



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:20 am BST

PDB ID : 6ERQ
Title : Structure of the human mitochondrial transcription initiation complex at the HSP promoter
Authors : Hillen, H.S.; Morozov, Y.I.; Sarfallah, A.; Temiakov, D.; Cramer, P.
Deposited on : 2017-10-18
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

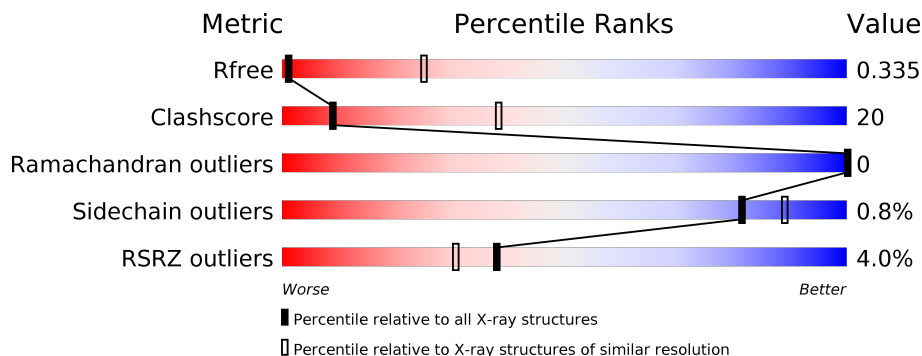
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

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






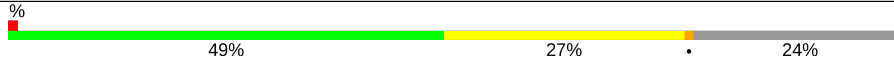
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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 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	C	205	
1	G	205	
2	D	50	
2	H	50	
3	E	50	
3	I	50	

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Mol	Chain	Length	Quality of chain
4	A	1128	 4% 59% 30% 10%
4	B	1128	 3% 57% 31% 11%
5	F	377	 3% 52% 24% 24%
5	J	377	 1% 49% 27% 24%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 27643 atoms, of which 42 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 Transcription factor A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	192	1615	1019	291	300	5	0	0	0
1	G	192	1615	1019	291	300	5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	41	ASN	-	expression tag	UNP Q00059
C	42	ALA	-	expression tag	UNP Q00059
C	49	SER	CYS	conflict	UNP Q00059
G	41	ASN	-	expression tag	UNP Q00059
G	42	ALA	-	expression tag	UNP Q00059
G	49	SER	CYS	conflict	UNP Q00059

- Molecule 2 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	46	924	440	175	264	45	0	0	0
2	H	46	924	440	175	264	45	0	0	0

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	45	938	444	171	279	44	0	0	0
3	I	45	938	444	171	279	44	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1011	Total	C	N	O	S	0	0	0
			8028	5107	1452	1418	51			
4	B	1002	Total	C	N	O	S	0	0	0
			7967	5069	1443	1404	51			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	-	expression tag	UNP O00411
A	104	ALA	-	expression tag	UNP O00411
A	555	ALA	GLU	conflict	UNP O00411
B	103	ASN	-	expression tag	UNP O00411
B	104	ALA	-	expression tag	UNP O00411
B	555	ALA	GLU	conflict	UNP O00411

- Molecule 5 is a protein called Dimethyladenosine transferase 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
5	F	288	Total	C	H	N	O	S	0	0	0
			2347	1506	21	397	408	15			
5	J	288	Total	C	H	N	O	S	0	0	0
			2347	1506	21	397	408	15			

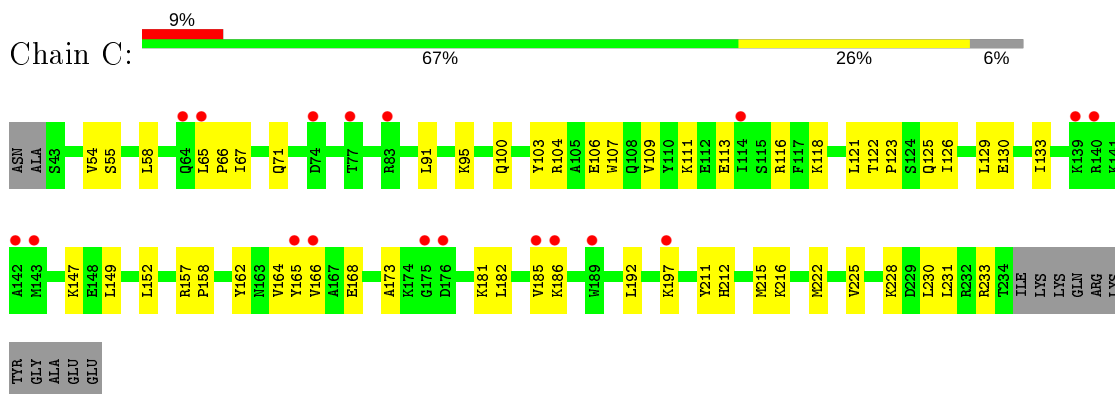
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	20	ASN	-	expression tag	UNP Q9H5Q4
F	21	ALA	-	expression tag	UNP Q9H5Q4
J	20	ASN	-	expression tag	UNP Q9H5Q4
J	21	ALA	-	expression tag	UNP Q9H5Q4

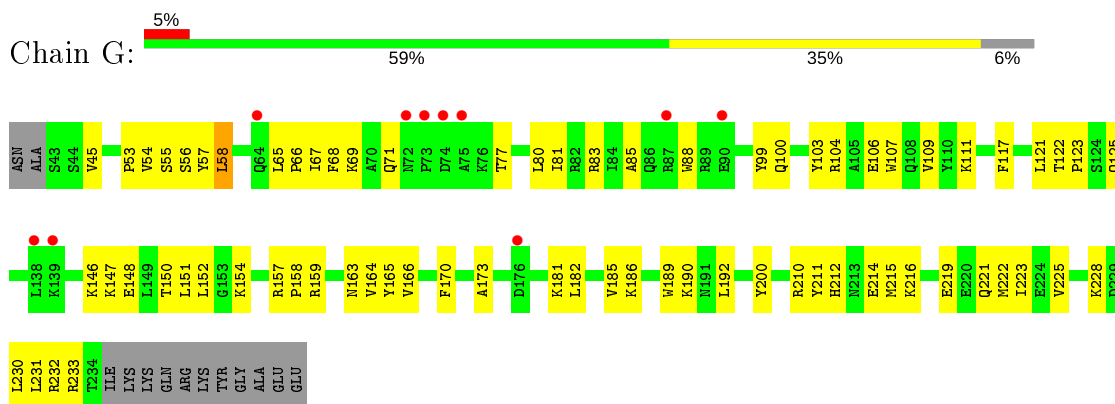
3 Residue-property plots [i](#)

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

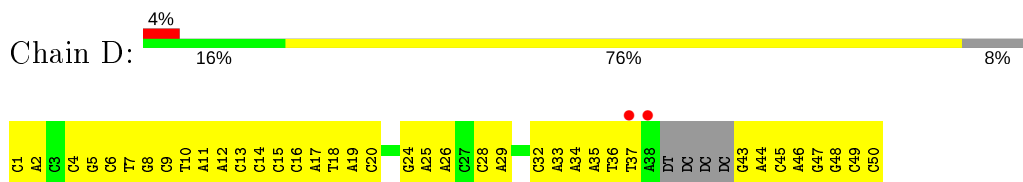
- Molecule 1: Transcription factor A, mitochondrial



- Molecule 1: Transcription factor A, mitochondrial



- Molecule 2: Non-Template DNA

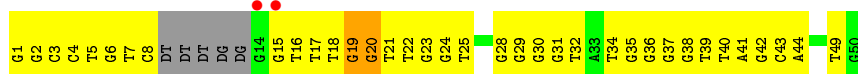


- Molecule 2: Non-Template DNA

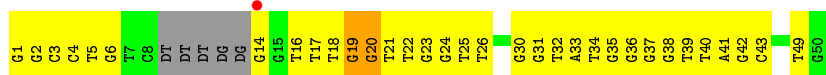




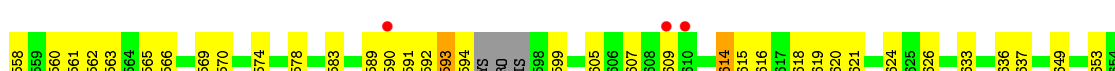
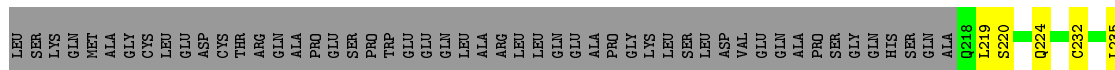
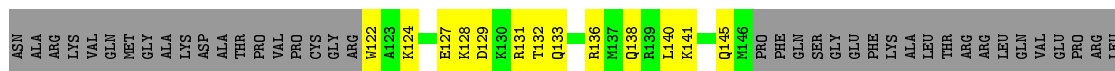
• Molecule 3: Template DNA

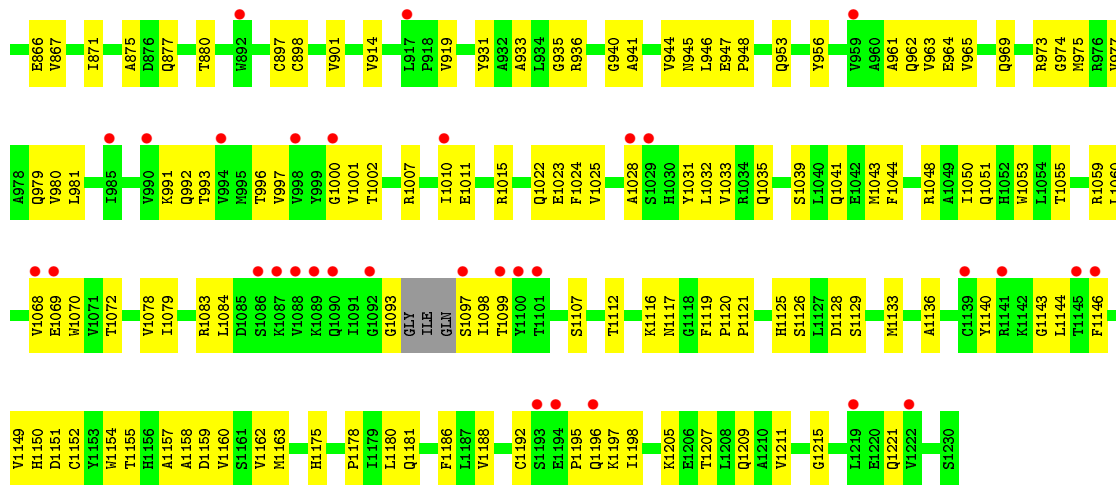


• Molecule 3: Template DNA

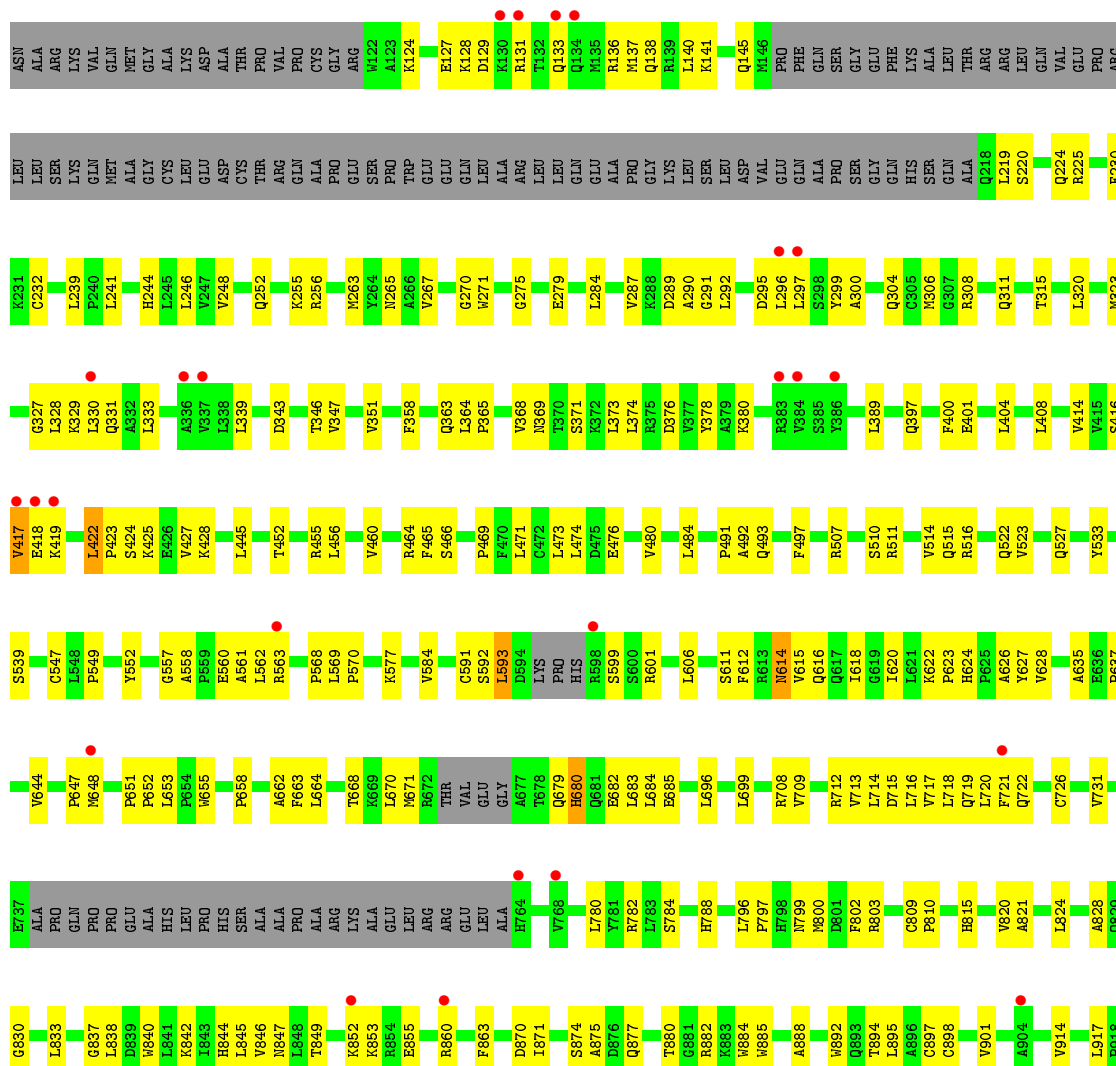


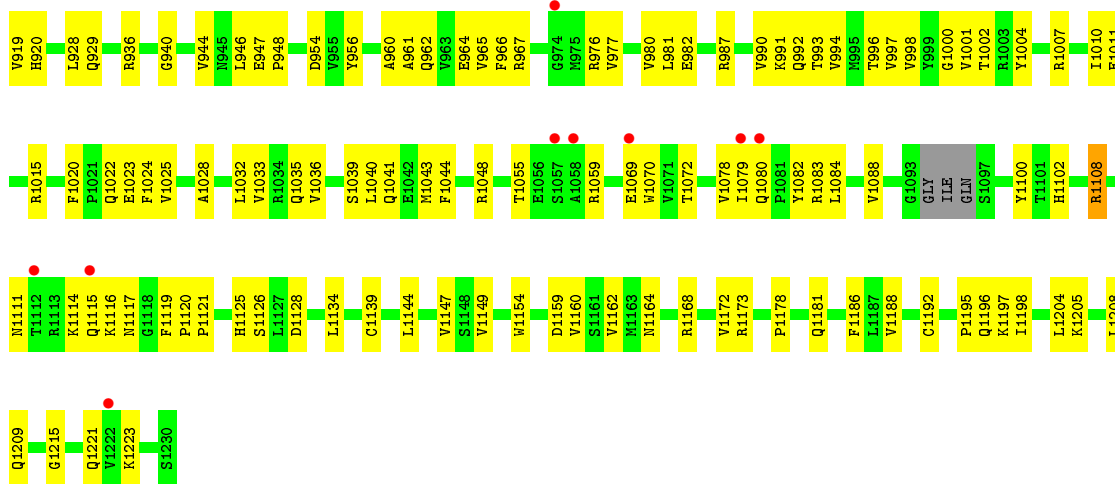
• Molecule 4: DNA-directed RNA polymerase, mitochondrial



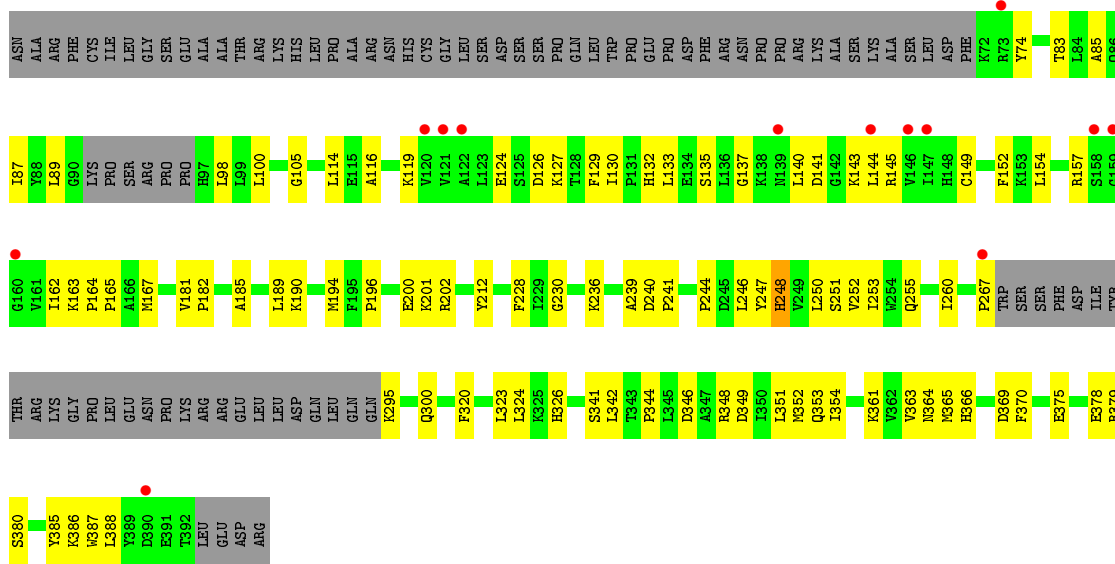


● Molecule 4: DNA-directed RNA polymerase, mitochondrial

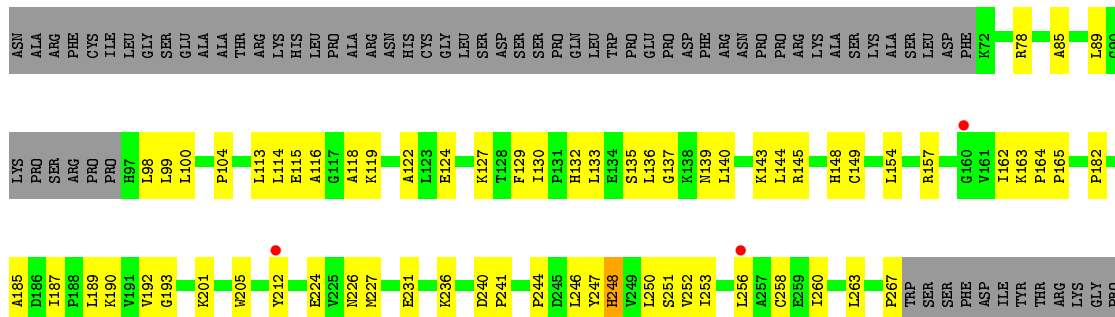




- Molecule 5: Dimethyladenosine transferase 2, mitochondrial



- Molecule 5: Dimethyladenosine transferase 2, mitochondrial



LEU	K295
GLU	L296
ASN	Y297
PRO	L298
LYS	L299
ARG	Q300
ARG	P303
GLU	L307
LEU	F368
LEU	T309
LEU	L312
ASP	H322
GLN	L323
LEU	H326
GLN	C327
GLN	F328
GLN	G329
GLN	R330
GLN	R331
GLN	L339
GLN	D346
GLU	D349
GLU	I350
ASP	L351
ASP	M352
ASP	Q353
ASP	K361
ASP	V362
ASP	V363
ASP	N364
ASP	M365
ASP	H366
ASP	D669
ASP	F370
ASP	K371

T372
L373
F374
E375
E378
R379
Y385
K386
W387
L388
Y389
D390
E391
T392
LEU
GLU
ASP
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.62Å 197.73Å 134.34Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	49.58 – 4.50 49.58 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.58-4.50) 99.2 (49.58-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 4.45Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.291 , 0.333 0.291 , 0.335	Depositor DCC
R_{free} test set	1573 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	248.7	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 252.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	27643	wwPDB-VP
Average B, all atoms (Å ²)	333.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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](#)

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	C	0.23	0/1646	0.35	0/2202
1	G	0.23	0/1646	0.35	0/2202
2	D	0.54	0/1035	0.87	0/1587
2	H	0.54	0/1035	0.88	0/1587
3	E	0.56	0/1051	1.07	4/1625 (0.2%)
3	I	0.57	0/1051	1.06	4/1625 (0.2%)
4	A	0.23	0/8213	0.38	0/11132
4	B	0.23	0/8150	0.38	0/11043
5	F	0.24	0/2380	0.38	0/3213
5	J	0.23	0/2380	0.38	0/3213
All	All	0.30	0/28587	0.52	8/39429 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	19	DG	OP2-P-O3'	-11.21	80.54	105.20
3	I	19	DG	OP2-P-O3'	-11.08	80.81	105.20
3	E	20	DG	OP1-P-OP2	9.01	133.11	119.60
3	I	19	DG	OP1-P-O3'	-8.61	86.26	105.20
3	I	20	DG	OP1-P-OP2	8.61	132.51	119.60
3	E	19	DG	OP1-P-O3'	-8.50	86.49	105.20
3	I	19	DG	O4'-C1'-N9	5.77	112.04	108.00
3	E	19	DG	O4'-C1'-N9	5.75	112.03	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	C	1615	0	1655	47	0
1	G	1615	0	1655	83	1
2	D	924	0	514	54	1
2	H	924	0	514	50	0
3	E	938	0	512	66	0
3	I	938	0	512	66	1
4	A	8028	0	8092	310	1
4	B	7967	0	8032	323	0
5	F	2326	21	2375	81	0
5	J	2326	21	2375	94	0
All	All	27601	42	26236	1087	2

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 20.

All (1087) 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:A:363:GLN:HB3	4:A:364:LEU:HG	1.30	1.13
4:B:422:LEU:HD12	4:B:427:VAL:HG23	1.19	1.12
4:A:422:LEU:HD12	4:A:427:VAL:HG23	1.29	1.11
3:E:16:DT:H4'	4:A:618:ILE:HG22	1.31	1.11
4:B:363:GLN:HB3	4:B:364:LEU:HG	1.26	1.09
4:B:422:LEU:HD22	4:B:423:PRO:HD2	1.39	1.05
3:E:15:DG:H2'	3:E:16:DT:H72	1.38	1.04
4:A:422:LEU:HD13	4:A:423:PRO:HD2	1.39	1.03
5:J:114:LEU:HB3	5:J:140:LEU:HD11	1.43	1.01
4:A:944:VAL:HG23	4:A:946:LEU:HD13	1.42	1.00
5:F:114:LEU:HB3	5:F:140:LEU:HD11	1.45	0.96
4:A:655:TRP:HB3	4:A:696:LEU:HD22	1.46	0.95
3:I:16:DT:H4'	4:B:618:ILE:HG22	1.46	0.95
4:B:419:LYS:HE2	4:B:422:LEU:HD23	1.49	0.94
1:G:214:GLU:OE2	4:B:133:GLN:NE2	2.03	0.92
4:B:655:TRP:HB3	4:B:696:LEU:HD22	1.51	0.91
4:B:592:SER:HB2	4:B:599:SER:HB2	1.51	0.90
5:J:114:LEU:HD11	5:J:144:LEU:HD22	1.55	0.89
1:C:121:LEU:HD12	1:C:125:GLN:HG2	1.54	0.89
3:I:41:DA:H2'	3:I:42:DG:C8	2.08	0.88
4:B:592:SER:CB	4:B:599:SER:HB2	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:718:LEU:O	4:A:722:GLN:HG3	1.74	0.87
4:B:944:VAL:HG23	4:B:946:LEU:HD13	1.55	0.87
5:F:349:ASP:HA	5:F:352:MET:HE2	1.55	0.87
4:B:256:ARG:HD3	4:B:290:ALA:HB2	1.57	0.86
4:B:796:LEU:HD22	4:B:810:PRO:HG2	1.56	0.86
4:B:611:SER:OG	5:J:391:GLU:OE1	1.95	0.83
4:B:516:ARG:HH22	4:B:562:LEU:HD22	1.44	0.83
1:C:231:LEU:O	1:C:233:ARG:NH1	2.11	0.82
5:F:89:LEU:HD11	5:F:116:ALA:HB1	1.59	0.82
4:A:246:LEU:HD22	4:A:267:VAL:HG21	1.62	0.82
2:D:43:DG:H4'	2:D:44:DA:OP1	1.80	0.82
4:A:936:ARG:HB2	4:A:1215:GLY:H	1.46	0.81
2:D:34:DA:H2''	2:D:35:DA:C8	2.15	0.81
3:I:14:DG:H22	4:B:1102:HIS:HA	1.45	0.81
4:A:422:LEU:HD13	4:A:423:PRO:CD	2.10	0.80
2:D:35:DA:N1	4:A:616:GLN:HG3	1.95	0.80
5:J:100:LEU:HD13	5:J:189:LEU:HD11	1.62	0.80
4:B:422:LEU:CD2	4:B:423:PRO:HD2	2.11	0.80
3:E:41:DA:H2'	3:E:42:DG:C8	2.15	0.80
1:C:121:LEU:HB2	1:C:125:GLN:CG	2.12	0.80
4:B:996:THR:O	4:B:1000:GLY:N	2.15	0.79
1:C:149:LEU:O	1:C:152:LEU:HG	1.82	0.79
3:E:36:DG:H2'	3:E:37:DG:C8	2.18	0.79
4:A:422:LEU:CD1	4:A:423:PRO:HD2	2.12	0.79
5:F:244:PRO:HB3	5:F:363:VAL:HG21	1.65	0.79
5:F:244:PRO:HB3	5:F:363:VAL:CG2	2.12	0.79
4:B:712:ARG:NH2	4:B:875:ALA:O	2.16	0.78
4:A:815:HIS:HD2	4:A:1149:VAL:HG22	1.48	0.78
4:B:422:LEU:HD12	4:B:427:VAL:CG2	2.08	0.78
3:I:39:DT:C6	3:I:40:DT:H72	2.18	0.78
4:A:718:LEU:HB3	4:A:722:GLN:HE21	1.48	0.78
4:B:363:GLN:HB3	4:B:364:LEU:CG	2.11	0.78
5:J:100:LEU:HD22	5:J:189:LEU:HD21	1.65	0.78
4:A:852:LYS:HD2	4:A:855:GLU:HG3	1.65	0.78
4:B:1069:GLU:HG2	4:B:1079:ILE:HG23	1.64	0.77
4:A:936:ARG:HB2	4:A:1215:GLY:N	2.00	0.77
3:I:17:DT:OP2	4:B:1100:TYR:HA	1.83	0.77
2:H:36:DT:H6	5:J:201:LYS:HZ3	1.33	0.77
5:J:349:ASP:OD1	5:J:353:GLN:NE2	2.17	0.77
4:B:363:GLN:CB	4:B:364:LEU:HG	2.12	0.76
4:A:417:VAL:HG11	4:A:718:LEU:HD22	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:DC:H2'	2:H:5:DG:C8	2.21	0.75
4:B:422:LEU:HD13	4:B:423:PRO:CD	2.18	0.74
5:F:349:ASP:O	5:F:353:GLN:HG2	1.88	0.74
4:A:363:GLN:HB3	4:A:364:LEU:CG	2.14	0.73
4:B:300:ALA:HB2	4:B:333:LEU:HD11	1.71	0.73
4:A:809:CYS:HB2	4:A:810:PRO:HD3	1.69	0.73
5:F:100:LEU:HD13	5:F:189:LEU:HD11	1.69	0.73
3:I:20:DG:C8	3:I:21:DT:H72	2.23	0.73
4:A:219:LEU:HD23	4:A:219:LEU:H	1.54	0.72
2:D:25:DA:H1'	2:D:26:DA:H5'	1.70	0.72
3:E:39:DT:H2''	3:E:40:DT:C5	2.24	0.72
5:F:114:LEU:HB3	5:F:140:LEU:CD1	2.20	0.72
5:J:137:GLY:HA2	5:J:144:LEU:HD23	1.71	0.72
4:A:1178:PRO:HB2	4:A:1181:GLN:HB2	1.71	0.72
4:A:940:GLY:O	4:A:944:VAL:HG22	1.89	0.72
1:G:107:TRP:CZ2	2:H:24:DG:H5''	2.24	0.72
3:E:39:DT:H2''	3:E:40:DT:C7	2.19	0.72
2:H:17:DA:H2''	2:H:18:DT:H71	1.71	0.72
4:A:363:GLN:CB	4:A:364:LEU:HG	2.15	0.72
4:B:1001:VAL:O	4:B:1002:THR:OG1	2.04	0.72
4:B:306:MET:HG2	4:B:311:GLN:HG3	1.70	0.72
4:A:369:ASN:ND2	4:A:690:THR:O	2.23	0.71
4:A:962:GLN:O	4:A:965:VAL:HG22	1.90	0.71
5:J:236:LYS:HG2	5:J:246:LEU:HD22	1.72	0.71
4:A:283:VAL:HA	4:A:286:MET:CE	2.20	0.71
4:B:809:CYS:HB2	4:B:810:PRO:HD3	1.71	0.71
2:D:18:DT:H2''	2:D:19:DA:C8	2.25	0.71
4:A:815:HIS:CD2	4:A:1149:VAL:HG22	2.24	0.71
4:B:658:PRO:HA	4:B:670:LEU:HD22	1.70	0.71
3:E:20:DG:C8	3:E:21:DT:H72	2.25	0.71
4:A:838:LEU:HG	4:A:842:LYS:HE3	1.73	0.71
4:A:992:GLN:HG3	4:A:1010:ILE:HG12	1.72	0.71
4:A:1001:VAL:O	4:A:1002:THR:OG1	2.03	0.71
4:A:422:LEU:CD1	4:A:427:VAL:HG23	2.14	0.71
4:B:962:GLN:O	4:B:965:VAL:HG22	1.91	0.70
1:G:58:LEU:HD22	3:I:30:DG:N3	2.05	0.70
4:A:803:ARG:HD3	4:A:1125:HIS:ND1	2.06	0.70
4:B:219:LEU:HD23	4:B:219:LEU:H	1.56	0.70
1:C:165:TYR:CE1	1:C:192:LEU:HD11	2.26	0.70
2:D:36:DT:H2''	2:D:37:DT:H5''	1.71	0.70
4:B:1004:TYR:HB2	4:B:1007:ARG:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:36:DG:H2'	3:I:37:DG:C8	2.26	0.70
4:A:239:LEU:HD11	4:A:270:GLY:HA3	1.73	0.70
3:I:21:DT:C2'	3:I:22:DT:H71	2.22	0.70
5:J:349:ASP:O	5:J:353:GLN:HG2	1.92	0.69
4:A:363:GLN:HA	4:A:365:PRO:HD3	1.73	0.69
4:B:424:SER:O	4:B:428:LYS:HG3	1.92	0.69
4:B:653:LEU:HG	4:B:664:LEU:HD23	1.72	0.69
5:F:114:LEU:HD11	5:F:144:LEU:HD22	1.75	0.69
3:E:5:DT:H2''	3:E:6:DG:C8	2.28	0.69
1:G:45:VAL:HG21	1:G:125:GLN:HB3	1.75	0.69
4:B:718:LEU:O	4:B:722:GLN:HG3	1.93	0.69
3:E:18:DT:OP2	4:A:1099:THR:N	2.26	0.69
2:D:37:DT:H72	5:F:202:ARG:HH11	1.57	0.69
4:B:419:LYS:CE	4:B:422:LEU:HD23	2.22	0.69
4:A:232:CYS:SG	4:A:473:LEU:HD11	2.34	0.68
4:B:849:THR:HA	4:B:888:ALA:HB1	1.76	0.68
4:B:416:SER:HB3	4:B:637:PRO:HA	1.74	0.68
4:B:1080:GLN:NE2	4:B:1115:GLN:OE1	2.27	0.68
3:E:19:DG:H1'	3:E:20:DG:OP1	1.93	0.68
4:B:417:VAL:HG22	4:B:784:SER:HA	1.75	0.68
1:G:107:TRP:CH2	2:H:24:DG:H5''	2.28	0.68
1:G:165:TYR:CE1	1:G:192:LEU:HD11	2.29	0.68
3:I:16:DT:C2	4:B:616:GLN:HB3	2.28	0.68
3:I:19:DG:H1'	3:I:20:DG:OP1	1.93	0.68
4:A:1011:GLU:O	4:A:1015:ARG:HG3	1.94	0.68
4:A:1070:TRP:HA	4:A:1186:PHE:CE1	2.28	0.68
4:B:422:LEU:HD13	4:B:423:PRO:HG2	1.76	0.67
3:E:35:DG:H2''	3:E:36:DG:C8	2.28	0.67
1:C:113:GLU:HG2	1:C:116:ARG:HH21	1.59	0.67
4:A:1043:MET:HG3	4:A:1044:PHE:CD2	2.30	0.67
4:A:467:LEU:HD12	4:A:578:LEU:CD1	2.23	0.67
5:F:200:GLU:OE2	5:F:230:GLY:N	2.23	0.67
5:F:100:LEU:HD22	5:F:189:LEU:HD21	1.75	0.67
5:F:240:ASP:HB2	5:F:241:PRO:HD2	1.76	0.67
3:I:5:DT:H2''	3:I:6:DG:C8	2.30	0.67
4:A:509:PHE:CE1	4:A:566:PRO:HA	2.29	0.67
4:A:300:ALA:HB2	4:A:333:LEU:HD11	1.77	0.67
4:A:718:LEU:C	4:A:722:GLN:HG3	2.15	0.67
4:B:256:ARG:NH2	4:B:289:ASP:OD2	2.27	0.67
1:G:221:GLN:NE2	4:B:140:LEU:HD13	2.09	0.67
4:A:1120:PRO:HB2	4:A:1121:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1083:ARG:NH1	4:B:1108:ARG:O	2.28	0.66
4:B:1070:TRP:HA	4:B:1186:PHE:CE1	2.30	0.66
2:H:35:DA:N1	4:B:616:GLN:HG3	2.10	0.66
1:G:146:LYS:HE2	3:I:39:DT:OP2	1.95	0.66
4:B:1120:PRO:HB2	4:B:1121:PRO:HD3	1.77	0.66
4:A:236:THR:HG23	4:A:473:LEU:HD23	1.78	0.66
4:B:592:SER:OG	4:B:599:SER:HB2	1.95	0.66
4:B:225:ARG:HD2	4:B:465:PHE:CE1	2.31	0.66
4:B:993:THR:HA	4:B:1010:ILE:CD1	2.26	0.66
4:B:239:LEU:HD11	4:B:270:GLY:HA3	1.77	0.66
4:B:726:CYS:H	4:B:731:VAL:HB	1.61	0.65
4:B:940:GLY:O	4:B:944:VAL:HG22	1.97	0.65
5:J:114:LEU:HB3	5:J:140:LEU:CD1	2.21	0.65
4:A:1125:HIS:HA	4:A:1128:ASP:OD2	1.96	0.65
4:B:1015:ARG:CZ	4:B:1025:VAL:HG11	2.26	0.65
4:B:993:THR:HA	4:B:1010:ILE:HD11	1.79	0.65
4:B:417:VAL:CG2	4:B:784:SER:HA	2.27	0.65
4:B:940:GLY:HA2	4:B:1044:PHE:HE1	1.63	0.64
4:A:138:GLN:HA	4:A:141:LYS:HE2	1.80	0.64
5:F:137:GLY:HA2	5:F:144:LEU:HD23	1.77	0.64
4:A:418:GLU:CG	4:A:722:GLN:HG2	2.26	0.64
4:B:956:TYR:CD1	4:B:991:LYS:HA	2.32	0.64
5:J:240:ASP:HB2	5:J:241:PRO:HD2	1.77	0.64
4:B:977:VAL:HA	4:B:980:VAL:HG22	1.79	0.64
4:B:954:ASP:OD1	4:B:987:ARG:NE	2.24	0.64
4:B:699:LEU:HD11	4:B:800:MET:HG3	1.80	0.64
4:B:833:LEU:HB3	4:B:837:GLY:HA3	1.80	0.64
2:D:35:DA:C2	4:A:616:GLN:HG3	2.32	0.64
4:A:1039:SER:O	4:A:1043:MET:HG2	1.98	0.64
4:A:832:PRO:O	4:A:1158:ALA:HB2	1.98	0.63
4:A:283:VAL:HA	4:A:286:MET:HE2	1.79	0.63
4:B:618:ILE:HG13	4:B:620:ILE:HD11	1.79	0.63
4:B:129:ASP:O	4:B:133:GLN:HG3	1.97	0.63
2:D:7:DT:H2'	2:D:8:DG:C8	2.33	0.63
4:B:1043:MET:HG3	4:B:1044:PHE:CD2	2.33	0.63
5:J:248:HIS:HA	5:J:328:PHE:CE1	2.33	0.63
4:B:1147:VAL:CG2	4:B:1154:TRP:HB2	2.29	0.63
3:E:18:DT:OP1	4:A:1098:ILE:HA	1.98	0.63
4:A:1072:THR:HG22	4:A:1126:SER:HB2	1.81	0.63
5:F:137:GLY:CA	5:F:144:LEU:HD23	2.28	0.63
5:F:164:PRO:HG2	5:F:165:PRO:HD3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1069:GLU:HG2	4:A:1079:ILE:HG23	1.78	0.62
4:A:522:GLN:OE1	4:A:561:ALA:HB1	1.99	0.62
3:E:16:DT:C2	4:A:616:GLN:HB3	2.34	0.62
5:F:236:LYS:O	5:F:251:SER:OG	2.17	0.62
3:I:31:DG:N7	3:I:32:DT:H73	2.14	0.62
4:A:241:LEU:HD11	4:A:460:VAL:HG11	1.81	0.62
4:A:418:GLU:CD	4:A:722:GLN:HG2	2.19	0.62
4:B:422:LEU:HD13	4:B:423:PRO:CG	2.29	0.62
5:J:322:HIS:HB3	5:J:389:TYR:CZ	2.35	0.62
4:A:1083:ARG:HD3	4:A:1107:SER:CB	2.30	0.62
4:A:607:TYR:CE1	5:F:388:LEU:HD13	2.34	0.62
1:C:212:HIS:NE2	1:C:216:LYS:HE3	2.14	0.62
4:A:414:VAL:HG13	4:A:788:HIS:HB2	1.81	0.62
4:B:232:CYS:SG	4:B:469:PRO:HB2	2.40	0.62
1:G:58:LEU:HG	3:I:31:DG:N3	2.14	0.62
5:J:137:GLY:CA	5:J:144:LEU:HD23	2.30	0.62
2:D:45:DC:H2''	2:D:46:DA:C8	2.34	0.62
4:B:680:HIS:NE2	4:B:802:PHE:HB2	2.15	0.62
4:B:838:LEU:HG	4:B:842:LYS:HE3	1.80	0.62
3:E:40:DT:OP2	3:E:40:DT:H71	1.99	0.62
5:J:164:PRO:HG2	5:J:165:PRO:HD3	1.82	0.62
5:F:240:ASP:HB2	5:F:241:PRO:CD	2.30	0.62
4:A:418:GLU:HG3	4:A:722:GLN:HA	1.82	0.61
1:C:233:ARG:HG2	3:E:49:DT:P	2.40	0.61
1:G:150:THR:HG21	3:I:38:DG:OP2	1.99	0.61
4:A:871:ILE:HG23	4:A:898:CYS:SG	2.40	0.61
3:E:34:DT:H2''	3:E:35:DG:C8	2.35	0.61
4:A:713:VAL:HG12	4:A:824:LEU:HD23	1.82	0.61
1:G:54:VAL:HG12	1:G:58:LEU:HB3	1.82	0.61
3:I:32:DT:H2''	3:I:33:DA:C8	2.35	0.61
5:J:240:ASP:HB2	5:J:241:PRO:CD	2.30	0.61
4:B:1059:ARG:HG2	4:B:1116:LYS:HD3	1.83	0.61
1:G:67:ILE:O	1:G:71:GLN:HG2	1.99	0.61
3:I:39:DT:H2'	3:I:40:DT:H72	1.83	0.61
2:H:4:DC:H2''	2:H:5:DG:O5'	2.01	0.61
5:F:344:PRO:HG3	5:F:385:TYR:CD2	2.35	0.61
1:G:159:ARG:HD3	2:H:8:DG:H5''	1.83	0.61
4:A:124:LYS:O	4:A:128:LYS:HG3	2.01	0.61
4:B:683:LEU:CD1	4:B:1079:ILE:HG12	2.31	0.61
4:B:1039:SER:O	4:B:1043:MET:HG2	2.00	0.60
4:B:124:LYS:O	4:B:128:LYS:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:236:THR:CG2	4:A:473:LEU:HD23	2.31	0.60
4:A:616:GLN:N	4:A:616:GLN:OE1	2.34	0.60
2:D:36:DT:O4'	4:A:615:VAL:HG13	2.00	0.60
4:A:456:LEU:O	4:A:460:VAL:HG23	2.00	0.60
4:B:1055:THR:O	4:B:1059:ARG:HG3	2.00	0.60
4:B:246:LEU:HD22	4:B:267:VAL:HG21	1.82	0.60
3:E:1:DG:H2''	3:E:2:DG:C8	2.35	0.60
2:D:47:DG:H2''	2:D:48:DG:C8	2.36	0.60
3:E:38:DG:C2'	3:E:39:DT:H71	2.32	0.60
4:B:422:LEU:HD13	4:B:423:PRO:HD2	1.82	0.60
3:I:21:DT:H2'	3:I:22:DT:H71	1.84	0.60
3:E:16:DT:C4'	4:A:618:ILE:HG22	2.20	0.60
4:A:852:LYS:CD	4:A:855:GLU:HG3	2.31	0.60
1:G:117:PHE:CZ	1:G:121:LEU:HD21	2.36	0.60
2:H:4:DC:H4'	2:H:5:DG:OP1	2.01	0.60
4:B:622:LYS:HD3	5:J:388:LEU:CD2	2.32	0.60
4:B:622:LYS:HD3	5:J:388:LEU:HD22	1.84	0.60
2:H:34:DA:H2''	2:H:35:DA:C8	2.36	0.60
4:A:355:LYS:HB3	4:A:358:PHE:HB2	1.83	0.60
4:B:1178:PRO:HB2	4:B:1181:GLN:HB2	1.83	0.60
5:F:349:ASP:HA	5:F:352:MET:CE	2.27	0.60
1:G:54:VAL:CG1	1:G:58:LEU:HB3	2.32	0.60
4:A:941:ALA:HA	4:A:946:LEU:HB2	1.83	0.60
2:D:4:DC:H2'	2:D:5:DG:C8	2.37	0.59
4:A:846:VAL:HG21	4:A:860:ARG:O	2.02	0.59
4:A:417:VAL:HG11	4:A:718:LEU:CD2	2.31	0.59
2:D:4:DC:H2''	2:D:5:DG:O5'	2.02	0.59
3:E:17:DT:C2'	3:E:18:DT:H71	2.33	0.59
3:E:7:DT:H2''	3:E:8:DC:C5	2.37	0.59
4:B:474:LEU:HD12	4:B:515:GLN:OE1	2.03	0.59
5:J:236:LYS:HA	5:J:246:LEU:HB3	1.85	0.59
4:A:1055:THR:O	4:A:1059:ARG:HG3	2.03	0.59
4:A:1150:HIS:NE2	4:A:1152:CYS:SG	2.73	0.59
4:B:993:THR:CG2	4:B:1036:VAL:HG21	2.33	0.59
1:C:122:THR:HB	1:C:123:PRO:CD	2.33	0.59
5:F:152:PHE:CZ	5:F:196:PRO:HD3	2.38	0.59
2:D:37:DT:H72	5:F:202:ARG:HD3	1.85	0.59
2:D:47:DG:OP1	4:A:1112:THR:HG21	2.02	0.58
1:C:121:LEU:CD1	1:C:125:GLN:HG2	2.30	0.58
1:C:168:GLU:OE2	4:A:122:TRP:NE1	2.37	0.58
4:B:844:HIS:CG	4:B:919:VAL:HG13	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:322:HIS:HB3	5:J:389:TYR:CE2	2.37	0.58
4:B:960:ALA:CB	4:B:990:VAL:HG21	2.33	0.58
1:C:54:VAL:CG1	1:C:58:LEU:HB3	2.33	0.58
1:G:57:TYR:OH	2:H:20:DC:H1'	2.03	0.58
4:A:241:LEU:HD11	4:A:460:VAL:CG1	2.34	0.58
4:A:940:GLY:HA2	4:A:1044:PHE:CE1	2.39	0.58
4:A:996:THR:O	4:A:1000:GLY:N	2.33	0.58
4:B:992:GLN:HG3	4:B:1010:ILE:HG12	1.86	0.58
4:B:653:LEU:HG	4:B:664:LEU:CD2	2.33	0.58
1:G:147:LYS:O	1:G:151:LEU:HD13	2.04	0.58
4:A:1155:THR:HB	4:A:1163:MET:SD	2.43	0.58
4:A:852:LYS:HB3	4:A:855:GLU:HB2	1.85	0.58
4:B:936:ARG:HB2	4:B:1215:GLY:H	1.69	0.58
4:B:680:HIS:O	4:B:684:LEU:HG	2.02	0.58
1:C:121:LEU:HB2	1:C:125:GLN:HG2	1.85	0.58
2:D:11:DA:H2''	2:D:12:DA:O4'	2.03	0.58
5:F:267:PRO:HA	5:F:295:LYS:HA	1.84	0.58
4:A:418:GLU:HG3	4:A:722:GLN:HG2	1.85	0.58
4:B:796:LEU:CD2	4:B:810:PRO:HG2	2.31	0.58
4:B:1144:LEU:HD11	4:B:1162:VAL:CG1	2.34	0.58
4:B:803:ARG:HD3	4:B:1125:HIS:ND1	2.18	0.58
1:G:117:PHE:CE2	1:G:121:LEU:HD11	2.38	0.58
1:C:164:VAL:HG13	4:A:122:TRP:CZ2	2.39	0.58
4:A:129:ASP:O	4:A:133:GLN:HG3	2.04	0.58
4:B:845:LEU:HD11	4:B:898:CYS:SG	2.44	0.58
4:A:1059:ARG:NE	4:A:1116:LYS:HD2	2.19	0.57
1:G:65:LEU:HD11	1:G:77:THR:HG23	1.86	0.57
4:B:616:GLN:OE1	4:B:616:GLN:N	2.37	0.57
2:H:36:DT:H71	5:J:201:LYS:NZ	2.19	0.57
4:B:1011:GLU:HG2	4:B:1025:VAL:HG22	1.85	0.57
2:D:13:DC:H2''	2:D:14:DC:C6	2.39	0.57
2:H:36:DT:O4'	4:B:615:VAL:HG13	2.05	0.57
5:J:162:ILE:O	5:J:163:LYS:HG3	2.04	0.57
4:A:969:GLN:O	4:A:973:ARG:HG3	2.05	0.57
4:B:1004:TYR:CB	4:B:1007:ARG:HB2	2.34	0.57
3:I:39:DT:H2''	3:I:40:DT:H5'	1.85	0.57
4:A:1041:GLN:HB3	4:A:1048:ARG:HD2	1.86	0.57
4:B:1004:TYR:HB3	4:B:1007:ARG:HD2	1.86	0.57
4:B:662:ALA:HB3	4:B:668:THR:OG1	2.04	0.57
1:G:164:VAL:HG12	1:G:200:TYR:HD1	1.69	0.57
5:J:263:LEU:HD11	5:J:300:GLN:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:683:LEU:HD12	4:B:1079:ILE:HG12	1.86	0.57
3:I:16:DT:H6	3:I:16:DT:OP1	1.87	0.57
2:D:37:DT:C7	5:F:202:ARG:HD3	2.34	0.57
3:I:1:DG:H2''	3:I:2:DG:C8	2.40	0.57
5:J:89:LEU:HD21	5:J:118:ALA:HB2	1.85	0.57
4:A:956:TYR:CD1	4:A:991:LYS:HA	2.39	0.57
3:E:39:DT:C2'	3:E:40:DT:C7	2.83	0.57
5:F:212:TYR:CE1	5:F:253:ILE:HG23	2.40	0.57
1:G:81:ILE:HG13	2:H:19:DA:C2	2.40	0.57
5:J:205:TRP:CE2	5:J:250:LEU:HD21	2.40	0.57
4:B:655:TRP:O	4:B:696:LEU:HB3	2.05	0.57
4:A:1119:PHE:HB3	4:A:1120:PRO:HD3	1.87	0.57
4:B:452:THR:HG23	4:B:455:ARG:NH2	2.20	0.57
4:B:547:CYS:SG	4:B:552:TYR:HB2	2.45	0.57
4:B:533:TYR:OH	4:B:549:PRO:HB3	2.04	0.57
4:B:1028:ALA:O	4:B:1032:LEU:HG	2.05	0.56
4:B:1088:VAL:O	4:B:1102:HIS:N	2.38	0.56
2:D:4:DC:H4'	2:D:5:DG:OP1	2.05	0.56
4:A:554:GLU:HA	4:A:558:ALA:HB2	1.87	0.56
4:A:944:VAL:CG2	4:A:946:LEU:HD13	2.25	0.56
4:B:940:GLY:HA2	4:B:1044:PHE:CE1	2.40	0.56
5:F:194:MET:HG2	5:F:228:PHE:CD2	2.41	0.56
4:A:574:GLU:O	4:A:578:LEU:HG	2.05	0.56
4:B:1041:GLN:HB3	4:B:1048:ARG:HD2	1.87	0.56
4:B:287:VAL:HG13	4:B:292:LEU:HB2	1.87	0.56
1:C:233:ARG:HG2	3:E:49:DT:OP1	2.04	0.56
2:H:18:DT:H2''	2:H:19:DA:C8	2.40	0.56
4:A:662:ALA:HB3	4:A:668:THR:HG21	1.87	0.56
4:B:327:GLY:O	4:B:329:LYS:HE2	2.05	0.56
1:G:69:LYS:NZ	3:I:34:DT:H5'	2.20	0.56
4:A:653:LEU:HG	4:A:664:LEU:HD23	1.86	0.56
5:F:375:GLU:O	5:F:379:ARG:HG3	2.05	0.56
1:G:170:PHE:HA	1:G:185:VAL:HG21	1.86	0.56
4:A:452:THR:HG23	4:A:455:ARG:NH2	2.20	0.56
4:B:363:GLN:HA	4:B:365:PRO:HD3	1.86	0.56
3:E:23:DG:H2''	3:E:24:DG:H5''	1.87	0.56
3:I:36:DG:H2'	3:I:37:DG:H8	1.68	0.56
4:A:690:THR:HA	4:A:693:HIS:CE1	2.41	0.56
4:A:607:TYR:CZ	5:F:388:LEU:HD13	2.40	0.56
1:G:233:ARG:HG2	3:I:49:DT:P	2.46	0.56
4:A:1149:VAL:HG12	4:A:1150:HIS:ND1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:708:ARG:HD3	4:A:828:ALA:HA	1.87	0.56
4:B:279:GLU:OE1	4:B:279:GLU:N	2.39	0.56
4:B:820:VAL:HG22	4:B:892:TRP:CD1	2.40	0.56
1:G:159:ARG:HG2	2:H:8:DG:H5'	1.88	0.56
2:H:45:DC:H2''	2:H:46:DA:C8	2.41	0.56
4:B:1011:GLU:O	4:B:1015:ARG:HG3	2.05	0.56
4:B:1119:PHE:HB3	4:B:1120:PRO:HD3	1.86	0.56
4:B:815:HIS:CD2	4:B:1149:VAL:HG22	2.41	0.56
4:B:138:GLN:HA	4:B:141:LYS:HE2	1.87	0.56
2:D:46:DA:H2''	2:D:47:DG:C8	2.40	0.56
3:E:4:DC:H2'	3:E:5:DT:H72	1.88	0.55
1:C:107:TRP:O	1:C:111:LYS:HG3	2.06	0.55
2:H:17:DA:H2''	2:H:18:DT:C7	2.36	0.55
5:J:78:ARG:NH2	5:J:115:GLU:OE1	2.39	0.55
4:A:422:LEU:HD22	4:A:423:PRO:HD2	1.88	0.55
4:A:1059:ARG:HE	4:A:1116:LYS:HD2	1.72	0.55
4:A:1068:VAL:HG11	4:A:1119:PHE:CD1	2.42	0.55
4:B:1125:HIS:HA	4:B:1128:ASP:OD2	2.06	0.55
4:B:1205:LYS:HE2	4:B:1209:GLN:NE2	2.21	0.55
5:F:239:ALA:O	5:F:255:GLN:NE2	2.35	0.55
1:G:186:LYS:HE2	3:I:43:DC:H4'	1.88	0.55
1:G:231:LEU:O	1:G:233:ARG:NH1	2.40	0.55
3:I:17:DT:C2'	3:I:18:DT:H71	2.37	0.55
5:J:244:PRO:HB3	5:J:363:VAL:CG2	2.37	0.55
4:A:467:LEU:HD12	4:A:578:LEU:HD11	1.89	0.55
4:A:712:ARG:NH2	4:A:875:ALA:O	2.38	0.55
4:B:655:TRP:HB3	4:B:696:LEU:CD2	2.33	0.55
4:B:844:HIS:HB2	4:B:919:VAL:HG13	1.87	0.55
4:B:852:LYS:HD2	4:B:855:GLU:HG3	1.89	0.55
4:B:929:GLN:HA	4:B:944:VAL:HG21	1.89	0.55
1:C:55:SER:HA	1:C:103:TYR:CD1	2.42	0.54
4:A:940:GLY:HA2	4:A:1044:PHE:HE1	1.72	0.54
4:B:219:LEU:HD12	4:B:224:GLN:NE2	2.22	0.54
2:H:47:DG:H2''	2:H:48:DG:C8	2.42	0.54
3:I:41:DA:H4'	3:I:42:DG:OP1	2.07	0.54
4:A:1015:ARG:CZ	4:A:1025:VAL:HG11	2.38	0.54
2:D:28:DC:H2''	2:D:29:DA:C8	2.43	0.54
3:E:3:DC:H2''	3:E:4:DC:C6	2.42	0.54
5:F:119:LYS:HE3	5:F:143:LYS:HB3	1.89	0.54
4:B:1147:VAL:HG23	4:B:1154:TRP:HB2	1.89	0.54
4:B:780:LEU:O	4:B:784:SER:OG	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:591:CYS:O	4:A:593:LEU:HD23	2.07	0.54
4:B:815:HIS:HD2	4:B:1149:VAL:HG22	1.73	0.54
4:B:830:GLY:HA3	4:B:914:VAL:HG12	1.90	0.54
1:C:173:ALA:O	1:C:181:LYS:HE3	2.08	0.54
3:E:17:DT:H2'	3:E:18:DT:H71	1.88	0.54
3:E:2:DG:H2''	3:E:3:DC:C6	2.43	0.54
5:F:248:HIS:NE2	5:F:250:LEU:HB2	2.23	0.54
4:A:414:VAL:HG22	4:A:788:HIS:CG	2.43	0.54
4:B:1084:LEU:HG	4:B:1111:ASN:HB2	1.90	0.54
4:B:300:ALA:CB	4:B:333:LEU:HD11	2.38	0.54
5:J:236:LYS:O	5:J:251:SER:OG	2.26	0.54
4:A:1093:GLY:HA2	4:A:1097:SER:CB	2.37	0.53
3:E:18:DT:P	4:A:1098:ILE:HA	2.48	0.53
4:A:808:PRO:CD	4:A:816:LEU:HD13	2.38	0.53
4:B:936:ARG:HB2	4:B:1215:GLY:N	2.22	0.53
1:C:122:THR:HB	1:C:123:PRO:HD2	1.90	0.53
4:A:589:MET:HB3	4:A:605:VAL:HG22	1.88	0.53
4:A:658:PRO:HA	4:A:670:LEU:HD22	1.90	0.53
4:A:680:HIS:O	4:A:684:LEU:HG	2.07	0.53
4:A:945:ASN:OD1	4:A:953:GLN:N	2.32	0.53
4:B:339:LEU:HB3	4:B:343:ASP:HB2	1.90	0.53
2:H:17:DA:C2'	2:H:18:DT:H71	2.38	0.53
4:A:283:VAL:HA	4:A:286:MET:HE3	1.87	0.53
4:B:1082:TYR:HB2	4:B:1115:GLN:HE21	1.73	0.53
4:B:224:GLN:OE1	4:B:568:PRO:HB3	2.08	0.53
4:A:265:ASN:HB3	4:A:297:LEU:HD23	1.90	0.53
1:G:107:TRP:O	1:G:111:LYS:HG3	2.08	0.53
4:A:590:PRO:HB3	4:A:599:SER:HB3	1.89	0.53
1:G:152:LEU:HD22	1:G:230:LEU:CD1	2.38	0.53
5:J:256:LEU:O	5:J:307:LEU:HD13	2.09	0.53
4:A:815:HIS:HD2	4:A:1149:VAL:CG2	2.21	0.53
5:F:144:LEU:HD12	5:F:145:ARG:H	1.73	0.53
4:A:956:TYR:CE1	4:A:991:LYS:HA	2.43	0.53
4:B:961:ALA:O	4:B:964:GLU:HB3	2.09	0.53
3:E:15:DG:H2'	3:E:16:DT:C7	2.27	0.53
4:B:1015:ARG:HA	4:B:1022:GLN:OE1	2.09	0.53
4:B:871:ILE:HG23	4:B:898:CYS:SG	2.49	0.53
3:E:4:DC:C2'	3:E:5:DT:H72	2.39	0.53
1:G:222:MET:HB2	1:G:231:LEU:HD11	1.91	0.53
4:A:609:VAL:HG12	5:F:341:SER:O	2.08	0.53
4:B:271:TRP:O	4:B:275:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:132:THR:O	4:A:136:ARG:HG3	2.08	0.52
4:B:419:LYS:HD3	4:B:635:ALA:HB1	1.90	0.52
4:A:1188:VAL:O	4:A:1192:CYS:HB2	2.08	0.52
4:A:992:GLN:HG3	4:A:1010:ILE:CG1	2.37	0.52
3:E:4:DC:H2''	3:E:5:DT:C6	2.44	0.52
1:G:166:VAL:HA	1:G:185:VAL:HG11	1.90	0.52
2:H:7:DT:H2'	2:H:8:DG:C8	2.44	0.52
4:A:467:LEU:HD12	4:A:578:LEU:HD12	1.90	0.52
1:C:121:LEU:HB2	1:C:125:GLN:HG3	1.90	0.52
1:C:158:PRO:HG3	1:C:211:TYR:CD2	2.44	0.52
5:F:320:PHE:CE2	5:F:324:LEU:HD11	2.44	0.52
5:J:144:LEU:HD12	5:J:145:ARG:H	1.74	0.52
5:J:263:LEU:CD1	5:J:300:GLN:HB2	2.39	0.52
4:B:304:GLN:HG3	4:B:346:THR:OG1	2.10	0.52
4:B:981:LEU:HD23	4:B:1020:PHE:CE2	2.45	0.52
1:G:225:VAL:HG12	1:G:225:VAL:O	2.10	0.52
4:B:562:LEU:HD23	4:B:563:ARG:N	2.24	0.52
5:F:260:ILE:HA	5:F:300:GLN:O	2.09	0.52
4:A:279:GLU:OE1	4:A:279:GLU:N	2.39	0.52
4:A:662:ALA:HB3	4:A:668:THR:OG1	2.10	0.52
1:G:170:PHE:HE2	2:H:10:DT:H4'	1.73	0.52
1:C:225:VAL:O	1:C:225:VAL:HG12	2.09	0.52
5:F:149:CYS:HB2	5:F:167:MET:SD	2.50	0.52
4:A:1150:HIS:HE2	4:A:1152:CYS:HG	1.53	0.52
4:A:655:TRP:CE3	4:A:670:LEU:HD13	2.45	0.52
4:A:671:MET:SD	4:A:684:LEU:HD11	2.50	0.52
4:A:679:GLN:O	4:A:682:GLU:HG2	2.09	0.52
4:B:671:MET:SD	4:B:680:HIS:ND1	2.82	0.52
1:C:157:ARG:HA	1:C:211:TYR:CE1	2.45	0.52
2:D:44:DA:H2''	2:D:45:DC:C6	2.45	0.52
1:G:45:VAL:HG21	1:G:125:GLN:CB	2.40	0.52
4:B:464:ARG:HA	4:B:464:ARG:HH11	1.75	0.52
3:E:41:DA:H4'	3:E:42:DG:OP1	2.09	0.52
1:G:211:TYR:O	1:G:215:MET:HG2	2.10	0.52
1:G:163:ASN:ND2	2:H:8:DG:H1'	2.24	0.52
4:B:291:GLY:O	4:B:292:LEU:HD23	2.10	0.52
1:G:159:ARG:HD3	2:H:8:DG:C5'	2.40	0.52
4:B:591:CYS:SG	4:B:601:ARG:NH2	2.73	0.51
4:B:960:ALA:HB2	4:B:990:VAL:HG21	1.90	0.51
1:C:182:LEU:HD21	3:E:43:DC:C2	2.45	0.51
4:A:590:PRO:CB	4:A:599:SER:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:376:ASP:OD2	4:B:1173:ARG:NH1	2.40	0.51
3:E:7:DT:H2''	3:E:8:DC:C6	2.45	0.51
5:F:137:GLY:O	5:F:141:ASP:N	2.21	0.51
2:H:46:DA:H2''	2:H:47:DG:C8	2.45	0.51
4:A:304:GLN:HG2	4:A:308:ARG:HH12	1.75	0.51
4:A:547:CYS:SG	4:A:552:TYR:HB2	2.50	0.51
4:A:833:LEU:HB3	4:A:837:GLY:HA3	1.91	0.51
4:B:846:VAL:HG21	4:B:860:ARG:O	2.11	0.51
4:B:844:HIS:CD2	4:B:920:HIS:H	2.28	0.51
4:A:419:LYS:N	4:A:420:PRO:HD3	2.25	0.51
4:A:400:PHE:CE1	4:A:664:LEU:HD13	2.45	0.51
4:B:295:ASP:HA	4:B:328:LEU:HD11	1.93	0.51
1:G:100:GLN:O	1:G:104:ARG:HG3	2.09	0.51
5:J:375:GLU:O	5:J:379:ARG:HG3	2.10	0.51
1:G:154:LYS:HE3	1:G:215:MET:HE1	1.92	0.51
4:A:351:VAL:HG11	4:A:358:PHE:CD2	2.44	0.51
5:J:247:TYR:OH	5:J:252:VAL:HG22	2.11	0.51
4:A:355:LYS:CB	4:A:358:PHE:HB2	2.41	0.51
2:D:35:DA:H2''	2:D:36:DT:H5'	1.93	0.51
5:J:244:PRO:HB3	5:J:363:VAL:HG21	1.93	0.51
4:A:562:LEU:HD23	4:A:563:ARG:N	2.25	0.51
4:A:931:TYR:CZ	4:A:1051:GLN:HG2	2.46	0.51
2:D:25:DA:C1'	2:D:26:DA:H5'	2.38	0.51
5:F:348:ARG:O	5:F:352:MET:HG3	2.11	0.51
5:J:212:TYR:CE1	5:J:253:ILE:HG23	2.45	0.51
5:J:378:GLU:OE2	5:J:387:TRP:NE1	2.40	0.51
4:B:612:PHE:HZ	5:J:326:HIS:HA	1.75	0.51
2:H:28:DC:H2''	2:H:29:DA:C8	2.46	0.50
5:J:98:LEU:O	5:J:189:LEU:HD12	2.11	0.50
4:B:1139:CYS:HB3	4:B:1144:LEU:HB2	1.93	0.50
5:F:149:CYS:SG	5:F:154:LEU:HD21	2.52	0.50
1:G:221:GLN:HE22	4:B:140:LEU:HD13	1.74	0.50
4:B:929:GLN:HG2	4:B:944:VAL:HB	1.92	0.50
3:E:21:DT:C2'	3:E:22:DT:H71	2.42	0.50
5:F:182:PRO:HG2	5:F:185:ALA:HB2	1.94	0.50
1:G:55:SER:HA	1:G:103:TYR:CD1	2.47	0.50
4:A:464:ARG:HH11	4:A:464:ARG:HA	1.76	0.50
4:A:944:VAL:HG23	4:A:946:LEU:CD1	2.28	0.50
4:A:977:VAL:HA	4:A:980:VAL:HG22	1.94	0.50
1:G:158:PRO:HG3	1:G:211:TYR:CD2	2.47	0.50
4:A:397:GLN:O	4:A:401:GLU:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:569:LEU:N	4:A:570:PRO:HD2	2.27	0.50
4:B:133:GLN:O	4:B:137:MET:HG2	2.11	0.50
1:C:211:TYR:O	1:C:215:MET:HG2	2.11	0.50
3:E:6:DG:H2"	3:E:7:DT:H71	1.93	0.50
4:A:455:ARG:O	4:A:459:GLU:HG3	2.12	0.50
4:B:343:ASP:O	4:B:347:VAL:HG23	2.12	0.50
4:B:870:ASP:HB3	4:B:884:TRP:CG	2.46	0.50
4:A:417:VAL:HG22	4:A:784:SER:HA	1.93	0.50
4:B:456:LEU:O	4:B:460:VAL:HG23	2.12	0.50
5:F:351:LEU:HD23	5:F:354:ILE:HD11	1.93	0.50
4:B:618:ILE:O	4:B:620:ILE:HD12	2.12	0.50
1:C:54:VAL:HG12	1:C:58:LEU:HB3	1.92	0.50
5:F:98:LEU:O	5:F:189:LEU:HD12	2.11	0.50
2:H:36:DT:C7	5:J:201:LYS:NZ	2.75	0.50
4:A:1023:GLU:HG3	4:A:1024:PHE:CD2	2.47	0.49
4:A:1053:TRP:CZ2	4:A:1211:VAL:HG22	2.47	0.49
4:A:802:PHE:O	4:A:1078:VAL:HG13	2.11	0.49
4:B:323:MET:SD	4:B:330:LEU:HD23	2.52	0.49
1:G:223:ILE:HD11	1:G:231:LEU:HD22	1.94	0.49
3:I:35:DG:H2"	3:I:36:DG:C8	2.46	0.49
4:A:464:ARG:NH1	4:A:465:PHE:H	2.09	0.49
4:A:470:PHE:HA	4:A:473:LEU:CD1	2.42	0.49
4:A:683:LEU:CD1	4:A:1079:ILE:HG12	2.42	0.49
4:A:845:LEU:O	4:A:849:THR:HG23	2.11	0.49
4:B:569:LEU:N	4:B:570:PRO:HD2	2.27	0.49
4:B:993:THR:O	4:B:996:THR:HB	2.13	0.49
1:C:118:LYS:O	1:C:125:GLN:HG3	2.12	0.49
5:J:339:LEU:HD21	5:J:373:LEU:HD21	1.94	0.49
4:A:469:PRO:O	4:A:473:LEU:HG	2.12	0.49
4:A:490:LEU:HD12	4:A:491:PRO:HD2	1.94	0.49
4:A:614:ASN:N	4:A:614:ASN:OD1	2.45	0.49
4:B:422:LEU:CD1	4:B:423:PRO:HD2	2.41	0.49
1:C:106:GLU:HA	1:C:109:VAL:HG12	1.94	0.49
3:I:37:DG:H2'	3:I:38:DG:C8	2.47	0.49
2:D:16:DC:H2"	2:D:17:DA:C8	2.47	0.49
5:F:162:ILE:O	5:F:163:LYS:HG3	2.13	0.49
1:G:158:PRO:HG3	1:G:211:TYR:CG	2.47	0.49
4:A:363:GLN:HB3	4:A:364:LEU:CA	2.43	0.49
4:A:530:TYR:CE1	4:A:534:LEU:HD21	2.47	0.49
4:B:418:GLU:HG3	4:B:721:PHE:CE2	2.48	0.49
4:B:671:MET:SD	4:B:684:LEU:HD11	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:20:DG:N9	3:I:21:DT:H72	2.28	0.49
4:A:1205:LYS:HE2	4:A:1209:GLN:OE1	2.12	0.49
4:A:808:PRO:HD2	4:A:816:LEU:HD22	1.94	0.49
4:B:510:SER:O	4:B:514:VAL:HG23	2.12	0.49
1:G:106:GLU:HA	1:G:109:VAL:HG12	1.94	0.49
1:G:152:LEU:HD22	1:G:230:LEU:HD13	1.95	0.49
1:G:173:ALA:O	1:G:181:LYS:HE3	2.12	0.49
4:A:1022:GLN:O	4:A:1025:VAL:HG12	2.11	0.49
4:A:446:CYS:SG	4:A:480:VAL:HG21	2.53	0.49
4:A:589:MET:CG	4:A:605:VAL:HG22	2.42	0.49
4:A:963:VAL:HG22	4:A:1039:SER:OG	2.12	0.49
3:I:16:DT:H2'	3:I:16:DT:OP1	2.13	0.49
5:J:309:THR:OG1	5:J:375:GLU:OE2	2.16	0.49
4:A:438:ARG:NH1	4:A:636:GLU:OE2	2.35	0.49
4:A:662:ALA:CB	4:A:668:THR:HG21	2.42	0.49
4:A:713:VAL:O	4:A:717:VAL:HG23	2.13	0.49
3:E:40:DT:C2	3:E:41:DA:N7	2.81	0.49
1:G:69:LYS:HZ1	3:I:34:DT:H5'	1.78	0.49
4:A:1024:PHE:O	4:A:1028:ALA:N	2.33	0.49
4:B:464:ARG:NH1	4:B:465:PHE:H	2.10	0.49
4:B:874:SER:HB3	4:B:885:TRP:HD1	1.78	0.49
1:C:100:GLN:O	1:C:104:ARG:HG3	2.12	0.49
5:F:132:HIS:O	5:F:135:SER:HB3	2.12	0.49
4:A:997:VAL:HG22	4:A:1033:VAL:HG13	1.94	0.49
1:C:129:LEU:HD11	1:C:133:ILE:HD11	1.95	0.49
5:F:248:HIS:CE1	5:F:250:LEU:HB2	2.48	0.49
5:F:74:TYR:CD1	5:F:105:GLY:HA3	2.48	0.49
5:J:144:LEU:HD12	5:J:145:ARG:N	2.28	0.49
4:A:1120:PRO:CB	4:A:1121:PRO:HD3	2.42	0.48
4:A:830:GLY:HA3	4:A:914:VAL:HG12	1.96	0.48
4:B:592:SER:O	4:B:593:LEU:HG	2.13	0.48
4:B:874:SER:HB3	4:B:885:TRP:CD1	2.48	0.48
1:C:67:ILE:O	1:C:71:GLN:HG2	2.13	0.48
2:D:11:DA:H2'	2:D:12:DA:C8	2.48	0.48
5:F:164:PRO:HG2	5:F:165:PRO:CD	2.42	0.48
1:G:53:PRO:HB3	1:G:106:GLU:HB3	1.95	0.48
2:D:15:DC:H2''	2:D:16:DC:C5	2.47	0.48
3:E:37:DG:H2'	3:E:38:DG:C8	2.48	0.48
5:F:89:LEU:HD11	5:F:116:ALA:CB	2.39	0.48
5:J:130:ILE:HD11	5:J:148:HIS:HB2	1.95	0.48
4:A:1136:ALA:HB2	4:A:1146:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1144:LEU:HD22	4:A:1159:ASP:CG	2.33	0.48
4:A:589:MET:HG2	4:A:605:VAL:HG22	1.94	0.48
4:B:232:CYS:SG	4:B:473:LEU:HD21	2.53	0.48
4:B:652:PRO:HB3	4:B:797:PRO:HB3	1.93	0.48
5:J:182:PRO:HG2	5:J:185:ALA:HB2	1.93	0.48
5:J:349:ASP:HA	5:J:352:MET:CE	2.43	0.48
4:A:127:GLU:O	4:A:131:ARG:HG3	2.14	0.48
4:B:1120:PRO:CB	4:B:1121:PRO:HD3	2.43	0.48
1:G:228:LYS:HA	1:G:231:LEU:HD13	1.96	0.48
4:A:808:PRO:HG3	4:A:815:HIS:CE1	2.48	0.48
4:A:838:LEU:CG	4:A:842:LYS:HE3	2.42	0.48
4:B:368:VAL:HG11	4:B:380:LYS:NZ	2.28	0.48
3:E:31:DG:N7	3:E:32:DT:H73	2.29	0.48
5:F:144:LEU:HD12	5:F:145:ARG:N	2.28	0.48
1:G:212:HIS:NE2	1:G:216:LYS:HE3	2.29	0.48
1:G:65:LEU:HB3	1:G:66:PRO:HD3	1.94	0.48
4:A:422:LEU:HD22	4:A:423:PRO:CD	2.43	0.48
1:G:80:LEU:CD2	1:G:83:ARG:HH21	2.27	0.48
4:A:1116:LYS:HG3	4:A:1117:ASN:N	2.29	0.48
4:A:349:LYS:O	4:A:353:LYS:HG2	2.13	0.48
4:B:241:LEU:HD11	4:B:460:VAL:CG1	2.44	0.48
4:B:680:HIS:CD2	4:B:802:PHE:HB2	2.49	0.48
3:E:23:DG:H2''	3:E:24:DG:C5'	2.44	0.48
5:F:129:PHE:O	5:F:133:LEU:HG	2.13	0.48
5:J:350:ILE:HA	5:J:353:GLN:HG2	1.95	0.48
4:B:584:VAL:HG22	4:B:606:LEU:HD12	1.96	0.48
5:J:260:ILE:HA	5:J:300:GLN:O	2.14	0.48
4:A:343:ASP:O	4:A:347:VAL:HG23	2.14	0.48
4:B:992:GLN:HG3	4:B:1010:ILE:CG1	2.42	0.48
4:B:1111:ASN:ND2	4:B:1114:LYS:HD2	2.28	0.48
4:B:1116:LYS:HG3	4:B:1117:ASN:N	2.28	0.48
4:B:347:VAL:O	4:B:351:VAL:HG23	2.13	0.48
4:B:708:ARG:HD3	4:B:828:ALA:HA	1.96	0.48
5:J:192:VAL:HA	5:J:226:ASN:O	2.13	0.48
4:A:961:ALA:O	4:A:964:GLU:HB3	2.14	0.48
4:B:820:VAL:O	4:B:824:LEU:HG	2.14	0.48
4:A:653:LEU:CD1	4:A:664:LEU:HA	2.44	0.47
4:A:808:PRO:CG	4:A:816:LEU:HD13	2.43	0.47
4:A:947:GLU:OE2	4:A:948:PRO:HD2	2.14	0.47
3:I:14:DG:N2	4:B:1102:HIS:HA	2.23	0.47
4:B:624:HIS:O	4:B:627:TYR:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:LEU:HD23	3:I:42:DG:N3	2.29	0.47
1:G:165:TYR:CD2	1:G:189:TRP:HB2	2.49	0.47
4:A:363:GLN:CB	4:A:364:LEU:HA	2.43	0.47
4:A:431:ARG:NH2	4:A:637:PRO:HD3	2.28	0.47
4:A:956:TYR:CZ	4:A:991:LYS:HG3	2.48	0.47
4:B:1084:LEU:HD11	4:B:1111:ASN:ND2	2.30	0.47
4:B:464:ARG:HA	4:B:464:ARG:NH1	2.28	0.47
3:E:39:DT:C2'	3:E:40:DT:H73	2.44	0.47
5:F:244:PRO:HB3	5:F:363:VAL:HG22	1.93	0.47
5:F:344:PRO:HG3	5:F:385:TYR:CE2	2.48	0.47
1:G:103:TYR:OH	2:H:23:DC:H4'	2.13	0.47
4:A:1002:THR:H	4:A:1007:ARG:NH2	2.11	0.47
4:B:658:PRO:CA	4:B:670:LEU:HD22	2.40	0.47
3:E:24:DG:H2''	3:E:25:DT:C6	2.48	0.47
4:A:981:LEU:HD13	4:A:1032:LEU:HD21	1.97	0.47
4:B:614:ASN:N	4:B:614:ASN:OD1	2.47	0.47
4:B:647:PRO:HG3	4:B:796:LEU:HD21	1.96	0.47
3:I:37:DG:C2'	3:I:38:DG:C8	2.97	0.47
3:I:4:DC:H2''	3:I:5:DT:C6	2.50	0.47
5:J:365:MET:HB2	5:J:370:PHE:CZ	2.49	0.47
4:A:690:THR:HA	4:A:693:HIS:NE2	2.29	0.47
4:B:136:ARG:O	4:B:140:LEU:HG	2.14	0.47
4:B:584:VAL:HA	4:B:606:LEU:HD12	1.95	0.47
5:F:323:LEU:HG	5:F:342:LEU:HD13	1.96	0.47
3:I:19:DG:C1'	3:I:20:DG:OP1	2.63	0.47
4:A:1059:ARG:HG2	4:A:1116:LYS:CB	2.44	0.47
4:A:268:MET:HG2	4:A:280:LEU:HG	1.96	0.47
4:A:518:ARG:HA	4:A:523:VAL:HG21	1.96	0.47
4:B:626:ALA:HB2	5:J:385:TYR:OH	2.14	0.47
4:B:679:GLN:O	4:B:682:GLU:HG2	2.14	0.47
3:I:39:DT:C2'	3:I:40:DT:H72	2.45	0.47
4:A:1144:LEU:HD11	4:A:1162:VAL:CG1	2.44	0.47
4:A:246:LEU:HD22	4:A:267:VAL:CG2	2.41	0.47
4:A:619:GLY:O	4:A:620:ILE:HD13	2.15	0.47
1:C:126:ILE:O	1:C:130:GLU:HG3	2.15	0.47
1:C:107:TRP:CZ2	2:D:24:DG:H5''	2.50	0.47
2:H:4:DC:H2''	2:H:5:DG:C5'	2.45	0.47
4:A:557:GLY:HA3	4:A:558:ALA:HA	1.47	0.47
4:B:1015:ARG:NH2	4:B:1025:VAL:HG11	2.29	0.47
4:B:422:LEU:CG	4:B:423:PRO:HD2	2.45	0.47
4:B:445:LEU:HD12	4:B:484:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:507:ARG:HB3	4:B:511:ARG:NH1	2.30	0.47
4:B:897:CYS:HA	4:B:917:LEU:HD22	1.97	0.47
1:G:215:MET:HB3	1:G:232:ARG:NH2	2.30	0.47
2:H:36:DT:C7	5:J:201:LYS:HZ3	2.27	0.47
4:A:683:LEU:HD12	4:A:1079:ILE:HG12	1.97	0.47
4:A:877:GLN:HB3	4:A:880:THR:OG1	2.15	0.47
4:A:941:ALA:CA	4:A:946:LEU:HB2	2.45	0.47
4:A:220:SER:O	4:A:224:GLN:HG3	2.14	0.46
4:A:363:GLN:HB3	4:A:364:LEU:HA	1.96	0.46
3:I:37:DG:C2'	3:I:38:DG:H8	2.27	0.46
5:J:164:PRO:HG2	5:J:165:PRO:CD	2.44	0.46
4:A:1059:ARG:HG2	4:A:1116:LYS:CD	2.45	0.46
1:C:107:TRP:CH2	2:D:24:DG:H4'	2.51	0.46
1:G:163:ASN:CB	2:H:8:DG:H1'	2.45	0.46
5:J:132:HIS:O	5:J:135:SER:HB3	2.15	0.46
4:A:422:LEU:CD2	4:A:423:PRO:HD2	2.45	0.46
4:A:426:GLU:OE2	4:A:633:LYS:HG2	2.15	0.46
4:A:507:ARG:HB3	4:A:511:ARG:NH1	2.30	0.46
1:C:58:LEU:HD22	3:E:30:DG:N3	2.30	0.46
1:C:186:LYS:HG3	3:E:44:DA:H5'	1.96	0.46
3:I:4:DC:H2'	3:I:5:DT:H72	1.98	0.46
5:J:149:CYS:SG	5:J:154:LEU:HD21	2.55	0.46
5:J:346:ASP:HB3	5:J:349:ASP:HB3	1.96	0.46
4:A:387:PRO:HD3	4:A:1143:GLY:HA2	1.98	0.46
4:A:592:SER:O	4:A:593:LEU:HG	2.15	0.46
4:B:476:GLU:O	4:B:480:VAL:HG23	2.15	0.46
1:G:56:SER:HA	1:G:99:TYR:HB3	1.96	0.46
3:I:16:DT:C2'	3:I:17:DT:H71	2.45	0.46
5:J:114:LEU:HD22	5:J:140:LEU:HD12	1.98	0.46
4:A:464:ARG:NH1	4:A:464:ARG:HA	2.30	0.46
4:A:400:PHE:HE1	4:A:664:LEU:HD13	1.80	0.46
4:B:491:PRO:HB2	4:B:493:GLN:CD	2.35	0.46
4:B:853:LYS:HD3	4:B:987:ARG:NH1	2.30	0.46
2:D:9:DC:H2''	2:D:10:DT:H5'	1.98	0.46
1:G:154:LYS:HE3	1:G:215:MET:CE	2.45	0.46
4:B:830:GLY:HA3	4:B:914:VAL:CG1	2.46	0.46
4:A:1059:ARG:CG	4:A:1116:LYS:HB2	2.46	0.46
4:A:844:HIS:CG	4:A:919:VAL:HG13	2.51	0.46
4:A:830:GLY:HA3	4:A:914:VAL:CG1	2.46	0.46
3:I:22:DT:H2''	3:I:23:DG:C8	2.51	0.46
3:I:23:DG:H2''	3:I:24:DG:H5''	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:119:LYS:HE3	5:J:143:LYS:HB3	1.96	0.46
5:J:129:PHE:O	5:J:133:LEU:HG	2.16	0.46
1:C:65:LEU:HB3	1:C:66:PRO:HD3	1.97	0.46
5:J:85:ALA:HA	5:J:113:LEU:CD2	2.46	0.46
4:A:491:PRO:HB2	4:A:493:GLN:CD	2.36	0.46
3:E:41:DA:H2''	3:E:42:DG:O5'	2.16	0.46
5:J:244:PRO:O	5:J:331:ARG:NH2	2.48	0.46
4:A:945:ASN:ND2	4:A:953:GLN:O	2.49	0.46
4:B:852:LYS:HE3	4:B:863:PHE:CG	2.51	0.46
2:D:34:DA:H2''	2:D:35:DA:H8	1.76	0.46
1:G:122:THR:HB	1:G:123:PRO:HD2	1.98	0.46
3:I:3:DC:H2''	3:I:4:DC:C6	2.51	0.46
4:A:523:VAL:O	4:A:527:GLN:HG3	2.16	0.45
4:B:1144:LEU:HD11	4:B:1162:VAL:HG12	1.97	0.45
4:B:300:ALA:HB2	4:B:333:LEU:CD1	2.43	0.45
4:B:671:MET:HA	4:B:800:MET:O	2.16	0.45
4:B:847:ASN:OD1	4:B:860:ARG:NH1	2.49	0.45
4:B:993:THR:HA	4:B:1010:ILE:HD13	1.95	0.45
2:D:4:DC:H2''	2:D:5:DG:C5'	2.46	0.45
3:E:19:DG:C1'	3:E:20:DG:OP1	2.62	0.45
5:F:346:ASP:HB3	5:F:349:ASP:HB3	1.97	0.45
5:F:378:GLU:OE2	5:F:387:TRP:NE1	2.48	0.45
4:B:363:GLN:HB3	4:B:364:LEU:CA	2.45	0.45
5:F:181:VAL:HB	5:F:182:PRO:HD2	1.99	0.45
4:A:235:LEU:HD13	4:A:512:HIS:NE2	2.32	0.45
4:B:557:GLY:HA3	4:B:558:ALA:HA	1.58	0.45
1:G:186:LYS:HD2	1:G:190:LYS:HE2	1.99	0.45
1:G:85:ALA:CB	2:H:20:DC:H4'	2.46	0.45
4:B:997:VAL:HG22	4:B:1033:VAL:HG13	1.99	0.45
4:B:1204:LEU:O	4:B:1208:LEU:HG	2.16	0.45
4:B:230:PHE:CD2	4:B:263:MET:HB3	2.51	0.45
4:B:720:LEU:HD12	4:B:892:TRP:HZ2	1.80	0.45
2:D:47:DG:H2''	2:D:48:DG:H8	1.79	0.45
5:F:247:TYR:OH	5:F:252:VAL:HG22	2.16	0.45
1:G:58:LEU:HD13	3:I:30:DG:N2	2.31	0.45
1:G:182:LEU:HD22	3:I:42:DG:C2	2.51	0.45
4:A:1041:GLN:HG2	4:A:1048:ARG:HB2	1.97	0.45
4:A:456:LEU:HD22	4:A:466:SER:HB2	1.98	0.45
4:B:141:LYS:O	4:B:145:GLN:HG3	2.16	0.45
4:B:522:GLN:OE1	4:B:561:ALA:HB1	2.17	0.45
4:B:956:TYR:CZ	4:B:991:LYS:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:19:DG:C4'	3:E:20:DG:OP1	2.63	0.45
5:F:127:LYS:HG3	5:F:130:ILE:HD12	1.98	0.45
5:F:351:LEU:HA	5:F:354:ILE:HG12	1.98	0.45
1:G:148:GLU:O	1:G:152:LEU:HG	2.17	0.45
4:A:470:PHE:HA	4:A:473:LEU:HG	1.99	0.45
4:A:594:ASP:OD2	4:A:633:LYS:NZ	2.28	0.45
4:A:993:THR:O	4:A:996:THR:HB	2.17	0.45
4:B:419:LYS:HD3	4:B:635:ALA:CB	2.46	0.45
4:B:644:VAL:HA	4:B:663:PHE:CE2	2.52	0.45
3:I:17:DT:H2'	3:I:18:DT:H71	1.97	0.45
4:A:347:VAL:O	4:A:351:VAL:HG23	2.16	0.45
4:B:1023:GLU:HG3	4:B:1024:PHE:CD2	2.51	0.45
4:B:1072:THR:HG22	4:B:1126:SER:HB2	1.99	0.45
4:B:497:PHE:CE2	4:B:577:LYS:HG2	2.52	0.45
5:F:365:MET:HB2	5:F:370:PHE:CZ	2.52	0.45
1:G:157:ARG:HH12	2:H:5:DG:N2	2.14	0.45
3:I:16:DT:H2''	3:I:17:DT:H71	1.99	0.45
4:A:1043:MET:HG3	4:A:1044:PHE:CE2	2.51	0.45
4:B:492:ALA:HB1	4:B:628:VAL:CG2	2.47	0.45
3:E:3:DC:H2''	3:E:4:DC:C5	2.52	0.45
5:F:89:LEU:CD1	5:F:116:ALA:HB1	2.39	0.45
5:F:164:PRO:N	5:F:165:PRO:HD2	2.32	0.45
2:H:46:DA:OP1	4:B:1059:ARG:NH2	2.49	0.45
5:J:231:GLU:OE2	5:J:297:TYR:OH	2.28	0.45
4:B:993:THR:HG21	4:B:1036:VAL:HG21	1.99	0.45
4:B:648:MET:SD	4:B:797:PRO:HG3	2.56	0.45
2:D:12:DA:H2''	2:D:13:DC:O5'	2.17	0.45
3:E:41:DA:H2'	3:E:42:DG:H8	1.77	0.45
5:F:189:LEU:HG	5:F:190:LYS:N	2.32	0.45
5:F:236:LYS:HG2	5:F:246:LEU:HD22	1.98	0.45
5:F:85:ALA:O	5:F:89:LEU:HG	2.17	0.45
5:J:366:HIS:O	5:J:369:ASP:HB2	2.17	0.45
4:A:1195:PRO:O	4:A:1198:ILE:HG13	2.17	0.45
4:B:1188:VAL:O	4:B:1192:CYS:HB2	2.17	0.45
4:B:948:PRO:HD3	4:B:1221:GLN:HB3	1.98	0.45
1:G:122:THR:HB	1:G:123:PRO:CD	2.46	0.45
5:J:205:TRP:CD2	5:J:250:LEU:HD21	2.52	0.45
4:A:1028:ALA:O	4:A:1032:LEU:HG	2.17	0.44
4:A:1083:ARG:O	4:A:1084:LEU:HD23	2.17	0.44
4:A:232:CYS:SG	4:A:473:LEU:HD21	2.57	0.44
4:B:244:HIS:O	4:B:248:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:612:PHE:CZ	5:J:326:HIS:HA	2.51	0.44
1:G:58:LEU:HG	3:I:31:DG:C4	2.52	0.44
4:A:1129:SER:O	4:A:1133:MET:HG3	2.17	0.44
4:B:1195:PRO:O	4:B:1198:ILE:HG13	2.17	0.44
4:B:265:ASN:HB3	4:B:297:LEU:HD23	2.00	0.44
1:C:113:GLU:HG2	1:C:116:ARG:NH2	2.30	0.44
5:J:189:LEU:HG	5:J:190:LYS:N	2.32	0.44
2:H:36:DT:H71	5:J:201:LYS:HZ3	1.81	0.44
4:A:690:THR:HA	4:A:693:HIS:CD2	2.52	0.44
4:B:416:SER:HB3	4:B:637:PRO:CA	2.45	0.44
5:F:126:ASP:HB3	5:F:129:PHE:HD2	1.82	0.44
5:F:114:LEU:HD22	5:F:140:LEU:HD12	1.99	0.44
4:A:497:PHE:CD1	4:A:621:LEU:HD11	2.52	0.44
4:A:607:TYR:HE2	4:A:624:HIS:HA	1.83	0.44
3:E:22:DT:H2''	3:E:23:DG:H8	1.81	0.44
3:E:39:DT:H2'	3:E:40:DT:H73	1.99	0.44
2:H:48:DG:H2''	2:H:49:DC:C6	2.52	0.44
4:A:300:ALA:CB	4:A:333:LEU:HD11	2.46	0.44
4:A:549:PRO:HB2	4:A:700:THR:HG21	2.00	0.44
4:B:252:GLN:HB2	4:B:255:LYS:HB2	1.99	0.44
4:B:782:ARG:HD2	4:B:821:ALA:HB2	1.99	0.44
5:F:164:PRO:CD	5:F:165:PRO:HD2	2.48	0.44
2:H:49:DC:H2''	2:H:50:DC:C6	2.52	0.44
5:J:127:LYS:HG3	5:J:130:ILE:HD12	2.00	0.44
4:A:1053:TRP:HZ3	4:A:1180:LEU:HD22	1.83	0.44
4:A:801:ASP:OD1	4:A:805:ARG:N	2.50	0.44
4:B:232:CYS:SG	4:B:473:LEU:HD11	2.58	0.44
1:G:57:TYR:HD1	1:G:88:TRP:CG	2.35	0.44
3:I:40:DT:C2	3:I:41:DA:N7	2.86	0.44
5:J:389:TYR:HB3	5:J:390:ASP:H	1.62	0.44
4:A:1041:GLN:NE2	4:A:1048:ARG:HH11	2.16	0.44
4:A:662:ALA:HB3	4:A:668:THR:CG2	2.48	0.44
4:A:808:PRO:HD3	4:A:816:LEU:HD13	1.99	0.44
4:B:1164:ASN:HB3	4:B:1168:ARG:NH1	2.32	0.44
4:B:306:MET:CE	4:B:315:THR:HG22	2.48	0.44
3:E:21:DT:H2'	3:E:22:DT:H71	2.00	0.44
5:F:194:MET:HG2	5:F:228:PHE:HD2	1.82	0.44
5:F:380:SER:O	5:F:386:LYS:HE2	2.18	0.44
1:G:56:SER:HB2	1:G:99:TYR:CB	2.48	0.44
5:J:85:ALA:HA	5:J:113:LEU:HD23	1.98	0.44
5:J:391:GLU:HG2	5:J:392:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:391:LEU:HD22	4:A:395:THR:HG21	1.99	0.44
4:B:523:VAL:O	4:B:527:GLN:HG3	2.17	0.44
4:B:994:VAL:HG13	4:B:1040:LEU:HD11	2.00	0.44
3:E:16:DT:H2''	3:E:17:DT:H71	2.00	0.44
3:E:21:DT:C2	3:E:22:DT:C5	3.06	0.44
3:E:22:DT:H2''	3:E:23:DG:C8	2.51	0.44
1:G:147:LYS:O	1:G:151:LEU:HB2	2.17	0.44
5:J:164:PRO:N	5:J:165:PRO:HD2	2.33	0.44
5:J:227:MET:O	5:J:299:ILE:HG12	2.18	0.44
4:B:655:TRP:CE3	4:B:670:LEU:HD13	2.52	0.44
4:B:713:VAL:O	4:B:717:VAL:HG23	2.18	0.44
4:B:967:ARG:NH2	4:B:982:GLU:HG3	2.32	0.44
3:E:19:DG:H4'	3:E:20:DG:OP2	2.18	0.44
1:G:219:GLU:O	1:G:223:ILE:HG12	2.18	0.44
3:I:4:DC:C2'	3:I:5:DT:H72	2.47	0.44
4:A:1150:HIS:CD2	4:A:1151:ASP:H	2.36	0.43
4:B:993:THR:HG22	4:B:1036:VAL:HG21	1.99	0.43
4:B:981:LEU:HD23	4:B:1020:PHE:HE2	1.83	0.43
4:B:241:LEU:HD11	4:B:460:VAL:HG11	1.99	0.43
3:E:17:DT:H2''	3:E:18:DT:C6	2.53	0.43
5:F:326:HIS:CG	5:F:342:LEU:HD21	2.53	0.43
2:H:16:DC:H2''	2:H:17:DA:H8	1.83	0.43
4:A:1060:LEU:HD11	4:A:1207:THR:HG21	2.00	0.43
4:A:1070:TRP:CE2	4:A:1078:VAL:HB	2.54	0.43
4:A:392:PRO:HG2	4:A:395:THR:OG1	2.18	0.43
4:A:404:LEU:O	4:A:408:LEU:HG	2.18	0.43
4:A:445:LEU:HD21	4:A:583:LEU:HD12	2.01	0.43
4:A:897:CYS:O	4:A:901:VAL:HG23	2.19	0.43
4:A:941:ALA:O	4:A:946:LEU:N	2.49	0.43
4:B:584:VAL:HG22	4:B:606:LEU:CD1	2.48	0.43
4:B:592:SER:HB2	4:B:599:SER:CB	2.35	0.43
4:B:897:CYS:HA	4:B:917:LEU:CD2	2.48	0.43
2:H:32:DC:H2''	2:H:33:DA:H8	1.82	0.43
3:I:25:DT:H2''	3:I:26:DT:H72	2.01	0.43
4:A:1031:TYR:O	4:A:1035:GLN:HG2	2.18	0.43
4:A:1059:ARG:HG2	4:A:1116:LYS:HB2	2.01	0.43
4:A:271:TRP:O	4:A:275:GLY:N	2.50	0.43
4:A:862:ALA:O	4:A:866:GLU:HG3	2.18	0.43
4:B:284:LEU:O	4:B:287:VAL:HB	2.19	0.43
4:B:422:LEU:HD22	4:B:423:PRO:CD	2.29	0.43
1:C:91:LEU:HG	1:C:95:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:219:LEU:HD12	4:A:224:GLN:NE2	2.33	0.43
4:B:870:ASP:OD1	4:B:882:ARG:NH1	2.51	0.43
2:D:36:DT:C2'	2:D:37:DT:H5''	2.42	0.43
3:I:33:DA:H2''	3:I:34:DT:C6	2.53	0.43
3:I:42:DG:H2''	3:I:43:DC:OP1	2.18	0.43
4:A:996:THR:OG1	4:A:1010:ILE:HD11	2.18	0.43
4:B:1070:TRP:CZ2	4:B:1078:VAL:HG11	2.53	0.43
4:B:1144:LEU:HD22	4:B:1159:ASP:CG	2.39	0.43
4:B:299:TYR:HB3	4:B:323:MET:CE	2.48	0.43
4:B:404:LEU:O	4:B:408:LEU:HG	2.18	0.43
4:B:425:LYS:HZ2	4:B:428:LYS:HD3	1.83	0.43
2:H:16:DC:H2''	2:H:17:DA:C8	2.53	0.43
1:G:57:TYR:HE2	2:H:20:DC:O2	2.00	0.43
4:A:935:GLY:HA3	4:A:1050:ILE:HD11	2.00	0.43
4:B:418:GLU:HB2	4:B:780:LEU:HD13	2.01	0.43
3:E:16:DT:C6	3:E:16:DT:OP1	2.72	0.43
3:I:32:DT:H2''	3:I:33:DA:N7	2.34	0.43
4:B:563:ARG:HH12	4:B:685:GLU:HG3	1.84	0.43
2:D:32:DC:H2''	2:D:33:DA:H8	1.83	0.43
2:D:46:DA:H2''	2:D:47:DG:H8	1.82	0.43
5:J:346:ASP:HB3	5:J:349:ASP:CB	2.49	0.43
4:A:1157:ALA:HA	4:A:1160:VAL:HG23	2.00	0.43
4:A:422:LEU:HB3	4:A:427:VAL:HG21	2.01	0.43
4:A:961:ALA:O	4:A:965:VAL:HG13	2.18	0.43
4:A:975:MET:O	4:A:979:GLN:HG3	2.18	0.43
4:B:852:LYS:HE3	4:B:863:PHE:CD1	2.54	0.43
3:I:2:DG:H2''	3:I:3:DC:C6	2.53	0.43
4:A:1059:ARG:HG2	4:A:1116:LYS:HD3	2.01	0.43
4:A:141:LYS:O	4:A:145:GLN:HG3	2.19	0.43
4:A:276:ALA:HB1	4:A:279:GLU:OE1	2.19	0.43
4:B:397:GLN:O	4:B:401:GLU:HG2	2.19	0.43
2:D:6:DC:C2'	2:D:7:DT:H71	2.48	0.43
3:E:1:DG:H2''	3:E:2:DG:H8	1.78	0.43
3:E:37:DG:C2'	3:E:38:DG:C8	3.02	0.43
2:H:34:DA:H2''	2:H:35:DA:H8	1.81	0.43
3:I:18:DT:H2''	3:I:19:DG:H8	1.84	0.43
4:A:339:LEU:HB3	4:A:343:ASP:HB2	2.01	0.42
4:B:651:PRO:HA	4:B:652:PRO:HD3	1.92	0.42
4:B:897:CYS:O	4:B:901:VAL:HG23	2.19	0.42
4:A:1041:GLN:CG	4:A:1048:ARG:HD2	2.49	0.42
4:A:374:LEU:HB3	4:A:378:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:384:VAL:HG21	4:A:546:PRO:HB2	2.02	0.42
4:B:1205:LYS:HE2	4:B:1209:GLN:HE22	1.83	0.42
4:B:373:LEU:HD13	4:B:1134:LEU:HD11	2.00	0.42
4:B:369:ASN:HB3	4:B:378:TYR:CD2	2.53	0.42
4:B:456:LEU:HD22	4:B:466:SER:HB2	2.01	0.42
2:D:1:DC:H2''	2:D:2:DA:H8	1.84	0.42
5:F:361:LYS:HB2	5:F:364:ASN:ND2	2.34	0.42
4:A:1041:GLN:CD	4:A:1048:ARG:HH11	2.22	0.42
4:B:1172:VAL:HG21	4:B:1223:LYS:HG3	2.01	0.42
4:B:713:VAL:HG12	4:B:824:LEU:HD23	2.00	0.42
2:D:13:DC:H2''	2:D:14:DC:C5	2.55	0.42
2:D:35:DA:H3'	5:F:201:LYS:HZ1	1.84	0.42
2:H:26:DA:H2''	2:H:27:DC:C5	2.55	0.42
2:H:6:DC:C2'	2:H:7:DT:H71	2.48	0.42
5:J:267:PRO:HA	5:J:295:LYS:HA	2.01	0.42
4:A:1151:ASP:N	4:A:1151:ASP:OD1	2.53	0.42
4:A:933:ALA:HB3	4:A:1175:HIS:CE1	2.55	0.42
4:B:1084:LEU:HD21	4:B:1111:ASN:HD22	1.85	0.42
4:B:230:PHE:CE2	4:B:263:MET:HB3	2.54	0.42
4:B:320:LEU:HD22	4:B:330:LEU:HD21	2.02	0.42
4:B:560:GLU:OE1	4:B:560:GLU:HA	2.19	0.42
4:B:977:VAL:HA	4:B:980:VAL:CG2	2.48	0.42
3:E:38:DG:H2'	3:E:39:DT:H71	2.01	0.42
4:A:497:PHE:HD1	4:A:621:LEU:HD11	1.84	0.42
4:A:518:ARG:HA	4:A:523:VAL:CG2	2.50	0.42
4:B:331:GLN:HG2	4:B:358:PHE:CZ	2.55	0.42
5:J:193:GLY:O	5:J:227:MET:HA	2.19	0.42
4:A:1196:GLN:HA	4:A:1197:LYS:HA	1.75	0.42
4:A:418:GLU:OE1	4:A:418:GLU:HA	2.19	0.42
4:A:699:LEU:HD11	4:A:800:MET:HG3	2.02	0.42
4:A:974:GLY:HA2	4:A:979:GLN:NE2	2.34	0.42
4:B:425:LYS:O	4:B:428:LYS:HB2	2.19	0.42
4:B:849:THR:HG22	4:B:894:THR:HG21	2.02	0.42
1:G:68:PHE:HB3	1:G:80:LEU:HD22	2.00	0.42
1:G:182:LEU:HB2	3:I:42:DG:H21	1.83	0.42
4:A:589:MET:CB	4:A:605:VAL:HG22	2.49	0.42
2:D:28:DC:H2''	2:D:29:DA:H8	1.85	0.42
2:D:36:DT:OP2	5:F:201:LYS:NZ	2.43	0.42
2:D:48:DG:H2''	2:D:49:DC:C6	2.53	0.42
2:H:11:DA:H2'	2:H:12:DA:C8	2.54	0.42
2:H:36:DT:H71	5:J:201:LYS:HZ2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:39:DT:H2'	3:I:40:DT:C7	2.49	0.42
4:B:967:ARG:NH1	4:B:982:GLU:HB2	2.35	0.42
2:D:33:DA:H2''	2:D:34:DA:H8	1.85	0.42
3:E:25:DT:H5''	4:A:254:GLN:HG2	2.02	0.42
1:G:54:VAL:HG22	3:I:31:DG:H5'	2.01	0.42
4:A:510:SER:O	4:A:514:VAL:HG23	2.18	0.42
4:A:562:LEU:HD23	4:A:563:ARG:C	2.40	0.42
4:A:948:PRO:HD3	4:A:1221:GLN:HB3	2.02	0.42
4:B:1084:LEU:HD21	4:B:1111:ASN:ND2	2.35	0.42
4:B:1070:TRP:CE3	4:B:1119:PHE:HE1	2.38	0.42
4:B:1147:VAL:HG22	4:B:1154:TRP:HB2	2.01	0.42
2:D:15:DC:H2''	2:D:16:DC:H5	1.85	0.42
3:E:23:DG:C2'	3:E:24:DG:H5''	2.50	0.42
5:J:312:LEU:HD23	5:J:371:LYS:HE3	2.01	0.42
4:A:468:TYR:N	4:A:469:PRO:HD2	2.35	0.42
4:A:813:PHE:CZ	4:A:825:LEU:HD21	2.54	0.42
4:B:296:LEU:HG	4:B:328:LEU:HD22	2.01	0.42
4:B:414:VAL:HG13	4:B:788:HIS:HB2	2.02	0.42
4:A:241:LEU:CD1	4:A:460:VAL:HG11	2.48	0.41
4:B:400:PHE:HE1	4:B:664:LEU:HD13	1.84	0.41
1:C:121:LEU:HB2	1:C:125:GLN:CB	2.50	0.41
2:H:35:DA:H2''	2:H:36:DT:H5'	2.02	0.41
5:J:361:LYS:HB2	5:J:364:ASN:ND2	2.35	0.41
4:B:1022:GLN:O	4:B:1025:VAL:HG12	2.20	0.41
4:B:491:PRO:HB2	4:B:493:GLN:NE2	2.35	0.41
4:B:845:LEU:HB2	4:B:897:CYS:SG	2.60	0.41
4:B:961:ALA:O	4:B:965:VAL:HG13	2.19	0.41
4:B:966:PHE:HB3	4:B:1035:GLN:HE21	1.85	0.41
1:C:107:TRP:CE2	2:D:24:DG:H5''	2.55	0.41
5:F:164:PRO:CG	5:F:165:PRO:CD	2.98	0.41
1:G:170:PHE:CE2	2:H:10:DT:H4'	2.53	0.41
5:J:136:LEU:O	5:J:139:ASN:HB2	2.20	0.41
5:J:162:ILE:HG22	5:J:162:ILE:O	2.20	0.41
5:J:258:CYS:SG	5:J:303:PRO:HA	2.60	0.41
4:B:371:SER:HB3	4:B:374:LEU:HB2	2.01	0.41
4:B:658:PRO:HA	4:B:670:LEU:HB2	2.01	0.41
3:E:28:DG:H2''	3:E:29:DG:C8	2.54	0.41
3:I:21:DT:C2	3:I:22:DT:C5	3.08	0.41
4:A:388:LYS:HD3	4:A:538:ALA:O	2.20	0.41
2:D:19:DA:H62	2:D:20:DC:N4	2.19	0.41
4:B:389:LEU:O	4:B:539:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:162:ILE:O	5:F:162:ILE:HG22	2.20	0.41
5:J:323:LEU:C	5:J:323:LEU:HD23	2.41	0.41
4:A:624:HIS:HD2	4:A:626:ALA:HB3	1.86	0.41
4:B:1108:ARG:HD3	4:B:1108:ARG:N	2.36	0.41
4:B:304:GLN:HG2	4:B:308:ARG:HH12	1.86	0.41
4:B:300:ALA:CA	4:B:333:LEU:HD11	2.50	0.41
4:B:400:PHE:CE1	4:B:664:LEU:HD13	2.56	0.41
4:B:662:ALA:HB3	4:B:668:THR:HG21	2.02	0.41
4:B:683:LEU:HD12	4:B:1079:ILE:CD1	2.50	0.41
4:B:844:HIS:CB	4:B:919:VAL:HG13	2.49	0.41
1:C:147:LYS:NZ	2:D:16:DC:H4'	2.35	0.41
5:F:83:THR:O	5:F:87:ILE:HG13	2.21	0.41
4:B:497:PHE:HE2	4:B:577:LYS:HG2	1.86	0.41
1:C:192:LEU:HB2	1:C:197:LYS:HE3	2.02	0.41
5:J:187:ILE:HD13	5:J:224:GLU:HB2	2.03	0.41
5:J:349:ASP:HA	5:J:352:MET:HE2	2.03	0.41
4:B:1116:LYS:NZ	4:B:1117:ASN:OD1	2.49	0.41
1:G:77:THR:HG21	3:I:33:DA:N3	2.36	0.41
5:J:104:PRO:HG3	5:J:122:ALA:HB1	2.03	0.41
4:A:136:ARG:O	4:A:140:LEU:HG	2.21	0.41
4:A:799:ASN:O	4:A:806:THR:HA	2.21	0.41
4:B:1196:GLN:HA	4:B:1197:LYS:HA	1.74	0.41
4:B:127:GLU:O	4:B:131:ARG:HG3	2.20	0.41
4:B:716:LEU:CD1	4:B:895:LEU:HD21	2.51	0.41
4:A:701:GLN:NE2	4:A:1140:TYR:HB2	2.36	0.41
4:B:220:SER:O	4:B:224:GLN:HG3	2.20	0.41
4:B:416:SER:HB3	4:B:637:PRO:C	2.42	0.41
4:B:928:LEU:HG	4:B:998:VAL:HG21	2.03	0.41
5:J:104:PRO:HD2	5:J:124:GLU:OE1	2.20	0.41
5:J:89:LEU:CD1	5:J:116:ALA:HB1	2.51	0.41
4:A:378:TYR:OH	4:A:693:HIS:HB3	2.21	0.41
4:B:363:GLN:CB	4:B:364:LEU:HA	2.49	0.41
4:B:369:ASN:HB3	4:B:378:TYR:CE2	2.56	0.41
4:B:622:LYS:HG3	4:B:623:PRO:HD2	2.02	0.41
2:D:37:DT:C5	5:F:202:ARG:HD3	2.57	0.41
1:G:215:MET:HB3	1:G:232:ARG:CZ	2.51	0.41
1:G:58:LEU:HD13	3:I:30:DG:C2	2.56	0.41
4:A:399:LEU:HB3	4:A:649:LEU:O	2.20	0.40
4:B:363:GLN:HB3	4:B:364:LEU:HA	2.02	0.40
4:B:418:GLU:HG3	4:B:721:PHE:HE2	1.84	0.40
4:B:840:TRP:CZ3	4:B:1160:VAL:HG11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:DT:C4	2:D:37:DT:H73	2.55	0.40
5:F:124:GLU:HG3	5:F:126:ASP:O	2.21	0.40
1:G:210:ARG:HD2	1:G:210:ARG:C	2.42	0.40
1:G:56:SER:HB2	1:G:99:TYR:HB2	2.03	0.40
5:J:164:PRO:CD	5:J:165:PRO:HD2	2.51	0.40
4:A:406:MET:HG3	4:A:412:VAL:HG22	2.02	0.40
4:A:500:LEU:HD23	4:A:621:LEU:CD1	2.51	0.40
4:A:562:LEU:C	4:A:562:LEU:HD23	2.41	0.40
4:A:718:LEU:O	4:A:722:GLN:N	2.25	0.40
4:B:1084:LEU:HD11	4:B:1111:ASN:CG	2.42	0.40
4:B:709:VAL:HG11	4:B:714:LEU:HD22	2.03	0.40
2:D:49:DC:H2''	2:D:50:DC:C6	2.56	0.40
3:I:18:DT:H5''	5:J:330:ARG:HG2	2.03	0.40
4:A:683:LEU:HD12	4:A:1079:ILE:CD1	2.51	0.40
4:A:363:GLN:HA	4:A:364:LEU:HA	1.90	0.40
4:A:560:GLU:OE1	4:A:560:GLU:HA	2.20	0.40
4:A:863:PHE:O	4:A:867:VAL:HG22	2.21	0.40
4:A:919:VAL:O	4:A:1154:TRP:HA	2.21	0.40
4:B:877:GLN:HB3	4:B:880:THR:OG1	2.21	0.40
1:C:181:LYS:O	1:C:185:VAL:HG23	2.22	0.40
1:C:228:LYS:HA	1:C:231:LEU:HD13	2.04	0.40
2:D:32:DC:H2''	2:D:33:DA:C8	2.55	0.40
3:E:42:DG:H2''	3:E:43:DC:OP1	2.21	0.40
5:J:130:ILE:CD1	5:J:148:HIS:HB2	2.51	0.40
5:J:99:LEU:HD23	5:J:190:LYS:HB3	2.03	0.40
4:A:997:VAL:CG2	4:A:1033:VAL:HG13	2.52	0.40
4:A:533:TYR:OH	4:A:549:PRO:HB3	2.21	0.40
4:B:456:LEU:HD12	4:B:471:LEU:HD12	2.03	0.40
4:B:715:ASP:O	4:B:719:GLN:HG3	2.20	0.40
4:B:947:GLU:OE2	4:B:948:PRO:HD2	2.22	0.40
5:F:366:HIS:O	5:F:369:ASP:HB2	2.22	0.40
2:H:17:DA:H2''	2:H:18:DT:C5	2.56	0.40
4:A:244:HIS:O	4:A:248:VAL:HG23	2.21	0.40
4:A:715:ASP:O	4:A:719:GLN:HG3	2.21	0.40
4:B:662:ALA:HB3	4:B:668:THR:HG1	1.86	0.40
1:C:162:TYR:O	1:C:166:VAL:HG23	2.21	0.40
1:C:222:MET:HE2	1:C:230:LEU:HD12	2.03	0.40
2:H:44:DA:H2''	2:H:45:DC:C6	2.56	0.40
3:I:19:DG:C4'	3:I:20:DG:OP1	2.66	0.40
4:B:976:ARG:NH2	5:J:162:ILE:HG22	2.36	0.40
5:J:244:PRO:HB3	5:J:363:VAL:HG22	2.04	0.40

All (2) 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)
2:D:1:DC:O5'	1:G:233:ARG:O[2_654]	2.02	0.18
3:I:40:DT:OP1	4:A:432:LYS:NZ[2_644]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	C	190/205 (93%)	185 (97%)	5 (3%)	0	100	100
1	G	190/205 (93%)	186 (98%)	4 (2%)	0	100	100
4	A	1001/1128 (89%)	962 (96%)	39 (4%)	0	100	100
4	B	990/1128 (88%)	949 (96%)	41 (4%)	0	100	100
5	F	282/377 (75%)	272 (96%)	10 (4%)	0	100	100
5	J	282/377 (75%)	272 (96%)	10 (4%)	0	100	100
All	All	2935/3420 (86%)	2826 (96%)	109 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	C	178/188 (95%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	178/188 (95%)	177 (99%)	1 (1%)	86	92
4	A	865/976 (89%)	859 (99%)	6 (1%)	84	90
4	B	859/976 (88%)	852 (99%)	7 (1%)	81	89
5	F	255/335 (76%)	253 (99%)	2 (1%)	81	89
5	J	255/335 (76%)	251 (98%)	4 (2%)	62	79
All	All	2590/2998 (86%)	2570 (99%)	20 (1%)	81	89

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	58	LEU
4	A	422	LEU
4	A	565	GLN
4	A	593	LEU
4	A	614	ASN
4	A	680	HIS
4	A	799	ASN
4	B	417	VAL
4	B	422	LEU
4	B	593	LEU
4	B	614	ASN
4	B	680	HIS
4	B	799	ASN
4	B	1108	ARG
5	F	157	ARG
5	F	248	HIS
5	J	157	ARG
5	J	248	HIS
5	J	388	LEU
5	J	391	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	221	GLN
4	A	722	GLN
4	A	815	HIS
4	A	979	GLN
4	B	624	HIS

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Mol	Chain	Res	Type
4	B	1111	ASN
4	B	1209	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

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	C	192/205 (93%)	0.35	18 (9%) 8 8	292, 364, 421, 433	0
1	G	192/205 (93%)	0.11	10 (5%) 27 24	335, 409, 458, 512	0
2	D	46/50 (92%)	-0.03	2 (4%) 35 29	344, 408, 562, 599	0
2	H	46/50 (92%)	0.31	4 (8%) 10 9	342, 419, 482, 500	0
3	E	45/50 (90%)	-0.02	2 (4%) 34 28	329, 373, 481, 547	0
3	I	45/50 (90%)	0.15	1 (2%) 62 52	336, 408, 504, 549	0
4	A	1011/1128 (89%)	0.18	40 (3%) 38 31	225, 300, 360, 402	0
4	B	1002/1128 (88%)	0.10	33 (3%) 46 37	245, 308, 366, 420	0
5	F	288/377 (76%)	0.03	13 (4%) 33 28	270, 328, 415, 455	0
5	J	288/377 (76%)	-0.06	3 (1%) 82 74	245, 321, 447, 510	0
All	All	3155/3620 (87%)	0.12	126 (3%) 38 31	225, 320, 426, 599	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	610	TYR	6.5
4	B	418	GLU	6.4
5	F	146	VAL	6.3
4	A	1090	GLN	5.6
4	A	1089	LYS	5.5
1	C	176	ASP	5.0
4	B	383	ARG	4.9
4	A	1101	THR	4.8
4	A	1087	LYS	4.4
4	B	384	VAL	4.2
2	D	38	DA	4.2
3	I	14	DG	4.2
4	B	974	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
4	B	1080	GLN	4.1
1	C	139	LYS	3.9
3	E	14	DG	3.8
4	A	1088	VAL	3.8
4	A	299	TYR	3.8
1	G	139	LYS	3.8
1	G	75	ALA	3.7
2	H	9	DC	3.7
1	C	166	VAL	3.5
1	G	87	ARG	3.5
4	B	337	VAL	3.5
1	C	175	GLY	3.5
4	A	1029	SER	3.5
1	C	142	ALA	3.4
4	B	904	ALA	3.4
4	A	1028	ALA	3.4
4	B	330	LEU	3.4
5	F	158	SER	3.3
4	A	1146	PHE	3.3
4	A	1194	GLU	3.3
4	B	1079	ILE	3.2
5	F	159	GLY	3.2
2	H	49	DC	3.1
4	A	1069	GLU	3.0
4	B	768	VAL	3.0
5	J	160	GLY	3.0
4	A	1097	SER	3.0
4	B	648	MET	2.9
4	B	417	VAL	2.9
4	A	1000	GLY	2.9
1	C	186	LYS	2.9
1	C	64	GLN	2.9
5	F	122	ALA	2.9
4	B	764	HIS	2.8
1	C	83	ARG	2.8
4	B	1069	GLU	2.8
4	A	985	ILE	2.8
4	A	1193	SER	2.8
4	B	133	GLN	2.7
2	H	50	DC	2.7
1	C	165	TYR	2.7
1	G	73	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
4	A	959	VAL	2.7
4	B	860	ARG	2.7
5	F	144	LEU	2.7
4	A	590	PRO	2.7
4	B	1115	GLN	2.6
1	C	77	THR	2.6
4	A	1219	LEU	2.6
1	C	74	ASP	2.6
4	A	1086	SER	2.5
5	F	147	ILE	2.5
4	A	1099	THR	2.5
4	A	1145	THR	2.5
2	D	37	DT	2.5
1	C	65	LEU	2.5
4	B	563	ARG	2.5
4	B	1057	SER	2.5
4	A	1141	ARG	2.5
4	A	917	LEU	2.5
5	F	73	ARG	2.5
4	B	336	ALA	2.4
4	B	598	ARG	2.4
1	G	64	GLN	2.4
1	G	74	ASP	2.4
4	B	296	LEU	2.4
5	J	256	LEU	2.4
1	C	140	ARG	2.4
4	B	131	ARG	2.4
1	G	138	LEU	2.3
4	B	134	GLN	2.3
4	A	296	LEU	2.3
1	C	143	MET	2.3
4	A	609	VAL	2.3
5	F	267	PRO	2.3
4	A	1100	TYR	2.3
4	B	386	TYR	2.3
3	E	15	DG	2.2
1	C	185	VAL	2.2
4	A	242	ALA	2.2
4	B	130	LYS	2.2
4	B	852	LYS	2.2
4	A	1092	GLY	2.2
4	A	892	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
4	A	998	VAL	2.2
5	F	390	ASP	2.2
4	B	297	LEU	2.2
4	A	1068	VAL	2.2
4	A	1196	GLN	2.2
5	J	212	TYR	2.1
5	F	139	ASN	2.1
4	A	994	VAL	2.1
1	G	176	ASP	2.1
4	B	419	LYS	2.1
4	B	1112	THR	2.1
4	A	1222	VAL	2.1
1	G	72	ASN	2.1
4	A	328	LEU	2.1
4	A	1139	CYS	2.1
4	A	990	VAL	2.1
1	C	114	ILE	2.1
4	B	1058	ALA	2.1
4	A	772	MET	2.0
1	G	90	GLU	2.0
5	F	120	VAL	2.0
2	H	48	DG	2.0
4	A	1010	ILE	2.0
4	B	1222	VAL	2.0
1	C	197	LYS	2.0
5	F	160	GLY	2.0
4	B	721	PHE	2.0
5	F	121	VAL	2.0
1	C	189	TRP	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](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.