



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:41 PM GMT

PDB ID : 4D1Q  
Title : Hermes transposase bound to its terminal inverted repeat  
Authors : Hickman, A.B.; Ewis, H.; Li, X.; Knapp, J.; Laver, T.; Doss, A.L.; Tolun, G.;  
Steven, A.; Grishaev, A.; Bax, A.; Atkinson, P.; Craig, N.L.; Dyda, F.  
Deposited on : 2014-05-04  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

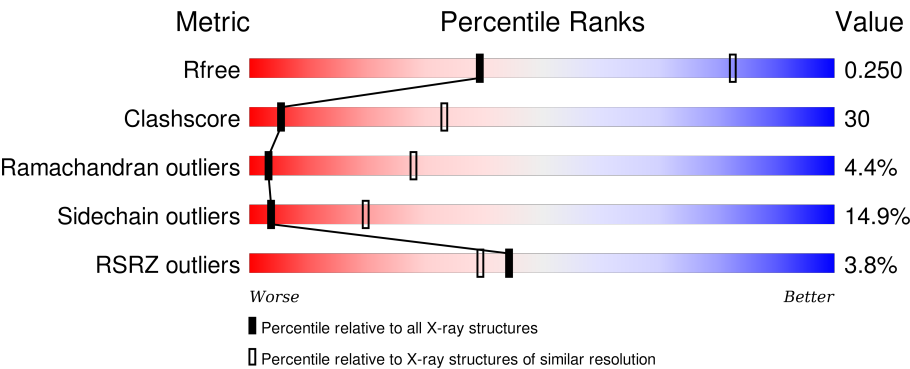
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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 <sub>free</sub>	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	536	<div><div>2%</div><div>38%44%11%6%</div></div>
1	B	536	<div><div>2%</div><div>45%39%10%6%</div></div>
1	G	536	<div><div>5%</div><div>42%43%7%7%</div></div>
1	H	536	<div><div>3%</div><div>45%42%8%5%</div></div>
2	C	15	<div><div>7%</div><div>20%60%13%7%</div></div>

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Mol	Chain	Length	Quality of chain
2	E	15	
2	I	15	
2	K	15	
3	D	16	
3	F	16	
3	J	16	
3	L	16	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	B	1610	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18737 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 TRANSPOSASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	0	0
			4041	2584	684	754	19			
1	B	505	Total	C	N	O	S	0	0	0
			4066	2599	689	758	20			
1	G	499	Total	C	N	O	S	0	0	0
			4013	2569	677	748	19			
1	H	509	Total	C	N	O	S	0	0	0
			4089	2613	691	765	20			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	HIS	-	EXPRESSION TAG	UNP Q25442
A	78	MET	-	EXPRESSION TAG	UNP Q25442
A	163	GLY	SER	CONFLICT	UNP Q25442
A	233	SER	LEU	ENGINEERED MUTATION	UNP Q25442
A	286	MET	VAL	ENGINEERED MUTATION	UNP Q25442
B	77	HIS	-	EXPRESSION TAG	UNP Q25442
B	78	MET	-	EXPRESSION TAG	UNP Q25442
B	163	GLY	SER	CONFLICT	UNP Q25442
B	233	SER	LEU	ENGINEERED MUTATION	UNP Q25442
B	286	MET	VAL	ENGINEERED MUTATION	UNP Q25442
B	519	CYS	CYS	CONFLICT	UNP Q25442
G	77	HIS	-	EXPRESSION TAG	UNP Q25442
G	78	MET	-	EXPRESSION TAG	UNP Q25442
G	163	GLY	SER	CONFLICT	UNP Q25442
G	233	SER	LEU	ENGINEERED MUTATION	UNP Q25442
G	286	MET	VAL	ENGINEERED MUTATION	UNP Q25442
H	77	HIS	-	EXPRESSION TAG	UNP Q25442
H	78	MET	-	EXPRESSION TAG	UNP Q25442
H	163	GLY	SER	CONFLICT	UNP Q25442
H	233	SER	LEU	ENGINEERED MUTATION	UNP Q25442
H	286	MET	VAL	ENGINEERED MUTATION	UNP Q25442

- Molecule 2 is a DNA chain called TERMINAL INVERTED REPEAT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			308	147	69	78	14			
2	E	15	Total	C	N	O	P	0	0	0
			308	147	69	78	14			
2	I	15	Total	C	N	O	P	0	0	0
			308	147	69	78	14			
2	K	15	Total	C	N	O	P	0	0	0
			308	147	69	78	14			

- Molecule 3 is a DNA chain called TERMINAL INVERTED REPEAT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	16	Total	C	N	O	P	0	0	0
			323	158	46	104	15			
3	F	16	Total	C	N	O	P	0	0	0
			323	158	46	104	15			
3	J	16	Total	C	N	O	P	0	0	0
			323	158	46	104	15			
3	L	16	Total	C	N	O	P	0	0	0
			323	158	46	104	15			

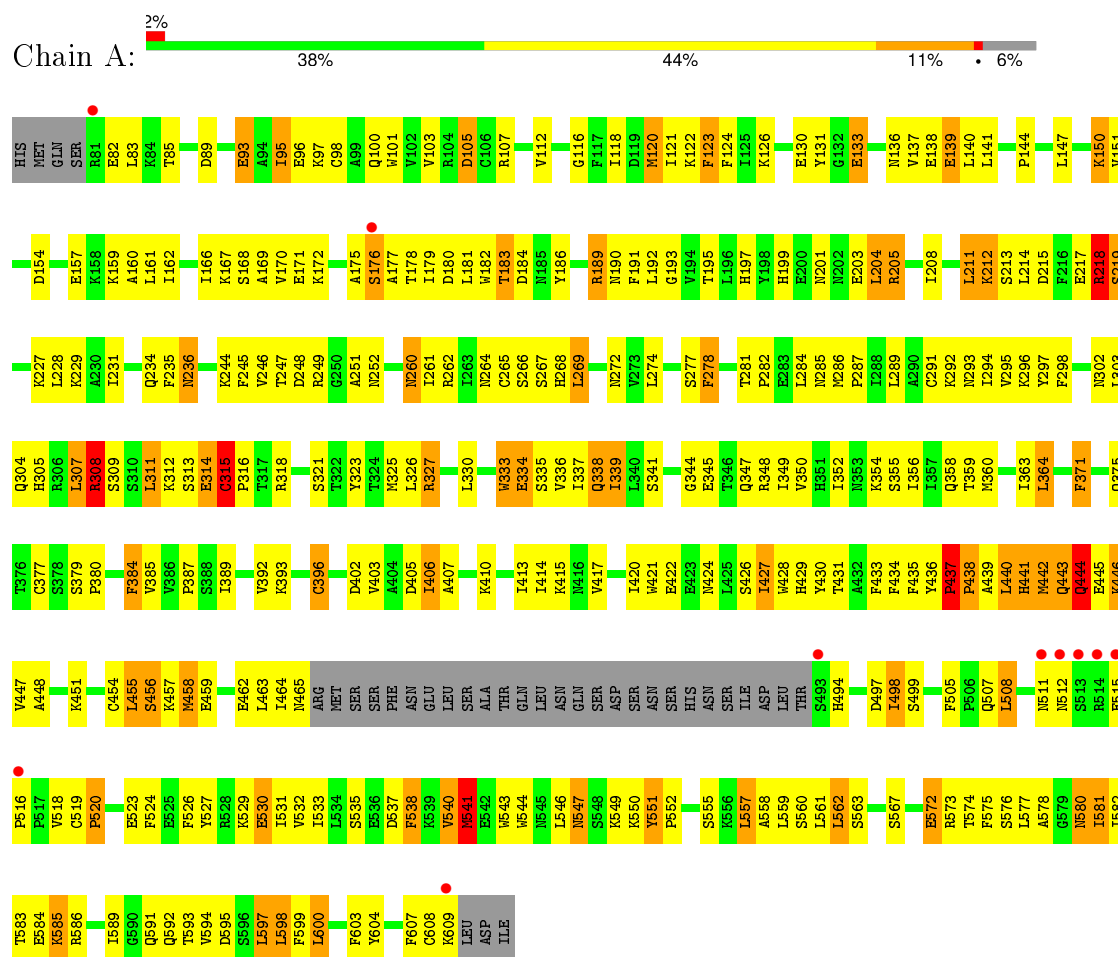
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Na	0	0
			1	1		
4	G	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		

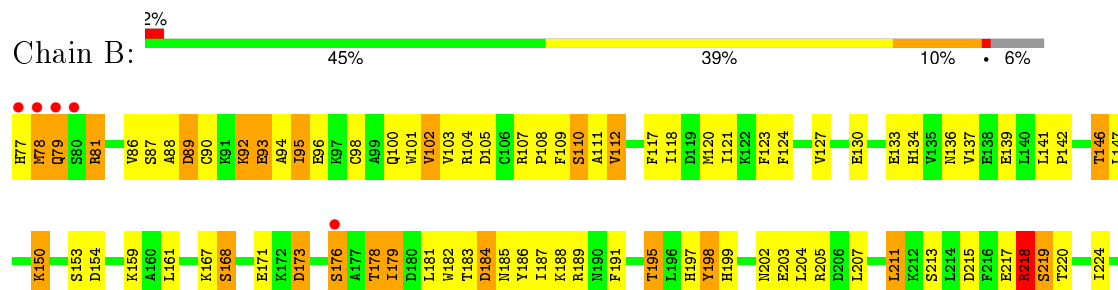
### 3 Residue-property plots

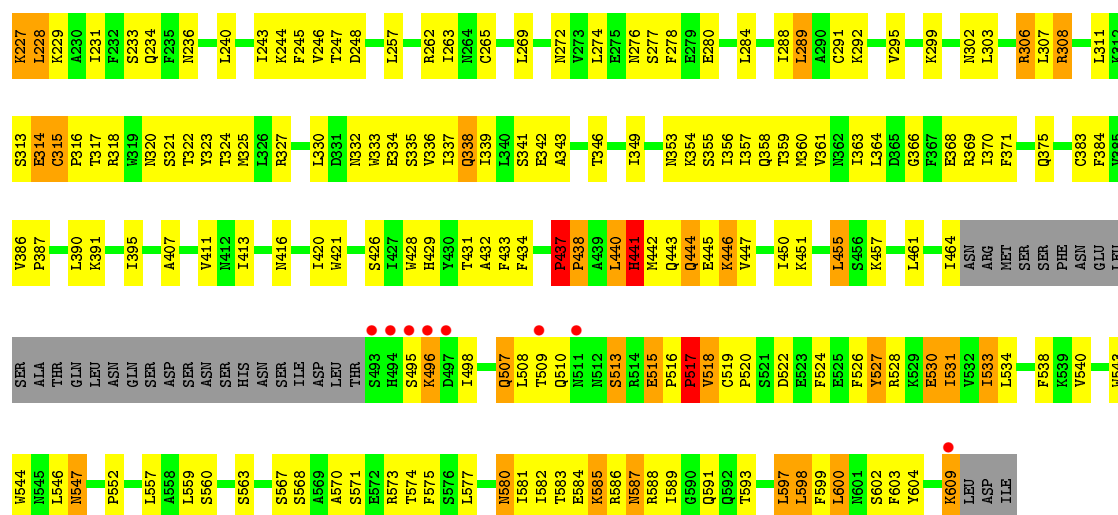
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: TRANSPOSASE

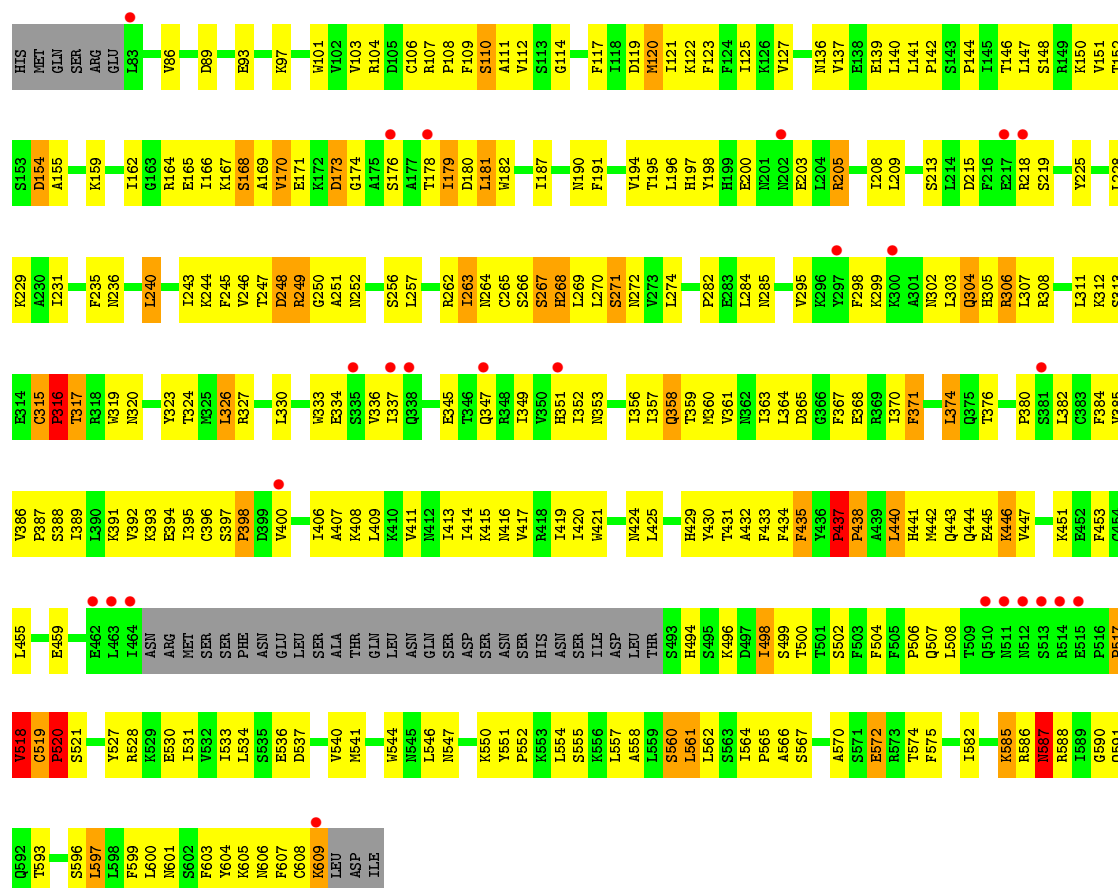


#### • Molecule 1: TRANSPOSASE

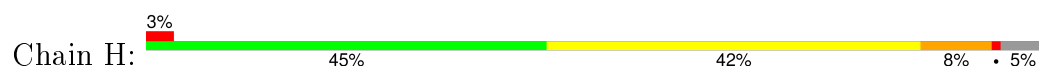


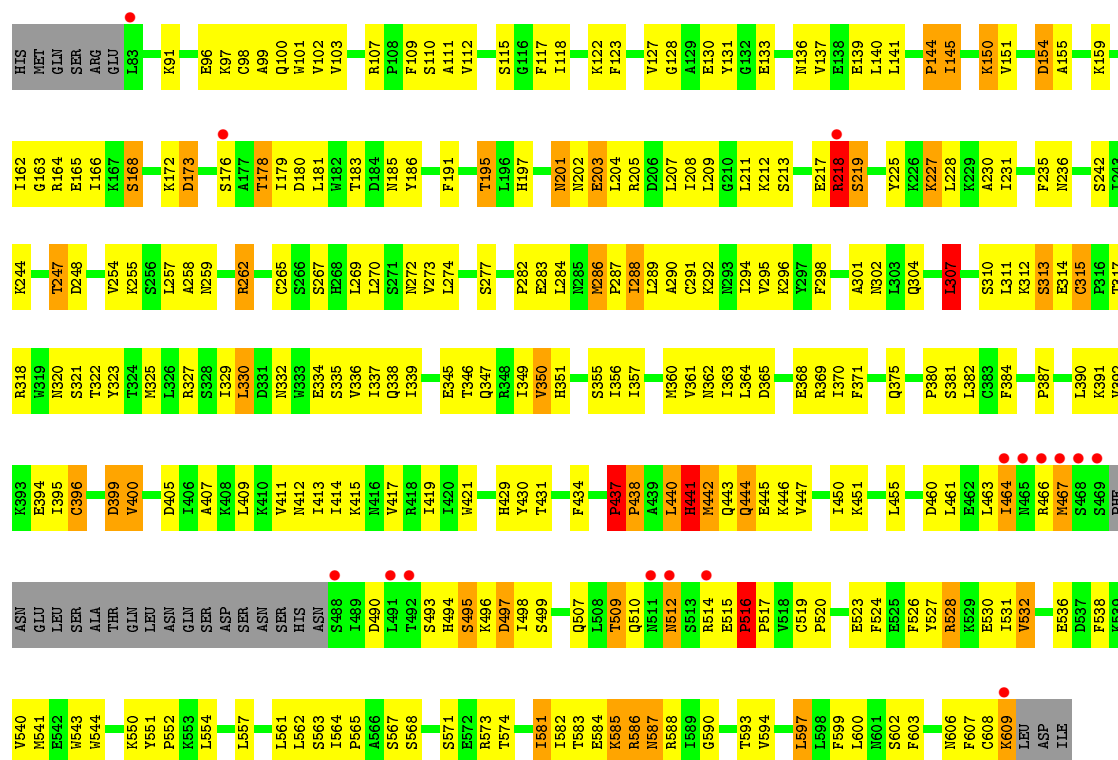


• Molecule 1: TRANSPOSASE



• Molecule 1: TRANSPOSASE

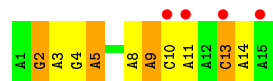




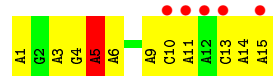
• Molecule 2: TERMINAL INVERTED REPEAT



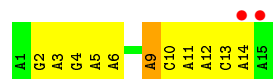
• Molecule 2: TERMINAL INVERTED REPEAT



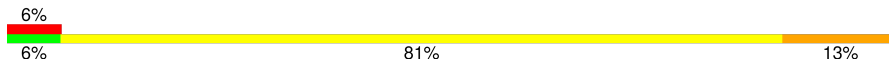
• Molecule 2: TERMINAL INVERTED REPEAT

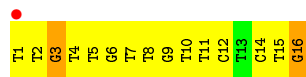


• Molecule 2: TERMINAL INVERTED REPEAT




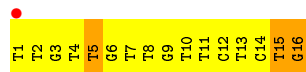
## ● Molecule 3: TERMINAL INVERTED REPEAT

Chain D:  6% 81% 13%



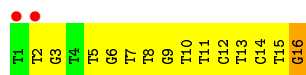
## ● Molecule 3: TERMINAL INVERTED REPEAT

Chain F:  6% 81% 19%

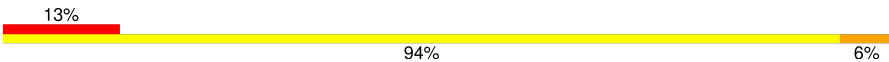


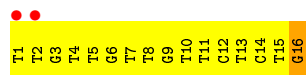
## ● Molecule 3: TERMINAL INVERTED REPEAT

Chain J:  13% 81% 6%



## ● Molecule 3: TERMINAL INVERTED REPEAT

Chain L:  13% 94% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	265.15Å 265.15Å 157.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.40 29.86 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-3.40) 98.9 (29.86-3.30)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.31Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.212 , 0.254 0.212 , 0.250	Depositor DCC
$R_{free}$ test set	870 reflections (1.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.4	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 93.2	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 94693 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	1.02	11/4120 (0.3%)	1.08	10/5561 (0.2%)
1	B	0.83	2/4146 (0.0%)	0.95	4/5595 (0.1%)
1	G	0.70	1/4092 (0.0%)	0.87	3/5524 (0.1%)
1	H	0.76	2/4168 (0.0%)	0.91	6/5626 (0.1%)
2	C	1.30	3/349 (0.9%)	1.08	2/536 (0.4%)
2	E	1.07	0/349	1.06	3/536 (0.6%)
2	I	0.68	0/349	0.86	1/536 (0.2%)
2	K	0.74	0/349	0.91	1/536 (0.2%)
3	D	1.35	2/358 (0.6%)	1.05	1/552 (0.2%)
3	F	1.04	0/358	1.08	2/552 (0.4%)
3	J	0.77	0/358	0.84	0/552
3	L	0.82	0/358	0.91	0/552
All	All	0.86	21/19354 (0.1%)	0.96	33/26658 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	G	0	2
1	H	0	3
2	C	0	3
2	E	0	2
2	I	0	1
2	K	0	1
3	D	0	1
3	F	0	1
3	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1
All	All	0	20

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	438	PRO	CA-C	8.22	1.69	1.52
1	B	78	MET	CG-SD	8.14	2.02	1.81
1	A	439	ALA	CA-CB	7.91	1.69	1.52
1	H	438	PRO	CA-C	7.14	1.67	1.52
1	B	438	PRO	CA-C	7.04	1.67	1.52
1	A	436	TYR	CE2-CZ	6.94	1.47	1.38
1	A	315	CYS	CB-SG	6.74	1.93	1.82
1	G	438	PRO	CA-C	6.58	1.66	1.52
1	H	467	MET	CG-SD	6.43	1.97	1.81
1	A	384	PHE	CB-CG	-6.31	1.40	1.51
3	D	16	DG	C2-N2	-6.13	1.28	1.34
3	D	16	DG	C5-C6	-5.79	1.36	1.42
2	C	2	DG	N3-C4	-5.69	1.31	1.35
1	A	551	TYR	CE2-CZ	5.58	1.45	1.38
2	C	2	DG	C2-N3	-5.46	1.28	1.32
1	A	541	MET	SD-CE	5.33	2.07	1.77
1	A	436	TYR	CE1-CZ	5.28	1.45	1.38
1	A	507	GLN	CG-CD	5.14	1.62	1.51
2	C	2	DG	C2-N2	-5.13	1.29	1.34
1	A	438	PRO	CB-CG	5.11	1.75	1.50
1	A	551	TYR	CE1-CZ	5.10	1.45	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	DA	C1'-O4'-C4'	-7.75	102.35	110.10
3	D	16	DG	C1'-O4'-C4'	-7.12	102.98	110.10
1	B	441	HIS	N-CA-C	6.82	129.41	111.00
3	F	15	DT	C5'-C4'-O4'	-6.77	96.44	109.30
1	A	318	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	A	438	PRO	C-N-CA	6.64	138.30	121.70
1	B	438	PRO	C-N-CA	6.31	137.47	121.70
1	A	396	CYS	CA-CB-SG	-6.26	102.73	114.00
1	H	399	ASP	N-CA-C	6.22	127.79	111.00
1	A	307	LEU	CA-CB-CG	-6.07	101.33	115.30
1	H	438	PRO	C-N-CA	5.96	136.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	13	DC	C1'-O4'-C4'	-5.91	104.19	110.10
3	F	5	DT	C1'-O4'-C4'	-5.87	104.23	110.10
1	A	546	LEU	CA-CB-CG	-5.82	101.90	115.30
2	C	13	DC	C1'-O4'-C4'	-5.75	104.35	110.10
1	A	204	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	G	518	VAL	N-CA-C	-5.70	95.60	111.00
2	E	5	DA	C1'-O4'-C4'	-5.68	104.42	110.10
1	H	133	GLU	N-CA-C	5.66	126.28	111.00
1	A	105	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	H	441	HIS	N-CA-C	5.58	126.08	111.00
1	G	181	LEU	CA-CB-CG	5.57	128.10	115.30
1	A	289	LEU	CA-CB-CG	-5.54	102.55	115.30
1	H	464	ILE	N-CA-C	-5.35	96.57	111.00
2	E	9	DA	C3'-C2'-C1'	-5.17	96.30	102.50
1	H	307	LEU	CA-CB-CG	5.16	127.18	115.30
1	B	289	LEU	CA-CB-CG	-5.13	103.50	115.30
2	K	9	DA	C1'-O4'-C4'	-5.13	104.97	110.10
1	A	464	ILE	N-CA-C	-5.09	97.27	111.00
1	G	587	ASN	N-CA-C	5.08	124.71	111.00
2	I	5	DA	C1'-O4'-C4'	-5.05	105.05	110.10
1	A	311	LEU	N-CA-C	-5.01	97.46	111.00
1	B	112	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	TYR	Sidechain
1	A	437	PRO	Mainchain
1	B	186	TYR	Sidechain
1	B	527	TYR	Sidechain
2	C	13	DC	Sidechain
2	C	3	DA	Sidechain
2	C	6	DA	Sidechain
3	D	3	DG	Sidechain
2	E	2	DG	Sidechain
2	E	9	DA	Sidechain
3	F	16	DG	Sidechain
1	G	437	PRO	Mainchain
1	G	527	TYR	Sidechain
1	H	186	TYR	Sidechain
1	H	225	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	H	437	PRO	Mainchain
2	I	5	DA	Sidechain
3	J	16	DG	Sidechain
2	K	6	DA	Sidechain
3	L	16	DG	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4041	0	4097	277	0
1	B	4066	0	4120	237	0
1	G	4013	0	4072	234	0
1	H	4089	0	4148	225	0
2	C	308	0	165	12	0
2	E	308	0	167	18	0
2	I	308	0	167	21	0
2	K	308	0	167	16	0
3	D	323	0	186	30	0
3	F	323	0	188	35	0
3	J	323	0	188	38	0
3	L	323	0	188	45	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
All	All	18737	0	17853	1096	0

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 30.

All (1096) 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:B:78:MET:SD	1:B:78:MET:CG	2.02	1.45
1:A:541:MET:SD	1:A:541:MET:CE	2.07	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:PRO:CB	1:A:438:PRO:CG	1.75	1.41
3:D:2:DT:H2''	3:D:3:DG:H5''	1.29	1.14
3:J:2:DT:H2''	3:J:3:DG:H5''	1.15	1.13
3:L:2:DT:H2''	3:L:3:DG:H5''	1.19	1.11
3:F:6:DG:H2''	3:F:7:DT:H5'	1.35	1.05
3:L:2:DT:H2''	3:L:3:DG:C5'	1.88	1.04
1:G:162:ILE:HD13	1:G:607:PHE:HE2	1.20	1.03
3:F:8:DT:H2''	3:F:9:DG:H5'	1.39	1.02
3:L:15:DT:H3'	3:L:16:DG:H5''	1.40	1.02
3:J:12:DC:H2'	3:J:13:DT:H5'	1.41	1.01
3:F:2:DT:H2''	3:F:3:DG:H5''	1.41	1.01
2:K:13:DC:H2''	2:K:14:DA:C8	1.97	0.99
3:F:6:DG:H2''	3:F:7:DT:C5'	1.92	0.99
3:J:2:DT:H2''	3:J:3:DG:C5'	1.95	0.97
2:I:9:DA:H2''	2:I:10:DC:H5''	1.47	0.96
3:L:12:DC:H2'	3:L:13:DT:H5'	1.47	0.95
2:I:4:DG:H8	2:I:4:DG:H5'	1.29	0.95
1:H:262:ARG:HG2	1:H:262:ARG:HH11	1.29	0.95
1:A:282:PRO:HA	1:A:285:ASN:HD22	1.29	0.95
2:C:13:DC:H2''	2:C:14:DA:C8	2.02	0.94
1:B:198:TYR:CE1	1:B:205:ARG:HG3	2.03	0.94
3:L:3:DG:H8	3:L:3:DG:H5'	1.34	0.92
1:H:430:TYR:HD1	1:H:442:MET:HE1	1.35	0.92
1:B:353:ASN:ND2	1:B:356:ILE:HG13	1.85	0.91
3:J:7:DT:H5'	3:J:7:DT:H6	1.36	0.91
3:L:2:DT:C2'	3:L:3:DG:H5''	2.00	0.91
3:D:14:DC:H2''	3:D:15:DT:H5''	1.52	0.91
1:G:162:ILE:HD13	1:G:607:PHE:CE2	2.06	0.91
2:I:4:DG:C8	2:I:4:DG:H5'	2.06	0.90
3:L:15:DT:C3'	3:L:16:DG:H5''	2.02	0.89
1:H:515:GLU:HB3	1:H:516:PRO:HD2	1.53	0.89
1:B:247:THR:HG22	1:B:262:ARG:HH11	1.38	0.88
3:L:12:DC:H2''	3:L:13:DT:H5''	1.54	0.88
3:J:2:DT:C2'	3:J:3:DG:H5''	2.03	0.88
1:G:111:ALA:HA	1:H:107:ARG:HH21	1.37	0.88
2:E:4:DG:C8	2:E:4:DG:H5'	2.09	0.88
3:D:14:DC:H2''	3:D:15:DT:C5'	2.04	0.87
1:B:437:PRO:HB2	1:B:438:PRO:HD3	1.57	0.86
1:G:247:THR:HG22	1:G:248:ASP:O	1.75	0.86
1:G:178:THR:HB	1:G:195:THR:OG1	1.75	0.86
3:D:7:DT:H5'	3:D:7:DT:H6	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:15:DT:C3'	3:F:16:DG:H5''	2.06	0.86
3:J:12:DC:C2'	3:J:13:DT:C5'	2.54	0.85
3:F:15:DT:H3'	3:F:16:DG:H5''	1.59	0.85
3:L:3:DG:C8	3:L:3:DG:H5'	2.10	0.85
1:G:263:ILE:HG22	1:G:429:HIS:HE1	1.42	0.84
3:L:12:DC:C2'	3:L:13:DT:C5'	2.56	0.84
3:D:2:DT:H2''	3:D:3:DG:C5'	2.07	0.84
2:I:3:DA:C2'	2:I:4:DG:H5''	2.08	0.84
1:G:270:LEU:HD11	1:G:367:PHE:HE2	1.42	0.83
2:I:13:DC:H2''	2:I:14:DA:C8	2.13	0.83
1:B:437:PRO:HG2	1:B:538:PHE:HZ	1.42	0.83
1:A:265:CYS:SG	1:A:567:SER:HB2	2.19	0.83
1:H:581:ILE:HD11	1:H:594:VAL:HG13	1.61	0.83
3:J:12:DC:H2'	3:J:13:DT:C5'	2.08	0.82
1:H:447:VAL:HG21	1:H:528:ARG:NH1	1.93	0.82
2:E:4:DG:H5'	2:E:4:DG:H8	1.41	0.82
3:D:11:DT:H2''	3:D:12:DC:H5''	1.61	0.82
3:J:12:DC:H2''	3:J:13:DT:H5''	1.59	0.82
3:F:11:DT:H2''	3:F:12:DC:H5''	1.62	0.81
1:A:136:ASN:ND2	1:A:139:GLU:HB3	1.95	0.81
1:A:555:SER:O	1:A:559:LEU:HD12	1.80	0.81
1:A:282:PRO:HA	1:A:285:ASN:ND2	1.95	0.80
1:A:327:ARG:HG2	1:A:327:ARG:HH11	1.45	0.80
3:L:15:DT:H5'	3:L:15:DT:C6	2.16	0.80
1:B:353:ASN:HD22	1:B:356:ILE:HG13	1.44	0.80
1:A:166:ILE:O	1:A:170:VAL:HG23	1.82	0.80
1:A:116:GLY:HA2	1:B:104:ARG:NH1	1.96	0.80
3:F:2:DT:H2''	3:F:3:DG:C5'	2.10	0.80
1:A:120:MET:HE1	1:B:98:CYS:SG	2.22	0.79
1:G:107:ARG:NH2	1:H:111:ALA:HA	1.97	0.79
3:J:11:DT:H2''	3:J:12:DC:H5''	1.65	0.79
3:L:12:DC:C2'	3:L:13:DT:H5'	2.12	0.79
1:A:281:THR:HG22	1:A:284:LEU:HD12	1.64	0.79
3:L:15:DT:H6	3:L:15:DT:H5'	1.47	0.79
3:F:14:DC:H2''	3:F:15:DT:H5''	1.66	0.78
1:A:281:THR:CG2	1:A:284:LEU:HD12	2.12	0.78
1:G:179:ILE:HD11	1:G:228:LEU:HD13	1.64	0.78
1:A:437:PRO:HB3	1:A:532:VAL:HG21	1.65	0.78
2:I:3:DA:H2'	2:I:4:DG:H5''	1.66	0.78
1:B:510:GLN:HB3	1:G:533:ILE:HG23	1.64	0.78
3:D:1:DT:H6	3:D:1:DT:H5'	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:12:DC:C2'	3:J:13:DT:H5'	2.13	0.77
2:E:10:DC:H5''	2:E:10:DC:H6	1.48	0.77
1:G:270:LEU:HD11	1:G:367:PHE:CE2	2.20	0.77
1:B:265:CYS:SG	1:B:567:SER:HB2	2.24	0.77
1:A:93:GLU:HB3	1:B:123:PHE:HE2	1.47	0.77
3:D:8:DT:H2''	3:D:9:DG:H5'	1.66	0.77
3:L:14:DC:H2''	3:L:15:DT:H5''	1.68	0.76
1:H:430:TYR:CD1	1:H:442:MET:HE1	2.21	0.76
1:G:123:PHE:O	1:G:127:VAL:HG23	1.85	0.76
1:G:123:PHE:HB2	1:H:97:LYS:HD3	1.68	0.76
1:G:122:LYS:HG2	1:H:137:VAL:HG21	1.68	0.76
1:H:162:ILE:HG21	1:H:607:PHE:CE2	2.20	0.76
3:F:8:DT:H2''	3:F:9:DG:C5'	2.14	0.76
1:G:106:CYS:SG	1:H:581:ILE:HG22	2.25	0.75
1:B:179:ILE:HD11	1:B:228:LEU:HG	1.68	0.75
1:A:330:LEU:HD21	1:A:358:GLN:HA	1.68	0.75
1:A:122:LYS:HG2	1:B:137:VAL:HG21	1.68	0.75
1:A:208:ILE:HD13	1:A:574:THR:HG23	1.67	0.74
1:G:249:ARG:HH21	1:G:272:ASN:HD22	1.36	0.74
1:B:603:PHE:HD1	1:B:604:TYR:HD1	1.35	0.74
3:L:13:DT:H6	3:L:13:DT:H5'	1.52	0.74
3:J:12:DC:C2'	3:J:13:DT:H5''	2.17	0.74
1:G:263:ILE:HG22	1:G:429:HIS:CE1	2.23	0.74
1:H:437:PRO:CB	1:H:532:VAL:HG11	2.18	0.74
1:G:265:CYS:SG	1:G:567:SER:HB2	2.27	0.73
2:I:10:DC:H2'	2:I:11:DA:C8	2.24	0.73
1:B:519:CYS:HB2	1:B:520:PRO:HD2	1.70	0.73
1:A:307:LEU:CD1	1:A:311:LEU:HD21	2.18	0.73
1:G:162:ILE:HG21	1:G:607:PHE:CE2	2.23	0.73
1:B:384:PHE:HA	1:B:387:PRO:HG2	1.70	0.73
1:G:323:TYR:CE2	1:G:368:GLU:HG3	2.24	0.73
3:D:5:DT:H2''	3:D:6:DG:H5'	1.69	0.73
1:G:159:LYS:HG2	1:G:599:PHE:CE2	2.24	0.73
3:J:3:DG:H8	3:J:3:DG:H5'	1.54	0.72
1:G:137:VAL:HG21	1:H:122:LYS:HG2	1.69	0.72
3:D:2:DT:C2'	3:D:3:DG:H5''	2.13	0.72
1:B:96:GLU:O	1:B:100:GLN:HG3	1.90	0.72
1:A:191:PHE:HB3	1:A:211:LEU:HD22	1.70	0.72
1:G:455:LEU:O	1:G:459:GLU:HG2	1.89	0.72
1:A:167:LYS:O	1:A:171:GLU:HG3	1.89	0.72
1:A:123:PHE:HE2	1:B:93:GLU:HB3	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LYS:O	1:A:154:ASP:HB2	1.90	0.72
1:B:437:PRO:HG2	1:B:538:PHE:CZ	2.25	0.72
2:E:10:DC:C5'	2:E:10:DC:H6	2.01	0.72
3:D:14:DC:C2'	3:D:15:DT:H5'	2.20	0.71
1:H:283:GLU:HB3	1:H:405:ASP:OD1	1.90	0.71
1:H:550:LYS:HE2	1:H:551:TYR:OH	1.91	0.71
1:A:304:GLN:NE2	1:A:311:LEU:H	1.88	0.71
1:B:323:TYR:CE2	1:B:368:GLU:HG3	2.24	0.71
1:G:112:VAL:HA	1:G:117:PHE:CE2	2.26	0.71
1:A:227:LYS:O	1:A:231:ILE:HG13	1.91	0.71
1:A:282:PRO:O	1:A:285:ASN:HB2	1.89	0.70
2:K:11:DA:C2	3:L:6:DG:N2	2.59	0.70
1:A:269:LEU:HD13	1:A:421:TRP:HA	1.73	0.70
1:G:111:ALA:HA	1:H:107:ARG:NH2	2.04	0.70
3:L:12:DC:C2'	3:L:13:DT:H5''	2.21	0.70
3:D:3:DG:H5'	3:D:3:DG:H8	1.56	0.70
1:B:437:PRO:HB2	1:B:438:PRO:CD	2.22	0.70
1:A:337:ILE:HG22	1:A:349:ILE:HD13	1.74	0.70
1:A:98:CYS:SG	1:B:120:MET:HE2	2.32	0.70
1:H:532:VAL:O	1:H:532:VAL:HG12	1.91	0.69
1:A:304:GLN:NE2	1:A:311:LEU:HD23	2.07	0.69
1:A:93:GLU:HB3	1:B:123:PHE:CE2	2.27	0.69
1:B:437:PRO:CB	1:B:438:PRO:HD3	2.22	0.69
1:G:435:PHE:HE2	1:G:557:LEU:HD13	1.58	0.68
1:A:392:VAL:HG11	1:A:417:VAL:HG21	1.76	0.68
1:B:191:PHE:HB3	1:B:211:LEU:HD22	1.75	0.68
1:B:407:ALA:O	1:B:411:VAL:HG23	1.92	0.68
1:B:583:THR:HG22	1:B:585:LYS:H	1.58	0.68
3:L:12:DC:H2'	3:L:13:DT:C5'	2.18	0.68
1:H:291:CYS:HB3	1:H:325:MET:HE1	1.75	0.68
2:K:4:DG:C8	2:K:4:DG:H5'	2.29	0.68
3:J:15:DT:C3'	3:J:16:DG:H5''	2.23	0.68
1:G:268:HIS:CE1	1:G:319:TRP:HZ2	2.12	0.68
1:H:330:LEU:HD23	1:H:357:ILE:HG22	1.76	0.68
1:A:581:ILE:HD11	1:A:594:VAL:HG13	1.74	0.68
1:A:131:TYR:HE2	1:B:86:VAL:HA	1.58	0.68
1:H:531:ILE:HG22	1:H:532:VAL:N	2.09	0.68
3:L:9:DG:H2''	3:L:10:DT:OP1	1.94	0.68
1:A:98:CYS:SG	1:B:120:MET:CE	2.83	0.67
1:H:262:ARG:HG2	1:H:262:ARG:NH1	2.05	0.67
3:D:14:DC:C2'	3:D:15:DT:C5'	2.71	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:PHE:HD1	1:B:604:TYR:CD1	2.13	0.67
1:G:121:ILE:HG21	1:H:141:LEU:HD21	1.77	0.67
1:H:509:THR:O	1:H:512:ASN:HB2	1.93	0.67
1:A:547:ASN:N	1:A:547:ASN:HD22	1.93	0.67
1:G:337:ILE:HG22	1:G:349:ILE:HD13	1.75	0.67
3:F:3:DG:C8	3:F:3:DG:H5'	2.30	0.67
3:F:12:DC:H2''	3:F:13:DT:H5'	1.77	0.67
1:G:265:CYS:SG	1:G:267:SER:HB2	2.34	0.67
1:A:444:GLN:O	1:A:446:LYS:N	2.28	0.66
1:A:131:TYR:CE2	1:B:86:VAL:HA	2.31	0.66
1:H:145:ILE:HD13	1:H:145:ILE:H	1.60	0.66
1:H:99:ALA:O	1:H:103:VAL:HG13	1.96	0.66
1:A:295:VAL:HG22	1:A:311:LEU:HB3	1.76	0.66
1:A:269:LEU:HD12	1:A:421:TRP:CD1	2.30	0.66
3:L:14:DC:C2'	3:L:15:DT:H5''	2.26	0.66
1:B:292:LYS:HE3	1:B:314:GLU:HG3	1.78	0.66
1:A:199:HIS:CD2	1:A:559:LEU:HD22	2.29	0.66
1:A:120:MET:CE	1:B:98:CYS:HA	2.26	0.66
1:G:360:MET:O	1:G:364:LEU:HD12	1.96	0.66
1:B:320:ASN:ND2	1:B:368:GLU:HG2	2.11	0.66
1:B:440:LEU:O	1:B:443:GLN:HG2	1.95	0.65
1:B:245:PHE:CD2	1:B:257:LEU:HD22	2.32	0.65
1:A:120:MET:CE	1:B:98:CYS:SG	2.84	0.65
1:H:607:PHE:O	1:H:608:CYS:SG	2.53	0.65
1:A:384:PHE:HA	1:A:387:PRO:HG2	1.78	0.65
1:H:584:GLU:O	1:H:587:ASN:HB3	1.97	0.65
1:B:220:THR:O	1:B:224:ILE:HG13	1.96	0.65
1:H:382:LEU:HD11	1:H:429:HIS:CD2	2.32	0.65
1:B:247:THR:HG21	1:B:262:ARG:HD2	1.79	0.65
2:C:10:DC:H6	2:C:10:DC:C5'	2.09	0.65
3:D:1:DT:H5'	3:D:1:DT:C6	2.31	0.65
3:L:7:DT:H6	3:L:7:DT:H5'	1.62	0.65
1:G:240:LEU:HD13	1:G:243:ILE:HD12	1.79	0.65
1:B:515:GLU:HB3	1:B:516:PRO:HD3	1.79	0.65
1:A:547:ASN:HB3	1:A:551:TYR:HD2	1.63	0.64
1:A:123:PHE:CE2	1:B:93:GLU:HB3	2.31	0.64
1:H:407:ALA:O	1:H:411:VAL:HG23	1.98	0.64
1:G:582:ILE:HG22	1:G:582:ILE:O	1.94	0.64
1:G:603:PHE:HD1	1:G:604:TYR:HD1	1.45	0.64
1:A:264:ASN:HD22	1:A:424:ASN:HB3	1.63	0.64
1:H:227:LYS:O	1:H:231:ILE:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:DA:H2'	2:C:1:DA:O5'	1.96	0.64
3:F:3:DG:H8	3:F:3:DG:H5'	1.63	0.64
1:H:531:ILE:O	1:H:532:VAL:HB	1.98	0.64
1:A:540:VAL:HG13	1:A:562:LEU:HD13	1.80	0.64
1:G:385:VAL:HG21	1:G:429:HIS:HD2	1.63	0.64
1:G:154:ASP:HB3	1:G:600:LEU:HD11	1.80	0.64
1:B:337:ILE:HG22	1:B:349:ILE:HD13	1.80	0.64
1:H:437:PRO:HB2	1:H:532:VAL:HG11	1.79	0.64
1:G:182:TRP:O	1:G:191:PHE:HB2	1.97	0.64
1:G:432:ALA:HB2	1:G:561:LEU:HD23	1.80	0.64
1:G:110:SER:OG	2:I:5:DA:H5''	1.98	0.64
3:L:15:DT:H3'	3:L:16:DG:C5'	2.22	0.63
1:H:179:ILE:HD11	1:H:228:LEU:HD13	1.79	0.63
1:B:547:ASN:N	1:B:547:ASN:HD22	1.95	0.63
3:J:3:DG:H5'	3:J:3:DG:C8	2.32	0.63
1:A:98:CYS:HA	1:B:120:MET:HE3	1.79	0.63
1:H:109:PHE:O	1:H:112:VAL:HG12	1.97	0.63
1:H:150:LYS:O	1:H:154:ASP:HB2	1.98	0.63
2:E:13:DC:C2'	2:E:14:DA:C8	2.82	0.63
1:G:120:MET:HE3	1:H:98:CYS:HA	1.81	0.63
1:G:540:VAL:HG13	1:G:562:LEU:HD13	1.79	0.63
1:H:437:PRO:HB3	1:H:532:VAL:HG11	1.80	0.63
1:B:320:ASN:HD22	1:B:368:GLU:HG2	1.63	0.63
2:K:3:DA:H2'	2:K:4:DG:H5''	1.81	0.63
1:A:573:ARG:O	1:A:576:SER:HB3	1.99	0.63
2:C:1:DA:C2'	2:C:1:DA:O5'	2.46	0.63
1:G:544:TRP:HH2	1:G:554:LEU:HD23	1.64	0.63
1:A:247:THR:HG22	1:A:262:ARG:HH11	1.63	0.63
1:A:585:LYS:NZ	1:B:580:ASN:HB3	2.14	0.62
1:H:444:GLN:O	1:H:447:VAL:HG12	1.99	0.62
3:F:14:DC:H2''	3:F:15:DT:C5'	2.29	0.62
1:H:98:CYS:O	1:H:101:TRP:HB3	1.99	0.62
1:B:110:SER:OG	2:E:5:DA:H5''	1.98	0.62
1:B:284:LEU:HD13	1:B:360:MET:CE	2.30	0.62
2:E:3:DA:C2'	2:E:4:DG:H5''	2.30	0.62
1:B:440:LEU:HD23	1:B:440:LEU:H	1.65	0.62
1:G:167:LYS:O	1:G:170:VAL:HG12	1.98	0.62
1:A:293:ASN:ND2	1:A:296:LYS:HE2	2.14	0.62
1:A:583:THR:HB	1:A:586:ARG:HB2	1.82	0.62
1:H:145:ILE:HD13	1:H:145:ILE:N	2.15	0.62
1:A:375:GLN:O	1:A:573:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:337:ILE:HD12	1:H:338:GLN:N	2.14	0.61
3:D:3:DG:C8	3:D:3:DG:H5'	2.36	0.61
1:B:191:PHE:HB3	1:B:211:LEU:CD2	2.30	0.61
1:A:95:ILE:HG22	1:A:96:GLU:N	2.15	0.61
1:A:327:ARG:HG2	1:A:327:ARG:NH1	2.15	0.61
3:J:11:DT:C2'	3:J:12:DC:H5''	2.30	0.61
1:G:263:ILE:CG2	1:G:429:HIS:CE1	2.84	0.61
1:G:136:ASN:HB3	1:G:139:GLU:HB3	1.82	0.61
3:J:6:DG:H2''	3:J:7:DT:C5'	2.30	0.61
1:G:431:THR:O	1:G:434:PHE:HB3	2.01	0.61
1:B:204:LEU:HD11	1:B:563:SER:HA	1.82	0.61
1:G:248:ASP:CB	1:G:268:HIS:CD2	2.83	0.60
1:G:174:GLY:HA2	1:G:560:SER:HB2	1.82	0.60
1:H:265:CYS:SG	1:H:567:SER:HB2	2.40	0.60
1:B:333:TRP:CE2	1:B:354:LYS:HD2	2.36	0.60
1:G:86:VAL:HG12	1:H:131:TYR:CE2	2.35	0.60
1:B:198:TYR:HE1	1:B:205:ARG:HG3	1.62	0.60
2:K:3:DA:C2'	2:K:4:DG:H5''	2.31	0.60
1:A:583:THR:HG22	1:A:585:LYS:H	1.65	0.60
1:G:257:LEU:HB2	1:G:262:ARG:HD3	1.82	0.60
1:H:207:LEU:HD12	1:H:606:ASN:ND2	2.17	0.60
1:B:330:LEU:HD21	1:B:358:GLN:HA	1.82	0.60
1:G:363:ILE:O	1:G:367:PHE:HD1	1.83	0.60
1:H:270:LEU:O	1:H:270:LEU:HD12	2.01	0.60
1:H:431:THR:O	1:H:434:PHE:HB3	2.02	0.60
1:B:437:PRO:HD2	1:B:540:VAL:HG23	1.83	0.60
1:A:97:LYS:HD2	1:B:123:PHE:HB2	1.83	0.60
1:A:247:THR:CG2	1:A:262:ARG:HH11	2.14	0.60
1:B:330:LEU:HD22	1:B:357:ILE:HG22	1.83	0.60
1:B:299:LYS:NZ	1:B:313:SER:HB3	2.17	0.60
1:H:391:LYS:HG3	1:H:395:ILE:CD1	2.31	0.60
3:J:15:DT:H3'	3:J:16:DG:H5''	1.83	0.60
1:G:437:PRO:HD2	1:G:540:VAL:HG23	1.84	0.60
3:F:6:DG:H2''	3:F:7:DT:H5''	1.82	0.59
1:G:120:MET:HE3	1:H:98:CYS:SG	2.42	0.59
1:A:333:TRP:CE2	1:A:354:LYS:HD2	2.37	0.59
1:G:544:TRP:CE3	1:G:555:SER:HA	2.37	0.59
1:G:359:THR:HG21	1:G:406:ILE:HD12	1.84	0.59
1:B:195:THR:HG21	1:B:570:ALA:HB1	1.84	0.59
1:A:218:ARG:O	1:A:219:SER:HB3	2.01	0.59
1:A:437:PRO:HB3	1:A:532:VAL:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:VAL:CG1	1:A:562:LEU:HD13	2.32	0.59
1:H:159:LYS:HG2	1:H:599:PHE:CE2	2.36	0.59
1:G:385:VAL:HG21	1:G:429:HIS:CD2	2.37	0.59
1:B:530:GLU:O	1:B:531:ILE:HG13	2.03	0.59
1:A:531:ILE:O	1:A:531:ILE:HG22	2.02	0.59
1:H:136:ASN:ND2	1:H:139:GLU:HB2	2.18	0.59
1:A:440:LEU:HD23	1:A:440:LEU:H	1.67	0.59
1:G:444:GLN:O	1:G:446:LYS:N	2.35	0.59
1:A:582:ILE:HG22	1:A:582:ILE:O	2.01	0.59
1:B:262:ARG:HG2	1:B:262:ARG:HH11	1.67	0.59
2:I:14:DA:H2''	2:I:15:DA:O5'	2.03	0.59
1:B:247:THR:CG2	1:B:262:ARG:HH11	2.13	0.59
1:A:217:GLU:O	1:A:219:SER:N	2.36	0.59
1:G:120:MET:CE	1:H:98:CYS:SG	2.91	0.58
1:A:454:CYS:O	1:A:458:MET:HE2	2.03	0.58
1:A:298:PHE:CZ	1:A:339:ILE:HD11	2.37	0.58
1:G:407:ALA:O	1:G:411:VAL:HG23	2.03	0.58
1:A:307:LEU:O	1:A:308:ARG:HB3	2.03	0.58
1:G:413:ILE:O	1:G:417:VAL:HG23	2.03	0.58
1:H:415:LYS:O	1:H:419:ILE:HG12	2.03	0.58
3:L:1:DT:H5'	3:L:1:DT:H6	1.68	0.58
3:J:7:DT:H5'	3:J:7:DT:C6	2.28	0.58
2:K:4:DG:H8	2:K:4:DG:H5'	1.67	0.58
1:G:148:SER:HA	1:H:109:PHE:CE1	2.39	0.58
1:G:307:LEU:HD11	1:G:311:LEU:HG	1.86	0.58
1:G:507:GLN:HG2	1:G:508:LEU:HD23	1.85	0.58
1:A:105:ASP:HB3	1:A:107:ARG:HE	1.68	0.58
1:H:582:ILE:O	1:H:582:ILE:HG22	2.02	0.58
1:G:416:ASN:HB3	1:G:420:ILE:HD12	1.85	0.58
1:B:284:LEU:HD13	1:B:360:MET:HE3	1.84	0.58
1:G:430:TYR:HD1	1:G:442:MET:HE3	1.69	0.58
1:H:168:SER:O	1:H:172:LYS:HG2	2.04	0.58
1:A:557:LEU:O	1:A:560:SER:HB3	2.04	0.58
3:L:15:DT:C3'	3:L:16:DG:C5'	2.80	0.58
2:E:13:DC:H2'	2:E:14:DA:C8	2.39	0.58
1:A:430:TYR:CD1	1:A:442:MET:HE1	2.39	0.58
1:G:326:LEU:N	1:G:326:LEU:HD23	2.19	0.58
1:G:136:ASN:ND2	1:G:139:GLU:HB2	2.19	0.57
1:B:507:GLN:O	1:B:508:LEU:HD23	2.04	0.57
1:B:269:LEU:HD13	1:B:421:TRP:HA	1.85	0.57
1:B:276:ASN:O	1:B:280:GLU:HG3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:15:DT:C2'	3:F:16:DG:H5''	2.33	0.57
2:C:10:DC:H5''	2:C:10:DC:H6	1.70	0.57
1:H:323:TYR:CE2	1:H:368:GLU:HG3	2.39	0.57
1:G:306:ARG:NE	1:G:306:ARG:HA	2.20	0.57
1:H:327:ARG:HH11	1:H:327:ARG:HG2	1.69	0.57
1:A:282:PRO:CA	1:A:285:ASN:HD22	2.09	0.57
1:G:391:LYS:O	1:G:395:ILE:HG13	2.04	0.57
3:D:7:DT:C6	3:D:7:DT:H5'	2.31	0.57
2:I:13:DC:H2''	2:I:14:DA:N7	2.18	0.57
1:A:269:LEU:CD1	1:A:421:TRP:HA	2.35	0.57
1:G:356:ILE:O	1:G:360:MET:HG3	2.04	0.57
1:A:547:ASN:HB3	1:A:551:TYR:CD2	2.40	0.57
1:A:179:ILE:HB	1:A:192:LEU:HD11	1.85	0.57
1:G:315:CYS:N	1:G:316:PRO:HD3	2.20	0.57
1:B:247:THR:HG23	1:B:248:ASP:O	2.04	0.57
3:D:14:DC:H2'	3:D:15:DT:H5'	1.87	0.57
1:H:350:VAL:O	1:H:350:VAL:HG12	2.04	0.57
1:A:269:LEU:HD12	1:A:421:TRP:HD1	1.68	0.57
1:A:459:GLU:O	1:A:462:GLU:HB2	2.05	0.57
1:B:133:GLU:HG3	1:B:134:HIS:ND1	2.20	0.57
1:A:523:GLU:O	1:A:526:PHE:HB2	2.05	0.57
1:H:155:ALA:HA	1:H:600:LEU:HD21	1.87	0.57
3:D:8:DT:C2'	3:D:9:DG:H5'	2.34	0.56
1:A:159:LYS:CE	1:A:234:GLN:NE2	2.68	0.56
1:H:451:LYS:HA	1:H:524:PHE:CE2	2.40	0.56
1:A:269:LEU:HD11	1:A:424:ASN:HB2	1.87	0.56
1:G:333:TRP:HA	1:G:336:VAL:HG12	1.88	0.56
1:A:139:GLU:HG3	1:A:140:LEU:N	2.21	0.56
2:E:10:DC:C6	2:E:10:DC:C5'	2.86	0.56
1:H:162:ILE:HD12	1:H:166:ILE:HD11	1.88	0.56
1:A:314:GLU:O	1:A:315:CYS:SG	2.63	0.56
3:F:15:DT:H5'	3:F:15:DT:C6	2.41	0.56
1:G:435:PHE:HE2	1:G:557:LEU:CD1	2.17	0.56
1:G:433:PHE:HB3	1:G:442:MET:SD	2.45	0.56
1:B:178:THR:HB	1:B:571:SER:OG	2.05	0.56
2:E:11:DA:C2	3:F:6:DG:N2	2.74	0.56
1:B:337:ILE:HG13	1:B:338:GLN:N	2.21	0.56
1:G:198:TYR:CZ	1:G:205:ARG:HG2	2.41	0.56
2:K:9:DA:N3	2:K:10:DC:H1'	2.21	0.56
1:G:326:LEU:O	1:G:330:LEU:HD13	2.06	0.56
1:A:112:VAL:HG11	1:B:147:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:527:TYR:O	1:H:530:GLU:HB2	2.04	0.56
1:B:102:VAL:HG22	1:B:107:ARG:O	2.06	0.56
1:G:208:ILE:HD13	1:G:574:THR:HG23	1.88	0.56
2:I:11:DA:N3	3:J:6:DG:N2	2.53	0.56
1:A:505:PHE:HB3	1:A:508:LEU:HD22	1.88	0.56
1:G:249:ARG:HH22	1:G:420:ILE:HG23	1.71	0.55
1:G:114:GLY:O	1:G:117:PHE:HB3	2.05	0.55
1:A:178:THR:HG22	1:A:246:VAL:HB	1.88	0.55
1:G:101:TRP:CD1	1:H:117:PHE:HB2	2.41	0.55
1:A:380:PRO:HB3	1:A:562:LEU:O	2.06	0.55
3:L:12:DC:H2"	3:L:13:DT:C5'	2.20	0.55
1:G:248:ASP:HB2	1:G:268:HIS:CD2	2.40	0.55
1:A:199:HIS:NE2	1:A:559:LEU:HD22	2.21	0.55
3:F:15:DT:H5'	3:F:15:DT:H6	1.72	0.55
1:H:550:LYS:HE2	1:H:551:TYR:CZ	2.40	0.55
1:B:582:ILE:O	1:B:582:ILE:HG22	2.04	0.55
3:F:2:DT:C2'	3:F:3:DG:H5"	2.28	0.55
1:B:265:CYS:SG	1:B:567:SER:CB	2.93	0.55
1:A:98:CYS:O	1:A:101:TRP:HB3	2.06	0.55
3:J:7:DT:C5'	3:J:7:DT:H6	2.15	0.55
1:A:359:THR:HG21	1:A:406:ILE:HG13	1.89	0.55
1:B:112:VAL:HA	1:B:117:PHE:CD2	2.42	0.55
1:G:249:ARG:NH2	1:G:272:ASN:HD22	2.04	0.55
3:J:6:DG:H2"	3:J:7:DT:H5"	1.88	0.55
1:B:330:LEU:HD13	1:B:357:ILE:HG21	1.88	0.55
1:B:246:VAL:HG12	1:B:263:ILE:HB	1.88	0.55
1:G:125:ILE:HG23	1:H:128:GLY:HA2	1.89	0.55
1:A:162:ILE:HD13	1:A:607:PHE:HE2	1.71	0.55
1:G:263:ILE:CG2	1:G:429:HIS:HE1	2.17	0.55
1:H:195:THR:HG22	1:H:207:LEU:O	2.07	0.55
1:H:320:ASN:ND2	1:H:368:GLU:HG2	2.22	0.55
1:G:586:ARG:O	1:G:588:ARG:N	2.39	0.54
1:H:213:SER:O	1:H:227:LYS:HE2	2.06	0.54
1:A:161:LEU:HD23	1:A:161:LEU:O	2.06	0.54
2:E:8:DA:C2	3:F:9:DG:N2	2.75	0.54
1:G:248:ASP:HB2	1:G:268:HIS:HD2	1.71	0.54
1:G:245:PHE:O	1:G:262:ARG:HA	2.08	0.54
1:G:389:ILE:HD11	1:G:425:LEU:HD11	1.88	0.54
1:H:540:VAL:HG11	1:H:562:LEU:HD22	1.88	0.54
1:B:159:LYS:HG2	1:B:599:PHE:CZ	2.43	0.54
1:H:365:ASP:O	1:H:368:GLU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:ARG:NH2	1:H:115:SER:HB3	2.23	0.54
1:A:437:PRO:HB2	1:A:438:PRO:HD3	1.90	0.54
1:G:435:PHE:CD2	1:G:558:ALA:HA	2.43	0.54
1:A:592:GLN:HG2	1:A:593:THR:N	2.23	0.54
1:B:78:MET:O	1:B:79:GLN:HB2	2.08	0.54
2:E:11:DA:H2'	2:E:11:DA:O5'	2.08	0.54
1:H:356:ILE:O	1:H:360:MET:HG3	2.08	0.54
1:H:581:ILE:O	1:H:581:ILE:HG13	2.08	0.54
1:H:363:ILE:HG22	1:H:364:LEU:N	2.23	0.54
1:G:519:CYS:HB2	1:G:520:PRO:HD2	1.88	0.54
1:G:196:LEU:HB2	1:G:209:LEU:HD11	1.90	0.54
1:G:330:LEU:HD22	1:G:361:VAL:HG11	1.90	0.53
1:H:247:THR:HG23	1:H:248:ASP:O	2.08	0.53
1:H:447:VAL:HG21	1:H:528:ARG:CZ	2.38	0.53
2:K:11:DA:C2	3:L:6:DG:C2	2.96	0.53
3:L:8:DT:H2''	3:L:9:DG:H5'	1.89	0.53
1:A:572:GLU:HG2	3:D:16:DG:H1'	1.90	0.53
1:A:406:ILE:HG22	1:A:407:ALA:N	2.23	0.53
1:H:400:VAL:O	1:H:400:VAL:HG12	2.08	0.53
1:G:219:SER:O	1:G:252:ASN:ND2	2.41	0.53
1:A:189:ARG:HG2	1:A:189:ARG:HH11	1.72	0.53
1:B:445:GLU:H	1:B:445:GLU:CD	2.12	0.53
1:H:586:ARG:O	1:H:588:ARG:N	2.42	0.53
1:B:262:ARG:NH1	1:B:262:ARG:HG2	2.23	0.53
1:G:295:VAL:HG22	1:G:311:LEU:HB3	1.89	0.53
1:A:183:THR:HG23	1:A:190:ASN:OD1	2.08	0.53
1:A:334:GLU:O	1:A:337:ILE:HG12	2.09	0.53
1:H:178:THR:CG2	1:H:568:SER:HA	2.38	0.53
2:C:3:DA:C2'	2:C:4:DG:H5'	2.39	0.53
1:B:227:LYS:O	1:B:231:ILE:HG13	2.09	0.53
1:A:213:SER:C	1:A:215:ASP:H	2.11	0.53
1:B:391:LYS:O	1:B:395:ILE:HG13	2.09	0.53
1:G:394:GLU:O	1:G:394:GLU:HG2	2.08	0.53
1:G:270:LEU:HD21	1:G:367:PHE:HD2	1.74	0.53
2:K:11:DA:N3	3:L:6:DG:N2	2.56	0.53
1:A:392:VAL:HG11	1:A:417:VAL:CG2	2.38	0.53
2:I:6:DA:H2'	2:I:6:DA:O5'	2.07	0.53
2:E:13:DC:H2'	2:E:14:DA:N7	2.24	0.53
3:F:7:DT:H5'	3:F:7:DT:H6	1.74	0.53
1:G:271:SER:HG	1:G:319:TRP:HD1	1.57	0.53
1:G:353:ASN:ND2	1:G:356:ILE:HG13	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:PHE:HB2	1:H:97:LYS:CD	2.39	0.53
2:I:1:DA:H5'	2:I:1:DA:H8	1.74	0.53
1:B:218:ARG:O	1:B:219:SER:HB3	2.08	0.53
1:H:235:PHE:O	1:H:236:ASN:HB2	2.09	0.53
1:B:444:GLN:C	1:B:446:LYS:N	2.62	0.53
1:B:199:HIS:CE1	1:B:559:LEU:HD13	2.44	0.53
1:A:120:MET:HE1	1:B:98:CYS:HA	1.90	0.52
1:A:281:THR:HG21	1:A:284:LEU:HD12	1.90	0.52
1:B:581:ILE:CD1	1:B:598:LEU:HD13	2.39	0.52
1:H:337:ILE:HD12	1:H:338:GLN:H	1.73	0.52
1:G:361:VAL:O	1:G:365:ASP:N	2.42	0.52
1:G:209:LEU:HD22	1:G:235:PHE:CE2	2.44	0.52
1:G:593:THR:O	1:G:597:LEU:HB2	2.09	0.52
1:H:583:THR:HG22	1:H:584:GLU:N	2.25	0.52
1:G:585:LYS:O	2:K:5:DA:H1'	2.09	0.52
1:H:527:TYR:O	1:H:530:GLU:CB	2.57	0.52
1:A:120:MET:HE3	1:B:98:CYS:HA	1.92	0.52
1:H:265:CYS:SG	1:H:267:SER:HB2	2.49	0.52
1:B:187:ILE:HG22	1:B:187:ILE:O	2.09	0.52
3:J:5:DT:H2''	3:J:6:DG:O4'	2.09	0.52
3:F:15:DT:H2'	3:F:16:DG:H5''	1.92	0.52
1:G:144:PRO:HG3	1:H:112:VAL:CG1	2.39	0.52
2:E:13:DC:H2''	2:E:14:DA:C8	2.45	0.52
1:G:506:PRO:HD2	1:G:507:GLN:OE1	2.09	0.52
1:A:277:SER:OG	1:A:413:ILE:HA	2.10	0.52
1:B:247:THR:HG22	1:B:262:ARG:NH1	2.15	0.52
1:G:264:ASN:HD22	1:G:424:ASN:HB3	1.75	0.52
1:H:201:ASN:O	1:H:203:GLU:N	2.43	0.52
1:H:304:GLN:NE2	1:H:311:LEU:H	2.08	0.52
1:G:248:ASP:HB3	1:G:268:HIS:CD2	2.44	0.52
3:F:14:DC:C2'	3:F:15:DT:C5'	2.88	0.52
1:A:123:PHE:CZ	1:B:94:ALA:HB2	2.45	0.52
1:G:315:CYS:N	1:G:316:PRO:CD	2.72	0.52
1:A:204:LEU:HD11	1:A:563:SER:HA	1.92	0.52
1:H:387:PRO:HA	1:H:390:LEU:HG	1.91	0.52
1:B:588:ARG:HD3	3:D:12:DC:H1'	1.92	0.52
1:G:107:ARG:HH21	1:H:111:ALA:HA	1.75	0.52
1:H:551:TYR:HB3	1:H:554:LEU:HB3	1.91	0.52
1:A:297:TYR:HD1	1:A:348:ARG:NH2	2.08	0.52
1:A:541:MET:CE	1:A:541:MET:CB	2.88	0.51
1:A:95:ILE:CG2	1:B:150:LYS:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:599:PHE:C	1:H:599:PHE:CD1	2.83	0.51
1:B:531:ILE:HD12	1:G:550:LYS:HE3	1.91	0.51
1:A:213:SER:HB3	1:A:591:GLN:OE1	2.10	0.51
1:B:543:TRP:HZ3	1:B:544:TRP:CD2	2.27	0.51
1:A:137:VAL:HG12	1:A:138:GLU:N	2.25	0.51
3:D:5:DT:H2''	3:D:6:DG:C5'	2.37	0.51
1:A:547:ASN:N	1:A:547:ASN:ND2	2.58	0.51
1:B:81:ARG:H	1:B:81:ARG:HD2	1.76	0.51
1:G:396:CYS:O	1:G:414:ILE:HD11	2.10	0.51
1:G:374:LEU:HD23	1:G:566:ALA:HB1	1.91	0.51
1:H:102:VAL:HG13	1:H:107:ARG:O	2.10	0.51
1:B:384:PHE:CA	1:B:387:PRO:HG2	2.40	0.51
1:B:197:HIS:HA	1:B:205:ARG:O	2.10	0.51
1:H:590:GLY:O	1:H:594:VAL:HG23	2.10	0.51
1:G:86:VAL:HA	1:H:131:TYR:CE2	2.45	0.51
1:G:315:CYS:O	1:G:317:THR:N	2.44	0.51
1:G:244:LYS:HD2	1:G:564:ILE:HD11	1.91	0.51
1:H:262:ARG:CG	1:H:262:ARG:HH11	2.13	0.51
3:L:2:DT:C2'	3:L:3:DG:C5'	2.75	0.51
1:B:495:SER:O	1:B:496:LYS:HB2	2.10	0.51
1:A:325:MET:CE	1:A:326:LEU:HD23	2.41	0.51
3:J:7:DT:H2'	3:J:8:DT:C6	2.45	0.51
1:B:518:VAL:HG12	1:B:519:CYS:N	2.26	0.51
1:B:384:PHE:HA	1:B:387:PRO:CG	2.37	0.51
1:A:581:ILE:CD1	1:A:594:VAL:HG13	2.41	0.51
1:B:442:MET:C	1:B:444:GLN:N	2.61	0.51
1:H:304:GLN:NE2	1:H:310:SER:HB2	2.26	0.51
1:A:600:LEU:HB3	1:B:103:VAL:HG11	1.92	0.51
1:B:142:PRO:HB2	1:B:146:THR:CG2	2.40	0.51
3:J:13:DT:H2'	3:J:14:DC:H6	1.76	0.51
1:A:314:GLU:C	1:A:315:CYS:SG	2.89	0.51
1:H:519:CYS:HB2	1:H:520:PRO:HD2	1.93	0.51
1:H:573:ARG:HD3	2:K:2:DG:O4'	2.11	0.51
1:H:369:ARG:HH11	1:H:369:ARG:HG2	1.76	0.51
1:G:225:TYR:CE1	1:G:229:LYS:HE2	2.46	0.51
2:I:11:DA:C2	3:J:6:DG:C2	2.99	0.50
1:G:107:ARG:HB3	1:G:108:PRO:HD2	1.94	0.50
1:G:142:PRO:HG2	1:G:147:LEU:HD21	1.93	0.50
1:G:364:LEU:HA	1:G:367:PHE:HB2	1.92	0.50
1:G:547:ASN:HD22	1:G:547:ASN:H	1.57	0.50
1:A:323:TYR:HB2	1:A:364:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:THR:HG21	1:G:570:ALA:HB1	1.93	0.50
1:B:603:PHE:CD1	1:B:604:TYR:HD1	2.23	0.50
1:A:307:LEU:HD12	1:A:311:LEU:CD2	2.41	0.50
1:G:389:ILE:CD1	1:G:425:LEU:HD11	2.40	0.50
1:H:145:ILE:H	1:H:145:ILE:CD1	2.20	0.50
1:A:169:ALA:HA	1:A:172:LYS:HE2	1.93	0.50
1:G:384:PHE:O	1:G:388:SER:OG	2.29	0.50
1:G:247:THR:CG2	1:G:248:ASP:N	2.74	0.50
1:B:583:THR:HG22	1:B:584:GLU:N	2.27	0.50
3:F:1:DT:H6	3:F:1:DT:H5''	1.77	0.50
3:L:14:DC:C2'	3:L:15:DT:C5'	2.89	0.50
1:B:437:PRO:CB	1:B:438:PRO:CD	2.88	0.50
1:A:123:PHE:C	1:A:123:PHE:CD1	2.84	0.50
1:B:577:LEU:HA	1:B:580:ASN:ND2	2.26	0.50
1:B:431:THR:O	1:B:434:PHE:HB3	2.10	0.50
1:A:103:VAL:HG11	1:B:600:LEU:HB3	1.92	0.50
1:A:518:VAL:HG13	1:A:518:VAL:O	2.11	0.50
1:H:218:ARG:O	1:H:219:SER:HB3	2.12	0.50
3:L:2:DT:H2''	3:L:3:DG:H5'	1.86	0.50
1:B:314:GLU:O	1:B:315:CYS:SG	2.70	0.50
1:G:498:ILE:HD11	1:G:502:SER:HB2	1.93	0.50
1:A:82:GLU:HA	1:A:82:GLU:OE1	2.11	0.50
1:H:550:LYS:C	1:H:552:PRO:HD3	2.32	0.49
1:B:444:GLN:O	1:B:446:LYS:N	2.45	0.49
1:G:264:ASN:HB3	1:G:269:LEU:HD21	1.92	0.49
1:G:164:ARG:HG2	1:G:165:GLU:N	2.27	0.49
1:H:269:LEU:O	1:H:272:ASN:HB2	2.12	0.49
1:A:307:LEU:O	1:A:308:ARG:CB	2.61	0.49
2:K:3:DA:H5''	2:K:3:DA:H8	1.77	0.49
1:A:175:ALA:O	1:A:244:LYS:HE3	2.12	0.49
1:A:180:ASP:HB3	1:A:575:PHE:CE2	2.47	0.49
1:H:320:ASN:HD22	1:H:368:GLU:HG2	1.76	0.49
1:H:96:GLU:O	1:H:100:GLN:HG3	2.12	0.49
1:B:341:SER:O	1:B:343:ALA:N	2.45	0.49
1:B:87:SER:C	1:B:89:ASP:H	2.16	0.49
1:G:451:LYS:O	1:G:455:LEU:HD13	2.13	0.49
3:L:1:DT:H5'	3:L:1:DT:C6	2.47	0.49
1:B:426:SER:O	1:B:429:HIS:HB2	2.12	0.49
1:H:288:ILE:HG22	1:H:289:LEU:N	2.26	0.49
1:G:176:SER:CB	1:G:565:PRO:HD3	2.42	0.49
1:H:345:GLU:O	1:H:347:GLN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASP:O	1:B:188:LYS:HA	2.12	0.49
1:G:151:VAL:HG11	1:G:597:LEU:HD22	1.93	0.49
1:H:413:ILE:O	1:H:417:VAL:HG23	2.12	0.49
1:H:286:MET:HB3	1:H:287:PRO:CD	2.41	0.49
1:H:204:LEU:HD11	1:H:563:SER:HA	1.93	0.49
1:A:147:LEU:O	1:A:151:VAL:HG23	2.12	0.49
1:A:586:ARG:O	1:A:589:ILE:HG22	2.13	0.49
1:B:284:LEU:O	1:B:288:ILE:HG13	2.12	0.49
1:A:126:LYS:HG2	1:A:126:LYS:O	2.13	0.49
1:H:370:ILE:HD11	1:H:391:LYS:HB3	1.94	0.49
1:B:130:GLU:O	1:B:130:GLU:HG2	2.11	0.49
3:L:11:DT:C4	3:L:12:DC:C5	3.01	0.49
1:A:307:LEU:CD1	1:A:311:LEU:CD2	2.89	0.49
1:A:101:TRP:O	1:A:105:ASP:HB2	2.13	0.49
1:B:433:PHE:CZ	1:B:441:HIS:HD2	2.31	0.49
1:A:580:ASN:HB3	1:B:585:LYS:HZ1	1.78	0.49
1:A:131:TYR:CE2	1:B:86:VAL:HG12	2.47	0.49
1:G:603:PHE:CD1	1:G:604:TYR:HD1	2.30	0.49
1:H:375:GLN:O	1:H:573:ARG:NH2	2.46	0.49
1:A:100:GLN:HG2	1:B:604:TYR:CE2	2.48	0.48
1:H:144:PRO:HB2	1:H:145:ILE:HD13	1.94	0.48
1:A:162:ILE:HG21	1:A:607:PHE:CE2	2.48	0.48
1:B:318:ARG:HA	3:F:16:DG:C8	2.48	0.48
1:B:182:TRP:HB2	1:B:575:PHE:CZ	2.48	0.48
1:G:248:ASP:HB3	1:G:268:HIS:NE2	2.29	0.48
1:G:263:ILE:HD13	1:G:263:ILE:N	2.28	0.48
1:A:304:GLN:HE22	1:A:311:LEU:H	1.58	0.48
2:C:11:DA:H2'	2:C:11:DA:O5'	2.12	0.48
1:A:589:ILE:HG12	1:A:594:VAL:HG23	1.94	0.48
1:B:330:LEU:HD13	1:B:357:ILE:CG2	2.43	0.48
1:H:460:ASP:O	1:H:463:LEU:HB2	2.13	0.48
1:H:185:ASN:OD1	1:H:185:ASN:N	2.45	0.48
1:G:606:ASN:O	1:G:607:PHE:HD1	1.96	0.48
3:J:8:DT:H2''	3:J:9:DG:H5'	1.96	0.48
1:H:162:ILE:HD13	1:H:607:PHE:HE2	1.77	0.48
1:A:304:GLN:HE22	1:A:311:LEU:HD23	1.75	0.48
1:A:392:VAL:CG1	1:A:417:VAL:HG21	2.43	0.48
1:A:315:CYS:N	1:A:316:PRO:HD3	2.27	0.48
1:A:607:PHE:C	1:A:608:CYS:SG	2.91	0.48
1:H:369:ARG:HG2	1:H:369:ARG:NH1	2.28	0.48
1:B:416:ASN:HB3	1:B:420:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:VAL:HG12	1:A:405:ASP:H	1.78	0.48
1:A:431:THR:O	1:A:434:PHE:HB3	2.12	0.48
1:H:176:SER:HA	1:H:244:LYS:O	2.13	0.48
3:J:13:DT:H5'	3:J:13:DT:H6	1.78	0.48
1:H:531:ILE:HG22	1:H:532:VAL:H	1.77	0.48
1:B:440:LEU:HG	1:B:441:HIS:H	1.78	0.48
1:A:189:ARG:NH1	1:A:189:ARG:HG2	2.27	0.48
1:B:442:MET:C	1:B:444:GLN:H	2.17	0.48
1:B:444:GLN:C	1:B:446:LYS:H	2.16	0.48
1:H:110:SER:OG	2:K:5:DA:H5"	2.13	0.48
1:G:266:SER:HB2	1:G:374:LEU:HD22	1.96	0.48
1:G:415:LYS:O	1:G:419:ILE:HG12	2.13	0.48
1:G:585:LYS:H	1:G:585:LYS:HD2	1.77	0.48
1:A:297:TYR:CD1	1:A:348:ARG:NH2	2.82	0.48
1:A:341:SER:O	1:A:344:GLY:N	2.43	0.48
1:H:332:ASN:O	1:H:336:VAL:HG22	2.13	0.48
1:B:303:LEU:O	1:B:306:ARG:HG2	2.13	0.48
1:H:531:ILE:CG2	1:H:532:VAL:N	2.76	0.48
1:A:298:PHE:HZ	1:A:339:ILE:HD11	1.78	0.48
1:H:399:ASP:O	1:H:400:VAL:HB	2.14	0.48
1:G:385:VAL:HG11	1:G:429:HIS:CD2	2.49	0.47
1:B:530:GLU:HG3	1:B:531:ILE:H	1.79	0.47
1:B:136:ASN:ND2	1:B:139:GLU:HB2	2.28	0.47
1:A:396:CYS:HA	1:A:410:LYS:HD3	1.95	0.47
1:H:431:THR:HG23	1:H:450:ILE:HG23	1.95	0.47
1:G:155:ALA:CA	1:G:600:LEU:HD21	2.43	0.47
1:B:337:ILE:HG13	1:B:338:GLN:H	1.77	0.47
1:B:527:TYR:O	1:B:530:GLU:HB2	2.14	0.47
1:A:600:LEU:HA	1:A:600:LEU:HD13	1.78	0.47
1:B:359:THR:O	1:B:363:ILE:HG13	2.14	0.47
1:G:608:CYS:O	1:G:609:LYS:HD3	2.14	0.47
3:D:4:DT:H2"	3:D:5:DT:O5'	2.13	0.47
1:B:323:TYR:HB2	1:B:364:LEU:HD13	1.95	0.47
1:G:112:VAL:O	1:G:117:PHE:HD2	1.98	0.47
1:A:389:ILE:HD13	1:A:422:GLU:HG2	1.97	0.47
1:B:213:SER:C	1:B:215:ASP:H	2.17	0.47
1:A:323:TYR:HB2	1:A:364:LEU:HD13	1.96	0.47
1:H:543:TRP:HZ3	1:H:544:TRP:CD2	2.31	0.47
1:B:315:CYS:N	1:B:316:PRO:HD3	2.28	0.47
1:A:599:PHE:C	1:A:599:PHE:CD1	2.88	0.47
2:I:11:DA:C2	3:J:6:DG:N2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LEU:HD12	1:A:311:LEU:HD21	1.95	0.47
1:B:516:PRO:HA	1:B:517:PRO:HD2	1.66	0.47
1:B:299:LYS:HZ1	1:B:313:SER:HB3	1.78	0.47
1:H:540:VAL:CG1	1:H:562:LEU:HD13	2.44	0.47
1:A:593:THR:O	1:A:597:LEU:HD22	2.15	0.47
1:G:151:VAL:O	1:G:596:SER:HB3	2.15	0.47
1:B:327:ARG:HH11	1:B:327:ARG:HG2	1.79	0.47
1:G:496:LYS:HD2	1:G:496:LYS:HA	1.73	0.47
1:B:384:PHE:N	1:B:384:PHE:CD1	2.79	0.47
1:B:211:LEU:HA	1:B:211:LEU:HD23	1.65	0.47
1:A:443:GLN:O	1:A:444:GLN:O	2.33	0.47
1:A:333:TRP:NE1	1:A:354:LYS:HD2	2.30	0.47
1:B:167:LYS:HD3	1:B:236:ASN:O	2.15	0.47
1:B:533:ILE:HD12	1:B:533:ILE:HA	1.80	0.47
3:D:11:DT:C2'	3:D:12:DC:H5''	2.37	0.47
1:G:112:VAL:HA	1:G:117:PHE:CD2	2.50	0.47
1:A:581:ILE:HD11	1:A:594:VAL:HG22	1.96	0.47
1:A:292:LYS:HE3	1:A:314:GLU:HG3	1.97	0.47
1:G:235:PHE:O	1:G:236:ASN:HB2	2.14	0.47
1:G:345:GLU:C	1:G:347:GLN:H	2.18	0.47
1:B:308:ARG:HE	1:B:308:ARG:HB3	1.67	0.47
1:G:194:VAL:HG21	1:G:231:ILE:HD12	1.97	0.47
2:I:3:DA:H2''	2:I:4:DG:H5''	1.95	0.47
1:G:271:SER:O	1:G:274:LEU:N	2.47	0.47
1:A:199:HIS:CD2	1:A:559:LEU:CD2	2.96	0.47
1:A:580:ASN:HB3	1:B:585:LYS:NZ	2.30	0.47
1:H:195:THR:HB	1:H:197:HIS:NE2	2.30	0.47
1:H:380:PRO:HB3	1:H:562:LEU:O	2.15	0.47
3:D:7:DT:H2'	3:D:8:DT:C6	2.50	0.47
1:A:264:ASN:ND2	1:A:424:ASN:HB3	2.27	0.47
1:B:101:TRP:O	1:B:105:ASP:HB2	2.15	0.47
3:L:9:DG:H2'	3:L:9:DG:O5'	2.15	0.46
1:A:433:PHE:HZ	1:A:441:HIS:HD2	1.60	0.46
1:H:532:VAL:O	1:H:532:VAL:CG1	2.62	0.46
1:B:383:CYS:HB3	1:B:432:ALA:O	2.16	0.46
1:B:179:ILE:HG21	1:B:179:ILE:HD13	1.65	0.46
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.43	0.46
2:C:3:DA:H2''	2:C:4:DG:H5'	1.96	0.46
1:A:511:ASN:O	1:A:512:ASN:HB2	2.15	0.46
1:A:543:TRP:HZ3	1:A:544:TRP:CE3	2.32	0.46
1:H:207:LEU:HD23	1:H:209:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:TYR:CE1	1:G:205:ARG:HG2	2.51	0.46
2:I:1:DA:C8	2:I:1:DA:H5'	2.51	0.46
1:B:240:LEU:HD22	1:B:243:ILE:HD12	1.98	0.46
1:G:531:ILE:HG22	1:G:531:ILE:O	2.15	0.46
1:H:495:SER:O	1:H:497:ASP:N	2.48	0.46
1:H:292:LYS:HE3	1:H:314:GLU:HG3	1.97	0.46
1:B:109:PHE:O	1:B:111:ALA:N	2.48	0.46
1:G:107:ARG:NH1	2:K:5:DA:OP2	2.49	0.46
1:G:368:GLU:O	1:G:371:PHE:N	2.48	0.46
1:G:86:VAL:HG21	1:H:140:LEU:HD13	1.97	0.46
1:G:386:VAL:N	1:G:387:PRO:HD2	2.31	0.46
3:F:5:DT:H2'	3:F:6:DG:C8	2.51	0.46
1:G:117:PHE:CE1	1:G:121:ILE:HD11	2.51	0.46
1:A:159:LYS:HE3	1:A:234:GLN:NE2	2.30	0.46
1:A:325:MET:HE2	1:A:326:LEU:CD2	2.45	0.46
1:G:140:LEU:O	1:H:91:LYS:HE3	2.15	0.46
1:B:176:SER:HB3	1:B:244:LYS:HB2	1.96	0.46
1:H:162:ILE:O	1:H:164:ARG:N	2.48	0.46
1:G:359:THR:CG2	1:G:406:ILE:HD12	2.45	0.46
1:A:245:PHE:HB2	1:A:261:ILE:O	2.15	0.46
1:A:538:PHE:C	1:A:538:PHE:CD1	2.88	0.46
1:B:141:LEU:HA	1:B:141:LEU:HD23	1.56	0.46
1:H:585:LYS:O	1:H:587:ASN:N	2.49	0.46
3:L:11:DT:C2	3:L:12:DC:C6	3.04	0.46
1:H:430:TYR:CD2	1:H:446:LYS:HE2	2.51	0.46
1:H:444:GLN:O	1:H:446:LYS:N	2.48	0.46
1:B:587:ASN:HD21	3:D:12:DC:C2'	2.28	0.46
1:B:95:ILE:HG22	1:B:96:GLU:N	2.31	0.46
1:G:582:ILE:CG2	1:G:582:ILE:O	2.64	0.46
1:B:547:ASN:ND2	1:B:547:ASN:N	2.62	0.46
1:G:380:PRO:HB3	1:G:562:LEU:O	2.16	0.46
1:B:431:THR:HG23	1:B:450:ILE:HG23	1.96	0.46
1:B:198:TYR:C	1:B:198:TYR:CD1	2.89	0.46
1:G:353:ASN:HB3	1:G:356:ILE:HD12	1.97	0.46
1:H:325:MET:O	1:H:325:MET:HE2	2.16	0.46
1:G:431:THR:HG1	1:G:453:PHE:HD2	1.58	0.46
1:G:356:ILE:O	1:G:356:ILE:HG22	2.16	0.45
1:G:155:ALA:HA	1:G:600:LEU:HD21	1.98	0.45
1:G:86:VAL:HA	1:H:131:TYR:HE2	1.81	0.45
1:H:178:THR:CB	1:H:195:THR:HG1	2.29	0.45
1:H:178:THR:HB	1:H:571:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:HD12	1:B:330:LEU:HA	1.64	0.45
1:G:392:VAL:HG11	1:G:417:VAL:HG21	1.98	0.45
1:B:451:LYS:HG2	1:B:455:LEU:HD22	1.98	0.45
1:H:438:PRO:HG3	1:H:532:VAL:HG12	1.98	0.45
1:B:581:ILE:HD11	1:B:598:LEU:HD13	1.99	0.45
2:I:5:DA:H2'	2:I:6:DA:C8	2.51	0.45
1:H:523:GLU:O	1:H:526:PHE:HB2	2.16	0.45
2:K:10:DC:N4	2:K:11:DA:N6	2.64	0.45
1:G:382:LEU:HD23	1:G:564:ILE:HB	1.97	0.45
1:B:526:PHE:HZ	1:G:547:ASN:HD21	1.63	0.45
1:B:182:TRP:HB2	1:B:575:PHE:CE2	2.52	0.45
1:B:274:LEU:HD23	1:B:274:LEU:HA	1.60	0.45
1:B:384:PHE:N	1:B:384:PHE:HD1	2.12	0.45
1:A:212:LYS:HB3	1:A:227:LYS:HD2	1.97	0.45
1:A:446:LYS:HA	1:A:446:LYS:HD2	1.88	0.45
1:H:519:CYS:HB2	1:H:520:PRO:CD	2.47	0.45
1:G:547:ASN:N	1:G:547:ASN:HD22	2.14	0.45
1:H:257:LEU:O	1:H:259:ASN:N	2.49	0.45
1:A:130:GLU:O	1:A:130:GLU:HG2	2.17	0.45
1:A:204:LEU:HD23	1:A:377:CYS:O	2.17	0.45
1:A:168:SER:OG	1:A:169:ALA:N	2.49	0.45
1:B:570:ALA:HA	1:B:573:ARG:NH1	2.31	0.45
3:D:7:DT:H2''	3:D:8:DT:O5'	2.16	0.45
1:G:435:PHE:CE2	1:G:557:LEU:CD1	2.98	0.45
1:B:583:THR:HB	1:B:586:ARG:H	1.82	0.45
1:B:517:PRO:O	1:B:522:ASP:HB2	2.16	0.45
1:H:178:THR:HG21	1:H:568:SER:HA	1.99	0.45
1:G:382:LEU:CD2	1:G:564:ILE:HB	2.47	0.45
1:G:200:GLU:O	1:G:203:GLU:HG2	2.16	0.45
1:H:295:VAL:HG12	1:H:296:LYS:N	2.31	0.45
1:B:245:PHE:O	1:B:262:ARG:HA	2.17	0.45
1:G:540:VAL:CG1	1:G:562:LEU:HD13	2.44	0.45
1:B:213:SER:O	1:B:227:LYS:HE2	2.16	0.45
1:A:428:TRP:HE3	1:A:561:LEU:HD22	1.82	0.45
1:B:277:SER:OG	1:B:413:ILE:HA	2.17	0.45
1:H:564:ILE:HA	1:H:565:PRO:HD3	1.68	0.45
1:A:252:ASN:N	1:A:252:ASN:OD1	2.49	0.45
3:F:4:DT:C2	3:F:5:DT:C6	3.05	0.45
1:H:262:ARG:CG	1:H:262:ARG:NH1	2.76	0.45
1:H:247:THR:CG2	1:H:248:ASP:O	2.64	0.45
1:H:217:GLU:O	1:H:219:SER:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLY:O	1:B:370:ILE:HG13	2.16	0.45
3:F:14:DC:C2'	3:F:15:DT:H5'	2.47	0.45
1:A:550:LYS:C	1:A:552:PRO:HD3	2.38	0.45
1:H:291:CYS:HB3	1:H:325:MET:CE	2.43	0.45
1:A:589:ILE:HG12	1:A:594:VAL:CG2	2.46	0.45
1:G:437:PRO:HB2	1:G:438:PRO:HD3	1.98	0.45
1:B:278:PHE:HE1	1:B:360:MET:HE2	1.82	0.45
1:A:161:LEU:C	1:A:161:LEU:HD23	2.36	0.45
1:B:142:PRO:HB2	1:B:146:THR:HG22	1.98	0.45
1:G:284:LEU:HD13	1:G:360:MET:CE	2.46	0.45
1:A:311:LEU:N	1:A:311:LEU:HD22	2.32	0.45
1:B:524:PHE:O	1:B:527:TYR:HB3	2.17	0.45
1:G:330:LEU:HD11	1:G:357:ILE:CG2	2.47	0.45
1:B:178:THR:CG2	1:B:568:SER:HA	2.47	0.45
1:A:505:PHE:HB3	1:A:508:LEU:CD2	2.46	0.45
1:G:151:VAL:HG11	1:G:597:LEU:CD2	2.47	0.45
1:A:291:CYS:HA	1:A:294:ILE:HG12	1.98	0.45
1:B:123:PHE:O	1:B:127:VAL:HG23	2.17	0.44
1:B:386:VAL:N	1:B:387:PRO:HD2	2.32	0.44
1:B:387:PRO:HB2	1:G:504:PHE:CD1	2.51	0.44
1:G:590:GLY:O	1:G:593:THR:N	2.50	0.44
1:A:312:LYS:O	1:A:325:MET:HG3	2.18	0.44
1:A:433:PHE:CZ	1:A:441:HIS:HD2	2.34	0.44
3:J:13:DT:C2'	3:J:14:DC:O5'	2.66	0.44
1:A:585:LYS:HZ1	1:B:580:ASN:HB3	1.79	0.44
1:B:442:MET:O	1:B:444:GLN:N	2.50	0.44
1:A:561:LEU:O	1:A:563:SER:N	2.51	0.44
1:H:314:GLU:O	1:H:315:CYS:CB	2.65	0.44
1:H:516:PRO:N	1:H:517:PRO:HD3	2.32	0.44
1:B:587:ASN:O	1:B:588:ARG:CB	2.66	0.44
1:B:168:SER:O	1:B:171:GLU:N	2.50	0.44
2:C:6:DA:H2''	2:C:7:DC:O5'	2.18	0.44
1:H:446:LYS:O	1:H:450:ILE:HG13	2.17	0.44
1:G:270:LEU:HD21	1:G:367:PHE:CD2	2.52	0.44
1:B:341:SER:C	1:B:343:ALA:H	2.20	0.44
1:A:543:TRP:HZ3	1:A:544:TRP:CD2	2.34	0.44
1:B:295:VAL:HG13	1:B:311:LEU:HB2	1.99	0.44
1:A:455:LEU:O	1:A:456:SER:C	2.56	0.44
1:G:397:SER:O	1:G:398:PRO:C	2.56	0.44
2:E:3:DA:H2'	2:E:4:DG:H5''	1.99	0.44
1:A:583:THR:CG2	1:A:584:GLU:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ILE:HG22	1:B:150:LYS:HD2	1.99	0.44
1:G:430:TYR:HD1	1:G:442:MET:CE	2.29	0.44
1:H:155:ALA:CA	1:H:600:LEU:HD21	2.47	0.44
2:C:11:DA:C2	3:D:6:DG:N2	2.86	0.44
1:A:440:LEU:O	1:A:443:GLN:NE2	2.51	0.44
1:H:282:PRO:C	1:H:284:LEU:H	2.21	0.44
1:H:609:LYS:HE2	1:H:609:LYS:HB2	1.86	0.44
1:G:601:ASN:OD1	1:G:605:LYS:HE3	2.18	0.44
1:H:585:LYS:C	1:H:587:ASN:H	2.21	0.44
2:I:4:DG:C5'	2:I:4:DG:C8	2.92	0.44
1:G:320:ASN:ND2	1:G:368:GLU:HG2	2.33	0.44
1:B:159:LYS:HG2	1:B:599:PHE:CE2	2.52	0.44
1:G:225:TYR:CD2	1:G:256:SER:O	2.70	0.44
1:A:537:ASP:O	1:A:538:PHE:C	2.56	0.44
1:G:171:GLU:C	1:G:173:ASP:H	2.21	0.44
2:E:11:DA:N3	3:F:6:DG:N2	2.66	0.44
3:J:9:DG:C2	3:J:10:DT:N3	2.86	0.44
1:H:438:PRO:HG3	1:H:532:VAL:O	2.17	0.44
1:B:171:GLU:C	1:B:173:ASP:H	2.21	0.44
1:A:515:GLU:N	1:A:516:PRO:HD3	2.33	0.44
1:A:83:LEU:HG	1:A:83:LEU:H	1.58	0.44
3:F:15:DT:H3'	3:F:16:DG:C5'	2.39	0.44
1:A:147:LEU:HD21	1:B:98:CYS:HB3	2.00	0.44
1:A:284:LEU:HD22	1:A:360:MET:CE	2.47	0.44
1:G:110:SER:OG	2:I:5:DA:H3'	2.17	0.44
1:A:333:TRP:CZ2	1:A:354:LYS:HB2	2.53	0.44
1:G:307:LEU:CD1	1:G:311:LEU:HG	2.48	0.44
1:B:178:THR:HG21	1:B:568:SER:HA	1.99	0.44
1:B:178:THR:HG23	1:B:246:VAL:HG23	1.99	0.44
1:A:527:TYR:HE1	1:A:543:TRP:CH2	2.36	0.44
1:A:121:ILE:HD13	1:A:121:ILE:HA	1.66	0.44
1:G:572:GLU:O	1:G:575:PHE:HB2	2.18	0.44
1:H:538:PHE:C	1:H:538:PHE:CD1	2.91	0.44
1:H:274:LEU:HD23	1:H:274:LEU:HA	1.60	0.44
1:H:162:ILE:O	1:H:165:GLU:N	2.51	0.43
3:L:5:DT:H2'	3:L:6:DG:C8	2.53	0.43
1:G:551:TYR:HB3	1:G:554:LEU:HB3	1.99	0.43
1:H:451:LYS:HA	1:H:524:PHE:HE2	1.82	0.43
1:A:359:THR:O	1:A:363:ILE:HG12	2.18	0.43
1:A:182:TRP:HB2	1:A:575:PHE:CE1	2.53	0.43
1:H:603:PHE:C	1:H:603:PHE:CD1	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3:DG:H2'	3:L:4:DT:H72	2.00	0.43
1:H:434:PHE:CD2	1:H:450:ILE:HG21	2.52	0.43
1:A:307:LEU:HD13	1:A:311:LEU:HD21	1.98	0.43
1:G:603:PHE:CD1	1:G:603:PHE:C	2.92	0.43
1:H:399:ASP:O	1:H:400:VAL:CB	2.67	0.43
3:L:15:DT:C2'	3:L:16:DG:H5''	2.48	0.43
1:G:323:TYR:CZ	1:G:327:ARG:HD2	2.52	0.43
1:A:247:THR:CG2	1:A:262:ARG:HD2	2.49	0.43
1:G:330:LEU:HD23	1:G:358:GLN:NE2	2.33	0.43
1:G:141:LEU:HD23	1:G:141:LEU:HA	1.67	0.43
1:B:593:THR:HG22	1:B:597:LEU:HD23	2.00	0.43
1:H:583:THR:HG22	1:H:584:GLU:H	1.82	0.43
1:H:118:ILE:O	1:H:122:LYS:HG3	2.18	0.43
1:A:298:PHE:CE2	1:A:339:ILE:HD11	2.54	0.43
1:B:335:SER:O	1:B:339:ILE:HG13	2.18	0.43
1:H:298:PHE:HE2	1:H:307:LEU:HD11	1.83	0.43
1:G:182:TRP:HD1	3:J:16:DG:OP2	2.02	0.43
1:A:118:ILE:O	1:A:121:ILE:N	2.52	0.43
1:G:299:LYS:NZ	1:G:313:SER:HB2	2.34	0.43
1:A:123:PHE:O	1:A:123:PHE:CD1	2.71	0.43
1:A:430:TYR:HD1	1:A:442:MET:HE1	1.82	0.43
1:B:247:THR:CG2	1:B:262:ARG:NH1	2.80	0.43
1:A:574:THR:O	1:A:577:LEU:HB2	2.17	0.43
1:B:603:PHE:CD1	1:B:604:TYR:CD1	3.01	0.43
1:A:371:PHE:O	1:A:375:GLN:HG3	2.19	0.43
1:G:392:VAL:HG12	1:G:393:LYS:N	2.33	0.43
1:A:607:PHE:C	1:A:608:CYS:HG	2.21	0.43
1:H:277:SER:OG	1:H:413:ILE:HA	2.19	0.43
3:J:6:DG:H2''	3:J:7:DT:H5'	2.01	0.43
1:H:130:GLU:O	1:H:131:TYR:CD1	2.72	0.43
1:B:369:ARG:HH21	1:G:500:THR:HA	1.84	0.43
1:A:260:ASN:ND2	1:A:260:ASN:N	2.66	0.43
1:H:446:LYS:HA	1:H:446:LYS:HD3	1.80	0.43
1:B:433:PHE:HZ	1:B:441:HIS:HD2	1.65	0.43
1:B:178:THR:HG23	1:B:246:VAL:CG2	2.48	0.43
1:B:159:LYS:HE3	1:B:234:GLN:OE1	2.18	0.43
2:E:11:DA:C2'	2:E:11:DA:O5'	2.67	0.43
1:B:112:VAL:HA	1:B:117:PHE:CE2	2.53	0.43
1:H:461:LEU:O	1:H:464:ILE:HG12	2.18	0.43
1:H:290:ALA:O	1:H:294:ILE:HG12	2.19	0.43
1:G:408:LYS:HE3	1:G:408:LYS:HB2	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HG12	1:A:393:LYS:N	2.33	0.42
1:A:581:ILE:HG13	1:A:589:ILE:HD13	2.01	0.42
1:A:508:LEU:HD12	1:A:508:LEU:HA	1.81	0.42
1:B:446:LYS:HD2	1:B:446:LYS:HA	1.75	0.42
1:A:325:MET:CE	1:A:326:LEU:CD2	2.97	0.42
1:A:325:MET:HE2	1:A:326:LEU:HD23	2.01	0.42
1:A:260:ASN:HD22	1:A:260:ASN:N	2.17	0.42
1:A:136:ASN:HD21	1:A:139:GLU:HB3	1.78	0.42
1:H:159:LYS:HG2	1:H:599:PHE:CZ	2.54	0.42
1:H:323:TYR:HB2	1:H:364:LEU:HB3	1.99	0.42
1:A:427:ILE:HG23	1:A:428:TRP:N	2.33	0.42
1:G:547:ASN:N	1:G:547:ASN:ND2	2.66	0.42
1:B:609:LYS:H	1:B:609:LYS:HD2	1.84	0.42
2:K:12:DA:H2''	2:K:13:DC:O5'	2.18	0.42
1:B:195:THR:HB	1:B:197:HIS:NE2	2.34	0.42
1:G:268:HIS:CE1	1:G:319:TRP:CZ2	2.99	0.42
1:A:266:SER:HA	1:A:269:LEU:HB2	1.99	0.42
1:G:168:SER:O	1:G:170:VAL:N	2.52	0.42
1:G:596:SER:O	1:G:597:LEU:C	2.56	0.42
1:A:426:SER:O	1:A:429:HIS:HB2	2.19	0.42
1:H:396:CYS:HB2	1:H:414:ILE:HD11	2.00	0.42
3:L:3:DG:C5'	3:L:3:DG:C8	2.94	0.42
3:F:7:DT:H2''	3:F:8:DT:O5'	2.19	0.42
3:J:7:DT:H2'	3:J:8:DT:H6	1.83	0.42
1:H:162:ILE:HD12	1:H:166:ILE:CD1	2.49	0.42
1:A:349:ILE:HA	1:A:352:ILE:HD12	2.01	0.42
1:A:583:THR:HG22	1:A:585:LYS:N	2.31	0.42
1:H:440:LEU:O	1:H:443:GLN:HB2	2.19	0.42
1:A:286:MET:N	1:A:287:PRO:HD2	2.34	0.42
1:A:235:PHE:O	1:A:236:ASN:HB2	2.19	0.42
1:H:593:THR:O	1:H:597:LEU:HB2	2.18	0.42
1:H:123:PHE:O	1:H:127:VAL:HG23	2.19	0.42
1:A:420:ILE:HG21	1:A:420:ILE:HD13	1.79	0.42
2:C:8:DA:C2	3:D:9:DG:N2	2.87	0.42
3:F:15:DT:C3'	3:F:16:DG:C5'	2.89	0.42
1:A:311:LEU:N	1:A:311:LEU:CD2	2.83	0.42
1:H:391:LYS:HG3	1:H:395:ILE:HD11	2.01	0.42
1:A:451:LYS:HE3	1:A:524:PHE:CD2	2.54	0.42
1:A:603:PHE:CD2	1:A:607:PHE:HD2	2.38	0.42
1:G:370:ILE:O	1:G:374:LEU:HD12	2.20	0.42
1:B:88:ALA:O	1:B:92:LYS:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:TRP:HH2	1:B:457:LYS:HE2	1.84	0.42
1:A:551:TYR:N	1:A:552:PRO:HD3	2.35	0.42
1:B:217:GLU:O	1:B:219:SER:N	2.52	0.42
1:G:382:LEU:HB2	1:G:564:ILE:O	2.19	0.42
1:B:327:ARG:HG2	1:B:327:ARG:NH1	2.34	0.42
1:A:278:PHE:HA	1:A:278:PHE:HD1	1.65	0.42
1:H:442:MET:C	1:H:444:GLN:H	2.22	0.42
1:G:585:LYS:H	1:G:585:LYS:CD	2.32	0.42
1:A:308:ARG:HG3	1:A:309:SER:N	2.33	0.42
3:L:7:DT:H2''	3:L:8:DT:O5'	2.19	0.42
2:C:10:DC:C6	2:C:10:DC:C5'	2.98	0.42
1:A:137:VAL:HG11	1:B:118:ILE:HG23	2.02	0.42
1:A:248:ASP:HB2	1:A:268:HIS:CD2	2.55	0.42
1:B:189:ARG:NH2	1:B:589:ILE:O	2.53	0.42
1:A:437:PRO:CB	1:A:438:PRO:HD3	2.49	0.42
3:J:13:DT:H2'	3:J:14:DC:C6	2.54	0.42
1:H:581:ILE:HD13	1:H:597:LEU:HB3	2.02	0.42
1:B:384:PHE:C	1:B:387:PRO:HG2	2.41	0.42
1:H:227:LYS:O	1:H:230:ALA:HB3	2.19	0.42
1:A:261:ILE:HD12	1:A:428:TRP:HZ2	1.85	0.42
1:A:325:MET:HE3	1:A:326:LEU:HD23	2.01	0.42
1:A:326:LEU:N	1:A:326:LEU:HD23	2.34	0.42
1:H:543:TRP:HZ3	1:H:544:TRP:CE2	2.38	0.42
1:A:498:ILE:HG23	1:A:498:ILE:O	2.20	0.42
1:H:551:TYR:N	1:H:552:PRO:HD3	2.35	0.42
3:L:8:DT:C2'	3:L:9:DG:H5'	2.50	0.42
1:B:531:ILE:HG22	1:B:531:ILE:O	2.20	0.42
1:G:550:LYS:O	1:G:552:PRO:HD3	2.19	0.42
1:A:603:PHE:HD1	1:A:604:TYR:CD1	2.38	0.42
1:G:103:VAL:HG23	1:G:104:ARG:N	2.33	0.42
1:G:209:LEU:HB3	1:G:235:PHE:HE2	1.85	0.42
1:B:92:LYS:HD3	1:B:92:LYS:HA	1.86	0.42
1:H:208:ILE:HD13	1:H:602:SER:HB2	2.02	0.42
1:H:584:GLU:CD	3:J:14:DC:H5'	2.40	0.41
1:G:274:LEU:HD23	1:G:274:LEU:HA	1.86	0.41
1:B:211:LEU:HD12	1:B:598:LEU:CD2	2.50	0.41
3:J:15:DT:C2'	3:J:16:DG:H5''	2.49	0.41
1:A:218:ARG:O	1:A:219:SER:CB	2.65	0.41
1:A:543:TRP:C	1:A:543:TRP:CE3	2.94	0.41
1:H:282:PRO:O	1:H:284:LEU:N	2.53	0.41
1:B:291:CYS:HB3	1:B:325:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:HIS:HA	1:A:205:ARG:O	2.20	0.41
1:B:375:GLN:O	1:B:573:ARG:NH2	2.53	0.41
1:H:127:VAL:O	1:H:131:TYR:HB2	2.20	0.41
1:B:269:LEU:O	1:B:272:ASN:HB2	2.20	0.41
1:A:121:ILE:HD12	1:B:124:PHE:HD2	1.83	0.41
1:H:298:PHE:CE2	1:H:307:LEU:HD11	2.55	0.41
3:L:11:DT:N3	3:L:12:DC:C5	2.88	0.41
1:G:406:ILE:O	1:G:409:LEU:HB3	2.21	0.41
1:A:179:ILE:HG13	1:A:179:ILE:O	2.20	0.41
1:G:519:CYS:CB	1:G:520:PRO:HD2	2.50	0.41
1:H:218:ARG:O	1:H:219:SER:CB	2.68	0.41
1:B:87:SER:C	1:B:89:ASP:N	2.72	0.41
1:H:498:ILE:HG13	1:H:498:ILE:O	2.20	0.41
1:G:162:ILE:HD12	1:G:166:ILE:HD11	2.03	0.41
1:G:421:TRP:CD1	1:G:425:LEU:HD21	2.55	0.41
1:H:269:LEU:HD12	1:H:421:TRP:CD1	2.55	0.41
1:H:295:VAL:HG11	1:H:313:SER:HA	2.02	0.41
1:A:249:ARG:HH21	1:A:272:ASN:ND2	2.18	0.41
1:H:254:VAL:HG23	1:H:255:LYS:N	2.35	0.41
1:A:124:PHE:CD2	1:B:121:ILE:HD12	2.55	0.41
3:D:9:DG:H2''	3:D:10:DT:OP1	2.20	0.41
1:B:123:PHE:C	1:B:123:PHE:CD1	2.93	0.41
1:A:586:ARG:HD2	1:B:108:PRO:HB3	2.02	0.41
1:G:144:PRO:HG3	1:H:112:VAL:HG12	2.02	0.41
1:B:571:SER:O	1:B:574:THR:HB	2.21	0.41
1:A:184:ASP:OD1	1:A:189:ARG:N	2.53	0.41
1:B:543:TRP:CZ3	1:B:544:TRP:CD2	3.08	0.41
1:G:176:SER:O	1:G:197:HIS:N	2.51	0.41
1:A:385:VAL:HG11	1:A:429:HIS:CD2	2.55	0.41
1:A:141:LEU:HA	1:A:141:LEU:HD23	1.86	0.41
1:G:190:ASN:O	1:G:213:SER:HA	2.21	0.41
2:I:6:DA:C2'	2:I:6:DA:O5'	2.66	0.41
1:G:304:GLN:NE2	1:G:311:LEU:H	2.19	0.41
1:G:176:SER:HB2	1:G:565:PRO:HD3	2.03	0.41
1:A:437:PRO:HD2	1:A:540:VAL:HG23	2.02	0.41
1:G:380:PRO:HD3	1:G:541:MET:HG3	2.02	0.41
1:B:299:LYS:HZ2	1:B:313:SER:HB3	1.85	0.41
1:G:176:SER:OG	1:G:564:ILE:HA	2.20	0.41
1:B:332:ASN:O	1:B:336:VAL:HG13	2.21	0.41
3:F:8:DT:C2'	3:F:9:DG:C5'	2.92	0.41
1:H:317:THR:O	3:L:16:DG:H8	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:ASN:O	1:B:588:ARG:HB2	2.21	0.41
1:A:330:LEU:HA	1:A:330:LEU:HD12	1.78	0.41
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.79	0.41
1:A:192:LEU:HD12	1:A:193:GLY:N	2.36	0.41
1:B:185:ASN:HA	1:B:188:LYS:HD3	2.03	0.41
2:E:2:DG:C4	2:E:3:DA:N7	2.88	0.41
1:G:268:HIS:ND1	1:G:319:TRP:HZ2	2.19	0.41
1:A:337:ILE:HG13	1:A:338:GLN:N	2.36	0.41
1:B:583:THR:CG2	1:B:584:GLU:N	2.84	0.41
1:A:247:THR:HG21	1:A:262:ARG:HD2	2.01	0.41
1:H:540:VAL:HG12	1:H:541:MET:N	2.36	0.41
1:H:247:THR:HG23	1:H:248:ASP:N	2.36	0.41
1:A:177:ALA:HA	1:A:195:THR:O	2.20	0.41
1:A:435:PHE:CD2	1:A:558:ALA:HA	2.55	0.41
1:H:409:LEU:O	1:H:412:ASN:N	2.54	0.41
1:G:268:HIS:ND1	1:G:319:TRP:CZ2	2.89	0.41
1:A:304:GLN:HE21	1:A:311:LEU:HD23	1.86	0.41
1:A:583:THR:HG22	1:A:584:GLU:N	2.36	0.41
1:A:443:GLN:O	1:A:444:GLN:C	2.57	0.41
1:G:101:TRP:NE1	1:H:117:PHE:HB2	2.36	0.41
1:G:282:PRO:O	1:G:285:ASN:HB2	2.21	0.41
1:B:161:LEU:HD23	1:B:161:LEU:C	2.40	0.41
1:B:207:LEU:HD12	1:B:602:SER:OG	2.21	0.41
1:H:191:PHE:CD1	1:H:211:LEU:HG	2.56	0.41
1:A:551:TYR:O	1:A:555:SER:HB3	2.20	0.40
1:H:330:LEU:CD2	1:H:357:ILE:HG22	2.48	0.40
1:A:126:LYS:HG3	1:B:133:GLU:OE1	2.20	0.40
1:G:162:ILE:HG21	1:G:607:PHE:HE2	1.77	0.40
1:H:515:GLU:O	1:H:516:PRO:C	2.58	0.40
1:H:151:VAL:HG11	1:H:597:LEU:CD2	2.52	0.40
1:G:431:THR:HG22	1:G:561:LEU:HD22	2.03	0.40
1:H:150:LYS:HG3	1:H:150:LYS:O	2.19	0.40
1:H:384:PHE:C	1:H:387:PRO:HD2	2.41	0.40
1:A:85:THR:HG23	1:B:139:GLU:HG2	2.03	0.40
1:H:466:ARG:HA	1:H:466:ARG:HD3	1.93	0.40
1:H:318:ARG:HA	3:L:16:DG:C8	2.56	0.40
1:B:438:PRO:HG2	1:B:534:LEU:HB2	2.03	0.40
1:H:581:ILE:HD11	1:H:594:VAL:HA	2.03	0.40
1:H:145:ILE:N	1:H:145:ILE:CD1	2.80	0.40
1:H:212:LYS:HB2	1:H:227:LYS:HD2	2.03	0.40
1:A:451:LYS:O	1:A:454:CYS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:322:THR:O	1:H:323:TYR:C	2.59	0.40
1:A:176:SER:HA	1:A:244:LYS:O	2.21	0.40
1:A:274:LEU:HA	1:A:274:LEU:HD23	1.96	0.40
3:J:9:DG:H2"	3:J:10:DT:OP1	2.20	0.40
1:G:109:PHE:C	1:G:111:ALA:H	2.23	0.40
1:G:385:VAL:HG11	1:G:429:HIS:HD2	1.86	0.40
3:D:5:DT:H2"	3:D:6:DG:O4'	2.21	0.40
1:H:270:LEU:O	1:H:273:VAL:HB	2.20	0.40
1:H:391:LYS:HD2	1:H:394:GLU:OE1	2.20	0.40
1:G:519:CYS:O	1:G:520:PRO:C	2.60	0.40
1:G:196:LEU:HB2	1:G:209:LEU:CD1	2.52	0.40
1:A:428:TRP:HE3	1:A:561:LEU:CD2	2.34	0.40
1:G:180:ASP:HB3	1:G:575:PHE:CE2	2.57	0.40
1:G:517:PRO:HB2	1:G:518:VAL:H	1.63	0.40
1:A:157:GLU:O	1:A:160:ALA:HB3	2.21	0.40
1:B:461:LEU:O	1:B:464:ILE:HG13	2.21	0.40
3:F:9:DG:H2"	3:F:10:DT:OP1	2.22	0.40
3:J:13:DT:H5'	3:J:13:DT:C6	2.56	0.40
3:L:11:DT:C2	3:L:12:DC:C5	3.10	0.40
1:A:530:GLU:OE1	1:A:551:TYR:OH	2.40	0.40
1:A:389:ILE:HG12	1:A:421:TRP:CE3	2.56	0.40
1:H:291:CYS:SG	1:H:329:ILE:HD12	2.62	0.40
1:H:178:THR:OG1	1:H:195:THR:OG1	2.36	0.40
1:H:390:LEU:HD23	1:H:390:LEU:N	2.37	0.40
1:H:392:VAL:HG11	1:H:417:VAL:CG2	2.50	0.40
1:G:194:VAL:CG2	1:G:231:ILE:HD12	2.52	0.40
1:A:345:GLU:C	1:A:347:GLN:H	2.25	0.40
1:A:578:ALA:HB2	1:A:598:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

## 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	498/536 (93%)	400 (80%)	80 (16%)	18 (4%)	4	34
1	B	501/536 (94%)	399 (80%)	83 (17%)	19 (4%)	4	32
1	G	495/536 (92%)	412 (83%)	61 (12%)	22 (4%)	3	28
1	H	505/536 (94%)	401 (79%)	75 (15%)	29 (6%)	2	20
All	All	1999/2144 (93%)	1612 (81%)	299 (15%)	88 (4%)	3	28

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ARG
1	A	219	SER
1	A	444	GLN
1	A	445	GLU
1	A	494	HIS
1	A	538	PHE
1	B	218	ARG
1	B	219	SER
1	B	342	GLU
1	B	437	PRO
1	B	444	GLN
1	B	517	PRO
1	G	302	ASN
1	G	316	PRO
1	G	437	PRO
1	G	441	HIS
1	G	445	GLU
1	G	517	PRO
1	G	520	PRO
1	G	587	ASN
1	H	202	ASN
1	H	218	ARG
1	H	219	SER
1	H	258	ALA
1	H	400	VAL
1	H	445	GLU
1	H	493	SER
1	H	496	LYS
1	H	514	ARG
1	H	516	PRO
1	H	536	GLU
1	A	133	GLU
1	A	305	HIS

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Mol	Chain	Res	Type
1	A	308	ARG
1	A	333	TRP
1	A	437	PRO
1	A	562	LEU
1	B	79	GLN
1	B	110	SER
1	B	496	LYS
1	B	513	SER
1	B	518	VAL
1	G	168	SER
1	G	169	ALA
1	G	173	ASP
1	G	251	ALA
1	G	308	ARG
1	G	400	VAL
1	H	163	GLY
1	H	302	ASN
1	H	346	THR
1	H	495	SER
1	H	586	ARG
1	H	587	ASN
1	B	314	GLU
1	B	509	THR
1	G	250	GLY
1	G	435	PHE
1	G	494	HIS
1	H	173	ASP
1	H	437	PRO
1	H	441	HIS
1	H	494	HIS
1	A	236	ASN
1	A	402	ASP
1	A	448	ALA
1	A	520	PRO
1	B	168	SER
1	B	531	ILE
1	G	218	ARG
1	H	201	ASN
1	H	301	ALA
1	H	313	SER
1	H	532	VAL
1	B	441	HIS

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Mol	Chain	Res	Type
1	B	552	PRO
1	G	110	SER
1	G	440	LEU
1	H	350	VAL
1	H	396	CYS
1	A	95	ILE
1	A	251	ALA
1	B	515	GLU
1	H	286	MET
1	B	498	ILE
1	G	187	ILE
1	G	447	VAL
1	H	315	CYS

### 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	461/494 (93%)	375 (81%)	86 (19%)	2	10
1	B	464/494 (94%)	395 (85%)	69 (15%)	4	20
1	G	458/494 (93%)	393 (86%)	65 (14%)	4	22
1	H	468/494 (95%)	412 (88%)	56 (12%)	6	29
All	All	1851/1976 (94%)	1575 (85%)	276 (15%)	4	20

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	93	GLU
1	A	120	MET
1	A	123	PHE
1	A	133	GLU
1	A	139	GLU
1	A	144	PRO
1	A	150	LYS

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Mol	Chain	Res	Type
1	A	176	SER
1	A	181	LEU
1	A	183	THR
1	A	189	ARG
1	A	201	ASN
1	A	203	GLU
1	A	205	ARG
1	A	211	LEU
1	A	212	LYS
1	A	214	LEU
1	A	218	ARG
1	A	228	LEU
1	A	229	LYS
1	A	260	ASN
1	A	267	SER
1	A	269	LEU
1	A	278	PHE
1	A	302	ASN
1	A	303	LEU
1	A	308	ARG
1	A	313	SER
1	A	314	GLU
1	A	315	CYS
1	A	321	SER
1	A	327	ARG
1	A	334	GLU
1	A	335	SER
1	A	336	VAL
1	A	338	GLN
1	A	339	ILE
1	A	350	VAL
1	A	355	SER
1	A	356	ILE
1	A	364	LEU
1	A	371	PHE
1	A	379	SER
1	A	406	ILE
1	A	414	ILE
1	A	415	LYS
1	A	427	ILE
1	A	437	PRO
1	A	440	LEU

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Mol	Chain	Res	Type
1	A	441	HIS
1	A	442	MET
1	A	443	GLN
1	A	444	GLN
1	A	446	LYS
1	A	447	VAL
1	A	455	LEU
1	A	456	SER
1	A	457	LYS
1	A	458	MET
1	A	463	LEU
1	A	465	ASN
1	A	497	ASP
1	A	498	ILE
1	A	499	SER
1	A	508	LEU
1	A	519	CYS
1	A	520	PRO
1	A	529	LYS
1	A	530	GLU
1	A	533	ILE
1	A	535	SER
1	A	540	VAL
1	A	541	MET
1	A	547	ASN
1	A	549	LYS
1	A	557	LEU
1	A	572	GLU
1	A	580	ASN
1	A	581	ILE
1	A	585	LYS
1	A	595	ASP
1	A	597	LEU
1	A	598	LEU
1	A	600	LEU
1	A	609	LYS
1	B	77	HIS
1	B	81	ARG
1	B	89	ASP
1	B	90	CYS
1	B	92	LYS
1	B	93	GLU

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Mol	Chain	Res	Type
1	B	95	ILE
1	B	102	VAL
1	B	146	THR
1	B	150	LYS
1	B	153	SER
1	B	154	ASP
1	B	173	ASP
1	B	176	SER
1	B	178	THR
1	B	179	ILE
1	B	181	LEU
1	B	183	THR
1	B	184	ASP
1	B	195	THR
1	B	198	TYR
1	B	202	ASN
1	B	203	GLU
1	B	211	LEU
1	B	218	ARG
1	B	227	LYS
1	B	228	LEU
1	B	229	LYS
1	B	233	SER
1	B	289	LEU
1	B	302	ASN
1	B	306	ARG
1	B	307	LEU
1	B	308	ARG
1	B	315	CYS
1	B	317	THR
1	B	321	SER
1	B	322	THR
1	B	324	THR
1	B	334	GLU
1	B	338	GLN
1	B	346	THR
1	B	355	SER
1	B	361	VAL
1	B	371	PHE
1	B	390	LEU
1	B	437	PRO
1	B	440	LEU

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Mol	Chain	Res	Type
1	B	446	LYS
1	B	447	VAL
1	B	455	LEU
1	B	507	GLN
1	B	513	SER
1	B	517	PRO
1	B	528	ARG
1	B	530	GLU
1	B	533	ILE
1	B	546	LEU
1	B	547	ASN
1	B	557	LEU
1	B	560	SER
1	B	580	ASN
1	B	585	LYS
1	B	587	ASN
1	B	591	GLN
1	B	597	LEU
1	B	598	LEU
1	B	600	LEU
1	B	609	LYS
1	G	89	ASP
1	G	93	GLU
1	G	97	LYS
1	G	119	ASP
1	G	120	MET
1	G	146	THR
1	G	150	LYS
1	G	152	THR
1	G	154	ASP
1	G	170	VAL
1	G	179	ILE
1	G	181	LEU
1	G	205	ARG
1	G	215	ASP
1	G	240	LEU
1	G	246	VAL
1	G	248	ASP
1	G	249	ARG
1	G	263	ILE
1	G	267	SER
1	G	268	HIS

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Mol	Chain	Res	Type
1	G	271	SER
1	G	298	PHE
1	G	303	LEU
1	G	304	GLN
1	G	305	HIS
1	G	306	ARG
1	G	312	LYS
1	G	315	CYS
1	G	316	PRO
1	G	317	THR
1	G	324	THR
1	G	326	LEU
1	G	334	GLU
1	G	351	HIS
1	G	352	ILE
1	G	358	GLN
1	G	371	PHE
1	G	374	LEU
1	G	376	THR
1	G	398	PRO
1	G	437	PRO
1	G	440	LEU
1	G	443	GLN
1	G	446	LYS
1	G	498	ILE
1	G	499	SER
1	G	518	VAL
1	G	519	CYS
1	G	520	PRO
1	G	521	SER
1	G	528	ARG
1	G	530	GLU
1	G	534	LEU
1	G	536	GLU
1	G	537	ASP
1	G	546	LEU
1	G	560	SER
1	G	561	LEU
1	G	572	GLU
1	G	585	LYS
1	G	587	ASN
1	G	591	GLN

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Mol	Chain	Res	Type
1	G	597	LEU
1	G	609	LYS
1	H	144	PRO
1	H	145	ILE
1	H	150	LYS
1	H	154	ASP
1	H	168	SER
1	H	173	ASP
1	H	178	THR
1	H	180	ASP
1	H	181	LEU
1	H	183	THR
1	H	195	THR
1	H	203	GLU
1	H	205	ARG
1	H	218	ARG
1	H	227	LYS
1	H	242	SER
1	H	247	THR
1	H	262	ARG
1	H	288	ILE
1	H	307	LEU
1	H	312	LYS
1	H	321	SER
1	H	330	LEU
1	H	334	GLU
1	H	335	SER
1	H	339	ILE
1	H	349	ILE
1	H	351	HIS
1	H	355	SER
1	H	361	VAL
1	H	362	ASN
1	H	371	PHE
1	H	381	SER
1	H	437	PRO
1	H	440	LEU
1	H	441	HIS
1	H	442	MET
1	H	444	GLN
1	H	455	LEU
1	H	467	MET

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Mol	Chain	Res	Type
1	H	490	ASP
1	H	497	ASP
1	H	499	SER
1	H	507	GLN
1	H	509	THR
1	H	510	GLN
1	H	512	ASN
1	H	516	PRO
1	H	528	ARG
1	H	557	LEU
1	H	561	LEU
1	H	574	THR
1	H	581	ILE
1	H	585	LYS
1	H	597	LEU
1	H	609	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	234	GLN
1	A	260	ASN
1	A	272	ASN
1	A	285	ASN
1	A	293	ASN
1	A	304	GLN
1	A	358	GLN
1	A	362	ASN
1	A	416	ASN
1	A	441	HIS
1	A	443	GLN
1	A	545	ASN
1	A	547	ASN
1	A	580	ASN
1	B	100	GLN
1	B	305	HIS
1	B	353	ASN
1	B	358	GLN
1	B	362	ASN
1	B	412	ASN
1	B	441	HIS

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Mol	Chain	Res	Type
1	B	449	GLN
1	B	545	ASN
1	B	547	ASN
1	B	591	GLN
1	B	601	ASN
1	G	197	HIS
1	G	272	ASN
1	G	304	GLN
1	G	353	ASN
1	G	358	GLN
1	G	362	ASN
1	G	412	ASN
1	G	416	ASN
1	G	429	HIS
1	G	441	HIS
1	G	547	ASN
1	H	234	GLN
1	H	260	ASN
1	H	293	ASN
1	H	304	GLN
1	H	358	GLN
1	H	412	ASN
1	H	449	GLN
1	H	465	ASN
1	H	512	ASN

### 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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	502/536 (93%)	-0.33	10 (1%) 68 62	16, 68, 129, 200	0
1	B	505/536 (94%)	-0.31	13 (2%) 59 54	45, 83, 137, 200	0
1	G	499/536 (93%)	-0.02	25 (5%) 32 29	63, 116, 168, 200	0
1	H	509/536 (94%)	-0.21	16 (3%) 52 48	48, 102, 159, 200	0
2	C	15/15 (100%)	0.34	1 (6%) 21 20	61, 82, 164, 170	0
2	E	15/15 (100%)	0.88	4 (26%) 1 1	66, 91, 159, 177	0
2	I	15/15 (100%)	1.11	5 (33%) 0 1	103, 127, 188, 191	0
2	K	15/15 (100%)	0.88	2 (13%) 4 4	82, 118, 185, 195	0
3	D	16/16 (100%)	0.19	1 (6%) 23 22	62, 94, 149, 162	0
3	F	16/16 (100%)	0.14	1 (6%) 23 22	64, 104, 162, 164	0
3	J	16/16 (100%)	1.06	2 (12%) 5 5	109, 141, 184, 190	0
3	L	16/16 (100%)	0.61	2 (12%) 5 5	84, 140, 178, 183	0
All	All	2139/2268 (94%)	-0.17	82 (3%) 44 39	16, 95, 161, 200	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	HIS	7.7
1	A	513	SER	7.3
1	A	515	GLU	7.2
1	A	512	ASN	6.3
1	B	493	SER	6.2
1	B	80	SER	5.3
3	J	1	DT	5.1
1	G	511	ASN	5.1
1	G	512	ASN	5.1
1	H	468	SER	5.1
1	B	79	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	H	512	ASN	4.3
1	A	511	ASN	4.2
1	A	516	PRO	4.2
1	H	469	SER	4.2
1	H	488	SER	4.1
1	B	78	MET	4.1
1	H	465	ASN	4.1
1	G	464	ILE	4.0
1	A	514	ARG	3.9
3	D	1	DT	3.9
3	L	1	DT	3.8
1	H	514	ARG	3.5
1	B	494	HIS	3.5
1	B	497	ASP	3.5
1	G	218	ARG	3.5
1	G	515	GLU	3.5
2	E	11	DA	3.4
1	A	81	ARG	3.3
2	K	15	DA	3.2
1	G	347	GLN	3.2
1	H	467	MET	3.2
2	I	13	DC	3.2
1	G	510	GLN	3.2
1	B	509	THR	3.1
3	J	2	DT	3.1
3	F	1	DT	3.0
1	G	351	HIS	3.0
1	H	466	ARG	2.9
1	G	400	VAL	2.9
1	G	300	LYS	2.9
1	H	511	ASN	2.9
1	G	514	ARG	2.9
1	H	83	LEU	2.9
1	G	176	SER	2.9
1	G	83	LEU	2.9
2	E	15	DA	2.8
2	I	11	DA	2.8
1	H	218	ARG	2.8
2	I	10	DC	2.8
1	A	176	SER	2.7
2	K	14	DA	2.7
1	G	609	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	15	DA	2.6
1	H	176	SER	2.6
1	G	217	GLU	2.5
2	E	10	DC	2.5
1	B	511	ASN	2.5
2	I	12	DA	2.5
1	G	338	GLN	2.4
1	A	493	SER	2.4
2	C	15	DA	2.4
1	B	609	LYS	2.3
1	G	381	SER	2.3
1	G	202	ASN	2.3
1	H	609	LYS	2.3
1	A	609	LYS	2.3
1	G	513	SER	2.3
1	G	462	GLU	2.3
1	G	463	LEU	2.2
1	H	492	THR	2.2
3	L	2	DT	2.2
1	G	335	SER	2.2
1	G	337	ILE	2.1
1	H	464	ILE	2.1
1	H	491	LEU	2.1
1	G	297	TYR	2.1
1	B	176	SER	2.1
1	B	495	SER	2.1
1	G	178	THR	2.0
1	B	496	LYS	2.0
2	E	13	DC	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NA	B	1610	1/1	0.87	0.24	2.48	57,57,57,57	0
4	NA	G	1610	1/1	0.80	0.19	-0.36	77,77,77,77	0
4	NA	H	1610	1/1	0.98	0.16	-0.95	58,58,58,58	0
4	NA	A	1610	1/1	0.87	0.14	-1.00	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.