



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:48 AM UTC

PDB ID : 2W9B / pdb_00002w9b
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

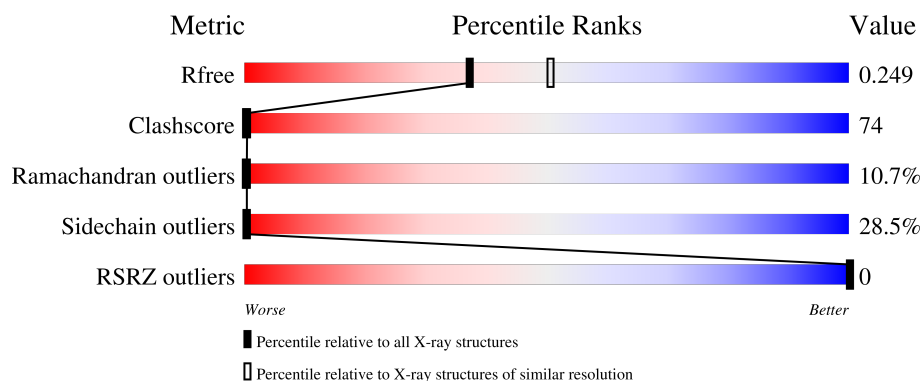
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

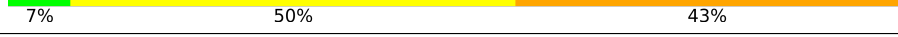
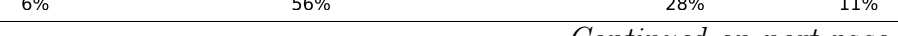
The reported resolution of this entry is 2.28 Å.

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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
2	B	358	
3	C	14	
3	D	14	
4	E	18	

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	-

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 (CCD ID: MG) (formula: Mg).

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

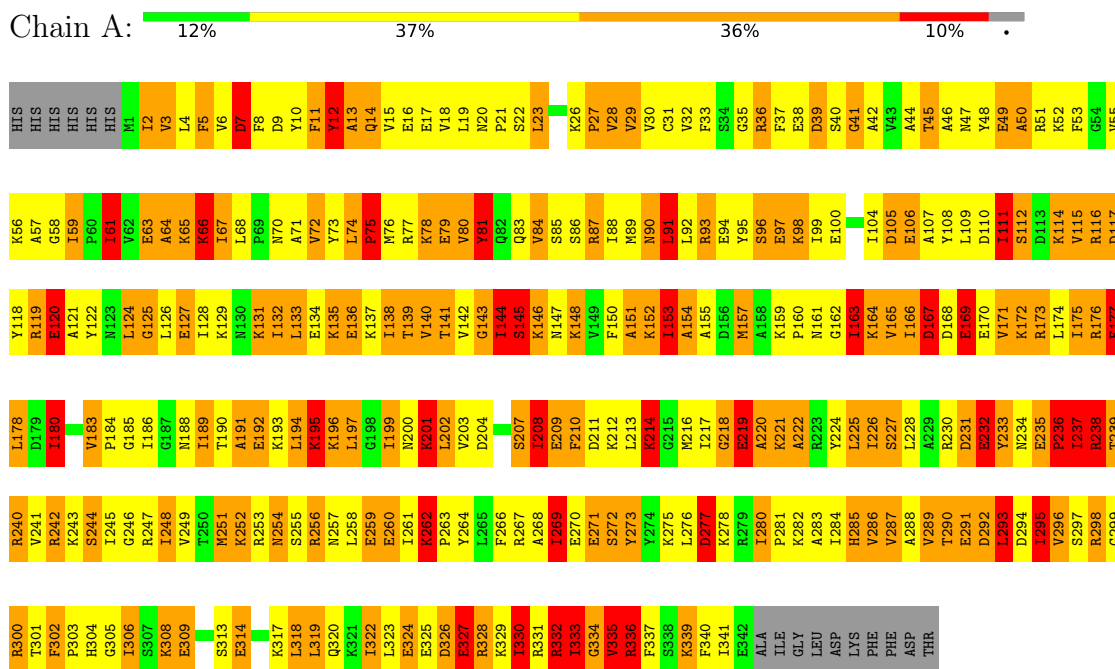
- Molecule 6 is water.

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

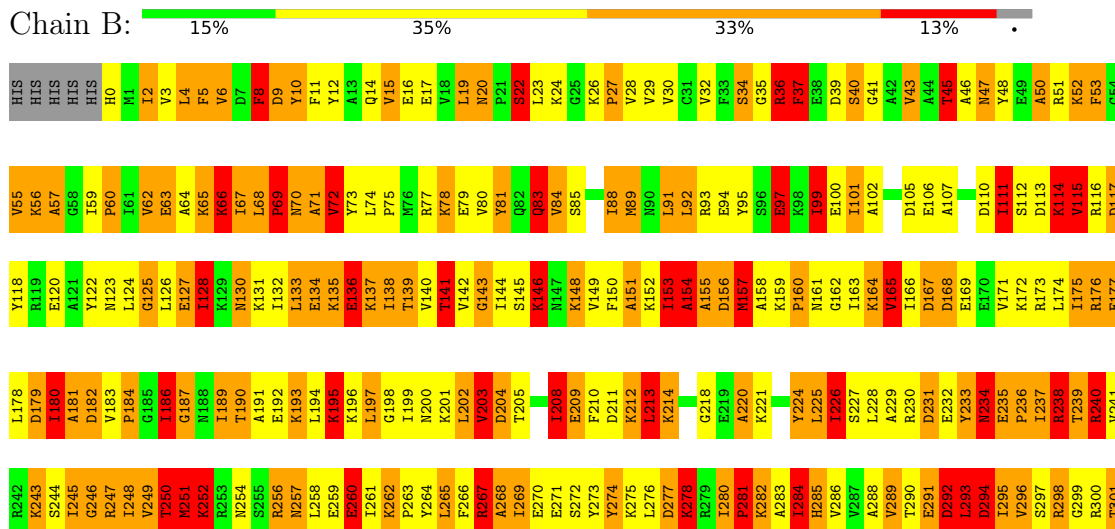
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 2: DNA POLYMERASE IV

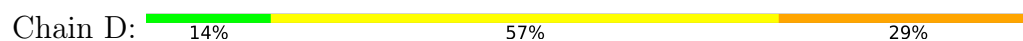




- Molecule 3: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP *TP*TP*CP*DOCP)-3'



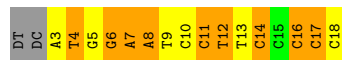
- Molecule 3: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP *TP*TP*CP*DOCP)-3'



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



- Molecule 4: 5'-D(*TP*CP*AP*TP*M2GP*GP*AP*AP*TP*CP*CP *TP*TP*CP*CP*CP*CP*CP*CP)-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 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.4 (28.75-2.28) 87.3 (28.75-2.28)	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 0.236 , 0.249	Depositor DCC
R_{free} test set	2231 reflections (4.88%)	wwPDB-VP
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 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.085 for -h,-l,-k 0.085 for -h,l,k 0.308 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	2.02	73/2785 (2.6%)	2.08	118/3741 (3.2%)
2	B	1.94	61/2794 (2.2%)	2.13	126/3753 (3.4%)
3	C	1.35	1/308 (0.3%)	1.87	5/476 (1.1%)
3	D	1.20	0/308	1.74	7/476 (1.5%)
4	E	1.17	1/327 (0.3%)	1.90	15/498 (3.0%)
4	F	1.21	1/327 (0.3%)	2.10	22/498 (4.4%)
All	All	1.86	137/6849 (2.0%)	2.07	293/9442 (3.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	43	VAL	CA-CB	12.77	1.67	1.53
1	A	84	VAL	CA-CB	-11.14	1.42	1.54
1	A	39	ASP	CA-C	10.97	1.67	1.53
2	B	249	VAL	CA-CB	10.38	1.67	1.54
2	B	30	VAL	CA-CB	-10.29	1.41	1.54
2	B	88	ILE	CA-CB	-10.20	1.39	1.54
1	A	14	GLN	C-O	-9.24	1.13	1.24
1	A	220	ALA	CA-CB	9.06	1.68	1.53
2	B	150	PHE	CA-C	-9.06	1.41	1.52
1	A	251	MET	CA-C	-9.03	1.42	1.52
1	A	155	ALA	CA-CB	9.01	1.67	1.53
1	A	332	ARG	N-CA	8.90	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	VAL	CA-CB	-8.80	1.43	1.54
2	B	141	THR	CA-CB	8.70	1.66	1.53
1	A	2	ILE	N-CA	8.68	1.57	1.46
2	B	314	GLU	CA-C	-8.56	1.41	1.52
1	A	183	VAL	CA-CB	8.40	1.61	1.54
2	B	15	VAL	CA-CB	-8.39	1.42	1.54
1	A	244	SER	CA-C	-8.26	1.42	1.52
1	A	68	LEU	CA-CB	-8.20	1.43	1.53
2	B	165	VAL	CA-CB	7.84	1.64	1.54
2	B	107	ALA	CA-CB	-7.84	1.40	1.53
1	A	165	VAL	CA-CB	7.84	1.63	1.54
4	E	4[E]	DT	P-OP2	7.81	1.64	1.48
1	A	70	ASN	CA-C	7.70	1.64	1.52
1	A	2	ILE	CA-CB	7.69	1.65	1.54
4	F	4[F]	DT	P-OP2	7.58	1.63	1.48
2	B	237	ILE	CA-C	7.54	1.60	1.53
1	A	16	GLU	CA-C	7.43	1.63	1.52
1	A	111	ILE	CA-CB	7.42	1.64	1.54
1	A	309	GLU	CA-C	-7.28	1.43	1.52
2	B	3	VAL	CA-CB	-7.25	1.45	1.54
1	A	155	ALA	C-O	-7.22	1.15	1.24
2	B	111	ILE	CA-CB	-7.20	1.44	1.54
1	A	314	GLU	CA-C	-7.18	1.42	1.52
1	A	208	ILE	CA-CB	7.10	1.64	1.54
1	A	202	LEU	CA-C	-7.03	1.43	1.52
1	A	145	SER	CA-C	7.02	1.62	1.52
1	A	289	VAL	CA-CB	-7.01	1.45	1.53
1	A	180	ILE	CA-CB	-6.98	1.46	1.54
2	B	285	HIS	CA-C	-6.89	1.45	1.52
2	B	186	ILE	CA-C	-6.79	1.45	1.52
2	B	57	ALA	CA-CB	-6.72	1.42	1.53
1	A	165	VAL	CA-C	6.71	1.60	1.52
1	A	44	ALA	N-CA	6.70	1.55	1.46
1	A	140	VAL	CA-CB	6.61	1.63	1.54
2	B	84	VAL	N-CA	-6.61	1.38	1.46
2	B	154	ALA	CA-CB	-6.59	1.42	1.53
1	A	313	SER	CA-C	6.54	1.61	1.52
1	A	286	VAL	CA-CB	-6.49	1.46	1.54
2	B	158	ALA	CA-C	6.44	1.61	1.52
1	A	68	LEU	CG-CD2	6.38	1.73	1.52
1	A	138	ILE	CG1-CD1	-6.37	1.26	1.51
1	A	141	THR	CA-CB	-6.32	1.41	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLU	N-CA	6.29	1.53	1.46
2	B	22	SER	CA-C	6.26	1.61	1.52
1	A	50	ALA	CA-CB	6.21	1.64	1.54
2	B	8	PHE	C-O	-6.20	1.16	1.23
2	B	132	ILE	N-CA	-6.15	1.39	1.46
2	B	73	TYR	N-CA	6.15	1.53	1.46
1	A	107	ALA	CA-CB	-6.09	1.44	1.53
2	B	189	ILE	CA-CB	6.08	1.61	1.54
2	B	102	ALA	CA-C	-6.07	1.44	1.52
1	A	58	GLY	C-O	6.06	1.32	1.23
2	B	69	PRO	CA-C	-6.01	1.43	1.52
1	A	330	ILE	CA-CB	5.99	1.61	1.54
2	B	268	ALA	CA-CB	-5.98	1.44	1.53
1	A	318	LEU	C-O	-5.93	1.17	1.24
1	A	327	GLU	CA-C	5.92	1.58	1.52
1	A	132	ILE	CA-CB	-5.89	1.46	1.54
2	B	286	VAL	CA-CB	-5.89	1.47	1.54
2	B	281	PRO	N-CA	-5.87	1.41	1.46
2	B	60	PRO	CA-C	-5.82	1.46	1.52
1	A	287	VAL	C-O	-5.79	1.17	1.24
1	A	332	ARG	CA-C	5.78	1.60	1.52
2	B	81	TYR	N-CA	5.73	1.53	1.46
2	B	34	SER	CA-C	5.71	1.60	1.52
1	A	164	LYS	CA-C	-5.71	1.45	1.52
2	B	151	ALA	CA-CB	5.70	1.62	1.53
1	A	45	THR	C-O	5.65	1.30	1.23
2	B	310	THR	CA-C	5.64	1.59	1.52
2	B	220	ALA	N-CA	-5.63	1.39	1.46
1	A	235	GLU	CA-CB	-5.63	1.44	1.54
1	A	283	ALA	CA-CB	-5.63	1.43	1.53
2	B	284	ILE	CA-C	5.61	1.59	1.52
1	A	313	SER	N-CA	5.61	1.52	1.46
1	A	75	PRO	N-CA	-5.60	1.40	1.47
2	B	311	ALA	CA-CB	-5.59	1.44	1.53
2	B	72	VAL	CA-CB	-5.57	1.47	1.54
2	B	139	THR	C-O	5.54	1.30	1.23
1	A	221	LYS	CB-CG	5.54	1.69	1.52
2	B	75	PRO	CA-C	-5.52	1.45	1.52
1	A	20	ASN	C-N	-5.51	1.28	1.34
2	B	239	THR	CA-C	-5.50	1.45	1.52
1	A	295	ILE	CA-CB	5.48	1.61	1.54
1	A	61	ILE	CA-CB	5.48	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	85	SER	CA-C	-5.47	1.45	1.52
2	B	155	ALA	CA-CB	5.46	1.62	1.53
1	A	199	ILE	CA-C	5.43	1.58	1.52
2	B	72	VAL	CA-C	-5.42	1.46	1.52
1	A	72	VAL	CA-CB	5.39	1.60	1.54
1	A	285	HIS	C-O	-5.39	1.17	1.24
1	A	13	ALA	CA-CB	5.39	1.61	1.53
2	B	89	MET	CA-C	-5.39	1.46	1.52
2	B	180	ILE	CA-CB	-5.38	1.47	1.54
1	A	231	ASP	N-CA	5.36	1.53	1.46
1	A	146	LYS	N-CA	5.30	1.53	1.46
1	A	237	ILE	CA-C	5.29	1.59	1.52
1	A	106	GLU	CB-CG	5.29	1.68	1.52
2	B	175	ILE	C-O	-5.28	1.18	1.24
2	B	83	GLN	C-O	5.27	1.30	1.24
2	B	115	VAL	CA-CB	5.26	1.61	1.54
2	B	67	ILE	N-CA	-5.25	1.39	1.46
2	B	84	VAL	CA-CB	-5.25	1.48	1.54
1	A	7	ASP	C-O	-5.22	1.16	1.23
1	A	154	ALA	CA-C	5.21	1.59	1.52
2	B	181	ALA	CA-C	5.20	1.59	1.52
2	B	175	ILE	CA-CB	5.20	1.60	1.54
2	B	249	VAL	CA-C	5.19	1.59	1.52
1	A	91	LEU	CA-C	5.18	1.59	1.52
1	A	248	ILE	CG1-CD1	5.18	1.72	1.51
2	B	29	VAL	CA-CB	-5.16	1.47	1.54
2	B	186	ILE	CA-CB	-5.16	1.48	1.53
2	B	250	THR	N-CA	5.16	1.52	1.46
1	A	57	ALA	CA-C	-5.15	1.46	1.52
2	B	212	LYS	CA-C	5.13	1.59	1.52
1	A	27	PRO	C-O	-5.12	1.17	1.23
1	A	90	ASN	C-O	-5.12	1.18	1.24
2	B	246	GLY	CA-C	-5.10	1.46	1.52
1	A	277	ASP	CB-CG	5.07	1.64	1.52
3	C	4	DG	P-OP2	5.06	1.58	1.48
1	A	333	ILE	CA-CB	-5.05	1.47	1.54
1	A	157	MET	N-CA	5.05	1.52	1.46
2	B	123	ASN	N-CA	-5.04	1.40	1.46
2	B	235	GLU	N-CA	5.04	1.53	1.46
1	A	6	VAL	CA-CB	5.02	1.61	1.54
1	A	153	ILE	C-O	5.01	1.30	1.24

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	322	ILE	CB-CA-C	-12.70	96.91	110.62
2	B	323	LEU	N-CA-C	-12.41	98.17	113.18
2	B	235	GLU	CA-C-N	11.73	131.84	119.76
2	B	235	GLU	C-N-CA	11.73	131.84	119.76
2	B	20	ASN	CA-C-N	-11.15	105.91	119.84
2	B	20	ASN	C-N-CA	-11.15	105.91	119.84
2	B	203	VAL	N-CA-C	-10.73	103.14	111.62
1	A	22	SER	N-CA-C	-10.55	99.67	112.54
1	A	269	ILE	N-CA-C	10.54	120.54	110.42
4	E	13	DT	C4'-C3'-O3'	-10.29	94.57	110.00
2	B	130	ASN	N-CA-C	10.27	124.49	111.24
2	B	233	TYR	N-CA-C	10.19	122.38	111.28
2	B	84	VAL	N-CA-C	-10.18	100.96	110.53
2	B	151	ALA	N-CA-C	-10.11	98.98	111.11
1	A	280	ILE	CA-C-N	10.08	132.63	120.23
1	A	280	ILE	C-N-CA	10.08	132.63	120.23
1	A	254	ASN	N-CA-C	-10.06	96.67	110.35
2	B	197	LEU	N-CA-C	-10.03	99.86	113.30
1	A	144	ILE	N-CA-C	9.88	121.94	108.11
1	A	84	VAL	CB-CA-C	-9.84	99.29	111.88
2	B	186	ILE	CB-CA-C	-9.61	99.04	111.25
2	B	72	VAL	CB-CA-C	-9.25	97.55	111.33
1	A	287	VAL	CB-CA-C	-9.23	100.85	111.09
1	A	142	VAL	CB-CA-C	-9.17	96.70	110.82
2	B	269	ILE	N-CA-C	-9.17	101.93	110.82
4	F	11	DC	C2'-C3'-O3'	9.08	125.11	111.50
2	B	175	ILE	N-CA-C	-9.01	100.90	110.36
2	B	187	GLY	N-CA-C	8.98	125.89	112.41
1	A	120	GLU	N-CA-C	-8.86	103.58	112.97
1	A	260	GLU	N-CA-C	-8.75	103.11	113.88
1	A	335	VAL	N-CA-C	8.75	119.26	108.06
1	A	115[A]	VAL	N-CA-C	8.73	120.46	107.80
1	A	313	SER	N-CA-C	8.68	125.61	111.37
1	A	29	VAL	N-CA-CB	-8.61	104.04	112.65
2	B	88	ILE	CB-CA-C	-8.61	99.52	111.65
1	A	199	ILE	N-CA-C	8.58	120.17	108.84
2	B	50	ALA	N-CA-C	-8.31	103.66	113.88
1	A	319	LEU	N-CA-C	8.29	119.94	111.07
1	A	163	ILE	CA-C-N	-8.26	111.32	122.72
1	A	163	ILE	C-N-CA	-8.26	111.32	122.72
1	A	74	LEU	N-CA-C	8.13	122.42	109.40
1	A	88	ILE	CA-C-N	-8.07	109.95	120.44
1	A	88	ILE	C-N-CA	-8.07	109.95	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	211	ASP	N-CA-C	-8.03	103.43	113.55
1	A	165	VAL	N-CA-C	8.02	119.83	108.36
1	A	23	LEU	N-CA-C	7.94	121.03	111.82
2	B	249	VAL	N-CA-C	7.89	119.15	108.11
2	B	24	LYS	N-CA-C	-7.80	98.73	110.28
4	F	8	DA	N9-C1'-C2'	-7.72	101.92	113.50
1	A	96	SER	N-CA-C	7.72	121.98	109.40
2	B	130	ASN	CA-C-N	7.71	130.95	120.54
2	B	130	ASN	C-N-CA	7.71	130.95	120.54
2	B	240	ARG	CA-C-N	-7.65	110.53	122.69
2	B	240	ARG	C-N-CA	-7.65	110.53	122.69
4	F	11	DC	O3'-P-O5'	7.62	115.43	104.00
1	A	226	ILE	N-CA-C	7.59	117.67	110.53
2	B	45	THR	N-CA-C	7.59	120.75	108.76
1	A	141	THR	CB-CA-C	-7.58	97.08	109.89
4	F	13	DT	O4'-C1'-N1	-7.56	97.06	108.40
3	C	1	DG	C4'-C3'-O3'	-7.54	98.69	110.00
2	B	295	ILE	CB-CA-C	-7.51	103.03	111.45
2	B	252	LYS	N-CA-C	-7.46	94.90	110.80
1	A	20	ASN	CA-C-N	-7.45	111.85	120.12
1	A	20	ASN	C-N-CA	-7.45	111.85	120.12
1	A	201	LYS	N-CA-C	7.42	118.31	108.07
2	B	143	GLY	N-CA-C	-7.41	95.61	113.18
4	E	13	DT	C2'-C3'-O3'	7.37	122.55	111.50
1	A	29	VAL	N-CA-C	7.27	117.40	106.42
1	A	189	ILE	CB-CA-C	-7.25	99.39	111.29
1	A	140	VAL	CA-C-N	7.21	133.90	121.64
1	A	140	VAL	C-N-CA	7.21	133.90	121.64
2	B	3	VAL	N-CA-C	7.20	118.49	108.12
1	A	64	ALA	N-CA-C	-7.17	103.15	112.68
3	C	5	DG	O4'-C1'-N9	7.15	119.13	108.40
1	A	259	GLU	N-CA-C	-7.15	104.30	113.16
1	A	194	LEU	N-CA-C	7.14	122.28	113.50
2	B	187	GLY	CA-C-O	7.10	129.38	122.28
1	A	143	GLY	O-C-N	7.03	128.93	123.23
2	B	280	ILE	CA-C-N	-7.02	113.01	120.66
2	B	280	ILE	C-N-CA	-7.02	113.01	120.66
1	A	225	LEU	CA-C-N	6.97	129.48	120.56
1	A	225	LEU	C-N-CA	6.97	129.48	120.56
1	A	151	ALA	N-CA-C	-6.95	102.27	111.24
2	B	27	PRO	CA-C-N	-6.95	113.33	122.99
2	B	27	PRO	C-N-CA	-6.95	113.33	122.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	TYR	N-CA-C	-6.90	103.45	110.97
4	E	8	DA	P-O5'-C5'	-6.90	109.65	120.00
1	A	138	ILE	N-CA-C	6.88	118.96	108.71
1	A	334	GLY	CA-C-O	-6.85	114.94	121.38
1	A	339	LYS	CA-C-N	6.79	130.40	120.82
1	A	339	LYS	C-N-CA	6.79	130.40	120.82
2	B	142	VAL	N-CA-C	-6.79	100.01	109.45
1	A	61	ILE	N-CA-C	-6.79	103.87	110.72
4	F	13	DT	C2'-C3'-O3'	6.78	121.66	111.50
1	A	42	ALA	CA-C-O	-6.72	113.24	121.11
2	B	292	ASP	N-CA-C	-6.71	100.27	110.14
1	A	163	ILE	N-CA-C	6.70	118.50	107.24
2	B	336	ARG	NE-CZ-NH1	-6.70	114.80	121.50
2	B	335	VAL	N-CA-C	6.68	117.78	108.23
1	A	125	GLY	N-CA-C	-6.66	97.39	113.18
2	B	70	ASN	CA-C-N	-6.65	110.63	122.74
2	B	70	ASN	C-N-CA	-6.65	110.63	122.74
2	B	156	ASP	CA-C-N	-6.60	109.58	121.14
2	B	156	ASP	C-N-CA	-6.60	109.58	121.14
4	E	12	DT	P-O5'-C5'	-6.60	110.10	120.00
2	B	209	GLU	N-CA-C	6.55	120.18	109.24
4	F	8	DA	C4'-C3'-O3'	-6.54	100.19	110.00
1	A	269	ILE	CB-CA-C	-6.53	103.61	111.97
4	E	16	DC	C5'-C4'-O4'	-6.51	99.64	109.40
2	B	36	ARG	CA-C-N	-6.50	113.58	122.16
2	B	36	ARG	C-N-CA	-6.50	113.58	122.16
2	B	125	GLY	N-CA-C	-6.50	97.77	113.18
2	B	9	ASP	N-CA-C	-6.47	100.90	110.48
2	B	236	PRO	N-CA-C	6.46	121.22	111.14
1	A	339	LYS	N-CA-C	6.45	120.30	111.39
2	B	5	PHE	CA-C-N	6.44	131.94	122.99
2	B	5	PHE	C-N-CA	6.44	131.94	122.99
2	B	168	ASP	CA-C-N	6.43	129.38	120.63
2	B	168	ASP	C-N-CA	6.43	129.38	120.63
1	A	59	ILE	CA-C-N	6.42	126.40	119.78
1	A	59	ILE	C-N-CA	6.42	126.40	119.78
4	E	15	DC	C2'-C3'-O3'	-6.42	101.87	111.50
2	B	289	VAL	CA-C-N	-6.40	109.56	120.95
2	B	289	VAL	C-N-CA	-6.40	109.56	120.95
4	F	13	DT	N1-C1'-C2'	6.39	123.08	113.50
1	A	18	VAL	N-CA-C	-6.35	106.61	112.96
2	B	153	ILE	N-CA-C	-6.33	104.16	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	235	GLU	O-C-N	6.29	128.55	121.32
1	A	7	ASP	CA-C-O	-6.27	113.75	121.78
4	E	18	DC	P-O5'-C5'	-6.23	110.65	120.00
1	A	28	VAL	CA-C-N	-6.23	117.05	122.96
1	A	28	VAL	C-N-CA	-6.23	117.05	122.96
3	C	13	DC	C2'-C3'-O3'	6.19	120.78	111.50
2	B	6	VAL	CB-CA-C	-6.15	101.35	110.33
1	A	195	LYS	N-CA-C	-6.15	105.61	113.23
2	B	71	ALA	CA-C-N	-6.14	112.63	120.98
2	B	71	ALA	C-N-CA	-6.14	112.63	120.98
2	B	231	ASP	N-CA-C	-6.13	103.47	111.74
1	A	306	ILE	N-CA-C	6.11	116.92	107.99
4	E	7	DA	P-O3'-C3'	-6.11	111.04	120.20
4	F	11	DC	P-O3'-C3'	6.10	129.35	120.20
1	A	72	VAL	N-CA-CB	6.07	117.92	111.00
4	F	12	DT	O4'-C1'-N1	6.06	117.48	108.40
3	D	10	DA	C4'-C3'-O3'	6.05	119.07	110.00
1	A	196	LYS	N-CA-C	-6.04	105.87	113.18
2	B	335	VAL	CB-CA-C	-6.02	99.97	110.38
1	A	29	VAL	CB-CA-C	6.01	117.31	111.23
1	A	166	ILE	N-CA-C	6.01	121.85	109.34
1	A	295	ILE	N-CA-C	6.00	117.37	109.21
2	B	236	PRO	CA-C-N	6.00	129.98	122.48
2	B	236	PRO	C-N-CA	6.00	129.98	122.48
1	A	236	PRO	N-CA-C	5.99	123.49	111.69
2	B	2	ILE	N-CA-C	5.99	116.56	108.17
3	D	7	DA	N9-C1'-C2'	5.97	122.45	113.50
1	A	293	LEU	N-CA-C	5.96	120.50	113.23
1	A	183	VAL	CB-CA-C	5.95	117.13	110.52
1	A	114	LYS	CA-C-N	-5.95	115.39	123.12
1	A	114	LYS	C-N-CA	-5.95	115.39	123.12
1	A	119[A]	ARG	N-CA-C	-5.87	102.57	111.56
2	B	334	GLY	CA-C-O	-5.87	115.22	121.38
2	B	75	PRO	CA-C-N	-5.86	113.04	121.42
2	B	75	PRO	C-N-CA	-5.86	113.04	121.42
1	A	324	GLU	N-CA-C	-5.86	98.32	110.80
2	B	138	ILE	N-CA-C	5.86	115.56	108.06
2	B	2	ILE	CB-CA-C	-5.85	102.11	110.83
2	B	97	GLU	N-CA-C	-5.84	104.51	111.69
2	B	140	VAL	N-CA-C	-5.83	99.90	108.23
1	A	219	GLU	O-C-N	5.83	129.44	122.27
2	B	211	ASP	CA-C-N	5.81	128.32	120.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	211	ASP	C-N-CA	5.81	128.32	120.65
1	A	50	ALA	CA-C-N	-5.80	112.71	120.54
1	A	50	ALA	C-N-CA	-5.80	112.71	120.54
3	D	9	DG	O3'-P-O5'	-5.78	95.33	104.00
4	F	16	DC	C4'-C3'-O3'	-5.78	101.33	110.00
1	A	336	ARG	CG-CD-NE	-5.77	99.31	112.00
2	B	203	VAL	CB-CA-C	5.77	116.18	111.05
4	F	8	DA	C3'-C2'-C1'	5.75	110.23	101.60
1	A	5	PHE	N-CA-C	-5.75	100.52	109.72
2	B	302	PHE	CA-C-N	-5.74	113.70	119.56
2	B	302	PHE	C-N-CA	-5.74	113.70	119.56
1	A	237	ILE	N-CA-C	5.71	121.23	109.34
4	E	7	DA	O4'-C1'-C2'	-5.71	97.84	106.40
2	B	116	ARG	N-CA-C	5.69	118.84	107.62
1	A	336	ARG	CB-CA-C	-5.69	99.47	109.71
1	A	75	PRO	CA-C-N	5.68	132.39	121.54
1	A	75	PRO	C-N-CA	5.68	132.39	121.54
2	B	320	GLN	N-CA-C	-5.68	104.99	111.07
1	A	262	LYS	N-CA-C	5.66	120.45	112.75
2	B	78	LYS	CB-CG-CD	5.66	124.31	111.30
2	B	17	GLU	N-CA-C	-5.65	104.59	112.45
3	D	7	DA	C4'-C3'-O3'	5.65	118.47	110.00
2	B	146	LYS	N-CA-C	5.63	120.31	113.38
4	F	13	DT	O5'-C5'-C4'	-5.63	102.35	110.80
1	A	29	VAL	CA-C-N	-5.63	112.74	121.18
1	A	29	VAL	C-N-CA	-5.63	112.74	121.18
1	A	314	GLU	N-CA-C	-5.59	105.56	112.38
1	A	67	ILE	CB-CA-C	-5.58	104.76	112.24
1	A	74	LEU	CA-C-N	-5.56	114.23	119.85
1	A	74	LEU	C-N-CA	-5.56	114.23	119.85
4	F	10	DC	C5'-C4'-C3'	-5.54	106.59	114.90
2	B	329	LYS	N-CA-C	-5.52	101.16	109.60
3	C	9	DG	O3'-P-O5'	-5.49	95.77	104.00
1	A	27	PRO	CB-CA-C	-5.49	104.73	111.64
4	F	17	DC	N1-C1'-C2'	5.47	121.71	113.50
2	B	99	ILE	CB-CA-C	-5.47	102.07	110.50
2	B	183	VAL	CA-C-N	5.46	126.67	119.84
2	B	183	VAL	C-N-CA	5.46	126.67	119.84
2	B	57	ALA	CA-C-O	-5.46	115.17	121.07
4	F	11	DC	C4'-C3'-O3'	-5.46	101.81	110.00
4	E	8	DA	O3'-P-O5'	-5.44	95.83	104.00
4	E	15	DC	C3'-C2'-C1'	-5.44	93.44	101.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ILE	O-C-N	5.42	127.28	121.10
1	A	45	THR	CB-CA-C	-5.42	100.25	110.16
2	B	195[B]	LYS	N-CA-C	-5.41	99.28	110.80
2	B	128	ILE	N-CA-C	5.41	115.61	110.53
2	B	28	VAL	N-CA-C	-5.39	100.35	108.12
3	D	7	DA	C5'-C4'-O4'	-5.39	101.31	109.40
1	A	145	SER	N-CA-C	5.39	122.28	110.80
1	A	189	ILE	N-CA-C	5.38	120.53	109.34
2	B	34	SER	N-CA-C	-5.37	105.56	113.61
1	A	335	VAL	CB-CA-C	-5.36	103.54	111.80
2	B	92	LEU	N-CA-C	-5.36	105.87	112.90
2	B	262	LYS	CA-C-N	-5.36	113.14	119.84
2	B	262	LYS	C-N-CA	-5.36	113.14	119.84
2	B	72	VAL	N-CA-C	-5.35	102.61	109.30
3	D	7	DA	C2'-C3'-O3'	5.35	119.52	111.50
1	A	218	GLY	N-CA-C	-5.34	106.31	112.29
2	B	267	ARG	N-CA-C	-5.34	105.86	112.38
1	A	144	ILE	CB-CA-C	-5.34	102.73	110.63
3	D	13	DC	N1-C1'-C2'	5.34	121.51	113.50
2	B	66	LYS	CA-CB-CG	5.33	124.76	114.10
2	B	101	ILE	CB-CA-C	-5.33	104.48	111.25
2	B	274	TYR	N-CA-C	-5.32	105.39	111.14
2	B	157	MET	CB-CG-SD	-5.32	96.74	112.70
2	B	226	ILE	N-CA-C	-5.32	104.70	110.23
4	F	7	DA	C5'-C4'-C3'	-5.29	106.96	114.90
1	A	65	LYS	N-CA-C	-5.28	105.94	112.38
4	F	9	DT	C4-C5-C7	-5.28	114.48	122.40
4	F	6	DG	C5'-C4'-O4'	-5.27	101.49	109.40
2	B	136	GLU	CA-C-N	-5.26	115.05	122.63
2	B	136	GLU	C-N-CA	-5.26	115.05	122.63
3	C	11	DT	P-O5'-C5'	-5.26	112.11	120.00
2	B	297	SER	N-CA-C	5.26	118.00	108.69
2	B	139	THR	N-CA-C	-5.25	101.16	109.76
2	B	53	PHE	N-CA-C	-5.24	106.67	114.64
1	A	208	ILE	N-CA-C	5.24	120.23	109.34
4	E	15	DC	O5'-C5'-C4'	-5.23	102.96	110.80
4	F	7	DA	O3'-P-O5'	-5.22	96.16	104.00
1	A	211	ASP	N-CA-C	-5.22	106.91	113.28
1	A	169	GLU	N-CA-C	-5.22	105.20	112.45
2	B	278	LYS	N-CA-C	5.22	121.91	110.80
4	E	10	DC	C5'-C4'-C3'	-5.22	107.08	114.90
2	B	250	THR	CB-CA-C	-5.21	101.06	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	16	DC	C5'-C4'-O4'	-5.20	101.60	109.40
1	A	81	TYR	N-CA-C	5.20	119.33	112.89
1	A	41	GLY	N-CA-C	5.18	117.74	110.38
1	A	66	LYS	CB-CA-C	-5.18	102.71	110.90
1	A	273	TYR	N-CA-C	5.18	118.86	112.54
2	B	175	ILE	N-CA-CB	5.18	116.26	110.51
1	A	171	VAL	N-CA-C	-5.18	105.45	110.42
4	E	13	DT	N1-C1'-C2'	5.18	121.27	113.50
1	A	12	TYR	CB-CA-C	-5.18	100.12	110.42
2	B	55	VAL	N-CA-C	-5.17	98.58	109.34
1	A	72	VAL	CB-CA-C	-5.17	104.70	110.96
2	B	94	GLU	N-CA-C	-5.17	107.26	113.21
1	A	16	GLU	O-C-N	-5.17	115.61	122.33
2	B	158	ALA	N-CA-C	5.17	119.67	112.90
1	A	12	TYR	N-CA-C	5.16	121.80	110.80
1	A	91	LEU	CA-CB-CG	5.16	134.37	116.30
2	B	177	GLU	CB-CA-C	-5.14	101.28	110.70
2	B	114	LYS	CB-CA-C	-5.13	102.67	110.88
1	A	220	ALA	CA-C-N	5.11	127.44	120.54
1	A	220	ALA	C-N-CA	5.11	127.44	120.54
2	B	282	LYS	CG-CD-CE	5.10	123.03	111.30
2	B	37	PHE	N-CA-C	5.10	118.08	108.65
4	F	14	DC	C2'-C3'-O3'	5.09	119.13	111.50
2	B	265	LEU	N-CA-C	-5.07	105.83	111.36
2	B	202	LEU	CA-C-N	-5.06	117.79	123.16
2	B	202	LEU	C-N-CA	-5.06	117.79	123.16
1	A	106	GLU	CA-CB-CG	5.05	124.21	114.10
1	A	300	ARG	CG-CD-NE	-5.05	100.89	112.00
1	A	164	LYS	N-CA-C	5.05	117.47	109.24
2	B	333	ILE	CB-CA-C	-5.04	102.62	110.69
2	B	27	PRO	CB-CA-C	-5.03	106.07	111.56
1	A	242	ARG	N-CA-C	-5.03	103.15	110.24
2	B	67	ILE	N-CA-C	-5.02	98.90	109.34
1	A	14	GLN	CA-C-O	-5.02	115.73	120.90
4	E	13	DT	C6-C5-C7	-5.01	116.48	124.00
2	B	234	ASN	N-CA-C	5.01	121.47	110.80
1	A	27	PRO	CA-C-N	-5.01	115.49	122.75
1	A	27	PRO	C-N-CA	-5.01	115.49	122.75
4	F	8	DA	C5'-C4'-O4'	5.01	116.91	109.40
2	B	224	TYR	CA-C-O	-5.00	115.55	120.70

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2746	0	2872	464	0
2	B	2754	0	2880	430	0
3	C	309	0	167	28	0
3	D	309	0	170	26	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	968	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 74.

All (968) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:NH1	1:A:93:ARG:HB2	1.60	1.16
2:B:114:LYS:HD2	2:B:114:LYS:H	1.07	1.15
2:B:195[B]:LYS:C	2:B:198:GLY:H	1.56	1.13
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:HH11	1:A:298:ARG:HG2	1.02	1.09
1:A:93:ARG:HB2	1:A:93:ARG:HH11	1.02	1.09
2:B:78:LYS:HA	2:B:81:TYR:HD2	1.09	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
1:A:10:TYR:HD1	1:A:13:ALA:HB3	1.20	1.02
2:B:332:ARG:HH12	4:F:5[F]:O2G:H2'A	0.91	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
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:HD2	1:A:210:PHE:O	1.50	0.94
2:B:322:ILE:HG22	2:B:322:ILE:O	1.68	0.93
1:A:228:LEU:HD23	1:A:233:TYR:HB2	1.49	0.93
2:B:324:GLU:C	2:B:325:GLU:OE1	2.11	0.93
1:A:197:LEU:HD13	1:A:212:LYS:NZ	1.83	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HG12	1:A:164:LYS:O	1.68	0.93
1:A:200:ASN:C	1:A:201:LYS:HD2	1.93	0.93
2:B:114:LYS:HD2	2:B:114:LYS:N	1.80	0.92
1:A:298:ARG:HG3	1:A:322:ILE:HG12	1.49	0.92
1:A:238:ARG:HH11	1:A:238:ARG:HG2	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:141:THR:HG23	2:B:162:GLY:H	1.34	0.92
2:B:228:LEU:HD21	2:B:233:TYR:CD1	2.04	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:126:LEU:O	2:B:130:ASN:HB2	1.72	0.90
2:B:195[B]:LYS:CA	2:B:198:GLY:H	1.84	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:301:THR:HG22	2:B:301:THR:O	1.70	0.89
2:B:181:ALA:HA	2:B:186:ILE:HG21	1.52	0.88
1:A:91:LEU:O	1:A:94:GLU:HB3	1.72	0.88
2:B:88:ILE:HG22	2:B:88:ILE:O	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
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:HG12	2:B:111:ILE:O	1.77	0.85
1:A:288:ALA:HB1	1:A:330:ILE:HG21	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:CD	1:A:79:GLU:H	1.85	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:N	1:A:327:GLU:OE1	2.11	0.84
2:B:228:LEU:HD23	2:B:233:TYR:HB2	1.60	0.84
2:B:99:ILE:HG23	2:B:99:ILE:O	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
2:B:43:VAL:HG12	2:B:57:ALA:HA	1.60	0.83
3:C:13:DC:H5'	3:C:14[B]:DOC:C5	2.09	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
1:A:285:HIS:CD2	1:A:299:GLY:HA3	2.14	0.82
2:B:79:GLU:N	2:B:79:GLU:OE1	2.11	0.82
2:B:192:GLU:O	2:B:195[B]:LYS:HG2	1.79	0.82
2:B:195[B]:LYS:C	2:B:198:GLY:N	2.36	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
1:A:227:SER:HA	1:A:230:ARG:HD2	1.62	0.81
2:B:231:ASP:OD1	2:B:231:ASP:O	1.97	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:280:ILE:CG2	1:A:305:GLY:HA3	2.10	0.81
2:B:55:VAL:HG21	2:B:68:LEU:HD12	1.63	0.81
2:B:250:THR:HA	2:B:332:ARG:CB	2.09	0.80
1:A:210:PHE:O	1:A:210:PHE:CD2	2.34	0.80
1:A:284:ILE:HG12	1:A:285:HIS:N	1.94	0.80
1:A:290:THR:HG21	1:A:328:ARG:HH22	1.47	0.80
2:B:0:HIS:NE2	2:B:2:ILE:HD11	1.97	0.80
1:A:186:ILE:HD11	1:A:225:LEU:HD21	1.64	0.80
2:B:290:THR:O	2:B:292:ASP:O	2.00	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:OE1	2:B:136:GLU:HA	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CG	1:A:298:ARG:NH1	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
1:A:127:GLU:OE1	1:A:127:GLU:C	2.28	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
1:A:115[A]:VAL:HG11	1:A:120:GLU:C	2.12	0.75
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
1:A:164:LYS:HZ3	1:A:166:ILE:HD11	1.49	0.75
1:A:170:GLU:HA	1:A:173:ARG:HB3	1.68	0.75
3:D:14[A]:DOC:OP1	6:D:2016:HOH:O	2.02	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:HG22	2:B:186:ILE:O	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
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:HD12	2:B:248:ILE:N	2.03	0.73
2:B:176:ARG:HA	2:B:203:VAL:CG1	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:77:ARG:C	2:B:81:TYR:CE2	2.67	0.73
1:A:175:ILE:HD12	1:A:202:LEU:HD13	1.71	0.73
2:B:209:GLU:C	2:B:213:LEU:HD12	2.13	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:CD1	2:B:248:ILE:N	2.52	0.72
1:A:127:GLU:OE1	1:A:128:ILE:HA	1.90	0.72
1:A:280:ILE:O	1:A:340:PHE:HA	1.90	0.71
2:B:228:LEU:HD23	2:B:233:TYR:CB	2.19	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
1:A:334:GLY:O	1:A:335:VAL:HG12	1.91	0.71
4:F:6:DG:H1'	4:F:7:DA:H5'	1.72	0.71
1:A:93:ARG:NH1	1:A:93:ARG:CB	2.47	0.70
1:A:164:LYS:NZ	1:A:166:ILE:HD11	2.06	0.70
1:A:324:GLU:C	1:A:326:ASP:H	1.99	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
1:A:108:TYR:OH	1:A:152:LYS:HD2	1.92	0.70
2:B:259:GLU:C	2:B:261:ILE:H	1.98	0.70
2:B:267:ARG:HB2	2:B:267:ARG:NH1	2.05	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:OP1	2.23	0.70
1:A:238:ARG:HG2	1:A:238:ARG:NH1	2.04	0.69
1:A:320:GLN:O	1:A:323:LEU:N	2.25	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
2:B:282:LYS:HD3	2:B:341:ILE:CG1	2.23	0.69
2:B:267:ARG:NH1	2:B:267:ARG:CB	2.55	0.69
2:B:319:LEU:HD12	2:B:319:LEU:O	1.92	0.69
1:A:27:PRO:HA	1:A:49:GLU:HB2	1.75	0.69
2:B:282:LYS:HG3	2:B:339:LYS:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:143:GLY:C	2:B:144:ILE:HG13	2.18	0.68
3:D:5:DG:H2''	3:D:6:DA:H8	1.58	0.68
1:A:197:LEU:HD23	1:A:216:MET:HG2	1.74	0.68
2:B:267:ARG:HH11	2:B:267:ARG:CB	2.06	0.68
2:B:115:VAL:HG12	2:B:115:VAL:O	1.93	0.68
2:B:23:LEU:HD22	2:B:72:VAL:HG21	1.76	0.68
2:B:319:LEU:HD12	2:B:319:LEU:C	2.19	0.68
1:A:248:ILE:CG2	1:A:334:GLY:HA3	2.18	0.68
1:A:289:VAL:HG12	1:A:289:VAL:O	1.94	0.67
2:B:312:TYR:O	2:B:313:SER:C	2.37	0.67
2:B:332:ARG:NH1	4:F:5[F]:O2G:C2'	2.51	0.67
2:B:251:MET:HE3	2:B:330:ILE:HG22	1.75	0.67
2:B:317:LYS:H	2:B:317:LYS:CD	2.06	0.67
1:A:127:GLU:OE1	1:A:128:ILE:CA	2.43	0.67
2:B:41:GLY:HA2	4:F:5[F]:O2G:H5'	1.74	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
1:A:285:HIS:HA	1:A:299:GLY:HA2	1.75	0.67
2:B:240:ARG:NH2	3:D:14[B]:DOC:O2	2.28	0.67
2:B:176:ARG:HA	2:B:203:VAL:HG11	1.76	0.67
1:A:183:VAL:O	1:A:184:PRO:C	2.35	0.66
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:290:THR:CG2	1:A:328:ARG:NH2	2.58	0.66
3:C:8:DG:H2''	3:C:9:DG:OP2	1.95	0.66
1:A:258:LEU:HD21	1:A:323:LEU:HD13	1.78	0.66
2:B:155:ALA:O	2:B:156:ASP:C	2.39	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
4:F:5[F]:O2G:H8	4:F:5[F]:O2G:P	2.36	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:208:ILE:HG22	2:B:213:LEU:HD11	1.77	0.66
2:B:273:TYR:HE2	6:B:2051:HOH:O	1.79	0.66
1:A:291:GLU:O	1:A:293:LEU:N	2.29	0.65
2:B:336:ARG:NH1	2:B:336:ARG:HB3	2.10	0.65
1:A:172:LYS:O	1:A:174:LEU:N	2.28	0.65
1:A:271:GLU:O	1:A:275:LYS:HG3	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:CZ	1:A:327:GLU:HA	2.27	0.65
2:B:281:PRO:CB	2:B:337:PHE:HB3	2.26	0.65
1:A:293:LEU:O	1:A:293:LEU:HD13	1.96	0.65
2:B:59:ILE:HD11	2:B:64:ALA:HB2	1.77	0.65
1:A:14:GLN:O	1:A:15:VAL:C	2.36	0.65
1:A:282:LYS:HB2	1:A:339:LYS:O	1.96	0.65
2:B:0:HIS:HD2	2:B:2:ILE:CD1	2.10	0.65
1:A:210:PHE:HD2	1:A:210:PHE:C	2.05	0.65
1:A:251:MET:HE2	1:A:253:ARG:O	1.96	0.65
2:B:280:ILE:N	2:B:280:ILE:HD12	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:28:VAL:HG23	1:A:47:ASN:ND2	2.12	0.64
1:A:298:ARG:HG3	1:A:322:ILE:CG1	2.24	0.64
2:B:227:SER:O	2:B:231:ASP:N	2.30	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
2:B:289:VAL:O	2:B:290:THR:C	2.37	0.64
1:A:180:ILE:HD13	1:A:201:LYS:C	2.21	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:324:GLU:C	1:A:326:ASP:N	2.54	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: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
1:A:209:GLU:CD	1:A:209:GLU:H	2.04	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
1:A:210:PHE:CD2	1:A:210:PHE:C	2.76	0.63
2:B:111:ILE:O	2:B:111:ILE:CG1	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
3:D:4:DG:H2"	3:D:5:DG:C8	2.34	0.62
1:A:5:PHE:CE1	1:A:106:GLU:HB3	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:PHE:CD1	2:B:8:PHE:N	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:41:GLY:C	1:A:61:ILE:HD12	2.24	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
2:B:93:ARG:HG2	2:B:99:ILE:HD12	1.81	0.62
2:B:233:TYR:C	2:B:233:TYR:CD2	2.78	0.62
2:B:324:GLU:O	2:B:325:GLU:OE1	2.17	0.62
1:A:144:ILE:O	1:A:145:SER:HB2	1.98	0.62
1:A:282:LYS:HE2	1:A:339:LYS:O	2.00	0.62
1:A:290:THR:OG1	1:A:294:ASP:N	2.21	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
1:A:332:ARG:HH21	4:E:6:DG:P	2.23	0.61
2:B:164:LYS:NZ	2:B:165:VAL:H	1.97	0.61
1:A:100:GLU:OE2	1:A:237:ILE:HA	1.99	0.61
1:A:232:GLU:HG2	1:A:233:TYR:N	2.15	0.61
2:B:59:ILE:HD12	2:B:59:ILE:C	2.25	0.61
2:B:240:ARG:NH2	6:B:2044:HOH:O	2.34	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:10:TYR:O	1:A:11:PHE:C	2.44	0.61
1:A:114:LYS:HD2	1:A:114:LYS:N	2.16	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:147:ASN:CB	6:A:2049:HOH:O	2.43	0.60
1:A:280:ILE:O	1:A:341:ILE:N	2.31	0.60
2:B:9:ASP:OD1	2:B:160:PRO:HA	2.00	0.60
1:A:291:GLU:HG3	1:A:329:LYS:HB2	1.81	0.60
2:B:288:ALA:HA	2:B:332:ARG:O	2.00	0.60
2:B:234:ASN:C	2:B:234:ASN:OD1	2.44	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: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:OP2	2.27	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
1:A:288:ALA:CB	1:A:330:ILE:HG21	2.31	0.59
1:A:291:GLU:C	1:A:293:LEU:H	2.11	0.59
2:B:298:ARG:HG2	3:D:8:DG:OP1	2.03	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
1:A:94:GLU:CG	1:A:94:GLU:O	2.50	0.58
1:A:292[A]:ASP:OD1	1:A:328:ARG:NH1	2.34	0.58
2:B:256:ARG:HG2	2:B:256:ARG:HH21	1.67	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
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
2:B:289:VAL:O	2:B:290:THR:O	2.22	0.58
1:A:175:ILE:HG22	1:A:203:VAL:HB	1.86	0.58
2:B:46:ALA:O	2:B:51:ARG:NH1	2.37	0.58
2:B:251:MET:HE3	2:B:330:ILE:CG2	2.33	0.58
2:B:301:THR:O	2:B:301:THR:CG2	2.42	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:O	1:A:262:LYS:HG3	2.04	0.57
1:A:258:LEU:HD13	1:A:319:LEU:HD21	1.86	0.57
2:B:70:ASN:ND2	6:B:2016:HOH:O	2.37	0.57
3:D:5:DG:N2	4:F:14:DC:N3	2.45	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
1:A:264:TYR:CD1	1:A:267:ARG:NH1	2.71	0.57
2:B:322:ILE:C	2:B:324:GLU:N	2.60	0.57
1:A:238:ARG:CD	1:A:240:ARG:N	2.67	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG11	1:A:81:TYR:HD1	1.70	0.57
1:A:258:LEU:HD13	1:A:319:LEU:CD2	2.35	0.57
2:B:93:ARG:HB3	6:B:2025:HOH:O	2.03	0.57
2:B:210:PHE:HA	2:B:213:LEU:HB2	1.86	0.57
1:A:53:PHE:O	1:A:67:ILE:HG21	2.04	0.57
1:A:238:ARG:CD	1:A:239:THR:H	2.12	0.57
2:B:12:TYR:HB2	2:B:45:THR:HG23	1.87	0.57
2:B:247:ARG:O	2:B:247:ARG:CG	2.53	0.57
1:A:75:PRO:O	1:A:75:PRO:HG2	2.03	0.56
1:A:28:VAL:H	1:A:47:ASN:ND2	2.03	0.56
1:A:235:GLU:HG2	1:A:236:PRO:CD	2.35	0.56
1:A:127:GLU:C	1:A:127:GLU:CD	2.73	0.56
1:A:151:ALA:O	1:A:154:ALA:HB3	2.06	0.56
1:A:217:ILE:HD12	1:A:221:LYS:HB3	1.87	0.56
2:B:55:VAL:CG2	2:B:68:LEU:HD12	2.33	0.56
2:B:115:VAL:O	2:B:115:VAL:CG1	2.53	0.56
2:B:166:ILE:HG22	2:B:171:VAL:CG2	2.32	0.56
2:B:190:THR:O	2:B:194:LEU:HG	2.05	0.56
3:C:13:DC:C5'	3:C:14[B]:DOC:H6	2.36	0.56
3:D:10:DA:H2'	3:D:10:DA:O5'	2.06	0.56
2:B:308:LYS:O	2:B:312:TYR:CD2	2.59	0.56
2:B:325:GLU:OE1	2:B:325:GLU:N	2.37	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
1:A:49:GLU:H	1:A:49:GLU:CD	2.11	0.56
1:A:291:GLU:CG	1:A:329:LYS:HB2	2.36	0.56
2:B:298:ARG:HG2	2:B:298:ARG:NH1	2.06	0.56
1:A:282:LYS:HB2	1:A:339:LYS:HB2	1.86	0.56
1:A:268:ALA:O	1:A:272:SER:OG	2.23	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:124:LEU:HA	1:A:127:GLU:CB	2.29	0.56
2:B:187:GLY:O	2:B:191:ALA:N	2.37	0.56
2:B:210:PHE:O	2:B:210:PHE:CG	2.58	0.56
1:A:50:ALA:O	1:A:51:ARG:C	2.44	0.56
1:A:133:LEU:O	1:A:137:LYS:N	2.24	0.56
2:B:175:ILE:HG22	2:B:203:VAL:HB	1.88	0.56
2:B:317:LYS:O	2:B:320:GLN:N	2.39	0.56
1:A:221:LYS:O	1:A:225:LEU:N	2.36	0.55
2:B:91:LEU:HD23	2:B:91:LEU:C	2.31	0.55
2:B:307:SER:O	2:B:308:LYS:C	2.48	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TYR:CE1	1:A:163:ILE:HG12	2.41	0.55
2:B:32:VAL:HG11	4:F:6:DG:C5'	2.36	0.55
2:B:100:GLU:HB3	2:B:237:ILE:HG23	1.88	0.55
2:B:208:ILE:HG22	2:B:209:GLU:N	2.19	0.55
1:A:290:THR:N	1:A:294:ASP:O	2.40	0.55
2:B:208:ILE:HG22	2:B:213:LEU:CD1	2.35	0.55
2:B:248:ILE:H	2:B:248:ILE:HD13	1.69	0.55
2:B:284:ILE:HG13	2:B:337:PHE:CE1	2.42	0.55
1:A:28:VAL:N	1:A:47:ASN:ND2	2.44	0.55
1:A:178:LEU:O	1:A:201:LYS:HB3	2.06	0.55
1:A:317:LYS:O	1:A:318:LEU:C	2.45	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
1:A:169:GLU:C	1:A:169:GLU:OE2	2.49	0.55
1:A:257:ASN:HB3	1:A:260:GLU:CD	2.32	0.55
2:B:176:ARG:HA	2:B:203:VAL:HG12	1.88	0.55
2:B:179:ASP:OD1	2:B:180:ILE:N	2.40	0.55
1:A:136:GLU:O	1:A:137:LYS:HB2	2.07	0.55
2:B:234:ASN:OD1	2:B:235:GLU:N	2.40	0.55
2:B:262:LYS:O	2:B:263:PRO:C	2.49	0.55
2:B:289:VAL:CG2	2:B:332:ARG:HD2	2.35	0.55
2:B:298:ARG:HA	3:D:8:DG:OP2	2.06	0.55
1:A:29:VAL:CG2	1:A:73:TYR:CD2	2.90	0.55
1:A:197:LEU:HD11	1:A:212:LYS:HG2	1.89	0.55
1:A:328:ARG:NH2	6:A:2087:HOH:O	2.39	0.55
1:A:189:ILE:O	1:A:189:ILE:HG22	2.06	0.55
2:B:269:ILE:HG22	2:B:273:TYR:HD1	1.71	0.55
1:A:189:ILE:O	1:A:193:LYS:HG3	2.07	0.54
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
2:B:210:PHE:CD1	2:B:210:PHE:C	2.81	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:273:TYR:OH	1:A:306:ILE:O	2.26	0.54
2:B:259:GLU:C	2:B:261:ILE:N	2.62	0.54
4:F:11:DC:H1'	4:F:12:DT:H5'	1.89	0.54
1:A:9:ASP:C	1:A:10:TYR:CD2	2.86	0.54
1:A:240:ARG:C	1:A:241:VAL:HG13	2.31	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:164:LYS:CE	2:B:165:VAL:N	2.47	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:ILE:HD11	2:B:225:LEU:HD21	1.89	0.54
1:A:191:ALA:O	1:A:192:GLU:C	2.50	0.54
1:A:335:VAL:O	1:A:335:VAL:CG2	2.54	0.54
1:A:19:LEU:HD12	1:A:19:LEU:N	2.23	0.54
1:A:296:VAL:HG22	1:A:296:VAL:O	2.08	0.54
2:B:4:LEU:HD23	2:B:5:PHE: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
2:B:199:ILE:HG12	2:B:204:ASP:HB3	1.90	0.54
2:B:218:GLY:C	2:B:220:ALA:H	2.15	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
2:B:65:LYS:O	2:B:69:PRO:HA	2.07	0.53
2:B:137:LYS:O	2:B:138:ILE:CG1	2.56	0.53
3:D:14[A]:DOC:H6	6:D:2019:HOH:O	2.08	0.53
1:A:132:ILE:O	1:A:136:GLU:HB3	2.08	0.53
1:A:263:PRO:O	1:A:267:ARG:HG3	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
2:B:37:PHE:HZ	4:F:4[F]:DT:OP2	1.92	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:240:ARG:HG2	6:A:2067:HOH:O	2.08	0.53
1:A:336:ARG:HH22	4:E:7:DA:H2'	1.71	0.53
1:A:49:GLU:CD	1:A:49:GLU:N	2.67	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
1:A:173:ARG:HG2	1:A:173:ARG:HH11	1.74	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
2:B:114:LYS:O	2:B:115:VAL:O	2.26	0.52
2:B:235:GLU:CG	2:B:236:PRO:HD2	2.37	0.52
2:B:328[B]:ARG:C	2:B:329:LYS:O	2.51	0.52
1:A:35:GLY:O	1:A:36:ARG:C	2.52	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:DT:H2''	3:C:12:DT:H72	1.91	0.52
1:A:48:TYR:N	1:A:48:TYR:CD2	2.73	0.52
1:A:240:ARG:C	1:A:241:VAL:CG1	2.83	0.52
2:B:259:GLU:O	2:B:261:ILE:N	2.42	0.52
1:A:257:ASN:OD1	1:A:257:ASN:C	2.52	0.52
2:B:290:THR:O	2:B:291:GLU:C	2.52	0.52
1:A:209:GLU:CD	1:A:209:GLU:N	2.68	0.52
2:B:117:ASP:OD2	2:B:118:TYR:N	2.43	0.52
1:A:36:ARG:HH12	1:A:254:ASN:ND2	2.08	0.52
1:A:48:TYR:O	1:A:52:LYS:HG2	2.09	0.52
1:A:334:GLY:C	1:A:335:VAL:CG1	2.82	0.52
1:A:147:ASN:HD21	1:A:150:PHE:HD2	1.57	0.52
1:A:248:ILE:HG12	4:E:7:DA:OP2	2.09	0.52
2:B:321:LYS:O	2:B:321:LYS:HG2	2.08	0.52
1:A:332:ARG:NH2	4:E:6:DG:OP2	2.43	0.52
2:B:195[B]:LYS:C	2:B:197:LEU:N	2.64	0.52
2:B:314:GLU:O	2:B:315:SER:C	2.52	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:OP2	2.58	0.51
2:B:20:ASN:OD1	2:B:22:SER:CB	2.57	0.51
2:B:290:THR:OG1	2:B:328[B]:ARG:HD2	2.10	0.51
4:E:15:DC:O5'	4:E:15:DC:C2'	2.57	0.51
1:A:193:LYS:NZ	3:C:11:DT:OP1	2.33	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:28:VAL:C	1:A:29:VAL:CG1	2.82	0.51
1:A:219:GLU:HA	1:A:222:ALA:CB	2.39	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:320:GLN:O	2:B:322:ILE:N	2.44	0.51
2:B:10:TYR:CE1	2:B:14:GLN:HB2	2.46	0.51
2:B:93:ARG:C	2:B:95:TYR:H	2.18	0.51
1:A:37:PHE:O	1:A:38:GLU:C	2.54	0.51
1:A:236:PRO:O	1:A:238:ARG:N	2.43	0.51
1:A:237:ILE:HD13	6:A:2038:HOH:O	2.11	0.51
1:A:9:ASP:O	1:A:10:TYR:C	2.54	0.51
1:A:64:ALA:C	1:A:66:LYS:N	2.67	0.51
2:B:47:ASN:O	2:B:50:ALA:HB3	2.11	0.51
3:D:3:DG:H2''	3:D:4:DG:H5'	1.93	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:N	1:A:309:GLU:OE1	2.41	0.51
1:A:92:LEU:C	1:A:94:GLU:H	2.19	0.50
2:B:149:VAL:HG12	2:B:153:ILE:HD12	1.93	0.50
1:A:80:VAL:O	1:A:84:VAL:HG23	2.12	0.50
1:A:276:LEU:O	1:A:277:ASP:O	2.28	0.50
1:A:282:LYS:CB	1:A:339:LYS:O	2.59	0.50
1:A:289:VAL:O	1:A:290:THR:O	2.29	0.50
3:C:13:DC:H5'	3:C:14[B]:DOC:C6	2.42	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
1:A:7:ASP:CG	1:A:8:PHE:N	2.70	0.50
1:A:180:ILE:O	1:A:186:ILE:HD12	2.11	0.50
2:B:59:ILE:O	2:B:60:PRO:C	2.51	0.50
2:B:80:VAL:O	2:B:84:VAL:HG23	2.12	0.50
1:A:172:LYS:O	1:A:175:ILE:N	2.44	0.50
1:A:185:GLY:O	3:C:12:DT:H5''	2.12	0.50
1:A:252:LYS:C	1:A:253:ARG:HG3	2.36	0.50
2:B:269:ILE:HG23	2:B:337:PHE:HZ	1.77	0.50
2:B:304:HIS:CD2	6:B:2050:HOH:O	2.65	0.50
1:A:241:VAL:O	1:A:243:LYS:HE3	2.12	0.50
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
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:28:VAL:HB	1:A:47:ASN:ND2	2.27	0.50
1:A:46:ALA:HB1	1:A:50:ALA:CB	2.40	0.50
1:A:126:LEU:O	1:A:127:GLU:C	2.54	0.50
1:A:217:ILE:HG13	1:A:218:GLY:N	2.26	0.50
2:B:0:HIS:CD2	2:B:0:HIS:O	2.65	0.50
2:B:226:ILE:CG2	2:B:227:SER:N	2.75	0.50
2:B:233:TYR:O	2:B:234:ASN:C	2.54	0.50
1:A:14:GLN:O	1:A:17:GLU:N	2.36	0.50
1:A:166:ILE:HG22	1:A:166:ILE:O	2.11	0.50
1:A:79:GLU:CD	1:A:79:GLU:N	2.64	0.49
1:A:190:THR:OG1	3:C:12:DT:OP1	2.21	0.49
1:A:284:ILE:CG1	1:A:285:HIS:N	2.70	0.49
2:B:209:GLU:O	2:B:213:LEU:HD12	2.12	0.49
1:A:28:VAL:C	1:A:29:VAL:HG13	2.37	0.49
1:A:93:ARG:HB2	1:A:93:ARG:CZ	2.30	0.49
1:A:291:GLU:CA	1:A:329:LYS:O	2.59	0.49
2:B:332:ARG:HH22	4:F:5[F]:O2G:H2'	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:339:LYS:O	2:B:340:PHE:C	2.55	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
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:32:VAL:CG1	4:F:6:DG:C5'	2.86	0.49
2:B:51:ARG:NH1	6:B:2012:HOH:O	2.46	0.49
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:52:LYS:HZ2	2:B:53:PHE:HE1	1.61	0.48
2:B:205:THR:OG1	2:B:229:ALA:CB	2.61	0.48
1:A:176:ARG:O	1:A:177:GLU:CB	2.45	0.48
2:B:289:VAL:C	2:B:290:THR:O	2.55	0.48
2:B:338:SER:O	2:B:339:LYS:C	2.55	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:28:VAL:CG2	1:A:47:ASN:ND2	2.76	0.48
1:A:87:ARG:HG3	1:A:87:ARG:HH11	1.79	0.48
1:A:93:ARG:CB	1:A:93:ARG:CZ	2.89	0.48
1:A:251:MET:HG2	1:A:264:TYR:CD2	2.49	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:10:TYR:CE1	1:A:14:GLN:HG3	2.49	0.48
1:A:74:LEU:O	1:A:75:PRO:C	2.52	0.48
1:A:147:ASN:CB	1:A:233:TYR:CD2	2.93	0.48
1:A:71:ALA:HB3	1:A:73:TYR:CE1	2.48	0.48
1:A:203:VAL:CG1	1:A:204:ASP:N	2.75	0.48
1:A:219:GLU:CA	1:A:222:ALA:HB3	2.42	0.48
1:A:262:LYS:HE2	1:A:266:PHE:CE2	2.49	0.48
1:A:287:VAL:HA	1:A:297:SER:CB	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:MET:O	2:B:93:ARG:HG3	2.14	0.48
2:B:296:VAL:O	2:B:296:VAL:CG1	2.62	0.48
1:A:77:ARG:O	1:A:81:TYR:CD2	2.67	0.48
1:A:135:LYS:CG	1:A:135:LYS:O	2.62	0.48
1:A:286:VAL:HG23	1:A:318:LEU:HB2	1.95	0.48
1:A:289:VAL:O	1:A:290:THR:C	2.57	0.48
1:A:214:LYS:O	1:A:218:GLY:N	2.46	0.48
1:A:262:LYS:O	1:A:266:PHE:N	2.42	0.48
1:A:302:PHE:HZ	1:A:314:GLU:HG2	1.78	0.48
1:A:327:GLU:N	1:A:327:GLU:CD	2.62	0.48
2:B:161:ASN:OD1	2:B:161:ASN:O	2.32	0.48
1:A:28:VAL:HB	1:A:47:ASN:HD22	1.78	0.47
1:A:261:ILE:CD1	1:A:330:ILE:HD12	2.44	0.47
2:B:280:ILE:N	2:B:280:ILE:CD1	2.78	0.47
1:A:150:PHE:CE2	1:A:228:LEU:HD22	2.48	0.47
2:B:152:LYS:NZ	3:D:14[B]:DOC:H5'	2.29	0.47
1:A:183:VAL:HB	1:A:186:ILE:HD12	1.95	0.47
2:B:15:VAL:O	2:B:15:VAL:HG12	2.13	0.47
2:B:133:LEU:O	2:B:137:LYS:CA	2.62	0.47
2:B:268:ALA:O	2:B:272:SER:OG	2.21	0.47
1:A:124:LEU:HD11	1:A:128:ILE:HD11	1.97	0.47
1:A:168[A]:ASP:OD2	1:A:171:VAL:HG21	2.14	0.47
2:B:141:THR:HG23	2:B:162:GLY:CA	2.43	0.47
2:B:148:LYS:HD3	2:B:237:ILE:HG13	1.96	0.47
2:B:193:LYS:HB3	2:B:193:LYS:HE3	1.25	0.47
1:A:63:GLU:HG3	6:A:2027:HOH:O	2.13	0.47
2:B:265:LEU:HD21	2:B:315:SER:OG	2.15	0.47
1:A:3:VAL:O	6:A:2001:HOH:O	2.21	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
2:B:78:LYS:HA	2:B:81:TYR:CE2	2.40	0.47
2:B:320:GLN:C	2:B:322:ILE:H	2.23	0.47
1:A:94:GLU:O	1:A:94:GLU:HG2	2.15	0.47
1:A:116[A]:ARG:HH11	1:A:116[A]:ARG:CG	2.28	0.47
1:A:224:TYR:CD1	1:A:224:TYR:C	2.89	0.47
1:A:287:VAL:CG1	1:A:295:ILE:HD12	2.44	0.47
1:A:333:ILE:O	1:A:333:ILE:CG2	2.62	0.47
2:B:114:LYS:H	2:B:114:LYS:CD	1.99	0.47
2:B:333:ILE:HG13	2:B:334:GLY:H	1.78	0.47
1:A:26:LYS:HB2	1:A:27:PRO:CD	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ASP:OD1	2:B:112:SER:OG	2.22	0.47
2:B:203:VAL:O	2:B:204:ASP:C	2.58	0.47
2:B:310:THR:O	2:B:311:ALA:C	2.57	0.47
2:B:247:ARG:HD3	2:B:275:LYS:NZ	2.30	0.47
1:A:11:PHE:O	1:A:12:TYR:C	2.56	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
1:A:232:GLU:O	1:A:233:TYR:HB3	2.14	0.46
2:B:122:TYR:CE1	2:B:163:ILE:HG12	2.49	0.46
2:B:146:LYS:HE3	2:B:146:LYS:HB2	1.69	0.46
1:A:48:TYR:OH	1:A:160:PRO:CG	2.62	0.46
2:B:316:VAL:O	2:B:317:LYS:C	2.57	0.46
1:A:21:PRO:C	1:A:23:LEU:N	2.67	0.46
1:A:273:TYR:HB3	1:A:308:LYS:HE2	1.97	0.46
1:A:167[A]:ASP:C	1:A:169:GLU:H	2.23	0.46
1:A:203:VAL:HG13	1:A:204:ASP:N	2.29	0.46
2:B:171:VAL:O	2:B:172:LYS:C	2.58	0.46
2:B:180:ILE:C	2:B:182:ASP:H	2.23	0.46
2:B:316:VAL:O	2:B:319:LEU:HB3	2.15	0.46
2:B:218:GLY:C	2:B:220:ALA:N	2.73	0.46
1:A:33:PHE:HE2	1:A:39:ASP:OD1	1.99	0.46
2:B:125:GLY:O	2:B:126:LEU:C	2.58	0.46
2:B:194:LEU:C	2:B:195[B]:LYS:HD2	2.40	0.46
1:A:258:LEU:CD1	1:A:319:LEU:CD2	2.93	0.46
2:B:136:GLU:O	2:B:137:LYS:C	2.54	0.46
2:B:203:VAL:C	2:B:205:THR:N	2.74	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: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
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
2:B:2:ILE:CG2	2:B:111:ILE:HD11	2.46	0.46
1:A:28:VAL:HG23	1:A:47:ASN:HD21	1.80	0.46
1:A:244:SER:OG	4:E:9:DT:OP2	2.31	0.46
1:A:99:ILE:CD1	1:A:109:LEU:HG	2.46	0.45
1:A:172:LYS:C	1:A:174:LEU:N	2.74	0.45
1:A:147:ASN:HA	6:A:2049:HOH:O	2.15	0.45
1:A:287:VAL:HG13	1:A:297:SER:HB3	1.98	0.45
1:A:291:GLU:C	1:A:291:GLU:OE1	2.59	0.45
1:A:301:THR:CG2	1:A:302:PHE:N	2.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:19:LEU:CD2	2:B:80:VAL:HG11	2.45	0.45
2:B:41:GLY:CA	4:F:5[F]:O2G:H5'	2.46	0.45
2:B:292:ASP:O	2:B:293:LEU:C	2.59	0.45
2:B:317:LYS:O	2:B:318:LEU:C	2.58	0.45
1:A:91:LEU:HD21	1:A:131:LYS:HG2	1.97	0.45
1:A:111:ILE:HD12	1:A:115[A]:VAL:HB	1.98	0.45
1:A:147:ASN:CG	1:A:233:TYR:CD2	2.95	0.45
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.57	0.45
1:A:197:LEU:CD2	1:A:216:MET:HG2	2.45	0.45
1:A:241:VAL:HG22	1:A:243:LYS:HE2	1.97	0.45
2:B:48:TYR:C	2:B:50:ALA:H	2.25	0.45
2:B:152:LYS:HZ3	3:D:14[B]:DOC:H5'	1.80	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
1:A:98:LYS:HE3	1:A:98:LYS:N	2.31	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
2:B:114:LYS:O	2:B:115:VAL:HB	2.15	0.45
1:A:92:LEU:C	1:A:94:GLU:N	2.74	0.45
2:B:22:SER:O	2:B:26:LYS:HE2	2.17	0.45
2:B:51:ARG:C	2:B:53:PHE:H	2.25	0.45
2:B:284:ILE:C	2:B:285:HIS:ND1	2.74	0.45
2:B:298:ARG:HD3	2:B:322:ILE:CG1	2.19	0.45
3:D:8:DG:H2''	3:D:9:DG:OP2	2.16	0.45
1:A:195:LYS:N	1:A:195:LYS:CD	2.78	0.45
2:B:65:LYS:O	2:B:69:PRO:CA	2.64	0.45
2:B:263:PRO:O	2:B:266:PHE:N	2.50	0.45
2:B:20:ASN:OD1	2:B:20:ASN:C	2.60	0.45
2:B:139:THR:HB	2:B:161:ASN:HD22	1.82	0.45
2:B:164:LYS:HD2	2:B:164:LYS:HA	1.75	0.45
2:B:263:PRO:O	2:B:264:TYR:C	2.60	0.45
2:B:269:ILE:HG22	2:B:273:TYR:CD1	2.51	0.45
1:A:226:ILE:CG2	1:A:230:ARG:HE	2.28	0.45
2:B:256:ARG:CG	2:B:329:LYS:HA	2.45	0.45
1:A:119[A]:ARG:HE	1:A:120:GLU:CD	2.25	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
4:F:5[F]:O2G:HM2A	4:F:6:DG:C2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:HB3	6:A:2033:HOH:O	2.16	0.44
2:B:64:ALA:C	2:B:66:LYS:N	2.75	0.44
2:B:151:ALA:O	2:B:152:LYS:C	2.59	0.44
2:B:153:ILE:O	2:B:156:ASP:HB2	2.18	0.44
2:B:208:ILE:HD13	2:B:208:ILE:HA	1.94	0.44
1:A:119[A]:ARG:C	1:A:121:ALA:H	2.24	0.44
1:A:192:GLU:C	1:A:194:LEU:H	2.25	0.44
1:A:192:GLU:O	1:A:194:LEU:N	2.50	0.44
1:A:240:ARG:CG	1:A:241:VAL:N	2.79	0.44
2:B:77:ARG:O	2:B:81:TYR:CE2	2.71	0.44
2:B:79:GLU:O	2:B:83:GLN:N	2.50	0.44
1:A:141:THR:HA	1:A:162:GLY:O	2.17	0.44
1:A:213:LEU:O	1:A:214:LYS:C	2.60	0.44
2:B:284:ILE:CG2	2:B:318:LEU:HD11	2.48	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
2:B:100:GLU:OE1	2:B:148:LYS:HE2	2.18	0.44
2:B:261:ILE:O	2:B:264:TYR:HB2	2.17	0.44
2:B:322:ILE:C	2:B:324:GLU:H	2.22	0.44
3:C:2:DG:H1	4:E:17:DC:H42	1.64	0.44
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.75	0.44
3:C:13:DC:C4'	3:C:14[B]:DOC:H6	2.45	0.44
1:A:29:VAL:HG22	1:A:72:VAL:O	2.18	0.44
1:A:189:ILE:HG22	1:A:193:LYS:HE3	1.99	0.44
1:A:280:ILE:HA	1:A:281:PRO:HD2	1.70	0.44
2:B:324:GLU:HB3	2:B:325:GLU:OE1	2.17	0.44
1:A:293:LEU:O	1:A:293:LEU:CD1	2.65	0.44
3:D:3:DG:C5	3:D:4:DG:N7	2.86	0.44
4:E:5[E]:O2G:H8	4:E:5[E]:O2G:P	2.58	0.44
1:A:334:GLY:C	1:A:335:VAL:HG12	2.43	0.44
2:B:12:TYR:HB2	2:B:45:THR:CG2	2.48	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:285:HIS:O	2:B:335:VAL:HA	2.18	0.44
2:B:298:ARG:NH2	2:B:325:GLU:OE2	2.51	0.44
1:A:251:MET:C	1:A:253:ARG:H	2.26	0.44
2:B:126:LEU:O	2:B:130:ASN:CB	2.55	0.44
2:B:164:LYS:HZ2	2:B:165:VAL:H	1.64	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:117:ASP:HB3	2:B:120:GLU:CG	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LYS:C	2:B:138:ILE:HG13	2.42	0.43
2:B:283:ALA:HA	2:B:300:ARG:O	2.18	0.43
2:B:307:SER:C	2:B:309:GLU:N	2.76	0.43
2:B:338:SER:HB2	2:B:339:LYS:H	1.52	0.43
2:B:128:ILE:C	2:B:130:ASN:N	2.72	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
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:48:TYR:C	2:B:50:ALA:N	2.74	0.43
2:B:266:PHE:HD1	2:B:269:ILE:HD12	1.83	0.43
2:B:267:ARG:NH1	2:B:267:ARG:HB3	2.31	0.43
2:B:299:GLY:HA2	2:B:318:LEU:HD13	2.00	0.43
1:A:36:ARG:HH22	1:A:254:ASN:N	2.16	0.43
1:A:192:GLU:C	1:A:194:LEU:N	2.76	0.43
2:B:293:LEU:O	2:B:294:ASP:CB	2.66	0.43
1:A:282:LYS:HG2	1:A:304:HIS:O	2.17	0.43
1:A:336:ARG:NH2	4:E:7:DA:C2'	2.68	0.43
1:A:226:ILE:HG23	1:A:230:ARG:HH21	1.83	0.43
1:A:241:VAL:O	1:A:242:ARG:C	2.61	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:114:LYS:N	1:A:114:LYS:CD	2.79	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
3:C:11:DT:C2'	3:C:12:DT:H72	2.49	0.43
1:A:19:LEU:N	1:A:19:LEU:CD1	2.82	0.43
2:B:212:LYS:O	2:B:213:LEU:C	2.62	0.43
2:B:274:TYR:O	2:B:275:LYS:C	2.61	0.43
2:B:11:PHE:O	2:B:12:TYR:C	2.61	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
2:B:114:LYS:O	2:B:115:VAL:CB	2.67	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
1:A:251:MET:HE1	1:A:255:SER:HB2	2.01	0.42
2:B:51:ARG:O	2:B:53:PHE:N	2.52	0.42
2:B:226:ILE:O	2:B:229:ALA:HB3	2.19	0.42
3:D:6:DA:H2''	3:D:7:DA:OP2	2.19	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:OP2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.83	0.42
2:B:56:LYS:O	2:B:57:ALA:C	2.63	0.42
2:B:62:VAL:HG21	4:F:3[F]:DA:C5'	2.48	0.42
2:B:250:THR:N	2:B:332:ARG:HB3	2.33	0.42
3:C:5:DG:H2''	3:C:6:DA:H8	1.79	0.42
1:A:302:PHE:N	1:A:302:PHE:CD1	2.87	0.42
2:B:228:LEU:CD2	2:B:233:TYR:HB2	2.41	0.42
2:B:261:ILE:HG21	2:B:319:LEU:HD21	2.00	0.42
1:A:41:GLY:HA3	1:A:61:ILE:CD1	2.47	0.42
2:B:251:MET:O	2:B:252:LYS:HD2	2.20	0.42
2:B:290:THR:O	2:B:292:ASP:N	2.53	0.42
1:A:144:ILE:HG13	1:A:165:VAL:CG1	2.42	0.42
2:B:34:SER:O	2:B:36:ARG:N	2.52	0.42
2:B:262:LYS:HE2	2:B:316:VAL:HG21	2.01	0.42
2:B:336:ARG:NE	6:F:2005:HOH:O	2.44	0.42
2:B:15:VAL:O	2:B:15:VAL:CG1	2.66	0.42
2:B:141:THR:CG2	2:B:162:GLY:C	2.93	0.42
1:A:30:VAL:CG1	1:A:76:MET:HA	2.50	0.42
1:A:118:TYR:HA	1:A:121:ALA:CB	2.50	0.42
1:A:244:SER:HA	1:A:337:PHE:O	2.19	0.42
2:B:97:GLU:O	2:B:99:ILE:N	2.53	0.42
1:A:37:PHE:O	1:A:40:SER:HB2	2.20	0.42
1:A:218:GLY:HA3	4:E:12:DT:OP1	2.20	0.42
1:A:246:GLY:CA	1:A:335:VAL:O	2.67	0.42
2:B:78:LYS:N	2:B:81:TYR:CE2	2.87	0.42
2:B:307:SER:O	2:B:309:GLU:N	2.53	0.42
2:B:336:ARG:NH2	6:F:2005:HOH:O	2.48	0.42
1:A:99:ILE:O	1:A:99:ILE:HG23	2.20	0.42
1:A:173:ARG:O	1:A:177:GLU:HB2	2.20	0.42
1:A:150:PHE:HA	1:A:153:ILE:HG13	2.02	0.41
1:A:247:ARG:HG2	1:A:271:GLU:HB3	2.01	0.41
2:B:226:ILE:HG22	2:B:227:SER:H	1.82	0.41
4:F:17:DC:H1'	4:F:18:DC:C6	2.55	0.41
1:A:8:PHE:CZ	1:A:89:MET:HE2	2.55	0.41
1:A:92:LEU:O	1:A:95:TYR:HB2	2.20	0.41
1:A:166:ILE:O	1:A:167[A]:ASP:C	2.62	0.41
1:A:296:VAL:O	1:A:322:ILE:HD13	2.20	0.41
2:B:178:LEU:O	2:B:179:ASP:O	2.38	0.41
1:A:172:LYS:O	1:A:173:ARG:C	2.64	0.41
1:A:290:THR:HG1	1:A:294:ASP:H	1.55	0.41
2:B:139:THR:CG2	2:B:161:ASN:HD22	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:320:GLN:C	2:B:322:ILE:N	2.78	0.41
2:B:336:ARG:CB	2:B:336:ARG:HH11	2.33	0.41
1:A:208:ILE:CG2	1:A:209:GLU:O	2.60	0.41
2:B:111:ILE:HD13	2:B:111:ILE:H	1.84	0.41
1:A:195:LYS:N	1:A:195:LYS:HD3	2.35	0.41
2:B:174:LEU:O	2:B:175:ILE:C	2.63	0.41
3:D:4:DG:C5'	6:D:2010:HOH:O	2.68	0.41
1:A:74:LEU:HD22	6:A:2008:HOH:O	2.21	0.41
1:A:197:LEU:O	1:A:208:ILE:HG13	2.20	0.41
2:B:77:ARG:NH1	6:B:2017:HOH:O	2.40	0.41
2:B:131:LYS:O	2:B:135:LYS:HB3	2.21	0.41
2:B:166:ILE:CG2	2:B:171:VAL:HG22	2.44	0.41
1:A:10:TYR:O	1:A:11:PHE:O	2.38	0.41
1:A:84:VAL:O	1:A:85:SER:C	2.62	0.41
1:A:97:GLU:HB3	1:A:98:LYS:CE	2.51	0.41
1:A:301:THR:C	1:A:302:PHE:CD1	2.99	0.41
2:B:155:ALA:O	2:B:157:MET:N	2.53	0.41
1:A:111:ILE:CG2	1:A:124:LEU:HD21	2.46	0.41
1:A:200:ASN:C	1:A:201:LYS:CD	2.79	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:277:ASP:O	1:A:278:LYS:HB2	2.21	0.41
1:A:322:ILE:C	1:A:324:GLU:H	2.29	0.41
2:B:115:VAL:HG21	6:B:2031:HOH:O	2.19	0.41
2:B:133:LEU:HB3	2:B:134:GLU:H	1.74	0.41
2:B:177:GLU:O	2:B:178:LEU:C	2.62	0.41
2:B:230:ARG:O	2:B:231:ASP:C	2.62	0.41
2:B:245:ILE:HB	2:B:340:PHE:HZ	1.86	0.41
3:C:3:DG:H2''	3:C:4:DG:O5'	2.19	0.41
1:A:124:LEU:O	1:A:125:GLY:C	2.61	0.41
1:A:235:GLU:HG2	1:A:236:PRO:HD2	2.02	0.41
1:A:261:ILE:HD13	1:A:330:ILE:HD12	2.03	0.41
1:A:5:PHE:HB2	1:A:108:TYR:CD2	2.56	0.40
1:A:147:ASN:HB2	1:A:233:TYR:CE2	2.56	0.40
1:A:314:GLU:O	1:A:317:LYS:HB2	2.21	0.40
1:A:332:ARG:CZ	4:E:6:DG:OP2	2.69	0.40
2:B:9:ASP:HB3	2:B:10:TYR:CD2	2.56	0.40
2:B:152:LYS:HG2	2:B:184:PRO:HG3	2.03	0.40
2:B:225:LEU:O	2:B:226:ILE:C	2.58	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:THR:O	2:B:240:ARG:O	2.39	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: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
1:A:8:PHE:HD2	1:A:11:PHE:CD1	2.39	0.40
1:A:170:GLU:HG3	1:A:173:ARG:HG2	2.04	0.40
1:A:197:LEU:HD12	1:A:208:ILE:HG21	2.02	0.40
1:A:131:LYS:HE2	1:A:131:LYS:HB2	1.92	0.40
1:A:148:LYS:N	6:A:2049:HOH:O	2.22	0.40
1:A:267:ARG:O	1:A:268:ALA:C	2.64	0.40
2:B:101:ILE:O	2:B:101:ILE:HG22	2.19	0.40
2:B:134:GLU:C	2:B:136:GLU:H	2.30	0.40
2:B:240:ARG:C	2:B:241:VAL:HG23	2.46	0.40
2:B:266:PHE:C	2:B:268:ALA:N	2.77	0.40
2:B:284:ILE:O	2:B:285:HIS:ND1	2.55	0.40
4:F:6:DG:C4	4:F:7:DA:N7	2.89	0.40
2:B:163:ILE:O	6:B:2037:HOH:O	2.22	0.40
2:B:293:LEU:O	2:B:294:ASP:OD2	2.40	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%)	0	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	218 (73%)	82 (27%)	0 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	301/315 (96%)	212 (70%)	89 (30%)	0	0
All	All	601/630 (95%)	430 (72%)	171 (28%)	0	0

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	7	ASP
1	A	31	CYS
1	A	32	VAL
1	A	49	GLU
1	A	56	LYS
1	A	59	ILE
1	A	61	ILE
1	A	63	GLU
1	A	65	LYS
1	A	66	LYS
1	A	75	PRO
1	A	78	LYS
1	A	79	GLU
1	A	81	TYR
1	A	83	GLN
1	A	87	ARG
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	120	GLU
1	A	124	LEU
1	A	129	LYS
1	A	131	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	153	ILE
1	A	163	ILE
1	A	167[A]	ASP
1	A	169	GLU
1	A	176	ARG
1	A	177	GLU
1	A	178	LEU
1	A	180	ILE
1	A	195	LYS
1	A	196	LYS
1	A	197	LEU
1	A	199	ILE
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	245	ILE
1	A	252	LYS
1	A	256	ARG
1	A	262	LYS
1	A	269	ILE
1	A	270	GLU
1	A	271	GLU
1	A	272	SER
1	A	291	GLU
1	A	293	LEU
1	A	295	ILE
1	A	296	VAL
1	A	298	ARG
1	A	302	PHE
1	A	322	ILE
1	A	326	ASP
1	A	327	GLU
1	A	330	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	332	ARG
1	A	333	ILE
1	A	335	VAL
1	A	336	ARG
2	B	4	LEU
2	B	6	VAL
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	72	VAL
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	127	GLU
2	B	128	ILE
2	B	133	LEU
2	B	136	GLU
2	B	137	LYS
2	B	141	THR
2	B	146	LYS
2	B	148	LYS
2	B	153	ILE
2	B	157	MET
2	B	160	PRO
2	B	164	LYS
2	B	165	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	213	LEU
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	243	LYS
2	B	245	ILE
2	B	248	ILE
2	B	249	VAL
2	B	250	THR
2	B	251	MET
2	B	256	ARG
2	B	257[B]	ASN
2	B	260	GLU
2	B	267	ARG
2	B	270	GLU
2	B	277[B]	ASP
2	B	278	LYS
2	B	281	PRO
2	B	284	ILE
2	B	292	ASP
2	B	293	LEU
2	B	294	ASP
2	B	295	ILE
2	B	298	ARG
2	B	301	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	308	LYS
2	B	314	GLU
2	B	323	LEU
2	B	324	GLU
2	B	325	GLU
2	B	329	LYS
2	B	330	ILE
2	B	332	ARG
2	B	333	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	90	ASN
1	A	254	ASN
1	A	285	HIS
2	B	0	HIS
2	B	82	GLN
2	B	161	ASN
2	B	200	ASN
2	B	320	GLN

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	D	14[B]	3	16,19,20	1.07	1 (6%)	20,26,29	1.52	2 (10%)
3	DOC	D	14[A]	4,3	16,19,20	1.55	2 (12%)	20,26,29	2.62	7 (35%)
3	DOC	C	14[A]	4,3	16,19,20	1.09	2 (12%)	20,26,29	1.85	6 (30%)
3	DOC	C	14[B]	3	16,19,20	0.69	0	20,26,29	0.93	1 (5%)

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	D	14[B]	3	-	1/7/18/19	0/2/2/2
3	DOC	D	14[A]	4,3	-	2/7/18/19	0/2/2/2
3	DOC	C	14[A]	4,3	-	4/7/18/19	0/2/2/2
3	DOC	C	14[B]	3	-	0/7/18/19	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	14[A]	DOC	C2-N1	4.69	1.49	1.40
3	D	14[B]	DOC	O4'-C4'	3.48	1.51	1.44
3	C	14[A]	DOC	O4'-C4'	-3.15	1.38	1.44
3	C	14[A]	DOC	C2-N1	2.20	1.44	1.40
3	D	14[A]	DOC	C2-N3	-2.06	1.32	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	14[A]	DOC	C1'-N1-C2	5.77	127.73	117.83
3	D	14[A]	DOC	C2'-C1'-N1	5.54	122.91	112.40
3	D	14[B]	DOC	O4'-C4'-C5'	-4.38	101.44	109.34
3	D	14[A]	DOC	O2-C2-N3	-4.17	115.76	122.33
3	D	14[B]	DOC	O4'-C4'-C3'	-4.05	98.14	104.81
3	D	14[A]	DOC	C1'-N1-C6	-4.01	113.65	121.53
3	C	14[A]	DOC	O4'-C4'-C5'	3.96	116.48	109.34
3	D	14[A]	DOC	O2-C2-N1	3.76	126.26	118.90
3	C	14[A]	DOC	O4'-C4'-C3'	3.68	110.86	104.81
3	C	14[B]	DOC	O4'-C4'-C5'	-3.30	103.39	109.34
3	D	14[A]	DOC	C3'-C2'-C1'	-3.07	99.34	102.87
3	C	14[A]	DOC	C2'-C1'-N1	2.95	118.00	112.40
3	C	14[A]	DOC	C2'-C3'-C4'	-2.80	97.55	102.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	14[A]	DOC	O2-C2-N3	-2.59	118.25	122.33
3	D	14[A]	DOC	O4'-C1'-C2'	-2.28	103.71	106.41
3	C	14[A]	DOC	C1'-N1-C2	2.17	121.56	117.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	14[A]	DOC	C3'-C4'-C5'-O5'
3	D	14[A]	DOC	O4'-C4'-C5'-O5'
3	C	14[A]	DOC	C2'-C1'-N1-C6
3	C	14[A]	DOC	O4'-C1'-N1-C6
3	C	14[A]	DOC	O4'-C1'-N1-C2
3	C	14[A]	DOC	C2'-C1'-N1-C2
3	D	14[B]	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 19 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-1.22	0 100 100	20, 31, 51, 63	11 (3%)
2	B	343/358 (95%)	-1.25	0 100 100	21, 32, 52, 67	5 (1%)
3	C	13/14 (92%)	-1.63	0 100 100	24, 33, 45, 47	0
3	D	13/14 (92%)	-1.55	0 100 100	23, 35, 54, 57	0
4	E	15/18 (83%)	-1.48	0 100 100	34, 45, 59, 62	1 (6%)
4	F	15/18 (83%)	-1.32	0 100 100	33, 50, 62, 64	2 (13%)
All	All	741/780 (95%)	-1.26	0 100 100	20, 32, 53, 67	19 (2%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
3	DOC	C	14[A]	18/19	0.97	0.09	37,42,44,45	18
3	DOC	C	14[B]	18/19	0.97	0.09	29,31,36,36	17
3	DOC	D	14[A]	18/19	0.98	0.09	32,38,39,39	17
3	DOC	D	14[B]	18/19	0.98	0.09	42,42,42,42	18
4	O2G	E	5[E]	24/25	0.98	0.08	68,71,78,79	13
4	O2G	F	5[F]	24/25	0.98	0.08	66,76,77,77	13

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	1342	1/1	0.98	0.03	42,42,42,42	0
5	MG	A	1343	1/1	0.98	0.06	53,53,53,53	0
5	MG	B	1342	1/1	0.98	0.08	47,47,47,47	0
5	MG	B	1343	1/1	0.98	0.09	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.