



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:49 am GMT

PDB ID : 4C2T  
Title : Crystal structure of full length Deinococcus radiodurans UvrD in complex with DNA  
Authors : Stelter, M.; Acajjaoui, S.; McSweeney, S.; Timmins, J.  
Deposited on : 2013-08-20  
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 : trunk28620  
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) : recalc28949

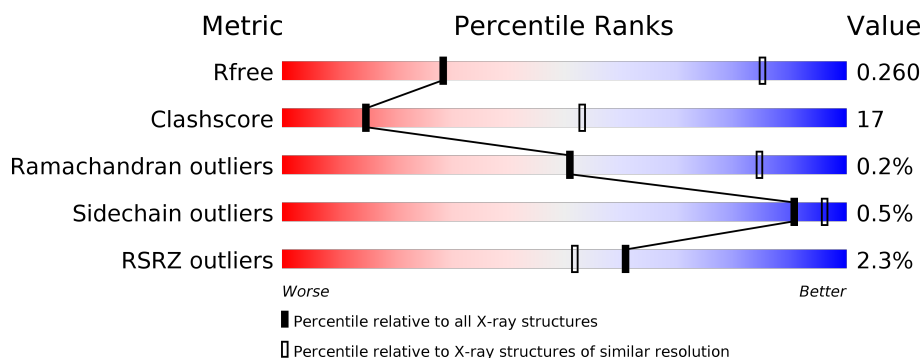
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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	A	745	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 62%, yellow 25%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>62%</span> <span>25%</span> <span>13%</span> </div> </div>
1	B	745	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 61%, yellow 26%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>61%</span> <span>26%</span> <span>13%</span> </div> </div>
1	C	745	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 63%, yellow 23%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>63%</span> <span>23%</span> <span>13%</span> </div> </div>
1	D	745	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 62%, yellow 24%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>62%</span> <span>24%</span> <span>13%</span> </div> </div>
2	M	28	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 18%, green 46%, yellow 25%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>18%</span> <span>46%</span> <span>25%</span> <span>11%</span> </div> </div>
2	P	28	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, green 64%, yellow 14%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>64%</span> <span>14%</span> <span>7%</span> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	N	28	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>7%11%61%18%11%</div></div>
3	O	28	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%21%46%25%7%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA HELICASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			5097	3190	923	969	15			
1	B	645	Total	C	N	O	S	0	0	0
			5057	3167	914	961	15			
1	C	651	Total	C	N	O	S	0	0	0
			5114	3200	923	976	15			
1	D	645	Total	C	N	O	S	0	0	0
			5069	3172	917	965	15			

- Molecule 2 is a DNA chain called DNA STRAND FOR28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	25	Total	C	N	O	P	0	0	0
			508	243	84	156	25			
2	P	26	Total	C	N	O	P	0	0	0
			530	253	89	162	26			

- Molecule 3 is a DNA chain called DNA STRAND REV28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	25	Total	C	N	O	P	0	0	0
			511	243	90	153	25			
3	O	26	Total	C	N	O	P	0	0	0
			531	253	92	160	26			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

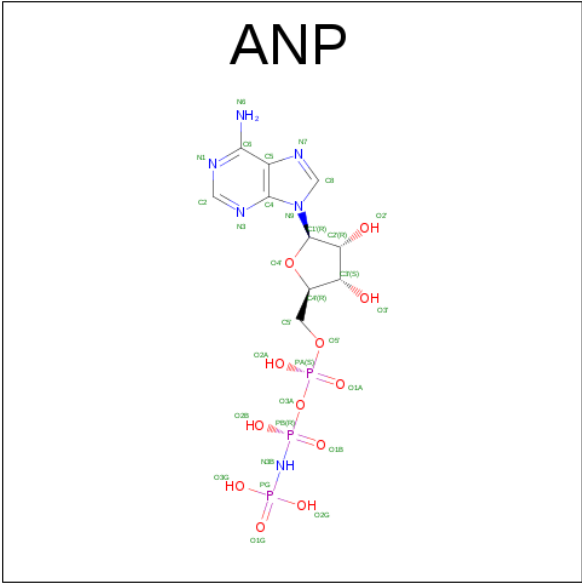
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 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>).

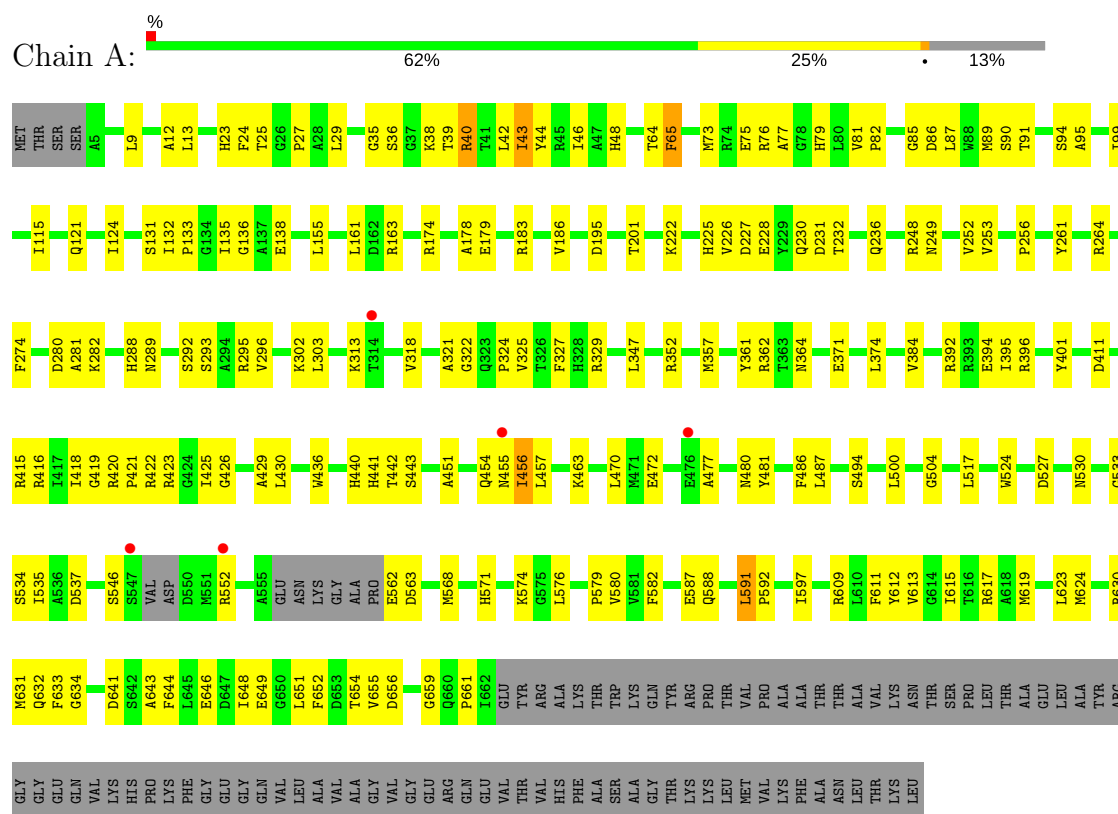


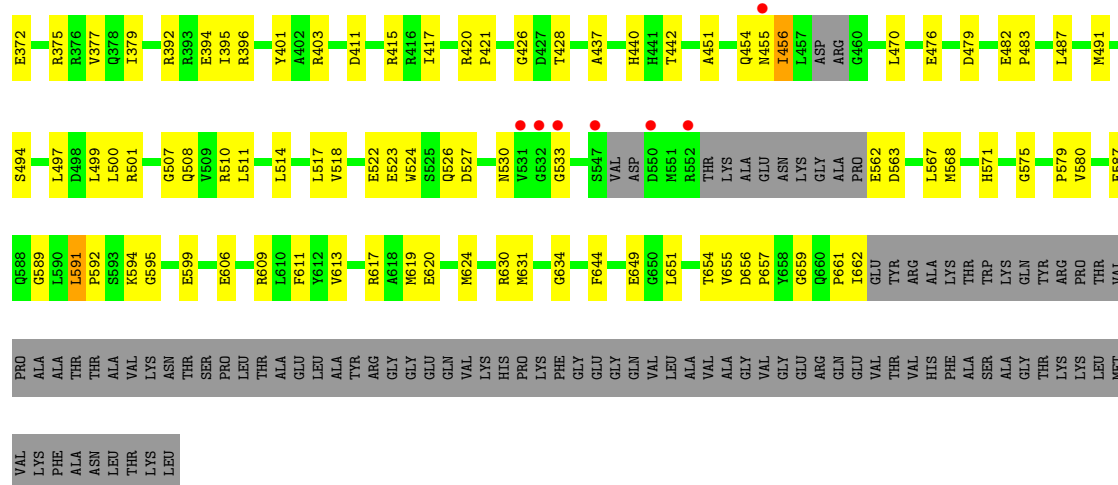
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

### 3 Residue-property plots [i](#)

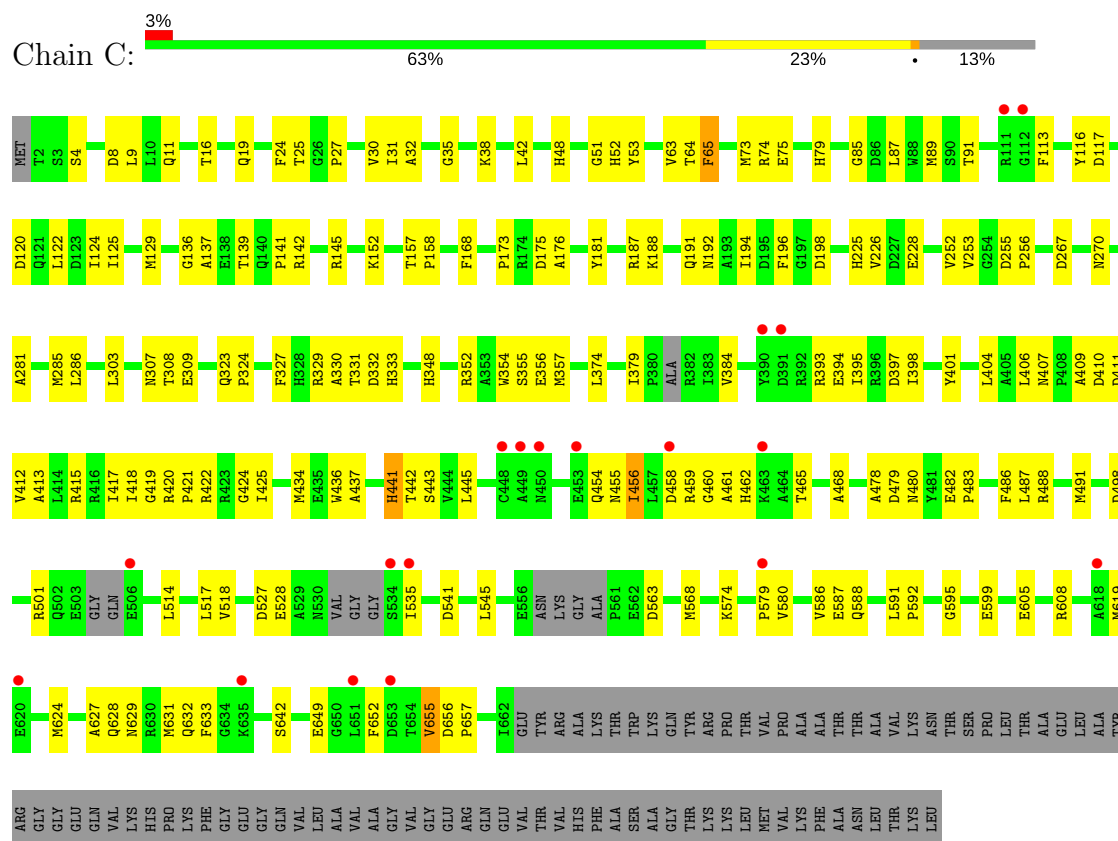
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: DNA HELICASE II

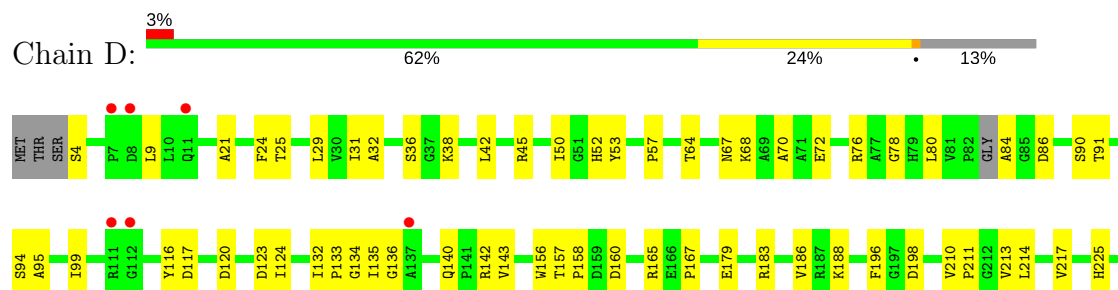


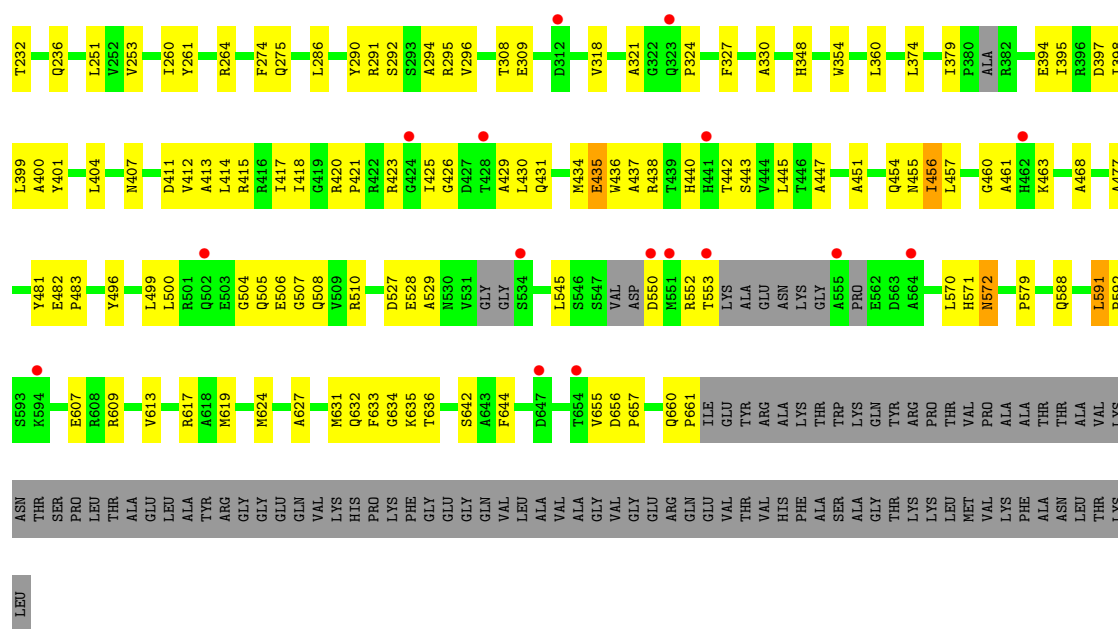


### • Molecule 1: DNA HELICASE II

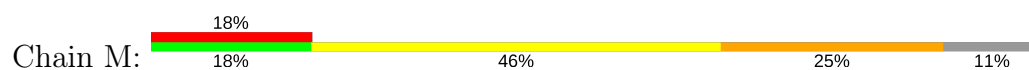


### • Molecule 1: DNA HELICASE II

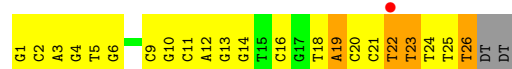
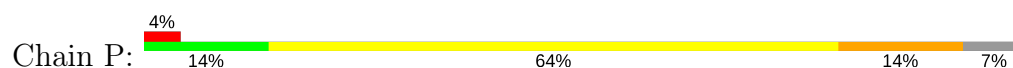




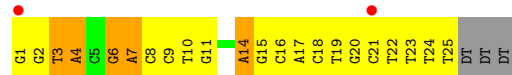
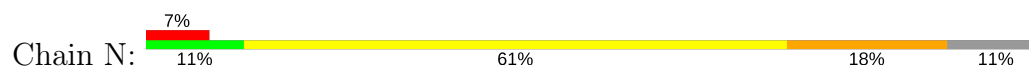
- Molecule 2: DNA STRAND FOR28



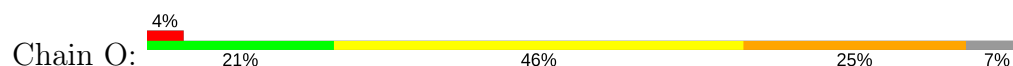
- Molecule 2: DNA STRAND FOR28



- Molecule 3: DNA STRAND REV28



- Molecule 3: DNA STRAND REV28





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.46Å 390.04Å 71.56Å 90.00° 106.13° 90.00°	Depositor
Resolution (Å)	46.15 – 4.00 46.11 – 3.99	Depositor EDS
% Data completeness (in resolution range)	94.5 (46.15-4.00) 99.3 (46.11-3.99)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 4.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.246 , 0.271 0.229 , 0.260	Depositor DCC
$R_{free}$ test set	1518 reflections (4.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	159.8	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 77.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.399 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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	A	0.27	1/5188 (0.0%)	0.55	5/7016 (0.1%)
1	B	0.27	0/5147	0.54	2/6960 (0.0%)
1	C	0.25	0/5204	0.52	0/7036
1	D	0.25	0/5156	0.52	0/6968
2	M	0.60	0/566	1.47	10/871 (1.1%)
2	P	0.53	0/591	1.45	8/910 (0.9%)
3	N	0.57	0/571	1.41	7/879 (0.8%)
3	O	0.55	0/593	1.52	14/913 (1.5%)
All	All	0.30	1/23016 (0.0%)	0.70	46/31553 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	ASP	C-N	-5.75	1.20	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	18	DT	O4'-C4'-C3'	-10.21	99.87	106.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	14	DA	C3'-C2'-C1'	-9.33	91.31	102.50
1	B	136	GLY	N-CA-C	-8.93	90.77	113.10
2	M	22	DT	O4'-C1'-N1	-8.89	101.78	108.00
3	O	4	DA	O4'-C1'-N9	8.65	114.05	108.00
2	P	22	DT	C1'-O4'-C4'	-8.24	101.86	110.10
2	M	2	DC	C1'-O4'-C4'	-8.16	101.94	110.10
3	O	4	DA	C3'-C2'-C1'	-7.56	93.43	102.50
3	O	4	DA	C1'-O4'-C4'	-7.40	102.70	110.10
3	O	11	DG	C3'-C2'-C1'	-7.37	93.66	102.50
2	P	22	DT	O4'-C4'-C3'	-7.32	101.57	104.50
3	O	17	DA	C3'-C2'-C1'	-7.05	94.03	102.50
2	P	26	DT	O4'-C1'-N1	7.05	112.94	108.00
2	P	19	DA	O4'-C1'-N9	6.72	112.70	108.00
3	O	10	DT	O4'-C4'-C3'	-6.57	101.87	104.50
3	N	3	DT	O4'-C1'-N1	6.53	112.57	108.00
3	N	14	DA	C1'-O4'-C4'	-6.31	103.79	110.10
1	A	43	ILE	CB-CA-C	-6.20	99.21	111.60
2	M	17	DG	C3'-C2'-C1'	-6.18	95.08	102.50
2	P	19	DA	C1'-O4'-C4'	-6.08	104.02	110.10
3	O	5	DC	O4'-C1'-N1	5.92	112.15	108.00
1	A	85	GLY	N-CA-C	5.91	127.87	113.10
2	M	22	DT	O4'-C4'-C3'	5.78	109.47	106.00
3	O	22	DT	O4'-C4'-C3'	-5.70	102.22	104.50
2	M	18	DT	C4'-C3'-C2'	-5.67	98.00	103.10
3	N	6	DG	O4'-C1'-N9	5.64	111.95	108.00
3	O	17	DA	O4'-C1'-N9	5.59	111.92	108.00
3	N	7	DA	C3'-C2'-C1'	-5.57	95.82	102.50
2	P	3	DA	C1'-O4'-C4'	-5.56	104.54	110.10
1	B	137	ALA	N-CA-C	-5.53	96.06	111.00
1	A	86	ASP	C-N-CA	5.51	135.47	121.70
3	N	3	DT	C1'-O4'-C4'	-5.46	104.64	110.10
2	P	19	DA	O4'-C1'-C2'	-5.40	101.58	105.90
2	M	3	DA	C1'-O4'-C4'	-5.38	104.72	110.10
3	O	5	DC	C1'-O4'-C4'	-5.28	104.82	110.10
3	O	17	DA	O4'-C1'-C2'	-5.21	101.73	105.90
3	O	11	DG	O4'-C1'-N9	5.20	111.64	108.00
1	A	87	LEU	N-CA-CB	5.15	120.70	110.40
2	M	21	DC	C1'-O4'-C4'	-5.12	104.98	110.10
3	N	4	DA	C1'-O4'-C4'	-5.12	104.98	110.10
3	O	17	DA	C1'-O4'-C4'	-5.11	104.99	110.10
3	O	8	DC	C1'-O4'-C4'	-5.10	105.00	110.10
1	A	87	LEU	N-CA-C	-5.09	97.27	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	DA	O4'-C1'-N9	5.03	111.52	108.00
2	P	23	DT	C1'-O4'-C4'	-5.03	105.08	110.10
2	M	15	DT	N3-C4-O4	5.00	122.90	119.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	591	LEU	Peptide
1	B	135	ILE	Peptide
1	B	591	LEU	Peptide
1	D	591	LEU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5097	0	5029	184	0
1	B	5057	0	4987	160	0
1	C	5114	0	5041	146	0
1	D	5069	0	4993	165	0
2	M	508	0	285	35	0
2	P	530	0	296	23	0
3	N	511	0	283	35	0
3	O	531	0	295	28	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	13	4	0
5	B	31	0	13	3	0
5	C	31	0	13	2	0
5	D	31	0	13	2	0
All	All	22545	0	21261	741	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 17.

All (741) 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:117:ASP:HA	1:D:196:PHE:CE2	1.25	1.59
1:D:117:ASP:CA	1:D:196:PHE:CE2	2.18	1.24
1:D:117:ASP:CA	1:D:196:PHE:HE2	1.49	1.23
1:D:117:ASP:HA	1:D:196:PHE:CZ	1.74	1.22
1:A:40:ARG:HG2	1:A:40:ARG:HH11	1.07	1.18
2:P:22:DT:H4'	2:P:23:DT:H5''	1.21	1.16
2:M:22:DT:H4'	2:M:23:DT:O5'	1.40	1.10
1:D:436:TRP:O	1:D:440:HIS:HB2	1.52	1.10
3:O:21:DC:H2''	3:O:22:DT:H5''	1.31	1.09
3:N:21:DC:H4'	3:N:22:DT:O5'	1.49	1.06
2:M:8:DT:H3	3:N:14:DA:N6	1.52	1.06
1:A:256:PRO:HD2	1:A:313:LYS:HZ1	1.25	1.02
1:A:43:ILE:HD11	1:A:76:ARG:HB3	1.40	1.02
1:A:395:ILE:HG23	1:A:517:LEU:HD12	1.39	1.01
1:B:291:ARG:HH22	5:B:1664:ANP:HNB1	1.02	1.00
1:B:656:ASP:HB3	1:B:662:ILE:HD11	1.42	1.00
1:A:75:GLU:HG3	1:A:79:HIS:HD2	1.26	0.98
3:O:21:DC:C2'	3:O:22:DT:H5''	1.94	0.98
1:D:505:GLN:HG3	1:D:506:GLU:H	1.30	0.97
1:A:480:ASN:O	1:A:481:TYR:CD1	2.17	0.97
1:A:13:LEU:HD23	1:A:40:ARG:HH12	1.32	0.94
1:B:291:ARG:NH2	5:B:1664:ANP:HNB1	1.64	0.94
2:M:8:DT:H3	3:N:14:DA:H61	1.00	0.93
3:O:22:DT:H4'	3:O:23:DT:OP2	1.65	0.93
2:P:22:DT:C4'	2:P:23:DT:H5''	1.97	0.93
1:B:43:ILE:HG21	1:B:76:ARG:HG3	1.50	0.92
1:A:591:LEU:HG	1:A:592:PRO:CD	2.00	0.92
1:B:43:ILE:HD13	1:B:76:ARG:HG2	1.50	0.91
1:D:423:ARG:H	1:D:425:ILE:HD11	1.33	0.91
2:M:21:DC:H3'	2:M:22:DT:H5''	1.53	0.90
1:A:256:PRO:HD2	1:A:313:LYS:NZ	1.86	0.89
1:B:500:LEU:HD22	1:B:511:LEU:HB3	1.53	0.88
1:D:418:ILE:HG13	1:D:425:ILE:HD12	1.53	0.87
1:D:67:ASN:ND2	1:D:91:THR:HG23	1.88	0.87
1:A:13:LEU:CD2	1:A:40:ARG:HH12	1.86	0.87
1:C:591:LEU:HB3	1:C:592:PRO:HD3	1.57	0.86
1:A:75:GLU:HG3	1:A:79:HIS:CD2	2.09	0.86
1:C:401:TYR:OH	1:C:421:PRO:HG3	1.77	0.84
1:A:40:ARG:NH1	1:A:40:ARG:HG2	1.86	0.84
1:C:168:PHE:HD1	1:C:173:PRO:HA	1.39	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:15:DG:H2''	3:N:16:DC:O5'	1.78	0.84
3:N:16:DC:H2''	3:N:17:DA:H5'	1.60	0.83
1:B:420:ARG:O	1:B:499:LEU:HD11	1.79	0.83
1:B:591:LEU:HG	1:B:592:PRO:CD	2.09	0.83
1:A:43:ILE:HD11	1:A:76:ARG:CB	2.07	0.83
2:M:15:DT:H3	3:N:7:DA:H61	1.24	0.82
1:C:454:GLN:HG3	1:C:455:ASN:H	1.42	0.82
1:C:482:GLU:HG2	1:C:483:PRO:HD2	1.61	0.82
1:A:480:ASN:O	1:A:481:TYR:HD1	1.61	0.81
1:A:43:ILE:CD1	1:A:76:ARG:HB3	2.10	0.81
1:B:188:LYS:HE2	1:B:194:ILE:HA	1.61	0.81
2:M:21:DC:C3'	2:M:22:DT:H5''	2.11	0.81
1:A:454:GLN:HG3	1:A:455:ASN:H	1.46	0.81
1:A:579:PRO:HA	1:A:619:MET:HB2	1.64	0.80
3:O:4:DA:H4'	3:O:5:DC:OP2	1.82	0.80
1:A:591:LEU:HG	1:A:592:PRO:HD3	1.61	0.80
1:B:426:GLY:HA3	3:N:11:DG:OP1	1.82	0.80
1:A:43:ILE:HG13	1:A:76:ARG:CZ	2.13	0.79
1:C:454:GLN:HG3	1:C:455:ASN:N	1.98	0.79
1:A:13:LEU:HD23	1:A:40:ARG:NH1	1.96	0.78
1:C:117:ASP:HA	1:C:196:PHE:CE2	2.18	0.78
1:D:655:VAL:HA	1:D:661:PRO:HA	1.66	0.77
1:B:579:PRO:HA	1:B:619:MET:HB2	1.67	0.77
1:D:291:ARG:NH2	5:D:1663:ANP:HNB1	1.82	0.77
1:B:591:LEU:HG	1:B:592:PRO:HD3	1.66	0.76
1:D:411:ASP:O	1:D:415:ARG:HG2	1.85	0.76
2:P:13:DG:H2''	2:P:14:DG:C8	2.20	0.76
1:D:454:GLN:HG3	1:D:455:ASN:H	1.51	0.75
1:B:500:LEU:HD21	1:B:507:GLY:O	1.86	0.75
1:B:392:ARG:HB3	1:B:394:GLU:OE1	1.86	0.75
1:D:436:TRP:HE3	1:D:447:ALA:HB1	1.50	0.75
1:D:117:ASP:C	1:D:196:PHE:HE2	1.89	0.75
2:M:21:DC:H3'	2:M:22:DT:C5'	2.16	0.75
1:A:43:ILE:HG13	1:A:76:ARG:NH1	2.02	0.74
1:C:422:ARG:HD3	3:O:13:DG:O5'	1.88	0.74
1:D:631:MET:HE3	1:D:634:GLY:HA2	1.69	0.74
2:M:2:DC:H2''	2:M:3:DA:C8	2.23	0.74
1:A:13:LEU:CD2	1:A:40:ARG:NH1	2.51	0.74
3:O:11:DG:OP2	3:O:11:DG:H2'	1.88	0.74
2:P:9:DC:H2''	2:P:10:DG:C8	2.23	0.74
1:B:523:GLU:O	1:B:527:ASP:HB2	1.87	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:TYR:HE2	1:A:364:ASN:HA	1.51	0.73
1:A:392:ARG:HB3	1:A:394:GLU:OE1	1.89	0.73
1:A:40:ARG:HA	1:A:76:ARG:NH2	2.03	0.73
1:B:65:PHE:CZ	1:B:264:ARG:NH1	2.55	0.73
2:M:21:DC:N3	3:N:1:DG:N2	2.35	0.73
1:B:65:PHE:HZ	1:B:264:ARG:NH1	1.87	0.73
1:B:500:LEU:CD2	1:B:511:LEU:HB3	2.18	0.73
1:B:295:ARG:HG2	1:B:321:ALA:HB1	1.71	0.73
1:A:357:MET:HG2	1:A:580:VAL:HB	1.70	0.73
1:B:119:ASP:HB3	1:B:396:ARG:NH2	2.05	0.72
3:N:1:DG:H2''	3:N:2:DG:C8	2.25	0.72
1:B:426:GLY:HA3	3:N:11:DG:P	2.29	0.72
1:B:65:PHE:HZ	1:B:264:ARG:HH12	1.37	0.72
1:B:161:LEU:HD23	1:B:178:ALA:HA	1.71	0.72
1:B:179:GLU:HG3	1:B:183:ARG:HD2	1.73	0.71
1:A:292:SER:HB3	1:A:296:VAL:CG2	2.21	0.71
3:N:20:DG:H1'	3:N:21:DC:OP1	1.90	0.71
1:A:65:PHE:O	1:A:65:PHE:HD1	1.74	0.71
3:N:7:DA:H2''	3:N:8:DC:OP2	1.91	0.70
1:A:426:GLY:HA3	1:A:429:ALA:HB3	1.71	0.70
3:O:21:DC:H2''	3:O:22:DT:C5'	2.18	0.70
1:A:131:SER:HB3	1:A:183:ARG:HH21	1.57	0.70
1:A:361:TYR:CE2	1:A:364:ASN:HA	2.27	0.69
1:B:411:ASP:O	1:B:415:ARG:HG2	1.92	0.69
1:C:9:LEU:HD11	1:C:48:HIS:CE1	2.27	0.69
1:B:38:LYS:HB3	1:B:253:VAL:HG11	1.74	0.69
3:N:17:DA:H2''	3:N:18:DC:OP2	1.93	0.69
1:D:504:GLY:O	1:D:508:GLN:HB2	1.92	0.69
1:A:362:ARG:NH2	2:M:23:DT:O2	2.26	0.69
1:D:456:ILE:HG23	1:D:456:ILE:O	1.92	0.69
1:A:35:GLY:H	5:A:1664:ANP:HNB1	1.39	0.69
1:B:487:LEU:O	1:B:491:MET:HG3	1.93	0.68
1:A:38:LYS:HB3	1:A:253:VAL:CG1	2.24	0.68
1:A:500:LEU:O	1:A:504:GLY:HA2	1.94	0.68
1:B:562:GLU:HG2	1:B:563:ASP:H	1.58	0.68
1:B:142:ARG:HH21	3:N:20:DG:H5''	1.58	0.68
1:C:442:THR:HG22	1:C:443:SER:O	1.93	0.68
1:D:426:GLY:HA3	1:D:429:ALA:HB3	1.76	0.67
1:D:454:GLN:HG3	1:D:455:ASN:N	2.08	0.67
1:C:35:GLY:H	5:C:1664:ANP:HNB1	1.42	0.67
1:B:222:LYS:O	1:B:249:ASN:HB2	1.93	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ALA:HA	1:B:442:THR:HG22	1.76	0.67
3:O:21:DC:H2''	3:O:22:DT:OP1	1.93	0.67
1:D:421:PRO:HB2	1:D:423:ARG:HH12	1.59	0.67
1:D:400:ALA:HB1	1:D:413:ALA:HB1	1.76	0.67
1:A:451:ALA:O	1:A:456:ILE:HA	1.94	0.67
1:D:588:GLN:HG2	1:D:642:SER:HA	1.75	0.67
1:D:499:LEU:HD12	1:D:500:LEU:N	2.10	0.66
1:D:360:LEU:HB3	1:D:570:LEU:HD23	1.77	0.66
1:D:117:ASP:CA	1:D:196:PHE:CZ	2.60	0.66
1:D:132:ILE:HG22	1:D:134:GLY:H	1.60	0.66
1:D:457:LEU:O	1:D:461:ALA:HB2	1.94	0.66
1:D:140:GLN:HB2	1:D:143:VAL:HG23	1.78	0.66
1:A:648:ILE:HA	1:A:651:LEU:HD12	1.76	0.66
1:B:357:MET:HG2	1:B:580:VAL:HB	1.78	0.66
1:C:142:ARG:HG3	1:C:145:ARG:HH21	1.61	0.66
2:M:15:DT:H2''	2:M:16:DC:O5'	1.96	0.66
1:A:43:ILE:CG1	1:A:76:ARG:HB3	2.26	0.66
1:D:117:ASP:HA	1:D:196:PHE:HE2	0.85	0.66
1:D:434:MET:O	1:D:437:ALA:N	2.28	0.66
1:C:329:ARG:HD3	1:C:628:GLN:HE21	1.61	0.65
1:A:40:ARG:HH11	1:A:40:ARG:CG	1.93	0.65
1:C:394:GLU:O	1:C:398:ILE:HG12	1.96	0.65
1:D:431:GLN:HA	1:D:434:MET:HB2	1.77	0.65
1:D:120:ASP:HA	1:D:412:VAL:HG11	1.78	0.65
1:A:232:THR:HA	1:A:236:GLN:NE2	2.12	0.65
1:D:609:ARG:O	1:D:613:VAL:HG23	1.97	0.65
1:C:632:GLN:HB3	1:C:633:PHE:CE1	2.32	0.65
1:D:505:GLN:HG3	1:D:506:GLU:N	2.08	0.64
1:A:454:GLN:HG3	1:A:455:ASN:N	2.10	0.64
1:A:477:ALA:O	1:A:481:TYR:HB2	1.97	0.64
1:D:445:LEU:HD11	1:D:468:ALA:HA	1.80	0.64
1:B:43:ILE:HG21	1:B:76:ARG:CG	2.26	0.64
1:D:291:ARG:HH22	5:D:1663:ANP:HNB1	1.44	0.64
2:M:23:DT:H2'	2:M:24:DT:O4'	1.97	0.64
1:A:64:THR:HG22	1:A:227:ASP:HB3	1.80	0.64
1:B:451:ALA:O	1:B:456:ILE:HA	1.97	0.64
1:D:38:LYS:HB3	1:D:253:VAL:CG1	2.28	0.63
3:N:8:DC:H2''	3:N:9:DC:O5'	1.97	0.63
1:B:42:LEU:HD11	1:B:225:HIS:HB3	1.79	0.63
1:B:655:VAL:CG1	1:B:659:GLY:HA2	2.29	0.63
1:D:327:PHE:HA	1:D:624:MET:O	1.98	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:THR:HG22	1:C:628:GLN:OE1	1.99	0.63
1:D:477:ALA:O	1:D:481:TYR:HB2	1.98	0.63
1:A:395:ILE:HG23	1:A:517:LEU:CD1	2.22	0.63
1:C:393:ARG:HH21	1:C:420:ARG:NH1	1.97	0.63
1:C:588:GLN:HG2	1:C:642:SER:HA	1.81	0.62
1:C:157:THR:HB	1:C:158:PRO:HD2	1.81	0.62
1:C:456:ILE:O	1:C:456:ILE:HG23	1.99	0.62
1:B:118:ASP:O	1:B:121:GLN:HG2	1.98	0.62
1:D:426:GLY:O	1:D:430:LEU:HB2	2.00	0.62
1:B:491:MET:HE1	1:B:514:LEU:HB3	1.80	0.62
1:D:188:LYS:HB3	1:D:188:LYS:NZ	2.15	0.62
2:M:2:DC:H2"	2:M:3:DA:H8	1.63	0.62
1:A:24:PHE:CD2	1:A:25:THR:HG23	2.35	0.62
1:C:437:ALA:O	1:C:441:HIS:N	2.33	0.62
1:C:168:PHE:CD1	1:C:173:PRO:HA	2.29	0.62
1:D:571:HIS:ND1	2:P:24:DT:H2"	2.15	0.62
1:B:327:PHE:HA	1:B:624:MET:O	2.00	0.62
1:B:64:THR:HG22	1:B:227:ASP:HB3	1.81	0.62
1:B:326:THR:HB	1:B:655:VAL:HG21	1.81	0.62
1:D:397:ASP:OD2	1:D:420:ARG:HG3	2.00	0.62
1:D:401:TYR:OH	1:D:421:PRO:HG2	2.00	0.62
1:C:482:GLU:CG	1:C:483:PRO:HD2	2.28	0.61
1:D:579:PRO:HA	1:D:619:MET:HB2	1.82	0.61
1:D:67:ASN:HD21	1:D:91:THR:H	1.48	0.61
1:A:524:TRP:O	1:A:527:ASP:HB3	2.00	0.61
1:B:524:TRP:O	1:B:530:ASN:ND2	2.28	0.61
1:C:38:LYS:HB3	1:C:253:VAL:CG1	2.29	0.61
1:C:355:SER:HB3	1:C:563:ASP:HA	1.82	0.61
1:A:420:ARG:HB2	1:A:421:PRO:HD3	1.81	0.61
1:A:411:ASP:O	1:A:415:ARG:HG2	2.00	0.61
1:A:155:LEU:HD12	1:A:201:THR:HG22	1.82	0.60
1:D:435:GLU:HA	1:D:438:ARG:HB3	1.81	0.60
1:C:579:PRO:HA	1:C:619:MET:HB2	1.83	0.60
1:A:609:ARG:O	1:A:613:VAL:HG23	2.02	0.60
1:C:188:LYS:HE3	1:C:198:ASP:OD2	2.01	0.60
2:M:20:DC:H2"	2:M:21:DC:OP2	2.01	0.60
1:B:40:ARG:HD3	5:B:1664:ANP:C8	2.32	0.60
1:C:401:TYR:OH	1:C:421:PRO:CG	2.49	0.59
1:A:24:PHE:HD2	1:A:25:THR:HG23	1.67	0.59
1:B:132:ILE:HD11	1:B:183:ARG:HD3	1.83	0.59
1:B:656:ASP:HB3	1:B:662:ILE:CD1	2.24	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:PRO:HB2	1:D:86:ASP:HB2	1.84	0.59
1:B:78:GLY:HA2	1:B:81:VAL:O	2.02	0.59
1:C:527:ASP:OD1	1:C:528:GLU:N	2.36	0.59
1:B:113:PHE:HA	1:B:192:ASN:O	2.03	0.59
1:B:591:LEU:HD11	1:B:611:PHE:HB2	1.84	0.59
2:M:4:DG:H2''	2:M:5:DT:OP2	2.02	0.59
1:A:327:PHE:HA	1:A:624:MET:O	2.03	0.59
1:C:267:ASP:HB3	1:C:270:ASN:OD1	2.03	0.59
1:C:42:LEU:HD11	1:C:225:HIS:HB3	1.85	0.59
1:C:331:THR:O	1:C:629:ASN:N	2.36	0.59
1:A:401:TYR:OH	1:A:421:PRO:HG2	2.03	0.59
1:B:401:TYR:CZ	1:B:417:ILE:HB	2.37	0.59
1:C:437:ALA:HA	1:C:442:THR:HB	1.83	0.59
3:O:22:DT:C4'	3:O:23:DT:OP2	2.44	0.59
1:C:16:THR:HA	1:C:19:GLN:NE2	2.17	0.58
1:C:384:VAL:HB	1:C:568:MET:HB3	1.85	0.58
1:D:420:ARG:CB	1:D:421:PRO:HD3	2.34	0.58
1:D:655:VAL:HA	1:D:661:PRO:CA	2.33	0.58
1:A:440:HIS:O	1:A:441:HIS:CG	2.56	0.58
1:B:38:LYS:HB3	1:B:253:VAL:CG1	2.32	0.58
1:A:395:ILE:HD12	1:A:517:LEU:HB2	1.84	0.58
1:B:591:LEU:O	1:B:592:PRO:O	2.21	0.58
1:C:136:GLY:HA3	1:C:139:THR:OG1	2.04	0.58
1:D:423:ARG:H	1:D:425:ILE:CD1	2.12	0.58
1:D:656:ASP:HB3	1:D:660:GLN:O	2.03	0.58
1:B:125:ILE:O	1:B:129:MET:HG3	2.04	0.58
1:A:132:ILE:HG23	1:A:133:PRO:HD2	1.84	0.58
1:B:440:HIS:HB3	1:B:442:THR:HB	1.86	0.58
1:C:157:THR:HB	1:C:158:PRO:CD	2.34	0.58
1:D:633:PHE:O	3:O:1:DG:C5	2.57	0.58
1:D:656:ASP:HB2	1:D:657:PRO:CD	2.34	0.58
1:A:38:LYS:HB3	1:A:253:VAL:HG11	1.86	0.57
1:B:126:LYS:HA	1:B:129:MET:HE2	1.86	0.57
1:C:413:ALA:O	1:C:417:ILE:HG13	2.04	0.57
1:C:327:PHE:HA	1:C:624:MET:O	2.03	0.57
1:D:436:TRP:CE3	1:D:447:ALA:HB1	2.37	0.57
1:C:422:ARG:HD3	3:O:13:DG:P	2.44	0.57
1:D:308:THR:O	1:D:309:GLU:HB2	2.04	0.57
1:A:231:ASP:OD2	1:A:261:TYR:HD2	1.88	0.57
1:D:64:THR:O	1:D:91:THR:HA	2.05	0.57
1:B:114:VAL:HG22	1:B:115:ILE:N	2.18	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:ILE:N	1:D:425:ILE:HD13	2.20	0.57
1:D:592:PRO:HD3	1:D:644:PHE:CE2	2.40	0.57
1:C:136:GLY:O	1:C:139:THR:N	2.38	0.56
1:D:50:ILE:HD13	1:D:57:PRO:HG3	1.87	0.56
1:B:352:ARG:NH2	1:B:620:GLU:HG3	2.20	0.56
1:D:656:ASP:N	1:D:660:GLN:O	2.38	0.56
1:A:43:ILE:CG1	1:A:76:ARG:CZ	2.83	0.56
3:N:3:DT:H2"	3:N:4:DA:C8	2.40	0.56
1:C:425:ILE:O	1:C:425:ILE:HD12	2.05	0.56
2:M:8:DT:H2"	2:M:9:DC:C5	2.41	0.56
1:C:395:ILE:HG12	1:C:517:LEU:HD12	1.86	0.56
1:D:135:ILE:HG23	1:D:136:GLY:H	1.71	0.56
1:A:23:HIS:ND1	1:A:282:LYS:HD3	2.21	0.56
1:A:40:ARG:HD3	5:A:1664:ANP:C8	2.36	0.56
1:D:527:ASP:CG	1:D:528:GLU:H	2.09	0.56
1:A:591:LEU:O	1:A:592:PRO:O	2.24	0.56
1:B:155:LEU:HD12	1:B:201:THR:HG22	1.87	0.56
1:C:38:LYS:HB3	1:C:253:VAL:HG11	1.86	0.56
1:D:421:PRO:HB2	1:D:423:ARG:NH1	2.21	0.56
1:B:592:PRO:HD3	1:B:644:PHE:CE2	2.41	0.56
1:C:591:LEU:HB3	1:C:592:PRO:CD	2.35	0.56
1:C:16:THR:HA	1:C:19:GLN:HE21	1.72	0.55
1:C:73:MET:HB3	1:C:89:MET:HE1	1.88	0.55
1:D:394:GLU:O	1:D:398:ILE:HG12	2.06	0.55
2:M:9:DC:H2"	2:M:10:DG:C8	2.41	0.55
3:O:7:DA:H2"	3:O:8:DC:C6	2.41	0.55
1:B:591:LEU:HD21	1:B:644:PHE:HD2	1.71	0.55
1:C:24:PHE:CE1	1:C:53:TYR:HB3	2.42	0.55
1:A:174:ARG:NH2	1:C:281:ALA:O	2.30	0.55
1:A:121:GLN:HA	1:A:124:ILE:HD12	1.88	0.55
1:C:445:LEU:HD11	1:C:468:ALA:HA	1.88	0.55
1:D:295:ARG:HD2	1:D:324:PRO:HA	1.89	0.55
1:A:39:THR:O	1:A:76:ARG:NH1	2.39	0.55
1:D:116:TYR:O	1:D:196:PHE:CE2	2.60	0.55
1:D:591:LEU:O	1:D:592:PRO:O	2.25	0.55
1:A:611:PHE:CE2	1:A:615:ILE:HD11	2.41	0.55
1:D:36:SER:O	1:D:286:LEU:HD23	2.06	0.55
1:C:418:ILE:HG13	1:C:425:ILE:HG21	1.89	0.55
1:A:418:ILE:HG12	1:A:425:ILE:HG21	1.89	0.55
1:A:436:TRP:O	1:A:440:HIS:HB2	2.07	0.55
1:D:38:LYS:HB3	1:D:253:VAL:HG11	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:LEU:HB3	1:D:552:ARG:HG3	1.89	0.55
1:A:222:LYS:O	1:A:249:ASN:HB2	2.07	0.54
1:B:132:ILE:HD11	1:B:180:ALA:HA	1.88	0.54
1:D:442:THR:HG22	1:D:443:SER:O	2.07	0.54
1:D:656:ASP:HB2	1:D:657:PRO:HD2	1.90	0.54
3:O:2:DG:H2''	3:O:3:DT:OP2	2.07	0.54
1:A:44:TYR:O	1:A:48:HIS:HB2	2.08	0.54
1:A:486:PHE:HD2	1:A:535:ILE:HD13	1.71	0.54
1:B:132:ILE:HG23	1:B:133:PRO:HD2	1.90	0.54
1:B:401:TYR:OH	1:B:421:PRO:HG2	2.07	0.54
3:O:20:DG:H1	2:P:2:DC:H42	1.56	0.54
1:A:40:ARG:NH1	1:A:40:ARG:CG	2.58	0.54
1:A:12:ALA:O	1:A:40:ARG:NH2	2.39	0.54
1:D:434:MET:O	1:D:438:ARG:N	2.38	0.54
3:N:9:DC:H2'	3:N:10:DT:H72	1.89	0.54
1:A:179:GLU:HA	1:A:179:GLU:OE1	2.08	0.54
1:B:122:LEU:HD12	1:B:141:PRO:HB2	1.89	0.54
1:B:497:LEU:HD23	1:B:501:ARG:HD2	1.89	0.54
1:A:77:ALA:O	1:A:81:VAL:HG12	2.08	0.54
1:B:107:ILE:HB	1:B:205:ARG:HH12	1.73	0.54
1:A:292:SER:HB3	1:A:296:VAL:HG21	1.89	0.54
1:C:333:HIS:CE1	1:C:631:MET:HG2	2.43	0.54
3:O:10:DT:C6	3:O:10:DT:H5'	2.42	0.54
1:A:295:ARG:HG2	1:A:321:ALA:HB1	1.90	0.54
1:D:260:ILE:HD12	1:D:571:HIS:HD2	1.72	0.53
1:D:423:ARG:N	1:D:425:ILE:HD11	2.14	0.53
1:A:592:PRO:HD3	1:A:644:PHE:CE2	2.43	0.53
1:B:655:VAL:HG12	1:B:656:ASP:O	2.08	0.53
1:C:649:GLU:HA	1:C:652:PHE:CE1	2.43	0.53
1:C:87:LEU:CD1	1:C:89:MET:HG3	2.38	0.53
2:P:12:DA:H2''	2:P:13:DG:C8	2.44	0.53
1:C:75:GLU:HG3	1:C:79:HIS:CE1	2.43	0.53
1:C:188:LYS:NZ	1:C:188:LYS:HB3	2.23	0.53
1:C:404:LEU:HA	1:C:407:ASN:O	2.08	0.53
1:A:648:ILE:CA	1:A:651:LEU:HD12	2.38	0.53
1:B:114:VAL:CG2	1:B:403:ARG:HD2	2.38	0.53
1:B:366:GLN:O	1:B:370:ILE:HG12	2.08	0.53
1:C:4:SER:HB3	1:C:51:GLY:O	2.09	0.53
1:D:354:TRP:CZ3	1:D:379:ILE:HG23	2.44	0.53
1:D:420:ARG:HB2	1:D:421:PRO:HD3	1.91	0.53
1:A:456:ILE:O	1:A:456:ILE:HG23	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD11	1:A:48:HIS:CE1	2.44	0.53
2:P:4:DG:H2''	2:P:5:DT:OP2	2.08	0.53
1:B:179:GLU:HA	1:B:179:GLU:OE1	2.08	0.53
1:B:232:THR:HA	1:B:236:GLN:NE2	2.24	0.53
1:C:142:ARG:HG3	1:C:145:ARG:NH2	2.24	0.53
2:M:15:DT:H3	3:N:7:DA:N6	2.00	0.53
1:B:609:ARG:O	1:B:613:VAL:HG23	2.09	0.53
1:B:302:LYS:HG2	1:B:651:LEU:HD11	1.91	0.53
1:C:116:TYR:OH	1:C:191:GLN:HG2	2.09	0.53
1:D:290:TYR:HA	1:D:318:VAL:CG2	2.39	0.53
1:D:454:GLN:CG	1:D:455:ASN:H	2.15	0.53
2:P:22:DT:H4'	2:P:23:DT:C5'	2.14	0.52
1:D:68:LYS:HE2	1:D:550:ASP:N	2.24	0.52
2:M:2:DC:H1'	2:M:3:DA:OP2	2.09	0.52
1:B:656:ASP:HB2	1:B:657:PRO:CD	2.39	0.52
1:D:90:SER:HB2	1:D:94:SER:HB2	1.92	0.52
2:P:5:DT:H2''	2:P:6:DG:C8	2.45	0.52
2:P:1:DG:H2''	2:P:2:DC:OP2	2.09	0.52
1:D:232:THR:HA	1:D:236:GLN:NE2	2.25	0.52
3:O:1:DG:H22	2:P:21:DC:H42	1.56	0.52
1:D:132:ILE:HG23	1:D:133:PRO:HD2	1.92	0.52
1:D:64:THR:HG21	1:D:70:ALA:HB2	1.92	0.52
1:D:142:ARG:HH21	2:P:21:DC:P	2.32	0.52
1:B:292:SER:HB3	1:B:296:VAL:CG2	2.40	0.52
1:D:157:THR:HB	1:D:158:PRO:HD2	1.92	0.52
1:D:635:LYS:HG3	1:D:635:LYS:O	2.10	0.52
2:M:23:DT:C2'	2:M:24:DT:O4'	2.57	0.52
2:M:2:DC:H4'	2:M:3:DA:OP1	2.05	0.52
1:A:121:GLN:HE21	1:A:195:ASP:HB2	1.75	0.51
1:A:396:ARG:HH12	1:A:416:ARG:HG3	1.75	0.51
1:C:120:ASP:HA	1:C:412:VAL:HG11	1.92	0.51
1:B:483:PRO:O	1:B:487:LEU:HG	2.10	0.51
1:B:482:GLU:OE1	1:B:483:PRO:HD2	2.10	0.51
1:C:649:GLU:HA	1:C:652:PHE:HE1	1.74	0.51
1:A:655:VAL:HG12	1:A:656:ASP:O	2.10	0.51
1:C:454:GLN:CG	1:C:455:ASN:H	2.09	0.51
2:P:22:DT:C3'	2:P:23:DT:H5''	2.41	0.51
1:A:426:GLY:O	1:A:430:LEU:HB2	2.11	0.51
1:A:231:ASP:CG	1:A:261:TYR:HD2	2.14	0.51
1:A:264:ARG:HG3	1:A:264:ARG:O	2.11	0.51
1:D:528:GLU:HG2	1:D:529:ALA:N	2.25	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LYS:HE3	1:B:198:ASP:OD2	2.10	0.51
1:B:571:HIS:NE2	3:N:23:DT:H1'	2.26	0.51
1:D:72:GLU:O	1:D:76:ARG:HG3	2.10	0.51
3:O:5:DC:H4'	3:O:6:DG:OP2	2.07	0.51
1:A:347:LEU:O	1:A:352:ARG:HB2	2.11	0.51
1:A:436:TRP:CH2	1:A:455:ASN:HB3	2.46	0.51
1:C:419:GLY:HA2	1:C:425:ILE:HG12	1.92	0.51
3:N:17:DA:H1'	3:N:18:DC:H5'	1.91	0.51
1:A:40:ARG:HD2	5:A:1664:ANP:H2'	1.93	0.51
1:A:591:LEU:HD21	1:A:644:PHE:HD2	1.76	0.51
1:A:90:SER:HB2	1:A:94:SER:HB2	1.92	0.51
1:B:29:LEU:HB2	1:B:274:PHE:CD2	2.46	0.51
1:C:152:LYS:HE3	1:C:181:TYR:HE1	1.75	0.51
1:C:24:PHE:CD2	1:C:25:THR:HG23	2.45	0.51
1:D:440:HIS:HB3	1:D:442:THR:OG1	2.11	0.51
1:D:656:ASP:CB	1:D:660:GLN:O	2.58	0.51
1:A:534:SER:O	1:A:537:ASP:HB2	2.11	0.50
1:C:117:ASP:HA	1:C:196:PHE:CZ	2.46	0.50
1:D:460:GLY:HA2	1:D:463:LYS:HG3	1.93	0.50
1:B:426:GLY:CA	3:N:11:DG:P	2.99	0.50
1:B:119:ASP:HB3	1:B:396:ARG:HH21	1.77	0.50
1:C:655:VAL:HG13	1:C:656:ASP:O	2.11	0.50
1:D:591:LEU:O	1:D:592:PRO:C	2.50	0.50
1:A:40:ARG:HA	1:A:76:ARG:CZ	2.41	0.50
3:O:16:DC:H2''	3:O:17:DA:C8	2.46	0.50
1:A:631:MET:HG3	1:A:634:GLY:O	2.11	0.50
1:A:163:ARG:HD3	1:C:285:MET:CE	2.42	0.50
3:O:21:DC:H2'	3:O:22:DT:H5''	1.90	0.50
1:B:132:ILE:CD1	1:B:180:ALA:HA	2.41	0.50
1:B:168:PHE:HA	1:B:172:LEU:O	2.12	0.50
1:A:64:THR:O	1:A:91:THR:HA	2.12	0.50
1:A:29:LEU:HB2	1:A:274:PHE:CD2	2.46	0.50
1:B:456:ILE:HG23	1:B:456:ILE:O	2.11	0.50
1:D:188:LYS:HE3	1:D:198:ASP:OD2	2.11	0.50
1:D:292:SER:HB3	1:D:296:VAL:HG23	1.94	0.50
1:A:163:ARG:HD3	1:C:285:MET:HE1	1.94	0.49
1:C:404:LEU:HD13	1:C:410:ASP:O	2.12	0.49
1:A:295:ARG:HD2	1:A:324:PRO:HA	1.93	0.49
1:A:486:PHE:CD2	1:A:535:ILE:HD13	2.46	0.49
1:C:487:LEU:O	1:C:491:MET:HG3	2.12	0.49
1:D:135:ILE:HG23	1:D:136:GLY:N	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:THR:HG22	1:D:443:SER:N	2.27	0.49
1:A:295:ARG:CG	1:A:321:ALA:HB1	2.43	0.49
1:A:632:GLN:HB3	1:A:633:PHE:CD1	2.47	0.49
1:B:121:GLN:HA	1:B:124:ILE:HD12	1.95	0.49
1:B:420:ARG:C	1:B:499:LEU:HD11	2.33	0.49
1:C:437:ALA:HA	1:C:442:THR:CB	2.42	0.49
1:A:43:ILE:O	1:A:46:ILE:N	2.45	0.49
1:B:152:LYS:HE3	1:B:181:TYR:HE1	1.77	0.49
1:C:498:ASP:N	1:C:498:ASP:OD1	2.45	0.49
3:N:8:DC:H1'	3:N:9:DC:OP2	2.11	0.49
1:B:428:THR:OG1	3:N:10:DT:H3'	2.11	0.49
1:D:418:ILE:HG13	1:D:425:ILE:CD1	2.33	0.49
3:N:16:DC:H2'	3:N:17:DA:C8	2.47	0.49
1:A:230:GLN:HE21	1:A:574:LYS:NZ	2.09	0.49
1:D:117:ASP:CB	1:D:196:PHE:CZ	2.95	0.49
1:A:582:PHE:HA	1:A:623:LEU:O	2.12	0.49
1:B:524:TRP:CH2	1:B:533:GLY:HA3	2.47	0.49
1:D:290:TYR:HA	1:D:318:VAL:HG22	1.95	0.49
1:D:436:TRP:CZ2	1:D:455:ASN:HB3	2.47	0.49
1:C:401:TYR:CE1	1:C:417:ILE:HD13	2.47	0.49
1:D:420:ARG:HB3	1:D:496:TYR:HE1	1.78	0.49
1:D:4:SER:HB2	1:D:52:HIS:CD2	2.47	0.49
1:A:303:LEU:CD2	1:A:611:PHE:HD2	2.26	0.49
1:C:352:ARG:NH1	1:C:356:GLU:OE1	2.46	0.49
2:M:21:DC:C3'	2:M:22:DT:C5'	2.84	0.49
3:N:16:DC:H2''	3:N:17:DA:C5'	2.39	0.48
1:B:518:VAL:O	1:B:522:GLU:HG3	2.13	0.48
1:B:654:THR:O	1:B:661:PRO:HA	2.13	0.48
1:C:307:ASN:OD1	1:C:605:GLU:HG2	2.12	0.48
1:D:165:ARG:O	1:D:167:PRO:HD3	2.12	0.48
1:D:179:GLU:OE1	1:D:179:GLU:HA	2.14	0.48
1:A:13:LEU:HD21	1:A:40:ARG:NH1	2.27	0.48
3:N:20:DG:C1'	3:N:21:DC:OP1	2.59	0.48
1:A:436:TRP:CZ3	1:A:455:ASN:HB3	2.49	0.48
1:C:308:THR:O	1:C:309:GLU:HB2	2.13	0.48
2:M:21:DC:H2''	2:M:22:DT:C6	2.49	0.48
3:O:14:DA:H2''	3:O:15:DG:C8	2.48	0.48
1:A:231:ASP:OD2	1:A:574:LYS:NZ	2.47	0.48
1:A:588:GLN:NE2	1:A:597:ILE:HD11	2.29	0.48
1:A:591:LEU:O	1:A:592:PRO:C	2.52	0.48
1:C:407:ASN:C	1:C:409:ALA:H	2.17	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:ASP:O	1:C:459:ARG:HB2	2.14	0.48
1:A:292:SER:HB3	1:A:296:VAL:HG23	1.93	0.48
1:C:436:TRP:HZ2	1:C:454:GLN:HG2	1.78	0.48
1:D:395:ILE:O	1:D:399:LEU:HG	2.14	0.48
1:B:575:GLY:H	1:B:617:ARG:NH1	2.12	0.48
1:C:330:ALA:O	1:C:627:ALA:HA	2.14	0.47
1:A:43:ILE:H	1:A:76:ARG:HH12	1.60	0.47
2:M:23:DT:H2'	2:M:24:DT:O5'	2.14	0.47
1:B:27:PRO:O	1:B:281:ALA:HA	2.13	0.47
1:B:293:SER:HB2	1:B:322:GLY:H	1.78	0.47
1:D:631:MET:HA	1:D:636:THR:HA	1.95	0.47
1:A:40:ARG:CD	5:A:1664:ANP:H2'	2.44	0.47
1:A:65:PHE:O	1:A:65:PHE:CD1	2.61	0.47
1:B:114:VAL:HG23	1:B:403:ARG:HD2	1.97	0.47
1:C:357:MET:HG2	1:C:580:VAL:HB	1.95	0.47
1:C:632:GLN:O	1:C:633:PHE:C	2.53	0.47
1:D:45:ARG:HD3	1:D:251:LEU:HD13	1.95	0.47
3:N:25:DT:H2'	3:N:25:DT:H6	1.60	0.47
1:B:345:THR:HG21	1:B:377:VAL:HG11	1.95	0.47
1:B:77:ALA:O	1:B:80:LEU:HB2	2.15	0.47
1:D:117:ASP:CB	1:D:196:PHE:HZ	2.28	0.47
1:B:420:ARG:CB	1:B:421:PRO:HD3	2.44	0.47
1:B:530:ASN:O	1:B:533:GLY:N	2.47	0.47
1:B:591:LEU:O	1:B:592:PRO:C	2.52	0.47
1:C:586:VAL:C	1:C:587:GLU:HG3	2.35	0.47
1:B:23:HIS:ND1	1:B:282:LYS:HD3	2.30	0.47
1:A:135:ILE:HG13	1:A:136:GLY:N	2.29	0.47
1:B:587:GLU:OE1	1:B:630:ARG:NH1	2.47	0.47
1:C:491:MET:CE	1:C:514:LEU:HB3	2.44	0.47
1:A:131:SER:CB	1:A:183:ARG:HH21	2.25	0.47
1:B:395:ILE:HD12	1:B:517:LEU:HB2	1.96	0.47
1:A:264:ARG:NH2	2:M:25:DT:O2	2.48	0.47
1:A:592:PRO:HG3	1:A:644:PHE:CZ	2.50	0.47
1:B:161:LEU:HD23	1:B:178:ALA:CA	2.43	0.47
1:C:113:PHE:HA	1:C:192:ASN:ND2	2.30	0.47
1:D:123:ASP:HB3	1:D:412:VAL:HG22	1.97	0.47
1:D:418:ILE:CG1	1:D:425:ILE:HD12	2.34	0.47
1:B:74:ARG:CG	1:B:84:ALA:HB1	2.44	0.47
1:D:123:ASP:CB	1:D:412:VAL:HG13	2.45	0.47
1:A:571:HIS:CE1	2:M:24:DT:H1'	2.50	0.47
1:B:507:GLY:O	1:B:510:ARG:HB2	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLU:O	1:B:526:GLN:HG2	2.15	0.46
1:C:517:LEU:HD23	1:C:517:LEU:C	2.35	0.46
1:C:64:THR:O	1:C:91:THR:HA	2.15	0.46
2:P:16:DC:OP2	2:P:16:DC:H6	1.97	0.46
1:A:457:LEU:H	1:A:457:LEU:HD12	1.80	0.46
1:C:48:HIS:CE1	1:C:52:HIS:CB	2.98	0.46
1:D:411:ASP:HA	1:D:414:LEU:CB	2.45	0.46
1:D:507:GLY:HA2	1:D:510:ARG:HD3	1.98	0.46
1:A:576:LEU:O	1:A:617:ARG:HD3	2.15	0.46
2:M:18:DT:H2''	2:M:19:DA:OP2	2.15	0.46
2:P:18:DT:H2''	2:P:19:DA:C8	2.51	0.46
1:A:442:THR:HG22	1:A:443:SER:N	2.30	0.46
1:D:68:LYS:NZ	1:D:553:THR:HG21	2.31	0.46
1:C:175:ASP:OD1	1:C:176:ALA:N	2.49	0.46
1:D:24:PHE:CE1	1:D:53:TYR:HB3	2.50	0.46
1:B:454:GLN:HG3	1:B:455:ASN:H	1.80	0.46
1:B:76:ARG:O	1:B:80:LEU:HD13	2.15	0.46
1:B:655:VAL:HG13	1:B:659:GLY:HA2	1.97	0.46
1:C:483:PRO:HA	1:C:486:PHE:HB3	1.97	0.46
1:C:87:LEU:HD12	1:C:89:MET:HG3	1.98	0.46
1:D:527:ASP:CG	1:D:528:GLU:N	2.69	0.46
1:C:354:TRP:CZ3	1:C:379:ILE:HG23	2.50	0.45
1:C:63:VAL:HG12	1:C:225:HIS:O	2.15	0.45
1:D:374:LEU:HB3	1:D:379:ILE:HB	1.98	0.45
1:D:211:PRO:O	1:D:214:LEU:HB3	2.15	0.45
1:A:591:LEU:HG	1:A:592:PRO:N	2.32	0.45
1:D:348:HIS:CE1	1:D:354:TRP:CE2	3.04	0.45
1:B:114:VAL:HG12	1:B:193:ALA:CB	2.47	0.45
1:C:407:ASN:C	1:C:409:ALA:N	2.67	0.45
1:D:156:TRP:HB3	1:D:160:ASP:HB2	1.98	0.45
2:M:15:DT:C2'	2:M:16:DC:O5'	2.64	0.45
1:C:436:TRP:HZ3	1:C:442:THR:HG21	1.82	0.45
1:D:179:GLU:O	1:D:183:ARG:HD3	2.17	0.45
1:A:43:ILE:HD11	1:A:76:ARG:CA	2.47	0.45
1:A:546:SER:O	1:A:552:ARG:HD3	2.17	0.45
1:A:588:GLN:HE22	1:A:597:ILE:HD11	1.80	0.45
1:B:631:MET:HE2	1:B:634:GLY:H	1.82	0.45
1:C:136:GLY:O	1:C:139:THR:OG1	2.30	0.45
1:C:411:ASP:HB3	1:C:415:ARG:NH1	2.32	0.45
1:C:255:ASP:HA	1:C:256:PRO:HD3	1.77	0.45
1:C:8:ASP:HB2	1:C:11:GLN:HB2	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ARG:HH22	1:B:620:GLU:HG3	1.81	0.45
1:A:470:LEU:HD21	1:A:494:SER:HA	1.99	0.45
1:C:65:PHE:HD1	1:C:65:PHE:HA	1.68	0.45
2:M:18:DT:C6	2:M:18:DT:H5'	2.51	0.45
1:B:345:THR:HG23	1:B:379:ILE:HD11	1.97	0.45
1:C:116:TYR:CE2	1:C:124:ILE:HD11	2.52	0.45
1:C:129:MET:CE	1:C:141:PRO:HG3	2.47	0.45
1:C:417:ILE:O	1:C:421:PRO:HD2	2.17	0.45
1:C:595:GLY:O	1:C:599:GLU:HG3	2.17	0.45
1:D:504:GLY:C	1:D:508:GLN:HB2	2.37	0.45
1:A:440:HIS:HB3	1:A:442:THR:OG1	2.17	0.44
1:A:73:MET:HE3	1:A:89:MET:HE2	2.00	0.44
1:B:348:HIS:CE1	1:B:354:TRP:CE2	3.05	0.44
1:C:458:ASP:C	1:C:460:GLY:H	2.20	0.44
1:D:24:PHE:CD2	1:D:25:THR:HG23	2.52	0.44
1:D:330:ALA:O	1:D:627:ALA:HA	2.17	0.44
1:A:115:ILE:O	1:A:115:ILE:HG23	2.17	0.44
1:A:95:ALA:O	1:A:99:ILE:HG13	2.18	0.44
1:B:454:GLN:HG3	1:B:455:ASN:N	2.33	0.44
2:M:23:DT:OP2	2:M:23:DT:O4'	2.35	0.44
1:D:572:ASN:HD21	2:P:25:DT:P	2.40	0.44
1:A:13:LEU:HD21	1:A:40:ARG:HH12	1.74	0.44
1:A:230:GLN:HE21	1:A:574:LYS:HZ2	1.65	0.44
1:A:587:GLU:OE1	1:A:630:ARG:NH1	2.50	0.44
1:C:356:GLU:HB3	1:C:579:PRO:HG2	2.00	0.44
1:D:117:ASP:HB3	1:D:196:PHE:HZ	1.81	0.44
1:A:609:ARG:O	1:A:612:TYR:HB3	2.18	0.44
1:B:295:ARG:HG3	1:B:322:GLY:N	2.32	0.44
1:D:32:ALA:CB	1:D:286:LEU:HB2	2.48	0.44
1:A:530:ASN:O	1:A:533:GLY:N	2.50	0.44
1:A:81:VAL:HG23	1:A:82:PRO:HD2	1.98	0.44
1:B:372:GLU:HA	1:B:375:ARG:HB3	1.99	0.44
1:B:591:LEU:CD1	1:B:611:PHE:HB2	2.46	0.44
1:C:27:PRO:HB2	1:C:281:ALA:HB2	1.99	0.44
1:D:411:ASP:HA	1:D:414:LEU:HB3	2.00	0.44
1:D:434:MET:C	1:D:436:TRP:N	2.70	0.44
1:A:261:TYR:O	1:A:264:ARG:HB3	2.17	0.44
1:A:562:GLU:HG2	1:A:563:ASP:H	1.82	0.44
1:C:397:ASP:O	1:C:417:ILE:HG21	2.18	0.44
1:C:462:HIS:HA	1:C:465:THR:OG1	2.18	0.44
1:B:264:ARG:HD3	3:N:24:DT:O2	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LEU:HD13	1:A:517:LEU:CD2	2.47	0.44
1:B:134:GLY:HA3	1:B:176:ALA:HB1	1.98	0.44
1:B:164:SER:O	1:B:174:ARG:NH1	2.50	0.44
1:A:261:TYR:O	1:A:264:ARG:N	2.49	0.44
1:B:656:ASP:HB2	1:B:657:PRO:HD2	2.00	0.44
1:C:226:VAL:HB	1:C:252:VAL:HG12	1.99	0.44
1:A:420:ARG:CB	1:A:421:PRO:HD3	2.46	0.44
1:B:295:ARG:HD2	1:B:324:PRO:HA	2.00	0.44
3:N:16:DC:H2'	3:N:17:DA:O4'	2.17	0.44
1:A:303:LEU:HD21	1:A:611:PHE:HD2	1.83	0.43
1:A:303:LEU:HD22	1:A:611:PHE:CD2	2.53	0.43
1:C:117:ASP:HA	1:C:196:PHE:HE2	1.73	0.43
1:D:404:LEU:HA	1:D:407:ASN:O	2.18	0.43
1:A:161:LEU:HD23	1:A:178:ALA:HA	2.00	0.43
1:A:440:HIS:O	1:A:441:HIS:ND1	2.51	0.43
1:A:472:GLU:OE1	1:A:472:GLU:HA	2.17	0.43
1:B:345:THR:HG21	1:B:377:VAL:CG1	2.48	0.43
1:B:589:GLY:HA2	1:B:594:LYS:HG2	1.99	0.43
1:B:595:GLY:O	1:B:599:GLU:HG3	2.18	0.43
1:D:183:ARG:O	1:D:186:VAL:HG22	2.18	0.43
1:A:426:GLY:HA2	2:M:12:DA:P	2.58	0.43
1:C:422:ARG:HB3	3:O:13:DG:OP2	2.18	0.43
1:A:36:SER:HA	1:A:288:HIS:O	2.18	0.43
1:C:459:ARG:NH2	3:O:10:DT:OP1	2.52	0.43
1:C:656:ASP:HB2	1:C:657:PRO:CD	2.48	0.43
2:M:20:DC:C2'	2:M:21:DC:OP2	2.66	0.43
3:N:22:DT:H2''	3:N:23:DT:O5'	2.19	0.43
1:A:296:VAL:HG12	1:A:325:VAL:CG1	2.49	0.43
1:A:42:LEU:HD11	1:A:225:HIS:HB3	2.00	0.43
1:A:327:PHE:HB3	1:A:652:PHE:CE2	2.54	0.43
1:D:31:ILE:O	1:D:31:ILE:HG23	2.19	0.43
1:D:570:LEU:CD1	1:D:591:LEU:HD11	2.48	0.43
1:B:84:ALA:HA	1:B:87:LEU:HD12	2.01	0.43
1:D:210:VAL:O	1:D:210:VAL:HG23	2.18	0.43
1:D:456:ILE:CG2	1:D:456:ILE:O	2.62	0.43
1:D:656:ASP:H	1:D:660:GLN:C	2.22	0.43
2:M:16:DC:H2''	2:M:17:DG:C8	2.53	0.43
1:B:326:THR:HB	1:B:655:VAL:CG2	2.47	0.43
1:C:303:LEU:O	1:C:608:ARG:HD3	2.19	0.43
1:C:31:ILE:HG23	1:C:31:ILE:O	2.19	0.43
1:A:228:GLU:HB3	1:A:574:LYS:HE3	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD21	1:A:48:HIS:ND1	2.34	0.43
1:D:420:ARG:HB3	1:D:496:TYR:CE1	2.54	0.43
1:A:371:GLU:O	1:A:374:LEU:HB2	2.18	0.43
1:A:655:VAL:HG13	1:A:659:GLY:CA	2.49	0.43
1:D:572:ASN:ND2	1:D:572:ASN:N	2.67	0.43
1:D:613:VAL:O	1:D:617:ARG:HG2	2.18	0.43
1:D:95:ALA:O	1:D:99:ILE:HG13	2.18	0.43
1:A:500:LEU:O	1:A:504:GLY:CA	2.64	0.42
1:B:72:GLU:O	1:B:76:ARG:HB2	2.18	0.42
1:A:654:THR:O	1:A:661:PRO:HA	2.19	0.42
1:C:424:GLY:O	3:O:12:DC:OP1	2.36	0.42
1:D:656:ASP:CB	1:D:657:PRO:CD	2.96	0.42
2:P:19:DA:H2''	2:P:20:DC:OP2	2.19	0.42
1:A:329:ARG:NH2	1:A:641:ASP:OD2	2.42	0.42
1:A:654:THR:HG22	1:A:655:VAL:N	2.34	0.42
1:C:74:ARG:HH21	1:C:89:MET:HG3	1.84	0.42
1:D:261:TYR:O	1:D:264:ARG:HG2	2.18	0.42
1:A:423:ARG:O	1:A:463:LYS:HD2	2.19	0.42
1:B:125:ILE:HA	1:B:128:VAL:HG22	2.01	0.42
1:B:24:PHE:CD2	1:B:25:THR:HG23	2.54	0.42
1:B:395:ILE:HD13	1:B:514:LEU:HD23	2.01	0.42
1:D:21:ALA:HA	1:D:45:ARG:HB2	2.01	0.42
1:A:384:VAL:HB	1:A:568:MET:HB3	2.00	0.42
1:B:136:GLY:C	1:B:138:GLU:N	2.64	0.42
1:B:65:PHE:HZ	1:B:264:ARG:CZ	2.32	0.42
1:B:73:MET:HB2	1:B:73:MET:HE3	1.85	0.42
1:C:136:GLY:O	1:C:137:ALA:C	2.58	0.42
1:C:30:VAL:HB	1:C:253:VAL:HG22	2.01	0.42
1:C:486:PHE:CD2	1:C:535:ILE:HD11	2.54	0.42
1:C:498:ASP:HA	1:C:501:ARG:HB2	2.02	0.42
1:D:592:PRO:HA	1:D:607:GLU:HG3	2.01	0.42
1:A:23:HIS:CE1	1:A:282:LYS:HD3	2.54	0.42
1:B:74:ARG:HG3	1:B:84:ALA:HB1	2.00	0.42
1:C:348:HIS:CE1	1:C:354:TRP:CE2	3.07	0.42
1:A:302:LYS:HG2	1:A:651:LEU:HD11	2.01	0.42
1:B:36:SER:HA	1:B:288:HIS:O	2.19	0.42
1:B:631:MET:CE	1:B:634:GLY:H	2.32	0.42
1:B:649:GLU:HG3	1:B:649:GLU:O	2.20	0.42
1:D:499:LEU:HD12	1:D:499:LEU:C	2.40	0.42
1:A:73:MET:HB3	1:A:89:MET:CE	2.50	0.42
1:B:138:GLU:OE1	1:B:138:GLU:HA	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LEU:HD22	1:C:478:ALA:HB1	2.02	0.42
3:O:21:DC:C2'	3:O:22:DT:C5'	2.83	0.42
1:A:27:PRO:HB2	1:A:281:ALA:HB2	2.02	0.42
1:A:632:GLN:HB3	1:A:633:PHE:CE1	2.54	0.42
1:B:14:ASN:HB2	1:B:15:PRO:HD2	2.02	0.42
1:B:508:GLN:O	1:B:511:LEU:HG	2.20	0.42
1:D:42:LEU:HD11	1:D:225:HIS:HB3	2.02	0.42
1:A:136:GLY:C	1:A:138:GLU:H	2.22	0.41
1:A:289:ASN:O	1:A:318:VAL:HG22	2.20	0.41
1:B:338:ASP:HA	1:B:341:ALA:HB3	2.02	0.41
1:B:362:ARG:NH2	3:N:22:DT:O2	2.53	0.41
1:B:81:VAL:O	1:B:81:VAL:HG13	2.20	0.41
1:C:122:LEU:HD23	1:C:125:ILE:HD12	2.01	0.41
1:C:332:ASP:OD1	1:C:333:HIS:N	2.53	0.41
1:C:479:ASP:OD1	1:C:480:ASN:N	2.54	0.41
1:C:656:ASP:HB2	1:C:657:PRO:HD2	2.01	0.41
2:M:23:DT:H4'	2:M:24:DT:OP1	2.20	0.41
1:A:643:ALA:O	1:A:646:GLU:HB3	2.20	0.41
1:C:455:ASN:O	1:C:456:ILE:HG22	2.20	0.41
1:D:294:ALA:HB3	1:D:321:ALA:HA	2.00	0.41
1:B:263:PHE:CZ	3:N:23:DT:H2'	2.55	0.41
2:P:20:DC:H4'	2:P:21:DC:OP2	2.20	0.41
1:B:567:LEU:O	1:B:568:MET:HB3	2.20	0.41
1:C:488:ARG:NH1	1:C:518:VAL:HG11	2.35	0.41
1:C:331:THR:HA	1:C:628:GLN:HB2	2.02	0.41
1:D:417:ILE:O	1:D:421:PRO:HD2	2.21	0.41
1:D:633:PHE:O	1:D:633:PHE:CD1	2.73	0.41
1:A:43:ILE:HG21	1:A:43:ILE:HD13	1.80	0.41
1:B:27:PRO:HB2	1:B:281:ALA:HB2	2.01	0.41
5:C:1664:ANP:O1G	5:C:1664:ANP:O1B	2.38	0.41
1:D:455:ASN:O	1:D:456:ILE:HG22	2.20	0.41
1:D:632:GLN:O	1:D:633:PHE:CG	2.74	0.41
1:A:248:ARG:NH2	1:A:280:ASP:OD2	2.53	0.41
1:A:347:LEU:HD13	1:A:580:VAL:HG11	2.02	0.41
1:A:655:VAL:CG1	1:A:659:GLY:HA2	2.50	0.41
1:C:461:ALA:O	1:C:465:THR:HG23	2.20	0.41
1:D:482:GLU:HB3	1:D:483:PRO:HD2	2.03	0.41
3:O:13:DG:H2''	3:O:14:DA:C8	2.55	0.41
1:B:107:ILE:HB	1:B:205:ARG:NH1	2.34	0.41
1:B:40:ARG:HA	1:B:43:ILE:HD12	2.03	0.41
1:B:654:THR:HG22	1:B:655:VAL:N	2.36	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:VAL:HG13	1:B:659:GLY:CA	2.50	0.41
1:C:188:LYS:HE2	1:C:194:ILE:HA	2.02	0.41
3:N:6:DG:H2''	3:N:7:DA:OP2	2.20	0.41
1:C:415:ARG:HH21	1:C:434:MET:HG2	1.85	0.41
1:A:419:GLY:O	1:A:422:ARG:HD3	2.21	0.41
1:B:114:VAL:CG2	1:B:115:ILE:N	2.83	0.41
1:B:9:LEU:HD21	1:B:48:HIS:CG	2.55	0.41
1:C:228:GLU:OE1	1:C:574:LYS:HD3	2.21	0.41
1:A:649:GLU:C	1:A:651:LEU:H	2.24	0.41
1:B:470:LEU:HD21	1:B:494:SER:HA	2.03	0.41
1:C:187:ARG:O	1:C:191:GLN:HB2	2.20	0.41
1:D:188:LYS:HB3	1:D:188:LYS:HZ2	1.86	0.41
2:P:11:DC:H2''	2:P:12:DA:C8	2.56	0.41
1:A:226:VAL:HB	1:A:252:VAL:HG12	2.03	0.41
1:A:487:LEU:HD13	1:A:517:LEU:HD21	2.03	0.41
1:B:476:GLU:O	1:B:479:ASP:OD1	2.39	0.41
1:C:323:GLN:HA	1:C:324:PRO:HD3	1.85	0.41
1:C:74:ARG:HD2	1:C:85:GLY:HA2	2.02	0.41
1:D:213:VAL:O	1:D:217:VAL:HG23	2.21	0.41
1:D:29:LEU:HD22	1:D:274:PHE:HB3	2.02	0.41
1:C:374:LEU:HB3	1:C:379:ILE:HB	2.03	0.40
1:D:655:VAL:CA	1:D:661:PRO:HA	2.43	0.40
3:O:1:DG:H22	2:P:21:DC:N4	2.19	0.40
1:A:422:ARG:HD2	2:M:13:DG:H3'	2.03	0.40
1:A:423:ARG:HE	1:A:470:LEU:HD23	1.86	0.40
1:B:289:ASN:O	1:B:318:VAL:HG22	2.21	0.40
1:D:451:ALA:O	1:D:456:ILE:HA	2.21	0.40
1:D:505:GLN:CG	1:D:506:GLU:H	2.14	0.40
1:D:78:GLY:HA2	1:D:84:ALA:HB2	2.03	0.40
3:N:18:DC:H2''	3:N:19:DT:C6	2.56	0.40
1:B:606:GLU:HA	1:B:609:ARG:NH1	2.36	0.40
1:C:32:ALA:CB	1:C:286:LEU:HB2	2.51	0.40
1:C:541:ASP:O	1:C:545:LEU:HG	2.22	0.40
3:N:17:DA:C2'	3:N:18:DC:OP2	2.66	0.40
1:A:183:ARG:HA	1:A:186:VAL:HG22	2.03	0.40
1:A:293:SER:HB2	1:A:322:GLY:H	1.86	0.40
1:B:182:ARG:O	1:B:186:VAL:HG13	2.21	0.40
1:C:9:LEU:HD11	1:C:48:HIS:ND1	2.36	0.40
1:D:157:THR:HB	1:D:158:PRO:CD	2.51	0.40
1:C:421:PRO:HG2	1:C:421:PRO:O	2.21	0.40
1:C:422:ARG:HD3	3:O:13:DG:OP2	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASP:O	1:D:124:ILE:HG13	2.22	0.40
1:D:633:PHE:O	3:O:1:DG:C4	2.75	0.40
2:P:25:DT:H2''	2:P:26:DT:O5'	2.21	0.40
2:P:25:DT:H2''	2:P:26:DT:OP2	2.19	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	644/745 (86%)	612 (95%)	31 (5%)	1 (0%)	51	84
1	B	637/745 (86%)	604 (95%)	32 (5%)	1 (0%)	51	84
1	C	641/745 (86%)	621 (97%)	19 (3%)	1 (0%)	51	84
1	D	632/745 (85%)	608 (96%)	23 (4%)	1 (0%)	51	84
All	All	2554/2980 (86%)	2445 (96%)	105 (4%)	4 (0%)	51	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	ILE
1	B	456	ILE
1	C	456	ILE
1	D	456	ILE

### 5.3.2 Protein sidechains [i](#)

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	523/598 (88%)	521 (100%)	2 (0%)	93	96
1	B	519/598 (87%)	518 (100%)	1 (0%)	94	97
1	C	528/598 (88%)	525 (99%)	3 (1%)	89	95
1	D	522/598 (87%)	517 (99%)	5 (1%)	80	90
All	All	2092/2392 (88%)	2081 (100%)	11 (0%)	91	96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	65	PHE
1	B	116	TYR
1	C	65	PHE
1	C	441	HIS
1	C	655	VAL
1	D	9	LEU
1	D	80	LEU
1	D	275	GLN
1	D	435	GLU
1	D	572	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	230	GLN
1	A	236	GLN
1	A	270	ASN
1	A	588	GLN
1	B	236	GLN
1	C	19	GLN
1	C	192	ASN
1	C	333	HIS
1	D	67	ASN
1	D	236	GLN
1	D	270	ASN
1	D	572	ASN



### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
5	ANP	A	1664	4	29,33,33	3.10	10 (34%)	28,52,52	2.08	5 (17%)
5	ANP	B	1664	4	29,33,33	3.07	10 (34%)	28,52,52	2.03	5 (17%)
5	ANP	C	1664	4	29,33,33	3.15	10 (34%)	28,52,52	1.96	3 (10%)
5	ANP	D	1663	4	29,33,33	3.10	10 (34%)	28,52,52	2.08	6 (21%)

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
5	ANP	A	1664	4	-	0/13/38/38	0/3/3/3
5	ANP	B	1664	4	-	0/13/38/38	0/3/3/3
5	ANP	C	1664	4	-	0/13/38/38	0/3/3/3
5	ANP	D	1663	4	-	0/13/38/38	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1664	ANP	C2'-C1'	-4.98	1.45	1.53
5	D	1663	ANP	C2'-C1'	-4.92	1.45	1.53
5	A	1664	ANP	C2'-C1'	-4.90	1.45	1.53
5	B	1664	ANP	C2'-C1'	-4.89	1.45	1.53
5	D	1663	ANP	PG-O3G	-3.22	1.47	1.56
5	B	1664	ANP	PG-O3G	-3.20	1.47	1.56
5	C	1664	ANP	PG-O3G	-3.17	1.48	1.56
5	A	1664	ANP	PG-O3G	-3.07	1.48	1.56
5	A	1664	ANP	C2'-C3'	-3.01	1.45	1.53
5	D	1663	ANP	C2'-C3'	-2.82	1.45	1.53
5	C	1664	ANP	C2'-C3'	-2.82	1.46	1.53
5	B	1664	ANP	C2'-C3'	-2.77	1.46	1.53
5	D	1663	ANP	O4'-C4'	-2.77	1.38	1.45
5	B	1664	ANP	O4'-C4'	-2.72	1.38	1.45
5	C	1664	ANP	O4'-C4'	-2.68	1.38	1.45
5	A	1664	ANP	O2'-C2'	-2.65	1.36	1.43
5	D	1663	ANP	O2'-C2'	-2.60	1.37	1.43
5	C	1664	ANP	O2'-C2'	-2.54	1.37	1.43
5	B	1664	ANP	O2'-C2'	-2.51	1.37	1.43
5	A	1664	ANP	O4'-C4'	-2.51	1.39	1.45
5	A	1664	ANP	C3'-C4'	-2.38	1.46	1.53
5	D	1663	ANP	C3'-C4'	-2.36	1.46	1.53
5	B	1664	ANP	C3'-C4'	-2.30	1.47	1.53
5	C	1664	ANP	C3'-C4'	-2.29	1.47	1.53
5	A	1664	ANP	C6-N6	3.40	1.48	1.34
5	B	1664	ANP	C6-N6	3.45	1.48	1.34
5	C	1664	ANP	C6-N6	3.45	1.48	1.34
5	D	1663	ANP	C6-N6	3.45	1.48	1.34
5	D	1663	ANP	O4'-C1'	4.90	1.48	1.41
5	B	1664	ANP	O4'-C1'	4.99	1.48	1.41
5	A	1664	ANP	O4'-C1'	5.06	1.48	1.41
5	C	1664	ANP	O4'-C1'	5.09	1.48	1.41
5	C	1664	ANP	PG-O1G	7.84	1.55	1.46
5	D	1663	ANP	PG-O1G	7.86	1.55	1.46
5	A	1664	ANP	PG-O1G	7.89	1.55	1.46
5	B	1664	ANP	PG-O1G	7.91	1.55	1.46
5	B	1664	ANP	PB-O1B	10.07	1.57	1.46
5	A	1664	ANP	PB-O1B	10.21	1.57	1.46
5	D	1663	ANP	PB-O1B	10.25	1.57	1.46
5	C	1664	ANP	PB-O1B	10.66	1.58	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1664	ANP	N3-C2-N1	-8.45	121.50	128.86
5	D	1663	ANP	N3-C2-N1	-8.22	121.70	128.86
5	B	1664	ANP	N3-C2-N1	-8.16	121.75	128.86
5	C	1664	ANP	N3-C2-N1	-8.09	121.81	128.86
5	A	1664	ANP	PA-O3A-PB	-3.49	120.07	132.38
5	B	1664	ANP	PA-O3A-PB	-2.97	121.91	132.38
5	D	1663	ANP	PA-O3A-PB	-2.94	121.99	132.38
5	D	1663	ANP	C4'-O4'-C1'	-2.92	106.66	109.77
5	A	1664	ANP	C4'-O4'-C1'	-2.84	106.75	109.77
5	B	1664	ANP	C4'-O4'-C1'	-2.59	107.01	109.77
5	C	1664	ANP	PA-O3A-PB	-2.39	123.93	132.38
5	A	1664	ANP	O1G-PG-N3B	-2.17	108.55	111.79
5	D	1663	ANP	C5'-C4'-C3'	-2.11	107.24	115.29
5	B	1664	ANP	O1G-PG-N3B	-2.08	108.68	111.79
5	D	1663	ANP	O5'-C5'-C4'	2.03	116.20	109.00
5	C	1664	ANP	C2'-C3'-C4'	2.17	106.84	102.62
5	B	1664	ANP	O5'-C5'-C4'	2.36	117.38	109.00
5	A	1664	ANP	O5'-C5'-C4'	2.38	117.43	109.00
5	D	1663	ANP	C2'-C3'-C4'	2.47	107.43	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1664	ANP	4	0
5	B	1664	ANP	3	0
5	C	1664	ANP	2	0
5	D	1663	ANP	2	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	A	650/745 (87%)	-0.39	5 (0%) 86 79	116, 179, 263, 334	0
1	B	645/745 (86%)	-0.36	7 (1%) 80 72	116, 182, 268, 324	0
1	C	651/745 (87%)	-0.21	19 (2%) 52 42	140, 212, 298, 369	0
1	D	645/745 (86%)	-0.18	22 (3%) 46 36	145, 217, 300, 385	0
2	M	25/28 (89%)	0.36	5 (20%) 1 2	137, 248, 287, 357	0
2	P	26/28 (92%)	-0.24	1 (3%) 41 32	173, 262, 307, 333	0
3	N	25/28 (89%)	-0.05	2 (8%) 13 11	141, 254, 293, 325	0
3	O	26/28 (92%)	-0.14	1 (3%) 41 32	156, 280, 323, 337	0
All	All	2693/3092 (87%)	-0.28	62 (2%) 61 52	116, 199, 291, 385	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	532	GLY	6.3
1	C	111	ARG	5.0
1	C	534	SER	4.4
1	C	458	ASP	4.2
1	D	553	THR	3.8
1	D	550	ASP	3.7
1	D	11	GLN	3.5
1	D	312	ASP	3.5
1	D	551	MET	3.4
1	B	533	GLY	3.4
1	C	448	CYS	3.3
1	D	502	GLN	3.2
1	D	7	PRO	3.2
1	C	506	GLU	3.2
1	D	111	ARG	3.1
1	A	552	ARG	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	M	22	DT	3.0
1	C	112	GLY	2.9
1	C	535	ILE	2.8
1	D	8	ASP	2.8
1	A	314	THR	2.8
1	C	390	TYR	2.7
1	B	455	ASN	2.7
1	A	455	ASN	2.7
1	D	323	GLN	2.7
1	D	428	THR	2.7
1	B	550	ASP	2.7
2	M	17	DG	2.6
1	D	441	HIS	2.6
1	C	635	LYS	2.6
1	D	424	GLY	2.5
3	O	22	DT	2.5
1	C	653	ASP	2.5
1	C	453	GLU	2.5
1	C	651	LEU	2.4
1	D	534	SER	2.4
1	D	647	ASP	2.4
1	C	450	ASN	2.4
2	M	15	DT	2.4
2	P	22	DT	2.3
1	B	547	SER	2.3
3	N	21	DC	2.3
1	D	112	GLY	2.3
1	C	463	LYS	2.2
1	C	620	GLU	2.2
3	N	1	DG	2.2
1	D	462	HIS	2.2
1	A	547	SER	2.2
1	D	555	ALA	2.2
1	C	449	ALA	2.2
1	C	391	ASP	2.2
1	D	654	THR	2.1
2	M	16	DC	2.1
1	D	137	ALA	2.1
1	B	552	ARG	2.1
1	A	476	GLU	2.1
2	M	6	DG	2.1
1	D	594	LYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	579	PRO	2.0
1	D	564	ALA	2.0
1	B	531	VAL	2.0
1	C	618	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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
5	ANP	A	1664	31/31	0.89	0.23	0.41	152,152,152,152	0
5	ANP	C	1664	31/31	0.88	0.24	0.14	187,187,187,187	0
5	ANP	D	1663	31/31	0.87	0.21	-0.26	193,193,193,193	0
5	ANP	B	1664	31/31	0.92	0.20	-0.57	140,140,140,140	0
4	MG	B	1663	1/1	0.98	0.25	-	92,92,92,92	0
4	MG	D	1662	1/1	0.91	0.21	-	105,105,105,105	0
4	MG	A	1663	1/1	0.99	0.26	-	97,97,97,97	0
4	MG	C	1663	1/1	0.94	0.29	-	123,123,123,123	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.