



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:46 PM GMT

PDB ID : 3V6D  
Title : Crystal structure of HIV-1 reverse transcriptase (RT) cross-linked with AZT-terminated DNA  
Authors : Das, K.; Martinez, S.E.; Arnold, E.  
Deposited on : 2011-12-19  
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

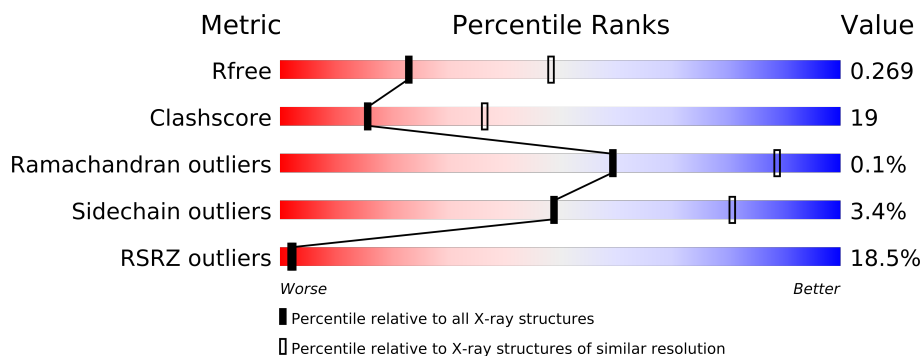
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance




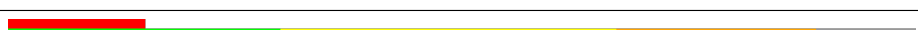

The reported resolution of this entry is 2.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	556	
1	C	556	
2	B	428	
2	D	428	
3	E	27	
3	T	27	
4	F	21	
4	P	21	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17627 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE P66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4511	2920	751	832	8			
1	C	554	Total	C	N	O	S	0	0	0
			4506	2917	750	831	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P03366
A	0	VAL	-	EXPRESSION TAG	UNP P03366
A	258	CYS	GLN	ENGINEERED MUTATION	UNP P03366
A	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
A	498	ASN	ASP	ENGINEERED MUTATION	UNP P03366
C	-1	MET	-	EXPRESSION TAG	UNP P03366
C	0	VAL	-	EXPRESSION TAG	UNP P03366
C	258	CYS	GLN	ENGINEERED MUTATION	UNP P03366
C	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
C	498	ASN	ASP	ENGINEERED MUTATION	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			
2	D	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
D	280	SER	CYS	ENGINEERED MUTATION	UNP P03366

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	24	Total 497	C 234	N 102	O 138	P 23	0	0	0
3	E	24	Total 497	C 234	N 102	O 138	P 23	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(\*AP\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(MRG)P\*CP\*GP\*CP\*CP\*(ATM))-3').

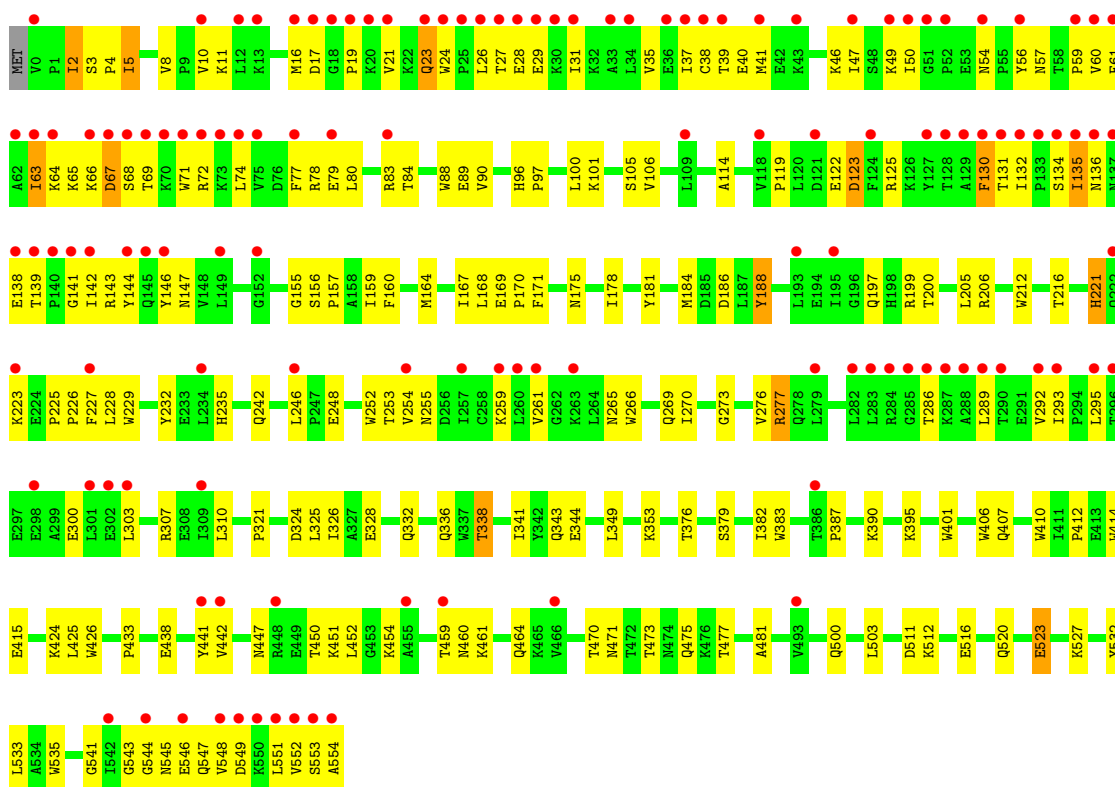
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	P	20	Total 408	C 195	N 72	O 121	P 19	S 1	0	0	0
4	F	20	Total 408	C 195	N 72	O 121	P 19	S 1	0	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

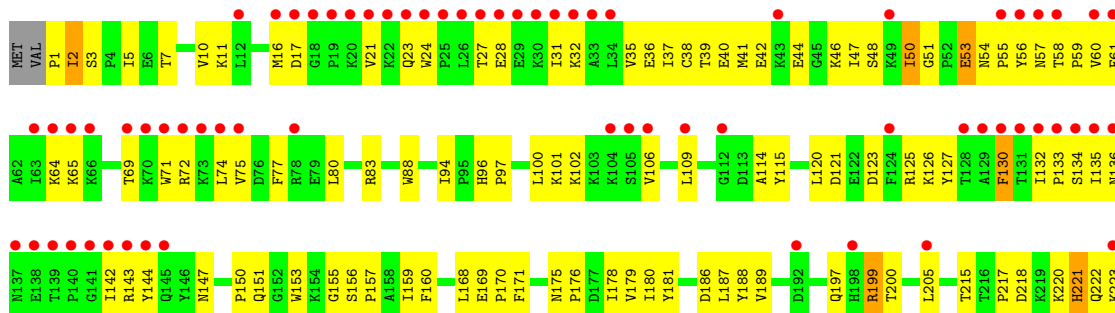
- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 subunit

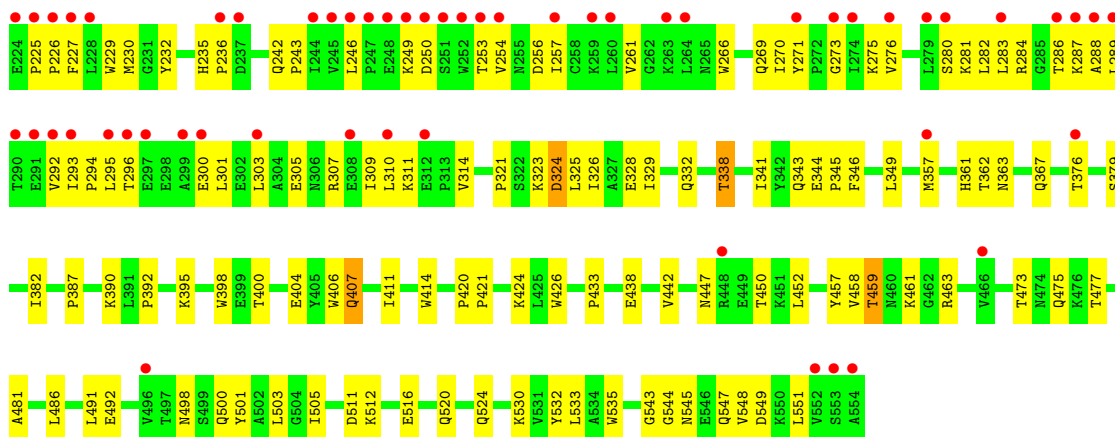
Chain A: 



- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 subunit

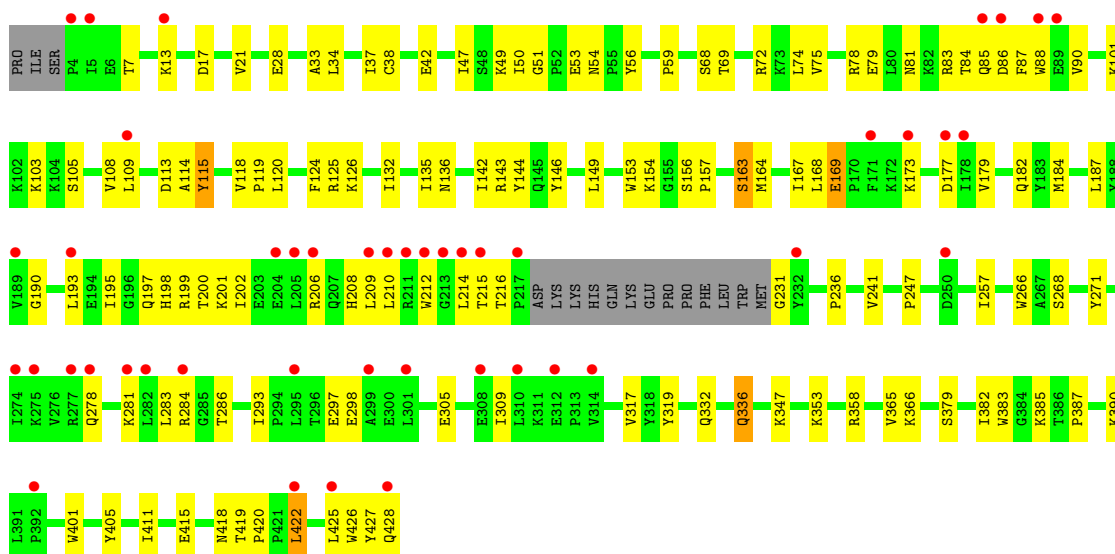
Chain C: 





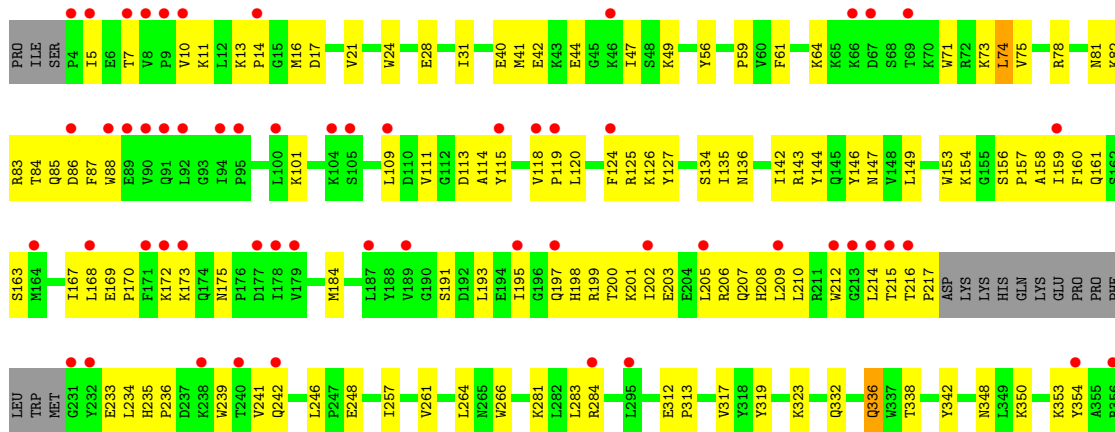
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 subunit

Chain B:



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 subunit

Chain D:





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

Chain T:



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

Chain E:



- Molecule 4: DNA (5'-D(\*AP\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(M RG)P\*CP\*GP\*CP\*CP\*(ATM))-3')

Chain P:



- Molecule 4: DNA (5'-D(\*AP\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(M RG)P\*CP\*GP\*CP\*CP\*(ATM))-3')

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.48Å 133.17Å 139.90Å 90.00° 98.67° 90.00°	Depositor
Resolution (Å)	44.30 – 2.70 48.21 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.30-2.70) 97.8 (48.21-2.71)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.233 , 0.268 0.234 , 0.269	Depositor DCC
$R_{free}$ test set	2607 reflections (3.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 86162 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17627	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATM, MRG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.46	0/4629	0.61	1/6290 (0.0%)
1	C	0.45	0/4624	0.58	0/6282
2	B	0.48	0/3497	0.60	0/4751
2	D	0.46	0/3497	0.61	0/4751
3	E	0.79	0/560	1.44	10/864 (1.2%)
3	T	0.80	0/560	1.48	11/864 (1.3%)
4	F	0.82	0/400	1.58	9/612 (1.5%)
4	P	0.78	0/400	1.52	6/612 (1.0%)
All	All	0.51	0/18167	0.76	37/25026 (0.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	810	DT	O4'-C1'-N1	9.89	114.92	108.00
4	F	807	DC	O4'-C1'-N1	8.96	114.27	108.00
4	P	816	DG	O4'-C1'-N9	8.78	114.14	108.00
3	E	721	DG	O4'-C1'-N9	-8.59	101.99	108.00
3	T	703	DG	O4'-C4'-C3'	-7.75	101.35	106.00
3	T	719	DG	C1'-O4'-C4'	-7.44	102.66	110.10
3	T	703	DG	O4'-C1'-N9	7.26	113.08	108.00
4	F	811	DG	O4'-C1'-N9	7.20	113.04	108.00
3	T	708	DG	O4'-C1'-N9	7.18	113.03	108.00
4	F	810	DT	N3-C4-O4	6.99	124.10	119.90
3	E	707	DG	O4'-C4'-C3'	-6.80	101.78	104.50
3	E	718	DA	O4'-C1'-N9	6.60	112.62	108.00
3	E	719	DG	C1'-O4'-C4'	-6.50	103.60	110.10
4	F	810	DT	C5-C4-O4	-6.46	120.38	124.90
3	T	708	DG	N9-C4-C5	6.41	107.96	105.40
4	F	812	DT	O4'-C1'-N1	-5.93	103.85	108.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	820	DC	O4'-C1'-N1	5.86	112.10	108.00
3	E	708	DG	N9-C4-C5	5.78	107.71	105.40
4	F	808	DC	C5'-C4'-C3'	-5.71	103.82	114.10
4	F	816	DG	O4'-C1'-N9	5.64	111.94	108.00
3	E	708	DG	C8-N9-C4	-5.62	104.15	106.40
4	P	807	DC	O4'-C1'-N1	5.55	111.89	108.00
3	E	703	DG	O4'-C1'-N9	5.55	111.88	108.00
3	E	711	DC	O4'-C1'-N1	5.49	111.84	108.00
3	T	708	DG	C8-N9-C4	-5.39	104.24	106.40
3	T	703	DG	C4'-C3'-C2'	-5.39	98.25	103.10
4	P	810	DT	C5-C4-O4	-5.33	121.17	124.90
4	F	820	DC	O4'-C1'-N1	5.23	111.66	108.00
3	E	707	DG	O4'-C1'-N9	5.18	111.63	108.00
3	T	718	DA	C3'-C2'-C1'	-5.18	96.28	102.50
4	F	814	DC	O4'-C1'-C2'	-5.18	101.76	105.90
1	A	4	PRO	N-CA-C	5.17	125.55	112.10
3	T	709	DC	C4'-C3'-C2'	-5.14	98.47	103.10
4	P	808	DC	C5'-C4'-C3'	-5.12	104.89	114.10
3	T	708	DG	C4'-C3'-C2'	-5.09	98.52	103.10
3	E	708	DG	N3-C2-N2	-5.06	116.36	119.90
3	T	720	DG	O4'-C1'-N9	-5.03	104.48	108.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4511	0	4570	174	0
1	C	4506	0	4568	182	0
2	B	3400	0	3433	117	0
2	D	3400	0	3433	135	0
3	E	497	0	268	14	0
3	T	497	0	268	15	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	408	0	231	27	0
4	P	408	0	231	20	0
All	All	17627	0	17002	643	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (643) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:223:LYS:O	1:C:225:PRO:HD3	1.53	1.09
1:A:541:GLY:HA2	1:A:546:GLU:HB2	1.41	1.01
1:C:500:GLN:HG2	2:D:422:LEU:HD22	1.44	1.00
1:A:459:THR:HG22	1:A:461:LYS:H	1.23	0.99
1:A:2:ILE:HD12	1:A:2:ILE:H	1.26	0.99
1:A:223:LYS:O	1:A:225:PRO:HD3	1.64	0.98
2:B:266:TRP:CD1	2:B:425:LEU:HD22	2.01	0.96
2:D:170:PRO:HB2	2:D:208:HIS:HE1	1.31	0.94
1:A:37:ILE:HD12	1:A:40:GLU:HG3	1.52	0.91
1:A:65:LYS:HB3	1:A:68:SER:HB2	1.52	0.91
1:A:5:ILE:HG22	1:A:212:TRP:HD1	1.37	0.90
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.08	0.89
1:A:199:ARG:NH2	1:A:223:LYS:HB3	1.89	0.88
1:C:175:ASN:HB3	1:C:178:ILE:HD13	1.55	0.87
1:C:125:ARG:HD3	1:C:147:ASN:HA	1.56	0.87
2:D:115:TYR:HD2	2:D:156:SER:HB3	1.40	0.86
4:P:807:DC:H2''	4:P:808:DC:H5''	1.56	0.85
2:B:109:LEU:HD22	2:B:216:THR:HG21	1.59	0.84
1:C:450:THR:HG21	1:C:452:LEU:HD12	1.60	0.84
1:C:23:GLN:HE22	1:C:60:VAL:HG12	1.43	0.84
1:C:253:THR:HG22	1:C:292:VAL:HG12	1.60	0.83
1:C:199:ARG:NH2	1:C:223:LYS:HB2	1.93	0.83
4:F:817:MRG:N3	4:F:817:MRG:H222	1.94	0.81
2:B:13:LYS:HD2	2:B:85:GLN:HB3	1.63	0.80
1:C:303:LEU:O	1:C:307:ARG:HG3	1.81	0.79
2:B:266:TRP:NE1	2:B:425:LEU:HD22	1.98	0.79
1:A:303:LEU:O	1:A:307:ARG:HG3	1.83	0.79
2:D:87:PHE:HZ	2:D:159:ILE:HG13	1.48	0.79
1:A:199:ARG:HH21	1:A:223:LYS:HB3	1.47	0.78
1:C:438:GLU:OE2	1:C:459:THR:HG21	1.83	0.78
4:F:807:DC:H2''	4:F:808:DC:C5'	2.12	0.78
1:A:459:THR:CG2	1:A:461:LYS:H	1.97	0.78
4:P:807:DC:H2''	4:P:808:DC:C5'	2.14	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:266:TRP:CD1	2:D:425:LEU:HD22	2.18	0.78
4:F:807:DC:H2"	4:F:808:DC:H5"	1.65	0.77
1:A:459:THR:HG22	1:A:461:LYS:N	1.97	0.77
1:C:254:VAL:HG21	1:C:286:THR:HG21	1.65	0.77
1:C:459:THR:HG22	1:C:461:LYS:H	1.49	0.77
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.84	0.77
1:A:5:ILE:HG22	1:A:212:TRP:CD1	2.20	0.76
2:D:319:TYR:OH	2:D:385:LYS:HD2	1.84	0.76
2:D:266:TRP:NE1	2:D:425:LEU:HD22	2.00	0.76
1:C:323:LYS:HE2	1:C:344:GLU:OE2	1.85	0.76
1:C:459:THR:CG2	1:C:461:LYS:H	1.98	0.76
2:B:281:LYS:HE3	2:B:284:ARG:NH2	2.01	0.76
1:C:273:GLY:HA2	1:C:338:THR:HG21	1.69	0.75
1:A:541:GLY:CA	1:A:546:GLU:HB2	2.16	0.75
2:B:182:GLN:HG3	2:B:187:LEU:HD12	1.68	0.75
1:A:78:ARG:HH21	3:T:705:DA:H5"	1.52	0.74
1:C:21:VAL:HG23	1:C:59:PRO:HD3	1.67	0.74
1:A:543:GLY:HA2	2:B:283:LEU:O	1.87	0.74
1:C:21:VAL:CG2	1:C:59:PRO:HD3	2.17	0.74
1:C:544:GLY:HA2	1:C:547:GLN:HE21	1.51	0.74
1:A:31:ILE:O	1:A:35:VAL:HG23	1.88	0.74
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.70	0.73
2:B:114:ALA:H	2:B:214:LEU:HD13	1.53	0.73
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.20	0.73
1:C:51:GLY:N	1:C:53:GLU:OE2	2.21	0.73
4:F:804:DA:H2'	4:F:805:DG:C8	2.24	0.73
2:D:209:LEU:HD22	2:D:214:LEU:HD23	1.70	0.73
3:E:721:DG:H2"	3:E:722:DA:OP2	1.87	0.72
1:A:21:VAL:HG23	1:A:59:PRO:HD3	1.71	0.72
1:A:511:ASP:OD2	1:A:512:LYS:NZ	2.21	0.72
2:B:33:ALA:O	2:B:37:ILE:HG12	1.89	0.72
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.52	0.72
1:A:252:TRP:O	1:A:292:VAL:HG23	1.90	0.72
2:D:358:ARG:HB2	2:D:370:GLU:OE2	1.90	0.72
1:A:66:LYS:NZ	1:A:67:ASP:OD2	2.24	0.71
1:A:543:GLY:N	2:B:283:LEU:O	2.23	0.71
1:C:543:GLY:HA2	2:D:283:LEU:O	1.89	0.71
1:A:125:ARG:HG2	1:A:146:TYR:O	1.91	0.71
2:B:68:SER:O	2:B:69:THR:HB	1.90	0.71
1:C:101:LYS:HE2	1:C:321:PRO:HG3	1.72	0.71
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.72	0.71
1:C:293:ILE:HG13	1:C:294:PRO:HD2	1.72	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:198:HIS:NE2	2:B:202:ILE:HD11	2.06	0.70
2:D:312:GLU:HB3	2:D:313:PRO:HD2	1.74	0.70
2:D:354:TYR:HE2	2:D:375:ILE:HG13	1.57	0.70
1:C:367:GLN:HE22	1:C:512:LYS:HD2	1.57	0.69
2:D:169:GLU:O	2:D:173:LYS:HG2	1.92	0.69
1:C:261:VAL:HG13	1:C:276:VAL:HG11	1.73	0.69
3:E:723:DC:OP1	3:E:723:DC:H4'	1.91	0.69
3:E:723:DC:H5''	3:E:723:DC:H6	1.58	0.69
1:C:77:PHE:CD1	1:C:80:LEU:HD23	2.28	0.69
3:E:716:DA:H2''	3:E:717:DC:OP2	1.91	0.69
1:C:215:THR:HG22	1:C:217:PRO:HD3	1.74	0.68
2:D:342:TYR:HB3	2:D:348:ASN:HD22	1.57	0.68
1:A:544:GLY:O	1:A:548:VAL:HG23	1.94	0.68
2:B:154:LYS:HG2	2:B:184:MET:SD	2.34	0.68
1:A:253:THR:HA	1:A:292:VAL:HA	1.76	0.68
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.29	0.68
3:T:724:DT:H3	4:P:804:DA:H61	1.42	0.68
2:D:47:ILE:HD12	2:D:144:TYR:CD1	2.28	0.68
1:C:459:THR:HG22	1:C:461:LYS:N	2.08	0.68
4:F:805:DG:H2''	4:F:806:DT:O5'	1.93	0.68
2:D:266:TRP:HD1	2:D:425:LEU:HD13	1.59	0.68
2:D:360:ALA:HA	2:D:367:GLN:NE2	2.08	0.68
2:D:157:PRO:HG3	2:D:184:MET:HA	1.75	0.68
1:C:2:ILE:HD12	1:C:2:ILE:N	2.09	0.68
4:F:804:DA:H2''	4:F:805:DG:O5'	1.94	0.68
1:C:287:LYS:HG3	1:C:288:ALA:H	1.58	0.68
1:A:135:ILE:HG12	1:A:136:ASN:H	1.58	0.67
2:B:336:GLN:HG2	2:B:353:LYS:HD2	1.77	0.67
2:D:115:TYR:CD2	2:D:156:SER:HB3	2.26	0.67
1:A:266:TRP:O	1:A:269:GLN:HG2	1.95	0.67
2:D:163:SER:O	2:D:167:ILE:HG13	1.94	0.67
1:C:246:LEU:HD11	1:C:310:LEU:HD22	1.76	0.67
1:A:41:MET:HB3	1:A:46:LYS:HB2	1.77	0.67
1:A:543:GLY:CA	2:B:283:LEU:O	2.43	0.66
2:B:332:GLN:HB2	2:B:336:GLN:HB3	1.76	0.66
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.76	0.66
2:D:86:ASP:OD1	2:D:87:PHE:N	2.29	0.66
2:D:214:LEU:HD12	2:D:215:THR:H	1.60	0.66
1:C:109:LEU:HD23	1:C:220:LYS:HD2	1.77	0.66
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.75	0.66
2:D:16:MET:HG3	2:D:83:ARG:HG2	1.76	0.66
1:C:100:LEU:HD11	1:C:229:TRP:CZ3	2.31	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:198:HIS:CD2	2:D:202:ILE:HD11	2.31	0.66
1:C:407:GLN:HE22	2:D:418:ASN:HA	1.60	0.66
1:A:500:GLN:HG2	2:B:422:LEU:CD1	2.26	0.66
1:C:32:LYS:O	1:C:36:GLU:HG3	1.97	0.65
4:F:803:DC:H2'	4:F:804:DA:C8	2.32	0.65
2:D:114:ALA:H	2:D:214:LEU:HD13	1.61	0.65
1:A:23:GLN:HG2	1:A:59:PRO:HA	1.79	0.65
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.79	0.65
2:B:115:TYR:O	2:B:149:LEU:HB2	1.95	0.65
1:A:332:GLN:OE1	1:A:338:THR:HG23	1.96	0.65
4:P:817:MRG:H222	4:P:817:MRG:N3	2.12	0.65
1:C:289:LEU:HD21	4:F:817:MRG:H4'	1.77	0.64
4:F:806:DT:H2'	4:F:807:DC:C6	2.32	0.64
1:C:543:GLY:O	1:C:547:GLN:NE2	2.30	0.64
2:B:114:ALA:N	2:B:214:LEU:HD13	2.12	0.64
2:D:338:THR:HG22	2:D:353:LYS:HG3	1.80	0.64
2:B:81:ASN:ND2	2:B:154:LYS:HG3	2.13	0.64
1:A:253:THR:HG22	1:A:292:VAL:HB	1.79	0.64
1:C:21:VAL:HG22	1:C:57:ASN:O	1.98	0.64
1:C:500:GLN:HG2	2:D:422:LEU:CD2	2.23	0.64
4:F:807:DC:C2'	4:F:808:DC:H5"	2.28	0.63
1:C:503:LEU:CD1	1:C:533:LEU:HG	2.29	0.63
1:C:31:ILE:O	1:C:35:VAL:HG23	1.98	0.63
1:A:276:VAL:O	1:A:276:VAL:HG12	1.96	0.63
1:C:275:LYS:HE2	1:C:332:GLN:NE2	2.13	0.63
1:C:186:ASP:HB2	4:F:822:ATM:N5'	2.13	0.63
2:D:115:TYR:O	2:D:149:LEU:HB2	1.99	0.63
4:P:807:DC:H2'	4:P:808:DC:C6	2.33	0.63
1:A:167:ILE:O	1:A:170:PRO:HD2	1.99	0.63
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.62	0.63
1:A:78:ARG:NH2	3:T:705:DA:H5"	2.14	0.62
1:A:125:ARG:HE	1:A:147:ASN:HA	1.61	0.62
1:A:60:VAL:HG11	1:A:130:PHE:HD1	1.64	0.62
2:B:193:LEU:HB3	2:B:197:GLN:HB2	1.81	0.62
2:D:78:ARG:O	2:D:82:LYS:HG3	1.99	0.62
3:T:716:DA:H2"	3:T:717:DC:OP2	2.00	0.62
1:A:545:ASN:O	1:A:549:ASP:HB2	2.00	0.62
1:C:226:PRO:HB3	1:C:235:HIS:CE1	2.35	0.62
2:B:195:ILE:HG22	2:B:199:ARG:HE	1.63	0.62
2:D:266:TRP:CD1	2:D:425:LEU:HD13	2.34	0.62
2:D:167:ILE:O	2:D:208:HIS:NE2	2.33	0.61
2:D:7:THR:HG22	2:D:119:PRO:HB2	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.24	0.61
1:C:395:LYS:NZ	1:C:414:TRP:O	2.34	0.61
1:A:61:PHE:CE1	3:T:704:DG:C8	2.89	0.61
2:B:169:GLU:O	2:B:173:LYS:HG2	2.00	0.60
1:A:500:GLN:HG2	2:B:422:LEU:HD11	1.84	0.60
3:T:718:DA:H2'	3:T:718:DA:OP2	2.02	0.60
1:C:307:ARG:O	1:C:311:LYS:HG3	2.00	0.60
2:D:13:LYS:HB2	2:D:16:MET:HE3	1.82	0.60
1:A:254:VAL:HG21	1:A:286:THR:HG21	1.82	0.60
1:A:135:ILE:CG2	1:A:138:GLU:HB2	2.31	0.60
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	2.90	0.60
4:F:807:DC:H2''	4:F:808:DC:O5'	2.01	0.60
1:C:61:PHE:HE1	1:C:74:LEU:HD12	1.67	0.59
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.84	0.59
1:C:109:LEU:CD2	1:C:220:LYS:HD2	2.32	0.59
2:D:40:GLU:HG2	2:D:44:GLU:OE1	2.02	0.59
1:C:37:ILE:O	1:C:40:GLU:HB2	2.02	0.59
2:B:86:ASP:OD1	2:B:87:PHE:N	2.35	0.59
3:T:725:DG:N2	4:P:803:DC:N3	2.39	0.59
2:D:13:LYS:HE3	2:D:16:MET:HE3	1.84	0.59
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.37	0.59
1:C:276:VAL:HG12	1:C:276:VAL:O	2.03	0.59
2:D:109:LEU:HD22	2:D:216:THR:HG21	1.85	0.59
4:F:814:DC:H2''	4:F:815:DG:C8	2.38	0.59
1:C:516:GLU:O	1:C:520:GLN:HG3	2.03	0.59
1:A:5:ILE:CG2	1:A:212:TRP:HD1	2.10	0.58
2:B:167:ILE:HG23	2:B:212:TRP:CG	2.37	0.58
2:B:317:VAL:HG12	2:B:347:LYS:CD	2.32	0.58
1:A:452:LEU:HD23	1:A:470:THR:HA	1.84	0.58
1:C:457:TYR:HE1	1:C:463:ARG:HG2	1.68	0.58
2:B:197:GLN:O	2:B:201:LYS:HG2	2.03	0.58
1:A:24:TRP:CD1	1:A:61:PHE:HE2	2.21	0.58
3:T:717:DC:H2''	3:T:718:DA:OP2	2.02	0.58
1:C:31:ILE:HG23	1:C:133:PRO:O	2.04	0.58
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.39	0.58
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.84	0.58
2:D:191:SER:OG	2:D:198:HIS:ND1	2.27	0.58
2:B:115:TYR:CD2	2:B:115:TYR:N	2.72	0.57
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.39	0.57
2:B:108:VAL:O	2:B:231:GLY:HA3	2.03	0.57
2:D:209:LEU:HD22	2:D:214:LEU:CD2	2.34	0.57
2:B:317:VAL:HG12	2:B:347:LYS:HD3	1.86	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.86	0.57
1:C:367:GLN:NE2	1:C:512:LYS:HD2	2.18	0.57
2:B:163:SER:O	2:B:167:ILE:HG13	2.04	0.57
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.85	0.57
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.39	0.57
2:B:206:ARG:HH21	2:B:210:LEU:HD11	1.68	0.57
2:B:209:LEU:HD22	2:B:214:LEU:HD23	1.85	0.57
2:D:13:LYS:HE3	2:D:16:MET:CE	2.34	0.57
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.87	0.57
2:B:336:GLN:HG2	2:B:427:TYR:CE1	2.40	0.57
1:C:305:GLU:O	1:C:309:ILE:HG13	2.05	0.57
2:B:266:TRP:CD1	2:B:425:LEU:CD2	2.81	0.56
3:T:713:DC:H2''	3:T:714:DG:H5'	1.88	0.56
2:D:233:GLU:O	2:D:234:LEU:HD23	2.05	0.56
1:A:5:ILE:HD11	1:A:119:PRO:HD2	1.87	0.56
2:D:114:ALA:N	2:D:214:LEU:HD13	2.20	0.56
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.19	0.56
1:A:464:GLN:NE2	1:A:551:LEU:HD11	2.20	0.56
2:B:88:TRP:CZ2	2:B:154:LYS:HD2	2.40	0.56
2:D:118:VAL:HG12	2:D:119:PRO:O	2.05	0.56
3:E:704:DG:H5''	3:E:704:DG:N3	2.20	0.56
1:C:23:GLN:NE2	1:C:60:VAL:HG12	2.18	0.56
1:C:407:GLN:NE2	2:D:418:ASN:HA	2.20	0.56
2:D:266:TRP:HE1	2:D:425:LEU:HD22	1.70	0.56
1:A:139:THR:HG22	1:A:141:GLY:H	1.71	0.56
1:C:328:GLU:HG3	1:C:390:LYS:HB2	1.88	0.56
1:A:441:TYR:O	1:A:548:VAL:HG21	2.06	0.55
1:C:155:GLY:O	1:C:159:ILE:HG13	2.07	0.55
4:P:807:DC:C2'	4:P:808:DC:H5''	2.31	0.55
2:D:336:GLN:HG2	2:D:427:TYR:CE1	2.42	0.55
1:C:75:VAL:HB	1:C:77:PHE:CE2	2.42	0.55
1:A:186:ASP:HB2	4:P:822:ATM:N5'	2.20	0.55
2:B:358:ARG:HG3	2:B:366:LYS:HD3	1.88	0.55
1:C:473:THR:O	1:C:477:THR:HG23	2.06	0.55
2:D:160:PHE:CD2	2:D:160:PHE:O	2.60	0.55
2:B:115:TYR:HD2	2:B:115:TYR:N	2.05	0.55
4:F:815:DG:H2'	4:F:815:DG:OP2	2.07	0.55
1:A:523:GLU:O	1:A:527:LYS:HG3	2.06	0.55
2:D:168:LEU:HB3	2:D:172:LYS:HE3	1.88	0.55
1:A:37:ILE:HA	1:A:40:GLU:CG	2.37	0.54
4:P:815:DG:H2''	4:P:816:DG:O5'	2.05	0.54
1:C:77:PHE:O	1:C:80:LEU:N	2.40	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:195:ILE:O	2:D:199:ARG:HG3	2.07	0.54
1:C:197:GLN:O	1:C:200:THR:HB	2.07	0.54
1:A:206:ARG:NH2	1:A:216:THR:O	2.40	0.54
1:C:295:LEU:HD22	1:C:300:GLU:OE1	2.07	0.54
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.43	0.54
1:C:301:LEU:O	1:C:305:GLU:HG2	2.08	0.54
1:C:97:PRO:HD3	1:C:232:TYR:CE2	2.43	0.54
2:B:195:ILE:HG21	2:B:199:ARG:HH21	1.73	0.54
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.89	0.54
1:A:49:LYS:HE3	1:A:142:ILE:HG23	1.89	0.54
2:D:425:LEU:HD23	2:D:426:TRP:CE2	2.42	0.54
1:C:180:ILE:HA	1:C:188:TYR:O	2.07	0.54
1:A:132:ILE:HB	1:A:142:ILE:O	2.07	0.54
1:A:516:GLU:O	1:A:520:GLN:HG3	2.08	0.54
1:C:130:PHE:CE2	1:C:144:TYR:HB2	2.43	0.53
1:C:287:LYS:HG3	1:C:288:ALA:N	2.23	0.53
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.89	0.53
4:F:817:MRG:H2'	4:F:818:DC:C6	2.43	0.53
2:D:175:ASN:OD1	2:D:201:LYS:NZ	2.34	0.53
2:D:56:TYR:HE2	2:D:126:LYS:HE2	1.73	0.53
1:C:406:TRP:CD1	1:C:407:GLN:HG2	2.44	0.53
1:C:503:LEU:HD11	1:C:533:LEU:HG	1.89	0.53
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.07	0.53
2:D:332:GLN:HB2	2:D:336:GLN:HB3	1.90	0.53
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.91	0.53
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.90	0.53
2:D:64:LYS:HE3	2:D:71:TRP:CZ2	2.44	0.53
1:C:41:MET:HB3	1:C:46:LYS:HB2	1.90	0.53
2:D:87:PHE:CZ	2:D:159:ILE:HG13	2.37	0.53
2:B:281:LYS:HE3	2:B:284:ARG:HH21	1.74	0.53
3:T:713:DC:H2'	3:T:714:DG:C8	2.44	0.53
2:D:210:LEU:HA	2:D:214:LEU:O	2.09	0.53
2:D:395:LYS:HE2	2:D:399:GLU:OE2	2.08	0.53
1:A:123:ASP:N	1:A:123:ASP:OD2	2.42	0.52
1:A:135:ILE:HG23	1:A:138:GLU:HB2	1.90	0.52
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.91	0.52
2:B:105:SER:O	2:B:190:GLY:HA2	2.09	0.52
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.91	0.52
1:A:246:LEU:HD11	1:A:310:LEU:HD22	1.89	0.52
1:A:155:GLY:O	1:A:159:ILE:HG13	2.08	0.52
1:C:199:ARG:HE	1:C:222:GLN:HG2	1.72	0.52
1:C:41:MET:HA	1:C:44:GLU:OE1	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:111:VAL:HG23	2:D:115:TYR:HE1	1.74	0.52
2:D:16:MET:CG	2:D:83:ARG:HG2	2.39	0.52
1:A:31:ILE:HG21	1:A:135:ILE:HA	1.90	0.52
1:A:390:LYS:HE2	1:A:415:GLU:OE2	2.08	0.52
1:A:464:GLN:NE2	1:A:551:LEU:HD21	2.24	0.52
1:C:24:TRP:CZ3	3:E:703:DG:N2	2.76	0.52
1:C:257:ILE:HG21	1:C:283:LEU:HD21	1.90	0.52
1:C:398:TRP:CZ2	1:C:411:ILE:HG13	2.44	0.52
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.91	0.52
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.39	0.52
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.44	0.52
1:C:178:ILE:HD12	1:C:178:ILE:N	2.25	0.51
1:C:249:LYS:HG2	1:C:256:ASP:OD2	2.10	0.51
1:C:21:VAL:HG21	1:C:59:PRO:HD3	1.92	0.51
2:D:419:THR:HG22	2:D:419:THR:O	2.09	0.51
1:A:379:SER:CB	1:A:387:PRO:HD3	2.40	0.51
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.75	0.51
2:D:214:LEU:HD12	2:D:215:THR:N	2.25	0.51
2:B:278:GLN:NE2	2:B:298:GLU:CB	2.74	0.51
1:A:450:THR:HB	1:A:452:LEU:HD12	1.92	0.51
1:C:362:THR:HG21	1:C:367:GLN:HE21	1.75	0.51
1:C:253:THR:CG2	1:C:292:VAL:HG12	2.36	0.51
2:D:198:HIS:O	2:D:202:ILE:HG13	2.10	0.51
1:C:31:ILE:HD12	1:C:133:PRO:HB2	1.93	0.51
1:C:10:VAL:O	1:C:11:LYS:HG3	2.11	0.51
4:F:806:DT:H2''	4:F:807:DC:OP1	2.09	0.51
4:F:804:DA:C2'	4:F:805:DG:C8	2.94	0.51
4:F:807:DC:H2'	4:F:808:DC:C6	2.46	0.51
1:C:186:ASP:CB	4:F:822:ATM:N5'	2.74	0.51
1:A:169:GLU:N	1:A:170:PRO:HD2	2.25	0.51
1:C:126:LYS:HG3	1:C:127:TYR:CD2	2.46	0.51
4:F:817:MRG:N3	4:F:817:MRG:C22	2.72	0.50
2:D:210:LEU:HD12	2:D:214:LEU:O	2.11	0.50
2:D:73:LYS:CE	2:D:146:TYR:OH	2.60	0.50
2:D:109:LEU:HD22	2:D:216:THR:CG2	2.41	0.50
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.93	0.50
2:B:317:VAL:O	2:B:317:VAL:HG23	2.11	0.50
2:D:31:ILE:HD12	2:D:135:ILE:HG12	1.92	0.50
1:A:295:LEU:HB2	1:A:300:GLU:OE2	2.11	0.50
2:D:42:GLU:OE2	2:D:49:LYS:HG3	2.11	0.50
2:D:167:ILE:HG23	2:D:212:TRP:CG	2.46	0.50
4:P:806:DT:H2'	4:P:807:DC:C6	2.47	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:354:TYR:CE2	2:D:375:ILE:HG13	2.43	0.50
1:A:473:THR:O	1:A:477:THR:HG23	2.12	0.50
2:D:241:VAL:HG12	2:D:242:GLN:H	1.75	0.50
4:P:803:DC:H2'	4:P:804:DA:C8	2.46	0.50
2:B:101:LYS:O	2:B:236:PRO:HB2	2.12	0.50
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.46	0.50
1:C:179:VAL:O	1:C:189:VAL:HA	2.12	0.50
1:C:94:ILE:HD11	3:E:708:DG:N2	2.26	0.50
1:A:64:LYS:HE3	1:A:69:THR:O	2.11	0.50
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.94	0.49
1:A:407:GLN:HE22	2:B:418:ASN:HA	1.76	0.49
2:B:305:GLU:O	2:B:309:ILE:HG13	2.11	0.49
1:A:184:MET:HG2	4:P:822:ATM:H1'	1.94	0.49
2:D:28:GLU:HA	2:D:135:ILE:HD11	1.93	0.49
1:C:329:ILE:O	1:C:392:PRO:HD3	2.12	0.49
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.49
1:A:63:ILE:O	1:A:72:ARG:HB3	2.12	0.49
1:A:37:ILE:HA	1:A:40:GLU:HG3	1.93	0.49
1:C:38:CYS:HB3	1:C:144:TYR:CE2	2.47	0.49
3:E:722:DA:H2''	3:E:723:DC:H5''	1.94	0.49
2:B:390:LYS:HE2	2:B:415:GLU:OE2	2.12	0.49
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.93	0.49
1:C:28:GLU:HB2	1:C:135:ILE:HG21	1.95	0.49
1:C:115:TYR:CD2	1:C:151:GLN:HG2	2.47	0.49
3:E:718:DA:H4'	3:E:719:DG:OP1	2.12	0.49
1:A:500:GLN:CD	2:B:422:LEU:HD11	2.32	0.49
1:A:328:GLU:HG3	1:A:390:LYS:CB	2.41	0.49
1:C:296:THR:O	1:C:300:GLU:HB2	2.12	0.49
4:F:819:DG:H2'	4:F:820:DC:C6	2.48	0.49
2:B:69:THR:O	2:B:69:THR:HG22	2.12	0.49
2:B:118:VAL:HG12	2:B:119:PRO:O	2.12	0.49
1:A:130:PHE:H	1:A:130:PHE:HD2	1.59	0.49
1:A:97:PRO:HD3	1:A:232:TYR:CE2	2.47	0.49
2:B:142:ILE:HG22	2:B:144:TYR:CE2	2.48	0.49
1:C:282:LEU:HB3	1:C:293:ILE:HD13	1.95	0.49
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.48	0.49
2:D:199:ARG:HA	2:D:202:ILE:HD12	1.94	0.49
1:A:433:PRO:HD3	1:A:532:TYR:CZ	2.48	0.49
1:A:17:ASP:OD2	1:A:56:TYR:HE1	1.96	0.49
2:B:336:GLN:CG	2:B:353:LYS:HD2	2.43	0.49
1:A:10:VAL:HG12	1:A:11:LYS:H	1.78	0.49
1:C:281:LYS:HG3	1:C:284:ARG:CZ	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:390:LYS:HE2	2:D:415:GLU:OE2	2.13	0.48
1:C:376:THR:HG21	2:D:401:TRP:CH2	2.48	0.48
1:C:361:HIS:CD2	1:C:505:ILE:HG12	2.48	0.48
1:C:223:LYS:O	1:C:223:LYS:HG2	2.13	0.48
1:A:2:ILE:CD1	1:A:2:ILE:N	2.73	0.48
1:C:276:VAL:HG12	1:C:280:SER:OG	2.12	0.48
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.96	0.48
2:B:281:LYS:O	2:B:284:ARG:HG3	2.14	0.48
2:D:360:ALA:C	2:D:362:THR:H	2.17	0.48
1:A:2:ILE:CD1	1:A:2:ILE:H	1.99	0.48
1:C:37:ILE:HD13	1:C:40:GLU:HG3	1.96	0.48
1:C:50:ILE:HG12	1:C:54:ASN:HD22	1.79	0.48
2:B:109:LEU:HD22	2:B:216:THR:CG2	2.37	0.48
1:A:135:ILE:HG22	1:A:138:GLU:HB2	1.95	0.48
1:A:24:TRP:O	1:A:26:LEU:HG	2.14	0.48
1:C:324:ASP:O	1:C:343:GLN:HG2	2.13	0.48
1:A:10:VAL:HG12	1:A:11:LYS:N	2.29	0.48
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.96	0.48
1:C:130:PHE:HD2	1:C:130:PHE:H	1.60	0.48
4:F:803:DC:H2'	4:F:804:DA:N7	2.28	0.48
2:B:206:ARG:NH2	2:B:210:LEU:HD11	2.29	0.48
2:D:85:GLN:HA	2:D:88:TRP:CE2	2.49	0.48
1:C:171:PHE:CZ	1:C:205:LEU:HB2	2.49	0.48
2:B:56:TYR:HE2	2:B:126:LYS:CE	2.26	0.48
2:B:124:PHE:HE2	2:B:153:TRP:CZ2	2.32	0.47
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.49	0.47
4:P:811:DG:H2''	4:P:812:DT:O5'	2.14	0.47
4:P:807:DC:H4'	4:P:808:DC:OP1	2.15	0.47
1:C:37:ILE:HA	1:C:40:GLU:HG3	1.95	0.47
1:C:115:TYR:HD2	1:C:151:GLN:HG2	1.79	0.47
1:C:545:ASN:O	1:C:549:ASP:HB2	2.14	0.47
1:A:276:VAL:CG1	1:A:276:VAL:O	2.62	0.47
1:C:64:LYS:NZ	1:C:69:THR:HA	2.30	0.47
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.95	0.47
1:C:221:HIS:ND1	1:C:221:HIS:N	2.63	0.47
2:D:84:THR:O	2:D:84:THR:HG22	2.14	0.47
1:A:122:GLU:OE2	1:A:125:ARG:NH1	2.48	0.47
2:D:419:THR:O	2:D:420:PRO:C	2.50	0.47
2:D:203:GLU:O	2:D:207:GLN:HG2	2.14	0.47
1:A:79:GLU:OE1	1:A:83:ARG:NH2	2.48	0.47
1:C:125:ARG:HH11	1:C:147:ASN:HB3	1.79	0.47
1:A:261:VAL:HG22	1:A:276:VAL:HG13	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:500:GLN:CG	2:B:422:LEU:HD11	2.44	0.47
2:B:164:MET:HE2	2:B:168:LEU:HD11	1.95	0.47
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.50	0.47
1:C:447:ASN:HB3	1:C:450:THR:HB	1.96	0.47
2:B:214:LEU:HD12	2:B:215:THR:H	1.80	0.47
2:D:17:ASP:O	2:D:83:ARG:HD3	2.15	0.47
1:C:406:TRP:CZ2	2:D:420:PRO:HG3	2.49	0.47
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.15	0.47
1:C:102:LYS:HE2	1:C:236:PRO:O	2.14	0.47
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.45	0.47
1:C:106:VAL:O	1:C:227:PHE:CZ	2.68	0.47
2:D:358:ARG:HB3	2:D:366:LYS:HE2	1.96	0.47
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.97	0.47
1:A:35:VAL:HA	1:A:38:CYS:HB2	1.97	0.46
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.50	0.46
1:A:8:VAL:O	1:A:10:VAL:HG23	2.16	0.46
1:A:135:ILE:HG12	1:A:136:ASN:N	2.27	0.46
1:C:398:TRP:CH2	1:C:411:ILE:HG13	2.50	0.46
1:C:242:GLN:HB3	1:C:243:PRO:HD2	1.96	0.46
1:A:106:VAL:O	1:A:227:PHE:CZ	2.68	0.46
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.97	0.46
1:A:228:LEU:HD22	1:A:242:GLN:NE2	2.31	0.46
1:C:65:LYS:HE2	1:C:72:ARG:HD3	1.98	0.46
1:C:64:LYS:HD3	1:C:71:TRP:CE2	2.50	0.46
1:A:226:PRO:HB3	1:A:235:HIS:NE2	2.30	0.46
1:C:120:LEU:HG	1:C:121:ASP:N	2.30	0.46
1:A:88:TRP:CD1	2:B:143:ARG:NH1	2.84	0.46
1:A:164:MET:HE2	1:A:168:LEU:HD11	1.96	0.46
2:D:235:HIS:N	2:D:236:PRO:HD3	2.30	0.46
2:B:182:GLN:HG3	2:B:187:LEU:CD1	2.41	0.46
1:C:53:GLU:H	1:C:53:GLU:HG3	1.37	0.46
1:C:548:VAL:HA	1:C:551:LEU:HD12	1.98	0.46
2:D:13:LYS:HB3	2:D:14:PRO:HD2	1.98	0.46
4:F:815:DG:OP2	4:F:815:DG:H8	1.99	0.46
1:A:325:LEU:HD11	1:A:383:TRP:CE3	2.51	0.46
1:C:254:VAL:CG2	1:C:286:THR:HG21	2.42	0.46
2:D:41:MET:HB3	2:D:47:ILE:HG12	1.98	0.46
1:A:186:ASP:CB	4:P:822:ATM:N5'	2.78	0.46
1:C:88:TRP:CD1	2:D:143:ARG:NH1	2.83	0.46
1:C:345:PRO:O	1:C:346:PHE:HB2	2.15	0.46
1:C:169:GLU:N	1:C:170:PRO:HD2	2.31	0.46
3:E:723:DC:H2''	3:E:724:DT:C6	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:87:PHE:CD2	2:B:87:PHE:C	2.88	0.46
2:B:17:ASP:O	2:B:83:ARG:HD3	2.15	0.46
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.15	0.46
1:A:100:LEU:HD11	1:A:229:TRP:CZ3	2.51	0.46
3:E:723:DC:H5''	3:E:723:DC:C6	2.46	0.45
2:B:197:GLN:O	2:B:200:THR:HB	2.16	0.45
2:B:379:SER:HB3	2:B:385:LYS:O	2.15	0.45
2:D:205:LEU:O	2:D:205:LEU:HD12	2.16	0.45
2:D:191:SER:HB2	2:D:193:LEU:HG	1.99	0.45
1:C:168:LEU:HD11	1:C:187:LEU:HD21	1.99	0.45
2:D:284:ARG:HG2	2:D:284:ARG:HH11	1.81	0.45
1:A:424:LYS:HE3	1:A:426:TRP:CZ3	2.51	0.45
1:A:60:VAL:HG11	1:A:130:PHE:CD1	2.47	0.45
1:A:221:HIS:ND1	1:A:221:HIS:N	2.63	0.45
1:A:8:VAL:HG12	1:A:8:VAL:O	2.16	0.45
1:A:131:THR:HA	1:A:143:ARG:HG2	1.98	0.45
1:C:130:PHE:CD2	1:C:130:PHE:N	2.85	0.45
3:T:725:DG:N2	4:P:803:DC:C2	2.84	0.45
1:A:547:GLN:O	1:A:551:LEU:HB2	2.17	0.45
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.99	0.45
1:A:64:LYS:HD3	1:A:71:TRP:NE1	2.31	0.45
1:A:80:LEU:O	1:A:84:THR:OG1	2.29	0.45
2:D:114:ALA:HB2	2:D:214:LEU:HD13	1.98	0.45
3:E:721:DG:C2'	3:E:722:DA:OP2	2.61	0.45
1:A:46:LYS:O	1:A:47:ILE:HG23	2.17	0.45
1:A:503:LEU:CD1	1:A:533:LEU:HD13	2.43	0.45
1:C:17:ASP:O	1:C:83:ARG:HD3	2.17	0.45
1:C:362:THR:CG2	1:C:367:GLN:HE21	2.29	0.45
2:B:268:SER:HA	2:B:271:TYR:O	2.16	0.45
3:E:706:DA:H2'	3:E:707:DG:C8	2.52	0.45
2:D:13:LYS:HD3	2:D:85:GLN:HB3	1.98	0.44
1:A:60:VAL:CG1	1:A:130:PHE:HD1	2.27	0.44
2:D:101:LYS:O	2:D:236:PRO:HB2	2.17	0.44
2:B:247:PRO:CA	2:B:428:GLN:HE22	2.30	0.44
1:A:27:THR:OG1	1:A:29:GLU:HB3	2.17	0.44
2:D:124:PHE:CE2	2:D:153:TRP:CZ2	3.05	0.44
2:D:323:LYS:O	2:D:385:LYS:NZ	2.50	0.44
2:D:78:ARG:HD3	2:D:411:ILE:O	2.17	0.44
1:C:120:LEU:HG	1:C:121:ASP:H	1.82	0.44
2:D:109:LEU:HA	2:D:109:LEU:HD23	1.87	0.44
1:A:77:PHE:O	1:A:80:LEU:N	2.49	0.44
1:C:47:ILE:HG12	1:C:144:TYR:HB3	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:21:VAL:CG2	1:C:58:THR:HA	2.48	0.44
4:P:818:DC:H2'	4:P:819:DG:H8	1.83	0.44
2:D:81:ASN:HB3	2:D:154:LYS:HD2	2.00	0.44
2:D:317:VAL:HG23	2:D:317:VAL:O	2.17	0.44
3:E:712:DC:H2''	3:E:713:DC:O5'	2.18	0.44
2:D:239:TRP:CH2	2:D:378:GLU:HA	2.53	0.44
2:B:69:THR:CG2	2:B:69:THR:O	2.65	0.44
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.98	0.44
1:C:253:THR:HG22	1:C:292:VAL:CG1	2.39	0.44
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.53	0.44
1:C:16:MET:CE	1:C:83:ARG:HG2	2.48	0.44
3:T:710:DG:H2'	3:T:711:DC:C6	2.53	0.44
3:T:711:DC:H2''	3:T:712:DC:O5'	2.18	0.44
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.99	0.44
2:B:42:GLU:OE2	2:B:49:LYS:HG3	2.18	0.44
1:A:37:ILE:HA	1:A:40:GLU:HG2	1.98	0.44
1:C:424:LYS:HE2	1:C:426:TRP:CZ3	2.53	0.44
4:F:819:DG:H2'	4:F:820:DC:H6	1.83	0.44
1:C:433:PRO:HD3	1:C:532:TYR:CZ	2.52	0.44
2:B:195:ILE:O	2:B:199:ARG:HG3	2.18	0.44
1:A:197:GLN:O	1:A:200:THR:HB	2.18	0.44
2:D:281:LYS:O	2:D:284:ARG:HG3	2.18	0.43
1:C:175:ASN:N	1:C:176:PRO:HD3	2.33	0.43
1:A:122:GLU:HB3	1:A:123:ASP:OD2	2.18	0.43
1:C:50:ILE:HD13	1:C:143:ARG:NH1	2.33	0.43
2:D:74:LEU:HD12	2:D:75:VAL:N	2.33	0.43
1:A:500:GLN:HG2	2:B:422:LEU:HD13	1.99	0.43
1:A:382:ILE:O	2:B:136:ASN:HB2	2.19	0.43
1:C:254:VAL:HG21	1:C:286:THR:CG2	2.44	0.43
1:A:259:LYS:HG3	4:P:819:DG:OP1	2.17	0.43
2:D:428:GLN:HA	2:D:428:GLN:OE1	2.18	0.43
1:A:130:PHE:N	1:A:130:PHE:CD2	2.87	0.43
1:A:171:PHE:CE1	1:A:175:ASN:ND2	2.86	0.43
1:A:277:ARG:HB3	1:A:336:GLN:OE1	2.19	0.43
2:B:157:PRO:HG3	2:B:184:MET:HA	1.99	0.43
2:D:198:HIS:NE2	2:D:202:ILE:HD11	2.33	0.43
1:C:27:THR:O	1:C:31:ILE:HG12	2.18	0.43
1:A:451:LYS:O	1:A:471:ASN:N	2.51	0.43
1:C:492:GLU:HG2	1:C:530:LYS:HB2	2.01	0.43
2:D:11:LYS:HA	2:D:11:LYS:HD3	1.83	0.43
1:C:1:PRO:HB2	1:C:2:ILE:H	1.59	0.43
4:F:812:DT:H2''	4:F:813:DT:O5'	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:132:ILE:HB	1:C:142:ILE:HG22	2.00	0.43
1:A:325:LEU:HD11	1:A:383:TRP:CD2	2.53	0.43
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.54	0.43
1:A:74:LEU:HD22	3:T:705:DA:C2	2.54	0.42
4:P:819:DG:H2'	4:P:820:DC:C6	2.53	0.42
2:D:158:ALA:O	2:D:161:GLN:HB2	2.19	0.42
1:A:475:GLN:NE2	1:A:475:GLN:H	2.17	0.42
2:B:74:LEU:HD12	2:B:75:VAL:N	2.33	0.42
2:B:210:LEU:HD23	2:B:214:LEU:O	2.18	0.42
2:D:209:LEU:HD13	2:D:214:LEU:HD23	2.02	0.42
1:C:2:ILE:HD12	1:C:2:ILE:H	1.84	0.42
1:C:400:THR:O	1:C:404:GLU:HG2	2.20	0.42
1:C:325:LEU:HD23	1:C:325:LEU:HA	1.89	0.42
2:D:169:GLU:HB3	2:D:170:PRO:HD3	2.00	0.42
1:A:464:GLN:HE21	1:A:551:LEU:HD21	1.82	0.42
1:C:491:LEU:HA	1:C:491:LEU:HD23	1.71	0.42
1:C:58:THR:HG21	1:C:77:PHE:CE1	2.55	0.42
2:B:195:ILE:HG22	2:B:199:ARG:NE	2.33	0.42
2:D:5:ILE:O	2:D:119:PRO:HG2	2.19	0.42
2:D:28:GLU:HG3	2:D:135:ILE:HD11	2.02	0.42
2:D:350:LYS:HE2	2:D:378:GLU:OE1	2.19	0.42
1:C:39:THR:HA	1:C:42:GLU:OE2	2.18	0.42
2:B:34:LEU:HD23	2:B:34:LEU:HA	1.80	0.42
1:C:31:ILE:CG2	1:C:134:SER:HA	2.50	0.42
1:C:230:MET:O	4:F:821:DC:H5'	2.18	0.42
1:A:441:TYR:CD2	2:B:286:THR:HG23	2.55	0.42
2:D:120:LEU:HB3	2:D:147:ASN:O	2.20	0.42
2:D:200:THR:O	2:D:203:GLU:HB3	2.20	0.42
1:C:486:LEU:HB3	1:C:524:GLN:HB3	2.02	0.42
1:A:401:TRP:HB2	1:A:425:LEU:HD11	2.02	0.42
1:A:134:SER:O	1:A:135:ILE:HB	2.19	0.42
2:B:317:VAL:HG12	2:B:347:LYS:HD2	2.02	0.42
1:A:454:LYS:HB2	1:A:552:VAL:O	2.19	0.42
1:C:150:PRO:HG2	1:C:153:TRP:HB2	2.02	0.42
2:B:419:THR:HG22	2:B:419:THR:O	2.18	0.42
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.01	0.42
1:A:41:MET:HB2	1:A:47:ILE:HD11	2.02	0.41
2:B:167:ILE:HG23	2:B:212:TRP:CD1	2.55	0.41
1:C:249:LYS:HD2	1:C:249:LYS:HA	1.81	0.41
2:D:207:GLN:OE1	2:D:207:GLN:HA	2.20	0.41
1:C:135:ILE:O	1:C:136:ASN:HB2	2.20	0.41
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.56	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:10:VAL:HG12	1:C:11:LYS:N	2.35	0.41
1:C:326:ILE:O	1:C:341:ILE:HA	2.20	0.41
1:C:156:SER:HB2	1:C:157:PRO:HD3	2.01	0.41
4:P:822:ATM:O5'	4:P:822:ATM:H6	2.21	0.41
1:A:16:MET:CE	1:A:83:ARG:HG2	2.50	0.41
1:C:17:ASP:OD2	1:C:56:TYR:HE1	2.04	0.41
2:B:425:LEU:HD23	2:B:426:TRP:CE2	2.56	0.41
1:C:261:VAL:CG1	1:C:276:VAL:HG11	2.47	0.41
1:C:458:VAL:HG23	1:C:548:VAL:HB	2.01	0.41
2:D:24:TRP:HZ2	2:D:61:PHE:CD2	2.39	0.41
3:T:719:DG:H2''	3:T:720:DG:C8	2.55	0.41
2:D:10:VAL:HG13	2:D:87:PHE:CD1	2.55	0.41
2:B:210:LEU:HA	2:B:214:LEU:O	2.20	0.41
1:C:36:GLU:O	1:C:40:GLU:HG2	2.21	0.41
2:B:428:GLN:HA	2:B:428:GLN:OE1	2.21	0.41
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.61	0.41
1:C:266:TRP:O	1:C:269:GLN:HG2	2.20	0.41
1:A:270:ILE:HA	1:A:270:ILE:HD12	1.76	0.41
1:A:23:GLN:HE21	1:A:23:GLN:HB3	1.64	0.41
1:C:31:ILE:HG21	1:C:134:SER:HA	2.02	0.41
1:C:171:PHE:CE2	1:C:205:LEU:HD13	2.55	0.41
1:C:271:TYR:CE1	1:C:314:VAL:HG22	2.55	0.41
1:A:21:VAL:N	1:A:57:ASN:O	2.48	0.41
2:D:312:GLU:HB3	2:D:313:PRO:CD	2.48	0.41
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.50	0.41
2:D:168:LEU:CB	2:D:172:LYS:HE3	2.50	0.41
1:C:535:TRP:CD2	2:D:422:LEU:HD21	2.56	0.41
1:C:60:VAL:HG11	1:C:130:PHE:HD1	1.85	0.41
2:D:357:MET:HB3	2:D:370:GLU:OE1	2.21	0.41
2:B:86:ASP:O	2:B:90:VAL:HB	2.21	0.41
4:F:815:DG:H2''	4:F:816:DG:OP2	2.21	0.41
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.21	0.41
2:D:73:LYS:HE3	2:D:146:TYR:OH	2.21	0.41
2:D:206:ARG:NH2	2:D:217:PRO:O	2.54	0.41
2:B:382:ILE:HG22	2:B:383:TRP:CE2	2.56	0.41
1:A:459:THR:CG2	1:A:460:ASN:N	2.84	0.41
1:A:326:ILE:O	1:A:341:ILE:HA	2.21	0.41
2:D:422:LEU:HA	2:D:422:LEU:HD12	1.77	0.40
1:C:130:PHE:HD2	1:C:130:PHE:N	2.18	0.40
1:C:54:ASN:HA	1:C:55:PRO:HD2	1.86	0.40
1:C:120:LEU:CG	1:C:121:ASP:H	2.34	0.40
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:50:ILE:HG13	2:B:51:GLY:N	2.35	0.40
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.20	0.40
1:A:28:GLU:CD	1:A:28:GLU:H	2.24	0.40
1:C:395:LYS:HD2	1:C:414:TRP:CH2	2.56	0.40
2:D:56:TYR:CE2	2:D:127:TYR:CE1	3.10	0.40
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.56	0.40
2:B:53:GLU:HG2	2:B:54:ASN:N	2.35	0.40
2:B:297:GLU:OE1	2:B:297:GLU:HA	2.21	0.40
2:D:142:ILE:HG22	2:D:144:TYR:CE2	2.56	0.40
2:B:84:THR:HG22	2:B:84:THR:O	2.22	0.40
1:A:135:ILE:HG22	1:A:138:GLU:CB	2.50	0.40
2:D:336:GLN:HB2	2:D:336:GLN:HE21	1.79	0.40
2:D:197:GLN:O	2:D:201:LYS:HG2	2.22	0.40
2:B:28:GLU:HB2	2:B:135:ILE:HD11	2.03	0.40
1:A:553:SER:O	1:A:554:ALA:C	2.59	0.40
1:A:132:ILE:HD12	1:A:144:TYR:CD2	2.56	0.40
1:C:379:SER:CB	1:C:387:PRO:HD3	2.51	0.40
1:C:382:ILE:O	2:D:136:ASN:HB2	2.21	0.40
1:C:420:PRO:HA	1:C:421:PRO:C	2.40	0.40
2:D:257:ILE:O	2:D:261:VAL:HG23	2.22	0.40
2:B:78:ARG:HD3	2:B:411:ILE:O	2.21	0.40
2:D:376:THR:HG21	2:D:410:TRP:CZ3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/556 (100%)	529 (96%)	23 (4%)	1 (0%)	56	86
1	C	552/556 (99%)	528 (96%)	24 (4%)	0	100	100
2	B	408/428 (95%)	399 (98%)	9 (2%)	0	100	100
2	D	408/428 (95%)	391 (96%)	17 (4%)	0	100	100
All	All	1921/1968 (98%)	1847 (96%)	73 (4%)	1 (0%)	59	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	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	495/497 (100%)	476 (96%)	19 (4%)	44	76
1	C	495/497 (100%)	475 (96%)	20 (4%)	42	75
2	B	374/390 (96%)	362 (97%)	12 (3%)	51	82
2	D	374/390 (96%)	366 (98%)	8 (2%)	66	91
All	All	1738/1774 (98%)	1679 (97%)	59 (3%)	49	81

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	SER
1	A	5	ILE
1	A	23	GLN
1	A	39	THR
1	A	63	ILE
1	A	67	ASP
1	A	90	VAL
1	A	105	SER
1	A	123	ASP
1	A	130	PHE
1	A	188	TYR
1	A	221	HIS
1	A	248	GLU
1	A	277	ARG
1	A	293	ILE
1	A	324	ASP
1	A	338	THR
1	A	523	GLU
2	B	72	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	113	ASP
2	B	115	TYR
2	B	163	SER
2	B	169	GLU
2	B	177	ASP
2	B	208	HIS
2	B	241	VAL
2	B	257	ILE
2	B	293	ILE
2	B	336	GLN
2	B	422	LEU
1	C	2	ILE
1	C	3	SER
1	C	5	ILE
1	C	7	THR
1	C	48	SER
1	C	50	ILE
1	C	53	GLU
1	C	123	ASP
1	C	130	PHE
1	C	199	ARG
1	C	218	ASP
1	C	221	HIS
1	C	250	ASP
1	C	270	ILE
1	C	324	ASP
1	C	338	THR
1	C	357	MET
1	C	407	GLN
1	C	459	THR
1	C	498	ASN
2	D	74	LEU
2	D	113	ASP
2	D	134	SER
2	D	248	GLU
2	D	336	GLN
2	D	379	SER
2	D	423	VAL
2	D	424	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	GLN
1	A	464	GLN
1	A	487	GLN
2	B	278	GLN
2	B	336	GLN
1	C	222	GLN
1	C	367	GLN
1	C	407	GLN
1	C	464	GLN
1	C	547	GLN
2	D	348	ASN
2	D	361	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 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
4	MRG	F	817	1,3,4	26,28,29	2.61	11 (42%)	33,39,42	1.71	7 (21%)
4	ATM	F	822	3,4	21,23,24	1.30	4 (19%)	24,32,35	2.32	7 (29%)
4	MRG	P	817	1,3,4	26,28,29	2.68	11 (42%)	33,39,42	1.73	9 (27%)
4	ATM	P	822	3,4	21,23,24	1.28	3 (14%)	24,32,35	2.10	7 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MRG	F	817	1,3,4	-	0/11/26/27	0/1/3/3
4	ATM	F	822	3,4	-	0/8/24/25	0/2/2/2
4	MRG	P	817	1,3,4	-	0/11/26/27	0/1/3/3
4	ATM	P	822	3,4	-	0/8/24/25	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	817	MRG	C2-N2	5.55	1.48	1.32
4	P	817	MRG	C2-N2	5.47	1.48	1.32
4	P	817	MRG	C4-N3	5.43	1.44	1.35
4	F	817	MRG	C4-N3	5.18	1.44	1.35
4	F	817	MRG	P-OP1	4.83	1.52	1.46
4	P	817	MRG	P-OP1	4.75	1.52	1.46
4	P	817	MRG	C6-C5	4.74	1.49	1.41
4	F	817	MRG	C6-C5	4.71	1.48	1.41
4	F	817	MRG	C2-N3	4.59	1.43	1.33
4	P	817	MRG	C2-N3	4.49	1.43	1.33
4	P	817	MRG	C2'-C3'	-3.27	1.43	1.52
4	F	817	MRG	C2'-C3'	-3.24	1.43	1.52
4	P	817	MRG	C6-N1	3.14	1.42	1.37
4	P	817	MRG	O3'-C3'	-3.12	1.36	1.43
4	P	817	MRG	C2-N1	2.99	1.43	1.36
4	F	822	ATM	N5'-N4'	2.97	1.26	1.15
4	P	822	ATM	C6-N1	2.81	1.41	1.34
4	F	817	MRG	C2-N1	2.76	1.43	1.36
4	F	817	MRG	O4'-C4'	-2.67	1.38	1.45
4	F	817	MRG	C6-N1	2.66	1.41	1.37
4	P	817	MRG	O4'-C4'	-2.61	1.38	1.45
4	P	822	ATM	N5'-N4'	2.59	1.25	1.15
4	P	817	MRG	C4-N9	-2.47	1.34	1.37
4	F	822	ATM	C6-N1	2.43	1.40	1.34
4	F	822	ATM	P-OP1	2.38	1.49	1.46
4	F	817	MRG	O3'-C3'	-2.35	1.38	1.43
4	P	822	ATM	P-OP1	2.29	1.49	1.46
4	F	817	MRG	C4-N9	-2.20	1.34	1.37
4	F	822	ATM	C4-N3	2.18	1.40	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	822	ATM	C6-N1-C2	-6.66	120.51	122.41
4	F	822	ATM	N3-C2-N1	5.76	120.78	115.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	822	ATM	C2'-C1'-N1	-5.36	100.15	114.08
4	P	822	ATM	N3-C2-N1	4.02	119.33	115.97
4	P	817	MRG	C6-C5-N7	-3.99	133.60	134.14
4	P	822	ATM	C6-N1-C2	-3.67	121.36	122.41
4	F	817	MRG	C2-N3-C4	3.57	119.85	115.03
4	F	817	MRG	C5-C4-N3	-3.50	120.87	125.94
4	F	817	MRG	C6-C5-N7	-3.41	133.68	134.14
4	P	817	MRG	O4'-C1'-N9	3.24	113.76	107.68
4	F	822	ATM	C4-N3-C2	-3.05	119.14	125.39
4	P	817	MRG	C22-C21-N2	3.04	119.71	111.26
4	F	817	MRG	C4-C5-N7	-3.02	106.93	109.52
4	F	817	MRG	O4'-C1'-N9	3.01	113.34	107.68
4	P	817	MRG	C2-N3-C4	2.99	119.06	115.03
4	F	817	MRG	N3-C4-N9	2.93	131.21	126.91
4	F	822	ATM	N5'-N4'-N3'	2.92	179.11	172.25
4	P	822	ATM	N5'-N4'-N3'	2.91	179.07	172.25
4	P	822	ATM	C4-N3-C2	-2.90	119.43	125.39
4	F	822	ATM	C5-C6-N1	-2.78	118.88	121.59
4	P	817	MRG	C5-C4-N3	-2.74	121.97	125.94
4	P	817	MRG	C4-C5-N7	-2.66	107.25	109.52
4	F	817	MRG	C22-C21-N2	2.59	118.46	111.26
4	P	822	ATM	C5-C6-N1	-2.56	119.10	121.59
4	P	817	MRG	N3-C4-N9	2.44	130.49	126.91
4	P	817	MRG	C8-N9-C4	2.42	108.74	106.90
4	F	822	ATM	C6-C5-C4	2.37	120.87	115.11
4	P	822	ATM	C5'-C4'-C3'	-2.31	106.22	114.50
4	F	822	ATM	O4'-C1'-N1	2.15	111.73	107.68
4	P	817	MRG	N7-C8-N9	-2.02	108.65	114.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	555/556 (99%)	1.60	128 (23%) 1 1	36, 83, 138, 149	0
1	C	554/556 (99%)	1.48	123 (22%) 1 1	34, 81, 136, 148	0
2	B	412/428 (96%)	1.02	45 (10%) 6 6	34, 66, 118, 131	0
2	D	412/428 (96%)	1.11	65 (15%) 3 3	40, 69, 125, 132	0
3	E	24/27 (88%)	0.91	4 (16%) 2 3	67, 104, 156, 164	0
3	T	24/27 (88%)	1.01	4 (16%) 2 3	69, 106, 158, 161	0
4	F	20/21 (95%)	0.60	2 (10%) 8 8	60, 92, 141, 142	0
4	P	20/21 (95%)	0.39	2 (10%) 8 8	68, 90, 142, 144	0
All	All	2021/2064 (97%)	1.31	373 (18%) 2 2	34, 75, 132, 164	0

All (373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	PRO	15.6
1	A	74	LEU	15.5
2	B	214	LEU	14.0
1	C	142	ILE	13.4
1	A	133	PRO	12.5
1	A	26	LEU	12.2
1	A	131	THR	11.9
1	A	30	LYS	11.5
1	A	61	PHE	10.8
1	C	252	TRP	10.5
2	D	4	PRO	10.4
1	C	135	ILE	10.3
2	B	215	THR	10.1
3	T	702	DT	10.1
1	A	549	ASP	9.4
1	A	140	PRO	9.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	287	LYS	9.2
2	D	231	GLY	9.1
1	A	34	LEU	8.9
1	C	130	PHE	8.7
1	A	289	LEU	8.3
1	A	286	THR	8.2
1	C	136	ASN	8.2
1	C	144	TYR	8.1
2	D	214	LEU	8.0
1	C	138	GLU	7.9
1	C	129	ALA	7.8
1	A	52	PRO	7.8
1	C	141	GLY	7.6
1	C	293	ILE	7.6
1	A	130	PHE	7.4
1	C	247	PRO	7.4
1	A	128	THR	7.4
1	C	132	ILE	7.4
1	A	553	SER	7.3
1	C	61	PHE	7.0
1	A	19	PRO	6.9
1	C	554	ALA	6.8
1	A	72	ARG	6.8
1	A	135	ILE	6.7
1	A	63	ILE	6.4
2	D	177	ASP	6.4
1	A	73	LYS	6.2
1	C	292	VAL	6.2
2	B	212	TRP	6.2
2	D	5	ILE	6.2
2	D	94	ILE	6.2
1	A	59	PRO	6.1
1	C	26	LEU	6.0
1	C	74	LEU	6.0
1	A	71	TRP	6.0
1	A	222	GLN	5.9
1	A	136	ASN	5.9
1	C	71	TRP	5.9
1	A	50	ILE	5.9
1	A	285	GLY	5.9
1	C	17	ASP	5.9
1	A	129	ALA	5.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	27	THR	5.8
1	A	141	GLY	5.8
1	A	132	ILE	5.8
2	B	204	GLU	5.8
1	C	140	PRO	5.8
2	D	178	ILE	5.8
1	C	246	LEU	5.8
2	B	5	ILE	5.8
1	C	134	SER	5.8
1	C	73	LYS	5.8
1	C	223	LYS	5.7
2	D	90	VAL	5.7
1	A	21	VAL	5.6
1	A	144	TYR	5.6
1	A	56	TYR	5.5
1	A	54	ASN	5.5
1	C	24	TRP	5.5
1	C	139	THR	5.5
1	A	127	TYR	5.5
1	A	25	PRO	5.5
1	C	30	LYS	5.5
2	D	197	GLN	5.4
1	A	18	GLY	5.4
1	C	288	ALA	5.3
1	A	23	GLN	5.3
1	A	33	ALA	5.2
1	A	62	ALA	5.2
1	C	251	SER	5.2
1	C	291	GLU	5.2
1	A	552	VAL	5.2
1	A	38	CYS	5.1
1	A	550	LYS	5.1
1	C	143	ARG	5.1
2	B	88	TRP	5.1
1	A	288	ALA	5.1
1	C	60	VAL	5.0
2	D	216	THR	5.0
2	B	4	PRO	4.9
1	A	145	GLN	4.9
1	C	25	PRO	4.9
1	C	260	LEU	4.9
1	C	248	GLU	4.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	21	VAL	4.9
1	A	37	ILE	4.8
2	D	168	LEU	4.8
1	C	72	ARG	4.8
1	A	139	THR	4.6
1	C	296	THR	4.6
2	D	8	VAL	4.6
1	A	68	SER	4.6
1	A	287	LYS	4.5
1	C	63	ILE	4.5
1	C	28	GLU	4.5
1	C	254	VAL	4.5
1	A	293	ILE	4.5
1	C	224	GLU	4.4
2	B	213	GLY	4.4
2	B	295	LEU	4.4
1	A	70	LYS	4.4
3	E	725	DG	4.3
1	A	137	ASN	4.3
1	C	22	LYS	4.3
2	D	95	PRO	4.3
2	D	67	ASP	4.3
1	A	146	TYR	4.3
1	A	60	VAL	4.3
1	C	104	LYS	4.3
2	D	92	LEU	4.2
2	D	89	GLU	4.2
1	A	283	LEU	4.2
2	D	171	PHE	4.2
1	A	551	LEU	4.1
1	C	34	LEU	4.1
2	B	209	LEU	4.1
1	A	29	GLU	4.1
2	D	354	TYR	4.1
1	C	75	VAL	4.0
1	C	448	ARG	4.0
2	D	357	MET	4.0
1	C	66	LYS	4.0
2	B	428	GLN	4.0
3	E	702	DT	4.0
1	C	226	PRO	4.0
1	C	109	LEU	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	303	LEU	4.0
2	B	250	ASP	3.9
1	A	254	VAL	3.9
2	D	172	LYS	3.9
1	A	448	ARG	3.9
1	C	128	THR	3.9
1	A	134	SER	3.8
1	C	137	ASN	3.8
1	A	223	LYS	3.8
2	D	232	TYR	3.8
1	A	51	GLY	3.8
2	D	124	PHE	3.7
1	C	264	LEU	3.7
2	D	421	PRO	3.7
1	C	253	THR	3.7
2	D	187	LEU	3.7
2	D	212	TRP	3.7
1	A	28	GLU	3.7
2	D	105	SER	3.7
1	C	357	MET	3.7
3	T	703	DG	3.7
1	A	69	THR	3.7
1	C	236	PRO	3.7
1	C	249	LYS	3.7
2	D	360	ALA	3.6
2	B	205	LEU	3.6
2	D	7	THR	3.5
1	C	237	ASP	3.5
2	B	281	LYS	3.5
1	C	124	PHE	3.5
2	B	425	LEU	3.5
1	C	69	THR	3.5
2	B	277	ARG	3.5
1	C	276	VAL	3.5
1	A	282	LEU	3.4
2	B	211	ARG	3.4
3	T	725	DG	3.4
2	B	232	TYR	3.4
1	C	19	PRO	3.4
1	C	299	ALA	3.4
1	A	246	LEU	3.4
1	A	261	VAL	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	23	GLN	3.3
2	B	310	LEU	3.3
1	C	312	GLU	3.3
1	A	257	ILE	3.3
2	D	9	PRO	3.3
2	D	10	VAL	3.3
1	A	142	ILE	3.3
2	B	210	LEU	3.3
2	D	209	LEU	3.3
2	D	91	GLN	3.2
1	C	131	THR	3.2
1	A	39	THR	3.2
2	D	66	LYS	3.2
1	C	310	LEU	3.2
1	C	32	LYS	3.2
2	D	238	LYS	3.2
2	B	278	GLN	3.2
1	C	257	ILE	3.2
1	A	284	ARG	3.2
2	B	171	PHE	3.1
1	C	145	GLN	3.1
2	B	217	PRO	3.1
1	C	198	HIS	3.1
1	A	24	TRP	3.1
2	B	193	LEU	3.1
4	F	803	DC	3.1
1	C	205	LEU	3.1
1	A	12	LEU	3.0
1	A	544	GLY	3.0
1	C	192	ASP	3.0
1	A	124	PHE	3.0
1	C	225	PRO	3.0
1	C	308	GLU	3.0
1	A	66	LYS	3.0
2	B	206	ARG	3.0
1	C	274	ILE	3.0
1	A	493	VAL	2.9
2	D	118	VAL	2.9
1	A	67	ASP	2.9
1	C	70	LYS	2.9
1	A	149	LEU	2.9
2	B	284	ARG	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	118	VAL	2.9
2	D	189	VAL	2.9
1	A	260	LEU	2.9
1	A	295	LEU	2.9
2	B	422	LEU	2.9
1	C	27	THR	2.9
2	D	284	ARG	2.9
2	D	215	THR	2.9
1	C	105	SER	2.9
2	D	119	PRO	2.9
2	D	173	LYS	2.9
1	A	554	ALA	2.8
2	D	426	TRP	2.8
1	A	296	THR	2.8
2	D	420	PRO	2.8
1	C	58	THR	2.8
1	A	263	LYS	2.8
2	D	358	ARG	2.8
1	C	297	GLU	2.8
1	C	244	ILE	2.8
3	T	724	DT	2.8
1	C	56	TYR	2.8
4	P	803	DC	2.7
1	A	36	GLU	2.7
1	A	41	MET	2.7
4	F	804	DA	2.7
2	D	69	THR	2.7
2	B	301	LEU	2.7
1	A	49	LYS	2.7
1	A	193	LEU	2.7
2	D	179	VAL	2.7
1	A	109	LEU	2.6
1	C	106	VAL	2.6
1	C	31	ILE	2.6
2	B	275	LYS	2.6
2	D	202	ILE	2.6
1	C	250	ASP	2.6
1	A	75	VAL	2.6
1	A	234	LEU	2.6
2	D	361	HIS	2.6
1	A	31	ILE	2.6
2	D	159	ILE	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	43	LYS	2.5
2	B	282	LEU	2.5
2	D	115	TYR	2.5
2	B	274	ILE	2.5
2	D	88	TRP	2.5
1	C	552	VAL	2.5
1	C	20	LYS	2.5
2	B	299	ALA	2.5
1	C	295	LEU	2.5
1	A	227	PHE	2.5
1	C	290	THR	2.5
1	A	290	THR	2.5
1	A	152	GLY	2.4
1	C	228	LEU	2.4
1	C	289	LEU	2.4
2	D	100	LEU	2.4
1	C	78	ARG	2.4
1	A	548	VAL	2.4
2	D	295	LEU	2.4
1	C	33	ALA	2.4
1	A	20	LYS	2.4
1	C	280	SER	2.4
1	A	466	VAL	2.3
1	A	459	THR	2.3
1	C	112	GLY	2.3
1	A	79	GLU	2.3
1	C	16	MET	2.3
1	A	47	ILE	2.3
2	D	86	ASP	2.3
1	A	441	TYR	2.3
1	C	227	PHE	2.3
1	A	0	VAL	2.3
2	D	164	MET	2.3
1	A	195	ILE	2.3
1	C	300	GLU	2.3
1	C	49	LYS	2.3
1	C	259	LYS	2.3
3	E	704	DG	2.3
1	C	55	PRO	2.3
1	C	286	THR	2.2
2	D	240	THR	2.2
2	B	178	ILE	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	13	LYS	2.2
1	C	263	LYS	2.2
1	A	17	ASP	2.2
1	A	121	ASP	2.2
1	A	386	THR	2.2
2	B	85	GLN	2.2
2	D	195	ILE	2.2
1	A	298	GLU	2.2
1	A	16	MET	2.2
1	A	302	GLU	2.2
2	B	13	LYS	2.2
2	B	173	LYS	2.2
2	D	109	LEU	2.2
1	A	309	ILE	2.2
1	A	77	PHE	2.2
3	E	724	DT	2.2
1	C	283	LEU	2.2
2	B	109	LEU	2.2
2	B	177	ASP	2.2
1	A	442	VAL	2.2
1	C	64	LYS	2.2
2	B	189	VAL	2.2
1	A	83	ARG	2.2
1	A	303	LEU	2.2
2	D	213	GLY	2.2
1	C	279	LEU	2.2
2	B	312	GLU	2.2
2	D	242	GLN	2.1
2	B	314	VAL	2.1
1	C	553	SER	2.1
1	A	138	GLU	2.1
1	C	496	VAL	2.1
2	B	392	PRO	2.1
2	D	14	PRO	2.1
1	C	65	LYS	2.1
1	A	279	LEU	2.1
1	C	12	LEU	2.1
1	C	29	GLU	2.1
2	B	89	GLU	2.1
1	C	18	GLY	2.1
2	B	308	GLU	2.1
2	D	356	ARG	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	205	LEU	2.1
1	A	455	ALA	2.1
1	C	466	VAL	2.1
1	C	273	GLY	2.1
1	A	10	VAL	2.1
2	D	104	LYS	2.1
4	P	804	DA	2.1
1	A	259	LYS	2.1
1	A	292	VAL	2.1
1	C	271	TYR	2.1
1	A	301	LEU	2.1
1	C	57	ASN	2.1
1	C	376	THR	2.0
1	A	43	LYS	2.0
2	D	46	LYS	2.0
2	D	422	LEU	2.0
2	B	86	ASP	2.0
1	A	64	LYS	2.0
1	A	542	ILE	2.0
1	A	546	GLU	2.0
1	C	245	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ATM	F	822	22/23	0.20	-0.54	71,78,87,95	0
4	MRG	P	817	26/27	0.18	-0.58	88,102,117,121	0
4	ATM	P	822	22/23	0.18	-0.73	71,82,95,95	0
4	MRG	F	817	26/27	0.18	-0.77	84,99,117,127	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.