



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 08:14 PM EDT

PDB ID : 2IS4  
Title : Crystal structure of UvrD-DNA-ADPNP ternary complex  
Authors : Yang, W.; Lee, J.Y.  
Deposited on : unknown  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

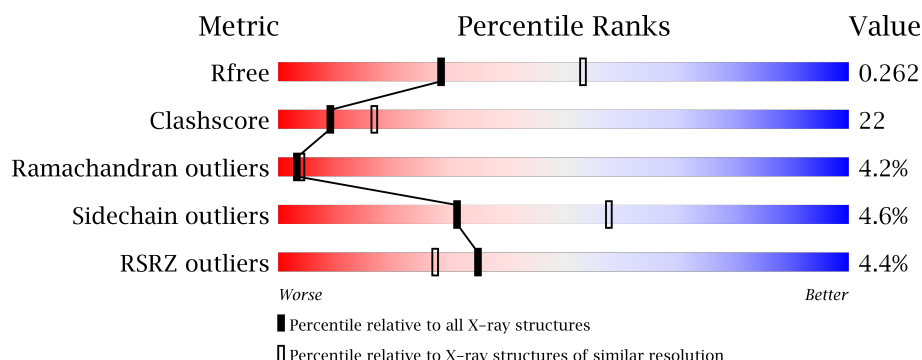
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	C	26	<div> <div>46%</div> <div>50%</div> <div>.</div> </div>
1	D	26	<div> <div>27%</div> <div>69%</div> <div>.</div> </div>
2	A	680	<div> <div>5%</div> <div>57%</div> <div>34%</div> <div>5%</div> </div>
2	B	680	<div> <div>4%</div> <div>53%</div> <div>35%</div> <div>5%</div> <div>7%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11148 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 25-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	25	Total	C	N	O	P	0	0	0
			506	244	89	150	23			
1	D	25	Total	C	N	O	P	0	0	0
			509	244	89	152	24			

- Molecule 2 is a protein called DNA helicase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	646	Total	C	N	O	S	0	0	0
			5006	3140	898	942	26			
2	B	632	Total	C	N	O	S	0	0	0
			4945	3101	896	923	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	VAL	ALA	ENGINEERED	UNP P03018
B	399	VAL	ALA	ENGINEERED	UNP P03018

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

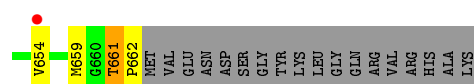


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

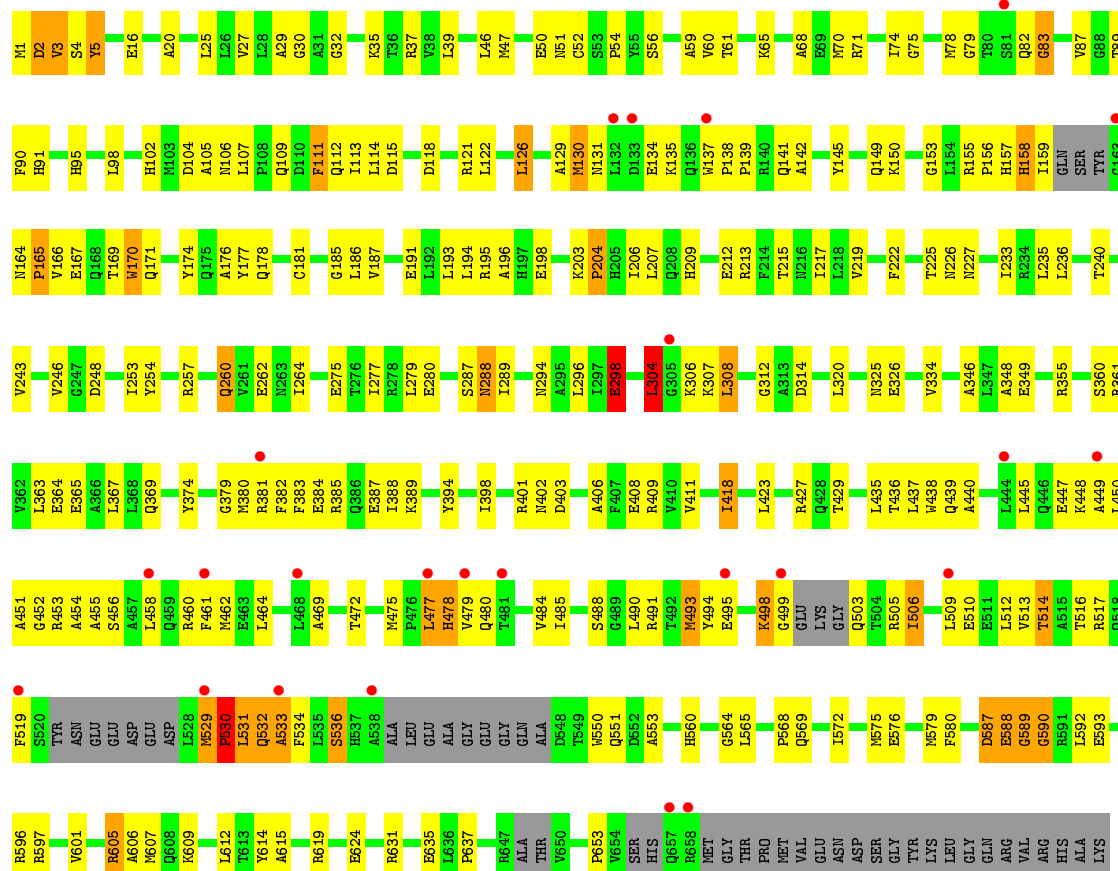
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	56	Total	O	0	0
			56	56		





• Molecule 2: DNA helicase II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.11Å 96.78Å 111.04Å 90.00° 93.85° 90.00°	Depositor
Resolution (Å)	29.84 – 2.60 48.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	85.3 (29.84-2.60) 85.2 (48.29-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.215 , 0.256 0.224 , 0.262	Depositor DCC
$R_{free}$ test set	5886 reflections (10.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.6	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	C	0.40	0/565	0.71	0/869
1	D	0.32	0/569	0.70	0/877
2	A	0.42	2/5099 (0.0%)	0.61	2/6913 (0.0%)
2	B	0.41	1/5032 (0.0%)	0.61	2/6807 (0.0%)
All	All	0.41	3/11265 (0.0%)	0.62	4/15466 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	134	GLU	CB-CG	-5.22	1.42	1.52
2	B	134	GLU	CB-CG	-5.17	1.42	1.52
2	A	511	GLU	CB-CG	-5.10	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	551	GLN	N-CA-C	-6.50	93.47	111.00
2	B	653	PRO	N-CA-CB	5.39	109.77	103.30
2	B	530	PRO	N-CA-CB	5.37	109.75	103.30
2	A	662	PRO	N-CA-CB	5.23	109.58	103.30

There are no chirality outliers.

There are no planarity outliers.

### 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	C	506	0	287	24	0
1	D	509	0	285	32	0
2	A	5006	0	4755	211	0
2	B	4945	0	4732	217	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	13	3	0
4	B	31	0	13	1	0
5	A	62	0	0	3	0
5	B	56	0	0	1	0
All	All	11148	0	10085	468	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 22.

All (468) 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)
1:D:15:DG:H2''	1:D:16:DC:H5''	1.28	1.15
2:B:478:HIS:HB2	2:B:517:ARG:HA	1.32	1.10
1:D:5:DG:H2''	1:D:6:DC:H5''	1.34	1.09
1:D:15:DG:H2''	1:D:16:DC:C5'	1.89	1.02
1:C:13:DG:H4'	2:A:453:ARG:HD2	1.37	1.01
2:A:25:LEU:HD21	2:A:277:ILE:HD12	1.50	0.94
1:C:20:DT:HO3'	1:C:22:DG:H8	1.17	0.93
2:B:382:PHE:HA	2:B:385:ARG:NH2	1.86	0.90
2:B:155:ARG:H	2:B:158:HIS:HD2	1.17	0.89
2:A:25:LEU:HD11	2:A:277:ILE:HG13	1.55	0.88
2:B:227:ASN:HD21	2:B:260:GLN:NE2	1.71	0.88
1:C:14:DT:H2''	1:C:15:DG:C8	2.09	0.86
2:A:23:SER:HA	2:A:242:LYS:HD2	1.58	0.85
2:A:382:PHE:O	2:A:385:ARG:HG3	1.76	0.85
1:D:19:DG:H2''	1:D:20:DT:OP2	1.75	0.84
2:A:659:MET:HB3	2:A:661:THR:HG22	1.59	0.84
2:A:416:ARG:NH2	2:A:464:LEU:HD23	1.92	0.83
1:D:6:DC:H2''	1:D:7:DA:C8	2.13	0.83
1:D:15:DG:C2'	1:D:16:DC:H5''	2.08	0.82
2:A:32:GLY:H	4:A:700:ANP:HNB1	1.24	0.81
2:B:65:LYS:HD2	2:B:565:LEU:HD11	1.63	0.81
2:A:475:MET:HE2	2:A:479:VAL:HG13	1.63	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:DT:O3'	1:C:22:DG:H8	1.64	0.79
1:D:18:DC:H4'	1:D:19:DG:OP1	1.80	0.78
2:A:226:ASN:HD21	2:A:229:GLN:HG3	1.49	0.78
2:B:346:ALA:HB3	2:B:349:GLU:HG3	1.66	0.77
2:B:32:GLY:H	4:B:701:ANP:HNB1	1.33	0.77
1:D:7:DA:H1'	1:D:8:DC:H5"	1.66	0.77
2:B:308:LEU:H	2:B:308:LEU:HD12	1.51	0.76
1:D:5:DG:C2'	1:D:6:DC:H5"	2.13	0.76
2:A:208:GLN:O	2:A:212:GLU:HG3	1.85	0.76
2:B:227:ASN:HD21	2:B:260:GLN:HE21	1.33	0.75
2:B:381:ARG:HA	2:B:384:GLU:HG2	1.69	0.74
1:D:10:DG:H3'	2:A:421:ARG:HG3	1.69	0.74
2:B:25:LEU:HD11	2:B:277:ILE:HG13	1.70	0.74
1:C:20:DT:O3'	1:C:22:DG:H2'	1.88	0.73
2:A:476:PRO:HG2	2:A:479:VAL:HG12	1.69	0.73
2:A:429:THR:O	2:A:433:ARG:HB2	1.88	0.73
1:C:15:DG:H1	1:D:6:DC:H42	1.37	0.73
2:B:475:MET:HB3	2:B:479:VAL:HG13	1.71	0.72
2:B:222:PHE:O	2:B:225:THR:HG23	1.89	0.72
2:A:421:ARG:NH1	2:A:421:ARG:HB3	2.04	0.72
2:A:290:LEU:HD11	2:A:308:LEU:HD13	1.71	0.72
1:C:26:DA:N7	2:B:380:MET:HG2	2.05	0.72
2:A:130:MET:HG2	2:A:431:ARG:HH21	1.55	0.71
2:B:503:GLN:O	2:B:506:ILE:HG23	1.90	0.71
2:B:532:GLN:HE21	2:B:532:GLN:CA	2.03	0.71
1:D:17:DT:H4'	1:D:18:DC:OP1	1.89	0.70
2:B:532:GLN:O	2:B:534:PHE:N	2.24	0.70
2:B:532:GLN:HE21	2:B:532:GLN:HA	1.56	0.70
2:A:459:GLN:O	2:A:463:GLU:HG3	1.92	0.69
2:B:382:PHE:HA	2:B:385:ARG:HH21	1.56	0.69
2:B:592:LEU:HD21	2:B:631:ARG:NH1	2.07	0.69
2:A:411:VAL:O	2:A:416:ARG:HD3	1.93	0.69
2:B:475:MET:HB3	2:B:479:VAL:CG1	2.23	0.69
2:A:133:ASP:HB3	2:A:136:GLN:HB2	1.75	0.69
2:B:102:HIS:HB2	2:B:107:LEU:O	1.91	0.69
2:B:478:HIS:HB2	2:B:517:ARG:CA	2.17	0.68
2:A:130:MET:HG2	2:A:431:ARG:NH2	2.09	0.68
2:A:476:PRO:O	2:A:480:GLN:HB2	1.94	0.67
2:B:478:HIS:CB	2:B:517:ARG:HA	2.18	0.67
2:A:411:VAL:HA	2:A:461:PHE:CZ	2.30	0.67
2:A:25:LEU:HD12	2:A:275:GLU:O	1.95	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:149:GLN:OE1	2:A:154:LEU:HD12	1.95	0.66
2:B:25:LEU:HD21	2:B:277:ILE:HD12	1.78	0.66
2:A:421:ARG:H	2:A:421:ARG:NE	1.95	0.64
2:B:114:LEU:CD1	2:B:118:ASP:HB3	2.26	0.64
2:A:416:ARG:HH22	2:A:464:LEU:HD23	1.58	0.64
2:B:59:ALA:HB3	2:B:87:VAL:HG22	1.79	0.64
2:A:153:GLY:HA2	2:A:194:LEU:HD13	1.78	0.64
2:A:601:VAL:O	2:A:605:ARG:HD2	1.97	0.64
2:B:564:GLY:H	2:B:605:ARG:HH21	1.45	0.64
2:B:576:GLU:HG3	2:B:579:MET:HG3	1.80	0.64
2:A:431:ARG:O	2:A:431:ARG:HD3	1.98	0.63
1:C:11:DC:H42	1:D:10:DG:H1	1.47	0.63
2:A:378:GLY:CA	2:A:381:ARG:HH12	2.12	0.63
1:C:26:DA:H5''	2:B:91:HIS:HB3	1.80	0.63
2:A:218:LEU:HD12	2:A:218:LEU:N	2.13	0.63
2:A:429:THR:OG1	2:A:444:LEU:HD11	1.99	0.62
2:A:421:ARG:HH11	2:A:421:ARG:HB3	1.64	0.62
2:A:43:ILE:HG23	2:A:57:ILE:HD13	1.81	0.62
2:B:472:THR:HG22	2:B:475:MET:SD	2.39	0.62
2:A:133:ASP:HB3	2:A:136:GLN:CB	2.30	0.62
2:B:453:ARG:HG3	2:B:453:ARG:HH11	1.64	0.62
2:A:416:ARG:HH22	2:A:464:LEU:CD2	2.11	0.62
2:A:564:GLY:H	2:A:605:ARG:NH2	1.99	0.61
2:A:303:ARG:HH11	2:A:303:ARG:HB2	1.66	0.61
2:A:408:GLU:O	2:A:411:VAL:HG12	2.01	0.60
2:B:114:LEU:HD12	2:B:118:ASP:HB3	1.82	0.60
1:D:15:DG:H2''	1:D:16:DC:H5'	1.77	0.60
2:B:104:ASP:HB3	2:B:203:LYS:HE3	1.83	0.60
2:B:514:THR:O	2:B:517:ARG:HB3	2.01	0.60
2:A:377:TYR:HE2	2:A:544:GLU:H	1.50	0.60
2:A:217:ILE:C	2:A:218:LEU:HD12	2.22	0.59
2:A:378:GLY:O	2:A:381:ARG:NH1	2.35	0.59
2:B:90:PHE:HE2	2:B:233:ILE:HD11	1.67	0.59
2:A:486:LYS:HA	2:A:491:ARG:CB	2.33	0.59
2:B:56:SER:HA	2:B:213:ARG:O	2.02	0.59
2:B:153:GLY:HA2	2:B:194:LEU:HD13	1.84	0.59
2:A:416:ARG:HH11	2:A:416:ARG:HG3	1.67	0.59
2:A:383:PHE:HA	2:A:388:ILE:HG21	1.84	0.58
1:C:20:DT:C3'	1:C:22:DG:H2'	2.32	0.58
2:A:105:ALA:O	2:A:106:ASN:HB3	2.02	0.58
2:A:601:VAL:O	2:A:605:ARG:CD	2.50	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:PRO:HA	2:B:171:GLN:NE2	2.19	0.58
2:B:485:ILE:HG22	2:B:491:ARG:HG3	1.84	0.58
2:A:433:ARG:O	2:A:434:GLN:HB2	2.04	0.58
2:A:389:LYS:HB3	2:A:409:ARG:NE	2.19	0.58
2:A:436:THR:OG1	2:A:439:GLN:HG3	2.04	0.58
2:A:461:PHE:CZ	2:A:465:ILE:HD11	2.38	0.58
2:A:433:ARG:HB3	2:A:435:LEU:HG	1.86	0.58
2:B:47:MET:CE	2:B:54:PRO:HG3	2.34	0.58
1:D:11:DC:OP2	2:A:421:ARG:HG2	2.04	0.57
2:B:30:GLY:HA2	2:B:248:ASP:OD2	2.04	0.57
2:B:364:GLU:HG3	2:B:374:TYR:OH	2.05	0.57
2:A:146:ILE:HD13	2:A:177:TYR:CD2	2.40	0.57
2:B:2:ASP:O	2:B:5:TYR:HD2	1.88	0.57
2:B:126:LEU:HD21	2:B:176:ALA:HB1	1.85	0.56
1:C:19:DG:H4'	1:C:20:DT:OP1	2.06	0.56
2:A:287:SER:HB3	2:A:314:ASP:HA	1.86	0.56
2:A:393:SER:OG	2:A:409:ARG:HD3	2.06	0.56
2:B:159:ILE:HB	2:B:171:GLN:OE1	2.04	0.56
2:B:435:LEU:HB3	2:B:439:GLN:HB3	1.87	0.56
2:A:130:MET:CG	2:A:431:ARG:HH21	2.19	0.56
2:A:157:HIS:H	2:A:157:HIS:CD2	2.23	0.56
2:B:135:LYS:NZ	2:B:135:LYS:HB3	2.20	0.56
2:A:194:LEU:O	2:A:198:GLU:HG3	2.06	0.56
2:A:614:TYR:CE2	2:A:629:PRO:HG3	2.41	0.56
2:B:320:LEU:HD11	2:B:614:TYR:CE1	2.41	0.56
2:A:25:LEU:HD21	2:A:277:ILE:CD1	2.31	0.56
2:B:155:ARG:H	2:B:158:HIS:CD2	2.08	0.56
2:B:150:LYS:NZ	2:B:178:GLN:HE22	2.04	0.56
2:B:401:ARG:HH22	2:B:469:ALA:CB	2.19	0.55
2:B:461:PHE:O	2:B:464:LEU:HB3	2.07	0.55
2:A:380:MET:O	2:A:384:GLU:HG3	2.07	0.55
2:B:170:TRP:HA	2:B:170:TRP:CE3	2.41	0.55
1:D:17:DT:H2''	1:D:18:DC:C6	2.42	0.55
2:A:362:VAL:HG23	5:A:1036:HOH:O	2.05	0.55
2:B:194:LEU:O	2:B:198:GLU:HG3	2.07	0.55
2:B:287:SER:HB3	2:B:314:ASP:HA	1.89	0.55
2:A:166:VAL:HG23	2:A:167:GLU:N	2.22	0.55
2:B:369:GLN:O	2:B:369:GLN:HG2	2.07	0.55
2:A:401:ARG:HH22	2:A:469:ALA:CB	2.20	0.55
2:B:129:ALA:C	2:B:131:ASN:H	2.09	0.55
1:C:16:DC:H42	1:D:5:DG:H1	1.55	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:503:GLN:O	2:A:506:ILE:HG22	2.07	0.54
2:B:506:ILE:HD12	2:B:506:ILE:O	2.07	0.54
2:B:529:MET:O	2:B:531:LEU:N	2.40	0.54
2:A:165:PRO:HG2	2:A:166:VAL:H	1.71	0.54
2:B:387:GLU:OE2	2:B:505:ARG:NH1	2.39	0.54
2:B:550:TRP:CE2	2:B:551:GLN:HG3	2.42	0.54
2:B:568:PRO:HA	2:B:607:MET:HB2	1.87	0.54
2:B:320:LEU:HD11	2:B:614:TYR:HE1	1.72	0.54
1:D:10:DG:H3'	2:A:421:ARG:CG	2.35	0.54
2:B:164:ASN:CB	2:B:165:PRO:HD2	2.38	0.54
1:C:16:DC:H1'	1:C:17:DT:O5'	2.07	0.54
2:B:1:MET:O	2:B:3:VAL:N	2.40	0.54
2:B:637:PRO:HA	5:B:1054:HOH:O	2.08	0.54
1:C:16:DC:H2''	1:C:17:DT:OP2	2.06	0.54
2:A:91:HIS:CE1	2:A:193:LEU:HD11	2.43	0.54
2:A:379:GLY:HA2	2:A:542:ALA:HB1	1.89	0.54
2:B:601:VAL:O	2:B:605:ARG:HD2	2.08	0.54
2:A:72:HIS:O	2:A:76:GLN:HG2	2.09	0.53
2:B:587:ASP:O	2:B:589:GLY:N	2.39	0.53
1:D:11:DC:H2''	1:D:12:DA:C5'	2.38	0.53
1:D:22:DG:H2''	1:D:23:DT:OP2	2.07	0.53
2:A:378:GLY:HA2	2:A:381:ARG:HH12	1.73	0.53
2:B:203:LYS:N	2:B:204:PRO:HD3	2.24	0.53
2:B:423:LEU:O	2:B:427:ARG:HG3	2.09	0.53
2:B:509:LEU:O	2:B:513:VAL:HG23	2.08	0.53
1:D:11:DC:H2''	1:D:12:DA:H5'	1.91	0.53
2:A:555:GLN:C	2:A:556:LEU:HD12	2.29	0.53
2:A:126:LEU:HD21	2:A:176:ALA:HB1	1.91	0.53
2:A:5:TYR:CD2	2:A:6:LEU:N	2.77	0.53
2:A:392:LEU:HD23	2:A:395:LEU:HD12	1.91	0.52
2:A:390:ASP:OD1	2:A:409:ARG:NE	2.42	0.52
2:A:207:LEU:HD21	2:A:211:ARG:HH21	1.74	0.52
2:A:407:PHE:CE1	2:A:461:PHE:HE2	2.27	0.52
2:A:56:SER:HA	2:A:213:ARG:O	2.10	0.52
2:B:207:LEU:HD22	2:B:235:LEU:HD21	1.91	0.52
2:B:288:ASN:HB2	2:B:314:ASP:O	2.09	0.52
2:B:450:LEU:CB	2:B:455:ALA:HB2	2.40	0.52
2:A:166:VAL:HG23	2:A:167:GLU:H	1.75	0.52
2:A:619:ARG:HA	2:A:623:LYS:O	2.09	0.52
2:B:493:MET:HG3	2:B:494:TYR:N	2.24	0.52
2:A:127:ILE:HD12	2:A:139:PRO:HG3	1.90	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:PHE:CE2	2:B:233:ILE:HD11	2.45	0.52
1:C:14:DT:H2"	1:C:15:DG:N7	2.25	0.52
2:B:619:ARG:HH12	2:B:624:GLU:HB3	1.75	0.52
2:A:401:ARG:NH1	2:A:465:ILE:HG22	2.24	0.51
2:A:592:LEU:HD11	2:A:631:ARG:NH1	2.24	0.51
2:B:411:VAL:HA	2:B:461:PHE:CZ	2.44	0.51
2:A:30:GLY:HA2	2:A:248:ASP:OD2	2.10	0.51
2:A:79:GLY:O	2:A:80:THR:C	2.49	0.51
2:B:382:PHE:HA	2:B:385:ARG:HH22	1.71	0.51
2:B:46:LEU:O	2:B:52:CYS:HB2	2.10	0.51
2:B:187:VAL:HG13	2:B:191:GLU:HB3	1.93	0.51
2:B:95:HIS:CE1	2:B:532:GLN:HG2	2.45	0.51
2:A:475:MET:HE2	2:A:479:VAL:CG1	2.38	0.51
2:A:110:ASP:O	2:A:111:PHE:C	2.48	0.51
2:B:16:GLU:O	2:B:20:ALA:HB2	2.10	0.51
2:A:114:LEU:HD13	2:A:186:LEU:HD13	1.93	0.51
2:A:226:ASN:HD22	2:A:226:ASN:C	2.13	0.51
2:A:179:GLU:O	2:A:183:ARG:HG3	2.11	0.51
2:A:318:ILE:HB	2:A:641:VAL:HG22	1.94	0.50
2:A:490:LEU:HD22	2:A:494:TYR:HE1	1.75	0.50
2:B:114:LEU:HD11	2:B:118:ASP:HB3	1.92	0.50
2:A:445:LEU:C	2:A:447:GLU:H	2.13	0.50
2:A:509:LEU:O	2:A:513:VAL:HG23	2.11	0.50
2:B:145:TYR:O	2:B:149:GLN:HG2	2.12	0.50
2:B:217:ILE:HB	2:B:243:VAL:HG22	1.92	0.50
2:B:408:GLU:HG2	2:B:437:LEU:CD1	2.42	0.50
2:B:529:MET:O	2:B:530:PRO:C	2.49	0.50
2:B:91:HIS:CE1	2:B:193:LEU:HD11	2.46	0.50
2:A:187:VAL:HG13	2:A:191:GLU:HB3	1.94	0.50
2:A:205:HIS:CE1	2:A:206:ILE:HG13	2.47	0.50
2:A:472:THR:HG22	2:A:483:ARG:HD2	1.94	0.50
1:D:12:DA:OP1	2:A:417:GLY:HA2	2.11	0.50
2:B:361:ARG:O	2:B:365:GLU:HG3	2.11	0.50
2:A:364:GLU:HG3	2:A:374:TYR:CZ	2.47	0.50
2:B:27:VAL:HB	2:B:246:VAL:HG12	1.94	0.50
2:B:385:ARG:HB3	2:B:387:GLU:OE1	2.12	0.50
2:B:82:GLN:O	2:B:83:GLY:C	2.50	0.50
2:A:61:THR:O	2:A:89:THR:HA	2.12	0.49
2:A:429:THR:HG22	2:A:440:ALA:HB1	1.93	0.49
2:A:458:LEU:HD12	2:A:458:LEU:O	2.12	0.49
2:B:530:PRO:O	2:B:531:LEU:O	2.30	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:226:ASN:ND2	2:A:229:GLN:HG3	2.23	0.49
2:A:480:GLN:O	2:A:484:VAL:HG23	2.12	0.49
2:B:569:GLN:NE2	2:B:609:LYS:HB3	2.27	0.49
2:B:47:MET:HE2	2:B:54:PRO:HG3	1.94	0.49
2:B:498:LYS:O	2:B:499:GLY:C	2.51	0.49
2:B:512:LEU:O	2:B:516:THR:HG23	2.12	0.49
2:A:23:SER:CA	2:A:242:LYS:HD2	2.36	0.49
2:B:170:TRP:HA	2:B:170:TRP:HE3	1.77	0.49
2:B:564:GLY:H	2:B:605:ARG:NH2	2.09	0.49
2:B:141:GLN:HG3	2:B:170:TRP:CZ2	2.48	0.49
2:B:187:VAL:HG13	2:B:191:GLU:CG	2.43	0.49
2:B:588:GLU:O	2:B:590:GLY:N	2.46	0.49
2:A:109:GLN:HG2	2:A:109:GLN:O	2.13	0.49
2:A:78:MET:O	2:A:79:GLY:O	2.31	0.49
2:B:155:ARG:N	2:B:158:HIS:HD2	1.99	0.49
2:B:289:ILE:HD13	2:B:606:ALA:HB3	1.95	0.49
2:B:438:TRP:CZ3	2:B:462:MET:HG2	2.48	0.48
2:A:191:GLU:OE2	2:A:195:ARG:HD3	2.13	0.48
2:A:303:ARG:CB	2:A:303:ARG:NH1	2.76	0.48
2:B:112:GLN:HB3	2:B:186:LEU:HD23	1.95	0.48
1:D:12:DA:H2''	1:D:13:DG:H8	1.77	0.48
2:A:55:TYR:HA	2:A:84:GLY:O	2.13	0.48
1:C:6:DC:H2''	1:C:7:DA:OP2	2.13	0.48
2:A:411:VAL:HG13	2:A:412:ASN:N	2.28	0.48
2:A:296:LEU:O	2:A:596:ARG:HD3	2.12	0.48
2:A:401:ARG:HH12	2:A:465:ILE:HG22	1.78	0.48
2:B:107:LEU:HB3	2:B:111:PHE:HD2	1.78	0.48
1:C:20:DT:HO3'	1:C:22:DG:H2'	1.77	0.48
2:A:389:LYS:HB3	2:A:409:ARG:CZ	2.44	0.48
2:A:2:ASP:O	2:A:3:VAL:C	2.51	0.48
2:A:150:LYS:NZ	2:A:178:GLN:HE22	2.12	0.48
2:B:348:ALA:HA	2:B:553:ALA:O	2.13	0.48
2:B:394:TYR:O	2:B:398:ILE:HG13	2.14	0.48
2:A:10:LEU:HD13	2:A:18:VAL:HG21	1.96	0.47
2:A:436:THR:HG23	2:A:439:GLN:OE1	2.14	0.47
1:D:15:DG:C2'	1:D:16:DC:C5'	2.76	0.47
2:A:378:GLY:CA	2:A:381:ARG:NH1	2.77	0.47
2:B:126:LEU:HD11	2:B:177:TYR:N	2.29	0.47
2:B:491:ARG:O	2:B:495:GLU:HG3	2.14	0.47
2:B:532:GLN:CD	2:B:536:SER:HB2	2.34	0.47
2:A:155:ARG:HB3	2:A:156:PRO:HD2	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:181:CYS:O	2:A:185:GLY:N	2.47	0.47
2:B:61:THR:O	2:B:89:THR:HA	2.14	0.47
2:A:10:LEU:CD1	2:A:18:VAL:HG21	2.45	0.47
2:A:407:PHE:O	2:A:411:VAL:HB	2.14	0.47
2:A:457:ALA:O	2:A:460:ARG:N	2.47	0.47
2:B:355:ARG:HD3	2:B:580:PHE:CD2	2.49	0.47
2:A:397:LEU:HD13	2:A:465:ILE:HD13	1.97	0.47
2:A:383:PHE:HA	2:A:388:ILE:CG2	2.45	0.47
2:A:102:HIS:HB2	2:A:107:LEU:O	2.15	0.47
2:A:200:TRP:HB3	2:A:207:LEU:HD13	1.97	0.47
2:B:95:HIS:CE1	2:B:113:ILE:HD11	2.50	0.47
2:A:126:LEU:O	2:A:130:MET:HG3	2.15	0.47
2:A:90:PHE:CZ	2:A:225:THR:HG22	2.50	0.46
2:A:399:VAL:O	2:A:400:ASN:HB2	2.16	0.46
2:A:159:ILE:O	2:A:160:GLN:CB	2.64	0.46
2:B:304:LEU:N	2:B:304:LEU:HD23	2.30	0.46
2:B:418:ILE:HD13	2:B:458:LEU:HD23	1.97	0.46
2:A:203:LYS:N	2:A:204:PRO:HD3	2.31	0.46
2:A:2:ASP:O	2:A:4:SER:N	2.48	0.46
2:B:104:ASP:HB3	2:B:203:LYS:HG3	1.96	0.46
2:B:254:TYR:HB3	2:B:257:ARG:HH21	1.79	0.46
2:A:438:TRP:HZ3	2:A:465:ILE:HD12	1.80	0.46
2:B:436:THR:OG1	2:B:439:GLN:HB2	2.15	0.46
2:A:420:ASP:HB3	2:A:421:ARG:HH21	1.81	0.46
2:A:191:GLU:O	2:A:195:ARG:HB2	2.16	0.46
2:A:549:THR:O	2:A:551:GLN:N	2.49	0.46
2:A:325:ASN:HA	2:A:617:THR:O	2.16	0.46
2:B:490:LEU:HA	2:B:493:MET:HG2	1.98	0.46
2:B:294:ASN:O	2:B:298:GLU:HB2	2.16	0.46
2:B:126:LEU:O	2:B:130:MET:HG3	2.16	0.45
2:B:530:PRO:O	2:B:531:LEU:C	2.54	0.45
2:A:202:ASN:O	2:A:203:LYS:HG2	2.16	0.45
2:A:397:LEU:HD21	2:A:407:PHE:N	2.31	0.45
2:A:618:ARG:O	2:A:625:VAL:HG22	2.16	0.45
1:D:26:DA:N7	2:A:380:MET:HG3	2.32	0.45
2:B:402:ASN:HB3	2:B:436:THR:HG21	1.96	0.45
2:B:389:LYS:HB3	2:B:409:ARG:NE	2.32	0.45
2:B:56:SER:HB2	2:B:215:THR:OG1	2.16	0.45
2:B:445:LEU:C	2:B:447:GLU:H	2.19	0.45
2:B:532:GLN:NE2	2:B:532:GLN:CA	2.75	0.45
2:B:532:GLN:C	2:B:532:GLN:HE21	2.20	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:DC:N4	1:D:10:DG:H1	2.11	0.45
2:B:209:HIS:O	2:B:212:GLU:HB2	2.16	0.45
2:B:418:ILE:CD1	2:B:458:LEU:HD23	2.47	0.45
2:A:217:ILE:HD11	2:A:236:LEU:HG	1.98	0.45
2:A:303:ARG:NH1	2:A:303:ARG:HB2	2.32	0.45
2:A:309:TRP:HZ3	2:A:311:ASP:OD2	1.99	0.45
2:B:95:HIS:HE1	2:B:532:GLN:HG2	1.80	0.45
2:A:496:GLN:O	2:A:498:LYS:N	2.49	0.45
2:A:375:ARG:HH12	2:A:544:GLU:HA	1.81	0.45
2:A:1:MET:O	2:A:3:VAL:N	2.50	0.45
2:A:356:SER:H	2:A:359:GLN:NE2	2.15	0.45
2:A:197:HIS:CD2	2:A:235:LEU:HD12	2.52	0.45
2:B:105:ALA:O	2:B:107:LEU:HG	2.17	0.45
2:B:121:ARG:CZ	2:B:409:ARG:HH22	2.30	0.45
2:B:181:CYS:O	2:B:185:GLY:N	2.49	0.45
1:D:8:DC:H2'	1:D:9:DT:H71	1.99	0.45
2:A:32:GLY:N	4:A:700:ANP:HNB1	2.04	0.44
2:B:374:TYR:HA	2:B:553:ALA:HB1	1.98	0.44
2:B:60:VAL:O	2:B:219:VAL:HA	2.17	0.44
2:A:281:GLN:HB2	2:A:309:TRP:CZ2	2.52	0.44
2:B:361:ARG:HH11	2:B:361:ARG:HG2	1.82	0.44
2:B:381:ARG:HA	2:B:384:GLU:CG	2.45	0.44
1:C:13:DG:H2''	1:C:14:DT:H5'	1.99	0.44
2:A:130:MET:HB2	2:A:132:LEU:HD12	1.99	0.44
2:A:39:LEU:C	2:A:39:LEU:HD23	2.37	0.44
2:B:477:LEU:HG	2:B:516:THR:HB	2.00	0.44
2:B:29:ALA:HB3	2:B:35:LYS:HD3	1.99	0.44
2:B:480:GLN:O	2:B:484:VAL:HG23	2.16	0.44
2:B:126:LEU:HD23	2:B:126:LEU:O	2.17	0.44
2:A:355:ARG:HD3	2:A:580:PHE:CD2	2.53	0.44
2:B:334:VAL:HG22	2:B:367:LEU:HD23	1.99	0.44
2:A:307:LYS:O	2:A:308:LEU:HB2	2.18	0.43
2:A:429:THR:CG2	2:A:440:ALA:HB1	2.48	0.43
2:B:217:ILE:HD11	2:B:236:LEU:HG	1.99	0.43
2:B:447:GLU:C	2:B:449:ALA:H	2.21	0.43
2:A:303:ARG:C	2:A:305:GLY:H	2.21	0.43
2:A:398:ILE:HG23	2:A:469:ALA:HA	2.00	0.43
2:B:203:LYS:O	2:B:206:ILE:N	2.47	0.43
2:B:325:ASN:HB2	2:B:326:GLU:OE1	2.18	0.43
2:A:207:LEU:HD21	2:A:211:ARG:NH2	2.33	0.43
2:A:123:LEU:O	2:A:127:ILE:HG13	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:150:LYS:NZ	2:A:188:ASP:OD2	2.52	0.43
2:B:29:ALA:CB	2:B:279:LEU:HB2	2.48	0.43
2:A:119:GLN:HG3	2:A:177:TYR:OH	2.18	0.43
2:A:491:ARG:O	2:A:495:GLU:HB2	2.18	0.43
2:B:142:ALA:HB2	2:B:170:TRP:CZ3	2.54	0.43
2:B:107:LEU:HD21	2:B:195:ARG:CZ	2.49	0.43
2:B:387:GLU:CD	2:B:387:GLU:H	2.17	0.43
2:B:325:ASN:HA	2:B:615:ALA:HB1	1.99	0.43
1:D:12:DA:H2"	1:D:13:DG:C8	2.53	0.43
2:B:113:ILE:HD12	2:B:532:GLN:OE1	2.17	0.43
2:B:25:LEU:HD12	2:B:275:GLU:O	2.19	0.43
2:A:13:LYS:NZ	5:A:1026:HOH:O	2.44	0.43
2:B:114:LEU:HD12	2:B:118:ASP:CB	2.48	0.43
2:B:129:ALA:C	2:B:131:ASN:N	2.71	0.43
2:A:157:HIS:CD2	2:A:157:HIS:N	2.85	0.43
2:A:303:ARG:HH11	2:A:303:ARG:CB	2.30	0.43
2:B:383:PHE:HA	2:B:388:ILE:HG21	2.00	0.43
2:B:157:HIS:O	2:B:159:ILE:N	2.52	0.43
1:D:16:DC:H2"	1:D:17:DT:C6	2.53	0.43
1:D:20:DT:C2	2:A:621:TYR:HD2	2.35	0.43
2:B:488:SER:OG	2:B:490:LEU:HG	2.19	0.43
2:B:532:GLN:O	2:B:533:ALA:C	2.57	0.43
2:A:475:MET:HE3	2:A:483:ARG:CZ	2.49	0.42
2:B:516:THR:HG22	2:B:534:PHE:CE2	2.54	0.42
2:A:145:TYR:CD2	2:A:170:TRP:HB3	2.54	0.42
2:A:654:VAL:HG13	2:A:654:VAL:O	2.18	0.42
2:B:111:PHE:C	2:B:111:PHE:CD1	2.92	0.42
2:B:203:LYS:N	2:B:204:PRO:CD	2.82	0.42
2:B:206:ILE:O	2:B:209:HIS:HB3	2.19	0.42
2:B:50:GLU:O	2:B:51:ASN:C	2.57	0.42
2:A:226:ASN:HA	2:A:259:ALA:HA	2.02	0.42
2:B:429:THR:HB	2:B:440:ALA:HB1	2.01	0.42
2:A:445:LEU:HD13	2:A:459:GLN:OE1	2.19	0.42
2:A:169:THR:O	2:A:172:LYS:N	2.51	0.42
2:A:174:TYR:C	2:A:174:TYR:CD1	2.93	0.42
2:A:273:GLY:O	2:A:274:ALA:C	2.57	0.42
2:A:284:ARG:HH22	4:A:700:ANP:HNB1	1.67	0.42
2:B:47:MET:O	2:B:51:ASN:HA	2.20	0.42
2:A:397:LEU:HD11	2:A:407:PHE:HA	2.01	0.42
2:A:647:ARG:NE	2:A:649:THR:O	2.51	0.42
1:C:13:DG:H5"	2:A:453:ARG:NH1	2.35	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:38:VAL:HG12	2:A:39:LEU:N	2.34	0.42
2:A:568:PRO:HA	2:A:607:MET:HB2	2.02	0.42
2:A:661:THR:HG23	2:A:661:THR:O	2.20	0.42
2:B:129:ALA:O	2:B:131:ASN:N	2.52	0.42
2:A:224:ASP:O	2:A:259:ALA:HB2	2.20	0.42
2:A:2:ASP:O	2:A:5:TYR:CD2	2.72	0.42
2:A:457:ALA:C	2:A:459:GLN:N	2.73	0.42
2:A:395:LEU:HD23	2:A:484:VAL:HG21	2.00	0.42
2:B:115:ASP:OD2	2:B:115:ASP:C	2.57	0.42
2:A:226:ASN:ND2	2:A:226:ASN:H	2.18	0.42
2:B:137:TRP:CZ3	2:B:169:THR:OG1	2.73	0.42
2:B:104:ASP:CB	2:B:203:LYS:HE3	2.48	0.42
2:B:70:MET:O	2:B:74:ILE:HG13	2.19	0.42
2:A:199:LEU:O	2:A:203:LYS:HB2	2.20	0.42
2:A:60:VAL:HG22	2:A:61:THR:N	2.34	0.42
2:A:242:LYS:HD3	2:A:242:LYS:HA	1.77	0.41
2:B:304:LEU:HD11	2:B:306:LYS:CE	2.50	0.41
2:B:253:ILE:HD12	2:B:560:HIS:CD2	2.55	0.41
2:B:575:MET:HG3	2:B:612:LEU:HB3	2.02	0.41
1:D:11:DC:H5"	2:A:417:GLY:O	2.19	0.41
2:A:331:ARG:HB3	2:A:331:ARG:HH21	1.84	0.41
2:A:82:GLN:O	2:A:83:GLY:O	2.38	0.41
2:B:260:GLN:HG3	2:B:260:GLN:H	1.55	0.41
2:B:296:LEU:O	2:B:596:ARG:HD3	2.19	0.41
2:B:514:THR:HG23	2:B:517:ARG:HH11	1.85	0.41
1:C:15:DG:H1	1:D:6:DC:N4	2.12	0.41
1:C:20:DT:H2"	1:C:22:DG:C2'	2.50	0.41
2:A:447:GLU:O	2:A:448:LYS:C	2.58	0.41
2:B:593:GLU:O	2:B:597:ARG:HG3	2.19	0.41
2:B:631:ARG:HG3	2:B:635:GLU:OE2	2.21	0.41
2:A:375:ARG:HD3	2:A:377:TYR:CZ	2.55	0.41
2:A:37:ARG:HD3	5:A:1005:HOH:O	2.19	0.41
2:A:130:MET:CG	2:A:431:ARG:NH2	2.81	0.41
2:B:138:PRO:HA	2:B:139:PRO:HD3	1.84	0.41
2:B:453:ARG:NH1	2:B:453:ARG:HG3	2.33	0.41
2:B:532:GLN:HA	2:B:532:GLN:NE2	2.31	0.41
2:B:550:TRP:CD2	2:B:551:GLN:HG3	2.55	0.41
2:A:60:VAL:O	2:A:219:VAL:HA	2.21	0.41
2:B:159:ILE:HB	2:B:171:GLN:CD	2.41	0.41
2:B:403:ASP:HB3	2:B:406:ALA:HB3	2.02	0.41
2:B:452:GLY:C	2:B:454:ALA:H	2.22	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:157:HIS:O	2:A:158:HIS:C	2.59	0.41
2:B:122:LEU:O	2:B:126:LEU:HB2	2.20	0.41
2:B:360:SER:HA	2:B:363:LEU:HD12	2.02	0.41
2:B:364:GLU:HG3	2:B:374:TYR:CZ	2.55	0.41
2:B:2:ASP:O	2:B:3:VAL:C	2.58	0.41
2:B:519:PHE:HZ	2:B:533:ALA:HB1	1.85	0.41
2:B:532:GLN:O	2:B:532:GLN:NE2	2.53	0.41
2:B:2:ASP:O	2:B:5:TYR:N	2.47	0.41
2:B:39:LEU:C	2:B:39:LEU:HD23	2.41	0.41
2:B:510:GLU:O	2:B:513:VAL:HB	2.21	0.41
2:B:114:LEU:HD13	2:B:186:LEU:HD13	2.03	0.41
2:B:2:ASP:O	2:B:4:SER:N	2.53	0.41
2:B:452:GLY:C	2:B:454:ALA:N	2.73	0.41
2:B:572:ILE:HB	2:B:612:LEU:HD23	2.03	0.41
2:B:68:ALA:HA	2:B:71:ARG:NH2	2.35	0.41
1:C:16:DC:H1'	1:C:17:DT:C5'	2.50	0.41
1:C:25:DT:H2'	1:C:25:DT:H6	1.51	0.41
2:A:19:ALA:HA	2:A:45:TRP:CE2	2.56	0.41
2:A:203:LYS:O	2:A:206:ILE:N	2.54	0.41
2:B:456:SER:O	2:B:460:ARG:CG	2.69	0.41
2:B:477:LEU:HD12	2:B:477:LEU:O	2.21	0.41
2:B:75:GLY:O	2:B:79:GLY:N	2.54	0.41
2:B:106:ASN:CG	2:B:106:ASN:O	2.59	0.41
2:B:98:LEU:HD21	2:B:196:ALA:HA	2.03	0.41
2:B:550:TRP:CZ2	2:B:551:GLN:HG3	2.56	0.41
2:A:426:VAL:HG11	2:A:441:CYS:SG	2.61	0.40
2:B:98:LEU:HD21	2:B:196:ALA:CA	2.51	0.40
2:B:78:MET:O	2:B:79:GLY:C	2.60	0.40
2:A:2:ASP:O	2:A:5:TYR:HD2	2.05	0.40
2:A:322:CYS:HB2	2:A:614:TYR:CZ	2.57	0.40
2:B:262:GLU:C	2:B:264:ILE:N	2.75	0.40
2:B:576:GLU:HG3	2:B:579:MET:CG	2.50	0.40
2:B:98:LEU:HD11	2:B:195:ARG:HB3	2.04	0.40
2:A:469:ALA:O	2:A:473:ALA:HB2	2.22	0.40
2:A:66:ALA:O	2:A:69:GLU:HB3	2.22	0.40
2:B:288:ASN:HA	2:B:288:ASN:HD22	1.63	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	638/680 (94%)	541 (85%)	72 (11%)	25 (4%)	3	4
2	B	618/680 (91%)	531 (86%)	59 (10%)	28 (4%)	3	3
All	All	1256/1360 (92%)	1072 (85%)	131 (10%)	53 (4%)	3	4

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2	ASP
2	A	81	SER
2	A	307	LYS
2	A	451	ALA
2	A	497	GLU
2	A	550	TRP
2	A	661	THR
2	B	2	ASP
2	B	307	LYS
2	B	418	ILE
2	B	529	MET
2	B	530	PRO
2	B	531	LEU
2	B	533	ALA
2	B	536	SER
2	B	589	GLY
2	A	3	VAL
2	A	79	GLY
2	A	83	GLY
2	A	400	ASN
2	A	475	MET
2	B	83	GLY
2	B	130	MET
2	B	158	HIS
2	B	165	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	304	LEU
2	B	312	GLY
2	B	379	GLY
2	B	451	ALA
2	B	477	LEU
2	A	80	THR
2	A	259	ALA
2	A	274	ALA
2	A	420	ASP
2	A	448	LYS
2	A	454	ALA
2	B	109	GLN
2	B	448	LYS
2	B	587	ASP
2	A	408	GLU
2	B	498	LYS
2	A	158	HIS
2	A	235	LEU
2	A	263	ASN
2	B	298	GLU
2	B	590	GLY
2	A	165	PRO
2	B	588	GLU
2	B	3	VAL
2	B	204	PRO
2	A	159	ILE
2	A	418	ILE
2	B	166	VAL

### 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	496/574 (86%)	472 (95%)	24 (5%)	30	55
2	B	493/574 (86%)	472 (96%)	21 (4%)	33	61
All	All	989/1148 (86%)	944 (95%)	45 (5%)	31	58

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	TYR
2	A	9	SER
2	A	23	SER
2	A	37	ARG
2	A	126	LEU
2	A	174	TYR
2	A	195	ARG
2	A	226	ASN
2	A	235	LEU
2	A	261	VAL
2	A	280	GLU
2	A	288	ASN
2	A	298	GLU
2	A	331	ARG
2	A	389	LYS
2	A	416	ARG
2	A	420	ASP
2	A	421	ARG
2	A	475	MET
2	A	492	THR
2	A	505	ARG
2	A	530	PRO
2	A	550	TRP
2	A	628	ARG
2	B	5	TYR
2	B	37	ARG
2	B	111	PHE
2	B	126	LEU
2	B	167	GLU
2	B	170	TRP
2	B	174	TYR
2	B	226	ASN
2	B	240	THR
2	B	260	GLN
2	B	280	GLU
2	B	288	ASN
2	B	298	GLU
2	B	304	LEU
2	B	308	LEU
2	B	478	HIS
2	B	493	MET
2	B	506	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	514	THR
2	B	532	GLN
2	B	605	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	119	GLN
2	A	136	GLN
2	A	147	ASN
2	A	157	HIS
2	A	178	GLN
2	A	197	HIS
2	A	205	HIS
2	A	226	ASN
2	A	227	ASN
2	A	288	ASN
2	A	359	GLN
2	A	508	ASN
2	B	119	GLN
2	B	147	ASN
2	B	158	HIS
2	B	178	GLN
2	B	226	ASN
2	B	260	GLN
2	B	288	ASN
2	B	359	GLN
2	B	508	ASN
2	B	518	GLN
2	B	560	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	ANP	A	700	3	29,33,33	4.32	12 (41%)	28,52,52	2.30	8 (28%)
4	ANP	B	701	3	29,33,33	4.34	13 (44%)	28,52,52	2.18	7 (25%)

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	ANP	A	700	3	-	0/13/38/38	0/3/3/3
4	ANP	B	701	3	-	0/13/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	ANP	C2'-C1'	-4.90	1.45	1.53
4	A	700	ANP	C2'-C1'	-4.80	1.46	1.53
4	B	701	ANP	PG-O3G	-4.45	1.44	1.56
4	A	700	ANP	PG-O3G	-3.79	1.46	1.56
4	A	700	ANP	PB-O2B	-3.60	1.46	1.56
4	B	701	ANP	PB-O2B	-3.48	1.47	1.56
4	A	700	ANP	C5-N7	-2.41	1.31	1.39
4	B	701	ANP	C5-N7	-2.34	1.31	1.39
4	B	701	ANP	PA-O2A	-2.11	1.44	1.55
4	A	700	ANP	PA-O2A	-2.10	1.44	1.55
4	B	701	ANP	O4'-C4'	-2.09	1.40	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	ANP	O3'-C3'	2.13	1.47	1.43
4	B	701	ANP	O4'-C1'	2.34	1.44	1.41
4	A	700	ANP	C2-N1	2.40	1.38	1.33
4	B	701	ANP	C2-N1	2.51	1.38	1.33
4	B	701	ANP	PB-N3B	2.71	1.70	1.63
4	A	700	ANP	O4'-C1'	2.86	1.45	1.41
4	B	701	ANP	C4-N3	3.72	1.41	1.35
4	A	700	ANP	C4-N3	3.80	1.41	1.35
4	B	701	ANP	C5-C4	4.00	1.49	1.40
4	A	700	ANP	C5-C4	4.09	1.49	1.40
4	A	700	ANP	C2-N3	4.17	1.39	1.32
4	B	701	ANP	C2-N3	4.79	1.40	1.32
4	B	701	ANP	PG-O1G	19.53	1.68	1.46
4	A	700	ANP	PG-O1G	19.66	1.68	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	ANP	N3-C2-N1	-8.32	121.61	128.86
4	B	701	ANP	N3-C2-N1	-8.03	121.86	128.86
4	A	700	ANP	C1'-N9-C4	-2.80	121.79	126.64
4	B	701	ANP	C1'-N9-C4	-2.61	122.13	126.64
4	A	700	ANP	O1B-PB-N3B	-2.56	107.96	111.79
4	B	701	ANP	O2G-PG-O1G	-2.39	107.33	113.41
4	A	700	ANP	O3'-C3'-C4'	-2.33	104.29	111.09
4	B	701	ANP	O3'-C3'-C4'	-2.29	104.41	111.09
4	B	701	ANP	C4-C5-N7	-2.09	107.39	109.41
4	A	700	ANP	O2G-PG-O1G	-2.07	108.14	113.41
4	A	700	ANP	C4-C5-N7	-2.06	107.42	109.41
4	B	701	ANP	O3G-PG-O2G	2.09	113.54	107.69
4	A	700	ANP	O3G-PG-O2G	2.33	114.22	107.69
4	B	701	ANP	O2B-PB-O1B	4.78	119.81	109.87
4	A	700	ANP	O2B-PB-O1B	4.97	120.20	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	ANP	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	ANP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	C	25/26 (96%)	0.12	0	100 100	51, 117, 165, 171	0
1	D	25/26 (96%)	0.12	0	100 100	59, 117, 150, 153	0
2	A	646/680 (95%)	0.17	35 (5%)	26 20	31, 73, 126, 140	1 (0%)
2	B	632/680 (92%)	0.13	24 (3%)	41 33	36, 68, 122, 179	1 (0%)
All	All	1328/1412 (94%)	0.15	59 (4%)	35 27	31, 72, 126, 179	2 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	658	ARG	16.0
2	B	657	GLN	9.7
2	A	499	GLY	6.2
2	B	519	PHE	5.1
2	A	137	TRP	4.7
2	B	132	LEU	4.1
2	A	464	LEU	3.9
2	A	468	LEU	3.8
2	A	1	MET	3.8
2	A	453	ARG	3.7
2	A	506	ILE	3.7
2	A	116	SER	3.3
2	B	81	SER	3.3
2	A	454	ALA	3.3
2	B	509	LEU	3.2
2	A	144	TRP	3.2
2	B	449	ALA	3.2
2	A	446	GLN	3.1
2	A	465	ILE	3.1
2	B	499	GLY	3.1
2	A	141	GLN	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	A	449	ALA	3.0
2	B	163	GLY	3.0
2	A	474	ASP	3.0
2	A	481	THR	2.9
2	B	458	LEU	2.7
2	A	472	THR	2.7
2	A	159	ILE	2.7
2	B	305	GLY	2.7
2	B	468	LEU	2.6
2	B	479	VAL	2.6
2	A	463	GLU	2.6
2	B	461	PHE	2.5
2	B	137	TRP	2.5
2	A	475	MET	2.4
2	A	470	GLN	2.4
2	B	444	LEU	2.4
2	A	425	VAL	2.4
2	A	485	ILE	2.4
2	A	445	LEU	2.3
2	B	381	ARG	2.3
2	B	538	ALA	2.3
2	A	80	THR	2.3
2	B	477	LEU	2.3
2	A	305	GLY	2.2
2	A	537	HIS	2.2
2	A	304	LEU	2.2
2	B	529	MET	2.2
2	B	481	THR	2.1
2	A	549	THR	2.1
2	B	133	ASP	2.1
2	B	533	ALA	2.1
2	A	483	ARG	2.1
2	A	444	LEU	2.1
2	A	450	LEU	2.1
2	A	654	VAL	2.0
2	A	459	GLN	2.0
2	A	384	GLU	2.0
2	B	495	GLU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ANP	A	700	31/31	0.97	0.18	1.12	43,48,56,58	0
4	ANP	B	701	31/31	0.97	0.19	0.35	45,52,58,61	0
3	MG	A	1001	1/1	0.99	0.16	-0.20	45,45,45,45	0
3	MG	B	1002	1/1	0.99	0.24	-	40,40,40,40	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.