



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 AM GMT

PDB ID : 2W9B
Title : BINARY COMPLEX OF DPO4 BOUND TO N2,N2-DIMETHYL-DEOXYGUANOSINE MODIFIED DNA
Authors : Eoff, R.L.; Zhang, H.; Kosekov, I.D.; Rizzo, C.J.; Egli, M.; Guengerich, F.P.
Deposited on : 2009-01-22
Resolution : 2.28 Å(reported)

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

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

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

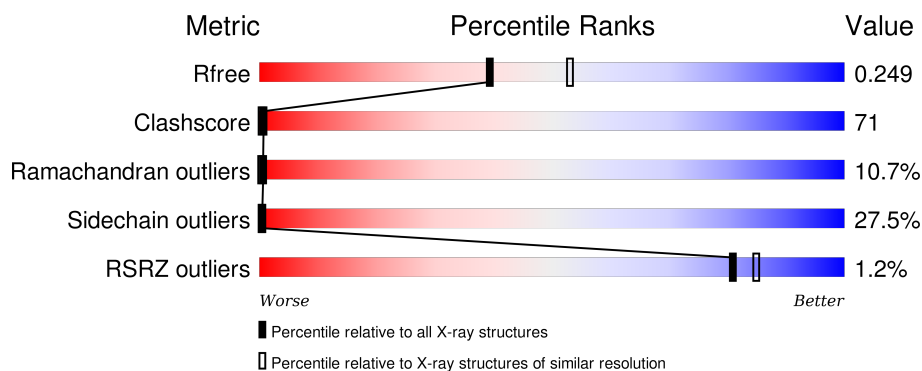
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	358	 14% 49% 27% 5% .
2	B	358	 19% 45% 26% 6% .
3	C	14	 21% 79%
3	D	14	 7% 21% 71%
4	E	18	 6% 50% 39% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	18	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DOC	C	14[B]	-	-	X	-
4	O2G	F	5[F]	-	-	X	-
5	MG	A	1343	-	-	-	X
5	MG	B	1343	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA POLYMERASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	12	1
			2746	1760	475	504	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ARG	LYS	CONFLICT	UNP Q97W02

- Molecule 2 is a protein called DNA POLYMERASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	343	Total	C	N	O	S	0	6	1
			2754	1766	476	505	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	P	0	1	0
			309	147	63	85	14			
3	D	14	Total	C	N	O	P	0	1	0
			309	147	63	85	14			

- Molecule 4 is a DNA chain called 5'-D(*TP*CP*AP*TP*M2GP*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	16	Total	C	N	O	P	0	3	0
			319	155	54	95	15			
4	F	16	Total	C	N	O	P	0	3	0
			319	155	54	95	15			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Mg 2	0	0
5	A	2	Total 2	Mg 2	0	0

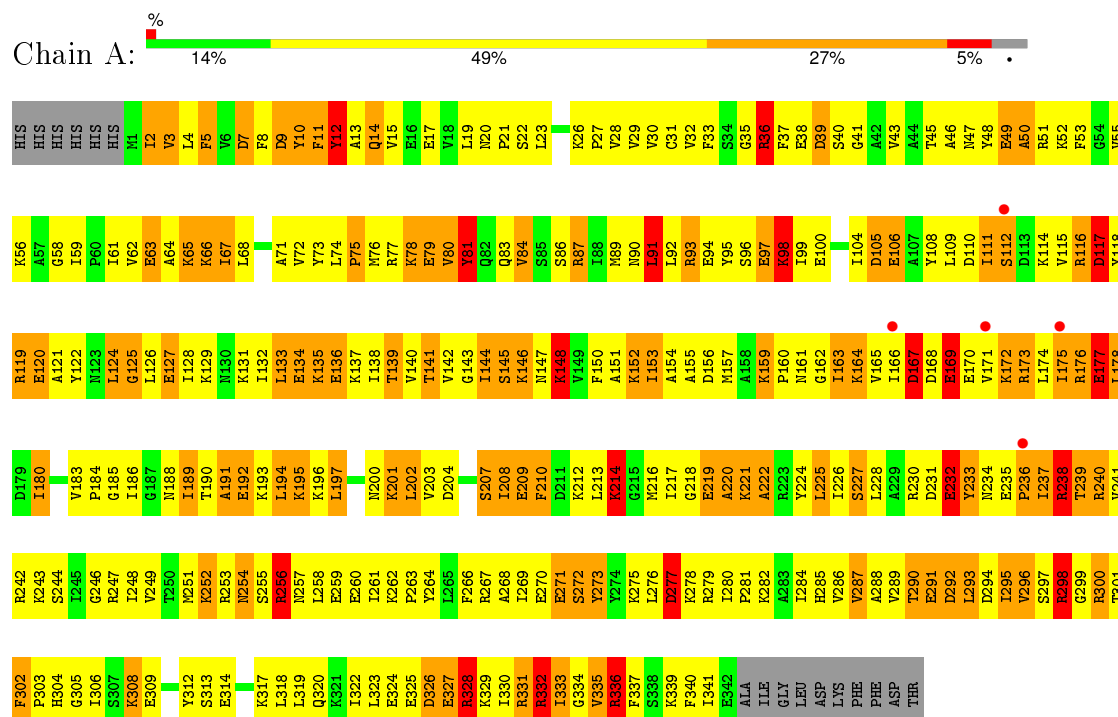
- Molecule 6 is water.

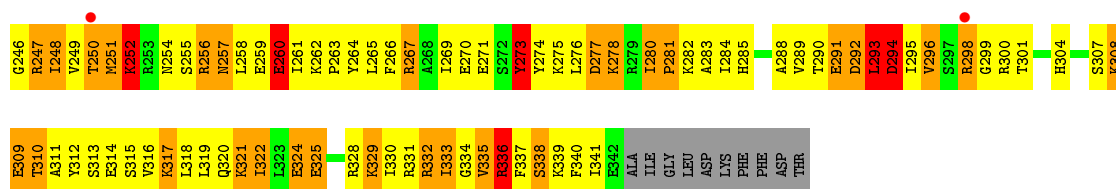
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	87	Total 87	O 87	0	0
6	B	56	Total 56	O 56	0	0
6	C	14	Total 14	O 14	0	0
6	D	20	Total 20	O 20	0	0
6	E	17	Total 17	O 17	0	0
6	F	9	Total 9	O 9	0	0

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: DNA POLYMERASE IV

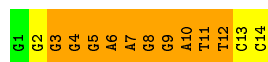




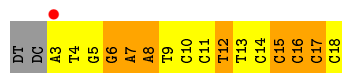
- Molecule 3: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP *TP*TP*CP*DOCP)-3'



- Molecule 3: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP *TP*TP*CP*DOCP)-3'



- Molecule 4: 5'-D(*TP*CP*AP*TP*M2GP*GP*AP*AP*TP*CP*CP *TP*TP*CP*CP*CP*CP*P*C)-3'



- Molecule 4: 5'-D(*TP*CP*AP*TP*M2GP*GP*AP*AP*TP*CP*CP *TP*TP*CP*CP*CP*CP*P*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.79Å 101.78Å 97.27Å 90.00° 91.95° 90.00°	Depositor
Resolution (Å)	28.75 – 2.28 28.75 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.4 (28.75-2.28) 86.5 (28.75-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.24Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.239 , 0.251 0.237 , 0.249	Depositor DCC
R_{free} test set	2231 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.5	EDS
Estimated twinning fraction	0.085 for -h,-l,-k 0.085 for -h,l,k 0.308 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 45673 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6963	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: O2G, MG, DOC

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	1.58	32/2785 (1.1%)	1.57	30/3741 (0.8%)
2	B	1.58	28/2794 (1.0%)	1.59	30/3753 (0.8%)
3	C	2.69	25/308 (8.1%)	2.81	33/476 (6.9%)
3	D	2.45	18/308 (5.8%)	2.43	26/476 (5.5%)
4	E	2.21	16/327 (4.9%)	2.44	23/498 (4.6%)
4	F	2.14	11/327 (3.4%)	2.85	38/498 (7.6%)
All	All	1.76	130/6849 (1.9%)	1.85	180/9442 (1.9%)

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	B	0	1

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	12	TYR	CD2-CE2	-9.92	1.24	1.39
2	B	122	TYR	CD2-CE2	-9.40	1.25	1.39
4	E	11	DC	C2-O2	-9.15	1.16	1.24
3	C	11	DT	C1'-N1	9.07	1.61	1.49
4	E	4[E]	DT	P-OP2	8.89	1.64	1.49
4	F	4[F]	DT	P-OP2	8.62	1.63	1.49
1	A	106	GLU	CB-CG	8.51	1.68	1.52
1	A	106	GLU	CG-CD	8.15	1.64	1.51
3	C	12	DT	C5-C6	-8.12	1.28	1.34
3	C	8	DG	N1-C2	-7.79	1.31	1.37
3	C	12	DT	C4-O4	-7.78	1.16	1.23
1	A	220	ALA	CA-CB	7.78	1.68	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	DG	N9-C4	7.68	1.44	1.38
4	F	12	DT	N1-C2	7.59	1.44	1.38
2	B	55	VAL	CB-CG2	7.45	1.68	1.52
2	B	84	VAL	CB-CG2	7.34	1.68	1.52
3	C	7	DA	C5-C6	7.30	1.47	1.41
3	D	11	DT	C2-O2	-7.28	1.16	1.22
3	C	11	DT	C4-O4	7.27	1.29	1.23
1	A	155	ALA	CA-CB	7.27	1.67	1.52
2	B	63	GLU	CG-CD	7.27	1.62	1.51
2	B	170	GLU	CB-CG	7.25	1.66	1.52
3	D	11	DT	C5-C7	-7.23	1.45	1.50
3	C	8	DG	C6-O6	-7.21	1.17	1.24
3	D	8	DG	C2-N3	7.21	1.38	1.32
3	D	12	DT	C2-O2	-7.20	1.16	1.22
3	D	2	DG	C6-N1	7.04	1.44	1.39
2	B	169	GLU	CG-CD	6.89	1.62	1.51
3	D	13	DC	N1-C2	6.78	1.47	1.40
3	C	8	DG	C5-C6	6.73	1.49	1.42
4	E	13	DT	N1-C6	-6.66	1.33	1.38
2	B	88	ILE	CA-CB	-6.55	1.39	1.54
1	A	79	GLU	CG-CD	6.44	1.61	1.51
3	C	3	DG	N7-C5	6.42	1.43	1.39
3	D	4	DG	N9-C4	6.37	1.43	1.38
4	E	6	DG	C5-C6	-6.35	1.35	1.42
2	B	30	VAL	CA-CB	-6.31	1.41	1.54
2	B	43	VAL	CB-CG2	-6.31	1.39	1.52
4	F	18	DC	C2-N3	6.25	1.40	1.35
3	C	1	DG	C5-C6	-6.23	1.36	1.42
2	B	150	PHE	CB-CG	-6.21	1.40	1.51
1	A	80	VAL	CB-CG2	6.19	1.65	1.52
3	D	3	DG	N1-C2	6.18	1.42	1.37
1	A	277	ASP	CB-CG	6.18	1.64	1.51
2	B	43	VAL	CA-CB	6.17	1.67	1.54
1	A	221	LYS	CB-CG	6.12	1.69	1.52
4	E	10	DC	C2-O2	6.09	1.29	1.24
3	C	3	DG	C2-N2	-6.08	1.28	1.34
3	C	10	DA	N3-C4	6.08	1.38	1.34
2	B	15	VAL	CA-CB	-6.07	1.42	1.54
1	A	84	VAL	CA-CB	-6.06	1.42	1.54
2	B	249	VAL	CA-CB	5.95	1.67	1.54
3	D	6	DA	C5-C6	5.95	1.46	1.41
2	B	107	ALA	CA-CB	-5.91	1.40	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	16	DC	C3'-O3'	-5.88	1.36	1.44
1	A	68	LEU	CG-CD2	5.88	1.73	1.51
3	D	2	DG	N1-C2	5.87	1.42	1.37
3	D	5	DG	C5-C6	5.87	1.48	1.42
4	E	6	DG	N9-C4	-5.80	1.33	1.38
3	C	9	DG	C8-N7	5.78	1.34	1.30
3	D	10	DA	C5-C6	5.77	1.46	1.41
4	E	10	DC	N1-C2	5.75	1.46	1.40
1	A	81	TYR	CD1-CE1	5.72	1.48	1.39
4	F	12	DT	C4-O4	-5.72	1.18	1.23
1	A	134	GLU	CG-CD	5.71	1.60	1.51
4	E	18	DC	C4-C5	-5.71	1.38	1.43
4	E	13	DT	C5-C7	-5.71	1.46	1.50
3	D	3	DG	C6-N1	5.70	1.43	1.39
2	B	224	TYR	CB-CG	5.67	1.60	1.51
3	C	4	DG	P-OP2	5.66	1.58	1.49
4	E	10	DC	C5-C6	-5.66	1.29	1.34
4	E	17	DC	N3-C4	-5.66	1.29	1.33
4	E	9	DT	C5-C7	-5.66	1.46	1.50
4	F	18	DC	N1-C2	-5.66	1.34	1.40
1	A	50	ALA	CA-CB	5.62	1.64	1.52
3	C	3	DG	N9-C4	5.61	1.42	1.38
1	A	169	GLU	CG-CD	5.60	1.60	1.51
3	C	7	DA	N7-C5	5.60	1.42	1.39
4	E	18	DC	N1-C2	-5.58	1.34	1.40
4	F	8	DA	C4'-O4'	5.58	1.50	1.45
1	A	10	TYR	CD2-CE2	-5.57	1.30	1.39
3	D	8	DG	N1-C2	5.55	1.42	1.37
3	D	5	DG	N9-C4	5.55	1.42	1.38
1	A	43	VAL	CB-CG1	5.48	1.64	1.52
1	A	169	GLU	CB-CG	5.47	1.62	1.52
1	A	39	ASP	CA-C	5.46	1.67	1.52
3	D	7	DA	C3'-O3'	5.45	1.51	1.44
2	B	55	VAL	CB-CG1	-5.44	1.41	1.52
3	D	13	DC	C2-N3	5.44	1.40	1.35
1	A	221	LYS	CD-CE	5.43	1.64	1.51
1	A	164	LYS	CD-CE	5.43	1.64	1.51
1	A	2	ILE	N-CA	5.42	1.57	1.46
2	B	233	TYR	CE2-CZ	-5.42	1.31	1.38
1	A	221	LYS	CE-NZ	5.40	1.62	1.49
1	A	80	VAL	CA-CB	-5.37	1.43	1.54
3	C	13	DC	C2-N3	-5.37	1.31	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	DG	C5-C6	-5.36	1.36	1.42
2	B	309	GLU	CG-CD	5.35	1.59	1.51
2	B	30	VAL	CB-CG2	5.34	1.64	1.52
4	F	6	DG	C5-C6	5.34	1.47	1.42
1	A	65	LYS	CE-NZ	5.34	1.62	1.49
1	A	156	ASP	CB-CG	5.33	1.62	1.51
4	F	18	DC	C1'-N1	-5.29	1.39	1.47
1	A	20	ASN	CB-CG	5.28	1.63	1.51
1	A	58	GLY	C-O	5.28	1.32	1.23
1	A	312	TYR	CD2-CE2	-5.28	1.31	1.39
4	F	15	DC	N1-C2	5.27	1.45	1.40
1	A	332	ARG	N-CA	5.26	1.56	1.46
1	A	14	GLN	C-O	-5.25	1.13	1.23
4	F	18	DC	N3-C4	5.24	1.37	1.33
2	B	273	TYR	CB-CG	-5.23	1.43	1.51
3	C	8	DG	C6-N1	-5.22	1.35	1.39
1	A	62	VAL	CB-CG1	5.21	1.63	1.52
3	C	10	DA	N7-C5	5.21	1.42	1.39
2	B	309	GLU	CB-CG	5.17	1.61	1.52
3	C	11	DT	C5-C6	5.14	1.38	1.34
4	E	18	DC	C5-C6	-5.13	1.30	1.34
1	A	106	GLU	CD-OE2	5.13	1.31	1.25
2	B	30	VAL	CB-CG1	-5.12	1.42	1.52
4	E	15	DC	N1-C2	5.10	1.45	1.40
3	D	5	DG	N1-C2	-5.09	1.33	1.37
2	B	141	THR	CA-CB	5.08	1.66	1.53
4	E	6	DG	C5-C4	-5.08	1.34	1.38
3	C	3	DG	C5-C6	5.06	1.47	1.42
2	B	10	TYR	CB-CG	-5.06	1.44	1.51
2	B	11	PHE	CD1-CE1	5.03	1.49	1.39
3	C	1	DG	N9-C4	-5.03	1.33	1.38
3	C	2	DG	P-OP2	5.03	1.57	1.49
2	B	38	GLU	CB-CG	5.01	1.61	1.52
2	B	29	VAL	CB-CG1	-5.01	1.42	1.52

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	DG	O4'-C1'-N9	15.90	119.13	108.00
4	F	13	DT	O4'-C1'-N1	-15.62	97.06	108.00
4	F	10	DC	O5'-P-OP1	-13.78	93.30	105.70
4	F	12	DT	O4'-C1'-N1	13.55	117.48	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	336	ARG	NE-CZ-NH1	-11.01	114.80	120.30
3	C	11	DT	O4'-C1'-N1	10.71	115.50	108.00
4	E	13	DT	C6-C5-C7	-10.70	116.48	122.90
4	F	11	DC	O5'-P-OP2	-10.40	96.34	105.70
3	C	8	DG	N1-C6-O6	-10.29	113.72	119.90
3	C	4	DG	O4'-C1'-N9	10.21	115.14	108.00
4	E	7	DA	O4'-C1'-C2'	-10.08	97.84	105.90
2	B	7	ASP	CB-CG-OD2	9.27	126.64	118.30
4	E	15	DC	N1-C2-O2	9.24	124.44	118.90
3	C	11	DT	C2-N3-C4	9.07	132.64	127.20
4	E	6	DG	O4'-C1'-N9	8.82	114.18	108.00
4	F	8	DA	O4'-C1'-N9	8.71	114.10	108.00
4	E	8	DA	O4'-C1'-N9	8.62	114.03	108.00
3	D	12	DT	O5'-P-OP1	-8.57	97.99	105.70
2	B	176	ARG	NE-CZ-NH1	8.34	124.47	120.30
3	C	10	DA	O4'-C1'-N9	8.33	113.83	108.00
1	A	91	LEU	CA-CB-CG	8.29	134.37	115.30
3	C	12	DT	C6-C5-C7	-8.22	117.97	122.90
4	F	11	DC	P-O3'-C3'	8.04	129.35	119.70
3	C	11	DT	C6-N1-C2	-8.00	117.30	121.30
4	F	9	DT	C5-C4-O4	-7.96	119.33	124.90
1	A	87	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	A	202	LEU	CB-CG-CD1	-7.92	97.54	111.00
3	C	12	DT	C4-C5-C7	7.90	123.74	119.00
2	B	182	ASP	CB-CG-OD2	7.77	125.30	118.30
1	A	142	VAL	CB-CA-C	-7.74	96.70	111.40
3	C	11	DT	C5-C6-N1	7.74	128.34	123.70
1	A	9	ASP	CB-CG-OD1	7.63	125.17	118.30
4	E	15	DC	C3'-C2'-C1'	-7.55	93.44	102.50
4	F	9	DT	C4-C5-C7	-7.53	114.48	119.00
3	D	6	DA	O4'-C1'-C2'	-7.52	99.89	105.90
4	F	15	DC	O4'-C1'-C2'	-7.46	99.93	105.90
2	B	322	ILE	CB-CA-C	-7.35	96.91	111.60
1	A	298	ARG	NE-CZ-NH1	-7.34	116.63	120.30
4	E	13	DT	C4-C5-C7	7.33	123.40	119.00
2	B	72	VAL	CB-CA-C	-7.29	97.55	111.40
4	F	8	DA	O4'-C1'-C2'	-7.23	100.12	105.90
4	E	7	DA	P-O3'-C3'	-7.22	111.04	119.70
3	D	9	DG	O4'-C1'-N9	7.21	113.05	108.00
3	D	6	DA	O4'-C1'-N9	-7.20	102.96	108.00
1	A	68	LEU	CB-CG-CD1	-7.19	98.78	111.00
4	F	9	DT	C2-N3-C4	-7.18	122.89	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	LEU	CA-CB-CG	7.17	131.78	115.30
3	D	4	DG	O4'-C1'-N9	7.15	113.00	108.00
1	A	331	ARG	NE-CZ-NH2	-7.13	116.74	120.30
2	B	230	ARG	NE-CZ-NH2	-7.11	116.75	120.30
4	F	18	DC	C1'-O4'-C4'	-7.10	103.00	110.10
4	F	6	DG	O5'-P-OP1	-7.10	99.31	105.70
4	F	10	DC	C4'-C3'-C2'	-7.09	96.72	103.10
3	D	2	DG	C1'-O4'-C4'	-7.08	103.02	110.10
4	E	8	DA	P-O5'-C5'	-7.03	109.65	120.90
2	B	143	GLY	N-CA-C	-7.00	95.61	113.10
4	F	11	DC	O5'-P-OP1	6.90	118.98	110.70
4	F	15	DC	O4'-C1'-N1	6.88	112.82	108.00
4	E	12	DT	P-O5'-C5'	-6.75	110.10	120.90
4	F	6	DG	O4'-C1'-C2'	-6.73	100.52	105.90
4	F	18	DC	O4'-C1'-N1	-6.72	103.30	108.00
1	A	256	ARG	NE-CZ-NH2	-6.71	116.94	120.30
3	C	10	DA	O5'-P-OP1	6.54	118.55	110.70
3	C	8	DG	C4-C5-C6	-6.54	114.88	118.80
3	D	5	DG	O4'-C1'-N9	6.51	112.56	108.00
4	E	7	DA	O5'-P-OP1	-6.45	99.90	105.70
4	F	8	DA	C3'-C2'-C1'	6.44	110.23	102.50
3	D	9	DG	O4'-C1'-C2'	6.42	111.03	105.90
4	E	16	DC	O4'-C1'-N1	-6.41	103.52	108.00
4	E	18	DC	P-O5'-C5'	-6.41	110.65	120.90
3	C	7	DA	N1-C6-N6	-6.38	114.77	118.60
1	A	84	VAL	CB-CA-C	-6.38	99.29	111.40
1	A	256	ARG	NE-CZ-NH1	6.37	123.49	120.30
3	D	12	DT	OP1-P-OP2	6.34	129.10	119.60
2	B	178	LEU	CB-CG-CD1	6.31	121.73	111.00
2	B	133	LEU	CB-CG-CD2	-6.31	100.28	111.00
3	C	10	DA	C4-C5-C6	-6.29	113.86	117.00
4	F	17	DC	O4'-C1'-N1	6.29	112.40	108.00
1	A	125	GLY	N-CA-C	-6.28	97.39	113.10
2	B	186	ILE	CB-CA-C	-6.28	99.04	111.60
3	C	11	DT	N1-C2-O2	6.26	128.11	123.10
3	D	9	DG	O5'-P-OP2	-6.26	100.07	105.70
3	D	11	DT	N3-C4-O4	6.25	123.65	119.90
3	C	9	DG	C5-C6-O6	6.18	132.31	128.60
2	B	125	GLY	N-CA-C	-6.13	97.77	113.10
4	F	10	DC	C1'-O4'-C4'	-6.11	103.99	110.10
3	D	2	DG	N1-C6-O6	6.11	123.56	119.90
1	A	189	ILE	CB-CA-C	-6.10	99.39	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	DG	N3-C2-N2	-6.10	115.63	119.90
2	B	197	LEU	CA-CB-CG	6.10	129.32	115.30
1	A	67	ILE	CG1-CB-CG2	6.08	124.78	111.40
3	C	8	DG	C6-C5-N7	6.08	134.05	130.40
3	C	11	DT	N3-C2-O2	-6.07	118.66	122.30
1	A	225	LEU	CB-CG-CD2	6.07	121.32	111.00
2	B	7	ASP	CB-CG-OD1	-6.07	112.83	118.30
4	E	13	DT	C4'-C3'-O3'	-6.05	94.57	109.70
2	B	88	ILE	CB-CA-C	-6.04	99.52	111.60
3	D	2	DG	N1-C2-N2	6.04	121.64	116.20
4	F	6	DG	O4'-C1'-N9	-6.04	103.78	108.00
4	E	15	DC	O4'-C4'-C3'	-6.03	102.09	104.50
2	B	335	VAL	CB-CA-C	-6.02	99.97	111.40
4	F	11	DC	O3'-P-O5'	6.01	115.43	104.00
1	A	225	LEU	CA-CB-CG	6.01	129.12	115.30
3	D	11	DT	C2-N3-C4	-6.01	123.59	127.20
3	C	1	DG	C5-C6-O6	-6.00	125.00	128.60
3	C	8	DG	C5-C6-O6	5.98	132.19	128.60
4	F	18	DC	N3-C2-O2	5.98	126.09	121.90
3	D	2	DG	C5-C6-O6	-5.97	125.02	128.60
3	C	1	DG	N1-C6-O6	5.96	123.48	119.90
2	B	252	LYS	N-CA-C	-5.96	94.90	111.00
1	A	336	ARG	CG-CD-NE	-5.95	99.31	111.80
1	A	36	ARG	NE-CZ-NH2	-5.89	117.35	120.30
2	B	20	ASN	C-N-CD	5.81	140.61	128.40
4	F	12	DT	C5-C4-O4	-5.79	120.85	124.90
3	D	8	DG	C4'-C3'-C2'	-5.78	97.90	103.10
4	E	7	DA	C3'-C2'-C1'	-5.75	95.59	102.50
4	F	7	DA	O4'-C1'-N9	-5.75	103.98	108.00
4	F	9	DT	N3-C4-O4	5.71	123.33	119.90
4	E	6	DG	C5-C6-O6	-5.71	125.17	128.60
4	F	14	DC	N1-C2-O2	-5.71	115.47	118.90
3	C	6	DA	O4'-C1'-N9	5.69	111.98	108.00
3	C	5	DG	C8-N9-C4	-5.66	104.14	106.40
3	D	11	DT	C5-C4-O4	-5.66	120.94	124.90
4	F	8	DA	N9-C1'-C2'	-5.62	101.92	112.60
3	D	11	DT	N1-C2-N3	5.58	117.95	114.60
1	A	287	VAL	CB-CA-C	-5.55	100.85	111.40
3	C	10	DA	N1-C2-N3	-5.55	126.53	129.30
2	B	280	ILE	C-N-CD	5.53	140.01	128.40
4	F	13	DT	N1-C1'-C2'	5.52	123.08	112.60
3	C	13	DC	N3-C4-N4	-5.50	114.15	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	DG	O4'-C1'-N9	5.50	111.85	108.00
3	C	11	DT	P-O5'-C5'	-5.50	112.11	120.90
3	D	4	DG	O5'-P-OP2	-5.49	100.76	105.70
4	E	8	DA	OP1-P-O3'	5.48	117.25	105.20
1	A	178	LEU	CA-CB-CG	-5.47	102.73	115.30
1	A	336	ARG	CB-CA-C	-5.46	99.47	110.40
3	C	9	DG	O4'-C1'-N9	5.44	111.81	108.00
3	C	11	DT	N3-C4-C5	-5.43	111.94	115.20
4	F	12	DT	C2-N3-C4	-5.42	123.95	127.20
1	A	313	SER	N-CA-C	5.41	125.61	111.00
1	A	141	THR	CB-CA-C	-5.38	97.08	111.60
2	B	310	THR	CA-CB-CG2	-5.37	104.88	112.40
3	C	7	DA	C5-C6-N6	5.37	128.00	123.70
3	C	2	DG	C1'-O4'-C4'	-5.36	104.74	110.10
4	F	7	DA	O5'-P-OP2	5.36	117.13	110.70
4	F	6	DG	OP1-P-O3'	5.36	116.98	105.20
4	F	9	DT	C5-C6-N1	-5.32	120.51	123.70
1	A	254	ASN	N-CA-C	-5.31	96.67	111.00
2	B	6	VAL	CB-CA-C	-5.29	101.35	111.40
4	E	13	DT	N3-C4-C5	-5.28	112.03	115.20
2	B	157	MET	CB-CG-SD	-5.22	96.74	112.40
4	F	16	DC	O4'-C1'-C2'	-5.22	101.72	105.90
2	B	202	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	A	300	ARG	CG-CD-NE	-5.20	100.89	111.80
3	D	7	DA	N9-C1'-C2'	5.18	122.45	112.60
2	B	119	ARG	NE-CZ-NH2	-5.17	117.71	120.30
3	C	8	DG	C5-C6-N1	5.17	114.08	111.50
2	B	66	LYS	CA-CB-CG	5.16	124.76	113.40
3	D	5	DG	N1-C6-O6	-5.16	116.81	119.90
4	F	14	DC	N3-C2-O2	5.16	125.51	121.90
1	A	12	TYR	CB-CA-C	-5.14	100.12	110.40
2	B	201	LYS	CD-CE-NZ	-5.13	99.89	111.70
4	F	18	DC	C6-N1-C2	5.13	122.35	120.30
4	E	16	DC	O4'-C1'-C2'	5.12	109.99	105.90
2	B	187	GLY	N-CA-C	5.12	125.89	113.10
3	D	11	DT	C5-C6-N1	-5.11	120.64	123.70
1	A	164	LYS	CD-CE-NZ	5.09	123.41	111.70
4	E	16	DC	C5'-C4'-O4'	-5.09	99.64	109.30
1	A	194	LEU	CA-CB-CG	5.08	126.99	115.30
2	B	190	THR	CA-CB-CG2	-5.08	105.29	112.40
1	A	279	ARG	NE-CZ-NH2	5.07	122.83	120.30
4	E	15	DC	C6-N1-C1'	-5.06	114.72	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	7	DA	O4'-C1'-C2'	5.06	109.95	105.90
2	B	4	LEU	CA-CB-CG	5.05	126.91	115.30
4	F	17	DC	C4'-C3'-C2'	-5.04	98.56	103.10
3	D	13	DC	C2-N1-C1'	5.04	124.34	118.80
1	A	98	LYS	CD-CE-NZ	5.03	123.28	111.70
3	C	10	DA	P-O5'-C5'	-5.03	112.85	120.90
4	E	7	DA	C5-C6-N6	5.03	127.72	123.70
3	D	3	DG	C3'-C2'-C1'	5.02	108.52	102.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	238	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2746	0	2872	446	0
2	B	2754	0	2880	407	0
3	C	309	0	167	28	0
3	D	309	0	170	25	0
4	E	319	0	181	33	0
4	F	319	0	181	37	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	87	0	0	21	0
6	B	56	0	0	14	0
6	C	14	0	0	2	0
6	D	20	0	0	5	0
6	E	17	0	0	0	0
6	F	9	0	0	4	0
All	All	6963	0	6451	928	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 71.

All (928) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:2010:HOH:O	3:D:14[A]:DOC:H3'2	1.28	1.27
1:A:144:ILE:HA	6:A:2001:HOH:O	1.28	1.25
1:A:115[A]:VAL:HG11	1:A:120:GLU:O	1.33	1.25
1:A:109:LEU:HA	6:A:2038:HOH:O	1.37	1.24
1:A:298:ARG:HH11	1:A:298:ARG:CG	1.49	1.23
2:B:159:LYS:HE3	6:B:2001:HOH:O	1.36	1.20
2:B:78:LYS:HA	2:B:81:TYR:CD2	1.76	1.20
1:A:93:ARG:NH1	1:A:93:ARG:HB2	1.60	1.16
2:B:114:LYS:H	2:B:114:LYS:HD2	1.07	1.15
1:A:48:TYR:CZ	1:A:160:PRO:HG3	1.84	1.13
2:B:164:LYS:HE3	2:B:165:VAL:H	1.15	1.12
2:B:298:ARG:HD3	2:B:322:ILE:HG12	1.26	1.12
2:B:250:THR:HA	2:B:332:ARG:HB3	1.21	1.11
2:B:332:ARG:NH1	4:F:5[F]:O2G:H2'A	1.64	1.10
1:A:298:ARG:HG2	1:A:298:ARG:HH11	1.02	1.09
1:A:93:ARG:HH11	1:A:93:ARG:HB2	1.02	1.09
2:B:78:LYS:HA	2:B:81:TYR:HD2	1.09	1.08
2:B:195[B]:LYS:C	2:B:198:GLY:H	1.56	1.08
1:A:288:ALA:HB1	1:A:330:ILE:CG2	1.84	1.06
2:B:164:LYS:HE3	2:B:165:VAL:N	1.70	1.05
1:A:248:ILE:HG22	1:A:334:GLY:HA3	1.37	1.04
2:B:332:ARG:HH12	4:F:5[F]:O2G:H2'A	0.91	1.02
1:A:10:TYR:HD1	1:A:13:ALA:HB3	1.20	1.02
2:B:62:VAL:O	2:B:66:LYS:HB3	1.56	1.02
1:A:238:ARG:HD3	1:A:239:THR:N	1.74	1.01
2:B:208:ILE:HG23	2:B:209:GLU:H	1.25	1.01
2:B:164:LYS:CE	2:B:165:VAL:H	1.73	1.01
1:A:197:LEU:CD1	1:A:212:LYS:HZ1	1.73	1.00
1:A:78:LYS:HB3	1:A:79:GLU:OE2	1.61	1.00
2:B:23:LEU:HA	2:B:26:LYS:HE3	1.41	0.99
1:A:176:ARG:O	1:A:177:GLU:HB2	1.61	0.99
2:B:298:ARG:CD	2:B:322:ILE:HG12	1.92	0.99
1:A:298:ARG:HG2	1:A:298:ARG:NH1	1.67	0.99
1:A:28:VAL:N	1:A:47:ASN:HD21	1.61	0.98
2:B:210:PHE:HE1	2:B:214:LYS:HB2	1.23	0.98
2:B:0:HIS:CD2	2:B:2:ILE:HD11	1.99	0.97
2:B:210:PHE:CE1	2:B:214:LYS:HB2	2.00	0.97
2:B:289:VAL:HA	2:B:294:ASP:O	1.65	0.96
2:B:298:ARG:HG2	2:B:298:ARG:HH11	1.29	0.96
2:B:133:LEU:O	2:B:137:LYS:N	1.98	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:DC:H5'	3:C:14[B]:DOC:H5	1.46	0.95
2:B:79:GLU:O	2:B:83:GLN:HB2	1.66	0.95
3:C:14[A]:DOC:OP2	6:C:2014:HOH:O	1.83	0.94
1:A:210:PHE:O	1:A:210:PHE:HD2	1.50	0.94
2:B:322:ILE:O	2:B:322:ILE:HG22	1.68	0.93
1:A:228:LEU:HD23	1:A:233:TYR:HB2	1.49	0.93
1:A:197:LEU:HD13	1:A:212:LYS:NZ	1.83	0.93
1:A:144:ILE:HG12	1:A:164:LYS:O	1.68	0.93
2:B:114:LYS:N	2:B:114:LYS:HD2	1.80	0.92
1:A:298:ARG:HG3	1:A:322:ILE:HG12	1.49	0.92
1:A:238:ARG:HG2	1:A:238:ARG:HH11	1.31	0.92
1:A:7:ASP:OD2	1:A:8:PHE:N	2.01	0.92
4:E:6:DG:H2''	4:E:7:DA:C8	2.03	0.92
2:B:228:LEU:HD21	2:B:233:TYR:CD1	2.04	0.92
2:B:141:THR:HG23	2:B:162:GLY:H	1.34	0.92
1:A:256:ARG:HG2	1:A:256:ARG:HH11	1.30	0.92
2:B:141:THR:HG23	2:B:162:GLY:N	1.84	0.91
1:A:197:LEU:CD1	1:A:212:LYS:NZ	2.32	0.91
1:A:336:ARG:HH22	4:E:7:DA:H2''	1.35	0.91
1:A:100:GLU:HB2	1:A:237:ILE:HG23	1.53	0.91
1:A:238:ARG:HD3	1:A:239:THR:H	1.32	0.90
1:A:288:ALA:HB1	1:A:330:ILE:HG23	1.50	0.90
2:B:195[B]:LYS:CA	2:B:198:GLY:H	1.84	0.90
2:B:126:LEU:O	2:B:130:ASN:HB2	1.72	0.90
1:A:124:LEU:HA	1:A:127:GLU:HB2	1.53	0.90
1:A:127:GLU:OE1	1:A:128:ILE:N	2.04	0.90
2:B:224:TYR:CE1	2:B:228:LEU:HD11	2.07	0.89
2:B:63:GLU:O	2:B:67:ILE:HG13	1.72	0.89
2:B:210:PHE:O	2:B:210:PHE:CD1	2.26	0.89
2:B:324:GLU:C	2:B:325:GLU:OE1	2.11	0.89
2:B:301:THR:O	2:B:301:THR:HG22	1.70	0.89
2:B:181:ALA:HA	2:B:186:ILE:HG21	1.52	0.88
1:A:200:ASN:C	1:A:201:LYS:HD2	1.93	0.88
1:A:91:LEU:O	1:A:94:GLU:HB3	1.72	0.88
2:B:88:ILE:O	2:B:88:ILE:HG22	1.72	0.88
2:B:167:ASP:O	2:B:171:VAL:HG23	1.72	0.88
2:B:23:LEU:HA	2:B:26:LYS:CE	2.03	0.87
1:A:336:ARG:HH22	4:E:7:DA:C2'	1.88	0.87
2:B:32:VAL:CG1	4:F:6:DG:H5''	2.03	0.87
2:B:194:LEU:O	2:B:195[B]:LYS:HD2	1.75	0.87
1:A:221:LYS:O	1:A:224:TYR:HB3	1.74	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ILE:O	2:B:59:ILE:HD12	1.75	0.87
1:A:284:ILE:HG12	1:A:285:HIS:H	1.39	0.86
2:B:332:ARG:HH12	4:F:5[F]:O2G:C2'	1.85	0.86
2:B:250:THR:CA	2:B:332:ARG:HB3	2.05	0.85
2:B:208:ILE:CG2	2:B:209:GLU:N	2.37	0.85
3:D:5:DG:H2"	3:D:6:DA:C8	2.12	0.85
2:B:111:ILE:O	2:B:111:ILE:HG12	1.77	0.85
1:A:288:ALA:HB1	1:A:330:ILE:HG21	1.60	0.84
2:B:174:LEU:HB3	2:B:178:LEU:HB2	1.59	0.84
1:A:147:ASN:HB2	6:A:2049:HOH:O	1.76	0.84
1:A:327:GLU:OE1	1:A:327:GLU:N	2.11	0.84
2:B:228:LEU:HD23	2:B:233:TYR:HB2	1.60	0.84
2:B:99:ILE:O	2:B:99:ILE:HG23	1.77	0.84
1:A:10:TYR:CD1	1:A:13:ALA:HB3	2.11	0.84
2:B:208:ILE:CG2	2:B:209:GLU:H	1.91	0.83
2:B:180:ILE:HG22	2:B:181:ALA:N	1.89	0.83
1:A:297:SER:O	1:A:298:ARG:HG2	1.79	0.83
3:C:13:DC:H5'	3:C:14[B]:DOC:C5	2.09	0.83
2:B:43:VAL:HG12	2:B:57:ALA:HA	1.60	0.83
2:B:117:ASP:HB3	2:B:120:GLU:HG3	1.61	0.83
1:A:197:LEU:HD13	1:A:212:LYS:HZ1	1.42	0.82
1:A:208:ILE:HG22	1:A:209:GLU:O	1.79	0.82
1:A:200:ASN:O	1:A:201:LYS:HD2	1.80	0.82
2:B:79:GLU:N	2:B:79:GLU:OE1	2.11	0.82
1:A:285:HIS:CD2	1:A:299:GLY:HA3	2.14	0.82
2:B:192:GLU:O	2:B:195[B]:LYS:HG2	1.79	0.82
2:B:289:VAL:HG21	2:B:332:ARG:HD2	1.62	0.82
2:B:251:MET:HB3	2:B:264:TYR:CE2	2.15	0.81
2:B:231:ASP:OD1	2:B:231:ASP:O	1.97	0.81
1:A:227:SER:HA	1:A:230:ARG:HD2	1.62	0.81
2:B:266:PHE:HA	2:B:269:ILE:HD12	1.62	0.81
2:B:267:ARG:HH11	2:B:267:ARG:HB2	1.45	0.81
1:A:164:LYS:HZ3	1:A:166:ILE:HD11	1.42	0.81
2:B:55:VAL:HG21	2:B:68:LEU:HD12	1.63	0.81
1:A:280:ILE:CG2	1:A:305:GLY:HA3	2.10	0.81
2:B:250:THR:HA	2:B:332:ARG:CB	2.09	0.80
1:A:210:PHE:CD2	1:A:210:PHE:O	2.34	0.80
1:A:284:ILE:HG12	1:A:285:HIS:N	1.94	0.80
2:B:0:HIS:NE2	2:B:2:ILE:HD11	1.97	0.80
1:A:290:THR:HG21	1:A:328:ARG:HH22	1.47	0.80
1:A:79:GLU:CD	1:A:79:GLU:H	1.85	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:THR:O	2:B:292:ASP:O	2.00	0.80
1:A:186:ILE:HD11	1:A:225:LEU:HD21	1.64	0.80
1:A:280:ILE:HG22	1:A:305:GLY:HA3	1.64	0.80
2:B:195[B]:LYS:O	2:B:198:GLY:N	2.16	0.79
2:B:23:LEU:O	2:B:26:LYS:HB2	1.83	0.79
1:A:285:HIS:CD2	1:A:299:GLY:CA	2.65	0.79
2:B:332:ARG:HH11	4:F:5[F]:O2G:P	2.06	0.79
2:B:136:GLU:HA	2:B:136:GLU:OE1	1.82	0.79
2:B:91:LEU:HD23	2:B:91:LEU:O	1.84	0.78
2:B:189:ILE:O	2:B:193:LYS:HG3	1.83	0.78
2:B:137:LYS:O	2:B:138:ILE:HG13	1.82	0.78
1:A:257:ASN:O	1:A:261:ILE:HG13	1.83	0.78
2:B:195[B]:LYS:C	2:B:198:GLY:N	2.36	0.77
2:B:88:ILE:O	2:B:88:ILE:CG2	2.32	0.77
2:B:248:ILE:H	2:B:248:ILE:CD1	1.97	0.77
1:A:285:HIS:NE2	1:A:299:GLY:HA3	2.00	0.77
1:A:298:ARG:NH1	1:A:298:ARG:CG	2.25	0.77
2:B:0:HIS:CD2	2:B:2:ILE:CD1	2.68	0.77
2:B:235:GLU:HG3	2:B:236:PRO:HD2	1.67	0.77
2:B:208:ILE:HG23	2:B:209:GLU:N	1.98	0.76
2:B:248:ILE:HA	2:B:334:GLY:HA3	1.65	0.76
1:A:290:THR:HG21	1:A:328:ARG:NH2	1.99	0.76
1:A:48:TYR:OH	1:A:160:PRO:HG3	1.85	0.76
2:B:257[B]:ASN:HB3	2:B:260:GLU:HB2	1.67	0.76
2:B:166:ILE:HG22	2:B:171:VAL:HG22	1.67	0.76
1:A:100:GLU:HB2	1:A:237:ILE:CG2	2.16	0.76
2:B:106:GLU:OE2	3:D:14[B]:DOC:OP2	2.04	0.76
3:C:13:DC:H4'	3:C:14[B]:DOC:H5'	1.67	0.76
2:B:99:ILE:O	2:B:99:ILE:CG2	2.34	0.75
2:B:195[B]:LYS:CA	2:B:198:GLY:N	2.49	0.75
3:D:5:DG:H1	4:F:14:DC:H42	1.35	0.75
3:D:14[A]:DOC:OP1	6:D:2016:HOH:O	2.02	0.75
1:A:170:GLU:HA	1:A:173:ARG:HB3	1.68	0.75
1:A:28:VAL:H	1:A:47:ASN:HD21	1.33	0.75
1:A:5:PHE:HZ	1:A:106:GLU:HG2	1.51	0.75
1:A:269:ILE:O	1:A:273:TYR:HB2	1.86	0.75
2:B:186:ILE:O	2:B:186:ILE:HG22	1.85	0.75
1:A:256:ARG:HG2	1:A:256:ARG:NH1	2.02	0.74
1:A:144:ILE:HG13	1:A:165:VAL:HG12	1.69	0.74
2:B:195[B]:LYS:CA	2:B:198:GLY:HA2	2.16	0.74
2:B:124:LEU:O	2:B:128:ILE:HG13	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.70	0.74
1:A:153:ILE:O	1:A:157:MET:HG2	1.87	0.74
4:E:6:DG:H2''	4:E:7:DA:H8	1.53	0.73
1:A:29:VAL:HG21	1:A:73:TYR:CE2	2.22	0.73
2:B:248:ILE:N	2:B:248:ILE:HD12	2.03	0.73
2:B:317:LYS:H	2:B:317:LYS:HD3	1.53	0.73
3:C:14[A]:DOC:O5'	6:C:2012:HOH:O	2.06	0.73
2:B:176:ARG:HA	2:B:203:VAL:CG1	2.18	0.73
1:A:290:THR:HG23	1:A:294:ASP:O	1.88	0.73
2:B:32:VAL:HG11	4:F:6:DG:H5''	1.71	0.73
1:A:175:ILE:HD12	1:A:202:LEU:HD13	1.71	0.73
1:A:291:GLU:HB2	1:A:329:LYS:O	1.88	0.72
1:A:148:LYS:HG2	6:A:2049:HOH:O	1.89	0.72
2:B:256:ARG:HG2	2:B:329:LYS:HA	1.71	0.72
2:B:141:THR:CG2	2:B:162:GLY:H	2.02	0.72
2:B:248:ILE:N	2:B:248:ILE:CD1	2.52	0.72
1:A:127:GLU:OE1	1:A:128:ILE:HA	1.90	0.72
2:B:228:LEU:HD23	2:B:233:TYR:CB	2.19	0.71
1:A:280:ILE:O	1:A:340:PHE:HA	1.90	0.71
1:A:298:ARG:HH11	1:A:298:ARG:HG3	1.54	0.71
2:B:180:ILE:CG2	2:B:181:ALA:N	2.54	0.71
1:A:292[A]:ASP:OD1	1:A:328:ARG:HG2	1.89	0.71
1:A:336:ARG:NH2	4:E:7:DA:H2''	2.04	0.71
4:F:6:DG:H1'	4:F:7:DA:H5'	1.72	0.71
1:A:115[A]:VAL:HG11	1:A:120:GLU:C	2.12	0.71
1:A:334:GLY:O	1:A:335:VAL:HG12	1.91	0.71
1:A:127:GLU:OE1	1:A:127:GLU:C	2.28	0.70
1:A:164:LYS:NZ	1:A:166:ILE:HD11	2.06	0.70
1:A:93:ARG:NH1	1:A:93:ARG:CB	2.47	0.70
3:C:5:DG:N2	4:E:14:DC:O2	2.24	0.70
1:A:256:ARG:NH2	1:A:327:GLU:HA	2.06	0.70
1:A:219:GLU:HA	1:A:222:ALA:HB3	1.74	0.70
4:F:3[F]:DA:H2''	4:F:4[F]:DT:OP2	1.91	0.70
2:B:267:ARG:NH1	2:B:267:ARG:HB2	2.05	0.70
1:A:108:TYR:OH	1:A:152:LYS:HD2	1.92	0.70
2:B:282:LYS:HD3	2:B:341:ILE:HG12	1.74	0.70
1:A:247:ARG:NH1	4:E:7:DA:OP2	2.23	0.70
1:A:320:GLN:O	1:A:323:LEU:N	2.25	0.69
1:A:238:ARG:NH1	1:A:238:ARG:HG2	2.04	0.69
3:C:13:DC:H4'	3:C:14[B]:DOC:H6	1.72	0.69
1:A:228:LEU:CD2	1:A:233:TYR:HB2	2.23	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LYS:HD3	2:B:341:ILE:CG1	2.23	0.69
2:B:267:ARG:CB	2:B:267:ARG:NH1	2.55	0.69
2:B:319:LEU:HD12	2:B:319:LEU:O	1.92	0.69
2:B:282:LYS:HG3	2:B:339:LYS:O	1.93	0.69
1:A:27:PRO:HA	1:A:49:GLU:HB2	1.75	0.69
2:B:333:ILE:HG13	2:B:334:GLY:N	2.07	0.69
1:A:4:LEU:HA	6:A:2001:HOH:O	1.93	0.68
1:A:41:GLY:HA3	1:A:61:ILE:HD12	1.75	0.68
3:D:5:DG:H2"	3:D:6:DA:H8	1.58	0.68
2:B:267:ARG:CB	2:B:267:ARG:HH11	2.06	0.68
1:A:197:LEU:HD23	1:A:216:MET:HG2	1.74	0.68
2:B:115:VAL:O	2:B:115:VAL:HG12	1.93	0.68
2:B:209:GLU:C	2:B:213:LEU:HD12	2.13	0.68
2:B:23:LEU:HD22	2:B:72:VAL:HG21	1.76	0.68
2:B:77:ARG:C	2:B:81:TYR:CE2	2.67	0.68
1:A:248:ILE:CG2	1:A:334:GLY:HA3	2.18	0.68
2:B:332:ARG:NH1	4:F:5[F]:O2G:C2'	2.51	0.67
1:A:289:VAL:HG12	1:A:289:VAL:O	1.94	0.67
2:B:317:LYS:CD	2:B:317:LYS:H	2.06	0.67
2:B:41:GLY:HA2	4:F:5[F]:O2G:H5'	1.74	0.67
1:A:127:GLU:OE1	1:A:128:ILE:CA	2.43	0.67
1:A:124:LEU:O	1:A:127:GLU:HB3	1.94	0.67
1:A:246:GLY:HA2	1:A:335:VAL:O	1.95	0.67
2:B:240:ARG:NH2	3:D:14[B]:DOC:O2	2.28	0.67
1:A:285:HIS:HA	1:A:299:GLY:HA2	1.75	0.67
2:B:176:ARG:HA	2:B:203:VAL:HG11	1.76	0.67
2:B:124:LEU:O	2:B:124:LEU:HD12	1.95	0.66
2:B:304:HIS:HB3	6:B:2050:HOH:O	1.94	0.66
1:A:12:TYR:HD2	1:A:45:THR:HG1	1.41	0.66
1:A:290:THR:CG2	1:A:328:ARG:NH2	2.58	0.66
3:C:8:DG:H2"	3:C:9:DG:OP1	1.95	0.66
1:A:258:LEU:HD21	1:A:323:LEU:HD13	1.78	0.66
4:F:5[F]:O2G:H8	4:F:5[F]:O2G:P	2.36	0.66
1:A:115[A]:VAL:HG13	1:A:120:GLU:HB3	1.77	0.66
2:B:195[B]:LYS:CA	2:B:198:GLY:CA	2.74	0.66
2:B:78:LYS:CA	2:B:81:TYR:CD2	2.68	0.66
2:B:181:ALA:HA	2:B:186:ILE:CG2	2.24	0.66
2:B:273:TYR:HE2	6:B:2051:HOH:O	1.79	0.66
2:B:208:ILE:HG22	2:B:213:LEU:HD11	1.77	0.66
1:A:324:GLU:C	1:A:326:ASP:H	1.99	0.66
1:A:291:GLU:O	1:A:293:LEU:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:GLU:C	2:B:261:ILE:H	1.98	0.65
2:B:336:ARG:HB3	2:B:336:ARG:NH1	2.10	0.65
1:A:271:GLU:O	1:A:275:LYS:HG3	1.96	0.65
1:A:172:LYS:O	1:A:174:LEU:N	2.28	0.65
1:A:251:MET:HE2	1:A:253:ARG:O	1.96	0.65
2:B:281:PRO:CB	2:B:337:PHE:HB3	2.26	0.65
1:A:256:ARG:CZ	1:A:327:GLU:HA	2.27	0.65
2:B:59:ILE:HD11	2:B:64:ALA:HB2	1.77	0.65
1:A:293:LEU:HD13	1:A:293:LEU:O	1.96	0.65
2:B:0:HIS:HD2	2:B:2:ILE:CD1	2.10	0.65
1:A:282:LYS:HB2	1:A:339:LYS:O	1.96	0.65
2:B:280:ILE:HD12	2:B:280:ILE:N	2.12	0.65
1:A:147:ASN:HB2	1:A:233:TYR:CD2	2.31	0.64
3:C:5:DG:H2"	3:C:6:DA:C8	2.31	0.64
1:A:298:ARG:HG3	1:A:322:ILE:CG1	2.24	0.64
1:A:28:VAL:HG23	1:A:47:ASN:ND2	2.12	0.64
2:B:227:SER:O	2:B:231:ASP:N	2.30	0.64
2:B:143:GLY:C	2:B:144:ILE:HG13	2.18	0.64
2:B:311:ALA:O	2:B:315:SER:HB2	1.97	0.64
2:B:136:GLU:O	2:B:137:LYS:HB2	1.96	0.64
1:A:267:ARG:HD2	6:A:2072:HOH:O	1.96	0.64
1:A:144:ILE:HG13	1:A:165:VAL:HA	1.79	0.64
1:A:111:ILE:HG21	1:A:124:LEU:HD21	1.78	0.64
2:B:282:LYS:HE2	6:B:2049:HOH:O	1.97	0.64
2:B:95:TYR:O	2:B:114:LYS:HG2	1.98	0.64
2:B:209:GLU:HG2	2:B:212:LYS:HD3	1.79	0.64
1:A:147:ASN:CB	1:A:233:TYR:HD2	2.11	0.63
2:B:308:LYS:O	2:B:312:TYR:HD2	1.81	0.63
1:A:144:ILE:O	1:A:145:SER:HB2	1.98	0.63
1:A:257:ASN:OD1	1:A:259:GLU:N	2.30	0.63
1:A:41:GLY:CA	1:A:61:ILE:HD12	2.29	0.63
2:B:246:GLY:HA3	6:F:2005:HOH:O	1.99	0.63
2:B:319:LEU:HD12	2:B:319:LEU:C	2.19	0.63
1:A:257:ASN:HB3	1:A:260:GLU:HB2	1.79	0.63
1:A:5:PHE:CZ	1:A:106:GLU:HG2	2.34	0.63
2:B:111:ILE:CG1	2:B:111:ILE:O	2.44	0.63
2:B:226:ILE:HG22	2:B:227:SER:N	2.14	0.63
2:B:298:ARG:NH1	3:D:8:DG:OP1	2.32	0.63
2:B:322:ILE:O	2:B:322:ILE:CG2	2.42	0.63
2:B:312:TYR:O	2:B:313:SER:C	2.37	0.63
3:D:4:DG:H2"	3:D:5:DG:C8	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:CE1	1:A:106:GLU:HB3	2.33	0.62
2:B:8:PHE:N	2:B:8:PHE:CD1	2.64	0.62
2:B:296:VAL:O	2:B:296:VAL:HG13	1.99	0.62
1:A:5:PHE:HE1	1:A:106:GLU:HB3	1.64	0.62
1:A:238:ARG:CD	1:A:240:ARG:H	2.11	0.62
1:A:332:ARG:NE	4:E:6:DG:OP2	2.31	0.62
1:A:232:GLU:HG2	1:A:233:TYR:N	2.15	0.62
2:B:93:ARG:HG2	2:B:99:ILE:HD12	1.81	0.62
2:B:324:GLU:O	2:B:325:GLU:OE1	2.17	0.62
1:A:183:VAL:O	1:A:184:PRO:C	2.35	0.62
1:A:290:THR:OG1	1:A:294:ASP:N	2.21	0.62
1:A:282:LYS:HE2	1:A:339:LYS:O	2.00	0.62
2:B:241:VAL:O	2:B:243:LYS:NZ	2.23	0.62
1:A:77:ARG:O	1:A:81:TYR:CE2	2.53	0.61
1:A:150:PHE:HE1	1:A:174:LEU:HD12	1.64	0.61
1:A:159:LYS:HE3	6:A:2021:HOH:O	1.99	0.61
2:B:164:LYS:NZ	2:B:165:VAL:H	1.97	0.61
1:A:332:ARG:HH21	4:E:6:DG:P	2.23	0.61
1:A:100:GLU:OE2	1:A:237:ILE:HA	1.99	0.61
2:B:240:ARG:NH2	6:B:2044:HOH:O	2.34	0.61
2:B:155:ALA:O	2:B:156:ASP:C	2.39	0.61
1:A:188:ASN:O	1:A:192:GLU:HG2	2.00	0.61
2:B:332:ARG:NH1	4:F:5[F]:O2G:P	2.73	0.61
1:A:247:ARG:NH2	1:A:249:VAL:HG12	2.16	0.61
2:B:228:LEU:CD2	2:B:233:TYR:CD1	2.84	0.61
1:A:114:LYS:HD2	1:A:114:LYS:N	2.16	0.61
1:A:147:ASN:CB	6:A:2049:HOH:O	2.43	0.60
1:A:180:ILE:HD13	1:A:201:LYS:C	2.21	0.60
2:B:9:ASP:OD1	2:B:160:PRO:HA	2.00	0.60
1:A:280:ILE:O	1:A:341:ILE:N	2.31	0.60
2:B:288:ALA:HA	2:B:332:ARG:O	2.00	0.60
1:A:291:GLU:HG3	1:A:329:LYS:HB2	1.81	0.60
1:A:14:GLN:O	1:A:15:VAL:C	2.36	0.60
1:A:210:PHE:C	1:A:210:PHE:HD2	2.05	0.60
1:A:147:ASN:HB2	1:A:233:TYR:HD2	1.67	0.60
1:A:291:GLU:CB	1:A:329:LYS:O	2.49	0.60
2:B:27:PRO:HB2	2:B:71:ALA:HB1	1.84	0.60
1:A:324:GLU:O	1:A:326:ASP:N	2.35	0.60
2:B:244:SER:HB3	4:F:8:DA:H3'	1.84	0.60
1:A:10:TYR:N	1:A:10:TYR:CD2	2.70	0.59
4:E:15:DC:H2'	4:E:15:DC:O5'	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:VAL:O	2:B:290:THR:C	2.37	0.59
2:B:34:SER:OG	2:B:40:SER:HB2	2.01	0.59
1:A:126:LEU:HG	1:A:163:ILE:HD13	1.82	0.59
1:A:336:ARG:NH1	4:E:8:DA:OP1	2.27	0.59
1:A:324:GLU:C	1:A:326:ASP:N	2.54	0.59
2:B:332:ARG:NH1	4:F:5[F]:O2G:OP2	2.34	0.59
2:B:37:PHE:CZ	4:F:4[F]:DT:OP2	2.55	0.59
1:A:154:ALA:HA	1:A:164:LYS:HG2	1.85	0.59
2:B:298:ARG:HG2	3:D:8:DG:OP1	2.03	0.59
1:A:288:ALA:CB	1:A:330:ILE:HG21	2.31	0.59
2:B:203:VAL:O	2:B:205:THR:N	2.36	0.59
1:A:170:GLU:O	1:A:174:LEU:HG	2.03	0.59
1:A:144:ILE:CG1	1:A:164:LYS:O	2.49	0.58
1:A:197:LEU:HD11	1:A:212:LYS:NZ	2.17	0.58
2:B:245:ILE:HG21	2:B:276:LEU:HG	1.84	0.58
2:B:256:ARG:HH21	2:B:256:ARG:HG2	1.67	0.58
1:A:94:GLU:O	1:A:94:GLU:CG	2.50	0.58
1:A:292[A]:ASP:OD1	1:A:328:ARG:NH1	2.34	0.58
1:A:210:PHE:CD2	1:A:210:PHE:C	2.76	0.58
1:A:209:GLU:H	1:A:209:GLU:CD	2.04	0.58
1:A:226:ILE:HG23	1:A:230:ARG:HE	1.68	0.58
1:A:333:ILE:HG23	1:A:333:ILE:O	2.03	0.58
2:B:289:VAL:O	2:B:290:THR:O	2.22	0.58
1:A:238:ARG:HD3	1:A:240:ARG:N	2.18	0.58
2:B:247:ARG:HG3	2:B:247:ARG:O	2.03	0.58
1:A:175:ILE:HG22	1:A:203:VAL:HB	1.86	0.58
2:B:301:THR:O	2:B:301:THR:CG2	2.42	0.58
2:B:46:ALA:O	2:B:51:ARG:NH1	2.37	0.58
1:A:247:ARG:NH2	6:A:2069:HOH:O	2.36	0.58
2:B:209:GLU:CG	2:B:212:LYS:HD3	2.33	0.58
4:F:16:DC:C4	4:F:17:DC:C4	2.92	0.58
2:B:254:ASN:HB3	2:B:331:ARG:HA	1.84	0.58
1:A:258:LEU:HD13	1:A:319:LEU:HD21	1.86	0.57
1:A:258:LEU:O	1:A:262:LYS:HG3	2.04	0.57
3:D:5:DG:N2	4:F:14:DC:N3	2.45	0.57
1:A:41:GLY:C	1:A:61:ILE:HD12	2.24	0.57
2:B:70:ASN:ND2	6:B:2016:HOH:O	2.37	0.57
2:B:23:LEU:CA	2:B:26:LYS:HE3	2.26	0.57
2:B:176:ARG:O	2:B:201:LYS:HB3	2.04	0.57
4:F:16:DC:N4	4:F:17:DC:N4	2.52	0.57
1:A:180:ILE:HG13	1:A:180:ILE:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:TYR:CD2	2:B:233:TYR:C	2.78	0.57
1:A:264:TYR:CD1	1:A:267:ARG:NH1	2.71	0.57
1:A:238:ARG:CD	1:A:240:ARG:N	2.67	0.57
2:B:93:ARG:HB3	6:B:2025:HOH:O	2.03	0.57
1:A:258:LEU:HD13	1:A:319:LEU:CD2	2.35	0.57
1:A:15:VAL:HG11	1:A:81:TYR:HD1	1.70	0.57
2:B:210:PHE:HA	2:B:213:LEU:HB2	1.86	0.57
1:A:238:ARG:CD	1:A:239:THR:H	2.12	0.57
2:B:59:ILE:C	2:B:59:ILE:HD12	2.25	0.57
2:B:247:ARG:O	2:B:247:ARG:CG	2.53	0.57
1:A:53:PHE:O	1:A:67:ILE:HG21	2.04	0.57
2:B:12:TYR:HB2	2:B:45:THR:HG23	1.87	0.57
1:A:75:PRO:O	1:A:75:PRO:HG2	2.03	0.56
1:A:235:GLU:HG2	1:A:236:PRO:CD	2.35	0.56
1:A:28:VAL:H	1:A:47:ASN:ND2	2.03	0.56
1:A:151:ALA:O	1:A:154:ALA:HB3	2.06	0.56
2:B:115:VAL:O	2:B:115:VAL:CG1	2.53	0.56
2:B:190:THR:O	2:B:194:LEU:HG	2.05	0.56
1:A:217:ILE:HD12	1:A:221:LYS:HB3	1.87	0.56
3:C:13:DC:C5'	3:C:14[B]:DOC:H6	2.36	0.56
2:B:166:ILE:HG22	2:B:171:VAL:CG2	2.32	0.56
2:B:55:VAL:CG2	2:B:68:LEU:HD12	2.33	0.56
3:D:10:DA:O5'	3:D:10:DA:H2'	2.06	0.56
2:B:325:GLU:N	2:B:325:GLU:OE1	2.37	0.56
1:A:10:TYR:O	1:A:11:PHE:C	2.44	0.56
2:B:308:LYS:O	2:B:312:TYR:CD2	2.59	0.56
1:A:147:ASN:CA	6:A:2049:HOH:O	2.52	0.56
2:B:238:ARG:HG3	2:B:238:ARG:HH11	1.70	0.56
2:B:298:ARG:HG2	2:B:298:ARG:NH1	2.06	0.56
1:A:291:GLU:CG	1:A:329:LYS:HB2	2.36	0.56
1:A:282:LYS:HB2	1:A:339:LYS:HB2	1.86	0.56
1:A:280:ILE:HG22	1:A:305:GLY:CA	2.35	0.56
3:D:11:DT:H2''	3:D:12:DT:OP2	2.06	0.56
1:A:268:ALA:O	1:A:272:SER:OG	2.23	0.56
1:A:124:LEU:HA	1:A:127:GLU:CB	2.29	0.56
2:B:210:PHE:O	2:B:210:PHE:CG	2.58	0.56
2:B:187:GLY:O	2:B:191:ALA:N	2.37	0.56
2:B:317:LYS:O	2:B:320:GLN:N	2.39	0.56
2:B:175:ILE:HG22	2:B:203:VAL:HB	1.88	0.56
1:A:133:LEU:O	1:A:137:LYS:N	2.24	0.56
1:A:221:LYS:O	1:A:225:LEU:N	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ASN:OD1	2:B:234:ASN:C	2.44	0.55
2:B:32:VAL:HG11	4:F:6:DG:C5'	2.36	0.55
1:A:122:TYR:CE1	1:A:163:ILE:HG12	2.41	0.55
2:B:208:ILE:HG22	2:B:209:GLU:N	2.19	0.55
2:B:100:GLU:HB3	2:B:237:ILE:HG23	1.88	0.55
2:B:284:ILE:HG13	2:B:337:PHE:CE1	2.42	0.55
2:B:208:ILE:HG22	2:B:213:LEU:CD1	2.35	0.55
1:A:290:THR:N	1:A:294:ASP:O	2.40	0.55
2:B:248:ILE:HD13	2:B:248:ILE:H	1.69	0.55
1:A:178:LEU:O	1:A:201:LYS:HB3	2.06	0.55
1:A:28:VAL:N	1:A:47:ASN:ND2	2.44	0.55
2:B:276:LEU:HD21	2:B:340:PHE:CE1	2.42	0.55
3:C:9:DG:H2''	3:C:10:DA:O5'	2.06	0.55
2:B:179:ASP:OD1	2:B:180:ILE:N	2.40	0.55
2:B:176:ARG:HA	2:B:203:VAL:HG12	1.88	0.55
2:B:289:VAL:CG2	2:B:332:ARG:HD2	2.35	0.55
2:B:234:ASN:OD1	2:B:235:GLU:N	2.40	0.55
1:A:136:GLU:O	1:A:137:LYS:HB2	2.07	0.55
2:B:298:ARG:HA	3:D:8:DG:OP2	2.06	0.55
1:A:197:LEU:HD11	1:A:212:LYS:HG2	1.89	0.55
1:A:29:VAL:CG2	1:A:73:TYR:CD2	2.90	0.55
1:A:328:ARG:NH2	6:A:2087:HOH:O	2.39	0.55
2:B:269:ILE:HG22	2:B:273:TYR:HD1	1.71	0.55
1:A:189:ILE:O	1:A:189:ILE:HG22	2.06	0.55
1:A:258:LEU:CD1	1:A:319:LEU:HD23	2.36	0.54
2:B:14:GLN:OE1	2:B:138:ILE:HA	2.07	0.54
1:A:189:ILE:O	1:A:193:LYS:HG3	2.07	0.54
1:A:45:THR:HG22	1:A:46:ALA:N	2.21	0.54
1:A:238:ARG:HD3	1:A:240:ARG:H	1.73	0.54
1:A:291:GLU:C	1:A:293:LEU:H	2.11	0.54
4:F:11:DC:H1'	4:F:12:DT:H5'	1.89	0.54
2:B:164:LYS:CE	2:B:165:VAL:N	2.47	0.54
1:A:7:ASP:O	1:A:140:VAL:HB	2.08	0.54
1:A:302:PHE:HB3	1:A:303:PRO:HD2	1.89	0.54
2:B:186:ILE:HD11	2:B:225:LEU:HD21	1.89	0.54
1:A:335:VAL:CG2	1:A:335:VAL:O	2.54	0.54
1:A:296:VAL:O	1:A:296:VAL:HG22	2.08	0.54
2:B:4:LEU:HD23	2:B:5:PHE:N	2.23	0.54
1:A:19:LEU:HD12	1:A:19:LEU:N	2.23	0.54
1:A:150:PHE:CE1	1:A:174:LEU:HD12	2.42	0.54
1:A:284:ILE:CG1	1:A:285:HIS:H	2.16	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ILE:HG12	2:B:204:ASP:HB3	1.90	0.54
2:B:41:GLY:HA2	4:F:5[F]:O2G:C5'	2.38	0.53
2:B:254:ASN:OD1	2:B:331:ARG:O	2.26	0.53
1:A:280:ILE:HG21	1:A:305:GLY:HA3	1.90	0.53
3:D:14[A]:DOC:H6	6:D:2019:HOH:O	2.08	0.53
2:B:137:LYS:O	2:B:138:ILE:CG1	2.56	0.53
2:B:65:LYS:O	2:B:69:PRO:HA	2.07	0.53
1:A:263:PRO:O	1:A:267:ARG:HG3	2.08	0.53
1:A:132:ILE:O	1:A:136:GLU:HB3	2.08	0.53
2:B:151:ALA:O	2:B:154:ALA:HB3	2.08	0.53
1:A:29:VAL:HG21	1:A:73:TYR:CD2	2.43	0.53
2:B:168:ASP:O	2:B:171:VAL:HB	2.09	0.53
1:A:49:GLU:CD	1:A:49:GLU:H	2.11	0.53
2:B:37:PHE:HZ	4:F:4[F]:DT:OP2	1.92	0.53
2:B:322:ILE:C	2:B:324:GLU:N	2.60	0.53
1:A:28:VAL:CB	1:A:47:ASN:ND2	2.72	0.53
1:A:89:MET:O	1:A:92:LEU:HB2	2.08	0.53
2:B:16:GLU:OE1	2:B:74:LEU:HD13	2.08	0.53
1:A:214:LYS:HG3	1:A:219:GLU:HG3	1.89	0.53
1:A:336:ARG:HH22	4:E:7:DA:H2'	1.71	0.53
1:A:240:ARG:HG2	6:A:2067:HOH:O	2.08	0.53
2:B:251:MET:HB3	2:B:264:TYR:CZ	2.43	0.53
2:B:264:TYR:HD1	2:B:267:ARG:HH21	1.56	0.53
2:B:114:LYS:O	2:B:115:VAL:O	2.26	0.52
1:A:173:ARG:HH11	1:A:173:ARG:HG2	1.74	0.52
2:B:235:GLU:CG	2:B:236:PRO:HD2	2.37	0.52
2:B:46:ALA:HB1	2:B:50:ALA:HB3	1.92	0.52
2:B:80:VAL:O	2:B:84:VAL:N	2.37	0.52
1:A:48:TYR:CE2	1:A:160:PRO:HG3	2.39	0.52
1:A:51:ARG:HA	1:A:55:VAL:O	2.09	0.52
1:A:300:ARG:HD2	1:A:301:THR:N	2.25	0.52
3:C:11:DT:H2''	3:C:12:DT:H72	1.91	0.52
1:A:48:TYR:CD2	1:A:48:TYR:N	2.73	0.52
2:B:259:GLU:O	2:B:261:ILE:N	2.42	0.52
2:B:259:GLU:C	2:B:261:ILE:N	2.62	0.52
2:B:117:ASP:OD2	2:B:118:TYR:N	2.43	0.52
1:A:48:TYR:O	1:A:52:LYS:HG2	2.09	0.52
1:A:36:ARG:HH12	1:A:254:ASN:ND2	2.08	0.52
1:A:248:ILE:HG12	4:E:7:DA:OP1	2.09	0.52
1:A:147:ASN:HD21	1:A:150:PHE:HD2	1.57	0.52
2:B:321:LYS:HG2	2:B:321:LYS:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:NH2	4:E:6:DG:OP2	2.43	0.52
1:A:124:LEU:O	1:A:124:LEU:HD12	2.10	0.51
3:C:8:DG:C2'	3:C:9:DG:OP1	2.58	0.51
2:B:290:THR:OG1	2:B:328[B]:ARG:HD2	2.10	0.51
2:B:20:ASN:OD1	2:B:22:SER:CB	2.57	0.51
4:E:15:DC:C2'	4:E:15:DC:O5'	2.57	0.51
1:A:50:ALA:O	1:A:51:ARG:C	2.44	0.51
1:A:227:SER:CA	1:A:230:ARG:HD2	2.37	0.51
3:C:3:DG:H1	4:E:16:DC:H42	1.58	0.51
1:A:219:GLU:HA	1:A:222:ALA:CB	2.39	0.51
2:B:320:GLN:O	2:B:322:ILE:N	2.44	0.51
1:A:118:TYR:HA	1:A:121:ALA:HB3	1.91	0.51
2:B:19:LEU:HD21	2:B:80:VAL:HG11	1.93	0.51
2:B:10:TYR:CE1	2:B:14:GLN:HB2	2.46	0.51
1:A:237:ILE:HD13	6:A:2038:HOH:O	2.11	0.51
1:A:236:PRO:O	1:A:238:ARG:N	2.43	0.51
2:B:307:SER:O	2:B:308:LYS:C	2.48	0.51
1:A:257:ASN:HB3	1:A:260:GLU:CD	2.32	0.51
3:D:3:DG:H2''	3:D:4:DG:H5'	1.93	0.51
2:B:91:LEU:HD23	2:B:91:LEU:C	2.31	0.51
2:B:47:ASN:O	2:B:50:ALA:HB3	2.11	0.51
1:A:164:LYS:HE2	1:A:165:VAL:O	2.11	0.51
1:A:224:TYR:CD1	1:A:224:TYR:O	2.63	0.51
1:A:309:GLU:OE1	1:A:309:GLU:N	2.41	0.51
2:B:149:VAL:HG12	2:B:153:ILE:HD12	1.93	0.50
3:C:13:DC:H5'	3:C:14[B]:DOC:C6	2.42	0.50
1:A:276:LEU:O	1:A:277:ASP:O	2.28	0.50
1:A:289:VAL:O	1:A:290:THR:O	2.29	0.50
1:A:282:LYS:CB	1:A:339:LYS:O	2.59	0.50
1:A:317:LYS:O	1:A:318:LEU:C	2.45	0.50
1:A:80:VAL:O	1:A:84:VAL:HG23	2.12	0.50
1:A:175:ILE:HG23	1:A:202:LEU:HB3	1.92	0.50
2:B:100:GLU:HB2	2:B:238:ARG:O	2.11	0.50
2:B:262:LYS:O	2:B:263:PRO:C	2.49	0.50
1:A:180:ILE:O	1:A:186:ILE:HD12	2.11	0.50
2:B:80:VAL:O	2:B:84:VAL:HG23	2.12	0.50
1:A:169:GLU:C	1:A:169:GLU:OE2	2.49	0.50
2:B:269:ILE:HG23	2:B:337:PHE:HZ	1.77	0.50
1:A:172:LYS:O	1:A:175:ILE:N	2.44	0.50
2:B:304:HIS:CD2	6:B:2050:HOH:O	2.65	0.50
1:A:185:GLY:O	3:C:12:DT:H5''	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:PHE:HD1	2:B:269:ILE:CD1	2.24	0.50
2:B:298:ARG:HD2	2:B:322:ILE:HG12	1.90	0.50
2:B:195[B]:LYS:C	2:B:197:LEU:N	2.64	0.50
1:A:241:VAL:O	1:A:243:LYS:HE3	2.12	0.50
1:A:2:ILE:HD11	1:A:145:SER:HA	1.94	0.50
1:A:14:GLN:OE1	1:A:139:THR:HG23	2.11	0.50
1:A:46:ALA:HB1	1:A:50:ALA:CB	2.40	0.50
1:A:28:VAL:HB	1:A:47:ASN:ND2	2.27	0.50
1:A:217:ILE:HG13	1:A:218:GLY:N	2.26	0.50
2:B:210:PHE:C	2:B:210:PHE:CD1	2.81	0.50
2:B:0:HIS:O	2:B:0:HIS:CD2	2.65	0.50
2:B:226:ILE:CG2	2:B:227:SER:N	2.75	0.50
1:A:166:ILE:O	1:A:166:ILE:HG22	2.11	0.50
1:A:14:GLN:O	1:A:17:GLU:N	2.36	0.50
1:A:240:ARG:C	1:A:241:VAL:HG13	2.31	0.50
2:B:209:GLU:O	2:B:213:LEU:HD12	2.12	0.49
1:A:284:ILE:CG1	1:A:285:HIS:N	2.70	0.49
1:A:190:THR:OG1	3:C:12:DT:OP2	2.21	0.49
1:A:9:ASP:C	1:A:10:TYR:CD2	2.86	0.49
1:A:273:TYR:OH	1:A:306:ILE:O	2.26	0.49
2:B:332:ARG:HH22	4:F:5[F]:O2G:H2'	1.76	0.49
1:A:93:ARG:CZ	1:A:93:ARG:HB2	2.30	0.49
1:A:291:GLU:CA	1:A:329:LYS:O	2.59	0.49
1:A:48:TYR:H	1:A:48:TYR:HD2	1.58	0.49
1:A:3:VAL:HG13	1:A:237:ILE:HD11	1.93	0.49
1:A:175:ILE:HG23	1:A:202:LEU:CB	2.42	0.49
1:A:290:THR:HG21	1:A:294:ASP:HB3	1.95	0.49
1:A:191:ALA:O	1:A:192:GLU:C	2.50	0.49
2:B:105:ASP:O	2:B:106:GLU:HG3	2.12	0.49
3:D:14[A]:DOC:H5"	6:D:2016:HOH:O	2.11	0.49
1:A:180:ILE:HD13	1:A:201:LYS:O	2.12	0.49
1:A:164:LYS:HE2	1:A:166:ILE:HG12	1.94	0.49
3:C:2:DG:H2"	3:C:3:DG:C8	2.48	0.49
2:B:267:ARG:O	2:B:271:GLU:HG3	2.13	0.49
2:B:281:PRO:HB2	2:B:337:PHE:HB3	1.94	0.49
2:B:316:VAL:O	2:B:320:GLN:N	2.40	0.49
3:D:4:DG:H2"	3:D:5:DG:H8	1.78	0.49
2:B:32:VAL:CG1	4:F:6:DG:C5'	2.86	0.49
1:A:257:ASN:OD1	1:A:258:LEU:N	2.46	0.49
2:B:20:ASN:OD1	2:B:22:SER:HB3	2.13	0.49
2:B:51:ARG:NH1	6:B:2012:HOH:O	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:HB2	1:A:27:PRO:HD2	1.95	0.48
1:A:232:GLU:CG	1:A:233:TYR:N	2.75	0.48
2:B:205:THR:OG1	2:B:229:ALA:CB	2.61	0.48
2:B:52:LYS:HZ2	2:B:53:PHE:HE1	1.61	0.48
1:A:176:ARG:O	1:A:177:GLU:CB	2.45	0.48
1:A:334:GLY:C	1:A:335:VAL:CG1	2.82	0.48
2:B:230:ARG:O	2:B:231:ASP:HB3	2.14	0.48
2:B:339:LYS:HB3	6:B:2049:HOH:O	2.12	0.48
1:A:93:ARG:CZ	1:A:93:ARG:CB	2.89	0.48
1:A:28:VAL:CG2	1:A:47:ASN:ND2	2.76	0.48
2:B:63:GLU:O	2:B:67:ILE:CG1	2.54	0.48
2:B:180:ILE:HG22	2:B:181:ALA:H	1.70	0.48
1:A:251:MET:HG2	1:A:264:TYR:CD2	2.49	0.48
1:A:87:ARG:HG3	1:A:87:ARG:HH11	1.79	0.48
1:A:10:TYR:CE1	1:A:14:GLN:HG3	2.49	0.48
1:A:147:ASN:CB	1:A:233:TYR:CD2	2.93	0.48
2:B:218:GLY:C	2:B:220:ALA:H	2.15	0.48
1:A:287:VAL:HA	1:A:297:SER:CB	2.44	0.48
2:B:89:MET:O	2:B:93:ARG:HG3	2.14	0.48
1:A:262:LYS:HE2	1:A:266:PHE:CE2	2.49	0.48
1:A:219:GLU:CA	1:A:222:ALA:HB3	2.42	0.48
1:A:203:VAL:CG1	1:A:204:ASP:N	2.75	0.48
1:A:71:ALA:HB3	1:A:73:TYR:CE1	2.48	0.48
2:B:296:VAL:O	2:B:296:VAL:CG1	2.62	0.48
2:B:328[B]:ARG:C	2:B:329:LYS:O	2.51	0.48
1:A:77:ARG:O	1:A:81:TYR:CD2	2.67	0.48
1:A:286:VAL:HG23	1:A:318:LEU:HB2	1.95	0.48
1:A:135:LYS:O	1:A:135:LYS:CG	2.62	0.48
1:A:262:LYS:O	1:A:266:PHE:N	2.42	0.48
1:A:214:LYS:O	1:A:218:GLY:N	2.46	0.48
1:A:302:PHE:HZ	1:A:314:GLU:HG2	1.78	0.48
2:B:161:ASN:O	2:B:161:ASN:OD1	2.32	0.48
1:A:261:ILE:CD1	1:A:330:ILE:HD12	2.44	0.47
1:A:28:VAL:HB	1:A:47:ASN:HD22	1.78	0.47
2:B:280:ILE:CD1	2:B:280:ILE:N	2.78	0.47
1:A:35:GLY:O	1:A:36:ARG:C	2.52	0.47
2:B:152:LYS:NZ	3:D:14[B]:DOC:H5'	2.29	0.47
1:A:150:PHE:CE2	1:A:228:LEU:HD22	2.48	0.47
2:B:290:THR:O	2:B:291:GLU:C	2.52	0.47
1:A:257:ASN:C	1:A:257:ASN:OD1	2.52	0.47
1:A:183:VAL:HB	1:A:186:ILE:HD12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LEU:O	2:B:137:LYS:CA	2.62	0.47
2:B:15:VAL:O	2:B:15:VAL:HG12	2.13	0.47
1:A:124:LEU:HD11	1:A:128:ILE:HD11	1.97	0.47
2:B:141:THR:HG23	2:B:162:GLY:CA	2.43	0.47
2:B:193:LYS:HE3	2:B:193:LYS:HB3	1.25	0.47
1:A:168[A]:ASP:OD2	1:A:171:VAL:HG21	2.14	0.47
2:B:148:LYS:HD3	2:B:237:ILE:HG13	1.96	0.47
1:A:127:GLU:CD	1:A:127:GLU:C	2.73	0.47
2:B:265:LEU:HD21	2:B:315:SER:OG	2.15	0.47
1:A:63:GLU:HG3	6:A:2027:HOH:O	2.13	0.47
1:A:3:VAL:O	6:A:2001:HOH:O	2.21	0.47
2:B:78:LYS:HA	2:B:81:TYR:CE2	2.40	0.47
1:A:180:ILE:HB	1:A:201:LYS:HA	1.96	0.47
1:A:197:LEU:CD1	1:A:212:LYS:HZ2	2.22	0.47
1:A:291:GLU:N	1:A:329:LYS:O	2.47	0.47
1:A:287:VAL:CG1	1:A:295:ILE:HD12	2.44	0.47
2:B:114:LYS:CD	2:B:114:LYS:H	1.99	0.47
1:A:94:GLU:O	1:A:94:GLU:HG2	2.15	0.47
2:B:333:ILE:HG13	2:B:334:GLY:H	1.78	0.47
1:A:49:GLU:CD	1:A:49:GLU:N	2.67	0.47
2:B:314:GLU:O	2:B:315:SER:C	2.52	0.47
1:A:333:ILE:CG2	1:A:333:ILE:O	2.62	0.47
1:A:116[A]:ARG:HH11	1:A:116[A]:ARG:CG	2.28	0.47
2:B:110:ASP:OD1	2:B:112:SER:OG	2.22	0.47
1:A:26:LYS:HB2	1:A:27:PRO:CD	2.45	0.47
1:A:21:PRO:C	1:A:23:LEU:N	2.67	0.47
2:B:247:ARG:HD3	2:B:275:LYS:NZ	2.30	0.47
1:A:209:GLU:CD	1:A:209:GLU:N	2.68	0.47
3:C:13:DC:C5'	3:C:14[B]:DOC:C6	2.93	0.47
1:A:124:LEU:O	1:A:125:GLY:O	2.33	0.46
2:B:93:ARG:C	2:B:95:TYR:H	2.18	0.46
1:A:232:GLU:O	1:A:233:TYR:HB3	2.14	0.46
2:B:146:LYS:HE3	2:B:146:LYS:HB2	1.69	0.46
2:B:122:TYR:CE1	2:B:163:ILE:HG12	2.49	0.46
1:A:48:TYR:OH	1:A:160:PRO:CG	2.62	0.46
1:A:240:ARG:C	1:A:241:VAL:CG1	2.83	0.46
1:A:28:VAL:C	1:A:29:VAL:CG1	2.82	0.46
1:A:273:TYR:HB3	1:A:308:LYS:HE2	1.97	0.46
1:A:74:LEU:O	1:A:75:PRO:C	2.52	0.46
2:B:316:VAL:O	2:B:319:LEU:HB3	2.15	0.46
1:A:203:VAL:HG13	1:A:204:ASP:N	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:O	1:A:38:GLU:C	2.54	0.46
1:A:9:ASP:O	1:A:10:TYR:C	2.54	0.46
1:A:33:PHE:HE2	1:A:39:ASP:OD1	1.99	0.46
1:A:258:LEU:CD1	1:A:319:LEU:CD2	2.93	0.46
2:B:282:LYS:HD3	2:B:341:ILE:HG13	1.96	0.46
3:D:11:DT:H5'	6:D:2012:HOH:O	2.15	0.46
1:A:64:ALA:C	1:A:66:LYS:N	2.67	0.46
2:B:59:ILE:O	2:B:60:PRO:C	2.51	0.46
1:A:292[A]:ASP:OD2	1:A:328:ARG:NH1	2.49	0.46
1:A:5:PHE:HZ	1:A:106:GLU:CG	2.27	0.46
2:B:2:ILE:CG2	2:B:111:ILE:HD11	2.46	0.46
1:A:92:LEU:C	1:A:94:GLU:H	2.19	0.46
1:A:276:LEU:HD11	1:A:281:PRO:HG3	1.98	0.46
1:A:286:VAL:CG2	1:A:318:LEU:HB2	2.45	0.46
1:A:28:VAL:HG23	1:A:47:ASN:HD21	1.80	0.46
1:A:99:ILE:CD1	1:A:109:LEU:HG	2.46	0.45
1:A:7:ASP:CG	1:A:8:PHE:N	2.70	0.45
1:A:252:LYS:C	1:A:253:ARG:HG3	2.36	0.45
1:A:287:VAL:HG13	1:A:297:SER:HB3	1.98	0.45
1:A:147:ASN:HA	6:A:2049:HOH:O	2.15	0.45
2:B:2:ILE:HG22	2:B:2:ILE:O	2.15	0.45
2:B:333:ILE:CG1	2:B:334:GLY:N	2.78	0.45
2:B:336:ARG:NH1	2:B:336:ARG:CB	2.78	0.45
1:A:301:THR:CG2	1:A:302:PHE:N	2.78	0.45
2:B:41:GLY:CA	4:F:5[F]:O2G:H5'	2.46	0.45
1:A:79:GLU:CD	1:A:79:GLU:N	2.64	0.45
2:B:19:LEU:CD2	2:B:80:VAL:HG11	2.45	0.45
1:A:111:ILE:HD12	1:A:115[A]:VAL:HB	1.98	0.45
1:A:126:LEU:O	1:A:127:GLU:C	2.54	0.45
1:A:241:VAL:HG22	1:A:243:LYS:HE2	1.97	0.45
1:A:197:LEU:CD2	1:A:216:MET:HG2	2.45	0.45
1:A:174:LEU:HA	1:A:174:LEU:HD23	1.57	0.45
1:A:91:LEU:HD21	1:A:131:LYS:HG2	1.97	0.45
2:B:243:LYS:H	2:B:243:LYS:HG2	1.58	0.45
4:F:11:DC:H6	4:F:11:DC:H2'	1.40	0.45
2:B:114:LYS:O	2:B:115:VAL:HB	2.15	0.45
1:A:221:LYS:O	1:A:224:TYR:CB	2.56	0.45
1:A:240:ARG:HG2	1:A:241:VAL:N	2.31	0.45
1:A:301:THR:HG22	1:A:302:PHE:N	2.31	0.45
1:A:98:LYS:N	1:A:98:LYS:HE3	2.31	0.45
2:B:298:ARG:HD3	2:B:322:ILE:CG1	2.19	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:8:DG:H2"	3:D:9:DG:OP1	2.16	0.45
2:B:22:SER:O	2:B:26:LYS:HE2	2.17	0.45
2:B:233:TYR:O	2:B:234:ASN:C	2.54	0.45
2:B:263:PRO:O	2:B:266:PHE:N	2.50	0.45
2:B:65:LYS:O	2:B:69:PRO:CA	2.64	0.45
1:A:195:LYS:N	1:A:195:LYS:CD	2.78	0.45
2:B:164:LYS:HA	2:B:164:LYS:HD2	1.75	0.45
2:B:269:ILE:HG22	2:B:273:TYR:CD1	2.51	0.45
1:A:28:VAL:C	1:A:29:VAL:HG13	2.37	0.45
2:B:139:THR:HB	2:B:161:ASN:HD22	1.82	0.45
2:B:256:ARG:CG	2:B:329:LYS:HA	2.45	0.45
1:A:226:ILE:CG2	1:A:230:ARG:HE	2.28	0.45
4:F:5[F]:O2G:HM2A	4:F:6:DG:C2	2.52	0.45
1:A:287:VAL:CG1	1:A:295:ILE:CD1	2.95	0.45
2:B:43:VAL:CG1	2:B:57:ALA:HA	2.41	0.45
2:B:208:ILE:HA	2:B:208:ILE:HD13	1.94	0.44
2:B:339:LYS:O	2:B:340:PHE:C	2.55	0.44
2:B:153:ILE:O	2:B:156:ASP:HB2	2.18	0.44
1:A:86:SER:HB3	6:A:2033:HOH:O	2.16	0.44
2:B:77:ARG:O	2:B:81:TYR:CE2	2.71	0.44
1:A:240:ARG:CG	1:A:241:VAL:N	2.79	0.44
2:B:79:GLU:O	2:B:83:GLN:N	2.50	0.44
1:A:192:GLU:O	1:A:194:LEU:N	2.50	0.44
2:B:284:ILE:CG2	2:B:318:LEU:HD11	2.48	0.44
1:A:141:THR:HA	1:A:162:GLY:O	2.17	0.44
2:B:261:ILE:O	2:B:264:TYR:HB2	2.17	0.44
1:A:258:LEU:HD21	1:A:323:LEU:CD1	2.45	0.44
2:B:4:LEU:HB2	2:B:111:ILE:HD12	2.00	0.44
3:C:2:DG:H1	4:E:17:DC:H42	1.64	0.44
2:B:100:GLU:OE1	2:B:148:LYS:HE2	2.18	0.44
3:C:13:DC:C4'	3:C:14[B]:DOC:H6	2.45	0.44
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.75	0.44
2:B:324:GLU:HB3	2:B:325:GLU:OE1	2.17	0.44
1:A:29:VAL:HG22	1:A:72:VAL:O	2.18	0.44
1:A:280:ILE:HA	1:A:281:PRO:HD2	1.70	0.44
1:A:189:ILE:HG22	1:A:193:LYS:HE3	1.99	0.44
1:A:11:PHE:O	1:A:12:TYR:C	2.56	0.44
3:D:3:DG:C5	3:D:4:DG:N7	2.86	0.44
4:E:5[E]:O2G:P	4:E:5[E]:O2G:H8	2.58	0.44
1:A:293:LEU:O	1:A:293:LEU:CD1	2.65	0.44
2:B:298:ARG:NH2	2:B:325:GLU:OE2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:HIS:O	2:B:335:VAL:HA	2.18	0.44
2:B:62:VAL:HG21	4:F:3[F]:DA:H5''	1.99	0.44
2:B:88:ILE:O	2:B:92:LEU:HG	2.18	0.44
2:B:12:TYR:HB2	2:B:45:THR:CG2	2.48	0.44
2:B:289:VAL:C	2:B:290:THR:O	2.55	0.44
2:B:164:LYS:HZ2	2:B:165:VAL:H	1.64	0.44
2:B:126:LEU:O	2:B:130:ASN:CB	2.55	0.44
1:A:8:PHE:HB2	1:A:105:ASP:HB2	1.98	0.43
1:A:105:ASP:OD1	1:A:106:GLU:OE2	2.35	0.43
2:B:283:ALA:HA	2:B:300:ARG:O	2.18	0.43
2:B:117:ASP:HB3	2:B:120:GLU:CG	2.39	0.43
2:B:338:SER:O	2:B:339:LYS:C	2.55	0.43
2:B:338:SER:HB2	2:B:339:LYS:H	1.52	0.43
2:B:300:ARG:HG2	2:B:301:THR:N	2.33	0.43
1:A:143:GLY:O	6:A:2001:HOH:O	2.21	0.43
2:B:267:ARG:HB3	2:B:267:ARG:NH1	2.31	0.43
2:B:266:PHE:HD1	2:B:269:ILE:HD12	1.83	0.43
1:A:173:ARG:HE	1:A:177:GLU:HG3	1.82	0.43
2:B:0:HIS:HD2	2:B:2:ILE:HD12	1.82	0.43
2:B:299:GLY:HA2	2:B:318:LEU:HD13	2.00	0.43
2:B:293:LEU:O	2:B:294:ASP:CB	2.66	0.43
1:A:36:ARG:HH22	1:A:254:ASN:N	2.16	0.43
1:A:336:ARG:NH2	4:E:7:DA:C2'	2.68	0.43
1:A:282:LYS:HG2	1:A:304:HIS:O	2.17	0.43
1:A:327:GLU:CD	1:A:327:GLU:N	2.62	0.43
2:B:128:ILE:C	2:B:130:ASN:N	2.72	0.43
1:A:226:ILE:HG23	1:A:230:ARG:HH21	1.83	0.43
1:A:289:VAL:O	1:A:290:THR:C	2.57	0.43
1:A:273:TYR:HD2	1:A:273:TYR:O	2.02	0.43
3:C:11:DT:H2''	3:C:12:DT:C7	2.48	0.43
1:A:201:LYS:HD2	1:A:201:LYS:N	2.32	0.43
2:B:127:GLU:O	2:B:130:ASN:HB3	2.18	0.43
1:A:114:LYS:CD	1:A:114:LYS:N	2.79	0.43
3:C:11:DT:C2'	3:C:12:DT:H72	2.49	0.43
1:A:19:LEU:CD1	1:A:19:LEU:N	2.82	0.43
2:B:114:LYS:O	2:B:115:VAL:CB	2.67	0.43
2:B:22:SER:O	2:B:26:LYS:CE	2.67	0.43
2:B:43:VAL:HG12	2:B:43:VAL:O	2.18	0.43
4:E:15:DC:C2	4:E:16:DC:C5	3.06	0.43
1:A:5:PHE:CZ	1:A:106:GLU:CG	3.02	0.42
3:D:6:DA:H2''	3:D:7:DA:OP2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:ILE:O	2:B:229:ALA:HB3	2.19	0.42
2:B:51:ARG:O	2:B:53:PHE:N	2.52	0.42
2:B:250:THR:N	2:B:332:ARG:HB3	2.33	0.42
1:A:213:LEU:O	1:A:214:LYS:O	2.36	0.42
1:A:247:ARG:HA	4:E:7:DA:OP1	2.19	0.42
2:B:62:VAL:HG21	4:F:3[F]:DA:C5'	2.48	0.42
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.83	0.42
3:C:5:DG:H2"	3:C:6:DA:H8	1.79	0.42
2:B:261:ILE:HG21	2:B:319:LEU:HD21	2.00	0.42
2:B:228:LEU:CD2	2:B:233:TYR:HB2	2.41	0.42
1:A:302:PHE:CD1	1:A:302:PHE:N	2.87	0.42
1:A:41:GLY:HA3	1:A:61:ILE:CD1	2.47	0.42
2:B:290:THR:O	2:B:292:ASP:N	2.53	0.42
2:B:251:MET:O	2:B:252:LYS:HD2	2.20	0.42
2:B:320:GLN:C	2:B:322:ILE:H	2.23	0.42
1:A:224:TYR:CD1	1:A:224:TYR:C	2.89	0.42
2:B:218:GLY:C	2:B:220:ALA:N	2.73	0.42
1:A:144:ILE:HG13	1:A:165:VAL:CG1	2.42	0.42
2:B:262:LYS:HE2	2:B:316:VAL:HG21	2.01	0.42
2:B:34:SER:O	2:B:36:ARG:N	2.52	0.42
2:B:203:VAL:O	2:B:204:ASP:C	2.58	0.42
1:A:290:THR:HG1	1:A:294:ASP:H	1.54	0.42
2:B:336:ARG:NE	6:F:2005:HOH:O	2.44	0.42
2:B:310:THR:O	2:B:311:ALA:C	2.57	0.42
2:B:15:VAL:CG1	2:B:15:VAL:O	2.66	0.42
2:B:97:GLU:O	2:B:99:ILE:N	2.53	0.42
1:A:118:TYR:HA	1:A:121:ALA:CB	2.50	0.42
1:A:30:VAL:CG1	1:A:76:MET:HA	2.50	0.42
1:A:244:SER:HA	1:A:337:PHE:O	2.19	0.42
2:B:78:LYS:N	2:B:81:TYR:CE2	2.87	0.42
1:A:218:GLY:HA3	4:E:12:DT:OP2	2.20	0.42
1:A:246:GLY:CA	1:A:335:VAL:O	2.67	0.42
2:B:336:ARG:NH2	6:F:2005:HOH:O	2.48	0.42
2:B:307:SER:O	2:B:309:GLU:N	2.53	0.42
1:A:37:PHE:O	1:A:40:SER:HB2	2.20	0.42
1:A:99:ILE:HG23	1:A:99:ILE:O	2.20	0.42
2:B:316:VAL:O	2:B:317:LYS:C	2.57	0.42
1:A:173:ARG:O	1:A:177:GLU:HB2	2.20	0.42
1:A:247:ARG:HG2	1:A:271:GLU:HB3	2.01	0.41
1:A:150:PHE:HA	1:A:153:ILE:HG13	2.02	0.41
2:B:226:ILE:HG22	2:B:227:SER:H	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:17:DC:H1'	4:F:18:DC:C6	2.55	0.41
1:A:296:VAL:O	1:A:322:ILE:HD13	2.20	0.41
1:A:146:LYS:NZ	1:A:232:GLU:O	2.52	0.41
2:B:178:LEU:O	2:B:179:ASP:O	2.38	0.41
2:B:180:ILE:C	2:B:182:ASP:H	2.23	0.41
1:A:92:LEU:O	1:A:95:TYR:HB2	2.20	0.41
2:B:171:VAL:O	2:B:172:LYS:C	2.58	0.41
1:A:167[A]:ASP:C	1:A:169:GLU:H	2.23	0.41
2:B:174:LEU:O	2:B:178:LEU:HB3	2.19	0.41
4:F:16:DC:H2''	4:F:17:DC:O5'	2.21	0.41
2:B:139:THR:CG2	2:B:161:ASN:HD22	2.33	0.41
2:B:194:LEU:C	2:B:195[B]:LYS:HD2	2.40	0.41
2:B:336:ARG:HH11	2:B:336:ARG:CB	2.33	0.41
1:A:208:ILE:CG2	1:A:209:GLU:O	2.60	0.41
2:B:111:ILE:H	2:B:111:ILE:HD13	1.84	0.41
2:B:125:GLY:O	2:B:126:LEU:C	2.58	0.41
2:B:136:GLU:O	2:B:137:LYS:C	2.54	0.41
3:D:4:DG:C5'	6:D:2010:HOH:O	2.68	0.41
2:B:203:VAL:C	2:B:205:THR:N	2.74	0.41
1:A:119[A]:ARG:C	1:A:121:ALA:H	2.24	0.41
1:A:195:LYS:N	1:A:195:LYS:HD3	2.35	0.41
2:B:77:ARG:NH1	6:B:2017:HOH:O	2.40	0.41
1:A:197:LEU:O	1:A:208:ILE:HG13	2.20	0.41
2:B:166:ILE:CG2	2:B:171:VAL:HG22	2.44	0.41
1:A:74:LEU:HD22	6:A:2008:HOH:O	2.21	0.41
2:B:131:LYS:O	2:B:135:LYS:HB3	2.21	0.41
1:A:10:TYR:O	1:A:11:PHE:O	2.38	0.41
2:B:155:ALA:O	2:B:157:MET:N	2.53	0.41
1:A:97:GLU:HB3	1:A:98:LYS:CE	2.51	0.41
1:A:111:ILE:CG2	1:A:124:LEU:HD21	2.46	0.41
2:B:115:VAL:HG21	6:B:2031:HOH:O	2.19	0.41
1:A:210:PHE:HA	1:A:213:LEU:HD12	2.03	0.41
1:A:240:ARG:O	6:A:2065:HOH:O	2.22	0.41
1:A:172:LYS:C	1:A:174:LEU:N	2.74	0.41
2:B:133:LEU:HB3	2:B:134:GLU:H	1.74	0.41
1:A:277:ASP:O	1:A:278:LYS:HB2	2.21	0.41
1:A:291:GLU:OE1	1:A:291:GLU:C	2.59	0.41
3:C:3:DG:H2''	3:C:4:DG:O5'	2.19	0.41
2:B:245:ILE:HB	2:B:340:PHE:HZ	1.86	0.41
2:B:48:TYR:C	2:B:50:ALA:N	2.74	0.41
2:B:292:ASP:O	2:B:293:LEU:C	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:LYS:O	2:B:318:LEU:C	2.58	0.41
1:A:261:ILE:HD13	1:A:330:ILE:HD12	2.03	0.41
1:A:235:GLU:HG2	1:A:236:PRO:HD2	2.02	0.41
2:B:152:LYS:HG2	2:B:184:PRO:HG3	2.03	0.40
2:B:239:THR:O	2:B:240:ARG:O	2.39	0.40
1:A:332:ARG:CZ	4:E:6:DG:OP2	2.69	0.40
1:A:5:PHE:HB2	1:A:108:TYR:CD2	2.56	0.40
1:A:147:ASN:CG	1:A:233:TYR:CD2	2.95	0.40
1:A:147:ASN:HB2	1:A:233:TYR:CE2	2.56	0.40
2:B:9:ASP:HB3	2:B:10:TYR:CD2	2.56	0.40
3:C:3:DG:H1	4:E:16:DC:N4	2.18	0.40
3:C:4:DG:H2"	3:C:5:DG:H5"	2.03	0.40
2:B:48:TYR:C	2:B:50:ALA:H	2.25	0.40
1:A:314:GLU:O	1:A:317:LYS:HB2	2.21	0.40
2:B:317:LYS:CD	2:B:317:LYS:N	2.77	0.40
3:C:5:DG:N2	4:E:14:DC:N3	2.56	0.40
2:B:284:ILE:C	2:B:285:HIS:ND1	2.74	0.40
1:A:8:PHE:HD2	1:A:11:PHE:CD1	2.39	0.40
1:A:197:LEU:HD12	1:A:208:ILE:HG21	2.02	0.40
1:A:170:GLU:HG3	1:A:173:ARG:HG2	2.04	0.40
4:F:6:DG:C4	4:F:7:DA:N7	2.89	0.40
2:B:284:ILE:O	2:B:285:HIS:ND1	2.55	0.40
1:A:148:LYS:N	6:A:2049:HOH:O	2.22	0.40
1:A:131:LYS:HB2	1:A:131:LYS:HE2	1.92	0.40
2:B:101:ILE:O	2:B:101:ILE:HG22	2.19	0.40
2:B:293:LEU:O	2:B:294:ASP:OD2	2.40	0.40
2:B:263:PRO:O	2:B:264:TYR:C	2.60	0.40
2:B:163:ILE:O	6:B:2037:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	340/358 (95%)	237 (70%)	65 (19%)	38 (11%)	0	0
2	B	341/358 (95%)	238 (70%)	68 (20%)	35 (10%)	1	0
All	All	681/716 (95%)	475 (70%)	133 (20%)	73 (11%)	0	0

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	36	ARG
1	A	117[A]	ASP
1	A	146	LYS
1	A	173	ARG
1	A	208	ILE
1	A	214	LYS
1	A	220	ALA
1	A	237	ILE
1	A	238	ARG
1	A	277	ASP
1	A	290	THR
1	A	328	ARG
2	B	179	ASP
2	B	204	ASP
2	B	208	ILE
2	B	234	ASN
2	B	240	ARG
2	B	291	GLU
2	B	294	ASP
2	B	321	LYS
1	A	161	ASN
1	A	172	LYS
1	A	175	ILE
1	A	177	GLU
1	A	234	ASN
1	A	292[A]	ASP
1	A	325	GLU
2	B	35[B]	GLY
2	B	180	ILE
2	B	213	LEU
2	B	251	MET
2	B	258	LEU
2	B	277[B]	ASP
1	A	12	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	112[A]	SER
1	A	127	GLU
1	A	136	GLU
1	A	145	SER
1	A	148	LYS
1	A	152	LYS
1	A	167[A]	ASP
1	A	191	ALA
1	A	192	GLU
1	A	207	SER
1	A	222	ALA
1	A	231	ASP
2	B	10	TYR
2	B	134	GLU
2	B	135	LYS
2	B	145	SER
2	B	247	ARG
2	B	260	GLU
2	B	293	LEU
2	B	296	VAL
1	A	232	GLU
1	A	233	TYR
2	B	52	LYS
2	B	167	ASP
2	B	252	LYS
1	A	104	ILE
1	A	308	LYS
2	B	22	SER
2	B	196	LYS
2	B	214	LYS
2	B	338	SER
2	B	39	ASP
2	B	115	VAL
2	B	117	ASP
2	B	154	ALA
2	B	68	LEU
1	A	111	ILE
2	B	111	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/315 (95%)	219 (73%)	81 (27%)	0	0
2	B	301/315 (96%)	217 (72%)	84 (28%)	0	0
All	All	601/630 (95%)	436 (72%)	165 (28%)	0	0

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	5	PHE
1	A	7	ASP
1	A	22	SER
1	A	31	CYS
1	A	32	VAL
1	A	49	GLU
1	A	56	LYS
1	A	59	ILE
1	A	63	GLU
1	A	65	LYS
1	A	66	LYS
1	A	75	PRO
1	A	78	LYS
1	A	81	TYR
1	A	83	GLN
1	A	90	ASN
1	A	91	LEU
1	A	93	ARG
1	A	96	SER
1	A	97	GLU
1	A	98	LYS
1	A	105	ASP
1	A	110[A]	ASP
1	A	116[A]	ARG
1	A	117[A]	ASP
1	A	119[A]	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	120	GLU
1	A	124	LEU
1	A	129	LYS
1	A	133	LEU
1	A	134	GLU
1	A	135	LYS
1	A	138	ILE
1	A	139	THR
1	A	144	ILE
1	A	148	LYS
1	A	153	ILE
1	A	159	LYS
1	A	163	ILE
1	A	167[A]	ASP
1	A	169	GLU
1	A	176	ARG
1	A	177	GLU
1	A	180	ILE
1	A	195	LYS
1	A	196	LYS
1	A	197	LEU
1	A	201	LYS
1	A	207	SER
1	A	209	GLU
1	A	210	PHE
1	A	214	LYS
1	A	219	GLU
1	A	227	SER
1	A	232	GLU
1	A	236	PRO
1	A	238	ARG
1	A	239	THR
1	A	240	ARG
1	A	242	ARG
1	A	252	LYS
1	A	255	SER
1	A	256	ARG
1	A	270	GLU
1	A	271	GLU
1	A	272	SER
1	A	273	TYR
1	A	291	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	293	LEU
1	A	295	ILE
1	A	296	VAL
1	A	298	ARG
1	A	302	PHE
1	A	326	ASP
1	A	327	GLU
1	A	328	ARG
1	A	332	ARG
1	A	333	ILE
1	A	335	VAL
1	A	336	ARG
2	B	4	LEU
2	B	8	PHE
2	B	19	LEU
2	B	22	SER
2	B	36	ARG
2	B	37	PHE
2	B	40	SER
2	B	45	THR
2	B	47	ASN
2	B	56	LYS
2	B	62	VAL
2	B	63	GLU
2	B	65	LYS
2	B	66	LYS
2	B	69	PRO
2	B	83	GLN
2	B	91	LEU
2	B	97	GLU
2	B	99	ILE
2	B	111	ILE
2	B	113	ASP
2	B	114	LYS
2	B	115	VAL
2	B	116	ARG
2	B	128	ILE
2	B	136	GLU
2	B	137	LYS
2	B	141	THR
2	B	146	LYS
2	B	153	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	157	MET
2	B	164	LYS
2	B	165	VAL
2	B	169	GLU
2	B	173	ARG
2	B	176	ARG
2	B	180	ILE
2	B	182	ASP
2	B	184	PRO
2	B	186	ILE
2	B	190	THR
2	B	193	LYS
2	B	195[B]	LYS
2	B	200	ASN
2	B	202	LEU
2	B	203	VAL
2	B	208	ILE
2	B	210	PHE
2	B	221	LYS
2	B	225	LEU
2	B	226	ILE
2	B	232	GLU
2	B	238	ARG
2	B	240	ARG
2	B	242	ARG
2	B	243	LYS
2	B	245	ILE
2	B	248	ILE
2	B	250	THR
2	B	255	SER
2	B	256	ARG
2	B	257[B]	ASN
2	B	260	GLU
2	B	267	ARG
2	B	270	GLU
2	B	273	TYR
2	B	274	TYR
2	B	277[B]	ASP
2	B	278	LYS
2	B	281	PRO
2	B	292	ASP
2	B	293	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	294	ASP
2	B	295	ILE
2	B	298	ARG
2	B	308	LYS
2	B	317	LYS
2	B	324	GLU
2	B	325	GLU
2	B	329	LYS
2	B	330	ILE
2	B	332	ARG
2	B	333	ILE
2	B	336	ARG

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

Mol	Chain	Res	Type
1	A	47	ASN
1	A	254	ASN
1	A	285	HIS
2	B	0	HIS
2	B	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DOC	C	14[A]	3	11,19,20	1.10	1 (9%)	14,26,29	2.28	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DOC	C	14[B]	3	11,19,20	0.85	0	14,26,29	1.54	2 (14%)
3	DOC	D	14[A]	3	11,19,20	1.16	1 (9%)	14,26,29	2.21	4 (28%)
3	DOC	D	14[B]	3	11,19,20	1.33	1 (9%)	14,26,29	2.16	3 (21%)
4	O2G	E	5[E]	4	17,26,27	2.35	5 (29%)	23,38,41	2.40	7 (30%)
4	O2G	F	5[F]	4	17,26,27	1.35	2 (11%)	23,38,41	2.05	7 (30%)

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
3	DOC	C	14[A]	3	-	0/3/18/19	0/2/2/2
3	DOC	C	14[B]	3	-	0/3/18/19	0/2/2/2
3	DOC	D	14[A]	3	-	0/3/18/19	0/2/2/2
3	DOC	D	14[B]	3	-	0/3/18/19	0/2/2/2
4	O2G	E	5[E]	4	-	0/7/25/26	0/3/3/3
4	O2G	F	5[F]	4	-	0/7/25/26	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5[E]	O2G	C6-C5	-5.78	1.29	1.41
4	E	5[E]	O2G	C4-N3	-3.91	1.29	1.35
3	C	14[A]	DOC	O4'-C4'	-2.61	1.38	1.44
3	D	14[A]	DOC	C6-C5	-2.18	1.33	1.38
4	E	5[E]	O2G	O6-C6	2.64	1.31	1.24
3	D	14[B]	DOC	O4'-C4'	3.08	1.51	1.44
4	F	5[F]	O2G	C2-N1	3.28	1.40	1.34
4	E	5[E]	O2G	C2-N1	3.32	1.40	1.34
4	E	5[E]	O2G	C6-N1	3.85	1.40	1.33
4	F	5[F]	O2G	C6-N1	3.85	1.40	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5[E]	O2G	C4-C5-N7	-5.57	104.36	109.48
3	D	14[B]	DOC	O4'-C4'-C5'	-5.49	101.44	109.54
4	E	5[E]	O2G	N3-C2-N1	-4.42	118.92	126.35
3	C	14[B]	DOC	O4'-C4'-C5'	-4.17	103.39	109.54
3	D	14[B]	DOC	O4'-C4'-C3'	-3.91	98.14	104.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5[F]	O2G	C5-C6-N1	-3.62	118.63	123.59
4	F	5[F]	O2G	N3-C2-N1	-3.61	120.27	126.35
3	D	14[A]	DOC	C3'-C2'-C1'	-3.01	99.34	102.71
3	D	14[A]	DOC	O4'-C1'-C2'	-2.73	103.71	106.67
3	C	14[A]	DOC	C2'-C3'-C4'	-2.58	97.55	102.59
4	E	5[E]	O2G	C6-C5-C4	-2.18	118.29	120.90
4	F	5[F]	O2G	C4-C5-N7	-2.17	107.48	109.48
4	F	5[F]	O2G	N3-C2-N2	2.19	119.63	117.16
4	F	5[F]	O2G	N1-C2-N2	2.43	119.90	117.16
4	E	5[E]	O2G	N3-C2-N2	2.58	120.08	117.16
3	C	14[A]	DOC	C2'-C1'-N1	2.72	118.00	112.49
3	D	14[B]	DOC	C2-N3-C4	2.97	119.80	115.61
4	E	5[E]	O2G	O4'-C1'-N9	3.12	113.12	107.72
3	C	14[B]	DOC	C2-N3-C4	3.16	120.07	115.61
4	E	5[E]	O2G	N1-C2-N2	3.38	120.97	117.16
3	C	14[A]	DOC	C2-N3-C4	3.61	120.70	115.61
3	C	14[A]	DOC	O4'-C4'-C3'	3.68	110.86	104.69
4	F	5[F]	O2G	O4'-C1'-N9	3.82	114.34	107.72
3	D	14[A]	DOC	C2-N3-C4	4.08	121.37	115.61
3	C	14[A]	DOC	O4'-C4'-C5'	4.70	116.48	109.54
3	D	14[A]	DOC	C2'-C1'-N1	5.15	122.91	112.49
4	F	5[F]	O2G	C2-N3-C4	5.64	121.89	115.09
4	E	5[E]	O2G	C2-N3-C4	6.25	122.61	115.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	14[A]	DOC	2	0
3	C	14[B]	DOC	8	0
3	D	14[A]	DOC	5	0
3	D	14[B]	DOC	3	0
4	E	5[E]	O2G	3	0
4	F	5[F]	O2G	17	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	342/358 (95%)	0.04	5 (1%) 76 81	21, 31, 52, 63	11 (3%)
2	B	343/358 (95%)	-0.03	2 (0%) 90 93	21, 32, 52, 67	5 (1%)
3	C	13/14 (92%)	-0.56	0 100 100	24, 33, 45, 47	0
3	D	13/14 (92%)	-0.53	0 100 100	23, 35, 54, 57	0
4	E	15/18 (83%)	-0.07	1 (6%) 21 27	34, 45, 68, 89	1 (6%)
4	F	15/18 (83%)	0.53	1 (6%) 21 27	33, 52, 69, 91	2 (13%)
All	All	741/780 (95%)	-0.00	9 (1%) 81 85	21, 33, 54, 91	19 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	3[F]	DA	12.1
4	E	3[E]	DA	4.7
2	B	250	THR	3.3
1	A	166	ILE	3.3
1	A	112[A]	SER	2.5
1	A	236	PRO	2.4
1	A	171	VAL	2.2
1	A	175	ILE	2.2
2	B	298	ARG	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	DOC	C	14[B]	18/19	0.81	0.28	-	29,31,36,36	17
4	O2G	F	5[F]	24/25	0.85	0.28	-	66,76,77,77	13
3	DOC	C	14[A]	18/19	0.81	0.28	-	37,42,44,45	18
3	DOC	D	14[B]	18/19	0.88	0.25	-	42,42,42,42	18
3	DOC	D	14[A]	18/19	0.88	0.25	-	32,38,39,39	17
4	O2G	E	5[E]	24/25	0.83	0.20	-	68,71,78,79	13

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MG	B	1343	1/1	0.98	0.26	4.92	42,42,42,42	0
5	MG	A	1343	1/1	0.91	0.20	4.72	53,53,53,53	0
5	MG	B	1342	1/1	0.94	0.16	0.86	47,47,47,47	0
5	MG	A	1342	1/1	0.97	0.09	-1.49	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.