



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:20 PM UTC

PDB ID : 2DY4 / pdb_00002dy4
Title : Crystal structure of RB69 GP43 in complex with DNA containing Thymine Glycol
Authors : Aller, P.; Rould, M.A.; Hogg, M.; Wallace, S.S.; Doublie, S.
Deposited on : 2006-09-06
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

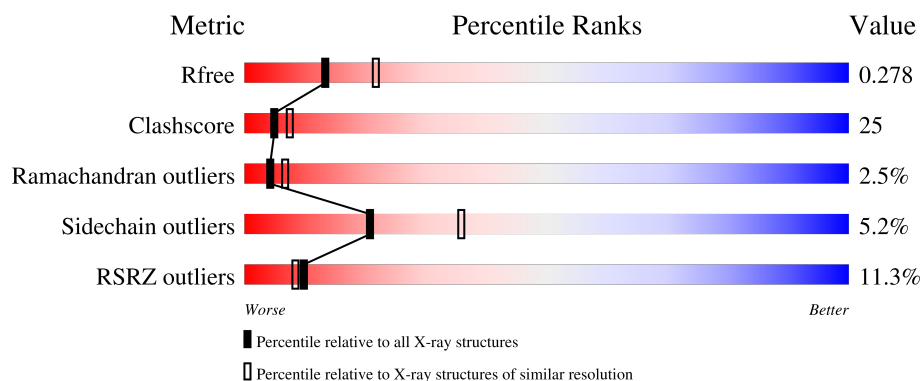
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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

Mol	Chain	Length	Quality of chain
1	E	18	28% 33% 61% 6%
1	G	18	22% 28% 50%
1	I	18	6% 33% 61%
1	K	18	28% 17% 83%
2	F	15	40% 7% 7% 80% 7%

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Mol	Chain	Length	Quality of chain
2	H	15	13% 47% 40%
2	J	15	40% 60%
2	L	15	40% 20% 80%
3	A	903	7% 57% 38%
3	B	903	5% 61% 32% 5%
3	C	903	4% 63% 33%
3	D	903	26% 45% 45% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31943 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	17	Total	C	N	O	P	0	0	0
			348	165	69	99	15			
1	G	18	Total	C	N	O	P	0	0	0
			372	175	74	106	17			
1	I	18	Total	C	N	O	P	0	0	0
			372	175	74	106	17			
1	K	18	Total	C	N	O	P	0	0	0
			372	175	74	106	17			

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	14	Total	C	N	O	P	0	0	0
			276	133	51	80	12			
2	H	15	Total	C	N	O	P	0	0	0
			299	143	53	89	14			
2	J	15	Total	C	N	O	P	0	0	0
			299	143	53	89	14			
2	L	15	Total	C	N	O	P	0	0	0
			299	143	53	89	14			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	902	Total	C	N	O	S	Se	0	0	0
			7302	4689	1213	1367	8	25			
3	B	888	Total	C	N	O	S	Se	0	0	0
			7175	4608	1193	1341	8	25			
3	C	900	Total	C	N	O	S	Se	0	0	0
			7300	4683	1214	1370	8	25			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	890	Total	C	N	O	S	Se	0	0	0
			6923	4449	1130	1313	8	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087

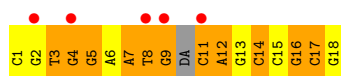
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	9	Total	O	0	0
			9	9		
4	F	5	Total	O	0	0
			5	5		
4	G	18	Total	O	0	0
			18	18		
4	H	9	Total	O	0	0
			9	9		
4	I	17	Total	O	0	0
			17	17		
4	J	4	Total	O	0	0
			4	4		
4	K	5	Total	O	0	0
			5	5		
4	L	2	Total	O	0	0
			2	2		
4	A	117	Total	O	0	0
			117	117		
4	B	205	Total	O	0	0
			205	205		
4	C	160	Total	O	0	0
			160	160		
4	D	55	Total	O	0	0
			55	55		

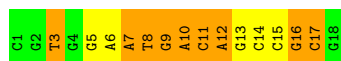
3 Residue-property plots [i](#)

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

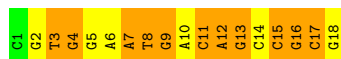
- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



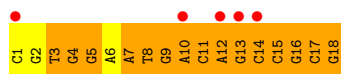
- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



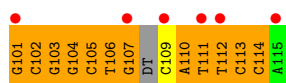
- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



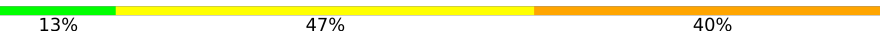
- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'



- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'

Chain H: 

G101	G102	G103	G104	G105	T106	G107	T108	C109	A110	T111	T112	C113	C114	A115
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- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'

Chain J: 

G101	C102	G103	G104	C105	T106	G107	T108	C109	A110	T111	T112	C113	C114	A115
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- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'

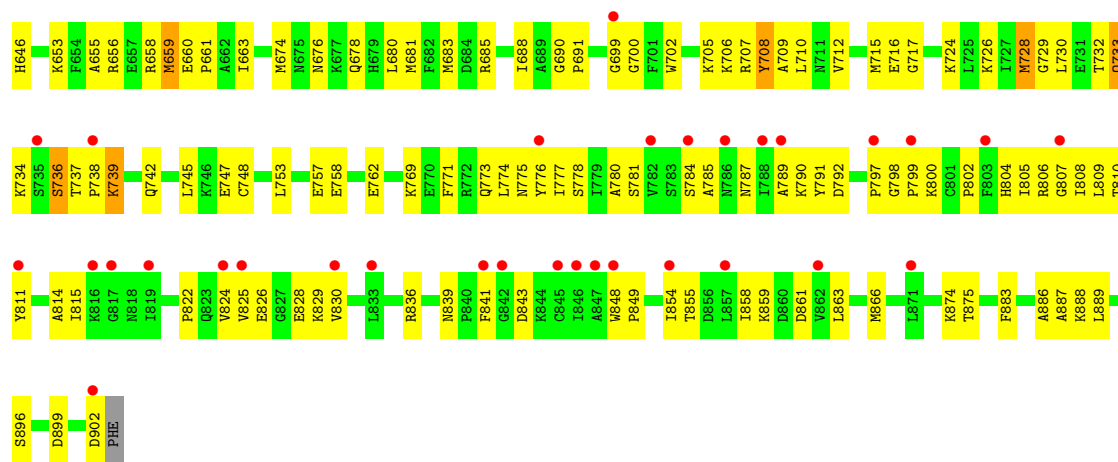
Chain L: 

G101	C102	G103	G104	C105	T106	G107	T108	C109	A110	T111	T112	C113	C114	A115
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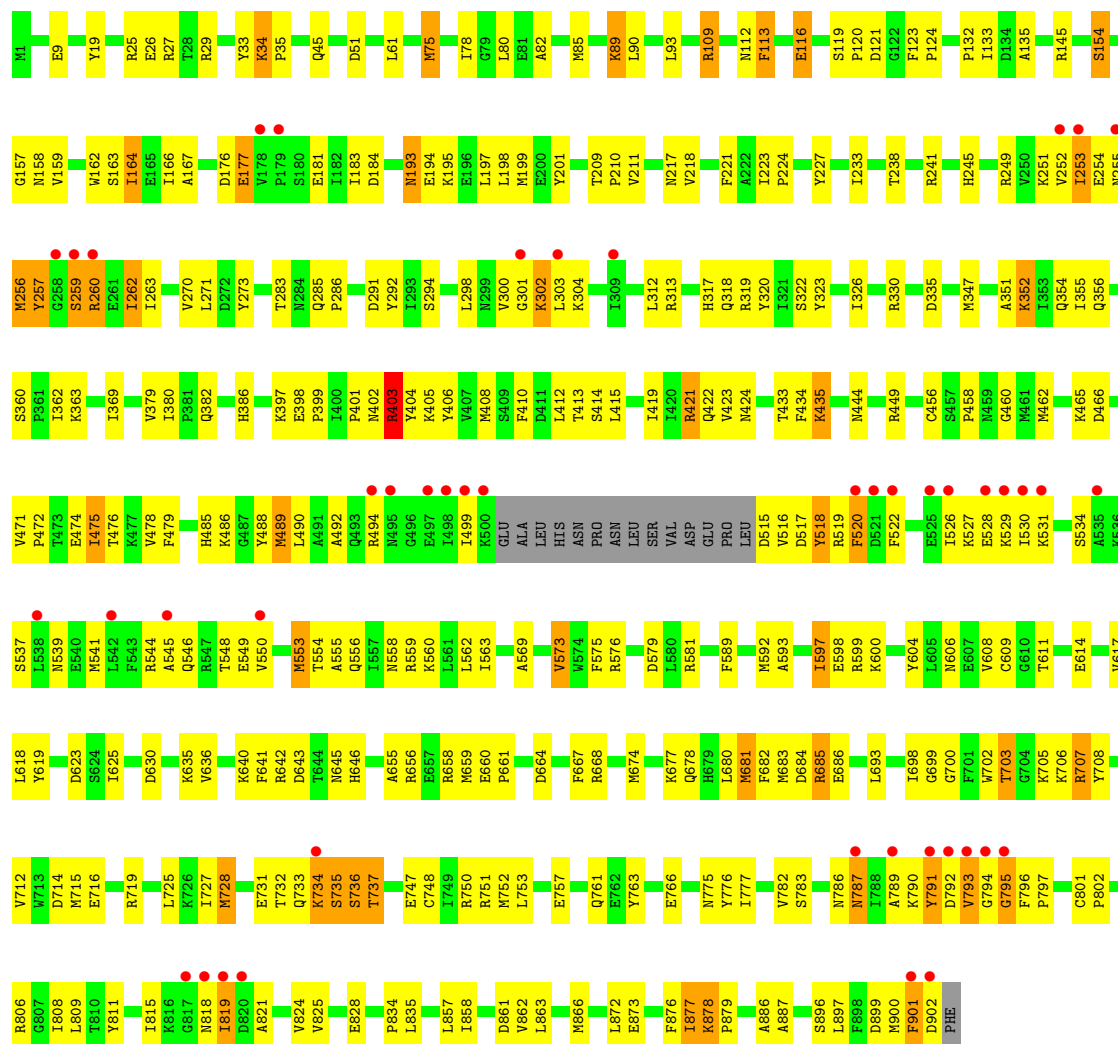
- Molecule 3: DNA polymerase

Chain A: 

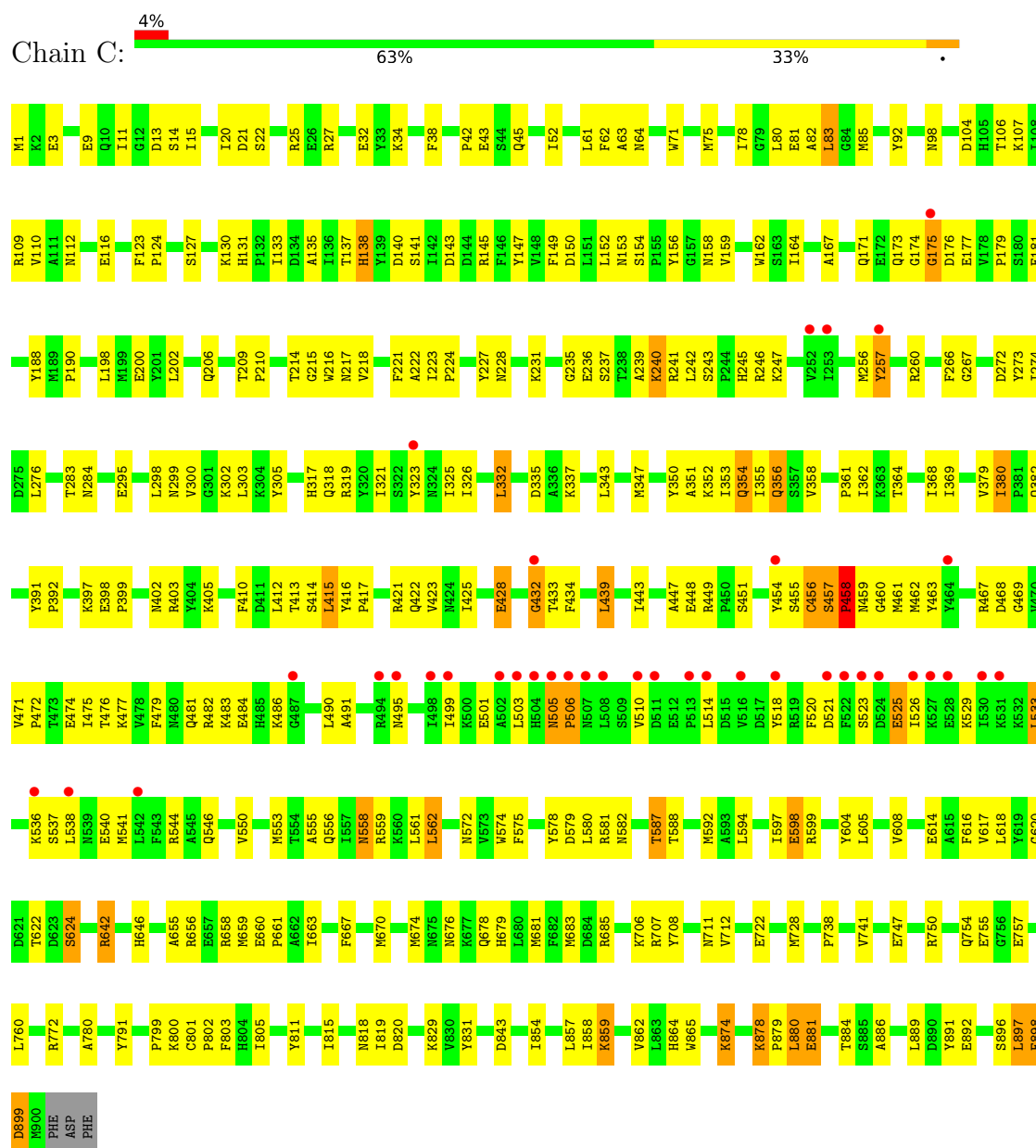
K1	K2	E3	L6	Q10	T11	G12	D13	S14	I15	F16	E17	R18	D21	S22	N23	G24	R25	E26	T28	R27	R29	E32	S36	L37	C41	A46	D51	K55	P56	C57	T58	N64	M65	R66	D67	W71	I72	K73	R74	E76	E81	A82	L83	G84	M85	D86								
L90	E100	I101	K102	Y103	D104	H105	T106	M112	F113	E116	P120	A121	E125	P126	A129	K130	H131	P132	I133	A135	D150	S154	P155	Y156	G157	M158	V159	S163	L170	Q171	D176	E177	V178	E181	Y188	M193	E194	K196	A196	L197	L198	M199												
L202	N203	F204	W205	G206	Q207	K208	V211	I212	L213	V216	N217	V218	F221	A222	I223	P224	Y225	R229	I230	K231	F234	G235	E236	K240	R241	L242	H245	K251	V252	I253	E254	G258	S259	I262	S269	Y273	L276	N284	S287	D291	Y292	S294												
L298	N299	V300	P302	G303	K302	L303	K304	P308	K311	H317	Q318	R319	I326	R330	V331	L332	D335	A336	K337	R338	F340	D346	K347	G348	Y349	I353	S357	V358	F359	S360	P361	I362	D366	A367	L373	Q376	R377	K378	V379	F379	N480	P381	Q382	H386	P387	V388								
Q389	P390	Y391	L490	R392	G393	A394	F395	V396	K397	P399	I400	N401	N402	R403	Y404	K405	Y406	V407	M408	L508	F410	D411	L412	T413	S414	L415	I419	Q422	V423	P438	L439	I443	S455	C456	S457	P458	D466	R467	D468	V471	P472	T476	K477	V478	F479	N480	Q481	R482	K483	E484	H485			
K486	M489	L490	A491	A492	Q493	R494	N495	I498	I499	F500	E501	A502	L503	H504	N505	P506	N507	S509	V510	D511	F512	P513	L514	D515	V516	E517	Y518	R519	F520	D521	F522	S523	I526	K527	E528	K529	I530	K531	K532	L533	S534	A535	K536	S537	L538	N539	E540	M541	T548	G552	M553	F641	R642	A555
G556	I557	N558	R559	K560	L561	I562	I563	L570	G571	N572	Y573	Y578	I586	T587	H592	A593	L594	Q595	V596	I597	N602	N606	E607	V608	T611	E612	G613	E614	A615	F616	V617	L618	V619	G620	D621	T622	I625	A629	D630	K631	I632	L633	D634	K635	V636	K640	F641	R642						



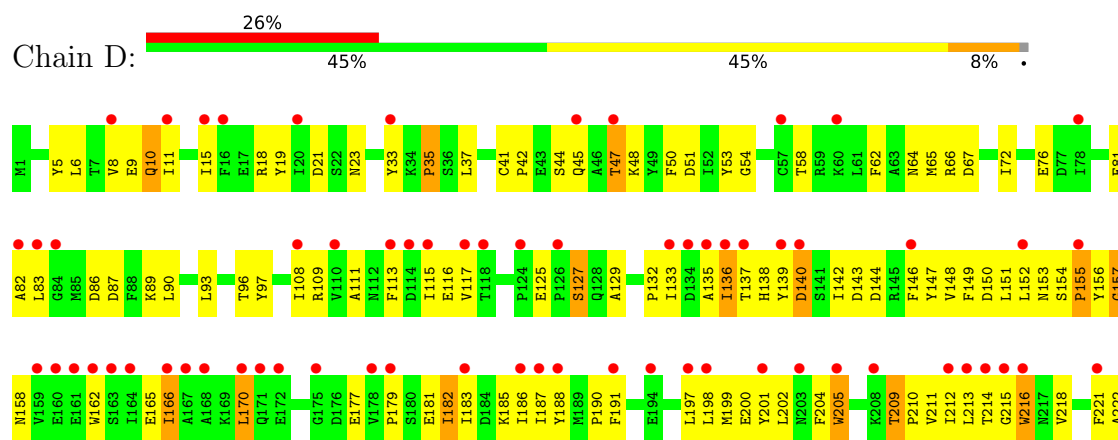
• Molecule 3: DNA polymerase

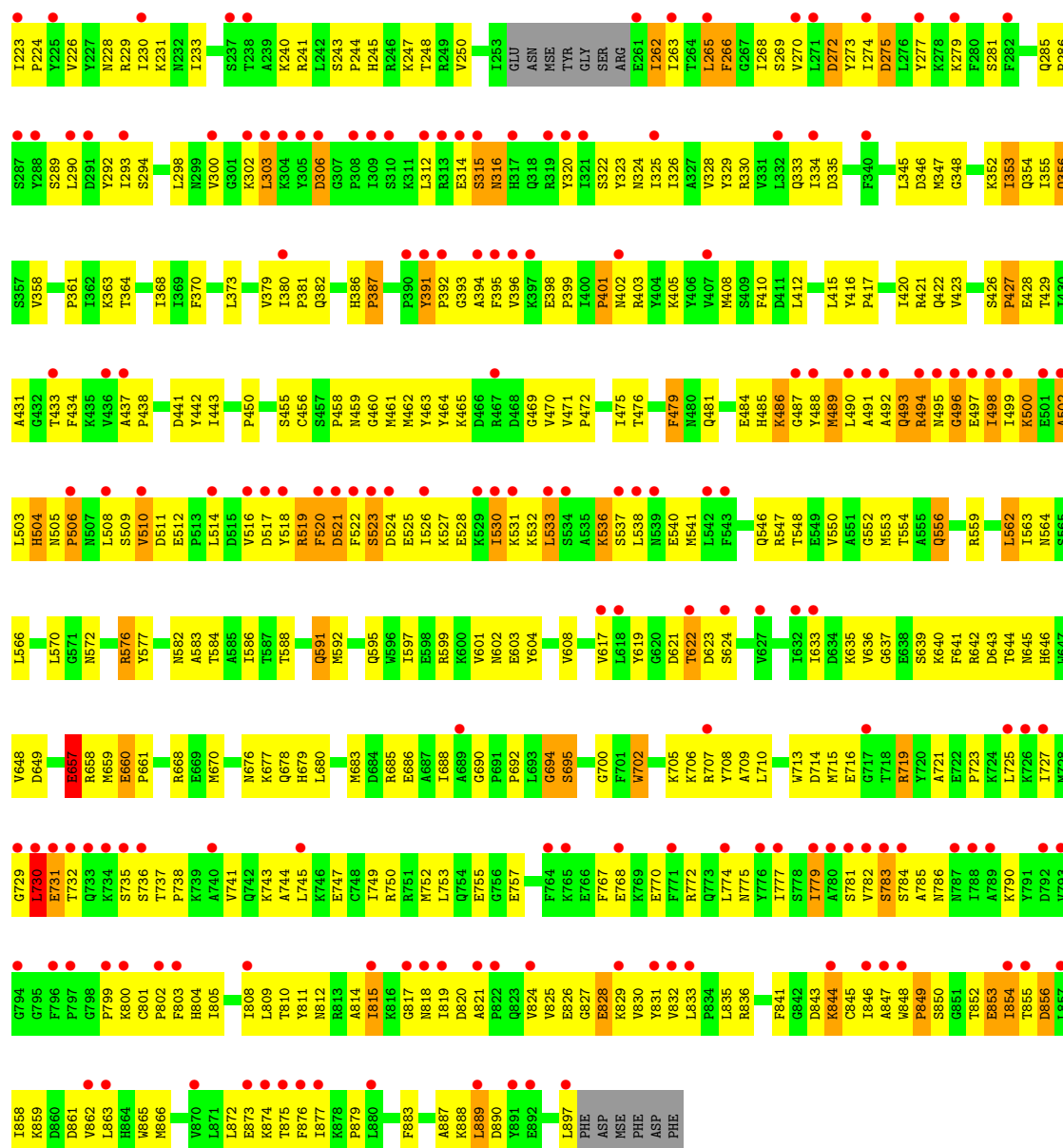


• Molecule 3: DNA polymerase



• Molecule 3: DNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.61Å 122.63Å 168.69Å 90.00° 96.31° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	88.3 (50.00-2.65) 92.1 (50.00-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.281 0.226 , 0.278	Depositor DCC
R_{free} test set	28873 reflections (9.49%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31943	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	E	0.23	0/365	1.46	13/558 (2.3%)
1	G	0.29	0/393	1.37	9/603 (1.5%)
1	I	0.35	0/393	1.38	14/603 (2.3%)
1	K	0.41	0/393	1.43	16/603 (2.7%)
2	F	0.25	0/307	1.40	12/468 (2.6%)
2	H	0.32	0/333	1.38	7/510 (1.4%)
2	J	0.33	0/333	1.39	12/510 (2.4%)
2	L	0.44	0/333	1.47	15/510 (2.9%)
3	A	0.46	0/7457	0.92	21/10050 (0.2%)
3	B	0.49	0/7326	0.94	18/9873 (0.2%)
3	C	0.48	0/7454	0.92	15/10045 (0.1%)
3	D	0.35	0/7072	0.86	18/9590 (0.2%)
All	All	0.44	0/32159	0.97	170/43923 (0.4%)

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	G	1	0
2	H	0	1
All	All	1	1

There are no bond length outliers.

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	211	VAL	N-CA-C	-13.19	99.08	111.48
1	G	12	DA	C2'-C3'-O3'	10.62	127.44	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	211	VAL	N-CA-C	-9.77	102.39	111.67
3	B	255	ASN	N-CA-C	-9.05	95.47	108.96
1	G	12	DA	C4'-C3'-O3'	9.00	123.50	110.00
1	E	1	DC	C2'-C3'-O3'	8.78	124.68	111.50
1	E	8	DT	C2'-C3'-O3'	8.61	124.42	111.50
1	E	7	DA	C2'-C3'-O3'	8.46	124.20	111.50
1	K	12	DA	C2'-C3'-O3'	8.30	123.95	111.50
2	F	106	DT	C2'-C3'-O3'	8.15	123.72	111.50
3	D	493	GLN	N-CA-C	-7.77	103.53	113.16
2	L	110	DA	C2'-C3'-O3'	7.40	122.59	111.50
3	A	456	CYS	N-CA-C	7.29	120.96	109.81
2	J	111	DT	C2'-C3'-O3'	7.25	122.38	111.50
1	E	14	DC	C2'-C3'-O3'	7.23	122.35	111.50
2	L	104	DG	C2'-C3'-O3'	7.18	122.27	111.50
2	L	110	DA	C4'-C3'-O3'	7.16	120.74	110.00
1	G	10	DA	C2'-C3'-O3'	7.11	122.16	111.50
1	I	11	DC	C2'-C3'-O3'	7.00	121.99	111.50
2	J	108	DT	C2'-C3'-O3'	6.96	121.95	111.50
3	C	403	ARG	N-CA-C	-6.85	100.38	110.52
2	F	102	DC	C2'-C3'-O3'	6.81	121.71	111.50
1	E	5	DG	C2'-C3'-O3'	6.79	121.69	111.50
1	E	14	DC	C4'-C3'-O3'	6.79	120.19	110.00
3	A	18	ARG	N-CA-C	-6.74	98.74	109.59
3	C	831	TYR	N-CA-C	-6.70	100.56	110.48
3	C	598	GLU	N-CA-C	-6.68	103.69	110.97
2	J	113	DC	C2'-C3'-O3'	6.66	121.50	111.50
3	C	457	SER	CA-C-N	6.65	128.15	119.84
3	C	457	SER	C-N-CA	6.65	128.15	119.84
1	K	10	DA	C2'-C3'-O3'	6.54	121.31	111.50
3	A	486	LYS	N-CA-C	-6.53	104.20	111.71
1	K	8	DT	C2'-C3'-O3'	6.51	121.27	111.50
3	C	712	VAL	N-CA-C	6.50	117.47	108.89
2	H	113	DC	C4'-C3'-O3'	6.49	119.74	110.00
1	K	18	DG	C2'-C3'-O3'	-6.45	101.83	111.50
1	K	10	DA	C4'-C3'-O3'	6.43	119.64	110.00
1	I	15	DC	C2'-C3'-O3'	6.41	121.11	111.50
3	D	139	TYR	N-CA-C	6.40	118.05	111.14
3	D	496	GLY	N-CA-C	-6.36	106.47	114.16
2	L	103	DG	C2'-C3'-O3'	6.34	121.01	111.50
1	K	17	DC	C2'-C3'-O3'	6.28	120.92	111.50
3	B	456	CYS	N-CA-C	6.25	119.73	109.85
2	L	109	DC	C2'-C3'-O3'	6.24	120.86	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	17	DC	C2'-C3'-O3'	6.22	120.83	111.50
2	L	106	DT	C2'-C3'-O3'	6.20	120.80	111.50
2	L	108	DT	C2'-C3'-O3'	6.20	120.79	111.50
1	G	11	DC	C2'-C3'-O3'	6.18	120.77	111.50
2	J	107	DG	C2'-C3'-O3'	6.16	120.73	111.50
2	F	105	DC	C2'-C3'-O3'	6.13	120.69	111.50
3	D	540	GLU	N-CA-C	-6.12	105.77	113.18
1	I	13	DG	C4'-C3'-O3'	6.11	119.17	110.00
2	L	101	DG	C2'-C3'-O3'	6.10	120.65	111.50
2	J	113	DC	C4'-C3'-O3'	6.08	119.12	110.00
2	H	114	DC	C2'-C3'-O3'	6.03	120.55	111.50
1	K	13	DG	C2'-C3'-O3'	6.03	120.55	111.50
1	I	13	DG	C2'-C3'-O3'	6.00	120.50	111.50
1	I	12	DA	C2'-C3'-O3'	5.98	120.48	111.50
2	F	111	DT	C2'-C3'-O3'	5.97	120.45	111.50
3	A	178	VAL	CA-C-N	5.97	127.30	119.84
3	A	178	VAL	C-N-CA	5.97	127.30	119.84
1	I	9	DG	N9-C1'-C2'	5.96	122.44	113.50
2	H	104	DG	C2'-C3'-O3'	5.96	120.44	111.50
2	L	114	DC	C2'-C3'-O3'	5.93	120.39	111.50
1	K	11	DC	C2'-C3'-O3'	5.91	120.36	111.50
1	E	17	DC	C2'-C3'-O3'	5.91	120.36	111.50
3	D	302	LYS	N-CA-C	5.88	118.73	109.96
3	D	500	LYS	N-CA-C	-5.86	105.03	111.82
2	L	106	DT	C4'-C3'-O3'	5.85	118.77	110.00
2	F	112	DT	C2'-C3'-O3'	5.85	120.27	111.50
1	K	7	DA	C2'-C3'-O3'	5.84	120.26	111.50
2	J	111	DT	C5'-C4'-C3'	-5.84	106.14	114.90
3	D	275	ASP	N-CA-C	-5.83	105.01	111.36
1	K	5	DG	C2'-C3'-O3'	5.82	120.22	111.50
2	L	107	DG	C2'-C3'-O3'	5.81	120.21	111.50
2	F	113	DC	C2'-C3'-O3'	5.80	120.20	111.50
3	C	405	LYS	N-CA-C	5.80	117.29	110.97
3	D	721	ALA	N-CA-C	-5.78	104.88	111.07
2	J	110	DA	C2'-C3'-O3'	5.78	120.17	111.50
3	B	254	GLU	CA-C-N	5.77	131.33	121.87
3	B	254	GLU	C-N-CA	5.77	131.33	121.87
2	F	101	DG	C2'-C3'-O3'	5.75	120.13	111.50
2	J	106	DT	C2'-C3'-O3'	5.74	120.11	111.50
3	B	703	THR	N-CA-C	-5.71	106.86	113.88
2	L	112	DT	C2'-C3'-O3'	5.71	120.06	111.50
3	A	204	PHE	N-CA-C	-5.71	104.97	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	9	DG	C2'-C3'-O3'	5.69	120.03	111.50
3	D	502	ALA	N-CA-C	-5.69	106.18	113.23
3	A	708	TYR	N-CA-C	5.66	115.32	107.73
3	B	403	ARG	N-CA-C	-5.65	101.34	110.32
3	D	547	ARG	N-CA-C	-5.65	105.50	112.90
2	H	105	DC	C4'-C3'-O3'	5.63	118.44	110.00
2	F	114	DC	C2'-C3'-O3'	5.61	119.92	111.50
3	B	201	TYR	N-CA-C	-5.61	105.17	111.28
3	C	398	GLU	CA-C-N	5.58	125.49	119.85
3	C	398	GLU	C-N-CA	5.58	125.49	119.85
2	H	110	DA	C2'-C3'-O3'	5.57	119.86	111.50
3	D	504	HIS	N-CA-C	-5.55	106.46	113.18
1	K	16	DG	C2'-C3'-O3'	5.54	119.81	111.50
3	C	380	ILE	CA-C-N	5.54	125.48	119.78
3	C	380	ILE	C-N-CA	5.54	125.48	119.78
1	K	14	DC	C2'-C3'-O3'	5.52	119.78	111.50
1	K	4	DG	C2'-C3'-O3'	5.52	119.77	111.50
3	D	494	ARG	N-CA-C	-5.52	104.80	113.02
3	B	253	ILE	N-CA-C	5.51	120.81	109.34
3	B	113	PHE	N-CA-C	5.51	117.79	109.41
2	F	104	DG	C2'-C3'-O3'	5.51	119.76	111.50
3	C	354	GLN	N-CA-C	-5.50	102.74	110.50
1	G	7	DA	C2'-C3'-O3'	5.50	119.75	111.50
2	J	104	DG	C2'-C3'-O3'	5.49	119.74	111.50
1	I	8	DT	C2'-C3'-O3'	5.48	119.72	111.50
3	A	728	MSE	N-CA-C	5.48	117.34	108.41
3	B	360	SER	N-CA-C	5.47	119.55	109.10
3	A	366	ASP	N-CA-C	-5.47	105.32	111.28
3	C	624	SER	N-CA-C	5.46	118.12	109.50
2	L	105	DC	C2'-C3'-O3'	5.45	119.68	111.50
3	A	336	ALA	N-CA-C	-5.44	105.45	111.71
3	A	380	ILE	CA-C-N	5.44	125.74	119.92
3	A	380	ILE	C-N-CA	5.44	125.74	119.92
1	E	4	DG	C2'-C3'-O3'	5.43	119.64	111.50
1	K	7	DA	C4'-C3'-O3'	5.41	118.11	110.00
2	J	105	DC	C2'-C3'-O3'	5.41	119.61	111.50
1	K	9	DG	C2'-C3'-O3'	5.41	119.61	111.50
3	B	553	MSE	N-CA-C	-5.38	104.76	112.13
1	G	16	DG	C2'-C3'-O3'	5.37	119.55	111.50
1	E	11	DC	C2'-C3'-O3'	5.36	119.54	111.50
2	L	102	DC	C2'-C3'-O3'	5.36	119.54	111.50
1	G	8	DT	C2'-C3'-O3'	5.36	119.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	712	VAL	N-CA-C	5.35	116.29	108.58
1	I	7	DA	C4'-C3'-O3'	5.33	117.99	110.00
1	I	17	DC	C2'-C3'-O3'	5.32	119.48	111.50
3	B	233	ILE	N-CA-C	5.28	115.50	110.53
1	I	4	DG	C5'-C4'-C3'	-5.28	106.98	114.90
2	L	111	DT	C2'-C3'-O3'	5.28	119.42	111.50
1	G	9	DG	C2'-C3'-O3'	5.27	119.41	111.50
2	F	107	DG	C2'-C3'-O3'	5.27	119.41	111.50
1	I	16	DG	C2'-C3'-O3'	5.25	119.38	111.50
2	J	108	DT	C4'-C3'-O3'	5.25	117.88	110.00
3	D	19	TYR	N-CA-C	5.24	115.46	108.38
1	E	12	DA	C2'-C3'-O3'	5.24	119.36	111.50
1	I	7	DA	C2'-C3'-O3'	5.24	119.36	111.50
3	A	133	ILE	N-CA-C	-5.23	100.23	108.23
3	A	596	TRP	N-CA-C	-5.23	105.49	111.14
3	D	694	GLY	N-CA-C	-5.23	106.86	111.67
2	H	113	DC	C2'-C3'-O3'	5.21	119.32	111.50
3	B	354	GLN	N-CA-C	-5.19	102.60	110.28
1	I	4	DG	C2'-C3'-O3'	5.18	119.27	111.50
3	A	276	LEU	N-CA-C	-5.18	105.53	111.07
3	D	657	GLU	N-CA-C	5.18	119.60	113.12
2	F	103	DG	C2'-C3'-O3'	5.17	119.25	111.50
3	A	55	LYS	CA-C-N	5.17	124.93	119.76
3	A	55	LYS	C-N-CA	5.17	124.93	119.76
1	E	1	DC	C4'-C3'-O3'	5.16	117.74	110.00
1	E	16	DG	C2'-C3'-O3'	5.16	119.24	111.50
3	B	735	SER	N-CA-C	5.15	116.35	108.42
1	K	15	DC	C2'-C3'-O3'	5.15	119.22	111.50
3	A	748	CYS	N-CA-C	-5.14	105.58	111.14
2	H	106	DT	C2'-C3'-O3'	5.14	119.21	111.50
3	A	586	ILE	CB-CA-C	-5.13	105.40	111.81
3	C	505	ASN	CA-C-N	5.11	126.23	119.84
3	C	505	ASN	C-N-CA	5.11	126.23	119.84
1	I	18	DG	C2'-C3'-O3'	-5.10	103.85	111.50
3	B	449	ARG	CA-C-N	5.10	124.54	119.24
3	B	449	ARG	C-N-CA	5.10	124.54	119.24
2	F	110	DA	C2'-C3'-O3'	5.09	119.13	111.50
3	A	608	VAL	N-CA-C	-5.08	108.88	113.71
3	D	486	LYS	N-CA-C	-5.06	106.94	113.01
3	D	548	THR	N-CA-C	-5.03	107.14	113.28
2	J	103	DG	C2'-C3'-O3'	5.03	119.04	111.50
3	D	526	ILE	N-CA-C	-5.00	107.98	113.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	12	DA	C3'

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	115	DA	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	E	348	0	195	40	0
1	G	372	0	204	26	0
1	I	372	0	204	39	0
1	K	372	0	204	38	0
2	F	276	0	155	22	0
2	H	299	0	165	23	0
2	J	299	0	165	28	0
2	L	299	0	165	26	0
3	A	7302	0	7141	316	0
3	B	7175	0	6995	318	0
3	C	7300	0	7144	260	0
3	D	6923	0	6512	433	0
4	A	117	0	0	28	0
4	B	205	0	0	19	0
4	C	160	0	0	14	0
4	D	55	0	0	27	0
4	E	9	0	0	2	0
4	F	5	0	0	1	0
4	G	18	0	0	0	0
4	H	9	0	0	2	0
4	I	17	0	0	3	0
4	J	4	0	0	0	0
4	K	5	0	0	1	0
4	L	2	0	0	0	0
All	All	31943	0	29249	1529	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 25.

All (1529) 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:I:14:DC:H2''	1:I:15:DC:H5''	1.21	1.17
2:J:111:DT:H2''	2:J:112:DT:H5'	1.16	1.13
3:B:164:ILE:HD12	3:B:164:ILE:H	1.13	1.09
2:L:104:DG:H2''	2:L:105:DC:H5''	1.32	1.07
1:G:11:DC:H2''	1:G:12:DA:H5''	1.34	1.05
3:B:347:MSE:HE1	3:B:562:LEU:HD11	1.43	1.00
3:B:556:GLN:HB3	4:B:990:HOH:O	1.61	0.99
3:D:212:ILE:HD11	3:D:345:LEU:HD21	1.45	0.98
1:I:15:DC:H2''	1:I:16:DG:H5'	1.45	0.97
3:D:619:TYR:HE1	3:D:621:ASP:HB2	1.30	0.96
3:B:82:ALA:H	3:B:382:GLN:HE21	1.06	0.96
2:J:111:DT:H2''	2:J:112:DT:C5'	1.95	0.95
3:C:112:ASN:HB3	3:C:214:THR:HG23	1.49	0.95
1:I:17:DC:H1'	4:I:435:HOH:O	1.67	0.94
3:C:897:LEU:HD23	3:C:897:LEU:H	1.31	0.94
3:D:218:VAL:HG12	3:D:223:ILE:HG13	1.48	0.93
3:D:356:GLN:H	3:D:356:GLN:HE21	0.94	0.93
3:A:863:LEU:HA	3:A:866:MSE:HE3	1.48	0.93
3:D:214:THR:HG22	3:D:215:GLY:H	1.30	0.93
3:D:356:GLN:H	3:D:356:GLN:NE2	1.66	0.92
3:B:736:SER:HA	4:B:910:HOH:O	1.68	0.92
3:B:793:VAL:HB	3:B:796:PHE:HB2	1.49	0.91
3:A:642:ARG:H	3:A:646:HIS:HD2	1.20	0.90
3:D:686:GLU:HB3	3:D:715:MSE:HE1	1.54	0.89
3:B:405:LYS:HA	3:B:699:GLY:HA3	1.55	0.89
1:I:10:DA:H2''	1:I:11:DC:H5'	1.55	0.89
3:B:530:ILE:HG13	3:B:531:LYS:H	1.38	0.89
3:B:732:THR:HG23	3:B:733:GLN:HE21	1.38	0.88
1:G:11:DC:C2'	1:G:12:DA:H5''	2.04	0.87
3:D:356:GLN:HE21	3:D:356:GLN:N	1.71	0.87
3:C:112:ASN:HD21	3:C:332:LEU:HD11	1.37	0.86
3:D:619:TYR:CE1	3:D:621:ASP:HB2	2.09	0.86
3:D:844:LYS:H	3:D:844:LYS:HD3	1.38	0.86
3:C:572:ASN:ND2	3:C:574:TRP:H	1.73	0.86
3:D:854:ILE:HD11	3:D:858:ILE:HD11	1.56	0.86
2:L:112:DT:H2''	2:L:113:DC:H5''	1.55	0.86
2:L:112:DT:C2'	2:L:113:DC:H5''	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:597:ILE:O	3:D:601:VAL:HG23	1.73	0.86
3:D:873:GLU:HA	3:D:877:ILE:HG12	1.57	0.85
3:A:495:ASN:HD21	3:A:521:ASP:HA	1.41	0.85
3:C:553:MSE:HA	4:C:1026:HOH:O	1.75	0.85
1:I:9:DG:H2''	1:I:10:DA:H5''	1.59	0.85
3:B:253:ILE:HD11	3:B:260:ARG:CZ	2.07	0.84
3:A:655:ALA:HA	3:A:659:MSE:HG3	1.60	0.84
1:E:6:DA:H2''	1:E:7:DA:C8	2.12	0.84
3:B:863:LEU:HA	3:B:866:MSE:HE3	1.60	0.84
3:D:489:MSE:HE3	3:D:490:LEU:HB2	1.57	0.84
1:G:7:DA:H2''	1:G:8:DT:H5'	1.58	0.84
3:D:6:LEU:HD22	3:D:211:VAL:HG11	1.60	0.83
3:A:90:LEU:HD22	3:A:353:ILE:HG22	1.59	0.83
2:J:104:DG:H2'	2:J:105:DC:C6	2.12	0.83
1:K:5:DG:H2''	1:K:6:DA:H5'	1.59	0.83
3:A:728:MSE:HG3	4:A:986:HOH:O	1.77	0.83
3:D:154:SER:HB3	3:D:155:PRO:HD2	1.60	0.83
3:D:137:THR:HB	3:D:328:VAL:HG21	1.58	0.83
1:I:14:DC:C2'	1:I:15:DC:H5''	2.07	0.83
2:L:105:DC:H2'	2:L:106:DT:H72	1.59	0.83
3:B:386:HIS:HB2	3:B:573:VAL:HG22	1.60	0.83
3:B:157:GLY:C	3:B:158:ASN:HD22	1.87	0.83
3:C:660:GLU:HB2	3:C:661:PRO:HD3	1.60	0.83
3:D:412:LEU:HD12	3:D:623:ASP:HA	1.61	0.82
3:A:486:LYS:HE3	3:A:556:GLN:HG2	1.62	0.82
2:L:104:DG:H2''	2:L:105:DC:C5'	2.08	0.82
3:B:75:MSE:HE3	3:B:75:MSE:HA	1.61	0.82
1:K:8:DT:H2''	1:K:9:DG:H5'	1.62	0.81
3:A:499:ILE:HD13	3:A:541:MSE:HG2	1.61	0.81
3:B:121:ASP:HA	3:B:819:ILE:HG21	1.62	0.81
3:D:303:LEU:HD23	3:D:303:LEU:H	1.44	0.81
1:I:12:DA:H2''	1:I:13:DG:C8	2.14	0.81
3:C:592:MSE:HE3	3:C:670:MSE:SE	2.30	0.81
3:A:660:GLU:HB2	3:A:661:PRO:HD3	1.63	0.81
3:A:738:PRO:HB3	3:A:780:ALA:O	1.80	0.80
2:F:106:DT:H2''	2:F:107:DG:H5''	1.63	0.80
3:C:412:LEU:HG	3:C:683:MSE:HE3	1.64	0.80
3:D:484:GLU:HG2	3:D:488:TYR:HE1	1.46	0.80
1:I:9:DG:H2''	1:I:10:DA:C5'	2.12	0.80
3:A:408:MSE:HE1	3:A:655:ALA:HB2	1.62	0.80
3:B:154:SER:HB3	3:B:313:ARG:HH12	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:503:LEU:HA	3:C:506:PRO:HG3	1.64	0.80
2:J:111:DT:C2'	2:J:112:DT:H5'	2.08	0.79
1:I:5:DG:H2''	1:I:6:DA:C5'	2.12	0.79
3:A:483:LYS:HE3	3:A:483:LYS:HA	1.64	0.79
3:C:392:PRO:O	3:C:587:THR:HG21	1.83	0.79
2:J:109:DC:H2''	2:J:110:DA:H5'	1.65	0.79
3:B:732:THR:HG23	3:B:733:GLN:NE2	1.98	0.78
3:C:240:LYS:HE3	3:C:246:ARG:HB3	1.64	0.78
1:I:5:DG:H2''	1:I:6:DA:H5'	1.65	0.77
3:A:347:MSE:HB2	3:A:558:ASN:HD21	1.50	0.77
3:D:137:THR:HG22	3:D:138:HIS:H	1.48	0.77
3:B:159:VAL:HG21	3:B:317:HIS:CD2	2.20	0.77
2:H:101:DG:H8	2:H:101:DG:HO5'	1.31	0.76
1:I:8:DT:H4'	4:I:192:HOH:O	1.86	0.76
3:B:224:PRO:HA	3:B:263:ILE:HD12	1.66	0.76
3:C:153:ASN:HD22	3:C:158:ASN:CG	1.93	0.76
1:G:9:DG:H2''	1:G:10:DA:H5'	1.68	0.76
3:A:739:LYS:HD3	3:A:778:SER:HA	1.65	0.76
1:E:13:DG:O5'	3:A:800:LYS:HG2	1.85	0.76
1:K:13:DG:H2''	1:K:14:DC:H5'	1.65	0.76
3:D:833:LEU:HD22	3:D:866:MSE:HE3	1.68	0.76
3:A:176:ASP:HA	3:A:319:ARG:HH21	1.51	0.75
3:A:507:ASN:C	3:A:508:LEU:HD22	2.10	0.75
3:C:523:SER:HB2	3:C:525:GLU:HG2	1.68	0.75
3:A:700:GLY:HA2	3:A:753:LEU:HD22	1.69	0.75
3:C:454:TYR:HD2	3:C:462:MSE:HE2	1.51	0.75
3:D:136:ILE:HG23	3:D:149:PHE:HB2	1.66	0.75
1:K:8:DT:H2'	1:K:9:DG:C8	2.22	0.75
3:A:775:ASN:HD21	3:A:777:ILE:HB	1.51	0.75
3:D:784:SER:HA	3:D:829:LYS:HA	1.67	0.75
3:A:514:LEU:HD21	3:A:529:LYS:HE2	1.67	0.75
3:C:221:PHE:O	3:C:224:PRO:HD2	1.86	0.75
3:D:824:VAL:HA	3:D:849:PRO:HB3	1.69	0.75
3:D:399:PRO:HB3	3:D:619:TYR:HD2	1.52	0.74
1:I:10:DA:H2''	1:I:11:DC:C5'	2.16	0.74
2:J:114:DC:H2''	2:J:115:DA:H5''	1.68	0.74
3:A:100:GLU:HG2	3:A:102:LYS:HE2	1.67	0.74
1:K:8:DT:H2'	1:K:9:DG:H8	1.52	0.74
3:A:848:TRP:HB2	3:A:849:PRO:HD2	1.69	0.74
3:B:116:GLU:HB2	3:B:135:ALA:HB3	1.69	0.74
3:B:735:SER:HB3	3:B:737:THR:HG23	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:739:LYS:CD	3:A:739:LYS:H	1.99	0.74
3:B:818:ASN:ND2	3:B:821:ALA:HB2	2.02	0.74
3:D:700:GLY:HA2	3:D:753:LEU:HD22	1.69	0.74
3:A:213:LEU:HD13	3:A:223:ILE:HD11	1.68	0.74
3:B:298:LEU:O	3:B:300:VAL:HG23	1.88	0.74
3:B:733:GLN:O	3:B:734:LYS:C	2.30	0.74
1:I:6:DA:H2''	1:I:7:DA:C8	2.23	0.73
3:D:730:LEU:HD23	3:D:730:LEU:H	1.52	0.73
3:A:392:PRO:O	3:A:587:THR:HG21	1.88	0.73
3:D:300:VAL:HG21	3:D:330:ARG:HH12	1.52	0.73
3:D:514:LEU:HB3	3:D:516:VAL:HG13	1.69	0.73
3:A:631:LYS:HB2	3:A:631:LYS:NZ	2.04	0.73
1:I:13:DG:H2''	1:I:14:DC:H5'	1.71	0.73
3:C:482:ARG:C	3:C:484:GLU:H	1.96	0.73
3:D:218:VAL:HG13	3:D:222:ALA:HB3	1.69	0.73
3:A:112:ASN:HB2	4:A:987:HOH:O	1.89	0.73
3:B:700:GLY:HA2	3:B:753:LEU:HD22	1.70	0.72
3:D:250:VAL:HG13	3:D:263:ILE:HG12	1.71	0.72
2:H:104:DG:H2''	2:H:105:DC:O5'	1.88	0.72
3:A:776:TYR:HB2	3:A:866:MSE:HE1	1.71	0.72
3:B:732:THR:CG2	3:B:733:GLN:HE21	2.03	0.72
2:L:106:DT:H2''	2:L:107:DG:H5''	1.72	0.72
3:A:443:ILE:HD13	3:A:595:GLN:HB2	1.71	0.72
3:B:163:SER:H	3:B:318:GLN:HE22	1.37	0.72
3:D:492:ALA:HA	3:D:495:ASN:HB3	1.72	0.72
3:D:790:LYS:O	3:D:790:LYS:HD3	1.89	0.72
2:F:106:DT:H2''	2:F:107:DG:C5'	2.20	0.72
3:B:223:ILE:HB	3:B:224:PRO:HD3	1.70	0.72
3:D:523:SER:HB2	3:D:527:LYS:CB	2.20	0.71
3:A:592:MSE:HE1	3:A:674:MSE:HG3	1.71	0.71
3:B:589:PHE:HE1	3:B:681:MSE:HE2	1.55	0.71
3:D:405:LYS:O	3:D:690:GLY:HA2	1.91	0.71
3:D:604:TYR:OH	3:D:658:ARG:HG3	1.89	0.71
3:D:347:MSE:HG2	3:D:358:VAL:HG13	1.72	0.71
3:A:422:GLN:HE22	3:A:681:MSE:HG2	1.56	0.71
3:A:468:ASP:HA	4:A:997:HOH:O	1.90	0.71
3:B:253:ILE:O	3:B:259:SER:HA	1.90	0.71
3:C:295:GLU:O	3:C:299:ASN:HA	1.91	0.71
3:D:202:LEU:HB3	3:D:241:ARG:HD3	1.72	0.71
3:B:435:LYS:H	3:B:435:LYS:HD3	1.54	0.70
3:D:486:LYS:HA	4:D:916:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:702:TRP:CE2	3:D:708:TYR:HB3	2.27	0.70
3:B:303:LEU:HD13	3:B:319:ARG:HD2	1.72	0.70
3:B:408:MSE:HE1	3:B:655:ALA:HB2	1.73	0.70
3:C:572:ASN:HD22	3:C:574:TRP:H	1.38	0.70
3:C:21:ASP:OD2	3:C:25:ARG:HG3	1.92	0.70
3:C:104:ASP:OD1	3:C:106:THR:HB	1.91	0.70
2:L:110:DA:H2''	2:L:111:DT:O4'	1.92	0.70
3:B:164:ILE:H	3:B:164:ILE:CD1	1.90	0.70
3:B:735:SER:CB	3:B:737:THR:HG23	2.22	0.70
3:D:370:PHE:HA	3:D:380:ILE:HD11	1.73	0.69
3:D:730:LEU:HG	3:D:731:GLU:H	1.57	0.69
3:A:218:VAL:HG23	3:A:222:ALA:HB3	1.74	0.69
3:D:803:PHE:CZ	3:D:845:CYS:HB3	2.27	0.69
3:D:326:ILE:O	3:D:330:ARG:HG2	1.92	0.69
3:D:802:PRO:HB2	3:D:804:HIS:CE1	2.27	0.69
2:H:107:DG:H5'	4:H:306:HOH:O	1.92	0.69
3:A:347:MSE:HE1	3:A:562:LEU:HD11	1.75	0.69
3:B:435:LYS:HD3	3:B:435:LYS:N	2.08	0.69
3:B:797:PRO:HG3	3:B:806:ARG:NH1	2.08	0.69
3:D:213:LEU:HB3	3:D:270:VAL:HG12	1.73	0.69
3:D:731:GLU:OE2	3:D:879:PRO:HB3	1.92	0.69
1:K:5:DG:H2''	1:K:6:DA:C5'	2.21	0.69
3:C:343:LEU:HG	4:C:1053:HOH:O	1.92	0.69
3:C:604:TYR:OH	3:C:658:ARG:HB3	1.93	0.69
3:D:8:VAL:HG11	3:D:93:LEU:HD13	1.75	0.69
3:D:779:ILE:HD11	3:D:866:MSE:HE1	1.73	0.69
3:D:117:VAL:HG12	3:D:133:ILE:HA	1.73	0.69
3:D:649:ASP:CG	3:D:719:ARG:HH22	2.01	0.69
2:H:110:DA:H2''	2:H:111:DT:H5'	1.74	0.68
3:B:303:LEU:HD12	3:B:323:TYR:HA	1.74	0.68
3:C:412:LEU:HD13	3:C:415:LEU:HD13	1.75	0.68
3:D:109:ARG:HB2	3:D:211:VAL:HG23	1.75	0.68
3:D:504:HIS:C	3:D:506:PRO:HD3	2.17	0.68
3:A:738:PRO:HB3	3:A:780:ALA:C	2.18	0.68
2:F:106:DT:C2'	2:F:107:DG:H5''	2.22	0.68
3:D:90:LEU:HG	3:D:353:ILE:HG22	1.75	0.68
2:F:111:DT:H1'	4:F:577:HOH:O	1.93	0.68
3:C:81:GLU:HG2	3:C:83:LEU:HD22	1.73	0.68
3:A:642:ARG:H	3:A:646:HIS:CD2	2.08	0.68
3:D:458:PRO:HG3	3:D:592:MSE:SE	2.43	0.68
3:A:739:LYS:HD2	3:A:778:SER:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:13:DG:H2''	1:I:14:DC:C5'	2.24	0.68
3:C:881:GLU:HG3	3:C:891:TYR:HE1	1.59	0.68
3:D:737:THR:HG22	3:D:875:THR:HB	1.76	0.68
4:E:449:HOH:O	2:F:110:DA:H1'	1.93	0.67
3:B:75:MSE:HA	3:B:75:MSE:CE	2.23	0.67
3:D:427:PRO:HG2	4:D:953:HOH:O	1.94	0.67
3:B:326:ILE:CG2	3:B:330:ARG:HE	2.06	0.67
3:C:52:ILE:HD12	3:C:428:GLU:HG3	1.77	0.67
3:D:830:VAL:HA	3:D:850:SER:H	1.58	0.67
1:I:9:DG:C2'	1:I:10:DA:H5''	2.23	0.67
3:A:485:HIS:HB3	3:A:556:GLN:HE21	1.58	0.67
3:C:171:GLN:HA	3:C:175:GLY:HA2	1.77	0.67
3:C:495:ASN:O	3:C:499:ILE:HG12	1.94	0.67
3:A:602:ASN:HD21	3:A:617:VAL:H	1.42	0.67
3:C:152:LEU:HD11	3:C:190:PRO:HB2	1.76	0.67
3:D:132:PRO:HB3	3:D:229:ARG:NH2	2.10	0.67
3:A:403:ARG:HD2	3:A:887:ALA:O	1.95	0.67
2:J:105:DC:H2''	2:J:106:DT:H5'	1.77	0.66
3:C:175:GLY:HA3	3:C:319:ARG:HH21	1.59	0.66
3:D:821:ALA:HB1	3:D:855:THR:HG21	1.78	0.66
3:A:559:ARG:O	3:A:563:ILE:HG13	1.94	0.66
3:C:130:LYS:HE3	3:C:131:HIS:CE1	2.29	0.66
2:L:105:DC:H2'	2:L:106:DT:C7	2.24	0.66
3:B:82:ALA:H	3:B:382:GLN:NE2	1.88	0.66
3:D:471:VAL:HB	3:D:472:PRO:HD3	1.77	0.66
1:E:18:DG:OP1	1:E:18:DG:H3'	1.96	0.66
2:H:107:DG:H2''	2:H:108:DT:O5'	1.94	0.66
2:H:110:DA:H2''	2:H:111:DT:C5'	2.26	0.66
3:B:164:ILE:HD12	3:B:164:ILE:N	1.98	0.66
3:C:298:LEU:HB2	3:C:300:VAL:HG12	1.78	0.66
3:A:338:ARG:HB3	3:A:340:PHE:CE1	2.30	0.66
3:C:78:ILE:HG13	3:C:80:LEU:HD23	1.77	0.66
1:E:2:DG:OP1	3:A:361:PRO:HD2	1.96	0.66
1:I:16:DG:H2''	1:I:17:DC:O5'	1.94	0.66
3:B:527:LYS:HA	3:B:530:ILE:HD11	1.76	0.66
3:C:391:TYR:HB2	3:C:392:PRO:HD2	1.76	0.66
1:K:8:DT:H4'	1:K:8:DT:OP1	1.96	0.66
3:B:458:PRO:HG3	3:B:592:MSE:SE	2.46	0.66
3:C:556:GLN:HB3	4:C:1026:HOH:O	1.96	0.66
3:B:326:ILE:O	3:B:330:ARG:HG2	1.95	0.65
3:B:593:ALA:CB	3:B:681:MSE:HE3	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:402:ASN:CG	3:D:403:ARG:H	2.04	0.65
3:D:191:PHE:HE2	3:D:200:GLU:HG3	1.61	0.65
3:C:540:GLU:O	3:C:544:ARG:HG2	1.96	0.65
3:A:170:LEU:HA	3:A:177:GLU:HG2	1.79	0.65
3:A:874:LYS:HB3	4:A:964:HOH:O	1.96	0.65
1:G:9:DG:H2''	1:G:10:DA:C5'	2.26	0.65
3:A:810:THR:OG1	3:A:843:ASP:HB2	1.96	0.65
3:D:768:GLU:HG2	3:D:872:LEU:HD21	1.79	0.65
2:L:112:DT:H2''	2:L:113:DC:O4'	1.97	0.65
3:D:244:PRO:HD3	3:D:268:ILE:HD11	1.79	0.64
3:A:193:ASN:HD21	3:A:196:GLU:HG3	1.61	0.64
3:A:554:THR:C	4:A:960:HOH:O	2.41	0.64
3:A:555:ALA:N	4:A:960:HOH:O	2.30	0.64
3:B:422:GLN:HG3	3:B:678:GLN:O	1.96	0.64
3:B:516:VAL:H	3:B:544:ARG:NH1	1.94	0.64
3:C:439:LEU:HD21	3:C:588:THR:HG23	1.78	0.64
1:E:5:DG:C2'	1:E:6:DA:H5''	2.27	0.64
3:C:458:PRO:HB2	3:C:588:THR:HG22	1.79	0.64
1:K:3:CTG:H2''	1:K:4:DG:C8	2.32	0.64
3:C:231:LYS:HE3	3:C:236:GLU:HG3	1.79	0.64
3:C:455:SER:OG	3:C:676:ASN:HA	1.98	0.64
3:D:592:MSE:HE3	3:D:670:MSE:SE	2.48	0.64
3:B:541:MSE:HE3	3:B:544:ARG:NH2	2.12	0.64
3:C:218:VAL:HG22	3:C:223:ILE:HG13	1.80	0.64
3:D:492:ALA:HA	3:D:495:ASN:CB	2.27	0.64
2:L:112:DT:H2''	2:L:113:DC:C5'	2.27	0.64
3:D:355:ILE:O	3:D:358:VAL:HG23	1.97	0.64
3:D:484:GLU:HG2	3:D:488:TYR:CE1	2.29	0.64
3:A:811:TYR:OH	3:A:822:PRO:HG2	1.98	0.64
3:B:303:LEU:C	3:B:304:LYS:HD2	2.23	0.64
3:B:668:ARG:HG3	3:B:668:ARG:HH11	1.62	0.64
3:D:416:TYR:O	3:D:420:ILE:HG13	1.98	0.64
3:D:668:ARG:NH1	3:D:668:ARG:HB2	2.12	0.64
2:F:106:DT:H1'	2:F:107:DG:H5''	1.80	0.64
3:A:83:LEU:HD12	3:A:83:LEU:H	1.62	0.64
3:B:757:GLU:O	3:B:761:GLN:HG3	1.97	0.64
2:H:113:DC:O5'	3:B:734:LYS:HB2	1.98	0.63
1:K:8:DT:H2''	1:K:9:DG:C5'	2.28	0.63
3:A:822:PRO:HD2	3:A:855:THR:HB	1.80	0.63
3:D:856:ASP:HA	3:D:859:LYS:HB3	1.80	0.63
3:A:13:ASP:OD1	3:A:66:ARG:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:231:LYS:HG3	3:A:236:GLU:HA	1.79	0.63
3:B:397:LYS:HD3	3:B:619:TYR:HA	1.81	0.63
3:B:598:GLU:HG3	3:B:617:VAL:HG11	1.80	0.63
1:E:11:DC:H2''	1:E:12:DA:H5'	1.79	0.63
1:E:9:DG:H2'	1:E:11:DC:C6	2.34	0.63
3:A:251:LYS:HD2	3:A:262:ILE:HD11	1.80	0.63
3:B:403:ARG:HH11	3:B:403:ARG:CB	2.12	0.63
3:B:658:ARG:NE	3:D:897:LEU:HD11	2.13	0.63
1:K:9:DG:H2''	1:K:10:DA:O5'	1.99	0.63
3:A:387:PRO:HB2	4:A:998:HOH:O	1.98	0.63
3:B:304:LYS:HD2	3:B:304:LYS:N	2.12	0.63
3:A:620:GLY:O	3:A:621:ASP:HB2	1.99	0.63
3:D:273:TYR:OH	3:D:335:ASP:HA	1.99	0.63
3:D:41:CYS:HB2	3:D:42:PRO:HD2	1.81	0.62
3:D:398:GLU:OE1	3:D:705:LYS:HE3	1.98	0.62
3:D:642:ARG:HG2	3:D:646:HIS:HD2	1.63	0.62
1:G:14:DC:H2''	1:G:15:DC:H5'	1.81	0.62
3:A:304:LYS:O	3:A:319:ARG:HD3	1.99	0.62
3:C:467:ARG:H	3:C:467:ARG:HD3	1.64	0.62
1:I:2:DG:OP2	3:C:361:PRO:HD2	2.00	0.62
3:D:166:ILE:HB	4:D:934:HOH:O	1.99	0.62
3:B:403:ARG:HH11	3:B:403:ARG:HB3	1.64	0.62
3:A:655:ALA:HA	3:A:659:MSE:CG	2.27	0.62
3:A:685:ARG:NH1	3:A:688:ILE:HG13	2.15	0.62
3:B:589:PHE:CE1	3:B:681:MSE:HE2	2.33	0.62
3:D:272:ASP:OD2	3:D:274:ILE:HG22	1.99	0.62
3:D:725:LEU:HD11	3:D:750:ARG:HG3	1.82	0.62
1:E:14:DC:H2''	1:E:15:DC:H5'	1.81	0.62
3:A:839:ASN:HD22	3:A:841:PHE:HB2	1.63	0.62
3:C:818:ASN:OD1	3:C:857:LEU:HD11	2.00	0.62
2:J:103:DG:H2''	2:J:104:DG:O5'	1.99	0.62
1:K:16:DG:H2''	1:K:17:DC:H5''	1.82	0.62
3:B:790:LYS:HE2	3:B:802:PRO:HD3	1.81	0.62
3:D:841:PHE:HZ	3:D:861:ASP:HB3	1.64	0.62
3:A:130:LYS:HE2	4:A:956:HOH:O	2.00	0.62
3:C:520:PHE:HA	4:C:937:HOH:O	2.00	0.61
3:D:520:PHE:HA	4:D:931:HOH:O	2.00	0.61
1:E:12:DA:H2''	1:E:13:DG:O5'	2.00	0.61
1:G:7:DA:H2''	1:G:8:DT:C5'	2.29	0.61
2:J:108:DT:H2''	2:J:109:DC:H5'	1.82	0.61
3:B:162:TRP:CZ3	3:B:164:ILE:HG13	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:82:ALA:O	3:A:382:GLN:HG3	2.00	0.61
3:C:164:ILE:N	4:C:983:HOH:O	2.27	0.61
3:B:303:LEU:HB2	3:B:323:TYR:CD1	2.36	0.61
3:B:541:MSE:HE3	3:B:544:ARG:HH22	1.65	0.61
3:C:181:GLU:CD	3:C:181:GLU:H	2.08	0.61
1:E:11:DC:H2''	1:E:12:DA:C5'	2.31	0.61
3:A:157:GLY:C	3:A:158:ASN:HD22	2.09	0.61
3:C:421:ARG:HD3	3:C:476:THR:OG1	1.99	0.61
3:D:686:GLU:CB	3:D:715:MSE:HE1	2.28	0.61
3:B:257:TYR:CE1	3:B:786:ASN:HB3	2.35	0.61
3:D:604:TYR:HH	3:D:658:ARG:HG3	1.63	0.61
3:D:496:GLY:O	3:D:499:ILE:HB	2.01	0.61
3:A:443:ILE:HD13	3:A:595:GLN:CB	2.30	0.61
3:D:277:TYR:O	3:D:281:SER:HB2	2.01	0.61
3:D:553:MSE:O	3:D:556:GLN:HG3	2.00	0.61
3:D:825:VAL:HB	3:D:828:GLU:HB2	1.81	0.61
3:A:85:MSE:HE1	3:A:366:ASP:OD2	2.01	0.61
3:A:606:ASN:OD1	3:A:616:PHE:HE1	1.84	0.61
2:L:114:DC:H2''	2:L:115:DA:O4'	2.01	0.60
3:A:707:ARG:HD3	3:A:729:GLY:HA3	1.83	0.60
3:D:465:LYS:HD2	3:D:677:LYS:HA	1.83	0.60
1:K:13:DG:H2''	1:K:14:DC:C5'	2.32	0.60
3:B:132:PRO:HA	3:B:194:GLU:OE2	2.01	0.60
3:B:197:LEU:C	3:B:197:LEU:HD23	2.26	0.60
3:B:421:ARG:HD3	3:B:475:ILE:HD12	1.82	0.60
3:C:343:LEU:HD11	3:C:558:ASN:ND2	2.15	0.60
1:K:2:DG:O6	3:D:279:LYS:HD2	2.01	0.60
3:A:347:MSE:HB2	3:A:558:ASN:ND2	2.16	0.60
3:B:159:VAL:HG11	3:B:317:HIS:HB2	1.83	0.60
3:D:9:GLU:O	3:D:15:ILE:HG13	2.01	0.60
3:D:714:ASP:HB2	3:D:719:ARG:HD3	1.83	0.60
1:E:6:DA:H2''	1:E:7:DA:N7	2.15	0.60
3:D:262:ILE:HD12	3:D:262:ILE:N	2.16	0.60
3:A:362:ILE:HD11	3:A:572:ASN:CG	2.26	0.60
3:A:606:ASN:HD21	3:A:614:GLU:H	1.47	0.60
3:B:494:ARG:CB	3:B:494:ARG:HH11	2.15	0.60
3:C:112:ASN:HD21	3:C:332:LEU:CD1	2.14	0.60
3:C:791:TYR:CD2	3:C:801:CYS:HA	2.36	0.60
3:D:142:ILE:HD12	3:D:143:ASP:N	2.17	0.60
2:H:106:DT:H2''	2:H:107:DG:H5'	1.83	0.60
1:I:7:DA:H2''	1:I:8:DT:O5'	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:405:LYS:HA	3:A:699:GLY:HA3	1.84	0.60
3:D:434:PHE:CZ	3:D:460:GLY:HA2	2.36	0.60
2:F:111:DT:H2''	2:F:112:DT:C5'	2.31	0.60
1:G:12:DA:H2''	1:G:13:DG:C8	2.36	0.60
3:B:294:SER:HB2	3:B:301:GLY:HA2	1.82	0.60
3:C:818:ASN:C	3:C:818:ASN:HD22	2.10	0.60
3:A:502:ALA:HA	3:A:538:LEU:HD23	1.82	0.60
3:A:784:SER:HB3	3:A:829:LYS:HG2	1.81	0.60
3:C:711:ASN:ND2	3:C:754:GLN:HE21	2.00	0.60
3:D:890:ASP:HB3	4:D:949:HOH:O	2.02	0.60
3:A:386:HIS:HB2	3:A:573:VAL:HB	1.84	0.59
3:A:625:ILE:HG12	3:A:683:MSE:HE1	1.83	0.59
3:C:655:ALA:O	3:C:660:GLU:HG2	2.02	0.59
3:B:285:GLN:HG3	3:B:286:PRO:HD2	1.84	0.59
3:B:636:VAL:O	3:B:640:LYS:HG3	2.02	0.59
3:D:730:LEU:HD12	3:D:883:PHE:CZ	2.37	0.59
3:A:81:GLU:OE2	3:A:83:LEU:HG	2.03	0.59
3:C:112:ASN:HB3	3:C:214:THR:CG2	2.30	0.59
2:F:102:DC:H2''	2:F:103:DG:OP2	2.02	0.59
2:J:101:DG:HO5'	2:J:101:DG:H8	1.50	0.59
1:I:6:DA:H2''	1:I:7:DA:H8	1.66	0.59
1:K:3:CTG:H2''	1:K:4:DG:H8	1.66	0.59
3:A:791:TYR:O	3:A:798:GLY:N	2.36	0.59
3:D:402:ASN:CG	3:D:403:ARG:N	2.60	0.59
3:D:497:GLU:C	3:D:499:ILE:H	2.11	0.59
3:D:510:VAL:O	3:D:533:LEU:HD13	2.02	0.59
2:J:105:DC:H2''	2:J:106:DT:C5'	2.32	0.59
1:K:13:DG:H2'	1:K:14:DC:C6	2.38	0.59
3:A:194:GLU:OE1	3:A:229:ARG:HD2	2.02	0.59
3:C:273:TYR:OH	3:C:335:ASP:HA	2.02	0.59
3:D:731:GLU:N	4:D:925:HOH:O	2.35	0.59
1:K:1:DC:H4'	3:D:572:ASN:HD21	1.68	0.59
3:B:82:ALA:N	3:B:382:GLN:HE21	1.90	0.59
3:C:1:MSE:HE1	3:C:107:LYS:HE3	1.84	0.59
2:L:105:DC:H4'	2:L:105:DC:OP1	2.03	0.58
3:B:731:GLU:HB3	3:B:737:THR:HG21	1.85	0.58
3:D:81:GLU:CD	3:D:83:LEU:HD21	2.28	0.58
3:D:708:TYR:O	3:D:730:LEU:HD22	2.03	0.58
3:C:757:GLU:HB2	3:C:889:LEU:HD22	1.84	0.58
3:A:90:LEU:CD2	3:A:353:ILE:HG22	2.31	0.58
3:A:513:PRO:HG3	3:A:537:SER:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:87:ASP:CG	3:D:90:LEU:HD13	2.28	0.58
3:D:202:LEU:HD13	3:D:241:ARG:HD2	1.86	0.58
3:D:306:ASP:HB2	3:D:315:SER:OG	2.03	0.58
3:D:330:ARG:O	3:D:334:ILE:HG13	2.02	0.58
3:D:844:LYS:HD3	3:D:844:LYS:N	2.15	0.58
1:I:2:DG:H2''	1:I:3:CTG:OP2	2.04	0.58
1:I:8:DT:H2'	1:I:9:DG:C8	2.37	0.58
3:A:791:TYR:HA	3:A:799:PRO:HD2	1.84	0.58
3:A:807:GLY:HA3	4:A:972:HOH:O	2.03	0.58
3:D:642:ARG:HG3	3:D:643:ASP:OD2	2.03	0.58
3:D:832:VAL:HB	4:D:957:HOH:O	2.02	0.58
3:A:896:SER:HB3	3:A:899:ASP:OD1	2.03	0.58
3:D:392:PRO:HD2	3:D:584:THR:HG22	1.86	0.58
3:D:496:GLY:HA2	3:D:499:ILE:HD12	1.84	0.58
3:A:129:ALA:HA	3:A:225:TYR:CE1	2.39	0.58
3:A:784:SER:HA	3:A:829:LYS:HA	1.85	0.58
3:A:734:LYS:HE2	3:A:737:THR:OG1	2.04	0.58
3:D:155:PRO:C	3:D:157:GLY:H	2.12	0.58
3:A:485:HIS:HB3	3:A:556:GLN:NE2	2.18	0.58
3:D:422:GLN:HG3	3:D:678:GLN:O	2.04	0.58
3:D:487:GLY:C	4:D:938:HOH:O	2.46	0.58
3:B:386:HIS:CD2	4:B:1064:HOH:O	2.56	0.58
3:D:10:GLN:HG3	3:D:65:MSE:SE	2.53	0.58
3:D:830:VAL:HG22	3:D:831:TYR:H	1.69	0.58
3:A:64:ASN:ND2	3:A:67:ASP:H	2.02	0.58
3:A:489:MSE:HE2	3:A:490:LEU:HG	1.86	0.58
3:B:435:LYS:O	3:B:435:LYS:HG2	2.04	0.58
3:C:897:LEU:H	3:C:897:LEU:CD2	2.11	0.58
3:A:775:ASN:ND2	3:A:777:ILE:HB	2.16	0.57
3:A:776:TYR:CB	3:A:866:MSE:HE1	2.34	0.57
3:B:271:LEU:HD11	3:B:356:GLN:HA	1.85	0.57
1:E:4:DG:H2''	1:E:5:DG:O5'	2.05	0.57
1:G:7:DA:H2'	1:G:8:DT:H72	1.86	0.57
1:G:14:DC:H2''	1:G:15:DC:C5'	2.34	0.57
2:L:103:DG:H2''	2:L:104:DG:C8	2.39	0.57
3:D:51:ASP:HA	3:D:379:VAL:HG22	1.85	0.57
3:D:495:ASN:HD22	3:D:521:ASP:HA	1.68	0.57
2:H:114:DC:OP1	3:B:728:MSE:HE3	2.04	0.57
1:I:5:DG:H2''	1:I:6:DA:H5''	1.86	0.57
3:A:739:LYS:CD	3:A:739:LYS:N	2.68	0.57
3:B:158:ASN:HD22	3:B:158:ASN:N	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:ILE:HB	3:C:428:GLU:HG2	1.85	0.57
3:A:254:GLU:CD	3:A:259:SER:HB2	2.29	0.57
3:B:421:ARG:HD2	3:B:476:THR:OG1	2.03	0.57
3:B:534:SER:OG	3:B:537:SER:HB2	2.05	0.57
3:B:685:ARG:NH2	3:B:714:ASP:OD1	2.37	0.57
3:C:555:ALA:O	3:C:559:ARG:HG2	2.04	0.57
3:D:509:SER:HB2	3:D:533:LEU:HA	1.87	0.57
3:A:896:SER:HB3	3:A:899:ASP:CG	2.29	0.57
3:B:183:ILE:HG23	3:B:184:ASP:N	2.19	0.57
3:B:227:TYR:CD2	3:B:263:ILE:HD13	2.40	0.57
3:B:312:LEU:HD12	3:B:320:TYR:HB2	1.86	0.57
3:B:703:THR:OG1	3:B:707:ARG:HD3	2.05	0.57
3:C:711:ASN:HD21	3:C:754:GLN:HE21	1.51	0.57
3:D:514:LEU:HD23	3:D:541:MSE:HE1	1.87	0.57
3:A:471:VAL:HB	3:A:472:PRO:CD	2.34	0.57
3:A:800:LYS:HB2	3:A:800:LYS:NZ	2.20	0.57
3:B:245:HIS:HE1	4:B:961:HOH:O	1.85	0.57
3:C:477:LYS:O	3:C:481:GLN:HG3	2.04	0.57
3:D:730:LEU:HD23	3:D:730:LEU:N	2.19	0.57
3:A:806:ARG:HA	3:A:809:LEU:HD12	1.86	0.57
3:D:396:VAL:HG21	3:D:706:LYS:HE2	1.86	0.57
3:D:833:LEU:CD2	3:D:866:MSE:HE3	2.35	0.57
1:E:9:DG:H2''	1:E:11:DC:O4'	2.05	0.57
3:B:593:ALA:HB1	3:B:681:MSE:HE3	1.87	0.57
3:A:807:GLY:CA	4:A:972:HOH:O	2.52	0.57
3:C:42:PRO:HG2	3:C:45:GLN:HG3	1.86	0.57
3:D:300:VAL:HG21	3:D:330:ARG:NH1	2.20	0.57
3:A:6:LEU:CD1	3:A:26:GLU:HG3	2.35	0.56
3:A:597:ILE:HD11	3:A:663:ILE:HG23	1.86	0.56
3:A:771:PHE:HA	3:A:774:LEU:HD12	1.86	0.56
3:B:478:VAL:HG13	3:B:559:ARG:HG3	1.87	0.56
3:C:221:PHE:C	3:C:224:PRO:HD2	2.29	0.56
2:L:106:DT:H5''	2:L:106:DT:H6	1.70	0.56
3:C:750:ARG:NH2	3:C:755:GLU:OE1	2.38	0.56
3:D:147:TYR:HA	3:D:187:ILE:HG23	1.87	0.56
3:D:517:ASP:C	3:D:519:ARG:H	2.12	0.56
3:D:831:TYR:HB2	3:D:848:TRP:CB	2.35	0.56
1:E:14:DC:H2'	1:E:15:DC:C6	2.40	0.56
3:A:163:SER:N	3:A:318:GLN:OE1	2.35	0.56
3:A:685:ARG:HH11	3:A:688:ILE:HG13	1.69	0.56
3:B:410:PHE:HB3	3:B:683:MSE:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:218:VAL:HA	3:C:222:ALA:HB3	1.86	0.56
3:D:35:PRO:HD2	3:D:64:ASN:O	2.06	0.56
3:D:116:GLU:HB3	3:D:135:ALA:HB3	1.87	0.56
3:D:212:ILE:CD1	3:D:345:LEU:HD21	2.29	0.56
3:D:873:GLU:HG2	3:D:877:ILE:CD1	2.35	0.56
1:K:11:DC:H2''	1:K:12:DA:H5'	1.87	0.56
3:A:101:ILE:HG21	3:A:349:TYR:HB3	1.88	0.56
3:B:660:GLU:HB3	3:B:661:PRO:HD3	1.87	0.56
3:C:523:SER:CB	3:C:525:GLU:HG2	2.35	0.56
3:C:599:ARG:HA	4:C:920:HOH:O	2.06	0.56
3:B:351:ALA:O	3:B:352:LYS:HB2	2.05	0.56
3:B:530:ILE:HG13	3:B:531:LYS:N	2.15	0.56
3:C:216:TRP:O	3:C:217:ASN:HB2	2.06	0.56
1:E:2:DG:OP2	3:A:362:ILE:HD12	2.05	0.56
3:C:503:LEU:HD21	3:C:538:LEU:HB3	1.86	0.56
3:D:530:ILE:HD13	3:D:530:ILE:N	2.19	0.56
3:D:803:PHE:CE1	3:D:845:CYS:HB3	2.41	0.56
2:L:106:DT:H2''	2:L:107:DG:C5'	2.35	0.56
3:A:712:VAL:HG22	3:A:724:LYS:O	2.06	0.56
3:B:221:PHE:O	3:B:224:PRO:HD2	2.05	0.56
3:D:546:GLN:HA	3:D:546:GLN:OE1	2.05	0.56
2:F:111:DT:H2''	2:F:112:DT:H5'	1.87	0.56
1:K:5:DG:H2'	1:K:6:DA:C8	2.40	0.56
3:A:231:LYS:O	3:A:234:PHE:O	2.23	0.56
3:A:410:PHE:HZ	3:A:659:MSE:HE3	1.69	0.56
3:B:528:GLU:C	3:B:530:ILE:H	2.14	0.56
3:C:175:GLY:CA	3:C:319:ARG:HH21	2.19	0.56
3:C:434:PHE:CE1	3:C:460:GLY:HA2	2.40	0.56
3:C:750:ARG:HH22	3:C:755:GLU:CD	2.13	0.56
3:D:223:ILE:HB	3:D:224:PRO:HD3	1.86	0.56
3:D:416:TYR:N	4:D:958:HOH:O	2.32	0.56
3:B:494:ARG:HH11	3:B:494:ARG:HB3	1.70	0.56
3:D:752:MSE:HE3	3:D:889:LEU:HD12	1.87	0.56
3:B:245:HIS:HD2	4:B:957:HOH:O	1.88	0.56
3:C:150:ASP:OD2	3:C:321:ILE:HG13	2.06	0.56
3:C:171:GLN:NE2	3:C:303:LEU:HD22	2.21	0.56
3:D:216:TRP:CZ2	3:D:293:ILE:HD13	2.41	0.56
3:D:222:ALA:O	3:D:226:VAL:HG23	2.06	0.56
3:D:329:TYR:O	3:D:333:GLN:HG3	2.05	0.56
3:D:421:ARG:NE	3:D:476:THR:OG1	2.39	0.56
3:D:518:TYR:C	3:D:520:PHE:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:588:THR:O	3:D:591:GLN:HB2	2.05	0.55
1:E:13:DG:H2''	1:E:14:DC:O5'	2.06	0.55
1:E:18:DG:N3	1:E:18:DG:H2'	2.22	0.55
3:A:116:GLU:HB2	3:A:135:ALA:HB3	1.87	0.55
3:A:739:LYS:HD2	3:A:739:LYS:N	2.21	0.55
3:D:146:PHE:HB2	3:D:186:ILE:HG22	1.88	0.55
3:D:348:GLY:HA2	3:D:353:ILE:CD1	2.37	0.55
3:A:113:PHE:CE1	3:A:218:VAL:HG21	2.41	0.55
3:C:482:ARG:HG3	3:C:559:ARG:HB2	1.86	0.55
3:D:566:LEU:O	3:D:570:LEU:HD23	2.06	0.55
3:D:801:CYS:SG	3:D:802:PRO:HD2	2.47	0.55
3:D:873:GLU:HG2	3:D:877:ILE:HD13	1.87	0.55
3:B:322:SER:O	3:B:326:ILE:HG12	2.07	0.55
3:C:25:ARG:HD2	4:C:958:HOH:O	2.06	0.55
3:D:469:GLY:C	3:D:472:PRO:HD2	2.31	0.55
3:D:493:GLN:HG2	3:D:546:GLN:HE22	1.72	0.55
3:A:394:ALA:N	4:A:1011:HOH:O	2.37	0.55
3:C:482:ARG:C	3:C:484:GLU:N	2.64	0.55
3:B:253:ILE:HD11	3:B:260:ARG:NH1	2.21	0.55
3:C:143:ASP:O	3:C:145:ARG:HG2	2.07	0.55
3:D:511:ASP:O	3:D:533:LEU:HD11	2.07	0.55
1:I:4:DG:H2''	1:I:5:DG:O5'	2.07	0.55
3:A:287:SER:HB3	3:A:292:TYR:CD1	2.41	0.55
3:C:457:SER:O	3:C:459:ASN:N	2.39	0.55
3:D:470:VAL:HG13	3:D:471:VAL:N	2.20	0.55
3:D:887:ALA:O	3:D:888:LYS:HB3	2.05	0.55
3:A:485:HIS:CB	3:A:556:GLN:HE21	2.19	0.55
3:A:489:MSE:C	3:A:491:ALA:H	2.14	0.55
3:A:726:LYS:HE3	3:A:728:MSE:CG	2.37	0.55
3:C:422:GLN:HG3	3:C:678:GLN:O	2.07	0.55
3:D:426:SER:O	3:D:428:GLU:N	2.40	0.55
3:D:443:ILE:HD13	3:D:595:GLN:HB2	1.89	0.55
3:A:221:PHE:O	3:A:224:PRO:HD2	2.07	0.55
3:B:121:ASP:HA	3:B:819:ILE:CG2	2.34	0.55
3:B:776:TYR:HB2	3:B:866:MSE:HE1	1.89	0.55
3:D:188:TYR:CD2	3:D:190:PRO:HD3	2.42	0.55
3:C:52:ILE:HG12	4:C:926:HOH:O	2.07	0.55
3:D:617:VAL:HG23	3:D:617:VAL:O	2.07	0.55
3:C:223:ILE:HB	3:C:224:PRO:HD3	1.89	0.54
3:C:237:SER:O	3:C:240:LYS:HG2	2.07	0.54
3:A:592:MSE:HE1	3:A:674:MSE:CG	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:653:LYS:HD2	3:A:653:LYS:C	2.32	0.54
3:D:64:ASN:HD21	3:D:67:ASP:H	1.55	0.54
3:D:137:THR:HG22	3:D:138:HIS:N	2.19	0.54
3:D:455:SER:OG	3:D:676:ASN:HA	2.06	0.54
3:A:37:LEU:HD21	3:A:72:ILE:HD11	1.88	0.54
3:A:631:LYS:HB2	3:A:631:LYS:HZ3	1.72	0.54
3:D:151:LEU:HD22	3:D:152:LEU:H	1.71	0.54
2:J:101:DG:H2''	2:J:102:DC:H6	1.72	0.54
1:K:4:DG:H4'	3:D:391:TYR:O	2.07	0.54
3:B:405:LYS:HA	3:B:699:GLY:CA	2.34	0.54
3:B:700:GLY:HA2	3:B:753:LEU:CD2	2.36	0.54
3:B:789:ALA:C	3:B:791:TYR:H	2.16	0.54
3:D:213:LEU:HD23	3:D:213:LEU:C	2.32	0.54
3:D:403:ARG:HA	4:D:917:HOH:O	2.08	0.54
3:D:485:HIS:HB3	3:D:556:GLN:HB3	1.90	0.54
3:A:376:GLN:HG3	3:A:378:LYS:HG3	1.90	0.54
3:B:34:LYS:HZ3	3:B:61:LEU:HD11	1.72	0.54
3:C:443:ILE:O	3:C:599:ARG:NH2	2.33	0.54
3:A:482:ARG:HE	3:A:560:LYS:HB2	1.72	0.54
3:B:291:ASP:HB2	3:B:302:LYS:HG3	1.89	0.54
3:C:656:ARG:HA	3:C:660:GLU:HG3	1.90	0.54
2:L:106:DT:H2''	2:L:107:DG:O4'	2.07	0.54
3:A:221:PHE:C	3:A:224:PRO:HD2	2.32	0.54
3:C:482:ARG:HG2	3:C:556:GLN:HG2	1.90	0.54
3:D:348:GLY:HA2	3:D:353:ILE:HD11	1.90	0.54
3:D:639:SER:C	3:D:641:PHE:H	2.16	0.54
3:B:256:MSE:HG2	3:B:257:TYR:CD2	2.42	0.54
3:B:818:ASN:HD22	3:B:857:LEU:CD1	2.20	0.54
3:C:167:ALA:HA	3:C:176:ASP:CB	2.38	0.54
3:D:599:ARG:HB3	3:D:599:ARG:NH1	2.23	0.54
2:F:104:DG:H2''	2:F:105:DC:O5'	2.08	0.54
1:G:12:DA:H2''	1:G:13:DG:H8	1.71	0.54
1:G:12:DA:C2'	1:G:13:DG:C8	2.90	0.54
3:B:433:THR:O	3:B:462:MSE:HE2	2.08	0.54
3:B:775:ASN:HD21	3:B:777:ILE:HB	1.73	0.54
3:D:685:ARG:NH1	3:D:688:ILE:HG13	2.23	0.54
1:K:12:DA:H2''	1:K:13:DG:O5'	2.07	0.54
3:A:491:ALA:C	3:A:493:GLN:H	2.15	0.54
3:D:64:ASN:HD22	3:D:66:ARG:H	1.56	0.54
3:D:484:GLU:C	3:D:486:LYS:H	2.14	0.54
3:D:637:GLY:HA2	4:D:956:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:DA:H2''	1:E:7:DA:H8	1.69	0.53
3:D:744:ALA:HB2	3:D:767:PHE:CE2	2.43	0.53
2:F:103:DG:H2''	2:F:104:DG:O5'	2.08	0.53
3:A:132:PRO:HD2	4:A:963:HOH:O	2.07	0.53
3:B:251:LYS:HB3	3:B:262:ILE:HG13	1.89	0.53
3:C:15:ILE:HD11	3:C:92:TYR:CZ	2.43	0.53
3:D:111:ALA:HB3	3:D:210:PRO:HB3	1.90	0.53
3:D:214:THR:HG22	3:D:215:GLY:N	2.10	0.53
3:D:582:ASN:O	3:D:586:ILE:HG13	2.07	0.53
2:L:105:DC:OP1	2:L:105:DC:C4'	2.57	0.53
3:A:373:LEU:HD12	3:A:380:ILE:HG22	1.90	0.53
3:B:163:SER:N	3:B:318:GLN:HE22	2.06	0.53
3:D:125:GLU:O	3:D:129:ALA:HB2	2.08	0.53
2:F:112:DT:H2''	2:F:113:DC:O5'	2.08	0.53
2:J:109:DC:H2''	2:J:110:DA:C5'	2.37	0.53
3:A:389:GLN:HB2	4:A:998:HOH:O	2.07	0.53
3:B:645:ASN:OD1	3:B:719:ARG:NH1	2.42	0.53
3:C:526:ILE:HG23	3:C:529:LYS:HD3	1.90	0.53
3:D:459:ASN:HD21	3:D:461:MSE:HB2	1.73	0.53
3:D:524:ASP:HB3	3:D:525:GLU:OE2	2.07	0.53
3:D:642:ARG:H	3:D:646:HIS:CD2	2.26	0.53
3:A:213:LEU:CD1	3:A:223:ILE:HD11	2.37	0.53
3:A:739:LYS:H	3:A:739:LYS:HD2	1.74	0.53
3:B:303:LEU:HB2	3:B:323:TYR:HD1	1.72	0.53
3:C:14:SER:HB3	3:C:32:GLU:OE1	2.09	0.53
3:D:533:LEU:HD12	3:D:537:SER:OG	2.08	0.53
3:D:730:LEU:H	3:D:730:LEU:CD2	2.21	0.53
3:D:809:LEU:HA	3:D:812:ASN:ND2	2.23	0.53
2:J:115:DA:OP1	3:C:708:TYR:OH	2.23	0.53
1:K:2:DG:H1'	1:K:3:CTG:O5	2.07	0.53
3:A:552:GLY:O	3:A:555:ALA:HB3	2.09	0.53
3:B:435:LYS:H	3:B:435:LYS:CD	2.21	0.53
3:D:490:LEU:O	3:D:490:LEU:HD23	2.08	0.53
3:A:825:VAL:HG23	3:A:828:GLU:HB2	1.90	0.53
3:D:247:LYS:O	3:D:266:PHE:HB2	2.09	0.53
3:D:679:HIS:O	3:D:680:LEU:HG	2.09	0.53
3:D:700:GLY:CA	3:D:753:LEU:HD22	2.38	0.53
1:G:16:DG:H2''	1:G:17:DC:H5''	1.90	0.53
2:H:107:DG:H8	4:H:306:HOH:O	1.92	0.53
3:A:738:PRO:HD3	3:A:781:SER:HA	1.91	0.53
3:B:154:SER:HB3	3:B:313:ARG:NH1	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:858:ILE:O	3:C:862:VAL:HG23	2.08	0.53
3:C:587:THR:HG22	3:C:588:THR:N	2.21	0.53
3:D:602:ASN:HD21	3:D:617:VAL:HG22	1.74	0.53
3:D:782:VAL:HG12	3:D:783:SER:N	2.24	0.53
3:B:133:ILE:HD12	3:B:198:LEU:HD21	1.90	0.53
3:C:461:MSE:HE3	3:C:581:ARG:HB3	1.91	0.53
3:C:706:LYS:C	3:C:707:ARG:HG2	2.34	0.53
3:D:528:GLU:C	3:D:530:ILE:HD13	2.34	0.53
1:E:13:DG:OP1	3:A:800:LYS:HA	2.10	0.52
3:B:475:ILE:HD13	3:B:475:ILE:C	2.33	0.52
3:C:351:ALA:O	3:C:352:LYS:HB2	2.08	0.52
3:C:355:ILE:O	3:C:358:VAL:HG13	2.08	0.52
3:C:681:MSE:HE2	3:C:681:MSE:HA	1.92	0.52
2:J:112:DT:H2''	2:J:113:DC:OP2	2.09	0.52
2:L:114:DC:H1'	3:D:706:LYS:HD3	1.90	0.52
3:A:12:GLY:O	3:A:13:ASP:HB2	2.10	0.52
3:A:902:ASP:HA	4:A:1014:HOH:O	2.10	0.52
3:B:465:LYS:HE3	3:B:677:LYS:HA	1.92	0.52
2:F:104:DG:H2'	2:F:105:DC:C6	2.44	0.52
3:A:64:ASN:HD22	3:A:67:ASP:H	1.57	0.52
3:D:47:THR:HG22	3:D:48:LYS:H	1.74	0.52
1:E:7:DA:H2'	1:E:8:DT:H72	1.91	0.52
1:G:6:DA:H2''	1:G:7:DA:OP2	2.10	0.52
2:H:110:DA:H1'	2:H:111:DT:H5''	1.90	0.52
1:K:7:DA:H2'	1:K:8:DT:C6	2.44	0.52
3:A:709:ALA:O	3:A:710:LEU:HD23	2.09	0.52
3:A:739:LYS:H	3:A:739:LYS:CE	2.22	0.52
3:B:791:TYR:HA	4:B:1086:HOH:O	2.10	0.52
3:C:145:ARG:HB2	3:C:147:TYR:CE1	2.45	0.52
3:D:21:ASP:HB3	3:D:23:ASN:OD1	2.09	0.52
3:A:557:ILE:HB	4:A:960:HOH:O	2.10	0.52
3:B:34:LYS:NZ	3:B:61:LEU:HD11	2.24	0.52
3:B:592:MSE:HE1	3:B:674:MSE:HG3	1.91	0.52
3:C:34:LYS:HE3	3:C:63:ALA:HA	1.91	0.52
3:C:369:ILE:HG12	3:C:474:GLU:HG3	1.92	0.52
3:C:898:PHE:O	3:C:899:ASP:HB3	2.09	0.52
1:E:11:DC:H2''	1:E:12:DA:O5'	2.10	0.52
1:K:17:DC:H6	1:K:17:DC:H5'	1.74	0.52
3:A:527:LYS:O	3:A:530:ILE:HG12	2.09	0.52
3:C:659:MSE:O	3:C:663:ILE:HG13	2.09	0.52
3:D:197:LEU:C	3:D:199:MSE:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:51:ASP:HB2	4:A:908:HOH:O	2.09	0.52
3:A:112:ASN:C	3:A:112:ASN:HD22	2.18	0.52
3:A:346:ASP:HB3	4:A:965:HOH:O	2.10	0.52
3:B:193:ASN:HD22	3:B:194:GLU:N	2.08	0.52
3:B:727:ILE:HG21	3:B:732:THR:HG21	1.91	0.52
3:D:116:GLU:HB2	3:D:324:ASN:HD22	1.74	0.52
3:B:486:LYS:HA	3:B:556:GLN:OE1	2.09	0.52
3:A:486:LYS:CE	3:A:556:GLN:HG2	2.38	0.52
3:B:434:PHE:CE2	3:B:460:GLY:HA2	2.45	0.52
3:C:397:LYS:O	3:C:399:PRO:HD3	2.10	0.52
3:D:364:THR:O	3:D:368:ILE:HG13	2.09	0.52
3:D:713:TRP:CZ3	3:D:723:PRO:HD3	2.45	0.52
1:I:9:DG:H2''	1:I:10:DA:H5'	1.92	0.51
3:C:110:VAL:O	3:C:141:SER:HB3	2.10	0.51
3:C:240:LYS:HD2	3:C:246:ARG:O	2.10	0.51
3:D:50:PHE:HD2	3:D:54:GLY:O	1.93	0.51
3:D:285:GLN:HE21	3:D:286:PRO:HD2	1.75	0.51
3:D:735:SER:HA	4:D:930:HOH:O	2.09	0.51
3:A:822:PRO:HB2	3:A:849:PRO:HG3	1.91	0.51
3:B:641:PHE:HD1	3:B:646:HIS:CD2	2.28	0.51
3:D:218:VAL:HG12	3:D:223:ILE:CG1	2.31	0.51
3:D:410:PHE:O	3:D:624:SER:HA	2.10	0.51
3:D:517:ASP:C	3:D:519:ARG:N	2.69	0.51
1:E:9:DG:O3'	3:A:874:LYS:HE3	2.11	0.51
3:A:197:LEU:HD23	3:A:197:LEU:C	2.35	0.51
3:A:739:LYS:NZ	3:A:780:ALA:O	2.43	0.51
3:C:20:ILE:HA	3:C:25:ARG:O	2.10	0.51
3:C:451:SER:HB3	3:C:456:CYS:SG	2.50	0.51
3:C:594:LEU:O	3:C:597:ILE:HG22	2.10	0.51
3:D:485:HIS:HA	3:D:488:TYR:HD1	1.74	0.51
3:A:458:PRO:HG3	3:A:592:MSE:SE	2.60	0.51
3:A:518:TYR:HE2	3:A:541:MSE:HG3	1.76	0.51
3:D:511:ASP:C	3:D:533:LEU:HD11	2.35	0.51
1:I:16:DG:H2''	1:I:17:DC:C5'	2.41	0.51
3:B:555:ALA:O	3:B:559:ARG:HD3	2.10	0.51
3:B:597:ILE:HD12	3:B:598:GLU:N	2.26	0.51
3:C:811:TYR:CE2	3:C:815:ILE:HD13	2.45	0.51
3:D:757:GLU:HB2	3:D:889:LEU:HD22	1.92	0.51
3:A:757:GLU:HB2	3:A:889:LEU:HD22	1.92	0.51
3:B:75:MSE:HE2	3:B:78:ILE:HG21	1.92	0.51
3:B:401:PRO:O	3:B:402:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:ILE:HD13	3:C:247:LYS:HD2	1.92	0.51
3:C:112:ASN:ND2	3:C:332:LEU:HD11	2.17	0.51
3:C:116:GLU:HB2	3:C:135:ALA:HB3	1.92	0.51
3:C:159:VAL:HG21	3:C:317:HIS:CD2	2.45	0.51
3:C:598:GLU:HG3	3:C:617:VAL:HG11	1.92	0.51
3:D:151:LEU:HD13	3:D:151:LEU:C	2.35	0.51
3:D:410:PHE:HB3	3:D:683:MSE:HE2	1.93	0.51
3:D:846:ILE:HD13	3:D:862:VAL:HG21	1.93	0.51
3:A:526:ILE:O	3:A:530:ILE:HG23	2.11	0.51
3:B:581:ARG:HD2	4:B:999:HOH:O	2.11	0.51
3:C:137:THR:HG21	3:C:325:ILE:HA	1.92	0.51
3:C:138:HIS:C	3:C:138:HIS:CD2	2.88	0.51
3:D:485:HIS:CG	4:D:918:HOH:O	2.63	0.51
3:D:489:MSE:HA	4:D:936:HOH:O	2.09	0.51
3:D:494:ARG:O	3:D:494:ARG:HG2	2.10	0.51
3:D:505:ASN:N	3:D:506:PRO:HD3	2.26	0.51
3:D:781:SER:HB2	4:D:957:HOH:O	2.10	0.51
3:B:402:ASN:HA	3:B:886:ALA:O	2.10	0.51
3:B:589:PHE:HE1	3:B:681:MSE:CE	2.24	0.51
3:B:793:VAL:C	3:B:795:GLY:H	2.18	0.51
3:B:793:VAL:O	3:B:796:PHE:HD2	1.93	0.51
3:C:738:PRO:HG2	3:C:741:VAL:HB	1.93	0.51
3:D:841:PHE:CZ	3:D:861:ASP:HB3	2.44	0.51
1:G:16:DG:H2''	1:G:17:DC:C5'	2.41	0.51
3:B:89:LYS:HB2	3:B:89:LYS:NZ	2.25	0.51
3:B:398:GLU:OE2	3:B:705:LYS:HE3	2.11	0.51
3:C:362:ILE:HD12	3:C:575:PHE:HB2	1.93	0.51
3:C:518:TYR:HA	4:C:1027:HOH:O	2.10	0.51
3:C:620:GLY:HA2	3:C:624:SER:O	2.11	0.51
3:D:354:GLN:HB3	3:D:356:GLN:NE2	2.26	0.51
3:D:599:ARG:O	3:D:603:GLU:HG3	2.11	0.51
3:A:700:GLY:HA2	3:A:753:LEU:CD2	2.41	0.51
3:B:241:ARG:NH2	4:B:1087:HOH:O	2.44	0.51
3:C:572:ASN:HD22	3:C:574:TRP:N	2.07	0.51
3:D:490:LEU:HD23	3:D:490:LEU:C	2.36	0.51
3:D:599:ARG:HB3	3:D:599:ARG:HH11	1.76	0.51
3:A:298:LEU:O	3:A:299:ASN:HB3	2.11	0.50
3:B:787:ASN:C	3:B:789:ALA:N	2.68	0.50
3:C:162:TRP:HB3	3:C:188:TYR:CZ	2.46	0.50
3:D:811:TYR:CZ	3:D:815:ILE:HD11	2.47	0.50
3:D:819:ILE:HG13	3:D:819:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:DA:H2''	1:E:8:DT:O5'	2.12	0.50
2:L:103:DG:H2''	2:L:104:DG:H8	1.74	0.50
3:C:154:SER:C	3:C:156:TYR:H	2.18	0.50
3:D:322:SER:O	3:D:326:ILE:HG23	2.11	0.50
3:A:732:THR:C	3:A:733:GLN:HE21	2.18	0.50
3:A:839:ASN:ND2	3:A:841:PHE:HB2	2.26	0.50
3:B:405:LYS:O	3:B:630:ASP:OD2	2.29	0.50
3:B:522:PHE:HB2	3:B:526:ILE:HD12	1.92	0.50
3:C:133:ILE:HD12	3:C:198:LEU:HD21	1.92	0.50
3:D:64:ASN:ND2	3:D:67:ASP:H	2.09	0.50
3:B:658:ARG:HG2	3:D:897:LEU:HD21	1.94	0.50
3:B:790:LYS:HA	4:B:1052:HOH:O	2.10	0.50
3:C:260:ARG:HG2	3:C:260:ARG:HH11	1.75	0.50
3:D:182:ILE:O	3:D:186:ILE:HG23	2.11	0.50
3:D:381:PRO:O	3:D:576:ARG:HD2	2.11	0.50
2:J:108:DT:H2''	2:J:109:DC:C5'	2.42	0.50
3:A:171:GLN:HE22	3:A:319:ARG:HH12	1.60	0.50
3:A:526:ILE:HA	3:A:529:LYS:HB3	1.92	0.50
3:B:599:ARG:HA	4:B:1083:HOH:O	2.11	0.50
3:C:239:ALA:C	3:C:241:ARG:H	2.20	0.50
3:C:447:ALA:HA	4:C:927:HOH:O	2.11	0.50
1:K:11:DC:H2''	1:K:12:DA:C5'	2.42	0.50
3:A:730:LEU:HD13	3:A:883:PHE:CE1	2.46	0.50
3:D:487:GLY:O	3:D:491:ALA:N	2.37	0.50
2:F:106:DT:C1'	2:F:107:DG:H5''	2.41	0.50
1:K:1:DC:H4'	3:D:572:ASN:ND2	2.27	0.50
3:A:245:HIS:HE1	4:A:949:HOH:O	1.94	0.50
3:A:733:GLN:HE21	3:A:733:GLN:N	2.09	0.50
3:B:608:VAL:HG11	3:D:897:LEU:HD22	1.94	0.50
3:D:479:PHE:CE1	3:D:563:ILE:HD13	2.47	0.50
3:D:484:GLU:C	3:D:486:LYS:N	2.67	0.50
1:I:10:DA:OP1	3:C:874:LYS:HD2	2.11	0.50
2:J:101:DG:H2''	2:J:102:DC:C6	2.46	0.50
3:A:236:GLU:HG2	3:A:240:LYS:HE2	1.93	0.50
3:A:439:LEU:HD22	4:A:988:HOH:O	2.12	0.50
3:B:218:VAL:HG22	3:B:223:ILE:HG13	1.94	0.50
3:B:326:ILE:HG23	3:B:330:ARG:HE	1.76	0.50
3:B:548:THR:C	3:B:550:VAL:H	2.19	0.50
3:D:127:SER:C	3:D:129:ALA:H	2.20	0.50
3:D:488:TYR:O	3:D:552:GLY:HA3	2.11	0.50
2:J:104:DG:H2'	2:J:105:DC:C5	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2:DG:OP2	3:D:361:PRO:HD2	2.11	0.50
3:B:221:PHE:C	3:B:224:PRO:HD2	2.37	0.50
3:C:818:ASN:HD22	3:C:819:ILE:N	2.09	0.50
3:D:144:ASP:OD1	3:D:185:LYS:HD3	2.11	0.50
3:D:854:ILE:HD11	3:D:858:ILE:CD1	2.37	0.50
3:B:413:THR:O	3:B:414:SER:C	2.55	0.49
3:B:471:VAL:O	3:B:475:ILE:HG22	2.11	0.49
3:D:642:ARG:HG2	3:D:646:HIS:CD2	2.46	0.49
3:D:809:LEU:HA	3:D:812:ASN:HD22	1.76	0.49
3:A:154:SER:HB2	3:A:155:PRO:HD2	1.94	0.49
3:A:338:ARG:HB3	3:A:340:PHE:CZ	2.47	0.49
3:C:179:PRO:HB3	3:C:181:GLU:OE1	2.12	0.49
1:E:14:DC:H5"	1:E:14:DC:H6	1.78	0.49
3:B:797:PRO:HG3	3:B:806:ARG:HH12	1.74	0.49
3:D:51:ASP:HB2	4:D:909:HOH:O	2.13	0.49
3:D:380:ILE:HD12	3:D:577:TYR:OH	2.11	0.49
3:B:355:ILE:N	3:B:355:ILE:HD12	2.26	0.49
3:B:116:GLU:CB	3:B:135:ALA:HB3	2.41	0.49
3:B:362:ILE:HD12	3:B:575:PHE:HB2	1.94	0.49
3:D:202:LEU:HD21	3:D:230:ILE:HD13	1.95	0.49
3:D:428:GLU:N	4:D:953:HOH:O	2.44	0.49
3:B:154:SER:CB	3:B:313:ARG:HH12	2.21	0.49
3:B:423:VAL:O	3:B:424:ASN:HB3	2.11	0.49
3:B:486:LYS:O	3:B:489:MSE:HG3	2.12	0.49
3:C:302:LYS:HE2	3:C:326:ILE:HG21	1.94	0.49
3:C:707:ARG:HD3	4:C:905:HOH:O	2.12	0.49
3:D:115:ILE:HD13	3:D:226:VAL:HG23	1.94	0.49
3:A:629:ALA:HA	3:A:632:ILE:HD12	1.94	0.49
3:B:183:ILE:CG2	3:B:184:ASP:N	2.76	0.49
3:B:218:VAL:O	3:B:223:ILE:HG13	2.13	0.49
3:B:499:ILE:HG22	4:B:1054:HOH:O	2.12	0.49
3:B:863:LEU:O	3:B:863:LEU:HD23	2.12	0.49
3:C:167:ALA:O	3:C:176:ASP:O	2.31	0.49
3:C:469:GLY:C	3:C:472:PRO:HD2	2.38	0.49
3:A:415:LEU:O	3:A:419:ILE:HG13	2.13	0.49
3:B:609:CYS:HA	3:B:635:LYS:HE3	1.94	0.49
3:C:272:ASP:OD1	3:C:274:ILE:HG22	2.13	0.49
3:B:645:ASN:HB2	4:B:1063:HOH:O	2.13	0.49
3:B:808:ILE:HD13	3:B:824:VAL:HG11	1.95	0.49
3:D:197:LEU:HD12	3:D:197:LEU:H	1.78	0.49
3:D:285:GLN:NE2	3:D:286:PRO:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:399:PRO:HB3	3:D:619:TYR:CD2	2.41	0.49
2:J:104:DG:H2'	2:J:105:DC:H6	1.73	0.49
3:B:193:ASN:ND2	3:B:193:ASN:C	2.71	0.49
3:B:193:ASN:ND2	3:B:194:GLU:N	2.61	0.49
3:B:792:ASP:CG	3:B:793:VAL:H	2.20	0.49
3:C:61:LEU:HD23	3:C:62:PHE:N	2.28	0.49
3:D:11:ILE:O	3:D:11:ILE:HG23	2.13	0.49
3:B:825:VAL:HB	3:B:828:GLU:CD	2.38	0.48
3:C:3:GLU:HG2	3:C:21:ASP:C	2.38	0.48
3:C:52:ILE:HD12	3:C:428:GLU:CG	2.41	0.48
3:C:471:VAL:HB	3:C:472:PRO:HD3	1.95	0.48
3:C:533:LEU:HB2	3:C:537:SER:HB2	1.95	0.48
3:C:880:LEU:HD22	3:C:884:THR:HG23	1.94	0.48
3:D:274:ILE:HG23	3:D:275:ASP:N	2.27	0.48
3:D:316:ASN:HD22	3:D:316:ASN:H	1.60	0.48
3:D:824:VAL:HG22	3:D:825:VAL:N	2.28	0.48
1:E:12:DA:O3'	3:A:800:LYS:HA	2.14	0.48
3:B:123:PHE:CD1	3:B:124:PRO:HD2	2.48	0.48
3:D:830:VAL:HG22	3:D:831:TYR:N	2.28	0.48
1:G:8:DT:H2"	1:G:9:DG:C8	2.48	0.48
3:A:159:VAL:HG21	3:A:317:HIS:CD2	2.48	0.48
3:A:685:ARG:NH2	3:A:717:GLY:H	2.10	0.48
3:A:739:LYS:H	3:A:739:LYS:HE3	1.78	0.48
3:C:605:LEU:HA	3:C:608:VAL:HG22	1.94	0.48
3:C:347:MSE:HE2	3:C:558:ASN:ND2	2.29	0.48
3:C:410:PHE:HB3	3:C:683:MSE:HG2	1.95	0.48
3:C:416:TYR:HB2	3:C:417:PRO:HD3	1.95	0.48
3:D:116:GLU:CB	3:D:135:ALA:HB3	2.43	0.48
3:A:776:TYR:CD1	3:A:863:LEU:HD11	2.49	0.48
3:B:727:ILE:HG21	3:B:732:THR:CG2	2.43	0.48
3:A:113:PHE:CE1	3:A:218:VAL:CG2	2.97	0.48
3:A:347:MSE:N	4:A:965:HOH:O	2.46	0.48
3:B:415:LEU:HD11	3:B:419:ILE:HD11	1.95	0.48
3:B:597:ILE:HG21	3:B:667:PHE:CE2	2.49	0.48
3:B:734:LYS:O	3:B:735:SER:OG	2.30	0.48
3:B:901:PHE:HB2	3:D:608:VAL:O	2.13	0.48
3:C:34:LYS:HB3	3:C:61:LEU:HD21	1.96	0.48
3:C:149:PHE:CD1	3:C:149:PHE:N	2.81	0.48
3:C:803:PHE:HA	4:C:922:HOH:O	2.14	0.48
3:D:64:ASN:ND2	3:D:66:ARG:H	2.12	0.48
3:D:213:LEU:HD21	3:D:218:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:438:PRO:HG2	3:D:441:ASP:CG	2.37	0.48
3:D:804:HIS:CD2	3:D:805:ILE:HG13	2.48	0.48
3:A:347:MSE:CB	3:A:558:ASN:HD21	2.23	0.48
3:A:405:LYS:O	3:A:690:GLY:HA2	2.13	0.48
3:B:900:MSE:SE	3:D:636:VAL:HA	2.64	0.48
3:C:486:LYS:O	3:C:490:LEU:HG	2.12	0.48
3:D:514:LEU:C	3:D:516:VAL:H	2.21	0.48
3:D:727:ILE:HG13	3:D:732:THR:HG21	1.96	0.48
3:D:732:THR:HG23	4:D:914:HOH:O	2.13	0.48
1:E:3:CTG:O6	1:E:3:CTG:H2'	2.12	0.48
3:A:158:ASN:HD22	3:A:158:ASN:N	2.12	0.48
3:D:316:ASN:HD22	3:D:316:ASN:N	2.11	0.48
2:L:107:DG:H2'	2:L:108:DT:C6	2.49	0.48
3:A:6:LEU:HD11	3:A:26:GLU:HG3	1.95	0.48
3:A:211:VAL:HG21	4:A:957:HOH:O	2.14	0.48
3:B:560:LYS:HE3	4:B:979:HOH:O	2.13	0.48
3:B:642:ARG:H	3:B:646:HIS:CD2	2.31	0.48
3:C:3:GLU:HG2	3:C:22:SER:N	2.29	0.48
3:C:302:LYS:HD2	3:C:323:TYR:CE1	2.48	0.48
3:C:592:MSE:HE1	3:C:674:MSE:HG3	1.96	0.48
3:D:487:GLY:O	3:D:491:ALA:HB3	2.13	0.48
1:K:10:DA:H3'	4:K:146:HOH:O	2.14	0.48
3:A:636:VAL:O	3:A:640:LYS:HG3	2.14	0.48
3:A:706:LYS:O	3:A:707:ARG:HD3	2.14	0.48
3:B:85:MSE:HA	3:B:380:ILE:HD11	1.96	0.48
3:B:163:SER:HB3	3:B:166:ILE:HD12	1.95	0.48
3:B:471:VAL:HB	3:B:472:PRO:CD	2.44	0.48
3:C:104:ASP:OD1	3:C:107:LYS:HG2	2.14	0.48
3:D:62:PHE:HB3	3:D:67:ASP:OD2	2.12	0.48
3:D:503:LEU:O	3:D:506:PRO:HG3	2.13	0.48
1:I:13:DG:H2''	1:I:14:DC:O5'	2.13	0.47
3:C:481:GLN:HE21	3:C:559:ARG:HD2	1.78	0.47
1:E:16:DG:H2''	1:E:17:DC:O5'	2.14	0.47
3:A:502:ALA:O	3:A:506:PRO:HB3	2.14	0.47
3:B:748:CYS:O	3:B:752:MSE:HG3	2.14	0.47
3:C:878:LYS:HB3	3:C:879:PRO:CD	2.45	0.47
3:D:248:THR:HG22	3:D:265:LEU:HA	1.96	0.47
1:G:5:DG:H1'	1:G:6:DA:H5'	1.96	0.47
3:A:489:MSE:C	3:A:491:ALA:N	2.71	0.47
3:B:858:ILE:O	3:B:862:VAL:HG23	2.13	0.47
3:C:667:PHE:HB3	3:C:679:HIS:HE1	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:102:DC:H2''	2:J:103:DG:O5'	2.15	0.47
2:J:111:DT:C2'	2:J:112:DT:C5'	2.79	0.47
3:A:790:LYS:HD3	3:A:791:TYR:CE1	2.49	0.47
3:B:403:ARG:NH1	3:B:887:ALA:O	2.47	0.47
3:C:81:GLU:HG2	3:C:83:LEU:CD2	2.44	0.47
3:D:660:GLU:CB	3:D:661:PRO:HD3	2.43	0.47
1:E:5:DG:H2'	1:E:6:DA:H5''	1.97	0.47
3:B:167:ALA:HA	3:B:176:ASP:HB2	1.97	0.47
3:B:664:ASP:OD2	3:B:668:ARG:NH1	2.48	0.47
3:D:824:VAL:HG22	3:D:825:VAL:H	1.80	0.47
1:G:3:CTG:O6	1:G:3:CTG:H2'	2.15	0.47
3:A:72:ILE:HG22	3:A:76:GLU:OE1	2.15	0.47
3:B:494:ARG:CB	3:B:494:ARG:NH1	2.77	0.47
3:B:787:ASN:C	3:B:789:ALA:H	2.21	0.47
3:C:305:TYR:HB3	3:C:323:TYR:OH	2.14	0.47
3:D:82:ALA:N	3:D:382:GLN:OE1	2.43	0.47
3:D:154:SER:HB3	3:D:155:PRO:CD	2.39	0.47
3:D:530:ILE:HG12	3:D:531:LYS:N	2.29	0.47
3:D:856:ASP:HA	3:D:859:LYS:CB	2.45	0.47
2:H:112:DT:H2''	2:H:113:DC:OP2	2.15	0.47
3:A:202:LEU:O	3:A:206:GLN:HG2	2.15	0.47
3:A:774:LEU:HB3	4:A:1004:HOH:O	2.14	0.47
3:A:797:PRO:N	3:A:809:LEU:HD13	2.30	0.47
3:D:201:TYR:O	3:D:204:PHE:HB3	2.15	0.47
1:I:2:DG:C8	3:C:361:PRO:HG2	2.50	0.47
3:A:413:THR:O	3:A:414:SER:C	2.57	0.47
3:A:822:PRO:HD3	4:A:933:HOH:O	2.15	0.47
3:D:197:LEU:HD12	3:D:197:LEU:N	2.30	0.47
3:D:399:PRO:O	3:D:401:PRO:HD3	2.15	0.47
3:D:685:ARG:C	3:D:685:ARG:HD2	2.40	0.47
3:A:347:MSE:HG2	3:A:358:VAL:HG23	1.96	0.47
3:C:15:ILE:HD11	3:C:92:TYR:CE2	2.49	0.47
3:C:392:PRO:C	3:C:587:THR:HG21	2.39	0.47
3:C:451:SER:OG	3:C:462:MSE:HE3	2.14	0.47
3:D:109:ARG:HD2	3:D:209:THR:O	2.14	0.47
3:D:151:LEU:HD22	3:D:152:LEU:N	2.30	0.47
3:D:170:LEU:HA	3:D:177:GLU:HG2	1.97	0.47
3:D:290:LEU:HD21	3:D:330:ARG:HB2	1.96	0.47
3:D:644:THR:O	3:D:648:VAL:HG23	2.15	0.47
3:D:730:LEU:HD11	3:D:749:ILE:HD13	1.97	0.47
2:H:104:DG:C2'	2:H:105:DC:O5'	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:730:LEU:HD22	3:A:883:PHE:HE1	1.80	0.47
3:B:362:ILE:HD13	3:B:569:ALA:HB1	1.96	0.47
3:D:153:ASN:HA	3:D:158:ASN:OD1	2.15	0.47
3:D:752:MSE:HG2	3:D:889:LEU:HD13	1.97	0.47
1:E:15:DC:H2''	1:E:16:DG:C8	2.50	0.46
3:A:412:LEU:HG	3:A:683:MSE:HG2	1.96	0.46
3:A:607:GLU:O	3:A:607:GLU:HG2	2.14	0.46
3:B:818:ASN:ND2	3:B:857:LEU:CD1	2.78	0.46
3:D:202:LEU:HD21	3:D:230:ILE:CD1	2.45	0.46
3:D:808:ILE:HA	3:D:847:ALA:HB3	1.96	0.46
3:A:357:SER:C	3:A:359:PHE:N	2.72	0.46
3:A:887:ALA:O	3:A:888:LYS:HB2	2.15	0.46
3:B:249:ARG:HG2	3:B:249:ARG:HH11	1.80	0.46
3:B:415:LEU:HD22	3:B:623:ASP:HB3	1.97	0.46
3:B:489:MSE:HE2	3:B:490:LEU:HG	1.97	0.46
3:B:787:ASN:O	3:B:789:ALA:N	2.48	0.46
3:D:386:HIS:HB3	3:D:387:PRO:HD2	1.96	0.46
3:D:818:ASN:C	3:D:820:ASP:H	2.22	0.46
3:A:875:THR:HA	4:A:955:HOH:O	2.15	0.46
3:B:641:PHE:HA	3:B:646:HIS:HD2	1.80	0.46
3:B:732:THR:CG2	3:B:733:GLN:N	2.77	0.46
3:C:448:GLU:O	3:C:449:ARG:C	2.57	0.46
3:D:416:TYR:HB2	3:D:417:PRO:HD3	1.96	0.46
3:A:482:ARG:HH11	3:A:483:LYS:NZ	2.13	0.46
3:C:412:LEU:HD13	3:C:415:LEU:CD1	2.43	0.46
3:C:482:ARG:HD2	3:C:556:GLN:HE21	1.79	0.46
3:C:514:LEU:HD23	3:C:541:MSE:HE1	1.98	0.46
3:D:33:TYR:HB3	3:D:65:MSE:CE	2.45	0.46
3:D:730:LEU:O	3:D:731:GLU:HB2	2.15	0.46
1:K:16:DG:H2''	1:K:17:DC:C5'	2.43	0.46
3:B:312:LEU:HD12	3:B:320:TYR:CB	2.45	0.46
3:B:319:ARG:HA	3:B:319:ARG:HD3	1.73	0.46
3:B:347:MSE:HB2	3:B:558:ASN:HD21	1.80	0.46
3:C:579:ASP:HB3	3:C:582:ASN:HB2	1.96	0.46
1:E:13:DG:P	3:A:800:LYS:HA	2.56	0.46
1:E:14:DC:H2'	1:E:15:DC:C5	2.50	0.46
3:A:326:ILE:O	3:A:330:ARG:HG2	2.15	0.46
3:A:523:SER:HB3	3:A:526:ILE:HG12	1.96	0.46
3:B:285:GLN:HG3	3:B:292:TYR:HE2	1.80	0.46
3:B:386:HIS:HD2	4:B:1064:HOH:O	1.98	0.46
3:C:162:TRP:HB3	3:C:188:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:818:ASN:C	3:C:818:ASN:ND2	2.71	0.46
3:D:10:GLN:H	3:D:89:LYS:HE2	1.80	0.46
3:D:730:LEU:HG	3:D:732:THR:H	1.80	0.46
2:H:105:DC:H2''	2:H:106:DT:H5'	1.98	0.46
3:A:797:PRO:HD3	3:A:809:LEU:HD13	1.98	0.46
3:C:413:THR:O	3:C:414:SER:C	2.59	0.46
3:C:881:GLU:HG3	3:C:891:TYR:CE1	2.44	0.46
3:D:391:TYR:CZ	3:D:583:ALA:HB1	2.51	0.46
3:D:660:GLU:HB3	3:D:661:PRO:HD3	1.96	0.46
1:E:14:DC:H2''	1:E:15:DC:C5'	2.46	0.46
1:K:7:DA:H2'	1:K:8:DT:H6	1.81	0.46
1:K:16:DG:C2'	1:K:17:DC:H5''	2.44	0.46
2:L:101:DG:N3	2:L:102:DC:C5	2.84	0.46
3:A:824:VAL:HG22	3:A:849:PRO:HD3	1.98	0.46
3:B:75:MSE:HE2	3:B:78:ILE:CG2	2.46	0.46
3:B:492:ALA:HB1	3:B:545:ALA:O	2.14	0.46
3:B:702:TRP:CD1	3:B:708:TYR:HB3	2.51	0.46
3:B:811:TYR:O	3:B:815:ILE:HG12	2.16	0.46
3:C:127:SER:HA	3:C:228:ASN:ND2	2.31	0.46
2:J:101:DG:H2''	2:J:102:DC:O5'	2.16	0.46
3:A:514:LEU:HB3	3:A:541:MSE:SE	2.65	0.46
3:B:252:VAL:HG23	3:B:252:VAL:O	2.15	0.46
3:B:747:GLU:OE2	3:B:750:ARG:NH2	2.49	0.46
3:C:526:ILE:HG22	3:C:526:ILE:O	2.15	0.46
3:D:183:ILE:O	3:D:186:ILE:HG12	2.15	0.46
3:D:216:TRP:CZ3	3:D:274:ILE:HD12	2.51	0.46
3:D:394:ALA:HB1	4:D:945:HOH:O	2.15	0.46
1:G:16:DG:H2''	1:G:17:DC:O5'	2.16	0.46
3:A:205:TRP:CE2	3:A:242:LEU:HD12	2.51	0.46
3:A:455:SER:OG	3:A:676:ASN:HA	2.15	0.46
3:A:758:GLU:O	3:A:762:GLU:HG3	2.16	0.46
3:B:9:GLU:HA	3:B:89:LYS:HD2	1.98	0.46
3:B:415:LEU:O	3:B:419:ILE:HG13	2.16	0.46
3:C:347:MSE:CE	3:C:562:LEU:HD13	2.46	0.46
3:C:432:GLY:C	3:C:433:THR:HG23	2.40	0.46
3:C:491:ALA:HB1	3:C:521:ASP:N	2.31	0.46
3:C:750:ARG:NH2	3:C:755:GLU:CD	2.73	0.46
3:D:136:ILE:HD11	3:D:201:TYR:CE2	2.51	0.46
3:D:293:ILE:HG13	3:D:294:SER:N	2.31	0.46
3:D:546:GLN:O	3:D:550:VAL:HG23	2.16	0.46
1:E:12:DA:H61	2:F:106:DT:H3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:691:PRO:HD3	3:A:699:GLY:HA2	1.98	0.45
3:B:347:MSE:SE	3:B:562:LEU:HG	2.66	0.45
3:D:226:VAL:O	3:D:230:ILE:HG13	2.16	0.45
3:D:428:GLU:OE2	3:D:470:VAL:HG12	2.15	0.45
3:D:775:ASN:OD1	3:D:777:ILE:HG12	2.16	0.45
3:A:308:PRO:CG	3:A:311:LYS:HD2	2.47	0.45
3:B:517:ASP:C	3:B:519:ARG:H	2.24	0.45
3:C:167:ALA:HA	3:C:176:ASP:HB3	1.98	0.45
3:C:738:PRO:HG2	3:C:741:VAL:CG2	2.46	0.45
3:C:854:ILE:CG2	3:C:859:LYS:HD3	2.47	0.45
3:D:37:LEU:HD11	3:D:72:ILE:HD11	1.97	0.45
3:D:113:PHE:HE1	3:D:213:LEU:HD21	1.81	0.45
3:D:429:THR:O	3:D:463:TYR:HA	2.16	0.45
3:D:443:ILE:HD13	3:D:595:GLN:CB	2.46	0.45
3:A:495:ASN:ND2	3:A:521:ASP:HA	2.21	0.45
3:B:257:TYR:HE1	3:B:786:ASN:CG	2.24	0.45
3:B:369:ILE:HG12	3:B:474:GLU:HG3	1.98	0.45
3:B:897:LEU:O	3:B:900:MSE:HG3	2.16	0.45
3:C:21:ASP:CG	3:C:25:ARG:HG3	2.40	0.45
3:D:410:PHE:CB	3:D:683:MSE:HE2	2.46	0.45
1:I:5:DG:C2'	1:I:6:DA:H5''	2.46	0.45
3:A:642:ARG:HG3	3:A:646:HIS:CD2	2.52	0.45
3:B:528:GLU:C	3:B:530:ILE:N	2.74	0.45
3:B:792:ASP:CG	3:B:793:VAL:N	2.75	0.45
3:B:835:LEU:HD23	3:B:866:MSE:HA	1.98	0.45
3:B:873:GLU:HA	3:B:877:ILE:HG13	1.98	0.45
3:D:433:THR:N	3:D:462:MSE:HE2	2.31	0.45
3:A:422:GLN:NE2	3:A:680:LEU:H	2.14	0.45
3:A:481:GLN:HA	3:A:484:GLU:HG2	1.99	0.45
3:B:273:TYR:OH	3:B:335:ASP:HA	2.16	0.45
3:B:516:VAL:H	3:B:544:ARG:CZ	2.29	0.45
3:B:600:LYS:NZ	4:B:960:HOH:O	2.49	0.45
3:B:818:ASN:ND2	3:B:857:LEU:HD12	2.32	0.45
3:D:155:PRO:O	3:D:156:TYR:HB2	2.16	0.45
1:E:13:DG:O4'	3:A:800:LYS:HD3	2.16	0.45
3:A:843:ASP:HA	4:A:1009:HOH:O	2.16	0.45
3:A:769:LYS:HD2	4:A:994:HOH:O	2.16	0.45
3:A:810:THR:HG22	4:A:999:HOH:O	2.16	0.45
3:C:578:TYR:CD1	3:C:578:TYR:C	2.95	0.45
3:D:412:LEU:HD23	3:D:683:MSE:HG2	1.99	0.45
3:C:109:ARG:NH1	3:C:140:ASP:OD2	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:660:GLU:HB2	3:C:661:PRO:CD	2.39	0.45
3:D:887:ALA:C	3:D:889:LEU:H	2.25	0.45
1:E:4:DG:OP1	3:A:390:PRO:HA	2.16	0.45
3:A:594:LEU:HD21	3:A:621:ASP:H	1.82	0.45
3:A:810:THR:HG23	3:A:841:PHE:O	2.17	0.45
3:B:193:ASN:ND2	3:B:195:LYS:H	2.14	0.45
3:B:435:LYS:O	3:B:435:LYS:CG	2.64	0.45
3:B:519:ARG:O	3:B:520:PHE:C	2.60	0.45
3:B:897:LEU:C	3:B:899:ASP:H	2.24	0.45
3:D:426:SER:C	3:D:428:GLU:H	2.25	0.45
3:D:533:LEU:HD12	3:D:537:SER:CB	2.47	0.45
3:D:692:PRO:HG3	3:D:713:TRP:HZ2	1.82	0.45
3:D:858:ILE:O	3:D:862:VAL:HG23	2.16	0.45
2:J:104:DG:H2''	2:J:105:DC:O5'	2.17	0.45
1:K:18:DG:O4'	3:A:36:SER:HB2	2.17	0.45
3:A:402:ASN:HA	3:A:886:ALA:O	2.17	0.45
3:A:471:VAL:HG11	3:A:570:LEU:HD11	1.99	0.45
3:A:491:ALA:C	3:A:493:GLN:N	2.75	0.45
3:B:901:PHE:HD2	3:D:635:LYS:HG2	1.82	0.45
3:D:709:ALA:HB1	3:D:727:ILE:HG22	1.99	0.45
3:D:786:ASN:OD1	3:D:805:ILE:HD11	2.17	0.45
1:G:5:DG:H2''	1:G:6:DA:O5'	2.17	0.44
1:I:7:DA:H2'	1:I:8:DT:H71	1.98	0.44
3:A:71:TRP:CZ2	3:A:75:MSE:HE2	2.53	0.44
3:B:113:PHE:CE1	3:B:218:VAL:CG2	3.00	0.44
3:B:181:GLU:CD	3:B:181:GLU:H	2.25	0.44
3:B:735:SER:HB2	3:B:737:THR:HG23	1.97	0.44
3:C:425:ILE:HG23	3:C:463:TYR:CE2	2.52	0.44
3:D:289:SER:HB2	3:D:292:TYR:CB	2.47	0.44
3:D:470:VAL:HG13	3:D:471:VAL:H	1.81	0.44
3:D:645:ASN:CG	3:D:719:ARG:HH21	2.24	0.44
1:I:11:DC:H2''	1:I:12:DA:O5'	2.18	0.44
2:J:109:DC:O4'	3:C:800:LYS:NZ	2.50	0.44
3:A:747:GLU:HA	4:A:916:HOH:O	2.16	0.44
3:B:435:LYS:HG3	4:B:1082:HOH:O	2.16	0.44
3:B:751:ARG:NE	3:B:763:TYR:HB2	2.33	0.44
3:B:872:LEU:HD12	3:B:876:PHE:HB3	1.99	0.44
3:C:154:SER:C	3:C:156:TYR:N	2.75	0.44
3:C:414:SER:O	3:C:415:LEU:C	2.59	0.44
3:D:240:LYS:HE2	3:D:248:THR:OG1	2.16	0.44
3:D:250:VAL:HG22	3:D:263:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:111:DT:H2''	2:F:112:DT:H5''	1.99	0.44
2:F:112:DT:H1'	2:F:113:DC:H5'	1.99	0.44
3:A:15:ILE:HG12	3:A:65:MSE:HE1	2.00	0.44
3:B:421:ARG:HB3	3:B:680:LEU:CD1	2.47	0.44
3:B:608:VAL:HG13	3:D:897:LEU:HB2	1.99	0.44
3:C:214:THR:OG1	3:C:215:GLY:N	2.50	0.44
3:D:33:TYR:HB3	3:D:65:MSE:HE1	1.99	0.44
3:D:741:VAL:O	3:D:745:LEU:HD13	2.18	0.44
2:H:111:DT:H2''	2:H:112:DT:C5'	2.47	0.44
3:B:408:MSE:CE	3:B:655:ALA:HB2	2.45	0.44
3:B:735:SER:C	3:B:737:THR:H	2.26	0.44
3:C:558:ASN:HD22	3:C:558:ASN:HA	1.62	0.44
3:C:738:PRO:HB3	3:C:780:ALA:O	2.18	0.44
3:D:150:ASP:HB3	3:D:188:TYR:CE1	2.53	0.44
3:D:434:PHE:CE1	3:D:460:GLY:HA2	2.53	0.44
3:A:176:ASP:OD2	3:A:318:GLN:NE2	2.51	0.44
3:A:406:TYR:CD2	3:A:633:ILE:HG13	2.53	0.44
3:A:553:MSE:HA	3:A:556:GLN:OE1	2.18	0.44
3:A:641:PHE:HA	3:A:646:HIS:CD2	2.52	0.44
3:A:715:MSE:O	3:A:716:GLU:HB2	2.18	0.44
3:B:257:TYR:CD2	3:B:257:TYR:N	2.85	0.44
3:D:243:SER:C	3:D:245:HIS:H	2.25	0.44
3:D:290:LEU:HD23	3:D:290:LEU:O	2.16	0.44
3:D:873:GLU:HB3	3:D:877:ILE:HD11	2.00	0.44
3:A:787:ASN:N	3:A:826:GLU:OE1	2.47	0.44
3:A:854:ILE:HG23	3:A:859:LYS:HB2	2.00	0.44
3:B:734:LYS:C	3:B:735:SER:HG	2.26	0.44
3:B:735:SER:C	4:B:1001:HOH:O	2.60	0.44
3:D:434:PHE:CE2	3:D:450:PRO:HB3	2.53	0.44
3:A:539:ASN:HD22	3:A:539:ASN:HA	1.61	0.44
3:A:800:LYS:HB2	3:A:800:LYS:HZ2	1.82	0.44
3:B:270:VAL:O	3:B:271:LEU:HD12	2.18	0.44
3:B:818:ASN:HD22	3:B:857:LEU:HD13	1.82	0.44
3:C:198:LEU:O	3:C:202:LEU:HB2	2.18	0.44
3:C:71:TRP:O	3:C:75:MSE:HG2	2.17	0.44
3:C:83:LEU:HB3	3:C:379:VAL:CG1	2.48	0.44
3:C:154:SER:O	3:C:156:TYR:N	2.51	0.44
3:C:284:ASN:ND2	3:C:829:LYS:NZ	2.66	0.44
3:C:491:ALA:O	3:C:495:ASN:HB2	2.18	0.44
3:D:151:LEU:HD23	3:D:191:PHE:O	2.18	0.44
1:I:15:DC:H2''	1:I:16:DG:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:112:DT:H2''	2:L:113:DC:C4'	2.47	0.44
3:A:357:SER:C	3:A:359:PHE:H	2.26	0.44
3:A:777:ILE:HD13	3:A:848:TRP:HZ2	1.83	0.44
3:C:482:ARG:O	3:C:484:GLU:N	2.50	0.44
3:D:8:VAL:HG11	3:D:93:LEU:CD1	2.46	0.44
3:D:314:GLU:HG3	3:D:314:GLU:O	2.18	0.44
3:D:481:GLN:HB3	3:D:559:ARG:HE	1.83	0.44
3:D:749:ILE:O	3:D:753:LEU:HG	2.18	0.44
3:D:848:TRP:CB	4:D:932:HOH:O	2.65	0.44
2:F:113:DC:H2''	2:F:114:DC:OP2	2.18	0.43
1:G:15:DC:H5'	1:G:15:DC:H6	1.81	0.43
2:J:105:DC:H2''	2:J:106:DT:O5'	2.17	0.43
3:B:686:GLU:HG3	3:B:715:MSE:SE	2.68	0.43
3:D:499:ILE:O	3:D:502:ALA:HB3	2.18	0.43
3:D:602:ASN:HD21	3:D:617:VAL:CG2	2.31	0.43
3:D:685:ARG:HD2	3:D:686:GLU:N	2.33	0.43
3:D:849:PRO:HG2	3:D:852:THR:OG1	2.18	0.43
3:D:853:GLU:O	3:D:854:ILE:HB	2.18	0.43
3:A:3:GLU:HG3	3:A:21:ASP:C	2.42	0.43
3:A:218:VAL:HG23	3:A:222:ALA:CB	2.46	0.43
3:A:734:LYS:HG2	3:A:736:SER:OG	2.17	0.43
3:A:814:ALA:HB1	3:A:858:ILE:HG21	2.00	0.43
3:B:494:ARG:NH1	3:B:494:ARG:HB2	2.33	0.43
3:B:606:ASN:HA	3:B:611:THR:OG1	2.19	0.43
3:A:516:VAL:HG22	3:A:517:ASP:N	2.33	0.43
3:A:737:THR:O	3:A:742:GLN:NE2	2.51	0.43
3:B:901:PHE:CD2	3:D:635:LYS:HG2	2.53	0.43
3:C:864:HIS:HD2	3:C:865:TRP:NE1	2.16	0.43
3:D:147:TYR:HA	3:D:187:ILE:CG2	2.48	0.43
3:D:487:GLY:HA2	3:D:490:LEU:HB3	2.00	0.43
3:D:694:GLY:O	3:D:695:SER:C	2.61	0.43
3:B:791:TYR:CD1	3:B:809:LEU:HD22	2.53	0.43
3:C:227:TYR:HD1	3:C:242:LEU:HD12	1.82	0.43
3:C:283:THR:HG23	3:C:283:THR:O	2.17	0.43
3:D:503:LEU:HA	3:D:538:LEU:HD13	2.01	0.43
3:D:700:GLY:HA2	3:D:753:LEU:CD2	2.44	0.43
3:A:83:LEU:HD12	3:A:83:LEU:N	2.31	0.43
3:A:401:PRO:O	3:A:402:ASN:HB2	2.17	0.43
3:B:604:TYR:O	3:B:608:VAL:HG23	2.17	0.43
3:B:643:ASP:OD2	3:B:646:HIS:HB2	2.18	0.43
3:B:660:GLU:CB	3:B:661:PRO:HD3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:792:ASP:C	3:B:794:GLY:H	2.26	0.43
3:B:878:LYS:HB3	3:B:879:PRO:CD	2.48	0.43
3:C:685:ARG:HD2	3:C:685:ARG:C	2.44	0.43
3:D:485:HIS:N	4:D:918:HOH:O	2.51	0.43
3:D:497:GLU:C	3:D:499:ILE:N	2.75	0.43
3:D:730:LEU:HB2	3:D:883:PHE:CE2	2.54	0.43
3:D:744:ALA:HB1	3:D:876:PHE:CE1	2.54	0.43
2:H:105:DC:H2'	2:H:106:DT:C6	2.53	0.43
3:A:36:SER:O	3:A:37:LEU:HD12	2.19	0.43
3:B:51:ASP:C	3:B:51:ASP:OD1	2.60	0.43
3:B:643:ASP:HB2	4:B:1024:HOH:O	2.18	0.43
3:B:834:PRO:O	3:B:866:MSE:HA	2.19	0.43
3:D:181:GLU:O	3:D:185:LYS:HD2	2.18	0.43
3:D:370:PHE:CD2	3:D:370:PHE:C	2.97	0.43
3:D:427:PRO:C	4:D:953:HOH:O	2.61	0.43
3:D:437:ALA:HB3	3:D:442:TYR:CE2	2.54	0.43
2:H:105:DC:H2''	2:H:106:DT:C5'	2.49	0.43
1:I:2:DG:P	3:C:361:PRO:HD2	2.59	0.43
3:A:606:ASN:OD1	3:A:616:PHE:CE1	2.69	0.43
3:B:668:ARG:HG3	3:B:668:ARG:NH1	2.30	0.43
3:C:25:ARG:HH21	3:C:27:ARG:HG2	1.84	0.43
3:D:228:ASN:HA	3:D:231:LYS:HD3	2.00	0.43
3:D:408:MSE:HE1	3:D:659:MSE:SE	2.69	0.43
3:D:493:GLN:C	4:D:939:HOH:O	2.60	0.43
3:D:738:PRO:HG2	3:D:741:VAL:HG23	2.00	0.43
3:D:846:ILE:HG21	3:D:862:VAL:CG1	2.48	0.43
2:H:114:DC:O2	3:B:706:LYS:NZ	2.52	0.43
1:K:6:DA:H5''	3:D:705:LYS:HD3	1.99	0.43
3:A:150:ASP:OD1	3:A:188:TYR:OH	2.30	0.43
3:A:386:HIS:HA	3:A:387:PRO:HD3	1.88	0.43
3:A:830:VAL:HG12	3:A:849:PRO:HA	2.01	0.43
3:B:145:ARG:HA	3:B:145:ARG:HD3	1.75	0.43
3:B:656:ARG:HD3	4:B:970:HOH:O	2.18	0.43
3:C:112:ASN:ND2	3:C:332:LEU:CD1	2.80	0.43
3:D:140:ASP:OD2	3:D:142:ILE:HD11	2.18	0.43
3:D:641:PHE:HB3	3:D:646:HIS:HB3	2.00	0.43
3:D:835:LEU:HA	3:D:865:TRP:O	2.19	0.43
3:A:41:CYS:O	3:A:56:PRO:HG2	2.19	0.43
3:A:199:MSE:HG2	3:A:234:PHE:CZ	2.53	0.43
3:A:353:ILE:HG21	3:A:367:ALA:HB2	2.01	0.43
3:B:541:MSE:CE	3:B:544:ARG:NH2	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:ASP:CG	3:C:64:ASN:HB2	2.44	0.43
3:C:818:ASN:ND2	3:C:820:ASP:H	2.16	0.43
3:C:878:LYS:HB3	3:C:879:PRO:HD3	2.00	0.43
3:D:421:ARG:HD2	3:D:475:ILE:HG23	2.01	0.43
3:D:485:HIS:C	3:D:487:GLY:N	2.77	0.43
2:J:101:DG:H8	2:J:101:DG:O5'	2.02	0.43
3:B:643:ASP:HA	3:B:693:LEU:HD23	2.00	0.43
3:B:698:ILE:HG12	3:B:752:MSE:O	2.19	0.43
3:C:240:LYS:O	3:C:246:ARG:HA	2.18	0.43
3:D:312:LEU:HG	3:D:320:TYR:CD2	2.54	0.43
3:D:511:ASP:OD1	3:D:536:LYS:HG2	2.18	0.43
3:D:642:ARG:H	3:D:646:HIS:HD2	1.67	0.43
3:D:710:LEU:HA	3:D:753:LEU:HD13	2.01	0.43
1:E:15:DC:H2''	1:E:16:DG:O5'	2.18	0.42
2:H:107:DG:H1'	2:H:108:DT:H5'	2.01	0.42
1:K:4:DG:H2'	1:K:5:DG:H8	1.84	0.42
2:L:113:DC:H2''	2:L:114:DC:O5'	2.19	0.42
3:A:17:GLU:O	3:A:28:THR:HA	2.19	0.42
3:A:422:GLN:HG3	3:A:678:GLN:O	2.19	0.42
3:A:785:ALA:HB2	3:A:808:ILE:HD11	1.99	0.42
3:B:19:TYR:HE1	3:B:29:ARG:HG2	1.84	0.42
3:B:423:VAL:O	3:B:424:ASN:CB	2.67	0.42
3:C:123:PHE:CD1	3:C:124:PRO:HD2	2.54	0.42
3:C:239:ALA:C	3:C:241:ARG:N	2.76	0.42
3:D:499:ILE:HD11	3:D:522:PHE:CE1	2.54	0.42
3:D:747:GLU:OE2	3:D:747:GLU:HA	2.19	0.42
2:J:107:DG:H2''	2:J:108:DT:O5'	2.19	0.42
2:J:113:DC:H2'	2:J:114:DC:C6	2.54	0.42
3:A:388:VAL:O	3:A:388:VAL:HG23	2.19	0.42
3:A:411:ASP:O	3:A:683:MSE:HA	2.19	0.42
3:A:532:LYS:O	3:A:533:LEU:HD22	2.18	0.42
3:A:728:MSE:HE2	3:A:728:MSE:HA	2.01	0.42
3:B:782:VAL:HG12	3:B:783:SER:N	2.33	0.42
3:D:564:ASN:N	3:D:564:ASN:HD22	2.15	0.42
3:D:715:MSE:O	3:D:716:GLU:HB2	2.18	0.42
1:E:2:DG:H2''	1:E:3:CTG:OP2	2.19	0.42
1:E:9:DG:N2	4:E:449:HOH:O	2.52	0.42
2:H:111:DT:H2''	2:H:112:DT:O5'	2.19	0.42
3:A:3:GLU:CG	3:A:21:ASP:HA	2.49	0.42
3:A:514:LEU:HD23	3:A:533:LEU:HD21	2.00	0.42
3:A:802:PRO:HG2	3:A:805:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:836:ARG:HG3	3:A:836:ARG:HH11	1.84	0.42
3:C:200:GLU:OE2	3:C:200:GLU:HA	2.19	0.42
3:C:350:TYR:OH	3:C:481:GLN:NE2	2.43	0.42
3:D:423:VAL:O	3:D:423:VAL:HG12	2.19	0.42
3:D:500:LYS:HA	4:D:942:HOH:O	2.19	0.42
3:D:743:LYS:HA	4:D:951:HOH:O	2.19	0.42
1:E:6:DA:OP1	3:A:705:LYS:NZ	2.52	0.42
1:K:14:DC:C4	1:K:15:DC:N4	2.88	0.42
3:A:10:GLN:HG3	3:A:65:MSE:SE	2.68	0.42
3:A:597:ILE:HD12	3:A:597:ILE:HA	1.82	0.42
3:B:176:ASP:O	3:B:177:GLU:C	2.62	0.42
3:C:176:ASP:OD1	3:C:318:GLN:HG3	2.20	0.42
3:C:799:PRO:HD2	4:C:952:HOH:O	2.19	0.42
3:D:707:ARG:HA	3:D:729:GLY:HA3	2.02	0.42
3:D:785:ALA:HB3	3:D:827:GLY:H	1.84	0.42
1:K:5:DG:P	3:D:393:GLY:H	2.43	0.42
3:A:21:ASP:C	3:A:21:ASP:OD2	2.62	0.42
3:A:573:VAL:HG12	3:A:578:TYR:CZ	2.54	0.42
3:B:75:MSE:CE	3:B:80:LEU:HD12	2.50	0.42
3:B:857:LEU:O	3:B:857:LEU:HD23	2.18	0.42
3:C:402:ASN:HA	3:C:886:ALA:O	2.20	0.42
3:D:323:TYR:HA	3:D:326:ILE:HG12	2.02	0.42
3:D:472:PRO:O	3:D:475:ILE:HG22	2.20	0.42
3:D:810:THR:HG23	3:D:841:PHE:O	2.19	0.42
3:A:476:THR:HG22	3:A:480:ASN:ND2	2.34	0.42
3:A:519:ARG:HA	3:A:548:THR:HG21	2.01	0.42
3:B:238:THR:O	3:B:241:ARG:HB2	2.20	0.42
3:B:362:ILE:CD1	3:B:575:PHE:HB2	2.49	0.42
3:B:515:ASP:HA	3:B:544:ARG:HH12	1.85	0.42
3:B:725:LEU:HD11	3:B:750:ARG:HG2	2.02	0.42
3:C:85:MSE:HA	3:C:380:ILE:HD11	2.00	0.42
3:C:354:GLN:HB3	3:C:356:GLN:OE1	2.18	0.42
3:C:642:ARG:HG3	3:C:646:HIS:CD2	2.55	0.42
3:D:6:LEU:HB2	3:D:18:ARG:O	2.19	0.42
3:D:6:LEU:HD21	3:D:108:ILE:HG12	2.00	0.42
3:D:298:LEU:HD13	3:D:333:GLN:OE1	2.20	0.42
3:D:485:HIS:C	3:D:487:GLY:H	2.26	0.42
3:D:824:VAL:HG13	3:D:826:GLU:H	1.84	0.42
1:E:13:DG:P	3:A:800:LYS:HG2	2.60	0.42
2:H:101:DG:H2''	2:H:102:DC:O5'	2.18	0.42
1:I:9:DG:H1'	1:I:10:DA:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:113:PHE:CE1	3:B:218:VAL:HG21	2.54	0.42
3:B:421:ARG:HG2	3:B:421:ARG:HH11	1.85	0.42
3:B:479:PHE:CE2	3:B:563:ILE:HD13	2.54	0.42
3:C:83:LEU:HD22	3:C:83:LEU:N	2.34	0.42
3:C:472:PRO:O	3:C:475:ILE:HG22	2.20	0.42
3:C:656:ARG:HA	3:C:660:GLU:CG	2.48	0.42
3:D:205:TRP:HH2	3:D:213:LEU:HD12	1.84	0.42
3:D:373:LEU:HD12	3:D:380:ILE:CD1	2.49	0.42
3:D:456:CYS:SG	3:D:462:MSE:HG2	2.60	0.42
3:D:770:GLU:O	3:D:774:LEU:HD23	2.19	0.42
3:D:811:TYR:O	3:D:814:ALA:HB3	2.20	0.42
1:I:11:DC:H5'	1:I:11:DC:H6	1.85	0.42
3:B:283:THR:HG23	3:B:283:THR:O	2.20	0.42
3:B:655:ALA:HA	3:B:659:MSE:HB2	2.01	0.42
3:C:423:VAL:HB	3:C:425:ILE:HG13	2.02	0.42
3:C:529:LYS:HE3	4:C:1047:HOH:O	2.20	0.42
3:D:231:LYS:C	3:D:233:ILE:H	2.27	0.42
1:G:15:DC:H2''	1:G:16:DG:O5'	2.20	0.42
3:A:181:GLU:H	3:A:181:GLU:CD	2.25	0.42
3:A:254:GLU:OE1	3:A:259:SER:HB2	2.20	0.42
3:A:494:ARG:NH2	3:A:521:ASP:OD1	2.53	0.42
3:A:789:ALA:HA	3:A:792:ASP:HB3	2.01	0.42
3:C:482:ARG:CD	3:C:556:GLN:HE21	2.33	0.42
3:C:605:LEU:HD21	3:C:659:MSE:HE3	2.02	0.42
3:C:898:PHE:N	3:C:898:PHE:CD2	2.83	0.42
3:D:262:ILE:N	3:D:262:ILE:CD1	2.82	0.42
3:D:859:LYS:O	3:D:863:LEU:HD13	2.20	0.42
3:A:775:ASN:HB3	3:A:778:SER:OG	2.20	0.42
3:B:466:ASP:OD1	3:B:466:ASP:N	2.53	0.42
3:B:790:LYS:HE2	3:B:801:CYS:HA	2.02	0.42
3:C:38:PHE:CD1	3:C:38:PHE:N	2.87	0.42
3:D:72:ILE:HG22	3:D:76:GLU:OE2	2.20	0.42
3:D:148:VAL:HG21	3:D:325:ILE:CD1	2.50	0.42
3:D:431:ALA:HA	3:D:464:TYR:CE1	2.55	0.42
2:F:109:DC:H2''	2:F:110:DA:O5'	2.20	0.41
2:H:113:DC:O5'	3:B:734:LYS:O	2.37	0.41
3:A:338:ARG:HD2	3:A:340:PHE:CZ	2.54	0.41
3:B:119:SER:HA	3:B:120:PRO:HD2	1.91	0.41
3:B:326:ILE:HG22	3:B:330:ARG:HG2	2.02	0.41
3:C:235:GLY:O	3:C:236:GLU:C	2.63	0.41
3:C:503:LEU:HD21	3:C:538:LEU:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:96:THR:HB	3:D:97:TYR:CD1	2.54	0.41
3:D:214:THR:CG2	3:D:215:GLY:H	2.11	0.41
3:D:352:LYS:O	3:D:353:ILE:HG23	2.19	0.41
3:D:368:ILE:CD1	3:D:562:LEU:HD21	2.50	0.41
3:D:489:MSE:CE	3:D:490:LEU:HB2	2.39	0.41
3:D:492:ALA:HA	3:D:495:ASN:HB2	2.02	0.41
3:D:779:ILE:CD1	3:D:866:MSE:HE1	2.45	0.41
1:G:6:DA:H1'	1:G:7:DA:C8	2.55	0.41
3:A:466:ASP:CG	3:A:467:ARG:H	2.28	0.41
3:C:510:VAL:O	3:C:533:LEU:HB3	2.19	0.41
3:A:120:PRO:HG2	3:A:156:TYR:CE1	2.55	0.41
3:B:195:LYS:O	3:B:199:MSE:HB2	2.20	0.41
3:B:355:ILE:N	3:B:355:ILE:CD1	2.83	0.41
3:C:171:GLN:C	3:C:173:GLN:H	2.26	0.41
3:C:239:ALA:O	3:C:241:ARG:N	2.53	0.41
3:C:501:GLU:C	3:C:503:LEU:H	2.28	0.41
3:A:51:ASP:HA	3:A:379:VAL:HG22	2.01	0.41
3:A:101:ILE:CG2	3:A:349:TYR:HB3	2.50	0.41
3:A:382:GLN:HE21	3:A:382:GLN:HB3	1.62	0.41
3:A:797:PRO:CD	3:A:809:LEU:HD13	2.50	0.41
3:B:380:ILE:HD12	3:B:576:ARG:CZ	2.50	0.41
3:B:404:TYR:CD1	3:B:618:LEU:HD22	2.55	0.41
3:B:489:MSE:SE	3:B:553:MSE:SE	3.38	0.41
3:B:546:GLN:C	3:B:548:THR:N	2.78	0.41
3:C:458:PRO:CG	3:C:592:MSE:SE	3.18	0.41
3:D:5:TYR:HB3	3:D:97:TYR:CE1	2.55	0.41
3:D:146:PHE:CE2	3:D:182:ILE:HG13	2.55	0.41
3:A:423:VAL:O	3:A:423:VAL:HG12	2.19	0.41
3:A:478:VAL:HG13	3:A:559:ARG:HD2	2.01	0.41
3:A:702:TRP:NE1	3:A:708:TYR:CD1	2.88	0.41
3:B:291:ASP:HA	3:B:302:LYS:HG3	2.02	0.41
3:B:579:ASP:OD1	3:B:581:ARG:HB2	2.20	0.41
3:C:364:THR:O	3:C:368:ILE:HG13	2.21	0.41
3:C:467:ARG:H	3:C:467:ARG:CD	2.31	0.41
3:D:827:GLY:HA2	4:D:921:HOH:O	2.21	0.41
2:F:102:DC:H1'	2:F:103:DG:C8	2.55	0.41
1:G:15:DC:H2''	1:G:16:DG:C8	2.55	0.41
2:L:104:DG:H1'	2:L:105:DC:O4'	2.20	0.41
3:A:100:GLU:CG	3:A:102:LYS:HE2	2.44	0.41
3:A:104:ASP:OD2	3:A:106:THR:HB	2.20	0.41
3:A:129:ALA:HA	3:A:225:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:212:ILE:HD13	3:A:269:SER:HB2	2.02	0.41
3:A:466:ASP:N	3:A:466:ASP:OD2	2.53	0.41
3:A:804:HIS:O	3:A:808:ILE:HG13	2.20	0.41
3:B:516:VAL:HB	3:B:544:ARG:NH2	2.36	0.41
3:C:546:GLN:O	3:C:550:VAL:HG23	2.21	0.41
3:C:854:ILE:HD13	3:C:862:VAL:HG21	2.03	0.41
3:D:621:ASP:O	3:D:622:THR:HB	2.19	0.41
3:A:507:ASN:O	3:A:508:LEU:HD22	2.17	0.41
3:B:82:ALA:O	3:B:382:GLN:HG3	2.21	0.41
3:B:209:THR:HA	3:B:210:PRO:HD3	1.94	0.41
3:B:444:ASN:HA	3:B:599:ARG:NE	2.35	0.41
3:C:9:GLU:OE2	3:C:266:PHE:HA	2.20	0.41
3:C:802:PRO:HB2	3:C:805:ILE:HG12	2.03	0.41
2:F:101:DG:H2''	2:F:102:DC:C6	2.55	0.41
3:A:216:TRP:O	3:A:217:ASN:HB2	2.21	0.41
3:A:739:LYS:CD	3:A:778:SER:HA	2.42	0.41
3:A:811:TYR:O	3:A:815:ILE:HG12	2.20	0.41
3:B:109:ARG:HB2	3:B:109:ARG:HH11	1.86	0.41
3:B:435:LYS:N	3:B:435:LYS:CD	2.82	0.41
3:B:492:ALA:HB1	3:B:549:GLU:HB2	2.02	0.41
3:C:243:SER:C	3:C:245:HIS:H	2.29	0.41
3:C:458:PRO:HG2	3:C:592:MSE:SE	2.71	0.41
3:D:6:LEU:CD2	3:D:108:ILE:HG12	2.51	0.41
3:D:429:THR:O	3:D:464:TYR:HD1	2.03	0.41
3:D:433:THR:OG1	3:D:434:PHE:N	2.53	0.41
3:A:21:ASP:OD1	3:A:25:ARG:HG2	2.20	0.41
3:A:41:CYS:HB3	3:A:58:THR:HG22	2.01	0.41
3:A:273:TYR:OH	3:A:335:ASP:HA	2.20	0.41
3:A:308:PRO:HG3	3:A:311:LYS:HD2	2.03	0.41
3:B:25:ARG:O	3:B:27:ARG:HG2	2.21	0.41
3:B:294:SER:CB	3:B:301:GLY:HA2	2.49	0.41
3:B:485:HIS:HA	3:B:488:TYR:CD2	2.56	0.41
3:B:731:GLU:OE2	3:B:731:GLU:N	2.38	0.41
3:C:82:ALA:O	3:C:382:GLN:HB2	2.21	0.41
3:C:891:TYR:CD2	3:C:892:GLU:HG3	2.55	0.41
3:D:51:ASP:C	3:D:53:TYR:H	2.29	0.41
3:D:228:ASN:HD22	3:D:231:LYS:HD3	1.86	0.41
3:D:657:GLU:O	3:D:661:PRO:HG2	2.21	0.41
2:F:105:DC:H2'	2:F:106:DT:H72	2.03	0.41
1:I:8:DT:P	4:I:192:HOH:O	2.79	0.41
1:I:12:DA:H2''	1:I:13:DG:N7	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:125:GLU:HA	3:A:126:PRO:HD3	1.91	0.41
3:A:204:PHE:CE1	3:A:208:LYS:HD2	2.56	0.41
3:A:395:PHE:CE2	3:A:595:GLN:HG2	2.56	0.41
3:B:19:TYR:CE1	3:B:29:ARG:HG2	2.56	0.41
3:B:320:TYR:O	3:B:323:TYR:HB3	2.21	0.41
3:B:554:THR:O	3:B:558:ASN:HB2	2.21	0.41
3:B:818:ASN:HD22	3:B:821:ALA:HB2	1.83	0.41
3:B:897:LEU:C	3:B:899:ASP:N	2.79	0.41
3:C:9:GLU:HG3	3:C:267:GLY:N	2.36	0.41
3:D:155:PRO:C	3:D:157:GLY:N	2.77	0.41
3:D:346:ASP:OD2	3:D:554:THR:HG22	2.22	0.41
3:D:668:ARG:HB2	3:D:668:ARG:CZ	2.51	0.41
3:A:405:LYS:O	3:A:699:GLY:HA3	2.22	0.40
3:B:33:TYR:O	3:B:35:PRO:HD3	2.21	0.40
3:B:412:LEU:HA	3:B:682:PHE:O	2.21	0.40
3:C:109:ARG:HD2	3:C:209:THR:O	2.21	0.40
3:C:202:LEU:O	3:C:206:GLN:HG2	2.20	0.40
3:C:433:THR:O	3:C:462:MSE:SE	2.88	0.40
3:C:505:ASN:N	3:C:506:PRO:HD3	2.36	0.40
3:D:702:TRP:NE1	3:D:708:TYR:HB3	2.35	0.40
1:G:12:DA:H2''	1:G:13:DG:O5'	2.21	0.40
1:K:6:DA:C2	1:K:7:DA:N6	2.90	0.40
3:A:176:ASP:HA	3:A:319:ARG:NH2	2.27	0.40
3:A:294:SER:HB3	3:A:301:GLY:HA2	2.03	0.40
3:A:438:PRO:O	3:A:439:LEU:C	2.65	0.40
3:B:379:VAL:O	3:B:379:VAL:HG13	2.21	0.40
3:B:593:ALA:HB2	3:B:681:MSE:HE3	2.00	0.40
3:C:454:TYR:HD2	3:C:462:MSE:CE	2.27	0.40
3:D:508:LEU:N	3:D:508:LEU:HD22	2.36	0.40
3:D:518:TYR:C	3:D:520:PHE:N	2.77	0.40
1:K:8:DT:C2'	1:K:9:DG:C8	2.99	0.40
2:L:101:DG:H2'	2:L:102:DC:C5	2.57	0.40
3:A:457:SER:HA	3:A:458:PRO:HD3	1.94	0.40
3:C:614:GLU:HB2	3:C:616:PHE:HE1	1.86	0.40
1:G:8:DT:H5'	1:G:8:DT:H6	1.86	0.40
1:I:15:DC:C2'	1:I:16:DG:H5'	2.33	0.40
3:A:494:ARG:HE	3:A:494:ARG:HB2	1.75	0.40
3:A:514:LEU:HD13	3:A:515:ASP:N	2.36	0.40
3:A:660:GLU:HB2	3:A:661:PRO:CD	2.42	0.40
3:B:686:GLU:OE2	3:B:716:GLU:CD	2.65	0.40
3:B:901:PHE:HB2	3:B:902:ASP:H	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:257:TYR:CD2	3:C:257:TYR:N	2.86	0.40
3:C:302:LYS:HD2	3:C:323:TYR:CD1	2.56	0.40
3:D:157:GLY:O	3:D:158:ASN:HB3	2.21	0.40
3:D:433:THR:O	3:D:462:MSE:HE2	2.21	0.40
3:D:730:LEU:N	4:D:925:HOH:O	2.54	0.40
2:H:110:DA:C2'	2:H:111:DT:C5'	2.98	0.40
1:K:11:DC:N3	2:L:107:DG:O6	2.55	0.40
3:A:397:LYS:O	3:A:399:PRO:HD3	2.21	0.40
3:B:397:LYS:O	3:B:399:PRO:HD3	2.21	0.40
3:B:518:TYR:CB	3:B:544:ARG:HG2	2.52	0.40
3:B:597:ILE:HD13	3:B:625:ILE:HD13	2.02	0.40
3:B:857:LEU:CD2	3:B:858:ILE:HG23	2.52	0.40
3:C:209:THR:HA	3:C:210:PRO:HD3	1.85	0.40
3:C:392:PRO:O	3:C:587:THR:CG2	2.62	0.40
3:C:772:ARG:HH11	3:C:772:ARG:HG3	1.87	0.40
3:D:188:TYR:CE2	3:D:190:PRO:HD3	2.55	0.40

There are no symmetry-related clashes.

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	
3	A	900/903 (100%)	804 (89%)	84 (9%)	12 (1%)	9	16
3	B	884/903 (98%)	802 (91%)	70 (8%)	12 (1%)	9	14
3	C	898/903 (99%)	830 (92%)	56 (6%)	12 (1%)	9	16
3	D	886/903 (98%)	701 (79%)	131 (15%)	54 (6%)	1	1
All	All	3568/3612 (99%)	3137 (88%)	341 (10%)	90 (2%)	4	7

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	519	ARG
3	A	611	THR
3	A	621	ASP
3	B	177	GLU
3	C	256	MSE
3	C	458	PRO
3	C	899	ASP
3	D	44	SER
3	D	170	LEU
3	D	265	LEU
3	D	489	MSE
3	D	498	ILE
3	D	521	ASP
3	D	532	LYS
3	D	731	GLU
3	D	736	SER
3	D	815	ILE
3	D	853	GLU
3	A	12	GLY
3	A	121	ASP
3	A	300	VAL
3	B	45	GLN
3	D	127	SER
3	D	155	PRO
3	D	165	GLU
3	D	179	PRO
3	D	221	PHE
3	D	387	PRO
3	D	427	PRO
3	D	506	PRO
3	D	523	SER
3	D	533	LEU
3	D	536	LYS
3	D	695	SER
3	D	800	LYS
3	D	817	GLY
3	D	836	ARG
3	D	854	ILE
3	A	303	LEU
3	B	352	LYS
3	B	406	TYR
3	B	518	TYR
3	B	795	GLY

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Mol	Chain	Res	Type
3	C	432	GLY
3	C	483	LYS
3	C	533	LEU
3	C	622	THR
3	D	45	GLN
3	D	140	ASP
3	D	315	SER
3	D	415	LEU
3	D	622	THR
3	D	843	ASP
3	D	874	LYS
3	A	338	ARG
3	A	490	LEU
3	A	509	SER
3	B	520	PHE
3	B	734	LYS
3	B	793	VAL
3	B	896	SER
3	C	174	GLY
3	C	415	LEU
3	C	506	PRO
3	D	198	LEU
3	D	262	ILE
3	D	272	ASP
3	D	401	PRO
3	D	512	GLU
3	D	640	LYS
3	D	730	LEU
3	D	783	SER
3	D	849	PRO
3	D	889	LEU
3	C	240	LYS
3	D	182	ILE
3	D	269	SER
3	D	391	TYR
3	D	395	PHE
3	D	510	VAL
3	A	622	THR
3	B	302	LYS
3	B	529	LYS
3	D	157	GLY
3	D	35	PRO

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Mol	Chain	Res	Type
3	D	799	PRO
3	C	175	GLY
3	A	388	VAL
3	D	166	ILE
3	D	779	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	785/775 (101%)	744 (95%)	41 (5%)	21	36
3	B	767/775 (99%)	724 (94%)	43 (6%)	19	32
3	C	786/775 (101%)	747 (95%)	39 (5%)	22	37
3	D	711/775 (92%)	675 (95%)	36 (5%)	21	36
All	All	3049/3100 (98%)	2890 (95%)	159 (5%)	21	36

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	14	SER
3	A	23	ASN
3	A	29	ARG
3	A	32	GLU
3	A	58	THR
3	A	64	ASN
3	A	73	LYS
3	A	86	ASP
3	A	112	ASN
3	A	116	GLU
3	A	121	ASP
3	A	213	LEU
3	A	229	ARG
3	A	231	LYS
3	A	242	LEU
3	A	291	ASP

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Mol	Chain	Res	Type
3	A	304	LYS
3	A	318	GLN
3	A	332	LEU
3	A	346	ASP
3	A	382	GLN
3	A	467	ARG
3	A	483	LYS
3	A	503	LEU
3	A	514	LEU
3	A	539	ASN
3	A	561	LEU
3	A	587	THR
3	A	612	GLU
3	A	618	LEU
3	A	631	LYS
3	A	635	LYS
3	A	656	ARG
3	A	658	ARG
3	A	659	MSE
3	A	733	GLN
3	A	736	SER
3	A	739	LYS
3	A	745	LEU
3	A	773	GLN
3	A	861	ASP
3	B	26	GLU
3	B	34	LYS
3	B	75	MSE
3	B	89	LYS
3	B	90	LEU
3	B	93	LEU
3	B	109	ARG
3	B	112	ASN
3	B	116	GLU
3	B	154	SER
3	B	164	ILE
3	B	193	ASN
3	B	217	ASN
3	B	256	MSE
3	B	257	TYR
3	B	259	SER
3	B	260	ARG

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Mol	Chain	Res	Type
3	B	262	ILE
3	B	363	LYS
3	B	403	ARG
3	B	421	ARG
3	B	435	LYS
3	B	475	ILE
3	B	489	MSE
3	B	539	ASN
3	B	573	VAL
3	B	597	ILE
3	B	614	GLU
3	B	681	MSE
3	B	684	ASP
3	B	685	ARG
3	B	707	ARG
3	B	728	MSE
3	B	736	SER
3	B	737	THR
3	B	766	GLU
3	B	787	ASN
3	B	791	TYR
3	B	819	ILE
3	B	861	ASP
3	B	877	ILE
3	B	878	LYS
3	B	901	PHE
3	C	43	GLU
3	C	83	LEU
3	C	98	ASN
3	C	138	HIS
3	C	177	GLU
3	C	257	TYR
3	C	276	LEU
3	C	332	LEU
3	C	337	LYS
3	C	353	ILE
3	C	356	GLN
3	C	428	GLU
3	C	439	LEU
3	C	456	CYS
3	C	458	PRO
3	C	468	ASP

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Mol	Chain	Res	Type
3	C	479	PHE
3	C	525	GLU
3	C	536	LYS
3	C	558	ASN
3	C	561	LEU
3	C	562	LEU
3	C	580	LEU
3	C	587	THR
3	C	618	LEU
3	C	642	ARG
3	C	722	GLU
3	C	728	MSE
3	C	747	GLU
3	C	760	LEU
3	C	843	ASP
3	C	859	LYS
3	C	874	LYS
3	C	878	LYS
3	C	880	LEU
3	C	881	GLU
3	C	896	SER
3	C	897	LEU
3	C	898	PHE
3	D	10	GLN
3	D	47	THR
3	D	58	THR
3	D	86	ASP
3	D	136	ILE
3	D	162	TRP
3	D	205	TRP
3	D	209	THR
3	D	216	TRP
3	D	266	PHE
3	D	303	LEU
3	D	306	ASP
3	D	316	ASN
3	D	353	ILE
3	D	356	GLN
3	D	363	LYS
3	D	479	PHE
3	D	498	ILE
3	D	519	ARG

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Mol	Chain	Res	Type
3	D	520	PHE
3	D	530	ILE
3	D	556	GLN
3	D	562	LEU
3	D	576	ARG
3	D	591	GLN
3	D	633	ILE
3	D	657	GLU
3	D	660	GLU
3	D	702	TRP
3	D	719	ARG
3	D	730	LEU
3	D	755	GLU
3	D	772	ARG
3	D	828	GLU
3	D	844	LYS
3	D	856	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	64	ASN
3	A	98	ASN
3	A	153	ASN
3	A	158	ASN
3	A	206	GLN
3	A	217	ASN
3	A	245	HIS
3	A	255	ASN
3	A	284	ASN
3	A	285	GLN
3	A	382	GLN
3	A	422	GLN
3	A	485	HIS
3	A	495	ASN
3	A	505	ASN
3	A	539	ASN
3	A	558	ASN
3	A	602	ASN
3	A	606	ASN
3	A	646	HIS
3	A	678	GLN

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Mol	Chain	Res	Type
3	A	733	GLN
3	A	742	GLN
3	A	773	GLN
3	A	775	ASN
3	A	839	ASN
3	B	70	GLN
3	B	98	ASN
3	B	105	HIS
3	B	153	ASN
3	B	158	ASN
3	B	193	ASN
3	B	203	ASN
3	B	217	ASN
3	B	245	HIS
3	B	284	ASN
3	B	316	ASN
3	B	318	GLN
3	B	324	ASN
3	B	354	GLN
3	B	376	GLN
3	B	382	GLN
3	B	389	GLN
3	B	493	GLN
3	B	539	ASN
3	B	591	GLN
3	B	595	GLN
3	B	646	HIS
3	B	733	GLN
3	B	742	GLN
3	B	775	ASN
3	B	818	ASN
3	C	45	GLN
3	C	98	ASN
3	C	112	ASN
3	C	131	HIS
3	C	153	ASN
3	C	158	ASN
3	C	173	GLN
3	C	203	ASN
3	C	207	GLN
3	C	217	ASN
3	C	284	ASN

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Mol	Chain	Res	Type
3	C	285	GLN
3	C	376	GLN
3	C	481	GLN
3	C	495	ASN
3	C	539	ASN
3	C	556	GLN
3	C	558	ASN
3	C	572	ASN
3	C	595	GLN
3	C	675	ASN
3	C	676	ASN
3	C	678	GLN
3	C	679	HIS
3	C	711	ASN
3	C	818	ASN
3	C	864	HIS
3	D	10	GLN
3	D	70	GLN
3	D	228	ASN
3	D	285	GLN
3	D	316	ASN
3	D	318	GLN
3	D	339	GLN
3	D	342	ASN
3	D	356	GLN
3	D	440	HIS
3	D	444	ASN
3	D	485	HIS
3	D	495	ASN
3	D	504	HIS
3	D	505	ASN
3	D	564	ASN
3	D	591	GLN
3	D	646	HIS
3	D	742	GLN
3	D	761	GLN
3	D	812	ASN
3	D	839	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CTG	E	3	1,2	18,23,24	0.75	0	21,35,38	1.10	2 (9%)
1	CTG	I	3	1,2	18,23,24	0.89	1 (5%)	21,35,38	1.19	3 (14%)
1	CTG	G	3	1,2	18,23,24	0.87	1 (5%)	21,35,38	1.11	1 (4%)
1	CTG	K	3	1	18,23,24	1.04	1 (5%)	21,35,38	1.06	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CTG	E	3	1,2	-	2/7/45/46	0/2/2/2
1	CTG	I	3	1,2	-	2/7/45/46	0/2/2/2
1	CTG	G	3	1,2	-	0/7/45/46	0/2/2/2
1	CTG	K	3	1	-	0/7/45/46	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	3	CTG	C5-C4	2.82	1.55	1.52
1	I	3	CTG	C1'-N1	2.41	1.48	1.45
1	G	3	CTG	C1'-N1	2.04	1.48	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	3	CTG	O3'-C3'-C2'	2.85	120.79	110.88
1	E	3	CTG	O3'-C3'-C2'	2.60	119.92	110.88
1	G	3	CTG	N3-C2-N1	-2.47	114.20	116.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	3	CTG	N3-C2-N1	-2.39	114.28	116.78
1	K	3	CTG	O3'-C3'-C2'	2.32	118.95	110.88
1	E	3	CTG	N3-C2-N1	-2.20	114.48	116.78
1	I	3	CTG	N3-C2-N1	-2.14	114.54	116.78
1	I	3	CTG	C2'-C3'-C4'	2.02	106.89	102.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	3	CTG	C3'-C4'-C5'-O5'
1	E	3	CTG	O4'-C4'-C5'-O5'
1	I	3	CTG	C3'-C4'-C5'-O5'
1	I	3	CTG	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	3	CTG	2	0
1	I	3	CTG	1	0
1	G	3	CTG	1	0
1	K	3	CTG	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	E	16/18 (88%)	1.90	5 (31%) 1 0	87, 109, 126, 131	0
1	G	17/18 (94%)	-0.35	0 100 100	34, 47, 76, 79	0
1	I	17/18 (94%)	0.22	0 100 100	35, 50, 84, 91	0
1	K	17/18 (94%)	1.73	5 (29%) 1 1	65, 80, 81, 81	0
2	F	14/15 (93%)	2.05	6 (42%) 0 0	106, 125, 133, 135	0
2	H	15/15 (100%)	-0.03	0 100 100	36, 49, 100, 100	0
2	J	15/15 (100%)	0.26	0 100 100	33, 65, 112, 113	0
2	L	15/15 (100%)	1.94	6 (40%) 1 0	78, 80, 82, 82	0
3	A	877/903 (97%)	0.33	66 (7%) 20 15	23, 51, 125, 141	0
3	B	863/903 (95%)	0.05	45 (5%) 33 25	16, 44, 116, 139	0
3	C	875/903 (96%)	0.13	38 (4%) 40 32	17, 47, 114, 142	0
3	D	867/903 (96%)	1.46	236 (27%) 1 1	54, 102, 140, 153	0
All	All	3608/3744 (96%)	0.51	407 (11%) 10 8	16, 58, 131, 153	0

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	498	ILE	10.3
3	C	526	ILE	6.7
3	A	846	ILE	6.4
3	D	135	ALA	6.1
3	C	498	ILE	5.7
3	B	792	ASP	5.3
3	A	847	ALA	5.2
3	C	495	ASN	5.0
3	D	303	LEU	4.9
3	D	315	SER	4.9
3	D	542	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
3	D	394	ALA	4.8
3	C	527	LYS	4.8
3	C	503	LEU	4.8
3	D	522	PHE	4.7
3	D	817	GLY	4.6
3	D	164	ILE	4.6
3	B	179	PRO	4.5
3	B	258	GLY	4.5
3	C	522	PHE	4.5
3	D	305	TYR	4.4
3	C	514	LEU	4.4
2	F	111	DT	4.4
3	D	517	ASP	4.4
3	C	502	ALA	4.4
3	D	782	VAL	4.3
3	D	309	ILE	4.3
3	A	510	VAL	4.2
3	D	803	PHE	4.2
3	A	503	LEU	4.2
3	D	115	ILE	4.2
3	D	800	LYS	4.2
3	D	771	PHE	4.2
3	D	312	LEU	4.1
3	D	829	LYS	4.1
3	D	175	GLY	4.0
3	D	526	ILE	4.0
3	D	230	ILE	4.0
3	D	490	LEU	4.0
3	B	178	VAL	4.0
3	D	8	VAL	4.0
3	D	313	ARG	4.0
3	D	530	ILE	4.0
3	A	902	ASP	3.9
3	B	787	ASN	3.9
3	B	530	ILE	3.9
3	B	252	VAL	3.9
3	D	133	ILE	3.9
3	D	395	PHE	3.9
3	D	491	ALA	3.8
3	D	518	TYR	3.8
3	C	530	ILE	3.8
3	D	523	SER	3.8

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Mol	Chain	Res	Type	RSRZ
3	D	831	TYR	3.8
3	B	498	ILE	3.8
3	D	889	LEU	3.7
3	D	730	LEU	3.7
3	D	497	GLU	3.7
3	D	152	LEU	3.7
3	C	505	ASN	3.7
3	D	622	THR	3.6
3	D	727	ILE	3.6
3	D	779	ILE	3.6
3	D	320	TYR	3.6
3	D	857	LEU	3.6
3	D	774	LEU	3.5
3	C	499	ILE	3.5
3	A	824	VAL	3.5
3	D	118	THR	3.5
1	E	11	DC	3.5
3	D	529	LYS	3.5
3	D	492	ALA	3.5
3	B	531	LYS	3.4
3	D	302	LYS	3.4
3	D	314	GLU	3.4
3	D	390	PRO	3.4
3	D	82	ALA	3.4
3	D	319	ARG	3.4
3	D	317	HIS	3.3
3	B	902	ASP	3.3
3	C	506	PRO	3.3
3	A	284	ASN	3.3
3	A	862	VAL	3.3
3	B	793	VAL	3.3
3	C	516	VAL	3.3
3	D	166	ILE	3.3
3	D	321	ILE	3.3
3	D	846	ILE	3.3
3	D	216	TRP	3.3
3	D	735	SER	3.3
3	B	253	ILE	3.3
3	C	510	VAL	3.3
1	E	9	DG	3.2
3	D	875	THR	3.2
3	A	498	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
3	B	734	LYS	3.2
3	D	844	LYS	3.2
3	D	732	THR	3.2
3	D	487	GLY	3.2
3	D	534	SER	3.2
3	D	780	ALA	3.2
3	D	863	LEU	3.2
3	A	799	PRO	3.2
3	D	179	PRO	3.2
3	B	499	ILE	3.2
3	D	136	ILE	3.2
3	B	521	ASP	3.1
3	D	397	LYS	3.1
3	D	514	LEU	3.1
3	D	11	ILE	3.1
3	D	632	ILE	3.1
3	D	793	VAL	3.1
3	D	201	TYR	3.1
3	D	897	LEU	3.1
3	C	523	SER	3.1
3	D	287	SER	3.1
3	D	870	VAL	3.1
3	D	539	ASN	3.1
3	A	502	ALA	3.1
3	D	467	ARG	3.1
3	B	522	PHE	3.1
3	D	178	VAL	3.1
3	B	791	TYR	3.0
3	D	274	ILE	3.0
3	A	535	ALA	3.0
3	D	113	PHE	3.0
3	D	396	VAL	3.0
3	D	796	PHE	3.0
3	A	514	LEU	3.0
3	C	513	PRO	3.0
3	D	821	ALA	3.0
3	D	117	VAL	3.0
3	D	854	ILE	3.0
3	B	794	GLY	3.0
3	D	84	GLY	3.0
3	B	538	LEU	2.9
3	D	290	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	A	509	SER	2.9
3	B	526	ILE	2.9
3	D	502	ALA	2.9
3	D	787	ASN	2.9
3	A	699	GLY	2.9
3	C	175	GLY	2.9
3	D	213	LEU	2.9
3	D	392	PRO	2.9
3	A	819	ILE	2.9
3	D	134	ASP	2.9
3	D	187	ILE	2.9
3	D	167	ALA	2.9
3	D	168	ALA	2.9
3	A	848	TRP	2.8
3	D	162	TRP	2.8
3	C	521	ASP	2.8
3	C	252	VAL	2.8
3	D	516	VAL	2.8
3	D	822	PRO	2.8
3	D	733	GLN	2.8
3	D	808	ILE	2.8
3	D	494	ARG	2.8
3	A	786	ASN	2.8
3	D	83	LEU	2.8
3	D	533	LEU	2.8
3	A	776	TYR	2.8
3	A	841	PHE	2.8
3	D	776	TYR	2.8
3	A	833	LEU	2.8
3	D	221	PHE	2.8
3	B	309	ILE	2.7
3	D	223	ILE	2.7
3	D	325	ILE	2.7
3	D	877	ILE	2.7
3	D	197	LEU	2.7
3	D	496	GLY	2.7
3	D	818	ASN	2.7
3	B	545	ALA	2.7
3	B	901	PHE	2.7
3	D	543	PHE	2.7
3	D	874	LYS	2.7
3	D	198	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	163	SER	2.7
3	D	161	GLU	2.7
3	B	535	ALA	2.7
3	D	300	VAL	2.7
3	D	789	ALA	2.7
3	A	520	PHE	2.7
3	A	532	LYS	2.7
3	A	505	ASN	2.7
3	D	876	PHE	2.7
3	B	528	GLU	2.7
3	B	520	PHE	2.7
3	D	510	VAL	2.7
3	D	183	ILE	2.6
3	D	707	ARG	2.6
3	D	261	GLU	2.6
3	D	729	GLY	2.6
3	C	536	LYS	2.6
3	D	832	VAL	2.6
3	A	513	PRO	2.6
3	D	799	PRO	2.6
2	F	115	DA	2.6
3	D	521	ASP	2.6
3	A	788	ILE	2.6
3	C	542	LEU	2.6
3	C	531	LYS	2.6
2	F	112	DT	2.6
2	F	109	DC	2.6
3	D	159	VAL	2.6
3	D	436	VAL	2.6
3	A	803	PHE	2.6
3	D	736	SER	2.6
3	D	633	ILE	2.6
3	D	788	ILE	2.6
3	D	407	VAL	2.6
3	D	203	ASN	2.6
3	D	495	ASN	2.6
3	A	253	ILE	2.5
3	D	15	ILE	2.5
2	L	115	DA	2.5
3	B	542	LEU	2.5
3	D	265	LEU	2.5
3	B	529	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	323	TYR	2.5
3	C	464	TYR	2.5
3	D	391	TYR	2.5
3	D	57	CYS	2.5
3	A	507	ASN	2.5
2	F	107	DG	2.5
3	D	848	TRP	2.5
3	B	820	ASP	2.5
3	D	306	ASP	2.5
3	D	524	ASP	2.5
3	D	78	ILE	2.5
3	D	186	ILE	2.5
3	D	60	LYS	2.5
3	D	160	GLU	2.5
3	D	891	TYR	2.5
3	D	824	VAL	2.5
3	A	511	ASP	2.5
3	A	526	ILE	2.5
3	D	205	TRP	2.5
3	C	511	ASP	2.5
3	D	170	LEU	2.5
3	D	745	LEU	2.5
2	F	101	DG	2.5
2	L	101	DG	2.5
3	C	432	GLY	2.5
3	D	794	GLY	2.5
3	D	137	THR	2.5
3	D	238	THR	2.5
3	A	784	SER	2.5
3	B	303	LEU	2.5
3	C	508	LEU	2.5
3	D	725	LEU	2.5
3	D	781	SER	2.5
3	B	525	GLU	2.5
1	K	13	DG	2.5
2	L	103	DG	2.5
3	A	554	THR	2.4
3	D	433	THR	2.4
3	B	818	ASN	2.4
3	D	334	ILE	2.4
3	D	215	GLY	2.4
3	D	33	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	488	TYR	2.4
1	E	2	DG	2.4
3	D	520	PHE	2.4
3	B	819	ILE	2.4
3	A	516	VAL	2.4
3	D	171	GLN	2.4
3	C	454	TYR	2.4
3	C	494	ARG	2.4
3	D	437	ALA	2.4
3	A	533	LEU	2.4
3	D	332	LEU	2.4
3	D	833	LEU	2.4
3	B	255	ASN	2.4
3	D	892	GLU	2.4
3	D	139	TYR	2.4
3	D	819	ILE	2.4
3	A	539	ASN	2.4
3	C	507	ASN	2.4
3	D	726	LYS	2.4
3	D	124	PRO	2.4
3	B	795	GLY	2.4
3	D	717	GLY	2.4
3	D	538	LEU	2.3
3	B	497	GLU	2.3
3	B	500	LYS	2.3
3	D	208	LYS	2.3
3	D	537	SER	2.3
3	D	797	PRO	2.3
1	K	12	DA	2.3
3	A	854	ILE	2.3
3	D	277	TYR	2.3
3	D	155	PRO	2.3
1	K	1	DC	2.3
2	L	107	DG	2.3
3	A	857	LEU	2.3
3	D	764	PHE	2.3
2	L	108	DT	2.3
3	D	740	ALA	2.3
3	D	293	ILE	2.3
3	D	380	ILE	2.3
3	D	815	ILE	2.3
3	D	279	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	114	ASP	2.3
3	D	126	PRO	2.3
3	A	538	LEU	2.3
2	L	102	DC	2.3
3	D	146	PHE	2.3
1	K	10	DA	2.3
3	A	536	LYS	2.3
3	A	811	TYR	2.3
3	D	624	SER	2.3
3	A	258	GLY	2.3
3	C	538	LEU	2.3
3	D	508	LEU	2.3
3	D	108	ILE	2.2
3	C	528	GLU	2.2
3	D	402	ASN	2.2
1	E	4	DG	2.2
3	D	310	SER	2.2
3	A	490	LEU	2.2
3	A	46	ALA	2.2
3	D	499	ILE	2.2
3	D	689	ALA	2.2
3	D	847	ALA	2.2
3	A	845	CYS	2.2
3	D	47	THR	2.2
3	D	194	GLU	2.2
3	A	518	TYR	2.2
3	B	495	ASN	2.2
3	D	506	PRO	2.2
3	D	140	ASP	2.2
3	B	550	VAL	2.2
3	A	530	ILE	2.2
3	C	253	ILE	2.2
3	D	16	PHE	2.2
3	C	518	TYR	2.2
3	A	842	GLY	2.2
3	B	817	GLY	2.2
3	C	487	GLY	2.2
3	A	735	SER	2.2
3	C	524	ASP	2.2
3	D	792	ASP	2.2
3	D	263	ILE	2.2
3	D	777	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	225	TYR	2.2
3	A	816	LYS	2.2
3	D	734	LYS	2.2
3	A	508	LEU	2.2
3	D	271	LEU	2.2
3	D	291	ASP	2.2
3	B	259	SER	2.2
3	D	783	SER	2.2
3	A	499	ILE	2.2
3	D	282	PHE	2.2
3	D	172	GLU	2.1
3	D	214	THR	2.1
3	D	855	THR	2.1
3	A	506	PRO	2.1
3	A	500	LYS	2.1
3	C	257	TYR	2.1
3	D	765	LYS	2.1
3	A	807	GLY	2.1
3	B	301	GLY	2.1
3	D	784	SER	2.1
3	A	789	ALA	2.1
3	D	501	GLU	2.1
3	D	731	GLU	2.1
3	D	880	LEU	2.1
3	C	504	HIS	2.1
3	D	270	VAL	2.1
3	D	768	GLU	2.1
3	D	531	LYS	2.1
3	A	556	GLN	2.1
3	A	504	HIS	2.1
3	D	288	TYR	2.1
3	D	627	VAL	2.1
1	E	8	DT	2.1
3	D	873	GLU	2.1
3	A	797	PRO	2.1
3	A	871	LEU	2.1
3	D	188	TYR	2.1
3	D	212	ILE	2.1
3	A	830	VAL	2.1
3	D	862	VAL	2.1
3	D	191	PHE	2.1
3	B	260	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	308	PRO	2.0
3	D	802	PRO	2.0
3	D	45	GLN	2.0
3	D	618	LEU	2.0
1	K	14	DC	2.0
3	A	817	GLY	2.0
3	A	782	VAL	2.0
3	A	825	VAL	2.0
3	D	617	VAL	2.0
3	B	494	ARG	2.0
3	D	340	PHE	2.0
3	A	492	ALA	2.0
3	B	789	ALA	2.0
3	D	304	LYS	2.0
3	D	237	SER	2.0
3	A	738	PRO	2.0
3	D	20	ILE	2.0
3	D	110	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CTG	K	3	22/23	0.67	0.16	75,79,85,88	0
1	CTG	E	3	22/23	0.84	0.15	110,111,113,114	0
1	CTG	I	3	22/23	0.94	0.08	58,61,62,63	0
1	CTG	G	3	22/23	0.97	0.07	32,41,42,43	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.