



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2AU0  
Title : Unmodified preinsertion binary complex  
Authors : Rechko, O.; Malinina, L.; Cheng, Y.; Kuryav, V.; Broyde, S.; Geacintov, N.E.; Patel, D.J.  
Deposited on : 2005-08-26  
Resolution : 2.70 Å(reported)

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

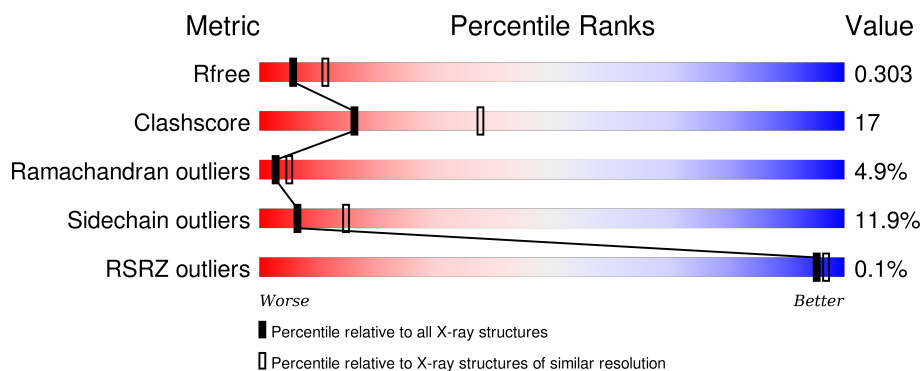
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

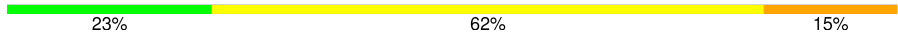
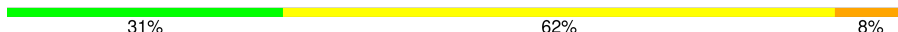
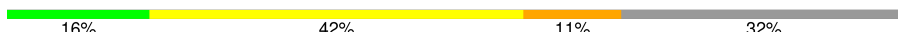


The reported resolution of this entry is 2.70 Å.

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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	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	 A horizontal bar chart showing the quality of chain B. The bar is divided into four segments: green (56%), yellow (33%), orange (6%), and grey (5%).

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6651 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\*TP\*AP\*AP\*CP\*G\*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 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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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	J	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0

- Molecule 5 is water.

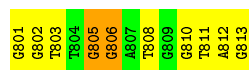
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	41	Total O 41 41	0	0
5	B	38	Total O 38 38	0	0
5	D	12	Total O 12 12	0	0
5	E	5	Total O 5 5	0	0
5	H	16	Total O 16 16	0	0
5	J	6	Total O 6 6	0	0

### 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\*G\*CP\*TP\*AP\*CP\*CP\*AP\*TP\*CP\*CP\*AP\*AP\*CP\*C)-3'

Chain E: 



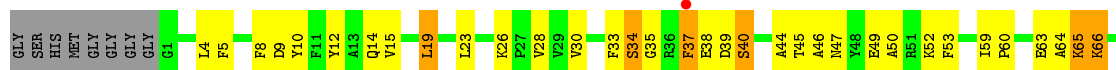
- Molecule 2: 5'-D(\*CP\*TP\*AP\*AP\*CP\*G\*CP\*TP\*AP\*CP\*CP\*AP\*TP\*CP\*CP\*AP\*AP\*CP\*C)-3'

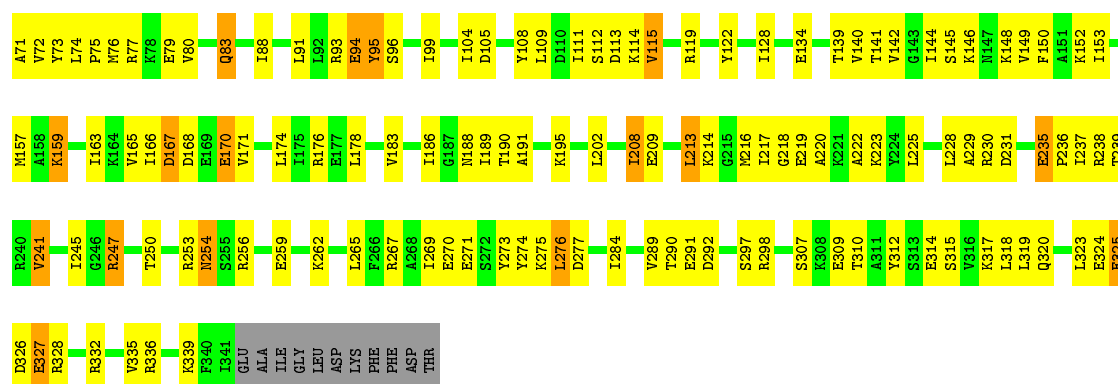
Chain J: 



- Molecule 3: Dpo4 polymerase IV

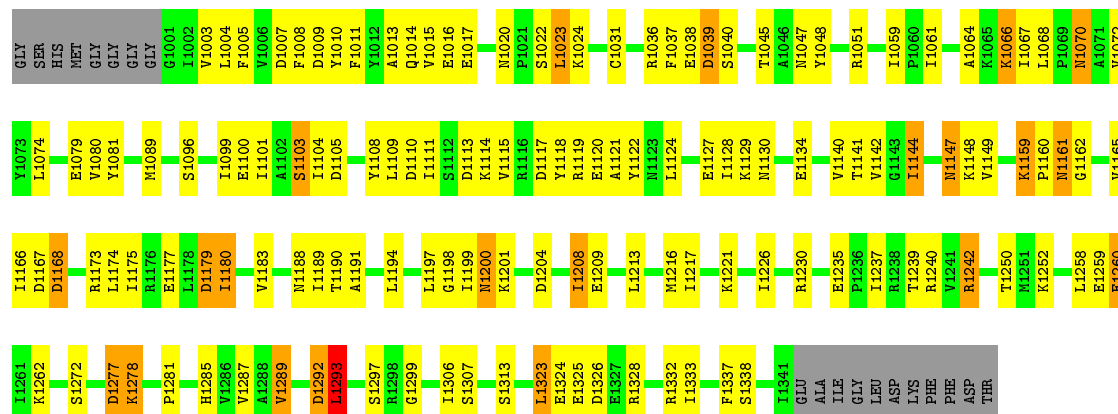
Chain A: 





• Molecule 3: Dpo4 polymerase IV

Chain B: 56% 33% 6% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.64Å 180.96Å 51.57Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 19.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.70) 99.1 (19.88-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.269 , 0.310 0.269 , 0.303	Depositor DCC
$R_{free}$ test set	1172 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.2	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 20.3	EDS
Estimated twinning fraction	0.400 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 27424 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.79	0/282	1.83	7/436 (1.6%)
1	H	0.87	0/282	1.78	10/436 (2.3%)
2	E	0.93	0/283	1.96	11/432 (2.5%)
2	J	0.93	1/283 (0.4%)	1.98	9/432 (2.1%)
3	A	0.54	0/2778	0.70	0/3731
3	B	0.55	0/2778	0.70	0/3731
All	All	0.62	1/6686 (0.0%)	1.03	37/9198 (0.4%)

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
3	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1910	DC	C3'-O3'	-6.38	1.35	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	918	DC	O4'-C1'-N1	15.70	118.99	108.00
2	J	1916	DA	O4'-C1'-N9	13.64	117.55	108.00
2	J	1912	DA	O4'-C1'-N9	11.47	116.03	108.00
2	J	1915	DC	O4'-C1'-N1	11.28	115.90	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	806	DG	O4'-C1'-N9	10.16	115.11	108.00
1	D	803	DT	O4'-C1'-N1	9.08	114.36	108.00
1	D	812	DA	O4'-C4'-C3'	-8.95	100.63	106.00
1	D	811	DT	C6-C5-C7	-8.80	117.62	122.90
1	H	1811	DT	O4'-C4'-C3'	-8.03	101.18	106.00
2	E	918	DC	O4'-C1'-C2'	-7.24	100.11	105.90
2	E	911	DC	O4'-C1'-N1	7.20	113.04	108.00
1	H	1808	DT	O4'-C1'-N1	7.19	113.03	108.00
2	J	1916	DA	C1'-O4'-C4'	-6.95	103.15	110.10
1	H	1808	DT	O4'-C1'-C2'	-6.55	100.66	105.90
2	J	1915	DC	P-O3'-C3'	6.53	127.53	119.70
2	E	916	DA	O4'-C1'-N9	6.48	112.53	108.00
1	H	1806	DG	O4'-C1'-N9	6.35	112.44	108.00
1	H	1804	DT	O4'-C1'-C2'	-6.27	100.89	105.90
2	E	908	DT	O4'-C1'-N1	6.25	112.38	108.00
1	D	805	DG	O4'-C1'-N9	6.07	112.25	108.00
1	D	808	DT	O4'-C1'-N1	6.06	112.25	108.00
1	H	1804	DT	O4'-C1'-N1	6.06	112.24	108.00
2	E	908	DT	O4'-C1'-C2'	-6.04	101.07	105.90
1	H	1812	DA	C4'-C3'-C2'	-5.91	97.78	103.10
2	E	913	DT	C1'-O4'-C4'	-5.85	104.25	110.10
2	J	1912	DA	O4'-C1'-C2'	-5.74	101.31	105.90
2	E	917	DA	N1-C6-N6	5.73	122.04	118.60
2	J	1911	DC	N1-C2-O2	5.71	122.33	118.90
2	J	1915	DC	O4'-C1'-C2'	-5.65	101.38	105.90
1	D	812	DA	C1'-O4'-C4'	-5.49	104.61	110.10
2	J	1910	DC	O4'-C1'-C2'	-5.32	101.64	105.90
2	E	912	DA	O4'-C1'-N9	5.27	111.69	108.00
2	E	910	DC	O4'-C1'-C2'	-5.22	101.72	105.90
1	H	1806	DG	O4'-C4'-C3'	-5.21	102.42	104.50
1	H	1808	DT	C3'-C2'-C1'	-5.17	96.29	102.50
1	H	1804	DT	N3-C4-O4	5.17	123.00	119.90
2	E	908	DT	P-O3'-C3'	5.10	125.83	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	235	GLU	Peptide
3	B	1099	ILE	Peptide

## 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	9	0
1	H	272	0	149	10	0
2	E	254	0	147	6	0
2	J	254	0	147	17	0
3	A	2739	0	2883	93	0
3	B	2739	0	2880	91	0
4	A	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
5	A	41	0	0	4	0
5	B	38	0	0	7	0
5	D	12	0	0	2	0
5	E	5	0	0	0	0
5	H	16	0	0	2	0
5	J	6	0	0	1	0
All	All	6651	0	6355	211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (211) 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:H:1813:DDG:H3'1	5:B:2:HOH:O	1.56	1.05
1:D:802:DG:H1	2:E:918:DC:H42	1.11	0.93
1:H:1802:DG:N2	2:J:1918:DC:N3	2.17	0.93
3:A:141:THR:OG1	3:A:159:LYS:O	1.99	0.80
3:B:1017:GLU:OE1	3:B:1024:LYS:NZ	2.13	0.79
3:A:23:LEU:HD21	3:A:74:LEU:HD11	1.65	0.79
1:D:802:DG:N2	2:E:918:DC:N3	2.30	0.78
3:B:1198:GLY:O	3:B:1200:ASN:ND2	2.17	0.78
1:H:1813:DDG:H3'1	5:B:85:HOH:O	1.84	0.78
3:A:326:ASP:OD2	3:A:328:ARG:N	2.18	0.76
3:B:1129:LYS:NZ	3:B:1161:ASN:OD1	2.15	0.73
3:A:245:ILE:HG21	3:A:275:LYS:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1813:DDG:H2''	3:B:1045:THR:HG23	1.70	0.72
3:B:1079:GLU:O	5:B:93:HOH:O	2.08	0.71
3:A:23:LEU:HD11	3:A:72:VAL:HG11	1.71	0.70
3:B:1129:LYS:HZ3	3:B:1162:GLY:N	1.89	0.70
3:A:4:LEU:HD21	3:A:128:ILE:HD13	1.74	0.69
3:B:1070:ASN:HD22	3:B:1070:ASN:C	1.96	0.69
3:B:1194:LEU:HD21	3:B:1217:ILE:HG21	1.75	0.68
3:A:188:ASN:O	3:A:191:ALA:N	2.27	0.67
2:J:1915:DC:H1'	2:J:1916:DA:OP2	1.95	0.67
3:B:1110:ASP:HB2	3:B:1237:ILE:HD13	1.76	0.66
3:B:1216:MET:O	5:B:3:HOH:O	2.14	0.65
3:A:324:GLU:N	3:A:324:GLU:OE2	2.30	0.64
3:A:202:LEU:CD2	3:A:229:ALA:HB2	2.28	0.64
3:B:1258:LEU:O	3:B:1260:GLU:N	2.29	0.63
1:D:802:DG:H1	2:E:918:DC:N4	1.90	0.62
3:A:149:VAL:HG11	3:A:228:LEU:HD21	1.80	0.62
3:B:1022:SER:O	3:B:1023:LEU:CB	2.46	0.62
3:B:1326:ASP:OD1	3:B:1328:ARG:HG2	2.00	0.61
1:H:1811:DT:OP1	3:B:1190:THR:HG22	2.00	0.61
3:B:1080:VAL:O	3:B:1080:VAL:HG12	2.00	0.61
3:B:1016:GLU:OE2	3:B:1081:TYR:OH	2.17	0.61
3:B:1201:LYS:N	3:B:1204:ASP:OD1	2.32	0.61
3:A:34:SER:OG	3:A:35:GLY:N	2.33	0.61
3:B:1038:GLU:O	3:B:1040:SER:N	2.34	0.61
3:A:5:PHE:CD2	3:A:152:LYS:HA	2.36	0.61
3:A:168:ASP:O	3:A:171:VAL:HB	2.00	0.60
3:B:1147:ASN:OD1	3:B:1147:ASN:C	2.40	0.60
3:A:191:ALA:O	3:A:195:LYS:N	2.25	0.59
3:A:37:PHE:O	3:A:39:ASP:O	2.20	0.59
3:B:1008:PHE:CD2	3:B:1105:ASP:HA	2.37	0.59
3:B:1066:LYS:HB3	3:B:1066:LYS:NZ	2.17	0.59
2:J:1907:DC:N4	5:J:87:HOH:O	2.26	0.58
3:A:44:ALA:O	3:A:45:THR:OG1	2.20	0.58
3:B:1213:LEU:HD23	3:B:1226:ILE:HD11	1.85	0.58
3:A:219:GLU:O	3:A:220:ALA:C	2.40	0.58
3:A:256:ARG:HD2	3:A:327:GLU:O	2.04	0.58
3:A:149:VAL:HG12	3:A:153:ILE:HD11	1.86	0.58
3:B:1194:LEU:HD21	3:B:1217:ILE:CG2	2.34	0.57
3:A:150:PHE:HA	3:A:153:ILE:HD12	1.86	0.57
3:A:202:LEU:HD23	3:A:202:LEU:O	2.05	0.56
3:A:111:ILE:O	3:A:113:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1022:SER:O	3:B:1023:LEU:HB2	2.05	0.56
3:A:167:ASP:O	3:A:171:VAL:HG23	2.06	0.56
3:B:1147:ASN:OD1	3:B:1148:LYS:N	2.40	0.55
3:B:1147:ASN:OD1	3:B:1149:VAL:N	2.36	0.55
3:A:23:LEU:HD21	3:A:74:LEU:CD1	2.35	0.55
3:A:149:VAL:HG11	3:A:228:LEU:CD2	2.37	0.55
3:B:1168:ASP:N	3:B:1168:ASP:OD1	2.40	0.54
3:A:166:ILE:HG23	3:A:170:GLU:HB3	1.89	0.54
3:A:28:VAL:HG23	3:A:47:ASN:HD21	1.71	0.54
3:B:1159:LYS:HB2	3:B:1160:PRO:HD3	1.90	0.54
3:A:9:ASP:O	3:A:10:TYR:C	2.47	0.53
3:B:1180:ILE:HB	3:B:1200:ASN:O	2.09	0.53
3:B:1011:PHE:O	3:B:1015:VAL:HG23	2.09	0.53
3:A:95:TYR:O	3:A:114:LYS:NZ	2.39	0.53
5:H:1509:HOH:O	2:J:1916:DA:H2	1.92	0.53
3:A:8:PHE:HB2	3:A:105:ASP:HB2	1.90	0.53
3:A:46:ALA:HB1	3:A:50:ALA:HB3	1.91	0.53
3:B:1089:MET:CE	3:B:1101:ILE:HG23	2.39	0.53
2:J:1915:DC:C1'	2:J:1916:DA:OP2	2.57	0.52
3:B:1323:LEU:O	3:B:1325:GLU:N	2.42	0.52
3:A:8:PHE:HA	3:A:140:VAL:HG12	1.92	0.52
3:B:1100:GLU:OE2	3:B:1240:ARG:NH2	2.43	0.52
1:H:1809:DG:N2	2:J:1912:DA:C2	2.78	0.52
3:A:319:LEU:HD12	3:A:319:LEU:O	2.11	0.51
3:A:176:ARG:NH2	5:A:537:HOH:O	2.43	0.51
3:A:237:ILE:N	3:A:237:ILE:HD12	2.25	0.51
3:B:1009:ASP:OD1	3:B:1141:THR:OG1	2.29	0.51
1:D:801:DG:H2''	1:D:802:DG:C8	2.46	0.51
3:B:1048:TYR:HA	3:B:1051:ARG:HG2	1.94	0.50
3:A:12:TYR:OH	3:A:104:ILE:HG21	2.12	0.50
3:A:235:GLU:HB3	3:A:236:PRO:CD	2.41	0.50
3:B:1003:VAL:HG22	3:B:1237:ILE:HD11	1.92	0.50
3:A:178:LEU:HB3	5:A:539:HOH:O	2.12	0.50
3:A:142:VAL:HG21	3:A:163:ILE:HD12	1.94	0.49
1:H:1801:DG:H1	2:J:1919:DC:H42	1.59	0.49
3:B:1272:SER:HB2	3:B:1337:PHE:HE2	1.78	0.49
3:B:1038:GLU:O	3:B:1039:ASP:C	2.51	0.49
3:A:241:VAL:HG13	5:A:530:HOH:O	2.12	0.49
3:A:269:ILE:HD13	3:A:312:TYR:HA	1.95	0.49
3:A:314:GLU:O	3:A:318:LEU:HG	2.12	0.49
3:B:1067:ILE:HG22	3:B:1068:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1010:TYR:CE1	3:B:1014:GLN:HB2	2.48	0.49
3:A:165:VAL:O	3:A:165:VAL:HG12	2.11	0.48
3:A:53:PHE:HE2	5:A:540:HOH:O	1.96	0.48
3:A:64:ALA:O	3:A:73:TYR:OH	2.31	0.48
3:A:14:GLN:HE22	3:A:139:THR:N	2.11	0.48
3:A:144:ILE:HB	3:A:165:VAL:HG22	1.95	0.48
3:B:1287:VAL:O	3:B:1333:ILE:HD12	2.12	0.48
3:A:186:ILE:HD12	3:A:190:THR:HG21	1.94	0.48
3:B:1199:ILE:HD11	3:B:1208:ILE:HG21	1.95	0.48
3:B:1144:ILE:HG21	3:B:1165:VAL:HG22	1.95	0.48
3:B:1072:VAL:HG12	3:B:1074:LEU:HD21	1.95	0.48
3:A:297:SER:O	3:A:298:ARG:HD3	2.14	0.48
3:A:93:ARG:HG3	3:A:99:ILE:HD13	1.95	0.48
3:A:319:LEU:O	3:A:320:GLN:C	2.52	0.48
3:A:307:SER:O	3:A:310:THR:HB	2.13	0.48
2:J:1915:DC:C2	2:J:1916:DA:C8	3.02	0.47
3:A:8:PHE:CZ	3:A:88:ILE:HG21	2.49	0.47
3:A:93:ARG:O	3:A:94:GLU:C	2.52	0.47
3:A:230:ARG:O	3:A:231:ASP:CB	2.62	0.47
3:A:63:GLU:HA	3:A:66:LYS:HG2	1.96	0.47
3:A:39:ASP:O	3:A:40:SER:CB	2.62	0.47
3:A:46:ALA:HB1	3:A:50:ALA:CB	2.44	0.47
2:J:1908:DT:H2'	2:J:1909:DA:C8	2.50	0.47
3:A:259:GLU:HA	3:A:262:LYS:HD3	1.96	0.47
3:B:1277:ASP:O	3:B:1278:LYS:HB2	2.14	0.47
3:B:1159:LYS:HB2	3:B:1159:LYS:NZ	2.30	0.47
3:A:174:LEU:O	3:A:178:LEU:N	2.48	0.47
3:B:1059:ILE:HD11	3:B:1064:ALA:HB2	1.97	0.47
3:A:267:ARG:O	3:A:270:GLU:HB2	2.15	0.47
3:A:45:THR:HG22	3:A:46:ALA:N	2.30	0.47
3:B:1003:VAL:CG2	3:B:1237:ILE:HD11	2.44	0.47
3:A:33:PHE:O	3:A:35:GLY:N	2.48	0.47
3:A:119:ARG:C	3:A:119:ARG:HD2	2.36	0.47
1:D:801:DG:O5'	5:D:33:HOH:O	2.21	0.46
3:B:1059:ILE:CD1	3:B:1064:ALA:HB2	2.44	0.46
3:A:247:ARG:CZ	3:A:271:GLU:OE2	2.64	0.46
3:B:1144:ILE:CG2	3:B:1165:VAL:HG22	2.45	0.46
3:B:1004:LEU:HD21	3:B:1142:VAL:HG13	1.97	0.46
1:D:806:DG:N2	5:D:67:HOH:O	2.26	0.46
3:A:219:GLU:O	3:A:222:ALA:N	2.48	0.46
3:B:1190:THR:HG21	3:B:1221:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:813:DDG:H1	2:E:907:DC:H42	1.64	0.46
3:B:1010:TYR:HD1	3:B:1013:ALA:HB3	1.81	0.46
3:B:1188:ASN:O	3:B:1189:ILE:C	2.55	0.46
3:B:1159:LYS:HB2	3:B:1159:LYS:HZ3	1.81	0.46
3:A:111:ILE:O	3:A:115:VAL:HG22	2.16	0.45
3:B:1281:PRO:CB	3:B:1337:PHE:HB3	2.46	0.45
1:D:805:DG:N2	2:E:915:DC:N3	2.60	0.45
3:A:202:LEU:HD23	3:A:229:ALA:HB2	1.97	0.45
3:B:1208:ILE:HD13	3:B:1209:GLU:O	2.16	0.45
3:B:1174:LEU:O	3:B:1175:ILE:C	2.55	0.45
3:A:30:VAL:CG1	3:A:76:MET:HG2	2.47	0.45
3:B:1179:ASP:O	3:B:1183:VAL:HG23	2.16	0.45
3:A:15:VAL:HG12	3:A:19:LEU:HD22	1.99	0.45
3:A:254:ASN:N	3:A:254:ASN:OD1	2.50	0.45
3:B:1258:LEU:HD21	3:B:1262:LYS:HE3	1.98	0.45
3:A:10:TYR:CE1	3:A:14:GLN:HG3	2.52	0.45
3:A:9:ASP:HB3	3:A:10:TYR:CE2	2.51	0.45
3:A:108:TYR:CD1	3:A:148:LYS:HG2	2.52	0.45
3:B:1130:ASN:ND2	5:B:51:HOH:O	2.49	0.45
3:B:1250:THR:HA	3:B:1332:ARG:HG2	1.99	0.45
3:B:1306:ILE:HG22	3:B:1307:SER:O	2.17	0.45
3:B:1045:THR:HG21	5:B:19:HOH:O	2.16	0.45
3:B:1174:LEU:O	3:B:1177:GLU:N	2.41	0.44
3:A:39:ASP:O	3:A:40:SER:HB3	2.18	0.44
3:A:8:PHE:CD2	3:A:105:ASP:HA	2.52	0.44
1:H:1802:DG:H1	2:J:1918:DC:H42	1.66	0.44
2:J:1915:DC:C2'	2:J:1916:DA:OP2	2.65	0.44
5:H:4:HOH:O	2:J:1912:DA:N6	2.50	0.44
2:J:1910:DC:H5''	3:B:1242:ARG:CZ	2.47	0.44
3:B:1070:ASN:C	3:B:1070:ASN:ND2	2.68	0.44
3:A:148:LYS:HD2	3:A:237:ILE:HG13	1.99	0.44
3:A:208:ILE:HD13	3:A:209:GLU:N	2.33	0.43
3:B:1118:TYR:O	3:B:1119:ARG:C	2.55	0.43
3:B:1031:CYS:HB3	3:B:1061:ILE:HD11	2.00	0.43
3:B:1066:LYS:HB3	3:B:1066:LYS:HZ2	1.80	0.43
3:A:250:THR:HA	3:A:332:ARG:HG2	1.99	0.43
3:B:1038:GLU:HA	5:B:27:HOH:O	2.18	0.43
3:B:1005:PHE:HD1	3:B:1108:TYR:CD1	2.37	0.43
1:H:1802:DG:N2	2:J:1918:DC:C2	2.84	0.43
3:B:1008:PHE:HA	3:B:1140:VAL:HG12	2.01	0.43
3:A:111:ILE:C	3:A:113:ASP:H	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:79:GLU:O	3:A:83:GLN:HG2	2.19	0.43
3:A:59:ILE:HA	3:A:60:PRO:HD2	1.88	0.42
3:B:1292:ASP:O	3:B:1293:LEU:HB2	2.19	0.42
2:J:1912:DA:H2''	2:J:1913:DT:OP2	2.20	0.42
3:A:314:GLU:OE1	3:A:317:LYS:NZ	2.24	0.42
3:B:1285:HIS:ND1	3:B:1299:GLY:HA3	2.35	0.42
3:A:335:VAL:HG22	3:A:336:ARG:N	2.35	0.42
3:A:30:VAL:HG12	3:A:76:MET:HG2	2.01	0.42
3:A:91:LEU:HD23	3:A:91:LEU:N	2.34	0.42
3:B:1023:LEU:HD11	3:B:1072:VAL:HG11	2.02	0.41
3:B:1190:THR:HG23	3:B:1190:THR:O	2.20	0.41
3:B:1201:LYS:O	3:B:1204:ASP:OD1	2.38	0.41
3:B:1103:SER:OG	3:B:1104:ILE:N	2.52	0.41
3:A:290:THR:O	3:A:292:ASP:O	2.38	0.41
2:J:1915:DC:H2''	2:J:1916:DA:OP2	2.20	0.41
3:B:1110:ASP:CB	3:B:1237:ILE:HD13	2.46	0.41
3:B:1004:LEU:HB2	3:B:1111:ILE:HD13	2.02	0.41
3:B:1117:ASP:O	3:B:1120:GLU:N	2.53	0.41
3:B:1005:PHE:CD1	3:B:1108:TYR:CE1	3.07	0.41
3:B:1166:ILE:O	3:B:1166:ILE:HG22	2.19	0.41
1:D:810:DG:P	3:A:189:ILE:HG21	2.59	0.41
3:A:65:LYS:HD2	3:A:73:TYR:CE2	2.55	0.41
2:E:917:DA:C6	2:E:918:DC:C4	3.08	0.41
3:B:1237:ILE:HD12	3:B:1237:ILE:H	1.85	0.41
1:H:1811:DT:OP2	3:B:1189:ILE:HB	2.19	0.41
3:B:1292:ASP:O	3:B:1293:LEU:CB	2.68	0.41
3:A:77:ARG:HB3	3:A:80:VAL:HG23	2.02	0.41
2:J:1916:DA:OP2	2:J:1916:DA:O4'	2.38	0.41
3:A:218:GLY:O	3:A:222:ALA:HB2	2.20	0.41
3:A:183:VAL:HG11	3:A:225:LEU:HD21	2.02	0.41
3:B:1117:ASP:O	3:B:1118:TYR:C	2.59	0.41
3:B:1289:VAL:HG12	3:B:1289:VAL:O	2.21	0.41
3:A:14:GLN:HE22	3:A:139:THR:H	1.68	0.40
3:B:1115:VAL:HG21	3:B:1121:ALA:HB2	2.02	0.40
3:B:1124:LEU:O	3:B:1128:ILE:HG13	2.22	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%)	258 (76%)	63 (19%)	18 (5%)	2	4
3	B	339/360 (94%)	279 (82%)	45 (13%)	15 (4%)	3	6
All	All	678/720 (94%)	537 (79%)	108 (16%)	33 (5%)	3	5

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	40	SER
3	A	276	LEU
3	A	277	ASP
3	B	1023	LEU
3	B	1036	ARG
3	B	1039	ASP
3	B	1252	LYS
3	B	1277	ASP
3	B	1293	LEU
3	A	112	SER
3	A	167	ASP
3	A	216	MET
3	A	291	GLU
3	B	1161	ASN
3	B	1278	LYS
3	B	1324	GLU
3	A	71	ALA
3	A	213	LEU
3	A	34	SER
3	A	38	GLU
3	A	157	MET
3	B	1047	ASN
3	B	1259	GLU
3	B	1260	GLU
3	A	145	SER

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Mol	Chain	Res	Type
3	A	339	LYS
3	B	1159	LYS
3	B	1167	ASP
3	B	1191	ALA
3	A	75	PRO
3	A	94	GLU
3	A	253	ARG
3	A	325	GLU

### 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%)	261 (87%)	38 (13%)	5	13
3	B	299/311 (96%)	266 (89%)	33 (11%)	8	18
All	All	598/622 (96%)	527 (88%)	71 (12%)	6	15

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	19	LEU
3	A	26	LYS
3	A	37	PHE
3	A	49	GLU
3	A	52	LYS
3	A	65	LYS
3	A	66	LYS
3	A	83	GLN
3	A	95	TYR
3	A	96	SER
3	A	109	LEU
3	A	115	VAL
3	A	122	TYR
3	A	134	GLU
3	A	146	LYS

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Mol	Chain	Res	Type
3	A	159	LYS
3	A	170	GLU
3	A	208	ILE
3	A	213	LEU
3	A	214	LYS
3	A	217	ILE
3	A	223	LYS
3	A	238	ARG
3	A	239	THR
3	A	241	VAL
3	A	247	ARG
3	A	254	ASN
3	A	265	LEU
3	A	273	TYR
3	A	274	TYR
3	A	276	LEU
3	A	284	ILE
3	A	289	VAL
3	A	309	GLU
3	A	315	SER
3	A	323	LEU
3	A	325	GLU
3	A	327	GLU
3	B	1007	ASP
3	B	1020	ASN
3	B	1037	PHE
3	B	1066	LYS
3	B	1070	ASN
3	B	1096	SER
3	B	1103	SER
3	B	1109	LEU
3	B	1113	ASP
3	B	1114	LYS
3	B	1122	TYR
3	B	1127	GLU
3	B	1134	GLU
3	B	1144	ILE
3	B	1147	ASN
3	B	1168	ASP
3	B	1173	ARG
3	B	1179	ASP
3	B	1180	ILE

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Mol	Chain	Res	Type
3	B	1197	LEU
3	B	1200	ASN
3	B	1208	ILE
3	B	1230	ARG
3	B	1235	GLU
3	B	1239	THR
3	B	1242	ARG
3	B	1289	VAL
3	B	1292	ASP
3	B	1293	LEU
3	B	1297	SER
3	B	1313	SER
3	B	1323	LEU
3	B	1338	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	14	GLN
3	A	285	HIS
3	B	1014	GLN
3	B	1070	ASN
3	B	1130	ASN
3	B	1188	ASN
3	B	1200	ASN

### 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	1.44	2 (13%)	16,33,36	2.88	4 (25%)
1	DDG	H	1813	1,2,4	15,23,24	1.23	2 (13%)	16,33,36	2.93	4 (25%)

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	D	813	DDG	C8-N7	-2.76	1.29	1.34
1	H	1813	DDG	C8-N7	-2.38	1.30	1.34
1	H	1813	DDG	C6-N1	3.42	1.39	1.33
1	D	813	DDG	C6-N1	4.23	1.41	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1813	DDG	C5-C6-N1	-8.59	111.84	123.59
1	D	813	DDG	C5-C6-N1	-8.36	112.16	123.59
1	H	1813	DDG	O4'-C4'-C5'	-2.75	105.48	109.54
1	H	1813	DDG	N3-C2-N1	-2.23	124.05	127.44
1	D	813	DDG	C4-C5-N7	2.21	111.51	109.48
1	D	813	DDG	C3'-C2'-C1'	2.34	105.33	102.71
1	D	813	DDG	C6-N1-C2	5.59	123.70	115.94
1	H	1813	DDG	C6-N1-C2	6.19	124.53	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	813	DDG	1	0
1	H	1813	DDG	3	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 [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	D	12/13 (92%)	-0.56	0	100 100	54, 60, 67, 69	0
1	H	12/13 (92%)	-0.63	0	100 100	47, 58, 67, 69	0
2	E	13/19 (68%)	-0.73	0	100 100	42, 53, 64, 66	0
2	J	13/19 (68%)	-0.65	0	100 100	48, 61, 64, 66	0
3	A	341/360 (94%)	-0.22	1 (0%)	94 95	41, 51, 60, 63	0
3	B	341/360 (94%)	-0.23	0	100 100	41, 51, 60, 65	0
All	All	732/784 (93%)	-0.25	1 (0%)	95 97	41, 52, 61, 69	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	37	PHE	2.3

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	DDG	D	813	21/22	0.89	0.15	-	51,51,61,63	0
1	DDG	H	1813	21/22	0.93	0.11	-	42,44,45,45	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	A	415	1/1	0.90	0.14	-0.34	43,43,43,43	0
4	CA	J	1416	1/1	0.93	0.35	-	74,74,74,74	0
4	CA	H	1415	1/1	0.84	0.07	-	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.