



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:50 PM UTC

PDB ID : 2AJQ / pdb_00002ajq
Title : Structure of replicative DNA polymerase provides insights into the mechanisms for processivity, frameshifting and editing
Authors : Briebe, L.; Ellenberger, T.
Deposited on : 2005-08-02
Resolution : 2.60 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

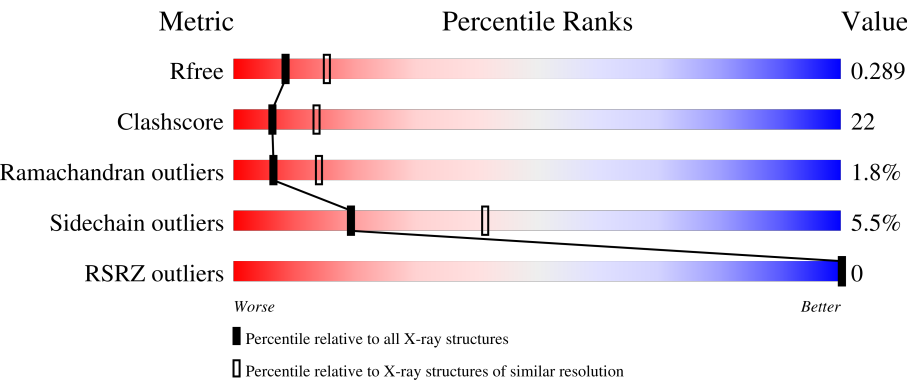
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	P	22	23%59%9%9%
1	X	22	32%55%9%5%
2	T	26	19%50%8%8%15%
2	Z	26	42%46%8%.
3	A	704	63%34%.

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Mol	Chain	Length	Quality of chain
3	F	704	
4	B	108	
4	I	108	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14791 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 DNA Primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	20	Total	C	N	O	P	0	0	1
			390	184	77	110	19			
1	X	21	Total	C	N	O	P	0	0	0
			432	204	87	120	21			

- Molecule 2 is a DNA chain called DNA Template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	22	Total	C	N	O	P	0	0	0
			453	215	79	137	22			
2	Z	25	Total	C	N	O	P	0	0	0
			514	244	89	156	25			

- Molecule 3 is a protein called T7 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	704	Total	C	N	O	S	0	0	0
			5541	3527	971	1019	24			
3	F	689	Total	C	N	O	S	0	0	0
			5459	3480	953	1003	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	ASP	engineered mutation	UNP P00581
A	7	ALA	GLU	engineered mutation	UNP P00581
F	5	ALA	ASP	engineered mutation	UNP P00581
F	7	ALA	GLU	engineered mutation	UNP P00581

- Molecule 4 is a protein called thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	105	Total 799	C 517	N 129	O 150	S 3	0	0	0
4	I	105	Total 789	C 512	N 126	O 148	S 3	0	0	0

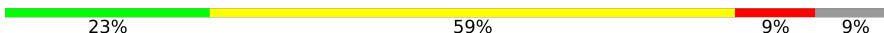
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	16	Total 16	O 16	0	0
5	T	21	Total 21	O 21	0	0
5	X	21	Total 21	O 21	0	0
5	Z	27	Total 27	O 27	0	0
5	A	158	Total 158	O 158	0	0
5	B	13	Total 13	O 13	0	0
5	F	142	Total 142	O 142	0	0
5	I	16	Total 16	O 16	0	0

3 Residue-property plots

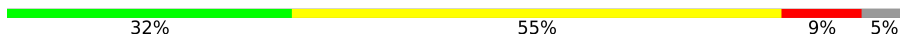
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

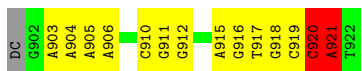
• Molecule 1: DNA Primer

Chain P: 

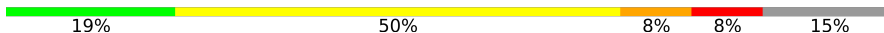


• Molecule 1: DNA Primer

Chain X: 



• Molecule 2: DNA Template

Chain T: 



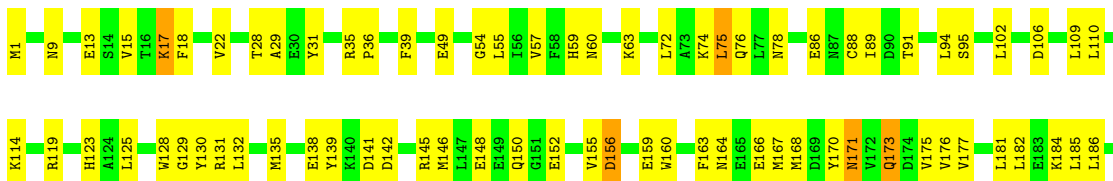
• Molecule 2: DNA Template

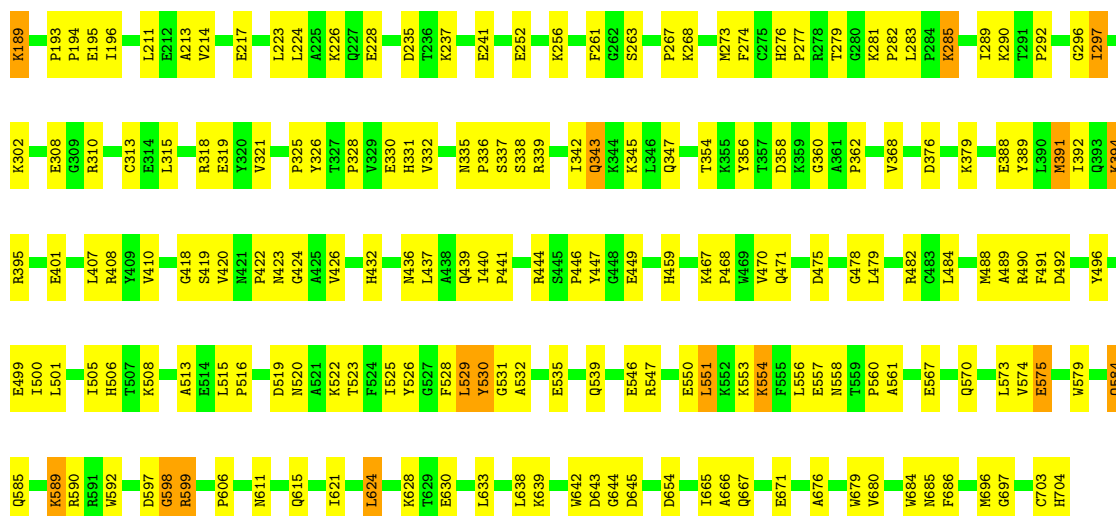
Chain Z: 



• Molecule 3: T7 DNA polymerase

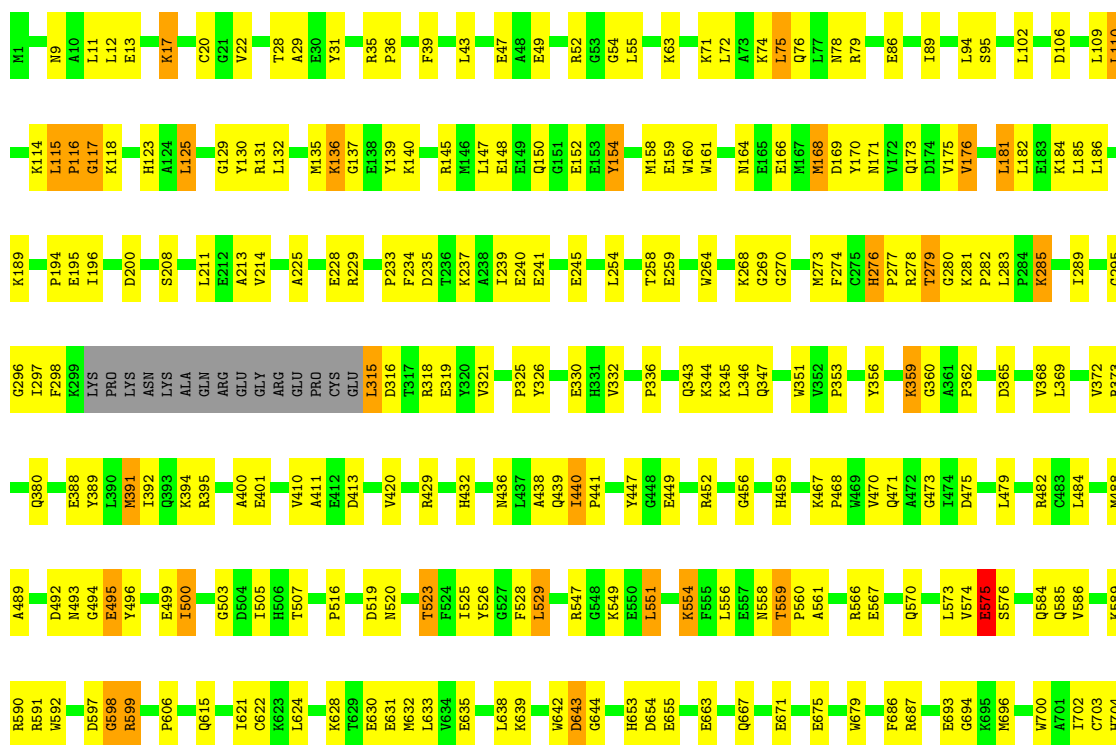
Chain A: 





• Molecule 3: T7 DNA polymerase

Chain F: 61% 32%



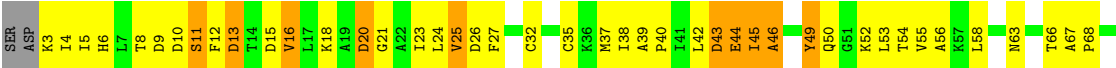
• Molecule 4: thioredoxin 1

Chain B: 50% 41% 6%





● Molecule 4: thioredoxin 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	168.31Å 169.24Å 179.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.97 – 2.60 45.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.97-2.60) 98.2 (45.97-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.284 0.245 , 0.289	Depositor DCC
R_{free} test set	4957 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	60.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.449 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14791	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: 2DT

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	P	0.46	1/417 (0.2%)	0.87	4/642 (0.6%)
1	X	0.32	0/465	0.74	2/715 (0.3%)
2	T	0.35	0/506	0.86	4/780 (0.5%)
2	Z	0.33	0/574	0.79	3/885 (0.3%)
3	A	0.47	0/5680	0.94	20/7693 (0.3%)
3	F	0.47	0/5594	0.96	29/7570 (0.4%)
4	B	0.36	0/814	0.88	2/1104 (0.2%)
4	I	0.39	0/803	0.87	1/1089 (0.1%)
All	All	0.45	1/14853 (0.0%)	0.92	65/20478 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	2
1	X	0	2
2	T	0	4
2	Z	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	803	DA	O3'-P	-5.70	1.52	1.61

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	503	GLY	N-CA-C	9.66	123.91	113.58
3	A	589	LYS	N-CA-C	-8.59	100.51	112.45
3	F	589	LYS	N-CA-C	-8.19	102.88	113.12
1	P	821	DA	N9-C1'-C2'	-7.62	102.08	113.50
3	F	573	LEU	N-CA-C	6.72	121.72	112.04
3	A	283	LEU	CA-C-N	6.71	126.50	119.05
3	A	283	LEU	C-N-CA	6.71	126.50	119.05
3	F	115	LEU	CA-C-N	6.57	128.06	119.84
3	F	115	LEU	C-N-CA	6.57	128.06	119.84
1	P	821	DA	C4'-C3'-O3'	6.40	119.60	110.00
3	A	574	VAL	N-CA-C	6.33	117.42	108.36
3	A	401	GLU	N-CA-C	6.33	121.19	112.90
3	F	574	VAL	N-CA-C	6.25	117.60	108.53
2	T	856	DT	C4'-C3'-O3'	6.23	119.34	110.00
3	A	598	GLY	N-CA-C	6.23	122.49	115.08
3	A	261	PHE	N-CA-C	-6.23	99.56	109.59
4	B	66	THR	N-CA-C	6.16	117.79	111.14
3	A	339	ARG	N-CA-C	-6.12	104.67	111.71
3	A	170	TYR	N-CA-C	-6.07	105.84	113.18
3	A	479	LEU	N-CA-C	5.98	117.80	111.28
3	F	586	VAL	N-CA-C	5.93	117.02	108.48
3	F	575	GLU	N-CA-C	-5.87	104.29	112.45
3	F	500	ILE	N-CA-C	-5.87	104.91	110.42
3	A	573	LEU	N-CA-C	5.86	120.45	113.12
3	F	225	ALA	N-CA-C	-5.86	104.80	111.07
3	F	283	LEU	CA-C-N	5.83	125.52	119.05
3	F	283	LEU	C-N-CA	5.83	125.52	119.05
3	A	424	GLY	N-CA-C	5.77	121.10	113.37
3	F	559	THR	CA-C-N	5.71	126.98	119.84
3	F	559	THR	C-N-CA	5.71	126.98	119.84
3	F	281	LYS	N-CA-C	5.66	117.02	109.83
4	I	66	THR	N-CA-C	5.62	117.20	111.14
1	P	820	DC	C4'-C3'-O3'	5.50	118.25	110.00
3	F	598	GLY	N-CA-C	5.46	122.31	115.21
3	F	507	THR	N-CA-C	-5.45	105.42	111.36
3	F	279	THR	N-CA-C	-5.44	101.27	109.60
3	F	401	GLU	N-CA-C	5.43	120.02	112.90
4	B	65	GLY	N-CA-C	5.39	119.67	112.77
3	F	479	LEU	N-CA-C	5.38	117.14	111.28
1	P	820	DC	C5'-C4'-C3'	-5.36	106.86	114.90
3	F	9	ASN	N-CA-C	5.33	119.40	113.01
3	F	208	SER	N-CA-C	5.32	116.76	111.07
3	F	171	ASN	N-CA-C	-5.31	105.57	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	955	DA	N9-C1'-C2'	-5.30	105.55	113.50
2	Z	957	DG	N9-C1'-C2'	-5.30	105.55	113.50
3	A	171	ASN	N-CA-C	-5.30	105.58	111.36
3	A	575	GLU	N-CA-C	-5.24	103.55	111.56
1	X	920	DC	N1-C1'-C2'	-5.24	105.65	113.50
3	A	530	TYR	N-CA-C	5.20	119.32	112.92
3	A	142	ASP	N-CA-C	-5.18	106.93	113.20
2	T	856	DT	C5'-C4'-C3'	-5.14	107.19	114.90
3	F	440	ILE	CB-CA-C	-5.11	106.19	110.94
3	F	136	LYS	N-CA-C	-5.09	107.45	113.97
3	A	263	SER	N-CA-C	-5.09	102.02	109.81
2	Z	955	DA	C4'-C3'-O3'	5.09	117.63	110.00
3	A	615	GLN	N-CA-C	-5.09	105.92	111.82
2	T	855	DA	C4'-C3'-O3'	5.05	117.58	110.00
2	T	863	DG	N9-C1'-C2'	5.04	121.06	113.50
3	F	643	ASP	N-CA-C	-5.04	107.15	113.15
3	A	531	GLY	N-CA-C	5.03	121.65	114.85
3	A	88	CYS	N-CA-C	5.02	117.68	109.59
3	F	276	HIS	CA-C-N	5.01	124.18	118.97
3	F	276	HIS	C-N-CA	5.01	124.18	118.97
1	X	921	DA	C5'-C4'-O4'	-5.00	101.89	109.40
3	F	400	ALA	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	820	DC	Sidechain
1	P	821	DA	Sidechain
2	T	854	DG	Sidechain
2	T	855	DA	Sidechain
2	T	856	DT	Sidechain
2	T	857	DG	Sidechain
1	X	920	DC	Sidechain
1	X	921	DA	Sidechain
2	Z	955	DA	Sidechain
2	Z	957	DG	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	P	390	0	212	36	0
1	X	432	0	234	29	0
2	T	453	0	250	22	0
2	Z	514	0	284	13	0
3	A	5541	0	5382	198	0
3	F	5459	0	5338	193	0
4	B	799	0	814	46	0
4	I	789	0	794	98	0
5	A	158	0	0	15	0
5	B	13	0	0	1	0
5	F	142	0	0	7	1
5	I	16	0	0	4	0
5	P	16	0	0	0	0
5	T	21	0	0	0	0
5	X	21	0	0	0	0
5	Z	27	0	0	0	0
All	All	14791	0	13308	608	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 22.

All (608) 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)
4:B:73:ARG:HH11	4:B:73:ARG:HB3	1.11	1.09
2:T:867:DG:H2''	2:T:868:DT:H5'	1.32	1.07
4:I:16:VAL:HA	4:I:23:ILE:HG21	1.36	1.04
1:P:807:DC:H2''	1:P:808:DG:H5'	1.38	1.03
4:B:73:ARG:HB3	4:B:73:ARG:NH1	1.79	0.96
4:I:80:LEU:H	4:I:89:THR:HG22	1.31	0.94
3:A:666:ALA:HB3	3:A:696:MET:HE2	1.48	0.94
1:X:917:DT:H2''	1:X:918:DG:H5'	1.50	0.93
1:P:817:DT:H2''	1:P:818:DG:H5'	1.51	0.92
4:I:25:VAL:HA	4:I:56:ALA:H	1.33	0.92
1:X:916:DG:H2''	1:X:917:DT:H5'	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:805:DA:H2''	1:P:806:DA:H5''	1.51	0.92
4:I:27:PHE:HE2	4:I:58:LEU:HD23	1.33	0.91
4:I:24:LEU:HD21	4:I:80:LEU:HD12	1.52	0.91
1:X:920:DC:H2''	1:X:921:DA:H5'	1.53	0.90
2:T:856:DT:H2''	2:T:857:DG:H5''	1.54	0.90
4:I:38:ILE:HD12	4:I:93:ALA:HA	1.54	0.89
4:B:27:PHE:HE2	4:B:58:LEU:HD23	1.37	0.89
3:F:321:VAL:HG21	4:I:94:LEU:HD21	1.55	0.89
4:B:38:ILE:HD12	4:B:93:ALA:HA	1.52	0.88
3:A:189:LYS:HG3	3:A:194:PRO:HG3	1.56	0.88
4:I:25:VAL:HG12	4:I:56:ALA:HB3	1.55	0.87
3:F:279:THR:HG22	3:F:280:GLY:H	1.37	0.86
4:I:24:LEU:HB2	4:I:55:VAL:HG22	1.57	0.85
1:X:920:DC:H2''	1:X:921:DA:C5'	2.07	0.85
4:I:24:LEU:HA	4:I:79:LEU:O	1.76	0.84
3:A:91:THR:HB	3:A:181:LEU:HD12	1.60	0.84
4:I:4:ILE:CG2	4:I:56:ALA:HA	2.08	0.83
3:F:164:ASN:OD1	3:F:166:GLU:HG2	1.78	0.83
3:F:315:LEU:HD23	3:F:316:ASP:H	1.44	0.83
3:A:321:VAL:HG21	4:B:94:LEU:HD21	1.61	0.83
4:I:23:ILE:O	4:I:80:LEU:HA	1.79	0.82
4:I:24:LEU:CB	4:I:55:VAL:HG22	2.09	0.82
1:X:921:DA:H5'	1:X:921:DA:H8	1.44	0.82
3:F:631:GLU:O	3:F:635:GLU:HG2	1.81	0.81
1:P:820:DC:H1'	5:A:5308:HOH:O	1.81	0.80
4:B:73:ARG:HH11	4:B:73:ARG:CB	1.93	0.80
4:B:27:PHE:HE1	4:B:79:LEU:HD22	1.47	0.79
2:T:856:DT:H2''	2:T:857:DG:C5'	2.12	0.79
4:I:12:PHE:HD1	4:I:13:ASP:H	1.30	0.79
3:A:276:HIS:HD2	3:A:279:THR:H	1.30	0.78
4:I:37:MET:O	4:I:40:PRO:HD2	1.81	0.78
2:Z:966:DC:H2''	2:Z:967:DG:C8	2.20	0.77
3:A:237:LYS:HA	3:A:237:LYS:HE2	1.67	0.77
3:A:22:VAL:HB	3:A:175:VAL:HG21	1.67	0.76
3:A:95:SER:OG	3:A:123:HIS:HD2	1.69	0.76
1:X:916:DG:H2''	1:X:917:DT:C5'	2.15	0.75
3:A:575:GLU:HG2	3:A:589:LYS:HG3	1.69	0.75
3:A:13:GLU:H	3:A:13:GLU:CD	1.96	0.74
4:B:27:PHE:CE2	4:B:58:LEU:HD23	2.22	0.74
3:F:343:GLN:HG3	3:F:362:PRO:HG2	1.70	0.74
3:A:189:LYS:CG	3:A:194:PRO:HG3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:436:ASN:HB3	3:A:439:GLN:HE21	1.53	0.74
3:F:55:LEU:HD13	3:F:89:ILE:HD11	1.70	0.74
3:A:570:GLN:HE22	3:A:606:PRO:HB3	1.52	0.73
3:F:13:GLU:H	3:F:13:GLU:CD	1.96	0.73
3:F:63:LYS:HE3	3:F:228:GLU:OE2	1.88	0.73
3:F:72:LEU:HA	3:F:75:LEU:CD2	2.18	0.73
3:F:49:GLU:OE2	3:F:54:GLY:HA3	1.88	0.73
1:X:910:DC:H2''	1:X:911:DG:H5''	1.71	0.73
3:F:516:PRO:HG2	3:F:520:ASN:HD22	1.53	0.73
3:A:376:ASP:HB3	3:A:379:LYS:HB2	1.69	0.73
4:I:44:GLU:HG3	4:I:45:ILE:H	1.53	0.73
4:B:53:LEU:HD21	4:B:103:LEU:HD13	1.70	0.72
1:P:805:DA:C2'	1:P:806:DA:H5''	2.19	0.72
1:X:919:DC:H1'	3:F:394:LYS:HE2	1.70	0.72
3:A:189:LYS:HD2	3:A:189:LYS:N	2.04	0.72
3:A:343:GLN:HG2	3:A:347:GLN:HE21	1.54	0.72
3:A:484:LEU:HD22	3:A:529:LEU:HD21	1.71	0.72
4:I:4:ILE:HG21	4:I:56:ALA:HA	1.71	0.72
1:X:910:DC:H2''	1:X:911:DG:C5'	2.20	0.71
4:I:52:LYS:HD2	4:I:107:LEU:HD13	1.72	0.71
3:A:72:LEU:HA	3:A:75:LEU:HD11	1.72	0.71
3:F:388:GLU:O	3:F:392:ILE:HG12	1.90	0.71
4:I:24:LEU:C	4:I:55:VAL:HA	2.16	0.71
3:A:318:ARG:HE	3:A:319:GLU:H	1.37	0.71
1:X:921:DA:H5'	1:X:921:DA:C8	2.25	0.71
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.71	0.71
3:F:95:SER:OG	3:F:123:HIS:HD2	1.73	0.70
3:A:585:GLN:HG2	5:A:5261:HOH:O	1.91	0.70
3:F:343:GLN:HG3	3:F:362:PRO:CG	2.21	0.70
1:P:807:DC:H2''	1:P:808:DG:C5'	2.20	0.70
2:T:858:DG:H2''	2:T:859:DC:H5'	1.73	0.70
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.20	0.70
4:B:37:MET:O	4:B:40:PRO:HD2	1.92	0.70
4:I:27:PHE:CE2	4:I:58:LEU:HD23	2.21	0.69
3:F:273:MET:HG2	3:F:282:PRO:HB3	1.73	0.69
3:A:129:GLY:HA3	3:A:135:MET:HG2	1.74	0.69
3:A:666:ALA:CB	3:A:696:MET:HE2	2.23	0.69
4:I:39:ALA:HB3	4:I:40:PRO:HD3	1.75	0.69
3:A:528:PHE:HZ	3:A:556:LEU:HD21	1.58	0.69
2:T:858:DG:H4'	3:A:432:HIS:O	1.92	0.68
3:A:436:ASN:HB3	3:A:439:GLN:NE2	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:575:GLU:HG3	3:F:576:SER:N	2.07	0.68
3:A:146:MET:HG2	3:A:150:GLN:HE21	1.57	0.68
3:F:359:LYS:N	3:F:359:LYS:HE2	2.09	0.68
3:A:128:TRP:CE3	3:A:131:ARG:HD2	2.28	0.68
3:A:488:MET:HE3	3:A:561:ALA:HB3	1.76	0.68
4:I:79:LEU:HA	4:I:89:THR:HB	1.75	0.67
3:F:279:THR:HG22	3:F:280:GLY:N	2.09	0.67
4:I:24:LEU:O	4:I:25:VAL:HG13	1.93	0.67
3:F:484:LEU:HD22	3:F:529:LEU:HD21	1.76	0.67
3:A:519:ASP:O	3:A:523:THR:HG22	1.95	0.67
3:A:579:TRP:CE2	3:A:584:GLN:HG3	2.29	0.67
3:A:228:GLU:CD	3:A:419:SER:HA	2.19	0.66
4:B:53:LEU:HD12	4:B:53:LEU:C	2.21	0.66
3:F:519:ASP:O	3:F:523:THR:HG22	1.96	0.66
3:F:145:ARG:HA	3:F:148:GLU:HG2	1.76	0.66
3:A:276:HIS:CD2	3:A:279:THR:H	2.13	0.65
3:F:189:LYS:NZ	3:F:194:PRO:HB3	2.12	0.65
4:I:23:ILE:C	4:I:24:LEU:HD12	2.20	0.65
3:A:516:PRO:HG2	3:A:520:ASN:HD22	1.61	0.65
1:P:808:DG:H1	2:T:869:DC:H42	1.44	0.65
3:F:488:MET:HE3	3:F:561:ALA:HB3	1.77	0.65
3:F:135:MET:HE2	3:F:135:MET:HA	1.79	0.65
3:F:43:LEU:O	3:F:47:GLU:HG3	1.96	0.65
4:I:80:LEU:HB3	4:I:88:ALA:O	1.97	0.65
3:F:22:VAL:HB	3:F:175:VAL:HG21	1.78	0.64
4:I:88:ALA:HB1	4:I:106:ASN:CB	2.28	0.64
4:B:8:THR:HG22	4:B:11:SER:OG	1.96	0.64
3:A:330:GLU:HG3	3:A:332:VAL:HG13	1.80	0.64
3:F:663:GLU:HB2	3:F:696:MET:SD	2.38	0.64
3:F:516:PRO:HG2	3:F:520:ASN:ND2	2.12	0.64
4:I:8:THR:HA	4:I:63:ASN:HD21	1.62	0.64
3:A:297:ILE:HD12	3:A:297:ILE:N	2.12	0.64
3:F:547:ARG:NH1	3:F:551:LEU:HD13	2.12	0.64
4:B:27:PHE:CE1	4:B:79:LEU:HD22	2.32	0.64
3:A:388:GLU:O	3:A:392:ILE:HG12	1.98	0.63
3:A:91:THR:HB	3:A:181:LEU:CD1	2.28	0.63
3:F:110:LEU:HD21	3:F:117:GLY:HA2	1.80	0.63
3:A:194:PRO:HD2	3:A:195:GLU:OE2	1.98	0.63
3:F:148:GLU:C	3:F:150:GLN:H	2.06	0.63
3:A:553:LYS:O	3:A:557:GLU:HG3	1.99	0.63
3:A:195:GLU:H	3:A:195:GLU:CD	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:285:LYS:NZ	3:F:285:LYS:HB3	2.14	0.63
4:B:79:LEU:HD23	4:B:81:PHE:HE1	1.64	0.63
4:I:58:LEU:HD11	4:I:63:ASN:ND2	2.14	0.63
2:T:856:DT:C2'	2:T:857:DG:H5''	2.28	0.62
3:F:633:LEU:HD22	3:F:638:LEU:HD12	1.80	0.62
3:F:336:PRO:HB2	3:F:389:TYR:CD1	2.33	0.62
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.81	0.62
3:A:135:MET:CE	3:A:173:GLN:HE22	2.12	0.62
3:A:489:ALA:HA	3:A:492:ASP:OD1	2.00	0.62
1:P:821:DA:H5'	1:P:821:DA:H8	1.63	0.62
3:A:516:PRO:HG2	3:A:520:ASN:ND2	2.15	0.62
1:P:820:DC:H2''	1:P:821:DA:OP2	1.99	0.62
3:A:345:LYS:HE2	3:A:345:LYS:HA	1.81	0.61
4:B:26:ASP:OD2	4:B:57:LYS:HD2	2.00	0.61
3:F:297:ILE:HD13	4:I:102:PHE:HA	1.82	0.61
4:I:24:LEU:HG	4:I:80:LEU:HB2	1.81	0.61
4:I:25:VAL:O	4:I:78:LEU:HA	2.01	0.61
3:F:189:LYS:HZ1	3:F:194:PRO:HB3	1.66	0.61
4:I:46:ALA:HA	5:I:5005:HOH:O	1.99	0.61
3:F:321:VAL:HG22	4:I:90:LYS:HE3	1.81	0.61
3:A:55:LEU:HD13	3:A:89:ILE:HD11	1.83	0.61
4:B:8:THR:HG23	4:B:11:SER:H	1.64	0.61
3:A:146:MET:HG2	3:A:150:GLN:NE2	2.16	0.61
4:I:53:LEU:O	4:I:53:LEU:HD23	1.99	0.61
4:I:5:ILE:HG22	4:I:6:HIS:N	2.16	0.60
3:A:547:ARG:NH1	3:A:551:LEU:HD13	2.17	0.60
3:A:667:GLN:HE21	3:A:671:GLU:HG3	1.66	0.60
3:A:22:VAL:HG23	3:A:171:ASN:OD1	2.01	0.60
3:F:79:ARG:HD3	5:F:5018:HOH:O	2.00	0.60
3:F:184:LYS:O	3:F:184:LYS:HD3	2.02	0.60
1:P:812:DG:H2''	1:P:813:DC:H5''	1.84	0.60
2:T:867:DG:H2''	2:T:868:DT:C5'	2.19	0.60
3:A:439:GLN:HB2	5:A:5308:HOH:O	2.01	0.60
2:T:868:DT:H1'	2:T:869:DC:H5''	1.84	0.60
3:A:391:MET:C	3:A:391:MET:HE2	2.27	0.60
1:X:916:DG:H1'	1:X:917:DT:H5''	1.84	0.59
1:P:812:DG:H2''	1:P:813:DC:C5'	2.32	0.59
1:P:806:DA:H1'	1:P:807:DC:OP1	2.02	0.59
4:I:4:ILE:HG23	4:I:56:ALA:HA	1.83	0.59
4:B:13:ASP:HA	4:B:17:LEU:HD12	1.84	0.59
4:I:24:LEU:O	4:I:55:VAL:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:26:ASP:N	4:I:56:ALA:O	2.33	0.59
3:A:285:LYS:NZ	3:A:285:LYS:HB3	2.18	0.59
3:F:496:TYR:O	3:F:500:ILE:HG12	2.03	0.59
3:A:315:LEU:HD23	3:A:315:LEU:H	1.67	0.59
3:A:703:CYS:O	3:A:704:HIS:HB2	2.01	0.59
3:F:28:THR:O	3:F:29:ALA:HB3	2.02	0.59
3:A:676:ALA:O	3:A:680:VAL:HG23	2.03	0.58
3:A:550:GLU:HG3	5:A:5421:HOH:O	2.03	0.58
3:F:289:ILE:HD12	3:F:325:PRO:HB2	1.84	0.58
1:P:807:DC:H5'	5:A:5117:HOH:O	2.04	0.58
3:F:484:LEU:O	3:F:488:MET:HG2	2.03	0.58
4:I:5:ILE:HG22	4:I:6:HIS:H	1.69	0.58
4:B:79:LEU:HD12	4:B:89:THR:HB	1.85	0.58
3:F:129:GLY:C	3:F:135:MET:HG2	2.27	0.58
3:F:136:LYS:HG3	3:F:173:GLN:HE21	1.69	0.58
3:A:106:ASP:CG	3:A:131:ARG:HH22	2.10	0.57
4:B:11:SER:O	4:B:15:ASP:HB2	2.03	0.57
1:P:817:DT:H2''	1:P:818:DG:C5'	2.31	0.57
3:A:132:LEU:HD21	3:A:184:LYS:HG3	1.86	0.57
1:P:812:DG:C2'	1:P:813:DC:H5''	2.35	0.57
1:X:910:DC:C2'	1:X:911:DG:H5''	2.33	0.57
2:Z:974:DT:H2''	2:Z:975:DC:C5	2.39	0.57
3:F:523:THR:HG21	5:F:5095:HOH:O	2.03	0.57
3:A:289:ILE:HD12	3:A:325:PRO:HB2	1.85	0.57
3:A:228:GLU:HG2	3:A:418:GLY:O	2.03	0.57
3:A:467:LYS:HE3	3:A:468:PRO:HD2	1.86	0.57
4:I:95:SER:OG	4:I:98:GLN:HG3	2.05	0.57
1:X:903:DA:H2''	1:X:904:DA:N7	2.19	0.56
3:F:268:LYS:HD2	3:F:330:GLU:CD	2.30	0.56
3:A:500:ILE:HD13	3:A:505:ILE:HD13	1.87	0.56
3:F:94:LEU:HD21	3:F:214:VAL:HG13	1.87	0.56
4:I:32:CYS:HB3	4:I:35:CYS:HB2	1.87	0.56
4:I:43:ASP:HB2	5:I:5012:HOH:O	2.05	0.56
3:F:13:GLU:CD	3:F:13:GLU:N	2.63	0.56
3:F:173:GLN:O	3:F:176:VAL:HG22	2.05	0.56
1:P:816:DG:H1'	1:P:817:DT:H5''	1.86	0.56
3:A:109:LEU:HD22	3:A:114:LYS:HD3	1.88	0.56
3:A:13:GLU:CD	3:A:13:GLU:N	2.64	0.56
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.05	0.56
4:B:79:LEU:HD23	4:B:81:PHE:CE1	2.41	0.56
3:F:547:ARG:HH12	3:F:551:LEU:HD13	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:130:TYR:CD1	3:A:135:MET:HG3	2.41	0.55
3:F:470:VAL:HG12	3:F:471:GLN:N	2.21	0.55
3:A:513:ALA:HB3	3:A:515:LEU:HD23	1.87	0.55
4:I:24:LEU:CA	4:I:79:LEU:O	2.51	0.55
2:T:869:DC:H2''	2:T:870:DG:C8	2.42	0.55
3:F:330:GLU:HG3	3:F:332:VAL:HG13	1.87	0.55
2:Z:961:DC:H2'	2:Z:962:DT:H71	1.89	0.55
3:A:74:LYS:O	3:A:78:ASN:HA	2.07	0.55
3:F:687:ARG:HH11	3:F:687:ARG:HB3	1.72	0.55
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.06	0.55
3:A:138:GLU:HB2	3:A:141:ASP:OD2	2.07	0.55
3:F:129:GLY:HA3	3:F:135:MET:HG2	1.89	0.55
3:F:74:LYS:O	3:F:78:ASN:HA	2.07	0.54
1:P:821:DA:H5'	1:P:821:DA:C8	2.41	0.54
2:T:864:DG:OP2	3:A:268:LYS:NZ	2.39	0.54
3:F:429:ARG:HD2	3:F:615:GLN:NE2	2.23	0.54
1:X:917:DT:C2'	1:X:918:DG:H5'	2.31	0.54
3:F:489:ALA:HA	3:F:492:ASP:OD1	2.07	0.54
3:F:639:LYS:NZ	3:F:643:ASP:OD1	2.40	0.54
1:X:917:DT:H2''	1:X:918:DG:C5'	2.30	0.54
4:B:3:LYS:HD3	4:B:50:GLN:NE2	2.22	0.54
3:F:195:GLU:H	3:F:195:GLU:CD	2.14	0.54
3:F:528:PHE:HZ	3:F:556:LEU:HD21	1.72	0.54
3:A:343:GLN:HG3	3:A:362:PRO:HG2	1.90	0.54
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.43	0.54
3:A:391:MET:HE1	3:A:447:TYR:CD2	2.43	0.54
3:F:703:CYS:O	3:F:704:HIS:ND1	2.40	0.54
4:I:8:THR:CA	4:I:63:ASN:HD21	2.20	0.54
3:F:20:CYS:HB2	3:F:168:MET:HE3	1.90	0.54
3:F:49:GLU:HA	3:F:52:ARG:NH1	2.23	0.54
4:I:44:GLU:HG3	4:I:45:ILE:N	2.21	0.54
4:I:80:LEU:C	4:I:80:LEU:HD23	2.33	0.54
1:X:915:DA:H2''	1:X:916:DG:H5'	1.88	0.53
3:A:224:LEU:HD12	3:A:422:PRO:HB3	1.88	0.53
3:A:488:MET:HE2	3:A:496:TYR:HB2	1.89	0.53
3:A:499:GLU:HG3	3:A:508:LYS:HE2	1.90	0.53
3:F:274:PHE:HE1	4:I:37:MET:HE2	1.74	0.53
3:F:130:TYR:CD1	3:F:135:MET:HG3	2.43	0.53
3:F:585:GLN:HE21	3:F:585:GLN:HA	1.73	0.53
3:A:290:LYS:HD2	3:A:328:PRO:HG3	1.89	0.53
1:X:919:DC:C1'	3:F:394:LYS:HE2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:971:DT:H2''	2:Z:972:DT:H71	1.89	0.53
3:A:376:ASP:OD2	3:A:379:LYS:HD3	2.08	0.53
3:F:235:ASP:HB2	3:F:459:HIS:CE1	2.44	0.53
1:P:807:DC:C2'	1:P:808:DG:H5'	2.27	0.53
2:Z:960:DA:H2''	2:Z:961:DC:H5'	1.90	0.53
3:A:315:LEU:HD23	3:A:315:LEU:N	2.23	0.53
3:F:391:MET:HE2	3:F:391:MET:O	2.08	0.53
4:I:79:LEU:HD12	4:I:89:THR:HG21	1.90	0.53
1:P:809:DA:H1'	1:P:810:DC:H5'	1.91	0.53
3:A:274:PHE:HE1	4:B:37:MET:HE2	1.73	0.53
3:A:546:GLU:HB3	5:A:5202:HOH:O	2.07	0.53
4:I:16:VAL:CA	4:I:23:ILE:HG21	2.25	0.53
1:P:805:DA:H2''	1:P:806:DA:O4'	2.09	0.53
3:A:290:LYS:HD3	3:A:326:TYR:OH	2.08	0.53
3:F:318:ARG:HH11	3:F:319:GLU:HG2	1.74	0.53
3:A:318:ARG:HE	3:A:319:GLU:N	2.05	0.52
4:B:37:MET:C	4:B:40:PRO:HD2	2.34	0.52
3:A:528:PHE:CZ	3:A:556:LEU:HD21	2.42	0.52
3:F:467:LYS:HE3	3:F:468:PRO:HD2	1.91	0.52
4:I:102:PHE:C	4:I:104:ASP:H	2.15	0.52
2:Z:958:DG:H4'	3:F:432:HIS:O	2.09	0.52
4:B:75:ILE:HB	4:B:76:PRO:HA	1.92	0.52
3:F:35:ARG:HB3	3:F:36:PRO:HD2	1.90	0.52
3:F:391:MET:HE2	3:F:391:MET:C	2.35	0.52
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.90	0.52
3:F:700:TRP:HE1	3:F:704:HIS:CE1	2.26	0.52
3:F:494:GLY:O	3:F:495:GLU:HB3	2.10	0.52
3:A:28:THR:O	3:A:29:ALA:HB3	2.10	0.52
4:I:81:PHE:HB3	4:I:84:GLY:H	1.75	0.52
4:B:39:ALA:N	4:B:40:PRO:CD	2.73	0.52
3:F:20:CYS:HB2	3:F:168:MET:CE	2.40	0.52
1:P:808:DG:H2''	1:P:809:DA:C8	2.45	0.52
3:A:164:ASN:OD1	3:A:166:GLU:HB2	2.09	0.51
3:A:492:ASP:HB3	3:A:561:ALA:HB2	1.91	0.51
3:F:181:LEU:HD22	3:F:185:LEU:HD11	1.92	0.51
3:A:696:MET:HE3	5:A:5084:HOH:O	2.10	0.51
4:B:38:ILE:HD12	4:B:93:ALA:CA	2.35	0.51
3:F:116:PRO:O	3:F:118:LYS:N	2.43	0.51
4:I:24:LEU:HB3	4:I:55:VAL:HG22	1.90	0.51
4:I:90:LYS:HD3	4:I:102:PHE:CZ	2.45	0.51
4:B:40:PRO:HA	4:B:43:ASP:OD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:72:LEU:O	3:A:76:GLN:HB2	2.11	0.51
3:F:181:LEU:O	3:F:185:LEU:HG	2.11	0.51
3:A:475:ASP:OD2	3:A:475:ASP:C	2.54	0.51
4:I:49:TYR:CE2	4:I:103:LEU:HB3	2.46	0.51
3:A:17:LYS:NZ	3:A:17:LYS:HB3	2.25	0.51
3:A:338:SER:O	3:A:342:ILE:HG13	2.10	0.51
3:A:484:LEU:O	3:A:488:MET:HG2	2.11	0.50
3:F:567:GLU:OE1	3:F:567:GLU:HA	2.10	0.50
4:B:5:ILE:HG22	4:B:6:HIS:O	2.11	0.50
4:I:24:LEU:O	4:I:54:THR:O	2.29	0.50
2:T:852:DT:H72	5:A:5032:HOH:O	2.11	0.50
2:T:865:DC:H2''	2:T:866:DC:O5'	2.11	0.50
3:A:321:VAL:CG2	4:B:94:LEU:HD21	2.39	0.50
3:A:331:HIS:HB3	5:A:5066:HOH:O	2.10	0.50
3:F:132:LEU:HD21	3:F:184:LYS:HG3	1.93	0.50
3:F:687:ARG:HB3	3:F:687:ARG:NH1	2.26	0.50
4:I:8:THR:C	4:I:63:ASN:HD21	2.20	0.50
3:F:11:LEU:HB3	3:F:13:GLU:OE1	2.11	0.50
4:I:100:LYS:NZ	4:I:100:LYS:HB3	2.26	0.50
1:P:807:DC:H1'	1:P:808:DG:H5''	1.94	0.50
1:P:808:DG:H1	2:T:869:DC:N4	2.10	0.50
3:F:655:GLU:OE2	3:F:704:HIS:HE1	1.94	0.50
3:A:391:MET:HE3	3:A:395:ARG:HG3	1.94	0.50
3:F:295:GLY:O	3:F:321:VAL:HA	2.12	0.50
3:A:624:LEU:HD12	3:A:684:TRP:CH2	2.47	0.50
4:I:107:LEU:HG	5:I:5013:HOH:O	2.12	0.50
1:X:920:DC:H5'	3:F:394:LYS:HE3	1.94	0.49
3:F:315:LEU:CD2	3:F:316:ASP:H	2.19	0.49
3:F:590:ARG:HD2	3:F:592:TRP:O	2.12	0.49
3:A:478:GLY:O	3:A:482:ARG:HG3	2.12	0.49
3:F:139:TYR:CE2	3:F:159:GLU:HB2	2.47	0.49
2:Z:960:DA:H2''	2:Z:961:DC:C5'	2.43	0.49
4:I:37:MET:HG3	4:I:38:ILE:N	2.28	0.49
1:P:806:DA:H2''	1:P:807:DC:C5	2.47	0.49
3:A:141:ASP:O	3:A:145:ARG:HG2	2.11	0.49
4:B:25:VAL:HG22	4:B:56:ALA:HB3	1.94	0.49
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.42	0.49
3:A:129:GLY:CA	3:A:135:MET:HG2	2.41	0.49
3:A:535:GLU:O	3:A:539:GLN:HG3	2.13	0.49
3:F:298:PHE:HA	3:F:315:LEU:C	2.38	0.49
3:F:452:ARG:HD2	5:F:5210:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:315:LEU:H	3:A:315:LEU:CD2	2.25	0.49
3:F:268:LYS:HD2	3:F:330:GLU:OE2	2.12	0.49
4:I:90:LYS:HD3	4:I:102:PHE:CE1	2.48	0.49
3:F:147:LEU:HD11	3:F:152:GLU:OE1	2.13	0.49
3:F:298:PHE:CD2	3:F:315:LEU:HA	2.48	0.48
3:A:102:LEU:HD12	3:A:123:HIS:CE1	2.48	0.48
3:A:119:ARG:HG3	3:A:119:ARG:HH11	1.78	0.48
3:F:39:PHE:CZ	3:F:43:LEU:HD11	2.48	0.48
3:F:655:GLU:OE2	3:F:704:HIS:CE1	2.67	0.48
4:I:52:LYS:CD	4:I:107:LEU:HD13	2.43	0.48
3:A:437:LEU:HA	3:A:440:ILE:CD1	2.42	0.48
3:F:200:ASP:HB2	5:F:5382:HOH:O	2.12	0.48
3:F:391:MET:CE	3:F:395:ARG:HG3	2.43	0.48
4:I:3:LYS:HE2	4:I:50:GLN:HE22	1.77	0.48
3:A:408:ARG:HG2	3:A:408:ARG:HH11	1.78	0.48
3:A:667:GLN:HE21	3:A:671:GLU:CG	2.25	0.48
2:T:868:DT:H2''	2:T:869:DC:C5'	2.44	0.48
3:A:135:MET:HE2	3:A:173:GLN:HE22	1.77	0.48
4:I:24:LEU:HG	4:I:80:LEU:CB	2.43	0.48
1:P:813:DC:H1'	1:P:814:DC:H5'	1.94	0.48
1:P:805:DA:H2''	1:P:806:DA:C5'	2.32	0.48
4:I:58:LEU:HD11	4:I:63:ASN:CG	2.38	0.48
4:I:80:LEU:HD23	4:I:80:LEU:O	2.13	0.48
1:P:816:DG:H2''	1:P:817:DT:C5'	2.44	0.47
1:X:911:DG:H2''	1:X:912:DG:C8	2.49	0.47
3:A:217:GLU:CD	3:A:599:ARG:HH22	2.22	0.47
3:F:494:GLY:O	3:F:495:GLU:CB	2.61	0.47
3:A:292:PRO:HA	5:A:5117:HOH:O	2.15	0.47
3:F:140:LYS:HE3	3:F:154:TYR:OH	2.14	0.47
3:F:159:GLU:HG2	3:F:160:TRP:CD1	2.48	0.47
1:P:805:DA:C3'	1:P:806:DA:H5''	2.45	0.47
3:A:128:TRP:CZ3	3:A:131:ARG:HD2	2.49	0.47
4:B:8:THR:HG23	4:B:11:SER:N	2.27	0.47
3:F:597:ASP:OD1	3:F:599:ARG:HD2	2.14	0.47
4:I:9:ASP:N	4:I:63:ASN:HD21	2.13	0.47
1:X:917:DT:H1'	1:X:918:DG:H5''	1.97	0.47
3:A:75:LEU:HD12	3:A:76:GLN:N	2.29	0.47
3:A:213:ALA:HA	3:A:597:ASP:OD2	2.15	0.47
3:A:326:TYR:HB3	4:B:92:GLY:HA2	1.95	0.47
3:F:702:ILE:C	3:F:704:HIS:H	2.22	0.47
3:A:9:ASN:HB3	3:A:17:LYS:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:570:GLN:HE22	3:F:606:PRO:HB3	1.80	0.47
3:A:35:ARG:HG3	3:A:35:ARG:HH11	1.79	0.47
3:F:556:LEU:HD11	3:F:566:ARG:NH2	2.30	0.47
1:P:816:DG:H2''	1:P:817:DT:H5'	1.96	0.46
3:F:72:LEU:HA	3:F:75:LEU:HD22	1.97	0.46
3:F:129:GLY:CA	3:F:135:MET:HG2	2.44	0.46
2:T:854:DG:H5''	3:A:532:ALA:HA	1.97	0.46
4:I:35:CYS:SG	4:I:76:PRO:HB3	2.56	0.46
3:A:114:LYS:HD2	5:A:5256:HOH:O	2.15	0.46
3:A:391:MET:HE2	3:A:391:MET:O	2.15	0.46
2:T:854:DG:H2''	2:T:855:DA:H8	1.80	0.46
1:X:916:DG:C2'	1:X:917:DT:C5'	2.89	0.46
5:A:5435:HOH:O	3:F:240:GLU:HG3	2.16	0.46
3:F:549:LYS:HD3	5:F:5409:HOH:O	2.15	0.46
3:A:211:LEU:HD21	3:A:598:GLY:C	2.41	0.46
3:A:444:ARG:HB2	5:A:5161:HOH:O	2.16	0.46
4:I:9:ASP:N	4:I:63:ASN:ND2	2.64	0.46
4:I:44:GLU:CG	4:I:45:ILE:H	2.20	0.46
3:A:109:LEU:CD2	3:A:114:LYS:HD3	2.45	0.46
3:A:159:GLU:HG2	3:A:160:TRP:CD1	2.50	0.46
3:F:31:TYR:CE2	3:F:176:VAL:HG12	2.50	0.46
3:F:318:ARG:NH1	3:F:319:GLU:HG2	2.30	0.46
3:A:31:TYR:OH	3:A:176:VAL:HG12	2.16	0.46
3:A:558:ASN:C	3:A:560:PRO:HD3	2.41	0.46
3:F:391:MET:HE1	3:F:447:TYR:CD2	2.51	0.46
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.98	0.46
3:F:72:LEU:HA	3:F:75:LEU:HD21	1.94	0.46
3:F:115:LEU:O	3:F:117:GLY:N	2.36	0.46
3:F:558:ASN:C	3:F:560:PRO:HD3	2.41	0.46
1:P:820:DC:H5'	3:A:394:LYS:HE2	1.98	0.46
3:F:106:ASP:OD2	3:F:131:ARG:NH2	2.48	0.46
3:F:297:ILE:HD13	4:I:102:PHE:CA	2.46	0.46
3:F:365:ASP:O	3:F:369:LEU:HB2	2.16	0.46
3:F:470:VAL:CG1	3:F:471:GLN:N	2.78	0.46
2:T:869:DC:H2''	2:T:870:DG:H8	1.81	0.45
3:F:136:LYS:CG	3:F:173:GLN:HE21	2.28	0.45
3:F:264:TRP:NE1	3:F:344:LYS:HE2	2.31	0.45
3:F:315:LEU:HD23	4:I:105:ALA:HB1	1.97	0.45
3:F:493:ASN:HD22	3:F:687:ARG:HH22	1.63	0.45
1:P:807:DC:H42	2:T:870:DG:H1	1.65	0.45
1:P:820:DC:C2'	1:P:821:DA:OP2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:966:DC:H2''	2:Z:967:DG:H8	1.76	0.45
4:B:45:ILE:HG13	4:B:99:LEU:CD1	2.46	0.45
3:F:693:GLU:OE2	3:F:693:GLU:HA	2.16	0.45
3:A:75:LEU:HD12	3:A:76:GLN:H	1.81	0.45
3:A:163:PHE:HE1	3:A:168:MET:HB2	1.80	0.45
3:F:351:TRP:CZ3	3:F:353:PRO:HG3	2.51	0.45
4:B:32:CYS:HB3	4:B:35:CYS:HB2	1.99	0.45
3:F:667:GLN:HE21	3:F:671:GLU:HG3	1.80	0.45
4:I:10:ASP:CG	4:I:11:SER:N	2.75	0.45
3:A:135:MET:HE1	3:A:173:GLN:HE22	1.81	0.45
3:F:436:ASN:OD1	3:F:438:ALA:HB3	2.17	0.45
3:F:628:LYS:HE2	3:F:679:TRP:CD2	2.51	0.45
4:I:25:VAL:N	4:I:55:VAL:HG13	2.32	0.45
4:I:44:GLU:O	4:I:46:ALA:N	2.49	0.45
3:A:59:HIS:O	3:A:60:ASN:HB3	2.17	0.45
3:F:449:GLU:HB3	5:F:5043:HOH:O	2.16	0.45
4:I:4:ILE:HG12	5:I:5003:HOH:O	2.16	0.45
4:I:102:PHE:C	4:I:104:ASP:N	2.75	0.45
3:A:285:LYS:HG2	5:A:5041:HOH:O	2.17	0.45
4:B:53:LEU:CD2	4:B:103:LEU:HD22	2.47	0.45
3:F:168:MET:O	3:F:168:MET:HG3	2.17	0.45
2:T:867:DG:C2'	2:T:868:DT:H5'	2.23	0.45
4:B:13:ASP:CG	4:B:17:LEU:HD12	2.42	0.45
3:F:391:MET:HE3	3:F:395:ARG:HG3	1.98	0.45
4:I:10:ASP:CG	4:I:11:SER:H	2.25	0.45
3:A:273:MET:HE2	3:A:273:MET:HB3	1.74	0.44
3:A:547:ARG:O	3:A:551:LEU:HB2	2.17	0.44
4:B:95:SER:OG	4:B:98:GLN:HG3	2.17	0.44
3:F:496:TYR:CZ	3:F:505:ILE:HD11	2.52	0.44
1:P:812:DG:H1'	1:P:813:DC:H5''	1.99	0.44
2:T:860:DA:H2''	2:T:861:DC:H5'	1.99	0.44
3:A:148:GLU:C	3:A:150:GLN:H	2.24	0.44
3:F:276:HIS:HA	3:F:277:PRO:HD3	1.88	0.44
1:X:921:DA:O4'	3:F:439:GLN:HA	2.16	0.44
3:A:146:MET:O	3:A:150:GLN:HG3	2.18	0.44
3:A:181:LEU:O	3:A:185:LEU:HG	2.17	0.44
3:F:326:TYR:HB3	4:I:92:GLY:HA2	1.98	0.44
1:X:903:DA:H2''	1:X:904:DA:C8	2.52	0.44
3:F:473:GLY:HA3	3:F:703:CYS:HB3	2.00	0.44
3:A:94:LEU:HD21	3:A:214:VAL:HG13	1.99	0.44
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:335:ASN:OD1	3:A:337:SER:HB2	2.17	0.44
3:A:525:ILE:HG23	3:A:526:TYR:N	2.32	0.44
3:F:234:PHE:CZ	3:F:239:ILE:HG13	2.53	0.44
3:F:642:TRP:C	3:F:644:GLY:H	2.26	0.44
1:X:910:DC:H2''	1:X:911:DG:H5'	1.94	0.44
3:A:267:PRO:HD3	4:B:31:TRP:CZ3	2.53	0.44
3:F:585:GLN:HA	3:F:585:GLN:NE2	2.31	0.44
4:I:42:LEU:O	4:I:43:ASP:CB	2.66	0.44
3:A:642:TRP:C	3:A:644:GLY:H	2.26	0.44
4:I:67:ALA:HB3	4:I:68:PRO:HD3	1.99	0.44
4:I:99:LEU:HD23	4:I:99:LEU:O	2.18	0.44
3:A:63:LYS:HE2	3:A:228:GLU:OE1	2.18	0.43
3:F:71:LYS:O	3:F:75:LEU:HD22	2.17	0.43
3:F:493:ASN:C	3:F:493:ASN:ND2	2.73	0.43
3:A:106:ASP:HA	3:A:109:LEU:HD12	2.00	0.43
3:F:12:LEU:HD21	3:F:229:ARG:HD3	2.00	0.43
3:F:28:THR:O	3:F:29:ALA:CB	2.66	0.43
3:A:318:ARG:NH1	3:A:319:GLU:HG2	2.33	0.43
3:A:407:LEU:HA	3:A:407:LEU:HD23	1.83	0.43
3:F:31:TYR:N	3:F:31:TYR:CD1	2.87	0.43
3:F:269:GLY:O	3:F:270:GLY:C	2.60	0.43
3:F:622:CYS:SG	3:F:654:ASP:HA	2.59	0.43
3:A:18:PHE:CD2	3:A:39:PHE:HB2	2.53	0.43
3:A:235:ASP:HB2	3:A:459:HIS:CE1	2.54	0.43
1:X:904:DA:H2''	1:X:905:DA:C8	2.54	0.43
3:A:252:GLU:HG3	3:A:256:LYS:NZ	2.33	0.43
3:A:506:HIS:CG	3:A:522:LYS:HG2	2.54	0.43
4:B:107:LEU:HB2	5:B:5187:HOH:O	2.18	0.43
3:F:373:ARG:HA	3:F:380:GLN:OE1	2.18	0.43
4:I:13:ASP:C	4:I:15:ASP:H	2.25	0.43
3:A:135:MET:HE2	3:A:135:MET:HA	2.01	0.43
3:F:233:PRO:HB2	3:F:456:GLY:O	2.18	0.43
3:A:17:LYS:HB3	3:A:17:LYS:HZ3	1.83	0.43
3:A:281:LYS:HA	3:A:282:PRO:HD3	1.93	0.43
1:P:806:DA:H2''	1:P:807:DC:C6	2.54	0.43
3:A:223:LEU:O	3:A:226:LYS:HB3	2.19	0.43
3:A:488:MET:HB2	3:A:561:ALA:HB1	2.01	0.43
3:A:621:ILE:HD11	3:A:686:PHE:CZ	2.54	0.43
3:A:633:LEU:HD22	3:A:638:LEU:HD12	2.00	0.43
4:I:42:LEU:O	4:I:43:ASP:HB2	2.19	0.43
3:A:15:VAL:HG22	3:A:72:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:173:GLN:O	3:A:177:VAL:HG23	2.19	0.43
3:F:297:ILE:O	3:F:297:ILE:HG22	2.19	0.43
3:F:321:VAL:HG22	4:I:90:LYS:CE	2.47	0.43
3:F:551:LEU:HD12	3:F:551:LEU:HA	1.84	0.43
3:A:72:LEU:HA	3:A:75:LEU:CD1	2.46	0.42
3:A:685:ASN:HB3	5:A:5046:HOH:O	2.19	0.42
3:F:182:LEU:O	3:F:186:LEU:HG	2.19	0.42
3:F:632:MET:HE1	3:F:675:GLU:HB3	2.01	0.42
4:I:45:ILE:CD1	4:I:99:LEU:HD13	2.49	0.42
4:I:99:LEU:O	4:I:103:LEU:HG	2.19	0.42
1:X:920:DC:H2''	1:X:921:DA:H5''	1.96	0.42
3:F:17:LYS:HA	3:F:76:GLN:NE2	2.34	0.42
3:A:184:LYS:O	3:A:184:LYS:HD3	2.20	0.42
3:F:213:ALA:HA	3:F:597:ASP:OD2	2.19	0.42
4:I:42:LEU:C	4:I:43:ASP:OD1	2.62	0.42
2:Z:974:DT:H2''	2:Z:975:DC:C6	2.55	0.42
3:A:155:VAL:O	3:A:156:ASP:C	2.61	0.42
3:A:182:LEU:O	3:A:186:LEU:HG	2.20	0.42
4:B:18:LYS:O	4:B:19:ALA:C	2.62	0.42
3:F:475:ASP:OD2	3:F:475:ASP:N	2.52	0.42
3:F:556:LEU:HD11	3:F:566:ARG:HH21	1.83	0.42
4:I:54:THR:O	4:I:54:THR:HG22	2.19	0.42
3:A:639:LYS:HZ1	3:A:643:ASP:CG	2.28	0.42
3:A:297:ILE:N	3:A:297:ILE:CD1	2.81	0.42
1:P:817:DT:C2'	1:P:818:DG:H5'	2.36	0.42
3:A:1:MET:HE2	3:A:89:ILE:HD12	2.02	0.42
3:A:160:TRP:CE3	3:A:167:MET:HE2	2.54	0.42
3:A:471:GLN:HB3	3:A:697:GLY:O	2.20	0.42
3:F:102:LEU:HD12	3:F:123:HIS:CE1	2.55	0.42
3:F:343:GLN:HG3	3:F:362:PRO:HG3	1.98	0.42
4:I:13:ASP:C	4:I:15:ASP:N	2.78	0.42
4:I:77:THR:HG22	4:I:79:LEU:HD22	2.02	0.42
4:B:8:THR:CG2	4:B:11:SER:H	2.30	0.42
3:F:31:TYR:H	3:F:31:TYR:HD1	1.68	0.42
3:F:136:LYS:HG3	3:F:173:GLN:NE2	2.34	0.42
3:F:237:LYS:O	3:F:241:GLU:HG3	2.19	0.42
3:A:196:ILE:HD12	3:A:196:ILE:N	2.35	0.42
3:F:264:TRP:CD1	3:F:344:LYS:HE2	2.55	0.42
4:I:12:PHE:CD1	4:I:13:ASP:N	2.81	0.42
3:F:356:TYR:HD2	3:F:360:GLY:O	2.03	0.41
3:F:109:LEU:HD13	3:F:131:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:285:LYS:HB3	3:F:285:LYS:HZ2	1.85	0.41
3:F:554:LYS:HD3	3:F:554:LYS:HA	1.83	0.41
3:F:621:ILE:HD11	3:F:686:PHE:CZ	2.55	0.41
2:Z:971:DT:H2''	2:Z:972:DT:C7	2.51	0.41
3:F:196:ILE:HD12	3:F:196:ILE:N	2.36	0.41
3:F:211:LEU:HD21	3:F:598:GLY:C	2.45	0.41
3:F:254:LEU:O	3:F:258:THR:HG23	2.19	0.41
3:F:591:ARG:HD2	5:F:5316:HOH:O	2.18	0.41
4:I:100:LYS:HB3	4:I:100:LYS:HZ3	1.86	0.41
1:P:807:DC:C2'	1:P:808:DG:C5'	2.95	0.41
2:T:868:DT:H2''	2:T:869:DC:H5'	2.02	0.41
3:A:628:LYS:HE2	3:A:679:TRP:CD2	2.56	0.41
3:F:137:GLY:C	3:F:170:TYR:HE1	2.28	0.41
3:F:635:GLU:HA	3:F:635:GLU:OE2	2.20	0.41
3:A:276:HIS:HA	3:A:277:PRO:HD3	1.94	0.41
3:A:290:LYS:HD2	3:A:328:PRO:CG	2.51	0.41
3:A:490:ARG:HD3	3:A:491:PHE:CZ	2.55	0.41
3:A:525:ILE:O	3:A:529:LEU:HB2	2.21	0.41
3:F:273:MET:HE2	3:F:273:MET:HB2	1.96	0.41
3:F:473:GLY:O	3:F:694:GLY:HA2	2.20	0.41
3:A:139:TYR:CE2	3:A:159:GLU:HB2	2.56	0.41
3:A:440:ILE:O	3:A:441:PRO:C	2.63	0.41
4:B:45:ILE:HG13	4:B:99:LEU:HD12	2.02	0.41
3:F:346:LEU:HD13	3:F:372:VAL:HG11	2.03	0.41
4:I:49:TYR:HE2	4:I:107:LEU:HD12	1.85	0.41
2:Z:967:DG:H2'	2:Z:968:DT:H72	2.02	0.41
3:F:440:ILE:O	3:F:441:PRO:C	2.63	0.41
4:I:79:LEU:HD22	4:I:79:LEU:N	2.36	0.41
3:A:129:GLY:C	3:A:135:MET:HG2	2.45	0.41
3:A:193:PRO:HB3	3:A:195:GLU:OE1	2.21	0.41
3:A:285:LYS:HB3	3:A:285:LYS:HZ2	1.83	0.41
3:A:590:ARG:HD2	3:A:592:TRP:O	2.21	0.41
4:B:48:GLU:OE2	4:B:96:LYS:NZ	2.49	0.41
3:F:343:GLN:O	3:F:347:GLN:HG3	2.21	0.41
3:A:168:MET:O	3:A:168:MET:HG3	2.20	0.41
3:A:296:GLY:C	3:A:297:ILE:HD12	2.46	0.41
4:I:20:ASP:HA	4:I:23:ILE:HG13	2.03	0.41
3:A:446:PRO:O	3:A:447:TYR:HB2	2.19	0.40
3:A:551:LEU:HD12	3:A:551:LEU:HA	1.91	0.40
3:F:106:ASP:HA	3:F:109:LEU:HD12	2.03	0.40
3:F:158:MET:HB2	3:F:161:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:228:GLU:OE1	3:F:420:VAL:N	2.47	0.40
3:A:530:TYR:CD1	3:A:611:ASN:HB2	2.56	0.40
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.61	0.40
3:F:274:PHE:CE1	4:I:37:MET:HE2	2.55	0.40
3:F:525:ILE:HG23	3:F:526:TYR:N	2.35	0.40
3:F:633:LEU:HD22	3:F:638:LEU:CD1	2.47	0.40
1:X:906:DA:H2	2:Z:972:DT:O2	2.04	0.40
1:X:915:DA:H2''	1:X:916:DG:C5'	2.50	0.40
3:A:57:VAL:HG21	3:A:182:LEU:HD22	2.03	0.40
3:A:356:TYR:HD2	3:A:360:GLY:O	2.04	0.40
3:F:35:ARG:HB3	3:F:36:PRO:CD	2.50	0.40
4:I:3:LYS:C	4:I:4:ILE:HG13	2.46	0.40
4:I:98:GLN:HA	4:I:101:GLU:HB3	2.02	0.40
2:Z:952:DT:O2	2:Z:952:DT:C2'	2.69	0.40
3:A:31:TYR:CD1	3:A:31:TYR:N	2.90	0.40
3:A:554:LYS:HD3	3:A:554:LYS:HA	1.85	0.40
3:F:345:LYS:HE2	3:F:345:LYS:HA	2.02	0.40
3:F:411:ALA:HB3	3:F:413:ASP:OD1	2.21	0.40
1:X:917:DT:C2'	1:X:918:DG:C5'	2.96	0.40
3:A:35:ARG:O	3:A:36:PRO:C	2.64	0.40
3:A:189:LYS:HG3	3:A:194:PRO:CG	2.40	0.40
4:B:7:LEU:HB2	4:B:58:LEU:HD13	2.02	0.40
3:F:125:LEU:HA	3:F:125:LEU:HD23	1.86	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)
5:F:5072:HOH:O	5:F:5072:HOH:O[3_555]	1.46	0.74

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	702/704 (100%)	657 (94%)	39 (6%)	6 (1%)	14	30
3	F	685/704 (97%)	635 (93%)	43 (6%)	7 (1%)	12	28
4	B	103/108 (95%)	89 (86%)	10 (10%)	4 (4%)	2	3
4	I	101/108 (94%)	71 (70%)	19 (19%)	11 (11%)	0	0
All	All	1591/1624 (98%)	1452 (91%)	111 (7%)	28 (2%)	6	14

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	302	LYS
3	A	310	ARG
4	B	18	LYS
4	B	19	ALA
3	F	114	LYS
4	I	11	SER
4	I	20	ASP
4	I	44	GLU
3	A	308	GLU
3	A	313	CYS
4	B	15	ASP
3	F	116	PRO
3	F	117	GLY
3	F	154	TYR
4	I	87	ALA
3	A	152	GLU
4	I	46	ALA
3	A	156	ASP
4	B	84	GLY
3	F	495	GLU
4	I	13	ASP
4	I	16	VAL
4	I	21	GLY
3	F	653	HIS
4	I	18	LYS
4	I	43	ASP
3	F	296	GLY
4	I	45	ILE

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	563/582 (97%)	531 (94%)	32 (6%)	18	40
3	F	559/582 (96%)	529 (95%)	30 (5%)	20	42
4	B	84/87 (97%)	77 (92%)	7 (8%)	10	23
4	I	81/87 (93%)	79 (98%)	2 (2%)	42	69
All	All	1287/1338 (96%)	1216 (94%)	71 (6%)	19	41

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	17	LYS
3	A	75	LEU
3	A	86	GLU
3	A	110	LEU
3	A	125	LEU
3	A	173	GLN
3	A	189	LYS
3	A	241	GLU
3	A	285	LYS
3	A	297	ILE
3	A	343	GLN
3	A	354	THR
3	A	358	ASP
3	A	368	VAL
3	A	391	MET
3	A	394	LYS
3	A	410	VAL
3	A	420	VAL
3	A	423	ASN
3	A	426	VAL
3	A	449	GLU
3	A	470	VAL
3	A	501	LEU
3	A	529	LEU

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Mol	Chain	Res	Type
3	A	551	LEU
3	A	554	LYS
3	A	567	GLU
3	A	584	GLN
3	A	599	ARG
3	A	624	LEU
3	A	630	GLU
3	A	654	ASP
4	B	36	LYS
4	B	37	MET
4	B	53	LEU
4	B	73	ARG
4	B	77	THR
4	B	79	LEU
4	B	80	LEU
3	F	17	LYS
3	F	75	LEU
3	F	86	GLU
3	F	110	LEU
3	F	125	LEU
3	F	168	MET
3	F	169	ASP
3	F	176	VAL
3	F	181	LEU
3	F	245	GLU
3	F	259	GLU
3	F	278	ARG
3	F	285	LYS
3	F	315	LEU
3	F	359	LYS
3	F	368	VAL
3	F	391	MET
3	F	410	VAL
3	F	482	ARG
3	F	499	GLU
3	F	523	THR
3	F	529	LEU
3	F	551	LEU
3	F	554	LYS
3	F	559	THR
3	F	575	GLU
3	F	584	GLN

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Mol	Chain	Res	Type
3	F	599	ARG
3	F	624	LEU
3	F	630	GLU
4	I	25	VAL
4	I	49	TYR

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

Mol	Chain	Res	Type
3	A	78	ASN
3	A	101	ASN
3	A	123	HIS
3	A	150	GLN
3	A	173	GLN
3	A	276	HIS
3	A	303	ASN
3	A	343	GLN
3	A	347	GLN
3	A	423	ASN
3	A	439	GLN
3	A	502	ASN
3	A	506	HIS
3	A	558	ASN
3	A	570	GLN
3	A	584	GLN
3	A	667	GLN
4	B	50	GLN
4	B	83	ASN
3	F	76	GLN
3	F	99	HIS
3	F	123	HIS
3	F	171	ASN
3	F	173	GLN
3	F	276	HIS
3	F	347	GLN
3	F	450	GLN
3	F	460	HIS
3	F	493	ASN
3	F	502	ASN
3	F	520	ASN
3	F	539	GLN
3	F	570	GLN

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Mol	Chain	Res	Type
3	F	584	GLN
3	F	585	GLN
3	F	611	ASN
3	F	615	GLN
3	F	667	GLN
4	I	50	GLN
4	I	59	ASN
4	I	62	GLN
4	I	63	ASN

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	$\# Z > 2$
1	2DT	P	822	2,1	17,20,21	0.39	0	22,28,31	0.61	0
1	2DT	X	922	2,1	17,20,21	0.33	0	22,28,31	0.68	0

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
1	2DT	P	822	2,1	-	0/7/18/19	0/2/2/2
1	2DT	X	922	2,1	-	0/7/18/19	0/2/2/2

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.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	81:PHE	C	82:LYS	N	5.61

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	P	19/22 (86%)	-1.45	0 100 100	50, 100, 170, 171	0
1	X	20/22 (90%)	-1.14	0 100 100	48, 100, 201, 201	0
2	T	22/26 (84%)	-1.51	0 100 100	49, 90, 145, 153	0
2	Z	25/26 (96%)	-1.34	0 100 100	49, 97, 183, 192	0
3	A	704/704 (100%)	-1.26	0 100 100	38, 61, 116, 153	0
3	F	689/704 (97%)	-1.27	0 100 100	38, 60, 105, 143	0
4	B	105/108 (97%)	-1.09	0 100 100	50, 93, 113, 116	0
4	I	105/108 (97%)	-0.85	0 100 100	51, 108, 147, 153	0
All	All	1689/1720 (98%)	-1.23	0 100 100	38, 64, 135, 201	0

There are no RSRZ outliers to report.

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
1	2DT	P	822	19/20	0.99	0.03	48,50,55,56	0
1	2DT	X	922	19/20	1.00	0.03	48,52,57,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.