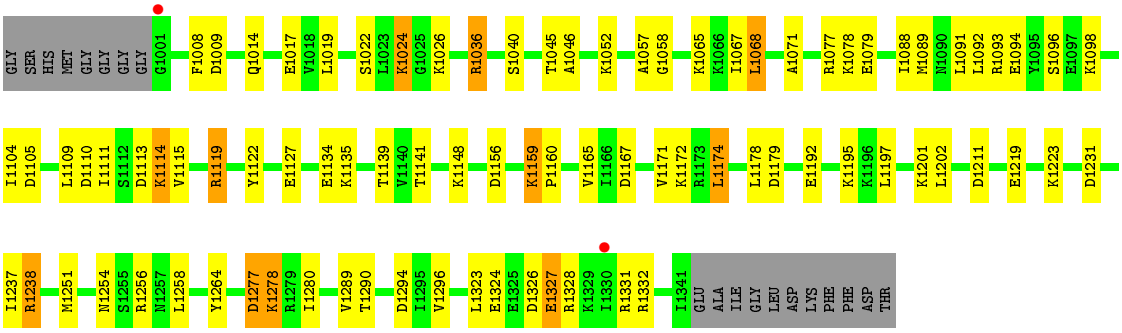
• Molecule 3: DNA polymerase IV

Chain A:





• Molecule 3: DNA polymerase IV



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.22Å 182.96Å 52.21Å 90.00° 107.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 19.96 – 2.35	Depositor EDS
% Data completeness (in resolution range)	88.7 (20.00-2.35) 88.7 (19.96-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.246 , 0.318 0.249 , 0.237	Depositor DCC
R_{free} test set	1878 reflections (5.76%)	DCC
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.8	EDS
Estimated twinning fraction	0.299 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 38149 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6677	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: CA, DDG

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	0.78	0/282	1.58	6/436 (1.4%)
1	H	0.87	0/282	1.57	3/436 (0.7%)
2	E	0.95	0/283	1.64	6/432 (1.4%)
2	J	0.84	0/283	1.58	4/432 (0.9%)
3	A	0.51	0/2778	0.62	0/3731
3	B	0.51	0/2778	0.64	0/3731
All	All	0.59	0/6686	0.89	19/9198 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	806	DG	O4'-C1'-N9	9.84	114.89	108.00
2	J	1911	DC	O4'-C1'-N1	8.52	113.97	108.00
1	D	805	DG	O4'-C1'-N9	7.97	113.58	108.00
1	H	1805	DG	O4'-C1'-N9	7.88	113.52	108.00
2	J	1915	DC	O4'-C1'-N1	7.26	113.08	108.00
2	E	918	DC	O4'-C1'-N1	7.21	113.05	108.00
1	D	808	DT	P-O3'-C3'	6.66	127.69	119.70
1	H	1806	DG	O4'-C4'-C3'	-6.41	101.94	104.50
1	D	811	DT	C6-C5-C7	-6.40	119.06	122.90
2	E	916	DA	O4'-C1'-N9	6.11	112.28	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	911	DC	O4'-C1'-N1	6.07	112.25	108.00
1	H	1801	DG	O4'-C1'-N9	6.02	112.22	108.00
2	E	909	DA	N1-C6-N6	5.91	122.14	118.60
2	J	1911	DC	P-O3'-C3'	5.67	126.50	119.70
2	J	1912	DA	C3'-C2'-C1'	-5.44	95.97	102.50
2	E	914	DC	P-O3'-C3'	5.29	126.05	119.70
1	D	804	DT	C1'-O4'-C4'	-5.22	104.88	110.10
2	E	910	DC	P-O3'-C3'	5.21	125.95	119.70
1	D	806	DG	C1'-O4'-C4'	-5.16	104.94	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	69	PRO	Peptide

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	D	272	0	149	4	0
1	H	272	0	149	11	0
2	E	254	0	147	7	0
2	J	254	0	147	7	0
3	A	2739	0	2883	51	0
3	B	2739	0	2880	46	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	A	45	0	0	3	0
5	B	61	0	0	5	0
5	D	11	0	0	0	0
5	E	9	0	0	1	0
5	H	10	0	0	0	0
5	J	8	0	0	2	0
All	All	6677	0	6355	116	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 9.

All (116) 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:B:1098:LYS:HD3	3:B:1110:ASP:HB3	1.55	0.89
3:A:238:ARG:HB2	3:A:238:ARG:HH21	1.48	0.79
3:B:1014:GLN:HE22	3:B:1139:THR:H	1.30	0.78
1:H:1809:DG:H2"	1:H:1810:DG:H5"	1.67	0.77
3:A:331:ARG:HH21	3:A:332:ARG:HE	1.32	0.76
2:J:1908:DT:OP2	3:B:1332:ARG:HD3	1.86	0.74
3:A:141:THR:OG1	3:A:159:LYS:O	2.06	0.73
1:D:805:DG:H1	2:E:915:DC:H42	1.35	0.72
3:A:256:ARG:HG3	3:A:329:LYS:HA	1.74	0.69
3:A:254:ASN:OD1	3:A:331:ARG:HG3	1.92	0.68
3:B:1096:SER:HB3	3:B:1109:LEU:HG	1.75	0.68
3:A:336:ARG:HH11	3:A:336:ARG:HB2	1.58	0.67
3:A:290:THR:O	5:A:543:HOH:O	2.11	0.66
2:J:1912:DA:N6	5:J:119:HOH:O	2.27	0.65
3:A:273:TYR:OH	3:A:306:ILE:O	2.14	0.65
1:H:1806:DG:H2'	1:H:1807:DA:C8	2.33	0.64
3:A:167:ASP:O	3:A:171:VAL:HG23	1.96	0.64
3:B:1036:ARG:NH2	3:B:1254:ASN:OD1	2.31	0.64
3:B:1078:LYS:HE2	3:B:1104:ILE:HD12	1.79	0.64
3:B:1156:ASP:HA	3:B:1159:LYS:HG3	1.81	0.63
3:A:152:LYS:HD3	3:A:184:PRO:HB3	1.80	0.61
1:D:805:DG:H1	2:E:915:DC:N4	1.99	0.61
3:B:1201:LYS:HB3	5:B:45:HOH:O	2.01	0.60
3:B:1174:LEU:O	3:B:1178:LEU:HB3	2.02	0.59
3:B:1119:ARG:NH2	5:B:69:HOH:O	2.34	0.59
3:B:1017:GLU:HB3	3:B:1024:LYS:HD2	1.85	0.58
3:B:1141:THR:HG21	3:B:1159:LYS:HA	1.85	0.58
3:A:38:GLU:O	3:A:39:ASP:HB2	2.04	0.58
3:B:1135:LYS:HE3	5:B:150:HOH:O	2.04	0.57
3:B:1141:THR:OG1	3:B:1159:LYS:O	2.13	0.57
1:D:807:DA:H2	2:E:913:DT:H3	1.53	0.57
3:B:1289:VAL:HB	3:B:1332:ARG:HB2	1.88	0.56
3:A:100:GLU:HG3	3:A:238:ARG:O	2.06	0.56
2:E:907:DC:N4	3:A:58:GLY:HA2	2.21	0.56
2:E:914:DC:H2'	5:E:505:HOH:O	2.05	0.55
1:H:1813:DDG:H8	1:H:1813:DDG:O5'	2.06	0.55
3:A:336:ARG:NH1	3:A:336:ARG:HB2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:69:PRO:O	3:A:71:ALA:N	2.40	0.54
3:B:1111:ILE:O	3:B:1115:VAL:HG22	2.08	0.54
3:A:238:ARG:HB2	3:A:238:ARG:NH2	2.20	0.53
3:A:93:ARG:HH21	3:A:101:ILE:HD11	1.71	0.53
3:A:14:GLN:HG2	3:A:138:ILE:HD13	1.89	0.53
3:B:1113:ASP:HB2	3:B:1114:LYS:HE2	1.91	0.53
1:H:1804:DT:H2'	1:H:1805:DG:C8	2.43	0.53
3:A:237:ILE:HG22	3:A:237:ILE:O	2.09	0.52
3:A:102:ALA:O	3:A:103:SER:HB3	2.10	0.52
3:A:291:GLU:OE1	3:A:329:LYS:HB2	2.09	0.51
2:E:908:DT:H5'	3:A:32:VAL:HG11	1.91	0.51
3:A:17:GLU:HB3	3:A:24:LYS:HE2	1.92	0.51
3:A:279:ARG:O	3:A:280:ILE:HD13	2.11	0.51
2:J:1907:DC:H2'	2:J:1908:DT:H71	1.93	0.50
3:A:76:MET:HG3	3:A:77:ARG:N	2.25	0.50
3:B:1014:GLN:NE2	3:B:1139:THR:H	2.04	0.50
1:H:1809:DG:H2"	1:H:1810:DG:C5'	2.39	0.50
3:B:1294:ASP:HB2	3:B:1328:ARG:HH12	1.76	0.50
3:A:277:ASP:O	3:A:278:LYS:HB2	2.11	0.50
3:B:1068:LEU:HD13	3:B:1071:ALA:HB2	1.93	0.50
3:B:1009:ASP:OD1	3:B:1141:THR:OG1	2.30	0.50
3:A:34:SER:OG	3:A:40:SER:HB2	2.12	0.49
3:B:1088:ILE:O	3:B:1092:LEU:HG	2.13	0.49
2:J:1916:DA:H2"	2:J:1917:DA:O5'	2.13	0.49
3:B:1008:PHE:CZ	3:B:1088:ILE:HG21	2.48	0.49
3:A:186:ILE:HG13	3:A:225:LEU:HD21	1.95	0.48
3:A:291:GLU:HG2	3:A:329:LYS:O	2.13	0.48
3:A:278:LYS:HA	5:A:518:HOH:O	2.12	0.48
3:B:1238:ARG:O	3:B:1238:ARG:HD2	2.13	0.48
3:B:1327:GLU:HG2	5:B:79:HOH:O	2.13	0.48
1:D:813:DDG:H1	2:E:907:DC:H42	1.62	0.48
3:B:1091:LEU:O	3:B:1094:GLU:HG2	2.14	0.48
3:A:36:ARG:NH2	3:A:331:ARG:HG3	2.29	0.47
3:A:108:TYR:OH	3:A:152:LYS:HD2	2.15	0.47
3:B:1251:MET:HA	3:B:1264:TYR:CE1	2.50	0.47
2:J:1907:DC:N4	3:B:1058:GLY:HA2	2.30	0.47
3:A:10:TYR:CD2	3:A:48:TYR:HE1	2.32	0.47
3:A:63:GLU:HA	3:A:66:LYS:HE3	1.96	0.47
1:H:1809:DG:C2'	1:H:1810:DG:H5"	2.41	0.46
3:B:1022:SER:O	3:B:1026:LYS:HE2	2.15	0.46
3:B:1219:GLU:O	3:B:1223:LYS:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:68:LEU:O	3:A:73:TYR:OH	2.30	0.46
3:B:1148:LYS:HD3	3:B:1237:ILE:HG13	1.98	0.46
1:H:1813:DDG:C6	3:B:1057:ALA:HB1	2.45	0.46
3:B:1172:LYS:HG2	5:B:27:HOH:O	2.16	0.46
3:B:1294:ASP:CB	3:B:1328:ARG:HH12	2.29	0.46
3:A:68:LEU:O	3:A:69:PRO:O	2.35	0.45
3:A:170:GLU:HG3	3:A:173:ARG:NH1	2.31	0.45
3:B:1008:PHE:CD2	3:B:1105:ASP:HA	2.51	0.45
3:A:147:ASN:OD1	3:A:150:PHE:HD2	1.99	0.45
3:A:238:ARG:HG3	3:A:238:ARG:H	1.64	0.45
3:B:1256:ARG:NH1	3:B:1328:ARG:O	2.50	0.45
3:A:90:ASN:HA	3:A:93:ARG:HD2	1.98	0.44
3:B:1277:ASP:O	3:B:1278:LYS:HB2	2.17	0.44
3:A:32:VAL:O	3:A:41:GLY:HA3	2.17	0.44
3:A:6:VAL:HG22	3:A:142:VAL:HG22	2.00	0.44
3:B:1167:ASP:O	3:B:1171:VAL:HG23	2.19	0.42
3:A:321:LYS:HG2	3:A:325:GLU:OE2	2.19	0.42
3:A:192:GLU:HA	3:A:195:LYS:HB3	2.01	0.42
3:B:1296:VAL:HG21	3:B:1326:ASP:OD2	2.19	0.42
3:A:46:ALA:HB1	3:A:50:ALA:HB3	2.00	0.42
3:B:1019:LEU:HD23	3:B:1077:ARG:HH22	1.85	0.42
3:A:194:LEU:HB3	3:A:199:ILE:HB	2.02	0.42
1:H:1804:DT:H2"	1:H:1805:DG:H5'	2.01	0.42
3:B:1045:THR:HG22	3:B:1046:ALA:N	2.35	0.42
3:B:1159:LYS:CB	3:B:1160:PRO:HD3	2.49	0.41
3:B:1159:LYS:HB3	3:B:1160:PRO:HD3	2.02	0.41
1:H:1802:DG:H2'	1:H:1803:DT:H72	2.03	0.41
3:A:2:ILE:HG22	3:A:111:ILE:HG13	2.02	0.41
3:A:244:SER:HB2	3:A:336:ARG:HE	1.85	0.41
3:B:1089:MET:O	3:B:1093:ARG:HG3	2.21	0.41
1:H:1804:DT:H2'	1:H:1805:DG:H8	1.84	0.41
3:A:50:ALA:O	3:A:55:VAL:HB	2.21	0.41
1:H:1809:DG:C2	2:J:1912:DA:C2	3.09	0.40
3:A:136:GLU:O	3:A:137:LYS:HB2	2.20	0.40
3:B:1122:TYR:HD1	3:B:1165:VAL:HG23	1.86	0.40
2:J:1908:DT:O4	5:J:43:HOH:O	2.16	0.40
3:A:289:VAL:HG12	5:A:543:HOH:O	2.21	0.40
3:B:1251:MET:HG3	3:B:1331:ARG:O	2.21	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%)	311 (92%)	21 (6%)	7 (2%)	9 6
3	B	339/360 (94%)	321 (95%)	14 (4%)	4 (1%)	16 15
All	All	678/720 (94%)	632 (93%)	35 (5%)	11 (2%)	12 10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	36	ARG
3	A	69	PRO
3	A	159	LYS
3	B	1159	LYS
3	B	1277	ASP
3	A	231	ASP
3	A	103	SER
3	B	1052	LYS
3	A	70	ASN
3	B	1278	LYS
3	A	104	ILE

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%)	275 (92%)	24 (8%)	15 16
3	B	299/311 (96%)	273 (91%)	26 (9%)	13 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	598/622 (96%)	548 (92%)	50 (8%)	14 14

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	19	LEU
3	A	23	LEU
3	A	24	LYS
3	A	67	ILE
3	A	70	ASN
3	A	76	MET
3	A	79	GLU
3	A	109	LEU
3	A	119	ARG
3	A	127	GLU
3	A	134	GLU
3	A	159	LYS
3	A	173	ARG
3	A	202	LEU
3	A	235	GLU
3	A	238	ARG
3	A	251	MET
3	A	253	ARG
3	A	273	TYR
3	A	284	ILE
3	A	309	GLU
3	A	324	GLU
3	A	327	GLU
3	A	336	ARG
3	B	1024	LYS
3	B	1036	ARG
3	B	1040	SER
3	B	1065	LYS
3	B	1067	ILE
3	B	1068	LEU
3	B	1079	GLU
3	B	1114	LYS
3	B	1119	ARG
3	B	1127	GLU
3	B	1134	GLU
3	B	1174	LEU
3	B	1179	ASP

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Mol	Chain	Res	Type
3	B	1192	GLU
3	B	1195	LYS
3	B	1197	LEU
3	B	1202	LEU
3	B	1211	ASP
3	B	1231	ASP
3	B	1238	ARG
3	B	1258	LEU
3	B	1280	ILE
3	B	1290	THR
3	B	1323	LEU
3	B	1324	GLU
3	B	1327	GLU

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	70	ASN
3	A	304	HIS
3	B	1014	GLN
3	B	1070	ASN
3	B	1304	HIS

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	1.20	1 (6%)	16,33,36	2.99	4 (25%)
1	DDG	H	1813	1,2,4	15,23,24	1.41	3 (20%)	16,33,36	2.99	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1813	DDG	C8-N7	-2.35	1.30	1.34
1	H	1813	DDG	C2-N1	2.08	1.39	1.35
1	D	813	DDG	C6-N1	3.45	1.39	1.33
1	H	1813	DDG	C6-N1	4.07	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	813	DDG	C5-C6-N1	-8.66	111.74	123.59
1	H	1813	DDG	C5-C6-N1	-8.49	111.98	123.59
1	D	813	DDG	N3-C2-N1	-2.37	123.83	127.44
1	H	1813	DDG	N3-C2-N1	-2.32	123.92	127.44
1	D	813	DDG	O4'-C1'-C2'	2.15	109.00	106.67
1	H	1813	DDG	C3'-C2'-C1'	2.47	105.47	102.71
1	H	1813	DDG	C4-C5-N7	2.56	111.83	109.48
1	H	1813	DDG	C6-N1-C2	5.94	124.19	115.94
1	D	813	DDG	C6-N1-C2	6.39	124.81	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	813	DDG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	1813	DDG	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 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	D	12/13 (92%)	-0.10	0 100 100	35, 57, 60, 60	0
1	H	12/13 (92%)	-0.07	0 100 100	34, 43, 51, 53	0
2	E	13/19 (68%)	-0.32	0 100 100	37, 53, 63, 63	0
2	J	13/19 (68%)	-0.21	0 100 100	32, 38, 56, 58	0
3	A	341/360 (94%)	0.38	9 (2%) 59 71	45, 55, 65, 70	0
3	B	341/360 (94%)	0.29	2 (0%) 90 95	45, 55, 64, 69	0
All	All	732/784 (93%)	0.30	11 (1%) 76 85	32, 55, 65, 70	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	2	ILE	3.5
3	A	323	LEU	2.6
3	B	1001	GLY	2.3
3	A	173	ARG	2.3
3	A	19	LEU	2.2
3	A	116	ARG	2.2
3	A	74	LEU	2.2
3	A	67	ILE	2.1
3	A	80	VAL	2.1
3	A	169	GLU	2.1
3	B	1330	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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
1	DDG	D	813	21/22	0.93	0.16	-	32,39,40,40	0
1	DDG	H	1813	21/22	0.95	0.13	-	38,38,41,48	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^{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
4	CA	B	1415	1/1	0.92	0.20	-	52,52,52,52	0
4	CA	E	416	1/1	0.95	0.07	-	75,75,75,75	0
4	CA	A	415	1/1	0.99	0.02	-	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.