



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:43 AM GMT

PDB ID : 3V21  
Title : Crystal structure of Type IIF restriction endonuclease Bse634I with cognate DNA  
Authors : Manakova, E.N.; Grazulis, S.; Golovenko, D.; Tamulaitiene, G.  
Deposited on : 2011-12-11  
Resolution : 2.70 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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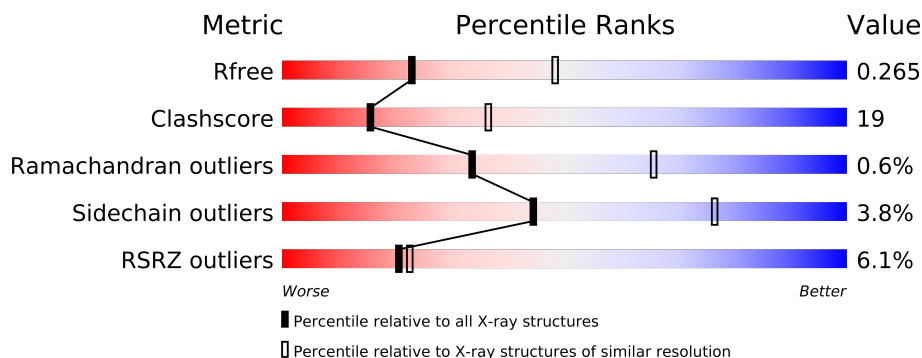
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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.




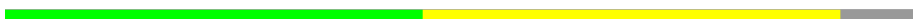


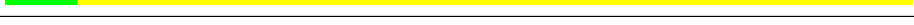

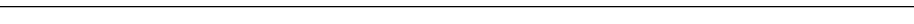

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. 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	A	293	
1	B	293	
1	C	293	
1	D	293	
1	E	293	
1	F	293	
1	G	293	
1	H	293	
2	I	13	
2	J	13	
2	K	13	
2	L	13	
2	M	13	
2	N	13	

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Mol	Chain	Length	Quality of chain
2	O	13	
2	P	13	
2	R	13	
2	S	13	
2	V	13	
2	X	13	
2	Y	13	
2	Z	13	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22656 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 protein called Endonuclease Bse634IR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	7	0	0
			2344	1495	404	439	6			
1	B	289	Total	C	N	O	S	2	0	0
			2344	1495	404	439	6			
1	C	288	Total	C	N	O	S	146	0	0
			2336	1491	402	437	6			
1	D	289	Total	C	N	O	S	264	0	0
			2344	1495	404	439	6			
1	E	289	Total	C	N	O	S	267	0	0
			2344	1495	404	439	6			
1	F	287	Total	C	N	O	S	359	0	0
			2328	1485	401	436	6			
1	G	289	Total	C	N	O	S	23	0	0
			2344	1495	404	439	6			
1	H	290	Total	C	N	O	S	11	0	0
			2351	1499	405	441	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
A	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
A	130	SER	THR	SEE REMARK 999	UNP Q8RT53
A	226	ALA	ARG	ENGINEERED MUTATION	UNP Q8RT53
B	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
B	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
B	130	SER	THR	SEE REMARK 999	UNP Q8RT53
B	226	ALA	ARG	ENGINEERED MUTATION	UNP Q8RT53
C	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
C	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
C	130	SER	THR	SEE REMARK 999	UNP Q8RT53
C	226	ALA	ARG	ENGINEERED MUTATION	UNP Q8RT53
D	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53

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Chain	Residue	Modelled	Actual	Comment	Reference
D	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
D	130	SER	THR	SEE REMARK 999	UNP Q8RT53
D	226	ALA	ARG	ENGINEERED MUTATION	UNP Q8RT53
E	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
E	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
E	130	SER	THR	SEE REMARK 999	UNP Q8RT53
E	226	ALA	ARG	ENGINEERED MUTATION	UNP Q8RT53
F	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
F	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
F	130	SER	THR	SEE REMARK 999	UNP Q8RT53
F	226	ALA	ARG	ENGINEERED MUTATION	UNP Q8RT53
G	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
G	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
G	130	SER	THR	SEE REMARK 999	UNP Q8RT53
G	226	ALA	ARG	ENGINEERED MUTATION	UNP Q8RT53
H	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
H	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
H	130	SER	THR	SEE REMARK 999	UNP Q8RT53
H	226	ALA	ARG	ENGINEERED MUTATION	UNP Q8RT53

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	13	Total 263	C 126	N 48	O 77	P 12	0	0	0
2	J	13	Total 263	C 126	N 48	O 77	P 12	9	0	0
2	K	13	Total 263	C 126	N 48	O 77	P 12	21	0	0
2	L	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	M	12	Total 243	C 116	N 46	O 70	P 11	82	0	0
2	N	12	Total 243	C 116	N 46	O 70	P 11	17	0	0
2	O	13	Total 263	C 126	N 48	O 77	P 12	0	0	0
2	P	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	R	12	Total 243	C 116	N 46	O 70	P 11	81	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	13	Total 263	C 126	N 48	O 77	P 12	62	0	0
2	V	13	Total 263	C 126	N 48	O 77	P 12	0	0	0
2	X	13	Total 263	C 126	N 48	O 77	P 12	0	0	0
2	Y	13	Total 263	C 126	N 48	O 77	P 12	0	0	0
2	Z	12	Total 243	C 116	N 46	O 70	P 11	36	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	44	Total 44	O 44	0	0
3	C	35	Total 35	O 35	0	0
3	D	22	Total 22	O 22	0	0
3	E	36	Total 36	O 36	0	0
3	F	25	Total 25	O 25	0	0
3	G	37	Total 37	O 37	0	0
3	H	50	Total 50	O 50	0	0
3	I	9	Total 9	O 9	0	0
3	J	12	Total 12	O 12	0	0
3	K	1	Total 1	O 1	0	0
3	L	2	Total 2	O 2	0	0
3	M	3	Total 3	O 3	0	0
3	N	1	Total 1	O 1	0	0

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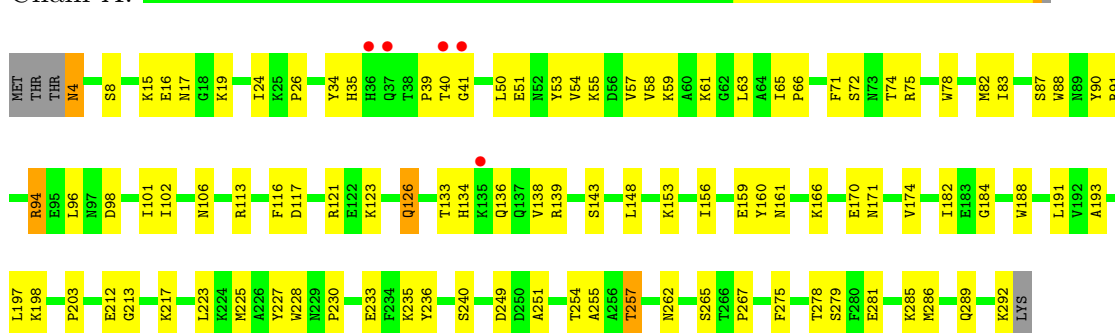
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	6	Total 6	O 6	0	0
3	P	3	Total 3	O 3	0	0
3	R	2	Total 2	O 2	0	0
3	S	5	Total 5	O 5	0	0
3	V	2	Total 2	O 2	0	0
3	X	4	Total 4	O 4	0	0
3	Y	3	Total 3	O 3	0	0
3	Z	2	Total 2	O 2	0	0

### 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.

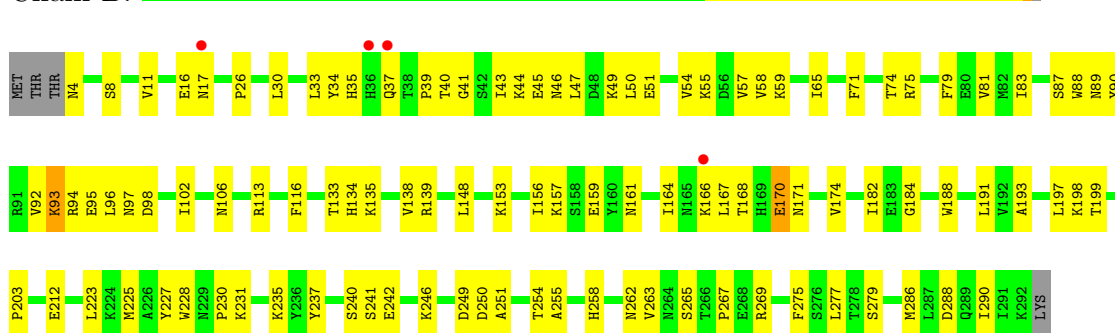
#### • Molecule 1: Endonuclease Bse634IR

Chain A:



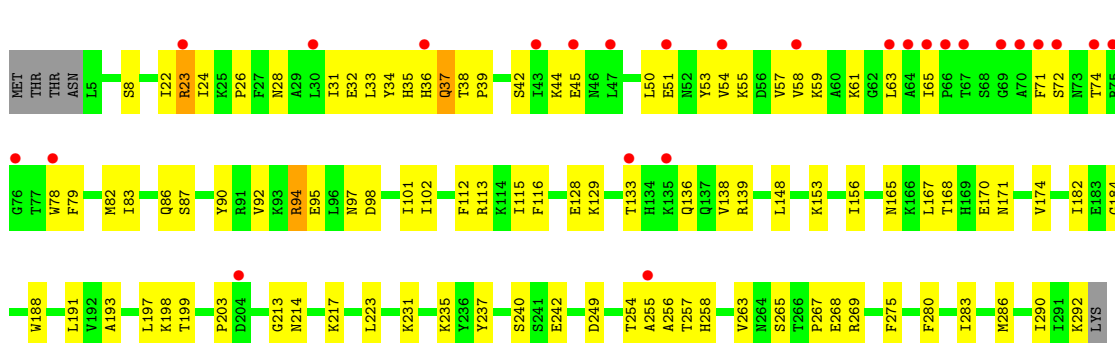
#### • Molecule 1: Endonuclease Bse634IR

Chain B:



#### • Molecule 1: Endonuclease Bse634IR

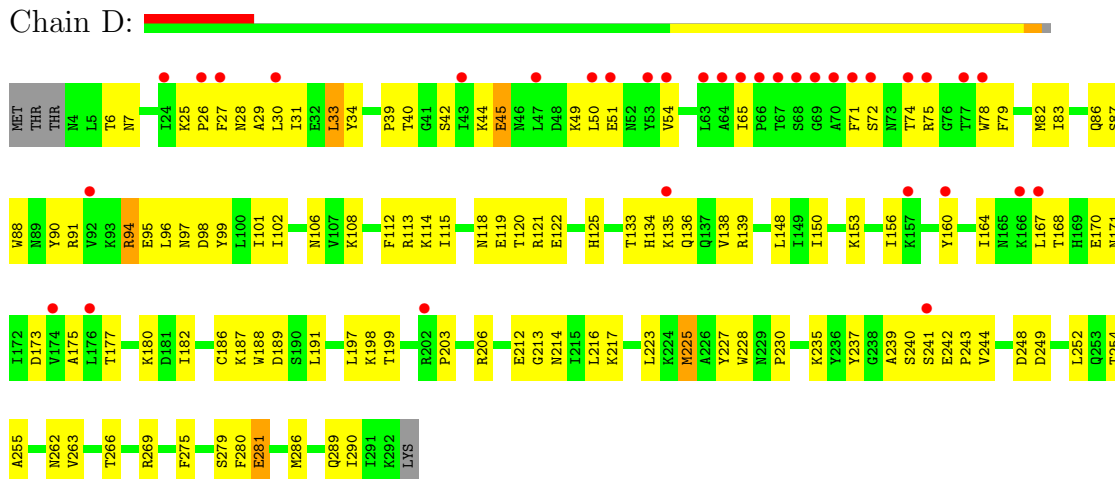
Chain C:





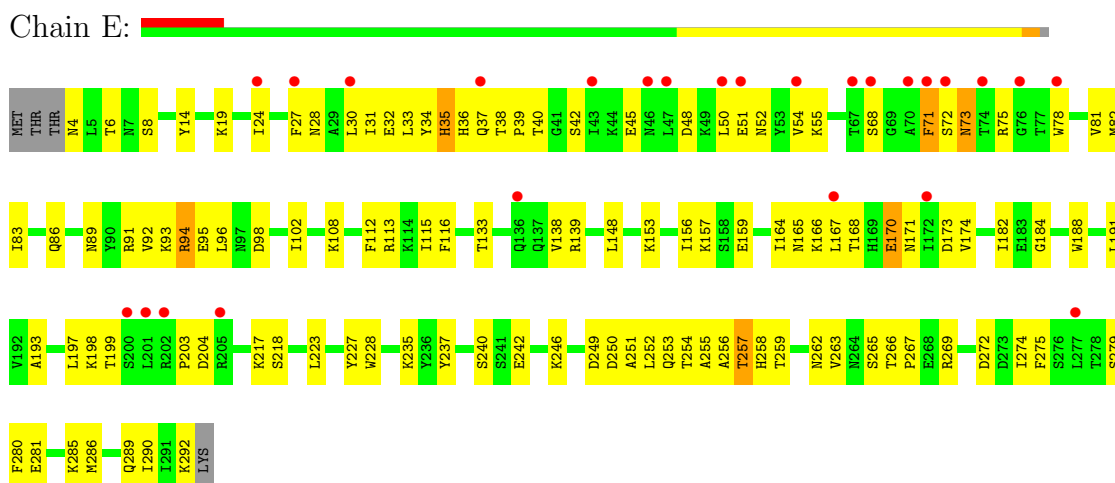
- Molecule 1: Endonuclease Bse634IR

Chain D:



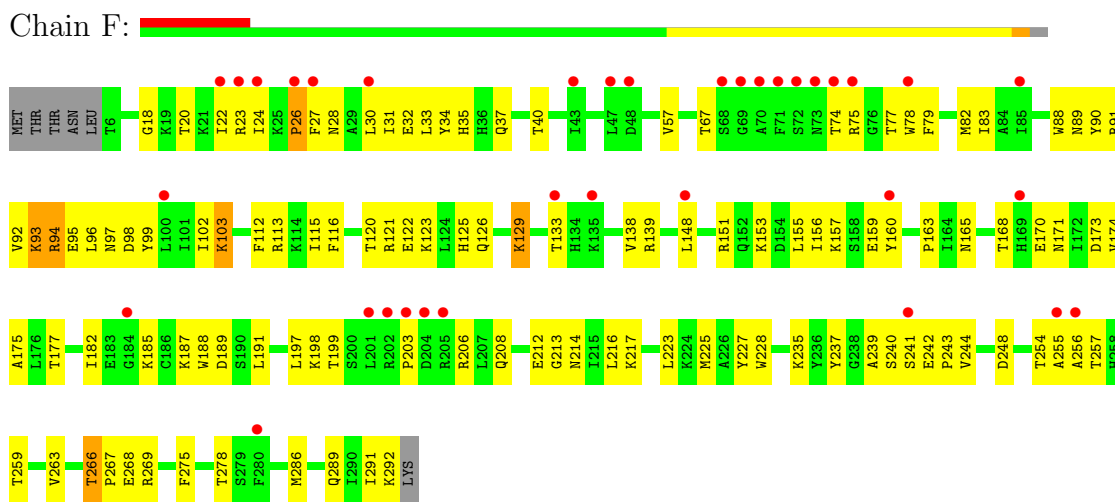
- Molecule 1: Endonuclease Bse634IR

Chain E:



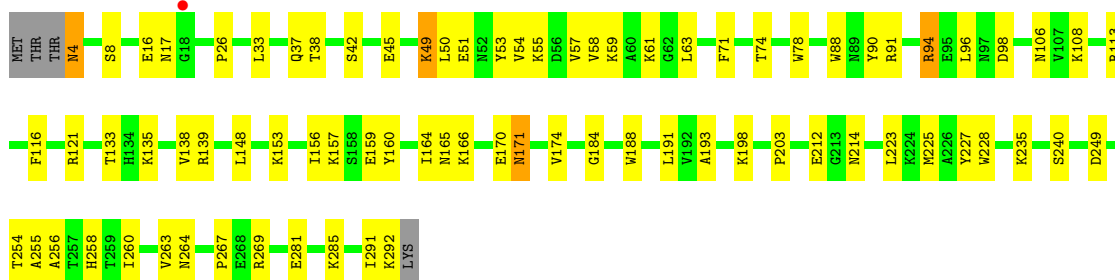
- Molecule 1: Endonuclease Bse634IR

Chain F:



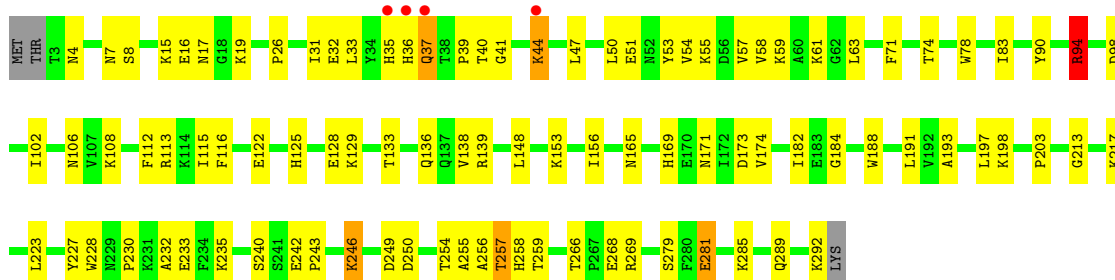
- Molecule 1: Endonuclease Bse634IR

Chain G: 



- Molecule 1: Endonuclease Bse634IR

Chain H: 



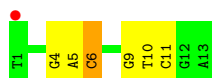
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain I: 



- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain J: 



- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain K: 



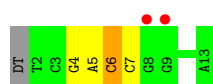
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain L: 



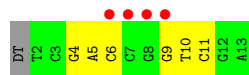
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain M: 



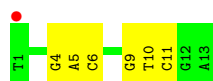
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain N:



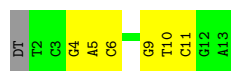
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain O:



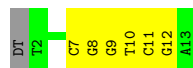
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain P:



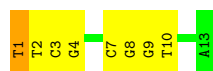
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain R:



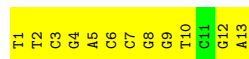
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain S:



- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain V:



- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain X:



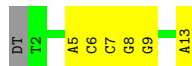
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain Y:



- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain Z: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.88Å 115.31Å 130.24Å 90.00° 112.50° 90.00°	Depositor
Resolution (Å)	65.09 – 2.70 65.09 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.09-2.70) 100.0 (65.09-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.230 , 0.267 0.228 , 0.265	Depositor DCC
$R_{free}$ test set	7973 reflections (11.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.3	EDS
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 80279 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/2389	0.65	0/3228
1	B	0.43	0/2389	0.64	0/3228
1	C	0.39	0/2381	0.63	0/3217
1	D	0.41	0/2389	0.63	0/3228
1	E	0.39	0/2389	0.62	0/3228
1	F	0.38	0/2373	0.62	0/3206
1	G	0.44	0/2389	0.62	0/3228
1	H	0.43	0/2396	0.63	1/3238 (0.0%)
2	I	0.49	0/294	0.72	0/452
2	J	0.47	0/294	0.70	0/452
2	K	0.43	0/294	0.72	0/452
2	L	0.35	0/272	0.70	0/418
2	M	0.41	0/272	0.75	0/418
2	N	0.37	0/272	0.71	0/418
2	O	0.53	0/294	0.72	0/452
2	P	0.49	0/272	0.76	0/418
2	R	0.41	0/272	0.72	0/418
2	S	0.49	0/294	0.75	0/452
2	V	0.43	0/294	0.70	0/452
2	X	0.41	0/294	0.68	0/452
2	Y	0.41	0/294	0.71	0/452
2	Z	0.37	0/272	0.66	0/418
All	All	0.42	0/23079	0.65	1/31925 (0.0%)

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
2	J	0	1
2	M	0	1
2	S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	94	ARG	NE-CZ-NH1	-5.42	117.59	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	6	DC	Sidechain
2	M	6	DC	Sidechain
2	S	1	DT	Sidechain

## 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	A	2344	0	2385	94	0
1	B	2344	0	2385	100	0
1	C	2336	0	2379	86	0
1	D	2344	0	2385	110	0
1	E	2344	0	2385	107	0
1	F	2328	0	2368	136	0
1	G	2344	0	2385	77	0
1	H	2351	0	2392	87	0
2	I	263	0	148	7	0
2	J	263	0	148	6	0
2	K	263	0	148	5	0
2	L	243	0	136	7	0
2	M	243	0	136	3	0
2	N	243	0	136	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	263	0	148	6	0
2	P	243	0	136	6	0
2	R	243	0	136	8	0
2	S	263	0	148	9	0
2	V	263	0	148	16	0
2	X	263	0	148	4	0
2	Y	263	0	148	8	0
2	Z	243	0	136	7	0
3	A	55	0	0	3	0
3	B	44	0	0	1	0
3	C	35	0	0	0	0
3	D	22	0	0	0	0
3	E	36	0	0	1	0
3	F	25	0	0	0	0
3	G	37	0	0	2	0
3	H	50	0	0	0	0
3	I	9	0	0	0	0
3	J	12	0	0	0	0
3	K	1	0	0	0	0
3	L	2	0	0	0	0
3	M	3	0	0	0	0
3	N	1	0	0	0	0
3	O	6	0	0	0	0
3	P	3	0	0	0	0
3	R	2	0	0	0	0
3	S	5	0	0	0	0
3	V	2	0	0	0	0
3	X	4	0	0	0	0
3	Y	3	0	0	0	0
3	Z	2	0	0	1	0
All	All	22656	0	21064	756	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 19.

All (756) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:138:VAL:CG1	1:H:255:ALA:HB2	1.30	1.55
1:E:255:ALA:HB2	1:F:138:VAL:CG1	1.56	1.33
1:A:138:VAL:CG1	1:B:255:ALA:HB2	1.60	1.31
1:E:138:VAL:CG1	1:F:255:ALA:HB2	1.66	1.25
1:A:255:ALA:HB2	1:B:138:VAL:CG1	1.72	1.20

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:138:VAL:HG13	1:H:255:ALA:HB2	1.25	1.16
1:G:138:VAL:HG11	1:H:255:ALA:CB	1.77	1.15
1:G:138:VAL:CG1	1:H:255:ALA:CB	2.26	1.13
1:A:255:ALA:HB2	1:B:138:VAL:HG11	1.30	1.11
1:C:255:ALA:HB2	1:D:138:VAL:CG1	1.80	1.11
1:F:133:THR:HG23	2:R:12:DG:H4'	1.30	1.11
1:A:138:VAL:HG11	1:B:255:ALA:HB2	1.16	1.10
1:E:138:VAL:HG11	1:F:255:ALA:CB	1.80	1.10
1:E:255:ALA:HB2	1:F:138:VAL:HG13	1.32	1.09
1:A:257:THR:HG22	1:B:258:HIS:HB3	1.09	1.08
1:E:138:VAL:CG1	1:F:255:ALA:CB	2.31	1.08
1:E:255:ALA:HB2	1:F:138:VAL:HG11	1.22	1.07
1:F:26:PRO:HB3	1:F:74:THR:HG23	1.36	1.04
1:A:225:MET:HE2	1:E:263:VAL:H	1.23	1.02
1:A:257:THR:HG21	1:B:258:HIS:ND1	1.75	1.01
1:C:26:PRO:HB3	1:C:74:THR:HG23	1.38	1.01
1:C:255:ALA:HB2	1:D:138:VAL:HG13	1.42	1.00
1:D:31:ILE:HG23	1:D:168:THR:HA	1.44	0.99
1:D:263:VAL:H	1:G:225:MET:HE2	1.27	0.99
1:A:262:ASN:HB3	3:A:308:HOH:O	1.64	0.98
1:E:138:VAL:HG11	1:F:255:ALA:HB2	1.39	0.97
1:A:257:THR:HG22	1:B:258:HIS:CB	1.94	0.96
1:E:138:VAL:HG13	1:F:255:ALA:HB2	1.46	0.96
1:F:31:ILE:HG23	1:F:168:THR:HA	1.44	0.96
1:A:262:ASN:HB2	1:A:265:SER:HB2	1.49	0.95
1:G:255:ALA:HB2	1:H:138:VAL:CG1	1.97	0.95
1:C:65:ILE:H	1:C:65:ILE:HD12	1.30	0.94
1:A:26:PRO:HB3	1:A:74:THR:HG23	1.50	0.93
1:E:255:ALA:CB	1:F:138:VAL:HG11	1.98	0.93
1:E:255:ALA:CB	1:F:138:VAL:CG1	2.47	0.92
1:A:138:VAL:HG13	1:B:255:ALA:HB2	1.50	0.92
1:G:138:VAL:HG11	1:H:255:ALA:HB2	0.94	0.92
1:B:263:VAL:H	1:F:225:MET:HE2	1.35	0.91
1:C:255:ALA:HB2	1:D:138:VAL:HG11	1.52	0.89
1:E:262:ASN:HB2	1:E:265:SER:HB2	1.55	0.88
1:G:26:PRO:HB3	1:G:74:THR:HG23	1.57	0.86
1:A:257:THR:CG2	1:B:258:HIS:HB3	2.02	0.86
1:D:42:SER:HB3	1:D:45:GLU:HB2	1.57	0.86
1:H:26:PRO:HB3	1:H:74:THR:HG23	1.56	0.85
1:F:26:PRO:HB3	1:F:74:THR:CG2	2.05	0.85
2:S:9:DG:H2''	2:S:10:DT:H5''	1.56	0.85
1:F:79:PHE:HA	1:F:82:MET:HE2	1.58	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Z:5:DA:H2''	2:Z:6:DC:H5'	1.60	0.83
1:G:4:ASN:N	1:G:4:ASN:HD22	1.74	0.83
1:E:170:GLU:O	1:E:174:VAL:HG13	1.77	0.83
1:B:225:MET:HE1	1:F:263:VAL:H	1.42	0.83
1:C:42:SER:HB3	1:C:45:GLU:HG3	1.60	0.82
1:E:138:VAL:HG11	1:F:255:ALA:HB3	1.61	0.81
1:E:138:VAL:HG13	1:F:255:ALA:CB	2.04	0.79
1:E:28:ASN:O	1:E:32:GLU:HG3	1.83	0.79
1:F:93:LYS:O	1:F:94:ARG:HD2	1.82	0.79
1:A:138:VAL:HG11	1:B:255:ALA:CB	2.05	0.79
1:F:255:ALA:HB1	1:F:268:GLU:O	1.83	0.79
1:A:257:THR:CG2	1:B:258:HIS:ND1	2.46	0.78
1:G:138:VAL:HG13	1:H:255:ALA:CB	2.03	0.78
1:F:255:ALA:HA	1:F:269:ARG:HA	1.66	0.78
1:F:90:TYR:O	1:F:94:ARG:HB2	1.82	0.78
1:G:255:ALA:HB2	1:H:138:VAL:HG11	1.65	0.78
1:C:138:VAL:CG1	1:D:255:ALA:HB2	2.14	0.77
1:C:256:ALA:HB1	1:C:258:HIS:CE1	2.20	0.76
1:A:148:LEU:HD22	1:A:191:LEU:HD11	1.68	0.76
1:G:170:GLU:O	1:G:174:VAL:HG13	1.86	0.75
1:B:26:PRO:HB3	1:B:74:THR:HG23	1.69	0.74
1:E:171:ASN:O	1:E:174:VAL:HG22	1.88	0.74
1:D:27:PHE:O	1:D:31:ILE:HG13	1.86	0.74
1:B:90:TYR:HA	1:B:93:LYS:HD3	1.68	0.74
1:C:138:VAL:HG11	1:D:255:ALA:HB2	1.68	0.73
1:E:27:PHE:O	1:E:31:ILE:HG13	1.89	0.73
1:B:157:LYS:HB3	1:B:159:GLU:OE1	1.89	0.73
1:A:4:ASN:HD22	1:A:4:ASN:N	1.85	0.73
1:D:133:THR:HG23	2:V:2:DT:H72	1.70	0.72
1:F:170:GLU:O	1:F:174:VAL:HG13	1.89	0.72
1:F:97:ASN:O	1:F:156:ILE:HG12	1.89	0.72
1:C:255:ALA:CB	1:D:138:VAL:HG11	2.20	0.71
1:D:164:ILE:HG23	1:D:171:ASN:OD1	1.89	0.71
1:E:255:ALA:CB	1:F:138:VAL:HG13	2.17	0.71
1:B:89:ASN:O	1:B:93:LYS:HD2	1.90	0.71
1:E:68:SER:HA	1:E:71:PHE:HB2	1.72	0.71
1:C:170:GLU:O	1:C:174:VAL:HG13	1.90	0.71
1:E:83:ILE:HD12	1:E:197:LEU:HD22	1.72	0.70
1:A:34:TYR:CE1	1:A:39:PRO:HB3	2.26	0.70
2:S:9:DG:H2''	2:S:10:DT:C5'	2.20	0.70
1:A:255:ALA:CB	1:B:138:VAL:HG11	2.17	0.70
2:S:3:DC:H2''	2:S:4:DG:C8	2.26	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:133:THR:HG23	2:V:2:DT:C7	2.21	0.70
1:C:255:ALA:CB	1:D:138:VAL:CG1	2.64	0.70
1:C:34:TYR:CE1	1:C:39:PRO:HB3	2.27	0.70
2:Z:8:DG:H2''	2:Z:9:DG:OP2	1.90	0.69
1:C:133:THR:HG22	1:C:133:THR:O	1.92	0.69
1:A:212:GLU:HG2	1:A:236:TYR:OH	1.91	0.69
1:E:86:GLN:OE1	1:E:280:PHE:HB3	1.92	0.69
1:D:133:THR:HG22	1:D:133:THR:O	1.91	0.69
2:S:9:DG:C2'	2:S:10:DT:H5''	2.22	0.69
1:A:16:GLU:O	1:A:17:ASN:HB2	1.93	0.69
1:D:198:LYS:O	1:D:240:SER:HA	1.92	0.69
1:G:281:GLU:HG2	1:G:285:LYS:HE3	1.74	0.69
1:H:4:ASN:HB3	1:H:7:ASN:ND2	2.07	0.68
1:E:148:LEU:HD22	1:E:191:LEU:HD11	1.74	0.68
1:A:278:THR:HG22	3:A:345:HOH:O	1.92	0.68
1:H:4:ASN:HB3	1:H:7:ASN:HD22	1.58	0.68
1:F:91:ARG:HG3	1:F:92:VAL:N	2.08	0.68
1:B:94:ARG:NH2	1:B:288:ASP:OD1	2.26	0.68
1:H:148:LEU:HD22	1:H:191:LEU:HD11	1.75	0.68
1:E:256:ALA:HB1	1:E:258:HIS:CE1	2.27	0.68
1:F:198:LYS:O	1:F:240:SER:HA	1.94	0.68
1:H:16:GLU:O	1:H:17:ASN:HB2	1.93	0.67
2:R:8:DG:H2''	2:R:9:DG:O5'	1.93	0.67
1:E:78:TRP:HB3	1:E:82:MET:CE	2.25	0.67
1:A:255:ALA:HB2	1:B:138:VAL:HG13	1.73	0.67
1:E:71:PHE:O	1:E:75:ARG:HG3	1.94	0.67
1:B:148:LEU:HD22	1:B:191:LEU:HD11	1.76	0.67
1:F:255:ALA:CB	1:F:268:GLU:O	2.43	0.67
2:V:9:DG:H2''	2:V:10:DT:OP2	1.94	0.67
1:F:148:LEU:HD22	1:F:191:LEU:HD11	1.75	0.66
2:Y:1:DT:H2''	2:Y:2:DT:O5'	1.94	0.66
1:H:39:PRO:O	1:H:40:THR:HG23	1.95	0.66
1:D:197:LEU:O	1:D:198:LYS:HG2	1.96	0.66
1:E:289:GLN:HG3	3:E:315:HOH:O	1.94	0.66
1:E:281:GLU:HG3	1:E:285:LYS:HE3	1.77	0.66
1:B:159:GLU:CD	1:B:159:GLU:H	1.99	0.66
1:B:16:GLU:O	1:B:17:ASN:HB2	1.95	0.66
2:R:9:DG:H2'	2:R:10:DT:H72	1.78	0.66
1:G:148:LEU:HD22	1:G:191:LEU:HD11	1.76	0.66
1:D:97:ASN:O	1:D:156:ILE:HG12	1.95	0.66
1:G:133:THR:HG22	1:G:133:THR:O	1.95	0.65
1:H:8:SER:HB3	1:H:57:VAL:CG1	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:199:THR:O	1:F:242:GLU:HG3	1.96	0.65
1:G:255:ALA:HB2	1:H:138:VAL:HG13	1.79	0.65
1:G:16:GLU:O	1:G:17:ASN:HB2	1.96	0.65
1:H:256:ALA:O	1:H:258:HIS:N	2.30	0.65
1:F:79:PHE:HA	1:F:82:MET:CE	2.26	0.64
1:D:199:THR:O	1:D:242:GLU:HG3	1.97	0.64
1:D:34:TYR:CZ	1:D:39:PRO:HB3	2.32	0.64
1:F:278:THR:HG23	1:H:285:LYS:HZ1	1.61	0.64
1:H:133:THR:O	1:H:133:THR:HG22	1.96	0.64
1:H:128:GLU:HG3	1:H:129:LYS:N	2.13	0.64
1:E:256:ALA:O	1:E:258:HIS:N	2.30	0.64
1:E:279:SER:OG	1:E:281:GLU:HB3	1.98	0.64
1:E:133:THR:O	1:E:133:THR:HG22	1.98	0.64
1:E:37:GLN:HA	1:E:165:ASN:O	1.97	0.64
1:A:138:VAL:CG1	1:B:255:ALA:CB	2.56	0.63
1:A:225:MET:CE	1:E:263:VAL:HG12	2.28	0.63
1:G:214:ASN:ND2	1:H:257:THR:HG21	2.13	0.63
1:C:22:ILE:HD13	1:C:63:LEU:HD13	1.79	0.63
1:F:30:LEU:O	1:F:34:TYR:HB2	1.97	0.63
1:C:65:ILE:H	1:C:65:ILE:CD1	2.07	0.63
1:E:34:TYR:CZ	1:E:39:PRO:HB3	2.33	0.63
1:B:170:GLU:O	1:B:174:VAL:HG13	1.99	0.62
1:B:30:LEU:HD13	1:B:81:VAL:HG11	1.80	0.62
1:A:8:SER:HB3	1:A:57:VAL:CG1	2.29	0.62
1:F:197:LEU:O	1:F:198:LYS:HG2	1.99	0.62
1:E:35:HIS:ND1	1:E:35:HIS:N	2.47	0.62
1:D:177:THR:HB	1:D:180:LYS:HE3	1.80	0.62
1:C:42:SER:CB	1:C:45:GLU:HG3	2.30	0.62
1:C:34:TYR:CZ	1:C:39:PRO:HB3	2.34	0.62
2:S:1:DT:H2''	2:S:2:DT:O5'	1.97	0.62
1:B:263:VAL:N	1:F:225:MET:HE2	2.13	0.62
1:E:31:ILE:HG23	1:E:168:THR:HA	1.81	0.62
2:Z:5:DA:H2''	2:Z:6:DC:C5'	2.29	0.61
1:C:148:LEU:HD22	1:C:191:LEU:HD11	1.82	0.61
1:E:138:VAL:CG2	1:F:255:ALA:HB2	2.30	0.61
1:C:255:ALA:HA	1:C:269:ARG:HA	1.82	0.61
2:I:9:DG:H2''	2:I:10:DT:O5'	2.01	0.61
1:D:263:VAL:N	1:G:225:MET:HE2	2.08	0.61
2:J:9:DG:H2''	2:J:10:DT:O5'	2.01	0.61
2:P:10:DT:H2'	2:P:11:DC:C5	2.36	0.61
1:F:79:PHE:CE1	1:F:241:SER:HB3	2.36	0.60
2:N:9:DG:H2''	2:N:10:DT:O5'	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:133:THR:HG22	1:F:133:THR:O	2.00	0.60
2:L:9:DG:H2"	2:L:10:DT:O5'	2.01	0.60
1:G:33:LEU:HD12	1:G:50:LEU:HD23	1.83	0.60
1:D:34:TYR:CD2	1:D:167:LEU:HD12	2.36	0.60
1:A:257:THR:CG2	1:B:258:HIS:CG	2.84	0.60
1:F:256:ALA:HB3	1:F:259:THR:HG23	1.83	0.60
1:E:138:VAL:CG1	1:F:255:ALA:HB3	2.19	0.60
1:H:281:GLU:HG3	1:H:285:LYS:HE3	1.84	0.60
1:D:135:LYS:HG3	2:Z:9:DG:OP2	2.02	0.60
1:D:148:LEU:HD22	1:D:191:LEU:HD11	1.83	0.60
1:B:133:THR:O	1:B:133:THR:HG22	2.00	0.60
1:F:103:LYS:O	1:F:103:LYS:HG3	2.00	0.60
1:H:44:LYS:HD2	1:H:44:LYS:O	2.00	0.60
2:K:9:DG:H2"	2:K:10:DT:O5'	2.02	0.60
1:A:133:THR:HG22	1:A:133:THR:O	2.01	0.60
1:G:4:ASN:ND2	1:G:4:ASN:N	2.48	0.59
2:K:10:DT:H2'	2:K:11:DC:C5	2.37	0.59
1:A:170:GLU:O	1:A:174:VAL:HG13	2.02	0.59
1:D:31:ILE:HG23	1:D:168:THR:CA	2.28	0.59
1:E:52:ASN:HA	1:E:55:LYS:HB3	1.84	0.59
1:F:88:TRP:HZ3	1:F:175:ALA:HA	1.66	0.59
2:V:8:DG:H2"	2:V:9:DG:OP2	2.01	0.59
1:H:36:HIS:CG	1:H:37:GLN:H	2.19	0.59
1:H:8:SER:HB3	1:H:57:VAL:HG11	1.84	0.59
1:D:39:PRO:O	1:D:40:THR:HG23	2.03	0.59
2:Y:6:DC:H1'	2:Y:7:DC:H5"	1.84	0.59
1:E:139:ARG:O	1:F:254:THR:HA	2.02	0.59
2:J:10:DT:H2'	2:J:11:DC:C5	2.37	0.59
1:C:128:GLU:HG2	1:C:129:LYS:N	2.17	0.59
2:S:7:DC:H2"	2:S:8:DG:C8	2.37	0.59
1:C:34:TYR:CD1	1:C:39:PRO:HD3	2.38	0.59
1:E:265:SER:O	1:E:267:PRO:HD3	2.03	0.58
1:B:225:MET:HE1	1:F:263:VAL:N	2.15	0.58
1:D:34:TYR:CE1	1:D:39:PRO:HB3	2.38	0.58
1:C:255:ALA:CB	1:D:138:VAL:HG13	2.26	0.58
1:F:79:PHE:O	1:F:83:ILE:HD12	2.02	0.58
1:F:197:LEU:HD23	1:F:239:ALA:HB3	1.85	0.58
1:A:136:GLN:HG2	1:B:269:ARG:HD3	1.85	0.58
1:G:166:LYS:O	1:G:171:ASN:OD1	2.21	0.58
1:F:278:THR:HG23	1:H:285:LYS:NZ	2.17	0.58
1:E:157:LYS:HB3	1:E:159:GLU:OE1	2.04	0.58
1:B:58:VAL:CG1	1:B:65:ILE:HD13	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:65:ILE:N	1:C:65:ILE:HD12	2.12	0.58
1:A:161:ASN:ND2	3:A:355:HOH:O	2.35	0.58
2:O:9:DG:H2"	2:O:10:DT:O5'	2.03	0.58
2:P:9:DG:H2"	2:P:10:DT:O5'	2.03	0.58
1:E:252:LEU:HD13	1:E:274:ILE:HB	1.85	0.58
2:Y:2:DT:O2	2:Z:13:DA:H5"	2.03	0.58
2:N:10:DT:H2'	2:N:11:DC:C5	2.38	0.58
2:V:5:DA:H1'	2:V:6:DC:H5'	1.84	0.57
2:L:10:DT:H2'	2:L:11:DC:C5	2.39	0.57
2:O:10:DT:H2'	2:O:11:DC:C5	2.39	0.57
1:C:263:VAL:O	1:H:230:PRO:HB3	2.05	0.57
1:D:244:VAL:HG13	1:D:248:ASP:HB2	1.87	0.57
1:B:251:ALA:O	1:B:254:THR:OG1	2.20	0.57
1:B:203:PRO:HG2	2:I:4:DG:C8	2.39	0.57
2:V:1:DT:H2"	2:V:2:DT:H5'	1.86	0.57
1:C:171:ASN:O	1:C:174:VAL:HG22	2.05	0.57
1:E:252:LEU:CD1	1:E:274:ILE:HB	2.34	0.57
1:H:4:ASN:CB	1:H:7:ASN:ND2	2.68	0.57
1:A:90:TYR:O	1:A:94:ARG:HB2	2.05	0.57
2:X:1:DT:H2"	2:X:2:DT:O5'	2.03	0.57
1:D:34:TYR:HB2	1:D:167:LEU:HB2	1.87	0.57
1:F:27:PHE:O	1:F:30:LEU:HB2	2.05	0.57
1:D:90:TYR:O	1:D:94:ARG:HB2	2.05	0.56
1:G:90:TYR:O	1:G:94:ARG:HB2	2.04	0.56
2:I:10:DT:H2'	2:I:11:DC:C5	2.40	0.56
2:Y:6:DC:H2"	2:Y:7:DC:H5'	1.85	0.56
1:H:116:PHE:O	1:H:184:GLY:HA2	2.05	0.56
1:C:168:THR:H	1:C:171:ASN:HB2	1.70	0.56
1:H:98:ASP:HB3	1:H:153:LYS:HG3	1.87	0.56
1:E:38:THR:HG23	1:E:165:ASN:C	2.26	0.56
2:R:10:DT:H2"	2:R:11:DC:H5'	1.87	0.56
1:G:291:ILE:HG22	1:G:292:LYS:HD2	1.88	0.56
1:C:23:ARG:CZ	1:C:23:ARG:HB2	2.36	0.56
1:A:225:MET:HE2	1:E:263:VAL:HG12	1.88	0.56
1:D:79:PHE:CE1	1:D:241:SER:HB3	2.41	0.56
2:V:3:DC:H5'	2:X:13:DA:H5'	1.88	0.56
1:F:256:ALA:HB3	1:F:259:THR:CG2	2.35	0.55
1:E:31:ILE:O	1:E:35:HIS:HB3	2.07	0.55
1:F:23:ARG:HG2	1:F:24:ILE:N	2.22	0.55
1:C:98:ASP:HB3	1:C:153:LYS:HG3	1.87	0.55
1:F:157:LYS:HE2	1:F:159:GLU:OE1	2.07	0.55
1:G:171:ASN:O	1:G:174:VAL:HG22	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:88:TRP:CZ2	1:G:160:TYR:HA	2.42	0.55
1:A:134:HIS:CE1	1:B:267:PRO:HG2	2.41	0.55
1:B:43:ILE:HD12	1:B:277:LEU:O	2.06	0.55
1:B:33:LEU:HD23	1:B:33:LEU:O	2.06	0.55
1:D:98:ASP:HB3	1:D:153:LYS:HG3	1.87	0.55
1:H:259:THR:HG21	1:H:268:GLU:HB3	1.89	0.55
1:G:98:ASP:HB3	1:G:153:LYS:HG3	1.88	0.55
1:E:262:ASN:O	1:E:265:SER:HB3	2.06	0.55
1:D:34:TYR:CD1	1:D:39:PRO:HD3	2.42	0.55
1:A:8:SER:HB3	1:A:57:VAL:HG11	1.88	0.55
2:R:7:DC:H42	2:S:8:DG:H1	1.54	0.55
1:E:102:ILE:CD1	1:E:182:ILE:HD13	2.37	0.55
1:F:244:VAL:HG13	1:F:248:ASP:HB2	1.88	0.55
1:F:278:THR:CG2	1:H:285:LYS:NZ	2.70	0.54
1:F:291:ILE:O	1:F:292:LYS:HB2	2.08	0.54
1:E:36:HIS:O	1:E:166:LYS:HB3	2.07	0.54
1:F:31:ILE:CG2	1:F:168:THR:HA	2.29	0.54
1:D:29:ALA:O	1:D:33:LEU:HB2	2.08	0.54
1:A:102:ILE:CD1	1:A:182:ILE:HD13	2.38	0.54
2:L:5:DA:H2"	2:L:6:DC:OP2	2.07	0.54
1:H:90:TYR:O	1:H:94:ARG:HB2	2.07	0.54
1:D:120:THR:OG1	1:D:188:TRP:HB3	2.08	0.54
1:D:197:LEU:HD23	1:D:239:ALA:HB3	1.89	0.54
1:D:31:ILE:CG2	1:D:168:THR:HA	2.30	0.54
1:E:38:THR:HG21	1:E:164:ILE:O	2.07	0.54
1:F:156:ILE:HD12	1:F:156:ILE:N	2.23	0.54
1:H:128:GLU:HG3	1:H:129:LYS:H	1.72	0.54
1:C:97:ASN:ND2	1:C:153:LYS:HE2	2.23	0.54
1:H:232:ALA:O	1:H:233:GLU:HG3	2.07	0.54
1:F:122:GLU:OE1	1:F:122:GLU:HA	2.07	0.54
1:H:4:ASN:CB	1:H:7:ASN:HD22	2.20	0.54
1:H:83:ILE:HD13	1:H:197:LEU:HD22	1.90	0.54
1:F:96:LEU:HB3	1:F:99:TYR:HB2	1.90	0.54
1:H:171:ASN:O	1:H:174:VAL:HG22	2.08	0.54
1:A:257:THR:HG22	1:B:258:HIS:CG	2.43	0.53
1:F:31:ILE:HG23	1:F:168:THR:CA	2.29	0.53
1:H:217:LYS:HD3	1:H:268:GLU:OE2	2.08	0.53
2:K:5:DA:H2"	2:K:6:DC:OP2	2.06	0.53
1:C:139:ARG:O	1:D:254:THR:HA	2.08	0.53
1:H:246:LYS:HE2	1:H:250:ASP:OD1	2.08	0.53
1:B:166:LYS:O	1:B:171:ASN:OD1	2.27	0.53
1:C:74:THR:HG22	1:C:78:TRP:CE2	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:164:ILE:HG23	1:B:171:ASN:CG	2.29	0.53
1:E:257:THR:HG21	1:F:214:ASN:ND2	2.23	0.53
1:F:78:TRP:O	1:F:82:MET:HG3	2.07	0.53
1:A:225:MET:CE	1:E:263:VAL:H	2.08	0.53
1:E:255:ALA:HA	1:E:269:ARG:HA	1.90	0.53
1:F:83:ILE:HD12	1:F:83:ILE:H	1.73	0.53
2:N:5:DA:H2"	2:N:6:DC:OP2	2.08	0.53
1:F:75:ARG:HB3	1:F:75:ARG:CZ	2.38	0.53
1:B:79:PHE:CE1	1:B:241:SER:HB3	2.44	0.53
1:G:269:ARG:HD3	1:H:136:GLN:HG3	1.91	0.53
1:D:114:LYS:HA	1:D:121:ARG:HH21	1.74	0.53
1:D:134:HIS:HD2	3:Z:286:HOH:O	1.90	0.53
1:D:225:MET:HG2	1:G:263:VAL:HG12	1.91	0.53
1:B:50:LEU:O	1:B:54:VAL:HG23	2.09	0.52
1:A:35:HIS:O	1:A:166:LYS:HB2	2.07	0.52
1:D:96:LEU:HB3	1:D:99:TYR:HB2	1.90	0.52
2:M:5:DA:H2"	2:M:6:DC:OP2	2.07	0.52
1:G:91:ARG:HA	1:G:96:LEU:HD12	1.90	0.52
1:H:256:ALA:N	1:H:268:GLU:O	2.41	0.52
1:D:50:LEU:O	1:D:54:VAL:HG23	2.09	0.52
1:C:92:VAL:O	1:C:95:GLU:HG3	2.09	0.52
1:G:8:SER:HB3	1:G:57:VAL:CG1	2.40	0.52
1:D:44:LYS:HE2	1:D:75:ARG:NH2	2.25	0.52
1:H:106:ASN:HB2	2:P:4:DG:O3'	2.10	0.52
1:H:106:ASN:OD1	1:H:108:LYS:HB3	2.10	0.52
1:C:265:SER:O	1:C:267:PRO:HD3	2.10	0.52
1:H:156:ILE:N	1:H:156:ILE:HD12	2.24	0.52
1:F:278:THR:CG2	1:H:285:LYS:HZ2	2.23	0.52
1:A:171:ASN:O	1:A:174:VAL:HG22	2.10	0.52
1:D:122:GLU:O	1:D:125:HIS:N	2.43	0.51
1:E:164:ILE:HG23	1:E:171:ASN:OD1	2.10	0.51
1:F:98:ASP:HB3	1:F:153:LYS:HG3	1.91	0.51
1:G:164:ILE:HG23	1:G:171:ASN:CG	2.31	0.51
1:G:106:ASN:HB2	2:O:4:DG:O3'	2.10	0.51
1:E:94:ARG:O	1:E:95:GLU:HB2	2.10	0.51
1:E:156:ILE:N	1:E:156:ILE:HD12	2.25	0.51
1:A:225:MET:HE3	1:E:263:VAL:HG12	1.93	0.51
1:B:92:VAL:HG22	1:B:161:ASN:HA	1.93	0.51
1:D:262:ASN:HA	1:G:225:MET:CE	2.41	0.51
1:B:106:ASN:HB2	2:J:4:DG:O3'	2.11	0.51
1:H:8:SER:HB3	1:H:57:VAL:HG13	1.92	0.51
1:E:198:LYS:O	1:E:240:SER:HA	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:138:VAL:HG13	1:F:255:ALA:H	1.75	0.51
2:X:1:DT:C6	2:X:2:DT:H72	2.46	0.51
1:G:198:LYS:O	1:G:240:SER:HA	2.10	0.51
1:B:113:ARG:HH11	1:B:113:ARG:HG3	1.76	0.51
1:F:28:ASN:C	1:F:30:LEU:H	2.15	0.51
1:B:33:LEU:HD11	1:B:49:LYS:HG2	1.93	0.51
2:J:5:DA:H2''	2:J:6:DC:OP2	2.11	0.51
1:A:58:VAL:CG2	1:A:63:LEU:HB2	2.41	0.51
1:G:203:PRO:HG2	2:P:4:DG:C8	2.46	0.51
2:X:7:DC:H2''	2:X:8:DG:C8	2.46	0.51
1:G:156:ILE:N	1:G:156:ILE:HD12	2.26	0.51
2:R:9:DG:H2'	2:R:10:DT:C7	2.40	0.50
2:V:3:DC:H2''	2:V:4:DG:C8	2.45	0.50
1:G:256:ALA:O	1:G:258:HIS:N	2.44	0.50
1:E:89:ASN:O	1:E:92:VAL:HB	2.12	0.50
1:F:168:THR:HG23	1:F:171:ASN:OD1	2.11	0.50
1:A:98:ASP:HB3	1:A:153:LYS:HG3	1.93	0.50
1:B:58:VAL:HG11	1:B:65:ILE:HA	1.94	0.50
1:E:218:SER:HB2	1:F:257:THR:CG2	2.42	0.50
1:F:188:TRP:HB2	1:F:223:LEU:HD13	1.92	0.50
1:D:74:THR:HG22	1:D:78:TRP:CE2	2.46	0.50
1:C:198:LYS:O	1:C:240:SER:HA	2.11	0.50
1:B:263:VAL:HB	1:F:225:MET:HG3	1.93	0.50
1:H:256:ALA:HB3	1:H:259:THR:HG23	1.93	0.50
1:G:55:LYS:O	1:G:59:LYS:HB2	2.12	0.50
1:C:188:TRP:HB2	1:C:223:LEU:HD13	1.93	0.50
2:P:5:DA:H2''	2:P:6:DC:OP2	2.12	0.50
2:R:7:DC:N3	2:S:8:DG:N2	2.52	0.50
1:A:8:SER:HB3	1:A:57:VAL:HG13	1.93	0.50
1:B:33:LEU:HD21	1:B:49:LYS:HE3	1.93	0.50
1:G:260:ILE:HG22	1:G:267:PRO:HB3	1.92	0.50
1:H:256:ALA:O	1:H:259:THR:N	2.24	0.50
1:C:90:TYR:O	1:C:94:ARG:HB2	2.11	0.50
1:D:156:ILE:HD12	1:D:156:ILE:N	2.27	0.49
1:B:41:GLY:O	1:B:279:SER:HA	2.12	0.49
1:C:156:ILE:N	1:C:156:ILE:HD12	2.26	0.49
1:A:230:PRO:HB3	1:E:263:VAL:O	2.12	0.49
1:F:102:ILE:CD1	1:F:182:ILE:HD13	2.42	0.49
1:B:156:ILE:HD12	1:B:156:ILE:N	2.27	0.49
1:H:125:HIS:HA	1:H:128:GLU:HG2	1.95	0.49
1:D:188:TRP:HB2	1:D:223:LEU:HD13	1.93	0.49
1:E:113:ARG:HG3	1:E:113:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:138:VAL:HG13	1:B:255:ALA:CB	2.32	0.49
1:C:255:ALA:HB1	1:C:268:GLU:O	2.10	0.49
1:H:198:LYS:O	1:H:240:SER:HA	2.13	0.49
1:E:116:PHE:O	1:E:184:GLY:HA2	2.12	0.49
1:A:83:ILE:HD13	1:A:197:LEU:HD22	1.94	0.49
2:I:5:DA:H2''	2:I:6:DC:OP2	2.12	0.49
1:B:59:LYS:HG2	1:B:65:ILE:HD11	1.95	0.49
1:G:42:SER:HB3	1:G:45:GLU:HG3	1.93	0.49
2:V:12:DG:H2''	2:V:13:DA:O5'	2.11	0.49
1:C:37:GLN:HG2	1:C:38:THR:N	2.28	0.49
1:G:108:LYS:HE3	3:G:308:HOH:O	2.12	0.49
1:C:116:PHE:O	1:C:184:GLY:HA2	2.13	0.49
1:H:55:LYS:O	1:H:58:VAL:HG12	2.13	0.49
2:O:5:DA:H2''	2:O:6:DC:OP2	2.13	0.49
1:G:74:THR:HG22	1:G:78:TRP:CE2	2.47	0.49
1:B:33:LEU:HD21	1:B:49:LYS:CE	2.43	0.49
1:D:87:SER:HB3	1:D:101:ILE:HG21	1.95	0.49
1:C:57:VAL:O	1:C:61:LYS:HG3	2.11	0.49
1:E:98:ASP:HB3	1:E:153:LYS:HG3	1.94	0.48
1:F:255:ALA:CA	1:F:268:GLU:O	2.61	0.48
1:E:24:ILE:HB	2:N:11:DC:H5''	1.94	0.48
1:B:102:ILE:CD1	1:B:182:ILE:HD13	2.43	0.48
1:H:102:ILE:CD1	1:H:182:ILE:HD13	2.43	0.48
1:B:44:LYS:O	1:B:47:LEU:N	2.46	0.48
1:H:113:ARG:HG3	1:H:113:ARG:HH11	1.77	0.48
1:C:50:LEU:O	1:C:54:VAL:HG23	2.12	0.48
1:F:155:LEU:HD21	1:F:185:LYS:HB3	1.94	0.48
1:B:159:GLU:N	1:B:159:GLU:CD	2.64	0.48
1:G:8:SER:HB3	1:G:57:VAL:HG11	1.95	0.48
1:C:53:TYR:O	1:C:57:VAL:HG23	2.14	0.48
1:A:255:ALA:CB	1:B:138:VAL:CG1	2.67	0.48
1:A:148:LEU:HD22	1:A:191:LEU:CD1	2.40	0.48
1:D:97:ASN:O	1:D:156:ILE:CG1	2.62	0.48
2:S:1:DT:H2'	2:S:2:DT:H72	1.95	0.48
1:D:119:GLU:O	1:D:122:GLU:HB3	2.13	0.48
1:D:235:LYS:HD3	1:D:237:TYR:OH	2.13	0.48
1:C:55:LYS:O	1:C:59:LYS:HB2	2.13	0.48
1:H:203:PRO:HG2	2:O:4:DG:C8	2.48	0.48
1:F:203:PRO:HG2	2:M:4:DG:C8	2.48	0.48
1:E:188:TRP:HB2	1:E:223:LEU:HD13	1.94	0.48
1:D:91:ARG:HA	1:D:96:LEU:HD12	1.96	0.48
1:G:116:PHE:O	1:G:184:GLY:HA2	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:10:DT:H4'	2:I:10:DT:OP1	2.14	0.48
1:B:188:TRP:HB2	1:B:223:LEU:HD13	1.96	0.48
1:G:113:ARG:HH11	1:G:113:ARG:HG3	1.79	0.48
1:D:279:SER:OG	1:D:281:GLU:HG3	2.14	0.48
1:A:74:THR:HG22	1:A:78:TRP:CE2	2.49	0.48
1:H:94:ARG:HG3	1:H:292:LYS:NZ	2.29	0.47
1:A:156:ILE:N	1:A:156:ILE:HD12	2.29	0.47
1:A:72:SER:HB3	2:I:7:DC:O4'	2.13	0.47
1:D:106:ASN:HB2	2:L:4:DG:O3'	2.14	0.47
1:A:50:LEU:O	1:A:54:VAL:HG23	2.13	0.47
1:E:251:ALA:O	1:E:254:THR:OG1	2.28	0.47
1:C:58:VAL:CG2	1:C:63:LEU:HB2	2.45	0.47
1:B:98:ASP:HB3	1:B:153:LYS:HG3	1.94	0.47
1:C:35:HIS:NE2	1:C:36:HIS:CE1	2.82	0.47
1:E:250:ASP:O	1:E:253:GLN:HB2	2.14	0.47
1:C:113:ARG:HH11	1:C:113:ARG:HG3	1.79	0.47
1:G:58:VAL:CG2	1:G:63:LEU:HB2	2.45	0.47
1:G:188:TRP:HB2	1:G:223:LEU:HD13	1.96	0.47
1:C:257:THR:HG21	1:D:214:ASN:ND2	2.30	0.47
1:H:255:ALA:HA	1:H:269:ARG:HA	1.97	0.47
1:A:113:ARG:HH11	1:A:113:ARG:HG3	1.78	0.47
1:A:257:THR:O	1:A:257:THR:HG22	2.15	0.47
1:B:55:LYS:O	1:B:59:LYS:HG3	2.15	0.47
1:A:58:VAL:HG23	1:A:63:LEU:HB2	1.96	0.47
1:E:50:LEU:O	1:E:54:VAL:HG12	2.14	0.47
1:D:213:GLY:O	1:D:217:LYS:HG3	2.15	0.47
1:C:87:SER:HB3	1:C:101:ILE:HG21	1.96	0.47
1:E:30:LEU:HD23	1:E:50:LEU:HD11	1.97	0.47
1:B:51:GLU:HG3	1:B:71:PHE:CE1	2.50	0.47
1:G:138:VAL:HG13	1:H:255:ALA:CA	2.45	0.47
1:F:278:THR:HG21	1:H:285:LYS:HZ2	1.80	0.47
1:B:58:VAL:HG12	1:B:65:ILE:HD13	1.97	0.47
1:D:34:TYR:HD2	1:D:167:LEU:HD12	1.80	0.46
1:E:51:GLU:O	1:E:55:LYS:HB2	2.15	0.46
1:H:55:LYS:O	1:H:59:LYS:HB2	2.16	0.46
1:F:74:THR:HG22	1:F:78:TRP:CZ2	2.50	0.46
1:B:33:LEU:CD2	1:B:49:LYS:HE3	2.45	0.46
1:D:230:PRO:HG3	1:G:263:VAL:HG22	1.97	0.46
1:C:83:ILE:HD13	1:C:197:LEU:HD22	1.96	0.46
1:H:50:LEU:O	1:H:54:VAL:HG23	2.15	0.46
1:B:230:PRO:HB3	1:F:263:VAL:O	2.15	0.46
1:D:173:ASP:O	1:D:177:THR:OG1	2.28	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:58:VAL:CG2	1:H:63:LEU:HB2	2.45	0.46
1:D:72:SER:HB3	2:L:7:DC:O4'	2.15	0.46
1:E:24:ILE:O	2:N:11:DC:H3'	2.15	0.46
2:V:5:DA:H2''	2:V:6:DC:O5'	2.14	0.46
1:A:83:ILE:CD1	1:A:197:LEU:HD22	2.46	0.46
1:E:33:LEU:CD1	1:E:50:LEU:HA	2.44	0.46
1:A:143:SER:O	1:A:212:GLU:OE2	2.33	0.46
1:D:91:ARG:HB2	1:D:96:LEU:HB2	1.97	0.46
1:A:55:LYS:O	1:A:59:LYS:HB2	2.15	0.46
1:D:115:ILE:O	1:D:186:CYS:HB2	2.15	0.46
1:B:94:ARG:O	1:B:95:GLU:HB2	2.15	0.46
1:F:97:ASN:O	1:F:156:ILE:CG1	2.60	0.46
1:F:242:GLU:HB3	1:F:243:PRO:CD	2.45	0.46
1:C:275:PHE:CD2	1:C:286:MET:HG3	2.51	0.46
1:F:235:LYS:HD3	1:F:237:TYR:OH	2.16	0.46
1:A:94:ARG:HA	1:A:94:ARG:HD3	1.68	0.46
1:A:203:PRO:HG2	2:J:4:DG:C8	2.50	0.46
1:B:71:PHE:O	1:B:75:ARG:HG3	2.16	0.46
1:A:188:TRP:HB2	1:A:223:LEU:HD13	1.97	0.46
1:A:78:TRP:O	1:A:82:MET:HG3	2.16	0.46
1:D:97:ASN:HD21	1:D:153:LYS:HE2	1.81	0.46
1:B:44:LYS:O	1:B:46:ASN:N	2.49	0.46
1:E:237:TYR:CE2	1:E:290:ILE:HG23	2.51	0.46
1:F:151:ARG:CG	1:F:151:ARG:O	2.63	0.46
1:F:74:THR:HG22	1:F:78:TRP:CE2	2.51	0.46
1:G:38:THR:HG23	1:G:165:ASN:C	2.37	0.46
1:C:231:LYS:HD3	2:V:10:DT:OP1	2.16	0.46
1:D:34:TYR:O	1:D:167:LEU:N	2.46	0.46
1:C:44:LYS:HD3	1:C:242:GLU:HG2	1.97	0.46
1:G:159:GLU:CD	1:G:159:GLU:H	2.20	0.46
1:B:90:TYR:HA	1:B:93:LYS:CD	2.42	0.46
1:F:88:TRP:O	1:F:92:VAL:HG23	2.16	0.46
1:G:157:LYS:HD3	1:G:160:TYR:OH	2.16	0.46
1:C:24:ILE:HG22	1:C:26:PRO:HD3	1.98	0.45
1:A:4:ASN:ND2	1:A:4:ASN:N	2.56	0.45
1:H:58:VAL:HG23	1:H:63:LEU:HB2	1.98	0.45
1:C:33:LEU:HD21	1:C:53:TYR:CZ	2.51	0.45
1:D:113:ARG:HG3	1:D:113:ARG:HH11	1.79	0.45
1:D:45:GLU:O	1:D:49:LYS:HB2	2.17	0.45
1:D:79:PHE:HA	1:D:82:MET:HE3	1.97	0.45
1:E:93:LYS:HG3	1:E:94:ARG:N	2.30	0.45
1:E:91:ARG:HA	1:E:96:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:113:ARG:HG3	1:F:113:ARG:HH11	1.81	0.45
1:B:116:PHE:O	1:B:184:GLY:HA2	2.16	0.45
1:C:237:TYR:CE2	1:C:290:ILE:HG23	2.51	0.45
1:E:48:ASP:O	1:E:51:GLU:HB3	2.16	0.45
1:D:225:MET:HG2	1:G:263:VAL:CG1	2.46	0.45
1:E:138:VAL:CB	1:F:255:ALA:HB2	2.40	0.45
1:F:92:VAL:HG11	1:F:163:PRO:HD3	1.97	0.45
1:D:34:TYR:HH	1:D:39:PRO:HB3	1.81	0.45
1:B:44:LYS:C	1:B:46:ASN:N	2.68	0.45
1:D:170:GLU:O	1:D:173:ASP:HB2	2.17	0.45
1:A:136:GLN:CG	1:B:269:ARG:HD3	2.45	0.45
1:F:263:VAL:HG22	1:F:263:VAL:O	2.15	0.45
2:Y:2:DT:H2'	2:Y:2:DT:H6	1.64	0.45
1:C:37:GLN:HA	1:C:165:ASN:O	2.16	0.45
1:F:255:ALA:HA	1:F:268:GLU:O	2.17	0.45
1:D:96:LEU:HD22	1:D:99:TYR:CD2	2.52	0.45
1:F:275:PHE:CD2	1:F:286:MET:HG3	2.52	0.45
1:B:198:LYS:O	1:B:240:SER:HA	2.16	0.45
1:E:73:ASN:OD1	1:E:73:ASN:C	2.54	0.45
1:F:213:GLY:O	1:F:217:LYS:HG3	2.17	0.45
2:N:10:DT:OP1	2:N:10:DT:H4'	2.17	0.45
1:H:36:HIS:CG	1:H:37:GLN:N	2.85	0.45
1:G:193:ALA:HA	1:G:235:LYS:O	2.16	0.45
1:F:91:ARG:HH11	1:F:160:TYR:HB3	1.81	0.45
2:Y:2:DT:H2''	2:Y:3:DC:OP2	2.16	0.45
1:C:203:PRO:HG2	2:L:4:DG:C8	2.52	0.45
1:A:138:VAL:HG22	1:B:269:ARG:HG3	1.99	0.45
1:C:138:VAL:HG13	1:D:255:ALA:HB2	1.97	0.45
1:E:275:PHE:CD2	1:E:286:MET:HG3	2.52	0.45
1:D:203:PRO:HA	1:D:206:ARG:CZ	2.47	0.45
1:H:41:GLY:O	1:H:279:SER:HA	2.17	0.45
1:E:199:THR:O	1:E:242:GLU:HG3	2.17	0.44
1:D:212:GLU:O	1:D:216:LEU:HG	2.16	0.44
2:Y:6:DC:H1'	2:Y:7:DC:C5'	2.47	0.44
1:F:23:ARG:HG2	1:F:24:ILE:H	1.82	0.44
1:E:254:THR:HA	1:F:139:ARG:O	2.17	0.44
1:C:102:ILE:CD1	1:C:182:ILE:HD13	2.47	0.44
1:D:94:ARG:O	1:D:95:GLU:HB2	2.18	0.44
1:B:168:THR:H	1:B:171:ASN:HB2	1.82	0.44
1:G:269:ARG:HG3	1:H:138:VAL:HG22	2.00	0.44
1:B:193:ALA:HA	1:B:235:LYS:O	2.17	0.44
1:G:37:GLN:HB2	3:G:305:HOH:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:138:VAL:HG13	1:F:255:ALA:N	2.32	0.44
1:F:90:TYR:CZ	1:F:94:ARG:HG2	2.52	0.44
1:D:242:GLU:HB3	1:D:243:PRO:CD	2.48	0.44
1:A:55:LYS:O	1:A:58:VAL:HG12	2.16	0.44
1:D:25:LYS:HA	1:D:26:PRO:HD2	1.82	0.44
1:A:275:PHE:CD2	1:A:286:MET:HG3	2.53	0.44
1:H:112:PHE:O	1:H:115:ILE:HG12	2.18	0.44
1:E:68:SER:O	1:E:72:SER:N	2.41	0.44
1:H:57:VAL:O	1:H:61:LYS:HG3	2.16	0.44
1:E:24:ILE:HG13	2:N:11:DC:OP1	2.18	0.44
2:O:10:DT:H4'	2:O:10:DT:OP1	2.18	0.44
2:Z:5:DA:H1'	2:Z:6:DC:H5''	1.98	0.44
1:C:42:SER:HB3	1:C:45:GLU:CG	2.39	0.44
1:E:256:ALA:C	1:E:258:HIS:N	2.71	0.44
1:B:44:LYS:O	1:B:45:GLU:C	2.55	0.44
1:E:42:SER:HB3	1:E:45:GLU:HB2	2.00	0.44
1:B:237:TYR:CE2	1:B:290:ILE:HG23	2.53	0.44
1:F:77:THR:O	1:F:78:TRP:C	2.56	0.44
2:Y:1:DT:H2'	2:Y:2:DT:H71	1.99	0.44
1:F:120:THR:OG1	1:F:188:TRP:HB3	2.18	0.44
1:E:227:TYR:O	1:E:228:TRP:C	2.55	0.44
1:H:256:ALA:O	1:H:257:THR:C	2.55	0.44
1:G:55:LYS:O	1:G:58:VAL:HG12	2.17	0.44
1:F:123:LYS:O	1:F:126:GLN:HB2	2.18	0.44
1:A:116:PHE:O	1:A:184:GLY:HA2	2.18	0.44
1:G:164:ILE:HG23	1:G:171:ASN:OD1	2.18	0.43
2:J:10:DT:OP1	2:J:10:DT:H4'	2.18	0.43
1:F:103:LYS:O	1:F:103:LYS:CG	2.66	0.43
1:D:44:LYS:HA	1:D:44:LYS:HD3	1.86	0.43
2:V:13:DA:OP1	2:V:13:DA:H4'	2.18	0.43
1:A:251:ALA:O	1:A:254:THR:OG1	2.25	0.43
1:B:34:TYR:HB2	1:B:167:LEU:HD12	1.98	0.43
1:A:123:LYS:O	1:A:126:GLN:HB2	2.18	0.43
1:B:4:ASN:HA	3:B:341:HOH:O	2.17	0.43
1:B:88:TRP:C	1:B:88:TRP:CD1	2.91	0.43
1:B:83:ILE:HD13	1:B:197:LEU:HD22	2.00	0.43
1:H:227:TYR:O	1:H:228:TRP:C	2.56	0.43
1:F:91:ARG:NH1	1:F:160:TYR:HB2	2.33	0.43
2:P:10:DT:OP1	2:P:10:DT:H4'	2.17	0.43
1:G:50:LEU:O	1:G:54:VAL:HG23	2.19	0.43
1:D:237:TYR:CE2	1:D:290:ILE:HG23	2.53	0.43
1:E:112:PHE:O	1:E:115:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:31:ILE:O	1:C:32:GLU:C	2.54	0.43
1:C:136:GLN:CG	1:D:269:ARG:HD3	2.48	0.43
1:A:41:GLY:O	1:A:279:SER:HA	2.18	0.43
1:A:51:GLU:HG3	1:A:71:PHE:CD1	2.53	0.43
1:F:168:THR:OG1	1:F:171:ASN:OD1	2.36	0.43
1:H:188:TRP:HB2	1:H:223:LEU:HD13	1.99	0.43
1:D:88:TRP:CZ2	1:D:160:TYR:HA	2.53	0.43
1:H:51:GLU:HG3	1:H:71:PHE:CD1	2.53	0.43
1:C:51:GLU:HG3	1:C:71:PHE:CD1	2.54	0.43
1:F:78:TRP:O	1:F:79:PHE:C	2.56	0.43
2:V:1:DT:H2''	2:V:2:DT:C5'	2.48	0.43
1:E:34:TYR:HB2	1:E:167:LEU:HD12	2.00	0.43
1:A:91:ARG:HA	1:A:96:LEU:HD12	2.00	0.43
1:E:72:SER:HB3	2:M:7:DC:O4'	2.19	0.43
1:B:58:VAL:HG11	1:B:65:ILE:HD13	1.99	0.43
1:B:227:TYR:O	1:B:228:TRP:C	2.56	0.43
1:C:79:PHE:HA	1:C:82:MET:HE3	2.00	0.43
1:B:246:LYS:NZ	1:B:250:ASP:OD1	2.45	0.43
1:F:187:LYS:HE2	1:F:187:LYS:HB3	1.81	0.43
1:H:32:GLU:OE1	1:H:53:TYR:OH	2.34	0.43
1:A:15:LYS:HA	1:A:19:LYS:O	2.19	0.43
1:C:193:ALA:HA	1:C:235:LYS:O	2.17	0.43
1:B:8:SER:HB3	1:B:57:VAL:HG11	1.99	0.43
1:D:83:ILE:CD1	1:D:197:LEU:HD22	2.49	0.43
1:H:256:ALA:C	1:H:258:HIS:N	2.72	0.43
1:C:58:VAL:HG23	1:C:63:LEU:HB2	2.01	0.43
1:B:8:SER:HB3	1:B:57:VAL:CG1	2.48	0.43
1:A:24:ILE:HD11	1:A:66:PRO:CB	2.49	0.43
1:C:55:LYS:O	1:C:58:VAL:HG12	2.19	0.43
1:A:198:LYS:O	1:A:240:SER:HA	2.19	0.43
1:C:254:THR:HA	1:D:139:ARG:O	2.19	0.43
1:F:91:ARG:HG3	1:F:92:VAL:H	1.81	0.42
1:F:291:ILE:O	1:F:292:LYS:CB	2.67	0.42
1:F:75:ARG:HH11	1:F:75:ARG:HG2	1.84	0.42
1:A:267:PRO:HG2	1:B:134:HIS:CE1	2.53	0.42
1:H:74:THR:HG22	1:H:78:TRP:CE2	2.54	0.42
1:E:218:SER:HB2	1:F:257:THR:HG21	2.00	0.42
1:G:58:VAL:HG23	1:G:63:LEU:HB2	2.00	0.42
1:A:88:TRP:CZ2	1:A:160:TYR:HA	2.54	0.42
1:A:193:ALA:HA	1:A:235:LYS:O	2.18	0.42
1:B:39:PRO:O	1:B:40:THR:HG23	2.18	0.42
1:C:74:THR:CG2	1:C:78:TRP:CZ2	3.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:55:LYS:HG2	1:E:55:LYS:O	2.19	0.42
1:C:112:PHE:O	1:C:115:ILE:HG12	2.19	0.42
1:G:135:LYS:HB2	2:V:8:DG:H5"	2.01	0.42
1:G:214:ASN:ND2	1:H:257:THR:CG2	2.80	0.42
1:D:188:TRP:CG	1:D:189:ASP:N	2.87	0.42
1:F:188:TRP:CG	1:F:189:ASP:N	2.87	0.42
1:H:242:GLU:HB3	1:H:243:PRO:CD	2.49	0.42
1:D:51:GLU:HG3	1:D:71:PHE:CD1	2.55	0.42
1:A:213:GLY:O	1:A:217:LYS:HG3	2.19	0.42
1:F:74:THR:CG2	1:F:78:TRP:CZ2	3.02	0.42
1:G:53:TYR:O	1:G:57:VAL:HG23	2.19	0.42
1:E:218:SER:CB	1:F:257:THR:HG22	2.50	0.42
1:H:169:HIS:O	1:H:173:ASP:OD2	2.37	0.42
1:D:86:GLN:OE1	1:D:280:PHE:HD2	2.03	0.42
2:K:10:DT:OP1	2:K:10:DT:H4'	2.20	0.42
1:G:57:VAL:O	1:G:61:LYS:HG3	2.19	0.42
1:F:223:LEU:O	1:F:227:TYR:HD2	2.03	0.42
1:D:281:GLU:HG3	1:D:281:GLU:H	1.50	0.42
1:B:98:ASP:N	1:B:98:ASP:OD1	2.50	0.42
1:C:44:LYS:HB3	1:C:44:LYS:HE3	1.86	0.42
1:G:139:ARG:O	1:H:254:THR:HA	2.19	0.42
2:L:10:DT:H4'	2:L:10:DT:OP1	2.20	0.42
1:B:54:VAL:O	1:B:58:VAL:HG23	2.19	0.42
1:C:263:VAL:HG22	1:H:230:PRO:HB3	2.01	0.42
1:A:51:GLU:OE1	1:A:75:ARG:HD2	2.20	0.42
1:D:28:ASN:C	1:D:30:LEU:N	2.72	0.42
1:A:281:GLU:HG3	1:A:285:LYS:HE3	2.02	0.42
1:E:193:ALA:HA	1:E:235:LYS:O	2.19	0.42
1:G:171:ASN:HA	1:G:171:ASN:HD22	1.52	0.42
1:F:88:TRP:CZ3	1:F:175:ALA:HA	2.52	0.42
1:E:256:ALA:HB3	1:E:259:THR:HG23	2.01	0.42
1:G:45:GLU:O	1:G:49:LYS:HB2	2.20	0.42
1:F:217:LYS:NZ	1:F:268:GLU:OE2	2.36	0.42
1:B:87:SER:O	1:B:90:TYR:HB3	2.20	0.42
1:F:203:PRO:HA	1:F:206:ARG:CZ	2.50	0.42
1:B:262:ASN:HB2	1:B:265:SER:HB2	2.02	0.42
1:D:275:PHE:CD2	1:D:286:MET:HG3	2.55	0.42
1:C:214:ASN:OD1	1:C:256:ALA:HA	2.20	0.41
1:F:197:LEU:C	1:F:198:LYS:HG2	2.41	0.41
1:B:11:VAL:HG11	1:B:58:VAL:CG2	2.50	0.41
1:G:42:SER:CB	1:G:45:GLU:HG3	2.50	0.41
1:A:223:LEU:HA	1:A:223:LEU:HD23	1.91	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:86:GLN:HG2	1:C:283:ILE:HD12	2.02	0.41
1:D:227:TYR:O	1:D:228:TRP:C	2.58	0.41
1:A:227:TYR:O	1:A:228:TRP:C	2.57	0.41
1:B:90:TYR:OH	1:B:288:ASP:OD1	2.28	0.41
1:D:197:LEU:C	1:D:198:LYS:HG2	2.40	0.41
1:A:57:VAL:O	1:A:61:LYS:HG3	2.18	0.41
1:H:44:LYS:HA	1:H:47:LEU:HD12	2.02	0.41
1:A:139:ARG:O	1:B:254:THR:HA	2.21	0.41
1:A:87:SER:HB3	1:A:101:ILE:HG21	2.02	0.41
1:F:94:ARG:O	1:F:95:GLU:HB2	2.21	0.41
1:E:30:LEU:CD1	1:E:81:VAL:HG11	2.51	0.41
1:A:136:GLN:HG2	1:B:269:ARG:CD	2.50	0.41
1:C:269:ARG:HD3	1:D:136:GLN:CG	2.51	0.41
1:F:79:PHE:CE1	1:F:83:ILE:HD11	2.55	0.41
1:D:133:THR:HG23	2:V:2:DT:H71	1.99	0.41
1:A:106:ASN:HB2	2:I:4:DG:O3'	2.20	0.41
1:E:257:THR:CG2	1:F:214:ASN:ND2	2.84	0.41
1:G:51:GLU:HG2	1:G:55:LYS:HE3	2.02	0.41
1:C:86:GLN:OE1	1:C:280:PHE:HD2	2.03	0.41
1:E:217:LYS:HZ1	1:E:272:ASP:CG	2.24	0.41
1:B:275:PHE:CD2	1:B:286:MET:HG3	2.55	0.41
1:D:65:ILE:HG23	1:D:65:ILE:O	2.20	0.41
1:F:89:ASN:O	1:F:93:LYS:HB2	2.21	0.41
1:F:175:ALA:C	1:F:177:THR:H	2.24	0.41
1:H:213:GLY:O	1:H:217:LYS:HG3	2.21	0.41
1:A:53:TYR:O	1:A:57:VAL:HG23	2.21	0.41
1:D:150:ILE:CD1	1:D:191:LEU:HD13	2.51	0.41
1:D:112:PHE:O	1:D:115:ILE:HG12	2.21	0.41
2:Z:6:DC:H2''	2:Z:7:DC:O5'	2.20	0.41
1:F:91:ARG:NH2	1:F:97:ASN:HA	2.35	0.41
1:F:28:ASN:C	1:F:30:LEU:N	2.73	0.41
1:F:125:HIS:O	1:F:129:LYS:HB2	2.20	0.41
2:R:9:DG:H2''	2:R:10:DT:O5'	2.20	0.41
1:H:53:TYR:O	1:H:57:VAL:HG23	2.20	0.41
1:A:65:ILE:HA	1:A:66:PRO:HD3	1.91	0.41
1:E:203:PRO:HG2	2:N:4:DG:C8	2.54	0.41
1:D:262:ASN:HA	1:G:225:MET:HE2	2.02	0.41
1:D:263:VAL:HG12	1:G:225:MET:CE	2.50	0.41
1:C:42:SER:O	1:C:45:GLU:HB2	2.21	0.41
1:C:138:VAL:HG22	1:D:269:ARG:HG3	2.03	0.41
1:G:38:THR:HG23	1:G:166:LYS:N	2.35	0.41
1:E:148:LEU:HD22	1:E:191:LEU:CD1	2.48	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:240:SER:C	1:F:242:GLU:H	2.23	0.41
2:V:6:DC:H2"	2:V:7:DC:OP2	2.20	0.41
1:C:23:ARG:HB2	1:C:23:ARG:NH1	2.35	0.41
1:E:30:LEU:HD13	1:E:81:VAL:HG11	2.03	0.41
1:F:266:THR:HA	1:F:267:PRO:HD3	1.95	0.41
1:F:112:PHE:O	1:F:115:ILE:HG12	2.21	0.41
1:G:227:TYR:O	1:G:228:TRP:C	2.58	0.41
1:G:51:GLU:HG3	1:G:71:PHE:CD1	2.55	0.41
1:C:213:GLY:O	1:C:217:LYS:HG3	2.21	0.41
1:H:193:ALA:HA	1:H:235:LYS:O	2.20	0.41
1:H:15:LYS:HA	1:H:19:LYS:O	2.21	0.41
1:F:79:PHE:O	1:F:83:ILE:CD1	2.67	0.40
1:F:227:TYR:O	1:F:228:TRP:C	2.59	0.40
1:C:199:THR:O	1:C:242:GLU:HG3	2.21	0.40
1:C:28:ASN:O	1:C:32:GLU:HG3	2.20	0.40
1:F:116:PHE:HB2	1:F:121:ARG:HG2	2.04	0.40
1:F:91:ARG:HB2	1:F:91:ARG:HE	1.68	0.40
1:D:175:ALA:C	1:D:177:THR:H	2.23	0.40
1:D:230:PRO:HG3	1:G:263:VAL:CG2	2.51	0.40
1:A:254:THR:HA	1:B:139:ARG:O	2.21	0.40
1:E:204:ASP:HB2	1:F:208:GLN:OE1	2.21	0.40
1:F:212:GLU:O	1:F:216:LEU:HG	2.20	0.40
1:D:102:ILE:CD1	1:D:182:ILE:HD13	2.51	0.40
1:E:52:ASN:O	1:E:55:LYS:N	2.54	0.40
1:D:44:LYS:HE2	1:D:75:ARG:HH22	1.86	0.40
1:D:106:ASN:OD1	1:D:108:LYS:HB2	2.21	0.40
1:C:72:SER:HB3	2:K:7:DC:O4'	2.21	0.40
1:A:117:ASP:O	1:A:121:ARG:HG3	2.21	0.40
1:E:108:LYS:HD3	1:E:108:LYS:HA	1.88	0.40
1:D:252:LEU:HD23	1:D:252:LEU:HA	1.88	0.40
1:F:168:THR:HG1	1:F:171:ASN:CG	2.25	0.40
1:C:34:TYR:HB2	1:C:167:LEU:HB2	2.02	0.40
1:H:31:ILE:O	1:H:35:HIS:HB3	2.22	0.40
1:F:91:ARG:NH1	1:F:160:TYR:CB	2.84	0.40
1:D:187:LYS:HG3	1:D:189:ASP:OD1	2.21	0.40
1:G:254:THR:HA	1:H:139:ARG:O	2.20	0.40
1:B:199:THR:O	1:B:242:GLU:HG3	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	
1	A	287/293 (98%)	278 (97%)	8 (3%)	1 (0%)	50	82
1	B	287/293 (98%)	268 (93%)	18 (6%)	1 (0%)	50	82
1	C	286/293 (98%)	267 (93%)	18 (6%)	1 (0%)	50	82
1	D	287/293 (98%)	267 (93%)	20 (7%)	0	100	100
1	E	287/293 (98%)	260 (91%)	24 (8%)	3 (1%)	22	51
1	F	285/293 (97%)	246 (86%)	33 (12%)	6 (2%)	11	27
1	G	287/293 (98%)	275 (96%)	12 (4%)	0	100	100
1	H	288/293 (98%)	278 (96%)	9 (3%)	1 (0%)	50	82
All	All	2294/2344 (98%)	2139 (93%)	142 (6%)	13 (1%)	33	66

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	257	THR
1	H	257	THR
1	A	257	THR
1	F	57	VAL
1	B	97	ASN
1	E	6	THR
1	F	18	GLY
1	F	32	GLU
1	C	8	SER
1	E	19	LYS
1	F	20	THR
1	F	67	THR
1	F	26	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of

similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/267 (98%)	254 (97%)	9 (3%)	49	81
1	B	263/267 (98%)	254 (97%)	9 (3%)	49	81
1	C	262/267 (98%)	257 (98%)	5 (2%)	69	92
1	D	263/267 (98%)	252 (96%)	11 (4%)	40	73
1	E	263/267 (98%)	249 (95%)	14 (5%)	32	62
1	F	261/267 (98%)	248 (95%)	13 (5%)	34	66
1	G	263/267 (98%)	255 (97%)	8 (3%)	53	84
1	H	264/267 (99%)	253 (96%)	11 (4%)	40	73
All	All	2102/2136 (98%)	2022 (96%)	80 (4%)	44	76

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	40	THR
1	A	94	ARG
1	A	126	GLN
1	A	159	GLU
1	A	233	GLU
1	A	249	ASP
1	A	289	GLN
1	A	292	LYS
1	B	35	HIS
1	B	37	GLN
1	B	93	LYS
1	B	96	LEU
1	B	135	LYS
1	B	170	GLU
1	B	212	GLU
1	B	231	LYS
1	B	249	ASP
1	C	23	ARG
1	C	37	GLN
1	C	94	ARG
1	C	249	ASP
1	C	292	LYS
1	D	6	THR

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Mol	Chain	Res	Type
1	D	7	ASN
1	D	33	LEU
1	D	45	GLU
1	D	94	ARG
1	D	118	ASN
1	D	225	MET
1	D	249	ASP
1	D	266	THR
1	D	281	GLU
1	D	289	GLN
1	E	4	ASN
1	E	8	SER
1	E	14	TYR
1	E	35	HIS
1	E	40	THR
1	E	71	PHE
1	E	73	ASN
1	E	94	ARG
1	E	170	GLU
1	E	173	ASP
1	E	246	LYS
1	E	249	ASP
1	E	266	THR
1	E	292	LYS
1	F	22	ILE
1	F	33	LEU
1	F	35	HIS
1	F	37	GLN
1	F	40	THR
1	F	93	LYS
1	F	94	ARG
1	F	103	LYS
1	F	129	LYS
1	F	165	ASN
1	F	173	ASP
1	F	266	THR
1	F	289	GLN
1	G	4	ASN
1	G	49	LYS
1	G	94	ARG
1	G	121	ARG
1	G	171	ASN

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Mol	Chain	Res	Type
1	G	212	GLU
1	G	249	ASP
1	G	264	ASN
1	H	33	LEU
1	H	37	GLN
1	H	44	LYS
1	H	94	ARG
1	H	122	GLU
1	H	165	ASN
1	H	246	LYS
1	H	249	ASP
1	H	266	THR
1	H	281	GLU
1	H	289	GLN

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

Mol	Chain	Res	Type
1	A	134	HIS
1	A	161	ASN
1	A	214	ASN
1	B	134	HIS
1	B	171	ASN
1	B	208	GLN
1	B	214	ASN
1	C	258	HIS
1	D	28	ASN
1	D	134	HIS
1	D	214	ASN
1	E	171	ASN
1	E	214	ASN
1	E	258	HIS
1	F	165	ASN
1	F	214	ASN
1	G	126	GLN
1	G	171	ASN
1	G	208	GLN
1	H	7	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 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 ⓘ

There are no ligands in this entry.

### 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(Å <sup>2</sup> )	Q<0.9
1	A	289/293 (98%)	0.20	5 (1%) 67 73	23, 40, 60, 76	2 (0%)
1	B	289/293 (98%)	0.10	4 (1%) 72 77	23, 45, 63, 79	1 (0%)
1	C	272/293 (92%)	0.40	26 (9%) 8 8	27, 47, 81, 89	5 (1%)
1	D	257/293 (87%)	0.76	34 (13%) 4 4	26, 56, 87, 98	3 (1%)
1	E	258/293 (88%)	0.47	26 (10%) 7 8	27, 53, 84, 90	8 (3%)
1	F	245/293 (83%)	0.72	35 (14%) 3 4	32, 63, 90, 94	9 (3%)
1	G	289/293 (98%)	0.06	1 (0%) 91 95	20, 41, 59, 68	7 (2%)
1	H	290/293 (98%)	0.14	4 (1%) 72 77	20, 39, 58, 82	4 (1%)
2	I	13/13 (100%)	0.11	0 100 100	28, 37, 61, 81	0
2	J	13/13 (100%)	0.33	1 (7%) 13 14	30, 41, 66, 93	1 (7%)
2	K	12/13 (92%)	0.79	0 100 100	47, 66, 87, 87	1 (8%)
2	L	12/13 (92%)	0.98	0 100 100	52, 69, 78, 84	0
2	M	8/13 (61%)	1.14	2 (25%) 1 1	55, 61, 73, 88	0
2	N	11/13 (84%)	1.40	4 (36%) 1 1	60, 81, 88, 89	0
2	O	13/13 (100%)	0.24	1 (7%) 13 14	27, 37, 79, 99	0
2	P	12/13 (92%)	0.01	0 100 100	26, 39, 50, 51	0
2	R	8/13 (61%)	0.44	0 100 100	54, 58, 82, 99	0
2	S	10/13 (76%)	0.27	0 100 100	45, 53, 86, 97	0
2	V	13/13 (100%)	1.05	0 100 100	80, 95, 100, 100	0
2	X	13/13 (100%)	0.13	0 100 100	55, 67, 86, 87	0
2	Y	13/13 (100%)	0.28	0 100 100	41, 69, 82, 84	0
2	Z	10/13 (76%)	0.59	0 100 100	68, 88, 98, 100	0
All	All	2350/2526 (93%)	0.36	143 (6%) 21 22	20, 48, 84, 100	41 (1%)



All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	69	GLY	8.9
1	D	65	ILE	7.7
1	D	66	PRO	7.2
1	F	71	PHE	6.3
1	F	70	ALA	6.2
1	F	47	LEU	5.8
1	F	43	ILE	5.5
1	D	68	SER	5.5
1	D	27	PHE	5.3
1	D	71	PHE	5.1
1	D	167	LEU	4.8
1	D	74	THR	4.6
1	D	24	ILE	4.4
1	E	71	PHE	4.3
1	C	63	LEU	4.3
1	C	70	ALA	4.2
1	E	167	LEU	4.2
1	C	71	PHE	4.1
1	C	64	ALA	4.1
1	C	78	TRP	4.0
1	F	73	ASN	4.0
1	F	69	GLY	3.9
1	F	135	LYS	3.9
1	H	35	HIS	3.8
2	J	1	DT	3.8
1	D	63	LEU	3.8
1	F	27	PHE	3.8
1	F	133	THR	3.7
1	D	51	GLU	3.7
1	A	37	GLN	3.7
1	D	78	TRP	3.7
1	D	174	VAL	3.7
1	D	30	LEU	3.6
1	D	75	ARG	3.6
1	F	22	ILE	3.6
1	A	36	HIS	3.6
1	D	67	THR	3.6
1	E	68	SER	3.6
1	E	47	LEU	3.6
1	F	75	ARG	3.5
1	D	157	LYS	3.4
1	D	241	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	18	GLY	3.3
1	C	51	GLU	3.3
1	E	200	SER	3.2
1	H	36	HIS	3.2
2	N	8	DG	3.1
1	D	176	LEU	3.1
1	D	50	LEU	3.1
1	C	36	HIS	3.1
1	E	136	GLN	3.1
2	M	9	DG	3.0
1	C	30	LEU	2.9
1	E	70	ALA	2.9
1	F	78	TRP	2.9
1	C	65	ILE	2.8
1	A	135	LYS	2.8
1	C	47	LEU	2.8
1	D	77	THR	2.8
1	F	241	SER	2.8
1	B	17	ASN	2.8
2	N	7	DC	2.8
1	D	47	LEU	2.7
1	D	69	GLY	2.7
1	D	43	ILE	2.7
1	F	204	ASP	2.7
1	C	23	ARG	2.7
1	B	36	HIS	2.7
1	A	40	THR	2.6
1	C	72	SER	2.6
1	C	43	ILE	2.6
2	O	1	DT	2.6
1	H	37	GLN	2.6
1	E	43	ILE	2.6
1	E	67	THR	2.6
1	E	50	LEU	2.5
1	E	37	GLN	2.5
1	E	202	ARG	2.5
1	F	26	PRO	2.5
1	D	135	LYS	2.5
1	D	166	LYS	2.5
1	F	255	ALA	2.5
1	D	53	TYR	2.5
1	E	172	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	201	LEU	2.4
1	E	46	ASN	2.4
1	E	51	GLU	2.4
1	E	277	LEU	2.4
1	D	72	SER	2.4
1	F	169	HIS	2.4
1	C	74	THR	2.4
1	D	64	ALA	2.4
2	M	8	DG	2.4
1	F	205	ARG	2.4
1	D	160	TYR	2.4
1	E	30	LEU	2.3
1	C	58	VAL	2.3
1	D	54	VAL	2.3
1	D	70	ALA	2.3
1	C	135	LYS	2.3
1	B	166	LYS	2.3
1	F	202	ARG	2.3
1	D	202	ARG	2.3
1	C	66	PRO	2.3
1	F	68	SER	2.3
1	F	74	THR	2.2
1	F	280	PHE	2.2
1	E	205	ARG	2.2
1	F	72	SER	2.2
1	H	44	LYS	2.2
1	F	23	ARG	2.2
1	F	100	LEU	2.2
1	E	24	ILE	2.2
1	F	24	ILE	2.2
1	E	27	PHE	2.2
1	F	184	GLY	2.2
2	N	6	DC	2.2
1	E	54	VAL	2.2
1	E	76	GLY	2.2
1	D	26	PRO	2.2
1	C	133	THR	2.1
1	F	160	TYR	2.1
2	N	9	DG	2.1
1	D	92	VAL	2.1
1	E	72	SER	2.1
1	F	48	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	41	GLY	2.1
1	F	85	ILE	2.1
1	F	30	LEU	2.1
1	E	78	TRP	2.1
1	C	75	ARG	2.1
1	F	203	PRO	2.1
1	F	148	LEU	2.1
1	F	256	ALA	2.1
1	B	37	GLN	2.1
1	E	74	THR	2.0
1	C	54	VAL	2.0
1	C	204	ASP	2.0
1	C	255	ALA	2.0
1	C	76	GLY	2.0
1	F	201	LEU	2.0
1	C	67	THR	2.0
1	C	45	GLU	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.