



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:19 PM UTC

PDB ID : 1N5Y / pdb_00001n5y
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

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:

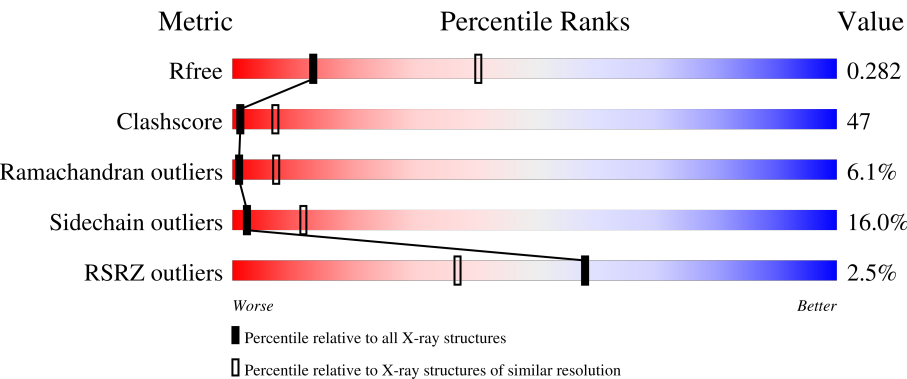
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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.



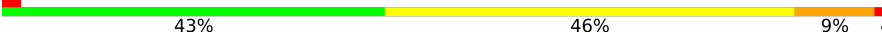
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	27	4% 48%26%22%
2	P	21	5% 43%48%5%
3	A	558	3% 35%47%15%
4	B	430	3% 28%51%19%

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Mol	Chain	Length	Quality of chain
5	L	211	 30% 59% 9% 2%
6	H	225	 2% 43% 46% 9%

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	-

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 mutation	UNP P03366
A	280	SER	CYS	engineered mutation	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 mutation	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 (CCD ID: MG) (formula: Mg).

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

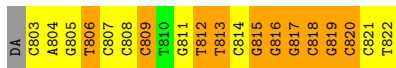
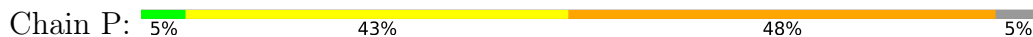
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

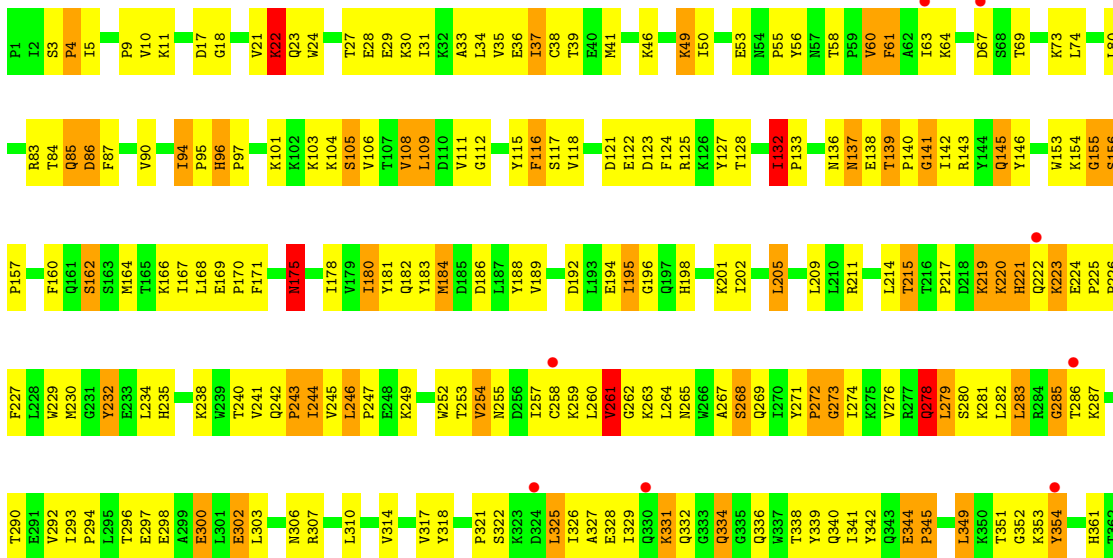
- Molecule 1: 5'-D(*AP*TP*GP*C*TP*AP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3'

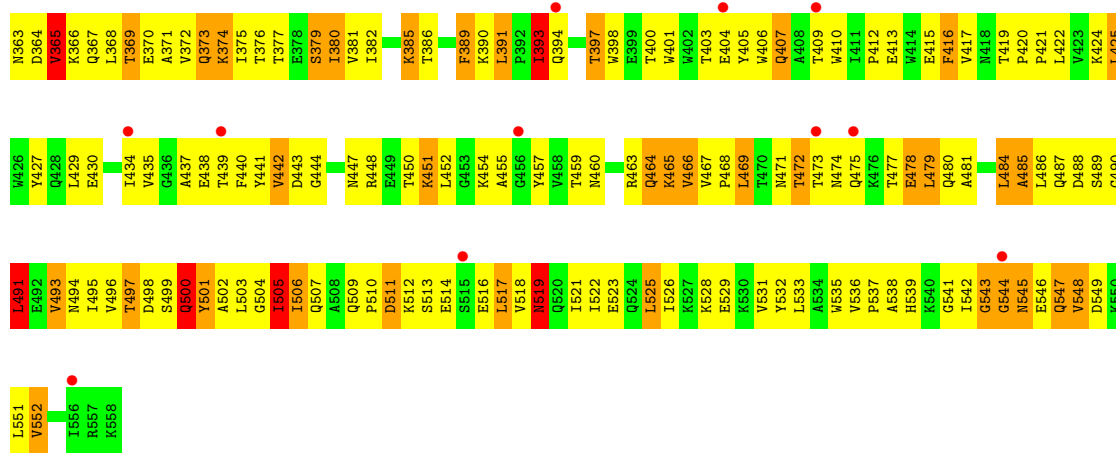


- Molecule 2: 5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*C P*GP*CP*CP*(ATM))-3'

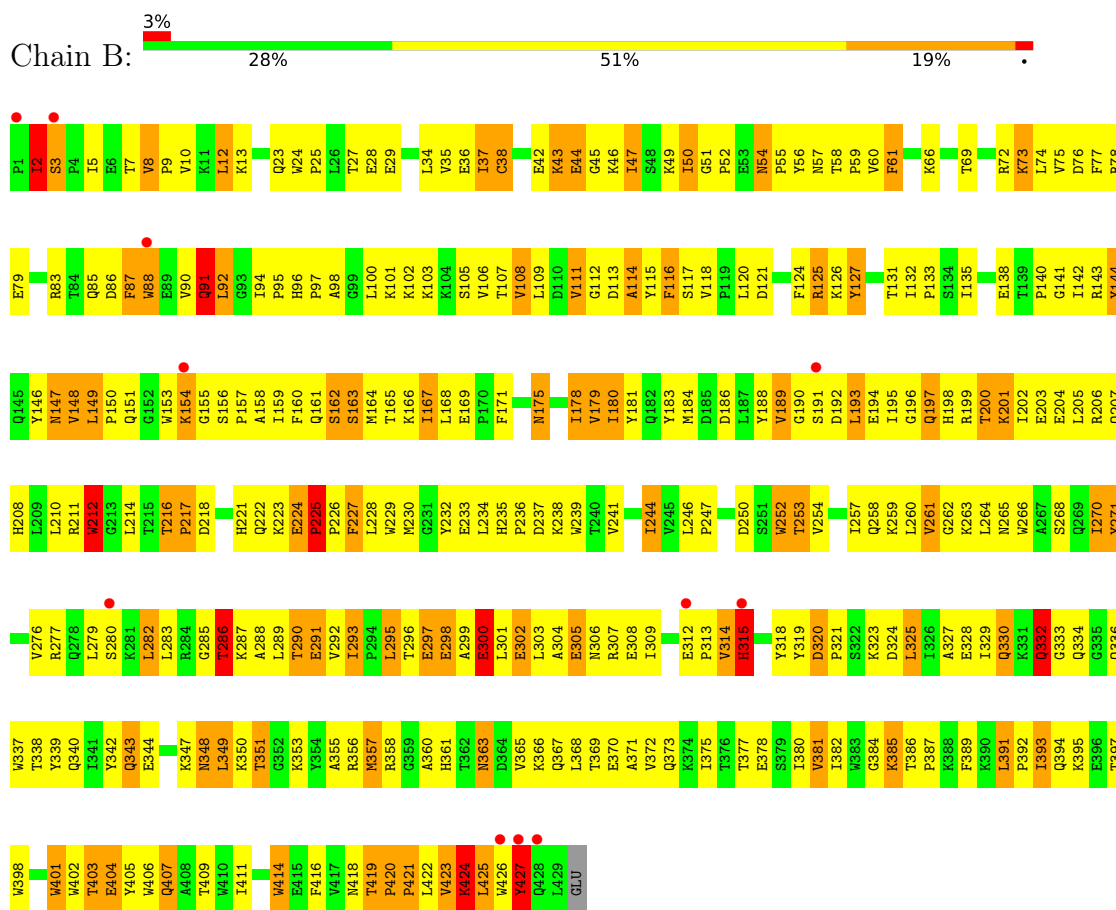


- Molecule 3: REVERSE TRANSCRIPTASE

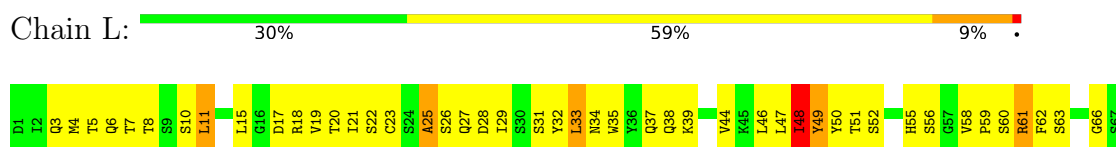


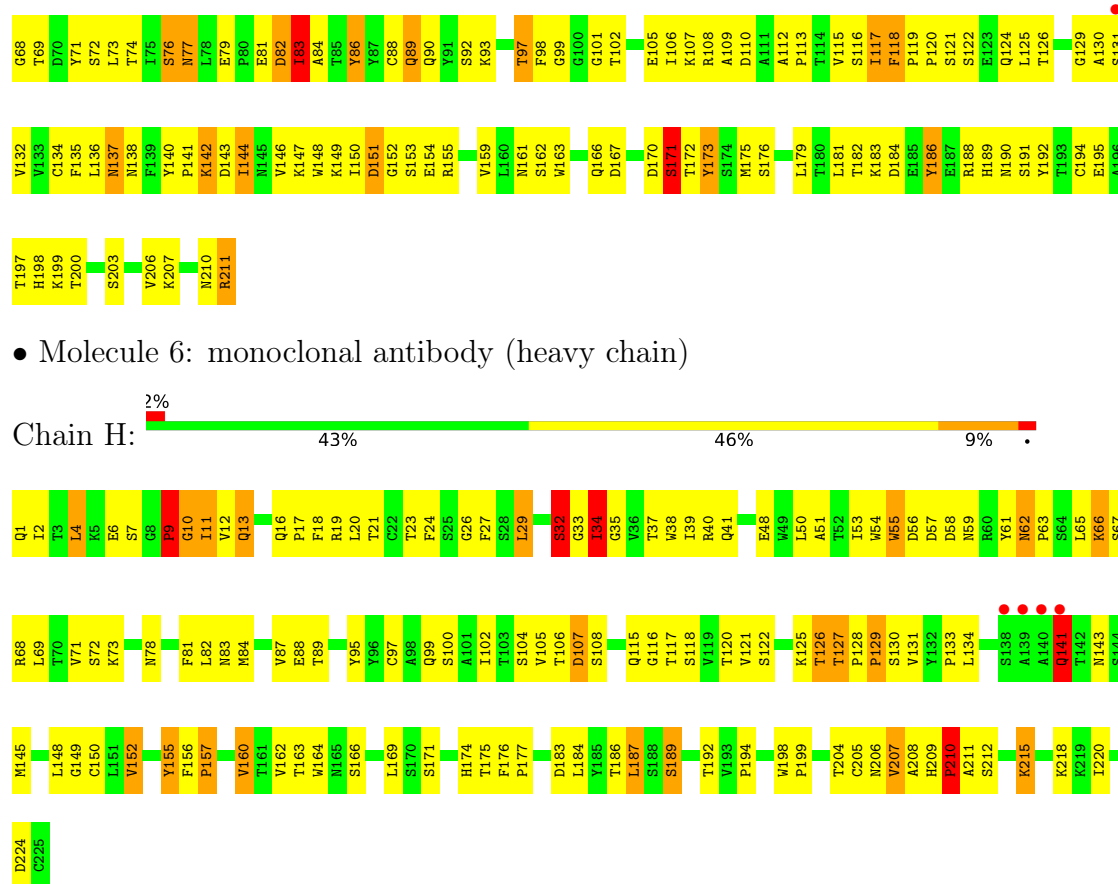


• Molecule 4: REVERSE TRANSCRIPTASE



• 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, α , β , γ	166.70Å 166.70Å 221.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.8 (20.00-3.10) 91.4 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	2502 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	85.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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, MRG, ATM

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	1.04	2/486 (0.4%)	1.46	10/749 (1.3%)
2	P	1.28	5/400 (1.2%)	1.86	15/612 (2.5%)
3	A	0.73	1/4600 (0.0%)	1.13	31/6259 (0.5%)
4	B	0.83	2/3639 (0.1%)	1.28	54/4949 (1.1%)
5	L	0.66	0/1681	1.10	12/2283 (0.5%)
6	H	0.80	0/1729	1.26	18/2372 (0.8%)
All	All	0.80	10/12535 (0.1%)	1.23	140/17224 (0.8%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	812	DT	C4-C5	8.87	1.62	1.44
2	P	806	DT	C4-C5	8.56	1.61	1.44
1	T	720	DG	C5-C6	8.19	1.58	1.42
4	B	393	ILE	CA-CB	-7.11	1.50	1.55
1	T	721	DG	C5-C6	6.19	1.54	1.42
3	A	118	VAL	CA-CB	-5.70	1.50	1.54
2	P	818	DC	P-OP1	-5.56	1.37	1.48
2	P	818	DC	O3'-P	5.35	1.69	1.61
2	P	813	DT	C4-C5	5.14	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	50	ILE	CA-CB	-5.12	1.51	1.55

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	816	DG	N9-C1'-C2'	14.69	135.53	113.50
2	P	815	DG	N9-C1'-C2'	14.48	135.22	113.50
4	B	225	PRO	N-CA-C	13.41	127.06	110.70
4	B	86	ASP	N-CA-C	-12.43	97.73	111.28
6	H	127	THR	CA-C-N	12.16	128.54	119.66
6	H	127	THR	C-N-CA	12.16	128.54	119.66
3	A	500	GLN	N-CA-C	-10.83	99.56	111.36
1	T	712	DC	C2'-C3'-O3'	-10.26	96.11	111.50
1	T	713	DC	N1-C1'-C2'	9.74	128.12	113.50
4	B	427	TYR	N-CA-C	9.56	131.16	110.80
5	L	112	ALA	N-CA-C	9.40	123.28	110.31
1	T	711	DC	N1-C1'-C2'	9.37	127.56	113.50
4	B	298	GLU	N-CA-C	-9.01	102.42	113.41
4	B	94	ILE	CA-C-N	8.80	130.84	119.84
4	B	94	ILE	C-N-CA	8.80	130.84	119.84
2	P	806	DT	N3-C4-O4	-8.79	109.42	122.60
4	B	224	GLU	CA-C-N	8.77	129.41	120.38
4	B	224	GLU	C-N-CA	8.77	129.41	120.38
6	H	141	GLN	N-CA-C	8.76	129.47	110.80
2	P	820	DC	C2'-C3'-O3'	-8.62	98.57	111.50
2	P	806	DT	C5-C4-O4	8.56	135.44	122.60
1	T	712	DC	N1-C1'-C2'	8.46	126.18	113.50
3	A	37	ILE	N-CA-C	8.29	118.38	110.42
4	B	66	LYS	N-CA-C	-8.15	103.33	113.28
1	T	713	DC	C2'-C3'-O3'	-7.73	99.91	111.50
3	A	519	ASN	N-CA-C	-7.67	104.05	113.41
3	A	349	LEU	N-CA-C	-7.65	102.51	112.68
4	B	43	LYS	N-CA-C	-7.59	102.70	110.97
4	B	50	ILE	CB-CA-C	-7.53	104.66	111.74
2	P	819	DG	C5'-C4'-C3'	-7.50	103.65	114.90
2	P	812	DT	C5-C4-O4	7.49	133.84	122.60
2	P	812	DT	N3-C4-O4	-7.39	111.52	122.60
5	L	137	ASN	N-CA-C	7.37	121.66	109.95
6	H	13	GLN	CA-C-N	7.36	127.41	119.90
6	H	13	GLN	C-N-CA	7.36	127.41	119.90
4	B	291	GLU	N-CA-C	7.32	119.70	109.15
4	B	216	THR	CA-C-N	7.29	128.96	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	216	THR	C-N-CA	7.29	128.96	119.84
4	B	54	ASN	CA-C-N	7.21	128.13	120.12
4	B	54	ASN	C-N-CA	7.21	128.13	120.12
4	B	8	VAL	CA-C-N	7.11	127.03	119.85
4	B	8	VAL	C-N-CA	7.11	127.03	119.85
4	B	125	ARG	N-CA-C	6.86	118.41	111.07
3	A	379	SER	N-CA-C	-6.85	102.30	111.96
4	B	175	ASN	CA-C-N	-6.84	112.65	119.56
4	B	175	ASN	C-N-CA	-6.84	112.65	119.56
2	P	812	DT	N1-C1'-C2'	6.82	123.72	113.50
3	A	325	LEU	N-CA-C	6.82	119.75	110.55
4	B	320	ASP	CA-C-N	6.81	126.95	119.87
4	B	320	ASP	C-N-CA	6.81	126.95	119.87
2	P	815	DG	C2'-C3'-O3'	-6.75	101.38	111.50
4	B	2	ILE	N-CA-C	6.72	123.31	109.34
4	B	147	ASN	N-CA-C	-6.71	105.65	114.31
3	A	391	LEU	N-CA-C	6.64	120.17	110.14
4	B	382	ILE	N-CA-C	6.60	116.73	110.53
4	B	252	TRP	N-CA-C	6.56	119.50	108.02
3	A	506	ILE	N-CA-C	6.55	116.58	110.42
3	A	298	GLU	N-CA-C	-6.52	105.18	113.01
6	H	62	ASN	CA-C-N	6.50	127.97	119.84
6	H	62	ASN	C-N-CA	6.50	127.97	119.84
3	A	184	MET	CB-CA-C	-6.47	109.13	116.63
4	B	261	VAL	N-CA-C	-6.42	105.48	111.45
3	A	493	VAL	N-CA-C	6.41	115.52	107.70
3	A	285	GLY	N-CA-C	-6.39	103.53	111.70
6	H	29	LEU	N-CA-C	-6.37	105.46	112.72
1	T	716	DA	N9-C1'-C2'	6.35	123.02	113.50
4	B	88	TRP	N-CA-C	6.31	120.08	112.38
3	A	132	ILE	CA-C-N	6.28	127.69	119.84
3	A	132	ILE	C-N-CA	6.28	127.69	119.84
3	A	21	VAL	N-CA-C	6.16	116.69	107.51
3	A	155	GLY	N-CA-C	6.11	120.59	112.77
4	B	343	GLN	N-CA-C	-6.09	106.39	113.88
3	A	365	VAL	N-CA-C	-6.04	96.78	109.34
2	P	818	DC	P-O5'-C5'	5.99	128.99	120.00
5	L	151	ASP	N-CA-C	-5.96	103.02	111.24
4	B	419	THR	CA-C-N	5.93	126.48	120.38
4	B	419	THR	C-N-CA	5.93	126.48	120.38
2	P	813	DT	N1-C1'-C2'	5.88	122.32	113.50
4	B	391	LEU	N-CA-C	5.87	118.13	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	381	VAL	CB-CA-C	-5.87	104.46	111.97
4	B	235	HIS	CA-C-N	5.83	127.13	119.84
4	B	235	HIS	C-N-CA	5.83	127.13	119.84
4	B	149	LEU	CA-C-N	5.80	126.29	120.14
4	B	149	LEU	C-N-CA	5.80	126.29	120.14
2	P	806	DT	N1-C1'-C2'	5.80	122.20	113.50
1	T	721	DG	N9-C1'-C2'	5.79	122.19	113.50
4	B	423	VAL	N-CA-C	-5.77	97.33	109.34
6	H	32	SER	N-CA-C	5.72	122.99	110.80
3	A	4	PRO	N-CA-C	-5.72	106.68	114.80
1	T	720	DG	N9-C1'-C2'	5.64	121.96	113.50
1	T	711	DC	C4'-C3'-O3'	-5.61	101.59	110.00
6	H	34	ILE	N-CA-C	5.59	120.97	109.34
3	A	491	LEU	N-CA-C	-5.57	105.83	113.30
4	B	61	PHE	N-CA-C	-5.52	99.92	108.42
6	H	131	VAL	N-CA-C	5.51	116.52	108.53
2	P	809	DC	N1-C1'-C2'	5.51	121.76	113.50
4	B	180	ILE	N-CA-C	5.50	115.92	107.77
6	H	59	ASN	N-CA-C	5.49	117.98	110.24
4	B	91	GLN	N-CA-C	5.46	116.92	110.97
3	A	96	HIS	CA-C-N	5.45	125.53	119.32
3	A	96	HIS	C-N-CA	5.45	125.53	119.32
6	H	224	ASP	N-CA-C	5.44	119.87	112.04
6	H	207	VAL	N-CA-C	5.42	115.67	107.75
3	A	175	ASN	CA-C-N	5.42	126.62	119.84
3	A	175	ASN	C-N-CA	5.42	126.62	119.84
4	B	420	PRO	CA-C-N	5.42	126.62	119.84
4	B	420	PRO	C-N-CA	5.42	126.62	119.84
3	A	28	GLU	N-CA-C	-5.41	105.30	112.34
2	P	813	DT	C5-C4-O4	5.41	130.71	122.60
4	B	3	SER	N-CA-C	5.41	116.99	108.23
4	B	127	TYR	N-CA-C	5.39	119.12	112.54
5	L	186	TYR	N-CA-C	-5.39	104.83	111.40
4	B	186	ASP	N-CA-C	5.38	117.86	109.52
5	L	110	ASP	N-CA-C	5.37	118.13	110.24
3	A	479	LEU	N-CA-C	-5.34	106.76	113.28
3	A	36	GLU	N-CA-C	-5.34	105.36	111.07
5	L	118	PHE	N-CA-C	5.32	118.34	109.09
5	L	22	SER	N-CA-C	5.31	117.90	109.24
4	B	297	GLU	N-CA-C	-5.28	106.79	113.18
5	L	48	ILE	N-CA-C	5.27	115.49	108.11
3	A	389	PHE	N-CA-C	5.27	118.58	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	115	GLN	N-CA-C	-5.24	107.55	114.31
4	B	414	TRP	N-CA-C	5.23	116.94	109.14
5	L	207	LYS	N-CA-C	-5.22	99.83	108.75
6	H	33	GLY	N-CA-C	5.18	118.91	112.64
4	B	90	VAL	N-CA-C	5.17	115.31	110.30
5	L	5	THR	N-CA-C	5.17	116.81	108.34
5	L	86	TYR	N-CA-C	5.16	117.86	109.24
3	A	493	VAL	CB-CA-C	-5.14	106.91	111.74
5	L	31	SER	N-CA-C	5.11	118.63	111.74
6	H	130	SER	N-CA-C	-5.11	100.92	109.24
4	B	73	LYS	N-CA-C	-5.10	102.94	110.48
1	T	710	DG	C2'-C3'-O3'	-5.07	103.89	111.50
3	A	156	SER	N-CA-C	5.04	120.95	109.81
6	H	107	ASP	N-CA-C	5.04	116.94	108.73
4	B	315	HIS	N-CA-C	5.03	121.52	110.80
3	A	211	ARG	N-CA-C	-5.02	105.94	111.71
4	B	51	GLY	CA-C-N	5.01	125.29	119.47
4	B	51	GLY	C-N-CA	5.01	125.29	119.47
3	A	340	GLN	N-CA-C	-5.01	100.87	109.24

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4482	0	4484	449	0
4	B	3534	0	3568	380	1
5	L	1643	0	1565	149	0
6	H	1685	0	1640	109	0
7	A	1	0	0	0	0
All	All	12185	0	11722	1106	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 47.

All (1106) 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:HD12	4:B:12:LEU:H	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:HD23	3:A:279:LEU:H	1.25	1.01
3:A:331:LYS:HB3	3:A:421:PRO:HG2	1.40	1.01
1:T:712:DC:H2''	1:T:713:DC:H5'	1.42	1.00
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.41	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:HD23	3:A:246:LEU:H	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:237:ASP:C	4:B:239:TRP:H	1.76	0.88
4:B:225:PRO:HB2	4:B:226:PRO:HD3	1.53	0.88
2:P:820:DC:H2''	2:P:821:DC:H5'	1.55	0.88
3:A:459:THR:HG22	3:A:463:ARG:HB3	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
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: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
4:B:423:VAL:C	4:B:425:LEU:H	1.82	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:H	3:A:22:LYS:HD3	1.43	0.83
3:A:489:SER:HB3	3:A:528:LYS:HZ3	1.42	0.83
4:B:58:THR:HG23	4:B:59:PRO:HD2	1.59	0.83
6:H:38:TRP:O	6:H:50:LEU:HB2	1.79	0.83
3:A:500:GLN:H	3:A:500:GLN:NE2	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:HG3	3:A:143:ARG:HH11	1.45	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:237:ASP:C	4:B:239:TRP:N	2.43	0.76
4:B:423:VAL:C	4:B:425:LEU:N	2.40	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
2:P:817:MRG:C2'	2:P:818:DC:O5'	2.35	0.74
3:A:310:LEU:HD23	3:A:310:LEU:O	1.87	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
3:A:406:TRP:CZ2	4:B:420:PRO:HG3	2.22	0.74
3:A:501:TYR:CD1	3:A:501:TYR:C	2.62	0.74
4:B:91:GLN:OE1	4:B:91:GLN:HA	1.85	0.74
4:B:111:VAL:HG23	4:B:111:VAL:O	1.85	0.74
4:B:12:LEU:HD12	4:B:12:LEU:N	2.01	0.74
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.68	0.74
3:A:279:LEU:HD23	3:A:279:LEU:N	2.02	0.74
4:B:299:ALA:C	4:B:301:LEU:H	1.94	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:299:ALA:O	4:B:301:LEU:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	4:B:244:ILE:CD1	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:387:PRO:HG2	4:B:389:PHE:CE1	2.25	0.71
4:B:2:ILE:HD12	4:B:2:ILE:O	1.91	0.71
4:B:426:TRP:HA	4:B:426:TRP:CE3	2.26	0.71
4:B:162:SER:O	4:B:165:THR:HG22	1.90	0.71
2:P:817:MRG:H2''	2:P:818:DC:C5'	2.21	0.70
3:A:420:PRO:HA	3:A:421:PRO:C	2.17	0.70
3:A:460:ASN:HD22	4:B:288:ALA:HB2	1.55	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:HD12	3:A:533:LEU:N	2.05	0.70
6:H:125:LYS:O	6:H:127:THR:HG23	1.91	0.70
4:B:8:VAL:HG11	4:B:159:ILE:HG12	1.73	0.70
4:B:206:ARG:NH1	4:B:217:PRO:O	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:817:MRG:H2''	2:P:818:DC:H5'	1.76	0.68
4:B:178:ILE:CD1	4:B:201:LYS:HG2	2.24	0.68
3:A:257:ILE:HG21	3:A:283:LEU:HD21	1.75	0.68
1:T:706:DA:H2'	1:T:707:DG:C8	2.29	0.68
3:A:9:PRO:HA	3:A:121:ASP:OD2	1.94	0.68
5:L:113:PRO:HG3	5:L:144:ILE:HD11	1.76	0.67
3:A:501:TYR:C	3:A:501:TYR:HD1	2.01	0.67
4:B:285:GLY:H	4:B:287:LYS:HZ3	1.43	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:43:LYS:C	4:B:45:GLY:H	2.02	0.66
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:457:TYR:HA	3:A:548:VAL:CG1	2.24	0.66
3:A:511:ASP:OD2	3:A:511:ASP:C	2.39	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
3:A:439:THR:CG2	4:B:288:ALA:HA	2.26	0.65
5:L:23:CYS:SG	5:L:33:LEU:HD11	2.37	0.65
6:H:34:ILE:CG2	6:H:35:GLY:N	2.59	0.65
3:A:354:TYR:CZ	3:A:374:LYS:HG2	2.30	0.65
3:A:486:LEU:HA	3:A:528:LYS:HZ2	1.59	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:440:PHE:HE2	3:A:489:SER:HG	1.45	0.64
4:B:395:LYS:HB2	4:B:416:PHE:CD2	2.32	0.64
4:B:87:PHE:CD2	4:B:88:TRP:N	2.65	0.64
4:B:403:THR:O	4:B:405:TYR:N	2.31	0.64
3:A:501:TYR:CE1	3:A:505:ILE:HD11	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:43:LYS:C	4:B:45:GLY:N	2.53	0.64
3:A:182:GLN:O	3:A:182:GLN:HG3	1.97	0.63
4:B:195:ILE:HG23	4:B:196:GLY:N	2.11	0.63
4:B:299:ALA:C	4:B:301:LEU:N	2.54	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:190:ASN:CG	5:L:210:ASN:HD22	2.07	0.63
5:L:19:VAL:O	5:L:74:THR:HA	1.97	0.63
4:B:393:ILE:HG12	4:B:394:GLN:N	2.12	0.63
5:L:38:GLN:HG3	5:L:44:VAL:CG2	2.28	0.63
6:H:53:ILE:HD12	6:H:71:VAL:HG12	1.81	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
2:P:812:DT:C6	2:P:813:DT:H73	2.34	0.62
3:A:465:LYS:NZ	3:A:488:ASP:OD2	2.31	0.62
4:B:120:LEU:HD12	4:B:121:ASP:H	1.64	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:416:PHE:CD1	3:A:416:PHE:C	2.76	0.61
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
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.82	0.61
6:H:162:VAL:HG22	6:H:207:VAL:HG22	1.81	0.61
1:T:715:DA:H2"	1:T:716:DA:H8	1.65	0.61
3:A:478:GLU:OE1	3:A:498:ASP:OD1	2.17	0.61
4:B:260:LEU:HD12	4:B:260:LEU:O	2.00	0.61
3:A:41:MET:HE1	3:A:73:LYS:CE	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:330:GLN:NE2	4:B:340:GLN:HE22	1.91	0.61
5:L:135:PHE:C	5:L:136:LEU:HD12	2.25	0.61
3:A:344:GLU:CB	3:A:345:PRO:HD2	2.29	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: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:225:PRO:HB3	5:L:32:TYR:CE1	2.36	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
3:A:162:SER:OG	4:B:52:PRO:HD3	2.01	0.61
4:B:34:LEU:CD1	4:B:73:LYS:HG3	2.30	0.61
4:B:210:LEU:C	4:B:212:TRP:H	2.09	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: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
5:L:89:GLN:HB2	5:L:98:PHE:CE1	2.35	0.60
5:L:117:ILE:HD13	5:L:194:CYS:HB2	1.82	0.60
6:H:183:ASP:O	6:H:184:LEU:HG	1.99	0.60
4:B:59:PRO:HG2	4:B:76:ASP:HB3	1.83	0.60
4:B:314:VAL:HG12	4:B:315:HIS:H	1.66	0.60
2:P:817:MRG:H2''	2:P:818:DC:O5'	2.01	0.60
3:A:115:TYR:C	3:A:117:SER:H	2.10	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
3:A:363:ASN:OD1	3:A:363:ASN:C	2.45	0.60
4:B:46:LYS:HD2	4:B:116:PHE:HB3	1.84	0.59
4:B:116:PHE:C	4:B:148:VAL:HG21	2.27	0.59
3:A:136:ASN:C	3:A:138:GLU:H	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:T:713:DC:H2''	1:T:714:DG:O5'	2.03	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
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
5:L:21:ILE:HD13	5:L:102:THR:HB	1.85	0.59
6:H:62:ASN:HD22	6:H:63:PRO:HD2	1.66	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:160:PHE:C	3:A:160:PHE:CD2	2.82	0.58
3:A:500:GLN:H	3:A:500:GLN:HE21	1.49	0.58
4:B:168:LEU:HD13	4:B:180:ILE:HG21	1.84	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
1:T:707:DG:C2'	1:T:708:DG:H5'	2.32	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
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
4:B:160:PHE:HE2	4:B:164:MET:HE2	1.68	0.58
3:A:5:ILE:CD1	3:A:167:ILE:HD11	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:171:PHE:CE1	4:B:205:LEU:HA	2.39	0.57
5:L:61:ARG:HG2	5:L:61:ARG:HH1	1.70	0.57
4:B:205:LEU:O	4:B:205:LEU:HD12	2.05	0.57
3:A:11:LYS:O	3:A:85:GLN:HG2	2.05	0.57
3:A:17:ASP:O	3:A:83:ARG:NH1	2.37	0.57
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
5:L:73:LEU:HD12	5:L:74:THR:N	2.20	0.57
5:L:120:PRO:CB	5:L:125:LEU:HD21	2.34	0.57
6:H:27:PHE:CE2	6:H:99:GLN:HG3	2.39	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
1:T:713:DC:H2'	1:T:714:DG:C8	2.39	0.56
4:B:58:THR:HG22	4:B:59:PRO:N	2.20	0.56
4:B:106:VAL:HA	4:B:190:GLY:HA2	1.87	0.56
4:B:112:GLY:HA3	4:B:151:GLN:NE2	2.19	0.56
3:A:459:THR:HG22	3:A:463:ARG:CB	2.32	0.56
3:A:518:VAL:O	3:A:518:VAL:HG12	2.04	0.56
4:B:120:LEU:HD12	4:B:121:ASP:N	2.20	0.56
5:L:81:GLU:N	5:L:81:GLU:OE1	2.37	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
4:B:121:ASP:OD1	4:B:121:ASP:C	2.49	0.56
5:L:35:TRP:CZ3	5:L:88:CYS:HB3	2.40	0.56
6:H:95:TYR:O	6:H:116:GLY:HA2	2.04	0.56
3:A:194:GLU:O	3:A:196:GLY:N	2.39	0.56
3:A:379:SER:O	3:A:380:ILE:C	2.49	0.56
3:A:438:GLU:HB3	3:A:459:THR:OG1	2.05	0.56
5:L:60:SER:C	5:L:62:PHE:H	2.13	0.56
5:L:182:THR:HG22	5:L:183:LYS:N	2.15	0.56
6:H:134:LEU:HD12	6:H:149:GLY:HA3	1.87	0.56
1:T:715:DA:C2	1:T:716:DA:C6	2.94	0.56
3:A:443:ASP:O	3:A:481:ALA:HB2	2.04	0.56
4:B:78:ARG:HD3	4:B:411:ILE:HG22	1.87	0.56
4:B:223:LYS:HD2	4:B:223:LYS:N	2.21	0.56
5:L:106:ILE:N	5:L:166:GLN:HE22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:47:ILE:HG23	4:B:144:TYR:HD1	1.70	0.55
4:B:252:TRP:CD1	4:B:252:TRP:N	2.75	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:263:LYS:HG2	4:B:423:VAL:HG12	1.88	0.55
4:B:356:ARG:HG2	4:B:357:MET:N	2.22	0.55
5:L:11:LEU:HG	5:L:11:LEU:O	2.05	0.55
3:A:466:VAL:HG12	3:A:466:VAL:O	2.06	0.55
4:B:302:GLU:HA	4:B:302:GLU:OE1	2.05	0.55
2:P:807:DC:H4'	3:A:448:ARG:HD2	1.88	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
3:A:545:ASN:O	3:A:546:GLU:C	2.49	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
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
1:T:720:DG:H2''	1:T:721:DG:OP2	2.07	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:198:HIS:O	4:B:199:ARG:C	2.49	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
3:A:447:ASN:HD22	3:A:450:THR:CG2	2.18	0.55
6:H:40:ARG:HD3	6:H:50:LEU:HD11	1.89	0.55
4:B:2:ILE:HD12	4:B:2:ILE:C	2.31	0.55
4:B:328:GLU:O	4:B:339:TYR:HA	2.07	0.55
2:P:819:DG:OP1	3:A:259:LYS:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:91:GLN:OE1	4:B:91:GLN:CA	2.53	0.55
4:B:131:THR:HG22	4:B:132:ILE:N	2.21	0.55
3:A:279:LEU:HA	3:A:282:LEU:HG	1.88	0.54
3:A:500:GLN:HE21	3:A:500:GLN:N	2.04	0.54
5:L:137:ASN:HB3	5:L:138:ASN:ND2	2.21	0.54
5:L:146:VAL:HG21	5:L:175:MET:HE1	1.89	0.54
1:T:709:DC:C2'	1:T:710:DG:O5'	2.55	0.54
1:T:724:DT:C2'	1:T:725:DG:C8	2.86	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
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: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:504:GLY:O	3:A:505:ILE:C	2.49	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
5:L:151:ASP:C	5:L:153:SER:H	2.15	0.54
2:P:812:DT:C6	2:P:813:DT:C7	2.91	0.54
3:A:479:LEU:O	3:A:521:ILE:HD11	2.08	0.54
3:A:512:LYS:HD2	3:A:513:SER:H	1.72	0.54
3:A:27:THR:OG1	3:A:29:GLU:HB3	2.07	0.54
3:A:440:PHE:CZ	3:A:488:ASP:O	2.60	0.54
3:A:451:LYS:O	3:A:471:ASN:N	2.39	0.54
5:L:23:CYS:HB2	5:L:35:TRP:CH2	2.43	0.54
1:T:712:DC:OP1	3:A:353:LYS:NZ	2.41	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
4:B:377:THR:O	4:B:381:VAL:HG23	2.07	0.54
4:B:394:GLN:O	4:B:395:LYS:C	2.49	0.54
4:B:113:ASP:O	4:B:114:ALA:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:138:GLU:OE1	3:A:139:THR:HG22	2.08	0.53
3:A:440:PHE:HE2	3:A:489:SER:OG	1.91	0.53
4:B:368:LEU:O	4:B:372:VAL:HG23	2.09	0.53
1:T:715:DA:H2''	1:T:716:DA:C8	2.43	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
3:A:439:THR:HG1	3:A:441:TYR:HE1	1.55	0.53
4:B:332:GLN:HA	4:B:332:GLN:OE1	2.08	0.53
6:H:69:LEU:HD22	6:H:82:LEU:HD11	1.90	0.53
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:225:PRO:HA	3:A:226:PRO:C	2.33	0.53
3:A:513:SER:OG	3:A:514:GLU:N	2.42	0.53
5:L:19:VAL:HG12	5:L:20:THR:N	2.24	0.53
6:H:198:TRP:CD1	6:H:199:PRO:HA	2.44	0.53
5:L:184:ASP:O	5:L:188:ARG:HD3	2.09	0.53
6:H:38:TRP:CZ3	6:H:97:CYS:HB3	2.44	0.53
1:T:722:DA:C4	1:T:723:DC:C5	2.97	0.53
3:A:450:THR:O	3:A:451:LYS:CG	2.57	0.53
3:A:523:GLU:HA	3:A:523:GLU:OE2	2.08	0.53
4:B:75:VAL:HG11	4:B:77:PHE:CE2	2.44	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:262:GLY:O	4:B:263:LYS:C	2.52	0.53
4:B:79:GLU:O	4:B:83:ARG:HG2	2.10	0.52
4:B:144:TYR:N	4:B:144:TYR:CD2	2.76	0.52
5:L:46:LEU:HD23	5:L:55:HIS:ND1	2.23	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:97:PRO:HD3	4:B:181:TYR:CD1	2.44	0.52
4:B:389:PHE:HB3	4:B:391:LEU:HD23	1.91	0.52
5:L:4:MET:HE2	5:L:90:GLN:HB2	1.92	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
3:A:493:VAL:C	3:A:494:ASN:HD22	2.17	0.52
5:L:3:GLN:O	5:L:26:SER:HB2	2.10	0.52
5:L:137:ASN:HB3	5:L:138:ASN:HD22	1.75	0.52
3:A:439:THR:HG21	4:B:288:ALA:HA	1.91	0.52
3:A:69:THR:O	3:A:69:THR:HG22	2.10	0.52
3:A:96:HIS:ND1	3:A:97:PRO:CD	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:503:LEU:CD2	3:A:535:TRP:HB2	2.40	0.52
4:B:312:GLU:HB3	4:B:313:PRO:CD	2.36	0.52
3:A:486:LEU:CD2	3:A:495:ILE:HD11	2.39	0.52
5:L:159:VAL:HG22	5:L:179:LEU:HD12	1.91	0.52
6:H:50:LEU:O	6:H:51:ALA:HB2	2.09	0.52
6:H:73:LYS:HG3	6:H:73:LYS:O	2.08	0.52
3:A:106:VAL:CB	3:A:227:PHE:HE1	2.19	0.52
3:A:329:ILE:CG1	3:A:391:LEU:HD22	2.39	0.52
3:A:372:VAL:HG13	3:A:389:PHE:CE2	2.44	0.52
3:A:478:GLU:OE1	3:A:498:ASP:CG	2.53	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
5:L:167:ASP:OD2	5:L:167:ASP:C	2.53	0.52
4:B:10:VAL:HG13	4:B:87:PHE:CD1	2.45	0.51
4:B:195:ILE:CG2	4:B:196:GLY:N	2.72	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: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
4:B:160:PHE:CD2	4:B:164:MET:HB2	2.45	0.51
3:A:27:THR:C	3:A:29:GLU:N	2.66	0.51
3:A:253:THR:O	3:A:254:VAL:C	2.53	0.51
4:B:113:ASP:C	4:B:115:TYR:N	2.66	0.51
4:B:306:ASN:O	4:B:309:ILE:HG12	2.11	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
2:P:817:MRG:H2'	2:P:818:DC:O5'	2.08	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:807:DC:C4	2:P:808:DC:N4	2.79	0.51
3:A:27:THR:CG2	3:A:30:LYS:HD2	2.41	0.51
3:A:306:ASN:O	3:A:307:ARG:C	2.54	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
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
4:B:166:LYS:O	4:B:167:ILE:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:816:DG:C2'	2:P:817:MRG:O5'	2.59	0.50
3:A:223:LYS:C	3:A:225:PRO:HD2	2.36	0.50
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
4:B:414:TRP:CD1	4:B:414:TRP:C	2.89	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
6:H:129:PRO:HB3	6:H:155:TYR:HB3	1.94	0.50
1:T:706:DA:C6	1:T:707:DG:C6	2.99	0.50
3:A:303:LEU:HD11	3:A:307:ARG:HD2	1.92	0.50
4:B:223:LYS:NZ	6:H:55:TRP:CH2	2.79	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
6:H:40:ARG:HB2	6:H:50:LEU:CD1	2.42	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:484:LEU:C	3:A:486:LEU:N	2.70	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
6:H:102:ILE:HG12	6:H:108:SER:HB2	1.93	0.50
3:A:61:PHE:N	3:A:61:PHE:CD2	2.78	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:405:TYR:CD1	3:A:406:TRP:N	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
6:H:65:LEU:O	6:H:66:LYS:C	2.54	0.50
1:T:709:DC:H2''	1:T:710:DG:C5'	2.42	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:325:LEU:HD12	4:B:343:GLN:HG2	1.92	0.50
3:A:143:ARG:HG3	3:A:143:ARG:NH1	2.19	0.49
4:B:309:ILE:N	4:B:309:ILE:HD13	2.27	0.49
6:H:2:ILE:HG12	6:H:26:GLY:HA3	1.93	0.49
1:T:709:DC:H2''	1:T:710:DG:H5'	1.94	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
2:P:817:MRG:H2'	2:P:818:DC:C6	2.47	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
3:A:60:VAL:O	3:A:60:VAL:HG13	2.12	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
4:B:325:LEU:HD22	4:B:385:LYS:HG2	1.93	0.49
5:L:90:GLN:CD	5:L:90:GLN:C	2.80	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:HD2	3:A:353:LYS:O	2.12	0.49
3:A:403:THR:HG23	3:A:404:GLU:N	2.26	0.49
4:B:244:ILE:HD13	4:B:244:ILE:N	2.03	0.49
1:T:713:DC:C2'	1:T:714:DG:O5'	2.61	0.49
4:B:46:LYS:CD	4:B:116:PHE:HB3	2.42	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
5:L:121:SER:O	5:L:122:SER:C	2.55	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:407:GLN:HG3	4:B:393:ILE:HA	1.94	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:344:GLU:HA	4:B:344:GLU:OE2	2.13	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
3:A:532:TYR:C	3:A:533:LEU:HD12	2.37	0.49
5:L:117:ILE:CD1	5:L:194:CYS:HB2	2.42	0.49
3:A:221:HIS:N	3:A:221:HIS:CD2	2.80	0.49
3:A:329:ILE:HG12	3:A:391:LEU:CD2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:260:LEU:HD11	4:B:264:LEU:HD11	1.95	0.49
1:T:713:DC:H2''	1:T:714:DG:C5'	2.43	0.48
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
3:A:184:MET:HE2	3:A:184:MET:HB2	1.73	0.48
4:B:85:GLN:C	4:B:87:PHE:N	2.66	0.48
4:B:286:THR:OG1	4:B:286:THR:O	2.30	0.48
4:B:401:TRP:O	4:B:402:TRP:C	2.53	0.48
5:L:186:TYR:C	5:L:188:ARG:H	2.21	0.48
6:H:69:LEU:HD21	6:H:84:MET:HE2	1.94	0.48
3:A:365:VAL:O	3:A:366:LYS:C	2.56	0.48
4:B:87:PHE:HD2	4:B:88:TRP:HB3	1.77	0.48
4:B:154:LYS:N	4:B:184:MET:HE3	2.28	0.48
5:L:146:VAL:HA	5:L:195:GLU:O	2.12	0.48
6:H:162:VAL:HA	6:H:206:ASN:O	2.13	0.48
2:P:820:DC:C2'	2:P:821:DC:O5'	2.61	0.48
3:A:501:TYR:HD1	3:A:501:TYR:O	1.95	0.48
4:B:282:LEU:N	4:B:282:LEU:HD23	2.27	0.48
4:B:403:THR:O	4:B:406:TRP:N	2.40	0.48
1:T:705:DT:H2''	1:T:706:DA:O5'	2.14	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
4:B:47:ILE:HD12	4:B:47:ILE:HA	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
6:H:69:LEU:CD2	6:H:84:MET:HE2	2.43	0.48
3:A:342:TYR:HD2	3:A:344:GLU:O	1.96	0.48
3:A:438:GLU:CD	3:A:463:ARG:HH21	2.22	0.48
4:B:363:ASN:HD22	4:B:363:ASN:C	2.21	0.48
4:B:403:THR:O	4:B:404:GLU:C	2.56	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
6:H:34:ILE:H	6:H:34:ILE:CD1	2.25	0.48
3:A:253:THR:HA	3:A:292:VAL:HA	1.96	0.48
3:A:367:GLN:O	3:A:368:LEU:C	2.55	0.48
4:B:24:TRP:O	4:B:25:PRO:C	2.56	0.48
4:B:125:ARG:HD3	4:B:147:ASN:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:131:THR:CG2	4:B:132:ILE:N	2.76	0.48
4:B:148:VAL:O	4:B:149:LEU:C	2.56	0.48
3:A:143:ARG:HH11	3:A:143:ARG:CG	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:207:GLN:O	4:B:208:HIS:C	2.57	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:183:TYR:CE2	3:A:230:MET:HE1	2.48	0.47
3:A:331:LYS:HD3	3:A:332:GLN:H	1.79	0.47
4:B:96:HIS:HE1	4:B:380:ILE:O	1.96	0.47
4:B:193:LEU:N	4:B:193:LEU:HD23	2.28	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
3:A:484:LEU:O	3:A:485:ALA:C	2.57	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
3:A:188:TYR:CD1	3:A:188:TYR:C	2.91	0.47
3:A:260:LEU:O	3:A:261:VAL:C	2.57	0.47
4:B:156:SER:O	4:B:158:ALA:N	2.48	0.47
4:B:210:LEU:C	4:B:212:TRP:N	2.72	0.47
4:B:306:ASN:CA	4:B:309:ILE:HG12	2.43	0.47
5:L:35:TRP:CE3	5:L:88:CYS:HB3	2.50	0.47
5:L:105:GLU:OE2	5:L:173:TYR:OH	2.32	0.47
3:A:344:GLU:HB3	3:A:345:PRO:CD	2.43	0.47
3:A:511:ASP:OD2	3:A:511:ASP:O	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
1:T:715:DA:N3	1:T:716:DA:C5	2.82	0.47
3:A:115:TYR:C	3:A:117:SER:N	2.71	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
3:A:265:ASN:HA	3:A:268:SER:OG	2.14	0.47
3:A:439:THR:CG2	4:B:289:LEU:H	2.09	0.47
3:A:473:THR:CG2	3:A:474:ASN:N	2.77	0.47
4:B:244:ILE:HD11	4:B:271:TYR:CZ	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:332:GLN:NE2	4:B:426:TRP:O	2.48	0.47
5:L:170:ASP:C	5:L:170:ASP:OD1	2.57	0.47
6:H:32:SER:O	6:H:55:TRP:CE2	2.68	0.47
6:H:134:LEU:HB2	6:H:149:GLY:CA	2.45	0.47
6:H:155:TYR:N	6:H:155:TYR:CD2	2.83	0.47
3:A:87:PHE:N	3:A:87:PHE:CD2	2.83	0.47
3:A:442:VAL:HG12	3:A:481:ALA:HB1	1.95	0.47
4:B:57:ASN:ND2	4:B:58:THR:N	2.62	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:12:LEU:H	4:B:12:LEU:CD1	1.99	0.47
4:B:13:LYS:HE2	4:B:85:GLN:HB3	1.96	0.47
4:B:97:PRO:O	4:B:98:ALA:C	2.56	0.47
4:B:207:GLN:O	4:B:210:LEU:N	2.48	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:498:ASP:OD1	3:A:498:ASP:N	2.47	0.46
3:A:507:GLN:C	3:A:509:GLN:H	2.22	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:194:GLU:C	3:A:196:GLY:H	2.23	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
4:B:425:LEU:C	4:B:427:TYR:N	2.73	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:215:THR:C	3:A:217:PRO:HD3	2.39	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:90:VAL:HG12	4:B:140:PRO:HB3	1.97	0.46
3:A:222:GLN:O	3:A:223:LYS:C	2.58	0.46
3:A:260:LEU:HD23	3:A:279:LEU:HD12	1.96	0.46
4:B:229:TRP:HA	4:B:232:TYR:CZ	2.49	0.46
1:T:716:DA:H1'	1:T:717:DC:H5'	1.97	0.46
3:A:116:PHE:N	3:A:116:PHE:CD1	2.83	0.46
3:A:441:TYR:CD2	3:A:544:GLY:C	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:460:ASN:ND2	4:B:288:ALA:HB2	2.25	0.46
3:A:516:GLU:O	3:A:517:LEU:C	2.59	0.46
4:B:69:THR:HG22	4:B:69:THR:O	2.16	0.46
4:B:360:ALA:CB	4:B:367:GLN:HE21	2.29	0.46
5:L:150:ILE:HG22	5:L:192:TYR:CD2	2.50	0.46
3:A:222:GLN:C	3:A:223:LYS:HG3	2.40	0.46
4:B:200:THR:O	4:B:201:LYS:C	2.58	0.46
4:B:225:PRO:HB2	4:B:226:PRO:CD	2.35	0.46
5:L:63:SER:O	5:L:73:LEU:HD12	2.16	0.46
5:L:105:GLU:HB3	5:L:106:ILE:H	1.62	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
5:L:15:LEU:H	5:L:15:LEU:CD1	2.19	0.46
5:L:176:SER:HB2	6:H:176:PHE:CD1	2.51	0.46
6:H:152:VAL:HB	6:H:187:LEU:HD12	1.98	0.46
1:T:706:DA:C6	1:T:707:DG:O6	2.69	0.46
2:P:815:DG:C6	2:P:816:DG:C6	3.04	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
3:A:38:CYS:O	3:A:39:THR:C	2.59	0.46
3:A:368:LEU:O	3:A:369:THR:C	2.58	0.46
3:A:494:ASN:HB3	4:B:289:LEU:CD1	2.45	0.46
4:B:111:VAL:O	4:B:111:VAL:CG2	2.59	0.46
4:B:112:GLY:C	4:B:151:GLN:HE21	2.24	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
3:A:302:GLU:O	3:A:303:LEU:C	2.58	0.45
4:B:55:PRO:HG2	4:B:56:TYR:CE1	2.51	0.45
4:B:343:GLN:HG3	4:B:349:LEU:HD11	1.98	0.45
5:L:148:TRP:CE3	5:L:179:LEU:HD22	2.50	0.45
2:P:805:DG:C6	2:P:806:DT:C4	3.05	0.45
3:A:31:ILE:C	3:A:33:ALA:N	2.73	0.45
3:A:132:ILE:O	3:A:132:ILE:HG12	2.17	0.45
4:B:115:TYR:OH	4:B:157:PRO:HB3	2.16	0.45
4:B:156:SER:O	4:B:157:PRO:C	2.58	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:H2''	2:P:806:DT:OP2	2.17	0.45
3:A:85:GLN:C	3:A:154:LYS:HZ2	2.21	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
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
3:A:412:PRO:O	3:A:413:GLU:C	2.59	0.45
5:L:125:LEU:CD2	5:L:130:ALA:HB2	2.46	0.45
1:T:706:DA:H2'	1:T:707:DG:H8	1.78	0.45
3:A:23:GLN:HE22	3:A:60:VAL:H	1.64	0.45
4:B:28:GLU:O	4:B:29:GLU:C	2.59	0.45
4:B:252:TRP:HB2	4:B:257:ILE:HD11	1.99	0.45
3:A:194:GLU:C	3:A:196:GLY:N	2.75	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
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
4:B:423:VAL:O	4:B:424:LYS:C	2.59	0.45
5:L:77:ASN:HD22	5:L:77:ASN:H	1.64	0.45
6:H:164:TRP:CH2	6:H:205:CYS:HB2	2.51	0.45
3:A:41:MET:HE1	3:A:73:LYS:HE2	1.98	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:87:PHE:HD2	4:B:88:TRP:N	2.13	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
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:224:GLU:O	3:A:225:PRO:C	2.58	0.44
3:A:454:LYS:HB2	3:A:552:VAL:HG13	1.98	0.44
3:A:539:HIS:N	3:A:539:HIS:CD2	2.83	0.44
4:B:115:TYR:C	4:B:117:SER:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:163:THR:O	6:H:206:ASN:HB2	2.18	0.44
3:A:160:PHE:CZ	3:A:164:MET:HE2	2.51	0.44
3:A:327:ALA:HB3	3:A:389:PHE:CD1	2.53	0.44
3:A:369:THR:HG22	3:A:370:GLU:N	2.31	0.44
3:A:397:THR:CG2	3:A:424:LYS:HA	2.44	0.44
3:A:410:TRP:CD2	4:B:363:ASN:OD1	2.70	0.44
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
5:L:38:GLN:HE22	6:H:41:GLN:CD	2.23	0.44
5:L:66:GLY:HA3	5:L:71:TYR:CG	2.51	0.44
6:H:89:THR:HA	6:H:121:VAL:HB	1.99	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:172:THR:C	5:L:173:TYR:CD1	2.96	0.44
6:H:210:PRO:O	6:H:211:ALA:C	2.60	0.44
3:A:457:TYR:C	3:A:457:TYR:CD2	2.96	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
6:H:129:PRO:HB2	6:H:152:VAL:HG12	1.98	0.44
3:A:94:ILE:HG13	3:A:95:PRO:O	2.17	0.44
3:A:116:PHE:N	3:A:116:PHE:HD1	2.15	0.44
3:A:257:ILE:HG21	3:A:283:LEU:CD2	2.42	0.44
3:A:310:LEU:HD23	3:A:310:LEU:C	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
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:N	5:L:77:ASN:ND2	2.66	0.44
6:H:125:LYS:O	6:H:126:THR:C	2.61	0.44
4:B:58:THR:CG2	4:B:59:PRO:CD	2.95	0.44
4:B:357:MET:HE3	4:B:370:GLU:OE1	2.18	0.44
4:B:369:THR:HG22	4:B:398:TRP:HZ3	1.80	0.44
5:L:189:HIS:O	5:L:211:ARG:NE	2.50	0.44
1:T:714:DG:OP1	3:A:285:GLY:N	2.42	0.44
2:P:812:DT:C5	2:P:813:DT:H73	2.53	0.44
3:A:222:GLN:C	3:A:224:GLU:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:373:GLN:HE22	4:B:397:THR:HG23	1.81	0.44
4:B:314:VAL:CG1	4:B:315:HIS:H	2.29	0.44
4:B:330:GLN:HG2	4:B:338:THR:OG1	2.17	0.44
2:P:814:DC:H2''	2:P:815:DG:C8	2.53	0.44
3:A:195:ILE:HG22	3:A:195:ILE:O	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:442:VAL:HG22	3:A:495:ILE:HG22	1.99	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
4:B:103:LYS:HD3	4:B:192:ASP:OD1	2.18	0.44
4:B:295:LEU:HD23	4:B:299:ALA:CB	2.47	0.44
5:L:144:ILE:HG13	5:L:198:HIS:ND1	2.32	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:156:SER:C	4:B:158:ALA:N	2.73	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
4:B:418:ASN:C	4:B:418:ASN:HD22	2.26	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:NE2	3:A:500:GLN:N	2.53	0.43
6:H:53:ILE:HD13	6:H:73:LYS:HB3	2.00	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:49:LYS:HB2	3:A:49:LYS:HZ2	1.81	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
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: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:31:ILE:C	3:A:33:ALA:H	2.25	0.43
3:A:180:ILE:HG23	3:A:189:VAL:HG22	2.00	0.43
3:A:398:TRP:O	3:A:401:TRP:N	2.52	0.43
4:B:357:MET:HG3	4:B:370:GLU:OE1	2.18	0.43
2:P:819:DG:H2''	2:P:820:DC:C5'	2.47	0.43
3:A:401:TRP:CZ2	3:A:405:TYR:CD2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:457:TYR:HA	3:A:548:VAL:HG11	1.99	0.43
4:B:2:ILE:HG23	4:B:3:SER:H	1.84	0.43
4:B:154:LYS:HA	4:B:184:MET:HE3	2.01	0.43
4:B:202:ILE:C	4:B:204:GLU:N	2.77	0.43
4:B:221:HIS:HB3	4:B:229:TRP:CE2	2.53	0.43
1:T:709:DC:H2''	1:T:710:DG:O5'	2.18	0.43
3:A:137:ASN:OD1	3:A:137:ASN:O	2.36	0.43
5:L:82:ASP:O	5:L:84:ALA:N	2.52	0.43
3:A:303:LEU:HD12	3:A:307:ARG:HG3	2.01	0.43
3:A:484:LEU:C	3:A:486:LEU:H	2.27	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
5:L:21:ILE:O	5:L:72:SER:HA	2.18	0.43
5:L:34:ASN:HB2	5:L:89:GLN:HE21	1.80	0.43
6:H:84:MET:HG2	6:H:87:VAL:HG12	2.00	0.43
1:T:705:DT:H2''	1:T:706:DA:H8	1.84	0.43
2:P:808:DC:H2''	2:P:809:DC:O5'	2.19	0.43
3:A:532:TYR:C	3:A:532:TYR:CD2	2.97	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
4:B:333:GLY:O	4:B:334:GLN:C	2.61	0.43
5:L:83:ILE:HG23	5:L:105:GLU:O	2.18	0.43
4:B:144:TYR:N	4:B:144:TYR:HD2	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
1:T:715:DA:H2''	1:T:716:DA:OP2	2.19	0.42
3:A:140:PRO:C	3:A:141:GLY:O	2.62	0.42
3:A:379:SER:C	3:A:381:VAL:N	2.76	0.42
3:A:498:ASP:CB	3:A:538:ALA:HB2	2.49	0.42
3:A:500:GLN:H	3:A:500:GLN:CD	2.24	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
6:H:99:GLN:OE1	6:H:99:GLN:O	2.37	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
5:L:60:SER:C	5:L:62:PHE:N	2.76	0.42
5:L:150:ILE:O	5:L:151:ASP:C	2.63	0.42
5:L:195:GLU:HG3	5:L:206:VAL:CG2	2.41	0.42
6:H:55:TRP:CE3	6:H:55:TRP:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:156:PHE:HA	6:H:157:PRO:HA	1.74	0.42
3:A:367:GLN:HA	3:A:370:GLU:CG	2.50	0.42
4:B:37:ILE:HG13	4:B:37:ILE:O	2.19	0.42
4:B:47:ILE:HG23	4:B:144:TYR:CD1	2.53	0.42
4:B:260:LEU:O	4:B:260:LEU:CD1	2.67	0.42
3:A:3:SER:HB3	3:A:5:ILE:CG1	2.48	0.42
3:A:103:LYS:O	3:A:104:LYS:C	2.61	0.42
3:A:241:VAL:HG13	3:A:241:VAL:O	2.19	0.42
3:A:400:THR:C	3:A:403:THR:HG22	2.44	0.42
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
2:P:815:DG:C6	2:P:816:DG:O6	2.72	0.42
3:A:46:LYS:HD3	3:A:46:LYS:N	2.34	0.42
3:A:543:GLY:C	3:A:545:ASN:N	2.78	0.42
4:B:8:VAL:HA	4:B:9:PRO:HD3	1.78	0.42
4:B:306:ASN:C	4:B:309:ILE:HG12	2.45	0.42
6:H:9:PRO:O	6:H:11:ILE:N	2.46	0.42
6:H:84:MET:HB2	6:H:84:MET:HE3	1.60	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
2:P:816:DG:H2''	2:P:817:MRG:O5'	2.20	0.42
3:A:18:GLY:H	3:A:56:TYR:HE2	1.66	0.42
3:A:168:LEU:O	3:A:169:GLU:C	2.61	0.42
3:A:221:HIS:CD2	3:A:221:HIS:H	2.38	0.42
3:A:410:TRP:HB3	4:B:365:VAL:HG23	2.00	0.42
4:B:124:PHE:O	4:B:124:PHE:CD1	2.72	0.42
5:L:105:GLU:C	5:L:106:ILE:HG13	2.44	0.42
6:H:145:MET:SD	6:H:194:PRO:HG3	2.60	0.42
3:A:27:THR:C	3:A:29:GLU:H	2.27	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:N	3:A:494:ASN:HD22	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
4:B:336:GLN:C	4:B:337:TRP:CD1	2.98	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:444:GLY:HA2	3:A:552:VAL:HG11	2.02	0.42
3:A:494:ASN:HB3	4:B:289:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:517:LEU:O	3:A:521:ILE:HG13	2.20	0.42
4:B:75:VAL:CG1	4:B:77:PHE:CE2	3.03	0.42
4:B:228:LEU:C	4:B:230:MET:N	2.76	0.42
4:B:266:TRP:CE3	4:B:423:VAL:HG23	2.55	0.42
5:L:58:VAL:HA	5:L:59:PRO:HD3	1.92	0.42
5:L:142:LYS:H	5:L:142:LYS:HG2	1.45	0.42
6:H:102:ILE:HG12	6:H:108:SER:CB	2.49	0.42
1:T:718:DA:C2	2:P:811:DG:C2	3.08	0.42
3:A:63:ILE:HG13	3:A:64:LYS:N	2.34	0.42
3:A:235:HIS:HB2	3:A:238:LYS:O	2.19	0.42
3:A:262:GLY:O	3:A:263:LYS:C	2.63	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
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
5:L:105:GLU:O	5:L:106:ILE:HG13	2.20	0.42
6:H:61:TYR:OH	6:H:71:VAL:N	2.53	0.42
6:H:155:TYR:CE1	6:H:160:VAL:HG13	2.55	0.42
3:A:334:GLN:HG2	3:A:512:LYS:NZ	2.35	0.41
4:B:87:PHE:CE2	4:B:155:GLY:HA2	2.53	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
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
5:L:115:VAL:HG12	5:L:116:SER:N	2.34	0.41
3:A:41:MET:HE1	3:A:73:LYS:HD3	2.02	0.41
3:A:363:ASN:O	3:A:367:GLN:HG3	2.20	0.41
3:A:420:PRO:CA	3:A:421:PRO:C	2.91	0.41
3:A:439:THR:HG21	4:B:289:LEU:HG	2.02	0.41
4:B:36:GLU:C	4:B:38:CYS:N	2.77	0.41
4:B:271:TYR:CD2	4:B:271:TYR:N	2.88	0.41
4:B:325:LEU:HB3	4:B:387:PRO:HA	2.02	0.41
4:B:360:ALA:HB1	4:B:367:GLN:HG2	2.02	0.41
5:L:34:ASN:HD22	5:L:89:GLN:HE22	1.66	0.41
6:H:10:GLY:HA2	6:H:118:SER:O	2.20	0.41
3:A:242:GLN:HA	3:A:243:PRO:HD2	1.78	0.41
3:A:254:VAL:O	3:A:255:ASN:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:56:ASP:O	6:H:57:ASP:HB2	2.21	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
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:281:LYS:O	3:A:282:LEU:C	2.61	0.41
3:A:516:GLU:HA	3:A:519:ASN:HB2	2.03	0.41
4:B:283:LEU:HA	4:B:287:LYS:HE2	2.03	0.41
5:L:170:ASP:O	5:L:171:SER:C	2.64	0.41
6:H:19:ARG:HH11	6:H:83:ASN:HD21	1.68	0.41
6:H:24:PHE:CE1	6:H:78:ASN:HB3	2.56	0.41
6:H:34:ILE:HD12	6:H:34:ILE:N	2.32	0.41
3:A:105:SER:HB2	3:A:198:HIS:ND1	2.35	0.41
3:A:229:TRP:CE2	3:A:230:MET:HG2	2.56	0.41
3:A:276:VAL:O	3:A:276:VAL:HG12	2.20	0.41
4:B:106:VAL:HA	4:B:189:VAL:O	2.21	0.41
4:B:208:HIS:C	4:B:208:HIS:CD2	2.96	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
5:L:27:GLN:O	5:L:29:ILE:HG23	2.21	0.41
5:L:77:ASN:H	5:L:77:ASN:ND2	2.18	0.41
6:H:24:PHE:CD1	6:H:78:ASN:HB3	2.55	0.41
3:A:3:SER:HA	3:A:4:PRO:HD3	1.70	0.41
3:A:201:LYS:O	3:A:202:ILE:C	2.64	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:332:GLN:HB2	3:A:336:GLN:C	2.45	0.41
3:A:442:VAL:CG2	3:A:495:ILE:CG2	2.98	0.41
4:B:304:ALA:C	4:B:307:ARG:HG2	2.46	0.41
6:H:54:TRP:HB3	6:H:55:TRP:CZ3	2.56	0.41
6:H:134:LEU:HB2	6:H:149:GLY:C	2.46	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:410:TRP:CE2	4:B:363:ASN:OD1	2.73	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
5:L:120:PRO:HG2	5:L:130:ALA:HB1	2.03	0.41
5:L:147:LYS:HZ1	5:L:149:LYS:HZ2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:37:THR:OG1	6:H:100:SER:HB2	2.19	0.41
6:H:220:ILE:HD12	6:H:220:ILE:HG23	1.89	0.41
1:T:707:DG:C2'	1:T:708:DG:C5'	2.99	0.41
2:P:817:MRG:S24	3:A:283:LEU:HD13	2.60	0.41
3:A:317:VAL:CG1	3:A:349:LEU:HD23	2.51	0.41
3:A:472:THR:CG2	3:A:477:THR:HG22	2.51	0.41
3:A:500:GLN:O	3:A:501:TYR:C	2.64	0.41
4:B:54:ASN:ND2	4:B:126:LYS:HB2	2.36	0.41
4:B:142:ILE:HG22	4:B:144:TYR:CE2	2.55	0.41
4:B:183:TYR:CD2	4:B:380:ILE:HD13	2.55	0.41
4:B:330:GLN:NE2	4:B:340:GLN:NE2	2.59	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
3:A:171:PHE:CZ	3:A:205:LEU:HD12	2.55	0.41
3:A:220:LYS:HB2	3:A:220:LYS:HE3	1.76	0.41
4:B:91:GLN:HG3	4:B:92:LEU:HG	2.03	0.41
4:B:166:LYS:C	4:B:168:LEU:N	2.78	0.41
4:B:265:ASN:O	4:B:268:SER:OG	2.31	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
6:H:39:ILE:CG2	6:H:40:ARG:N	2.84	0.41
3:A:86:ASP:HA	3:A:154:LYS:HZ2	1.86	0.40
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
4:B:159:ILE:C	4:B:161:GLN:H	2.29	0.40
4:B:228:LEU:C	4:B:230:MET:H	2.28	0.40
6:H:155:TYR:HD2	6:H:155:TYR:H	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:503:LEU:HD12	3:A:503:LEU:O	2.21	0.40
3:A:541:GLY:O	3:A:542:ILE:C	2.64	0.40
4:B:301:LEU:O	4:B:305:GLU:HB2	2.21	0.40
4:B:406:TRP:C	4:B:407:GLN:HE21	2.29	0.40
3:A:454:LYS:C	3:A:552:VAL:CG1	2.95	0.40
3:A:543:GLY:O	3:A:544:GLY:C	2.65	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
5:L:140:TYR:CE2	5:L:141:PRO:HG3	2.56	0.40
5:L:198:HIS:C	5:L:200:THR:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:B:225:PRO:HG2	5:L:92:SER:CA	2.48	0.40
4:B:258:GLN:O	4:B:259:LYS:C	2.65	0.40
4:B:266:TRP:CE3	4:B:423:VAL:CG2	3.04	0.40
5:L:81:GLU:O	5:L:82:ASP:C	2.64	0.40
5:L:83:ILE:HG21	5:L:106:ILE:CD1	2.51	0.40
6:H:187:LEU:C	6:H:187:LEU:CD1	2.95	0.40
3:A:278:GLN:H	3:A:278:GLN:HG2	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%)	1	9
4	B	427/430 (99%)	317 (74%)	77 (18%)	33 (8%)	1	4
5	L	209/211 (99%)	165 (79%)	32 (15%)	12 (6%)	1	8
6	H	223/225 (99%)	191 (86%)	21 (9%)	11 (5%)	1	11
All	All	1415/1424 (99%)	1097 (78%)	232 (16%)	86 (6%)	1	7

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	401 (83%)	84 (17%)	2	9
4	B	388/392 (99%)	322 (83%)	66 (17%)	2	10
5	L	190/190 (100%)	168 (88%)	22 (12%)	5	22
6	H	196/196 (100%)	166 (85%)	30 (15%)	3	12
All	All	1259/1276 (99%)	1057 (84%)	202 (16%)	2	12

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	VAL
3	A	22	LYS
3	A	24	TRP
3	A	49	LYS
3	A	55	PRO
3	A	58	THR
3	A	60	VAL
3	A	61	PHE
3	A	67	ASP
3	A	74	LEU
3	A	80	LEU
3	A	85	GLN
3	A	86	ASP
3	A	94	ILE
3	A	105	SER
3	A	108	VAL
3	A	109	LEU
3	A	122	GLU
3	A	132	ILE
3	A	145	GLN

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Mol	Chain	Res	Type
3	A	162	SER
3	A	175	ASN
3	A	180	ILE
3	A	186	ASP
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	244	ILE
3	A	245	VAL
3	A	246	LEU
3	A	261	VAL
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	322	SER
3	A	325	LEU
3	A	331	LYS
3	A	334	GLN
3	A	344	GLU
3	A	365	VAL
3	A	369	THR
3	A	373	GLN
3	A	374	LYS
3	A	377	THR
3	A	385	LYS
3	A	393	ILE
3	A	397	THR
3	A	407	GLN
3	A	409	THR
3	A	415	GLU
3	A	416	PHE
3	A	419	THR
3	A	425	LEU

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Mol	Chain	Res	Type
3	A	442	VAL
3	A	451	LYS
3	A	452	LEU
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	491	LEU
3	A	497	THR
3	A	500	GLN
3	A	501	TYR
3	A	505	ILE
3	A	511	ASP
3	A	517	LEU
3	A	519	ASN
3	A	525	LEU
3	A	545	ASN
3	A	547	GLN
3	A	548	VAL
3	A	552	VAL
4	B	5	ILE
4	B	7	THR
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	95	PRO
4	B	105	SER
4	B	108	VAL
4	B	109	LEU
4	B	111	VAL
4	B	144	TYR
4	B	148	VAL
4	B	162	SER
4	B	163	SER

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Mol	Chain	Res	Type
4	B	178	ILE
4	B	179	VAL
4	B	189	VAL
4	B	191	SER
4	B	193	LEU
4	B	197	GLN
4	B	212	TRP
4	B	216	THR
4	B	218	ASP
4	B	225	PRO
4	B	233	GLU
4	B	241	VAL
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	286	THR
4	B	293	ILE
4	B	295	LEU
4	B	300	GLU
4	B	302	GLU
4	B	305	GLU
4	B	315	HIS
4	B	318	TYR
4	B	325	LEU
4	B	330	GLN
4	B	332	GLN
4	B	347	LYS
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
4	B	401	TRP
4	B	403	THR

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Mol	Chain	Res	Type
4	B	407	GLN
4	B	409	THR
4	B	419	THR
4	B	424	LYS
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	83	ILE
5	L	89	GLN
5	L	97	THR
5	L	117	ILE
5	L	126	THR
5	L	142	LYS
5	L	143	ASP
5	L	144	ILE
5	L	171	SER
5	L	173	TYR
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	11	ILE
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	117	THR
6	H	120	THR
6	H	129	PRO
6	H	152	VAL

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Mol	Chain	Res	Type
6	H	155	TYR
6	H	157	PRO
6	H	160	VAL
6	H	169	LEU
6	H	171	SER
6	H	175	THR
6	H	186	THR
6	H	187	LEU
6	H	189	SER
6	H	192	THR
6	H	204	THR
6	H	210	PRO
6	H	215	LYS
6	H	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	GLN
3	A	85	GLN
3	A	145	GLN
3	A	161	GLN
3	A	221	HIS
3	A	235	HIS
3	A	265	ASN
3	A	269	GLN
3	A	306	ASN
3	A	315	HIS
3	A	447	ASN
3	A	464	GLN
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	235	HIS
4	B	242	GLN

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Mol	Chain	Res	Type
4	B	330	GLN
4	B	363	ASN
4	B	418	ASN
5	L	38	GLN
5	L	77	ASN
5	L	89	GLN
5	L	90	GLN
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	79	GLN
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	ATM	P	822	2,1	20,23,24	2.51	7 (35%)	26,32,35	2.91	12 (46%)
2	MRG	P	817	2,1,3	25,28,29	1.79	6 (24%)	32,39,42	2.01	9 (28%)

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	ATM	P	822	2,1	-	3/10/24/25	0/2/2/2
2	MRG	P	817	2,1,3	-	2/12/26/27	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	822	ATM	C6-C5	6.87	1.45	1.34
2	P	822	ATM	N4'-N3'	5.26	1.36	1.23
2	P	817	MRG	C2-N2	5.15	1.45	1.34
2	P	822	ATM	C1'-N1	-3.87	1.38	1.48
2	P	817	MRG	C21-N2	-3.07	1.39	1.46
2	P	822	ATM	O4-C4	2.84	1.29	1.23
2	P	817	MRG	C2-N1	2.67	1.40	1.36
2	P	817	MRG	C2-N3	-2.50	1.27	1.32
2	P	822	ATM	O2-C2	2.39	1.27	1.23
2	P	817	MRG	C8-N7	-2.37	1.25	1.32
2	P	822	ATM	C4-C5	-2.32	1.41	1.44
2	P	822	ATM	C5A-C5	2.25	1.56	1.50
2	P	817	MRG	C8-N9	-2.05	1.32	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	822	ATM	C5A-C5-C4	9.02	128.41	118.78
2	P	817	MRG	C22-C23-S24	7.50	136.04	113.10
2	P	822	ATM	C5A-C5-C6	-5.35	115.61	122.85
2	P	822	ATM	C5-C4-N3	4.96	119.64	115.32
2	P	822	ATM	C3'-C2'-C1'	4.68	108.22	103.21
2	P	822	ATM	O2-C2-N1	-3.39	118.39	122.80
2	P	822	ATM	O4'-C1'-N1	3.18	113.50	107.86
2	P	817	MRG	C5-C4-N3	3.10	133.32	128.39
2	P	817	MRG	O4'-C1'-N9	2.86	112.93	107.86
2	P	817	MRG	N9-C4-N3	-2.86	120.25	125.95
2	P	817	MRG	C2'-C3'-C4'	-2.57	97.58	102.80
2	P	817	MRG	C2'-C1'-N9	2.56	120.22	113.81
2	P	822	ATM	O4-C4-C5	-2.51	122.04	124.92
2	P	822	ATM	O4'-C4'-C5'	2.49	117.30	109.33
2	P	822	ATM	C6-C5-C4	-2.47	115.98	118.02
2	P	822	ATM	C5-C6-N1	-2.47	120.64	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	822	ATM	N3-C2-N1	2.32	117.92	114.89
2	P	822	ATM	C4-N3-C2	-2.24	124.41	127.34
2	P	817	MRG	O4'-C4'-C3'	2.23	110.73	105.65
2	P	817	MRG	C3'-C2'-C1'	2.19	107.96	102.60
2	P	817	MRG	C22-C21-N2	-2.11	106.27	112.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	822	ATM	C4'-C3'-N3'-N4'
2	P	822	ATM	C3'-N3'-N4'-N5'
2	P	817	MRG	C21-C22-C23-S24
2	P	817	MRG	C3'-C4'-C5'-O5'
2	P	822	ATM	C2'-C3'-N3'-N4'

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 oligosaccharides 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

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	21/27 (77%)	0.58	1 (4%) 35 19	64, 84, 98, 107	0
2	P	18/21 (85%)	0.61	0 100 100	75, 83, 100, 103	0
3	A	556/558 (99%)	0.03	19 (3%) 48 28	44, 91, 110, 110	1 (0%)
4	B	428/430 (99%)	-0.02	11 (2%) 57 36	30, 79, 110, 110	2 (0%)
5	L	211/211 (100%)	0.02	1 (0%) 87 73	56, 88, 110, 110	0
6	H	225/225 (100%)	-0.14	4 (1%) 67 47	51, 78, 105, 110	0
All	All	1459/1472 (99%)	-0.00	36 (2%) 58 37	30, 84, 110, 110	3 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	556	ILE	5.2
3	A	354	TYR	4.5
4	B	315	HIS	4.1
6	H	140	ALA	4.0
4	B	428	GLN	3.9
3	A	258	CYS	3.6
4	B	3	SER	3.5
4	B	312	GLU	3.4
6	H	141	GLN	3.3
4	B	426	TRP	3.1
3	A	473	THR	3.1
3	A	434	ILE	3.1
6	H	138	SER	3.0
3	A	67	ASP	2.9
3	A	394	GLN	2.9
3	A	544	GLY	2.8
4	B	1	PRO	2.6
1	T	725	DG	2.6
3	A	286	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	404	GLU	2.6
4	B	191	SER	2.5
3	A	330	GLN	2.5
3	A	475	GLN	2.5
3	A	439	THR	2.4
3	A	456	GLY	2.4
3	A	63	ILE	2.3
3	A	324	ASP	2.3
4	B	280	SER	2.2
3	A	515	SER	2.2
4	B	427	TYR	2.1
4	B	88	TRP	2.1
5	L	131	SER	2.0
3	A	409	THR	2.0
6	H	139	ALA	2.0
3	A	222	GLN	2.0
4	B	154	LYS	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. 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
2	MRG	P	817	26/27	0.78	0.19	92,92,92,92	0
2	ATM	P	822	22/23	0.88	0.15	62,68,87,87	0

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($\text{\AA}^2$)	Q<0.9
7	MG	A	1001	1/1	0.81	0.36	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.