



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:08 AM GMT

PDB ID : 2PI4
Title : T7RNAP complexed with a phi10 protein and initiating GTPs.
Authors : Kennedy, W.P.; Momand, J.R.; Yin, Y.W.
Deposited on : 2007-04-12
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

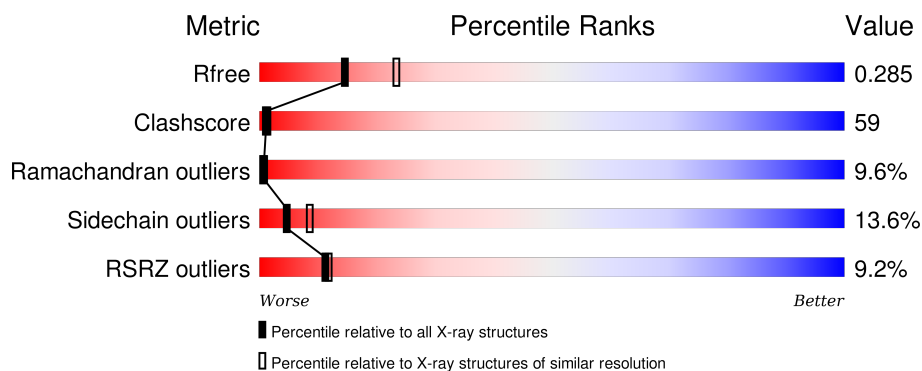
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

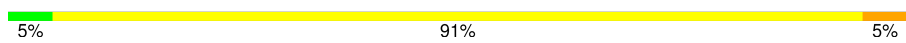
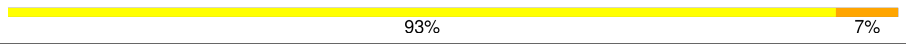
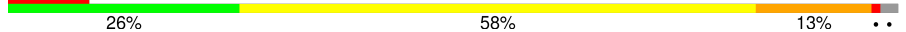
The reported resolution of this entry is 2.50 Å.

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 ≥ 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	T	22	
2	P	14	
3	A	878	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7722 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	22	Total	C	N	O	P	0	0	0
			446	216	75	134	21			

- Molecule 2 is a DNA chain called 5'-D(*TP*AP*AP*TP*AP*CP*GP*AP*CP*TP*CP*AP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	14	Total	C	N	O	P	0	0	0
			280	136	50	81	13			

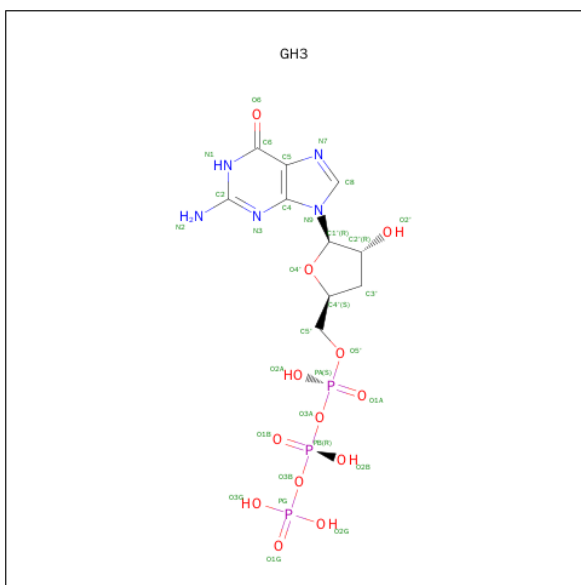
- Molecule 3 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	862	Total	C	N	O	S	0	0	0
			6803	4334	1178	1254	37			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is 3'-DEOXY-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GH3) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	A	1	Total 31	C 10	N 5	O 13	P 3	0	0

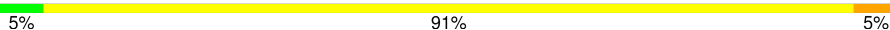
- Molecule 6 is water.

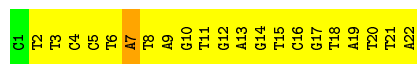
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	115	Total O 115 115	0	0
6	P	7	Total O 7 7	0	0
6	T	7	Total O 7 7	0	0

3 Residue-property plots

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

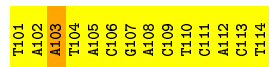
- Molecule 1: 5'-D(*CP*TP*TP*CP*CP*TP*AP*TP*AP*GP*TP*GP*AP*GP*TP*CP*GP*TP*AP*TP*TP*A)-3'

Chain T: 



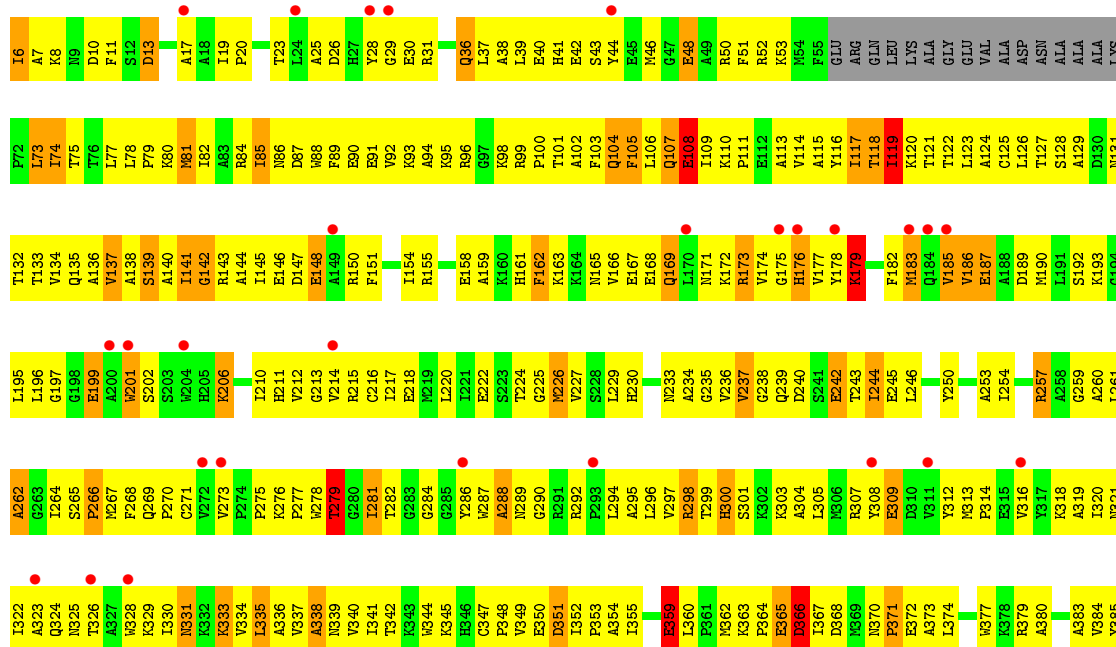
- Molecule 2: 5'-D(*TP*AP*AP*TP*AP*CP*GP*AP*CP*TP*CP*AP*CP*T)-3'

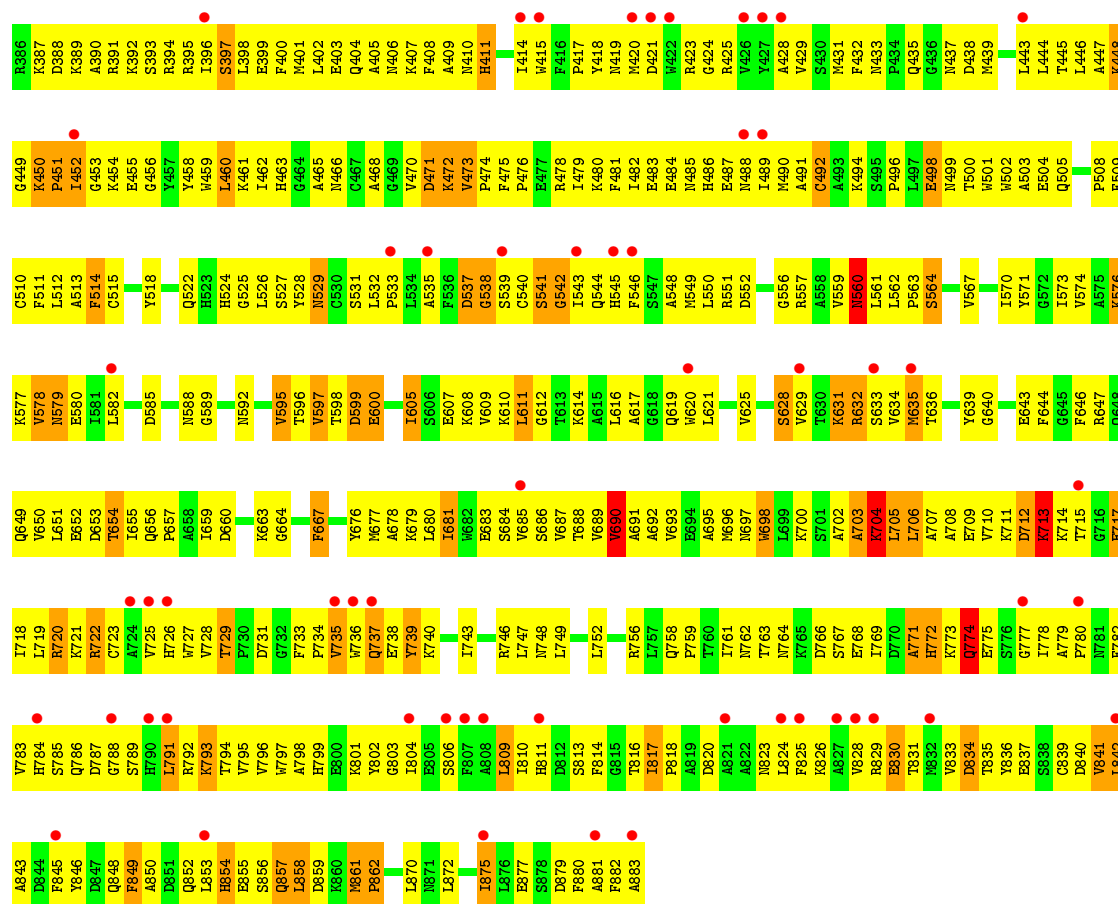
Chain P: 



- Molecule 3: DNA-directed RNA polymerase

Chain A: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	224.45Å 73.79Å 80.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 2.50 39.04 – 2.50	Depositor EDS
% Data completeness (in resolution range)	78.0 (39.04-2.50) 97.8 (39.04-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.265 , 0.297 0.285 , 0.285	Depositor DCC
R_{free} test set	2301 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 2.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 46159 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7722	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, GH3

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	T	0.68	0/498	0.85	0/767
2	P	0.69	0/313	0.87	0/480
3	A	0.58	1/6959 (0.0%)	0.66	0/9416
All	All	0.59	1/7770 (0.0%)	0.68	0/10663

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	T	0	2
2	P	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	222	GLU	CG-CD	5.41	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	103	DA	Sidechain
1	T	6	DT	Sidechain
1	T	7	DA	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	446	0	253	34	0
2	P	280	0	160	23	0
3	A	6803	0	6764	831	1
4	A	2	0	0	0	0
5	A	62	0	24	0	0
6	A	115	0	0	33	0
6	P	7	0	0	0	0
6	T	7	0	0	0	0
All	All	7722	0	7201	873	1

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 59.

All (873) 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)
3:A:452:ILE:CD1	3:A:456:GLY:HA3	1.59	1.31
3:A:402:LEU:HD11	6:A:931:HOH:O	1.34	1.27
3:A:267:MET:CE	6:A:984:HOH:O	1.83	1.25
3:A:452:ILE:HD11	3:A:456:GLY:CA	1.73	1.19
3:A:304:ALA:HB1	6:A:937:HOH:O	1.45	1.14
3:A:452:ILE:HD13	3:A:818:PRO:HB2	1.19	1.10
3:A:798:ALA:HB1	3:A:804:ILE:HD12	1.34	1.09
3:A:402:LEU:CD1	6:A:931:HOH:O	1.88	1.07
3:A:578:VAL:HG22	3:A:680:LEU:HB3	1.36	1.07
1:T:14:DG:H2''	1:T:15:DT:H5'	1.26	1.06
3:A:473:VAL:HG22	3:A:474:PRO:HD2	1.40	1.03
3:A:253:ALA:HB1	3:A:257:ARG:HE	1.22	1.03
3:A:861:MET:H	3:A:862:PRO:HD2	1.22	1.03
3:A:141:ILE:HG22	3:A:145:ILE:HD11	1.37	1.02
1:T:19:DA:H2''	1:T:20:DT:H5'	1.41	1.02
3:A:693:VAL:HG12	3:A:697:ASN:HD21	1.21	1.00
2:P:112:DA:H2''	2:P:113:DC:H5''	1.44	0.99
3:A:677:MET:O	3:A:681:ILE:HG13	1.63	0.98
3:A:210:ILE:O	3:A:214:VAL:HG23	1.64	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:281:ILE:H	3:A:281:ILE:HD13	1.28	0.96
3:A:269:GLN:HE21	3:A:404:GLN:NE2	1.61	0.96
3:A:269:GLN:NE2	3:A:404:GLN:HE22	1.63	0.95
3:A:131:ASN:ND2	6:A:980:HOH:O	1.99	0.95
3:A:269:GLN:HE21	3:A:404:GLN:HE22	1.01	0.94
3:A:726:HIS:CD2	6:A:982:HOH:O	2.20	0.94
3:A:740:LYS:HA	3:A:769:ILE:HA	1.51	0.93
3:A:137:VAL:HG21	3:A:244:ILE:HD13	1.51	0.92
3:A:739:TYR:HB2	3:A:774:GLN:NE2	1.85	0.92
3:A:452:ILE:HD13	3:A:818:PRO:CB	1.99	0.92
3:A:579:ASN:HA	3:A:582:LEU:HD12	1.51	0.92
3:A:557:ARG:NH2	3:A:562:LEU:HD13	1.84	0.92
3:A:452:ILE:CD1	3:A:818:PRO:HB2	2.01	0.91
3:A:726:HIS:NE2	6:A:982:HOH:O	2.01	0.91
3:A:333:LYS:H	3:A:333:LYS:HD2	1.35	0.90
3:A:725:VAL:HB	3:A:737:GLN:HB2	1.53	0.90
3:A:849:PHE:HB2	3:A:853:LEU:HB2	1.52	0.90
3:A:816:THR:HG22	3:A:817:ILE:H	1.38	0.88
3:A:855:GLU:HG3	3:A:856:SER:H	1.38	0.88
3:A:452:ILE:HD11	3:A:456:GLY:HA3	0.89	0.88
3:A:123:LEU:HA	3:A:126:LEU:HD12	1.55	0.88
3:A:557:ARG:HB2	3:A:562:LEU:HD12	1.56	0.87
3:A:663:LYS:HG2	3:A:664:GLY:H	1.40	0.86
3:A:748:ASN:HD21	3:A:756:ARG:HH21	1.18	0.86
3:A:145:ILE:HD13	3:A:212:VAL:HG12	1.56	0.85
2:P:107:DG:H2''	2:P:108:DA:H5'	1.58	0.85
3:A:303:LYS:HD3	3:A:303:LYS:H	1.38	0.85
3:A:329:LYS:NZ	6:A:968:HOH:O	2.09	0.85
3:A:629:VAL:HG13	3:A:654:THR:HG21	1.57	0.85
3:A:475:PHE:O	3:A:479:ILE:HD12	1.75	0.84
3:A:261:LEU:N	3:A:261:LEU:HD12	1.93	0.84
3:A:77:LEU:H	3:A:77:LEU:HD12	1.42	0.84
3:A:120:LYS:HG2	3:A:264:ILE:HG23	1.57	0.83
3:A:560:ASN:HB3	3:A:881:ALA:HB2	1.60	0.83
3:A:711:LYS:HA	3:A:718:ILE:HG22	1.58	0.83
3:A:276:LYS:HE3	3:A:287:TRP:HA	1.60	0.83
3:A:367:ILE:HG23	3:A:368:ASP:H	1.43	0.81
3:A:227:VAL:HG12	3:A:246:LEU:HA	1.62	0.81
3:A:213:GLY:O	3:A:217:ILE:HG12	1.79	0.81
3:A:678:ALA:HA	3:A:681:ILE:HD12	1.63	0.81
3:A:236:VAL:O	3:A:240:ASP:HB2	1.81	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:649:GLN:O	3:A:653:ASP:HB2	1.81	0.80
3:A:861:MET:N	3:A:862:PRO:HD2	1.97	0.80
3:A:605:ILE:HD13	3:A:605:ILE:O	1.83	0.79
3:A:23:THR:HG23	6:A:1010:HOH:O	1.82	0.78
3:A:177:VAL:HB	3:A:179:LYS:HD2	1.63	0.78
3:A:261:LEU:H	3:A:261:LEU:HD12	1.46	0.78
3:A:417:PRO:HG2	3:A:429:VAL:HB	1.65	0.78
3:A:377:TRP:HA	3:A:380:ALA:HB3	1.65	0.78
3:A:448:LYS:HD3	3:A:448:LYS:N	1.99	0.77
3:A:185:VAL:HG22	3:A:186:VAL:H	1.49	0.77
3:A:576:LYS:O	3:A:580:GLU:HG3	1.84	0.77
3:A:339:ASN:HA	3:A:402:LEU:HD21	1.66	0.77
3:A:677:MET:HG3	3:A:681:ILE:HD11	1.65	0.77
3:A:452:ILE:CD1	3:A:818:PRO:CB	2.62	0.77
3:A:841:VAL:HG23	3:A:842:LEU:H	1.50	0.76
3:A:324:GLN:HE21	3:A:418:TYR:H	1.31	0.76
3:A:345:LYS:HD3	3:A:355:ILE:HD11	1.68	0.76
3:A:73:LEU:HD22	3:A:260:ALA:HB1	1.68	0.76
3:A:816:THR:HG22	3:A:817:ILE:HG13	1.68	0.75
3:A:872:LEU:O	3:A:875:ILE:HD13	1.87	0.75
3:A:253:ALA:HB1	3:A:257:ARG:NE	1.98	0.75
3:A:253:ALA:CB	3:A:257:ARG:HE	2.00	0.75
3:A:303:LYS:HD3	3:A:303:LYS:N	2.01	0.75
3:A:131:ASN:CG	6:A:980:HOH:O	2.23	0.75
3:A:159:ALA:HA	3:A:162:PHE:CD2	2.20	0.75
1:T:15:DT:H1'	1:T:16:DC:H5''	1.68	0.75
3:A:281:ILE:H	3:A:281:ILE:CD1	2.00	0.74
3:A:363:LYS:HD2	3:A:364:PRO:HD2	1.68	0.74
3:A:141:ILE:HG22	3:A:145:ILE:CD1	2.15	0.74
1:T:10:DG:C6	3:A:237:VAL:HG13	2.23	0.73
3:A:746:ARG:HA	3:A:759:PRO:O	1.88	0.73
3:A:145:ILE:HD13	3:A:212:VAL:CG1	2.18	0.73
3:A:267:MET:HE2	6:A:984:HOH:O	1.66	0.73
3:A:461:LYS:HB3	3:A:482:ILE:HG13	1.70	0.73
3:A:791:LEU:HD23	3:A:792:ARG:N	2.04	0.73
3:A:141:ILE:HG13	3:A:217:ILE:HD11	1.68	0.73
3:A:573:ILE:HG13	3:A:574:VAL:N	2.04	0.73
3:A:739:TYR:HB2	3:A:774:GLN:HE21	1.53	0.73
3:A:333:LYS:N	3:A:333:LYS:HD2	2.04	0.72
3:A:474:PRO:HA	3:A:880:PHE:HZ	1.53	0.72
3:A:300:HIS:CD2	3:A:300:HIS:H	2.06	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:206:LYS:O	3:A:210:ILE:HG12	1.89	0.72
3:A:393:SER:O	3:A:397:SER:OG	2.06	0.72
3:A:363:LYS:HE3	3:A:367:ILE:HD12	1.71	0.72
3:A:44:TYR:HD2	3:A:148:GLU:HG2	1.53	0.72
3:A:816:THR:HG22	3:A:817:ILE:N	2.04	0.72
3:A:756:ARG:HB3	3:A:758:GLN:HE22	1.52	0.72
3:A:540:CYS:H	3:A:544:GLN:HE21	1.34	0.72
1:T:13:DA:H1'	1:T:14:DG:H5''	1.69	0.72
3:A:475:PHE:CE2	3:A:879:ASP:HB2	2.25	0.72
3:A:798:ALA:O	3:A:804:ILE:HG13	1.88	0.71
3:A:28:TYR:OH	3:A:185:VAL:HA	1.90	0.71
3:A:166:VAL:HG12	3:A:167:GLU:H	1.55	0.71
1:T:20:DT:H2''	1:T:21:DT:H5''	1.71	0.71
3:A:747:LEU:HD13	3:A:759:PRO:HG2	1.71	0.71
3:A:775:GLU:O	3:A:778:ILE:HG22	1.91	0.71
3:A:118:THR:HG22	3:A:220:LEU:HD22	1.72	0.71
3:A:330:ILE:HD12	3:A:330:ILE:N	2.05	0.71
3:A:633:SER:HB2	6:A:910:HOH:O	1.91	0.71
3:A:185:VAL:HG12	3:A:325:ASN:HD21	1.57	0.70
3:A:110:LYS:O	3:A:114:VAL:HG23	1.90	0.70
1:T:14:DG:C2'	1:T:15:DT:H5'	2.15	0.70
3:A:452:ILE:HD12	3:A:456:GLY:HA3	1.71	0.69
2:P:102:DA:H2''	2:P:103:DA:OP2	1.90	0.69
3:A:408:PHE:HA	3:A:411:HIS:HD2	1.57	0.69
3:A:709:GLU:HA	3:A:720:ARG:HE	1.56	0.69
3:A:448:LYS:CD	3:A:448:LYS:H	2.06	0.69
3:A:703:ALA:O	3:A:706:LEU:HG	1.93	0.69
3:A:236:VAL:HG12	3:A:239:GLN:H	1.56	0.69
3:A:118:THR:O	3:A:122:THR:N	2.18	0.69
3:A:557:ARG:HH21	3:A:562:LEU:HD13	1.57	0.69
3:A:703:ALA:HA	3:A:706:LEU:HG	1.73	0.69
3:A:448:LYS:H	3:A:448:LYS:HD3	1.58	0.69
3:A:445:THR:HG23	3:A:532:LEU:HA	1.75	0.69
3:A:425:ARG:NH2	6:A:903:HOH:O	2.25	0.69
3:A:159:ALA:HA	3:A:162:PHE:CE2	2.26	0.69
3:A:740:LYS:HG2	3:A:769:ILE:HG13	1.76	0.68
3:A:551:ARG:HG2	3:A:870:LEU:O	1.94	0.68
3:A:417:PRO:O	3:A:429:VAL:HG23	1.94	0.68
3:A:265:SER:HB3	3:A:269:GLN:NE2	2.09	0.68
2:P:105:DA:H1'	2:P:106:DC:H5''	1.74	0.68
3:A:692:ALA:O	3:A:696:MET:HG3	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:269:GLN:HG2	3:A:404:GLN:OE1	1.94	0.67
3:A:439:MET:HA	3:A:509:PHE:CG	2.29	0.67
3:A:328:TRP:CE3	3:A:445:THR:O	2.48	0.67
3:A:29:GLY:HA3	3:A:175:GLY:HA2	1.76	0.67
3:A:578:VAL:CG2	3:A:680:LEU:HB3	2.18	0.67
3:A:659:ILE:HG13	3:A:660:ASP:OD2	1.93	0.67
3:A:244:ILE:HD12	3:A:244:ILE:H	1.60	0.67
3:A:19:ILE:HB	3:A:20:PRO:HD3	1.76	0.67
1:T:5:DC:H4'	3:A:423:ARG:HD2	1.76	0.67
3:A:308:TYR:CE2	3:A:734:PRO:HG2	2.29	0.67
3:A:388:ASP:O	3:A:392:LYS:HG3	1.95	0.67
3:A:743:ILE:HG13	3:A:763:THR:OG1	1.95	0.67
1:T:14:DG:H2''	1:T:15:DT:C5'	2.16	0.66
3:A:828:VAL:HG23	3:A:829:ARG:H	1.60	0.66
3:A:154:ILE:HG22	3:A:290:GLY:HA2	1.77	0.66
3:A:303:LYS:H	3:A:303:LYS:CD	2.09	0.66
3:A:318:LYS:O	3:A:322:ILE:HG13	1.96	0.66
3:A:117:ILE:HG22	3:A:118:THR:N	2.11	0.66
3:A:330:ILE:HD12	3:A:330:ILE:H	1.59	0.66
3:A:612:GLY:O	3:A:616:LEU:HD13	1.95	0.66
3:A:328:TRP:HE3	3:A:445:THR:O	1.79	0.66
3:A:278:TRP:HE1	3:A:324:GLN:HE22	1.44	0.66
3:A:747:LEU:O	3:A:758:GLN:HA	1.95	0.65
3:A:236:VAL:HG11	3:A:239:GLN:HB2	1.79	0.65
3:A:616:LEU:HD23	3:A:676:TYR:HB2	1.78	0.65
3:A:331:ASN:ND2	3:A:334:VAL:H	1.94	0.65
3:A:353:PRO:HD3	3:A:394:ARG:NH1	2.12	0.65
1:T:9:DA:O4'	3:A:762:ASN:ND2	2.29	0.65
3:A:84:ARG:HH12	3:A:88:TRP:HB2	1.61	0.65
3:A:651:LEU:HD12	3:A:655:ILE:HB	1.78	0.65
3:A:578:VAL:HG23	3:A:684:SER:OG	1.98	0.64
2:P:103:DA:H2''	2:P:104:DT:H5''	1.77	0.64
3:A:794:THR:HA	3:A:831:THR:HG21	1.80	0.64
1:T:21:DT:H2''	1:T:22:DA:C8	2.33	0.64
3:A:313:MET:HB2	3:A:316:VAL:HG23	1.78	0.64
3:A:711:LYS:HD2	3:A:712:ASP:H	1.63	0.64
3:A:276:LYS:CE	3:A:287:TRP:HA	2.28	0.64
3:A:804:ILE:HG23	3:A:820:ASP:OD2	1.98	0.63
3:A:39:LEU:O	3:A:42:GLU:HB2	1.97	0.63
3:A:693:VAL:HG12	3:A:697:ASN:ND2	2.05	0.63
3:A:802:TYR:CG	3:A:823:ASN:HB3	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:37:LEU:HG	3:A:288:ALA:HB2	1.80	0.63
3:A:479:ILE:HG22	3:A:483:GLU:OE1	1.98	0.63
3:A:475:PHE:N	3:A:476:PRO:HD2	2.12	0.63
3:A:132:THR:O	3:A:244:ILE:HD12	1.99	0.63
3:A:335:LEU:N	3:A:443:LEU:HD21	2.14	0.63
3:A:768:GLU:CD	3:A:769:ILE:H	2.02	0.63
3:A:229:LEU:HD21	3:A:242:GLU:OE1	1.99	0.63
3:A:538:GLY:HA3	3:A:883:ALA:HB3	1.81	0.63
2:P:111:DC:H2''	2:P:112:DA:H5'	1.81	0.62
3:A:120:LYS:O	3:A:124:ALA:N	2.28	0.62
3:A:709:GLU:H	3:A:722:ARG:HE	1.47	0.62
3:A:73:LEU:O	3:A:77:LEU:HD12	2.00	0.62
3:A:688:THR:O	3:A:690:VAL:HG22	1.99	0.62
3:A:739:TYR:H	3:A:774:GLN:HE22	1.48	0.62
3:A:341:ILE:HA	3:A:344:TRP:NE1	2.14	0.62
3:A:579:ASN:O	3:A:582:LEU:HB2	2.00	0.62
3:A:663:LYS:HG2	3:A:664:GLY:N	2.11	0.61
3:A:872:LEU:HA	3:A:875:ILE:HD13	1.80	0.61
3:A:229:LEU:HD11	3:A:242:GLU:HG2	1.81	0.61
3:A:585:ASP:O	3:A:614:LYS:HA	2.00	0.61
3:A:144:ALA:O	3:A:147:ASP:N	2.32	0.61
3:A:617:ALA:O	3:A:621:LEU:HG	2.00	0.61
3:A:782:PHE:O	3:A:786:GLN:HG2	2.00	0.61
3:A:828:VAL:HG23	3:A:829:ARG:HG2	1.82	0.61
3:A:650:VAL:O	3:A:654:THR:HG23	2.01	0.61
3:A:227:VAL:HG12	3:A:246:LEU:CA	2.31	0.61
3:A:324:GLN:HE21	3:A:418:TYR:N	1.98	0.61
3:A:620:TRP:CZ2	3:A:677:MET:HB2	2.35	0.61
3:A:371:PRO:HG2	3:A:372:GLU:H	1.65	0.61
3:A:6:ILE:N	3:A:6:ILE:HD13	2.16	0.61
3:A:703:ALA:O	3:A:706:LEU:N	2.31	0.61
3:A:341:ILE:HA	3:A:344:TRP:CD1	2.35	0.61
3:A:576:LYS:NZ	3:A:577:LYS:HB2	2.16	0.61
3:A:799:HIS:O	3:A:803:GLY:HA2	2.00	0.61
3:A:448:LYS:CD	3:A:448:LYS:N	2.61	0.61
3:A:118:THR:HA	3:A:141:ILE:HD12	1.83	0.60
3:A:339:ASN:N	6:A:931:HOH:O	2.33	0.60
3:A:559:VAL:HG23	3:A:561:LEU:HB2	1.82	0.60
3:A:333:LYS:O	3:A:336:ALA:HB3	1.99	0.60
3:A:747:LEU:HD12	3:A:747:LEU:N	2.16	0.60
3:A:450:LYS:HE2	3:A:817:ILE:CD1	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:185:VAL:HG22	3:A:186:VAL:N	2.16	0.60
3:A:628:SER:O	3:A:631:LYS:HB2	2.01	0.60
3:A:120:LYS:HD3	3:A:265:SER:H	1.67	0.60
3:A:644:PHE:HA	3:A:647:ARG:NH2	2.17	0.60
3:A:705:LEU:HD22	6:A:904:HOH:O	2.00	0.60
3:A:446:LEU:HD22	3:A:806:SER:HB3	1.83	0.60
3:A:448:LYS:H	3:A:448:LYS:CE	2.15	0.60
3:A:452:ILE:O	3:A:452:ILE:HD12	2.02	0.60
3:A:574:VAL:HG13	3:A:684:SER:HB2	1.83	0.59
3:A:169:GLN:NE2	3:A:172:LYS:H	1.99	0.59
3:A:265:SER:HB3	3:A:269:GLN:CD	2.22	0.59
3:A:121:THR:CG2	3:A:141:ILE:HD13	2.33	0.59
3:A:154:ILE:H	3:A:154:ILE:HD12	1.67	0.59
3:A:341:ILE:HA	3:A:344:TRP:CE2	2.37	0.59
3:A:458:TYR:CE1	3:A:479:ILE:HD11	2.37	0.59
3:A:410:ASN:O	3:A:411:HIS:C	2.39	0.59
3:A:539:SER:H	3:A:544:GLN:NE2	2.00	0.59
3:A:397:SER:O	3:A:400:PHE:HB2	2.03	0.59
3:A:320:ILE:HD11	3:A:420:MET:HE2	1.84	0.59
3:A:324:GLN:NE2	3:A:418:TYR:H	1.99	0.59
3:A:634:VAL:HG23	6:A:910:HOH:O	2.02	0.59
3:A:359:GLU:OE1	3:A:360:LEU:HD23	2.03	0.59
3:A:855:GLU:HG3	3:A:856:SER:N	2.15	0.59
3:A:449:GLY:HA2	3:A:817:ILE:HG21	1.85	0.59
3:A:367:ILE:HG23	3:A:368:ASP:N	2.16	0.59
3:A:401:MET:HE1	3:A:432:PHE:HA	1.83	0.59
3:A:220:LEU:O	3:A:224:THR:O	2.21	0.58
3:A:652:GLU:HA	3:A:656:GLN:HB3	1.84	0.58
3:A:463:HIS:CD2	3:A:535:ALA:H	2.20	0.58
3:A:78:LEU:O	3:A:82:ILE:HG13	2.03	0.58
3:A:363:LYS:HE3	3:A:367:ILE:HA	1.84	0.58
3:A:552:ASP:HB2	3:A:691:ALA:HB2	1.85	0.58
3:A:842:LEU:HG	3:A:843:ALA:H	1.66	0.58
3:A:195:LEU:O	3:A:196:LEU:HD12	2.03	0.58
3:A:261:LEU:H	3:A:261:LEU:CD1	2.15	0.58
3:A:705:LEU:CD2	6:A:904:HOH:O	2.51	0.58
3:A:562:LEU:HD21	3:A:870:LEU:HD11	1.85	0.58
3:A:44:TYR:CD2	3:A:148:GLU:HG2	2.37	0.58
3:A:353:PRO:HD3	3:A:394:ARG:HH11	1.68	0.58
3:A:313:MET:HE3	3:A:316:VAL:HG11	1.86	0.58
3:A:234:ALA:HA	3:A:240:ASP:OD2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:538:GLY:H	3:A:883:ALA:HB2	1.67	0.58
3:A:450:LYS:HE2	3:A:817:ILE:HD12	1.86	0.58
3:A:185:VAL:HG21	3:A:277:PRO:HD3	1.86	0.58
3:A:359:GLU:CD	3:A:360:LEU:H	2.07	0.58
3:A:492:CYS:SG	3:A:499:ASN:HB3	2.43	0.58
3:A:120:LYS:NZ	3:A:267:MET:SD	2.73	0.58
3:A:639:TYR:HE1	3:A:784:HIS:CE1	2.21	0.58
3:A:116:TYR:HA	3:A:119:ILE:CD1	2.34	0.57
3:A:577:LYS:HA	3:A:580:GLU:OE1	2.04	0.57
3:A:792:ARG:O	3:A:795:VAL:HG22	2.03	0.57
3:A:845:PHE:O	3:A:848:GLN:HB2	2.04	0.57
1:T:3:DT:H5''	3:A:640:GLY:O	2.04	0.57
3:A:695:ALA:O	3:A:698:TRP:HB3	2.05	0.57
3:A:768:GLU:CD	3:A:769:ILE:N	2.57	0.57
3:A:557:ARG:CZ	3:A:562:LEU:HD13	2.34	0.57
3:A:532:LEU:HD12	3:A:533:PRO:HD2	1.86	0.57
3:A:84:ARG:NH1	3:A:88:TRP:HB2	2.18	0.57
3:A:475:PHE:HE2	3:A:879:ASP:HB2	1.67	0.57
3:A:545:HIS:NE2	3:A:787:ASP:HA	2.19	0.57
3:A:408:PHE:HA	3:A:411:HIS:CD2	2.40	0.57
2:P:108:DA:H2''	2:P:109:DC:H5'	1.85	0.57
3:A:842:LEU:H	3:A:842:LEU:HD23	1.69	0.57
3:A:872:LEU:C	3:A:875:ILE:HD13	2.25	0.57
3:A:38:ALA:HB2	3:A:162:PHE:HE1	1.70	0.57
3:A:350:GLU:CD	3:A:350:GLU:N	2.58	0.57
3:A:394:ARG:HH11	3:A:394:ARG:HG2	1.68	0.57
3:A:706:LEU:C	3:A:720:ARG:HH22	2.07	0.57
3:A:79:PRO:HA	3:A:82:ILE:HD12	1.85	0.57
3:A:244:ILE:N	3:A:244:ILE:HD12	2.20	0.57
3:A:646:PHE:O	3:A:650:VAL:HG12	2.05	0.57
3:A:297:VAL:HA	3:A:420:MET:O	2.05	0.57
3:A:556:GLY:HA2	3:A:559:VAL:HG22	1.85	0.57
3:A:491:ALA:HA	3:A:494:LYS:HE2	1.85	0.57
3:A:503:ALA:HA	3:A:508:PRO:HB3	1.86	0.56
3:A:861:MET:H	3:A:862:PRO:CD	2.04	0.56
2:P:111:DC:H2''	2:P:112:DA:C8	2.40	0.56
3:A:512:LEU:O	3:A:513:ALA:C	2.43	0.56
3:A:454:LYS:HD3	3:A:455:GLU:N	2.19	0.56
3:A:124:ALA:HB1	6:A:984:HOH:O	2.05	0.56
3:A:261:LEU:HD21	3:A:396:ILE:HD12	1.86	0.56
3:A:331:ASN:HD22	3:A:331:ASN:C	2.09	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:398:LEU:HD21	3:A:402:LEU:HD22	1.87	0.56
3:A:474:PRO:HB2	3:A:476:PRO:HD2	1.87	0.56
3:A:639:TYR:HE1	3:A:784:HIS:HE1	1.53	0.56
3:A:234:ALA:O	3:A:236:VAL:HG23	2.05	0.56
3:A:142:GLY:CA	3:A:145:ILE:HD12	2.36	0.56
3:A:659:ILE:HA	3:A:663:LYS:O	2.06	0.56
3:A:828:VAL:HG23	3:A:829:ARG:N	2.21	0.56
3:A:229:LEU:HD21	3:A:242:GLU:CD	2.25	0.56
3:A:335:LEU:O	3:A:339:ASN:OD1	2.23	0.56
3:A:702:ALA:C	3:A:706:LEU:HD23	2.26	0.56
3:A:90:GLU:O	3:A:93:LYS:N	2.39	0.56
3:A:729:THR:HG22	3:A:733:PHE:H	1.70	0.56
3:A:74:ILE:CD1	3:A:78:LEU:HB2	2.36	0.56
3:A:176:HIS:NE2	3:A:178:TYR:HA	2.20	0.56
3:A:19:ILE:HG22	3:A:195:LEU:HD11	1.88	0.56
3:A:560:ASN:OD1	3:A:880:PHE:HB2	2.07	0.55
3:A:141:ILE:CG2	3:A:145:ILE:HD11	2.24	0.55
3:A:353:PRO:HD3	3:A:394:ARG:HG2	1.87	0.55
3:A:706:LEU:HD12	3:A:706:LEU:C	2.26	0.55
3:A:300:HIS:H	3:A:300:HIS:HD2	1.52	0.55
3:A:849:PHE:HB2	3:A:853:LEU:CB	2.31	0.55
3:A:190:MET:SD	6:A:1010:HOH:O	2.59	0.55
3:A:229:LEU:HD21	3:A:242:GLU:CG	2.37	0.55
3:A:480:LYS:HA	3:A:480:LYS:NZ	2.21	0.55
3:A:271:CYS:O	3:A:414:ILE:HA	2.07	0.55
3:A:48:GLU:OE1	6:A:912:HOH:O	2.18	0.55
3:A:756:ARG:CB	3:A:758:GLN:HE22	2.19	0.55
3:A:576:LYS:HG3	3:A:577:LYS:H	1.72	0.55
3:A:574:VAL:HG13	3:A:684:SER:CB	2.37	0.55
3:A:722:ARG:NH1	3:A:771:ALA:HB2	2.22	0.55
3:A:108:GLU:C	3:A:109:ILE:HD13	2.27	0.55
3:A:573:ILE:O	3:A:576:LYS:HG3	2.05	0.54
2:P:107:DG:H2''	2:P:108:DA:C5'	2.32	0.54
3:A:313:MET:HB2	3:A:316:VAL:CG2	2.37	0.54
3:A:73:LEU:HB3	3:A:260:ALA:O	2.07	0.54
1:T:5:DC:H4'	3:A:423:ARG:CD	2.37	0.54
1:T:4:DC:H2''	1:T:5:DC:H5'	1.89	0.54
3:A:747:LEU:O	3:A:758:GLN:HG3	2.08	0.54
3:A:711:LYS:HD2	3:A:712:ASP:N	2.21	0.54
3:A:8:LYS:C	3:A:10:ASP:H	2.11	0.54
3:A:74:ILE:HD11	3:A:78:LEU:HD22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:769:ILE:HD12	3:A:769:ILE:N	2.22	0.54
2:P:103:DA:H2"	2:P:104:DT:C5'	2.38	0.54
3:A:474:PRO:HA	3:A:880:PHE:CZ	2.39	0.54
3:A:816:THR:CG2	3:A:817:ILE:H	2.16	0.54
3:A:213:GLY:O	3:A:216:CYS:HB2	2.08	0.54
1:T:18:DT:H2"	1:T:19:DA:C8	2.42	0.54
3:A:446:LEU:HD12	3:A:531:SER:O	2.07	0.54
3:A:447:ALA:H	3:A:448:LYS:NZ	2.06	0.54
3:A:330:ILE:CD1	3:A:330:ILE:H	2.20	0.54
3:A:488:ASN:HB3	3:A:501:TRP:CZ3	2.43	0.54
3:A:475:PHE:CZ	3:A:879:ASP:HB2	2.42	0.54
3:A:700:LYS:HD3	3:A:700:LYS:O	2.07	0.54
3:A:129:ALA:HB2	3:A:393:SER:CB	2.38	0.53
3:A:351:ASP:OD1	3:A:351:ASP:N	2.39	0.53
3:A:245:GLU:OE2	3:A:389:LYS:HE2	2.08	0.53
3:A:335:LEU:CA	3:A:443:LEU:HD21	2.38	0.53
3:A:562:LEU:CD2	3:A:563:PRO:HD2	2.38	0.53
3:A:308:TYR:HE2	3:A:734:PRO:HG2	1.72	0.53
3:A:393:SER:O	3:A:396:ILE:HG22	2.08	0.53
3:A:74:ILE:HD11	3:A:78:LEU:HB2	1.90	0.53
3:A:330:ILE:CD1	3:A:330:ILE:N	2.71	0.53
3:A:492:CYS:HA	3:A:499:ASN:CB	2.38	0.53
3:A:861:MET:N	3:A:862:PRO:CD	2.68	0.53
3:A:544:GLN:HG2	3:A:559:VAL:HB	1.90	0.53
1:T:2:DT:H2"	3:A:644:PHE:CD2	2.44	0.53
3:A:169:GLN:HE21	3:A:172:LYS:H	1.56	0.53
3:A:541:SER:O	3:A:543:ILE:N	2.41	0.53
3:A:576:LYS:HG3	3:A:577:LYS:N	2.24	0.53
3:A:445:THR:HG22	3:A:446:LEU:H	1.72	0.53
3:A:211:HIS:O	3:A:215:ARG:HD3	2.08	0.53
3:A:31:ARG:HB2	3:A:173:ARG:HH21	1.74	0.53
3:A:595:VAL:HG21	3:A:597:VAL:HG23	1.90	0.53
3:A:174:VAL:HG11	3:A:177:VAL:HG22	1.89	0.53
3:A:374:LEU:HA	3:A:377:TRP:HB2	1.90	0.53
3:A:748:ASN:ND2	3:A:756:ARG:HH21	1.97	0.53
3:A:729:THR:HG22	3:A:733:PHE:N	2.24	0.53
3:A:708:ALA:O	3:A:720:ARG:NH2	2.42	0.53
3:A:539:SER:H	3:A:544:GLN:HE22	1.57	0.53
3:A:721:LYS:O	3:A:723:CYS:N	2.41	0.52
3:A:632:ARG:NH1	3:A:632:ARG:HB3	2.24	0.52
3:A:108:GLU:O	3:A:109:ILE:HD13	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:7:DA:OP2	3:A:298:ARG:HD3	2.09	0.52
3:A:706:LEU:HD12	3:A:706:LEU:O	2.10	0.52
3:A:254:ILE:HG23	3:A:261:LEU:HD11	1.91	0.52
3:A:438:ASP:CG	3:A:509:PHE:HB2	2.30	0.52
1:T:21:DT:H2"	1:T:22:DA:N7	2.24	0.52
3:A:816:THR:HG22	3:A:817:ILE:CG1	2.38	0.52
3:A:688:THR:C	3:A:690:VAL:H	2.12	0.52
3:A:458:TYR:HE1	3:A:479:ILE:HD11	1.75	0.52
2:P:112:DA:C2'	2:P:113:DC:H5"	2.27	0.52
3:A:171:ASN:O	3:A:174:VAL:HG12	2.09	0.52
3:A:725:VAL:O	3:A:736:TRP:HA	2.09	0.52
3:A:573:ILE:CG1	3:A:574:VAL:N	2.73	0.52
3:A:176:HIS:O	3:A:179:LYS:HB2	2.09	0.52
3:A:278:TRP:H	3:A:321:ASN:HD21	1.58	0.52
3:A:137:VAL:O	3:A:140:ALA:N	2.42	0.52
3:A:545:HIS:HB3	3:A:836:TYR:OH	2.09	0.52
3:A:715:THR:HG22	3:A:717:GLU:OE2	2.09	0.52
3:A:229:LEU:CG	3:A:242:GLU:HG2	2.40	0.52
3:A:451:PRO:HA	3:A:529:ASN:HA	1.91	0.52
3:A:259:GLY:O	3:A:262:ALA:HB2	2.09	0.52
3:A:789:SER:HA	3:A:792:ARG:NH2	2.24	0.52
3:A:229:LEU:HD21	3:A:242:GLU:HG2	1.92	0.52
3:A:86:ASN:HA	3:A:89:PHE:CD2	2.44	0.52
1:T:10:DG:H2"	1:T:11:DT:OP2	2.10	0.52
3:A:703:ALA:CA	3:A:706:LEU:HG	2.37	0.51
3:A:446:LEU:HB3	3:A:448:LYS:HZ3	1.74	0.51
3:A:324:GLN:HG3	3:A:417:PRO:HA	1.93	0.51
3:A:576:LYS:HZ1	3:A:577:LYS:HB2	1.73	0.51
3:A:846:TYR:HA	3:A:849:PHE:CZ	2.46	0.51
3:A:639:TYR:HA	3:A:780:PRO:HB3	1.91	0.51
3:A:703:ALA:O	3:A:704:LYS:C	2.48	0.51
3:A:636:THR:HA	3:A:639:TYR:CD2	2.45	0.51
3:A:151:PHE:O	3:A:155:ARG:HB2	2.10	0.51
3:A:107:GLN:C	3:A:109:ILE:H	2.14	0.51
3:A:143:ARG:HD3	6:A:966:HOH:O	2.10	0.51
3:A:40:GLU:OE2	3:A:286:TYR:HB3	2.11	0.51
3:A:703:ALA:O	3:A:707:ALA:N	2.43	0.51
3:A:841:VAL:HG23	3:A:842:LEU:N	2.24	0.51
3:A:711:LYS:HG2	3:A:717:GLU:O	2.11	0.51
3:A:103:PHE:O	3:A:105:PHE:N	2.43	0.51
3:A:254:ILE:HG22	3:A:399:GLU:HG3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:402:LEU:CD2	6:A:931:HOH:O	2.57	0.51
3:A:79:PRO:O	3:A:80:LYS:C	2.49	0.51
1:T:20:DT:C2'	1:T:21:DT:H5''	2.41	0.51
3:A:308:TYR:CD2	3:A:734:PRO:HG2	2.46	0.51
3:A:826:LYS:O	3:A:830:GLU:HG3	2.11	0.51
3:A:740:LYS:HB3	3:A:768:GLU:O	2.10	0.51
3:A:676:TYR:O	3:A:679:LYS:HB3	2.11	0.51
1:T:22:DA:H4'	3:A:94:ALA:O	2.10	0.51
3:A:281:ILE:N	3:A:281:ILE:HD13	2.12	0.51
3:A:712:ASP:O	3:A:714:LYS:N	2.44	0.51
3:A:632:ARG:HH11	3:A:632:ARG:HB3	1.76	0.51
3:A:511:PHE:O	3:A:514:PHE:HB3	2.10	0.51
3:A:320:ILE:HD11	3:A:420:MET:CE	2.41	0.51
3:A:193:LYS:O	3:A:196:LEU:HD13	2.10	0.51
3:A:169:GLN:NE2	3:A:171:ASN:N	2.59	0.50
3:A:810:ILE:HB	3:A:813:SER:HB3	1.93	0.50
3:A:743:ILE:HG13	3:A:763:THR:HG1	1.75	0.50
3:A:133:THR:HA	3:A:243:THR:HG22	1.93	0.50
3:A:525:GLY:C	3:A:527:SER:H	2.13	0.50
3:A:452:ILE:CD1	3:A:456:GLY:CA	2.54	0.50
3:A:121:THR:HG22	3:A:141:ILE:HD13	1.93	0.50
3:A:275:PRO:HD3	3:A:415:TRP:CG	2.46	0.50
3:A:872:LEU:CA	3:A:875:ILE:HD13	2.41	0.50
2:P:109:DC:H2''	2:P:110:DT:H5'	1.92	0.50
3:A:281:ILE:HD12	3:A:309:GLU:HA	1.92	0.50
3:A:447:ALA:C	3:A:449:GLY:H	2.13	0.50
3:A:595:VAL:CG2	3:A:597:VAL:HG23	2.41	0.50
3:A:169:GLN:HE21	3:A:172:LYS:N	2.08	0.50
3:A:424:GLY:O	3:A:425:ARG:C	2.49	0.50
3:A:225:GLY:O	3:A:226:MET:C	2.49	0.50
3:A:596:THR:OG1	3:A:608:LYS:HG2	2.11	0.50
3:A:791:LEU:O	3:A:794:THR:HB	2.11	0.50
3:A:390:ALA:O	3:A:393:SER:HB3	2.11	0.50
3:A:330:ILE:HD13	3:A:408:PHE:O	2.10	0.50
3:A:150:ARG:O	3:A:151:PHE:HB2	2.11	0.50
3:A:227:VAL:HB	3:A:244:ILE:HG22	1.92	0.50
3:A:195:LEU:C	3:A:196:LEU:HD12	2.32	0.50
3:A:39:LEU:O	3:A:42:GLU:N	2.44	0.50
3:A:77:LEU:HD23	3:A:224:THR:HG21	1.94	0.50
3:A:120:LYS:HD2	3:A:265:SER:O	2.12	0.50
3:A:338:ALA:O	3:A:342:THR:HG23	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:443:LEU:O	3:A:444:LEU:HD23	2.12	0.50
3:A:875:ILE:N	3:A:875:ILE:CD1	2.75	0.50
3:A:107:GLN:O	3:A:109:ILE:N	2.45	0.50
3:A:342:THR:HG21	3:A:439:MET:HE1	1.94	0.50
3:A:709:GLU:HB3	3:A:722:ARG:HG3	1.93	0.50
3:A:561:LEU:HD23	3:A:561:LEU:O	2.11	0.50
3:A:784:HIS:HA	3:A:787:ASP:OD1	2.12	0.50
3:A:405:ALA:O	3:A:406:ASN:C	2.51	0.49
3:A:234:ALA:C	3:A:236:VAL:H	2.15	0.49
3:A:685:VAL:HG23	3:A:686:SER:N	2.27	0.49
3:A:856:SER:C	3:A:858:LEU:HD22	2.33	0.49
3:A:141:ILE:C	3:A:145:ILE:HD12	2.33	0.49
3:A:334:VAL:HB	3:A:443:LEU:HD23	1.93	0.49
2:P:101:DT:H1'	2:P:102:DA:H5'	1.93	0.49
3:A:779:ALA:N	3:A:780:PRO:HD2	2.26	0.49
3:A:792:ARG:O	3:A:793:LYS:C	2.48	0.49
3:A:51:PHE:HE1	3:A:75:THR:HA	1.77	0.49
3:A:771:ALA:O	3:A:772:HIS:C	2.50	0.49
3:A:710:VAL:HG22	3:A:711:LYS:N	2.27	0.49
3:A:773:LYS:O	3:A:775:GLU:N	2.46	0.49
3:A:445:THR:HG22	3:A:446:LEU:N	2.27	0.49
3:A:374:LEU:HD12	3:A:377:TRP:HB3	1.93	0.49
3:A:17:ALA:HB1	3:A:158:GLU:HA	1.94	0.49
3:A:78:LEU:HD13	3:A:119:ILE:HD11	1.95	0.49
3:A:300:HIS:CG	6:A:913:HOH:O	2.66	0.49
3:A:13:ASP:OD2	3:A:13:ASP:N	2.45	0.49
3:A:337:VAL:O	3:A:340:VAL:HB	2.11	0.49
3:A:267:MET:SD	3:A:267:MET:N	2.85	0.49
3:A:341:ILE:HG13	3:A:342:THR:N	2.28	0.49
3:A:778:ILE:HG23	3:A:779:ALA:N	2.28	0.49
3:A:217:ILE:O	3:A:220:LEU:HB3	2.13	0.49
3:A:275:PRO:HD3	3:A:415:TRP:CB	2.43	0.49
3:A:116:TYR:HA	3:A:119:ILE:HD11	1.94	0.49
3:A:398:LEU:HD23	3:A:398:LEU:C	2.33	0.49
3:A:404:GLN:O	3:A:407:LYS:HB3	2.13	0.49
3:A:775:GLU:C	3:A:777:GLY:H	2.16	0.49
3:A:174:VAL:HG13	3:A:176:HIS:H	1.76	0.49
1:T:12:DG:OP1	3:A:242:GLU:OE2	2.31	0.49
3:A:481:PHE:HA	3:A:484:GLU:OE1	2.12	0.49
3:A:142:GLY:HA2	3:A:145:ILE:HD12	1.95	0.49
3:A:73:LEU:CD2	3:A:260:ALA:HB1	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:237:VAL:HG12	3:A:237:VAL:O	2.11	0.49
3:A:452:ILE:CD1	3:A:818:PRO:HB3	2.43	0.48
3:A:779:ALA:HB3	3:A:780:PRO:CD	2.42	0.48
3:A:552:ASP:HB2	3:A:691:ALA:CB	2.42	0.48
1:T:7:DA:H2''	1:T:8:DT:O4'	2.12	0.48
3:A:81:MET:HB3	3:A:115:ALA:HB1	1.95	0.48
3:A:124:ALA:O	3:A:125:CYS:C	2.52	0.48
1:T:19:DA:H2'	1:T:20:DT:H71	1.96	0.48
3:A:562:LEU:HD22	3:A:563:PRO:HD2	1.94	0.48
3:A:439:MET:HA	3:A:509:PHE:CD2	2.48	0.48
3:A:771:ALA:O	3:A:774:GLN:HB3	2.14	0.48
2:P:102:DA:H1'	2:P:103:DA:C8	2.49	0.48
1:T:19:DA:C2'	1:T:20:DT:H5'	2.29	0.48
3:A:479:ILE:O	3:A:483:GLU:OE1	2.31	0.48
3:A:620:TRP:CE3	3:A:677:MET:HE3	2.48	0.48
3:A:421:ASP:CG	3:A:423:ARG:HD3	2.34	0.48
3:A:841:VAL:HG23	3:A:842:LEU:HD23	1.96	0.48
3:A:81:MET:O	3:A:85:ILE:HG12	2.13	0.48
3:A:347:CYS:SG	3:A:348:PRO:HD2	2.54	0.48
3:A:257:ARG:O	3:A:260:ALA:HB2	2.14	0.48
3:A:261:LEU:HB3	3:A:264:ILE:HB	1.96	0.48
3:A:474:PRO:C	3:A:476:PRO:HD2	2.33	0.48
3:A:449:GLY:C	3:A:450:LYS:HD3	2.34	0.48
3:A:711:LYS:HZ3	3:A:714:LYS:HA	1.77	0.48
3:A:373:ALA:O	3:A:377:TRP:HB2	2.13	0.48
3:A:229:LEU:CD1	3:A:242:GLU:HG2	2.44	0.48
3:A:398:LEU:HD22	3:A:399:GLU:OE2	2.13	0.48
3:A:579:ASN:HA	3:A:582:LEU:CD1	2.34	0.48
3:A:460:LEU:HD21	3:A:518:TYR:HB2	1.95	0.48
3:A:192:SER:O	3:A:195:LEU:HD12	2.14	0.48
3:A:360:LEU:HD13	3:A:385:TYR:HE1	1.79	0.48
3:A:142:GLY:HA2	3:A:145:ILE:CD1	2.44	0.48
3:A:518:TYR:O	3:A:522:GLN:HG3	2.13	0.48
3:A:195:LEU:HA	3:A:289:ASN:HD21	1.79	0.48
3:A:254:ILE:CG2	3:A:399:GLU:HG3	2.44	0.48
1:T:22:DA:O4'	3:A:96:ARG:HB3	2.13	0.48
3:A:350:GLU:C	3:A:352:ILE:H	2.16	0.48
3:A:448:LYS:O	3:A:450:LYS:HD3	2.14	0.48
3:A:401:MET:HE1	3:A:431:MET:O	2.14	0.48
3:A:496:PRO:O	3:A:498:GLU:N	2.47	0.47
3:A:543:ILE:HG22	3:A:559:VAL:HG11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:468:ALA:HA	3:A:505:GLN:CG	2.44	0.47
3:A:796:VAL:O	3:A:799:HIS:HB3	2.14	0.47
3:A:90:GLU:O	3:A:92:VAL:N	2.47	0.47
3:A:433:ASN:ND2	6:A:905:HOH:O	2.30	0.47
3:A:230:HIS:HA	6:A:963:HOH:O	2.14	0.47
3:A:299:THR:OG1	3:A:305:LEU:HB2	2.14	0.47
3:A:446:LEU:HD11	3:A:533:PRO:HB3	1.94	0.47
3:A:713:LYS:HD2	3:A:713:LYS:O	2.14	0.47
3:A:116:TYR:O	3:A:117:ILE:O	2.32	0.47
3:A:126:LEU:HD11	3:A:227:VAL:HG11	1.95	0.47
3:A:846:TYR:HA	3:A:849:PHE:CE1	2.49	0.47
3:A:786:GLN:C	3:A:788:GLY:H	2.16	0.47
3:A:278:TRP:HZ3	3:A:282:THR:HA	1.80	0.47
3:A:486:HIS:HD2	3:A:518:TYR:OH	1.96	0.47
3:A:124:ALA:CB	6:A:984:HOH:O	2.61	0.47
3:A:144:ALA:O	3:A:147:ASP:HB2	2.14	0.47
3:A:402:LEU:HD13	6:A:931:HOH:O	1.82	0.47
3:A:740:LYS:CB	3:A:768:GLU:O	2.62	0.47
3:A:702:ALA:O	3:A:706:LEU:HD23	2.14	0.47
3:A:775:GLU:C	3:A:777:GLY:N	2.67	0.47
3:A:20:PRO:HG2	3:A:289:ASN:HB2	1.97	0.47
1:T:9:DA:C4'	3:A:762:ASN:HD21	2.28	0.47
3:A:478:ARG:O	3:A:481:PHE:HB3	2.15	0.47
3:A:459:TRP:HA	3:A:462:ILE:HB	1.96	0.47
3:A:835:THR:C	3:A:837:GLU:H	2.18	0.47
3:A:141:ILE:O	3:A:142:GLY:C	2.53	0.47
3:A:117:ILE:HD12	3:A:144:ALA:HB1	1.97	0.47
3:A:39:LEU:O	3:A:40:GLU:C	2.52	0.47
3:A:349:VAL:CG1	3:A:352:ILE:HG12	2.44	0.47
3:A:465:ALA:HB1	3:A:470:VAL:HB	1.95	0.47
3:A:108:GLU:HG3	3:A:108:GLU:H	1.31	0.47
3:A:116:TYR:O	3:A:117:ILE:C	2.51	0.47
3:A:740:LYS:HE2	3:A:767:SER:O	2.14	0.47
3:A:401:MET:CE	3:A:432:PHE:HA	2.44	0.47
1:T:7:DA:H2''	1:T:8:DT:O5'	2.15	0.47
3:A:573:ILE:HD11	3:A:688:THR:HG21	1.96	0.47
3:A:370:ASN:N	3:A:371:PRO:CD	2.77	0.47
3:A:452:ILE:C	3:A:452:ILE:HD12	2.34	0.46
3:A:137:VAL:HG21	3:A:244:ILE:CD1	2.34	0.46
3:A:254:ILE:O	3:A:254:ILE:HG22	2.15	0.46
3:A:545:HIS:O	3:A:549:MET:HG2	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:454:LYS:HD3	3:A:454:LYS:C	2.36	0.46
3:A:51:PHE:CE1	3:A:75:THR:HA	2.49	0.46
3:A:134:VAL:HA	3:A:244:ILE:HD11	1.97	0.46
1:T:3:DT:P	1:T:3:DT:H3'	2.55	0.46
3:A:250:TYR:O	3:A:254:ILE:HG13	2.14	0.46
3:A:338:ALA:C	6:A:931:HOH:O	2.53	0.46
3:A:579:ASN:CA	3:A:582:LEU:HD12	2.35	0.46
3:A:829:ARG:HH21	3:A:882:PHE:HA	1.80	0.46
3:A:154:ILE:HD12	3:A:154:ILE:N	2.29	0.46
3:A:90:GLU:OE2	3:A:90:GLU:HA	2.15	0.46
3:A:746:ARG:C	3:A:747:LEU:HD12	2.36	0.46
3:A:351:ASP:O	3:A:394:ARG:NH1	2.48	0.46
3:A:582:LEU:HB3	3:A:621:LEU:HD21	1.97	0.46
3:A:316:VAL:O	3:A:319:ALA:HB3	2.15	0.46
3:A:809:LEU:HD12	3:A:809:LEU:O	2.15	0.46
3:A:266:PRO:C	3:A:268:PHE:H	2.19	0.46
3:A:387:LYS:HD3	3:A:387:LYS:O	2.15	0.46
3:A:226:MET:HA	3:A:250:TYR:CE2	2.51	0.46
2:P:113:DC:H3'	2:P:114:DT:H4'	1.98	0.46
3:A:174:VAL:HG13	3:A:175:GLY:N	2.31	0.46
3:A:524:HIS:HB2	3:A:528:TYR:HB2	1.98	0.46
3:A:850:ALA:HA	3:A:854:HIS:NE2	2.30	0.46
3:A:711:LYS:HD2	3:A:712:ASP:O	2.15	0.46
3:A:679:LYS:O	3:A:683:GLU:HG3	2.15	0.46
3:A:224:THR:HG22	3:A:250:TYR:OH	2.16	0.46
3:A:773:LYS:C	3:A:775:GLU:N	2.68	0.46
3:A:775:GLU:O	3:A:777:GLY:N	2.49	0.46
3:A:148:GLU:CD	3:A:155:ARG:HD3	2.36	0.46
3:A:631:LYS:O	3:A:634:VAL:HG23	2.15	0.46
2:P:105:DA:OP1	3:A:95:LYS:HE2	2.16	0.46
2:P:105:DA:N3	3:A:98:LYS:HE2	2.31	0.46
3:A:677:MET:HG3	3:A:681:ILE:CD1	2.43	0.46
3:A:726:HIS:CD2	3:A:852:GLN:HE22	2.34	0.46
3:A:345:LYS:CD	3:A:355:ILE:HD11	2.40	0.46
3:A:830:GLU:O	3:A:834:ASP:HB3	2.16	0.46
3:A:496:PRO:C	3:A:498:GLU:N	2.70	0.46
3:A:703:ALA:HA	3:A:706:LEU:CG	2.45	0.45
3:A:371:PRO:HG2	3:A:373:ALA:H	1.81	0.45
3:A:651:LEU:HA	3:A:655:ILE:HB	1.97	0.45
3:A:849:PHE:O	3:A:850:ALA:C	2.53	0.45
3:A:425:ARG:CZ	6:A:903:HOH:O	2.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:729:THR:HG21	3:A:733:PHE:HB3	1.99	0.45
3:A:176:HIS:CD2	3:A:178:TYR:HA	2.51	0.45
3:A:269:GLN:HE21	3:A:404:GLN:CD	2.18	0.45
3:A:687:VAL:HA	3:A:690:VAL:HG13	1.99	0.45
3:A:771:ALA:O	3:A:774:GLN:N	2.49	0.45
3:A:107:GLN:HG3	3:A:108:GLU:H	1.81	0.45
3:A:135:GLN:N	3:A:135:GLN:OE1	2.46	0.45
3:A:861:MET:O	3:A:862:PRO:O	2.35	0.45
3:A:210:ILE:HG13	3:A:761:ILE:HD13	1.98	0.45
3:A:359:GLU:O	3:A:384:VAL:HG11	2.17	0.45
3:A:458:TYR:HE1	3:A:479:ILE:CD1	2.29	0.45
3:A:711:LYS:NZ	3:A:714:LYS:HA	2.32	0.45
3:A:875:ILE:N	3:A:875:ILE:HD12	2.31	0.45
3:A:489:ILE:HA	3:A:492:CYS:HB2	1.98	0.45
3:A:502:TRP:CE3	3:A:512:LEU:HB2	2.51	0.45
3:A:488:ASN:HB3	3:A:501:TRP:CE3	2.52	0.45
3:A:496:PRO:C	3:A:498:GLU:H	2.19	0.45
3:A:727:TRP:CD1	3:A:728:VAL:N	2.85	0.45
3:A:141:ILE:HG13	3:A:217:ILE:CD1	2.44	0.45
3:A:393:SER:O	3:A:396:ILE:CG2	2.65	0.45
3:A:545:HIS:CE1	3:A:787:ASP:HB3	2.52	0.45
3:A:20:PRO:HA	3:A:195:LEU:HD21	1.99	0.45
3:A:734:PRO:HB2	3:A:736:TRP:CH2	2.52	0.45
3:A:492:CYS:HA	3:A:499:ASN:HB2	1.97	0.45
2:P:103:DA:C2'	2:P:104:DT:H5''	2.46	0.45
3:A:557:ARG:CB	3:A:562:LEU:HD12	2.38	0.45
3:A:712:ASP:CG	3:A:713:LYS:N	2.69	0.45
3:A:159:ALA:C	3:A:161:HIS:N	2.70	0.45
3:A:77:LEU:H	3:A:77:LEU:CD1	2.21	0.45
3:A:786:GLN:C	3:A:788:GLY:N	2.71	0.45
3:A:25:ALA:HA	3:A:29:GLY:O	2.17	0.45
3:A:611:LEU:CD2	3:A:612:GLY:H	2.30	0.45
3:A:756:ARG:HB3	3:A:758:GLN:NE2	2.25	0.44
3:A:537:ASP:O	3:A:882:PHE:HD2	2.01	0.44
3:A:31:ARG:HG2	3:A:31:ARG:HH11	1.83	0.44
3:A:118:THR:CG2	3:A:220:LEU:HD22	2.43	0.44
3:A:28:TYR:CD1	3:A:183:MET:HG3	2.52	0.44
3:A:192:SER:HB3	3:A:195:LEU:CD1	2.47	0.44
3:A:196:LEU:HB3	3:A:197:GLY:H	1.57	0.44
3:A:126:LEU:C	3:A:128:SER:H	2.20	0.44
3:A:576:LYS:HA	3:A:579:ASN:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:103:DA:H5'	3:A:96:ARG:NH2	2.32	0.44
3:A:772:HIS:O	3:A:775:GLU:HB3	2.17	0.44
3:A:779:ALA:HB3	3:A:780:PRO:HD3	2.00	0.44
3:A:639:TYR:CE1	3:A:784:HIS:HE1	2.34	0.44
3:A:300:HIS:HB3	6:A:913:HOH:O	2.17	0.44
3:A:300:HIS:O	3:A:301:SER:HB2	2.17	0.44
3:A:631:LYS:HE2	3:A:635:MET:SD	2.58	0.44
3:A:574:VAL:O	3:A:578:VAL:HB	2.18	0.44
3:A:227:VAL:HA	3:A:246:LEU:HA	2.00	0.44
3:A:739:TYR:H	3:A:774:GLN:NE2	2.13	0.44
3:A:532:LEU:HD12	3:A:533:PRO:CD	2.47	0.44
3:A:278:TRP:CE2	3:A:284:GLY:HA3	2.52	0.44
3:A:709:GLU:N	3:A:722:ARG:HG2	2.33	0.44
3:A:748:ASN:O	3:A:749:LEU:HD23	2.18	0.44
3:A:556:GLY:HA2	3:A:559:VAL:CG2	2.48	0.44
3:A:391:ARG:O	3:A:392:LYS:C	2.55	0.44
3:A:719:LEU:N	3:A:719:LEU:HD12	2.31	0.44
3:A:119:ILE:O	3:A:123:LEU:HG	2.17	0.44
3:A:224:THR:HG22	3:A:226:MET:H	1.81	0.44
1:T:16:DC:H2"	1:T:17:DG:C8	2.52	0.44
3:A:423:ARG:HH22	3:A:784:HIS:CD2	2.35	0.44
3:A:562:LEU:C	3:A:564:SER:H	2.21	0.44
3:A:363:LYS:HZ3	3:A:364:PRO:HG2	1.82	0.44
3:A:394:ARG:NH1	3:A:394:ARG:HG2	2.31	0.44
3:A:512:LEU:O	3:A:515:CYS:N	2.50	0.44
3:A:105:PHE:HA	3:A:108:GLU:OE1	2.18	0.44
3:A:472:LYS:C	3:A:567:VAL:HG21	2.38	0.44
3:A:842:LEU:HG	3:A:843:ALA:N	2.32	0.44
3:A:313:MET:SD	3:A:734:PRO:HD2	2.58	0.44
2:P:105:DA:H1'	2:P:106:DC:C5'	2.44	0.44
3:A:475:PHE:N	3:A:476:PRO:CD	2.81	0.44
3:A:704:LYS:C	3:A:706:LEU:H	2.21	0.44
3:A:605:ILE:HD11	3:A:608:LYS:HD2	1.99	0.44
3:A:245:GLU:HG3	3:A:389:LYS:HD3	2.00	0.44
3:A:186:VAL:HB	3:A:187:GLU:H	1.70	0.43
3:A:461:LYS:HG2	3:A:482:ILE:HG21	1.99	0.43
1:T:17:DG:N2	2:P:107:DG:C2	2.86	0.43
3:A:795:VAL:HG23	3:A:796:VAL:N	2.33	0.43
3:A:826:LYS:HB3	3:A:826:LYS:HZ2	1.84	0.43
3:A:428:ALA:H	3:A:435:GLN:HE22	1.67	0.43
3:A:809:LEU:HD12	3:A:809:LEU:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:505:GLN:O	3:A:508:PRO:HD3	2.18	0.43
3:A:501:TRP:HA	3:A:504:GLU:OE2	2.17	0.43
3:A:402:LEU:HD21	6:A:931:HOH:O	2.18	0.43
3:A:297:VAL:O	3:A:299:THR:HG23	2.17	0.43
3:A:167:GLU:O	3:A:167:GLU:HG3	2.18	0.43
3:A:17:ALA:HB1	3:A:158:GLU:HG3	2.00	0.43
3:A:50:ARG:O	3:A:53:LYS:HB3	2.17	0.43
3:A:377:TRP:C	3:A:379:ARG:N	2.72	0.43
3:A:785:SER:O	3:A:789:SER:HB2	2.18	0.43
3:A:211:HIS:O	3:A:215:ARG:HB2	2.18	0.43
3:A:835:THR:O	3:A:839:CYS:HB2	2.18	0.43
3:A:138:ALA:O	3:A:139:SER:C	2.54	0.43
3:A:73:LEU:O	3:A:77:LEU:CD1	2.66	0.43
3:A:798:ALA:HB1	3:A:804:ILE:CD1	2.26	0.43
3:A:549:MET:SD	3:A:841:VAL:HG21	2.59	0.43
3:A:828:VAL:O	3:A:831:THR:OG1	2.35	0.43
3:A:501:TRP:HB2	6:A:935:HOH:O	2.18	0.43
3:A:142:GLY:N	3:A:145:ILE:HD12	2.34	0.43
3:A:363:LYS:CE	3:A:367:ILE:HA	2.49	0.43
3:A:374:LEU:HA	3:A:377:TRP:CB	2.49	0.43
3:A:731:ASP:OD2	3:A:789:SER:OG	2.32	0.43
3:A:491:ALA:HB3	3:A:499:ASN:OD1	2.18	0.43
3:A:512:LEU:HA	3:A:512:LEU:HD12	1.76	0.43
3:A:723:CYS:HB3	3:A:853:LEU:CD1	2.49	0.43
3:A:187:GLU:N	3:A:187:GLU:CD	2.72	0.43
3:A:643:GLU:CD	3:A:679:LYS:HA	2.39	0.43
3:A:136:ALA:O	3:A:137:VAL:C	2.57	0.43
3:A:161:HIS:C	3:A:163:LYS:H	2.20	0.43
3:A:631:LYS:HB3	3:A:632:ARG:H	1.73	0.43
3:A:36:GLN:HE21	3:A:40:GLU:HG3	1.84	0.43
3:A:855:GLU:O	3:A:858:LEU:HD21	2.19	0.42
3:A:465:ALA:O	3:A:466:ASN:C	2.57	0.42
3:A:610:LYS:HD2	3:A:610:LYS:HA	1.79	0.42
3:A:473:VAL:CG2	3:A:474:PRO:HD2	2.29	0.42
3:A:849:PHE:HA	3:A:852:GLN:HB3	2.00	0.42
3:A:278:TRP:O	3:A:279:THR:HG23	2.19	0.42
3:A:355:ILE:HG22	3:A:395:ARG:HH21	1.85	0.42
3:A:559:VAL:C	3:A:561:LEU:H	2.22	0.42
3:A:425:ARG:HD3	3:A:811:HIS:CD2	2.54	0.42
3:A:465:ALA:HA	3:A:468:ALA:HB3	2.00	0.42
3:A:729:THR:CG2	3:A:733:PHE:HB3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:824:LEU:O	3:A:826:LYS:N	2.52	0.42
3:A:201:TRP:HE3	3:A:202:SER:H	1.68	0.42
3:A:403:GLU:O	3:A:407:LYS:N	2.51	0.42
2:P:110:DT:H2'	2:P:110:DT:H6	1.74	0.42
3:A:545:HIS:O	3:A:548:ALA:HB3	2.19	0.42
3:A:718:ILE:HD12	3:A:718:ILE:C	2.39	0.42
3:A:169:GLN:HE21	3:A:171:ASN:N	2.17	0.42
3:A:28:TYR:HD1	3:A:183:MET:HB2	1.84	0.42
3:A:286:TYR:HD2	3:A:294:LEU:HD21	1.84	0.42
3:A:465:ALA:O	3:A:468:ALA:N	2.53	0.42
3:A:295:ALA:O	3:A:419:ASN:OD1	2.37	0.42
3:A:383:ALA:O	3:A:387:LYS:HB2	2.19	0.42
3:A:335:LEU:HA	3:A:443:LEU:HD21	2.01	0.42
3:A:774:GLN:HA	3:A:774:GLN:HE21	1.84	0.42
3:A:855:GLU:CG	3:A:856:SER:H	2.14	0.42
3:A:323:ALA:O	3:A:326:THR:OG1	2.32	0.42
3:A:471:ASP:HA	3:A:478:ARG:HH21	1.85	0.42
3:A:616:LEU:HD23	3:A:676:TYR:CG	2.55	0.42
3:A:438:ASP:OD2	3:A:509:PHE:HB2	2.19	0.42
3:A:693:VAL:HA	3:A:696:MET:HE2	2.01	0.42
3:A:349:VAL:HG12	3:A:352:ILE:HG12	2.02	0.42
3:A:133:THR:HB	3:A:135:GLN:OE1	2.20	0.42
3:A:646:PHE:HB2	3:A:678:ALA:CB	2.50	0.42
3:A:549:MET:O	3:A:550:LEU:HD23	2.20	0.42
3:A:103:PHE:O	3:A:104:GLN:C	2.58	0.42
3:A:485:ASN:O	3:A:488:ASN:HB2	2.19	0.42
3:A:298:ARG:HE	3:A:419:ASN:HD22	1.67	0.42
3:A:147:ASP:OD1	3:A:292:ARG:HD3	2.19	0.42
3:A:344:TRP:N	3:A:344:TRP:CD1	2.88	0.42
1:T:17:DG:H2''	1:T:18:DT:H5''	2.02	0.42
3:A:857:GLN:O	3:A:858:LEU:HB2	2.20	0.42
3:A:460:LEU:HD23	3:A:461:LYS:N	2.34	0.42
3:A:174:VAL:HG13	3:A:177:VAL:H	1.82	0.42
3:A:159:ALA:HA	3:A:162:PHE:HD2	1.80	0.42
3:A:269:GLN:HE22	3:A:407:LYS:HE3	1.85	0.41
3:A:740:LYS:HB3	3:A:766:ASP:OD2	2.20	0.41
3:A:595:VAL:HG23	3:A:596:THR:N	2.35	0.41
3:A:177:VAL:HB	3:A:179:LYS:CD	2.43	0.41
3:A:154:ILE:O	3:A:158:GLU:HB2	2.20	0.41
3:A:261:LEU:HD21	3:A:396:ILE:CD1	2.49	0.41
3:A:365:GLU:HB2	3:A:366:ASP:H	1.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:360:LEU:HB3	3:A:384:VAL:HG21	2.02	0.41
3:A:312:TYR:C	3:A:314:PRO:HD3	2.40	0.41
3:A:693:VAL:O	3:A:697:ASN:ND2	2.53	0.41
1:T:8:DT:OP1	1:T:8:DT:H4'	2.20	0.41
3:A:452:ILE:HG22	3:A:528:TYR:O	2.20	0.41
3:A:560:ASN:CB	3:A:881:ALA:HB2	2.41	0.41
3:A:620:TRP:CH2	3:A:677:MET:HB2	2.56	0.41
3:A:371:PRO:HG2	3:A:372:GLU:N	2.35	0.41
3:A:84:ARG:HD2	3:A:84:ARG:HA	1.91	0.41
3:A:42:GLU:HG2	3:A:50:ARG:NH1	2.35	0.41
3:A:133:THR:C	3:A:135:GLN:N	2.74	0.41
3:A:487:GLU:HA	3:A:490:MET:HG2	2.03	0.41
3:A:453:GLY:HA2	3:A:526:LEU:O	2.20	0.41
3:A:308:TYR:CE2	3:A:736:TRP:HZ3	2.38	0.41
3:A:275:PRO:O	3:A:277:PRO:HD3	2.20	0.41
3:A:542:GLY:HA2	3:A:783:VAL:HG13	2.03	0.41
3:A:120:LYS:HA	3:A:123:LEU:HD12	2.03	0.41
3:A:159:ALA:O	3:A:163:LYS:HG2	2.21	0.41
3:A:452:ILE:HG23	3:A:453:GLY:N	2.35	0.41
3:A:570:ILE:HG23	3:A:571:TYR:N	2.35	0.41
3:A:879:ASP:N	3:A:879:ASP:OD1	2.54	0.41
3:A:725:VAL:CB	3:A:737:GLN:HB2	2.38	0.41
3:A:324:GLN:C	3:A:326:THR:H	2.24	0.41
3:A:88:TRP:O	3:A:92:VAL:HG23	2.21	0.41
3:A:505:GLN:OE1	3:A:505:GLN:N	2.54	0.41
3:A:826:LYS:CB	3:A:826:LYS:HZ2	2.33	0.41
3:A:396:ILE:O	3:A:396:ILE:HG13	2.20	0.41
2:P:106:DC:H2''	2:P:107:DG:C8	2.54	0.41
3:A:297:VAL:HG11	3:A:308:TYR:CE1	2.56	0.41
3:A:537:ASP:OD1	3:A:813:SER:HB2	2.21	0.41
3:A:651:LEU:O	3:A:656:GLN:N	2.51	0.41
3:A:105:PHE:CD1	3:A:105:PHE:N	2.89	0.41
3:A:570:ILE:O	3:A:573:ILE:HG12	2.21	0.41
1:T:17:DG:C2'	1:T:18:DT:H5''	2.51	0.41
3:A:546:PHE:CZ	3:A:696:MET:HG2	2.56	0.41
3:A:773:LYS:O	3:A:774:GLN:C	2.59	0.41
3:A:234:ALA:C	3:A:236:VAL:N	2.74	0.41
3:A:30:GLU:HG2	3:A:166:VAL:HG21	2.03	0.41
3:A:215:ARG:NH1	3:A:218:GLU:OE1	2.54	0.41
3:A:111:PRO:C	3:A:113:ALA:N	2.74	0.41
3:A:797:TRP:HZ2	3:A:801:LYS:HZ2	1.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:121:THR:HA	3:A:267:MET:HE3	2.03	0.41
3:A:339:ASN:N	3:A:339:ASN:OD1	2.54	0.41
3:A:646:PHE:HB2	3:A:678:ALA:HB1	2.03	0.41
3:A:784:HIS:O	3:A:788:GLY:N	2.54	0.41
3:A:364:PRO:O	3:A:366:ASP:N	2.54	0.41
3:A:468:ALA:HA	3:A:505:GLN:HB3	2.02	0.41
3:A:100:PRO:O	3:A:103:PHE:HB3	2.21	0.41
3:A:329:LYS:HG2	3:A:330:ILE:N	2.36	0.40
3:A:359:GLU:OE1	3:A:360:LEU:N	2.54	0.40
3:A:639:TYR:HA	3:A:780:PRO:CB	2.52	0.40
3:A:739:TYR:HB2	3:A:774:GLN:HE22	1.77	0.40
3:A:238:GLY:C	3:A:239:GLN:HE21	2.25	0.40
3:A:652:GLU:O	3:A:657:PRO:HD3	2.20	0.40
3:A:6:ILE:N	3:A:6:ILE:CD1	2.82	0.40
3:A:480:LYS:O	3:A:484:GLU:HG3	2.20	0.40
3:A:599:ASP:HB3	3:A:600:GLU:H	1.72	0.40
3:A:331:ASN:ND2	3:A:331:ASN:C	2.75	0.40
3:A:475:PHE:C	3:A:479:ILE:HD12	2.41	0.40
3:A:655:ILE:HD12	3:A:667:PHE:CE1	2.56	0.40
3:A:542:GLY:CA	3:A:783:VAL:HG13	2.52	0.40
3:A:78:LEU:HB3	3:A:79:PRO:CD	2.51	0.40
3:A:308:TYR:OH	3:A:735:VAL:HA	2.22	0.40
3:A:809:LEU:HA	3:A:813:SER:O	2.21	0.40
3:A:882:PHE:O	3:A:883:ALA:C	2.59	0.40
3:A:195:LEU:N	3:A:195:LEU:HD12	2.36	0.40
3:A:350:GLU:C	3:A:352:ILE:N	2.75	0.40
3:A:8:LYS:C	3:A:10:ASP:N	2.75	0.40
3:A:102:ALA:C	3:A:106:LEU:HD12	2.42	0.40
3:A:41:HIS:C	3:A:43:SER:N	2.74	0.40
3:A:267:MET:HE1	6:A:984:HOH:O	1.80	0.40
3:A:335:LEU:HD22	3:A:406:ASN:OD1	2.21	0.40
3:A:582:LEU:O	3:A:617:ALA:HB1	2.22	0.40
3:A:816:THR:CG2	3:A:817:ILE:N	2.75	0.40
3:A:234:ALA:O	3:A:236:VAL:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:498:GLU:OE1	3:A:619:GLN:NE2[3_646]	2.08	0.12

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
3	A	858/878 (98%)	558 (65%)	218 (25%)	82 (10%)	1 0

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	362	MET
3	A	371	PRO
3	A	595	VAL
3	A	598	THR
3	A	609	VAL
3	A	704	LYS
3	A	722	ARG
3	A	861	MET
3	A	862	PRO
3	A	104	GLN
3	A	108	GLU
3	A	119	ILE
3	A	137	VAL
3	A	176	HIS
3	A	189	ASP
3	A	354	ALA
3	A	359	GLU
3	A	365	GLU
3	A	366	ASP
3	A	541	SER
3	A	592	ASN
3	A	689	VAL
3	A	690	VAL
3	A	713	LYS
3	A	7	ALA
3	A	91	GLU
3	A	117	ILE
3	A	118	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	165	ASN
3	A	182	PHE
3	A	262	ALA
3	A	279	THR
3	A	288	ALA
3	A	338	ALA
3	A	409	ALA
3	A	411	HIS
3	A	448	LYS
3	A	538	GLY
3	A	560	ASN
3	A	667	PHE
3	A	738	GLU
3	A	764	ASN
3	A	774	GLN
3	A	825	PHE
3	A	830	GLU
3	A	841	VAL
3	A	36	GLN
3	A	142	GLY
3	A	169	GLN
3	A	179	LYS
3	A	199	GLU
3	A	226	MET
3	A	270	PRO
3	A	309	GLU
3	A	625	VAL
3	A	681	ILE
3	A	703	ALA
3	A	705	LEU
3	A	772	HIS
3	A	834	ASP
3	A	73	LEU
3	A	185	VAL
3	A	257	ARG
3	A	266	PRO
3	A	298	ARG
3	A	451	PRO
3	A	628	SER
3	A	771	ALA
3	A	833	VAL
3	A	849	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	857	GLN
3	A	859	ASP
3	A	141	ILE
3	A	233	ASN
3	A	564	SER
3	A	607	GLU
3	A	235	GLY
3	A	237	VAL
3	A	85	ILE
3	A	589	GLY
3	A	597	VAL
3	A	542	GLY

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
3	A	714/724 (99%)	617 (86%)	97 (14%)	5 8

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	ILE
3	A	11	PHE
3	A	13	ASP
3	A	26	ASP
3	A	46	MET
3	A	48	GLU
3	A	52	ARG
3	A	74	ILE
3	A	81	MET
3	A	87	ASP
3	A	99	ARG
3	A	101	THR
3	A	105	PHE
3	A	107	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	108	GLU
3	A	119	ILE
3	A	127	THR
3	A	139	SER
3	A	146	GLU
3	A	148	GLU
3	A	162	PHE
3	A	168	GLU
3	A	173	ARG
3	A	179	LYS
3	A	183	MET
3	A	186	VAL
3	A	187	GLU
3	A	199	GLU
3	A	201	TRP
3	A	206	LYS
3	A	242	GLU
3	A	244	ILE
3	A	273	VAL
3	A	279	THR
3	A	281	ILE
3	A	296	LEU
3	A	300	HIS
3	A	307	ARG
3	A	331	ASN
3	A	333	LYS
3	A	335	LEU
3	A	351	ASP
3	A	359	GLU
3	A	366	ASP
3	A	397	SER
3	A	437	ASN
3	A	450	LYS
3	A	452	ILE
3	A	460	LEU
3	A	471	ASP
3	A	472	LYS
3	A	473	VAL
3	A	492	CYS
3	A	498	GLU
3	A	500	THR
3	A	510	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	514	PHE
3	A	529	ASN
3	A	537	ASP
3	A	560	ASN
3	A	576	LYS
3	A	578	VAL
3	A	579	ASN
3	A	588	ASN
3	A	599	ASP
3	A	600	GLU
3	A	605	ILE
3	A	611	LEU
3	A	631	LYS
3	A	632	ARG
3	A	635	MET
3	A	654	THR
3	A	690	VAL
3	A	698	TRP
3	A	704	LYS
3	A	706	LEU
3	A	712	ASP
3	A	713	LYS
3	A	717	GLU
3	A	720	ARG
3	A	729	THR
3	A	735	VAL
3	A	737	GLN
3	A	739	TYR
3	A	752	LEU
3	A	774	GLN
3	A	791	LEU
3	A	793	LYS
3	A	809	LEU
3	A	814	PHE
3	A	817	ILE
3	A	840	ASP
3	A	842	LEU
3	A	854	HIS
3	A	858	LEU
3	A	875	ILE
3	A	877	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such

sidechains are listed below:

Mol	Chain	Res	Type
3	A	22	ASN
3	A	36	GLN
3	A	107	GLN
3	A	169	GLN
3	A	239	GLN
3	A	269	GLN
3	A	289	ASN
3	A	321	ASN
3	A	324	GLN
3	A	325	ASN
3	A	331	ASN
3	A	435	GLN
3	A	485	ASN
3	A	486	HIS
3	A	544	GLN
3	A	560	ASN
3	A	648	GLN
3	A	697	ASN
3	A	737	GLN
3	A	748	ASN
3	A	754	GLN
3	A	758	GLN
3	A	762	ASN
3	A	774	GLN
3	A	781	ASN
3	A	784	HIS
3	A	852	GLN
3	A	857	GLN

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 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
5	GH3	A	901	4	25,33,33	1.55	4 (16%)	29,52,52	2.66	11 (37%)
5	GH3	A	902	-	25,33,33	1.64	4 (16%)	29,52,52	2.58	8 (27%)

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	GH3	A	901	4	-	0/18/34/34	0/3/3/3
5	GH3	A	902	-	-	0/18/34/34	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	902	GH3	C8-N7	-2.10	1.30	1.34
5	A	901	GH3	O2'-C2'	2.08	1.48	1.43
5	A	901	GH3	O4'-C1'	2.28	1.44	1.41
5	A	902	GH3	O2'-C2'	2.44	1.48	1.43
5	A	901	GH3	C2-N1	2.58	1.40	1.35
5	A	902	GH3	C2-N1	3.52	1.41	1.35
5	A	901	GH3	C6-N1	3.77	1.40	1.33
5	A	902	GH3	C6-N1	4.13	1.40	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	902	GH3	C5-C6-N1	-7.37	113.51	123.59
5	A	901	GH3	C5-C6-N1	-7.25	113.67	123.59
5	A	902	GH3	N3-C2-N1	-4.03	121.31	127.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	GH3	N3-C2-N1	-3.67	121.86	127.44
5	A	902	GH3	PB-O3B-PG	-3.56	120.74	132.67
5	A	901	GH3	PB-O3B-PG	-2.94	122.79	132.67
5	A	901	GH3	C6-C5-C4	-2.43	117.99	120.90
5	A	901	GH3	C3'-C4'-C5'	-2.16	110.03	113.91
5	A	901	GH3	C1'-N9-C4	-2.03	123.88	126.94
5	A	902	GH3	O2A-PA-O3A	2.18	114.98	105.09
5	A	901	GH3	O2G-PG-O1G	2.27	117.89	110.58
5	A	901	GH3	O2A-PA-O3A	2.42	116.08	105.09
5	A	902	GH3	O2G-PG-O1G	2.45	118.45	110.58
5	A	902	GH3	O4'-C4'-C3'	2.81	108.88	105.04
5	A	901	GH3	O4'-C4'-C3'	3.35	109.61	105.04
5	A	902	GH3	O4'-C4'-C5'	4.22	115.77	109.54
5	A	901	GH3	O4'-C4'-C5'	5.76	118.05	109.54
5	A	902	GH3	C6-N1-C2	6.43	124.87	115.94
5	A	901	GH3	C6-N1-C2	6.45	124.89	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	T	22/22 (100%)	-0.26	0	100 100	48, 60, 79, 120	0
2	P	14/14 (100%)	-0.72	0	100 100	37, 47, 95, 126	0
3	A	862/878 (98%)	0.55	83 (9%)	10 11	0, 58, 121, 160	0
All	All	898/914 (98%)	0.51	83 (9%)	11 12	0, 58, 121, 160	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	273	VAL	5.9
3	A	629	VAL	4.9
3	A	845	PHE	4.9
3	A	175	GLY	4.5
3	A	543	ILE	4.5
3	A	200	ALA	4.3
3	A	24	LEU	4.2
3	A	535	ALA	4.0
3	A	176	HIS	3.9
3	A	533	PRO	3.8
3	A	788	GLY	3.8
3	A	881	ALA	3.7
3	A	725	VAL	3.6
3	A	178	TYR	3.5
3	A	633	SER	3.5
3	A	780	PRO	3.5
3	A	825	PHE	3.4
3	A	821	ALA	3.4
3	A	827	ALA	3.3
3	A	415	TRP	3.2
3	A	28	TYR	3.2
3	A	715	THR	3.1
3	A	308	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	737	GLN	3.1
3	A	777	GLY	3.1
3	A	875	ILE	3.1
3	A	546	PHE	3.1
3	A	685	VAL	3.1
3	A	828	VAL	3.0
3	A	724	ALA	3.0
3	A	620	TRP	3.0
3	A	414	ILE	3.0
3	A	807	PHE	2.9
3	A	539	SER	2.9
3	A	286	TYR	2.8
3	A	791	LEU	2.8
3	A	804	ILE	2.7
3	A	545	HIS	2.6
3	A	853	LEU	2.6
3	A	214	VAL	2.6
3	A	488	ASN	2.6
3	A	426	VAL	2.6
3	A	201	TRP	2.6
3	A	183	MET	2.6
3	A	427	TYR	2.5
3	A	736	TRP	2.5
3	A	326	THR	2.5
3	A	452	ILE	2.5
3	A	883	ALA	2.4
3	A	582	LEU	2.4
3	A	184	GLN	2.4
3	A	832	MET	2.4
3	A	420	MET	2.4
3	A	784	HIS	2.4
3	A	635	MET	2.3
3	A	323	ALA	2.3
3	A	422	TRP	2.2
3	A	726	HIS	2.2
3	A	806	SER	2.2
3	A	293	PRO	2.2
3	A	316	VAL	2.2
3	A	149	ALA	2.2
3	A	328	TRP	2.2
3	A	396	ILE	2.2
3	A	842	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	311	VAL	2.2
3	A	44	TYR	2.2
3	A	204	TRP	2.2
3	A	185	VAL	2.1
3	A	811	HIS	2.1
3	A	170	LEU	2.1
3	A	824	LEU	2.1
3	A	428	ALA	2.1
3	A	735	VAL	2.1
3	A	829	ARG	2.1
3	A	489	ILE	2.1
3	A	790	HIS	2.1
3	A	421	ASP	2.1
3	A	808	ALA	2.1
3	A	443	LEU	2.1
3	A	17	ALA	2.1
3	A	29	GLY	2.0
3	A	272	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GH3	A	901	31/31	0.87	0.24	-0.07	70,78,90,91	0
5	GH3	A	902	31/31	0.85	0.20	-0.27	60,63,70,72	0
4	MG	A	884	1/1	0.27	0.28	-	23,23,23,23	0
4	MG	A	885	1/1	0.16	2.30	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.