



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:12 AM GMT

PDB ID : 1Q2R  
Title : Chemical trapping and crystal structure of a catalytic tRNA guanine transglycosylase covalent intermediate  
Authors : Xie, W.; Liu, X.; Huang, R.H.  
Deposited on : 2003-07-25  
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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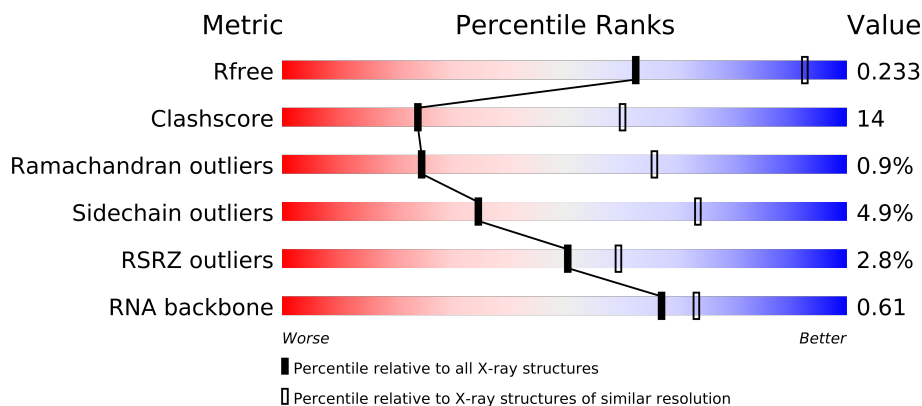
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	20	
1	F	20	
2	A	386	
2	B	386	
2	C	386	
2	D	386	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	9DG	B	387	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12672 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RNA chain called RNA (5'-R(\*AP\*GP\*CP\*AP\*CP\*GP\*GP\*CP\*UP\*(N)P\*UP\*AP\*AP\*AP\*CP\*CP\*GP\*UP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	20	Total	C	N	O	P	0	0	0
			414	186	74	135	19			
1	F	20	Total	C	N	O	P	0	0	0
			414	186	74	135	19			

- Molecule 2 is a protein called Queuine tRNA-ribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	376	Total	C	N	O	S	0	0	0
			2933	1833	534	545	21			
2	B	372	Total	C	N	O	S	0	0	0
			2902	1817	526	538	21			
2	C	376	Total	C	N	O	S	0	0	0
			2933	1833	534	545	21			
2	D	372	Total	C	N	O	S	0	0	0
			2902	1817	526	538	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P28720
B	1	MET	-	INITIATING METHIONINE	UNP P28720
C	1	MET	-	INITIATING METHIONINE	UNP P28720
D	1	MET	-	INITIATING METHIONINE	UNP P28720

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

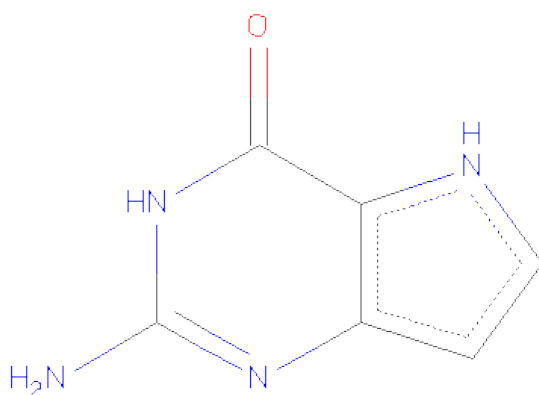
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0

- Molecule 4 is 9-DEAZAGUANINE (three-letter code: 9DG) (formula: C<sub>6</sub>H<sub>6</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 11	C 6	N 4	O 1	0	0
4	B	1	Total 11	C 6	N 4	O 1	0	0
4	C	1	Total 11	C 6	N 4	O 1	0	0
4	D	1	Total 11	C 6	N 4	O 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total 39	O 39	0	0
5	B	17	Total 17	O 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	31	Total 31	O 31	0	0
5	D	26	Total 26	O 26	0	0
5	E	8	Total 8	O 8	0	0
5	F	5	Total 5	O 5	0	0

### 3 Residue-property plots

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.

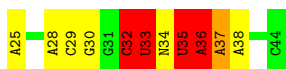
- Molecule 1: RNA (5'-R(\*AP\*GP\*CP\*AP\*CP\*GP\*GP\*CP\*UP\*(N)P\*UP\*AP\*AP\*AP\*CP\*CP\*GP\*UP\*GP\*C)-3')

Chain E: 



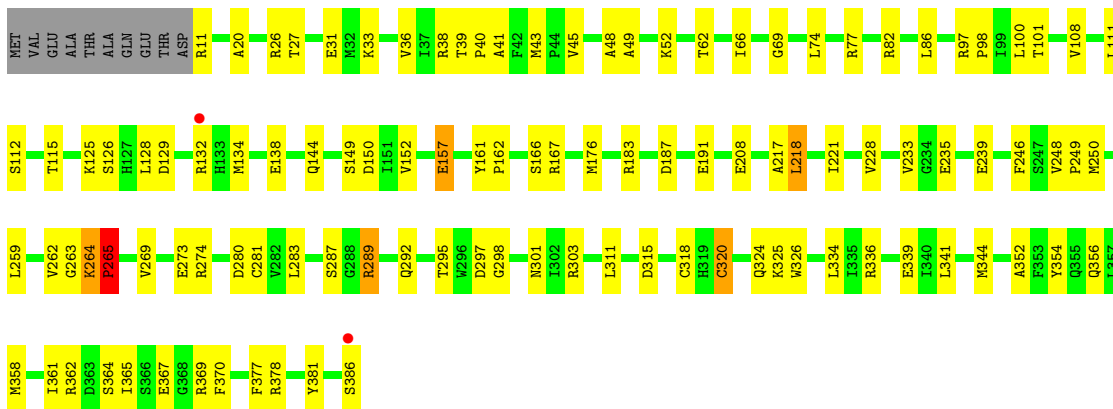
- Molecule 1: RNA (5'-R(\*AP\*GP\*CP\*AP\*CP\*GP\*GP\*CP\*UP\*(N)P\*UP\*AP\*AP\*AP\*CP\*CP\*GP\*UP\*GP\*C)-3')

Chain F: 



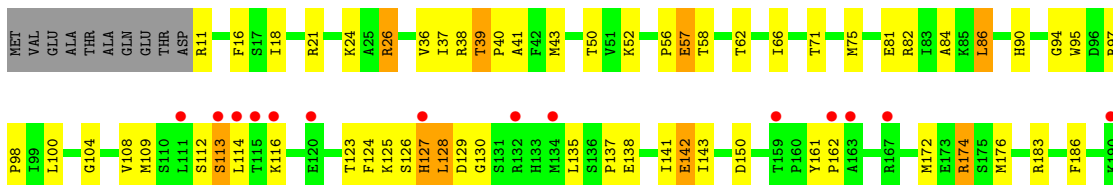
- Molecule 2: Queuine tRNA-ribosyltransferase

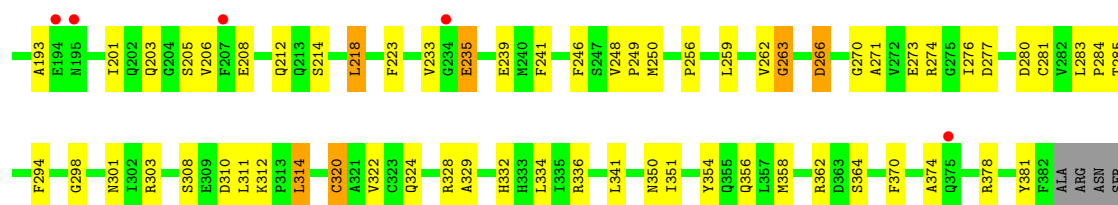
Chain A: 



- Molecule 2: Queuine tRNA-ribosyltransferase

Chain B: 





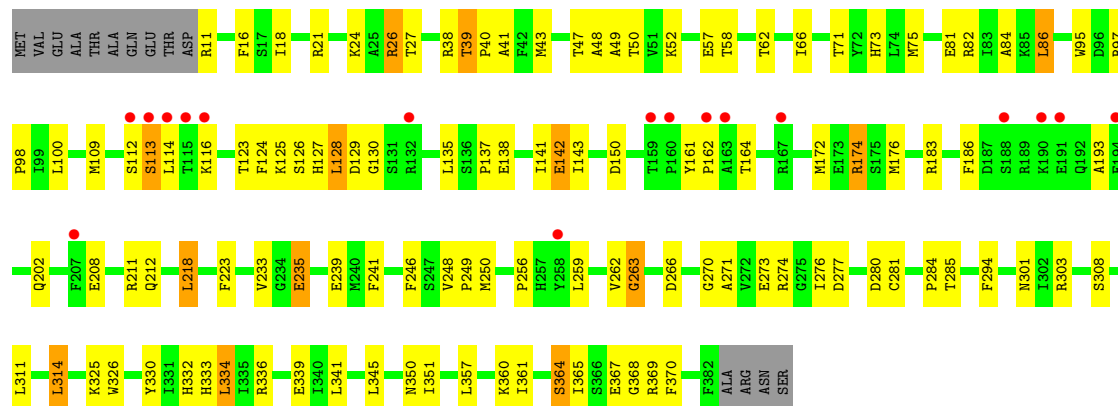
### • Molecule 2: Queuine tRNA-ribosyltransferase

Chain C:



### • Molecule 2: Queuine tRNA-ribosyltransferase

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.86Å 264.86Å 55.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.90) 97.1 (29.61-2.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.79 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.181 , 0.230 0.189 , 0.233	Depositor DCC
$R_{free}$ test set	3455 reflections (8.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 12.0	EDS
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43549 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 9DG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	E	0.50	0/448	1.10	5/694 (0.7%)
1	F	0.50	0/448	1.07	8/694 (1.2%)
2	A	0.38	0/2995	0.63	2/4032 (0.0%)
2	B	0.37	0/2964	0.56	0/3992
2	C	0.40	0/2995	0.63	2/4032 (0.0%)
2	D	0.38	0/2964	0.56	0/3992
All	All	0.39	0/12814	0.65	17/17436 (0.1%)

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
1	F	1	0

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	36	A	C2'-C3'-O3'	9.35	130.06	109.50
2	C	289	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	E	35	U	C2'-C3'-O3'	8.62	128.46	109.50
1	F	35	U	C2'-C3'-O3'	8.08	127.28	109.50
1	F	37	A	C2'-C3'-O3'	8.02	127.14	109.50
2	A	289	ARG	NE-CZ-NH1	-7.77	116.42	120.30
2	A	289	ARG	NE-CZ-NH2	7.76	124.18	120.30
2	C	289	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	F	33	U	C5'-C4'-C3'	-7.24	104.42	116.00
1	E	37	A	N9-C1'-C2'	6.84	122.89	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	32	C	C5'-C4'-C3'	-6.09	106.25	116.00
1	E	33	U	N1-C1'-C2'	5.72	121.43	114.00
1	E	36	A	N9-C1'-C2'	5.69	121.39	114.00
1	F	36	A	N9-C1'-C2'	5.60	121.28	114.00
1	F	35	U	C4'-C3'-O3'	5.45	123.89	113.00
1	F	35	U	C4'-C3'-C2'	5.33	107.93	102.60
1	F	37	A	C4'-C3'-C2'	5.23	107.83	102.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	35	U	C3'

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	414	0	215	7	0
1	F	414	0	215	11	0
2	A	2933	0	2877	82	0
2	B	2902	0	2848	102	0
2	C	2933	0	2877	78	0
2	D	2902	0	2848	86	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	11	0	6	0	0
4	B	11	0	6	0	0
4	C	11	0	6	0	0
4	D	11	0	6	0	0
5	A	39	0	0	2	0
5	B	17	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	31	0	0	2	0
5	D	26	0	0	3	0
5	E	8	0	0	0	0
5	F	5	0	0	2	0
All	All	12672	0	11904	346	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (346) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:36:A:H5''	2:A:111:LEU:HD21	1.56	0.87
2:D:334:LEU:HD21	2:D:341:LEU:HD23	1.59	0.84
2:C:112:SER:O	2:C:115:THR:HG22	1.80	0.81
2:A:112:SER:O	2:A:115:THR:HG22	1.81	0.80
2:A:318:CYS:SG	2:A:320:CYS:HB3	2.21	0.79
2:B:174:ARG:HH11	2:B:174:ARG:HB2	1.47	0.79
2:D:364:SER:OG	2:D:370:PHE:HA	1.82	0.78
2:D:174:ARG:HB2	2:D:174:ARG:HH11	1.49	0.77
2:C:183:ARG:HD2	2:C:187:ASP:OD2	1.86	0.76
2:A:11:ARG:HG2	2:A:33:LYS:HA	1.68	0.75
2:B:334:LEU:HD21	2:B:341:LEU:HG	1.68	0.75
2:C:11:ARG:HG2	2:C:33:LYS:HA	1.69	0.75
2:A:38:ARG:O	2:A:41:ALA:HB2	1.87	0.74
2:B:71:THR:HG23	2:B:143:ILE:HG21	1.70	0.74
2:A:289:ARG:HD3	5:A:390:HOH:O	1.88	0.73
2:C:38:ARG:O	2:C:41:ALA:HB2	1.89	0.72
2:A:354:TYR:O	2:A:358:MET:HG2	1.89	0.72
2:B:11:ARG:HG2	2:B:11:ARG:HH11	1.54	0.71
2:D:71:THR:HG23	2:D:143:ILE:HG21	1.70	0.70
2:A:183:ARG:HD2	2:A:187:ASP:OD2	1.90	0.70
2:D:97:ARG:HB3	2:D:98:PRO:HD2	1.73	0.69
2:B:320:CYS:O	2:B:324:GLN:HG2	1.92	0.69
2:A:208:GLU:HB3	2:A:246:PHE:CZ	2.27	0.69
2:A:273:GLU:OE1	2:A:378:ARG:NH2	2.27	0.68
2:D:208:GLU:HG2	5:D:395:HOH:O	1.93	0.67
2:C:312:LYS:O	2:C:328:ARG:HG3	1.94	0.67
2:B:113:SER:HB3	2:B:125:LYS:HB3	1.77	0.67
2:C:352:ALA:O	2:C:356:GLN:HG3	1.95	0.67
2:C:332:HIS:CE1	2:C:336:ARG:HD2	2.29	0.66
2:A:52:LYS:HB3	5:A:390:HOH:O	1.96	0.66
2:C:208:GLU:HB3	2:C:246:PHE:CZ	2.31	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:284:PRO:HB2	2:C:351:ILE:HD12	1.76	0.66
2:C:39:THR:HA	2:C:40:PRO:C	2.17	0.65
2:A:39:THR:HA	2:A:40:PRO:C	2.17	0.65
2:A:97:ARG:HB3	2:A:98:PRO:HD2	1.79	0.65
2:B:38:ARG:O	2:B:41:ALA:HB2	1.96	0.65
2:C:273:GLU:OE1	2:C:378:ARG:NH2	2.28	0.64
2:C:43:MET:HG2	2:C:66:ILE:HG23	1.78	0.64
2:A:301:ASN:OD1	2:A:303:ARG:HD3	1.98	0.64
2:B:241:PHE:HB3	2:B:274:ARG:NH2	2.13	0.64
2:C:301:ASN:OD1	2:C:303:ARG:HD3	1.98	0.64
2:A:43:MET:CG	2:A:66:ILE:HG23	2.28	0.64
2:D:116:LYS:HB3	2:D:123:THR:HB	1.79	0.64
2:C:97:ARG:HB3	2:C:98:PRO:HD2	1.81	0.63
2:B:39:THR:HA	2:B:40:PRO:C	2.19	0.63
2:B:97:ARG:HB3	2:B:98:PRO:HD2	1.79	0.63
2:A:43:MET:HG2	2:A:66:ILE:HG23	1.80	0.63
2:D:241:PHE:HB3	2:D:274:ARG:NH2	2.14	0.63
2:D:11:ARG:HH11	2:D:11:ARG:HG2	1.63	0.63
2:A:263:GLY:O	2:A:264:LYS:HB2	1.99	0.63
2:D:128:LEU:HD12	2:D:129:ASP:N	2.13	0.63
2:B:116:LYS:HB3	2:B:123:THR:HB	1.80	0.63
1:E:25:A:H8	1:E:25:A:HO5'	1.46	0.62
2:B:259:LEU:HD21	2:B:262:VAL:HG21	1.81	0.62
2:D:284:PRO:HB2	2:D:351:ILE:HD12	1.81	0.61
2:B:137:PRO:O	2:B:141:ILE:HG12	1.99	0.61
2:C:43:MET:CG	2:C:66:ILE:HG23	2.31	0.61
2:C:263:GLY:O	2:C:264:LYS:HB2	1.98	0.61
2:A:40:PRO:HD2	2:A:362:ARG:HG2	1.83	0.61
2:D:113:SER:HB3	2:D:125:LYS:HB3	1.83	0.60
2:B:208:GLU:HB3	2:B:246:PHE:CZ	2.36	0.60
1:F:28:A:H1'	5:F:101:HOH:O	2.01	0.60
2:C:263:GLY:O	2:C:264:LYS:CB	2.50	0.60
2:D:38:ARG:O	2:D:41:ALA:HB2	2.02	0.60
1:F:36:A:H5''	2:C:111:LEU:HD21	1.83	0.59
2:D:39:THR:HA	2:D:40:PRO:C	2.23	0.59
2:A:274:ARG:HH11	2:A:274:ARG:HG3	1.68	0.59
2:A:263:GLY:O	2:A:264:LYS:CB	2.50	0.59
2:B:43:MET:HG2	2:B:66:ILE:HG23	1.83	0.59
2:B:128:LEU:HD12	2:B:129:ASP:N	2.17	0.58
2:B:259:LEU:CD2	2:B:262:VAL:HG21	2.34	0.58
2:D:259:LEU:HD21	2:D:262:VAL:HG21	1.84	0.58
2:C:287:SER:HB3	2:C:292:GLN:HB3	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:274:ARG:HH11	2:C:274:ARG:HG3	1.68	0.57
2:B:16:PHE:CD2	2:B:256:PRO:HD3	2.39	0.57
2:D:43:MET:HG2	2:D:66:ILE:HG23	1.87	0.57
2:B:183:ARG:HH21	2:B:223:PHE:HA	1.69	0.57
2:B:126:SER:HB3	2:B:130:GLY:H	1.70	0.57
2:B:172:MET:O	2:B:176:MET:HG2	2.04	0.57
2:A:31:GLU:HG2	2:A:36:VAL:HG22	1.87	0.56
1:E:28:A:OP2	2:A:336:ARG:NH2	2.26	0.56
1:F:28:A:OP2	2:C:336:ARG:NH2	2.39	0.56
2:B:233:VAL:O	2:B:233:VAL:HG22	2.05	0.56
2:B:11:ARG:HG2	2:B:11:ARG:NH1	2.15	0.56
2:D:126:SER:HB3	2:D:130:GLY:H	1.71	0.56
2:B:271:ALA:HB1	2:B:276:ILE:HG13	1.86	0.56
2:D:98:PRO:HA	2:D:150:ASP:OD2	2.06	0.56
2:C:295:THR:HB	2:C:315:ASP:OD1	2.06	0.56
2:D:208:GLU:HB3	2:D:246:PHE:CZ	2.40	0.56
2:A:361:ILE:O	2:A:365:ILE:HG13	2.06	0.55
2:D:137:PRO:O	2:D:141:ILE:HG12	2.06	0.55
2:A:62:THR:HB	2:A:352:ALA:HA	1.86	0.55
1:F:25:A:N3	1:F:25:A:O5'	2.27	0.55
2:B:116:LYS:O	2:B:116:LYS:HD3	2.05	0.55
1:F:35:U:H3	2:C:289:ARG:HH22	1.54	0.55
2:D:116:LYS:O	2:D:116:LYS:HD3	2.05	0.55
2:A:364:SER:HB2	2:A:370:PHE:HA	1.89	0.55
1:F:32:C:O2'	2:C:286:ARG:HD2	2.06	0.54
2:D:176:MET:SD	2:D:218:LEU:HD13	2.47	0.54
2:D:259:LEU:CD2	2:D:262:VAL:HG21	2.37	0.54
2:A:325:LYS:HD3	2:A:326:TRP:CZ2	2.42	0.54
2:C:357:LEU:O	2:C:361:ILE:HG13	2.08	0.54
1:E:36:A:C5'	2:A:111:LEU:HD21	2.31	0.53
2:C:308:SER:HA	2:C:332:HIS:CD2	2.43	0.53
2:D:183:ARG:HH21	2:D:223:PHE:HA	1.73	0.53
2:A:297:ASP:HB2	2:A:386:SER:HB2	1.90	0.53
2:D:11:ARG:NH1	2:D:11:ARG:HG2	2.22	0.53
2:D:332:HIS:O	2:D:336:ARG:HB2	2.09	0.53
2:D:248:VAL:HB	2:D:249:PRO:HD3	1.91	0.53
2:B:176:MET:SD	2:B:218:LEU:HD13	2.49	0.52
2:B:112:SER:HB3	2:B:124:PHE:HB2	1.91	0.52
2:C:334:LEU:HD21	2:C:341:LEU:HD23	1.91	0.52
2:D:186:PHE:CE1	2:D:193:ALA:HA	2.44	0.52
2:D:27:THR:HG22	2:D:365:ILE:HG22	1.92	0.52
1:E:30:G:O6	2:A:303:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:295:THR:HB	2:A:315:ASP:OD1	2.09	0.52
2:A:320:CYS:O	2:A:324:GLN:HG2	2.09	0.52
2:D:95:TRP:NE1	2:D:97:ARG:HB2	2.25	0.52
2:B:294:PHE:H	2:B:350:ASN:HD21	1.58	0.52
2:D:71:THR:HG22	2:D:75:MET:HE2	1.92	0.52
2:D:112:SER:HB3	2:D:124:PHE:HB2	1.92	0.52
2:C:248:VAL:HB	2:C:249:PRO:HD3	1.92	0.52
2:B:36:VAL:HG22	5:B:401:HOH:O	2.10	0.52
2:D:208:GLU:HB3	2:D:246:PHE:CE1	2.45	0.51
2:B:208:GLU:HB3	2:B:246:PHE:CE1	2.45	0.51
2:A:352:ALA:O	2:A:356:GLN:HG3	2.11	0.51
2:D:172:MET:O	2:D:176:MET:HG2	2.10	0.51
2:B:320:CYS:SG	2:B:322:VAL:HB	2.51	0.51
2:D:212:GLN:HA	2:D:250:MET:SD	2.50	0.51
2:C:144:GLN:OE1	2:C:152:VAL:HG13	2.11	0.51
2:B:248:VAL:HB	2:B:249:PRO:HD3	1.92	0.51
2:C:62:THR:HB	2:C:352:ALA:HA	1.93	0.51
2:A:311:LEU:CD1	2:B:86:LEU:HD12	2.40	0.51
2:C:364:SER:HB2	2:C:370:PHE:HA	1.93	0.51
5:F:116:HOH:O	2:C:52:LYS:HB2	2.11	0.51
2:A:98:PRO:HA	2:A:150:ASP:OD2	2.11	0.50
2:D:294:PHE:H	2:D:350:ASN:HD21	1.59	0.50
2:A:108:VAL:HG11	2:A:157:GLU:HG2	1.93	0.50
2:B:212:GLN:HA	2:B:250:MET:SD	2.51	0.50
2:D:82:ARG:O	2:D:86:LEU:HD22	2.12	0.50
2:B:100:LEU:HD23	2:B:100:LEU:C	2.32	0.50
2:D:357:LEU:O	2:D:361:ILE:HG13	2.11	0.50
2:B:259:LEU:HG	2:B:262:VAL:CG2	2.42	0.50
2:D:259:LEU:HG	2:D:262:VAL:CG2	2.41	0.50
2:A:161:TYR:CD1	2:A:162:PRO:HA	2.47	0.50
2:C:40:PRO:HD2	2:C:362:ARG:HG2	1.94	0.49
2:B:26:ARG:HH11	2:B:26:ARG:HG3	1.77	0.49
2:C:161:TYR:CD1	2:C:162:PRO:HA	2.46	0.49
2:B:312:LYS:O	2:B:328:ARG:HG3	2.12	0.49
2:B:186:PHE:CE1	2:B:193:ALA:HA	2.47	0.49
2:B:201:ILE:HG22	2:B:203:GLN:NE2	2.27	0.49
2:D:263:GLY:HA3	2:D:281:CYS:CB	2.42	0.49
2:A:86:LEU:HD21	2:B:329:ALA:HB1	1.94	0.49
2:B:82:ARG:O	2:B:86:LEU:HD22	2.13	0.49
2:A:287:SER:HB3	2:A:292:GLN:HB3	1.95	0.49
2:A:208:GLU:HB3	2:A:246:PHE:CE1	2.47	0.49
2:A:325:LYS:HE2	2:B:94:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:217:ALA:O	2:A:221:ILE:HG13	2.13	0.49
2:A:367:GLU:CD	2:A:369:ARG:HE	2.16	0.49
2:D:71:THR:HG23	2:D:143:ILE:CG2	2.39	0.49
1:E:34:N:O2'	2:A:45:VAL:HG22	2.12	0.49
2:C:372:GLN:HG3	2:C:376:ASP:OD2	2.12	0.49
2:A:367:GLU:HB2	2:A:369:ARG:HG2	1.94	0.48
2:D:263:GLY:HA3	2:D:281:CYS:HB2	1.95	0.48
2:D:114:LEU:HD12	2:D:125:LYS:HD2	1.95	0.48
2:A:259:LEU:HG	2:A:262:VAL:HG21	1.95	0.48
2:C:52:LYS:HB3	5:C:389:HOH:O	2.12	0.48
2:B:235:GLU:O	2:B:239:GLU:HB2	2.13	0.48
2:C:208:GLU:HB3	2:C:246:PHE:CE1	2.48	0.48
2:D:308:SER:HA	2:D:332:HIS:CD2	2.48	0.48
2:D:271:ALA:HB1	2:D:276:ILE:HG13	1.94	0.48
2:B:263:GLY:HA3	2:B:281:CYS:CB	2.44	0.48
2:D:233:VAL:O	2:D:233:VAL:HG22	2.14	0.48
2:A:311:LEU:HD11	2:B:86:LEU:HD12	1.95	0.48
2:B:235:GLU:H	2:B:235:GLU:CD	2.17	0.48
2:A:43:MET:CE	2:A:100:LEU:HD13	2.44	0.48
2:B:266:ASP:HB2	5:B:393:HOH:O	2.13	0.48
2:C:235:GLU:O	2:C:239:GLU:HB2	2.13	0.48
2:A:43:MET:HG3	2:A:66:ILE:HG23	1.95	0.48
2:A:235:GLU:O	2:A:239:GLU:HB2	2.14	0.47
2:D:24:LYS:HB2	2:D:273:GLU:O	2.13	0.47
2:B:18:ILE:HD11	2:B:26:ARG:NH1	2.29	0.47
2:A:339:GLU:HG3	2:B:50:THR:HG21	1.95	0.47
2:A:265:PRO:HB3	2:A:377:PHE:HZ	1.79	0.47
2:A:66:ILE:HG13	2:A:98:PRO:O	2.15	0.47
2:C:246:PHE:O	2:C:250:MET:HG3	2.14	0.47
2:D:26:ARG:HH11	2:D:26:ARG:HG3	1.80	0.47
2:C:284:PRO:HB2	2:C:351:ILE:CD1	2.42	0.47
2:B:126:SER:HB3	2:B:129:ASP:HB3	1.97	0.47
2:B:263:GLY:HA3	2:B:281:CYS:HB2	1.97	0.47
2:A:233:VAL:HG22	2:A:233:VAL:O	2.15	0.47
2:C:298:GLY:HA2	2:C:381:TYR:CE1	2.50	0.47
2:B:174:ARG:HB2	2:B:174:ARG:NH1	2.24	0.46
2:A:274:ARG:NH1	2:A:274:ARG:HG3	2.30	0.46
2:D:235:GLU:H	2:D:235:GLU:CD	2.18	0.46
2:A:298:GLY:HA2	2:A:381:TYR:CE1	2.49	0.46
2:C:31:GLU:HG2	2:C:36:VAL:HG22	1.97	0.46
2:D:21:ARG:HB3	2:D:26:ARG:CB	2.46	0.46
2:B:273:GLU:HG2	2:B:370:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:112:SER:O	2:D:113:SER:HB2	2.15	0.46
2:B:112:SER:O	2:B:113:SER:HB2	2.15	0.46
2:B:71:THR:HG23	2:B:143:ILE:CG2	2.40	0.46
2:B:98:PRO:HA	2:B:150:ASP:OD2	2.15	0.46
2:B:183:ARG:NH2	2:B:223:PHE:HA	2.31	0.46
2:A:265:PRO:O	2:A:269:VAL:HG23	2.16	0.46
2:B:24:LYS:HB2	2:B:273:GLU:O	2.16	0.46
2:D:48:ALA:O	2:D:49:ALA:HB3	2.15	0.46
2:A:248:VAL:HB	2:A:249:PRO:HD3	1.98	0.46
2:B:308:SER:HA	2:B:332:HIS:CD2	2.51	0.46
2:C:259:LEU:HG	2:C:262:VAL:HG21	1.98	0.46
2:B:71:THR:HG22	2:B:75:MET:HE2	1.98	0.46
2:B:114:LEU:HD12	2:B:125:LYS:HD2	1.98	0.46
1:F:36:A:C5'	2:C:111:LEU:HD21	2.46	0.46
2:A:48:ALA:O	2:A:49:ALA:HB3	2.16	0.46
2:D:16:PHE:CD2	2:D:256:PRO:HD3	2.51	0.46
1:F:29:C:O2'	1:F:30:G:H5'	2.15	0.46
2:A:246:PHE:O	2:A:250:MET:HG3	2.15	0.45
2:C:274:ARG:HG3	2:C:274:ARG:NH1	2.30	0.45
2:C:318:CYS:SG	2:C:356:GLN:NE2	2.84	0.45
1:F:33:U:O2'	2:C:261:GLY:O	2.28	0.45
2:B:95:TRP:NE1	2:B:97:ARG:HB2	2.31	0.45
2:D:285:THR:HG23	2:D:351:ILE:HD11	1.99	0.45
2:A:132:ARG:NH1	2:A:132:ARG:HG3	2.32	0.45
2:C:217:ALA:O	2:C:221:ILE:HG13	2.16	0.45
2:D:361:ILE:HG23	2:D:370:PHE:CE1	2.51	0.45
2:B:40:PRO:HA	2:B:277:ASP:O	2.17	0.45
2:A:228:VAL:HG23	2:A:259:LEU:HA	1.99	0.45
2:C:128:LEU:HD12	2:C:129:ASP:HB2	1.98	0.45
2:C:233:VAL:O	2:C:233:VAL:HG22	2.17	0.45
2:B:332:HIS:CE1	2:B:336:ARG:HD2	2.52	0.45
2:B:310:ASP:HB3	2:B:328:ARG:HB2	1.98	0.45
2:A:367:GLU:OE2	2:A:369:ARG:NH2	2.48	0.45
2:B:273:GLU:HG2	2:B:370:PHE:CE2	2.51	0.45
2:A:176:MET:SD	2:A:218:LEU:HD13	2.57	0.45
2:B:241:PHE:CZ	2:B:270:GLY:HA3	2.52	0.45
2:B:364:SER:HB2	2:B:370:PHE:HA	1.97	0.45
1:E:25:A:H2'	1:E:26:G:H5'	1.99	0.44
2:C:128:LEU:HD12	2:C:129:ASP:N	2.31	0.44
2:A:125:LYS:O	2:A:126:SER:C	2.55	0.44
2:B:58:THR:O	2:B:62:THR:HG23	2.17	0.44
2:A:326:TRP:HZ2	2:B:56:PRO:HD2	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:108:VAL:HG11	2:A:157:GLU:CG	2.47	0.44
2:C:98:PRO:HA	2:C:150:ASP:OD2	2.17	0.44
2:B:354:TYR:O	2:B:358:MET:HG2	2.18	0.44
2:A:43:MET:HE1	2:A:100:LEU:HD13	2.00	0.44
2:B:303:ARG:HB3	2:B:303:ARG:HE	1.57	0.44
2:A:97:ARG:CB	2:A:98:PRO:HD2	2.47	0.44
2:A:128:LEU:HD12	2:A:129:ASP:HB2	1.99	0.44
2:C:228:VAL:HG23	2:C:259:LEU:HA	1.99	0.44
2:B:138:GLU:O	2:B:142:GLU:HB2	2.17	0.44
2:D:27:THR:HG22	2:D:365:ILE:CG2	2.48	0.44
2:C:66:ILE:HG13	2:C:98:PRO:O	2.19	0.43
2:D:40:PRO:HA	2:D:277:ASP:O	2.18	0.43
2:B:37:ILE:HD11	2:B:66:ILE:HD12	2.00	0.43
2:B:214:SER:O	2:B:218:LEU:HB2	2.18	0.43
2:B:21:ARG:HB3	2:B:26:ARG:CB	2.48	0.43
2:D:239:GLU:HG2	5:D:414:HOH:O	2.17	0.43
2:D:100:LEU:C	2:D:100:LEU:HD23	2.38	0.43
2:A:128:LEU:HD12	2:A:129:ASP:N	2.34	0.43
2:D:58:THR:O	2:D:62:THR:HG23	2.18	0.43
2:B:374:ALA:HB1	2:B:378:ARG:HH12	1.83	0.43
2:B:298:GLY:HA2	2:B:381:TYR:CE1	2.54	0.43
2:D:345:LEU:N	2:D:345:LEU:CD1	2.82	0.43
2:D:367:GLU:C	2:D:369:ARG:H	2.22	0.43
2:C:101:THR:HG23	2:C:149:SER:HB3	2.00	0.43
2:D:126:SER:HB3	2:D:129:ASP:HB3	2.01	0.43
2:D:246:PHE:O	2:D:250:MET:HG3	2.19	0.43
2:B:18:ILE:HD11	2:B:26:ARG:HH12	1.84	0.43
2:A:82:ARG:O	2:A:86:LEU:HD13	2.19	0.43
2:C:186:PHE:CE1	2:C:193:ALA:HA	2.54	0.43
2:B:205:SER:OG	2:B:206:VAL:N	2.49	0.43
2:A:20:ALA:HB3	2:A:27:THR:CG2	2.49	0.43
2:D:241:PHE:CZ	2:D:270:GLY:HA3	2.54	0.43
2:A:281:CYS:SG	2:A:283:LEU:HB2	2.59	0.43
2:C:20:ALA:HB3	2:C:27:THR:CG2	2.49	0.43
2:B:75:MET:HE3	2:B:135:LEU:HD22	2.01	0.42
2:B:37:ILE:CD1	2:B:66:ILE:HD12	2.49	0.42
2:A:259:LEU:HG	2:A:262:VAL:CG2	2.48	0.42
2:D:26:ARG:NH1	2:D:26:ARG:HG3	2.34	0.42
2:D:202:GLN:OE1	2:D:211:ARG:HD2	2.18	0.42
1:F:32:C:O2'	2:C:286:ARG:CD	2.67	0.42
2:B:358:MET:O	2:B:362:ARG:HG3	2.18	0.42
2:D:81:GLU:O	2:D:84:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:18:ILE:HD11	2:D:26:ARG:NH1	2.35	0.42
2:D:314:LEU:HA	2:D:314:LEU:HD12	1.86	0.42
2:D:339:GLU:HA	2:D:339:GLU:OE1	2.19	0.42
2:C:108:VAL:HG11	2:C:157:GLU:HG2	2.02	0.42
2:C:218:LEU:HD12	2:C:218:LEU:HA	1.81	0.42
2:D:164:THR:HB	5:D:413:HOH:O	2.19	0.42
2:C:361:ILE:O	2:C:365:ILE:HG13	2.19	0.42
2:D:235:GLU:O	2:D:239:GLU:HB2	2.19	0.42
2:A:341:LEU:HA	2:A:344:MET:SD	2.60	0.42
2:C:62:THR:HG21	2:C:351:ILE:HG22	2.01	0.42
2:A:325:LYS:HD3	2:A:326:TRP:CH2	2.55	0.42
2:C:176:MET:SD	2:C:218:LEU:HD13	2.60	0.42
2:A:69:GLY:O	2:A:101:THR:HA	2.20	0.42
2:D:360:LYS:O	2:D:364:SER:HB2	2.20	0.42
2:B:374:ALA:HB1	2:B:378:ARG:NH1	2.35	0.42
2:B:314:LEU:HA	2:B:314:LEU:HD12	1.83	0.42
2:C:68:LEU:C	2:C:68:LEU:HD23	2.40	0.42
2:B:246:PHE:O	2:B:250:MET:HG3	2.19	0.41
2:B:301:ASN:OD1	2:B:303:ARG:HG3	2.20	0.41
2:D:161:TYR:CD1	2:D:162:PRO:HA	2.55	0.41
2:B:56:PRO:HD2	2:B:57:GLU:OE1	2.20	0.41
2:C:259:LEU:HG	2:C:262:VAL:CG2	2.50	0.41
2:B:294:PHE:H	2:B:350:ASN:ND2	2.18	0.41
2:D:47:THR:HG23	2:D:73:HIS:CD2	2.55	0.41
2:B:11:ARG:CG	2:B:11:ARG:NH1	2.81	0.41
2:C:132:ARG:NH1	2:C:132:ARG:HG3	2.36	0.41
2:B:161:TYR:CD1	2:B:162:PRO:HA	2.54	0.41
2:D:75:MET:HE3	2:D:135:LEU:HD22	2.02	0.41
2:C:40:PRO:HA	2:C:277:ASP:O	2.21	0.41
2:B:201:ILE:HG22	2:B:203:GLN:HE22	1.84	0.41
2:C:108:VAL:HG11	2:C:157:GLU:CG	2.51	0.41
2:D:183:ARG:HD3	2:D:183:ARG:O	2.21	0.41
2:C:341:LEU:HG	2:C:345:LEU:HD22	2.01	0.41
2:D:95:TRP:CE2	2:D:97:ARG:HB2	2.56	0.41
2:C:97:ARG:CB	2:C:98:PRO:HD2	2.48	0.41
2:A:132:ARG:HH11	2:A:132:ARG:HG3	1.86	0.41
2:C:183:ARG:HA	2:C:183:ARG:HD3	1.99	0.41
2:C:128:LEU:C	2:C:128:LEU:HD12	2.42	0.41
2:B:90:HIS:HB2	5:B:391:HOH:O	2.20	0.41
2:C:56:PRO:HD2	2:D:326:TRP:HZ2	1.86	0.41
2:B:285:THR:CG2	2:B:351:ILE:HD11	2.51	0.41
2:A:167:ARG:HG2	2:A:167:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:144:GLN:OE1	2:A:152:VAL:HG13	2.20	0.41
2:B:104:GLY:O	2:B:108:VAL:HG23	2.21	0.41
2:D:125:LYS:HG3	2:D:130:GLY:O	2.21	0.40
2:B:26:ARG:HG3	2:B:26:ARG:NH1	2.32	0.40
2:C:374:ALA:HB1	2:C:378:ARG:NH2	2.35	0.40
2:D:301:ASN:OD1	2:D:303:ARG:HG3	2.21	0.40
2:D:365:ILE:HA	2:D:370:PHE:HB2	2.04	0.40
2:B:183:ARG:O	2:B:183:ARG:HD3	2.21	0.40
2:A:101:THR:HG23	2:A:149:SER:HB3	2.03	0.40
2:D:330:TYR:O	2:D:333:HIS:HB3	2.22	0.40
2:B:127:HIS:CD2	2:B:128:LEU:HG	2.57	0.40
2:D:367:GLU:O	2:D:369:ARG:N	2.54	0.40
1:F:34:N:O2'	2:C:68:LEU:HD22	2.22	0.40
2:B:283:LEU:N	2:B:284:PRO:HD2	2.36	0.40
2:C:48:ALA:O	2:C:49:ALA:HB3	2.21	0.40
2:B:81:GLU:O	2:B:84:ALA:HB3	2.21	0.40
2:B:126:SER:CB	2:B:129:ASP:HB3	2.51	0.40
2:D:138:GLU:O	2:D:142:GLU:HB2	2.21	0.40
2:A:74:LEU:HA	2:A:77:ARG:O	2.22	0.40
2:C:202:GLN:HE21	2:C:215:ALA:HB2	1.85	0.40
2:C:205:SER:HA	5:C:395:HOH: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	
2	A	374/386 (97%)	352 (94%)	20 (5%)	2 (0%)	38	79
2	B	370/386 (96%)	347 (94%)	20 (5%)	3 (1%)	27	68
2	C	374/386 (97%)	353 (94%)	18 (5%)	3 (1%)	27	68
2	D	370/386 (96%)	344 (93%)	21 (6%)	5 (1%)	16	52
All	All	1488/1544 (96%)	1396 (94%)	79 (5%)	13 (1%)	25	66

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	264	LYS
2	C	264	LYS
2	D	52	LYS
2	A	265	PRO
2	B	52	LYS
2	B	113	SER
2	D	113	SER
2	C	52	LYS
2	C	265	PRO
2	D	325	LYS
2	B	263	GLY
2	D	263	GLY
2	D	368	GLY

### 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	
2	A	307/315 (98%)	296 (96%)	11 (4%)	47	85
2	B	304/315 (96%)	287 (94%)	17 (6%)	30	66
2	C	307/315 (98%)	293 (95%)	14 (5%)	37	76
2	D	304/315 (96%)	286 (94%)	18 (6%)	28	64
All	All	1222/1260 (97%)	1162 (95%)	60 (5%)	35	73

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	26	ARG
2	A	134	MET
2	A	138	GLU
2	A	157	GLU
2	A	166	SER
2	A	191	GLU
2	A	218	LEU
2	A	265	PRO

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Mol	Chain	Res	Type
2	A	280	ASP
2	A	320	CYS
2	A	334	LEU
2	B	26	ARG
2	B	39	THR
2	B	57	GLU
2	B	86	LEU
2	B	109	MET
2	B	127	HIS
2	B	128	LEU
2	B	142	GLU
2	B	174	ARG
2	B	218	LEU
2	B	235	GLU
2	B	266	ASP
2	B	280	ASP
2	B	311	LEU
2	B	314	LEU
2	B	320	CYS
2	B	356	GLN
2	C	26	ARG
2	C	43	MET
2	C	134	MET
2	C	138	GLU
2	C	157	GLU
2	C	191	GLU
2	C	218	LEU
2	C	238	ASP
2	C	265	PRO
2	C	280	ASP
2	C	319	HIS
2	C	345	LEU
2	C	351	ILE
2	C	375	GLN
2	D	26	ARG
2	D	39	THR
2	D	50	THR
2	D	57	GLU
2	D	86	LEU
2	D	109	MET
2	D	127	HIS
2	D	128	LEU

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Mol	Chain	Res	Type
2	D	142	GLU
2	D	174	ARG
2	D	218	LEU
2	D	235	GLU
2	D	266	ASP
2	D	280	ASP
2	D	311	LEU
2	D	314	LEU
2	D	334	LEU
2	D	364	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	213	GLN
2	A	257	HIS
2	A	304	ASN
2	A	372	GLN
2	A	375	GLN
2	B	73	HIS
2	B	127	HIS
2	B	203	GLN
2	B	257	HIS
2	B	324	GLN
2	B	350	ASN
2	C	213	GLN
2	C	257	HIS
2	C	304	ASN
2	C	372	GLN
2	D	73	HIS
2	D	127	HIS
2	D	203	GLN
2	D	257	HIS
2	D	350	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	18/20 (90%)	3 (16%)	3 (16%)
1	F	18/20 (90%)	6 (33%)	2 (11%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	36/40 (90%)	9 (25%)	5 (13%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	35	U
1	E	36	A
1	E	37	A
1	F	32	C
1	F	33	U
1	F	35	U
1	F	36	A
1	F	37	A
1	F	38	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	33	U
1	E	35	U
1	E	36	A
1	F	35	U
1	F	37	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	9DG	A	387	-	12,12,12	1.90	3 (25%)	11,17,17	1.83	3 (27%)
4	9DG	B	387	-	12,12,12	1.99	4 (33%)	11,17,17	1.84	3 (27%)
4	9DG	C	387	-	12,12,12	1.98	3 (25%)	11,17,17	1.87	3 (27%)
4	9DG	D	387	-	12,12,12	2.00	4 (33%)	11,17,17	1.87	4 (36%)

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	9DG	A	387	-	-	0/0/0/0	0/0/2/2
4	9DG	B	387	-	-	0/0/0/0	0/0/2/2
4	9DG	C	387	-	-	0/0/0/0	0/0/2/2
4	9DG	D	387	-	-	0/0/0/0	0/0/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	387	9DG	C9-C4	-4.24	1.31	1.41
4	B	387	9DG	C9-C4	-4.24	1.31	1.41
4	D	387	9DG	C9-C4	-4.22	1.31	1.41
4	A	387	9DG	C9-C4	-4.19	1.32	1.41
4	D	387	9DG	C2-N1	3.29	1.42	1.36
4	B	387	9DG	C2-N1	3.22	1.41	1.36
4	C	387	9DG	C2-N1	3.18	1.41	1.36
4	A	387	9DG	C2-N1	2.92	1.41	1.36
4	C	387	9DG	C6-N1	2.83	1.42	1.37
4	B	387	9DG	C6-N1	2.75	1.41	1.37
4	D	387	9DG	C6-N1	2.63	1.41	1.37
4	A	387	9DG	C6-N1	2.42	1.41	1.37
4	D	387	9DG	C2-N3	2.14	1.36	1.33
4	B	387	9DG	C2-N3	2.09	1.36	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	387	9DG	C9-C4-C5	-3.44	104.57	106.29
4	B	387	9DG	C9-C4-C5	-3.35	104.61	106.29
4	A	387	9DG	C9-C4-C5	-3.30	104.64	106.29
4	C	387	9DG	C9-C4-C5	-3.27	104.66	106.29
4	C	387	9DG	C4-C5-N7	3.13	108.49	106.01
4	A	387	9DG	C4-C5-N7	3.02	108.40	106.01
4	D	387	9DG	C4-C5-N7	2.97	108.37	106.01
4	B	387	9DG	C4-C5-N7	2.97	108.36	106.01
4	C	387	9DG	C9-C8-N7	2.11	111.72	108.17
4	A	387	9DG	C9-C8-N7	2.09	111.70	108.17
4	D	387	9DG	C9-C8-N7	2.05	111.62	108.17
4	B	387	9DG	C9-C8-N7	2.04	111.61	108.17
4	D	387	9DG	N2-C2-N1	2.01	120.08	117.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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(Å²)	Q<0.9	
1	E	20/20 (100%)	0.15	0	100	100	12, 20, 31, 37	0
1	F	20/20 (100%)	0.27	0	100	100	12, 22, 37, 44	0
2	A	376/386 (97%)	-0.35	2 (0%)	88	93	7, 21, 35, 48	0
2	B	372/386 (96%)	0.12	19 (5%)	27	33	11, 37, 59, 79	0
2	C	376/386 (97%)	-0.34	5 (1%)	74	82	7, 22, 36, 59	0
2	D	372/386 (96%)	0.03	17 (4%)	31	38	6, 32, 57, 79	0
All	All	1536/1584 (96%)	-0.13	43 (2%)	50	59	6, 27, 54, 79	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	114	LEU	6.0
2	B	114	LEU	5.2
2	D	113	SER	4.8
2	B	115	THR	4.5
2	D	116	LYS	3.8
2	C	386	SER	3.7
2	D	112	SER	3.7
2	A	386	SER	3.5
2	B	116	LYS	3.5
2	B	167	ARG	3.5
2	D	160	PRO	3.1
2	B	194	GLU	3.0
2	D	194	GLU	2.9
2	D	115	THR	2.9
2	B	162	PRO	2.9
2	B	113	SER	2.9
2	B	120	GLU	2.9
2	D	188	SER	2.9
2	D	162	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	190	LYS	2.6
2	B	134	MET	2.6
2	D	159	THR	2.6
2	C	190	LYS	2.6
2	B	132	ARG	2.5
2	B	127	HIS	2.4
2	D	167	ARG	2.4
2	D	258	TYR	2.4
2	B	234	GLY	2.4
2	B	159	THR	2.4
2	D	191	GLU	2.3
2	B	111	LEU	2.3
2	D	207	PHE	2.3
2	A	132	ARG	2.3
2	D	132	ARG	2.3
2	B	190	LYS	2.3
2	B	375	GLN	2.2
2	B	163	ALA	2.2
2	D	163	ALA	2.2
2	C	385	ASN	2.1
2	C	162	PRO	2.1
2	C	191	GLU	2.1
2	B	207	PHE	2.1
2	B	195	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	9DG	B	387	11/11	0.34	2.82	83,84,85,85	0
4	9DG	C	387	11/11	0.20	1.17	16,20,21,24	0
4	9DG	A	387	11/11	0.16	-0.10	12,13,13,15	0
4	9DG	D	387	11/11	0.22	-0.16	44,45,45,47	0
3	ZN	D	404	1/1	0.07	-1.67	19,19,19,19	0
3	ZN	C	403	1/1	0.04	-2.14	25,25,25,25	0
3	ZN	B	402	1/1	0.07	-3.11	22,22,22,22	0
3	ZN	A	401	1/1	0.04	-4.57	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.