



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:12 AM UTC

PDB ID : 2PI4 / pdb_00002pi4
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

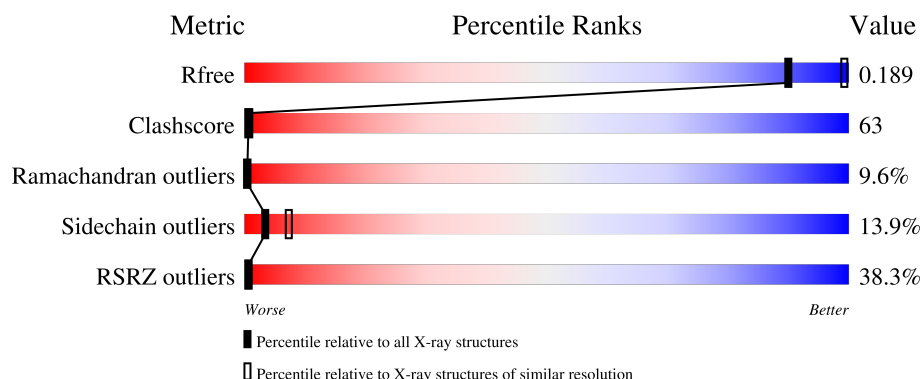
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	22	5% 5% 82% 9% 5%
2	P	14	86% 7% 7%
3	A	878	39% 24% 58% 15% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	885	-	-	-	X

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			

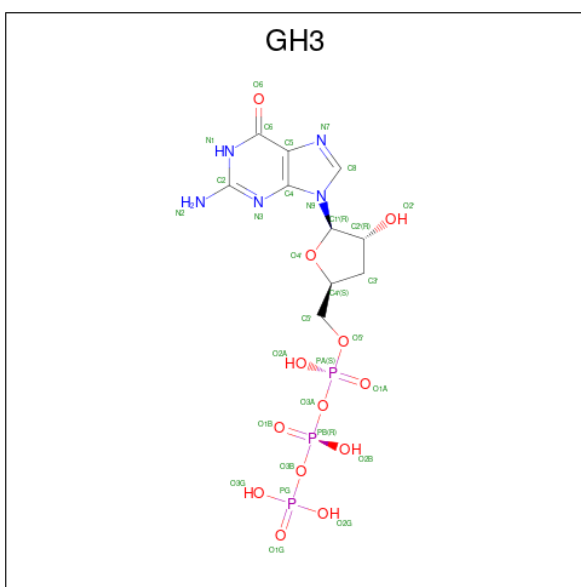
- Molecule 3 is a protein called DNA-directed RNA polymerase.

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 (CCD ID: 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 (CCD ID: 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

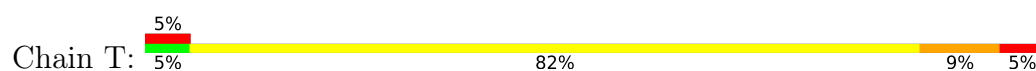
- Molecule 6 is water.

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

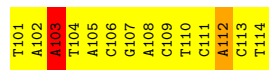
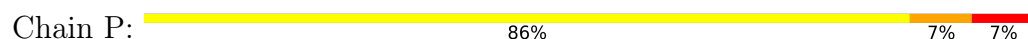
3 Residue-property plots

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

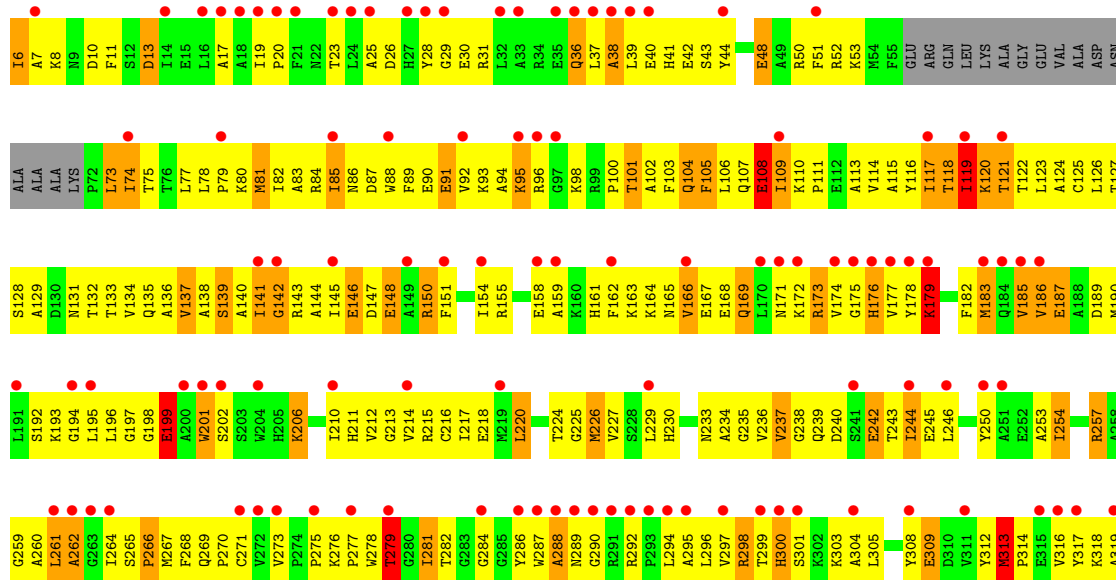
- Molecule 1: 5'-D(*CP*TP*TP*CP*CP*TP*AP*TP*AP*GP*TP*GP*AP*GP*TP*CP*GP*TP*AP*TP*TP*A)-3'

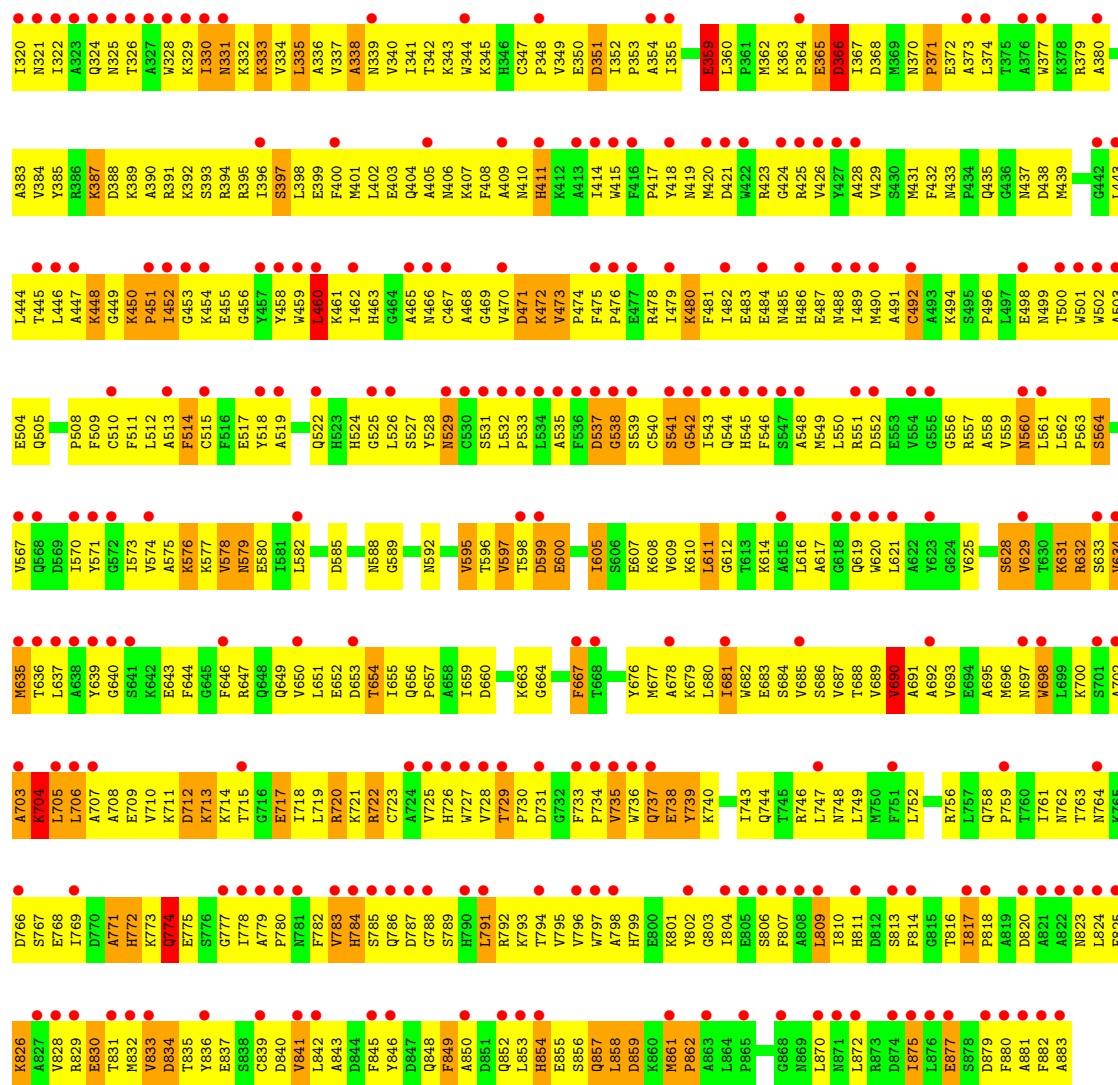


- Molecule 2: 5'-D(*TP*AP*AP*TP*AP*CP*GP*AP*CP*TP*CP*AP*CP*T)-3'



- Molecule 3: DNA-directed RNA polymerase





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) 96.2 (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 (Not available) , 0.189	Depositor DCC
R_{free} test set	2301 reflections (4.98%)	wwPDB-VP
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 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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, 0.333 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, 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	0.43	0/498	0.99	4/767 (0.5%)
2	P	0.44	0/313	0.98	2/480 (0.4%)
3	A	0.72	0/6959	0.96	15/9416 (0.2%)
All	All	0.69	0/7770	0.96	21/10663 (0.2%)

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

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	103	DA	C2'-C3'-O3'	8.69	124.53	111.50
1	T	4	DC	C2'-C3'-O3'	6.37	121.05	111.50
3	A	426	VAL	N-CA-C	6.35	117.64	107.73
1	T	7	DA	N9-C1'-C2'	-6.28	104.08	113.50
1	T	13	DA	C2'-C3'-O3'	6.27	120.90	111.50
3	A	121	THR	CA-C-N	-5.80	112.56	120.44
3	A	121	THR	C-N-CA	-5.80	112.56	120.44
3	A	146	GLU	N-CA-C	-5.74	105.11	111.36
3	A	313	MET	CA-C-N	5.69	125.16	119.24
3	A	313	MET	C-N-CA	5.69	125.16	119.24
2	P	112	DA	C2'-C3'-O3'	5.67	120.00	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	13	DA	C4'-C3'-O3'	5.56	118.34	110.00
3	A	744	GLN	N-CA-C	5.56	117.70	110.53
3	A	254	ILE	N-CA-C	-5.47	108.17	113.53
3	A	783	VAL	CB-CA-C	-5.47	104.97	111.81
3	A	38	ALA	N-CA-C	-5.44	105.26	111.14
3	A	460	LEU	N-CA-C	-5.32	105.38	111.07
3	A	634	VAL	N-CA-C	5.29	115.55	110.74
3	A	784	HIS	N-CA-C	-5.17	105.53	111.07
3	A	220	LEU	N-CA-C	-5.15	106.50	112.89
3	A	150	ARG	N-CA-C	-5.03	102.62	110.42

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	892	1
4	A	2	0	0	0	0
5	A	62	0	24	0	0
6	A	115	0	0	35	0
6	P	7	0	0	0	0
6	T	7	0	0	0	0
All	All	7722	0	7201	934	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 63.

All (934) 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
3:A:332:LYS:NZ	6:A:925:HOH:O	1.83	0.97
3:A:281:ILE:HD13	3:A:281:ILE:H	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:557:ARG:NH2	3:A:562:LEU:HD13	1.84	0.92
3:A:579:ASN:HA	3:A:582:LEU:HD12	1.51	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:123:LEU:HA	3:A:126:LEU:HD12	1.55	0.88
3:A:452:ILE:HD11	3:A:456:GLY:HA3	0.89	0.88
3:A:557:ARG:HB2	3:A:562:LEU:HD12	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	3:A:303:LYS:HD3	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:HD12	3:A:261:LEU:N	1.93	0.84
3:A:77:LEU:HD12	3:A:77:LEU:H	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
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:131:ASN:CG	6:A:980:HOH:O	2.23	0.79
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:HD12	3:A:261:LEU:H	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:324:GLN:HE21	3:A:418:TYR:H	1.31	0.76
3:A:841:VAL:HG23	3:A:842:LEU:H	1.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:124:ALA:HB2	3:A:267:MET:HE1	1.67	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: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:HD2	3:A:333:LYS:N	2.04	0.72
3:A:300:HIS:H	3:A:300:HIS:CD2	2.06	0.72
3:A:474:PRO:HA	3:A:880:PHE:HZ	1.53	0.72
3:A:206:LYS:O	3:A:210:ILE:HG12	1.89	0.72
3:A:363:LYS:HE3	3:A:367:ILE:HD12	1.71	0.72
3:A:393:SER:O	3:A:397:SER:OG	2.06	0.72
3:A:44:TYR:HD2	3:A:148:GLU:HG2	1.53	0.72
3:A:756:ARG:HB3	3:A:758:GLN:HE22	1.52	0.72
3:A:816:THR:HG22	3:A:817:ILE:N	2.04	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
2:P:102:DA:H2''	2:P:103:DA:OP2	1.90	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:408:PHE:HA	3:A:411:HIS:HD2	1.57	0.69
3:A:452:ILE:HD12	3:A:456:GLY:HA3	1.71	0.69
3:A:448:LYS:CD	3:A:448:LYS:H	2.06	0.69
3:A:709:GLU:HA	3:A:720:ARG:HE	1.56	0.69
3:A:236:VAL:HG12	3:A:239:GLN:H	1.56	0.69
3:A:703:ALA:O	3:A:706:LEU:HG	1.93	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:448:LYS:HD3	3:A:448:LYS:H	1.58	0.69
3:A:703:ALA:HA	3:A:706:LEU:HG	1.73	0.69
3:A:425:ARG:NH2	6:A:903:HOH:O	2.25	0.69
3:A:445:THR:HG23	3:A:532:LEU:HA	1.75	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:417:PRO:O	3:A:429:VAL:HG23	1.94	0.68
3:A:551:ARG:HG2	3:A:870:LEU:O	1.94	0.68
2:P:105:DA:H1'	2:P:106:DC:H5''	1.74	0.68
3:A:265:SER:HB3	3:A:269:GLN:NE2	2.09	0.68
3:A:692:ALA:O	3:A:696:MET:HG3	1.94	0.68
3:A:269:GLN:HG2	3:A:404:GLN:OE1	1.94	0.67
3:A:29:GLY:HA3	3:A:175:GLY:HA2	1.76	0.67
3:A:328:TRP:CE3	3:A:445:THR:O	2.48	0.67
3:A:439:MET:HA	3:A:509:PHE:CG	2.29	0.67
3:A:768:GLU:CD	3:A:769:ILE:H	2.02	0.67
3:A:313:MET:HE3	3:A:316:VAL:HG21	1.77	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: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:278:TRP:HE1	3:A:324:GLN:HE22	1.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:328:TRP:HE3	3:A:445:THR:O	1.79	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
3:A:117:ILE:HG22	3:A:118:THR:N	2.11	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:265:SER:HB3	3:A:269:GLN:CD	2.22	0.64
2:P:103:DA:H2''	2:P:104:DT:H5''	1.77	0.64
3:A:410:ASN:O	3:A:411:HIS:C	2.39	0.64
3:A:578:VAL:HG23	3:A:684:SER:OG	1.98	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:276:LYS:CE	3:A:287:TRP:HA	2.28	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: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:37:LEU:HG	3:A:288:ALA:HB2	1.80	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
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:229:LEU:HD21	3:A:242:GLU:OE1	1.99	0.63
3:A:335:LEU:N	3:A:443:LEU:HD21	2.14	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:768:GLU:CD	3:A:769:ILE:N	2.57	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:359:GLU:CD	3:A:360:LEU:H	2.07	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:872:LEU:C	3:A:875:ILE:HD13	2.25	0.62
3:A:350:GLU:N	3:A:350:GLU:CD	2.58	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:579:ASN:O	3:A:582:LEU:HB2	2.00	0.62
3:A:706:LEU:C	3:A:720:ARG:HH22	2.07	0.62
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:872:LEU:HA	3:A:875:ILE:HD13	1.80	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:512:LEU:O	3:A:513:ALA:C	2.43	0.61
3:A:620:TRP:CZ2	3:A:677:MET:HB2	2.35	0.61
3:A:6:ILE:HD13	3:A:6:ILE:N	2.16	0.61
3:A:313:MET:HE3	3:A:316:VAL:HG11	1.83	0.61
3:A:331:ASN:HD22	3:A:331:ASN:C	2.09	0.61
3:A:371:PRO:HG2	3:A:372:GLU:H	1.65	0.61
3:A:703:ALA:O	3:A:706:LEU:N	2.31	0.61
3:A:124:ALA:CB	3:A:267:MET:HE1	2.29	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:N	3:A:448:LYS:CD	2.61	0.61
3:A:702:ALA:C	3:A:706:LEU:HD23	2.26	0.61
3:A:118:THR:HA	3:A:141:ILE:HD12	1.83	0.60
3:A:267:MET:HE2	6:A:984:HOH:O	1.68	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:229:LEU:HD21	3:A:242:GLU:CD	2.25	0.60
3:A:747:LEU:HD12	3:A:747:LEU:N	2.16	0.60
3:A:185:VAL:HG22	3:A:186:VAL:N	2.16	0.60
3:A:450:LYS:HE2	3:A:817:ILE:CD1	2.32	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:706:LEU:C	3:A:706:LEU:HD12	2.26	0.60
3:A:448:LYS:H	3:A:448:LYS:CE	2.15	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:452:ILE:HD12	3:A:452:ILE:O	2.02	0.60
3:A:169:GLN:NE2	3:A:172:LYS:H	1.99	0.59
3:A:574:VAL:HG13	3:A:684:SER:HB2	1.83	0.59
3:A:663:LYS:HG2	3:A:664:GLY:N	2.11	0.59
3:A:108:GLU:C	3:A:109:ILE:HD13	2.27	0.59
3:A:121:THR:CG2	3:A:141:ILE:HD13	2.33	0.59
3:A:154:ILE:HD12	3:A:154:ILE:H	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: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:632:ARG:NH2	3:A:635:MET:HE2	2.17	0.59
3:A:8:LYS:C	3:A:10:ASP:H	2.11	0.59
3:A:324:GLN:NE2	3:A:418:TYR:H	1.99	0.59
3:A:359:GLU:OE1	3:A:360:LEU:HD23	2.03	0.59
3:A:634:VAL:HG23	6:A:910:HOH:O	2.02	0.59
3:A:855:GLU:HG3	3:A:856:SER:N	2.15	0.59
3:A:367:ILE:HG23	3:A:368:ASP:N	2.16	0.59
3:A:449:GLY:HA2	3:A:817:ILE:HG21	1.85	0.59
3:A:220:LEU:O	3:A:224:THR:O	2.21	0.58
3:A:463:HIS:CD2	3:A:535:ALA:H	2.20	0.58
3:A:652:GLU:HA	3:A:656:GLN:HB3	1.84	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:195:LEU:O	3:A:196:LEU:HD12	2.03	0.58
3:A:842:LEU:HG	3:A:843:ALA:H	1.66	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:797:TRP:HZ2	3:A:801:LYS:HZ2	1.50	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:234:ALA:HA	3:A:240:ASP:OD2	2.03	0.58
3:A:538:GLY:H	3:A:883:ALA:HB2	1.67	0.58
3:A:185:VAL:HG21	3:A:277:PRO:HD3	1.86	0.58
3:A:450:LYS:HE2	3:A:817:ILE:HD12	1.86	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
1:T:3:DT:H5"	3:A:640:GLY:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:695:ALA:O	3:A:698:TRP:HB3	2.05	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
3:A:84:ARG:NH1	3:A:88:TRP:HB2	2.18	0.57
3:A:532:LEU:HD12	3:A:533:PRO:HD2	1.86	0.57
3:A:557:ARG:CZ	3:A:562:LEU:HD13	2.34	0.57
3:A:408:PHE:HA	3:A:411:HIS:CD2	2.40	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
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:38:ALA:HB2	3:A:162:PHE:HE1	1.70	0.57
3:A:394:ARG:HH11	3:A:394:ARG:HG2	1.68	0.57
3:A:438:ASP:CG	3:A:509:PHE:HB2	2.30	0.57
3:A:688:THR:C	3:A:690:VAL:H	2.12	0.57
3:A:79:PRO:HA	3:A:82:ILE:HD12	1.85	0.57
3:A:244:ILE:HD12	3:A:244:ILE:N	2.20	0.57
3:A:297:VAL:HA	3:A:420:MET:O	2.05	0.57
3:A:491:ALA:HA	3:A:494:LYS:HE2	1.85	0.57
3:A:556:GLY:HA2	3:A:559:VAL:HG22	1.85	0.57
3:A:646:PHE:O	3:A:650:VAL:HG12	2.05	0.57
3:A:503:ALA:HA	3:A:508:PRO:HB3	1.86	0.56
2:P:111:DC:H2''	2:P:112:DA:C8	2.40	0.56
3:A:454:LYS:HD3	3:A:455:GLU:N	2.19	0.56
3:A:861:MET:H	3:A:862:PRO:CD	2.04	0.56
3:A:124:ALA:HB1	6:A:984:HOH:O	2.05	0.56
3:A:234:ALA:O	3:A:236:VAL:HG23	2.05	0.56
3:A:261:LEU:HD21	3:A:396:ILE:HD12	1.86	0.56
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: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:703:ALA:O	3:A:704:LYS:C	2.48	0.56
3:A:107:GLN:C	3:A:109:ILE:H	2.14	0.56
3:A:335:LEU:O	3:A:339:ASN:OD1	2.23	0.56
3:A:90:GLU:O	3:A:93:LYS:N	2.39	0.56
3:A:596:THR:C	3:A:608:LYS:HZ1	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:729:THR:HG22	3:A:733:PHE:H	1.70	0.56
3:A:19:ILE:HG22	3:A:195:LEU:HD11	1.88	0.56
3:A:74:ILE:CD1	3:A:78:LEU:HB2	2.36	0.56
3:A:79:PRO:O	3:A:80:LYS:C	2.49	0.56
3:A:176:HIS:NE2	3:A:178:TYR:HA	2.20	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:525:GLY:C	3:A:527:SER:H	2.13	0.55
3:A:300:HIS:H	3:A:300:HIS:HD2	1.52	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:271:CYS:O	3:A:414:ILE:HA	2.07	0.55
3:A:320:ILE:HD11	3:A:420:MET:HE2	1.88	0.55
3:A:480:LYS:HA	3:A:480:LYS:NZ	2.21	0.55
3:A:849:PHE:HB2	3:A:853:LEU:CB	2.31	0.55
3:A:225:GLY:O	3:A:226:MET:C	2.49	0.55
3:A:424:GLY:O	3:A:425:ARG:C	2.49	0.55
3:A:48:GLU:OE1	6:A:912:HOH:O	2.18	0.55
3:A:447:ALA:C	3:A:449:GLY:H	2.13	0.55
3:A:195:LEU:C	3:A:196:LEU:HD12	2.32	0.55
3:A:756:ARG:CB	3:A:758:GLN:HE22	2.19	0.55
3:A:574:VAL:HG13	3:A:684:SER:CB	2.37	0.55
3:A:576:LYS:HG3	3:A:577:LYS:H	1.72	0.55
3:A:722:ARG:NH1	3:A:771:ALA:HB2	2.22	0.55
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:573:ILE:O	3:A:576:LYS:HG3	2.05	0.54
1:T:4:DC:H2''	1:T:5:DC:H5'	1.89	0.54
1:T:5:DC:H4'	3:A:423:ARG:CD	2.37	0.54
3:A:73:LEU:HB3	3:A:260:ALA:O	2.07	0.54
3:A:405:ALA:O	3:A:406:ASN:C	2.51	0.54
3:A:711:LYS:HD2	3:A:712:ASP:N	2.21	0.54
3:A:747:LEU:O	3:A:758:GLN:HG3	2.08	0.54
3:A:74:ILE:HD11	3:A:78:LEU:HD22	1.89	0.54
3:A:769:ILE:N	3:A:769:ILE:HD12	2.22	0.54
3:A:856:SER:C	3:A:858:LEU:HD22	2.33	0.54
3:A:141:ILE:C	3:A:145:ILE:HD12	2.33	0.54
3:A:792:ARG:O	3:A:793:LYS:C	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:816:THR:CG2	3:A:817:ILE:H	2.16	0.54
1:T:18:DT:H2"	1:T:19:DA:C8	2.42	0.54
3:A:213:GLY:O	3:A:216:CYS:HB2	2.08	0.54
3:A:330:ILE:H	3:A:330:ILE:CD1	2.20	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: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:O	3:A:700:LYS:HD3	2.07	0.54
3:A:129:ALA:HB2	3:A:393:SER:CB	2.38	0.53
3:A:245:GLU:OE2	3:A:389:LYS:HE2	2.08	0.53
3:A:351:ASP:OD1	3:A:351:ASP:N	2.39	0.53
3:A:775:GLU:C	3:A:777:GLY:H	2.16	0.53
3:A:350:GLU:C	3:A:352:ILE:H	2.16	0.53
3:A:308:TYR:HE2	3:A:734:PRO:HG2	1.72	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:771:ALA:O	3:A:772:HIS:C	2.50	0.53
3:A:74:ILE:HD11	3:A:78:LEU:HB2	1.90	0.53
3:A:124:ALA:O	3:A:125:CYS:C	2.52	0.53
3:A:330:ILE:N	3:A:330:ILE:CD1	2.71	0.53
3:A:393:SER:O	3:A:396:ILE:HG22	2.08	0.53
3:A:492:CYS:HA	3:A:499:ASN:CB	2.38	0.53
1:T:2:DT:H2"	3:A:644:PHE:CD2	2.44	0.53
3:A:234:ALA:C	3:A:236:VAL:H	2.15	0.53
3:A:544:GLN:HG2	3:A:559:VAL:HB	1.90	0.53
3:A:861:MET:N	3:A:862:PRO:CD	2.68	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:31:ARG:HB2	3:A:173:ARG:HH21	1.74	0.53
3:A:211:HIS:O	3:A:215:ARG:HD3	2.08	0.53
3:A:421:ASP:CG	3:A:423:ARG:HD3	2.34	0.53
3:A:445:THR:HG22	3:A:446:LEU:H	1.72	0.53
3:A:474:PRO:C	3:A:476:PRO:HD2	2.33	0.53
3:A:576:LYS:HG3	3:A:577:LYS:N	2.24	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:595:VAL:HG21	3:A:597:VAL:HG23	1.90	0.53
3:A:398:LEU:HD23	3:A:398:LEU:C	2.33	0.53
3:A:446:LEU:HB3	3:A:448:LYS:HZ3	1.73	0.53
3:A:729:THR:HG22	3:A:733:PHE:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:748:ASN:ND2	3:A:756:ARG:HH21	1.97	0.53
3:A:449:GLY:C	3:A:450:LYS:HD3	2.34	0.53
3:A:539:SER:H	3:A:544:GLN:HE22	1.57	0.53
3:A:708:ALA:O	3:A:720:ARG:NH2	2.42	0.53
1:T:7:DA:OP2	3:A:298:ARG:HD3	2.09	0.52
3:A:108:GLU:O	3:A:109:ILE:HD13	2.08	0.52
3:A:632:ARG:NH1	3:A:632:ARG:HB3	2.24	0.52
3:A:721:LYS:O	3:A:723:CYS:N	2.41	0.52
3:A:706:LEU:HD12	3:A:706:LEU:O	2.10	0.52
1:T:21:DT:H2''	1:T:22:DA:N7	2.24	0.52
3:A:254:ILE:HG23	3:A:261:LEU:HD11	1.91	0.52
3:A:816:THR:HG22	3:A:817:ILE:CG1	2.38	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:313:MET:HE3	3:A:316:VAL:CB	2.40	0.52
3:A:458:TYR:HE1	3:A:479:ILE:HD11	1.75	0.52
3:A:725:VAL:O	3:A:736:TRP:HA	2.09	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:573:ILE:CG1	3:A:574:VAL:N	2.73	0.52
3:A:137:VAL:O	3:A:140:ALA:N	2.42	0.52
3:A:229:LEU:CG	3:A:242:GLU:HG2	2.40	0.52
3:A:259:GLY:O	3:A:262:ALA:HB2	2.09	0.52
3:A:451:PRO:HA	3:A:529:ASN:HA	1.91	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:86:ASN:HA	3:A:89:PHE:CD2	2.44	0.52
3:A:229:LEU:HD21	3:A:242:GLU:HG2	1.92	0.52
3:A:775:GLU:C	3:A:777:GLY:N	2.67	0.52
3:A:786:GLN:C	3:A:788:GLY:H	2.16	0.52
3:A:789:SER:HA	3:A:792:ARG:NH2	2.24	0.52
1:T:10:DG:H2''	1:T:11:DT:OP2	2.10	0.52
3:A:39:LEU:O	3:A:40:GLU:C	2.52	0.51
3:A:324:GLN:HG3	3:A:417:PRO:HA	1.93	0.51
3:A:452:ILE:HD12	3:A:452:ILE:C	2.34	0.51
3:A:496:PRO:C	3:A:498:GLU:H	2.19	0.51
3:A:703:ALA:CA	3:A:706:LEU:HG	2.37	0.51
3:A:835:THR:C	3:A:837:GLU:H	2.18	0.51
3:A:116:TYR:O	3:A:117:ILE:C	2.51	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:141:ILE:O	3:A:142:GLY:C	2.53	0.51
3:A:143:ARG:HD3	6:A:966:HOH:O	2.10	0.51
3:A:151:PHE:O	3:A:155:ARG:HB2	2.10	0.51
3:A:454:LYS:HD3	3:A:454:LYS:C	2.36	0.51
3:A:636:THR:HA	3:A:639:TYR:CD2	2.45	0.51
3:A:40:GLU:OE2	3:A:286:TYR:HB3	2.11	0.51
3:A:338:ALA:C	6:A:931:HOH:O	2.53	0.51
3:A:103:PHE:O	3:A:105:PHE:N	2.43	0.51
3:A:703:ALA:O	3:A:707:ALA:N	2.43	0.51
3:A:711:LYS:HG2	3:A:717:GLU:O	2.11	0.51
3:A:841:VAL:HG23	3:A:842:LEU:N	2.24	0.51
1:T:20:DT:C2'	1:T:21:DT:H5''	2.41	0.51
3:A:254:ILE:HG22	3:A:399:GLU:HG3	1.93	0.51
3:A:308:TYR:CD2	3:A:734:PRO:HG2	2.46	0.51
3:A:402:LEU:CD2	6:A:931:HOH:O	2.57	0.51
3:A:746:ARG:C	3:A:747:LEU:HD12	2.36	0.51
3:A:826:LYS:O	3:A:830:GLU:HG3	2.11	0.51
3:A:148:GLU:CD	3:A:155:ARG:HD3	2.36	0.51
3:A:676:TYR:O	3:A:679:LYS:HB3	2.11	0.51
3:A:740:LYS:HB3	3:A:768:GLU:O	2.10	0.51
1:T:22:DA:H4'	3:A:94:ALA:O	2.10	0.51
3:A:266:PRO:C	3:A:268:PHE:H	2.19	0.51
3:A:281:ILE:HD13	3:A:281:ILE:N	2.12	0.51
3:A:511:PHE:O	3:A:514:PHE:HB3	2.10	0.51
3:A:632:ARG:HB3	3:A:632:ARG:HH11	1.76	0.51
3:A:712:ASP:O	3:A:714:LYS:N	2.44	0.51
3:A:193:LYS:O	3:A:196:LEU:HD13	2.10	0.51
3:A:320:ILE:HD11	3:A:420:MET:CE	2.41	0.51
3:A:693:VAL:HA	3:A:696:MET:HE2	1.91	0.51
3:A:133:THR:HA	3:A:243:THR:HG22	1.93	0.50
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: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:452:ILE:CD1	3:A:456:GLY:CA	2.54	0.50
3:A:773:LYS:C	3:A:775:GLU:N	2.68	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:169:GLN:HE21	3:A:172:LYS:N	2.08	0.50
3:A:281:ILE:HD12	3:A:309:GLU:HA	1.92	0.50
3:A:595:VAL:CG2	3:A:597:VAL:HG23	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:150:ARG:O	3:A:151:PHE:HB2	2.11	0.50
3:A:330:ILE:HD13	3:A:408:PHE:O	2.10	0.50
3:A:390:ALA:O	3:A:393:SER:HB3	2.11	0.50
3:A:401:MET:HE1	3:A:432:PHE:HA	1.92	0.50
3:A:849:PHE:O	3:A:850:ALA:C	2.53	0.50
3:A:39:LEU:O	3:A:42:GLU:N	2.44	0.50
3:A:227:VAL:HB	3:A:244:ILE:HG22	1.92	0.50
3:A:77:LEU:HD23	3:A:224:THR:HG21	1.94	0.50
3:A:107:GLN:O	3:A:109:ILE:N	2.45	0.50
3:A:120:LYS:HD2	3:A:265:SER:O	2.12	0.50
3:A:269:GLN:HE21	3:A:404:GLN:CD	2.18	0.50
3:A:338:ALA:O	3:A:342:THR:HG23	2.12	0.50
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:561:LEU:HD23	3:A:561:LEU:O	2.11	0.50
3:A:709:GLU:HB3	3:A:722:ARG:HG3	1.93	0.50
3:A:784:HIS:HA	3:A:787:ASP:OD1	2.12	0.50
3:A:685:VAL:HG23	3:A:686:SER:N	2.27	0.49
2:P:101:DT:H1'	2:P:102:DA:H5'	1.93	0.49
3:A:51:PHE:HE1	3:A:75:THR:HA	1.77	0.49
3:A:334:VAL:HB	3:A:443:LEU:HD23	1.93	0.49
3:A:401:MET:HE1	3:A:431:MET:O	2.12	0.49
3:A:712:ASP:CG	3:A:713:LYS:N	2.69	0.49
3:A:779:ALA:N	3:A:780:PRO:HD2	2.26	0.49
3:A:710:VAL:HG22	3:A:711:LYS:N	2.27	0.49
3:A:17:ALA:HB1	3:A:158:GLU:HA	1.94	0.49
3:A:374:LEU:HD12	3:A:377:TRP:HB3	1.93	0.49
3:A:445:THR:HG22	3:A:446:LEU:N	2.27	0.49
3:A:773:LYS:O	3:A:775:GLU:N	2.46	0.49
3:A:13:ASP:OD2	3:A:13:ASP:N	2.45	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: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:313:MET:HE3	3:A:316:VAL:CG2	2.41	0.49
3:A:778:ILE:HG23	3:A:779:ALA:N	2.28	0.49
3:A:126:LEU:C	3:A:128:SER:H	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:12:DG:OP1	3:A:242:GLU:OE2	2.31	0.49
3:A:116:TYR:HA	3:A:119:ILE:HD11	1.94	0.49
3:A:174:VAL:HG13	3:A:176:HIS:H	1.76	0.49
3:A:404:GLN:O	3:A:407:LYS:HB3	2.13	0.49
3:A:481:PHE:HA	3:A:484:GLU:OE1	2.12	0.49
3:A:73:LEU:CD2	3:A:260:ALA:HB1	2.39	0.49
3:A:142:GLY:HA2	3:A:145:ILE:HD12	1.95	0.49
3:A:237:VAL:O	3:A:237:VAL:HG12	2.11	0.49
3:A:391:ARG:O	3:A:392:LYS:C	2.55	0.49
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:452:ILE:CD1	3:A:818:PRO:HB3	2.43	0.48
3:A:472:LYS:C	3:A:567:VAL:HG21	2.38	0.48
3:A:552:ASP:HB2	3:A:691:ALA:CB	2.42	0.48
3:A:562:LEU:C	3:A:564:SER:H	2.21	0.48
3:A:779:ALA:HB3	3:A:780:PRO:CD	2.42	0.48
1:T:19:DA:H2'	1:T:20:DT:H71	1.96	0.48
3:A:161:HIS:C	3:A:163:LYS:H	2.20	0.48
3:A:562:LEU:HD22	3:A:563:PRO:HD2	1.94	0.48
3:A:704:LYS:C	3:A:706:LEU:H	2.21	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
1:T:19:DA:C2'	1:T:20:DT:H5'	2.29	0.48
2:P:102:DA:H1'	2:P:103:DA:C8	2.49	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:479:ILE:O	3:A:483:GLU:OE1	2.31	0.48
3:A:841:VAL:HG23	3:A:842:LEU:HD23	1.96	0.48
3:A:229:LEU:CD1	3:A:242:GLU:HG2	2.44	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:267:MET:HE3	6:A:984:HOH:O	1.76	0.48
3:A:373:ALA:O	3:A:377:TRP:HB2	2.13	0.48
3:A:711:LYS:HZ3	3:A:714:LYS:HA	1.77	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:398:LEU:HD22	3:A:399:GLU:OE2	2.13	0.48
3:A:460:LEU:HD21	3:A:518:TYR:HB2	1.95	0.48
3:A:579:ASN:HA	3:A:582:LEU:CD1	2.34	0.48
3:A:138:ALA:O	3:A:139:SER:C	2.54	0.48
3:A:142:GLY:HA2	3:A:145:ILE:CD1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:195:LEU:HA	3:A:289:ASN:HD21	1.79	0.48
3:A:518:TYR:O	3:A:522:GLN:HG3	2.13	0.48
1:T:22:DA:O4'	3:A:96:ARG:HB3	2.13	0.48
3:A:254:ILE:CG2	3:A:399:GLU:HG3	2.44	0.48
3:A:401:MET:CE	3:A:432:PHE:HA	2.44	0.48
3:A:448:LYS:O	3:A:450:LYS:HD3	2.14	0.48
3:A:187:GLU:N	3:A:187:GLU:CD	2.72	0.47
3:A:496:PRO:O	3:A:498:GLU:N	2.47	0.47
3:A:718:ILE:HD12	3:A:718:ILE:C	2.39	0.47
3:A:136:ALA:O	3:A:137:VAL:C	2.57	0.47
3:A:341:ILE:HG13	3:A:342:THR:N	2.28	0.47
3:A:468:ALA:HA	3:A:505:GLN:CG	2.44	0.47
3:A:543:ILE:HG22	3:A:559:VAL:HG11	1.96	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:796:VAL:O	3:A:799:HIS:HB3	2.14	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:465:ALA:O	3:A:466:ASN:C	2.57	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: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:559:VAL:C	3:A:561:LEU:H	2.22	0.47
3:A:846:TYR:HA	3:A:849:PHE:CE1	2.49	0.47
1:T:9:DA:C4'	3:A:762:ASN:HD21	2.28	0.47
3:A:20:PRO:HG2	3:A:289:ASN:HB2	1.97	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:459:TRP:HA	3:A:462:ILE:HB	1.96	0.47
3:A:478:ARG:O	3:A:481:PHE:HB3	2.15	0.47
3:A:702:ALA:O	3:A:706:LEU:HD23	2.14	0.47
3:A:740:LYS:CB	3:A:768:GLU:O	2.62	0.47
3:A:108:GLU:H	3:A:108:GLU:HG3	1.31	0.47
3:A:117:ILE:HD12	3:A:144:ALA:HB1	1.97	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:643:GLU:CD	3:A:679:LYS:HA	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:7:DA:H2''	1:T:8:DT:O5'	2.15	0.47
3:A:740:LYS:HE2	3:A:767:SER:O	2.14	0.47
3:A:103:PHE:O	3:A:104:GLN:C	2.58	0.47
3:A:370:ASN:N	3:A:371:PRO:CD	2.77	0.47
3:A:573:ILE:HD11	3:A:688:THR:HG21	1.96	0.47
3:A:51:PHE:CE1	3:A:75:THR:HA	2.49	0.46
3:A:137:VAL:HG21	3:A:244:ILE:CD1	2.34	0.46
3:A:254:ILE:HG22	3:A:254:ILE:O	2.15	0.46
3:A:545:HIS:O	3:A:549:MET:HG2	2.14	0.46
1:T:3:DT:P	1:T:3:DT:H3'	2.55	0.46
3:A:134:VAL:HA	3:A:244:ILE:HD11	1.97	0.46
3:A:90:GLU:OE2	3:A:90:GLU:HA	2.15	0.46
3:A:154:ILE:HD12	3:A:154:ILE:N	2.29	0.46
3:A:250:TYR:O	3:A:254:ILE:HG13	2.14	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:351:ASP:O	3:A:394:ARG:NH1	2.48	0.46
3:A:496:PRO:C	3:A:498:GLU:N	2.70	0.46
3:A:576:LYS:HZ1	3:A:577:LYS:HB2	1.80	0.46
3:A:316:VAL:O	3:A:319:ALA:HB3	2.15	0.46
3:A:387:LYS:O	3:A:387:LYS:HD3	2.15	0.46
3:A:452:ILE:HD11	3:A:456:GLY:C	2.39	0.46
3:A:582:LEU:HB3	3:A:621:LEU:HD21	1.97	0.46
3:A:809:LEU:HD12	3:A:809:LEU:O	2.15	0.46
2:P:113:DC:H3'	2:P:114:DT:H4'	1.98	0.46
3:A:133:THR:C	3:A:135:GLN:N	2.74	0.46
3:A:174:VAL:HG13	3:A:175:GLY:N	2.31	0.46
3:A:226:MET:HA	3:A:250:TYR:CE2	2.51	0.46
3:A:524:HIS:HB2	3:A:528:TYR:HB2	1.98	0.46
3:A:679:LYS:O	3:A:683:GLU:HG3	2.15	0.46
3:A:711:LYS:HD2	3:A:712:ASP:O	2.15	0.46
3:A:850:ALA:HA	3:A:854:HIS:NE2	2.30	0.46
3:A:159:ALA:C	3:A:161:HIS:N	2.70	0.46
3:A:224:THR:HG22	3:A:250:TYR:OH	2.16	0.46
3:A:324:GLN:C	3:A:326:THR:H	2.24	0.46
3:A:363:LYS:HZ1	3:A:367:ILE:HA	1.81	0.46
3:A:631:LYS:O	3:A:634:VAL:HG23	2.15	0.46
3:A:775:GLU:O	3:A:777:GLY:N	2.49	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:345:LYS:CD	3:A:355:ILE:HD11	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:786:GLN:C	3:A:788:GLY:N	2.71	0.46
3:A:830:GLU:O	3:A:834:ASP:HB3	2.16	0.46
3:A:234:ALA:C	3:A:236:VAL:N	2.74	0.45
3:A:313:MET:HE3	3:A:316:VAL:CG1	2.46	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:703:ALA:HA	3:A:706:LEU:CG	2.45	0.45
3:A:773:LYS:O	3:A:774:GLN:C	2.59	0.45
3:A:312:TYR:C	3:A:314:PRO:HD3	2.40	0.45
3:A:425:ARG:CZ	6:A:903:HOH:O	2.63	0.45
3:A:729:THR:HG21	3:A:733:PHE:HB3	1.99	0.45
3:A:743:ILE:HG13	3:A:763:THR:HG1	1.80	0.45
3:A:176:HIS:CD2	3:A:178:TYR:HA	2.51	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: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:111:PRO:C	3:A:113:ALA:N	2.74	0.45
3:A:177:VAL:C	3:A:179:LYS:H	2.24	0.45
3:A:210:ILE:HG13	3:A:761:ILE:HD13	1.98	0.45
3:A:238:GLY:C	3:A:239:GLN:HE21	2.25	0.45
3:A:359:GLU:O	3:A:384:VAL:HG11	2.17	0.45
3:A:861:MET:O	3:A:862:PRO:O	2.35	0.45
3:A:458:TYR:HE1	3:A:479:ILE:CD1	2.29	0.45
3:A:475:PHE:C	3:A:479:ILE:HD12	2.41	0.45
3:A:488:ASN:HB3	3:A:501:TRP:CE3	2.52	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:711:LYS:NZ	3:A:714:LYS:HA	2.32	0.45
3:A:727:TRP:CD1	3:A:728:VAL:N	2.85	0.45
3:A:875:ILE:N	3:A:875:ILE:HD12	2.31	0.45
3:A:882:PHE:O	3:A:883:ALA:C	2.59	0.45
3:A:8:LYS:C	3:A:10:ASP:N	2.75	0.45
3:A:20:PRO:HA	3:A:195:LEU:HD21	1.99	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:377:TRP:C	3:A:379:ARG:N	2.72	0.45
3:A:492:CYS:HA	3:A:499:ASN:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:734:PRO:HB2	3:A:736:TRP:CH2	2.52	0.45
2:P:103:DA:C2'	2:P:104:DT:H5''	2.46	0.45
3:A:350:GLU:C	3:A:352:ILE:N	2.75	0.45
3:A:557:ARG:CB	3:A:562:LEU:HD12	2.38	0.45
3:A:25:ALA:HA	3:A:29:GLY:O	2.17	0.45
3:A:77:LEU:H	3:A:77:LEU:CD1	2.21	0.45
3:A:216:CYS:O	3:A:217:ILE:C	2.60	0.45
3:A:575:ALA:O	3:A:576:LYS:C	2.60	0.45
3:A:611:LEU:CD2	3:A:612:GLY:H	2.30	0.45
3:A:731:ASP:OD2	3:A:789:SER:OG	2.32	0.45
3:A:31:ARG:HG2	3:A:31:ARG:HH11	1.83	0.44
3:A:101:THR:O	3:A:102:ALA:C	2.59	0.44
3:A:537:ASP:O	3:A:882:PHE:HD2	2.01	0.44
3:A:756:ARG:HB3	3:A:758:GLN:NE2	2.25	0.44
3:A:28:TYR:CD1	3:A:183:MET:HG3	2.52	0.44
3:A:102:ALA:C	3:A:106:LEU:HD12	2.42	0.44
3:A:118:THR:CG2	3:A:220:LEU:HD22	2.43	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:421:ASP:C	3:A:423:ARG:H	2.26	0.44
3:A:737:GLN:HE21	3:A:774:GLN:CD	2.26	0.44
2:P:103:DA:H5'	3:A:96:ARG:NH2	2.32	0.44
3:A:300:HIS:HB3	6:A:913:HOH:O	2.17	0.44
3:A:576:LYS:HA	3:A:579:ASN:HB2	1.99	0.44
3:A:631:LYS:HE2	3:A:635:MET:SD	2.58	0.44
3:A:639:TYR:CE1	3:A:784:HIS:HE1	2.34	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:574:VAL:O	3:A:578:VAL:HB	2.18	0.44
3:A:828:VAL:O	3:A:831:THR:OG1	2.35	0.44
3:A:227:VAL:HA	3:A:246:LEU:HA	2.00	0.44
3:A:259:GLY:O	3:A:260:ALA:C	2.60	0.44
3:A:278:TRP:CE2	3:A:284:GLY:HA3	2.52	0.44
3:A:532:LEU:HD12	3:A:533:PRO:CD	2.47	0.44
3:A:739:TYR:H	3:A:774:GLN:NE2	2.13	0.44
3:A:90:GLU:C	3:A:92:VAL:N	2.74	0.44
3:A:300:HIS:O	3:A:301:SER:HB2	2.17	0.44
3:A:556:GLY:HA2	3:A:559:VAL:CG2	2.48	0.44
3:A:709:GLU:N	3:A:722:ARG:HG2	2.33	0.44
3:A:719:LEU:N	3:A:719:LEU:HD12	2.31	0.44
3:A:748:ASN:O	3:A:749:LEU:HD23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:16:DC:H2''	1:T:17:DG:C8	2.52	0.44
3:A:105:PHE:HA	3:A:108:GLU:OE1	2.18	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
3:A:394:ARG:NH1	3:A:394:ARG:HG2	2.31	0.44
3:A:423:ARG:HH22	3:A:784:HIS:CD2	2.35	0.44
3:A:512:LEU:O	3:A:515:CYS:N	2.50	0.44
3:A:41:HIS:C	3:A:43:SER:N	2.74	0.44
3:A:313:MET:SD	3:A:734:PRO:HD2	2.58	0.44
3:A:525:GLY:C	3:A:527:SER:N	2.74	0.44
3:A:842:LEU:HG	3:A:843:ALA:N	2.32	0.44
2:P:105:DA:H1'	2:P:106:DC:C5'	2.44	0.44
3:A:245:GLU:HG3	3:A:389:LYS:HD3	2.00	0.44
3:A:475:PHE:N	3:A:476:PRO:CD	2.81	0.44
3:A:605:ILE:HD11	3:A:608:LYS:HD2	1.99	0.44
3:A:737:GLN:O	3:A:738:GLU:C	2.61	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
3:A:857:GLN:C	3:A:859:ASP:H	2.26	0.43
1:T:17:DG:N2	2:P:107:DG:C2	2.86	0.43
3:A:428:ALA:H	3:A:435:GLN:HE22	1.67	0.43
3:A:795:VAL:HG23	3:A:796:VAL:N	2.33	0.43
3:A:501:TRP:HA	3:A:504:GLU:OE2	2.17	0.43
3:A:505:GLN:O	3:A:508:PRO:HD3	2.18	0.43
3:A:809:LEU:HD12	3:A:809:LEU:N	2.33	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:167:GLU:O	3:A:167:GLU:HG3	2.18	0.43
3:A:297:VAL:O	3:A:299:THR:HG23	2.17	0.43
3:A:402:LEU:HD21	6:A:931:HOH:O	2.18	0.43
3:A:681:ILE:O	3:A:682:TRP:C	2.61	0.43
3:A:118:THR:O	3:A:119:ILE:C	2.60	0.43
3:A:211:HIS:O	3:A:215:ARG:HB2	2.18	0.43
3:A:333:LYS:NZ	6:A:968:HOH:O	2.52	0.43
3:A:687:VAL:C	3:A:690:VAL:HG13	2.44	0.43
3:A:713:LYS:O	3:A:714:LYS:C	2.62	0.43
3:A:785:SER:O	3:A:789:SER:HB2	2.18	0.43
3:A:835:THR:O	3:A:839:CYS:HB2	2.18	0.43
3:A:73:LEU:O	3:A:77:LEU:CD1	2.66	0.43
3:A:501:TRP:HB2	6:A:935:HOH:O	2.18	0.43
3:A:546:PHE:C	3:A:548:ALA:N	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:549:MET:SD	3:A:841:VAL:HG21	2.59	0.43
3:A:798:ALA:HB1	3:A:804:ILE:CD1	2.26	0.43
3:A:881:ALA:O	3:A:882:PHE:C	2.62	0.43
3:A:142:GLY:N	3:A:145:ILE:HD12	2.34	0.43
3:A:317:TYR:O	3:A:318:LYS:C	2.62	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:491:ALA:HB3	3:A:499:ASN:OD1	2.18	0.43
3:A:512:LEU:HD12	3:A:512:LEU:HA	1.76	0.43
3:A:723:CYS:HB3	3:A:853:LEU:CD1	2.49	0.43
3:A:433:ASN:C	3:A:435:GLN:H	2.26	0.43
3:A:36:GLN:HE21	3:A:40:GLU:HG3	1.84	0.43
3:A:192:SER:C	3:A:194:GLY:N	2.77	0.43
3:A:631:LYS:HB3	3:A:632:ARG:H	1.73	0.43
3:A:467:CYS:C	3:A:469:GLY:H	2.26	0.42
3:A:266:PRO:C	3:A:268:PHE:N	2.77	0.42
3:A:610:LYS:HD2	3:A:610:LYS:HA	1.79	0.42
3:A:784:HIS:O	3:A:785:SER:C	2.61	0.42
3:A:855:GLU:O	3:A:858:LEU:HD21	2.19	0.42
3:A:201:TRP:HE3	3:A:202:SER:H	1.68	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: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:473:VAL:CG2	3:A:474:PRO:HD2	2.29	0.42
3:A:546:PHE:C	3:A:548:ALA:H	2.27	0.42
3:A:729:THR:CG2	3:A:733:PHE:HB3	2.49	0.42
3:A:824:LEU:O	3:A:826:LYS:N	2.52	0.42
3:A:849:PHE:HA	3:A:852:GLN:HB3	2.00	0.42
2:P:110:DT:H6	2:P:110:DT:H2'	1.74	0.42
3:A:28:TYR:HD1	3:A:183:MET:HB2	1.84	0.42
3:A:169:GLN:HE21	3:A:171:ASN:N	2.17	0.42
3:A:286:TYR:HD2	3:A:294:LEU:HD21	1.84	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:403:GLU:O	3:A:407:LYS:N	2.51	0.42
3:A:465:ALA:O	3:A:468:ALA:N	2.53	0.42
3:A:545:HIS:O	3:A:548:ALA:HB3	2.19	0.42
3:A:335:LEU:HA	3:A:443:LEU:HD21	2.01	0.42
3:A:405:ALA:C	3:A:407:LYS:N	2.76	0.42
3:A:471:ASP:HA	3:A:478:ARG:HH21	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:774:GLN:HE21	3:A:774:GLN:HA	1.84	0.42
3:A:855:GLU:CG	3:A:856:SER:H	2.14	0.42
3:A:875:ILE:C	3:A:877:GLU:N	2.77	0.42
3:A:417:PRO:C	3:A:429:VAL:HG23	2.45	0.42
3:A:616:LEU:HD23	3:A:676:TYR:CG	2.55	0.42
3:A:126:LEU:C	3:A:128:SER:N	2.77	0.42
3:A:133:THR:HB	3:A:135:GLN:OE1	2.20	0.42
3:A:213:GLY:O	3:A:214:VAL:C	2.62	0.42
3:A:349:VAL:HG12	3:A:352:ILE:HG12	2.02	0.42
3:A:438:ASP:OD2	3:A:509:PHE:HB2	2.19	0.42
3:A:824:LEU:C	3:A:826:LYS:N	2.75	0.42
3:A:831:THR:O	3:A:832:MET:C	2.63	0.42
3:A:90:GLU:O	3:A:91:GLU:C	2.63	0.42
3:A:298:ARG:HE	3:A:419:ASN:HD22	1.67	0.42
3:A:341:ILE:C	3:A:343:LYS:N	2.77	0.42
3:A:447:ALA:H	3:A:448:LYS:HZ3	1.65	0.42
3:A:485:ASN:O	3:A:488:ASN:HB2	2.19	0.42
3:A:549:MET:O	3:A:550:LEU:HD23	2.20	0.42
3:A:646:PHE:HB2	3:A:678:ALA:CB	2.50	0.42
3:A:704:LYS:C	3:A:706:LEU:N	2.77	0.42
1:T:17:DG:H2''	1:T:18:DT:H5''	2.02	0.42
3:A:147:ASP:OD1	3:A:292:ARG:HD3	2.19	0.42
3:A:334:VAL:O	3:A:335:LEU:C	2.62	0.42
3:A:344:TRP:CD1	3:A:344:TRP:N	2.88	0.42
3:A:460:LEU:HD23	3:A:461:LYS:N	2.34	0.42
3:A:857:GLN:O	3:A:858:LEU:HB2	2.20	0.42
3:A:159:ALA:HA	3:A:162:PHE:HD2	1.80	0.42
3:A:174:VAL:HG13	3:A:177:VAL:H	1.82	0.42
3:A:214:VAL:O	3:A:215:ARG:C	2.63	0.42
3:A:154:ILE:O	3:A:158:GLU:HB2	2.20	0.41
3:A:177:VAL:HB	3:A:179:LYS:CD	2.43	0.41
3:A:269:GLN:HE22	3:A:407:LYS:HE3	1.85	0.41
3:A:595:VAL:HG23	3:A:596:THR:N	2.35	0.41
3:A:703:ALA:C	3:A:706:LEU:HG	2.44	0.41
3:A:740:LYS:HB3	3:A:766:ASP:OD2	2.20	0.41
3:A:833:VAL:O	3:A:834:ASP:C	2.62	0.41
3:A:137:VAL:O	3:A:138:ALA:C	2.62	0.41
3:A:261:LEU:HD21	3:A:396:ILE:CD1	2.49	0.41
3:A:360:LEU:HB3	3:A:384:VAL:HG21	2.02	0.41
3:A:365:GLU:HB2	3:A:366:ASP:H	1.67	0.41
1:T:8:DT:H4'	1:T:8:DT:OP1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:693:VAL:O	3:A:697:ASN:ND2	2.53	0.41
3:A:42:GLU:HG2	3:A:50:ARG:NH1	2.35	0.41
3:A:84:ARG:HD2	3:A:84:ARG:HA	1.91	0.41
3:A:371:PRO:HG2	3:A:372:GLU:N	2.35	0.41
3:A:452:ILE:HG22	3:A:528:TYR:O	2.20	0.41
3:A:487:GLU:HA	3:A:490:MET:HG2	2.03	0.41
3:A:517:GLU:C	3:A:519:ALA:N	2.77	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:677:MET:C	3:A:681:ILE:HG13	2.41	0.41
3:A:791:LEU:HD23	3:A:791:LEU:C	2.45	0.41
3:A:275:PRO:O	3:A:277:PRO:HD3	2.20	0.41
3:A:308:TYR:CE2	3:A:736:TRP:HZ3	2.38	0.41
3:A:453:GLY:HA2	3:A:526:LEU:O	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:88:TRP:O	3:A:92:VAL:HG23	2.21	0.41
3:A:377:TRP:C	3:A:379:ARG:H	2.28	0.41
3:A:452:ILE:HG23	3:A:453:GLY:N	2.35	0.41
3:A:505:GLN:OE1	3:A:505:GLN:N	2.54	0.41
3:A:570:ILE:HG23	3:A:571:TYR:N	2.35	0.41
3:A:688:THR:C	3:A:690:VAL:N	2.78	0.41
3:A:725:VAL:CB	3:A:737:GLN:HB2	2.38	0.41
3:A:879:ASP:N	3:A:879:ASP:OD1	2.54	0.41
2:P:106:DC:H2"	2:P:107:DG:C8	2.54	0.41
3:A:105:PHE:N	3:A:105:PHE:CD1	2.89	0.41
3:A:297:VAL:HG11	3:A:308:TYR:CE1	2.56	0.41
3:A:396:ILE:O	3:A:396:ILE:HG13	2.20	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:857:GLN:C	3:A:858:LEU:HD22	2.45	0.41
1:T:17:DG:C2'	1:T:18:DT:H5"	2.51	0.41
3:A:30:GLU:HG2	3:A:166:VAL:HG21	2.03	0.41
3:A:83:ALA:O	3:A:84:ARG:C	2.63	0.41
3:A:215:ARG:NH1	3:A:218:GLU:OE1	2.54	0.41
3:A:341:ILE:C	3:A:343:LYS:H	2.27	0.41
3:A:421:ASP:C	3:A:423:ARG:N	2.79	0.41
3:A:546:PHE:CZ	3:A:696:MET:HG2	2.56	0.41
3:A:570:ILE:O	3:A:573:ILE:HG12	2.21	0.41
3:A:100:PRO:O	3:A:103:PHE:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:287:TRP:O	3:A:288:ALA:C	2.64	0.41
3:A:339:ASN:N	3:A:339:ASN:OD1	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: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: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:558:ALA:C	3:A:560:ASN:H	2.29	0.40
3:A:6:ILE:N	3:A:6:ILE:CD1	2.82	0.40
3:A:147:ASP:CG	3:A:292:ARG:HD3	2.47	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:639:TYR:HA	3:A:780:PRO:CB	2.52	0.40
3:A:652:GLU:O	3:A:657:PRO:HD3	2.20	0.40
3:A:739:TYR:HB2	3:A:774:GLN:HE22	1.77	0.40
3:A:806:SER:C	3:A:807:PHE:CD1	2.99	0.40
3:A:542:GLY:CA	3:A:783:VAL:HG13	2.52	0.40
3:A:655:ILE:HD12	3:A:667:PHE:CE1	2.56	0.40
3:A:677:MET:O	3:A:678:ALA:C	2.64	0.40
3:A:78:LEU:HB3	3:A:79:PRO:CD	2.51	0.40
3:A:195:LEU:HD12	3:A:195:LEU:N	2.36	0.40
3:A:198:GLY:O	3:A:199:GLU:C	2.64	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:840:ASP:O	3:A:841:VAL:C	2.65	0.40
3:A:107:GLN:C	3:A:109:ILE:N	2.77	0.40
3:A:234:ALA:O	3:A:236:VAL:N	2.55	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:635:MET:C	3:A:637:LEU:N	2.75	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%)	0 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%)	615 (86%)	99 (14%)	3 7

All (99) 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	48	GLU
3	A	52	ARG
3	A	74	ILE
3	A	81	MET
3	A	87	ASP
3	A	95	LYS
3	A	101	THR
3	A	105	PHE
3	A	108	GLU
3	A	109	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	119	ILE
3	A	120	LYS
3	A	127	THR
3	A	139	SER
3	A	146	GLU
3	A	148	GLU
3	A	164	LYS
3	A	166	VAL
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	261	LEU
3	A	273	VAL
3	A	279	THR
3	A	281	ILE
3	A	296	LEU
3	A	300	HIS
3	A	313	MET
3	A	330	ILE
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	387	LYS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	480	LYS
3	A	492	CYS
3	A	500	THR
3	A	510	CYS
3	A	514	PHE
3	A	529	ASN
3	A	537	ASP
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	629	VAL
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	717	GLU
3	A	720	ARG
3	A	729	THR
3	A	730	PRO
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	809	LEU
3	A	814	PHE
3	A	817	ILE
3	A	826	LYS
3	A	854	HIS
3	A	858	LEU
3	A	875	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	877	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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	300	HIS
3	A	321	ASN
3	A	324	GLN
3	A	325	ASN
3	A	331	ASN
3	A	435	GLN
3	A	486	HIS
3	A	544	GLN
3	A	560	ASN
3	A	648	GLN
3	A	649	GLN
3	A	672	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	823	ASN
3	A	848	GLN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	902	-	31,33,33	2.16	3 (9%)	44,52,52	1.35	5 (11%)
5	GH3	A	901	4	31,33,33	2.87	4 (12%)	44,52,52	1.53	5 (11%)

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	902	-	-	6/22/34/34	0/3/3/3
5	GH3	A	901	4	-	4/22/34/34	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	GH3	PA-O3A	13.42	1.74	1.59
5	A	902	GH3	PA-O3A	9.74	1.70	1.59
5	A	901	GH3	PB-O3A	5.99	1.66	1.59
5	A	902	GH3	PB-O3A	3.79	1.63	1.59
5	A	901	GH3	PB-O3B	3.08	1.62	1.59
5	A	902	GH3	O2'-C2'	2.63	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	GH3	O2'-C2'	2.24	1.48	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	GH3	O4'-C4'-C5'	4.83	118.05	109.34
5	A	901	GH3	O4'-C4'-C3'	3.58	109.61	105.07
5	A	902	GH3	O4'-C4'-C5'	3.57	115.77	109.34
5	A	901	GH3	O2A-PA-O3A	3.26	116.08	107.27
5	A	902	GH3	O4'-C4'-C3'	3.00	108.88	105.07
5	A	902	GH3	O2A-PA-O3A	2.85	114.98	107.27
5	A	901	GH3	O3B-PB-O1B	-2.57	102.96	110.70
5	A	902	GH3	O3B-PB-O1B	-2.49	103.22	110.70
5	A	902	GH3	O2G-PG-O3B	2.41	112.72	104.64
5	A	901	GH3	O2G-PG-O3B	2.02	111.42	104.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

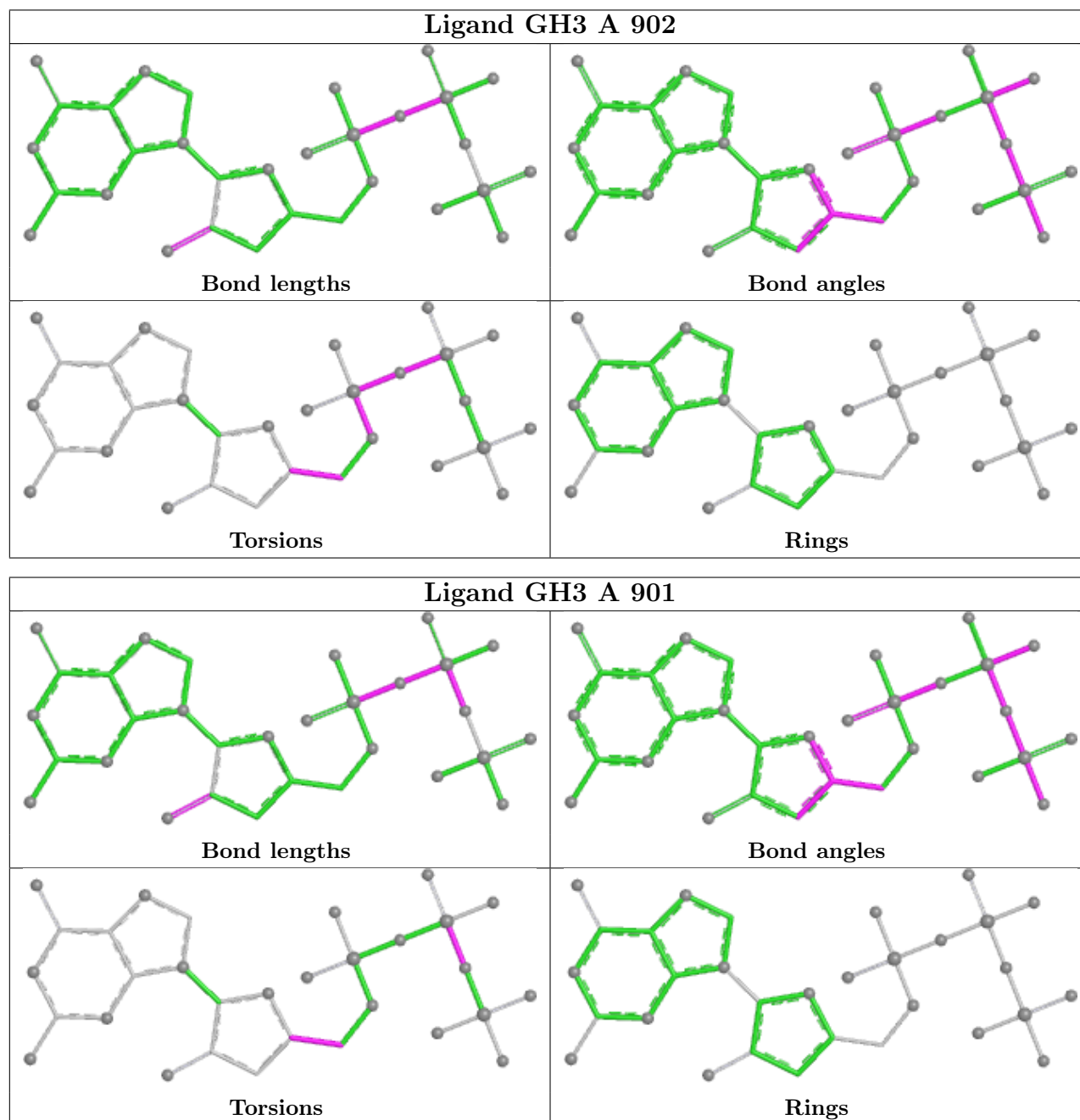
Mol	Chain	Res	Type	Atoms
5	A	901	GH3	C3'-C4'-C5'-O5'
5	A	902	GH3	PB-O3A-PA-O5'
5	A	901	GH3	O4'-C4'-C5'-O5'
5	A	902	GH3	O4'-C4'-C5'-O5'
5	A	902	GH3	C3'-C4'-C5'-O5'
5	A	902	GH3	C5'-O5'-PA-O1A
5	A	901	GH3	PG-O3B-PB-O2B
5	A	902	GH3	PA-O3A-PB-O2B
5	A	901	GH3	PG-O3B-PB-O1B
5	A	902	GH3	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.96	1 (4%) 38 33	48, 60, 79, 120	0
2	P	14/14 (100%)	0.40	0 100 100	37, 47, 95, 126	0
3	A	862/878 (98%)	1.84	343 (39%) 1 0	0, 58, 121, 160	0
All	All	898/914 (98%)	1.80	344 (38%) 1 0	0, 58, 121, 160	0

All (344) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	543	ILE	7.8
3	A	308	TYR	6.3
3	A	273	VAL	6.2
3	A	539	SER	6.0
3	A	875	ILE	6.0
3	A	881	ALA	6.0
3	A	316	VAL	5.9
3	A	37	LEU	5.7
3	A	821	ALA	5.5
3	A	788	GLY	5.4
3	A	422	TRP	5.0
3	A	452	ILE	5.0
3	A	715	THR	5.0
3	A	533	PRO	5.0
3	A	97	GLY	5.0
3	A	545	HIS	4.9
3	A	323	ALA	4.8
3	A	635	MET	4.8
3	A	825	PHE	4.8
3	A	883	ALA	4.7
3	A	489	ILE	4.7
3	A	24	LEU	4.6
3	A	320	ILE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	827	ALA	4.6
3	A	286	TYR	4.6
3	A	794	THR	4.5
3	A	685	VAL	4.5
3	A	317	TYR	4.5
3	A	538	GLY	4.5
3	A	194	GLY	4.4
3	A	542	GLY	4.4
3	A	16	LEU	4.4
3	A	544	GLN	4.4
3	A	414	ILE	4.4
3	A	804	ILE	4.4
3	A	178	TYR	4.4
3	A	872	LEU	4.3
3	A	832	MET	4.3
3	A	177	VAL	4.3
3	A	824	LEU	4.3
3	A	526	LEU	4.3
3	A	275	PRO	4.3
3	A	650	VAL	4.3
3	A	829	ARG	4.3
3	A	882	PHE	4.2
3	A	842	LEU	4.2
3	A	19	ILE	4.2
3	A	287	TRP	4.2
3	A	791	LEU	4.2
3	A	546	PHE	4.2
3	A	535	ALA	4.2
3	A	396	ILE	4.2
3	A	201	TRP	4.1
3	A	807	PHE	4.1
3	A	845	PHE	4.1
3	A	28	TYR	4.1
3	A	841	VAL	4.1
3	A	778	ILE	4.0
3	A	836	TYR	4.0
3	A	145	ILE	4.0
3	A	311	VAL	4.0
3	A	518	TYR	4.0
3	A	326	THR	3.9
3	A	777	GLY	3.8
3	A	541	SER	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	328	TRP	3.8
3	A	170	LEU	3.8
3	A	377	TRP	3.8
3	A	532	LEU	3.8
3	A	458	TYR	3.8
3	A	570	ILE	3.8
3	A	425	ARG	3.7
3	A	374	LEU	3.7
3	A	300	HIS	3.7
3	A	548	ALA	3.7
3	A	736	TRP	3.7
3	A	808	ALA	3.6
3	A	261	LEU	3.6
3	A	185	VAL	3.6
3	A	38	ALA	3.6
3	A	175	GLY	3.6
3	A	250	TYR	3.6
3	A	415	TRP	3.6
3	A	149	ALA	3.6
3	A	780	PRO	3.6
3	A	44	TYR	3.6
3	A	629	VAL	3.6
3	A	421	ASP	3.5
3	A	641	SER	3.5
3	A	162	PHE	3.5
3	A	870	LEU	3.5
3	A	443	LEU	3.5
3	A	547	SER	3.5
3	A	633	SER	3.5
3	A	183	MET	3.4
3	A	293	PRO	3.4
3	A	805	GLU	3.4
3	A	176	HIS	3.4
3	A	492	CYS	3.4
3	A	798	ALA	3.4
3	A	21	PHE	3.3
3	A	29	GLY	3.3
3	A	25	ALA	3.3
3	A	503	ALA	3.3
3	A	637	LEU	3.3
3	A	729	THR	3.3
3	A	288	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	833	VAL	3.3
3	A	706	LEU	3.3
3	A	373	ALA	3.3
3	A	289	ASN	3.2
3	A	457	TYR	3.2
3	A	724	ALA	3.2
3	A	411	HIS	3.2
3	A	330	ILE	3.2
3	A	459	TRP	3.2
3	A	701	SER	3.2
3	A	806	SER	3.2
3	A	820	ASP	3.2
3	A	460	LEU	3.2
3	A	446	LEU	3.1
3	A	534	LEU	3.1
3	A	828	VAL	3.1
3	A	846	TYR	3.1
3	A	783	VAL	3.1
3	A	681	ILE	3.1
3	A	510	CYS	3.1
3	A	348	PRO	3.1
3	A	475	PHE	3.1
3	A	814	PHE	3.1
3	A	698	TRP	3.1
3	A	324	GLN	3.0
3	A	304	ALA	3.0
3	A	315	GLU	3.0
3	A	33	ALA	3.0
3	A	418	TYR	3.0
3	A	639	TYR	3.0
3	A	802	TYR	3.0
3	A	823	ASN	3.0
3	A	119	ILE	3.0
3	A	519	ALA	3.0
3	A	271	CYS	3.0
3	A	158	GLU	3.0
3	A	797	TRP	3.0
3	A	638	ALA	3.0
3	A	784	HIS	3.0
3	A	427	TYR	3.0
3	A	787	ASP	3.0
3	A	839	CYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	174	VAL	2.9
3	A	204	TRP	2.9
3	A	327	ALA	2.9
3	A	818	PRO	2.9
3	A	667	PHE	2.9
3	A	811	HIS	2.9
3	A	640	GLY	2.9
3	A	567	VAL	2.9
3	A	571	TYR	2.9
3	A	702	ALA	2.8
3	A	779	ALA	2.8
3	A	32	LEU	2.8
3	A	202	SER	2.8
3	A	355	ILE	2.8
3	A	272	VAL	2.8
3	A	17	ALA	2.8
3	A	428	ALA	2.8
3	A	735	VAL	2.8
3	A	376	ALA	2.8
3	A	536	PHE	2.8
3	A	790	HIS	2.8
3	A	880	PHE	2.8
3	A	364	PRO	2.7
3	A	759	PRO	2.7
3	A	453	GLY	2.7
3	A	865	PRO	2.7
3	A	426	VAL	2.7
3	A	809	LEU	2.7
3	A	853	LEU	2.7
3	A	380	ALA	2.7
3	A	284	GLY	2.7
3	A	424	GLY	2.7
3	A	817	ILE	2.7
3	A	241	SER	2.7
3	A	876	LEU	2.7
3	A	96	ARG	2.7
3	A	294	LEU	2.7
3	A	785	SER	2.7
3	A	36	GLN	2.7
3	A	416	PHE	2.6
3	A	319	ALA	2.6
3	A	692	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	420	MET	2.6
3	A	195	LEU	2.6
3	A	705	LEU	2.6
3	A	707	ALA	2.6
3	A	74	ILE	2.6
3	A	154	ILE	2.6
3	A	322	ILE	2.6
3	A	530	CYS	2.6
3	A	582	LEU	2.6
3	A	466	ASN	2.6
3	A	263	GLY	2.6
3	A	290	GLY	2.6
3	A	488	ASN	2.6
3	A	634	VAL	2.6
3	A	725	VAL	2.6
3	A	409	ALA	2.6
3	A	500	THR	2.6
3	A	291	ARG	2.5
3	A	88	TRP	2.5
3	A	85	ILE	2.5
3	A	484	GLU	2.5
3	A	159	ALA	2.5
3	A	95	LYS	2.5
3	A	726	HIS	2.5
3	A	796	VAL	2.5
3	A	447	ALA	2.5
3	A	813	SER	2.5
3	A	142	GLY	2.5
3	A	498	GLU	2.5
3	A	537	ASP	2.5
3	A	297	VAL	2.5
3	A	822	ALA	2.5
3	A	552	ASP	2.5
3	A	151	PHE	2.5
3	A	646	PHE	2.5
1	T	5	DC	2.4
3	A	766	ASP	2.4
3	A	477	GLU	2.4
3	A	467	CYS	2.4
3	A	117	ILE	2.4
3	A	619	GLN	2.4
3	A	186	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	413	ALA	2.4
3	A	513	ALA	2.4
3	A	555	GLY	2.4
3	A	731	ASP	2.4
3	A	184	GLN	2.4
3	A	454	LYS	2.4
3	A	301	SER	2.4
3	A	14	ILE	2.4
3	A	141	ILE	2.4
3	A	39	LEU	2.4
3	A	747	LEU	2.4
3	A	295	ALA	2.4
3	A	451	PRO	2.3
3	A	502	TRP	2.4
3	A	854	HIS	2.3
3	A	171	ASN	2.3
3	A	560	ASN	2.3
3	A	40	GLU	2.3
3	A	121	THR	2.3
3	A	531	SER	2.3
3	A	264	ILE	2.3
3	A	769	ILE	2.3
3	A	214	VAL	2.3
3	A	321	ASN	2.3
3	A	871	ASN	2.3
3	A	251	ALA	2.3
3	A	525	GLY	2.3
3	A	620	TRP	2.3
3	A	727	TRP	2.3
3	A	490	MET	2.3
3	A	874	ASP	2.3
3	A	92	VAL	2.3
3	A	574	VAL	2.3
3	A	728	VAL	2.3
3	A	465	ALA	2.3
3	A	551	ARG	2.3
3	A	27	HIS	2.3
3	A	737	GLN	2.3
3	A	344	TRP	2.3
3	A	482	ILE	2.3
3	A	51	PHE	2.3
3	A	850	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	863	ALA	2.2
3	A	636	THR	2.2
3	A	572	GLY	2.2
3	A	229	LEU	2.2
3	A	599	ASP	2.2
3	A	653	ASP	2.2
3	A	18	ALA	2.2
3	A	445	THR	2.2
3	A	522	GLN	2.2
3	A	568	GLN	2.2
3	A	598	THR	2.2
3	A	786	GLN	2.2
3	A	179	LYS	2.2
3	A	479	ILE	2.2
3	A	751	PHE	2.2
3	A	20	PRO	2.2
3	A	331	ASN	2.2
3	A	764	ASN	2.2
3	A	219	MET	2.2
3	A	246	LEU	2.2
3	A	442	GLY	2.2
3	A	210	ILE	2.2
3	A	200	ALA	2.2
3	A	262	ALA	2.2
3	A	781	ASN	2.2
3	A	852	GLN	2.2
3	A	462	ILE	2.2
3	A	877	GLU	2.2
3	A	476	PRO	2.2
3	A	172	LYS	2.2
3	A	329	LYS	2.2
3	A	400	PHE	2.2
3	A	861	MET	2.1
3	A	668	THR	2.1
3	A	244	ILE	2.1
3	A	166	VAL	2.1
3	A	325	ASN	2.1
3	A	23	THR	2.1
3	A	561	LEU	2.1
3	A	621	LEU	2.1
3	A	734	PRO	2.1
3	A	486	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	354	ALA	2.1
3	A	339	ASN	2.1
3	A	299	THR	2.1
3	A	277	PRO	2.1
3	A	470	VAL	2.1
3	A	678	ALA	2.1
3	A	501	TRP	2.1
3	A	697	ASN	2.1
3	A	831	THR	2.1
3	A	554	VAL	2.0
3	A	7	ALA	2.0
3	A	292	ARG	2.0
3	A	405	ALA	2.0
3	A	615	ALA	2.0
3	A	191	LEU	2.0
3	A	35	GLU	2.0
3	A	618	GLY	2.0
3	A	109	ILE	2.0
3	A	279	THR	2.0
3	A	79	PRO	2.0
3	A	623	TYR	2.0
3	A	515	CYS	2.0
3	A	733	PHE	2.0
3	A	703	ALA	2.0
3	A	529	ASN	2.0
3	A	868	GLY	2.0
3	A	879	ASP	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 oligosaccharides in this entry.

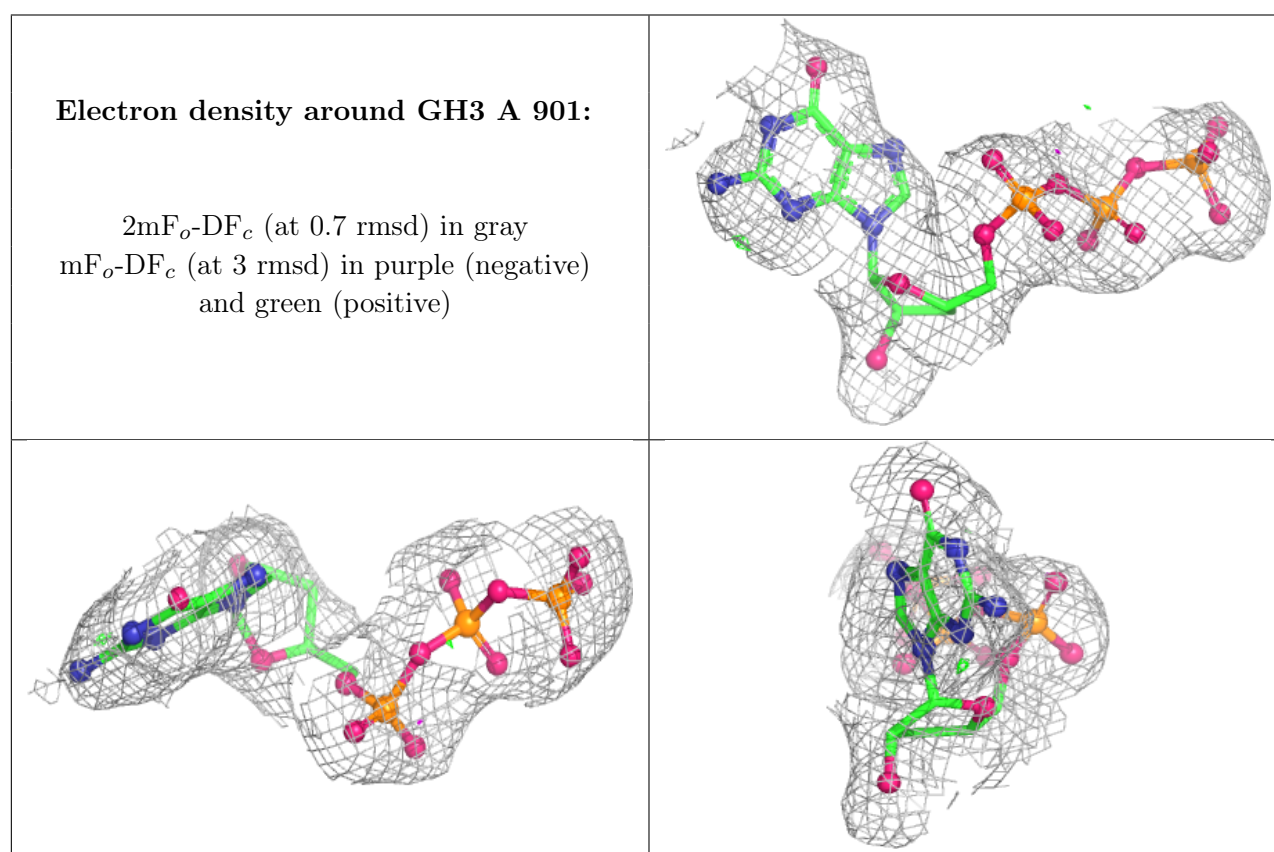
6.4 Ligands [i](#)

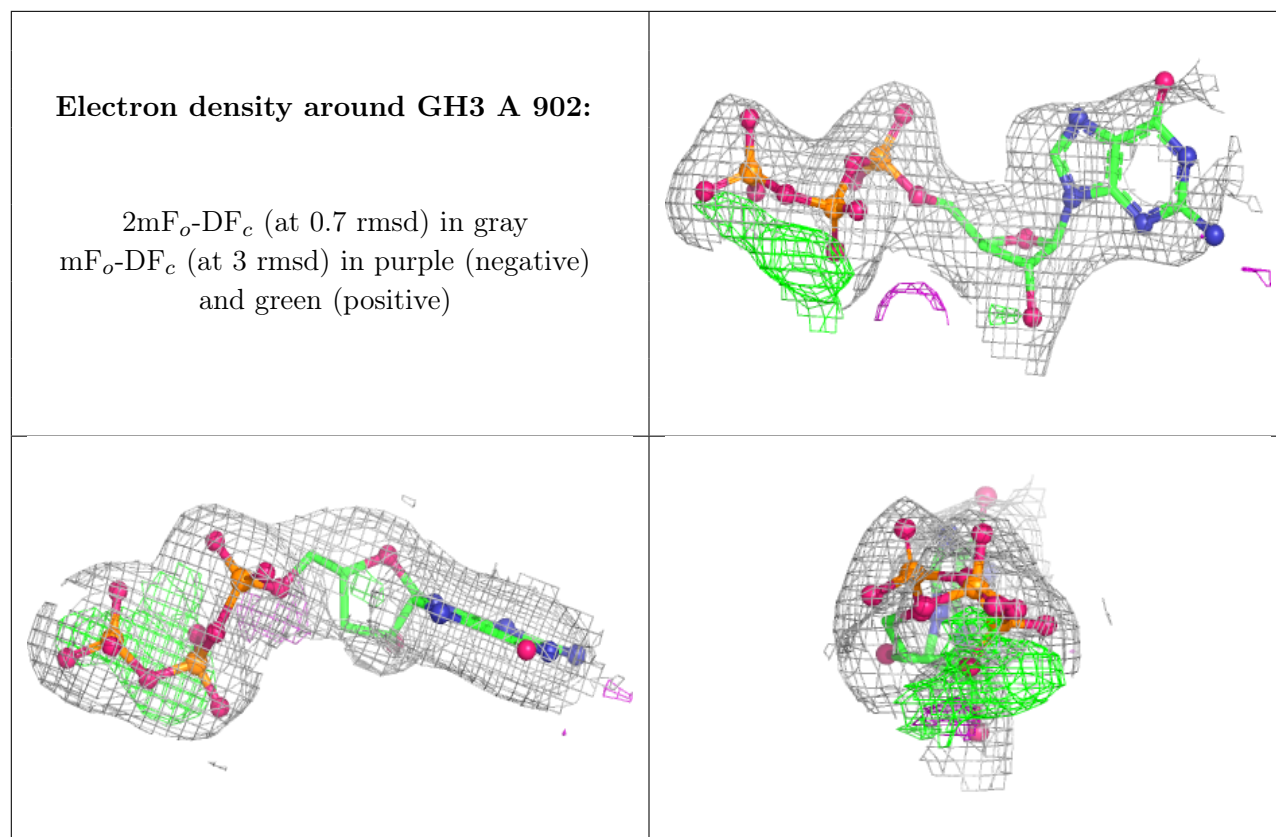
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	B-factors(Å ²)	Q<0.9
4	MG	A	885	1/1	0.30	0.79	42,42,42,42	0
4	MG	A	884	1/1	0.62	0.20	23,23,23,23	0
5	GH3	A	901	31/31	0.77	0.14	70,78,90,91	0
5	GH3	A	902	31/31	0.80	0.16	60,63,70,72	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.