



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 04:48 AM EST

PDB ID : 5TCT
Title : The Structure of SV40 Large T Hexameric Helicase in Complex with AT-rich Origin DNA
Authors : Gai, D.; Wang, D.; Li, S.X.; Chen, X.S.
Deposited on : 2016-09-15
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

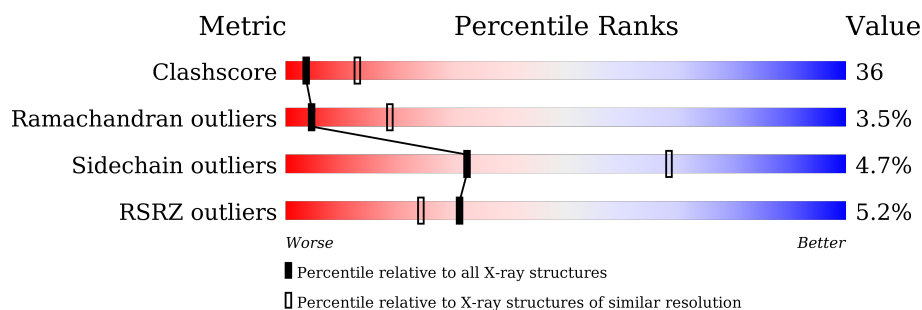
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	362	
1	B	362	
1	C	362	
1	D	362	
1	E	362	
1	F	362	
2	W	33	

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Mol	Chain	Length	Quality of chain
3	K	33	<div> <div>30%</div> <div>6%76%18%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19123 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 protein called Large T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	B	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	E	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	F	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	C	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	D	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	TYR	PHE	ENGINEERED MUTATION	UNP P03070
A	549	PRO	ALA	ENGINEERED MUTATION	UNP P03070
B	531	TYR	PHE	ENGINEERED MUTATION	UNP P03070
B	549	PRO	ALA	ENGINEERED MUTATION	UNP P03070
E	531	TYR	PHE	ENGINEERED MUTATION	UNP P03070
E	549	PRO	ALA	ENGINEERED MUTATION	UNP P03070
F	531	TYR	PHE	ENGINEERED MUTATION	UNP P03070
F	549	PRO	ALA	ENGINEERED MUTATION	UNP P03070
C	531	TYR	PHE	ENGINEERED MUTATION	UNP P03070
C	549	PRO	ALA	ENGINEERED MUTATION	UNP P03070
D	531	TYR	PHE	ENGINEERED MUTATION	UNP P03070
D	549	PRO	ALA	ENGINEERED MUTATION	UNP P03070

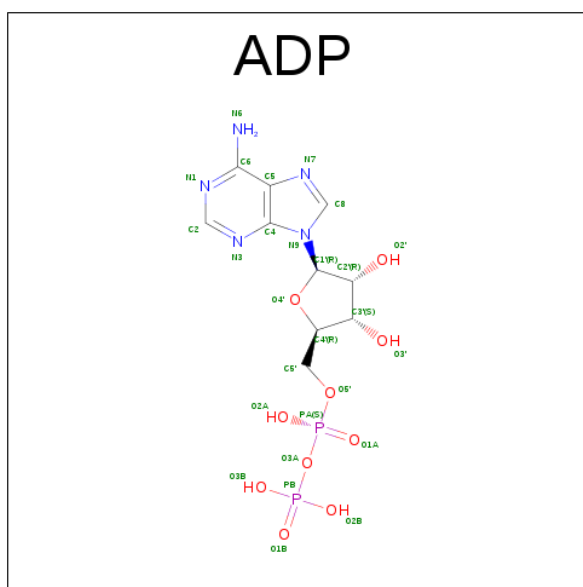
- Molecule 2 is a DNA chain called AT-rich Origin DNA (33-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	33	Total	C	N	O	P	0	0	0
			677	323	127	194	33			

- Molecule 3 is a DNA chain called AT-rich Origin DNA (33-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	33	Total	C	N	O	P	0	0	0
			677	325	113	206	33			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Zn 1 1	0	0
5	E	1	Total Zn 1 1	0	0
5	B	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0
5	A	1	Total Zn 1 1	0	0
5	F	1	Total Zn 1 1	0	0

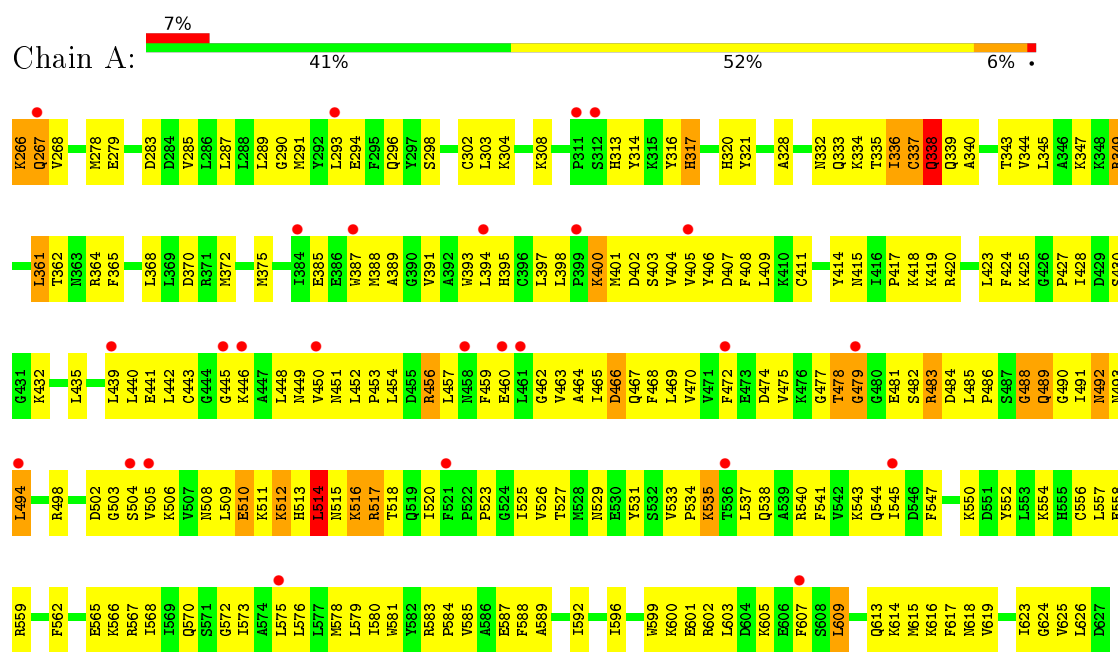
- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mn 1 1	0	0
6	D	1	Total Mn 1 1	0	0
6	F	1	Total Mn 1 1	0	0

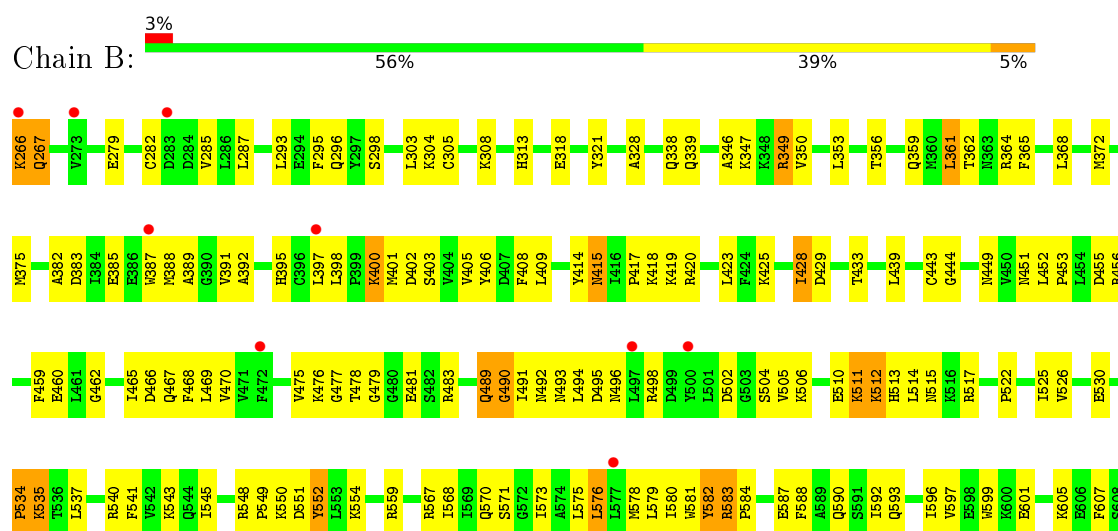
3 Residue-property plots

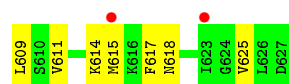
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Large T antigen

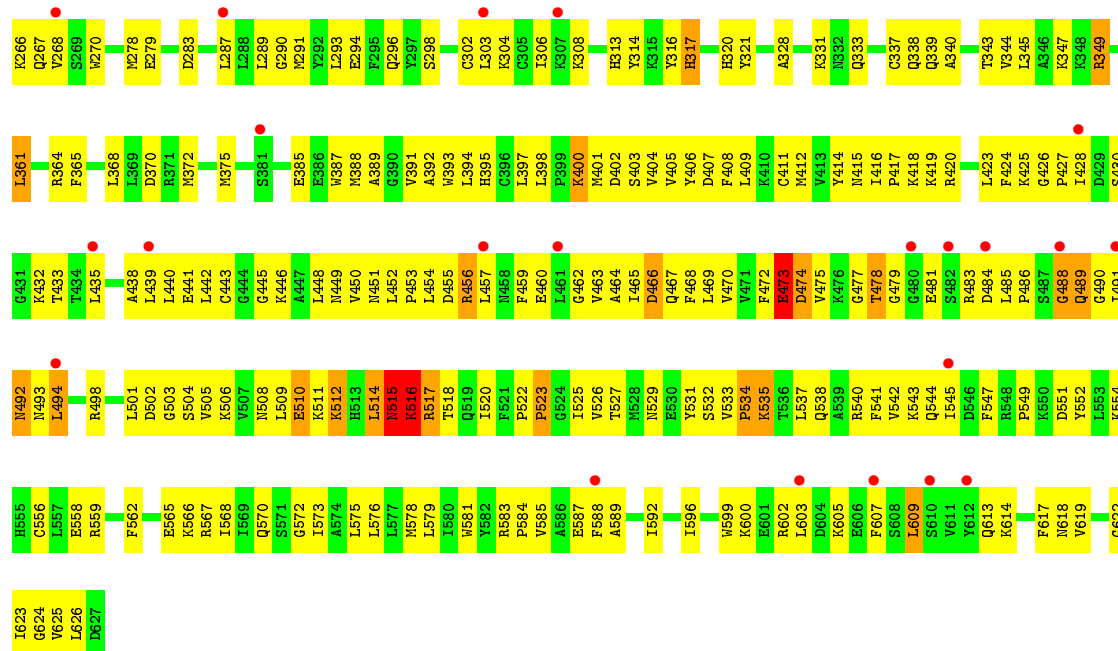
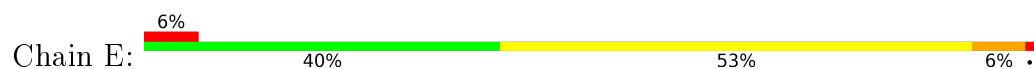


• Molecule 1: Large T antigen

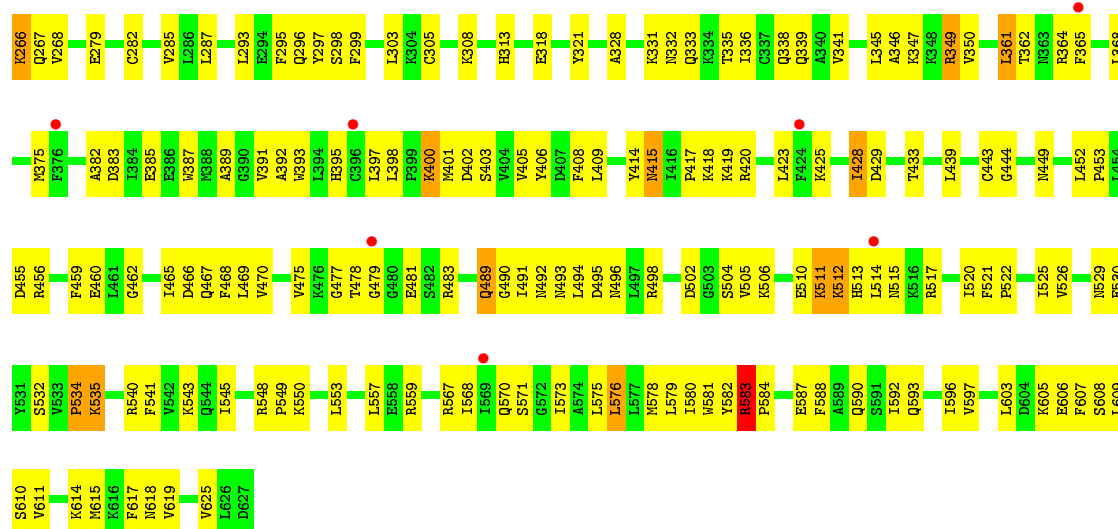




• Molecule 1: Large T antigen

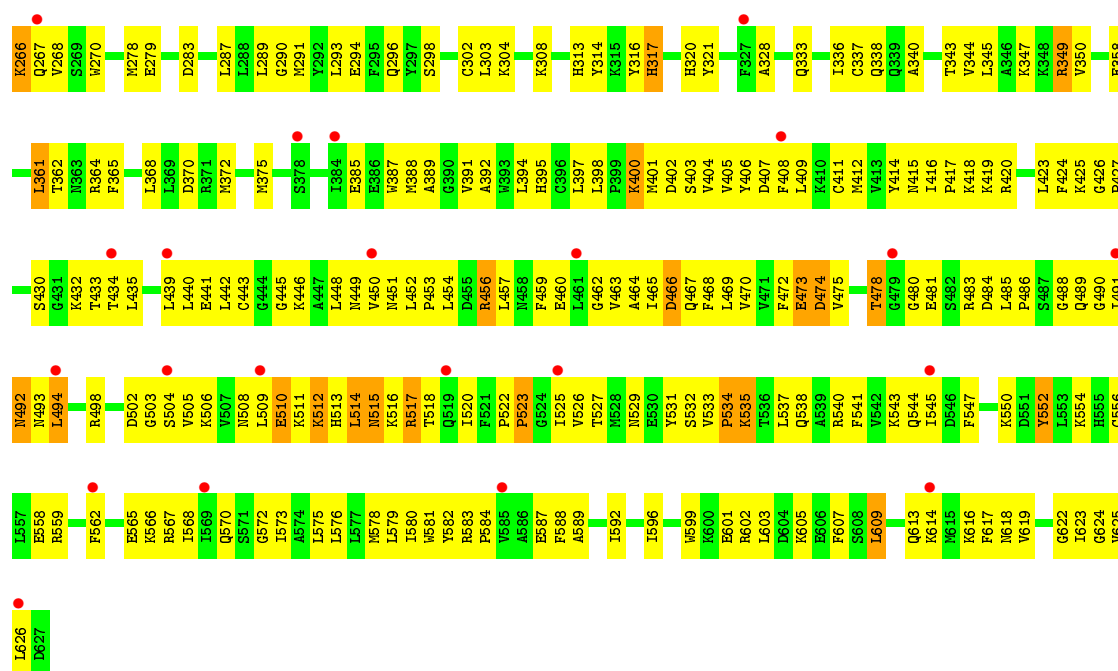


• Molecule 1: Large T antigen

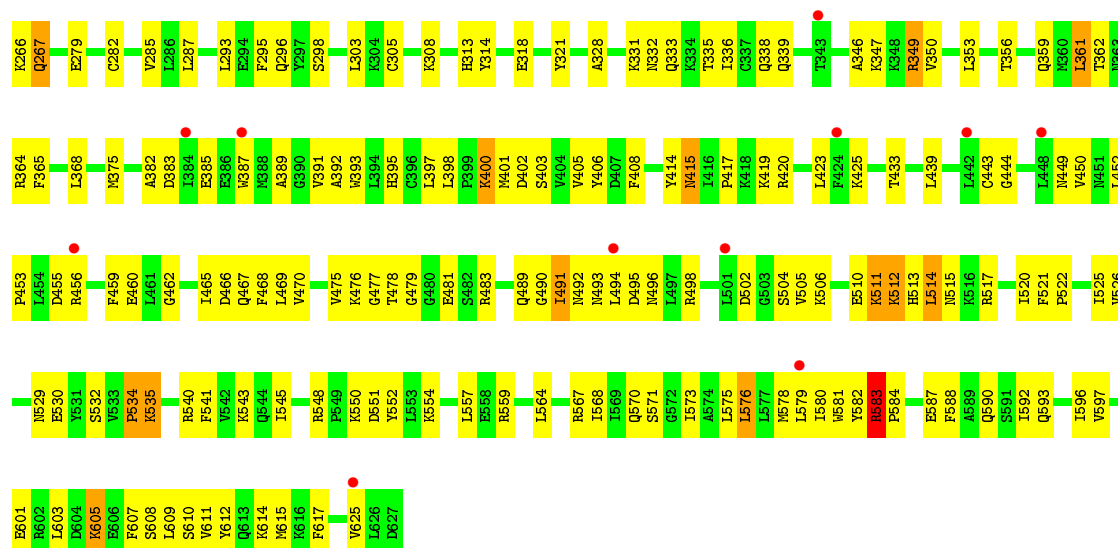


• Molecule 1: Large T antigen

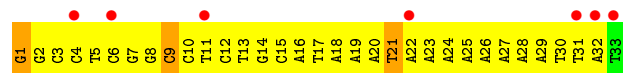




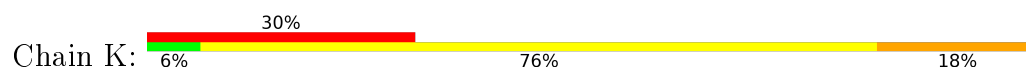
• Molecule 1: Large T antigen

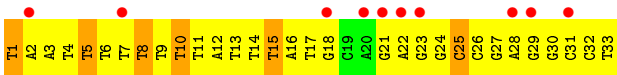


• Molecule 2: AT-rich Origin DNA (33-MER)



• Molecule 3: AT-rich Origin DNA (33-MER)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	107.48Å 107.59Å 107.87Å 107.13° 106.95° 106.86°	Depositor
Resolution (Å)	50.00 – 2.90 49.87 – 2.91	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-2.90) 75.8 (49.87-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.304 0.271 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	88.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.447 for k,l,h 0.447 for l,h,k 0.023 for -k,-h,-l 0.024 for -l,-k,-h 0.023 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19123	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN, ADP

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	A	0.35	0/2992	0.70	6/4030 (0.1%)
1	B	0.37	0/2992	0.57	0/4030
1	C	0.35	0/2992	0.58	2/4030 (0.0%)
1	D	0.35	0/2992	0.56	0/4030
1	E	0.33	0/2992	0.60	2/4030 (0.0%)
1	F	0.36	0/2992	0.57	0/4030
2	W	0.85	2/760 (0.3%)	0.78	0/1168
3	K	0.74	1/756 (0.1%)	0.79	0/1164
All	All	0.40	3/19468 (0.0%)	0.62	10/26512 (0.0%)

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	W	0	2
3	K	0	5
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1	DT	OP3-P	-7.22	1.52	1.61
2	W	1	DG	OP3-P	-6.06	1.53	1.61
2	W	1	DG	P-O5'	5.00	1.64	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	GLN	N-CA-CB	15.53	138.55	110.60
1	A	483	ARG	N-CA-C	-15.15	70.09	111.00
1	E	516	LYS	N-CA-CB	14.36	136.46	110.60
1	A	483	ARG	CB-CA-C	13.24	136.88	110.40
1	C	480	GLY	N-CA-C	9.14	135.95	113.10
1	E	516	LYS	N-CA-C	-7.51	90.72	111.00
1	A	484	ASP	N-CA-CB	-7.40	97.27	110.60
1	A	338	GLN	N-CA-C	-6.48	93.49	111.00
1	C	474	ASP	N-CA-C	-5.73	95.53	111.00
1	A	484	ASP	N-CA-C	-5.59	95.90	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	10	DT	Sidechain
3	K	15	DT	Sidechain
3	K	25	DC	Sidechain
3	K	5	DT	Sidechain
3	K	8	DT	Sidechain
2	W	21	DT	Sidechain
2	W	9	DC	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	A	2933	0	2982	235	1
1	B	2933	0	2981	164	0
1	C	2933	0	2982	226	0
1	D	2933	0	2981	176	0
1	E	2933	0	2981	234	0
1	F	2933	0	2981	168	0
2	W	677	0	372	129	0
3	K	677	0	378	118	1
4	A	27	0	12	0	0
4	B	27	0	12	2	0
4	C	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	27	0	12	0	0
4	E	27	0	12	0	0
4	F	27	0	12	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
All	All	19123	0	18710	1337	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 36.

All (1337) 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)
1:D:476:LYS:O	1:D:490:GLY:HA3	1.19	1.30
1:D:477:GLY:CA	1:D:490:GLY:O	1.88	1.22
1:D:476:LYS:O	1:D:490:GLY:CA	1.89	1.21
1:D:477:GLY:HA3	1:D:490:GLY:O	1.45	1.13
1:C:517:ARG:HH11	1:C:517:ARG:HB3	1.15	1.11
1:B:583:ARG:HG3	1:B:583:ARG:HH11	1.05	1.10
2:W:30:DT:N3	3:K:3:DA:H2	1.48	1.10
1:C:473:GLU:O	1:C:527:THR:HB	1.50	1.09
2:W:26:DA:H61	3:K:7:DT:H1'	1.18	1.08
3:K:10:DT:H2''	3:K:11:DT:H5'	1.30	1.07
1:A:517:ARG:HB3	1:A:517:ARG:HH11	1.14	1.06
1:E:517:ARG:HB3	1:E:517:ARG:HH11	1.16	1.04
2:W:29:DA:N1	3:K:4:DT:N3	2.05	1.02
2:W:27:DA:H2''	2:W:28:DA:H5'	1.36	1.02
2:W:24:DA:N1	3:K:9:DT:N3	2.08	1.01
1:E:475:VAL:HG21	1:E:491:ILE:HD13	1.41	1.00
2:W:30:DT:N3	3:K:3:DA:C2	2.27	0.99
2:W:29:DA:H2	3:K:4:DT:O2	1.46	0.97
2:W:21:DT:H2'	2:W:22:DA:C8	1.98	0.97
1:D:453:PRO:HA	1:D:489:GLN:HE22	1.29	0.96
2:W:25:DA:N6	3:K:8:DT:H3	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:8:DT:H2"	3:K:9:DT:OP2	1.67	0.94
2:W:26:DA:N6	3:K:7:DT:H1'	1.81	0.94
1:B:583:ARG:NH1	1:B:583:ARG:HG3	1.80	0.94
1:E:331:LYS:HZ1	1:F:267:GLN:HE22	1.15	0.94
2:W:31:DT:N3	3:K:2:DA:N1	2.15	0.93
2:W:32:DA:N1	3:K:1:DT:N3	2.15	0.93
1:A:535:LYS:HD2	1:A:535:LYS:H	1.34	0.93
2:W:25:DA:H61	3:K:8:DT:H3	1.04	0.92
2:W:5:DT:H3	3:K:28:DA:H61	1.06	0.92
1:D:453:PRO:HA	1:D:489:GLN:NE2	1.83	0.92
1:C:372:MET:SD	1:C:576:LEU:HD23	2.10	0.92
3:K:32:DC:H1'	3:K:33:DT:H2'	1.51	0.92
2:W:27:DA:C2'	2:W:28:DA:H5'	2.01	0.91
1:C:450:VAL:HG11	1:C:494:LEU:HD23	1.52	0.91
1:C:453:PRO:HG2	1:C:456:ARG:HB2	1.53	0.90
2:W:15:DC:H2"	2:W:16:DA:H5'	1.53	0.89
1:A:450:VAL:HG11	1:A:494:LEU:HD23	1.52	0.88
1:E:472:PHE:HB2	1:E:526:VAL:HG23	1.55	0.88
2:W:30:DT:H3	3:K:3:DA:H2	0.88	0.88
3:K:15:DT:H2"	3:K:16:DA:H5'	1.56	0.88
2:W:30:DT:C4	3:K:3:DA:H2	1.92	0.88
1:C:472:PHE:HB2	1:C:526:VAL:HG23	1.55	0.88
1:A:517:ARG:HB3	1:A:517:ARG:NH1	1.89	0.87
1:A:534:PRO:HD2	1:A:537:LEU:HD23	1.57	0.87
3:K:25:DC:H2'	3:K:26:DC:C6	2.10	0.87
1:E:372:MET:SD	1:E:576:LEU:HD23	2.14	0.86
1:C:517:ARG:HB3	1:C:517:ARG:NH1	1.91	0.86
1:B:266:LYS:O	1:B:267:GLN:HB2	1.74	0.86
1:B:535:LYS:H	1:B:535:LYS:HD2	1.40	0.86
2:W:19:DA:N6	3:K:14:DT:O2	2.09	0.85
1:F:535:LYS:H	1:F:535:LYS:HD2	1.40	0.85
2:W:29:DA:C2	3:K:4:DT:O2	2.28	0.85
1:A:482:SER:C	1:A:483:ARG:O	1.98	0.85
1:E:517:ARG:HB3	1:E:517:ARG:NH1	1.91	0.85
1:E:535:LYS:HD2	1:E:535:LYS:H	1.40	0.85
1:A:472:PHE:HB2	1:A:526:VAL:HG23	1.59	0.85
1:A:372:MET:SD	1:A:576:LEU:HD23	2.16	0.84
1:E:331:LYS:NZ	1:F:267:GLN:NE2	2.25	0.84
1:E:450:VAL:HG11	1:E:494:LEU:HD23	1.56	0.84
3:K:31:DC:H2"	3:K:32:DC:H5'	1.60	0.84
1:F:465:ILE:HD12	1:F:511:LYS:HB2	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:27:DA:N6	3:K:5:DT:O2	2.11	0.84
1:B:465:ILE:HD12	1:B:511:LYS:HB2	1.57	0.84
1:C:535:LYS:HD2	1:C:535:LYS:H	1.41	0.84
2:W:7:DG:N1	3:K:26:DC:O2	2.08	0.83
2:W:11:DT:H3	3:K:22:DA:H61	1.25	0.83
2:W:4:DC:H4'	2:W:5:DT:OP1	1.77	0.83
1:A:397:LEU:HG	1:A:398:LEU:HD13	1.60	0.83
1:A:498:ARG:HG3	1:A:540:ARG:HH21	1.44	0.83
1:D:465:ILE:HD12	1:D:511:LYS:HB2	1.59	0.83
1:D:535:LYS:H	1:D:535:LYS:HD2	1.41	0.83
2:W:20:DA:H61	3:K:13:DT:H3	1.27	0.83
1:D:477:GLY:N	1:D:490:GLY:O	2.12	0.82
3:K:2:DA:H2''	3:K:3:DA:C8	2.13	0.82
1:E:475:VAL:HG21	1:E:491:ILE:CD1	2.09	0.82
1:D:490:GLY:O	1:D:491:ILE:HB	1.79	0.82
1:E:331:LYS:NZ	1:F:267:GLN:HE22	1.76	0.82
3:K:3:DA:H2'	3:K:4:DT:C6	2.15	0.81
3:K:12:DA:H4'	3:K:13:DT:OP1	1.77	0.81
1:C:449:ASN:HD21	1:C:451:ASN:HB2	1.47	0.81
1:C:498:ARG:HG3	1:C:540:ARG:HH21	1.43	0.81
1:A:449:ASN:HD22	1:A:452:LEU:HD23	1.46	0.80
1:A:505:VAL:HG21	1:F:433:THR:HG22	1.62	0.80
1:B:581:TRP:O	1:B:582:TYR:CG	2.34	0.80
1:B:583:ARG:HG3	1:B:587:GLU:OE1	1.80	0.80
1:C:449:ASN:HD22	1:C:452:LEU:HD23	1.46	0.80
1:E:462:GLY:HA3	1:E:511:LYS:HB2	1.64	0.80
2:W:21:DT:H2''	2:W:22:DA:O5'	1.82	0.80
3:K:10:DT:C2'	3:K:11:DT:H5'	2.11	0.79
1:E:452:LEU:HB3	1:E:453:PRO:HD2	1.64	0.79
1:B:517:ARG:NH1	1:B:517:ARG:HB3	1.97	0.79
1:E:449:ASN:HD22	1:E:452:LEU:HD23	1.47	0.79
1:D:349:ARG:HH11	1:D:349:ARG:HB2	1.48	0.79
2:W:11:DT:H3	3:K:22:DA:N6	1.81	0.79
1:A:452:LEU:HB3	1:A:453:PRO:HD2	1.64	0.78
1:B:453:PRO:HA	1:B:489:GLN:HE22	1.47	0.78
1:D:266:LYS:O	1:D:267:GLN:CB	2.32	0.78
1:B:349:ARG:HH11	1:B:349:ARG:HB2	1.48	0.78
1:F:453:PRO:HA	1:F:489:GLN:HE22	1.49	0.78
1:B:425:LYS:NZ	1:B:530:GLU:HA	1.97	0.78
1:F:517:ARG:HB3	1:F:517:ARG:NH1	1.98	0.78
1:A:449:ASN:HD21	1:A:451:ASN:HB2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:ARG:HB3	1:D:517:ARG:NH1	1.99	0.77
2:W:1:DG:H2''	2:W:2:DG:OP2	1.82	0.77
1:C:452:LEU:HB3	1:C:453:PRO:HD2	1.67	0.77
1:B:581:TRP:O	1:B:582:TYR:CB	2.31	0.77
1:F:511:LYS:HE2	1:F:511:LYS:HA	1.67	0.76
1:D:425:LYS:NZ	1:D:530:GLU:HA	2.00	0.76
3:K:6:DT:H1'	3:K:7:DT:O4'	1.84	0.76
1:B:387:TRP:CZ3	1:B:573:ILE:HB	2.20	0.76
1:B:415:ASN:HD21	1:B:420:ARG:HH11	1.32	0.76
1:D:398:LEU:HD21	1:D:545:ILE:HG21	1.68	0.76
1:D:476:LYS:C	1:D:490:GLY:HA3	2.05	0.76
1:E:498:ARG:HG3	1:E:540:ARG:HH21	1.49	0.76
2:W:25:DA:N1	3:K:8:DT:O2	2.19	0.76
1:A:559:ARG:HB2	1:A:559:ARG:NH1	2.01	0.75
1:E:559:ARG:HB2	1:E:559:ARG:NH1	2.01	0.75
1:E:449:ASN:HD21	1:E:451:ASN:HB2	1.51	0.75
1:E:397:LEU:O	1:E:398:LEU:HD12	1.87	0.75
1:F:387:TRP:CZ3	1:F:573:ILE:HB	2.21	0.75
1:B:578:MET:O	1:B:581:TRP:O	2.04	0.75
1:C:559:ARG:HB2	1:C:559:ARG:NH1	2.02	0.75
2:W:16:DA:H2''	2:W:17:DT:C7	2.17	0.75
1:C:451:ASN:ND2	1:C:490:GLY:HA2	2.01	0.75
1:D:387:TRP:CZ3	1:D:573:ILE:HB	2.21	0.75
1:B:415:ASN:ND2	1:B:420:ARG:HD2	2.01	0.75
1:C:397:LEU:O	1:C:398:LEU:HD12	1.87	0.74
1:A:475:VAL:HG21	1:A:491:ILE:HD13	1.69	0.74
1:B:398:LEU:HD21	1:B:545:ILE:HG21	1.68	0.74
1:D:266:LYS:O	1:D:267:GLN:HB2	1.86	0.74
1:D:490:GLY:O	1:D:491:ILE:CB	2.34	0.74
1:F:425:LYS:NZ	1:F:530:GLU:HA	2.01	0.74
1:D:511:LYS:HA	1:D:511:LYS:HE2	1.68	0.74
1:F:415:ASN:HD21	1:F:420:ARG:HH11	1.35	0.74
2:W:20:DA:N6	3:K:13:DT:H3	1.86	0.74
1:F:349:ARG:HH11	1:F:349:ARG:HB2	1.49	0.74
1:A:488:GLY:O	1:A:489:GLN:HG3	1.88	0.74
1:F:398:LEU:HD21	1:F:545:ILE:HG21	1.68	0.74
1:C:475:VAL:HG21	1:C:491:ILE:HD13	1.69	0.73
2:W:28:DA:H1'	2:W:29:DA:O5'	1.87	0.73
1:B:511:LYS:HE2	1:B:511:LYS:HA	1.70	0.73
1:B:570:GLN:HE21	1:C:504:SER:HB3	1.53	0.73
1:A:556:CYS:SG	1:A:619:VAL:HG22	2.28	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:15:DT:C2'	3:K:16:DA:H5'	2.19	0.73
1:D:415:ASN:HD21	1:D:420:ARG:HH11	1.36	0.73
1:C:397:LEU:HG	1:C:398:LEU:HD13	1.68	0.73
2:W:5:DT:H3	3:K:28:DA:N6	1.84	0.73
1:E:488:GLY:O	1:E:489:GLN:HB2	1.89	0.72
1:A:267:GLN:HE22	1:F:331:LYS:HD3	1.54	0.72
2:W:16:DA:H2''	2:W:17:DT:C5	2.23	0.72
1:D:467:GLN:HA	1:D:467:GLN:NE2	2.04	0.72
1:D:467:GLN:HA	1:D:467:GLN:HE21	1.53	0.72
1:A:516:LYS:HG3	1:A:517:ARG:HG3	1.72	0.72
1:E:570:GLN:HE21	1:F:504:SER:HB3	1.53	0.72
1:D:395:HIS:HD2	1:D:401:MET:HB3	1.55	0.72
1:E:488:GLY:O	1:E:489:GLN:CB	2.37	0.72
1:A:462:GLY:HA3	1:A:511:LYS:HB2	1.72	0.71
1:E:473:GLU:OE2	1:E:474:ASP:OD1	2.07	0.71
2:W:27:DA:H1'	2:W:28:DA:C5'	2.20	0.71
1:C:516:LYS:HG3	1:C:517:ARG:HG3	1.72	0.71
1:E:516:LYS:HG3	1:E:517:ARG:HG3	1.73	0.71
3:K:31:DC:C2'	3:K:32:DC:H5'	2.20	0.71
1:F:467:GLN:HA	1:F:467:GLN:HE21	1.56	0.71
1:F:584:PRO:HG2	1:F:587:GLU:HG3	1.72	0.71
1:A:453:PRO:HG2	1:A:456:ARG:HB2	1.72	0.71
1:D:584:PRO:HG2	1:D:587:GLU:HG3	1.73	0.70
1:A:570:GLN:HE21	1:B:504:SER:HB3	1.56	0.70
1:E:394:LEU:O	1:E:401:MET:HG2	1.90	0.70
1:F:467:GLN:HA	1:F:467:GLN:NE2	2.05	0.70
1:A:534:PRO:HD2	1:A:537:LEU:CD2	2.22	0.70
1:B:453:PRO:HA	1:B:489:GLN:NE2	2.07	0.70
1:E:584:PRO:HG2	1:E:587:GLU:HG3	1.74	0.70
1:B:584:PRO:HG2	1:B:587:GLU:HG3	1.73	0.70
2:W:15:DC:C2'	2:W:16:DA:H5'	2.22	0.70
1:A:488:GLY:O	1:A:489:GLN:CB	2.39	0.69
1:B:581:TRP:O	1:B:582:TYR:HB2	1.90	0.69
1:F:512:LYS:HG3	3:K:5:DT:OP2	1.92	0.69
2:W:28:DA:H1'	2:W:29:DA:C5'	2.22	0.69
1:D:295:PHE:HE1	1:D:313:HIS:HD1	1.39	0.69
1:F:295:PHE:HE1	1:F:313:HIS:HD1	1.40	0.69
1:B:581:TRP:O	1:B:582:TYR:CD2	2.46	0.69
1:E:505:VAL:HG21	1:D:433:THR:HG22	1.72	0.69
1:B:266:LYS:O	1:B:267:GLN:CB	2.41	0.69
1:C:570:GLN:HE21	1:D:504:SER:HB3	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLN:NE2	1:F:331:LYS:HD3	2.07	0.69
1:B:467:GLN:NE2	1:B:467:GLN:HA	2.07	0.69
2:W:10:DC:H2"	2:W:11:DT:C7	2.23	0.69
1:B:295:PHE:HE1	1:B:313:HIS:HD1	1.39	0.69
1:B:433:THR:HG22	1:C:505:VAL:HG21	1.74	0.69
3:K:1:DT:H2"	3:K:2:DA:N7	2.08	0.68
2:W:19:DA:H1'	2:W:20:DA:H5'	1.75	0.68
1:A:584:PRO:HG2	1:A:587:GLU:HG3	1.75	0.68
1:F:285:VAL:HG21	1:F:338:GLN:HE22	1.59	0.68
1:A:397:LEU:O	1:A:398:LEU:HD12	1.93	0.68
1:B:425:LYS:HZ3	1:B:530:GLU:HA	1.58	0.68
1:C:440:LEU:HD11	1:C:445:GLY:O	1.94	0.68
1:C:457:LEU:HD21	1:C:493:ASN:HB3	1.76	0.68
1:C:443:CYS:HB3	1:C:468:PHE:CD2	2.30	0.67
1:C:512:LYS:HG3	2:W:29:DA:OP1	1.94	0.67
2:W:28:DA:H2"	2:W:29:DA:C8	2.29	0.67
1:C:425:LYS:HD2	1:C:544:GLN:OE1	1.95	0.67
1:E:443:CYS:HB3	1:E:468:PHE:CD2	2.30	0.67
1:A:285:VAL:HG13	1:A:337:CYS:O	1.95	0.67
1:B:467:GLN:HE21	1:B:467:GLN:HA	1.58	0.67
1:A:406:TYR:HE2	1:A:587:GLU:HB3	1.60	0.67
1:C:454:LEU:HD23	1:C:454:LEU:O	1.94	0.67
1:E:425:LYS:HD2	1:E:544:GLN:OE1	1.95	0.67
1:F:584:PRO:HD2	1:F:587:GLU:OE1	1.95	0.67
1:B:534:PRO:HG2	1:B:537:LEU:HB3	1.76	0.66
1:D:584:PRO:HD2	1:D:587:GLU:OE1	1.96	0.66
1:C:394:LEU:O	1:C:401:MET:HG2	1.96	0.66
1:C:584:PRO:HG2	1:C:587:GLU:HG3	1.76	0.66
1:D:498:ARG:NH1	1:D:498:ARG:HB3	2.10	0.66
1:E:298:SER:O	1:E:302:CYS:HB2	1.94	0.66
1:A:298:SER:O	1:A:302:CYS:HB2	1.95	0.66
1:A:443:CYS:HB3	1:A:468:PHE:CD2	2.31	0.66
1:F:583:ARG:HD2	1:F:583:ARG:H	1.61	0.66
1:A:430:SER:H	1:A:432:LYS:HZ1	1.43	0.66
1:B:347:LYS:HA	1:B:350:VAL:HG12	1.78	0.66
1:F:267:GLN:HG3	1:F:268:VAL:N	2.10	0.66
3:K:1:DT:H2"	3:K:2:DA:C8	2.31	0.66
1:B:498:ARG:HB3	1:B:498:ARG:NH1	2.11	0.66
1:D:425:LYS:HZ3	1:D:530:GLU:HA	1.60	0.66
1:F:590:GLN:HA	1:F:593:GLN:HE21	1.61	0.66
1:A:488:GLY:O	1:A:489:GLN:CG	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:SER:O	1:C:302:CYS:HB2	1.94	0.65
1:F:285:VAL:HG21	1:F:338:GLN:NE2	2.10	0.65
1:C:462:GLY:HA3	1:C:511:LYS:HB2	1.78	0.65
1:B:387:TRP:HZ3	1:B:573:ILE:HB	1.61	0.65
3:K:22:DA:H2"	3:K:23:DG:C8	2.32	0.65
3:K:3:DA:H2'	3:K:4:DT:C5	2.30	0.65
2:W:27:DA:N3	2:W:28:DA:O4'	2.29	0.65
1:A:451:ASN:ND2	1:A:490:GLY:HA2	2.12	0.65
1:C:448:LEU:HD22	1:C:460:GLU:HG3	1.79	0.65
1:A:477:GLY:O	1:A:531:TYR:HD2	1.79	0.65
1:A:425:LYS:HD2	1:A:544:GLN:OE1	1.96	0.65
1:C:554:LYS:O	1:C:558:GLU:HG3	1.95	0.65
1:A:440:LEU:HD11	1:A:445:GLY:O	1.96	0.65
1:D:364:ARG:HH12	1:D:444:GLY:CA	2.09	0.65
1:A:454:LEU:O	1:A:454:LEU:HD23	1.96	0.65
1:E:448:LEU:HD22	1:E:460:GLU:HG3	1.79	0.65
2:W:18:DA:H2"	2:W:19:DA:H5'	1.78	0.65
1:C:333:GLN:HG3	1:D:339:GLN:OE1	1.97	0.64
1:E:427:PRO:HD2	1:E:547:PHE:O	1.98	0.64
1:E:473:GLU:HA	1:E:473:GLU:OE1	1.97	0.64
1:E:406:TYR:HE2	1:E:587:GLU:HB3	1.60	0.64
1:C:406:TYR:HE2	1:C:587:GLU:HB3	1.61	0.64
1:E:451:ASN:ND2	1:E:490:GLY:HA2	2.12	0.64
3:K:25:DC:H2'	3:K:26:DC:C5	2.32	0.64
2:W:27:DA:C1'	2:W:28:DA:H5'	2.27	0.64
1:B:590:GLN:HA	1:B:593:GLN:HE21	1.61	0.64
1:E:485:LEU:HD13	1:E:531:TYR:CZ	2.33	0.64
1:E:397:LEU:HG	1:E:398:LEU:HD13	1.78	0.64
1:D:590:GLN:HA	1:D:593:GLN:HE21	1.62	0.64
1:F:498:ARG:NH1	1:F:498:ARG:HB3	2.12	0.64
1:A:481:GLU:O	1:A:483:ARG:O	2.16	0.64
1:A:485:LEU:HD13	1:A:531:TYR:CZ	2.32	0.64
1:D:583:ARG:H	1:D:583:ARG:HD2	1.62	0.64
1:E:406:TYR:CE2	1:E:587:GLU:HB3	2.33	0.64
1:F:387:TRP:HZ3	1:F:573:ILE:HB	1.63	0.64
1:A:428:ILE:N	1:A:529:ASN:HD22	1.95	0.63
1:C:485:LEU:HD13	1:C:531:TYR:CZ	2.33	0.63
1:E:467:GLN:HE21	1:E:467:GLN:HA	1.63	0.63
2:W:13:DT:H2"	2:W:14:DG:C8	2.33	0.63
1:D:347:LYS:HA	1:D:350:VAL:HG12	1.79	0.63
2:W:27:DA:H1'	2:W:28:DA:H5"	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLN:HE21	1:A:328:ALA:HB2	1.63	0.63
1:C:473:GLU:HA	1:C:473:GLU:OE1	1.99	0.63
1:F:462:GLY:O	1:F:465:ILE:HG13	1.98	0.63
1:F:583:ARG:N	1:F:583:ARG:HD2	2.13	0.63
1:A:477:GLY:O	1:A:478:THR:C	2.37	0.63
1:C:525:ILE:HG22	1:C:526:VAL:N	2.13	0.63
1:E:504:SER:HB3	1:D:570:GLN:HE21	1.63	0.63
1:D:387:TRP:HZ3	1:D:573:ILE:HB	1.62	0.63
2:W:1:DG:O6	3:K:32:DC:O2	2.17	0.63
1:A:406:TYR:CE2	1:A:587:GLU:HB3	2.33	0.63
1:C:467:GLN:HA	1:C:467:GLN:HE21	1.64	0.63
1:E:454:LEU:HD23	1:E:454:LEU:O	1.99	0.63
1:B:584:PRO:HD2	1:B:587:GLU:OE1	1.99	0.63
1:D:490:GLY:O	1:D:491:ILE:HG12	1.98	0.63
1:C:430:SER:H	1:C:432:LYS:HZ2	1.47	0.62
1:C:556:CYS:SG	1:C:619:VAL:HG22	2.39	0.62
1:F:453:PRO:HA	1:F:489:GLN:NE2	2.13	0.62
1:F:548:ARG:HH11	1:F:548:ARG:HG2	1.64	0.62
1:A:448:LEU:HD22	1:A:460:GLU:HG3	1.81	0.62
1:A:467:GLN:HA	1:A:467:GLN:HE21	1.63	0.62
1:E:525:ILE:HG22	1:E:526:VAL:N	2.14	0.62
3:K:31:DC:H1'	3:K:32:DC:H5'	1.81	0.62
2:W:10:DC:H2''	2:W:11:DT:H71	1.82	0.62
1:A:267:GLN:HG3	1:A:268:VAL:N	2.14	0.62
1:F:347:LYS:HA	1:F:350:VAL:HG12	1.80	0.62
1:A:394:LEU:O	1:A:401:MET:HG2	1.99	0.62
1:C:296:GLN:HE21	1:C:328:ALA:HB2	1.63	0.62
1:E:526:VAL:HG11	1:E:541:PHE:CZ	2.34	0.62
1:C:406:TYR:CE2	1:C:587:GLU:HB3	2.34	0.62
1:D:548:ARG:HG2	1:D:548:ARG:HH11	1.65	0.62
1:A:504:SER:HB3	1:F:570:GLN:HE21	1.65	0.62
1:B:583:ARG:CG	1:B:583:ARG:NH1	2.57	0.62
1:D:583:ARG:N	1:D:583:ARG:HD2	2.13	0.62
1:A:525:ILE:HG22	1:A:526:VAL:N	2.15	0.61
1:E:459:PHE:O	1:E:511:LYS:HD3	2.00	0.61
1:F:387:TRP:O	1:F:391:VAL:HG23	2.01	0.61
2:W:23:DA:C2	3:K:10:DT:O2	2.54	0.61
1:E:556:CYS:SG	1:E:619:VAL:HG22	2.40	0.61
1:A:449:ASN:ND2	1:A:451:ASN:HB2	2.16	0.61
1:A:535:LYS:CD	1:A:535:LYS:H	2.09	0.61
1:C:449:ASN:ND2	1:C:451:ASN:HB2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:395:HIS:HD2	1:F:401:MET:HB3	1.64	0.61
1:B:548:ARG:HG2	1:B:548:ARG:HH11	1.64	0.61
2:W:27:DA:H1'	2:W:28:DA:H5'	1.80	0.61
1:A:526:VAL:HG11	1:A:541:PHE:CZ	2.35	0.61
1:B:387:TRP:O	1:B:391:VAL:HG23	2.01	0.61
1:E:388:MET:HA	1:E:391:VAL:HG23	1.83	0.61
1:E:462:GLY:CA	1:E:511:LYS:HB2	2.31	0.61
3:K:14:DT:H2''	3:K:15:DT:H73	1.83	0.61
3:K:24:DG:H2''	3:K:25:DC:H5''	1.83	0.61
1:A:488:GLY:O	1:A:489:GLN:HB2	1.99	0.60
1:C:526:VAL:HG11	1:C:541:PHE:CZ	2.35	0.60
1:D:387:TRP:O	1:D:391:VAL:HG23	2.01	0.60
1:E:488:GLY:O	1:E:489:GLN:HG3	2.01	0.60
1:F:332:ASN:HD22	3:K:12:DA:H3'	1.65	0.60
1:E:296:GLN:HE21	1:E:328:ALA:HB2	1.65	0.60
1:D:467:GLN:HE21	1:D:467:GLN:CA	2.14	0.60
1:E:440:LEU:HD11	1:E:445:GLY:O	2.00	0.60
1:F:477:GLY:N	1:F:491:ILE:HG12	2.16	0.60
1:F:375:MET:O	1:F:382:ALA:HB3	2.01	0.60
1:F:364:ARG:HH12	1:F:444:GLY:CA	2.14	0.60
1:B:395:HIS:HD2	1:B:401:MET:HB3	1.65	0.60
2:W:29:DA:C2	3:K:4:DT:C2	2.89	0.60
1:A:388:MET:HA	1:A:391:VAL:HG23	1.83	0.60
1:E:428:ILE:N	1:E:529:ASN:HD22	1.99	0.60
1:A:424:PHE:HB3	1:A:547:PHE:HE2	1.67	0.60
1:C:388:MET:HA	1:C:391:VAL:HG23	1.83	0.60
3:K:1:DT:H1'	3:K:2:DA:C8	2.37	0.60
1:E:424:PHE:HB3	1:E:547:PHE:HE2	1.67	0.60
1:F:425:LYS:HZ3	1:F:530:GLU:HA	1.65	0.60
1:B:415:ASN:HD21	1:B:420:ARG:HD2	1.67	0.60
1:D:375:MET:O	1:D:382:ALA:HB3	2.02	0.60
1:D:400:LYS:HD2	1:D:400:LYS:N	2.16	0.60
2:W:13:DT:H2''	2:W:14:DG:N7	2.17	0.60
1:B:364:ARG:HH12	1:B:444:GLY:CA	2.15	0.59
1:B:400:LYS:N	1:B:400:LYS:HD2	2.17	0.59
1:E:430:SER:H	1:E:432:LYS:HZ2	1.49	0.59
1:C:467:GLN:HA	1:C:467:GLN:NE2	2.18	0.59
1:E:398:LEU:HD11	1:E:547:PHE:HD1	1.68	0.59
3:K:2:DA:H2''	3:K:3:DA:N7	2.17	0.59
1:C:298:SER:HA	1:C:321:TYR:CE2	2.38	0.59
3:K:15:DT:H1'	3:K:16:DA:H5'	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:CYS:HB3	1:C:468:PHE:HD2	1.67	0.59
1:C:368:LEU:O	1:C:372:MET:HG3	2.03	0.59
3:K:17:DT:H4'	3:K:18:DG:OP1	2.02	0.59
1:A:349:ARG:NH1	1:A:349:ARG:HB2	2.18	0.59
1:C:398:LEU:HD11	1:C:547:PHE:HD1	1.68	0.59
1:A:467:GLN:HA	1:A:467:GLN:NE2	2.17	0.58
1:D:364:ARG:HH12	1:D:444:GLY:HA3	1.67	0.58
1:E:298:SER:HA	1:E:321:TYR:CE2	2.38	0.58
1:E:467:GLN:NE2	1:E:467:GLN:HA	2.17	0.58
1:E:417:PRO:HA	1:E:502:ASP:O	2.03	0.58
1:B:361:LEU:HD22	1:B:365:PHE:CE1	2.38	0.58
1:B:477:GLY:N	1:B:491:ILE:HG12	2.18	0.58
1:C:424:PHE:HB3	1:C:547:PHE:HE2	1.68	0.58
1:C:417:PRO:HA	1:C:502:ASP:O	2.04	0.58
1:E:449:ASN:HD22	1:E:452:LEU:CD2	2.16	0.58
1:C:473:GLU:O	1:C:527:THR:CB	2.40	0.58
1:F:293:LEU:HD21	1:F:333:GLN:HE22	1.68	0.58
1:F:293:LEU:HD21	1:F:333:GLN:NE2	2.19	0.58
1:F:361:LEU:HD22	1:F:365:PHE:CE1	2.39	0.58
3:K:4:DT:O2	3:K:4:DT:O4'	2.22	0.58
2:W:14:DG:H2''	2:W:15:DC:C6	2.39	0.58
1:B:462:GLY:O	1:B:465:ILE:HG13	2.03	0.58
1:A:457:LEU:HD21	1:A:493:ASN:HB3	1.85	0.58
1:D:476:LYS:C	1:D:490:GLY:O	2.41	0.58
2:W:2:DG:H2''	2:W:3:DC:O5'	2.04	0.58
1:A:298:SER:HA	1:A:321:TYR:CE2	2.38	0.58
1:A:515:ASN:O	1:A:517:ARG:N	2.37	0.58
1:C:432:LYS:HE2	1:C:529:ASN:ND2	2.19	0.57
1:E:443:CYS:HB3	1:E:468:PHE:HD2	1.68	0.57
1:A:459:PHE:CG	3:K:2:DA:H4'	2.40	0.57
1:C:395:HIS:HB3	1:C:616:LYS:HZ3	1.69	0.57
1:E:449:ASN:ND2	1:E:451:ASN:HB2	2.19	0.57
1:E:483:ARG:HG3	1:E:483:ARG:HH11	1.69	0.57
1:A:505:VAL:HG21	1:F:433:THR:CG2	2.33	0.57
1:A:449:ASN:HD22	1:A:452:LEU:CD2	2.14	0.57
2:W:30:DT:C4	3:K:3:DA:C2	2.83	0.57
1:A:398:LEU:HD11	1:A:547:PHE:HD1	1.69	0.57
1:A:533:VAL:CG2	1:A:538:GLN:HB2	2.34	0.57
1:B:467:GLN:CA	1:B:467:GLN:HE21	2.17	0.57
1:C:525:ILE:HG22	1:C:526:VAL:H	1.68	0.57
1:F:415:ASN:ND2	1:F:420:ARG:HD2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:364:ARG:HH12	1:F:444:GLY:HA3	1.70	0.57
2:W:28:DA:H1'	2:W:29:DA:H5'	1.85	0.57
1:A:417:PRO:HA	1:A:502:ASP:O	2.03	0.57
1:E:333:GLN:HG3	1:F:339:GLN:OE1	2.04	0.57
1:B:517:ARG:HH11	1:B:517:ARG:HB3	1.69	0.57
1:C:405:VAL:HG21	1:C:578:MET:HE1	1.86	0.57
1:D:462:GLY:O	1:D:465:ILE:HG13	2.04	0.57
3:K:14:DT:N1	3:K:15:DT:H72	2.20	0.57
1:A:475:VAL:HG21	1:A:491:ILE:CD1	2.35	0.57
1:C:494:LEU:O	1:C:494:LEU:HD13	2.05	0.57
1:D:477:GLY:HA3	1:D:491:ILE:HB	1.86	0.57
1:E:488:GLY:O	1:E:489:GLN:CG	2.53	0.57
1:B:583:ARG:CG	1:B:587:GLU:OE1	2.51	0.56
1:D:611:VAL:O	1:D:614:LYS:HB3	2.05	0.56
1:F:494:LEU:O	1:F:494:LEU:HD13	2.04	0.56
1:F:583:ARG:HH11	1:F:583:ARG:HG3	1.70	0.56
1:A:459:PHE:CD2	3:K:2:DA:H4'	2.41	0.56
1:E:525:ILE:HG22	1:E:526:VAL:H	1.70	0.56
1:F:400:LYS:N	1:F:400:LYS:HD2	2.19	0.56
1:B:465:ILE:CD1	1:B:511:LYS:HB2	2.32	0.56
1:E:387:TRP:CZ3	1:E:573:ILE:HB	2.40	0.56
1:D:548:ARG:O	1:D:550:LYS:HG3	2.05	0.56
2:W:7:DG:O6	3:K:26:DC:N3	2.39	0.56
1:A:443:CYS:HB3	1:A:468:PHE:HD2	1.69	0.56
1:A:554:LYS:O	1:A:558:GLU:HG3	2.05	0.56
1:D:415:ASN:ND2	1:D:420:ARG:HD2	2.20	0.56
1:E:510:GLU:HB3	1:E:515:ASN:HA	1.88	0.56
1:F:403:SER:HA	1:F:583:ARG:HH21	1.71	0.56
1:A:533:VAL:HG21	1:A:538:GLN:HB2	1.87	0.56
1:D:398:LEU:HD21	1:D:545:ILE:CG2	2.36	0.56
1:D:583:ARG:HG3	1:D:587:GLU:OE1	2.05	0.56
2:W:11:DT:H2''	2:W:12:DC:O4'	2.06	0.56
2:W:18:DA:C2	3:K:15:DT:O2	2.59	0.56
1:A:389:ALA:HB1	1:A:625:VAL:HG11	1.88	0.56
1:A:448:LEU:O	1:A:472:PHE:HA	2.06	0.56
1:A:494:LEU:HD13	1:A:494:LEU:O	2.05	0.56
1:A:515:ASN:O	1:A:516:LYS:C	2.44	0.56
2:W:1:DG:H1'	2:W:2:DG:O4'	2.06	0.56
1:B:364:ARG:HH12	1:B:444:GLY:HA3	1.71	0.56
1:C:451:ASN:HD21	1:C:490:GLY:HA2	1.68	0.56
1:D:583:ARG:HG3	1:D:583:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:LYS:HE2	1:E:529:ASN:HD21	1.70	0.56
1:E:389:ALA:HB1	1:E:625:VAL:HG11	1.88	0.56
1:F:517:ARG:HB3	1:F:517:ARG:HH11	1.69	0.56
1:C:475:VAL:HG21	1:C:491:ILE:CD1	2.35	0.55
1:D:361:LEU:HD22	1:D:365:PHE:CE1	2.40	0.55
1:C:398:LEU:HD11	1:C:547:PHE:CD1	2.42	0.55
1:B:415:ASN:ND2	1:B:420:ARG:CD	2.69	0.55
1:B:513:HIS:NE2	2:W:27:DA:H5''	2.21	0.55
1:D:581:TRP:HZ3	1:D:603:LEU:HB3	1.70	0.55
1:F:583:ARG:HG3	1:F:587:GLU:OE1	2.06	0.55
1:A:525:ILE:HG22	1:A:526:VAL:H	1.71	0.55
1:C:387:TRP:CZ3	1:C:573:ILE:HB	2.40	0.55
1:C:389:ALA:HB1	1:C:625:VAL:HG11	1.89	0.55
1:F:362:THR:HG23	1:F:592:ILE:HD13	1.88	0.55
2:W:6:DC:H2''	2:W:7:DG:H5'	1.88	0.55
1:C:349:ARG:NH1	1:C:349:ARG:HB2	2.22	0.55
1:B:570:GLN:NE2	1:C:504:SER:HB3	2.21	0.55
1:A:398:LEU:HD21	1:A:545:ILE:CG2	2.37	0.55
1:A:550:LYS:HD3	1:A:552:TYR:OH	2.07	0.55
1:C:449:ASN:HD22	1:C:452:LEU:CD2	2.15	0.55
1:C:550:LYS:HD3	1:C:552:TYR:OH	2.07	0.55
1:E:388:MET:HA	1:E:391:VAL:CG2	2.37	0.55
1:F:483:ARG:HH11	1:F:483:ARG:HG3	1.72	0.55
1:C:475:VAL:HG12	1:C:527:THR:O	2.05	0.55
1:D:490:GLY:O	1:D:491:ILE:CG1	2.55	0.55
1:D:494:LEU:O	1:D:494:LEU:HD13	2.06	0.55
1:E:349:ARG:NH1	1:E:349:ARG:HB2	2.22	0.55
1:F:581:TRP:HZ3	1:F:603:LEU:HB3	1.70	0.55
1:F:611:VAL:O	1:F:614:LYS:HB3	2.07	0.55
2:W:30:DT:O4	3:K:3:DA:H2	1.88	0.55
2:W:12:DC:H2'	2:W:13:DT:H71	1.89	0.55
1:B:494:LEU:HD13	1:B:494:LEU:O	2.07	0.55
1:C:361:LEU:O	1:C:364:ARG:HB3	2.07	0.55
1:A:388:MET:HA	1:A:391:VAL:CG2	2.37	0.55
1:D:567:ARG:HH11	1:D:567:ARG:HG3	1.72	0.55
1:A:335:THR:HG23	3:K:11:DT:OP2	2.07	0.55
1:B:398:LEU:HD21	1:B:545:ILE:CG2	2.36	0.55
1:C:303:LEU:HD23	1:C:303:LEU:C	2.27	0.55
1:C:398:LEU:HD21	1:C:545:ILE:CG2	2.37	0.55
1:D:403:SER:HA	1:D:583:ARG:HH21	1.71	0.55
1:E:494:LEU:HD13	1:E:494:LEU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:TRP:CZ3	1:A:573:ILE:HB	2.40	0.54
1:B:285:VAL:HG21	1:B:338:GLN:NE2	2.22	0.54
1:B:375:MET:O	1:B:382:ALA:HB3	2.07	0.54
1:C:448:LEU:O	1:C:472:PHE:HA	2.06	0.54
1:F:465:ILE:CD1	1:F:511:LYS:HB2	2.32	0.54
1:D:588:PHE:CE2	1:D:596:ILE:HG21	2.43	0.54
1:E:398:LEU:HD21	1:E:545:ILE:CG2	2.37	0.54
3:K:31:DC:C1'	3:K:32:DC:H5'	2.37	0.54
2:W:12:DC:H2''	2:W:13:DT:H5'	1.88	0.54
1:B:611:VAL:O	1:B:614:LYS:HB3	2.07	0.54
1:D:581:TRP:CZ3	1:D:603:LEU:HB3	2.43	0.54
1:E:398:LEU:HD11	1:E:547:PHE:CD1	2.42	0.54
1:F:467:GLN:HE21	1:F:467:GLN:CA	2.16	0.54
1:F:417:PRO:HA	1:F:502:ASP:O	2.07	0.54
1:A:395:HIS:HA	1:A:401:MET:HB3	1.89	0.54
1:A:513:HIS:O	1:A:514:LEU:HB2	2.07	0.54
1:B:534:PRO:HG2	1:B:537:LEU:CB	2.38	0.54
1:E:477:GLY:O	1:E:531:TYR:HD2	1.91	0.54
1:E:559:ARG:HB2	1:E:559:ARG:HH11	1.73	0.54
1:D:362:THR:HG23	1:D:592:ILE:HD13	1.89	0.54
2:W:18:DA:N1	3:K:15:DT:C2	2.76	0.54
1:A:459:PHE:O	1:A:511:LYS:HD3	2.08	0.54
1:A:432:LYS:HE2	1:A:529:ASN:ND2	2.22	0.54
1:B:417:PRO:HA	1:B:502:ASP:O	2.08	0.54
1:D:498:ARG:HH11	1:D:498:ARG:CB	2.20	0.54
1:F:615:MET:HB3	1:F:625:VAL:HG13	1.90	0.54
1:A:340:ALA:O	1:A:343:THR:HB	2.08	0.54
2:W:31:DT:H2''	2:W:32:DA:H5'	1.90	0.54
1:D:406:TYR:CE2	1:D:587:GLU:HB3	2.43	0.54
1:E:331:LYS:HZ1	1:F:267:GLN:NE2	1.88	0.54
2:W:20:DA:N1	3:K:13:DT:O2	2.41	0.54
1:A:475:VAL:HG12	1:A:527:THR:O	2.07	0.54
1:B:305:CYS:O	1:B:308:LYS:HD2	2.08	0.54
1:E:451:ASN:HD21	1:E:490:GLY:HA2	1.73	0.54
1:E:331:LYS:HZ3	1:F:267:GLN:NE2	2.02	0.54
1:F:305:CYS:O	1:F:308:LYS:HD2	2.07	0.54
1:F:498:ARG:HH11	1:F:498:ARG:CB	2.21	0.54
2:W:8:DG:H2''	2:W:9:DC:H5''	1.90	0.54
1:A:408:PHE:CE2	1:A:439:LEU:HD13	2.43	0.53
1:C:388:MET:HA	1:C:391:VAL:CG2	2.37	0.53
1:D:285:VAL:HG21	1:D:338:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:GLN:HG3	1:E:268:VAL:N	2.23	0.53
1:E:338:GLN:O	1:E:338:GLN:HG3	2.08	0.53
1:E:432:LYS:HB3	1:E:527:THR:HG22	1.91	0.53
1:F:581:TRP:CZ3	1:F:603:LEU:HB3	2.43	0.53
2:W:29:DA:N1	3:K:4:DT:C2	2.75	0.53
1:A:398:LEU:HD11	1:A:547:PHE:CD1	2.42	0.53
1:A:559:ARG:HB2	1:A:559:ARG:HH11	1.73	0.53
1:A:439:LEU:HD23	1:A:575:LEU:HD13	1.89	0.53
1:B:498:ARG:CB	1:B:498:ARG:HH11	2.21	0.53
1:C:424:PHE:CE2	1:C:435:LEU:HD23	2.43	0.53
1:C:439:LEU:HD23	1:C:575:LEU:HD13	1.89	0.53
2:W:20:DA:H1'	2:W:21:DT:O4'	2.07	0.53
2:W:25:DA:N6	3:K:8:DT:N3	2.35	0.53
2:W:11:DT:H2"	2:W:12:DC:C6	2.43	0.53
1:C:409:LEU:HD21	1:C:442:LEU:HD21	1.90	0.53
1:C:427:PRO:HD2	1:C:547:PHE:O	2.09	0.53
1:D:305:CYS:O	1:D:308:LYS:HD2	2.07	0.53
1:E:303:LEU:C	1:E:303:LEU:HD23	2.29	0.53
1:F:406:TYR:CE2	1:F:587:GLU:HB3	2.44	0.53
2:W:22:DA:H1'	2:W:23:DA:H5'	1.91	0.53
1:E:340:ALA:O	1:E:343:THR:HB	2.08	0.53
1:F:568:ILE:O	1:F:571:SER:HB3	2.08	0.53
1:C:513:HIS:NE2	2:W:28:DA:O3'	2.42	0.53
1:A:285:VAL:HG11	1:A:334:LYS:HD2	1.89	0.53
1:A:511:LYS:NZ	3:K:2:DA:H5"	2.24	0.53
1:D:393:TRP:HE1	1:D:557:LEU:HG	1.74	0.53
1:D:476:LYS:O	1:D:490:GLY:N	2.40	0.53
2:W:12:DC:N3	3:K:21:DG:O6	2.42	0.53
1:E:395:HIS:HA	1:E:401:MET:CB	2.39	0.53
1:E:407:ASP:O	1:E:411:CYS:HB2	2.08	0.53
1:F:614:LYS:O	1:F:617:PHE:HB3	2.09	0.53
2:W:6:DC:N3	3:K:27:DG:O6	2.41	0.53
2:W:18:DA:H1'	2:W:19:DA:H5'	1.90	0.53
1:B:452:LEU:HD11	1:B:460:GLU:OE1	2.09	0.53
1:E:505:VAL:HG21	1:D:433:THR:CG2	2.39	0.53
1:D:498:ARG:HG3	1:D:540:ARG:NE	2.24	0.53
1:E:455:ASP:HB3	1:E:456:ARG:HE	1.73	0.53
1:F:397:LEU:CD1	4:F:702:ADP:HN61	2.22	0.53
2:W:8:DG:H1'	2:W:9:DC:H5"	1.91	0.53
1:A:303:LEU:C	1:A:303:LEU:HD23	2.29	0.53
1:A:361:LEU:O	1:A:364:ARG:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:HD21	1:A:442:LEU:HD21	1.91	0.53
1:A:467:GLN:HE21	1:A:467:GLN:CA	2.22	0.53
1:C:462:GLY:CA	1:C:511:LYS:HB2	2.39	0.53
1:E:439:LEU:HD23	1:E:575:LEU:HD13	1.89	0.53
1:A:407:ASP:O	1:A:411:CYS:HB2	2.09	0.52
1:B:583:ARG:CG	1:B:583:ARG:HH11	1.93	0.52
1:C:465:ILE:O	1:C:467:GLN:HG2	2.08	0.52
1:E:424:PHE:CE2	1:E:435:LEU:HD23	2.43	0.52
1:F:588:PHE:CE2	1:F:596:ILE:HG21	2.44	0.52
2:W:19:DA:H4'	2:W:20:DA:OP1	2.08	0.52
1:B:406:TYR:CE2	1:B:587:GLU:HB3	2.44	0.52
1:C:408:PHE:CE2	1:C:439:LEU:HD13	2.45	0.52
1:C:559:ARG:HB2	1:C:559:ARG:HH11	1.74	0.52
1:D:417:PRO:HA	1:D:502:ASP:O	2.10	0.52
1:E:395:HIS:CD2	1:E:401:MET:HB3	2.45	0.52
1:F:583:ARG:NH1	1:F:583:ARG:HG3	2.25	0.52
2:W:5:DT:H1'	2:W:6:DC:O4'	2.09	0.52
1:A:293:LEU:O	1:A:296:GLN:HG2	2.10	0.52
1:F:267:GLN:HG3	1:F:268:VAL:H	1.72	0.52
1:A:478:THR:HG22	1:A:479:GLY:N	2.24	0.52
1:C:512:LYS:NZ	1:D:514:LEU:HD12	2.25	0.52
1:D:615:MET:HB3	1:D:625:VAL:HG13	1.89	0.52
1:F:498:ARG:HG3	1:F:540:ARG:NE	2.24	0.52
2:W:23:DA:H2	3:K:10:DT:O2	1.92	0.52
1:A:535:LYS:N	1:A:535:LYS:HD2	2.12	0.52
1:B:588:PHE:CE2	1:B:596:ILE:HG21	2.45	0.52
1:C:552:TYR:HB2	1:C:619:VAL:O	2.10	0.52
1:D:469:LEU:C	1:D:469:LEU:HD12	2.29	0.52
1:D:517:ARG:HB3	1:D:517:ARG:HH11	1.71	0.52
1:E:321:TYR:C	1:E:321:TYR:CD1	2.83	0.52
1:F:567:ARG:HG3	1:F:567:ARG:HH11	1.74	0.52
3:K:5:DT:H2''	3:K:6:DT:C5	2.45	0.52
2:W:16:DA:H2''	2:W:17:DT:H71	1.92	0.52
1:C:409:LEU:HD21	1:C:442:LEU:CD2	2.39	0.52
1:E:361:LEU:O	1:E:364:ARG:HB3	2.08	0.52
2:W:21:DT:C2'	2:W:22:DA:C8	2.83	0.52
1:B:615:MET:HB3	1:B:625:VAL:HG13	1.91	0.52
1:D:583:ARG:HG3	1:D:583:ARG:NH1	2.25	0.52
1:D:614:LYS:O	1:D:617:PHE:HB3	2.10	0.52
1:E:425:LYS:O	1:E:547:PHE:N	2.39	0.52
1:F:398:LEU:HD21	1:F:545:ILE:CG2	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:2:DA:H2"	3:K:3:DA:OP2	2.09	0.52
1:B:517:ARG:CB	1:B:517:ARG:HH11	2.23	0.52
1:B:568:ILE:O	1:B:571:SER:HB3	2.10	0.52
1:B:362:THR:HG23	1:B:592:ILE:HD13	1.90	0.52
1:B:614:LYS:O	1:B:617:PHE:HB3	2.10	0.52
1:D:483:ARG:HG3	1:D:483:ARG:HH11	1.75	0.52
1:B:498:ARG:HB3	1:B:498:ARG:HH11	1.75	0.52
1:B:549:PRO:HA	4:B:701:ADP:N1	2.25	0.52
1:C:407:ASP:O	1:C:411:CYS:HB2	2.10	0.52
1:C:467:GLN:CA	1:C:467:GLN:HE21	2.23	0.52
1:E:408:PHE:CE2	1:E:439:LEU:HD13	2.45	0.52
1:F:470:VAL:HG13	1:F:522:PRO:HG2	1.92	0.52
3:K:15:DT:C1'	3:K:16:DA:H5'	2.40	0.52
3:K:29:DG:H2"	3:K:30:DG:OP2	2.10	0.52
2:W:10:DC:N3	3:K:23:DG:O6	2.43	0.52
2:W:30:DT:O4	3:K:3:DA:C2	2.62	0.52
1:A:428:ILE:HA	1:A:529:ASN:ND2	2.24	0.51
1:A:515:ASN:OD1	1:A:517:ARG:O	2.28	0.51
1:B:423:LEU:HB2	1:B:541:PHE:CD2	2.45	0.51
1:E:293:LEU:O	1:E:296:GLN:HG2	2.10	0.51
1:B:403:SER:HA	1:B:583:ARG:HH21	1.74	0.51
1:C:293:LEU:O	1:C:296:GLN:HG2	2.09	0.51
1:C:321:TYR:CD1	1:C:321:TYR:C	2.84	0.51
1:E:361:LEU:O	1:E:365:PHE:HD1	1.94	0.51
1:F:361:LEU:HD22	1:F:365:PHE:HE1	1.75	0.51
1:F:469:LEU:HD12	1:F:469:LEU:C	2.30	0.51
1:A:321:TYR:C	1:A:321:TYR:CD1	2.83	0.51
1:A:409:LEU:HD21	1:A:442:LEU:CD2	2.40	0.51
1:A:424:PHE:CE2	1:A:435:LEU:HD23	2.45	0.51
1:D:477:GLY:HA2	1:D:490:GLY:O	2.02	0.51
2:W:32:DA:H2	3:K:1:DT:O2	1.92	0.51
1:A:267:GLN:HE22	1:F:331:LYS:CD	2.23	0.51
1:B:361:LEU:HD22	1:B:365:PHE:HE1	1.74	0.51
1:D:452:LEU:HD11	1:D:460:GLU:OE1	2.10	0.51
1:D:568:ILE:O	1:D:571:SER:HB3	2.11	0.51
1:F:517:ARG:HH11	1:F:517:ARG:CB	2.23	0.51
2:W:23:DA:N1	3:K:10:DT:C2	2.78	0.51
2:W:22:DA:H61	3:K:11:DT:H3	1.59	0.51
1:C:395:HIS:HD2	1:C:401:MET:HB3	1.76	0.51
1:E:405:VAL:HG21	1:E:578:MET:HE1	1.93	0.51
1:E:465:ILE:O	1:E:467:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:423:LEU:HB2	1:F:541:PHE:CD2	2.46	0.51
2:W:27:DA:H62	3:K:5:DT:H3	1.59	0.51
1:C:506:LYS:HG2	1:C:520:ILE:HG22	1.93	0.51
1:D:465:ILE:CD1	1:D:511:LYS:HB2	2.35	0.51
1:D:593:GLN:O	1:D:597:VAL:HG23	2.11	0.51
1:A:451:ASN:HD21	1:A:490:GLY:HA2	1.76	0.51
1:A:465:ILE:O	1:A:467:GLN:HG2	2.11	0.51
1:C:469:LEU:HD12	1:C:469:LEU:C	2.31	0.51
1:E:395:HIS:HA	1:E:401:MET:HB3	1.92	0.51
1:F:347:LYS:O	1:F:350:VAL:HG12	2.11	0.51
1:B:498:ARG:HG3	1:B:540:ARG:NE	2.26	0.51
1:D:385:GLU:HA	1:D:607:PHE:HZ	1.76	0.51
3:K:5:DT:H2''	3:K:6:DT:C6	2.45	0.51
1:C:513:HIS:CD2	2:W:28:DA:O3'	2.64	0.51
1:D:517:ARG:CB	1:D:517:ARG:HH11	2.25	0.51
1:E:554:LYS:O	1:E:558:GLU:HG3	2.11	0.51
1:F:543:LYS:NZ	1:F:543:LYS:HB2	2.25	0.51
3:K:6:DT:H2'	3:K:6:DT:OP2	2.11	0.51
1:B:525:ILE:HG22	1:B:526:VAL:N	2.25	0.50
1:B:567:ARG:HG3	1:B:567:ARG:HH11	1.76	0.50
1:B:368:LEU:HD22	1:B:573:ILE:HD13	1.92	0.50
1:E:368:LEU:O	1:E:372:MET:HG3	2.11	0.50
1:A:395:HIS:HA	1:A:401:MET:CB	2.41	0.50
1:C:453:PRO:CG	1:C:456:ARG:HB2	2.33	0.50
1:D:477:GLY:N	1:D:491:ILE:HG12	2.27	0.50
1:E:409:LEU:HD21	1:E:442:LEU:CD2	2.41	0.50
1:E:506:LYS:HG2	1:E:520:ILE:HG22	1.92	0.50
1:F:383:ASP:OD1	1:F:385:GLU:HB3	2.11	0.50
2:W:18:DA:C2'	2:W:19:DA:H5'	2.40	0.50
2:W:2:DG:O6	3:K:31:DC:N3	2.44	0.50
1:D:295:PHE:O	1:D:321:TYR:HA	2.11	0.50
1:D:347:LYS:O	1:D:350:VAL:HG12	2.11	0.50
1:D:525:ILE:HG22	1:D:526:VAL:N	2.26	0.50
1:E:457:LEU:HD21	1:E:493:ASN:HB3	1.92	0.50
1:F:452:LEU:HD11	1:F:460:GLU:OE1	2.12	0.50
1:A:408:PHE:CD2	1:A:439:LEU:HD13	2.46	0.50
1:A:506:LYS:HG2	1:A:520:ILE:HG22	1.93	0.50
1:B:347:LYS:O	1:B:350:VAL:HG12	2.11	0.50
1:E:409:LEU:HD21	1:E:442:LEU:HD21	1.92	0.50
1:E:469:LEU:HD12	1:E:469:LEU:C	2.32	0.50
1:F:368:LEU:HD22	1:F:573:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:29:DA:OP2	2:W:29:DA:H8	1.94	0.50
1:A:401:MET:HG3	1:A:578:MET:CE	2.41	0.50
1:B:548:ARG:NH1	1:B:548:ARG:HG2	2.27	0.50
1:B:576:LEU:O	1:B:580:ILE:HG12	2.12	0.50
1:C:535:LYS:CD	1:C:535:LYS:H	2.19	0.50
1:C:543:LYS:NZ	1:C:543:LYS:HB2	2.26	0.50
1:D:368:LEU:HD22	1:D:573:ILE:HD13	1.92	0.50
1:F:332:ASN:ND2	3:K:12:DA:H3'	2.26	0.50
1:F:395:HIS:CD2	1:F:401:MET:HB3	2.47	0.50
1:A:408:PHE:O	1:A:411:CYS:HB3	2.11	0.50
1:B:543:LYS:HB2	1:B:543:LYS:NZ	2.26	0.50
1:C:556:CYS:HB2	1:C:622:GLY:HA2	1.94	0.50
1:F:295:PHE:O	1:F:321:TYR:HA	2.12	0.50
1:F:483:ARG:NH1	1:F:483:ARG:HG3	2.26	0.50
2:W:12:DC:H2'	2:W:13:DT:C7	2.41	0.50
2:W:24:DA:H2	3:K:9:DT:O2	1.94	0.50
1:C:361:LEU:O	1:C:365:PHE:HD1	1.95	0.50
1:D:492:ASN:O	1:D:495:ASP:HB3	2.11	0.50
1:E:543:LYS:NZ	1:E:543:LYS:HB2	2.27	0.50
1:C:609:LEU:HD22	1:C:613:GLN:OE1	2.12	0.50
1:D:282:CYS:SG	1:D:287:LEU:HD23	2.51	0.50
1:D:543:LYS:HB2	1:D:543:LYS:NZ	2.27	0.50
1:A:477:GLY:O	1:A:531:TYR:CD2	2.64	0.50
1:B:489:GLN:CB	1:B:493:ASN:HD21	2.25	0.50
1:D:478:THR:HA	1:D:481:GLU:OE1	2.12	0.50
1:E:408:PHE:CD2	1:E:439:LEU:HD13	2.47	0.50
1:F:449:ASN:N	1:F:460:GLU:OE2	2.43	0.50
1:F:548:ARG:O	1:F:550:LYS:HG3	2.12	0.50
3:K:2:DA:C2'	3:K:3:DA:N7	2.75	0.50
1:B:492:ASN:O	1:B:495:ASP:HB3	2.11	0.49
1:C:340:ALA:O	1:C:343:THR:HB	2.11	0.49
1:C:415:ASN:ND2	1:C:523:PRO:HD3	2.27	0.49
1:D:383:ASP:OD1	1:D:385:GLU:HB3	2.12	0.49
3:K:1:DT:C2'	3:K:2:DA:C8	2.95	0.49
1:A:425:LYS:O	1:A:547:PHE:N	2.37	0.49
1:A:609:LEU:HD22	1:A:613:GLN:OE1	2.12	0.49
1:C:417:PRO:HG3	1:C:503:GLY:O	2.11	0.49
1:E:372:MET:HA	1:E:375:MET:HG2	1.94	0.49
1:E:588:PHE:CD2	1:E:596:ILE:HG13	2.48	0.49
1:E:609:LEU:HD22	1:E:613:GLN:OE1	2.11	0.49
1:F:498:ARG:HB3	1:F:498:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:GLU:HA	1:F:607:PHE:HZ	1.76	0.49
3:K:14:DT:H2"	3:K:15:DT:C7	2.42	0.49
1:B:383:ASP:OD1	1:B:385:GLU:HB3	2.11	0.49
1:C:372:MET:HA	1:C:375:MET:HG2	1.93	0.49
1:A:533:VAL:O	1:A:533:VAL:HG13	2.12	0.49
1:B:478:THR:HG22	1:B:479:GLY:N	2.27	0.49
1:C:400:LYS:N	1:C:400:LYS:HD2	2.28	0.49
1:C:408:PHE:CD2	1:C:439:LEU:HD13	2.47	0.49
1:E:453:PRO:HG2	1:E:456:ARG:HB2	1.94	0.49
1:E:483:ARG:O	1:E:484:ASP:HB3	2.11	0.49
2:W:22:DA:H4'	2:W:23:DA:C5'	2.42	0.49
2:W:3:DC:O2	3:K:30:DG:N2	2.45	0.49
1:B:449:ASN:N	1:B:460:GLU:OE2	2.44	0.49
1:C:584:PRO:HD2	1:C:587:GLU:OE1	2.13	0.49
1:A:372:MET:HA	1:A:375:MET:HG2	1.94	0.49
1:A:498:ARG:NH1	1:A:498:ARG:HB3	2.27	0.49
1:C:298:SER:HA	1:C:321:TYR:CD2	2.48	0.49
1:C:498:ARG:HG3	1:C:540:ARG:NH2	2.22	0.49
1:D:496:ASN:C	1:D:498:ARG:H	2.16	0.49
1:E:556:CYS:HB2	1:E:622:GLY:HA2	1.94	0.49
3:K:32:DC:C4'	3:K:33:DT:H5'	2.42	0.49
2:W:27:DA:N6	3:K:5:DT:C2	2.81	0.49
1:A:287:LEU:HG	1:A:291:MET:CE	2.43	0.49
1:B:295:PHE:O	1:B:321:TYR:HA	2.13	0.49
1:B:469:LEU:C	1:B:469:LEU:HD12	2.32	0.49
1:E:400:LYS:HD2	1:E:400:LYS:N	2.28	0.49
1:E:467:GLN:HE21	1:E:467:GLN:CA	2.21	0.49
1:A:442:LEU:HD12	1:A:572:GLY:O	2.12	0.49
1:B:483:ARG:HG3	1:B:483:ARG:HH11	1.76	0.49
1:C:439:LEU:CD2	1:C:575:LEU:HD13	2.43	0.49
1:C:534:PRO:HD2	1:C:537:LEU:HD23	1.93	0.49
1:C:401:MET:HG3	1:C:578:MET:CE	2.43	0.49
1:D:393:TRP:CZ3	1:D:397:LEU:HD13	2.48	0.49
1:D:423:LEU:HB2	1:D:541:PHE:CD2	2.47	0.49
1:E:498:ARG:HB3	1:E:498:ARG:NH1	2.27	0.49
1:F:478:THR:HA	1:F:481:GLU:OE1	2.13	0.49
1:F:576:LEU:O	1:F:580:ILE:HG12	2.13	0.49
1:A:398:LEU:HD21	1:A:545:ILE:HG21	1.94	0.49
1:B:414:TYR:O	1:B:415:ASN:C	2.49	0.49
1:B:609:LEU:O	1:B:609:LEU:HD23	2.13	0.49
1:C:349:ARG:NH2	1:C:516:LYS:HE3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:MET:HG3	1:E:578:MET:CE	2.42	0.49
1:E:584:PRO:HD2	1:E:587:GLU:OE1	2.12	0.49
1:F:513:HIS:O	1:F:515:ASN:N	2.46	0.49
3:K:12:DA:H1'	3:K:13:DT:O5'	2.13	0.49
1:D:293:LEU:O	1:D:296:GLN:HG2	2.13	0.49
1:A:364:ARG:O	1:A:368:LEU:HG	2.12	0.48
1:E:439:LEU:CD2	1:E:575:LEU:HD13	2.43	0.48
1:F:548:ARG:HG2	1:F:548:ARG:NH1	2.27	0.48
1:A:504:SER:HB3	1:F:570:GLN:NE2	2.28	0.48
1:A:298:SER:HA	1:A:321:TYR:CD2	2.48	0.48
1:A:361:LEU:O	1:A:365:PHE:HD1	1.96	0.48
1:D:513:HIS:O	1:D:515:ASN:N	2.45	0.48
1:E:442:LEU:HD12	1:E:572:GLY:O	2.13	0.48
1:A:368:LEU:O	1:A:372:MET:HG3	2.11	0.48
1:B:478:THR:HA	1:B:481:GLU:OE1	2.13	0.48
1:C:408:PHE:O	1:C:411:CYS:HB3	2.13	0.48
1:D:470:VAL:HG13	1:D:522:PRO:HG2	1.94	0.48
1:D:476:LYS:O	1:D:490:GLY:C	2.50	0.48
1:D:483:ARG:NH1	1:D:483:ARG:HG3	2.28	0.48
1:F:535:LYS:H	1:F:535:LYS:CD	2.21	0.48
3:K:15:DT:O2	3:K:16:DA:O4'	2.31	0.48
1:A:439:LEU:CD2	1:A:575:LEU:HD13	2.43	0.48
1:A:543:LYS:NZ	1:A:543:LYS:HB2	2.27	0.48
1:B:496:ASN:C	1:B:498:ARG:H	2.17	0.48
1:F:593:GLN:O	1:F:597:VAL:HG23	2.12	0.48
3:K:32:DC:H1'	3:K:33:DT:C2'	2.36	0.48
1:A:405:VAL:HG21	1:A:578:MET:HE1	1.96	0.48
1:A:287:LEU:HD13	1:B:353:LEU:HD12	1.96	0.48
1:D:548:ARG:NH1	1:D:548:ARG:HG2	2.28	0.48
1:E:448:LEU:O	1:E:472:PHE:HA	2.13	0.48
1:A:339:GLN:NE2	1:F:333:GLN:H	2.11	0.48
1:A:290:GLY:CA	1:B:346:ALA:HB1	2.44	0.48
1:A:469:LEU:HD12	1:A:469:LEU:C	2.33	0.48
1:B:389:ALA:HB1	1:B:625:VAL:HG11	1.96	0.48
1:C:398:LEU:HD21	1:C:545:ILE:HG21	1.95	0.48
1:C:588:PHE:CD2	1:C:596:ILE:HG13	2.49	0.48
1:D:465:ILE:O	1:D:467:GLN:HG2	2.13	0.48
1:E:408:PHE:O	1:E:411:CYS:HB3	2.14	0.48
1:F:496:ASN:C	1:F:498:ARG:H	2.16	0.48
2:W:17:DT:H71	2:W:17:DT:OP2	2.14	0.48
1:F:492:ASN:O	1:F:495:ASP:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:GLU:HA	1:B:607:PHE:HZ	1.77	0.48
1:E:534:PRO:HD2	1:E:537:LEU:HD23	1.95	0.48
1:F:525:ILE:HG22	1:F:526:VAL:N	2.28	0.48
1:A:584:PRO:HD2	1:A:587:GLU:OE1	2.13	0.48
1:A:333:GLN:HG3	1:B:339:GLN:OE1	2.13	0.48
1:B:513:HIS:O	1:B:515:ASN:N	2.47	0.48
1:C:469:LEU:HD12	1:C:470:VAL:N	2.28	0.48
1:D:361:LEU:HD22	1:D:365:PHE:HE1	1.78	0.48
1:F:408:PHE:CZ	1:F:525:ILE:HD11	2.49	0.48
1:F:425:LYS:HZ2	1:F:530:GLU:HA	1.75	0.48
1:B:513:HIS:NE2	2:W:27:DA:C5'	2.77	0.48
1:A:588:PHE:CD2	1:A:596:ILE:HG13	2.48	0.48
1:B:470:VAL:HG13	1:B:522:PRO:HG2	1.96	0.48
1:B:593:GLN:O	1:B:597:VAL:HG23	2.13	0.48
1:C:364:ARG:O	1:C:368:LEU:HG	2.14	0.48
1:C:392:ALA:O	1:C:395:HIS:N	2.45	0.48
1:E:398:LEU:HD21	1:E:545:ILE:HG21	1.95	0.48
1:A:403:SER:O	1:A:407:ASP:OD2	2.31	0.47
1:A:432:LYS:HE2	1:A:529:ASN:HD21	1.79	0.47
1:C:432:LYS:HD2	1:C:527:THR:CG2	2.44	0.47
1:E:599:TRP:O	1:E:603:LEU:HD13	2.14	0.47
1:B:293:LEU:O	1:B:296:GLN:HG2	2.14	0.47
1:C:395:HIS:CD2	1:C:401:MET:HB3	2.48	0.47
1:C:405:VAL:HG21	1:C:578:MET:CE	2.44	0.47
1:C:443:CYS:HB3	1:C:468:PHE:CE2	2.49	0.47
1:E:283:ASP:HB2	1:E:345:LEU:HD21	1.96	0.47
1:F:452:LEU:HB3	1:F:453:PRO:HD2	1.96	0.47
1:B:548:ARG:O	1:B:550:LYS:HG3	2.14	0.47
1:C:287:LEU:HG	1:C:291:MET:CE	2.44	0.47
1:C:425:LYS:O	1:C:547:PHE:N	2.38	0.47
1:C:430:SER:H	1:C:432:LYS:NZ	2.12	0.47
1:C:589:ALA:HB3	1:C:592:ILE:HG13	1.97	0.47
1:D:498:ARG:HB3	1:D:498:ARG:HH11	1.75	0.47
1:E:430:SER:H	1:E:432:LYS:NZ	2.11	0.47
2:W:8:DG:C2'	2:W:9:DC:H5''	2.44	0.47
1:A:614:LYS:O	1:A:617:PHE:HB3	2.14	0.47
1:E:504:SER:HB3	1:D:570:GLN:NE2	2.29	0.47
1:A:469:LEU:HD12	1:A:470:VAL:N	2.30	0.47
1:C:290:GLY:CA	1:D:346:ALA:HB1	2.45	0.47
1:E:298:SER:HA	1:E:321:TYR:CD2	2.49	0.47
1:A:415:ASN:ND2	1:A:420:ARG:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:GLY:CA	1:A:511:LYS:HB2	2.42	0.47
1:E:417:PRO:C	1:E:419:LYS:H	2.18	0.47
1:E:443:CYS:HB3	1:E:468:PHE:CE2	2.49	0.47
1:E:535:LYS:CD	1:E:535:LYS:H	2.19	0.47
3:K:32:DC:O4'	3:K:32:DC:O2	2.32	0.47
1:B:517:ARG:CZ	1:B:517:ARG:HB3	2.44	0.47
1:C:442:LEU:HD12	1:C:572:GLY:O	2.14	0.47
1:F:389:ALA:HB1	1:F:625:VAL:HG11	1.97	0.47
1:A:465:ILE:HD11	1:A:509:LEU:O	2.15	0.47
1:C:403:SER:O	1:C:407:ASP:OD2	2.32	0.47
1:C:423:LEU:HD13	1:C:541:PHE:CE2	2.50	0.47
1:E:385:GLU:OE2	1:E:626:LEU:HD22	2.14	0.47
1:A:400:LYS:N	1:A:400:LYS:HD2	2.29	0.47
1:A:432:LYS:HB3	1:A:527:THR:HG22	1.96	0.47
1:E:405:VAL:HG21	1:E:578:MET:CE	2.45	0.47
1:E:614:LYS:O	1:E:617:PHE:HB3	2.15	0.47
1:E:623:ILE:O	1:E:623:ILE:HG13	2.14	0.47
1:B:452:LEU:HB3	1:B:453:PRO:HD2	1.96	0.47
1:C:614:LYS:O	1:C:617:PHE:HB3	2.15	0.47
1:C:287:LEU:HD13	1:D:353:LEU:HD12	1.97	0.47
1:D:489:GLN:O	1:D:493:ASN:ND2	2.48	0.47
1:E:417:PRO:HG3	1:E:503:GLY:O	2.14	0.47
1:E:584:PRO:HG2	1:E:587:GLU:CG	2.43	0.47
1:F:393:TRP:HE1	1:F:557:LEU:HG	1.80	0.47
1:F:609:LEU:HD23	1:F:609:LEU:O	2.15	0.47
1:A:332:ASN:O	1:A:336:ILE:HG13	2.15	0.47
1:B:433:THR:CG2	1:C:505:VAL:HG21	2.42	0.47
1:C:581:TRP:HB2	1:C:603:LEU:HD23	1.96	0.47
1:D:489:GLN:CB	1:D:493:ASN:HD21	2.28	0.47
1:E:364:ARG:O	1:E:368:LEU:HG	2.14	0.47
1:E:393:TRP:HZ3	1:E:397:LEU:HD22	1.80	0.47
1:A:581:TRP:HB2	1:A:603:LEU:HD23	1.95	0.46
1:D:576:LEU:O	1:D:580:ILE:HG12	2.15	0.46
1:E:514:LEU:HD11	1:D:511:LYS:CG	2.44	0.46
1:F:298:SER:HA	1:F:321:TYR:CE2	2.50	0.46
1:F:402:ASP:HB3	1:F:582:TYR:CD2	2.50	0.46
3:K:16:DA:H1'	3:K:17:DT:OP2	2.14	0.46
1:A:443:CYS:HB3	1:A:468:PHE:CE2	2.49	0.46
1:B:535:LYS:H	1:B:535:LYS:CD	2.20	0.46
1:C:510:GLU:O	1:C:510:GLU:OE1	2.33	0.46
1:E:567:ARG:HG3	1:E:567:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:581:TRP:HB2	1:E:603:LEU:HD23	1.96	0.46
1:A:385:GLU:OE2	1:A:626:LEU:HD22	2.15	0.46
1:B:405:VAL:HG21	1:B:578:MET:HE1	1.97	0.46
1:B:483:ARG:HG3	1:B:483:ARG:NH1	2.29	0.46
1:C:623:ILE:HG13	1:C:623:ILE:O	2.15	0.46
1:E:432:LYS:HE2	1:E:529:ASN:ND2	2.30	0.46
1:A:304:LYS:HB3	1:A:313:HIS:CD2	2.51	0.46
1:B:298:SER:HA	1:B:321:TYR:CE2	2.50	0.46
1:C:267:GLN:HG3	1:C:268:VAL:N	2.30	0.46
1:D:511:LYS:O	1:D:512:LYS:HE2	2.15	0.46
2:W:31:DT:H2'	2:W:32:DA:N7	2.30	0.46
1:A:394:LEU:HD13	1:A:575:LEU:HD23	1.97	0.46
1:A:456:ARG:HG2	3:K:1:DT:H5'	1.97	0.46
1:A:599:TRP:O	1:A:603:LEU:HD13	2.14	0.46
1:A:623:ILE:HG13	1:A:623:ILE:O	2.15	0.46
1:B:408:PHE:CE2	1:B:439:LEU:HD13	2.51	0.46
1:B:551:ASP:O	1:B:554:LYS:HB3	2.16	0.46
1:D:575:LEU:O	1:D:579:LEU:HG	2.16	0.46
1:E:304:LYS:HB3	1:E:313:HIS:CD2	2.50	0.46
2:W:6:DC:O2	3:K:27:DG:N1	2.44	0.46
1:A:618:ASN:HB3	1:A:624:GLY:O	2.16	0.46
1:B:575:LEU:O	1:B:579:LEU:HG	2.15	0.46
1:C:287:LEU:O	1:C:291:MET:HG3	2.16	0.46
1:C:567:ARG:HG3	1:C:567:ARG:HH11	1.80	0.46
1:D:408:PHE:CZ	1:D:525:ILE:HD11	2.50	0.46
1:E:589:ALA:HB3	1:E:592:ILE:HG13	1.97	0.46
2:W:17:DT:O2	3:K:16:DA:H2	1.99	0.46
1:C:498:ARG:NH1	1:C:498:ARG:HB3	2.31	0.46
1:C:559:ARG:HB2	1:C:559:ARG:CZ	2.46	0.46
3:K:25:DC:C2'	3:K:26:DC:C6	2.93	0.46
2:W:10:DC:H2''	2:W:11:DT:C5	2.51	0.46
1:A:283:ASP:HB2	1:A:345:LEU:HD21	1.98	0.46
1:A:289:LEU:HD11	1:A:293:LEU:HD11	1.98	0.46
1:A:338:GLN:HG3	1:A:338:GLN:O	2.16	0.46
1:A:559:ARG:CZ	1:A:559:ARG:HB2	2.46	0.46
1:B:395:HIS:CD2	1:B:401:MET:HB3	2.49	0.46
1:B:456:ARG:HG2	1:B:456:ARG:HH11	1.80	0.46
1:C:465:ILE:HD11	1:C:509:LEU:O	2.16	0.46
1:C:512:LYS:NZ	1:D:514:LEU:HB2	2.30	0.46
1:C:394:LEU:HD13	1:C:575:LEU:HD23	1.98	0.46
1:D:449:ASN:N	1:D:460:GLU:OE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:LEU:HD12	1:E:470:VAL:N	2.30	0.46
2:W:22:DA:N1	3:K:11:DT:O2	2.49	0.46
3:K:13:DT:H3'	3:K:13:DT:OP2	2.15	0.46
1:B:451:ASN:HD21	1:B:476:LYS:H	1.64	0.46
1:D:609:LEU:O	1:D:609:LEU:HD23	2.15	0.46
1:E:423:LEU:HD13	1:E:541:PHE:CE2	2.51	0.46
1:E:398:LEU:HD21	1:E:547:PHE:CE1	2.51	0.46
1:A:287:LEU:O	1:A:291:MET:HG3	2.16	0.46
1:E:387:TRP:O	1:E:391:VAL:HG23	2.16	0.46
1:E:477:GLY:O	1:E:478:THR:C	2.53	0.46
1:A:405:VAL:HG21	1:A:578:MET:CE	2.45	0.45
1:A:584:PRO:HG2	1:A:587:GLU:CG	2.44	0.45
1:C:304:LYS:HB3	1:C:313:HIS:CD2	2.51	0.45
1:D:452:LEU:HB3	1:D:453:PRO:HD2	1.98	0.45
1:C:512:LYS:HZ2	1:D:514:LEU:HD12	1.80	0.45
1:E:592:ILE:O	1:E:596:ILE:HG12	2.16	0.45
1:C:512:LYS:CG	2:W:29:DA:OP1	2.62	0.45
1:A:417:PRO:C	1:A:419:LYS:H	2.19	0.45
1:A:464:ALA:HB1	1:A:470:VAL:HG11	1.98	0.45
1:B:475:VAL:HG11	1:B:526:VAL:CG1	2.46	0.45
1:C:441:GLU:O	1:C:441:GLU:HG2	2.17	0.45
1:C:385:GLU:OE2	1:C:626:LEU:HD22	2.15	0.45
1:D:402:ASP:HB3	1:D:582:TYR:CD2	2.51	0.45
1:D:395:HIS:CE1	1:D:582:TYR:CZ	3.04	0.45
1:E:287:LEU:HG	1:E:291:MET:CE	2.46	0.45
3:K:32:DC:H4'	3:K:33:DT:OP1	2.16	0.45
2:W:12:DC:H2''	2:W:13:DT:C6	2.51	0.45
2:W:22:DA:C4'	2:W:23:DA:C5'	2.94	0.45
1:D:425:LYS:HZ2	1:D:530:GLU:HA	1.79	0.45
1:E:533:VAL:CG1	1:E:538:GLN:HB2	2.47	0.45
1:E:552:TYR:HB2	1:E:619:VAL:O	2.16	0.45
1:F:392:ALA:O	1:F:395:HIS:N	2.49	0.45
2:W:19:DA:C1'	2:W:20:DA:H5'	2.44	0.45
1:A:395:HIS:NE2	1:A:402:ASP:OD1	2.50	0.45
1:A:592:ILE:O	1:A:596:ILE:HG12	2.16	0.45
1:B:392:ALA:O	1:B:395:HIS:N	2.49	0.45
1:C:417:PRO:C	1:C:419:LYS:H	2.20	0.45
1:F:489:GLN:CB	1:F:493:ASN:HD21	2.30	0.45
1:A:589:ALA:HB3	1:A:592:ILE:HG13	1.97	0.45
1:C:283:ASP:HB2	1:C:345:LEU:HD21	1.97	0.45
1:C:599:TRP:O	1:C:603:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:SER:HA	1:D:321:TYR:CE2	2.51	0.45
1:B:443:CYS:HB3	1:B:468:PHE:CD2	2.52	0.45
1:B:408:PHE:CZ	1:B:525:ILE:HD11	2.52	0.45
1:C:468:PHE:O	1:C:522:PRO:HB2	2.16	0.45
1:D:517:ARG:HB3	1:D:517:ARG:CZ	2.46	0.45
1:E:415:ASN:ND2	1:E:420:ARG:HD2	2.31	0.45
1:E:559:ARG:HB2	1:E:559:ARG:CZ	2.45	0.45
1:A:481:GLU:C	1:A:483:ARG:O	2.55	0.45
1:A:513:HIS:O	1:A:514:LEU:CB	2.64	0.45
1:B:489:GLN:HB3	1:B:493:ASN:HD21	1.81	0.45
1:C:448:LEU:HD11	1:C:464:ALA:HB2	1.99	0.45
1:C:459:PHE:O	1:C:511:LYS:HD3	2.16	0.45
1:C:514:LEU:O	1:C:515:ASN:C	2.55	0.45
1:D:389:ALA:HB1	1:D:625:VAL:HG11	1.98	0.45
1:E:415:ASN:ND2	1:E:523:PRO:HD3	2.32	0.45
1:B:510:GLU:HG2	1:B:510:GLU:O	2.17	0.45
1:C:308:LYS:HA	1:C:314:TYR:CD2	2.51	0.45
1:C:464:ALA:HB1	1:C:470:VAL:HG11	1.98	0.45
1:C:483:ARG:O	1:C:484:ASP:HB3	2.16	0.45
1:E:267:GLN:HE22	1:D:331:LYS:HD3	1.81	0.45
1:E:403:SER:O	1:E:407:ASP:OD2	2.34	0.45
1:E:453:PRO:O	1:E:457:LEU:HB2	2.16	0.45
1:E:465:ILE:HD11	1:E:509:LEU:O	2.16	0.45
1:E:559:ARG:CB	1:E:559:ARG:HH11	2.30	0.45
1:D:590:GLN:HA	1:D:593:GLN:NE2	2.31	0.45
1:E:395:HIS:NE2	1:E:402:ASP:OD1	2.50	0.45
1:E:427:PRO:CG	1:E:549:PRO:HD3	2.47	0.45
1:A:602:ARG:HA	1:A:605:LYS:HE3	1.98	0.45
1:C:592:ILE:O	1:C:596:ILE:HG12	2.17	0.45
1:E:290:GLY:CA	1:F:346:ALA:HB1	2.46	0.45
1:E:475:VAL:HG13	1:E:475:VAL:O	2.17	0.45
1:E:567:ARG:NH1	1:E:567:ARG:HG3	2.32	0.45
1:F:456:ARG:HG2	1:F:456:ARG:HH11	1.82	0.45
3:K:15:DT:H1'	3:K:16:DA:C5'	2.47	0.45
1:B:397:LEU:CD1	4:B:701:ADP:HN61	2.30	0.44
1:B:590:GLN:HA	1:B:593:GLN:NE2	2.30	0.44
1:C:414:TYR:O	1:C:415:ASN:C	2.56	0.44
1:C:415:ASN:ND2	1:C:420:ARG:HD2	2.32	0.44
1:D:443:CYS:HB3	1:D:468:PHE:CD2	2.52	0.44
1:E:308:LYS:HA	1:E:314:TYR:CD2	2.52	0.44
1:E:427:PRO:HG2	1:E:549:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:618:ASN:HB3	1:E:624:GLY:O	2.16	0.44
1:F:293:LEU:O	1:F:296:GLN:HG2	2.17	0.44
1:A:283:ASP:HB3	1:A:344:VAL:HG11	1.98	0.44
1:C:287:LEU:HG	1:C:291:MET:HE2	1.99	0.44
1:C:316:TYR:O	1:C:317:HIS:C	2.56	0.44
1:C:387:TRP:O	1:C:391:VAL:HG23	2.17	0.44
1:D:335:THR:O	1:D:336:ILE:C	2.55	0.44
1:D:475:VAL:HG11	1:D:526:VAL:CG1	2.46	0.44
1:E:294:GLU:OE2	1:E:304:LYS:HE3	2.17	0.44
1:E:508:ASN:OD1	1:E:518:THR:HG23	2.17	0.44
1:C:294:GLU:OE2	1:C:304:LYS:HE3	2.17	0.44
1:C:283:ASP:HB3	1:C:344:VAL:HG11	1.99	0.44
1:C:584:PRO:HG2	1:C:587:GLU:CG	2.44	0.44
1:E:446:LYS:HG3	1:E:463:VAL:HG22	2.00	0.44
1:A:387:TRP:O	1:A:391:VAL:HG23	2.17	0.44
1:D:456:ARG:HH11	1:D:456:ARG:HG2	1.81	0.44
1:D:535:LYS:H	1:D:535:LYS:CD	2.21	0.44
1:E:401:MET:C	1:E:403:SER:H	2.19	0.44
1:E:473:GLU:OE1	1:E:473:GLU:CA	2.64	0.44
1:E:475:VAL:CG2	1:E:491:ILE:CD1	2.89	0.44
2:W:2:DG:H2'	2:W:3:DC:C6	2.52	0.44
1:A:308:LYS:HA	1:A:314:TYR:CD2	2.53	0.44
1:A:334:LYS:O	1:A:337:CYS:O	2.36	0.44
1:A:441:GLU:HG2	1:A:441:GLU:O	2.17	0.44
1:A:510:GLU:HB3	1:A:515:ASN:ND2	2.32	0.44
1:C:401:MET:C	1:C:403:SER:H	2.20	0.44
1:E:298:SER:HA	1:E:321:TYR:HE2	1.82	0.44
1:A:298:SER:HA	1:A:321:TYR:HE2	1.82	0.44
1:B:428:ILE:HG12	1:B:429:ASP:N	2.33	0.44
1:C:398:LEU:HD21	1:C:547:PHE:CE1	2.52	0.44
1:C:618:ASN:HB3	1:C:624:GLY:O	2.17	0.44
1:D:402:ASP:HA	1:D:578:MET:HE3	1.99	0.44
1:D:615:MET:HB3	1:D:625:VAL:CG1	2.48	0.44
2:W:22:DA:H1'	2:W:23:DA:C8	2.53	0.44
1:A:296:GLN:HE21	1:A:328:ALA:CB	2.30	0.44
1:A:559:ARG:CB	1:A:559:ARG:HH11	2.31	0.44
1:B:601:GLU:O	1:B:605:LYS:HB2	2.18	0.44
1:F:529:ASN:O	1:F:530:GLU:HB2	2.18	0.44
1:F:405:VAL:HG21	1:F:578:MET:HE1	1.98	0.44
3:K:14:DT:C1'	3:K:15:DT:H72	2.48	0.44
2:W:1:DG:OP1	2:W:1:DG:H4'	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:TYR:O	1:A:415:ASN:C	2.56	0.44
1:A:448:LEU:HD11	1:A:464:ALA:HB2	1.98	0.44
1:B:347:LYS:CA	1:B:350:VAL:HG12	2.46	0.44
1:C:602:ARG:HA	1:C:605:LYS:HE3	1.99	0.44
1:D:408:PHE:CE2	1:D:439:LEU:HD13	2.53	0.44
1:E:465:ILE:HG22	1:E:466:ASP:N	2.32	0.44
1:F:443:CYS:HB3	1:F:468:PHE:CD2	2.53	0.44
1:F:517:ARG:HB3	1:F:517:ARG:CZ	2.47	0.44
1:F:475:VAL:HG11	1:F:526:VAL:CG1	2.48	0.44
1:B:443:CYS:HB3	1:B:468:PHE:HD2	1.83	0.44
1:B:465:ILE:O	1:B:467:GLN:HG2	2.17	0.44
1:D:392:ALA:O	1:D:395:HIS:N	2.51	0.44
1:D:417:PRO:C	1:D:419:LYS:H	2.20	0.44
1:D:601:GLU:O	1:D:605:LYS:HB2	2.18	0.44
1:E:441:GLU:O	1:E:441:GLU:HG2	2.18	0.44
1:E:448:LEU:HD11	1:E:464:ALA:HB2	2.00	0.44
1:E:409:LEU:HD11	1:E:579:LEU:HD11	2.00	0.44
1:A:339:GLN:HE22	1:F:333:GLN:H	1.64	0.43
1:A:398:LEU:HD21	1:A:547:PHE:CE1	2.52	0.43
1:A:401:MET:C	1:A:403:SER:H	2.20	0.43
1:A:417:PRO:HG3	1:A:503:GLY:O	2.17	0.43
1:C:401:MET:HG3	1:C:578:MET:HE3	2.00	0.43
1:E:289:LEU:HD11	1:E:293:LEU:HD11	2.00	0.43
1:F:575:LEU:O	1:F:579:LEU:HG	2.17	0.43
1:C:395:HIS:HB3	1:C:616:LYS:NZ	2.33	0.43
1:C:465:ILE:HG22	1:C:466:ASP:N	2.32	0.43
1:E:465:ILE:CG2	1:E:466:ASP:N	2.82	0.43
2:W:9:DC:H2''	2:W:10:DC:O5'	2.18	0.43
1:A:428:ILE:CA	1:A:529:ASN:ND2	2.81	0.43
1:E:483:ARG:NH1	1:E:483:ARG:HG3	2.32	0.43
1:E:472:PHE:CB	1:E:526:VAL:HG23	2.36	0.43
1:F:282:CYS:SG	1:F:287:LEU:HD23	2.58	0.43
2:W:18:DA:H1'	2:W:19:DA:C5'	2.47	0.43
1:C:424:PHE:HE2	1:C:435:LEU:HD23	1.83	0.43
1:C:559:ARG:CB	1:C:559:ARG:HH11	2.32	0.43
1:D:443:CYS:HB3	1:D:468:PHE:HD2	1.83	0.43
1:E:510:GLU:OE1	1:E:510:GLU:O	2.36	0.43
1:E:468:PHE:O	1:E:522:PRO:HB2	2.19	0.43
1:A:316:TYR:O	1:A:317:HIS:C	2.57	0.43
1:A:567:ARG:HH11	1:A:567:ARG:HG3	1.82	0.43
1:E:602:ARG:HA	1:E:605:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:511:LYS:O	1:F:512:LYS:HE2	2.18	0.43
3:K:14:DT:C2	3:K:15:DT:H72	2.54	0.43
1:B:425:LYS:HZ2	1:B:530:GLU:HA	1.76	0.43
1:C:567:ARG:HG3	1:C:567:ARG:NH1	2.32	0.43
1:E:393:TRP:CZ3	1:E:397:LEU:HD22	2.53	0.43
1:E:424:PHE:HE2	1:E:435:LEU:HD23	1.83	0.43
1:F:414:TYR:O	1:F:415:ASN:C	2.56	0.43
1:A:538:GLN:HG3	1:A:538:GLN:O	2.18	0.43
1:C:270:TRP:CE2	1:C:336:ILE:HG12	2.53	0.43
1:B:428:ILE:HD11	1:C:498:ARG:HD2	2.01	0.43
1:D:510:GLU:O	1:D:510:GLU:HG2	2.18	0.43
1:D:395:HIS:CE1	1:D:582:TYR:HH	2.30	0.43
1:F:266:LYS:HD2	1:F:266:LYS:HA	1.28	0.43
1:F:335:THR:HG22	1:F:335:THR:O	2.18	0.43
1:A:400:LYS:O	1:A:404:VAL:HG23	2.19	0.43
1:A:427:PRO:HD2	1:A:547:PHE:O	2.18	0.43
1:F:550:LYS:HB2	1:F:553:LEU:HD12	2.01	0.43
1:F:395:HIS:CE1	1:F:582:TYR:CZ	3.06	0.43
1:A:283:ASP:HB2	1:A:345:LEU:CD2	2.49	0.43
1:C:296:GLN:HE21	1:C:328:ALA:CB	2.31	0.43
1:D:347:LYS:CA	1:D:350:VAL:HG12	2.47	0.43
1:E:283:ASP:HB3	1:E:344:VAL:HG11	2.00	0.43
1:E:287:LEU:O	1:E:291:MET:HG3	2.19	0.43
1:E:506:LYS:HG2	1:E:520:ILE:CG2	2.49	0.43
1:A:361:LEU:HD13	1:A:365:PHE:CE1	2.54	0.43
1:B:614:LYS:O	1:B:618:ASN:OD1	2.37	0.43
1:C:283:ASP:HB2	1:C:345:LEU:CD2	2.49	0.43
1:C:417:PRO:O	1:C:418:LYS:HB2	2.19	0.43
1:D:550:LYS:HB3	1:D:552:TYR:CE1	2.54	0.43
1:E:433:THR:C	1:E:435:LEU:N	2.72	0.43
2:W:31:DT:C4	3:K:2:DA:N1	2.85	0.43
1:A:430:SER:H	1:A:432:LYS:NZ	2.14	0.42
1:A:567:ARG:NH1	1:A:567:ARG:HG3	2.33	0.42
1:B:417:PRO:C	1:B:419:LYS:H	2.21	0.42
1:C:266:LYS:HA	1:C:266:LYS:HD2	1.51	0.42
1:C:409:LEU:HD11	1:C:579:LEU:HD11	2.01	0.42
1:E:320:HIS:O	1:E:321:TYR:C	2.57	0.42
1:E:392:ALA:O	1:E:395:HIS:N	2.51	0.42
1:A:320:HIS:O	1:A:321:TYR:C	2.57	0.42
1:B:498:ARG:CB	1:B:498:ARG:NH1	2.80	0.42
1:B:511:LYS:O	1:B:512:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ILE:CG2	1:C:466:ASP:N	2.81	0.42
1:C:508:ASN:OD1	1:C:518:THR:HG23	2.18	0.42
1:E:339:GLN:NE2	1:D:333:GLN:H	2.17	0.42
1:D:612:TYR:HA	1:D:615:MET:HE3	2.01	0.42
1:E:337:CYS:C	1:E:339:GLN:H	2.23	0.42
1:A:417:PRO:O	1:A:418:LYS:HB2	2.20	0.42
1:B:282:CYS:SG	1:B:287:LEU:HD23	2.59	0.42
1:C:278:MET:CE	1:C:347:LYS:HD2	2.50	0.42
1:D:489:GLN:HB3	1:D:493:ASN:HD21	1.84	0.42
1:E:316:TYR:O	1:E:317:HIS:C	2.58	0.42
1:F:417:PRO:O	1:F:418:LYS:HB2	2.19	0.42
1:F:510:GLU:HG2	1:F:510:GLU:O	2.18	0.42
1:B:296:GLN:HE21	1:B:328:ALA:CB	2.33	0.42
1:B:402:ASP:HA	1:B:578:MET:HE3	2.01	0.42
1:C:349:ARG:HG3	1:C:349:ARG:O	2.20	0.42
1:C:532:SER:O	1:C:534:PRO:HD3	2.20	0.42
1:E:267:GLN:NE2	1:D:331:LYS:HD3	2.34	0.42
1:D:332:ASN:O	1:D:336:ILE:HG13	2.18	0.42
1:D:551:ASP:O	1:D:554:LYS:HB3	2.18	0.42
1:E:361:LEU:O	1:E:365:PHE:CD1	2.73	0.42
2:W:28:DA:C1'	2:W:29:DA:O5'	2.62	0.42
1:A:294:GLU:OE2	1:A:304:LYS:HE3	2.19	0.42
1:A:362:THR:HG23	1:A:592:ILE:HD11	2.01	0.42
1:A:465:ILE:HG22	1:A:466:ASP:N	2.34	0.42
1:A:525:ILE:CG2	1:A:526:VAL:N	2.83	0.42
1:B:321:TYR:C	1:B:321:TYR:CD1	2.93	0.42
1:B:415:ASN:HD21	1:B:420:ARG:CD	2.30	0.42
1:C:511:LYS:O	1:C:512:LYS:HE3	2.20	0.42
1:D:321:TYR:C	1:D:321:TYR:CD1	2.92	0.42
1:E:349:ARG:NH2	1:E:516:LYS:HE3	2.34	0.42
1:F:321:TYR:CD1	1:F:321:TYR:C	2.93	0.42
1:F:417:PRO:C	1:F:419:LYS:H	2.22	0.42
1:B:408:PHE:CD2	1:B:439:LEU:HD13	2.55	0.42
1:C:424:PHE:CE1	1:C:525:ILE:HG23	2.54	0.42
1:C:433:THR:C	1:C:435:LEU:N	2.73	0.42
1:C:580:ILE:CD1	1:C:596:ILE:HG23	2.50	0.42
1:E:283:ASP:HB2	1:E:345:LEU:CD2	2.50	0.42
1:F:332:ASN:O	1:F:336:ILE:HG13	2.19	0.42
1:F:590:GLN:HA	1:F:593:GLN:NE2	2.30	0.42
2:W:18:DA:H2	3:K:15:DT:O2	2.01	0.42
1:A:510:GLU:OE1	1:A:510:GLU:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:LYS:HG3	1:C:463:VAL:HG22	2.01	0.42
1:E:450:VAL:C	1:E:451:ASN:HD22	2.22	0.42
1:E:491:ILE:O	1:E:491:ILE:HG22	2.20	0.42
1:E:603:LEU:O	1:E:607:PHE:HB2	2.20	0.42
2:W:12:DC:H2'	2:W:13:DT:C5	2.55	0.42
1:A:395:HIS:CD2	1:A:401:MET:HB3	2.55	0.42
1:A:585:VAL:HG22	1:A:600:LYS:HD2	2.02	0.42
1:C:298:SER:HA	1:C:321:TYR:HE2	1.81	0.42
1:D:476:LYS:C	1:D:490:GLY:C	2.79	0.42
1:D:505:VAL:HG12	1:D:506:LYS:N	2.34	0.42
1:E:412:MET:SD	1:E:523:PRO:HB2	2.60	0.42
1:F:549:PRO:HA	4:F:702:ADP:N1	2.34	0.42
2:W:21:DT:O4	3:K:12:DA:N1	2.52	0.42
1:A:446:LYS:HG3	1:A:463:VAL:HG22	2.01	0.42
1:B:339:GLN:HB2	1:B:339:GLN:HE21	1.59	0.42
1:C:337:CYS:O	1:C:340:ALA:N	2.51	0.42
1:C:450:VAL:C	1:C:451:ASN:HD22	2.23	0.42
1:C:478:THR:HG23	1:C:481:GLU:CG	2.50	0.42
1:C:603:LEU:O	1:C:607:PHE:HB2	2.20	0.42
2:W:22:DA:C2	3:K:11:DT:O2	2.72	0.42
1:C:491:ILE:C	1:C:493:ASN:H	2.24	0.42
1:C:533:VAL:CG1	1:C:538:GLN:HB2	2.49	0.42
1:F:339:GLN:HE21	1:F:339:GLN:HB2	1.59	0.42
1:F:347:LYS:CA	1:F:350:VAL:HG12	2.49	0.42
1:F:535:LYS:N	1:F:535:LYS:HD2	2.21	0.42
2:W:25:DA:H2''	2:W:26:DA:OP2	2.20	0.42
1:B:409:LEU:HD11	1:B:579:LEU:HD11	2.02	0.41
1:C:289:LEU:HD11	1:C:293:LEU:HD11	2.02	0.41
1:C:320:HIS:O	1:C:321:TYR:C	2.57	0.41
1:C:400:LYS:O	1:C:404:VAL:HG23	2.19	0.41
1:E:270:TRP:CD1	1:E:270:TRP:N	2.88	0.41
1:A:278:MET:CE	1:A:347:LYS:HD2	2.50	0.41
1:A:409:LEU:HD11	1:A:579:LEU:HD11	2.01	0.41
1:A:423:LEU:HD13	1:A:541:PHE:CE2	2.55	0.41
1:A:450:VAL:C	1:A:451:ASN:HD22	2.23	0.41
1:A:393:TRP:HE1	1:A:557:LEU:HG	1.85	0.41
1:B:368:LEU:O	1:B:372:MET:HG3	2.20	0.41
1:D:266:LYS:O	1:D:267:GLN:HB3	2.18	0.41
1:D:476:LYS:C	1:D:490:GLY:CA	2.74	0.41
1:E:424:PHE:CE1	1:E:525:ILE:HG23	2.55	0.41
1:E:481:GLU:OE1	1:E:485:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:532:SER:O	1:E:534:PRO:HD3	2.19	0.41
1:F:532:SER:O	1:F:534:PRO:HD3	2.20	0.41
1:F:615:MET:HB3	1:F:625:VAL:CG1	2.49	0.41
1:A:465:ILE:CG2	1:A:466:ASP:N	2.83	0.41
1:A:490:GLY:C	1:A:492:ASN:N	2.74	0.41
1:A:491:ILE:C	1:A:493:ASN:H	2.24	0.41
1:A:603:LEU:O	1:A:607:PHE:HB2	2.20	0.41
1:B:470:VAL:HG13	1:B:522:PRO:CG	2.51	0.41
1:B:388:MET:HG3	1:B:607:PHE:CE2	2.56	0.41
1:B:615:MET:HB3	1:B:625:VAL:CG1	2.50	0.41
1:C:395:HIS:HA	1:C:401:MET:CB	2.51	0.41
1:C:562:PHE:HA	1:C:565:GLU:HB2	2.02	0.41
1:D:356:THR:OG1	1:D:359:GLN:HG3	2.19	0.41
1:D:395:HIS:CD2	1:D:401:MET:HB3	2.44	0.41
1:E:414:TYR:O	1:E:415:ASN:C	2.58	0.41
1:E:525:ILE:CG2	1:E:526:VAL:N	2.82	0.41
1:F:408:PHE:CD2	1:F:439:LEU:HD13	2.56	0.41
1:A:349:ARG:HH11	1:A:349:ARG:HB2	1.84	0.41
1:A:508:ASN:OD1	1:A:518:THR:HG23	2.21	0.41
1:A:562:PHE:HA	1:A:565:GLU:HB2	2.02	0.41
1:C:372:MET:SD	1:C:576:LEU:CD2	2.98	0.41
1:C:405:VAL:O	1:C:408:PHE:HB3	2.21	0.41
1:C:418:LYS:N	1:C:502:ASP:O	2.44	0.41
1:D:582:TYR:O	1:D:583:ARG:O	2.38	0.41
1:E:417:PRO:O	1:E:418:LYS:HB2	2.20	0.41
1:E:438:ALA:HA	1:E:570:GLN:O	2.21	0.41
1:F:408:PHE:CE2	1:F:439:LEU:HD13	2.54	0.41
1:F:582:TYR:O	1:F:583:ARG:O	2.37	0.41
3:K:24:DG:H1'	3:K:25:DC:O4'	2.20	0.41
1:A:498:ARG:HH11	1:A:498:ARG:CB	2.34	0.41
1:B:550:LYS:HB3	1:B:552:TYR:CE1	2.55	0.41
1:C:491:ILE:HG22	1:C:491:ILE:O	2.20	0.41
1:D:520:ILE:O	1:D:521:PHE:C	2.57	0.41
1:E:388:MET:SD	1:E:391:VAL:HG21	2.61	0.41
1:F:341:VAL:O	1:F:345:LEU:HG	2.21	0.41
1:F:402:ASP:HA	1:F:578:MET:HE3	2.02	0.41
1:F:583:ARG:N	1:F:583:ARG:CD	2.83	0.41
3:K:6:DT:H1'	3:K:7:DT:C4'	2.50	0.41
1:A:490:GLY:C	1:A:492:ASN:H	2.24	0.41
1:A:566:LYS:HB2	1:A:568:ILE:HG13	2.03	0.41
1:C:362:THR:HG23	1:C:592:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ILE:HG21	1:A:537:LEU:HD22	2.03	0.41
1:D:414:TYR:O	1:D:415:ASN:C	2.59	0.41
1:E:498:ARG:HH11	1:E:498:ARG:CB	2.34	0.41
1:E:426:GLY:O	1:E:529:ASN:HA	2.20	0.41
1:E:566:LYS:HB2	1:E:568:ILE:HG13	2.02	0.41
1:F:296:GLN:HE21	1:F:328:ALA:CB	2.33	0.41
1:F:409:LEU:HD11	1:F:579:LEU:HD11	2.02	0.41
1:F:505:VAL:HG12	1:F:506:LYS:N	2.34	0.41
1:A:406:TYR:CD2	1:A:583:ARG:NH1	2.89	0.41
1:A:395:HIS:HB3	1:A:616:LYS:HZ3	1.85	0.41
1:B:583:ARG:N	1:B:583:ARG:HD2	2.35	0.41
1:C:412:MET:SD	1:C:523:PRO:HB2	2.61	0.41
1:D:405:VAL:HG21	1:D:578:MET:HE1	2.02	0.41
2:W:22:DA:C4'	2:W:23:DA:H5''	2.51	0.41
1:A:349:ARG:HG3	1:A:349:ARG:O	2.20	0.41
1:B:356:THR:OG1	1:B:359:GLN:HG3	2.21	0.41
1:B:513:HIS:H	1:B:513:HIS:HD1	1.69	0.41
1:C:347:LYS:O	1:C:350:VAL:N	2.54	0.41
1:D:408:PHE:CD2	1:D:439:LEU:HD13	2.56	0.41
1:D:529:ASN:O	1:D:530:GLU:HB2	2.19	0.41
1:E:361:LEU:HD13	1:E:365:PHE:CE1	2.54	0.41
1:F:470:VAL:HG13	1:F:522:PRO:CG	2.51	0.41
1:F:608:SER:C	1:F:610:SER:N	2.74	0.41
1:A:491:ILE:HG22	1:A:491:ILE:O	2.20	0.41
1:A:511:LYS:O	1:A:512:LYS:HE3	2.21	0.41
1:A:580:ILE:CD1	1:A:596:ILE:HG23	2.51	0.41
1:B:417:PRO:O	1:B:418:LYS:HB2	2.21	0.41
1:D:387:TRP:HZ3	1:D:571:SER:HG	1.69	0.41
1:D:603:LEU:C	1:D:605:LYS:H	2.24	0.41
1:E:302:CYS:O	1:E:306:ILE:HG13	2.21	0.41
1:E:403:SER:HA	1:E:583:ARG:HH21	1.86	0.41
1:F:443:CYS:HB3	1:F:468:PHE:HD2	1.84	0.41
1:F:520:ILE:HG13	1:F:520:ILE:O	2.20	0.41
1:A:395:HIS:HD2	1:A:401:MET:HB3	1.86	0.41
1:C:538:GLN:O	1:C:538:GLN:HG3	2.20	0.41
1:F:299:PHE:CD1	1:F:299:PHE:N	2.85	0.41
1:A:601:GLU:O	1:A:605:LYS:HB2	2.21	0.40
1:B:304:LYS:HB3	1:B:313:HIS:CD2	2.56	0.40
1:B:505:VAL:HG12	1:B:506:LYS:N	2.35	0.40
1:B:552:TYR:HD1	1:B:552:TYR:H	1.69	0.40
1:C:403:SER:HA	1:C:583:ARG:HH21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:LYS:O	1:E:404:VAL:HG23	2.21	0.40
1:F:297:TYR:O	1:F:321:TYR:HD2	2.04	0.40
1:F:397:LEU:HD11	4:F:702:ADP:HN61	1.85	0.40
2:W:17:DT:O2	3:K:16:DA:C2	2.74	0.40
1:A:266:LYS:HA	1:A:266:LYS:HD3	1.87	0.40
1:B:476:LYS:O	1:B:490:GLY:HA3	2.21	0.40
1:B:489:GLN:HB3	1:B:493:ASN:ND2	2.36	0.40
1:C:472:PHE:O	1:C:473:GLU:C	2.58	0.40
1:C:426:GLY:O	1:C:529:ASN:HA	2.21	0.40
1:D:296:GLN:HE21	1:D:328:ALA:CB	2.35	0.40
1:E:296:GLN:HE21	1:E:328:ALA:CB	2.32	0.40
1:E:414:TYR:HB3	1:E:416:ILE:HG13	2.04	0.40
1:E:511:LYS:O	1:E:512:LYS:HE3	2.21	0.40
1:F:520:ILE:O	1:F:521:PHE:C	2.60	0.40
1:F:619:VAL:HG22	1:F:625:VAL:HG22	2.03	0.40
1:C:402:ASP:HB3	1:C:582:TYR:CD2	2.57	0.40
1:C:414:TYR:HB3	1:C:416:ILE:HG13	2.04	0.40
1:C:566:LYS:HB2	1:C:568:ILE:HG13	2.04	0.40
1:D:520:ILE:HG13	1:D:520:ILE:O	2.22	0.40
1:D:532:SER:O	1:D:534:PRO:HD3	2.22	0.40
1:D:564:LEU:HD23	1:D:564:LEU:HA	1.89	0.40
1:D:608:SER:C	1:D:610:SER:N	2.74	0.40
1:E:538:GLN:O	1:E:538:GLN:HG3	2.20	0.40
1:E:562:PHE:HA	1:E:565:GLU:HB2	2.03	0.40
1:E:585:VAL:HG22	1:E:600:LYS:HD2	2.03	0.40
1:F:428:ILE:HG12	1:F:429:ASP:N	2.36	0.40
1:F:614:LYS:O	1:F:618:ASN:OD1	2.39	0.40
3:K:2:DA:P	3:K:2:DA:H8	2.45	0.40
2:W:22:DA:H4'	2:W:23:DA:H5''	2.03	0.40
1:A:615:MET:C	1:A:617:PHE:H	2.24	0.40
1:B:266:LYS:HA	1:B:266:LYS:HD2	1.73	0.40
1:C:490:GLY:C	1:C:492:ASN:H	2.25	0.40
1:C:601:GLU:O	1:C:605:LYS:HB2	2.21	0.40
1:E:278:MET:CE	1:E:347:LYS:HD2	2.51	0.40
1:E:501:LEU:HD12	1:E:540:ARG:HG3	2.02	0.40
2:W:31:DT:N3	3:K:2:DA:C2	2.77	0.40
2:W:22:DA:N6	3:K:11:DT:H3	2.18	0.40
2:W:29:DA:O5'	2:W:29:DA:C8	2.74	0.40
1:B:580:ILE:HG21	1:B:599:TRP:HB3	2.04	0.40
1:C:358:GLU:O	1:C:362:THR:OG1	2.18	0.40
1:C:395:HIS:HA	1:C:401:MET:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:VAL:HG13	1:D:522:PRO:CG	2.51	0.40
1:D:551:ASP:O	1:D:554:LYS:N	2.55	0.40
1:E:490:GLY:C	1:E:492:ASN:N	2.74	0.40
1:E:542:VAL:O	1:E:542:VAL:HG22	2.22	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)
1:A:488:GLY:O	3:K:33:DT:OP1[1_444]	2.16	0.04

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	
1	A	360/362 (99%)	285 (79%)	60 (17%)	15 (4%)	3	13
1	B	360/362 (99%)	302 (84%)	48 (13%)	10 (3%)	6	24
1	C	360/362 (99%)	288 (80%)	59 (16%)	13 (4%)	4	18
1	D	360/362 (99%)	302 (84%)	48 (13%)	10 (3%)	6	24
1	E	360/362 (99%)	286 (79%)	59 (16%)	15 (4%)	3	13
1	F	360/362 (99%)	305 (85%)	43 (12%)	12 (3%)	5	20
All	All	2160/2172 (99%)	1768 (82%)	317 (15%)	75 (4%)	4	18

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	GLN
1	A	474	ASP
1	A	478	THR
1	A	489	GLN

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Mol	Chain	Res	Type
1	B	267	GLN
1	B	514	LEU
1	B	582	TYR
1	E	473	GLU
1	E	489	GLN
1	E	516	LYS
1	F	514	LEU
1	F	583	ARG
1	C	473	GLU
1	D	267	GLN
1	D	491	ILE
1	D	514	LEU
1	D	583	ARG
1	A	336	ILE
1	A	516	LYS
1	B	415	ASN
1	B	490	GLY
1	E	523	PRO
1	E	534	PRO
1	F	490	GLY
1	F	534	PRO
1	F	606	GLU
1	C	515	ASN
1	C	534	PRO
1	D	466	ASP
1	A	337	CYS
1	A	466	ASP
1	A	523	PRO
1	E	466	ASP
1	E	551	ASP
1	F	466	ASP
1	F	605	LYS
1	C	466	ASP
1	C	488	GLY
1	C	514	LEU
1	C	523	PRO
1	D	534	PRO
1	A	479	GLY
1	B	466	ASP
1	B	489	GLN
1	B	512	LYS
1	B	534	PRO

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Mol	Chain	Res	Type
1	E	317	HIS
1	E	514	LEU
1	E	515	ASN
1	F	415	ASN
1	F	479	GLY
1	F	489	GLN
1	F	512	LYS
1	C	317	HIS
1	C	478	THR
1	C	492	ASN
1	D	479	GLY
1	D	512	LYS
1	A	317	HIS
1	A	488	GLY
1	A	492	ASN
1	E	478	THR
1	E	492	ASN
1	C	338	GLN
1	D	415	ASN
1	A	514	LEU
1	C	489	GLN
1	B	428	ILE
1	E	479	GLY
1	F	428	ILE
1	C	486	PRO
1	A	486	PRO
1	E	488	GLY
1	E	486	PRO
1	D	450	VAL

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
1	A	323/323 (100%)	308 (95%)	15 (5%)	33 69
1	B	323/323 (100%)	308 (95%)	15 (5%)	33 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	323/323 (100%)	307 (95%)	16 (5%)	30	65
1	D	323/323 (100%)	308 (95%)	15 (5%)	33	69
1	E	323/323 (100%)	307 (95%)	16 (5%)	30	65
1	F	323/323 (100%)	309 (96%)	14 (4%)	35	71
All	All	1938/1938 (100%)	1847 (95%)	91 (5%)	32	68

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	LYS
1	A	267	GLN
1	A	279	GLU
1	A	349	ARG
1	A	361	LEU
1	A	370	ASP
1	A	400	LYS
1	A	456	ARG
1	A	494	LEU
1	A	510	GLU
1	A	512	LYS
1	A	514	LEU
1	A	517	ARG
1	A	535	LYS
1	A	609	LEU
1	B	266	LYS
1	B	279	GLU
1	B	303	LEU
1	B	318	GLU
1	B	349	ARG
1	B	361	LEU
1	B	400	LYS
1	B	455	ASP
1	B	459	PHE
1	B	511	LYS
1	B	535	LYS
1	B	552	TYR
1	B	559	ARG
1	B	576	LEU
1	B	583	ARG
1	E	266	LYS
1	E	279	GLU

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Mol	Chain	Res	Type
1	E	349	ARG
1	E	361	LEU
1	E	370	ASP
1	E	400	LYS
1	E	456	ARG
1	E	473	GLU
1	E	474	ASP
1	E	494	LEU
1	E	510	GLU
1	E	512	LYS
1	E	515	ASN
1	E	517	ARG
1	E	535	LYS
1	E	609	LEU
1	F	266	LYS
1	F	279	GLU
1	F	303	LEU
1	F	318	GLU
1	F	349	ARG
1	F	361	LEU
1	F	400	LYS
1	F	455	ASP
1	F	459	PHE
1	F	511	LYS
1	F	535	LYS
1	F	559	ARG
1	F	576	LEU
1	F	583	ARG
1	C	266	LYS
1	C	279	GLU
1	C	349	ARG
1	C	361	LEU
1	C	370	ASP
1	C	400	LYS
1	C	434	THR
1	C	456	ARG
1	C	474	ASP
1	C	494	LEU
1	C	510	GLU
1	C	512	LYS
1	C	517	ARG
1	C	535	LYS

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Mol	Chain	Res	Type
1	C	552	TYR
1	C	609	LEU
1	D	279	GLU
1	D	303	LEU
1	D	314	TYR
1	D	318	GLU
1	D	349	ARG
1	D	361	LEU
1	D	400	LYS
1	D	455	ASP
1	D	459	PHE
1	D	511	LYS
1	D	535	LYS
1	D	559	ARG
1	D	576	LEU
1	D	583	ARG
1	D	605	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	296	GLN
1	A	338	GLN
1	A	339	GLN
1	A	363	ASN
1	A	415	ASN
1	A	449	ASN
1	A	451	ASN
1	A	467	GLN
1	A	492	ASN
1	A	529	ASN
1	B	267	GLN
1	B	296	GLN
1	B	338	GLN
1	B	363	ASN
1	B	415	ASN
1	B	451	ASN
1	B	467	GLN
1	B	492	ASN
1	B	493	ASN
1	B	593	GLN

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Mol	Chain	Res	Type
1	E	296	GLN
1	E	339	GLN
1	E	363	ASN
1	E	415	ASN
1	E	449	ASN
1	E	451	ASN
1	E	467	GLN
1	E	492	ASN
1	E	529	ASN
1	E	590	GLN
1	F	267	GLN
1	F	296	GLN
1	F	333	GLN
1	F	338	GLN
1	F	363	ASN
1	F	415	ASN
1	F	451	ASN
1	F	467	GLN
1	F	492	ASN
1	F	493	ASN
1	F	593	GLN
1	F	613	GLN
1	C	296	GLN
1	C	338	GLN
1	C	363	ASN
1	C	415	ASN
1	C	449	ASN
1	C	451	ASN
1	C	467	GLN
1	C	492	ASN
1	C	529	ASN
1	D	296	GLN
1	D	338	GLN
1	D	363	ASN
1	D	415	ASN
1	D	451	ASN
1	D	467	GLN
1	D	489	GLN
1	D	492	ASN
1	D	493	ASN
1	D	593	GLN
1	D	613	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ADP	A	701	-	24,29,29	1.40	4 (16%)	23,45,45	2.17	1 (4%)
4	ADP	B	701	6	24,29,29	1.30	3 (12%)	23,45,45	2.15	1 (4%)
4	ADP	C	701	-	24,29,29	1.53	5 (20%)	23,45,45	2.18	1 (4%)
4	ADP	D	701	6	24,29,29	1.45	4 (16%)	23,45,45	2.14	2 (8%)
4	ADP	E	701	-	24,29,29	1.39	4 (16%)	23,45,45	2.19	1 (4%)
4	ADP	F	702	6	24,29,29	1.28	3 (12%)	23,45,45	2.20	2 (8%)

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
4	ADP	A	701	-	-	0/12/32/32	0/3/3/3
4	ADP	B	701	6	-	0/12/32/32	0/3/3/3
4	ADP	C	701	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	701	6	-	0/12/32/32	0/3/3/3
4	ADP	E	701	-	-	0/12/32/32	0/3/3/3
4	ADP	F	702	6	-	0/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	ADP	C8-N7	-2.39	1.30	1.34
4	D	701	ADP	C8-N7	-2.25	1.30	1.34
4	C	701	ADP	C8-N7	-2.23	1.30	1.34
4	E	701	ADP	PB-O2B	-2.19	1.47	1.54
4	B	701	ADP	C8-N7	-2.18	1.30	1.34
4	E	701	ADP	C8-N7	-2.12	1.30	1.34
4	C	701	ADP	PB-O2B	-2.10	1.47	1.54
4	A	701	ADP	PB-O2B	-2.09	1.47	1.54
4	F	702	ADP	C8-N7	-2.09	1.30	1.34
4	B	701	ADP	O4'-C1'	2.41	1.44	1.41
4	F	702	ADP	O4'-C1'	2.55	1.44	1.41
4	D	701	ADP	O4'-C1'	2.58	1.44	1.41
4	D	701	ADP	PA-O1A	2.67	1.61	1.51
4	C	701	ADP	PA-O1A	2.89	1.61	1.51
4	F	702	ADP	PB-O1B	3.06	1.60	1.50
4	D	701	ADP	PB-O1B	3.07	1.60	1.50
4	B	701	ADP	PB-O1B	3.10	1.60	1.50
4	E	701	ADP	PB-O1B	3.25	1.61	1.50
4	A	701	ADP	PB-O1B	3.29	1.61	1.50
4	A	701	ADP	O4'-C1'	3.36	1.46	1.41
4	C	701	ADP	PB-O1B	3.38	1.61	1.50
4	E	701	ADP	O4'-C1'	3.51	1.46	1.41
4	C	701	ADP	O4'-C1'	3.58	1.46	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	701	ADP	N3-C2-N1	-9.58	121.35	128.87
4	C	701	ADP	N3-C2-N1	-9.54	121.38	128.87
4	F	702	ADP	N3-C2-N1	-9.47	121.43	128.87
4	A	701	ADP	N3-C2-N1	-9.45	121.44	128.87
4	B	701	ADP	N3-C2-N1	-9.30	121.56	128.87
4	D	701	ADP	N3-C2-N1	-9.23	121.62	128.87
4	D	701	ADP	O4'-C4'-C3'	2.01	109.23	105.16
4	F	702	ADP	O4'-C4'-C3'	2.02	109.26	105.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	ADP	2	0
4	F	702	ADP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
1	A	362/362 (100%)	0.26	26 (7%)	18	12	88, 148, 197, 205	0
1	B	362/362 (100%)	0.09	11 (3%)	54	47	82, 122, 157, 176	0
1	C	362/362 (100%)	0.21	22 (6%)	25	18	87, 148, 197, 205	0
1	D	362/362 (100%)	0.09	11 (3%)	54	47	83, 122, 157, 176	0
1	E	362/362 (100%)	0.23	22 (6%)	25	18	88, 148, 197, 205	0
1	F	362/362 (100%)	0.05	7 (1%)	70	66	84, 122, 157, 176	0
2	W	33/33 (100%)	0.79	7 (21%)	1	1	98, 152, 202, 215	32 (96%)
3	K	33/33 (100%)	1.84	10 (30%)	1	0	88, 160, 237, 250	32 (96%)
All	All	2238/2238 (100%)	0.19	116 (5%)	31	24	82, 133, 185, 250	64 (2%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	20	DA	14.4
1	C	494	LEU	8.4
1	A	312	SER	8.2
3	K	21	DG	8.2
3	K	22	DA	7.1
1	A	450	VAL	6.2
1	E	494	LEU	5.7
1	E	480	GLY	5.5
1	A	607	PHE	5.0
3	K	7	DT	4.6
1	C	509	LEU	4.3
2	W	31	DT	4.3
1	A	293	LEU	4.2
1	F	514	LEU	4.2
1	E	545	ILE	4.2
1	A	405	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	457	LEU	4.1
1	E	484	ASP	4.0
1	A	387	TRP	3.8
1	B	500	TYR	3.7
1	D	494	LEU	3.7
1	A	446	LYS	3.7
3	K	23	DG	3.7
1	A	479	GLY	3.6
1	A	575	LEU	3.6
1	B	397	LEU	3.6
1	A	494	LEU	3.5
1	B	623	ILE	3.5
1	A	394	LEU	3.5
1	C	585	VAL	3.4
1	A	472	PHE	3.3
2	W	33	DT	3.3
1	A	439	LEU	3.2
1	D	448	LEU	3.2
2	W	32	DA	3.2
1	C	267	GLN	3.1
1	A	311	PRO	3.1
1	F	569	ILE	3.1
1	D	625	VAL	3.0
3	K	29	DG	3.0
1	D	579	LEU	3.0
1	F	376	PHE	3.0
1	C	434	THR	3.0
1	E	607	PHE	3.0
1	C	408	PHE	2.9
1	E	268	VAL	2.9
1	C	569	ILE	2.9
3	K	2	DA	2.9
3	K	28	DA	2.9
1	A	384	ILE	2.9
1	A	505	VAL	2.8
1	C	461	LEU	2.8
1	D	387	TRP	2.7
1	A	267	GLN	2.7
1	E	287	LEU	2.7
1	C	479	GLY	2.7
1	A	521	PHE	2.7
1	C	562	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	W	6	DC	2.6
1	C	614	LYS	2.6
1	A	399	PRO	2.6
1	C	525	ILE	2.6
1	B	472	PHE	2.5
1	E	488	GLY	2.5
1	A	460	GLU	2.5
1	E	491	ILE	2.5
1	E	610	SER	2.5
1	E	482	SER	2.5
1	B	273	VAL	2.5
2	W	11	DT	2.4
1	E	428	ILE	2.4
1	C	545	ILE	2.4
1	B	283	ASP	2.4
1	E	603	LEU	2.4
1	E	435	LEU	2.4
1	F	479	GLY	2.4
1	C	491	ILE	2.4
1	A	536	THR	2.4
1	A	545	ILE	2.4
1	C	450	VAL	2.4
3	K	31	DC	2.3
1	A	504	SER	2.3
1	B	615	MET	2.3
1	A	458	ASN	2.3
1	C	327	PHE	2.3
1	B	577	LEU	2.3
1	D	343	THR	2.3
2	W	4	DC	2.3
3	K	18	DG	2.3
1	C	504	SER	2.3
1	E	307	LYS	2.3
1	D	501	LEU	2.2
1	A	445	GLY	2.2
1	F	365	PHE	2.2
1	C	519	GLN	2.2
1	F	424	PHE	2.2
1	D	456	ARG	2.2
2	W	22	DA	2.2
1	C	626	LEU	2.2
1	F	396	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	439	LEU	2.1
1	A	461	LEU	2.1
1	E	439	LEU	2.1
1	E	612	TYR	2.1
1	E	461	LEU	2.1
1	B	387	TRP	2.1
1	C	384	ILE	2.1
1	B	497	LEU	2.1
1	C	378	SER	2.1
1	D	424	PHE	2.1
1	D	442	LEU	2.0
1	D	384	ILE	2.0
1	B	266	LYS	2.0
1	E	303	LEU	2.0
1	E	588	PHE	2.0
1	E	381	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ZN	E	702	1/1	0.56	0.21	1.59	160,160,160,160	0
5	ZN	D	702	1/1	0.90	0.25	0.79	112,112,112,112	0
4	ADP	D	701	27/27	0.91	0.23	0.30	110,129,134,135	0
4	ADP	B	701	27/27	0.93	0.22	0.05	109,129,135,136	0
6	MN	B	703	1/1	0.98	0.19	-0.01	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ADP	F	702	27/27	0.92	0.21	-0.11	111,127,136,136	0
4	ADP	C	701	27/27	0.89	0.20	-0.26	150,157,166,167	0
4	ADP	A	701	27/27	0.92	0.17	-0.36	150,157,164,165	0
4	ADP	E	701	27/27	0.94	0.19	-0.56	152,161,169,169	0
6	MN	F	701	1/1	0.93	0.13	-1.14	103,103,103,103	0
6	MN	D	703	1/1	0.96	0.15	-1.42	103,103,103,103	0
5	ZN	C	702	1/1	0.89	0.23	-	160,160,160,160	0
5	ZN	F	703	1/1	0.86	0.23	-	109,109,109,109	0
5	ZN	A	702	1/1	0.94	0.13	-	162,162,162,162	0
5	ZN	B	702	1/1	0.96	0.22	-	112,112,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.