



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:44 am GMT

PDB ID : 1N5Y  
Title : HIV-1 Reverse Transcriptase Crosslinked to Post-Translocation AZTMP-Terminated DNA (Complex P)  
Authors : Sarafianos, S.G.; Clark Jr., A.D.; Das, K.; Tuske, S.; Birktoft, J.J.; Ilankumaran, P.; Ramesha, A.R.; Sayer, J.M.; Jerina, D.M.; Boyer, P.L.; Hughes, S.H.; Arnold, E.  
Deposited on : 2002-11-07  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

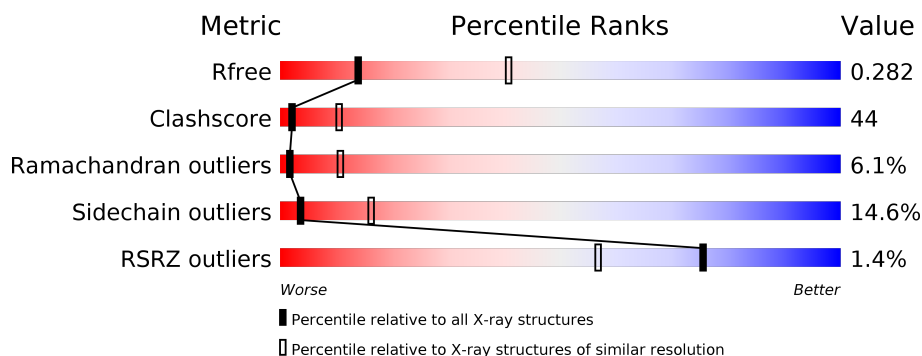
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	27	
2	P	21	
3	A	558	
4	B	430	
5	L	211	
6	H	225	

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
2	MRG	P	817	-	-	X	-
7	MG	A	1001	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12185 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(\*AP\*TP\*GP\*C\*TP\*AP\*GP\*GP\*CP\*GP\*CP\*CP\*CP\*GP\*AP\*AP\*CP\*AP\*GP\*GP\*GP\*AP\*CP\*TP\*GP\*TP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	21	Total	C	N	O	P	0	0	0
			432	204	87	121	20			

- Molecule 2 is a DNA chain called 5'-D(\*A\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(MRG)P\*CP\*GP\*CP\*CP\*(ATM))-3'.

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

- Molecule 3 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	558	Total	C	N	O	S	15	0	0
			4482	2901	741	832	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	CYS	GLN	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 4 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	429	Total	C	N	O	S	18	0	0
			3534	2304	586	637	7			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 5 is a protein called monoclonal antibody (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	211	Total	C	N	O	S	0	0	0
			1643	1025	270	342	6			

- Molecule 6 is a protein called monoclonal antibody (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	225	Total	C	N	O	S	0	0	0
			1685	1060	276	340	9			

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

### 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 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(\*AP\*TP\*GP\*C\*TP\*AP\*GP\*GP\*CP\*GP\*CP\*CP\*GP\*AP\*AP\*CP\*AP\*GP\*GP\*GP\*AP\*CP\*TP\*GP\*TP\*G)-3'

Chain T: 




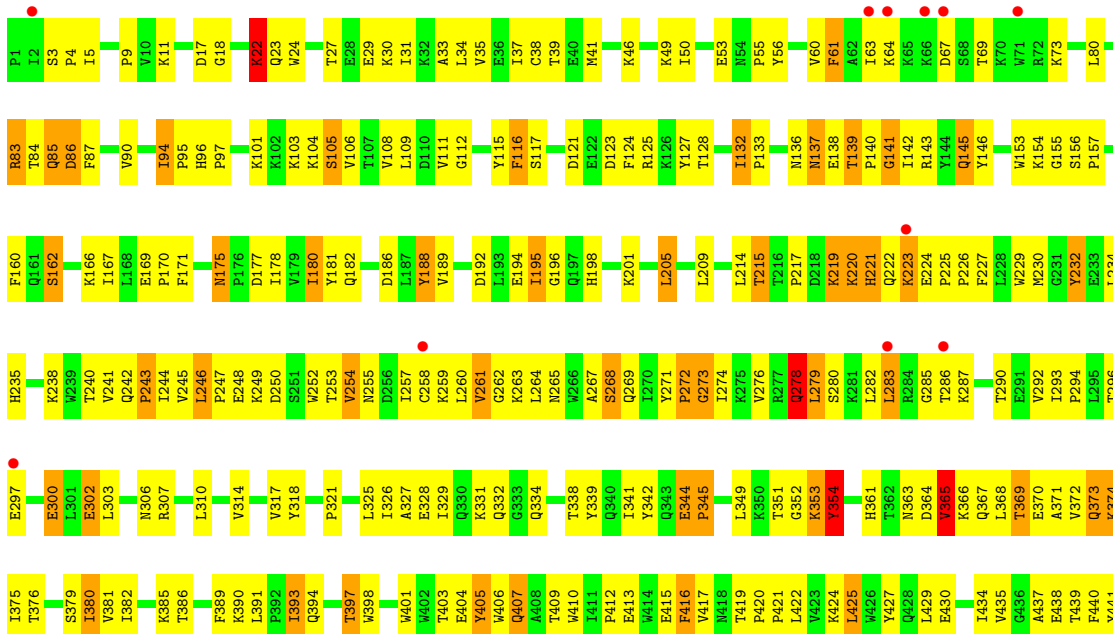
- Molecule 2: 5'-D(\*A\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(MRG)P\*C P\*GP\*CP\*CP\*(ATM))-3'

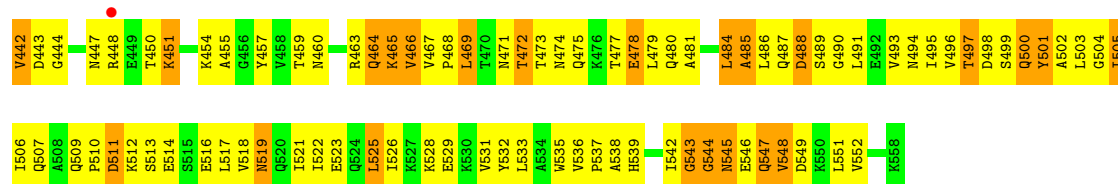
Chain P: 



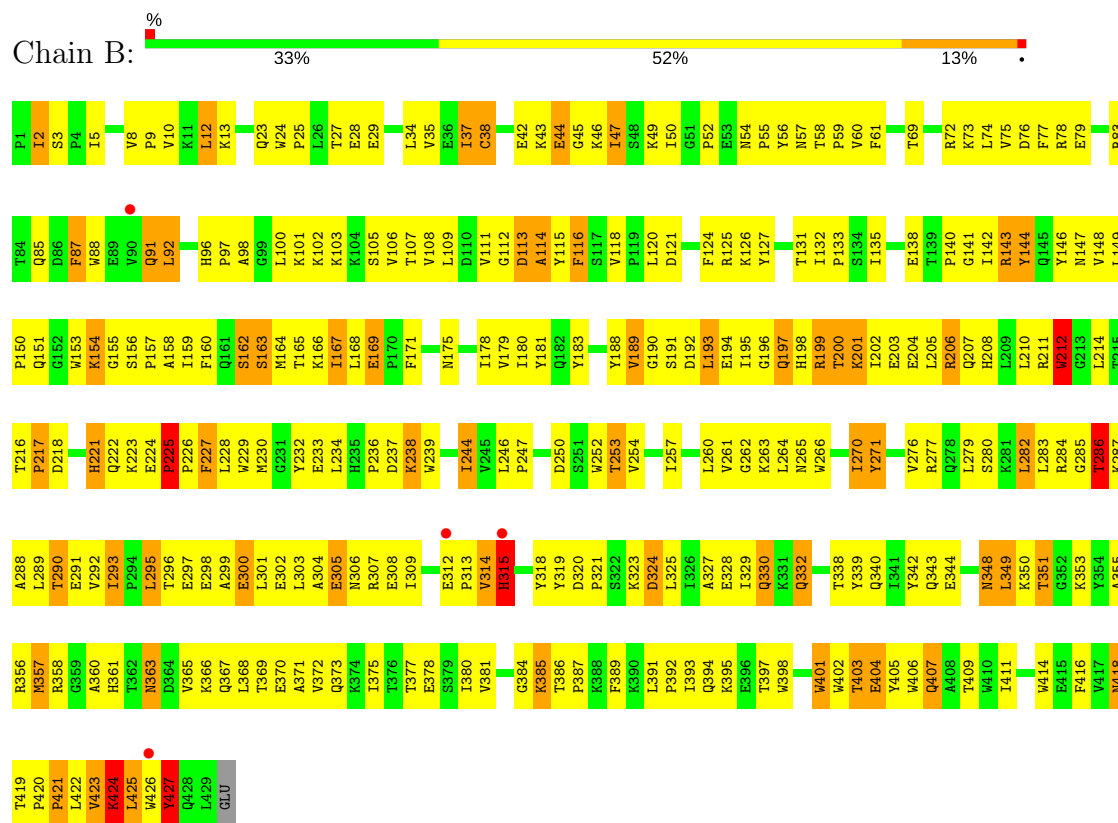
- Molecule 3: REVERSE TRANSCRIPTASE

Chain A: 

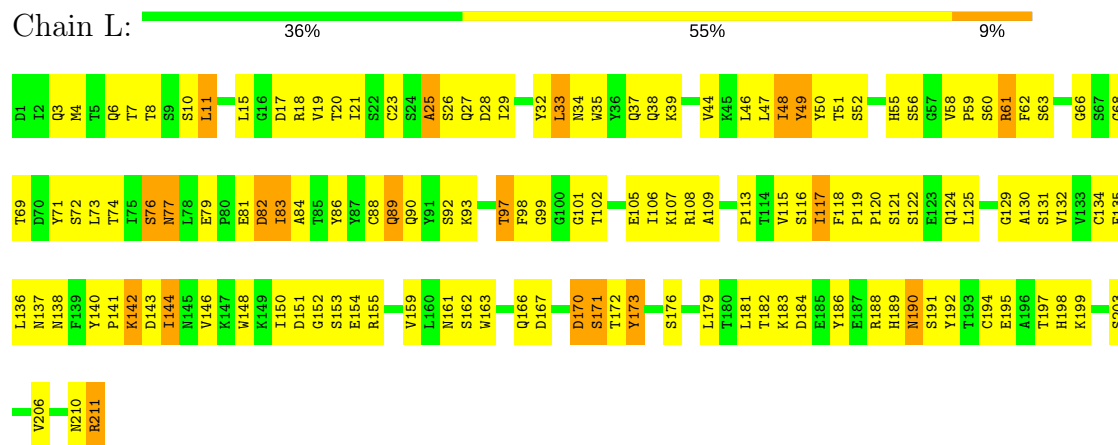




### • Molecule 4: REVERSE TRANSCRIPTASE

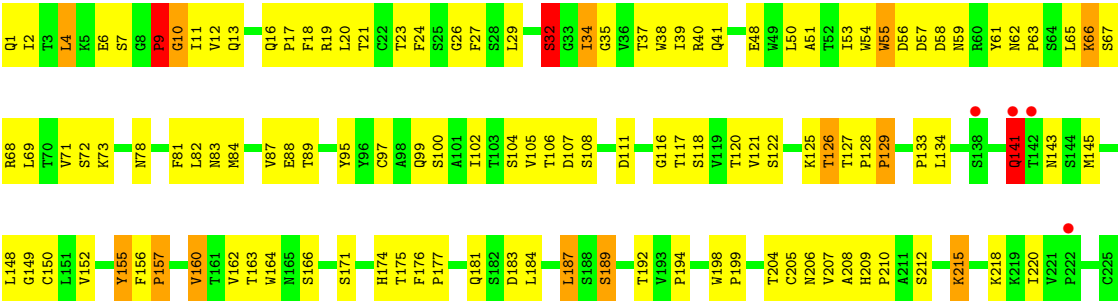


### • Molecule 5: monoclonal antibody (light chain)



### • Molecule 6: monoclonal antibody (heavy chain)







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.70Å 166.70Å 221.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10 34.36 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.8 (20.00-3.10) 91.7 (34.36-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 3.12Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.255 , 0.285 0.253 , 0.282	Depositor DCC
$R_{free}$ test set	2376 reflections (4.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	T	2.09	16/486 (3.3%)	1.80	20/749 (2.7%)
2	P	2.68	28/400 (7.0%)	2.60	44/612 (7.2%)
3	A	0.62	1/4600 (0.0%)	0.77	1/6259 (0.0%)
4	B	0.69	0/3639	0.83	3/4949 (0.1%)
5	L	0.58	0/1681	0.78	0/2283
6	H	0.63	0/1729	0.84	1/2372 (0.0%)
All	All	0.88	45/12535 (0.4%)	0.98	69/17224 (0.4%)

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
2	P	1	0
3	A	0	1
5	L	0	1
All	All	1	2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	812	DT	C4-C5	19.16	1.62	1.45
2	P	806	DT	C4-C5	18.46	1.61	1.45
1	T	720	DG	C5-C6	15.98	1.58	1.42
1	T	721	DG	C5-C6	11.98	1.54	1.42
2	P	813	DT	C4-C5	10.86	1.54	1.45
2	P	818	DC	N3-C4	10.35	1.41	1.33
2	P	806	DT	C2-N3	-9.41	1.30	1.37
2	P	816	DG	C5-C6	9.41	1.51	1.42
2	P	808	DC	N1-C2	8.34	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	809	DC	N1-C2	8.25	1.48	1.40
1	T	724	DT	N1-C2	7.90	1.44	1.38
2	P	820	DC	N3-C4	7.87	1.39	1.33
2	P	821	DC	C3'-O3'	7.82	1.54	1.44
2	P	818	DC	N1-C6	-7.66	1.32	1.37
3	A	248	GLU	CD-OE2	7.58	1.33	1.25
1	T	711	DC	N1-C2	-7.27	1.32	1.40
2	P	818	DC	C2'-C1'	7.20	1.59	1.52
2	P	809	DC	C4-C5	6.98	1.48	1.43
2	P	818	DC	P-OP1	-6.83	1.37	1.49
2	P	818	DC	O3'-P	6.68	1.69	1.61
2	P	808	DC	C4-C5	6.54	1.48	1.43
1	T	716	DA	C5-C6	6.44	1.46	1.41
2	P	818	DC	C3'-O3'	6.37	1.52	1.44
1	T	720	DG	C6-O6	6.36	1.29	1.24
1	T	723	DC	N1-C2	-6.34	1.33	1.40
1	T	709	DC	N1-C2	-6.31	1.33	1.40
2	P	818	DC	C2-N3	6.07	1.40	1.35
2	P	810	DT	C4-C5	6.03	1.50	1.45
1	T	720	DG	N9-C4	5.96	1.42	1.38
1	T	721	DG	N1-C2	-5.67	1.33	1.37
1	T	717	DC	N1-C2	-5.65	1.34	1.40
1	T	723	DC	N3-C4	5.57	1.37	1.33
2	P	804	DA	C6-N1	5.57	1.39	1.35
1	T	724	DT	C1'-N1	5.54	1.56	1.49
2	P	806	DT	N1-C2	5.50	1.42	1.38
1	T	723	DC	C5-C6	-5.46	1.29	1.34
2	P	816	DG	N1-C2	-5.45	1.33	1.37
2	P	816	DG	C8-N7	5.35	1.34	1.30
2	P	816	DG	N9-C8	5.20	1.41	1.37
2	P	809	DC	C5-C6	5.17	1.38	1.34
1	T	717	DC	N3-C4	5.15	1.37	1.33
1	T	723	DC	C4-C5	-5.07	1.38	1.43
2	P	808	DC	N3-C4	-5.05	1.30	1.33
2	P	812	DT	C4-O4	5.03	1.27	1.23
2	P	812	DT	N1-C2	5.01	1.42	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	806	DT	N3-C4-O4	-17.47	109.42	119.90
2	P	806	DT	C5-C4-O4	15.05	135.44	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	812	DT	N3-C4-O4	-13.97	111.52	119.90
2	P	812	DT	C5-C4-O4	12.77	133.84	124.90
2	P	816	DG	N9-C1'-C2'	12.07	135.53	112.60
2	P	815	DG	N9-C1'-C2'	11.90	135.22	112.60
2	P	812	DT	C4-C5-C7	11.06	125.63	119.00
2	P	806	DT	C4-C5-C7	10.71	125.43	119.00
2	P	818	DC	O4'-C1'-N1	8.74	114.12	108.00
2	P	806	DT	N3-C2-O2	-8.39	117.26	122.30
2	P	808	DC	N3-C4-N4	-8.34	112.16	118.00
1	T	720	DG	C5-C6-O6	8.32	133.59	128.60
2	P	813	DT	C5-C4-O4	8.30	130.71	124.90
1	T	713	DC	N1-C1'-C2'	8.17	128.12	112.60
2	P	809	DC	N3-C4-N4	-8.00	112.40	118.00
1	T	723	DC	O4'-C1'-N1	7.89	113.53	108.00
1	T	711	DC	N1-C1'-C2'	7.87	127.56	112.60
2	P	808	DC	C5-C4-N4	7.87	125.71	120.20
1	T	721	DG	C5-C6-O6	7.73	133.24	128.60
2	P	812	DT	C6-C5-C7	-7.64	118.31	122.90
2	P	813	DT	N3-C4-O4	-7.57	115.36	119.90
2	P	809	DC	C5-C4-N4	7.55	125.48	120.20
4	B	427	TYR	N-CA-C	7.47	131.16	111.00
1	T	721	DG	N1-C6-O6	-7.38	115.47	119.90
1	T	712	DC	N1-C1'-C2'	7.15	126.18	112.60
1	T	720	DG	N1-C6-O6	-7.09	115.64	119.90
6	H	141	GLN	N-CA-C	6.84	129.47	111.00
1	T	723	DC	N3-C4-N4	6.74	122.72	118.00
2	P	806	DT	C6-C5-C7	-6.72	118.87	122.90
2	P	813	DT	C4-C5-C7	6.50	122.90	119.00
1	T	709	DC	O4'-C1'-N1	6.47	112.53	108.00
1	T	723	DC	C5-C4-N4	-6.42	115.71	120.20
2	P	815	DG	O4'-C1'-C2'	6.40	111.02	105.90
2	P	816	DG	N1-C2-N2	-6.29	110.54	116.20
2	P	816	DG	O5'-P-OP1	6.09	118.00	110.70
2	P	808	DC	N3-C2-O2	-6.07	117.65	121.90
1	T	717	DC	C5-C4-N4	-5.93	116.05	120.20
2	P	812	DT	N1-C1'-C2'	5.85	123.72	112.60
2	P	816	DG	C5-C6-O6	5.83	132.09	128.60
1	T	717	DC	N3-C4-N4	5.82	122.07	118.00
2	P	819	DG	C5'-C4'-C3'	-5.81	103.65	114.10
2	P	818	DC	C5-C4-N4	-5.78	116.15	120.20
4	B	225	PRO	N-CA-C	5.75	127.06	112.10
2	P	820	DC	C2-N3-C4	-5.68	117.06	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	820	DC	C5-C4-N4	-5.59	116.29	120.20
2	P	808	DC	N1-C2-O2	5.57	122.24	118.90
1	T	720	DG	N1-C2-N2	-5.54	111.22	116.20
1	T	716	DA	N9-C1'-C2'	5.49	123.02	112.60
2	P	809	DC	N3-C2-O2	-5.46	118.08	121.90
1	T	717	DC	O4'-C1'-N1	5.43	111.80	108.00
2	P	806	DT	O4'-C1'-N1	-5.37	104.24	108.00
2	P	816	DG	N1-C6-O6	-5.36	116.69	119.90
2	P	815	DG	O4'-C1'-N9	5.33	111.73	108.00
2	P	816	DG	N3-C2-N2	5.33	123.63	119.90
2	P	818	DC	OP1-P-O3'	5.28	116.81	105.20
3	A	365	VAL	N-CA-C	-5.27	96.78	111.00
2	P	818	DC	N3-C4-N4	5.21	121.65	118.00
1	T	721	DG	N1-C2-N2	-5.16	111.56	116.20
1	T	721	DG	C6-C5-N7	5.15	133.49	130.40
2	P	818	DC	C6-N1-C2	5.15	122.36	120.30
2	P	813	DT	O4'-C1'-N1	-5.13	104.41	108.00
2	P	813	DT	N1-C1'-C2'	5.12	122.32	112.60
2	P	813	DT	C6-C5-C7	-5.10	119.84	122.90
1	T	720	DG	C6-C5-N7	5.08	133.45	130.40
4	B	423	VAL	N-CA-C	-5.06	97.33	111.00
2	P	812	DT	N3-C2-O2	-5.06	119.26	122.30
2	P	818	DC	P-O5'-C5'	5.05	128.99	120.90
2	P	806	DT	N1-C1'-C2'	5.05	122.20	112.60
1	T	721	DG	N9-C1'-C2'	5.04	122.19	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	P	815	DG	C1'

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	354	TYR	Sidechain
5	L	49	TYR	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	432	0	235	38	0
2	P	408	0	230	35	0
3	A	4482	0	4484	419	0
4	B	3534	0	3568	359	1
5	L	1643	0	1565	137	0
6	H	1685	0	1640	103	0
7	A	1	0	0	0	0
All	All	12185	0	11722	1038	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 44.

All (1038) 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)
5:L:61:ARG:HB2	5:L:76:SER:HB3	1.25	1.17
6:H:166:SER:H	6:H:206:ASN:ND2	1.51	1.07
6:H:166:SER:N	6:H:206:ASN:HD21	1.52	1.05
3:A:441:TYR:CE2	3:A:544:GLY:HA3	1.91	1.05
4:B:244:ILE:HD13	4:B:244:ILE:H	1.18	1.04
4:B:12:LEU:H	4:B:12:LEU:HD12	1.22	1.03
3:A:293:ILE:HD12	3:A:294:PRO:HD2	1.39	1.02
3:A:439:THR:HG21	4:B:289:LEU:H	1.19	1.01
3:A:254:VAL:HG13	3:A:255:ASN:H	1.26	1.01
3:A:279:LEU:H	3:A:279:LEU:HD23	1.25	1.01
3:A:331:LYS:HB3	3:A:421:PRO:HG2	1.40	1.01
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.41	1.00
1:T:712:DC:H2''	1:T:713:DC:H5'	1.42	1.00
4:B:371:ALA:O	4:B:375:ILE:HG13	1.60	0.99
6:H:53:ILE:HB	6:H:71:VAL:HG11	1.42	0.99
3:A:138:GLU:HG2	3:A:139:THR:H	1.29	0.97
3:A:246:LEU:H	3:A:246:LEU:HD23	1.31	0.95
4:B:363:ASN:ND2	4:B:366:LYS:H	1.66	0.94
1:T:724:DT:H2''	1:T:725:DG:C8	2.02	0.94
4:B:330:GLN:HE22	4:B:340:GLN:HE22	1.14	0.94
3:A:354:TYR:CE1	3:A:374:LYS:HB3	2.02	0.93
5:L:90:GLN:HE21	5:L:92:SER:H	0.93	0.91
2:P:819:DG:H2''	2:P:820:DC:O5'	1.70	0.91
5:L:170:ASP:O	5:L:172:THR:HG23	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:296:THR:HG22	4:B:298:GLU:H	1.31	0.90
5:L:90:GLN:HE21	5:L:92:SER:N	1.69	0.89
3:A:317:VAL:HG22	3:A:318:TYR:H	1.38	0.89
4:B:363:ASN:O	4:B:367:GLN:HG3	1.72	0.89
4:B:257:ILE:O	4:B:261:VAL:HG23	1.73	0.89
3:A:469:LEU:HD21	3:A:480:GLN:HG2	1.55	0.88
4:B:225:PRO:HB2	4:B:226:PRO:HD3	1.53	0.88
3:A:459:THR:HG22	3:A:463:ARG:HB3	1.55	0.88
2:P:820:DC:H2''	2:P:821:DC:H5'	1.55	0.88
2:P:818:DC:H2''	2:P:819:DG:O5'	1.72	0.87
3:A:215:THR:O	3:A:217:PRO:HD3	1.74	0.86
3:A:394:GLN:HG2	3:A:416:PHE:CE2	2.09	0.86
3:A:279:LEU:H	3:A:279:LEU:CD2	1.86	0.86
4:B:222:GLN:HG3	4:B:224:GLU:H	1.40	0.86
4:B:237:ASP:C	4:B:239:TRP:H	1.76	0.86
1:T:707:DG:H2''	1:T:708:DG:H5'	1.58	0.85
4:B:225:PRO:CG	5:L:92:SER:HA	2.07	0.85
3:A:459:THR:CG2	3:A:463:ARG:HB3	2.07	0.84
5:L:34:ASN:OD1	5:L:49:TYR:HA	1.77	0.84
3:A:447:ASN:HD22	3:A:450:THR:HG23	1.41	0.84
3:A:489:SER:HB3	3:A:528:LYS:HZ3	1.41	0.84
3:A:501:TYR:HE1	3:A:505:ILE:HD11	1.41	0.84
3:A:366:LYS:O	3:A:370:GLU:HG2	1.76	0.84
3:A:106:VAL:HB	3:A:227:PHE:HE1	1.41	0.84
2:P:818:DC:H2'	2:P:819:DG:H8	1.43	0.83
3:A:22:LYS:HD3	3:A:22:LYS:H	1.43	0.83
4:B:58:THR:HG23	4:B:59:PRO:HD2	1.59	0.83
4:B:423:VAL:C	4:B:425:LEU:H	1.82	0.83
6:H:38:TRP:O	6:H:50:LEU:HB2	1.79	0.83
3:A:500:GLN:NE2	3:A:500:GLN:H	1.77	0.82
5:L:182:THR:HG22	5:L:183:LYS:H	1.43	0.82
5:L:90:GLN:NE2	5:L:92:SER:H	1.77	0.82
3:A:434:ILE:HG22	3:A:494:ASN:HD21	1.43	0.82
3:A:90:VAL:HG12	4:B:141:GLY:H	1.43	0.81
5:L:15:LEU:HD12	5:L:15:LEU:H	1.44	0.81
5:L:38:GLN:HG3	5:L:44:VAL:HG22	1.60	0.81
5:L:89:GLN:HB2	5:L:98:PHE:CD1	2.15	0.81
3:A:439:THR:HG21	4:B:289:LEU:N	1.96	0.80
5:L:61:ARG:CB	5:L:76:SER:HB3	2.08	0.80
1:T:722:DA:N6	2:P:806:DT:O4	2.15	0.79
3:A:143:ARG:HH11	3:A:143:ARG:HG3	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:33:LEU:HD21	5:L:88:CYS:HB2	1.65	0.78
3:A:441:TYR:CD2	3:A:544:GLY:HA3	2.17	0.78
2:P:818:DC:H2'	2:P:819:DG:C8	2.18	0.78
4:B:253:THR:O	4:B:257:ILE:HG12	1.84	0.78
2:P:819:DG:C2'	2:P:820:DC:O5'	2.31	0.78
5:L:17:ASP:O	5:L:77:ASN:HA	1.84	0.77
5:L:34:ASN:HB2	5:L:89:GLN:NE2	1.98	0.77
5:L:195:GLU:HG3	5:L:206:VAL:HG22	1.63	0.77
4:B:312:GLU:HB3	4:B:313:PRO:HD2	1.66	0.77
3:A:209:LEU:HB3	3:A:214:LEU:HB2	1.66	0.77
1:T:716:DA:N6	2:P:812:DT:O4	2.16	0.77
4:B:163:SER:O	4:B:167:ILE:HG13	1.85	0.77
6:H:148:LEU:HD13	6:H:220:ILE:HG21	1.67	0.77
4:B:393:ILE:HD13	4:B:398:TRP:HB2	1.66	0.76
3:A:489:SER:HB3	3:A:528:LYS:NZ	2.00	0.76
1:T:724:DT:H2''	1:T:725:DG:H8	1.50	0.76
3:A:344:GLU:HB3	3:A:345:PRO:HD2	1.67	0.76
3:A:405:TYR:HD1	3:A:406:TRP:H	1.34	0.76
3:A:132:ILE:HG23	3:A:142:ILE:HB	1.68	0.76
4:B:369:THR:HG22	4:B:398:TRP:CZ3	2.19	0.76
4:B:363:ASN:HD21	4:B:365:VAL:HB	1.51	0.76
4:B:423:VAL:O	4:B:425:LEU:N	2.19	0.76
3:A:371:ALA:O	3:A:375:ILE:HG12	1.87	0.75
3:A:460:ASN:HA	4:B:286:THR:OG1	1.87	0.75
3:A:310:LEU:O	3:A:310:LEU:HD23	1.87	0.74
2:P:817:MRG:C2'	2:P:818:DC:O5'	2.35	0.74
3:A:136:ASN:O	3:A:138:GLU:N	2.21	0.74
3:A:397:THR:HG21	3:A:424:LYS:HA	1.68	0.74
4:B:111:VAL:HG23	4:B:111:VAL:O	1.85	0.74
3:A:406:TRP:CZ2	4:B:420:PRO:HG3	2.22	0.74
4:B:91:GLN:HA	4:B:91:GLN:OE1	1.85	0.74
4:B:12:LEU:N	4:B:12:LEU:HD12	2.01	0.74
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.68	0.74
3:A:279:LEU:N	3:A:279:LEU:HD23	2.02	0.74
4:B:365:VAL:O	4:B:369:THR:HG23	1.87	0.74
3:A:297:GLU:HA	3:A:300:GLU:HB2	1.69	0.73
3:A:50:ILE:CG2	3:A:145:GLN:HB3	2.18	0.73
3:A:450:THR:O	3:A:451:LYS:HG2	1.87	0.73
6:H:141:GLN:HE22	6:H:199:PRO:HD3	1.54	0.73
5:L:120:PRO:HB2	5:L:125:LEU:HD21	1.71	0.73
4:B:423:VAL:C	4:B:425:LEU:N	2.40	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:299:ALA:O	4:B:301:LEU:N	2.22	0.73
2:P:820:DC:H2''	2:P:821:DC:C5'	2.18	0.72
6:H:53:ILE:HB	6:H:71:VAL:CG1	2.19	0.72
3:A:254:VAL:HG13	3:A:255:ASN:N	2.03	0.72
4:B:285:GLY:H	4:B:287:LYS:NZ	1.87	0.72
4:B:279:LEU:HD11	4:B:302:GLU:HB2	1.70	0.72
4:B:229:TRP:HA	4:B:232:TYR:CE1	2.25	0.72
4:B:244:ILE:CD1	4:B:244:ILE:H	1.98	0.72
3:A:30:LYS:O	3:A:33:ALA:HB3	1.90	0.72
3:A:406:TRP:HE1	4:B:418:ASN:ND2	1.87	0.72
3:A:435:VAL:HG22	4:B:290:THR:HG21	1.72	0.72
3:A:27:THR:HG23	3:A:30:LYS:HD2	1.70	0.71
3:A:484:LEU:O	3:A:486:LEU:N	2.23	0.71
4:B:237:ASP:C	4:B:239:TRP:N	2.43	0.71
4:B:387:PRO:HG2	4:B:389:PHE:CE1	2.25	0.71
3:A:501:TYR:C	3:A:501:TYR:CD1	2.62	0.71
4:B:2:ILE:HD12	4:B:2:ILE:O	1.91	0.71
4:B:426:TRP:CE3	4:B:426:TRP:HA	2.26	0.71
4:B:162:SER:O	4:B:165:THR:HG22	1.90	0.71
3:A:440:PHE:HE2	3:A:489:SER:HG	1.38	0.70
3:A:460:ASN:HD22	4:B:288:ALA:HB2	1.55	0.70
2:P:817:MRG:H2''	2:P:818:DC:C5'	2.21	0.70
4:B:225:PRO:HG3	5:L:92:SER:HA	1.73	0.70
5:L:83:ILE:HG21	5:L:106:ILE:HG13	1.71	0.70
5:L:162:SER:OG	6:H:177:PRO:HG2	1.92	0.70
5:L:38:GLN:NE2	6:H:41:GLN:HE22	1.90	0.70
3:A:317:VAL:HG22	3:A:318:TYR:N	2.06	0.70
3:A:533:LEU:N	3:A:533:LEU:HD12	2.05	0.70
6:H:125:LYS:O	6:H:127:THR:HG23	1.91	0.70
4:B:206:ARG:NH1	4:B:217:PRO:O	2.25	0.70
4:B:8:VAL:HG11	4:B:159:ILE:HG12	1.73	0.70
2:P:818:DC:C2'	2:P:819:DG:O5'	2.39	0.69
3:A:354:TYR:HE1	3:A:374:LYS:HB3	1.54	0.69
4:B:263:LYS:HA	4:B:423:VAL:HG11	1.74	0.69
4:B:363:ASN:HD22	4:B:366:LYS:H	1.41	0.69
5:L:38:GLN:HE22	6:H:41:GLN:HE22	1.39	0.69
2:P:803:DC:H2''	2:P:804:DA:C8	2.28	0.69
3:A:376:THR:HG23	3:A:386:THR:HG23	1.73	0.69
4:B:266:TRP:CH2	4:B:422:LEU:HB3	2.27	0.69
3:A:138:GLU:HG2	3:A:139:THR:N	2.06	0.69
3:A:90:VAL:CG1	4:B:141:GLY:H	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:285:GLY:O	4:B:287:LYS:HG2	1.93	0.69
5:L:86:TYR:O	5:L:101:GLY:HA2	1.94	0.68
3:A:501:TYR:HE1	3:A:505:ILE:CD1	2.06	0.68
4:B:299:ALA:C	4:B:301:LEU:H	1.94	0.68
4:B:178:ILE:CD1	4:B:201:LYS:HG2	2.24	0.68
2:P:817:MRG:H2''	2:P:818:DC:H5'	1.76	0.68
3:A:257:ILE:HG21	3:A:283:LEU:HD21	1.75	0.68
3:A:9:PRO:HA	3:A:121:ASP:OD2	1.94	0.68
1:T:706:DA:H2'	1:T:707:DG:C8	2.29	0.68
5:L:113:PRO:HG3	5:L:144:ILE:HD11	1.76	0.67
4:B:320:ASP:OD2	4:B:323:LYS:HG3	1.94	0.67
3:A:3:SER:HB3	3:A:5:ILE:HG13	1.75	0.67
3:A:437:ALA:HB1	3:A:493:VAL:HA	1.75	0.67
5:L:106:ILE:H	5:L:166:GLN:HE22	1.42	0.67
4:B:106:VAL:HG13	4:B:234:LEU:HB2	1.77	0.66
5:L:151:ASP:HA	5:L:191:SER:HB3	1.78	0.66
3:A:518:VAL:O	3:A:522:ILE:HG13	1.94	0.66
3:A:246:LEU:H	3:A:246:LEU:CD2	2.06	0.66
4:B:166:LYS:HA	4:B:169:GLU:OE1	1.94	0.66
3:A:22:LYS:HD3	3:A:22:LYS:N	2.09	0.66
4:B:225:PRO:HG2	5:L:92:SER:HA	1.77	0.66
3:A:420:PRO:HA	3:A:421:PRO:C	2.17	0.66
3:A:457:TYR:HA	3:A:548:VAL:CG1	2.24	0.66
4:B:244:ILE:HD11	4:B:271:TYR:OH	1.95	0.66
6:H:54:TRP:HB3	6:H:55:TRP:CE3	2.30	0.66
4:B:285:GLY:H	4:B:287:LYS:HZ3	1.42	0.66
3:A:439:THR:CG2	4:B:288:ALA:HA	2.26	0.65
6:H:34:ILE:CG2	6:H:35:GLY:N	2.59	0.65
5:L:23:CYS:SG	5:L:33:LEU:HD11	2.37	0.65
3:A:354:TYR:CZ	3:A:374:LYS:HG2	2.30	0.65
4:B:195:ILE:HG23	4:B:196:GLY:N	2.11	0.65
3:A:293:ILE:CD1	3:A:294:PRO:HD2	2.21	0.65
3:A:430:GLU:HB2	3:A:532:TYR:HB2	1.79	0.65
3:A:486:LEU:HA	3:A:528:LYS:NZ	2.12	0.65
4:B:47:ILE:HD12	4:B:146:TYR:HA	1.77	0.64
3:A:96:HIS:ND1	3:A:97:PRO:HD2	2.12	0.64
5:L:11:LEU:HD21	5:L:19:VAL:HG11	1.78	0.64
3:A:254:VAL:CG1	3:A:255:ASN:H	2.06	0.64
3:A:486:LEU:HA	3:A:528:LYS:HZ2	1.60	0.64
4:B:395:LYS:HB2	4:B:416:PHE:CD2	2.32	0.64
4:B:403:THR:O	4:B:405:TYR:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:87:PHE:CD2	4:B:88:TRP:N	2.65	0.64
3:A:501:TYR:CE1	3:A:505:ILE:HD11	2.29	0.64
5:L:38:GLN:HE22	6:H:41:GLN:NE2	1.96	0.64
3:A:271:TYR:CE1	3:A:314:VAL:HG22	2.33	0.64
3:A:182:GLN:O	3:A:182:GLN:HG3	1.97	0.63
5:L:108:ARG:HG2	5:L:109:ALA:N	2.13	0.63
6:H:12:VAL:HG21	6:H:18:PHE:HB3	1.80	0.63
6:H:27:PHE:CZ	6:H:99:GLN:HG3	2.33	0.63
6:H:34:ILE:HD12	6:H:34:ILE:H	1.62	0.63
4:B:224:GLU:HB3	4:B:225:PRO:HD2	1.80	0.63
5:L:19:VAL:O	5:L:74:THR:HA	1.97	0.63
3:A:501:TYR:C	3:A:501:TYR:HD1	2.01	0.63
4:B:393:ILE:HG12	4:B:394:GLN:N	2.12	0.63
6:H:53:ILE:HD12	6:H:71:VAL:HG12	1.81	0.63
5:L:38:GLN:HG3	5:L:44:VAL:CG2	2.28	0.63
3:A:542:ILE:HD11	4:B:261:VAL:HG11	1.80	0.63
3:A:463:ARG:HG3	3:A:464:GLN:H	1.62	0.62
5:L:35:TRP:HB2	5:L:48:ILE:HD12	1.80	0.62
3:A:109:LEU:HD23	3:A:220:LYS:HB2	1.81	0.62
3:A:447:ASN:ND2	3:A:450:THR:HG23	2.13	0.62
4:B:263:LYS:HG2	4:B:423:VAL:CG1	2.29	0.62
3:A:473:THR:HG22	3:A:474:ASN:N	2.14	0.62
4:B:120:LEU:HD12	4:B:121:ASP:H	1.64	0.62
2:P:812:DT:C6	2:P:813:DT:H73	2.34	0.62
5:L:33:LEU:HD23	5:L:34:ASN:H	1.63	0.62
5:L:33:LEU:CD2	5:L:88:CYS:HB2	2.27	0.62
3:A:111:VAL:HG11	3:A:214:LEU:HD12	1.81	0.62
6:H:209:HIS:HD2	6:H:212:SER:OG	1.83	0.62
3:A:420:PRO:HG3	3:A:422:LEU:HG	1.82	0.61
4:B:227:PHE:O	4:B:230:MET:HB2	2.00	0.61
6:H:162:VAL:HG22	6:H:207:VAL:HG22	1.81	0.61
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.82	0.61
3:A:478:GLU:OE1	3:A:498:ASP:OD1	2.17	0.61
3:A:465:LYS:NZ	3:A:488:ASP:OD2	2.31	0.61
4:B:260:LEU:O	4:B:260:LEU:HD12	2.00	0.61
1:T:715:DA:H2"	1:T:716:DA:H8	1.65	0.61
4:B:260:LEU:O	4:B:264:LEU:HD12	2.01	0.61
3:A:219:LYS:O	3:A:219:LYS:HG3	2.00	0.61
4:B:330:GLN:NE2	4:B:340:GLN:HE22	1.91	0.61
4:B:43:LYS:C	4:B:45:GLY:H	2.02	0.61
3:A:344:GLU:CB	3:A:345:PRO:HD2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:511:ASP:OD2	3:A:511:ASP:C	2.39	0.61
4:B:293:ILE:HD13	4:B:293:ILE:N	2.15	0.61
4:B:323:LYS:HB2	4:B:343:GLN:NE2	2.16	0.61
3:A:104:LYS:HB2	3:A:192:ASP:HA	1.82	0.61
4:B:299:ALA:C	4:B:301:LEU:N	2.54	0.61
4:B:330:GLN:HE22	4:B:340:GLN:NE2	1.94	0.61
5:L:73:LEU:HD12	5:L:74:THR:H	1.66	0.61
4:B:306:ASN:HA	4:B:309:ILE:HG12	1.82	0.61
4:B:340:GLN:HG3	4:B:351:THR:HG22	1.83	0.61
4:B:225:PRO:HB3	5:L:32:TYR:CE1	2.36	0.61
4:B:262:GLY:O	4:B:265:ASN:N	2.33	0.61
4:B:302:GLU:HA	4:B:305:GLU:HB2	1.81	0.61
4:B:34:LEU:CD1	4:B:73:LYS:HG3	2.30	0.61
3:A:162:SER:OG	4:B:52:PRO:HD3	2.01	0.61
4:B:79:GLU:OE1	4:B:83:ARG:NH1	2.34	0.60
6:H:133:PRO:O	6:H:134:LEU:HD23	2.00	0.60
4:B:60:VAL:CG1	4:B:75:VAL:HG22	2.24	0.60
6:H:183:ASP:O	6:H:184:LEU:HG	1.99	0.60
5:L:117:ILE:HD13	5:L:194:CYS:HB2	1.82	0.60
5:L:89:GLN:HB2	5:L:98:PHE:CE1	2.35	0.60
3:A:86:ASP:HA	3:A:154:LYS:HZ2	1.66	0.60
4:B:314:VAL:HG12	4:B:315:HIS:H	1.66	0.60
4:B:59:PRO:HG2	4:B:76:ASP:HB3	1.83	0.60
2:P:817:MRG:H2''	2:P:818:DC:O5'	2.01	0.60
3:A:479:LEU:HD21	3:A:518:VAL:CG2	2.32	0.60
5:L:6:GLN:OE1	5:L:101:GLY:N	2.29	0.60
3:A:493:VAL:HG22	3:A:494:ASN:N	2.15	0.60
4:B:225:PRO:CB	4:B:226:PRO:HD3	2.28	0.60
3:A:109:LEU:HD23	3:A:220:LYS:CB	2.32	0.60
4:B:46:LYS:HD2	4:B:116:PHE:HB3	1.84	0.59
4:B:43:LYS:C	4:B:45:GLY:N	2.53	0.59
4:B:155:GLY:O	4:B:158:ALA:HB3	2.02	0.59
6:H:39:ILE:HG22	6:H:40:ARG:N	2.18	0.59
3:A:257:ILE:O	3:A:261:VAL:HG12	2.02	0.59
3:A:379:SER:O	3:A:382:ILE:N	2.31	0.59
3:A:548:VAL:O	3:A:552:VAL:HG23	2.02	0.59
4:B:34:LEU:HD11	4:B:73:LYS:HG3	1.84	0.59
3:A:31:ILE:O	3:A:35:VAL:HG23	2.03	0.59
5:L:173:TYR:N	5:L:173:TYR:CD1	2.70	0.59
4:B:314:VAL:HG12	4:B:315:HIS:N	2.17	0.59
6:H:55:TRP:HE3	6:H:55:TRP:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:713:DC:H2''	1:T:714:DG:O5'	2.03	0.59
3:A:373:GLN:NE2	4:B:397:THR:HG23	2.17	0.59
3:A:494:ASN:OD1	4:B:289:LEU:HD12	2.03	0.59
6:H:62:ASN:HD22	6:H:63:PRO:HD2	1.66	0.59
5:L:21:ILE:HD13	5:L:102:THR:HB	1.85	0.59
3:A:497:THR:HG22	3:A:498:ASP:H	1.68	0.59
3:A:175:ASN:OD1	3:A:201:LYS:HE3	2.03	0.58
3:A:361:HIS:CD2	3:A:505:ILE:HD13	2.38	0.58
4:B:43:LYS:O	4:B:45:GLY:N	2.35	0.58
4:B:87:PHE:HE2	4:B:155:GLY:HA2	1.68	0.58
5:L:66:GLY:HA3	5:L:71:TYR:CD2	2.38	0.58
3:A:500:GLN:HE21	3:A:500:GLN:H	1.49	0.58
4:B:168:LEU:HD13	4:B:180:ILE:HG21	1.84	0.58
5:L:190:ASN:CG	5:L:210:ASN:HD22	2.07	0.58
3:A:429:LEU:HD22	3:A:533:LEU:HD13	1.85	0.58
5:L:34:ASN:O	5:L:88:CYS:HA	2.03	0.58
3:A:543:GLY:O	3:A:545:ASN:N	2.37	0.58
4:B:113:ASP:O	4:B:115:TYR:N	2.37	0.58
4:B:100:LEU:HD23	4:B:100:LEU:O	2.04	0.58
6:H:209:HIS:CD2	6:H:212:SER:OG	2.56	0.58
1:T:707:DG:C2'	1:T:708:DG:H5'	2.32	0.58
3:A:166:LYS:O	3:A:169:GLU:HB3	2.02	0.58
3:A:317:VAL:CG2	3:A:318:TYR:H	2.15	0.58
5:L:33:LEU:HD23	5:L:89:GLN:O	2.03	0.58
3:A:280:SER:O	3:A:283:LEU:HG	2.04	0.58
3:A:363:ASN:OD1	3:A:364:ASP:N	2.37	0.58
4:B:112:GLY:HA3	4:B:151:GLN:HE21	1.68	0.58
3:A:475:GLN:HB3	3:A:501:TYR:CE2	2.39	0.58
3:A:34:LEU:HA	3:A:37:ILE:HD12	1.86	0.58
3:A:354:TYR:OH	3:A:374:LYS:HG2	2.03	0.58
3:A:5:ILE:CD1	3:A:167:ILE:HD11	2.34	0.58
4:B:58:THR:HG23	4:B:59:PRO:CD	2.33	0.57
4:B:58:THR:CG2	4:B:59:PRO:N	2.66	0.57
3:A:499:SER:OG	3:A:502:ALA:HB3	2.03	0.57
4:B:171:PHE:HE1	4:B:205:LEU:HA	1.68	0.57
6:H:40:ARG:HB2	6:H:50:LEU:HD11	1.86	0.57
3:A:439:THR:HG1	3:A:441:TYR:HE1	1.51	0.57
4:B:171:PHE:CE1	4:B:205:LEU:HA	2.39	0.57
5:L:61:ARG:HG2	5:L:61:ARG:HH11	1.70	0.57
3:A:416:PHE:CD1	3:A:416:PHE:C	2.76	0.57
4:B:205:LEU:HD12	4:B:205:LEU:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:417:VAL:O	3:A:417:VAL:HG13	2.05	0.57
3:A:463:ARG:HG3	3:A:464:GLN:N	2.20	0.57
3:A:521:ILE:O	3:A:525:LEU:HD13	2.05	0.57
3:A:17:ASP:O	3:A:83:ARG:NH1	2.37	0.57
3:A:11:LYS:O	3:A:85:GLN:HG2	2.05	0.57
6:H:27:PHE:CE2	6:H:99:GLN:HG3	2.39	0.57
5:L:120:PRO:CB	5:L:125:LEU:HD21	2.34	0.57
5:L:135:PHE:C	5:L:136:LEU:HD12	2.25	0.57
5:L:73:LEU:HD12	5:L:74:THR:N	2.20	0.57
3:A:466:VAL:HG21	3:A:551:LEU:HG	1.87	0.57
5:L:154:GLU:HG2	5:L:155:ARG:N	2.20	0.57
3:A:338:THR:HG22	3:A:339:TYR:N	2.20	0.57
4:B:234:LEU:HD21	4:B:377:THR:HG21	1.87	0.57
6:H:6:GLU:OE1	6:H:116:GLY:N	2.34	0.56
4:B:112:GLY:HA3	4:B:151:GLN:NE2	2.19	0.56
4:B:106:VAL:HA	4:B:190:GLY:HA2	1.87	0.56
4:B:58:THR:HG22	4:B:59:PRO:N	2.20	0.56
1:T:713:DC:H2'	1:T:714:DG:C8	2.39	0.56
4:B:120:LEU:HD12	4:B:121:ASP:N	2.20	0.56
5:L:81:GLU:OE1	5:L:81:GLU:N	2.37	0.56
3:A:459:THR:HG22	3:A:463:ARG:CB	2.32	0.56
3:A:518:VAL:HG12	3:A:518:VAL:O	2.04	0.56
3:A:261:VAL:HG13	3:A:262:GLY:H	1.70	0.56
5:L:61:ARG:CZ	5:L:79:GLU:HG3	2.35	0.56
3:A:460:ASN:HA	4:B:286:THR:O	2.05	0.56
6:H:95:TYR:O	6:H:116:GLY:HA2	2.04	0.56
5:L:35:TRP:CZ3	5:L:88:CYS:HB3	2.40	0.56
3:A:194:GLU:O	3:A:196:GLY:N	2.39	0.56
3:A:438:GLU:HB3	3:A:459:THR:OG1	2.05	0.56
6:H:134:LEU:HD12	6:H:149:GLY:HA3	1.87	0.56
5:L:182:THR:HG22	5:L:183:LYS:N	2.15	0.56
3:A:443:ASP:O	3:A:481:ALA:HB2	2.04	0.56
4:B:210:LEU:C	4:B:212:TRP:H	2.09	0.56
4:B:223:LYS:HD2	4:B:223:LYS:N	2.21	0.56
4:B:78:ARG:HD3	4:B:411:ILE:HG22	1.87	0.56
5:L:106:ILE:N	5:L:166:GLN:HE22	2.04	0.56
1:T:715:DA:C2	1:T:716:DA:C6	2.94	0.56
4:B:34:LEU:O	4:B:38:CYS:HB2	2.05	0.56
5:L:46:LEU:HD23	5:L:55:HIS:CG	2.40	0.56
3:A:108:VAL:HG22	3:A:188:TYR:HA	1.88	0.56
6:H:34:ILE:HG22	6:H:35:GLY:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:65:LEU:HD22	6:H:68:ARG:HH21	1.70	0.56
3:A:264:LEU:O	3:A:267:ALA:HB3	2.06	0.56
6:H:164:TRP:CZ3	6:H:205:CYS:HB2	2.41	0.56
3:A:115:TYR:C	3:A:117:SER:H	2.10	0.55
3:A:439:THR:HG23	4:B:288:ALA:HA	1.87	0.55
3:A:502:ALA:O	3:A:506:ILE:HG12	2.06	0.55
3:A:536:VAL:HG13	3:A:537:PRO:HD2	1.88	0.55
4:B:252:TRP:CD1	4:B:252:TRP:N	2.75	0.55
4:B:47:ILE:HG23	4:B:144:TYR:HD1	1.70	0.55
3:A:457:TYR:CZ	3:A:465:LYS:HB3	2.41	0.55
4:B:171:PHE:CD1	4:B:205:LEU:HD13	2.41	0.55
4:B:356:ARG:HG2	4:B:357:MET:N	2.22	0.55
4:B:263:LYS:HG2	4:B:423:VAL:HG12	1.88	0.55
5:L:11:LEU:HG	5:L:11:LEU:O	2.05	0.55
3:A:466:VAL:O	3:A:466:VAL:HG12	2.06	0.55
4:B:302:GLU:HA	4:B:302:GLU:OE1	2.05	0.55
3:A:405:TYR:HD1	3:A:406:TRP:N	2.04	0.55
3:A:442:VAL:CG2	3:A:495:ILE:HG22	2.37	0.55
4:B:175:ASN:HD21	4:B:201:LYS:NZ	2.04	0.55
6:H:4:LEU:HD23	6:H:24:PHE:HB3	1.89	0.55
2:P:807:DC:H4'	3:A:448:ARG:HD2	1.88	0.55
3:A:363:ASN:OD1	3:A:363:ASN:C	2.45	0.55
3:A:394:GLN:HG2	3:A:416:PHE:CD2	2.42	0.55
3:A:429:LEU:HD22	3:A:533:LEU:CD1	2.36	0.55
4:B:237:ASP:O	4:B:239:TRP:N	2.40	0.55
3:A:427:TYR:CE2	3:A:525:LEU:HD23	2.42	0.55
4:B:118:VAL:O	4:B:148:VAL:HG23	2.06	0.55
4:B:312:GLU:CB	4:B:313:PRO:HD2	2.35	0.55
5:L:33:LEU:HD23	5:L:34:ASN:N	2.22	0.55
1:T:720:DG:H2''	1:T:721:DG:OP2	2.07	0.55
3:A:447:ASN:HD22	3:A:450:THR:CG2	2.18	0.55
4:B:116:PHE:C	4:B:148:VAL:HG21	2.27	0.55
6:H:40:ARG:HD3	6:H:50:LEU:HD11	1.89	0.55
3:A:136:ASN:C	3:A:138:GLU:H	2.09	0.55
4:B:328:GLU:O	4:B:339:TYR:HA	2.07	0.55
3:A:244:ILE:HG13	3:A:263:LYS:HD3	1.89	0.55
3:A:469:LEU:CD2	3:A:480:GLN:HG2	2.32	0.55
4:B:131:THR:HG22	4:B:132:ILE:N	2.21	0.55
4:B:91:GLN:OE1	4:B:91:GLN:CA	2.53	0.55
2:P:819:DG:OP1	3:A:259:LYS:HG3	2.07	0.55
3:A:279:LEU:HA	3:A:282:LEU:HG	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:500:GLN:N	3:A:500:GLN:HE21	2.04	0.54
5:L:137:ASN:HB3	5:L:138:ASN:ND2	2.21	0.54
1:T:709:DC:C2'	1:T:710:DG:O5'	2.55	0.54
4:B:101:LYS:O	4:B:236:PRO:HB2	2.08	0.54
5:L:161:ASN:HB2	5:L:163:TRP:CH2	2.42	0.54
1:T:724:DT:C2'	1:T:725:DG:C8	2.86	0.54
3:A:278:GLN:HG3	3:A:302:GLU:CB	2.38	0.54
3:A:479:LEU:HD21	3:A:518:VAL:HG22	1.88	0.54
3:A:5:ILE:HD11	3:A:167:ILE:HD11	1.88	0.54
3:A:61:PHE:H	3:A:61:PHE:HD2	1.55	0.54
3:A:49:LYS:HB2	3:A:49:LYS:NZ	2.22	0.54
4:B:425:LEU:O	4:B:427:TYR:N	2.38	0.54
3:A:512:LYS:HD2	3:A:513:SER:H	1.72	0.54
3:A:479:LEU:O	3:A:521:ILE:HD11	2.08	0.54
2:P:812:DT:C6	2:P:813:DT:C7	2.91	0.54
3:A:27:THR:OG1	3:A:29:GLU:HB3	2.07	0.54
3:A:451:LYS:O	3:A:471:ASN:N	2.39	0.54
3:A:440:PHE:CZ	3:A:488:ASP:O	2.60	0.54
5:L:23:CYS:HB2	5:L:35:TRP:CH2	2.43	0.54
3:A:50:ILE:HG21	3:A:145:GLN:HB3	1.89	0.54
4:B:75:VAL:HG11	4:B:77:PHE:CZ	2.43	0.54
6:H:104:SER:O	6:H:106:THR:N	2.41	0.54
1:T:712:DC:OP1	3:A:353:LYS:NZ	2.41	0.54
3:A:160:PHE:CD2	3:A:160:PHE:C	2.82	0.54
4:B:377:THR:O	4:B:381:VAL:HG23	2.07	0.54
5:L:107:LYS:HA	5:L:140:TYR:OH	2.08	0.54
3:A:156:SER:HB2	3:A:157:PRO:HD3	1.89	0.53
3:A:484:LEU:O	3:A:487:GLN:N	2.40	0.53
3:A:435:VAL:HG22	4:B:290:THR:CG2	2.37	0.53
6:H:16:GLN:O	6:H:87:VAL:HG22	2.08	0.53
3:A:272:PRO:O	3:A:273:GLY:O	2.26	0.53
3:A:493:VAL:CG2	3:A:494:ASN:N	2.71	0.53
4:B:112:GLY:CA	4:B:151:GLN:HE21	2.20	0.53
6:H:20:LEU:HD12	6:H:82:LEU:HD23	1.89	0.53
3:A:138:GLU:OE1	3:A:139:THR:HG22	2.08	0.53
4:B:368:LEU:O	4:B:372:VAL:HG23	2.09	0.53
3:A:416:PHE:CD1	3:A:417:VAL:N	2.77	0.53
3:A:438:GLU:OE2	3:A:463:ARG:NH2	2.42	0.53
1:T:715:DA:H2''	1:T:716:DA:C8	2.43	0.53
4:B:332:GLN:OE1	4:B:332:GLN:HA	2.08	0.53
6:H:69:LEU:HD22	6:H:82:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:261:VAL:O	3:A:264:LEU:HB2	2.09	0.53
3:A:473:THR:HG22	3:A:474:ASN:H	1.74	0.53
4:B:149:LEU:HD13	4:B:156:SER:HA	1.91	0.53
3:A:513:SER:OG	3:A:514:GLU:N	2.42	0.53
6:H:198:TRP:CD1	6:H:199:PRO:HA	2.44	0.53
5:L:19:VAL:HG12	5:L:20:THR:N	2.24	0.53
6:H:38:TRP:CZ3	6:H:97:CYS:HB3	2.44	0.53
5:L:184:ASP:O	5:L:188:ARG:HD3	2.09	0.53
3:A:450:THR:O	3:A:451:LYS:CG	2.57	0.53
3:A:523:GLU:OE2	3:A:523:GLU:HA	2.08	0.53
4:B:226:PRO:O	4:B:228:LEU:HG	2.08	0.53
4:B:260:LEU:HD21	4:B:303:LEU:HD13	1.91	0.53
4:B:75:VAL:HG11	4:B:77:PHE:CE2	2.44	0.53
1:T:722:DA:C4	1:T:723:DC:C5	2.97	0.53
4:B:144:TYR:CD2	4:B:144:TYR:N	2.76	0.52
4:B:79:GLU:O	4:B:83:ARG:HG2	2.10	0.52
5:L:46:LEU:HD23	5:L:55:HIS:ND1	2.23	0.52
4:B:97:PRO:HD3	4:B:181:TYR:CD1	2.44	0.52
1:T:711:DC:H2'	1:T:712:DC:C6	2.43	0.52
1:T:712:DC:H2''	1:T:713:DC:C5'	2.27	0.52
4:B:389:PHE:HB3	4:B:391:LEU:HD23	1.91	0.52
3:A:434:ILE:HG22	3:A:494:ASN:ND2	2.18	0.52
5:L:117:ILE:HD12	5:L:134:CYS:HB2	1.92	0.52
5:L:137:ASN:HB3	5:L:138:ASN:HD22	1.75	0.52
5:L:3:GLN:O	5:L:26:SER:HB2	2.10	0.52
3:A:439:THR:HG21	4:B:288:ALA:HA	1.91	0.52
3:A:503:LEU:CD2	3:A:535:TRP:HB2	2.40	0.52
3:A:69:THR:HG22	3:A:69:THR:O	2.10	0.52
3:A:96:HIS:ND1	3:A:97:PRO:CD	2.72	0.52
4:B:312:GLU:HB3	4:B:313:PRO:CD	2.36	0.52
3:A:440:PHE:HE2	3:A:489:SER:OG	1.91	0.52
3:A:486:LEU:CD2	3:A:495:ILE:HD11	2.39	0.52
6:H:50:LEU:O	6:H:51:ALA:HB2	2.09	0.52
6:H:73:LYS:O	6:H:73:LYS:HG3	2.08	0.52
5:L:159:VAL:HG22	5:L:179:LEU:HD12	1.91	0.52
3:A:106:VAL:CB	3:A:227:PHE:HE1	2.19	0.52
3:A:372:VAL:HG13	3:A:389:PHE:CE2	2.44	0.52
3:A:329:ILE:CG1	3:A:391:LEU:HD22	2.39	0.52
3:A:84:THR:HG22	3:A:85:GLN:O	2.10	0.52
4:B:195:ILE:HG12	4:B:199:ARG:CD	2.40	0.52
4:B:380:ILE:O	4:B:384:GLY:HA2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:195:ILE:CG2	4:B:196:GLY:N	2.72	0.51
4:B:10:VAL:HG13	4:B:87:PHE:CD1	2.45	0.51
5:L:20:THR:HA	5:L:73:LEU:O	2.09	0.51
3:A:101:LYS:O	3:A:103:LYS:HG2	2.10	0.51
4:B:121:ASP:OD1	4:B:121:ASP:C	2.49	0.51
4:B:295:LEU:HD22	4:B:300:GLU:N	2.25	0.51
3:A:368:LEU:CD2	3:A:393:ILE:HG21	2.40	0.51
3:A:379:SER:O	3:A:380:ILE:C	2.49	0.51
4:B:160:PHE:CD2	4:B:164:MET:HB2	2.45	0.51
4:B:306:ASN:O	4:B:309:ILE:HG12	2.11	0.51
5:L:60:SER:C	5:L:62:PHE:H	2.13	0.51
5:L:90:GLN:NE2	5:L:92:SER:N	2.46	0.51
3:A:258:CYS:HA	3:A:261:VAL:CG1	2.40	0.51
4:B:422:LEU:O	4:B:423:VAL:HG23	2.09	0.51
3:A:440:PHE:HD2	3:A:493:VAL:HG21	1.76	0.51
4:B:195:ILE:HG12	4:B:199:ARG:NE	2.26	0.51
4:B:342:TYR:HB3	4:B:348:ASN:HA	1.93	0.51
2:P:817:MRG:H2'	2:P:818:DC:O5'	2.08	0.51
3:A:27:THR:CG2	3:A:30:LYS:HD2	2.41	0.51
3:A:427:TYR:CZ	3:A:525:LEU:HD23	2.45	0.51
4:B:175:ASN:ND2	4:B:201:LYS:HD2	2.26	0.51
2:P:807:DC:C4	2:P:808:DC:N4	2.79	0.51
3:A:254:VAL:O	3:A:257:ILE:HG13	2.11	0.51
3:A:441:TYR:CD2	3:A:544:GLY:CA	2.91	0.51
4:B:107:THR:HG22	4:B:108:VAL:N	2.25	0.51
6:H:166:SER:N	6:H:206:ASN:ND2	2.29	0.51
3:A:27:THR:OG1	3:A:30:LYS:HG3	2.11	0.51
3:A:457:TYR:HA	3:A:548:VAL:HG13	1.91	0.51
4:B:49:LYS:O	4:B:50:ILE:HG23	2.11	0.51
4:B:61:PHE:CZ	4:B:74:LEU:HD13	2.46	0.51
6:H:68:ARG:O	6:H:84:MET:HA	2.11	0.51
3:A:331:LYS:CB	3:A:421:PRO:HG2	2.26	0.50
4:B:178:ILE:CG2	4:B:179:VAL:N	2.73	0.50
4:B:393:ILE:CG1	4:B:394:GLN:N	2.74	0.50
6:H:129:PRO:HB3	6:H:155:TYR:HB3	1.94	0.50
5:L:124:GLN:HG2	5:L:129:GLY:O	2.10	0.50
5:L:150:ILE:N	5:L:153:SER:O	2.43	0.50
2:P:816:DG:C2'	2:P:817:MRG:O5'	2.59	0.50
3:A:303:LEU:HD11	3:A:307:ARG:HD2	1.92	0.50
3:A:545:ASN:O	3:A:546:GLU:C	2.49	0.50
4:B:223:LYS:NZ	6:H:55:TRP:CH2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:706:DA:C6	1:T:707:DG:C6	2.99	0.50
6:H:40:ARG:HB2	6:H:50:LEU:CD1	2.42	0.50
1:T:714:DG:H2''	1:T:715:DA:OP2	2.10	0.50
1:T:715:DA:C2	1:T:716:DA:C5	2.99	0.50
3:A:303:LEU:O	3:A:307:ARG:HG3	2.11	0.50
3:A:443:ASP:OD1	3:A:478:GLU:OE1	2.29	0.50
3:A:262:GLY:HA2	3:A:265:ASN:HD22	1.76	0.50
3:A:416:PHE:CE1	3:A:417:VAL:O	2.63	0.50
3:A:486:LEU:HD21	3:A:495:ILE:HD11	1.92	0.50
3:A:507:GLN:O	3:A:509:GLN:HG3	2.12	0.50
4:B:198:HIS:O	4:B:199:ARG:C	2.49	0.50
6:H:102:ILE:HG12	6:H:108:SER:HB2	1.93	0.50
3:A:247:PRO:O	3:A:252:TRP:HH2	1.94	0.50
3:A:296:THR:HG22	3:A:297:GLU:H	1.77	0.50
3:A:403:THR:HG23	3:A:404:GLU:N	2.26	0.50
3:A:405:TYR:CD1	3:A:406:TRP:N	2.78	0.50
3:A:61:PHE:N	3:A:61:PHE:CD2	2.78	0.50
4:B:200:THR:HG22	4:B:201:LYS:N	2.26	0.50
6:H:21:THR:HG23	6:H:81:PHE:CE2	2.47	0.50
3:A:115:TYR:O	3:A:117:SER:N	2.44	0.50
4:B:12:LEU:HD11	4:B:127:TYR:CE2	2.46	0.50
4:B:2:ILE:HD12	4:B:2:ILE:C	2.31	0.50
1:T:709:DC:H2''	1:T:710:DG:C5'	2.42	0.50
4:B:360:ALA:HB1	4:B:367:GLN:HE21	1.77	0.50
3:A:139:THR:OG1	3:A:140:PRO:HD2	2.12	0.50
3:A:504:GLY:O	3:A:505:ILE:C	2.49	0.50
4:B:325:LEU:HD12	4:B:343:GLN:HG2	1.92	0.50
3:A:143:ARG:NH1	3:A:143:ARG:HG3	2.19	0.49
4:B:309:ILE:HD13	4:B:309:ILE:N	2.27	0.49
6:H:2:ILE:HG12	6:H:26:GLY:HA3	1.93	0.49
4:B:254:VAL:HB	4:B:289:LEU:HA	1.95	0.49
4:B:257:ILE:HB	4:B:283:LEU:HD21	1.93	0.49
1:T:709:DC:H2''	1:T:710:DG:H5'	1.94	0.49
3:A:328:GLU:HG3	3:A:390:LYS:HB2	1.94	0.49
3:A:425:LEU:HD13	3:A:509:GLN:OE1	2.12	0.49
3:A:465:LYS:HD2	3:A:467:VAL:HG13	1.94	0.49
6:H:122:SER:HB3	6:H:156:PHE:CZ	2.47	0.49
2:P:817:MRG:H2'	2:P:818:DC:C6	2.47	0.49
3:A:227:PHE:HB2	3:A:234:LEU:HB2	1.93	0.49
3:A:416:PHE:HD1	3:A:417:VAL:N	2.09	0.49
3:A:60:VAL:O	3:A:60:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:325:LEU:HD22	4:B:385:LYS:HG2	1.93	0.49
3:A:106:VAL:HB	3:A:227:PHE:CE1	2.33	0.49
3:A:121:ASP:OD1	3:A:123:ASP:N	2.45	0.49
3:A:353:LYS:O	3:A:353:LYS:HD2	2.12	0.49
4:B:244:ILE:HD13	4:B:244:ILE:N	2.03	0.49
4:B:46:LYS:CD	4:B:116:PHE:HB3	2.42	0.49
1:T:713:DC:C2'	1:T:714:DG:O5'	2.61	0.49
3:A:283:LEU:N	3:A:283:LEU:HD23	2.28	0.49
3:A:523:GLU:O	3:A:526:ILE:HG22	2.12	0.49
4:B:221:HIS:HA	4:B:229:TRP:CD1	2.48	0.49
4:B:394:GLN:O	4:B:395:LYS:C	2.49	0.49
6:H:12:VAL:HG12	6:H:13:GLN:O	2.11	0.49
3:A:338:THR:CG2	3:A:339:TYR:N	2.75	0.49
3:A:478:GLU:HG2	3:A:499:SER:HB3	1.95	0.49
3:A:485:ALA:O	3:A:489:SER:HB2	2.13	0.49
3:A:501:TYR:CE1	3:A:505:ILE:CD1	2.92	0.49
4:B:113:ASP:O	4:B:114:ALA:C	2.50	0.49
4:B:344:GLU:OE2	4:B:344:GLU:HA	2.13	0.49
3:A:407:GLN:HG3	4:B:393:ILE:HA	1.94	0.49
5:L:61:ARG:HG2	5:L:61:ARG:NH1	2.27	0.49
5:L:89:GLN:HA	5:L:97:THR:O	2.12	0.49
5:L:117:ILE:CD1	5:L:194:CYS:HB2	2.42	0.49
3:A:221:HIS:CD2	3:A:221:HIS:N	2.80	0.49
3:A:329:ILE:HG12	3:A:391:LEU:CD2	2.41	0.49
4:B:260:LEU:HD11	4:B:264:LEU:HD11	1.95	0.49
3:A:232:TYR:N	3:A:232:TYR:CD1	2.81	0.48
3:A:257:ILE:CG2	3:A:283:LEU:HD21	2.40	0.48
3:A:517:LEU:HD13	3:A:521:ILE:HG13	1.93	0.48
1:T:713:DC:H2''	1:T:714:DG:C5'	2.43	0.48
4:B:286:THR:O	4:B:286:THR:OG1	2.30	0.48
4:B:87:PHE:HD2	4:B:88:TRP:HB3	1.77	0.48
6:H:162:VAL:HA	6:H:206:ASN:O	2.13	0.48
5:L:146:VAL:HA	5:L:195:GLU:O	2.12	0.48
3:A:501:TYR:O	3:A:501:TYR:HD1	1.95	0.48
4:B:282:LEU:HD23	4:B:282:LEU:N	2.27	0.48
4:B:403:THR:O	4:B:406:TRP:N	2.40	0.48
2:P:820:DC:C2'	2:P:821:DC:O5'	2.61	0.48
3:A:261:VAL:HA	3:A:264:LEU:HD12	1.96	0.48
3:A:329:ILE:HG13	3:A:391:LEU:HD22	1.94	0.48
4:B:406:TRP:O	4:B:407:GLN:NE2	2.47	0.48
1:T:705:DT:H2''	1:T:706:DA:O5'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:225:PRO:HA	3:A:226:PRO:C	2.33	0.48
4:B:47:ILE:HA	4:B:47:ILE:HD12	1.65	0.48
6:H:39:ILE:HG23	6:H:48:GLU:O	2.13	0.48
6:H:65:LEU:O	6:H:67:SER:N	2.46	0.48
3:A:342:TYR:HD2	3:A:344:GLU:O	1.96	0.48
5:L:190:ASN:O	5:L:210:ASN:HA	2.13	0.48
3:A:50:ILE:HG23	3:A:145:GLN:HB3	1.96	0.48
3:A:339:TYR:CZ	3:A:352:GLY:HA3	2.49	0.48
3:A:533:LEU:N	3:A:533:LEU:CD1	2.77	0.48
4:B:262:GLY:O	4:B:263:LYS:C	2.52	0.48
6:H:34:ILE:CD1	6:H:34:ILE:H	2.25	0.48
3:A:253:THR:HA	3:A:292:VAL:HA	1.96	0.48
4:B:131:THR:CG2	4:B:132:ILE:N	2.76	0.48
4:B:125:ARG:HD3	4:B:147:ASN:HA	1.95	0.48
3:A:143:ARG:CG	3:A:143:ARG:HH11	2.21	0.48
3:A:491:LEU:HD23	3:A:529:GLU:OE1	2.13	0.48
4:B:165:THR:HG23	4:B:166:LYS:N	2.29	0.48
4:B:423:VAL:HG12	4:B:425:LEU:H	1.78	0.48
5:L:151:ASP:O	5:L:153:SER:N	2.38	0.48
3:A:112:GLY:O	3:A:215:THR:HG23	2.14	0.47
3:A:331:LYS:HD3	3:A:332:GLN:H	1.79	0.47
4:B:193:LEU:HD23	4:B:193:LEU:N	2.28	0.47
4:B:96:HIS:HE1	4:B:380:ILE:O	1.96	0.47
3:A:493:VAL:C	3:A:494:ASN:HD22	2.17	0.47
4:B:113:ASP:O	4:B:116:PHE:N	2.43	0.47
4:B:223:LYS:HE3	6:H:58:ASP:HB3	1.96	0.47
4:B:113:ASP:C	4:B:115:TYR:N	2.66	0.47
4:B:254:VAL:HB	4:B:289:LEU:O	2.14	0.47
5:L:83:ILE:HG21	5:L:106:ILE:CG1	2.42	0.47
4:B:156:SER:O	4:B:158:ALA:N	2.48	0.47
4:B:306:ASN:CA	4:B:309:ILE:HG12	2.43	0.47
5:L:105:GLU:OE2	5:L:173:TYR:OH	2.32	0.47
5:L:35:TRP:CE3	5:L:88:CYS:HB3	2.50	0.47
3:A:344:GLU:HB3	3:A:345:PRO:CD	2.43	0.47
3:A:511:ASP:O	3:A:511:ASP:OD2	2.31	0.47
4:B:210:LEU:HD12	4:B:210:LEU:HA	1.59	0.47
4:B:244:ILE:HD11	4:B:271:TYR:CE2	2.50	0.47
4:B:302:GLU:HA	4:B:305:GLU:CB	2.44	0.47
6:H:53:ILE:HG23	6:H:53:ILE:O	2.15	0.47
3:A:128:THR:OG1	3:A:146:TYR:HB2	2.15	0.47
3:A:169:GLU:HB3	3:A:170:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:265:ASN:HA	3:A:268:SER:OG	2.14	0.47
3:A:478:GLU:OE1	3:A:498:ASP:CG	2.53	0.47
4:B:244:ILE:HD11	4:B:271:TYR:CZ	2.50	0.47
3:A:439:THR:CG2	4:B:289:LEU:H	2.09	0.47
4:B:291:GLU:HG2	4:B:293:ILE:CD1	2.45	0.47
4:B:320:ASP:N	4:B:343:GLN:OE1	2.40	0.47
6:H:134:LEU:HB2	6:H:149:GLY:CA	2.45	0.47
6:H:155:TYR:CD2	6:H:155:TYR:N	2.83	0.47
1:T:715:DA:N3	1:T:716:DA:C5	2.82	0.47
3:A:473:THR:CG2	3:A:474:ASN:N	2.77	0.47
4:B:332:GLN:NE2	4:B:426:TRP:O	2.48	0.47
6:H:32:SER:O	6:H:55:TRP:CE2	2.68	0.47
5:L:167:ASP:C	5:L:167:ASP:OD2	2.53	0.47
3:A:442:VAL:HG12	3:A:481:ALA:HB1	1.95	0.47
3:A:87:PHE:N	3:A:87:PHE:CD2	2.83	0.47
4:B:166:LYS:O	4:B:168:LEU:N	2.48	0.47
4:B:329:ILE:HA	4:B:338:THR:O	2.15	0.47
4:B:57:ASN:ND2	4:B:58:THR:N	2.62	0.47
4:B:12:LEU:H	4:B:12:LEU:CD1	1.99	0.47
4:B:207:GLN:O	4:B:210:LEU:N	2.48	0.47
4:B:13:LYS:HE2	4:B:85:GLN:HB3	1.96	0.47
5:L:151:ASP:C	5:L:153:SER:H	2.15	0.47
3:A:27:THR:O	3:A:30:LYS:N	2.45	0.47
4:B:101:LYS:HG3	4:B:102:LYS:HG3	1.97	0.47
5:L:131:SER:HA	5:L:179:LEU:O	2.15	0.47
5:L:132:VAL:HG12	5:L:148:TRP:HH2	1.80	0.47
3:A:253:THR:O	3:A:254:VAL:C	2.53	0.46
3:A:498:ASP:OD1	3:A:498:ASP:N	2.47	0.46
4:B:56:TYR:O	4:B:143:ARG:NH2	2.47	0.46
3:A:153:TRP:CZ3	3:A:155:GLY:HA3	2.50	0.46
3:A:181:TYR:CD2	4:B:138:GLU:HG3	2.50	0.46
3:A:430:GLU:HG2	3:A:531:VAL:O	2.15	0.46
3:A:536:VAL:HG13	3:A:542:ILE:HG13	1.98	0.46
4:B:420:PRO:HB3	4:B:421:PRO:HD2	1.96	0.46
6:H:174:HIS:O	6:H:189:SER:HA	2.15	0.46
3:A:115:TYR:CE2	3:A:156:SER:HB3	2.50	0.46
3:A:27:THR:C	3:A:29:GLU:N	2.66	0.46
3:A:389:PHE:HB3	3:A:391:LEU:HD21	1.98	0.46
3:A:475:GLN:HB3	3:A:501:TYR:HE2	1.78	0.46
4:B:47:ILE:CD1	4:B:146:TYR:HA	2.43	0.46
3:A:260:LEU:HD23	3:A:279:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:90:VAL:HG12	4:B:140:PRO:HB3	1.97	0.46
4:B:229:TRP:HA	4:B:232:TYR:CZ	2.49	0.46
3:A:116:PHE:CD1	3:A:116:PHE:N	2.83	0.46
3:A:306:ASN:O	3:A:307:ARG:C	2.54	0.46
4:B:166:LYS:O	4:B:167:ILE:C	2.54	0.46
3:A:460:ASN:ND2	4:B:288:ALA:HB2	2.25	0.46
4:B:360:ALA:CB	4:B:367:GLN:HE21	2.29	0.46
4:B:69:THR:HG22	4:B:69:THR:O	2.16	0.46
5:L:150:ILE:HG22	5:L:192:TYR:CD2	2.50	0.46
1:T:716:DA:H1'	1:T:717:DC:H5'	1.97	0.46
4:B:225:PRO:HB2	4:B:226:PRO:CD	2.35	0.46
5:L:105:GLU:HB3	5:L:106:ILE:H	1.62	0.46
5:L:63:SER:O	5:L:73:LEU:HD12	2.16	0.46
3:A:140:PRO:O	3:A:141:GLY:O	2.33	0.46
3:A:459:THR:HG21	3:A:463:ARG:HB3	1.91	0.46
4:B:202:ILE:O	4:B:205:LEU:N	2.48	0.46
4:B:85:GLN:C	4:B:87:PHE:N	2.66	0.46
6:H:152:VAL:HB	6:H:187:LEU:HD12	1.98	0.46
5:L:176:SER:HB2	6:H:176:PHE:CD1	2.51	0.46
5:L:15:LEU:CD1	5:L:15:LEU:H	2.19	0.46
3:A:86:ASP:OD2	3:A:86:ASP:N	2.48	0.46
3:A:90:VAL:CG1	4:B:141:GLY:N	2.75	0.46
4:B:279:LEU:HD12	4:B:279:LEU:N	2.31	0.46
2:P:815:DG:C6	2:P:816:DG:C6	3.04	0.46
1:T:706:DA:C6	1:T:707:DG:O6	2.69	0.46
4:B:111:VAL:CG2	4:B:111:VAL:O	2.59	0.46
3:A:494:ASN:HB3	4:B:289:LEU:CD1	2.45	0.46
4:B:414:TRP:CD1	4:B:414:TRP:C	2.89	0.46
6:H:18:PHE:CD2	6:H:87:VAL:HG11	2.50	0.46
6:H:208:ALA:HB2	6:H:215:LYS:HD2	1.98	0.46
3:A:296:THR:O	3:A:300:GLU:HB2	2.15	0.46
3:A:317:VAL:HG13	3:A:349:LEU:HD23	1.97	0.46
4:B:280:SER:O	4:B:283:LEU:HD12	2.16	0.46
4:B:343:GLN:HG3	4:B:349:LEU:HD11	1.98	0.45
4:B:55:PRO:HG2	4:B:56:TYR:CE1	2.51	0.45
5:L:148:TRP:CE3	5:L:179:LEU:HD22	2.50	0.45
3:A:132:ILE:O	3:A:132:ILE:HG12	2.17	0.45
3:A:223:LYS:C	3:A:225:PRO:HD2	2.36	0.45
3:A:484:LEU:C	3:A:486:LEU:N	2.70	0.45
4:B:115:TYR:OH	4:B:157:PRO:HB3	2.16	0.45
5:L:188:ARG:O	5:L:189:HIS:CG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:805:DG:C6	2:P:806:DT:C4	3.05	0.45
3:A:180:ILE:HA	3:A:188:TYR:O	2.16	0.45
4:B:307:ARG:HG3	4:B:308:GLU:N	2.30	0.45
4:B:372:VAL:HG13	4:B:389:PHE:CE2	2.51	0.45
2:P:805:DG:H2''	2:P:806:DT:OP2	2.17	0.45
3:A:125:ARG:HB3	3:A:145:GLN:HG3	1.98	0.45
3:A:420:PRO:HB3	3:A:421:PRO:HA	1.98	0.45
3:A:473:THR:CG2	3:A:474:ASN:H	2.28	0.45
4:B:23:GLN:HG2	4:B:133:PRO:HG3	1.99	0.45
4:B:296:THR:HG22	4:B:297:GLU:N	2.31	0.45
6:H:65:LEU:O	6:H:66:LYS:C	2.54	0.45
5:L:125:LEU:CD2	5:L:130:ALA:HB2	2.46	0.45
3:A:23:GLN:HE22	3:A:60:VAL:H	1.64	0.45
4:B:252:TRP:HB2	4:B:257:ILE:HD11	1.99	0.45
1:T:706:DA:H2'	1:T:707:DG:H8	1.78	0.45
3:A:379:SER:O	3:A:381:VAL:N	2.49	0.45
3:A:531:VAL:HG12	3:A:532:TYR:N	2.32	0.45
3:A:41:MET:HE1	3:A:73:LYS:HD3	1.99	0.45
5:L:179:LEU:HD23	5:L:181:LEU:HD11	1.98	0.45
3:A:175:ASN:HB3	3:A:178:ILE:HD12	1.98	0.45
3:A:354:TYR:HD2	3:A:354:TYR:HA	1.50	0.45
3:A:416:PHE:HE1	3:A:417:VAL:O	2.00	0.45
6:H:164:TRP:CH2	6:H:205:CYS:HB2	2.51	0.45
5:L:77:ASN:H	5:L:77:ASN:HD22	1.64	0.45
3:A:222:GLN:O	3:A:224:GLU:HG3	2.17	0.45
3:A:326:ILE:O	3:A:341:ILE:HA	2.16	0.45
3:A:447:ASN:HB3	3:A:450:THR:OG1	2.17	0.45
4:B:116:PHE:HA	4:B:148:VAL:HG21	1.99	0.45
4:B:369:THR:O	4:B:373:GLN:HG3	2.17	0.45
4:B:424:LYS:HD2	4:B:424:LYS:HA	1.86	0.45
4:B:87:PHE:HD2	4:B:88:TRP:N	2.13	0.45
3:A:132:ILE:CG2	3:A:142:ILE:HB	2.44	0.45
3:A:246:LEU:HD12	3:A:307:ARG:HE	1.82	0.45
4:B:23:GLN:NE2	4:B:60:VAL:O	2.44	0.45
3:A:539:HIS:N	3:A:539:HIS:CD2	2.83	0.44
3:A:454:LYS:HB2	3:A:552:VAL:HG13	1.98	0.44
6:H:163:THR:O	6:H:206:ASN:HB2	2.18	0.44
3:A:369:THR:HG22	3:A:370:GLU:N	2.31	0.44
3:A:327:ALA:HB3	3:A:389:PHE:CD1	2.53	0.44
3:A:410:TRP:CD2	4:B:363:ASN:OD1	2.70	0.44
3:A:397:THR:CG2	3:A:424:LYS:HA	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:455:ALA:HA	3:A:552:VAL:HG11	1.98	0.44
4:B:193:LEU:HD13	4:B:197:GLN:OE1	2.17	0.44
4:B:200:THR:O	4:B:202:ILE:N	2.50	0.44
4:B:291:GLU:O	4:B:293:ILE:HD13	2.16	0.44
4:B:320:ASP:O	4:B:343:GLN:NE2	2.40	0.44
6:H:89:THR:HA	6:H:121:VAL:HB	1.99	0.44
5:L:66:GLY:HA3	5:L:71:TYR:CG	2.51	0.44
3:A:498:ASP:OD2	3:A:538:ALA:HB2	2.17	0.44
4:B:44:GLU:OE1	4:B:46:LYS:NZ	2.33	0.44
5:L:121:SER:O	5:L:122:SER:C	2.55	0.44
6:H:129:PRO:HB2	6:H:152:VAL:HG12	1.98	0.44
5:L:118:PHE:HA	5:L:119:PRO:HD3	1.77	0.44
5:L:136:LEU:HD12	5:L:136:LEU:N	2.33	0.44
3:A:116:PHE:HD1	3:A:116:PHE:N	2.15	0.44
3:A:257:ILE:HG21	3:A:283:LEU:CD2	2.42	0.44
3:A:372:VAL:HG13	3:A:389:PHE:CZ	2.53	0.44
3:A:486:LEU:HD21	3:A:495:ILE:CD1	2.48	0.44
3:A:509:GLN:N	3:A:510:PRO:CD	2.80	0.44
3:A:532:TYR:C	3:A:533:LEU:HD12	2.37	0.44
3:A:94:ILE:HG13	3:A:95:PRO:O	2.17	0.44
4:B:327:ALA:HA	4:B:340:GLN:O	2.17	0.44
4:B:366:LYS:O	4:B:370:GLU:HG3	2.17	0.44
5:L:18:ARG:HA	5:L:76:SER:O	2.17	0.44
5:L:77:ASN:ND2	5:L:77:ASN:N	2.66	0.44
4:B:369:THR:HG22	4:B:398:TRP:HZ3	1.80	0.44
4:B:58:THR:CG2	4:B:59:PRO:CD	2.95	0.44
5:L:189:HIS:O	5:L:211:ARG:NE	2.50	0.44
3:A:373:GLN:HE22	4:B:397:THR:HG23	1.81	0.44
3:A:385:LYS:HZ2	3:A:385:LYS:CB	2.31	0.44
4:B:314:VAL:CG1	4:B:315:HIS:H	2.29	0.44
2:P:812:DT:C5	2:P:813:DT:H73	2.53	0.44
1:T:714:DG:OP1	3:A:285:GLY:N	2.42	0.44
4:B:330:GLN:HG2	4:B:338:THR:OG1	2.17	0.44
4:B:401:TRP:O	4:B:402:TRP:C	2.53	0.44
5:L:186:TYR:C	5:L:188:ARG:H	2.21	0.44
3:A:195:ILE:O	3:A:195:ILE:HG22	2.18	0.44
3:A:269:GLN:HA	3:A:351:THR:O	2.18	0.44
3:A:354:TYR:CE1	3:A:374:LYS:CB	2.90	0.44
3:A:365:VAL:O	3:A:366:LYS:C	2.56	0.44
3:A:442:VAL:HG22	3:A:495:ILE:HG22	1.99	0.44
4:B:103:LYS:HD3	4:B:192:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:295:LEU:HD23	4:B:299:ALA:CB	2.47	0.44
4:B:2:ILE:HG23	4:B:3:SER:N	2.32	0.44
4:B:47:ILE:CG2	4:B:144:TYR:HD1	2.31	0.44
4:B:56:TYR:O	4:B:57:ASN:HB2	2.17	0.44
5:L:144:ILE:HG13	5:L:198:HIS:ND1	2.32	0.44
2:P:814:DC:H2''	2:P:815:DG:C8	2.53	0.44
3:A:442:VAL:HG23	3:A:496:VAL:O	2.18	0.43
4:B:135:ILE:HD12	4:B:135:ILE:O	2.18	0.43
4:B:214:LEU:HD12	4:B:214:LEU:N	2.33	0.43
4:B:225:PRO:CB	4:B:226:PRO:CD	2.96	0.43
5:L:58:VAL:HG13	5:L:59:PRO:HD2	2.00	0.43
3:A:460:ASN:HD22	4:B:288:ALA:CB	2.28	0.43
3:A:500:GLN:N	3:A:500:GLN:NE2	2.53	0.43
6:H:53:ILE:HD13	6:H:73:LYS:HB3	2.00	0.43
4:B:363:ASN:HD22	4:B:363:ASN:C	2.21	0.43
5:L:4:MET:SD	5:L:25:ALA:HA	2.58	0.43
5:L:90:GLN:NE2	5:L:93:LYS:H	2.15	0.43
3:A:138:GLU:O	3:A:139:THR:O	2.36	0.43
3:A:339:TYR:CD2	3:A:375:ILE:HD11	2.53	0.43
4:B:106:VAL:HG13	4:B:234:LEU:CB	2.46	0.43
4:B:115:TYR:CD1	4:B:156:SER:HB3	2.53	0.43
4:B:403:THR:O	4:B:404:GLU:C	2.56	0.43
6:H:126:THR:HA	6:H:156:PHE:O	2.18	0.43
3:A:296:THR:O	3:A:300:GLU:N	2.51	0.43
3:A:438:GLU:CD	3:A:463:ARG:HH21	2.22	0.43
3:A:459:THR:HG22	3:A:463:ARG:N	2.33	0.43
4:B:72:ARG:HG3	4:B:73:LYS:O	2.19	0.43
3:A:180:ILE:HG23	3:A:189:VAL:HG22	2.00	0.43
3:A:367:GLN:O	3:A:368:LEU:C	2.55	0.43
3:A:398:TRP:O	3:A:401:TRP:N	2.52	0.43
4:B:148:VAL:O	4:B:149:LEU:C	2.56	0.43
4:B:24:TRP:O	4:B:25:PRO:C	2.56	0.43
4:B:357:MET:HG3	4:B:370:GLU:OE1	2.18	0.43
3:A:401:TRP:CZ2	3:A:405:TYR:CD2	3.06	0.43
3:A:457:TYR:HA	3:A:548:VAL:HG11	1.99	0.43
4:B:207:GLN:O	4:B:208:HIS:C	2.57	0.43
4:B:221:HIS:HB3	4:B:229:TRP:CE2	2.53	0.43
4:B:2:ILE:HG23	4:B:3:SER:H	1.84	0.43
2:P:819:DG:H2''	2:P:820:DC:C5'	2.47	0.43
3:A:137:ASN:OD1	3:A:137:ASN:O	2.36	0.43
3:A:63:ILE:HG13	3:A:64:LYS:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:82:ASP:O	5:L:84:ALA:N	2.52	0.43
1:T:709:DC:H2''	1:T:710:DG:O5'	2.18	0.43
3:A:303:LEU:HD12	3:A:307:ARG:HG3	2.01	0.43
4:B:146:TYR:CG	4:B:150:PRO:HB3	2.54	0.43
4:B:246:LEU:HD12	4:B:307:ARG:HA	2.00	0.43
6:H:84:MET:HG2	6:H:87:VAL:HG12	2.00	0.43
5:L:34:ASN:HB2	5:L:89:GLN:HE21	1.80	0.43
5:L:21:ILE:O	5:L:72:SER:HA	2.18	0.43
4:B:101:LYS:O	4:B:236:PRO:CB	2.67	0.43
4:B:156:SER:N	4:B:157:PRO:HD2	2.34	0.43
5:L:83:ILE:HG23	5:L:105:GLU:O	2.18	0.43
2:P:808:DC:H2''	2:P:809:DC:O5'	2.19	0.43
1:T:705:DT:H2''	1:T:706:DA:H8	1.84	0.43
3:A:484:LEU:O	3:A:485:ALA:C	2.57	0.42
4:B:144:TYR:HD2	4:B:144:TYR:N	2.16	0.42
4:B:175:ASN:HD21	4:B:201:LYS:CE	2.32	0.42
4:B:266:TRP:CZ3	4:B:422:LEU:HB3	2.53	0.42
4:B:350:LYS:HE2	4:B:378:GLU:OE1	2.18	0.42
6:H:148:LEU:HD13	6:H:220:ILE:CG2	2.43	0.42
3:A:188:TYR:C	3:A:188:TYR:CD1	2.91	0.42
3:A:260:LEU:O	3:A:261:VAL:C	2.57	0.42
3:A:498:ASP:CB	3:A:538:ALA:HB2	2.49	0.42
4:B:210:LEU:C	4:B:212:TRP:N	2.72	0.42
4:B:270:ILE:HB	4:B:271:TYR:CD2	2.54	0.42
4:B:296:THR:HG22	4:B:298:GLU:N	2.15	0.42
4:B:425:LEU:C	4:B:427:TYR:N	2.73	0.42
6:H:99:GLN:O	6:H:99:GLN:OE1	2.37	0.42
1:T:715:DA:H2''	1:T:716:DA:OP2	2.19	0.42
3:A:344:GLU:OE1	3:A:344:GLU:HA	2.18	0.42
4:B:181:TYR:HB3	4:B:188:TYR:HB2	2.01	0.42
6:H:156:PHE:HA	6:H:157:PRO:HA	1.74	0.42
6:H:55:TRP:CE3	6:H:55:TRP:N	2.88	0.42
6:H:69:LEU:CD2	6:H:84:MET:HE2	2.49	0.42
5:L:195:GLU:HG3	5:L:206:VAL:CG2	2.41	0.42
3:A:367:GLN:HA	3:A:370:GLU:CG	2.50	0.42
4:B:260:LEU:O	4:B:260:LEU:CD1	2.67	0.42
4:B:37:ILE:O	4:B:37:ILE:HG13	2.19	0.42
4:B:47:ILE:HG23	4:B:144:TYR:CD1	2.53	0.42
5:L:170:ASP:OD1	5:L:170:ASP:C	2.57	0.42
3:A:241:VAL:HG13	3:A:241:VAL:O	2.19	0.42
3:A:3:SER:HB3	3:A:5:ILE:CG1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:463:ARG:CG	3:A:464:GLN:N	2.82	0.42
4:B:329:ILE:O	4:B:392:PRO:HG3	2.18	0.42
5:L:179:LEU:CD2	5:L:181:LEU:HD11	2.50	0.42
3:A:46:LYS:HD3	3:A:46:LYS:N	2.34	0.42
3:A:85:GLN:O	3:A:154:LYS:NZ	2.51	0.42
4:B:8:VAL:HA	4:B:9:PRO:HD3	1.78	0.42
6:H:122:SER:HB3	6:H:156:PHE:HZ	1.84	0.42
6:H:128:PRO:HA	6:H:209:HIS:CD2	2.54	0.42
6:H:9:PRO:O	6:H:11:ILE:N	2.46	0.42
2:P:815:DG:C6	2:P:816:DG:O6	2.72	0.42
3:A:18:GLY:H	3:A:56:TYR:HE2	1.66	0.42
3:A:221:HIS:CD2	3:A:221:HIS:H	2.38	0.42
4:B:124:PHE:CD1	4:B:124:PHE:O	2.72	0.42
3:A:410:TRP:HB3	4:B:365:VAL:HG23	2.00	0.42
4:B:97:PRO:O	4:B:98:ALA:C	2.56	0.42
6:H:145:MET:SD	6:H:194:PRO:HG3	2.60	0.42
2:P:816:DG:H2''	2:P:817:MRG:O5'	2.20	0.42
3:A:115:TYR:C	3:A:117:SER:N	2.71	0.42
3:A:363:ASN:OD1	3:A:365:VAL:HG23	2.20	0.42
3:A:439:THR:OG1	3:A:441:TYR:HE1	2.03	0.42
3:A:494:ASN:HD22	3:A:494:ASN:N	2.16	0.42
4:B:9:PRO:HA	4:B:121:ASP:OD2	2.20	0.42
4:B:88:TRP:CG	4:B:154:LYS:HB3	2.53	0.42
4:B:96:HIS:HA	4:B:97:PRO:HD3	1.74	0.42
5:L:38:GLN:NE2	6:H:41:GLN:NE2	2.58	0.42
3:A:417:VAL:O	3:A:417:VAL:CG1	2.67	0.42
3:A:494:ASN:HB3	4:B:289:LEU:HD11	2.01	0.42
3:A:517:LEU:O	3:A:521:ILE:HG13	2.20	0.42
3:A:444:GLY:HA2	3:A:552:VAL:HG11	2.02	0.42
4:B:156:SER:C	4:B:158:ALA:N	2.73	0.42
4:B:266:TRP:CE3	4:B:423:VAL:HG23	2.55	0.42
4:B:75:VAL:CG1	4:B:77:PHE:CE2	3.03	0.42
6:H:102:ILE:HG12	6:H:108:SER:CB	2.49	0.42
5:L:142:LYS:H	5:L:142:LYS:HG2	1.45	0.42
5:L:58:VAL:HA	5:L:59:PRO:HD3	1.92	0.42
3:A:194:GLU:C	3:A:196:GLY:H	2.23	0.42
3:A:235:HIS:HB2	3:A:238:LYS:O	2.19	0.42
3:A:273:GLY:O	3:A:274:ILE:HD13	2.20	0.42
3:A:439:THR:HA	3:A:494:ASN:HB2	2.02	0.42
4:B:202:ILE:O	4:B:204:GLU:N	2.53	0.42
4:B:305:GLU:OE1	4:B:309:ILE:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:314:VAL:CG1	4:B:315:HIS:N	2.83	0.42
4:B:407:GLN:CA	4:B:407:GLN:HE21	2.32	0.42
6:H:155:TYR:CE1	6:H:160:VAL:HG13	2.55	0.42
6:H:61:TYR:OH	6:H:71:VAL:N	2.53	0.42
5:L:105:GLU:O	5:L:106:ILE:HG13	2.20	0.42
1:T:718:DA:C2	2:P:811:DG:C2	3.08	0.42
3:A:215:THR:C	3:A:217:PRO:HD3	2.39	0.41
3:A:334:GLN:HG2	3:A:512:LYS:NZ	2.35	0.41
4:B:132:ILE:HA	4:B:133:PRO:HD3	1.77	0.41
4:B:146:TYR:CD2	4:B:150:PRO:HB3	2.54	0.41
4:B:87:PHE:CE2	4:B:155:GLY:HA2	2.53	0.41
5:L:115:VAL:HG12	5:L:116:SER:N	2.34	0.41
5:L:26:SER:O	5:L:27:GLN:HB3	2.20	0.41
5:L:83:ILE:H	5:L:83:ILE:HG12	1.71	0.41
3:A:222:GLN:C	3:A:223:LYS:HG3	2.40	0.41
3:A:222:GLN:O	3:A:223:LYS:C	2.58	0.41
3:A:363:ASN:O	3:A:367:GLN:HG3	2.20	0.41
3:A:439:THR:HG21	4:B:289:LEU:HG	2.02	0.41
4:B:271:TYR:CD2	4:B:271:TYR:N	2.88	0.41
4:B:360:ALA:HB1	4:B:367:GLN:HG2	2.02	0.41
4:B:325:LEU:HB3	4:B:387:PRO:HA	2.02	0.41
6:H:10:GLY:HA2	6:H:118:SER:O	2.20	0.41
5:L:34:ASN:HD22	5:L:89:GLN:HE22	1.66	0.41
3:A:242:GLN:HA	3:A:243:PRO:HD2	1.78	0.41
3:A:441:TYR:CD2	3:A:544:GLY:C	2.94	0.41
3:A:507:GLN:C	3:A:509:GLN:H	2.22	0.41
3:A:516:GLU:O	3:A:517:LEU:C	2.59	0.41
4:B:194:GLU:OE2	4:B:195:ILE:HG22	2.20	0.41
4:B:389:PHE:HB3	4:B:391:LEU:CD2	2.50	0.41
6:H:150:CYS:HB2	6:H:164:TRP:CH2	2.55	0.41
6:H:150:CYS:HB2	6:H:164:TRP:CZ2	2.56	0.41
6:H:56:ASP:O	6:H:57:ASP:HB2	2.21	0.41
3:A:124:PHE:CD1	3:A:127:TYR:HD2	2.38	0.41
3:A:143:ARG:NH1	3:A:143:ARG:CG	2.82	0.41
3:A:516:GLU:HA	3:A:519:ASN:HB2	2.03	0.41
4:B:200:THR:O	4:B:201:LYS:C	2.58	0.41
4:B:283:LEU:HA	4:B:287:LYS:HE2	2.03	0.41
6:H:24:PHE:CE1	6:H:78:ASN:HB3	2.56	0.41
6:H:34:ILE:N	6:H:34:ILE:HD12	2.32	0.41
6:H:19:ARG:HH11	6:H:83:ASN:HD21	1.68	0.41
3:A:105:SER:HB2	3:A:198:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:229:TRP:CE2	3:A:230:MET:HG2	2.56	0.41
3:A:276:VAL:HG12	3:A:276:VAL:O	2.20	0.41
4:B:106:VAL:HA	4:B:189:VAL:O	2.21	0.41
4:B:325:LEU:HD12	4:B:325:LEU:HA	1.85	0.41
4:B:391:LEU:HA	4:B:392:PRO:HD2	1.97	0.41
6:H:24:PHE:CD1	6:H:78:ASN:HB3	2.55	0.41
6:H:59:ASN:ND2	6:H:59:ASN:N	2.69	0.41
5:L:27:GLN:O	5:L:29:ILE:HG23	2.21	0.41
5:L:77:ASN:ND2	5:L:77:ASN:H	2.18	0.41
3:A:261:VAL:HG23	3:A:276:VAL:HG11	2.03	0.41
3:A:296:THR:HG22	3:A:297:GLU:N	2.34	0.41
3:A:442:VAL:CG2	3:A:495:ILE:CG2	2.98	0.41
3:A:3:SER:HA	3:A:4:PRO:HD3	1.70	0.41
6:H:54:TRP:HB3	6:H:55:TRP:CZ3	2.56	0.41
3:A:5:ILE:HD13	3:A:167:ILE:HD11	2.03	0.41
3:A:171:PHE:O	3:A:175:ASN:ND2	2.42	0.41
3:A:368:LEU:O	3:A:369:THR:C	2.58	0.41
3:A:38:CYS:O	3:A:39:THR:C	2.59	0.41
3:A:410:TRP:CE2	4:B:363:ASN:OD1	2.73	0.41
4:B:112:GLY:C	4:B:151:GLN:HE21	2.24	0.41
4:B:304:ALA:HA	4:B:307:ARG:HG2	2.02	0.41
4:B:319:TYR:CZ	4:B:321:PRO:HA	2.55	0.41
4:B:372:VAL:HG13	4:B:389:PHE:CD2	2.56	0.41
3:A:385:LYS:HB2	3:A:385:LYS:NZ	2.36	0.41
4:B:295:LEU:HD23	4:B:299:ALA:HB3	2.02	0.41
6:H:220:ILE:HD12	6:H:220:ILE:HG23	1.89	0.41
6:H:37:THR:OG1	6:H:100:SER:HB2	2.19	0.41
5:L:120:PRO:HG2	5:L:130:ALA:HB1	2.03	0.41
3:A:302:GLU:O	3:A:303:LEU:C	2.58	0.41
3:A:317:VAL:CG1	3:A:349:LEU:HD23	2.51	0.41
3:A:31:ILE:C	3:A:33:ALA:N	2.73	0.41
3:A:472:THR:CG2	3:A:477:THR:HG22	2.51	0.41
4:B:183:TYR:CD2	4:B:380:ILE:HD13	2.55	0.41
5:L:115:VAL:CG1	5:L:116:SER:N	2.84	0.41
5:L:151:ASP:CA	5:L:191:SER:HB3	2.48	0.41
2:P:817:MRG:S24	3:A:283:LEU:HD13	2.60	0.41
1:T:707:DG:C2'	1:T:708:DG:C5'	2.99	0.41
4:B:142:ILE:HG22	4:B:144:TYR:CE2	2.55	0.41
4:B:330:GLN:NE2	4:B:340:GLN:NE2	2.59	0.41
4:B:54:ASN:ND2	4:B:126:LYS:HB2	2.36	0.41
3:A:171:PHE:CZ	3:A:205:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:220:LYS:HE3	3:A:220:LYS:HB2	1.76	0.41
4:B:156:SER:O	4:B:157:PRO:C	2.58	0.41
4:B:91:GLN:HG3	4:B:92:LEU:HG	2.03	0.41
6:H:39:ILE:CG2	6:H:40:ARG:N	2.84	0.41
5:L:50:TYR:O	5:L:52:SER:N	2.53	0.41
5:L:55:HIS:CD2	5:L:56:SER:N	2.89	0.41
3:A:220:LYS:HE2	3:A:222:GLN:HB3	2.02	0.40
3:A:385:LYS:HG2	3:A:386:THR:N	2.36	0.40
3:A:393:ILE:HG23	3:A:393:ILE:O	2.21	0.40
4:B:47:ILE:HD11	4:B:146:TYR:CD1	2.56	0.40
6:H:155:TYR:H	6:H:155:TYR:HD2	1.67	0.40
3:A:167:ILE:O	3:A:170:PRO:HD2	2.21	0.40
3:A:246:LEU:HD12	3:A:307:ARG:NE	2.36	0.40
3:A:412:PRO:O	3:A:413:GLU:C	2.59	0.40
3:A:503:LEU:HD12	3:A:503:LEU:O	2.21	0.40
4:B:301:LEU:O	4:B:305:GLU:HB2	2.21	0.40
4:B:118:VAL:H	4:B:148:VAL:HG23	1.86	0.40
4:B:153:TRP:O	4:B:155:GLY:N	2.54	0.40
4:B:28:GLU:O	4:B:29:GLU:C	2.59	0.40
5:L:140:TYR:CE2	5:L:141:PRO:HG3	2.56	0.40
3:A:194:GLU:C	3:A:196:GLY:N	2.75	0.40
3:A:171:PHE:CE2	3:A:205:LEU:HD12	2.57	0.40
3:A:459:THR:CG2	3:A:463:ARG:CB	2.91	0.40
4:B:225:PRO:HG2	5:L:92:SER:CA	2.48	0.40
4:B:266:TRP:CE3	4:B:423:VAL:CG2	3.04	0.40
4:B:47:ILE:CG2	4:B:144:TYR:CD1	3.04	0.40
4:B:54:ASN:HA	4:B:55:PRO:HD2	1.94	0.40
5:L:83:ILE:HG21	5:L:106:ILE:CD1	2.51	0.40
3:A:278:GLN:HG2	3:A:278:GLN:H	1.48	0.40
4:B:195:ILE:CG2	4:B:196:GLY:H	2.34	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)
4:B:2:ILE:CD1	4:B:2:ILE:CD1[6_565]	1.62	0.58



## 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	556/558 (100%)	424 (76%)	102 (18%)	30 (5%)	2	14
4	B	427/430 (99%)	317 (74%)	77 (18%)	33 (8%)	1	6
5	L	209/211 (99%)	165 (79%)	32 (15%)	12 (6%)	2	12
6	H	223/225 (99%)	191 (86%)	21 (9%)	11 (5%)	2	16
All	All	1415/1424 (99%)	1097 (78%)	232 (16%)	86 (6%)	2	11

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	137	ASN
3	A	139	THR
3	A	249	LYS
3	A	254	VAL
3	A	273	GLY
3	A	393	ILE
3	A	485	ALA
4	B	2	ILE
4	B	87	PHE
4	B	225	PRO
4	B	247	PRO
4	B	286	THR
4	B	315	HIS
4	B	404	GLU
5	L	51	THR
5	L	76	SER
6	H	32	SER
6	H	105	VAL
6	H	141	GLN
6	H	143	ASN
3	A	22	LYS
3	A	116	PHE

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Mol	Chain	Res	Type
3	A	195	ILE
3	A	278	GLN
3	A	287	LYS
3	A	490	GLY
3	A	543	GLY
3	A	544	GLY
4	B	114	ALA
4	B	116	PHE
4	B	154	LYS
4	B	270	ILE
4	B	300	GLU
4	B	314	VAL
4	B	332	GLN
4	B	361	HIS
4	B	424	LYS
5	L	83	ILE
6	H	34	ILE
6	H	66	LYS
3	A	243	PRO
3	A	321	PRO
3	A	345	PRO
3	A	505	ILE
4	B	355	ALA
4	B	421	PRO
4	B	425	LEU
5	L	28	ASP
5	L	61	ARG
5	L	171	SER
5	L	199	LYS
3	A	53	GLU
3	A	141	GLY
3	A	302	GLU
3	A	484	LEU
3	A	547	GLN
3	A	549	ASP
4	B	201	LYS
4	B	203	GLU
4	B	227	PHE
4	B	238	LYS
5	L	152	GLY
6	H	126	THR
3	A	133	PRO

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Mol	Chain	Res	Type
3	A	466	VAL
4	B	44	GLU
4	B	200	THR
4	B	211	ARG
4	B	212	TRP
4	B	217	PRO
4	B	290	THR
4	B	292	VAL
4	B	427	TYR
5	L	82	ASP
6	H	210	PRO
3	A	380	ILE
4	B	324	ASP
5	L	25	ALA
6	H	9	PRO
6	H	10	GLY
5	L	68	GLY
6	H	17	PRO
4	B	167	ILE
3	A	261	VAL
3	A	272	PRO
5	L	99	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	485/498 (97%)	414 (85%)	71 (15%)	3	16
4	B	388/392 (99%)	324 (84%)	64 (16%)	2	12
5	L	190/190 (100%)	168 (88%)	22 (12%)	6	26
6	H	196/196 (100%)	169 (86%)	27 (14%)	4	19
All	All	1259/1276 (99%)	1075 (85%)	184 (15%)	3	16

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	22	LYS
3	A	24	TRP
3	A	55	PRO
3	A	61	PHE
3	A	67	ASP
3	A	80	LEU
3	A	83	ARG
3	A	85	GLN
3	A	86	ASP
3	A	94	ILE
3	A	105	SER
3	A	132	ILE
3	A	145	GLN
3	A	162	SER
3	A	175	ASN
3	A	177	ASP
3	A	180	ILE
3	A	186	ASP
3	A	188	TYR
3	A	205	LEU
3	A	215	THR
3	A	219	LYS
3	A	220	LYS
3	A	221	HIS
3	A	223	LYS
3	A	232	TYR
3	A	240	THR
3	A	245	VAL
3	A	246	LEU
3	A	250	ASP
3	A	268	SER
3	A	278	GLN
3	A	279	LEU
3	A	283	LEU
3	A	286	THR
3	A	290	THR
3	A	300	GLU
3	A	325	LEU
3	A	344	GLU
3	A	353	LYS
3	A	354	TYR
3	A	365	VAL
3	A	369	THR

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Mol	Chain	Res	Type
3	A	373	GLN
3	A	374	LYS
3	A	397	THR
3	A	405	TYR
3	A	407	GLN
3	A	409	THR
3	A	415	GLU
3	A	416	PHE
3	A	419	THR
3	A	425	LEU
3	A	442	VAL
3	A	451	LYS
3	A	464	GLN
3	A	465	LYS
3	A	468	PRO
3	A	469	LEU
3	A	472	THR
3	A	478	GLU
3	A	488	ASP
3	A	497	THR
3	A	500	GLN
3	A	501	TYR
3	A	511	ASP
3	A	519	ASN
3	A	525	LEU
3	A	545	ASN
3	A	547	GLN
3	A	548	VAL
4	B	5	ILE
4	B	12	LEU
4	B	27	THR
4	B	35	VAL
4	B	37	ILE
4	B	38	CYS
4	B	42	GLU
4	B	47	ILE
4	B	91	GLN
4	B	92	LEU
4	B	105	SER
4	B	109	LEU
4	B	113	ASP
4	B	143	ARG

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Mol	Chain	Res	Type
4	B	144	TYR
4	B	162	SER
4	B	163	SER
4	B	169	GLU
4	B	189	VAL
4	B	191	SER
4	B	193	LEU
4	B	197	GLN
4	B	199	ARG
4	B	206	ARG
4	B	212	TRP
4	B	216	THR
4	B	218	ASP
4	B	221	HIS
4	B	225	PRO
4	B	233	GLU
4	B	238	LYS
4	B	244	ILE
4	B	250	ASP
4	B	253	THR
4	B	271	TYR
4	B	276	VAL
4	B	277	ARG
4	B	282	LEU
4	B	284	ARG
4	B	286	THR
4	B	293	ILE
4	B	295	LEU
4	B	305	GLU
4	B	315	HIS
4	B	318	TYR
4	B	324	ASP
4	B	330	GLN
4	B	348	ASN
4	B	349	LEU
4	B	351	THR
4	B	353	LYS
4	B	357	MET
4	B	358	ARG
4	B	363	ASN
4	B	385	LYS
4	B	386	THR

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Mol	Chain	Res	Type
4	B	401	TRP
4	B	403	THR
4	B	407	GLN
4	B	409	THR
4	B	418	ASN
4	B	419	THR
4	B	424	LYS
4	B	427	TYR
5	L	7	THR
5	L	8	THR
5	L	10	SER
5	L	11	LEU
5	L	33	LEU
5	L	39	LYS
5	L	48	ILE
5	L	69	THR
5	L	77	ASN
5	L	89	GLN
5	L	97	THR
5	L	117	ILE
5	L	142	LYS
5	L	143	ASP
5	L	144	ILE
5	L	170	ASP
5	L	171	SER
5	L	173	TYR
5	L	190	ASN
5	L	197	THR
5	L	203	SER
5	L	211	ARG
6	H	1	GLN
6	H	4	LEU
6	H	7	SER
6	H	9	PRO
6	H	23	THR
6	H	29	LEU
6	H	32	SER
6	H	55	TRP
6	H	72	SER
6	H	88	GLU
6	H	107	ASP
6	H	111	ASP

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Mol	Chain	Res	Type
6	H	117	THR
6	H	120	THR
6	H	129	PRO
6	H	155	TYR
6	H	157	PRO
6	H	160	VAL
6	H	171	SER
6	H	175	THR
6	H	181	GLN
6	H	187	LEU
6	H	189	SER
6	H	192	THR
6	H	204	THR
6	H	215	LYS
6	H	218	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	GLN
3	A	161	GLN
3	A	207	GLN
3	A	221	HIS
3	A	235	HIS
3	A	265	ASN
3	A	306	ASN
3	A	447	ASN
3	A	471	ASN
3	A	480	GLN
3	A	494	ASN
3	A	500	GLN
3	A	520	GLN
3	A	539	HIS
4	B	57	ASN
4	B	137	ASN
4	B	151	GLN
4	B	175	ASN
4	B	182	GLN
4	B	235	HIS
4	B	242	GLN
4	B	330	GLN
4	B	340	GLN

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Mol	Chain	Res	Type
4	B	363	ASN
4	B	394	GLN
4	B	418	ASN
5	L	38	GLN
5	L	77	ASN
5	L	89	GLN
5	L	90	GLN
5	L	137	ASN
5	L	138	ASN
5	L	166	GLN
5	L	190	ASN
5	L	210	ASN
6	H	59	ASN
6	H	62	ASN
6	H	141	GLN
6	H	174	HIS
6	H	181	GLN
6	H	206	ASN
6	H	209	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MRG	P	817	1,3,2	21,28,29	2.61	7 (33%)	24,39,42	3.22	11 (45%)
2	ATM	P	822	1,2	14,23,24	2.06	5 (35%)	18,32,35	3.68	7 (38%)

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
2	MRG	P	817	1,3,2	-	0/8/26/27	0/3/3/3
2	ATM	P	822	1,2	-	0/6/24/25	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	817	MRG	C8-N7	-4.67	1.25	1.34
2	P	817	MRG	C5-C4	-3.08	1.33	1.40
2	P	817	MRG	C21-N2	-2.99	1.39	1.46
2	P	817	MRG	C4-N3	-2.57	1.31	1.35
2	P	817	MRG	C2-N3	-2.37	1.27	1.34
2	P	822	ATM	C4-N3	2.13	1.36	1.33
2	P	822	ATM	C6-C5	2.22	1.45	1.40
2	P	822	ATM	C5A-C5	2.73	1.56	1.51
2	P	822	ATM	O5'-C5'	3.47	1.49	1.44
2	P	822	ATM	N4'-N3'	4.96	1.36	1.23
2	P	817	MRG	C6-N1	5.27	1.42	1.33
2	P	817	MRG	C2-N2	6.86	1.45	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	817	MRG	C5-C6-N1	-9.23	110.34	123.48
2	P	822	ATM	C5-C4-N3	-5.08	119.64	125.24
2	P	817	MRG	C23-C22-C21	-4.95	96.94	112.67
2	P	817	MRG	C2-N3-C4	-3.80	110.78	115.11
2	P	817	MRG	C6-C5-C4	-3.22	117.64	120.84
2	P	817	MRG	C2'-C3'-C4'	-2.42	97.58	102.73
2	P	817	MRG	O4'-C4'-C3'	2.10	110.73	105.68
2	P	817	MRG	C3'-C2'-C1'	2.14	107.96	102.48
2	P	822	ATM	O4'-C4'-C5'	2.34	117.30	109.40
2	P	822	ATM	O4'-C4'-C3'	2.47	108.58	105.42
2	P	817	MRG	C2'-C1'-N9	2.54	120.22	114.23
2	P	817	MRG	O4'-C1'-N9	3.06	112.93	107.78
2	P	822	ATM	O4'-C1'-N1	3.39	113.50	107.78
2	P	817	MRG	C6-N1-C2	4.24	122.77	115.18
2	P	822	ATM	C3'-C2'-C1'	4.87	108.22	103.19
2	P	822	ATM	C5A-C5-C4	7.14	128.41	120.17
2	P	817	MRG	C22-C23-S24	7.17	136.04	112.91
2	P	822	ATM	C4-N3-C2	10.58	124.41	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	817	MRG	9	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	T	21/27 (77%)	0.15	0	100 100	64, 84, 98, 107	0
2	P	18/21 (85%)	0.01	0	100 100	75, 83, 100, 103	0
3	A	556/558 (99%)	-0.13	12 (2%)	62 41	44, 91, 110, 110	1 (0%)
4	B	428/430 (99%)	-0.14	4 (0%)	84 69	35, 80, 110, 110	2 (0%)
5	L	211/211 (100%)	-0.10	0	100 100	56, 88, 110, 110	0
6	H	225/225 (100%)	-0.24	4 (1%)	69 47	51, 78, 105, 110	0
All	All	1459/1472 (99%)	-0.14	20 (1%)	75 57	35, 85, 110, 110	3 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	H	141	GLN	5.1
3	A	67	ASP	4.4
4	B	315	HIS	3.7
3	A	448	ARG	3.5
3	A	64	LYS	3.5
6	H	138	SER	3.4
4	B	90	VAL	3.1
3	A	223	LYS	2.6
3	A	258	CYS	2.5
6	H	222	PRO	2.5
3	A	66	LYS	2.4
6	H	142	THR	2.4
4	B	426	TRP	2.4
3	A	283	LEU	2.4
3	A	286	THR	2.3
4	B	312	GLU	2.3
3	A	2	ILE	2.2
3	A	297	GLU	2.2
3	A	71	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	63	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MRG	P	817	26/27	0.87	0.20	-	92,92,92,92	0
2	ATM	P	822	22/23	0.92	0.20	-	62,68,87,87	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	MG	A	1001	1/1	0.98	0.61	6.39	62,62,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.