



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:35 AM UTC

PDB ID : 1D0E / pdb_00001d0e
Title : CRYSTAL STRUCTURES OF THE N-TERMINAL FRAGMENT FROM
MOLONEY MURINE LEUKEMIA VIRUS REVERSE TRANSCRIPTASE
COMPLEXED WITH NUCLEIC ACID: FUNCTIONAL IMPLICATIONS
FOR TEMPLATE-PRIMER BINDING TO THE FINGERS DOMAIN
Authors : Najmudin, S.; Cote, M.L.; Sun, D.; Yohannan, S.; Montano, S.P.; Gu, J.;
Georgiadis, M.M.
Deposited on : 1999-09-09
Resolution : 3.00 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
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

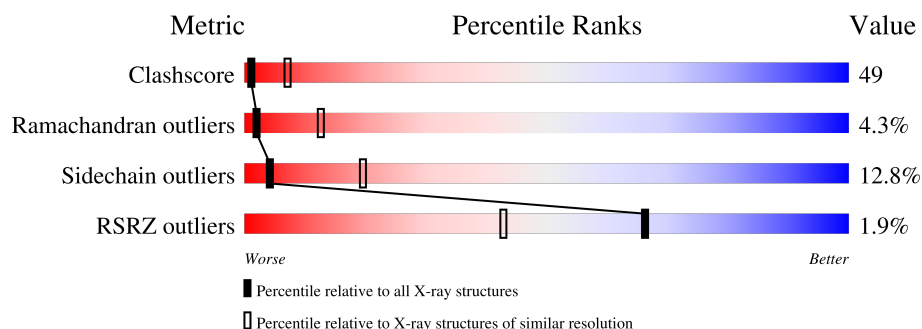
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	E	11	
1	F	11	
2	A	259	
2	B	259	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4570 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called 5'-D(*TP*TP*TP*CP*AP*TP*GP*CP*AP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	11	Total	C	N	O	P	0	0	0
			221	108	36	67	10			
1	F	11	Total	C	N	O	P	0	0	0
			221	108	36	67	10			

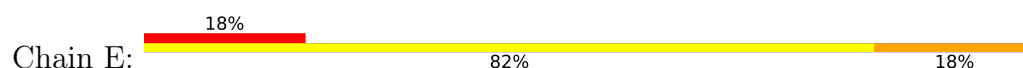
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	259	Total	C	N	O	S	0	0	0
			2069	1327	362	372	8			
2	B	257	Total	C	N	O	S	0	0	0
			2059	1322	360	369	8			

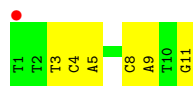
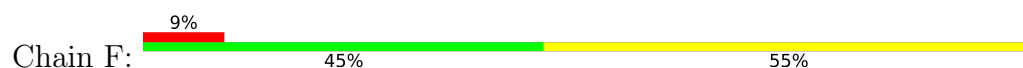
3 Residue-property plots [i](#)

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.

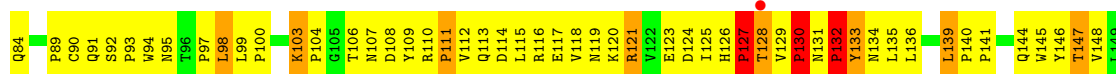
- Molecule 1: 5'-D(*TP*TP*TP*CP*AP*TP*GP*CP*AP*TP*G)-3'



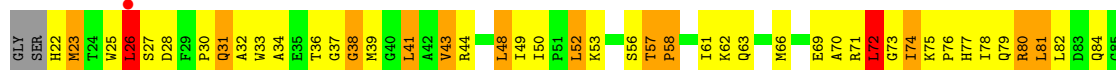
- Molecule 1: 5'-D(*TP*TP*TP*CP*AP*TP*GP*CP*AP*TP*G)-3'

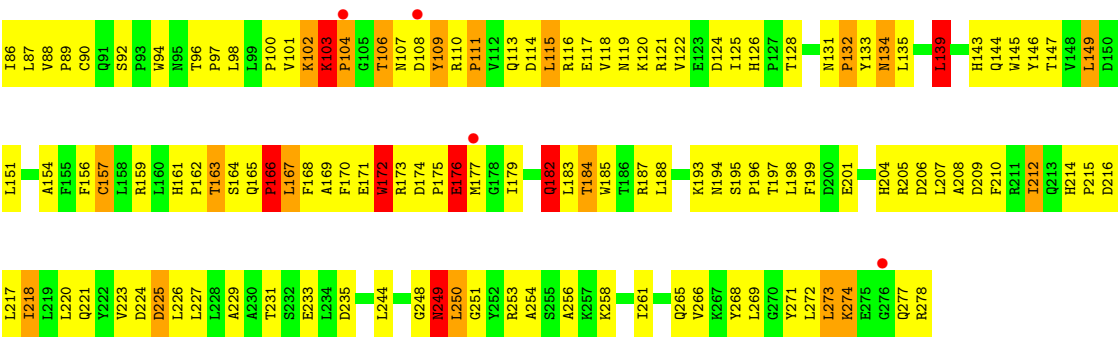


- Molecule 2: REVERSE TRANSCRIPTASE



- Molecule 2: REVERSE TRANSCRIPTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.16Å 63.54Å 73.50Å 90.00° 103.85° 90.00°	Depositor
Resolution (Å)	500.00 – 3.00 71.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (500.00-3.00) 95.7 (71.36-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.298 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4570	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.34	0/246	0.75	0/378
1	F	0.35	0/246	0.76	0/378
2	A	0.95	9/2126 (0.4%)	1.41	39/2896 (1.3%)
2	B	0.75	5/2116 (0.2%)	1.30	24/2883 (0.8%)
All	All	0.82	14/4734 (0.3%)	1.30	63/6535 (1.0%)

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

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	273	LEU	CA-C	19.29	1.76	1.52
2	A	274	LYS	N-CA	13.03	1.62	1.46
2	A	261	ILE	C-N	-10.42	1.19	1.33
2	A	273	LEU	C-N	9.66	1.46	1.33
2	B	107	ASN	N-CA	9.37	1.58	1.46
2	A	127	PRO	N-CA	9.22	1.59	1.47
2	B	109	TYR	N-CA	6.97	1.53	1.45
2	B	106	THR	C-N	6.92	1.43	1.33
2	A	126	HIS	CA-C	6.82	1.60	1.52
2	B	176	GLU	N-CA	-6.16	1.38	1.46
2	A	129	VAL	N-CA	5.79	1.50	1.46
2	A	126	HIS	C-N	5.73	1.42	1.33
2	B	104	PRO	N-CA	5.67	1.54	1.47
2	A	272	LEU	N-CA	5.07	1.52	1.46

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27	SER	N-CA-CB	-18.45	78.10	110.39
2	A	127	PRO	CA-N-CD	-12.19	94.94	112.00
2	A	127	PRO	N-CA-C	11.47	130.84	113.75
2	A	126	HIS	CA-C-N	10.91	131.76	119.32
2	A	126	HIS	C-N-CA	10.91	131.76	119.32
2	B	27	SER	N-CA-C	10.80	125.97	113.01
2	A	274	LYS	N-CA-C	10.73	122.97	111.28
2	A	260	GLN	CA-C-N	10.69	136.93	122.93
2	A	260	GLN	C-N-CA	10.69	136.93	122.93
2	B	26	LEU	CB-CA-C	10.51	131.33	110.42
2	A	273	LEU	N-CA-C	10.18	129.87	114.09
2	A	265	GLN	OE1-CD-NE2	-10.15	112.45	122.60
2	B	31	GLN	OE1-CD-NE2	-10.03	112.57	122.60
2	A	139	LEU	CA-C-N	9.94	126.92	119.66
2	A	139	LEU	C-N-CA	9.94	126.92	119.66
2	A	277	GLN	OE1-CD-NE2	-9.54	113.06	122.60
2	B	182	GLN	OE1-CD-NE2	-9.45	113.15	122.60
2	A	165	GLN	OE1-CD-NE2	-9.45	113.16	122.60
2	A	261	ILE	N-CA-C	9.18	121.18	107.51
2	A	273	LEU	CA-C-O	-7.22	110.63	118.79
2	B	31	GLN	CG-CD-NE2	6.99	126.89	116.40
2	A	73	GLY	N-CA-C	-6.91	106.09	114.66
2	A	265	GLN	CG-CD-NE2	6.78	126.56	116.40
2	B	109	TYR	N-CA-C	6.73	120.86	110.42
2	A	165	GLN	CG-CD-NE2	6.66	126.39	116.40
2	A	127	PRO	CA-C-N	-6.61	112.93	123.91
2	A	127	PRO	C-N-CA	-6.61	112.93	123.91
2	A	277	GLN	CG-CD-NE2	6.55	126.22	116.40
2	A	277	GLN	N-CA-C	6.50	116.44	107.73
2	A	128	THR	CA-C-N	6.49	127.26	122.59
2	A	128	THR	C-N-CA	6.49	127.26	122.59
2	B	182	GLN	CG-CD-NE2	6.34	125.91	116.40
2	B	273	LEU	N-CA-C	6.28	118.69	108.26
2	B	106	THR	CA-C-N	6.25	133.48	121.54
2	B	106	THR	C-N-CA	6.25	133.48	121.54
2	A	273	LEU	CA-C-N	6.14	128.51	120.28
2	A	273	LEU	C-N-CA	6.14	128.51	120.28
2	A	273	LEU	O-C-N	-6.12	115.42	122.09
2	B	108	ASP	CA-CB-CG	6.10	118.70	112.60
2	B	103	LYS	N-CA-C	-5.92	102.89	108.22
2	B	250	LEU	N-CA-C	-5.92	106.39	113.97
2	A	260	GLN	O-C-N	-5.88	114.16	122.87
2	B	171	GLU	N-CA-C	5.87	118.33	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	24	THR	N-CA-C	-5.84	105.00	111.36
2	B	111	PRO	CB-CA-C	5.81	119.02	111.64
2	A	129	VAL	N-CA-C	5.80	113.62	107.76
2	B	111	PRO	CA-C-N	-5.68	114.92	122.98
2	B	111	PRO	C-N-CA	-5.68	114.92	122.98
2	A	128	THR	N-CA-CB	-5.59	104.23	112.78
2	B	139	LEU	CA-C-N	5.54	126.08	120.38
2	B	139	LEU	C-N-CA	5.54	126.08	120.38
2	B	107	ASN	N-CA-C	5.53	122.58	110.80
2	A	43	VAL	N-CA-C	5.47	116.97	111.00
2	A	121	ARG	N-CA-C	-5.47	107.85	114.75
2	B	157	CYS	N-CA-C	-5.43	106.15	112.89
2	A	175	PRO	N-CA-C	-5.31	105.88	113.47
2	B	144	GLN	N-CA-C	-5.25	106.26	113.30
2	A	130	PRO	CA-N-CD	-5.21	104.70	112.00
2	B	48	LEU	N-CA-C	5.20	118.03	109.76
2	A	273	LEU	N-CA-CB	-5.09	103.07	111.01
2	A	182	GLN	N-CA-C	5.06	117.40	108.75
2	A	132	PRO	CB-CA-C	5.04	119.88	111.56
2	A	127	PRO	N-CD-CG	5.04	110.76	103.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	5	DA	Sidechain
1	E	7	DG	Sidechain

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	E	221	0	128	19	0
1	F	221	0	128	11	0
2	A	2069	0	2080	219	0
2	B	2059	0	2072	201	0
All	All	4570	0	4408	438	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 49.

All (438) 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)
2:A:273:LEU:C	2:A:273:LEU:CA	1.76	1.58
2:A:264:LYS:O	2:A:274:LYS:HB2	1.39	1.20
2:A:68:GLN:HE21	2:A:69:GLU:HG3	1.18	1.08
2:B:74:ILE:HG13	2:B:111:PRO:HG3	1.40	1.01
2:B:39:MET:HE3	2:B:86:ILE:HD11	1.41	0.99
2:A:266:VAL:HG22	2:A:273:LEU:HD21	1.44	0.97
2:A:165:GLN:HE21	2:A:186:THR:HA	1.25	0.97
2:B:131:ASN:HB3	2:B:134:ASN:HB3	1.44	0.97
2:B:201:GLU:HG2	2:B:205:ARG:HH22	1.30	0.95
2:B:71:ARG:HH22	2:B:75:LYS:HZ3	1.13	0.94
1:E:5:DA:H2''	1:E:6:DT:H5'	1.50	0.93
2:B:74:ILE:CD1	2:B:111:PRO:HD3	2.00	0.92
1:E:6:DT:H3	1:F:9:DA:H61	1.12	0.91
2:B:26:LEU:HD11	2:B:36:THR:HG23	1.52	0.90
2:B:74:ILE:HD11	2:B:111:PRO:HD3	1.54	0.88
2:A:232:SER:HB3	2:A:235:ASP:OD2	1.72	0.88
1:E:9:DA:H4'	1:E:10:DT:OP1	1.74	0.86
2:B:71:ARG:NH2	2:B:75:LYS:HZ3	1.72	0.86
2:A:214:HIS:HB3	2:A:217:LEU:HD12	1.57	0.86
2:A:68:GLN:NE2	2:A:69:GLU:HG3	1.91	0.86
2:B:61:ILE:HD11	2:B:117:GLU:HG3	1.57	0.86
2:A:266:VAL:CG2	2:A:273:LEU:HD21	2.05	0.86
2:A:266:VAL:O	2:A:273:LEU:HD22	1.76	0.85
2:A:261:ILE:HD12	2:A:261:ILE:H	1.42	0.83
2:B:101:VAL:O	2:B:109:TYR:CD1	2.31	0.83
2:B:101:VAL:O	2:B:109:TYR:HD1	1.61	0.83
2:B:66:MET:HE2	2:B:100:PRO:CD	2.09	0.82
2:B:66:MET:HE2	2:B:100:PRO:HD3	1.62	0.81
2:A:31:GLN:HE21	2:A:31:GLN:HA	1.46	0.81
2:B:71:ARG:HH22	2:B:75:LYS:NZ	1.77	0.81
2:B:149:LEU:O	2:B:149:LEU:HD12	1.79	0.81
2:A:113:GLN:HE21	2:A:170:PHE:HB3	1.46	0.81
2:A:91:GLN:HG3	2:A:91:GLN:O	1.80	0.81
2:A:21:SER:OG	2:A:24:THR:HG23	1.81	0.80
2:A:266:VAL:H	2:A:273:LEU:CD2	1.93	0.80
2:B:43:VAL:CG2	2:B:44:ARG:HH11	1.94	0.80
2:B:74:ILE:CG1	2:B:111:PRO:HG3	2.13	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:266:VAL:H	2:A:273:LEU:HD23	1.49	0.77
2:B:225:ASP:O	2:B:226:LEU:HD23	1.85	0.77
2:A:48:LEU:HD13	2:A:198:LEU:HD13	1.66	0.77
1:F:9:DA:H8	1:F:9:DA:OP2	1.68	0.77
2:B:118:VAL:O	2:B:122:VAL:HG23	1.84	0.77
2:A:77:HIS:O	2:A:81:LEU:HD23	1.84	0.76
2:A:130:PRO:O	2:A:131:ASN:C	2.24	0.76
2:B:266:VAL:O	2:B:272:LEU:HD12	1.85	0.76
2:A:41:LEU:HD13	2:B:43:VAL:HB	1.65	0.76
1:F:8:DC:H2"	1:F:9:DA:OP2	1.84	0.76
2:B:272:LEU:O	2:B:273:LEU:HD23	1.86	0.76
2:A:146:TYR:CE2	2:A:273:LEU:HG	2.20	0.76
2:A:130:PRO:HB2	2:A:135:LEU:HD22	1.69	0.75
2:A:39:MET:SD	2:A:84:GLN:HG3	2.26	0.75
2:A:70:ALA:O	2:A:74:ILE:HG12	1.85	0.75
2:A:165:GLN:NE2	2:A:186:THR:HA	2.02	0.73
2:A:266:VAL:O	2:A:273:LEU:CD2	2.37	0.73
1:E:6:DT:H2"	1:E:7:DG:N7	2.04	0.73
2:A:203:LEU:HD11	2:A:207:LEU:HD11	1.71	0.72
2:B:43:VAL:HG21	2:B:44:ARG:HH11	1.55	0.72
2:A:155:PHE:HB3	2:A:188:LEU:HB3	1.70	0.72
2:B:26:LEU:CD1	2:B:36:THR:HG23	2.19	0.72
2:A:22:HIS:HB3	2:A:23:MET:HE3	1.71	0.71
2:B:159:ARG:HA	2:B:187:ARG:HA	1.72	0.71
2:A:273:LEU:C	2:A:273:LEU:CB	2.63	0.71
2:A:127:PRO:O	2:A:128:THR:OG1	2.09	0.71
2:B:38:GLY:O	2:B:253:ARG:HG3	1.90	0.71
2:B:102:LYS:O	2:B:102:LYS:HD3	1.91	0.70
2:A:114:ASP:CG	2:A:116:ARG:HE	1.99	0.70
2:A:41:LEU:HD21	2:A:159:ARG:HD2	1.72	0.70
2:B:218:ILE:HB	2:B:229:ALA:HB3	1.72	0.70
2:B:74:ILE:HD11	2:B:111:PRO:CD	2.22	0.69
2:A:152:LYS:HG3	2:A:153:ASP:OD1	1.92	0.69
2:A:162:PRO:C	2:A:164:SER:H	2.01	0.69
2:B:90:CYS:SG	2:B:184:THR:HB	2.31	0.69
2:B:214:HIS:HB3	2:B:217:LEU:HD12	1.73	0.69
2:A:161:HIS:CD2	2:A:163:THR:OG1	2.45	0.69
2:B:73:GLY:O	2:B:76:PRO:HD2	1.93	0.69
2:B:61:ILE:CD1	2:B:117:GLU:HG3	2.22	0.69
2:A:273:LEU:C	2:A:273:LEU:HA	2.08	0.67
2:A:214:HIS:CB	2:A:217:LEU:HD12	2.24	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:GLN:NE2	2:B:170:PHE:HB3	2.10	0.66
2:A:26:LEU:HD22	2:A:33:TRP:CD1	2.31	0.66
2:A:90:CYS:SG	2:A:184:THR:HB	2.36	0.66
2:A:92:SER:CB	2:A:166:PRO:HB3	2.25	0.66
2:A:39:MET:HE3	2:A:80:ARG:HH21	1.61	0.66
2:B:34:ALA:HA	2:B:253:ARG:HB3	1.78	0.65
2:B:113:GLN:HE21	2:B:170:PHE:HB3	1.61	0.65
2:B:98:LEU:O	2:B:100:PRO:HD3	1.96	0.65
2:B:206:ASP:O	2:B:208:ALA:N	2.28	0.65
2:B:90:CYS:O	2:B:182:GLN:HG3	1.97	0.65
2:A:71:ARG:HH22	2:A:173:ARG:H	1.45	0.65
2:A:106:THR:C	2:A:108:ASP:H	2.05	0.64
2:A:146:TYR:CG	2:A:273:LEU:HD11	2.33	0.64
2:A:80:ARG:HG3	2:A:81:LEU:HD22	1.79	0.64
2:A:203:LEU:O	2:A:207:LEU:HG	1.98	0.64
2:B:156:PHE:HA	2:B:187:ARG:HB3	1.80	0.64
2:B:53:LYS:HE3	2:B:122:VAL:O	1.98	0.64
2:B:195:SER:HB2	2:B:196:PRO:HD3	1.80	0.64
2:A:83:ASP:OD1	2:B:161:HIS:HE1	1.80	0.64
2:A:161:HIS:HD2	2:A:163:THR:OG1	1.80	0.64
2:A:148:VAL:HB	2:A:260:GLN:HB2	1.80	0.64
2:B:201:GLU:HG2	2:B:205:ARG:NH2	2.09	0.64
2:A:39:MET:HE3	2:A:80:ARG:NH2	2.13	0.63
2:B:205:ARG:HG3	2:B:205:ARG:HH11	1.63	0.63
1:E:2:DT:H3	1:E:4:DC:H41	1.46	0.63
1:F:4:DC:H2''	1:F:5:DA:H5'	1.81	0.63
1:F:9:DA:OP2	1:F:9:DA:C8	2.50	0.63
2:A:113:GLN:NE2	2:A:170:PHE:HB3	2.15	0.62
2:B:161:HIS:HD2	2:B:163:THR:HB	1.64	0.62
2:B:175:PRO:O	2:B:176:GLU:C	2.42	0.62
1:E:5:DA:C2'	1:E:6:DT:H5'	2.27	0.62
2:A:164:SER:O	2:A:167:LEU:HG	1.99	0.62
2:B:22:HIS:HD2	2:B:23:MET:H	1.48	0.62
2:A:261:ILE:H	2:A:261:ILE:CD1	2.00	0.61
2:A:132:PRO:O	2:A:133:TYR:C	2.42	0.61
2:B:56:SER:OG	2:B:121:ARG:HB3	1.99	0.61
2:B:133:TYR:O	2:B:135:LEU:N	2.34	0.61
1:E:6:DT:H3	1:F:9:DA:N6	1.92	0.61
2:A:43:VAL:HG22	2:A:250:LEU:O	2.00	0.61
2:A:147:THR:HA	2:A:260:GLN:O	2.00	0.61
2:B:33:TRP:CD2	2:B:256:ALA:HB2	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:GLN:HB2	2:B:166:PRO:HD3	1.83	0.60
2:A:121:ARG:HG3	2:A:121:ARG:HH11	1.67	0.60
2:A:22:HIS:HB3	2:A:23:MET:CE	2.31	0.60
2:A:125:ILE:O	2:A:127:PRO:HD3	2.02	0.60
2:B:101:VAL:O	2:B:109:TYR:HA	2.00	0.60
2:B:74:ILE:HA	2:B:77:HIS:ND1	2.15	0.60
2:A:74:ILE:HD13	2:A:100:PRO:HB3	1.82	0.60
2:A:79:GLN:CD	2:A:177:MET:HE2	2.27	0.60
2:B:61:ILE:HD11	2:B:117:GLU:CG	2.31	0.60
2:A:115:LEU:O	2:A:119:ASN:ND2	2.35	0.59
2:B:50:ILE:HG12	2:B:164:SER:HB3	1.84	0.59
2:B:162:PRO:HA	2:B:165:GLN:HG3	1.84	0.59
2:A:26:LEU:HA	2:A:33:TRP:CD1	2.37	0.59
2:A:157:CYS:C	2:A:158:LEU:HD12	2.28	0.59
2:A:266:VAL:CG2	2:A:273:LEU:CD2	2.80	0.59
2:A:92:SER:HB3	2:A:166:PRO:HB3	1.83	0.59
2:B:41:LEU:O	2:B:251:GLY:HA3	2.03	0.59
2:A:114:ASP:OD2	2:A:116:ARG:NE	2.32	0.58
2:B:26:LEU:CD1	2:B:36:THR:CG2	2.79	0.58
2:A:49:ILE:O	2:A:50:ILE:HD13	2.03	0.58
2:B:72:LEU:HD13	2:B:73:GLY:H	1.67	0.58
2:B:102:LYS:HD3	2:B:102:LYS:C	2.28	0.58
2:B:272:LEU:HD12	2:B:273:LEU:H	1.68	0.58
2:A:127:PRO:C	2:A:128:THR:OG1	2.45	0.58
2:B:221:GLN:HB2	2:B:226:LEU:HD22	1.86	0.58
2:A:32:ALA:O	2:A:253:ARG:HA	2.03	0.58
2:A:79:GLN:NE2	2:A:177:MET:SD	2.77	0.58
2:A:136:LEU:HD12	2:A:136:LEU:N	2.18	0.58
2:B:115:LEU:O	2:B:119:ASN:ND2	2.37	0.57
2:A:145:TRP:O	2:A:229:ALA:HA	2.04	0.57
2:B:151:LEU:HD23	2:B:254:ALA:HB2	1.85	0.57
2:A:89:PRO:HG3	2:A:179:ILE:HD12	1.87	0.57
1:E:1:DT:O5'	2:A:104:PRO:HG3	2.04	0.57
2:A:71:ARG:O	2:A:74:ILE:HG13	2.04	0.56
2:A:58:PRO:HG3	2:A:94:TRP:HE1	1.69	0.56
2:A:200:ASP:HB2	2:A:223:VAL:HG22	1.86	0.56
2:B:221:GLN:HB2	2:B:226:LEU:CD2	2.34	0.56
2:A:266:VAL:N	2:A:273:LEU:CD2	2.66	0.56
2:A:66:MET:HE3	2:A:71:ARG:HG3	1.87	0.56
2:A:98:LEU:HD23	2:A:170:PHE:HB2	1.87	0.56
2:A:174:ASP:OD1	2:A:176:GLU:HB3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:269:LEU:C	2:A:271:TYR:H	2.14	0.56
2:B:22:HIS:CD2	2:B:23:MET:N	2.74	0.55
2:A:277:GLN:CD	2:A:278:ARG:H	2.14	0.55
2:A:91:GLN:HG2	2:B:89:PRO:HG2	1.88	0.55
2:A:261:ILE:O	2:A:262:CYS:C	2.47	0.55
2:B:133:TYR:C	2:B:135:LEU:H	2.15	0.55
2:B:204:HIS:N	2:B:221:GLN:HE22	2.04	0.55
2:A:165:GLN:HB3	2:A:185:TRP:O	2.07	0.55
2:A:29:PHE:N	2:A:30:PRO:HD3	2.21	0.55
2:A:49:ILE:N	2:A:49:ILE:HD12	2.21	0.55
2:A:158:LEU:O	2:A:187:ARG:HA	2.07	0.55
2:A:64:TYR:CE2	2:A:99:LEU:HD21	2.42	0.55
2:B:175:PRO:O	2:B:177:MET:N	2.40	0.55
2:B:175:PRO:C	2:B:177:MET:N	2.65	0.54
2:A:64:TYR:HE2	2:A:99:LEU:HD21	1.73	0.54
2:A:26:LEU:HD11	2:A:36:THR:OG1	2.08	0.54
2:A:192:PHE:HB3	2:A:195:SER:OG	2.07	0.54
1:E:8:DC:H2''	1:E:9:DA:C8	2.43	0.54
2:A:273:LEU:CA	2:A:273:LEU:O	2.48	0.54
2:A:119:ASN:O	2:A:193:LYS:NZ	2.32	0.54
2:A:273:LEU:HD23	2:A:273:LEU:H	1.72	0.54
2:B:39:MET:CE	2:B:86:ILE:HD11	2.26	0.54
2:B:78:ILE:HG23	2:B:87:LEU:CD1	2.37	0.54
2:B:125:ILE:HG12	2:B:194:ASN:OD1	2.08	0.54
2:B:197:THR:O	2:B:201:GLU:HB2	2.08	0.54
2:A:71:ARG:NH2	2:A:173:ARG:H	2.05	0.54
2:B:72:LEU:HD13	2:B:73:GLY:N	2.22	0.54
2:B:258:LYS:HB3	2:B:258:LYS:NZ	2.23	0.54
2:A:178:GLY:C	2:A:179:ILE:HD13	2.33	0.53
2:B:139:LEU:HD13	2:B:220:LEU:HD21	1.90	0.53
2:A:31:GLN:HE21	2:A:31:GLN:CA	2.19	0.53
2:A:226:LEU:HD12	2:A:226:LEU:N	2.23	0.53
2:B:66:MET:SD	2:B:100:PRO:HG3	2.49	0.53
1:F:11:DG:O3'	2:A:115:LEU:N	2.42	0.53
2:B:206:ASP:C	2:B:208:ALA:H	2.16	0.53
2:B:74:ILE:HA	2:B:77:HIS:HD1	1.74	0.53
2:B:92:SER:N	2:B:182:GLN:OE1	2.41	0.53
2:B:179:ILE:HD13	2:B:183:LEU:HD21	1.91	0.53
2:B:74:ILE:HD12	2:B:111:PRO:HD3	1.87	0.53
2:A:79:GLN:OE1	2:A:177:MET:HE2	2.08	0.52
2:A:200:ASP:HB2	2:A:223:VAL:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ILE:HG13	2:B:111:PRO:CG	2.27	0.52
2:B:154:ALA:HB1	2:B:199:PHE:CZ	2.44	0.52
1:E:1:DT:H3'	1:E:2:DT:C5'	2.40	0.52
2:A:42:ALA:O	2:A:159:ARG:NH1	2.42	0.52
1:F:3:DT:H2''	1:F:4:DC:OP2	2.09	0.52
2:A:266:VAL:N	2:A:273:LEU:HD21	2.25	0.52
2:A:92:SER:HB2	2:A:166:PRO:HB3	1.91	0.52
2:A:117:GLU:OE1	2:A:117:GLU:HA	2.08	0.52
2:B:22:HIS:HD2	2:B:23:MET:N	2.08	0.52
2:B:168:PHE:HB3	2:B:185:TRP:HD1	1.75	0.52
2:A:266:VAL:H	2:A:273:LEU:HD21	1.74	0.52
2:A:146:TYR:HA	2:A:228:LEU:O	2.10	0.52
2:B:37:GLY:O	2:B:38:GLY:O	2.27	0.52
2:A:26:LEU:HA	2:A:33:TRP:NE1	2.25	0.51
2:B:103:LYS:HE3	2:B:104:PRO:HD2	1.90	0.51
2:A:193:LYS:HG3	2:A:194:ASN:N	2.25	0.51
2:B:66:MET:HB3	2:B:70:ALA:HB3	1.92	0.51
2:A:83:ASP:OD1	2:B:161:HIS:CE1	2.61	0.51
2:B:258:LYS:HB3	2:B:258:LYS:HZ3	1.74	0.51
2:B:30:PRO:HA	2:B:36:THR:OG1	2.11	0.51
2:B:71:ARG:HH12	2:B:75:LYS:HE2	1.74	0.51
2:A:53:LYS:HD2	2:A:121:ARG:HA	1.93	0.51
2:B:209:ASP:HA	2:B:212:ILE:CD1	2.40	0.51
2:A:173:ARG:HB2	2:A:173:ARG:NH1	2.26	0.51
2:B:133:TYR:C	2:B:135:LEU:N	2.69	0.51
2:B:176:GLU:OE1	2:B:176:GLU:N	2.44	0.51
2:B:215:PRO:HG2	2:B:216:ASP:OD1	2.10	0.51
2:A:58:PRO:HG3	2:A:94:TRP:NE1	2.26	0.51
2:B:49:ILE:HD12	2:B:49:ILE:N	2.26	0.51
2:A:66:MET:HE3	2:A:71:ARG:HH11	1.76	0.51
2:A:120:LYS:O	2:A:120:LYS:HG3	2.11	0.51
2:B:75:LYS:N	2:B:76:PRO:HD2	2.26	0.51
2:A:44:ARG:HA	2:B:31:GLN:NE2	2.26	0.50
2:B:249:ASN:N	2:B:249:ASN:ND2	2.58	0.50
2:A:223:VAL:HG12	2:A:224:ASP:N	2.26	0.50
2:A:74:ILE:HG23	2:A:109:TYR:HB3	1.93	0.50
2:B:41:LEU:HD21	2:B:159:ARG:NH1	2.26	0.50
2:B:268:TYR:CE2	2:B:269:LEU:HD22	2.47	0.50
2:A:35:GLU:OE2	2:A:257:LYS:HD3	2.11	0.50
2:A:136:LEU:H	2:A:136:LEU:CD1	2.24	0.50
2:A:72:LEU:HA	2:A:75:LYS:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ARG:O	2:B:84:GLN:HG3	2.12	0.50
2:B:204:HIS:CE1	2:B:221:GLN:HG2	2.47	0.50
2:A:56:SER:HB3	2:A:121:ARG:HB3	1.94	0.50
2:B:57:THR:HG23	2:B:58:PRO:HD2	1.93	0.50
2:A:221:GLN:O	2:A:221:GLN:HG3	2.11	0.50
2:A:128:THR:OG1	2:A:197:THR:HG23	2.12	0.49
1:F:4:DC:H2''	1:F:5:DA:C5'	2.42	0.49
2:B:71:ARG:O	2:B:72:LEU:C	2.56	0.49
2:A:68:GLN:O	2:A:72:LEU:HG	2.12	0.49
2:A:95:ASN:HA	2:A:169:ALA:O	2.13	0.49
2:A:98:LEU:HD23	2:A:170:PHE:CB	2.42	0.49
2:A:150:ASP:OD2	2:A:152:LYS:NZ	2.46	0.49
2:B:209:ASP:HA	2:B:212:ILE:HD12	1.95	0.49
2:B:106:THR:HG23	2:B:106:THR:O	2.13	0.48
2:B:227:LEU:HB2	2:B:268:TYR:CE1	2.48	0.48
2:A:123:GLU:CD	2:A:124:ASP:H	2.21	0.48
2:A:195:SER:HB2	2:A:196:PRO:HD3	1.95	0.48
2:B:143:HIS:CE1	2:B:231:THR:HG23	2.47	0.48
2:A:35:GLU:OE1	2:A:35:GLU:N	2.41	0.48
2:B:172:TRP:HA	2:B:172:TRP:CE3	2.48	0.48
1:E:4:DC:O5'	1:E:4:DC:H6	1.97	0.48
2:A:106:THR:C	2:A:108:ASP:N	2.72	0.48
2:A:58:PRO:HA	2:A:94:TRP:CE2	2.49	0.48
2:B:71:ARG:HH12	2:B:75:LYS:CE	2.27	0.48
2:A:61:ILE:O	2:A:95:ASN:ND2	2.40	0.48
2:B:79:GLN:O	2:B:80:ARG:C	2.56	0.48
2:B:53:LYS:NZ	2:B:120:LYS:O	2.39	0.47
2:A:240:THR:O	2:A:244:LEU:HG	2.14	0.47
2:B:66:MET:HE2	2:B:98:LEU:O	2.14	0.47
2:B:72:LEU:O	2:B:73:GLY:C	2.57	0.47
2:B:205:ARG:HH11	2:B:205:ARG:CG	2.27	0.47
2:A:162:PRO:O	2:A:164:SER:N	2.47	0.47
2:A:67:SER:O	2:A:68:GLN:C	2.58	0.47
2:A:140:PRO:HD2	2:A:218:ILE:CD1	2.45	0.47
2:B:74:ILE:O	2:B:77:HIS:HB2	2.14	0.47
2:A:53:LYS:HB2	2:A:56:SER:OG	2.15	0.47
2:B:71:ARG:NH1	2:B:75:LYS:HE2	2.29	0.47
1:E:5:DA:H2''	1:E:6:DT:C5'	2.35	0.47
2:A:97:PRO:HD2	2:A:114:ASP:HB3	1.97	0.47
2:A:123:GLU:HA	2:A:123:GLU:OE2	2.14	0.47
2:A:136:LEU:N	2:A:136:LEU:CD1	2.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:199:PHE:HE2	2:A:223:VAL:O	1.98	0.47
2:A:269:LEU:C	2:A:271:TYR:N	2.71	0.47
2:B:114:ASP:OD1	2:B:114:ASP:O	2.32	0.47
2:B:116:ARG:HA	2:B:119:ASN:HD22	1.80	0.47
2:B:98:LEU:O	2:B:100:PRO:CD	2.61	0.47
2:B:32:ALA:O	2:B:253:ARG:HA	2.15	0.47
2:B:248:GLY:C	2:B:250:LEU:H	2.23	0.47
2:B:269:LEU:C	2:B:271:TYR:H	2.22	0.47
2:A:41:LEU:N	2:A:251:GLY:O	2.44	0.46
2:B:169:ALA:HA	2:B:183:LEU:O	2.15	0.46
1:E:6:DT:O2	1:F:9:DA:N1	2.48	0.46
2:B:143:HIS:ND1	2:B:231:THR:HG23	2.30	0.46
2:B:249:ASN:N	2:B:249:ASN:HD22	2.13	0.46
2:B:96:THR:OG1	2:B:113:GLN:NE2	2.48	0.46
2:A:192:PHE:CE2	2:A:194:ASN:HB2	2.51	0.46
2:B:69:GLU:H	2:B:69:GLU:CD	2.22	0.46
2:A:173:ARG:CZ	2:A:173:ARG:CB	2.94	0.46
1:E:9:DA:H1'	1:E:10:DT:H5'	1.96	0.46
2:B:78:ILE:HG22	2:B:82:LEU:CD2	2.46	0.46
2:A:98:LEU:HD23	2:A:170:PHE:CG	2.51	0.46
2:B:66:MET:HE2	2:B:100:PRO:CG	2.45	0.46
2:B:125:ILE:O	2:B:126:HIS:C	2.58	0.46
2:B:265:GLN:HG3	2:B:274:LYS:HG3	1.98	0.46
1:F:3:DT:O2	1:F:3:DT:O4'	2.34	0.46
2:A:173:ARG:CZ	2:A:173:ARG:HB3	2.45	0.46
2:A:211:ARG:HD3	2:A:219:LEU:HB3	1.96	0.46
2:A:267:LYS:HE3	2:A:267:LYS:O	2.15	0.46
2:B:172:TRP:HA	2:B:172:TRP:HE3	1.79	0.46
2:B:188:LEU:HD21	2:B:198:LEU:HB2	1.97	0.46
2:B:205:ARG:HB2	2:B:205:ARG:CZ	2.46	0.46
2:B:73:GLY:O	2:B:76:PRO:CD	2.64	0.45
2:A:139:LEU:C	2:A:139:LEU:HD23	2.42	0.45
2:B:272:LEU:C	2:B:273:LEU:HD23	2.42	0.45
2:B:33:TRP:CZ3	2:B:256:ALA:HA	2.52	0.45
2:B:71:ARG:HH12	2:B:75:LYS:NZ	2.15	0.45
2:B:227:LEU:HB2	2:B:268:TYR:CD1	2.52	0.45
2:A:59:VAL:HG13	2:A:59:VAL:O	2.17	0.45
2:A:218:ILE:HG22	2:A:220:LEU:CD1	2.47	0.45
2:A:266:VAL:HG23	2:A:273:LEU:CD2	2.46	0.45
2:B:146:TYR:HB2	2:B:266:VAL:HG11	1.98	0.45
2:B:154:ALA:O	2:B:157:CYS:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:LEU:H	2:B:167:LEU:HD13	1.81	0.45
2:B:89:PRO:O	2:B:90:CYS:HB3	2.17	0.45
2:B:154:ALA:HB1	2:B:199:PHE:CE2	2.52	0.45
1:E:3:DT:H4'	1:E:4:DC:OP1	2.15	0.45
2:A:141:PRO:O	2:A:144:GLN:HG3	2.17	0.45
2:A:246:THR:HG22	2:A:250:LEU:HD12	1.98	0.45
2:B:174:ASP:OD2	2:B:174:ASP:C	2.59	0.45
2:B:227:LEU:C	2:B:227:LEU:HD23	2.42	0.45
2:A:222:TYR:O	2:A:223:VAL:HB	2.17	0.44
2:B:101:VAL:O	2:B:109:TYR:CA	2.65	0.44
2:A:245:GLN:NE2	2:A:249:ASN:OD1	2.43	0.44
2:B:78:ILE:O	2:B:81:LEU:HB2	2.17	0.44
2:B:86:ILE:HG22	2:B:86:ILE:O	2.17	0.44
2:A:110:ARG:HH12	2:A:112:VAL:HG22	1.80	0.44
2:B:48:LEU:HD12	2:B:188:LEU:HD13	1.99	0.44
2:B:22:HIS:CD2	2:B:23:MET:H	2.31	0.44
2:B:139:LEU:HD13	2:B:220:LEU:CD2	2.47	0.44
2:A:273:LEU:HD23	2:A:273:LEU:N	2.32	0.44
2:A:57:THR:HG23	2:A:58:PRO:HD2	1.99	0.44
2:A:66:MET:SD	2:A:74:ILE:HD11	2.58	0.44
2:A:211:ARG:NE	2:A:219:LEU:HD23	2.33	0.44
2:A:136:LEU:HD12	2:A:136:LEU:H	1.79	0.44
2:B:22:HIS:HB3	2:B:25:TRP:CD1	2.52	0.44
2:B:33:TRP:CG	2:B:256:ALA:HB2	2.52	0.44
2:B:165:GLN:N	2:B:166:PRO:CD	2.80	0.44
2:A:49:ILE:HG22	2:A:50:ILE:N	2.32	0.44
2:A:237:GLN:HA	2:A:262:CYS:SG	2.57	0.44
2:A:269:LEU:O	2:A:271:TYR:N	2.51	0.44
2:B:258:LYS:NZ	2:B:258:LYS:CB	2.80	0.44
2:A:26:LEU:CD1	2:A:36:THR:OG1	2.66	0.44
2:A:195:SER:N	2:A:196:PRO:CD	2.80	0.44
2:B:61:ILE:HD11	2:B:117:GLU:CB	2.48	0.44
2:B:176:GLU:CD	2:B:176:GLU:H	2.26	0.44
2:B:63:GLN:HE22	2:B:98:LEU:H	1.65	0.43
2:B:165:GLN:N	2:B:166:PRO:HD2	2.33	0.43
2:A:70:ALA:CB	2:A:109:TYR:CE2	3.01	0.43
2:A:120:LYS:NZ	2:A:121:ARG:HH12	2.17	0.43
2:B:147:THR:HG23	2:B:261:ILE:HA	1.99	0.43
2:B:124:ASP:HA	2:B:193:LYS:HE3	2.00	0.43
2:A:121:ARG:HG3	2:A:121:ARG:NH1	2.32	0.43
2:A:225:ASP:HB3	2:A:268:TYR:HE1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:VAL:HG21	2:B:44:ARG:NH1	2.26	0.43
2:A:227:LEU:C	2:A:227:LEU:HD23	2.43	0.43
2:B:199:PHE:HE2	2:B:224:ASP:HA	1.82	0.43
1:E:9:DA:C4'	1:E:10:DT:OP1	2.55	0.43
2:B:26:LEU:HD13	2:B:26:LEU:HA	1.81	0.43
2:B:97:PRO:HG2	2:B:114:ASP:HB3	1.99	0.43
2:A:26:LEU:HD11	2:A:36:THR:CG2	2.49	0.43
2:A:62:LYS:HA	2:A:62:LYS:HD3	1.86	0.43
2:A:89:PRO:HG2	2:B:162:PRO:HB3	2.00	0.43
2:A:94:TRP:CE3	2:A:118:VAL:HG22	2.53	0.43
2:A:263:GLN:NE2	2:A:264:LYS:H	2.17	0.43
2:B:66:MET:CE	2:B:100:PRO:HD3	2.42	0.43
2:A:199:PHE:O	2:A:200:ASP:C	2.60	0.43
2:A:203:LEU:HD23	2:A:223:VAL:O	2.19	0.42
2:A:243:LEU:O	2:A:244:LEU:C	2.61	0.42
2:B:26:LEU:HD11	2:B:36:THR:CG2	2.32	0.42
2:B:77:HIS:O	2:B:81:LEU:HD22	2.18	0.42
2:A:106:THR:OG1	2:A:108:ASP:HB2	2.19	0.42
2:B:103:LYS:HE3	2:B:103:LYS:HA	2.00	0.42
2:A:230:ALA:HB1	2:A:235:ASP:HB2	2.00	0.42
2:B:248:GLY:O	2:B:250:LEU:N	2.52	0.42
2:A:117:GLU:O	2:A:118:VAL:C	2.61	0.42
2:A:68:GLN:NE2	2:A:69:GLU:N	2.68	0.42
2:A:70:ALA:CB	2:A:109:TYR:HE2	2.32	0.42
2:A:139:LEU:HD23	2:A:139:LEU:O	2.20	0.42
2:A:162:PRO:C	2:A:164:SER:N	2.70	0.42
2:A:82:LEU:CD1	2:B:162:PRO:HG2	2.50	0.42
2:A:133:TYR:CD2	2:A:134:ASN:N	2.88	0.42
2:A:176:GLU:O	2:A:176:GLU:HG2	2.19	0.42
2:B:143:HIS:HA	2:B:231:THR:HA	2.01	0.42
2:A:30:PRO:O	2:A:37:GLY:HA3	2.20	0.41
2:A:53:LYS:HB2	2:A:56:SER:HG	1.85	0.41
2:A:165:GLN:H	2:A:165:GLN:HG3	1.46	0.41
2:B:71:ARG:HG2	2:B:71:ARG:HH11	1.85	0.41
2:B:52:LEU:HD21	2:B:167:LEU:HD21	2.02	0.41
2:B:145:TRP:CZ2	2:B:233:GLU:HB2	2.54	0.41
2:A:165:GLN:O	2:A:166:PRO:C	2.62	0.41
2:B:209:ASP:O	2:B:210:PHE:C	2.62	0.41
2:A:80:ARG:CG	2:A:81:LEU:HD22	2.48	0.41
2:A:98:LEU:CD1	2:A:111:PRO:HB2	2.51	0.41
2:A:265:GLN:C	2:A:266:VAL:HG13	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:LEU:O	2:B:75:LYS:HB3	2.20	0.41
2:B:143:HIS:O	2:B:146:TYR:HE1	2.04	0.41
1:E:5:DA:H1'	1:E:6:DT:H5''	2.03	0.41
2:B:70:ALA:O	2:B:71:ARG:C	2.63	0.41
2:B:151:LEU:CD2	2:B:254:ALA:HB2	2.50	0.41
2:A:103:LYS:O	2:A:106:THR:HG22	2.21	0.41
2:A:277:GLN:O	2:A:278:ARG:C	2.63	0.41
2:B:122:VAL:O	2:B:193:LYS:NZ	2.51	0.41
2:A:146:TYR:CD2	2:A:273:LEU:HD11	2.55	0.41
2:B:131:ASN:OD1	2:B:132:PRO:HD2	2.21	0.41
2:B:265:GLN:HA	2:B:273:LEU:O	2.21	0.41
1:E:5:DA:H1'	1:E:6:DT:C5'	2.51	0.41
2:A:158:LEU:HD12	2:A:158:LEU:N	2.35	0.41
2:A:268:TYR:CE1	2:A:269:LEU:HD13	2.55	0.41
2:B:80:ARG:NH1	2:B:80:ARG:HG2	2.36	0.41
2:B:94:TRP:CE2	2:B:167:LEU:HD12	2.56	0.41
2:A:261:ILE:HD12	2:A:261:ILE:N	2.22	0.41
2:A:268:TYR:O	2:A:271:TYR:HB2	2.21	0.41
2:B:32:ALA:HB2	2:B:244:LEU:O	2.22	0.40
2:B:72:LEU:C	2:B:72:LEU:HD22	2.45	0.40
2:B:81:LEU:HD12	2:B:86:ILE:HB	2.03	0.40
1:E:10:DT:H2''	1:E:11:DG:OP2	2.20	0.40
2:A:60:SER:HB2	2:A:93:PRO:O	2.20	0.40
2:A:127:PRO:O	2:A:128:THR:C	2.61	0.40
2:A:218:ILE:HG22	2:A:220:LEU:HD12	2.03	0.40
2:B:25:TRP:O	2:B:26:LEU:C	2.64	0.40
2:A:40:GLY:N	2:A:253:ARG:HG3	2.36	0.40
2:B:212:ILE:H	2:B:212:ILE:HG13	1.55	0.40
2:B:215:PRO:C	2:B:217:LEU:H	2.30	0.40
2:A:94:TRP:HE3	2:A:118:VAL:HG22	1.87	0.40
2:A:158:LEU:N	2:A:158:LEU:CD1	2.84	0.40
2:A:211:ARG:CD	2:A:219:LEU:HB3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	257/259 (99%)	215 (84%)	32 (12%)	10 (4%)	2	14
2	B	255/259 (98%)	201 (79%)	42 (16%)	12 (5%)	2	11
All	All	512/518 (99%)	416 (81%)	74 (14%)	22 (4%)	2	12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	132	PRO
2	A	133	TYR
2	A	163	THR
2	B	72	LEU
2	B	207	LEU
2	A	54	ALA
2	A	223	VAL
2	B	38	GLY
2	B	134	ASN
2	B	249	ASN
2	B	277	GLN
2	A	37	GLY
2	B	172	TRP
2	B	223	VAL
2	A	176	GLU
2	A	107	ASN
2	A	130	PRO
2	B	115	LEU
2	B	132	PRO
2	B	166	PRO
2	A	215	PRO
2	B	58	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	227/227 (100%)	203 (89%)	24 (11%)	6	27
2	B	226/227 (100%)	192 (85%)	34 (15%)	3	14
All	All	453/454 (100%)	395 (87%)	58 (13%)	4	19

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	26	LEU
2	A	31	GLN
2	A	44	ARG
2	A	65	PRO
2	A	74	ILE
2	A	82	LEU
2	A	98	LEU
2	A	103	LYS
2	A	111	PRO
2	A	127	PRO
2	A	132	PRO
2	A	147	THR
2	A	152	LYS
2	A	160	LEU
2	A	162	PRO
2	A	165	GLN
2	A	188	LEU
2	A	204	HIS
2	A	211	ARG
2	A	257	LYS
2	A	261	ILE
2	A	267	LYS
2	A	269	LEU
2	A	277	GLN
2	B	23	MET
2	B	26	LEU
2	B	28	ASP
2	B	41	LEU
2	B	43	VAL
2	B	52	LEU
2	B	57	THR
2	B	62	LYS
2	B	72	LEU
2	B	74	ILE
2	B	80	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	81	LEU
2	B	88	VAL
2	B	102	LYS
2	B	103	LYS
2	B	110	ARG
2	B	128	THR
2	B	139	LEU
2	B	149	LEU
2	B	163	THR
2	B	166	PRO
2	B	167	LEU
2	B	172	TRP
2	B	173	ARG
2	B	176	GLU
2	B	182	GLN
2	B	184	THR
2	B	212	ILE
2	B	218	ILE
2	B	225	ASP
2	B	235	ASP
2	B	249	ASN
2	B	274	LYS
2	B	278	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	31	GLN
2	A	68	GLN
2	A	84	GLN
2	A	113	GLN
2	A	134	ASN
2	A	161	HIS
2	A	165	GLN
2	A	182	GLN
2	A	194	ASN
2	A	237	GLN
2	A	245	GLN
2	A	249	ASN
2	A	263	GLN
2	B	22	HIS
2	B	31	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	68	GLN
2	B	113	GLN
2	B	161	HIS
2	B	204	HIS
2	B	221	GLN
2	B	237	GLN
2	B	245	GLN
2	B	249	ASN
2	B	265	GLN
2	B	277	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	261:ILE	C	262:CYS	N	1.19

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	E	11/11 (100%)	0.68	2 (18%) 3 2	15, 40, 98, 98	0
1	F	11/11 (100%)	0.47	1 (9%) 15 8	15, 26, 99, 100	0
2	A	259/259 (100%)	-0.29	2 (0%) 82 64	3, 16, 44, 74	0
2	B	257/259 (99%)	-0.07	5 (1%) 66 43	5, 25, 64, 91	0
All	All	538/540 (99%)	-0.15	10 (1%) 66 43	3, 20, 55, 100	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	273	LEU	3.6
2	B	108	ASP	3.1
1	F	1	DT	2.8
2	B	26	LEU	2.8
1	E	2	DT	2.7
2	B	104	PRO	2.7
2	A	128	THR	2.6
2	B	276	GLY	2.5
1	E	3	DT	2.2
2	B	177	MET	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.