



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:30 AM UTC

PDB ID : 2DTU / pdb_00002dtu
Title : Crystal structure of the beta hairpin loop deletion variant of RB69 gp43 in complex with DNA containing an abasic site analog
Authors : Aller, P.; Hogg, M.; Konigsberg, W.; Wallace, S.S.; Doublié, S.
Deposited on : 2006-07-15
Resolution : 2.37 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

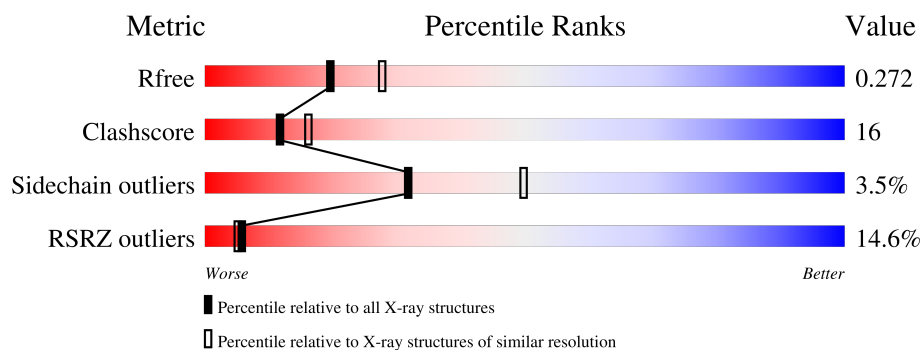
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	6% 11% 28% 56% 6%
1	G	18	11% 17% 28% 50% 6%
1	I	18	6% 22% 44% 28% 6%
1	K	18	6% 11% 44% 44%
2	F	15	13% 53% 47%
2	H	15	13% 7% 40% 53%

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Mol	Chain	Length	Quality of chain
2	J	15	13% 47% 47% 7%
2	L	15	7% 40% 60%
3	A	896	6% 73% 26%
3	B	896	18% 70% 28%
3	C	896	4% 75% 23%
3	D	896	31% 59% 39%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32454 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*(3DR)P*CP*TP*TP*AP*TP*GP*AP*C P*AP*GP*CP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	G	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	I	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	K	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*A P*AP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	H	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	J	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	L	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	896	Total	C	N	O	S	0	0	0
			7281	4678	1209	1362	32			
3	B	896	Total	C	N	O	S	0	0	0
			7235	4649	1201	1353	32			
3	C	892	Total	C	N	O	S	0	0	0
			7238	4650	1200	1357	31			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	891	Total	C	N	O	S	0	0	0
			7191	4619	1192	1349	31			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	253	GLY	ILE	engineered mutation	UNP Q38087
A	?	-	GLU	deletion	UNP Q38087
A	?	-	ASN	deletion	UNP Q38087
A	?	-	MET	deletion	UNP Q38087
A	?	-	TYR	deletion	UNP Q38087
A	?	-	GLY	deletion	UNP Q38087
A	?	-	SER	deletion	UNP Q38087
A	?	-	ARG	deletion	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	253	GLY	ILE	engineered mutation	UNP Q38087
B	?	-	GLU	deletion	UNP Q38087
B	?	-	ASN	deletion	UNP Q38087
B	?	-	MET	deletion	UNP Q38087
B	?	-	TYR	deletion	UNP Q38087
B	?	-	GLY	deletion	UNP Q38087
B	?	-	SER	deletion	UNP Q38087
B	?	-	ARG	deletion	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	253	GLY	ILE	engineered mutation	UNP Q38087
C	?	-	GLU	deletion	UNP Q38087
C	?	-	ASN	deletion	UNP Q38087
C	?	-	MET	deletion	UNP Q38087
C	?	-	TYR	deletion	UNP Q38087
C	?	-	GLY	deletion	UNP Q38087
C	?	-	SER	deletion	UNP Q38087
C	?	-	ARG	deletion	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	253	GLY	ILE	engineered mutation	UNP Q38087
D	?	-	GLU	deletion	UNP Q38087
D	?	-	ASN	deletion	UNP Q38087
D	?	-	MET	deletion	UNP Q38087
D	?	-	TYR	deletion	UNP Q38087

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	deletion	UNP Q38087
D	?	-	SER	deletion	UNP Q38087
D	?	-	ARG	deletion	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	9	Total 9	O 9	0	0
4	F	10	Total 10	O 10	0	0
4	G	15	Total 15	O 15	0	0
4	H	8	Total 8	O 8	0	0
4	I	31	Total 31	O 31	0	0
4	J	18	Total 18	O 18	0	0
4	K	10	Total 10	O 10	0	0
4	A	251	Total 251	O 251	0	0
4	B	195	Total 195	O 195	0	0
4	C	272	Total 272	O 272	0	0
4	D	38	Total 38	O 38	0	0

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.

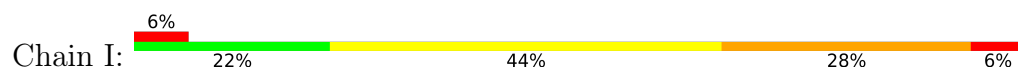
- Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'



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



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



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

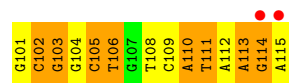


- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'





• Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'



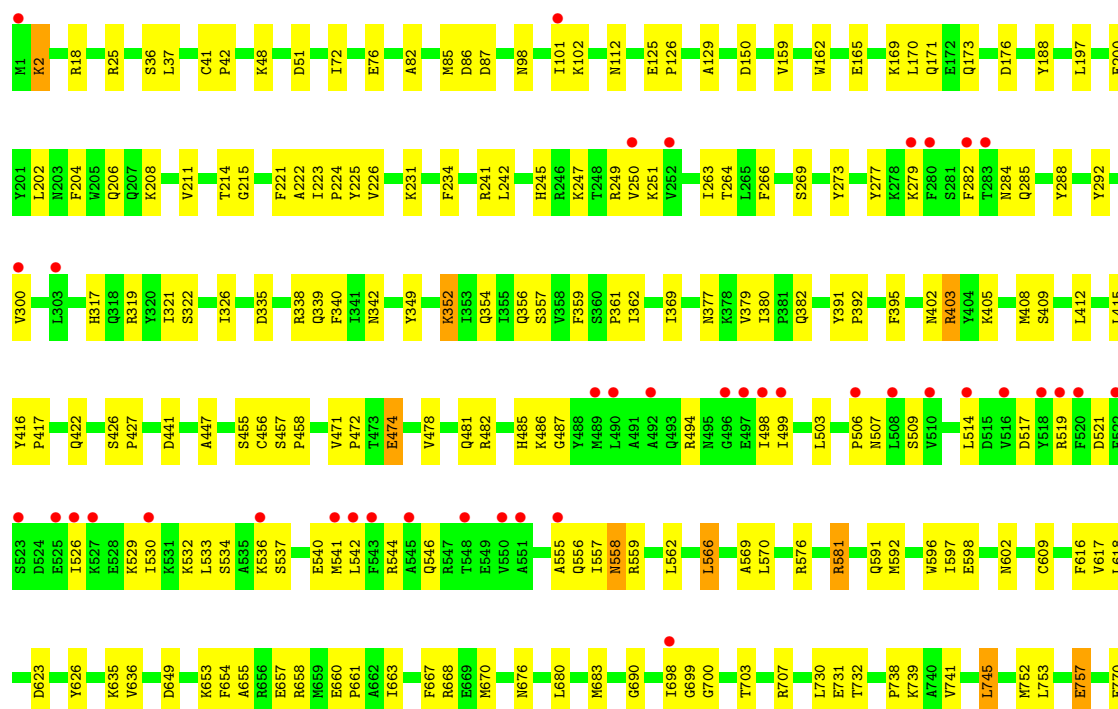
• Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

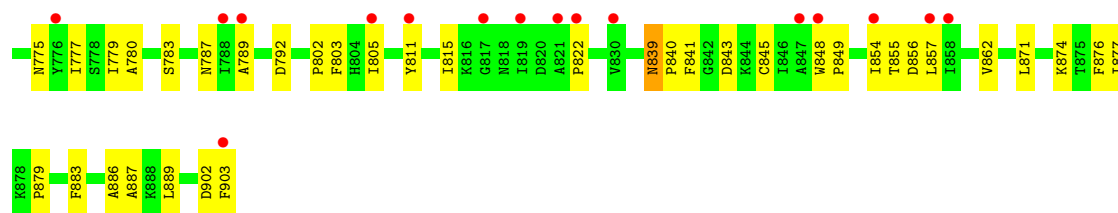


• Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

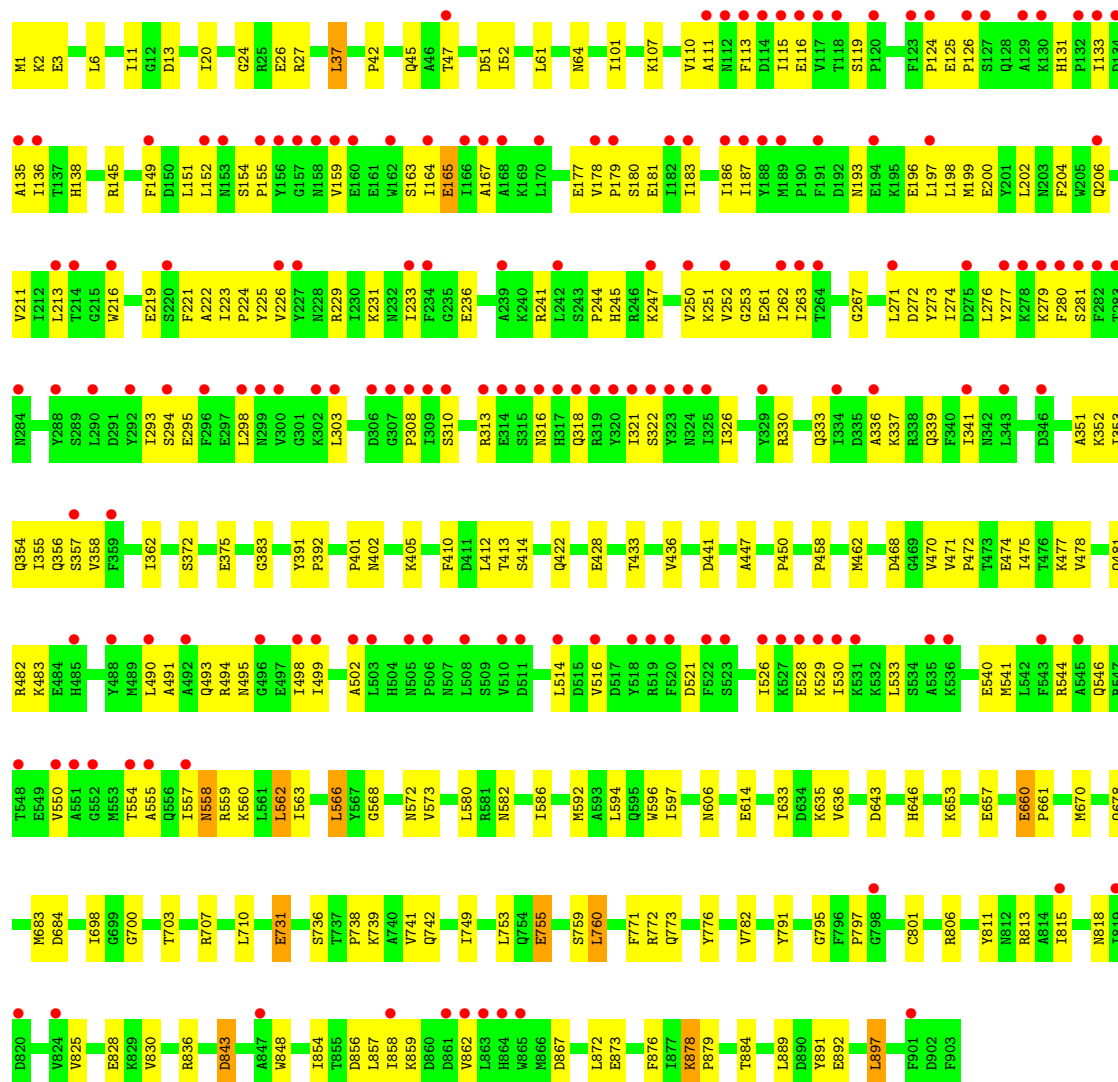


• Molecule 3: DNA polymerase

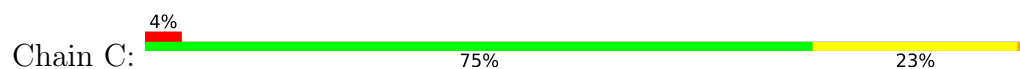


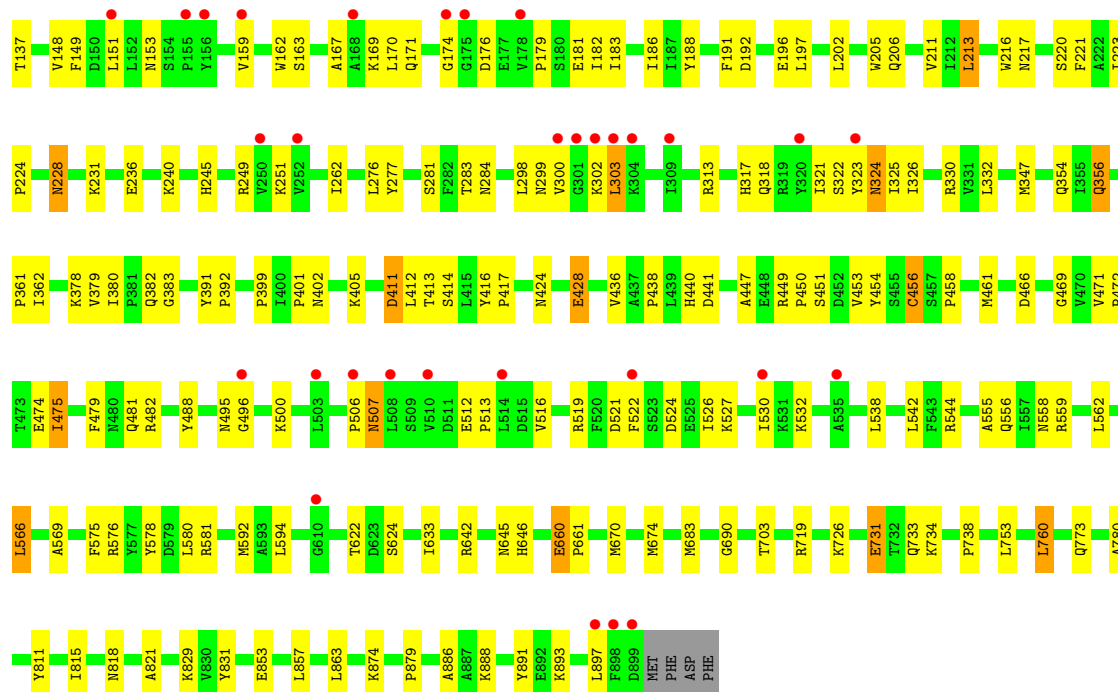


● Molecule 3: DNA polymerase

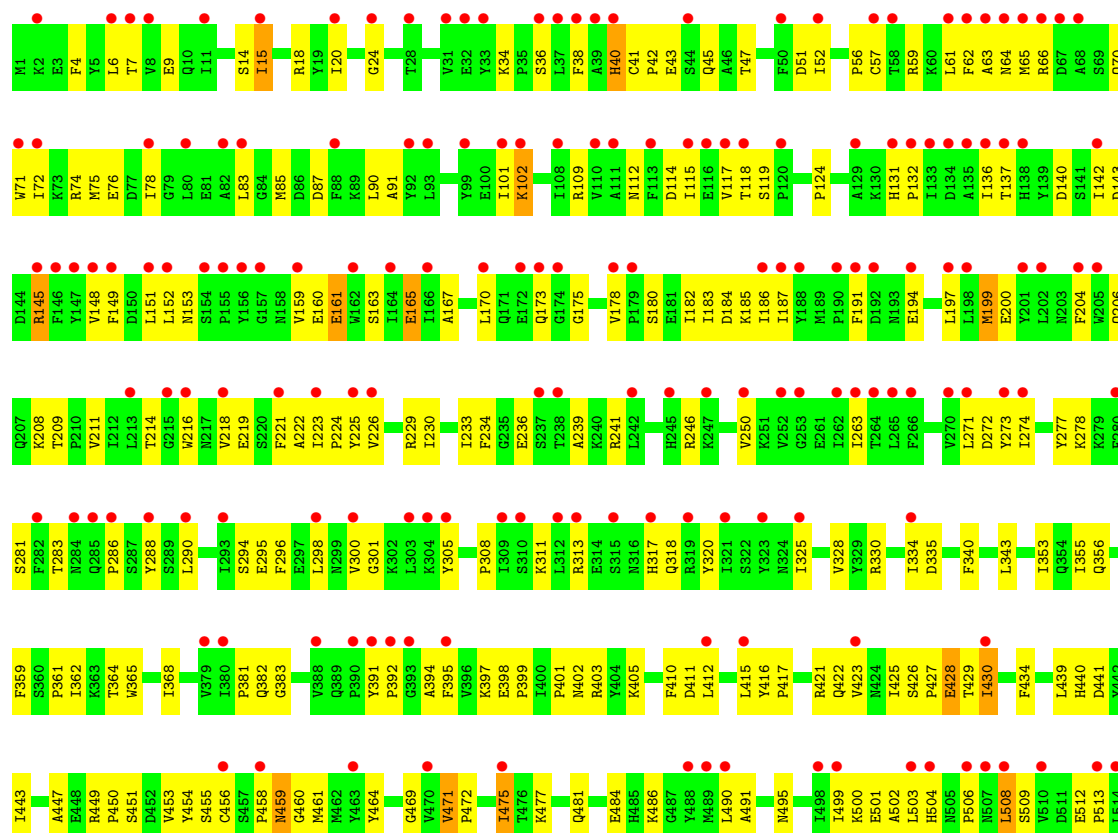


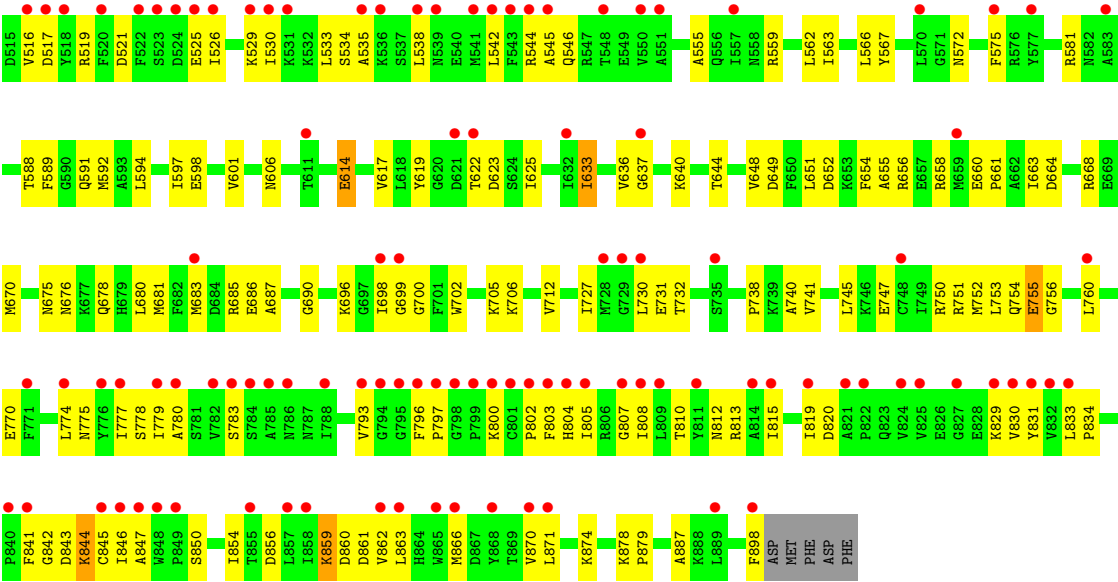
● Molecule 3: DNA polymerase





• 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	133.07Å 123.06Å 164.56Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	50.00 – 2.37 50.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.37) 87.8 (50.00-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.268 0.227 , 0.272	Depositor DCC
R_{free} test set	37523 reflections (9.47%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.1	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	0.94	EDS
Total number of atoms	32454	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: 3DR

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	0.26	0/384	1.43	15/588 (2.6%)
1	G	0.31	0/384	1.61	15/588 (2.6%)
1	I	0.35	0/384	1.49	14/588 (2.4%)
1	K	0.22	0/384	1.33	10/588 (1.7%)
2	F	0.24	0/346	1.36	10/533 (1.9%)
2	H	0.26	0/346	1.30	10/533 (1.9%)
2	J	0.39	0/346	1.48	13/533 (2.4%)
2	L	0.20	0/346	1.25	10/533 (1.9%)
3	A	0.48	0/7461	0.87	8/10092 (0.1%)
3	B	0.43	0/7414	0.83	6/10036 (0.1%)
3	C	0.49	0/7416	0.85	7/10032 (0.1%)
3	D	0.32	0/7369	0.76	4/9980 (0.0%)
All	All	0.43	0/32580	0.90	122/44624 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
1	I	0	1
2	J	0	2
All	All	0	5

There are no bond length outliers.

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	211	VAL	N-CA-C	-10.49	101.71	111.67
1	G	6	DT	C2'-C3'-O3'	9.75	126.12	111.50
1	G	7	DA	C4'-C3'-O3'	9.72	124.58	110.00
3	B	211	VAL	N-CA-C	-8.66	104.11	111.56
1	I	7	DA	C4'-C3'-O3'	8.46	122.69	110.00
1	G	6	DT	C4'-C3'-O3'	8.36	122.54	110.00
1	G	7	DA	C2'-C3'-O3'	8.10	123.64	111.50
1	K	17	DC	C2'-C3'-O3'	7.98	123.47	111.50
1	G	8	DT	C2'-C3'-O3'	7.85	123.27	111.50
1	G	4	DC	C2'-C3'-O3'	7.65	122.98	111.50
1	E	7	DA	C4'-C3'-O3'	7.65	121.47	110.00
2	J	105	DC	C2'-C3'-O3'	7.50	122.74	111.50
3	A	456	CYS	N-CA-C	7.33	121.42	109.85
1	G	4	DC	C4'-C3'-O3'	7.15	120.72	110.00
1	I	10	DA	C2'-C3'-O3'	7.09	122.14	111.50
1	I	7	DA	C2'-C3'-O3'	7.01	122.02	111.50
3	C	211	VAL	N-CA-C	-6.85	105.17	111.67
1	I	14	DC	C2'-C3'-O3'	6.60	121.40	111.50
2	F	112	DA	C2'-C3'-O3'	6.56	121.34	111.50
1	I	13	DG	C2'-C3'-O3'	6.55	121.33	111.50
2	J	113	DA	C2'-C3'-O3'	6.50	121.25	111.50
2	J	104	DG	C2'-C3'-O3'	6.47	121.21	111.50
1	G	5	DT	C2'-C3'-O3'	6.45	121.17	111.50
1	I	4	DC	C4'-C3'-O3'	6.44	119.65	110.00
2	J	102	DC	C2'-C3'-O3'	6.32	120.99	111.50
2	J	112	DA	C2'-C3'-O3'	6.28	120.91	111.50
2	F	111	DT	C2'-C3'-O3'	6.27	120.90	111.50
2	H	111	DT	C2'-C3'-O3'	6.26	120.89	111.50
1	K	6	DT	C2'-C3'-O3'	6.24	120.86	111.50
2	H	105	DC	C4'-C3'-O3'	6.21	119.31	110.00
1	E	7	DA	C2'-C3'-O3'	6.19	120.79	111.50
1	I	16	DG	C2'-C3'-O3'	6.19	120.79	111.50
1	E	17	DC	C2'-C3'-O3'	6.13	120.70	111.50
1	E	11	DC	C2'-C3'-O3'	6.12	120.67	111.50
1	E	10	DA	C2'-C3'-O3'	6.07	120.61	111.50
3	A	703	THR	N-CA-C	-6.05	106.44	113.88
1	I	15	DC	C2'-C3'-O3'	6.00	120.50	111.50
1	K	4	DC	C2'-C3'-O3'	5.98	120.47	111.50
1	E	5	DT	C2'-C3'-O3'	5.98	120.46	111.50
3	B	383	GLY	N-CA-C	-5.97	104.37	111.36
1	G	16	DG	C2'-C3'-O3'	5.96	120.44	111.50
2	F	105	DC	C2'-C3'-O3'	5.94	120.41	111.50
1	G	17	DC	C2'-C3'-O3'	5.93	120.39	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	105	DC	C4'-C3'-O3'	5.92	118.88	110.00
2	F	114	DG	C2'-C3'-O3'	5.89	120.34	111.50
1	I	15	DC	C4'-C3'-O3'	5.85	118.77	110.00
2	J	103	DG	C2'-C3'-O3'	5.84	120.26	111.50
2	L	111	DT	C2'-C3'-O3'	5.83	120.25	111.50
2	F	102	DC	C2'-C3'-O3'	5.83	120.24	111.50
1	K	15	DC	C2'-C3'-O3'	5.77	120.16	111.50
1	E	4	DC	C2'-C3'-O3'	5.75	120.13	111.50
1	I	9	DG	N9-C1'-C2'	5.75	122.12	113.50
2	H	110	DA	C2'-C3'-O3'	5.73	120.09	111.50
2	J	104	DG	C4'-C3'-O3'	5.71	118.57	110.00
2	F	113	DA	C2'-C3'-O3'	5.71	120.06	111.50
3	C	831	TYR	N-CA-C	-5.68	102.11	110.52
1	E	14	DC	C2'-C3'-O3'	5.68	120.02	111.50
1	K	5	DT	C2'-C3'-O3'	5.67	120.00	111.50
3	C	436	VAL	N-CA-C	5.65	116.44	108.36
2	J	105	DC	C4'-C3'-O3'	5.64	118.46	110.00
2	L	112	DA	C2'-C3'-O3'	5.59	119.88	111.50
1	E	6	DT	C4'-C3'-O3'	5.59	118.38	110.00
1	G	14	DC	C2'-C3'-O3'	5.58	119.88	111.50
2	F	101	DG	C2'-C3'-O3'	5.58	119.87	111.50
2	H	114	DG	C2'-C3'-O3'	5.57	119.86	111.50
2	H	101	DG	C2'-C3'-O3'	5.57	119.85	111.50
2	F	106	DT	C2'-C3'-O3'	5.56	119.83	111.50
2	H	102	DC	C2'-C3'-O3'	5.53	119.79	111.50
1	G	8	DT	C4'-C3'-O3'	5.52	118.28	110.00
2	H	106	DT	C2'-C3'-O3'	5.52	119.78	111.50
2	J	101	DG	C2'-C3'-O3'	5.50	119.76	111.50
2	L	102	DC	C2'-C3'-O3'	5.48	119.72	111.50
3	D	712	VAL	N-CA-C	5.47	116.64	109.58
1	K	1	DC	C2'-C3'-O3'	5.47	119.70	111.50
3	B	295	GLU	N-CA-C	-5.47	106.65	113.38
3	C	753	LEU	N-CA-C	5.46	118.16	111.82
2	L	110	DA	C2'-C3'-O3'	5.43	119.64	111.50
2	L	113	DA	C2'-C3'-O3'	5.43	119.64	111.50
1	K	2	DG	C2'-C3'-O3'	5.40	119.60	111.50
1	K	8	DT	C2'-C3'-O3'	5.38	119.57	111.50
3	D	508	LEU	CB-CA-C	-5.38	109.91	117.23
1	I	11	DC	C2'-C3'-O3'	5.37	119.56	111.50
3	C	853	GLU	N-CA-C	-5.37	103.30	110.55
3	D	502	ALA	N-CA-C	-5.37	106.90	113.50
3	B	101	ILE	N-CA-C	5.34	116.41	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	103	DG	C2'-C3'-O3'	5.33	119.50	111.50
2	J	106	DT	C2'-C3'-O3'	5.33	119.49	111.50
1	E	13	DG	C2'-C3'-O3'	5.32	119.48	111.50
2	L	105	DC	C2'-C3'-O3'	5.32	119.48	111.50
3	A	877	ILE	N-CA-C	5.32	115.52	110.42
1	E	12	DA	C2'-C3'-O3'	5.30	119.46	111.50
2	F	103	DG	C2'-C3'-O3'	5.29	119.44	111.50
1	E	6	DT	C2'-C3'-O3'	5.29	119.44	111.50
3	C	703	THR	N-CA-C	-5.27	107.22	113.97
1	K	7	DA	C2'-C3'-O3'	5.27	119.40	111.50
3	C	324	ASN	N-CA-C	-5.26	106.36	112.89
2	L	101	DG	C2'-C3'-O3'	5.25	119.38	111.50
1	I	1	DC	C2'-C3'-O3'	5.24	119.36	111.50
1	G	1	DC	C2'-C3'-O3'	5.23	119.34	111.50
2	H	113	DA	C2'-C3'-O3'	5.20	119.31	111.50
2	J	107	DG	C2'-C3'-O3'	5.20	119.30	111.50
1	E	5	DT	C4'-C3'-O3'	5.19	117.79	110.00
1	K	16	DG	C2'-C3'-O3'	5.19	119.29	111.50
2	L	109	DC	C2'-C3'-O3'	5.19	119.29	111.50
3	A	18	ARG	N-CA-C	-5.19	101.23	109.59
1	G	2	DG	C2'-C3'-O3'	5.19	119.28	111.50
1	I	4	DC	C2'-C3'-O3'	5.18	119.27	111.50
3	D	471	VAL	CB-CA-C	-5.16	108.80	113.70
3	B	703	THR	N-CA-C	-5.14	107.55	113.88
2	L	105	DC	C4'-C3'-O3'	5.12	117.68	110.00
3	A	757	GLU	N-CA-C	5.12	117.25	111.11
1	G	15	DC	C2'-C3'-O3'	5.10	119.16	111.50
2	L	114	DG	C2'-C3'-O3'	5.10	119.14	111.50
2	H	105	DC	C2'-C3'-O3'	5.09	119.14	111.50
1	I	9	DG	C2'-C3'-O3'	5.09	119.13	111.50
1	E	14	DC	C4'-C3'-O3'	5.08	117.63	110.00
3	B	110	VAL	CB-CA-C	-5.08	106.89	112.68
2	J	112	DA	C4'-C3'-O3'	5.06	117.59	110.00
3	A	839	ASN	CA-C-N	5.03	124.75	119.82
3	A	839	ASN	C-N-CA	5.03	124.75	119.82
1	E	15	DC	C2'-C3'-O3'	5.03	119.04	111.50
2	J	111	DT	C2'-C3'-O3'	5.02	119.03	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	7	DA	Sidechain
1	G	7	DA	Sidechain
1	I	7	DA	Sidechain
2	J	112	DA	Sidechain
2	J	114	DG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	355	0	200	17	0
1	G	355	0	200	16	0
1	I	355	0	200	10	0
1	K	355	0	200	19	0
2	F	308	0	170	17	0
2	H	308	0	170	20	0
2	J	308	0	170	21	0
2	L	308	0	170	16	0
3	A	7281	0	7136	189	0
3	B	7235	0	7052	205	0
3	C	7238	0	7101	158	0
3	D	7191	0	7005	300	0
4	A	251	0	0	18	0
4	B	195	0	0	18	0
4	C	272	0	0	18	0
4	D	38	0	0	9	0
4	E	9	0	0	0	0
4	F	10	0	0	1	0
4	G	15	0	0	1	0
4	H	8	0	0	3	0
4	I	31	0	0	1	0
4	J	18	0	0	5	0
4	K	10	0	0	4	0
All	All	32454	0	29774	976	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 16.

All (976) 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)
3:A:395:PHE:HB2	3:A:591:GLN:HG3	1.43	1.01
1:G:6:DT:H2'	1:G:7:DA:H5''	1.40	1.00
1:G:6:DT:C2'	1:G:7:DA:H5''	1.91	1.00
2:J:108:DT:H2''	2:J:109:DC:H5''	1.46	0.97
3:B:481:GLN:HE21	3:B:559:ARG:HE	1.13	0.97
3:A:2:LYS:H	3:A:2:LYS:HD2	1.33	0.91
3:D:194:GLU:HG2	3:D:229:ARG:HH21	1.35	0.91
3:C:356:GLN:H	3:C:356:GLN:HE21	1.16	0.89
1:I:3:3DR:H2''	1:I:4:DC:H5'	1.55	0.88
3:A:698:ILE:O	3:A:698:ILE:HG13	1.75	0.87
3:D:112:ASN:HB3	3:D:214:THR:HG23	1.55	0.86
3:B:606:ASN:HD21	3:B:614:GLU:H	1.19	0.86
3:B:499:ILE:HA	3:B:530:ILE:HD11	1.57	0.86
3:D:412:LEU:HB2	3:D:623:ASP:HB2	1.58	0.86
3:C:163:SER:H	3:C:318:GLN:HE22	1.23	0.85
3:D:422:GLN:HE22	3:D:681:MET:HG2	1.42	0.83
3:B:115:ILE:HD11	3:B:133:ILE:HG21	1.59	0.83
3:C:74:ARG:HD3	4:C:1164:HOH:O	1.77	0.83
3:D:819:ILE:HG22	3:D:820:ASP:H	1.44	0.82
3:A:85:MET:HE2	3:A:87:ASP:H	1.43	0.82
3:B:261:GLU:HG3	3:B:262:ILE:H	1.44	0.82
3:C:303:LEU:HD22	3:C:303:LEU:H	1.45	0.81
2:H:103:DG:H2''	2:H:104:DG:H5'	1.62	0.81
2:J:110:DA:H2''	2:J:111:DT:H5''	1.64	0.80
3:B:475:ILE:HD13	3:B:566:LEU:HD12	1.63	0.80
3:C:356:GLN:H	3:C:356:GLN:NE2	1.79	0.80
3:D:461:MET:HE1	3:D:581:ARG:HH21	1.48	0.79
3:D:295:GLU:HG2	3:D:301:GLY:HA2	1.64	0.79
3:B:2:LYS:HD3	4:B:1077:HOH:O	1.82	0.78
3:C:167:ALA:HA	3:C:176:ASP:HB2	1.66	0.78
3:B:481:GLN:NE2	3:B:559:ARG:HE	1.80	0.78
3:D:458:PRO:HB2	3:D:588:THR:HG22	1.64	0.78
3:B:116:GLU:HB2	3:B:135:ALA:HB3	1.64	0.78
2:J:108:DT:H2''	2:J:109:DC:C5'	2.13	0.78
3:D:751:ARG:HA	3:D:755:GLU:HG3	1.66	0.78
3:B:559:ARG:O	3:B:563:ILE:HG12	1.84	0.77
3:A:792:ASP:HB2	4:A:927:HOH:O	1.84	0.77
3:C:302:LYS:HA	3:C:302:LYS:HE2	1.66	0.77
3:A:481:GLN:HE21	3:A:559:ARG:HE	1.33	0.77
3:D:402:ASN:ND2	3:D:403:ARG:H	1.83	0.76
3:C:298:LEU:HB2	3:C:300:VAL:HG12	1.65	0.76
3:B:897:LEU:H	3:B:897:LEU:HD23	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:495:ASN:HD21	3:C:522:PHE:H	1.33	0.76
3:B:321:ILE:HD12	4:B:1074:HOH:O	1.87	0.75
1:E:6:DT:H2''	1:E:7:DA:H5''	1.69	0.74
3:B:223:ILE:HB	3:B:224:PRO:HD3	1.69	0.74
3:B:273:TYR:HA	3:B:276:LEU:HD12	1.68	0.74
3:C:354:GLN:HB3	3:C:356:GLN:HE22	1.53	0.74
3:A:206:GLN:NE2	3:A:241:ARG:HE	1.86	0.73
3:C:482:ARG:HE	3:C:556:GLN:HE21	1.36	0.73
3:A:698:ILE:C	4:A:998:HOH:O	2.29	0.73
3:A:699:GLY:N	4:A:998:HOH:O	2.21	0.73
3:B:222:ALA:O	3:B:226:VAL:HG23	1.89	0.73
3:A:602:ASN:HD21	3:A:617:VAL:H	1.35	0.72
3:B:133:ILE:HD11	3:B:198:LEU:HD21	1.70	0.72
3:C:78:ILE:HG13	3:C:80:LEU:HD23	1.71	0.72
3:B:336:ALA:HB3	3:B:337:LYS:HE3	1.70	0.72
3:D:500:LYS:HA	3:D:503:LEU:HD12	1.71	0.72
3:D:597:ILE:HG21	3:D:683:MET:HE1	1.71	0.72
3:C:231:LYS:HG3	3:C:236:GLU:HA	1.69	0.72
3:D:740:ALA:HB2	3:D:778:SER:HB3	1.71	0.71
3:B:231:LYS:HG3	3:B:236:GLU:HA	1.72	0.71
3:A:581:ARG:HD3	4:A:1102:HOH:O	1.90	0.71
3:B:273:TYR:HB3	4:B:1083:HOH:O	1.91	0.70
3:C:411:ASP:OD1	3:C:624:SER:HB3	1.91	0.70
3:D:308:PRO:HG2	3:D:311:LYS:HB2	1.74	0.70
3:D:298:LEU:HB2	3:D:300:VAL:HG12	1.72	0.70
3:A:698:ILE:O	3:A:753:LEU:HA	1.92	0.69
3:C:116:GLU:HB2	3:C:135:ALA:HB3	1.74	0.69
3:D:530:ILE:HA	3:D:533:LEU:HD13	1.73	0.69
1:E:5:DT:H2''	1:E:6:DT:H5'	1.73	0.69
3:C:516:VAL:HG11	3:C:526:ILE:HD13	1.74	0.69
3:D:85:MET:HE2	3:D:87:ASP:H	1.56	0.69
1:E:6:DT:H2''	1:E:7:DA:C5'	2.22	0.69
2:H:112:DA:H2''	2:H:113:DA:H5'	1.74	0.69
3:A:471:VAL:HB	3:A:472:PRO:HD3	1.75	0.69
3:A:649:ASP:O	3:A:653:LYS:HG2	1.92	0.69
3:B:11:ILE:HD13	3:B:247:LYS:HG3	1.74	0.69
3:D:170:LEU:HD12	3:D:170:LEU:H	1.58	0.69
3:D:660:GLU:HG2	4:D:915:HOH:O	1.92	0.68
3:D:399:PRO:HB3	3:D:619:TYR:HD2	1.58	0.68
1:K:5:DT:H2''	1:K:6:DT:H5'	1.74	0.68
3:C:441:ASP:HB3	3:C:447:ALA:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:167:ALA:HA	3:B:177:GLU:OE2	1.93	0.68
2:J:108:DT:C2'	2:J:109:DC:H5''	2.21	0.68
1:K:6:DT:H1'	3:D:706:LYS:HE3	1.75	0.68
3:A:775:ASN:OD1	3:A:777:ILE:HG22	1.94	0.68
3:D:530:ILE:HG13	3:D:533:LEU:HD22	1.74	0.68
3:A:540:GLU:O	3:A:544:ARG:HD3	1.93	0.68
1:K:15:DC:H5''	4:K:457:HOH:O	1.94	0.67
1:I:10:DA:H2''	1:I:11:DC:H5''	1.75	0.67
3:D:223:ILE:HB	3:D:224:PRO:HD3	1.74	0.67
3:D:731:GLU:HG3	3:D:879:PRO:HB3	1.75	0.67
4:F:120:HOH:O	3:A:783:SER:HA	1.95	0.67
3:D:598:GLU:HG3	3:D:617:VAL:HG11	1.76	0.67
3:D:833:LEU:HD21	3:D:866:MET:HE3	1.74	0.67
3:A:354:GLN:HB3	3:A:356:GLN:HE22	1.59	0.67
3:C:526:ILE:HD12	4:C:1045:HOH:O	1.94	0.67
3:D:516:VAL:HG11	3:D:526:ILE:HG21	1.77	0.67
3:D:860:ASP:H	3:D:863:LEU:HD23	1.60	0.67
3:A:602:ASN:ND2	3:A:616:PHE:H	1.92	0.66
3:C:148:VAL:HG13	4:C:1125:HOH:O	1.96	0.66
3:D:830:VAL:HA	3:D:850:SER:HB3	1.78	0.66
3:A:72:ILE:O	3:A:76:GLU:HG3	1.95	0.66
3:A:481:GLN:NE2	3:A:559:ARG:HE	1.93	0.66
3:C:81:GLU:HG2	3:C:83:LEU:CD1	2.26	0.66
3:A:526:ILE:HG23	3:A:529:LYS:HD2	1.77	0.65
3:B:738:PRO:HG2	3:B:741:VAL:HB	1.77	0.65
3:D:738:PRO:HG2	3:D:741:VAL:HB	1.77	0.65
1:G:6:DT:H5''	1:G:6:DT:H6	1.62	0.65
3:D:41:CYS:HB2	3:D:45:GLN:HG3	1.78	0.65
2:H:112:DA:H2''	2:H:113:DA:C5'	2.25	0.65
3:D:118:THR:HG21	3:D:313:ARG:HB3	1.79	0.65
3:D:700:GLY:HA2	3:D:753:LEU:HD22	1.79	0.65
3:B:119:SER:HB3	3:B:124:PRO:HD3	1.77	0.65
3:C:283:THR:HB	4:C:1145:HOH:O	1.95	0.65
3:D:606:ASN:HD21	3:D:614:GLU:H	1.45	0.65
2:J:114:DG:H2''	2:J:115:DA:O5'	1.96	0.64
3:D:149:PHE:HB3	3:D:197:LEU:HD21	1.79	0.64
2:F:110:DA:H1'	2:F:111:DT:H5''	1.79	0.64
3:C:277:TYR:O	3:C:281:SER:HB3	1.97	0.64
3:D:398:GLU:OE1	3:D:705:LYS:HE3	1.97	0.64
3:B:540:GLU:HB3	3:B:544:ARG:NH1	2.13	0.64
3:A:848:TRP:HB2	3:A:849:PRO:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:512:GLU:HG3	3:D:513:PRO:HD2	1.78	0.64
2:J:110:DA:H2''	2:J:111:DT:C5'	2.28	0.64
3:A:598:GLU:HG3	3:A:617:VAL:HG11	1.79	0.64
1:E:5:DT:H2'	1:E:6:DT:H71	1.80	0.64
1:K:5:DT:H2''	1:K:6:DT:C5'	2.28	0.63
2:F:113:DA:H3'	2:F:114:DG:H5''	1.80	0.63
3:B:52:ILE:HD12	3:B:428:GLU:HG3	1.81	0.63
3:A:422:GLN:NE2	3:A:680:LEU:H	1.96	0.63
3:A:653:LYS:O	3:A:657:GLU:HG2	1.98	0.63
3:A:514:LEU:HD12	3:A:530:ILE:HG12	1.80	0.63
3:C:60:LYS:C	4:C:1100:HOH:O	2.41	0.63
2:F:110:DA:H2''	2:F:111:DT:C5'	2.28	0.63
2:J:112:DA:H2'	4:J:405:HOH:O	1.98	0.63
3:A:85:MET:CE	3:A:87:ASP:H	2.12	0.63
3:A:2:LYS:H	3:A:2:LYS:CD	2.06	0.62
3:A:408:MET:HE1	3:A:655:ALA:HB2	1.80	0.62
2:F:103:DG:H2''	2:F:104:DG:H5'	1.82	0.62
3:A:82:ALA:O	3:A:382:GLN:HB2	1.99	0.62
3:B:606:ASN:ND2	3:B:614:GLU:H	1.95	0.62
3:C:223:ILE:HB	3:C:224:PRO:HD3	1.80	0.62
3:C:530:ILE:HG23	3:C:538:LEU:HD21	1.80	0.62
2:H:105:DC:H2'	2:H:106:DT:H72	1.80	0.62
3:C:482:ARG:HH21	3:C:556:GLN:NE2	1.97	0.62
3:D:660:GLU:HB2	3:D:661:PRO:HD3	1.82	0.62
3:C:191:PHE:HD2	3:C:196:GLU:HG3	1.63	0.62
3:A:2:LYS:HG2	3:A:102:LYS:HE3	1.81	0.62
3:A:395:PHE:HB2	3:A:591:GLN:CG	2.25	0.62
3:B:482:ARG:NH2	3:B:560:LYS:HD3	2.14	0.61
3:D:434:PHE:CZ	3:D:460:GLY:HA2	2.35	0.61
3:C:1:MET:HG2	3:C:22:SER:O	2.00	0.61
3:C:888:LYS:HE3	4:C:918:HOH:O	1.99	0.61
3:D:362:ILE:HG23	3:D:575:PHE:HD1	1.63	0.61
2:J:115:DA:H2'	4:J:414:HOH:O	1.98	0.61
2:H:104:DG:H2''	2:H:105:DC:O5'	2.00	0.61
3:D:230:ILE:HG23	3:D:234:PHE:HD2	1.66	0.61
3:D:51:ASP:HB2	4:D:912:HOH:O	2.01	0.61
2:L:112:DA:H2''	2:L:113:DA:H5'	1.82	0.61
3:B:635:LYS:HG2	3:D:898:PHE:CD2	2.35	0.61
3:C:148:VAL:HG22	4:C:1125:HOH:O	2.00	0.61
3:C:401:PRO:O	3:C:402:ASN:HB2	2.01	0.61
3:D:151:LEU:HD11	3:D:194:GLU:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:812:ASN:HA	3:D:815:ILE:HG12	1.83	0.61
3:B:514:LEU:HG	3:B:533:LEU:HD21	1.82	0.61
3:D:859:LYS:HD3	3:D:860:ASP:HB2	1.81	0.61
2:F:103:DG:H2'	2:F:104:DG:C8	2.35	0.61
1:K:17:DC:H2''	1:K:18:DG:OP1	2.01	0.60
3:B:606:ASN:HD21	3:B:614:GLU:N	1.97	0.60
3:D:286:PRO:O	3:D:829:LYS:HD2	2.01	0.60
1:K:4:DC:H42	2:L:114:DG:H1	1.49	0.60
3:B:202:LEU:O	3:B:206:GLN:HG2	2.01	0.60
3:D:401:PRO:HA	3:D:702:TRP:O	2.01	0.60
3:B:24:GLY:HA3	3:B:107:LYS:HE3	1.83	0.60
3:B:490:LEU:HA	3:B:493:GLN:HG2	1.83	0.60
3:C:169:LYS:HE2	3:C:174:GLY:H	1.66	0.60
3:C:424:ASN:HD21	3:C:469:GLY:H	1.48	0.60
3:D:535:ALA:HA	3:D:538:LEU:HB2	1.84	0.60
3:B:154:SER:HB2	3:B:155:PRO:HD2	1.82	0.60
3:A:176:ASP:HA	3:A:319:ARG:NH2	2.16	0.60
3:B:582:ASN:O	3:B:586:ILE:HG13	2.02	0.60
3:D:140:ASP:HB3	3:D:143:ASP:HB2	1.84	0.60
3:D:271:LEU:HD21	3:D:356:GLN:HA	1.84	0.60
3:B:825:VAL:HB	3:B:828:GLU:HG3	1.84	0.60
3:D:87:ASP:OD1	3:D:90:LEU:HD13	2.01	0.60
2:J:101:DG:H2'	2:J:102:DC:C5	2.36	0.60
2:J:110:DA:C2'	2:J:111:DT:H5''	2.32	0.60
3:C:815:ILE:HG23	3:C:821:ALA:HB3	1.84	0.60
3:A:441:ASP:HB3	3:A:447:ALA:HB2	1.83	0.59
3:B:391:TYR:HB2	3:B:392:PRO:HD2	1.83	0.59
3:D:416:TYR:HB2	3:D:417:PRO:HD3	1.83	0.59
1:E:5:DT:H2''	1:E:6:DT:C5'	2.32	0.59
3:C:52:ILE:HD12	3:C:428:GLU:HG3	1.82	0.59
3:D:434:PHE:CE1	3:D:460:GLY:HA2	2.37	0.59
3:D:449:ARG:HH21	3:D:675:ASN:HB2	1.65	0.59
3:A:556:GLN:HE22	3:A:557:ILE:HD13	1.67	0.59
3:B:261:GLU:HG3	3:B:262:ILE:N	2.17	0.59
3:C:10:GLN:HG3	3:C:65:MET:HE1	1.85	0.59
3:D:131:HIS:HB3	3:D:132:PRO:HD2	1.85	0.59
3:D:698:ILE:HG12	3:D:752:MET:O	2.02	0.59
3:A:698:ILE:CA	4:A:998:HOH:O	2.49	0.59
3:B:772:ARG:HG2	4:B:1043:HOH:O	2.03	0.59
3:D:854:ILE:HD12	3:D:859:LYS:HB2	1.85	0.59
3:B:136:ILE:HG23	3:B:149:PHE:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:405:LYS:O	3:D:690:GLY:HA2	2.03	0.58
3:D:471:VAL:HB	3:D:472:PRO:HD3	1.86	0.58
3:D:90:LEU:HG	3:D:353:ILE:HG22	1.85	0.58
3:C:469:GLY:C	3:C:472:PRO:HD2	2.29	0.58
3:D:102:LYS:HB2	3:D:102:LYS:NZ	2.18	0.58
2:H:110:DA:H2''	2:H:111:DT:O5'	2.02	0.58
2:F:110:DA:H2''	2:F:111:DT:H5'	1.84	0.58
3:C:284:ASN:HD21	3:C:829:LYS:HZ2	1.52	0.58
3:A:41:CYS:HB2	3:A:42:PRO:HD2	1.84	0.58
3:D:503:LEU:O	3:D:506:PRO:HD3	2.04	0.58
3:A:354:GLN:HB3	3:A:356:GLN:NE2	2.17	0.58
3:A:403:ARG:HD2	3:A:887:ALA:O	2.04	0.58
3:A:839:ASN:HD22	3:A:841:PHE:HB2	1.69	0.58
3:B:797:PRO:HG3	3:B:806:ARG:NH1	2.19	0.58
3:D:395:PHE:HB2	3:D:591:GLN:HG2	1.86	0.58
1:I:10:DA:H2''	1:I:11:DC:C5'	2.34	0.58
3:A:530:ILE:HG23	3:A:541:MET:HE3	1.85	0.57
3:B:470:VAL:O	3:B:474:GLU:HG2	2.04	0.57
3:D:115:ILE:HG22	3:D:136:ILE:HG12	1.86	0.57
3:B:514:LEU:N	3:B:541:MET:HE1	2.19	0.57
3:B:760:LEU:HD13	3:B:891:TYR:HA	1.87	0.57
3:C:78:ILE:CG1	3:C:80:LEU:HD23	2.34	0.57
3:A:202:LEU:O	3:A:206:GLN:HG2	2.05	0.57
3:B:322:SER:O	3:B:326:ILE:HG12	2.03	0.57
3:A:731:GLU:H	3:A:731:GLU:CD	2.10	0.57
3:C:216:TRP:O	3:C:217:ASN:HB2	2.05	0.57
3:B:339:GLN:HB3	4:B:1056:HOH:O	2.04	0.57
3:A:395:PHE:CB	3:A:591:GLN:HG3	2.26	0.57
3:B:219:GLU:HG2	3:B:262:ILE:HG23	1.86	0.56
3:D:359:PHE:O	3:D:361:PRO:HD3	2.05	0.56
3:B:178:VAL:HB	3:B:179:PRO:HA	1.86	0.56
3:B:199:MET:HE2	3:B:199:MET:HA	1.86	0.56
3:D:236:GLU:HA	3:D:239:ALA:HB3	1.88	0.56
3:D:664:ASP:O	3:D:668:ARG:HG3	2.05	0.56
2:J:101:DG:H2'	2:J:102:DC:C6	2.41	0.56
3:B:279:LYS:HE3	3:B:280:PHE:CZ	2.39	0.56
3:D:405:LYS:O	3:D:699:GLY:HA3	2.05	0.56
3:D:698:ILE:O	3:D:753:LEU:HA	2.05	0.56
3:C:302:LYS:HG2	3:C:330:ARG:HH12	1.71	0.56
1:E:18:DG:OP1	1:E:18:DG:H3'	2.06	0.56
3:B:897:LEU:HD12	3:D:636:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:VAL:HG21	3:C:317:HIS:CD2	2.40	0.56
3:D:696:LYS:O	3:D:756:GLY:HA2	2.05	0.56
1:I:7:DA:H2'	1:I:8:DT:H72	1.88	0.56
3:A:402:ASN:HA	3:A:886:ALA:O	2.06	0.56
3:D:545:ALA:HB1	4:D:923:HOH:O	2.04	0.56
2:J:111:DT:H2''	2:J:112:DA:H8	1.71	0.56
3:A:51:ASP:HA	3:A:379:VAL:HG22	1.87	0.56
3:A:362:ILE:HD11	3:A:569:ALA:HA	1.88	0.56
4:K:596:HOH:O	3:D:800:LYS:HG3	2.06	0.56
3:C:481:GLN:HE21	3:C:559:ARG:HE	1.53	0.56
3:C:507:ASN:N	3:C:507:ASN:HD22	2.04	0.56
3:A:112:ASN:HB3	4:A:1119:HOH:O	2.05	0.55
3:B:316:ASN:C	3:B:318:GLN:H	2.14	0.55
3:D:597:ILE:O	3:D:601:VAL:HG23	2.06	0.55
3:D:856:ASP:HA	3:D:859:LYS:HG2	1.88	0.55
3:A:159:VAL:HG21	3:A:317:HIS:CD2	2.42	0.55
3:A:249:ARG:HB3	3:A:264:THR:HG23	1.89	0.55
3:B:326:ILE:O	3:B:330:ARG:HG2	2.06	0.55
3:D:805:ILE:HA	3:D:808:ILE:HD12	1.88	0.55
3:C:148:VAL:HG23	3:C:188:TYR:HA	1.88	0.55
3:C:221:PHE:C	3:C:224:PRO:HD2	2.31	0.55
2:H:109:DC:H2''	2:H:110:DA:H5'	1.89	0.55
3:A:48:LYS:HZ3	3:A:377:ASN:CG	2.15	0.55
3:A:202:LEU:CD1	3:A:242:LEU:HD13	2.36	0.55
3:A:249:ARG:HH11	3:A:251:LYS:HE2	1.71	0.55
3:D:272:ASP:OD1	3:D:274:ILE:HG22	2.06	0.55
3:C:61:LEU:N	4:C:1100:HOH:O	2.39	0.55
3:C:303:LEU:HB2	3:C:323:TYR:OH	2.07	0.55
1:G:8:DT:H2'	1:G:9:DG:C8	2.42	0.55
3:D:109:ARG:HB3	3:D:211:VAL:HG23	1.87	0.55
3:A:654:PHE:O	3:A:658:ARG:HB2	2.07	0.55
3:D:206:GLN:HE22	3:D:241:ARG:HE	1.55	0.55
3:D:426:SER:OG	3:D:427:PRO:HD2	2.07	0.55
3:B:336:ALA:CB	3:B:337:LYS:HE3	2.37	0.55
3:D:250:VAL:HG12	3:D:263:ILE:HD12	1.89	0.55
3:A:482:ARG:HE	3:A:556:GLN:HE21	1.54	0.54
3:B:356:GLN:C	3:B:358:VAL:H	2.14	0.54
3:A:223:ILE:HB	3:A:224:PRO:HD3	1.89	0.54
3:A:732:THR:HG22	3:A:745:LEU:HB3	1.87	0.54
3:C:475:ILE:HG12	3:C:566:LEU:HD12	1.90	0.54
2:F:103:DG:H2''	2:F:104:DG:C5'	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:482:ARG:HE	3:A:556:GLN:HG2	1.72	0.54
3:A:779:ILE:O	3:A:871:LEU:HD21	2.07	0.54
3:A:25:ARG:HD2	4:A:926:HOH:O	2.08	0.54
3:B:2:LYS:HA	4:B:1077:HOH:O	2.07	0.54
3:B:47:THR:HB	4:B:1059:HOH:O	2.08	0.54
3:B:897:LEU:HD23	3:B:897:LEU:N	2.22	0.54
3:C:313:ARG:O	3:C:317:HIS:HB2	2.08	0.54
3:D:66:ARG:HH21	3:D:70:GLN:NE2	2.05	0.54
1:G:15:DC:H5''	4:G:515:HOH:O	2.08	0.54
3:A:555:ALA:O	3:A:559:ARG:HG2	2.08	0.54
3:A:822:PRO:HD2	3:A:855:THR:HB	1.88	0.54
3:C:412:LEU:HG	3:C:683:MET:HE3	1.90	0.54
3:D:229:ARG:NE	3:D:233:ILE:HD11	2.22	0.54
3:D:509:SER:HA	3:D:534:SER:HB3	1.89	0.54
3:D:151:LEU:HD23	3:D:152:LEU:N	2.22	0.54
3:A:85:MET:HE2	3:A:87:ASP:N	2.18	0.54
3:D:4:PHE:HB3	3:D:101:ILE:HG21	1.90	0.54
3:D:165:GLU:CD	3:D:165:GLU:H	2.15	0.54
3:D:216:TRP:H	3:D:218:VAL:HG13	1.73	0.54
3:D:364:THR:O	3:D:368:ILE:HG13	2.08	0.54
3:A:542:LEU:O	3:A:546:GLN:HG3	2.07	0.54
3:B:1:MET:HE1	3:B:20:ILE:CG2	2.37	0.54
3:B:26:GLU:O	3:B:27:ARG:HG2	2.08	0.54
3:B:516:VAL:HG11	3:B:526:ILE:HD13	1.89	0.54
3:D:469:GLY:C	3:D:472:PRO:HD2	2.33	0.54
1:K:2:DG:C3'	1:K:3:3DR:H5'	2.38	0.54
3:A:98:ASN:HB3	4:A:1126:HOH:O	2.07	0.54
3:A:222:ALA:O	3:A:226:VAL:HG23	2.08	0.54
2:J:105:DC:P	4:J:206:HOH:O	2.66	0.53
2:L:105:DC:H2'	2:L:106:DT:H72	1.91	0.53
2:F:112:DA:H2''	2:F:113:DA:O4'	2.08	0.53
2:H:105:DC:H2'	2:H:106:DT:C7	2.39	0.53
3:D:368:ILE:HD13	3:D:562:LEU:HD21	1.91	0.53
3:D:441:ASP:HB3	3:D:447:ALA:HB2	1.90	0.53
1:K:5:DT:H2'	1:K:6:DT:H71	1.90	0.53
3:C:438:PRO:HD2	3:C:441:ASP:OD1	2.08	0.53
3:D:182:ILE:O	3:D:186:ILE:HG13	2.08	0.53
1:E:6:DT:H2''	1:E:7:DA:O5'	2.08	0.53
3:B:326:ILE:CG2	3:B:330:ARG:HE	2.22	0.53
3:C:354:GLN:HB3	3:C:356:GLN:NE2	2.23	0.53
3:D:241:ARG:CZ	3:D:241:ARG:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:472:PRO:O	3:B:475:ILE:HG22	2.08	0.53
3:C:458:PRO:HD3	3:C:674:MET:HE2	1.90	0.53
3:A:85:MET:HE2	3:A:87:ASP:HB3	1.89	0.53
3:A:284:ASN:HA	3:A:288:TYR:OH	2.08	0.53
3:B:478:VAL:HG13	3:B:559:ARG:HD2	1.90	0.52
3:B:731:GLU:HG3	3:B:879:PRO:CB	2.39	0.52
3:C:299:ASN:HB3	4:C:927:HOH:O	2.07	0.52
3:C:475:ILE:CG1	3:C:566:LEU:HD12	2.38	0.52
3:C:731:GLU:CD	3:C:731:GLU:H	2.17	0.52
3:D:397:LYS:O	3:D:399:PRO:HD3	2.09	0.52
3:D:422:GLN:NE2	3:D:681:MET:HG2	2.18	0.52
3:B:250:VAL:HA	3:B:263:ILE:HG22	1.90	0.52
3:C:27:ARG:HH11	3:C:27:ARG:HB3	1.74	0.52
3:C:471:VAL:HB	3:C:472:PRO:HD3	1.91	0.52
3:C:516:VAL:CG1	3:C:526:ILE:HD13	2.39	0.52
3:A:507:ASN:HD22	3:A:532:LYS:HA	1.74	0.52
3:A:839:ASN:ND2	3:A:841:PHE:HB2	2.24	0.52
3:B:333:GLN:O	3:B:337:LYS:HG2	2.08	0.52
3:A:101:ILE:HD11	3:A:349:TYR:O	2.09	0.52
3:A:338:ARG:HB3	3:A:340:PHE:CE1	2.44	0.52
3:B:219:GLU:HA	3:B:223:ILE:HD12	1.90	0.52
3:B:514:LEU:HD13	3:B:526:ILE:HG23	1.90	0.52
3:A:245:HIS:HE1	4:A:938:HOH:O	1.92	0.52
3:A:285:GLN:HB3	3:A:292:TYR:HE2	1.75	0.52
3:B:145:ARG:HD2	3:B:187:ILE:HD11	1.91	0.52
3:B:294:SER:O	3:B:298:LEU:HB2	2.10	0.52
3:C:874:LYS:HB2	4:C:1151:HOH:O	2.07	0.52
3:D:271:LEU:HD11	3:D:355:ILE:HG22	1.90	0.52
3:C:738:PRO:HB3	3:C:780:ALA:O	2.10	0.52
3:D:194:GLU:HG2	3:D:229:ARG:NH2	2.15	0.52
3:D:656:ARG:HA	3:D:660:GLU:HG3	1.91	0.52
3:A:609:CYS:HA	3:A:635:LYS:HE3	1.91	0.52
3:B:755:GLU:HB3	3:B:759:SER:HB3	1.91	0.52
3:C:78:ILE:CD1	3:C:80:LEU:HD23	2.39	0.52
3:C:221:PHE:O	3:C:224:PRO:HD2	2.10	0.52
3:C:642:ARG:HH11	3:C:646:HIS:CD2	2.27	0.52
3:B:1:MET:HE1	3:B:20:ILE:HG22	1.91	0.52
3:B:355:ILE:C	3:B:356:GLN:O	2.51	0.52
3:B:491:ALA:HA	3:B:494:ARG:HH11	1.73	0.52
3:C:81:GLU:HG2	3:C:83:LEU:HD11	1.91	0.52
3:D:36:SER:HB3	3:D:59:ARG:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:594:LEU:O	3:D:597:ILE:HG22	2.09	0.52
3:C:495:ASN:ND2	3:C:522:PHE:H	2.05	0.52
3:D:167:ALA:HB2	3:D:318:GLN:HE22	1.74	0.52
3:A:566:LEU:O	3:A:570:LEU:HD23	2.10	0.51
3:B:441:ASP:HB3	3:B:447:ALA:HB2	1.91	0.51
3:D:148:VAL:HG21	3:D:325:ILE:HD11	1.93	0.51
3:D:403:ARG:HD2	3:D:887:ALA:O	2.10	0.51
1:E:15:DC:H2''	1:E:16:DG:O5'	2.09	0.51
3:C:592:MET:HE3	3:C:670:MET:SD	2.50	0.51
3:D:793:VAL:HG22	3:D:796:PHE:O	2.10	0.51
3:D:863:LEU:HD22	3:D:863:LEU:H	1.74	0.51
3:B:700:GLY:HA3	3:B:710:LEU:HD23	1.92	0.51
3:B:818:ASN:HD21	3:B:857:LEU:HD11	1.74	0.51
3:A:556:GLN:NE2	3:A:557:ILE:HD13	2.26	0.51
3:D:109:ARG:NH1	3:D:142:ILE:HD11	2.25	0.51
2:H:114:DG:H2''	2:H:115:DA:C8	2.46	0.51
2:J:113:DA:H2''	2:J:114:DG:H5''	1.93	0.51
3:A:356:GLN:NE2	3:A:356:GLN:H	2.08	0.51
3:B:163:SER:H	3:B:318:GLN:HE21	1.57	0.51
3:C:760:LEU:HD13	3:C:891:TYR:HA	1.92	0.51
3:D:802:PRO:HD2	3:D:805:ILE:HG13	1.92	0.51
3:C:284:ASN:HD21	3:C:829:LYS:NZ	2.07	0.51
3:D:475:ILE:HD13	3:D:475:ILE:O	2.10	0.51
3:D:517:ASP:OD2	3:D:519:ARG:HB2	2.09	0.51
1:G:7:DA:H2'	1:G:8:DT:H72	1.93	0.51
3:A:698:ILE:O	3:A:698:ILE:CG1	2.54	0.51
3:D:132:PRO:HG2	4:D:920:HOH:O	2.09	0.51
3:A:85:MET:HE2	3:A:87:ASP:CB	2.41	0.50
3:A:730:LEU:HD22	3:A:883:PHE:CE1	2.46	0.50
3:B:356:GLN:O	3:B:357:SER:HB2	2.11	0.50
3:B:450:PRO:HG2	4:B:965:HOH:O	2.09	0.50
3:C:451:SER:HB3	3:C:456:CYS:SG	2.51	0.50
3:C:179:PRO:HB3	3:C:181:GLU:OE1	2.10	0.50
3:C:555:ALA:O	3:C:559:ARG:HG2	2.12	0.50
3:D:273:TYR:OH	3:D:335:ASP:HA	2.10	0.50
3:B:731:GLU:HG3	3:B:879:PRO:HB3	1.93	0.50
3:C:645:ASN:ND2	3:C:719:ARG:HH11	2.09	0.50
3:A:482:ARG:HG2	3:A:482:ARG:HH11	1.76	0.50
3:B:313:ARG:HG2	3:B:313:ARG:HH11	1.77	0.50
3:D:47:THR:HG21	3:D:57:CYS:H	1.75	0.50
3:D:72:ILE:HG22	3:D:76:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:277:TYR:O	3:D:281:SER:HB2	2.12	0.50
3:D:637:GLY:O	3:D:640:LYS:HB2	2.11	0.50
2:H:109:DC:H2''	2:H:110:DA:C5'	2.42	0.50
3:A:412:LEU:HG	3:A:683:MET:HG2	1.93	0.50
3:C:424:ASN:HD22	3:C:472:PRO:HG2	1.77	0.50
3:D:7:THR:HG22	3:D:18:ARG:HB2	1.92	0.50
3:D:197:LEU:HD23	3:D:197:LEU:O	2.12	0.50
3:D:439:LEU:O	3:D:443:ILE:HG13	2.12	0.50
3:D:508:LEU:N	3:D:508:LEU:HD22	2.27	0.50
3:B:499:ILE:HA	3:B:530:ILE:CD1	2.37	0.50
3:C:726:LYS:HE3	4:C:1054:HOH:O	2.12	0.50
2:H:102:DC:H2''	2:H:103:DG:C8	2.46	0.50
3:A:517:ASP:OD2	3:A:519:ARG:HB2	2.11	0.50
3:C:171:GLN:HE22	3:C:303:LEU:HB3	1.77	0.50
3:D:863:LEU:HD22	3:D:863:LEU:N	2.27	0.50
2:F:108:DT:H2''	2:F:109:DC:O5'	2.12	0.50
1:K:11:DC:H4'	3:D:803:PHE:HB2	1.94	0.50
3:A:221:PHE:O	3:A:224:PRO:HD2	2.12	0.50
3:C:496:GLY:O	3:C:500:LYS:HG2	2.12	0.50
3:D:109:ARG:HD2	3:D:209:THR:O	2.12	0.50
3:D:330:ARG:O	3:D:334:ILE:HG13	2.12	0.50
3:D:458:PRO:HG3	3:D:592:MET:SD	2.51	0.50
3:C:302:LYS:HD2	3:C:326:ILE:HD13	1.93	0.50
3:D:542:LEU:O	3:D:546:GLN:HG3	2.11	0.50
3:B:273:TYR:HA	3:B:276:LEU:HB2	1.94	0.49
3:B:660:GLU:HB3	3:B:661:PRO:HD3	1.93	0.49
2:J:112:DA:H2''	2:J:113:DA:H5'	1.94	0.49
3:B:159:VAL:HG13	3:B:313:ARG:HH12	1.78	0.49
3:D:738:PRO:HB3	3:D:780:ALA:C	2.36	0.49
3:D:411:ASP:HB2	3:D:686:GLU:OE1	2.11	0.49
3:C:191:PHE:CD2	3:C:196:GLU:HG3	2.46	0.49
3:D:422:GLN:HG3	3:D:678:GLN:O	2.13	0.49
3:D:566:LEU:HD13	3:D:566:LEU:C	2.37	0.49
2:H:112:DA:C2'	2:H:113:DA:H5'	2.41	0.49
3:B:483:LYS:NZ	3:B:483:LYS:HB3	2.27	0.49
3:B:555:ALA:O	3:B:559:ARG:HG2	2.13	0.49
3:C:300:VAL:O	3:C:300:VAL:HG13	2.11	0.49
3:C:322:SER:O	3:C:326:ILE:HG23	2.12	0.49
3:C:362:ILE:HD13	3:C:569:ALA:HB1	1.95	0.49
3:A:481:GLN:HE21	3:A:559:ARG:NE	2.07	0.49
3:D:145:ARG:HG2	3:D:187:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:831:TYR:CD1	3:D:850:SER:HA	2.48	0.49
3:B:707:ARG:HD2	4:B:1050:HOH:O	2.12	0.49
3:A:101:ILE:HG12	4:A:1047:HOH:O	2.12	0.49
3:D:71:TRP:O	3:D:75:MET:HG2	2.12	0.49
3:D:222:ALA:O	3:D:226:VAL:HG23	2.11	0.49
3:D:633:ILE:HG13	3:D:651:LEU:HD21	1.94	0.49
1:E:12:DA:H2''	1:E:13:DG:O5'	2.13	0.49
3:A:731:GLU:HG3	3:A:879:PRO:CB	2.43	0.49
3:D:191:PHE:HB2	3:D:197:LEU:HD12	1.94	0.49
3:A:277:TYR:C	3:A:279:LYS:H	2.20	0.49
3:A:856:ASP:O	3:A:857:LEU:HB2	2.13	0.49
3:B:405:LYS:HA	3:B:698:ILE:O	2.12	0.49
3:C:488:TYR:CD1	3:C:519:ARG:HB3	2.48	0.49
3:A:48:LYS:NZ	3:A:377:ASN:CG	2.71	0.48
3:B:303:LEU:H	3:B:303:LEU:HD22	1.78	0.48
3:B:458:PRO:HG3	3:B:592:MET:SD	2.52	0.48
3:C:197:LEU:HD23	3:C:197:LEU:C	2.38	0.48
3:D:204:PHE:HE1	3:D:208:LYS:HD2	1.78	0.48
3:D:313:ARG:HD3	3:D:320:TYR:CE2	2.48	0.48
3:D:362:ILE:HD11	3:D:572:ASN:HD22	1.78	0.48
3:D:509:SER:HA	3:D:534:SER:CB	2.43	0.48
3:D:727:ILE:HG23	3:D:730:LEU:HD12	1.95	0.48
1:K:14:DC:H2''	1:K:15:DC:O5'	2.14	0.48
3:A:530:ILE:HA	3:A:533:LEU:HD13	1.95	0.48
3:B:372:SER:O	3:B:375:GLU:HG2	2.13	0.48
3:C:453:VAL:HG23	3:C:454:TYR:CG	2.48	0.48
3:A:405:LYS:O	3:A:690:GLY:HA2	2.14	0.48
3:D:137:THR:HG21	3:D:325:ILE:HA	1.95	0.48
3:A:757:GLU:HB2	3:A:889:LEU:HD22	1.93	0.48
3:C:361:PRO:HG3	4:C:1143:HOH:O	2.12	0.48
1:G:2:DG:H5'	1:G:3:3DR:H5'	1.95	0.48
3:A:362:ILE:CD1	3:A:569:ALA:HA	2.43	0.48
3:B:412:LEU:HG	3:B:683:MET:HE3	1.95	0.48
3:D:813:ARG:NH2	3:D:842:GLY:HA3	2.28	0.48
2:F:115:DA:H62	3:A:282:PHE:HE2	1.62	0.48
1:G:3:3DR:H2''	1:G:4:DC:O4'	2.13	0.48
3:C:11:ILE:HD12	3:C:16:PHE:CD2	2.48	0.48
1:G:10:DA:H1'	1:G:11:DC:H5'	1.94	0.48
2:L:102:DC:H2''	2:L:103:DG:C8	2.49	0.48
3:A:802:PRO:HG2	3:A:805:ILE:HD12	1.94	0.48
3:B:193:ASN:ND2	3:B:196:GLU:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:102:LYS:O	3:D:102:LYS:HD3	2.14	0.48
3:D:219:GLU:O	3:D:219:GLU:HG2	2.14	0.48
3:D:300:VAL:O	3:D:300:VAL:HG13	2.14	0.48
3:B:124:PRO:HB2	3:B:225:TYR:CE1	2.47	0.48
3:B:554:THR:O	3:B:557:ILE:HG22	2.14	0.48
3:C:52:ILE:HB	3:C:428:GLU:HG2	1.95	0.48
3:D:450:PRO:HB2	3:D:456:CYS:SG	2.53	0.48
3:B:45:GLN:O	3:B:45:GLN:HG3	2.14	0.48
3:B:401:PRO:O	3:B:402:ASN:HB2	2.13	0.48
3:C:12:GLY:O	3:C:13:ASP:HB2	2.13	0.48
3:D:750:ARG:HG3	3:D:754:GLN:NE2	2.29	0.48
2:H:108:DT:H5''	4:H:575:HOH:O	2.13	0.47
1:K:13:DG:H2''	1:K:14:DC:C6	2.48	0.47
3:C:382:GLN:HG2	3:C:383:GLY:N	2.28	0.47
3:C:495:ASN:HD21	3:C:522:PHE:N	2.04	0.47
3:D:402:ASN:ND2	3:D:403:ARG:N	2.59	0.47
3:D:503:LEU:HG	3:D:538:LEU:HB3	1.95	0.47
1:E:4:DC:H2'	1:E:5:DT:H71	1.96	0.47
4:K:745:HOH:O	3:D:361:PRO:HD2	2.14	0.47
3:B:354:GLN:HG3	4:B:907:HOH:O	2.14	0.47
3:D:38:PHE:CZ	3:D:59:ARG:HG2	2.48	0.47
3:D:41:CYS:CB	3:D:45:GLN:HG3	2.43	0.47
3:D:61:LEU:HD23	3:D:62:PHE:N	2.29	0.47
3:D:481:GLN:HB3	3:D:559:ARG:HE	1.79	0.47
2:H:110:DA:H2'	2:H:111:DT:H71	1.96	0.47
3:B:164:ILE:HG23	3:B:165:GLU:OE1	2.14	0.47
3:B:277:TYR:O	3:B:281:SER:HB2	2.15	0.47
3:B:660:GLU:CB	3:B:661:PRO:HD3	2.44	0.47
3:D:15:ILE:HD13	3:D:15:ILE:C	2.40	0.47
3:A:197:LEU:HD23	3:A:197:LEU:C	2.39	0.47
3:A:369:ILE:HG12	3:A:474:GLU:HG2	1.96	0.47
3:B:164:ILE:HG13	3:B:183:ILE:HD11	1.96	0.47
3:C:202:LEU:O	3:C:206:GLN:HG2	2.14	0.47
3:D:52:ILE:HD12	3:D:428:GLU:HG3	1.96	0.47
3:D:484:GLU:HG2	4:D:927:HOH:O	2.15	0.47
2:H:112:DA:H2''	2:H:113:DA:H5''	1.97	0.47
3:A:415:LEU:HD22	3:A:623:ASP:HB3	1.95	0.47
3:B:251:LYS:C	3:B:253:GLY:H	2.22	0.47
3:C:27:ARG:HB3	3:C:27:ARG:NH1	2.30	0.47
2:J:105:DC:H2'	2:J:106:DT:C6	2.50	0.47
3:B:355:ILE:O	3:B:356:GLN:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:529:LYS:O	3:B:533:LEU:HG	2.15	0.47
3:C:20:ILE:HD13	3:C:26:GLU:HA	1.97	0.47
3:C:137:THR:OG1	3:C:324:ASN:ND2	2.48	0.47
3:C:362:ILE:HD12	3:C:575:PHE:HB2	1.96	0.47
3:C:402:ASN:HA	3:C:886:ALA:O	2.14	0.47
3:D:362:ILE:HD11	3:D:572:ASN:ND2	2.29	0.47
3:D:423:VAL:HB	3:D:425:ILE:HG13	1.96	0.47
1:K:10:DA:OP1	3:D:878:LYS:HG2	2.14	0.47
3:B:272:ASP:OD1	3:B:274:ILE:HG22	2.15	0.47
3:D:455:SER:OG	3:D:676:ASN:HA	2.13	0.47
2:F:113:DA:H2'	2:F:114:DG:C8	2.50	0.47
3:A:902:ASP:O	3:A:903:PHE:HB2	2.14	0.47
3:D:18:ARG:HH12	3:D:209:THR:HB	1.80	0.47
3:D:819:ILE:HG22	3:D:820:ASP:N	2.23	0.47
3:B:596:TRP:CE2	3:B:670:MET:HB2	2.50	0.47
1:G:4:DC:H2'	1:G:5:DT:C6	2.50	0.47
3:A:485:HIS:C	3:A:487:GLY:H	2.21	0.47
3:B:351:ALA:O	3:B:352:LYS:HB2	2.14	0.47
3:D:38:PHE:CE2	3:D:59:ARG:HG2	2.49	0.47
3:D:180:SER:O	3:D:183:ILE:HG22	2.14	0.47
3:D:459:ASN:N	3:D:459:ASN:HD22	2.13	0.47
3:D:834:PRO:HD2	3:D:871:LEU:HD13	1.97	0.47
1:E:7:DA:H2''	1:E:8:DT:C6	2.51	0.46
3:A:221:PHE:C	3:A:224:PRO:HD2	2.39	0.46
3:C:231:LYS:HG3	3:C:236:GLU:CA	2.42	0.46
3:A:269:SER:OG	3:A:356:GLN:NE2	2.48	0.46
3:C:83:LEU:HB3	3:C:379:VAL:HG12	1.97	0.46
3:C:731:GLU:HA	3:C:734:LYS:HG3	1.98	0.46
3:D:85:MET:HE2	3:D:87:ASP:HB3	1.98	0.46
3:D:810:THR:HG23	3:D:813:ARG:HH21	1.81	0.46
3:A:514:LEU:H	3:A:541:MET:HE1	1.80	0.46
3:D:52:ILE:HG12	4:D:912:HOH:O	2.15	0.46
1:K:6:DT:O2	3:D:706:LYS:HE3	2.15	0.46
3:C:481:GLN:NE2	3:C:559:ARG:HE	2.12	0.46
3:C:660:GLU:CB	3:C:661:PRO:HD3	2.45	0.46
3:D:458:PRO:HG2	3:D:589:PHE:HA	1.96	0.46
3:D:775:ASN:OD1	3:D:777:ILE:HG13	2.14	0.46
1:K:4:DC:H2'	1:K:5:DT:C6	2.51	0.46
3:B:52:ILE:HD12	3:B:428:GLU:CG	2.44	0.46
3:B:151:LEU:HD23	3:B:152:LEU:N	2.30	0.46
3:B:252:VAL:HG12	3:B:252:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:362:ILE:HD11	3:B:572:ASN:HB3	1.98	0.46
3:C:303:LEU:H	3:C:303:LEU:CD2	2.23	0.46
3:D:159:VAL:HB	3:D:317:HIS:CD2	2.51	0.46
3:D:281:SER:OG	3:D:283:THR:HG22	2.14	0.46
3:D:412:LEU:HD13	3:D:415:LEU:HD13	1.98	0.46
3:A:247:LYS:HG3	3:A:266:PHE:CD1	2.50	0.46
3:A:263:ILE:HD12	3:A:263:ILE:N	2.31	0.46
3:A:494:ARG:HD2	3:A:521:ASP:OD1	2.16	0.46
3:B:633:ILE:O	3:B:636:VAL:HG22	2.15	0.46
3:C:284:ASN:ND2	3:C:829:LYS:HZ2	2.12	0.46
3:C:458:PRO:HG3	3:C:592:MET:SD	2.55	0.46
3:D:191:PHE:HZ	3:D:200:GLU:HG2	1.81	0.46
3:D:398:GLU:CD	3:D:705:LYS:HE3	2.40	0.46
3:A:241:ARG:NE	4:A:1105:HOH:O	2.49	0.46
3:A:566:LEU:HD13	3:A:570:LEU:HD23	1.98	0.46
3:B:791:TYR:CD2	3:B:801:CYS:HA	2.50	0.46
3:C:170:LEU:HD23	4:C:1112:HOH:O	2.15	0.46
3:C:594:LEU:HD22	3:C:622:THR:O	2.16	0.46
3:D:391:TYR:HB2	3:D:392:PRO:HD2	1.97	0.46
3:D:512:GLU:CG	3:D:513:PRO:HD2	2.44	0.46
3:A:206:GLN:HE21	3:A:241:ARG:HE	1.63	0.46
3:B:494:ARG:HG3	3:B:495:ASN:N	2.30	0.46
3:B:568:GLY:HA3	4:B:1016:HOH:O	2.16	0.46
3:D:41:CYS:SG	3:D:45:GLN:HG3	2.56	0.46
1:K:13:DG:H2''	1:K:14:DC:H6	1.81	0.46
3:A:129:ALA:HA	3:A:225:TYR:CE1	2.51	0.46
3:A:811:TYR:O	3:A:815:ILE:HG12	2.16	0.46
3:C:236:GLU:HG2	3:C:240:LYS:HZ2	1.79	0.46
3:C:893:LYS:HE3	4:C:1134:HOH:O	2.16	0.46
3:D:206:GLN:NE2	3:D:241:ARG:HE	2.13	0.46
3:D:430:ILE:HG22	4:D:936:HOH:O	2.16	0.46
3:D:807:GLY:HA2	3:D:845:CYS:O	2.15	0.46
1:K:10:DA:H2''	1:K:11:DC:O5'	2.15	0.46
3:D:453:VAL:HG23	3:D:454:TYR:CD2	2.51	0.46
1:G:6:DT:C3'	1:G:7:DA:H5''	2.46	0.45
3:A:86:ASP:OD1	3:A:86:ASP:N	2.49	0.45
3:A:636:VAL:HG12	3:A:636:VAL:O	2.16	0.45
3:D:544:ARG:HH11	3:D:544:ARG:HG3	1.81	0.45
3:A:352:LYS:CE	4:A:1069:HOH:O	2.63	0.45
2:J:113:DA:H2'	4:J:629:HOH:O	2.17	0.45
3:D:34:LYS:HG3	3:D:64:ASN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:145:ARG:HG3	3:D:185:LYS:O	2.17	0.45
3:D:199:MET:HE1	3:D:234:PHE:CZ	2.51	0.45
3:D:516:VAL:HG11	3:D:526:ILE:CG2	2.46	0.45
3:D:625:ILE:O	3:D:625:ILE:HG13	2.16	0.45
3:B:180:SER:O	3:B:183:ILE:HG22	2.16	0.45
3:B:231:LYS:HG3	3:B:236:GLU:CA	2.43	0.45
3:B:471:VAL:N	3:B:472:PRO:HD2	2.31	0.45
3:C:506:PRO:C	3:C:507:ASN:HD22	2.25	0.45
3:C:578:TYR:CD1	3:C:578:TYR:C	2.95	0.45
3:D:398:GLU:HA	3:D:705:LYS:HE2	1.98	0.45
3:D:644:THR:O	3:D:648:VAL:HG23	2.17	0.45
3:A:533:LEU:HB3	3:A:537:SER:OG	2.16	0.45
3:B:494:ARG:HG3	3:B:495:ASN:ND2	2.32	0.45
3:C:149:PHE:CD1	3:C:149:PHE:N	2.84	0.45
3:C:558:ASN:HD22	3:C:558:ASN:HA	1.66	0.45
3:D:295:GLU:CG	3:D:301:GLY:HA2	2.42	0.45
3:D:422:GLN:NE2	3:D:680:LEU:H	2.13	0.45
3:D:451:SER:HB3	3:D:456:CYS:SG	2.56	0.45
2:F:104:DG:H2''	2:F:105:DC:O5'	2.15	0.45
1:G:6:DT:C2'	1:G:7:DA:C5'	2.80	0.45
3:A:530:ILE:C	3:A:532:LYS:H	2.24	0.45
3:B:251:LYS:HG3	3:B:252:VAL:H	1.82	0.45
3:D:102:LYS:HB2	3:D:102:LYS:HZ3	1.81	0.45
3:D:429:THR:O	3:D:464:TYR:HD1	1.99	0.45
2:H:103:DG:H2''	2:H:104:DG:C5'	2.40	0.45
3:D:439:LEU:HD11	3:D:592:MET:HB2	1.98	0.45
3:D:738:PRO:HB3	3:D:780:ALA:O	2.17	0.45
3:B:684:ASP:HB2	4:B:1051:HOH:O	2.16	0.45
3:B:771:PHE:CE2	3:B:872:LEU:HB2	2.52	0.45
3:D:85:MET:HG2	3:D:91:ALA:HB2	1.99	0.45
3:D:239:ALA:C	3:D:241:ARG:H	2.24	0.45
3:D:430:ILE:CG2	3:D:461:MET:HE2	2.46	0.45
3:A:745:LEU:HD13	3:A:876:PHE:CD1	2.52	0.45
3:B:197:LEU:C	3:B:197:LEU:HD23	2.42	0.45
3:B:573:VAL:HG13	4:B:989:HOH:O	2.16	0.45
3:B:749:ILE:O	3:B:753:LEU:HG	2.17	0.45
3:D:365:TRP:CE2	3:D:566:LEU:HD23	2.52	0.45
3:D:800:LYS:HD2	3:D:800:LYS:N	2.32	0.45
1:I:7:DA:H2'	1:I:8:DT:C7	2.46	0.45
3:A:802:PRO:CG	3:A:805:ILE:HD12	2.48	0.45
3:B:273:TYR:HE2	3:B:341:ILE:HG12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:405:LYS:O	3:C:690:GLY:HA2	2.17	0.45
3:D:278:LYS:HG2	3:D:288:TYR:CE2	2.52	0.45
3:D:830:VAL:HG22	3:D:831:TYR:N	2.31	0.45
2:L:111:DT:H2''	2:L:112:DA:C8	2.52	0.44
3:B:119:SER:HB2	3:B:124:PRO:HB3	1.99	0.44
3:B:221:PHE:C	3:B:224:PRO:HD2	2.42	0.44
3:B:339:GLN:HB2	4:B:1092:HOH:O	2.16	0.44
3:B:472:PRO:HA	3:B:475:ILE:HG22	1.99	0.44
3:B:546:GLN:O	3:B:550:VAL:HG23	2.16	0.44
3:C:302:LYS:CG	3:C:330:ARG:HH12	2.28	0.44
3:D:112:ASN:HB3	3:D:214:THR:CG2	2.38	0.44
3:D:655:ALA:O	3:D:660:GLU:HG3	2.17	0.44
2:H:113:DA:H5'	4:H:758:HOH:O	2.15	0.44
1:K:13:DG:H2''	1:K:14:DC:O5'	2.15	0.44
2:L:108:DT:H2''	2:L:109:DC:O5'	2.17	0.44
3:A:231:LYS:O	3:A:234:PHE:O	2.35	0.44
3:A:653:LYS:HD3	4:A:1043:HOH:O	2.17	0.44
3:B:494:ARG:HD2	3:B:521:ASP:CG	2.42	0.44
3:D:4:PHE:HB3	3:D:101:ILE:CG2	2.48	0.44
1:I:7:DA:H2''	1:I:8:DT:C6	2.53	0.44
1:K:6:DT:H2''	1:K:7:DA:O5'	2.18	0.44
2:L:114:DG:H2''	2:L:115:DA:O5'	2.17	0.44
3:B:3:GLU:HG3	3:B:20:ILE:O	2.18	0.44
3:B:353:ILE:O	3:B:354:GLN:C	2.59	0.44
3:C:130:LYS:HG3	3:C:131:HIS:N	2.31	0.44
3:D:20:ILE:HD11	3:D:24:GLY:HA2	1.99	0.44
3:D:486:LYS:O	3:D:490:LEU:HG	2.18	0.44
2:F:105:DC:H2'	2:F:106:DT:H72	1.99	0.44
3:A:745:LEU:HD12	3:A:745:LEU:HA	1.83	0.44
3:D:6:LEU:HB2	3:D:18:ARG:O	2.17	0.44
3:D:109:ARG:HH12	3:D:142:ILE:HD11	1.83	0.44
3:D:779:ILE:O	3:D:871:LEU:HD21	2.17	0.44
2:L:101:DG:H2''	2:L:102:DC:C6	2.53	0.44
3:A:506:PRO:HG3	4:A:1153:HOH:O	2.16	0.44
3:A:698:ILE:HG12	3:A:752:MET:O	2.17	0.44
3:B:6:LEU:CD1	3:B:26:GLU:HG3	2.48	0.44
3:C:125:GLU:HG3	4:C:1142:HOH:O	2.17	0.44
3:D:163:SER:HB3	3:D:165:GLU:OE1	2.17	0.44
3:D:652:ASP:OD1	3:D:656:ARG:NH1	2.46	0.44
2:F:113:DA:H3'	2:F:114:DG:C5'	2.45	0.44
3:B:876:PHE:O	3:B:879:PRO:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:818:ASN:ND2	3:C:857:LEU:HD11	2.32	0.44
3:D:841:PHE:CZ	3:D:862:VAL:HG22	2.52	0.44
2:L:115:DA:H2''	3:D:567:TYR:HD2	1.82	0.44
3:A:101:ILE:HD12	3:A:349:TYR:HD1	1.83	0.44
3:B:51:ASP:C	3:B:51:ASP:OD1	2.61	0.44
3:B:326:ILE:HG23	3:B:330:ARG:HE	1.81	0.44
3:B:528:GLU:C	3:B:530:ILE:H	2.24	0.44
3:A:322:SER:O	3:A:326:ILE:HG12	2.16	0.44
3:A:338:ARG:HB3	3:A:340:PHE:CD1	2.53	0.44
3:C:512:GLU:HB3	3:C:513:PRO:HD2	1.99	0.44
3:D:40:HIS:ND1	3:D:83:LEU:HD11	2.32	0.44
3:D:731:GLU:HG3	3:D:879:PRO:CB	2.46	0.44
3:D:844:LYS:HD3	3:D:844:LYS:N	2.33	0.44
1:E:14:DC:H2'	1:E:15:DC:C5	2.53	0.44
3:A:660:GLU:HB2	3:A:661:PRO:HD3	1.99	0.44
3:B:594:LEU:O	3:B:597:ILE:HG22	2.18	0.44
3:B:811:TYR:O	3:B:815:ILE:HG12	2.17	0.44
3:D:63:ALA:HB3	3:D:66:ARG:HG2	1.99	0.44
3:D:525:GLU:O	3:D:529:LYS:HG3	2.17	0.44
3:D:783:SER:O	3:D:829:LYS:HB3	2.17	0.44
1:E:8:DT:H4'	3:A:707:ARG:CD	2.47	0.43
1:G:7:DA:H2'	1:G:8:DT:C7	2.48	0.43
1:G:10:DA:H2''	1:G:11:DC:O5'	2.18	0.43
1:G:16:DG:H2''	1:G:17:DC:O5'	2.18	0.43
3:A:165:GLU:H	3:A:165:GLU:CD	2.25	0.43
3:B:356:GLN:C	3:B:358:VAL:N	2.75	0.43
3:B:858:ILE:O	3:B:862:VAL:HG23	2.17	0.43
3:D:178:VAL:HG11	3:D:186:ILE:HD11	1.99	0.43
3:D:859:LYS:C	3:D:861:ASP:N	2.76	0.43
3:A:36:SER:O	3:A:37:LEU:HD23	2.18	0.43
3:B:42:PRO:HG2	3:B:45:GLN:HG2	2.00	0.43
3:C:186:ILE:HG23	4:C:1125:HOH:O	2.18	0.43
3:C:251:LYS:HB2	3:C:262:ILE:HG13	1.99	0.43
3:C:380:ILE:HD12	3:C:576:ARG:NE	2.32	0.43
3:D:14:SER:HA	3:D:65:MET:HG2	1.99	0.43
3:D:495:ASN:O	3:D:499:ILE:HG13	2.18	0.43
3:D:530:ILE:O	3:D:533:LEU:HB2	2.18	0.43
3:D:597:ILE:HD11	3:D:663:ILE:HG23	2.00	0.43
3:B:245:HIS:O	3:B:247:LYS:HG2	2.18	0.43
3:C:428:GLU:H	3:C:428:GLU:CD	2.26	0.43
3:D:72:ILE:O	3:D:76:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:114:ASP:HB3	3:D:328:VAL:HG13	2.00	0.43
3:D:143:ASP:OD2	3:D:208:LYS:HE2	2.16	0.43
3:D:151:LEU:HD23	3:D:153:ASN:H	1.82	0.43
3:D:459:ASN:HD22	3:D:459:ASN:H	1.66	0.43
2:J:111:DT:H2''	2:J:112:DA:C8	2.51	0.43
3:A:730:LEU:HB3	3:A:883:PHE:CZ	2.53	0.43
3:C:81:GLU:HG2	3:C:83:LEU:HD12	1.99	0.43
3:D:117:VAL:HG13	3:D:124:PRO:HG3	2.00	0.43
3:D:221:PHE:O	3:D:225:TYR:HB2	2.19	0.43
3:D:410:PHE:CD2	3:D:685:ARG:HA	2.54	0.43
1:E:8:DT:H4'	3:A:707:ARG:HD2	2.00	0.43
3:A:300:VAL:O	3:A:300:VAL:HG23	2.18	0.43
3:B:410:PHE:HB3	3:B:683:MET:HG2	1.99	0.43
3:B:795:GLY:O	3:B:813:ARG:HD3	2.19	0.43
3:C:347:MET:HE2	3:C:558:ASN:ND2	2.33	0.43
3:D:160:GLU:HB3	3:D:161:GLU:H	1.62	0.43
2:H:113:DA:H2''	2:H:114:DG:O5'	2.18	0.43
3:A:249:ARG:HG2	3:A:250:VAL:N	2.33	0.43
3:D:294:SER:C	3:D:296:PHE:H	2.27	0.43
3:D:878:LYS:N	3:D:879:PRO:HD2	2.33	0.43
3:B:111:ALA:HB1	3:B:138:HIS:NE2	2.33	0.43
3:B:308:PRO:C	3:B:310:SER:H	2.27	0.43
3:C:205:TRP:HH2	3:C:213:LEU:HD11	1.84	0.43
3:C:461:MET:CE	3:C:581:ARG:HD2	2.49	0.43
3:D:555:ALA:O	3:D:559:ARG:HG2	2.18	0.43
2:H:113:DA:H3'	4:H:758:HOH:O	2.18	0.43
3:B:251:LYS:C	3:B:253:GLY:N	2.77	0.43
3:B:271:LEU:HB3	3:B:276:LEU:HD11	2.01	0.43
3:B:279:LYS:HE3	3:B:280:PHE:CE2	2.54	0.43
3:C:10:GLN:HG3	3:C:65:MET:CE	2.48	0.43
3:C:105:HIS:HA	3:C:108:ILE:HD12	2.01	0.43
3:C:416:TYR:HB2	3:C:417:PRO:HD3	2.00	0.43
3:D:477:LYS:O	3:D:481:GLN:HG3	2.18	0.43
3:A:458:PRO:HG3	3:A:592:MET:SD	2.59	0.43
3:A:596:TRP:CE2	3:A:670:MET:HB2	2.54	0.43
3:A:700:GLY:HA2	3:A:753:LEU:HD22	2.00	0.43
3:B:131:HIS:HB2	3:B:225:TYR:OH	2.19	0.43
3:C:495:ASN:HD21	3:C:521:ASP:HA	1.83	0.43
3:C:532:LYS:HD2	3:C:532:LYS:N	2.34	0.43
3:D:458:PRO:HB2	3:D:588:THR:CG2	2.42	0.43
3:A:214:THR:OG1	3:A:215:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:405:LYS:HA	4:A:998:HOH:O	2.19	0.43
3:A:494:ARG:O	3:A:498:ILE:HG12	2.19	0.43
3:A:789:ALA:HA	3:A:792:ASP:CG	2.44	0.43
3:B:356:GLN:O	3:B:358:VAL:N	2.52	0.43
3:B:830:VAL:HB	3:B:848:TRP:O	2.18	0.43
3:C:262:ILE:HG13	3:C:262:ILE:O	2.19	0.43
3:C:391:TYR:HB2	3:C:392:PRO:HD2	1.99	0.43
3:D:559:ARG:O	3:D:563:ILE:HG13	2.19	0.43
3:A:482:ARG:HG2	3:A:482:ARG:NH1	2.34	0.42
3:A:536:LYS:HD3	3:A:536:LYS:C	2.44	0.42
3:B:244:PRO:HG2	3:B:267:GLY:HA3	2.01	0.42
3:C:284:ASN:ND2	3:C:829:LYS:NZ	2.66	0.42
3:D:340:PHE:HD1	3:D:343:LEU:HD12	1.84	0.42
3:D:381:PRO:HG3	4:D:912:HOH:O	2.19	0.42
3:D:394:ALA:HB1	3:D:622:THR:HA	2.01	0.42
3:D:456:CYS:HA	3:D:461:MET:O	2.18	0.42
1:I:6:DT:H2''	1:I:7:DA:H5''	2.01	0.42
1:K:2:DG:H3'	1:K:3:3DR:H5'	2.01	0.42
4:K:745:HOH:O	3:D:362:ILE:HG13	2.18	0.42
2:L:104:DG:H2''	2:L:105:DC:O5'	2.19	0.42
2:L:106:DT:H2''	2:L:107:DG:C8	2.54	0.42
3:A:129:ALA:HA	3:A:225:TYR:CZ	2.54	0.42
3:A:391:TYR:HB2	3:A:392:PRO:HD2	2.00	0.42
3:B:739:LYS:HD3	3:B:742:GLN:OE1	2.19	0.42
3:A:542:LEU:HD12	3:A:542:LEU:C	2.44	0.42
3:B:202:LEU:HD23	3:B:241:ARG:HH21	1.83	0.42
3:B:313:ARG:HG2	3:B:313:ARG:NH1	2.33	0.42
3:B:422:GLN:HG3	3:B:678:GLN:O	2.20	0.42
3:B:468:ASP:HB2	4:B:957:HOH:O	2.20	0.42
3:D:461:MET:HE1	3:D:581:ARG:NH2	2.25	0.42
3:A:170:LEU:HB2	3:A:173:GLN:HE21	1.84	0.42
3:A:380:ILE:HD12	3:A:576:ARG:CZ	2.49	0.42
3:B:186:ILE:HG22	4:B:1053:HOH:O	2.18	0.42
3:B:806:ARG:HD3	3:B:843:ASP:OD1	2.20	0.42
3:D:230:ILE:HG23	3:D:234:PHE:CD2	2.51	0.42
3:D:500:LYS:O	3:D:503:LEU:HB2	2.19	0.42
2:H:104:DG:H2''	2:H:105:DC:C5'	2.49	0.42
2:L:107:DG:H2''	2:L:108:DT:O5'	2.20	0.42
3:A:822:PRO:HA	4:A:1106:HOH:O	2.18	0.42
3:C:449:ARG:HA	3:C:450:PRO:HD2	1.88	0.42
3:D:732:THR:HG22	3:D:745:LEU:HB2	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:804:HIS:O	3:D:808:ILE:HG13	2.20	0.42
3:A:126:PRO:HB3	3:A:224:PRO:HB2	2.00	0.42
3:B:229:ARG:O	3:B:233:ILE:HG13	2.20	0.42
3:D:65:MET:O	3:D:65:MET:HG3	2.19	0.42
1:E:2:DG:OP2	3:A:361:PRO:HD2	2.19	0.42
3:A:485:HIS:C	3:A:487:GLY:N	2.76	0.42
3:A:738:PRO:HB3	3:A:780:ALA:C	2.45	0.42
3:B:13:ASP:CG	3:B:64:ASN:HB2	2.45	0.42
3:B:494:ARG:O	3:B:498:ILE:HG12	2.19	0.42
3:C:153:ASN:HB2	3:C:192:ASP:O	2.18	0.42
3:A:357:SER:C	3:A:359:PHE:N	2.77	0.42
3:A:422:GLN:HE21	3:A:422:GLN:HB2	1.70	0.42
3:B:806:ARG:HH11	3:B:843:ASP:CG	2.27	0.42
3:C:162:TRP:HB3	3:C:188:TYR:CE1	2.55	0.42
3:D:191:PHE:CZ	3:D:200:GLU:HG2	2.55	0.42
1:G:8:DT:H2''	1:G:9:DG:H5'	2.00	0.42
1:I:15:DC:P	4:I:440:HOH:O	2.78	0.42
3:B:653:LYS:HG3	3:B:657:GLU:OE2	2.19	0.42
3:B:856:ASP:HA	3:B:859:LYS:HB2	2.02	0.42
3:C:40:HIS:HE1	3:C:51:ASP:OD2	2.03	0.42
3:D:119:SER:OG	3:D:124:PRO:HD3	2.20	0.42
1:I:6:DT:H2''	1:I:7:DA:C5'	2.50	0.42
3:A:426:SER:OG	3:A:427:PRO:HD2	2.19	0.42
2:L:103:DG:H2''	2:L:104:DG:C8	2.55	0.41
2:L:105:DC:H2'	2:L:106:DT:C7	2.50	0.41
3:A:352:LYS:NZ	4:A:1069:HOH:O	2.53	0.41
3:A:803:PHE:CZ	3:A:845:CYS:HB3	2.55	0.41
3:B:413:THR:O	3:B:414:SER:C	2.63	0.41
3:C:500:LYS:HE3	3:C:542:LEU:HD11	2.02	0.41
3:A:741:VAL:HG12	3:A:745:LEU:HD22	2.02	0.41
3:B:37:LEU:HD12	3:B:37:LEU:HA	1.79	0.41
3:B:159:VAL:HG13	3:B:313:ARG:NH1	2.35	0.41
3:C:179:PRO:O	3:C:183:ILE:HG12	2.20	0.41
3:C:633:ILE:HD13	3:C:633:ILE:HA	1.87	0.41
3:D:142:ILE:HG13	3:D:143:ASP:OD1	2.20	0.41
3:D:216:TRP:CD1	3:D:290:LEU:HB2	2.54	0.41
3:D:430:ILE:H	3:D:430:ILE:HG13	1.55	0.41
3:D:440:HIS:HA	3:D:443:ILE:HD12	2.02	0.41
3:D:592:MET:HE3	3:D:670:MET:SD	2.60	0.41
3:D:664:ASP:OD1	3:D:668:ARG:HD2	2.21	0.41
3:B:436:VAL:HG12	4:B:1021:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:739:LYS:HD3	3:B:739:LYS:HA	1.87	0.41
3:B:891:TYR:CD2	3:B:892:GLU:HG3	2.55	0.41
3:C:524:ASP:HA	3:C:527:LYS:HE3	2.00	0.41
3:D:74:ARG:O	3:D:78:ILE:HG13	2.21	0.41
3:D:241:ARG:HB3	4:D:929:HOH:O	2.19	0.41
3:A:162:TRP:HB3	3:A:188:TYR:CE1	2.55	0.41
3:A:273:TYR:OH	3:A:335:ASP:HA	2.20	0.41
3:A:558:ASN:O	3:A:562:LEU:HD13	2.20	0.41
3:B:125:GLU:HA	3:B:126:PRO:HD3	1.94	0.41
3:B:562:LEU:HD12	3:B:562:LEU:HA	1.88	0.41
3:D:15:ILE:HD13	3:D:15:ILE:O	2.20	0.41
3:D:491:ALA:HA	3:D:521:ASP:OD1	2.20	0.41
3:D:878:LYS:HB3	3:D:879:PRO:HD3	2.01	0.41
1:E:16:DG:H2'	1:E:17:DC:C6	2.56	0.41
3:A:292:TYR:HB2	4:A:1131:HOH:O	2.20	0.41
3:A:486:LYS:O	3:A:486:LYS:HG2	2.19	0.41
3:A:499:ILE:CG2	3:A:541:MET:HB3	2.50	0.41
3:A:854:ILE:CD1	3:A:862:VAL:HG11	2.49	0.41
3:B:355:ILE:HD13	3:B:355:ILE:HA	1.80	0.41
3:B:499:ILE:HD12	3:B:530:ILE:HG13	2.03	0.41
3:B:836:ARG:HG2	3:B:867:ASP:CG	2.45	0.41
3:C:228:ASN:HD22	3:C:228:ASN:HA	1.64	0.41
3:C:326:ILE:HD11	4:C:1076:HOH:O	2.20	0.41
3:C:897:LEU:HD13	4:C:1114:HOH:O	2.20	0.41
3:D:9:GLU:O	3:D:15:ILE:HG12	2.21	0.41
3:D:183:ILE:HG23	3:D:184:ASP:N	2.36	0.41
3:D:382:GLN:HG2	3:D:383:GLY:N	2.35	0.41
3:D:475:ILE:HD11	3:D:563:ILE:HG23	2.01	0.41
3:D:770:GLU:O	3:D:774:LEU:HG	2.20	0.41
3:D:796:PHE:HB3	3:D:797:PRO:HD2	2.03	0.41
3:D:812:ASN:CA	3:D:815:ILE:HG12	2.50	0.41
3:D:859:LYS:C	3:D:861:ASP:H	2.27	0.41
1:I:4:DC:H2'	1:I:5:DT:H72	2.03	0.41
3:B:873:GLU:O	3:B:878:LYS:HB2	2.20	0.41
3:C:249:ARG:HD3	3:C:251:LYS:HZ1	1.84	0.41
3:D:64:ASN:O	3:D:65:MET:HB2	2.19	0.41
3:D:846:ILE:HG12	3:D:847:ALA:N	2.36	0.41
3:A:356:GLN:H	3:A:356:GLN:HE21	1.69	0.41
3:A:457:SER:HA	3:A:458:PRO:HD3	1.92	0.41
3:B:558:ASN:HD22	3:B:558:ASN:HA	1.57	0.41
3:B:731:GLU:HG3	3:B:879:PRO:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:PHE:HB3	3:C:245:HIS:CE1	2.55	0.41
3:C:182:ILE:O	3:C:186:ILE:HG13	2.21	0.41
3:D:843:ASP:C	3:D:845:CYS:H	2.29	0.41
3:A:150:ASP:OD2	3:A:321:ILE:HD11	2.21	0.41
3:A:171:GLN:HE22	3:A:319:ARG:HH12	1.69	0.41
3:A:339:GLN:HE21	3:A:339:GLN:HB3	1.68	0.41
3:B:884:THR:HB	3:B:889:LEU:O	2.20	0.41
3:C:321:ILE:O	3:C:325:ILE:HG13	2.20	0.41
3:D:686:GLU:HB3	3:D:687:ALA:H	1.75	0.41
2:F:107:DG:C8	2:F:108:DT:H72	2.56	0.41
3:A:125:GLU:HA	3:A:126:PRO:HD3	1.94	0.41
3:A:204:PHE:CE1	3:A:208:LYS:HD2	2.56	0.41
3:A:507:ASN:HD22	3:A:532:LYS:CA	2.34	0.41
3:A:663:ILE:HG21	3:A:683:MET:HB2	2.03	0.41
3:B:113:PHE:CE1	3:B:213:LEU:HD11	2.55	0.41
3:B:113:PHE:H	3:B:113:PHE:HD1	1.68	0.41
3:B:303:LEU:HD22	3:B:303:LEU:N	2.35	0.41
3:B:433:THR:O	3:B:462:MET:HE2	2.21	0.41
3:B:514:LEU:HD11	3:B:529:LYS:HB3	2.03	0.41
3:B:776:TYR:OH	3:B:854:ILE:HG22	2.20	0.41
3:D:145:ARG:NH2	3:D:185:LYS:HG2	2.36	0.41
3:D:241:ARG:HH12	3:D:246:ARG:CB	2.33	0.41
3:D:700:GLY:HA2	3:D:753:LEU:CD2	2.48	0.41
2:F:108:DT:H1'	2:F:109:DC:H5'	2.03	0.41
2:J:113:DA:H2''	2:J:114:DG:C5'	2.51	0.41
3:B:1:MET:HG2	3:B:2:LYS:N	2.36	0.41
3:B:124:PRO:HB2	3:B:225:TYR:HE1	1.86	0.41
3:B:124:PRO:HG2	3:B:221:PHE:HE2	1.86	0.41
3:B:477:LYS:O	3:B:481:GLN:HG3	2.21	0.41
3:C:458:PRO:CG	3:C:592:MET:SD	3.09	0.41
3:C:731:GLU:HG3	3:C:879:PRO:CB	2.51	0.41
3:D:199:MET:HE1	3:D:234:PHE:CE1	2.55	0.41
3:D:421:ARG:HD3	3:D:475:ILE:HG23	2.03	0.41
3:D:597:ILE:HA	3:D:597:ILE:HD12	1.86	0.41
3:D:747:GLU:OE2	3:D:747:GLU:HA	2.21	0.41
2:L:110:DA:H2''	2:L:111:DT:O5'	2.21	0.40
3:A:597:ILE:HB	3:A:667:PHE:CZ	2.56	0.40
3:A:730:LEU:HD22	3:A:883:PHE:HE1	1.86	0.40
3:B:216:TRP:HE3	4:B:1083:HOH:O	2.04	0.40
3:D:43:GLU:HA	3:D:56:PRO:HG3	2.02	0.40
3:D:173:GLN:C	3:D:175:GLY:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:250:VAL:HG12	3:D:263:ILE:CD1	2.50	0.40
3:D:870:VAL:O	3:D:874:LYS:HG2	2.22	0.40
3:A:509:SER:O	3:A:534:SER:HB3	2.21	0.40
3:B:502:ALA:HB3	3:B:530:ILE:HG12	2.03	0.40
3:B:736:SER:HA	3:B:782:VAL:HB	2.03	0.40
3:C:530:ILE:HG23	3:C:538:LEU:CD2	2.48	0.40
3:D:42:PRO:HG2	3:D:45:GLN:HG2	2.03	0.40
3:D:118:THR:HG21	3:D:313:ARG:CB	2.48	0.40
1:E:10:DA:H2''	1:E:11:DC:C5'	2.51	0.40
3:A:416:TYR:HB2	3:A:417:PRO:HD3	2.02	0.40
3:A:455:SER:OG	3:A:676:ASN:HA	2.22	0.40
3:A:478:VAL:HG13	3:A:559:ARG:HD2	2.04	0.40
3:A:822:PRO:HB2	3:A:849:PRO:HG3	2.04	0.40
3:A:839:ASN:HA	3:A:840:PRO:HD3	1.92	0.40
3:C:149:PHE:HB3	3:C:197:LEU:HG	2.03	0.40
3:D:654:PHE:O	3:D:658:ARG:HB2	2.21	0.40
2:J:105:DC:H5''	2:J:105:DC:H6	1.85	0.40
2:J:114:DG:H2'	4:J:750:HOH:O	2.21	0.40
3:A:409:SER:HB3	3:A:626:TYR:CD2	2.56	0.40
3:B:149:PHE:N	3:B:149:PHE:CD1	2.90	0.40
3:B:216:TRP:CH2	3:B:293:ILE:HG21	2.56	0.40
3:B:643:ASP:OD1	3:B:646:HIS:HB2	2.20	0.40
3:C:51:ASP:OD1	3:C:51:ASP:C	2.65	0.40
2:F:111:DT:H2''	2:F:112:DA:O5'	2.21	0.40
2:L:106:DT:H2''	2:L:107:DG:H8	1.86	0.40
3:A:503:LEU:C	3:A:506:PRO:HD3	2.47	0.40
3:A:738:PRO:HB3	3:A:780:ALA:O	2.22	0.40
3:B:138:HIS:ND1	3:B:204:PHE:HE2	2.20	0.40
3:C:42:PRO:HD2	3:C:45:GLN:HE21	1.87	0.40
3:C:811:TYR:O	3:C:815:ILE:HG12	2.21	0.40
3:D:501:GLU:HA	3:D:504:HIS:HD2	1.87	0.40
3:D:878:LYS:HB3	3:D:879:PRO:CD	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	482/793 (61%)	464 (96%)	18 (4%)	30	47
3	B	655/793 (83%)	638 (97%)	17 (3%)	40	60
3	C	718/793 (90%)	682 (95%)	36 (5%)	22	35
3	D	739/793 (93%)	720 (97%)	19 (3%)	40	60
All	All	2594/3172 (82%)	2504 (96%)	90 (4%)	32	50

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2	LYS
3	A	169	LYS
3	A	200	GLU
3	A	342	ASN
3	A	352	LYS
3	A	403	ARG
3	A	474	GLU
3	A	558	ASN
3	A	566	LEU
3	A	581	ARG
3	A	618	LEU
3	A	668	ARG
3	A	739	LYS
3	A	745	LEU
3	A	770	GLU
3	A	787	ASN
3	A	843	ASP
3	A	874	LYS
3	B	37	LEU
3	B	61	LEU
3	B	165	GLU
3	B	181	GLU
3	B	200	GLU
3	B	558	ASN

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Mol	Chain	Res	Type
3	B	562	LEU
3	B	566	LEU
3	B	580	LEU
3	B	660	GLU
3	B	731	GLU
3	B	755	GLU
3	B	760	LEU
3	B	773	GLN
3	B	843	ASP
3	B	878	LYS
3	B	897	LEU
3	C	14	SER
3	C	27	ARG
3	C	90	LEU
3	C	100	GLU
3	C	128	GLN
3	C	151	LEU
3	C	213	LEU
3	C	220	SER
3	C	228	ASN
3	C	276	LEU
3	C	303	LEU
3	C	332	LEU
3	C	356	GLN
3	C	378	LYS
3	C	399	PRO
3	C	411	ASP
3	C	413	THR
3	C	414	SER
3	C	428	GLU
3	C	440	HIS
3	C	456	CYS
3	C	466	ASP
3	C	474	GLU
3	C	475	ILE
3	C	479	PHE
3	C	507	ASN
3	C	544	ARG
3	C	562	LEU
3	C	566	LEU
3	C	580	LEU
3	C	660	GLU

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Mol	Chain	Res	Type
3	C	731	GLU
3	C	733	GLN
3	C	760	LEU
3	C	773	GLN
3	C	863	LEU
3	D	15	ILE
3	D	40	HIS
3	D	102	LYS
3	D	145	ARG
3	D	161	GLU
3	D	165	GLU
3	D	199	MET
3	D	305	TYR
3	D	428	GLU
3	D	430	ILE
3	D	459	ASN
3	D	475	ILE
3	D	614	GLU
3	D	633	ILE
3	D	649	ASP
3	D	755	GLU
3	D	760	LEU
3	D	844	LYS
3	D	859	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	10	GLN
3	A	98	ASN
3	A	173	GLN
3	A	206	GLN
3	A	339	GLN
3	A	342	ASN
3	A	371	ASN
3	A	377	ASN
3	A	422	GLN
3	A	481	GLN
3	A	558	ASN
3	A	595	GLN
3	A	602	ASN
3	A	678	GLN

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Mol	Chain	Res	Type
3	A	812	ASN
3	B	40	HIS
3	B	153	ASN
3	B	299	ASN
3	B	318	GLN
3	B	324	ASN
3	B	333	GLN
3	B	339	GLN
3	B	481	GLN
3	B	485	HIS
3	B	495	ASN
3	B	546	GLN
3	B	558	ASN
3	B	591	GLN
3	B	595	GLN
3	B	606	ASN
3	B	773	GLN
3	B	812	ASN
3	B	818	ASN
3	C	10	GLN
3	C	40	HIS
3	C	45	GLN
3	C	171	GLN
3	C	173	GLN
3	C	203	ASN
3	C	217	ASN
3	C	228	ASN
3	C	232	ASN
3	C	245	HIS
3	C	284	ASN
3	C	299	ASN
3	C	317	HIS
3	C	318	GLN
3	C	324	ASN
3	C	356	GLN
3	C	377	ASN
3	C	424	ASN
3	C	481	GLN
3	C	485	HIS
3	C	495	ASN
3	C	507	ASN
3	C	539	ASN

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Mol	Chain	Res	Type
3	C	546	GLN
3	C	556	GLN
3	C	558	ASN
3	C	591	GLN
3	C	595	GLN
3	C	645	ASN
3	C	679	HIS
3	C	773	GLN
3	C	818	ASN
3	C	864	HIS
3	D	45	GLN
3	D	70	GLN
3	D	131	HIS
3	D	173	GLN
3	D	207	GLN
3	D	232	ASN
3	D	245	HIS
3	D	316	ASN
3	D	318	GLN
3	D	324	ASN
3	D	339	GLN
3	D	342	ASN
3	D	371	ASN
3	D	389	GLN
3	D	402	ASN
3	D	422	GLN
3	D	459	ASN
3	D	504	HIS
3	D	505	ASN
3	D	546	GLN
3	D	558	ASN
3	D	564	ASN
3	D	572	ASN
3	D	591	GLN
3	D	606	ASN
3	D	676	ASN
3	D	679	HIS
3	D	733	GLN
3	D	761	GLN

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	3DR	E	3	1	8,11,12	0.47	0	7,14,17	1.80	1 (14%)
1	3DR	I	3	1	8,11,12	0.45	0	7,14,17	1.83	1 (14%)
1	3DR	G	3	1	8,11,12	0.49	0	7,14,17	1.99	1 (14%)
1	3DR	K	3	1	8,11,12	0.47	0	7,14,17	1.76	1 (14%)

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	3DR	E	3	1	-	0/3/15/16	0/1/1/1
1	3DR	I	3	1	-	0/3/15/16	0/1/1/1
1	3DR	G	3	1	-	0/3/15/16	0/1/1/1
1	3DR	K	3	1	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3	3DR	O3'-C3'-C2'	4.18	121.23	111.43
1	I	3	3DR	O3'-C3'-C2'	3.90	120.58	111.43
1	K	3	3DR	O3'-C3'-C2'	3.65	120.00	111.43
1	E	3	3DR	O3'-C3'-C2'	3.64	119.98	111.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	3	3DR	1	0
1	G	3	3DR	2	0
1	K	3	3DR	2	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	E	17/18 (94%)	0.56	1 (5%) 28 27	54, 75, 126, 146	0
1	G	17/18 (94%)	0.38	2 (11%) 9 8	45, 57, 133, 148	0
1	I	17/18 (94%)	-0.11	1 (5%) 28 27	35, 42, 101, 115	0
1	K	17/18 (94%)	0.98	1 (5%) 28 27	45, 123, 161, 169	0
2	F	15/15 (100%)	1.05	2 (13%) 7 6	68, 99, 128, 141	0
2	H	15/15 (100%)	0.55	2 (13%) 7 6	56, 71, 126, 152	0
2	J	15/15 (100%)	0.38	2 (13%) 7 6	38, 57, 91, 96	0
2	L	15/15 (100%)	1.05	1 (6%) 24 22	126, 131, 153, 157	0
3	A	896/896 (100%)	0.32	57 (6%) 25 24	30, 47, 125, 149	0
3	B	896/896 (100%)	0.84	161 (17%) 3 3	28, 62, 154, 165	0
3	C	892/896 (99%)	0.25	33 (3%) 45 45	23, 48, 83, 106	0
3	D	891/896 (99%)	1.61	279 (31%) 1 1	53, 117, 153, 160	0
All	All	3703/3716 (99%)	0.75	542 (14%) 6 5	23, 62, 148, 169	0

All (542) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	178	VAL	7.1
3	D	514	LEU	6.6
3	D	117	VAL	6.5
3	B	277	TYR	6.0
3	B	117	VAL	5.9
3	B	309	ILE	5.7
3	B	134	ASP	5.7
3	D	174	GLY	5.4
3	D	833	LEU	5.3
3	D	779	ILE	5.2
3	D	99	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
3	B	170	LEU	5.2
3	B	115	ILE	5.2
3	D	65	MET	5.1
3	A	542	LEU	5.1
3	B	135	ALA	5.1
3	B	113	PHE	5.1
3	D	101	ILE	4.9
3	A	510	VAL	4.8
3	D	522	PHE	4.7
3	D	262	ILE	4.6
3	B	233	ILE	4.6
3	D	8	VAL	4.6
3	D	61	LEU	4.5
3	D	510	VAL	4.5
3	B	197	LEU	4.5
3	D	498	ILE	4.5
3	D	113	PHE	4.4
3	D	809	LEU	4.3
3	D	526	ILE	4.3
3	B	300	VAL	4.3
3	D	250	VAL	4.3
3	B	182	ILE	4.3
3	B	282	PHE	4.2
3	D	513	PRO	4.2
3	D	542	LEU	4.2
3	D	800	LYS	4.2
3	D	797	PRO	4.2
3	B	179	PRO	4.2
3	D	535	ALA	4.2
3	D	319	ARG	4.2
3	D	393	GLY	4.1
3	A	530	ILE	4.1
3	D	303	LEU	4.1
3	D	803	PHE	4.1
3	D	66	ARG	4.1
3	D	550	VAL	4.1
3	D	799	PRO	4.1
3	B	498	ILE	4.0
3	C	323	TYR	4.0
3	D	846	ILE	4.0
3	D	825	VAL	4.0
3	A	821	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
3	B	123	PHE	4.0
3	D	282	PHE	4.0
3	D	147	TYR	4.0
3	D	68	ALA	3.9
3	D	72	ILE	3.9
3	C	155	PRO	3.9
3	D	135	ALA	3.9
3	D	252	VAL	3.9
3	A	847	ALA	3.9
3	A	280	PHE	3.8
3	A	857	LEU	3.8
3	B	187	ILE	3.8
3	B	118	THR	3.8
3	B	522	PHE	3.8
3	D	796	PHE	3.8
3	D	637	GLY	3.8
3	B	168	ALA	3.8
3	B	316	ASN	3.8
3	D	808	ILE	3.8
3	B	320	TYR	3.7
3	A	854	ILE	3.7
3	D	37	LEU	3.7
3	B	550	VAL	3.7
3	B	126	PRO	3.7
3	B	317	HIS	3.7
3	D	858	ILE	3.7
3	D	288	TYR	3.7
3	D	516	VAL	3.6
3	C	303	LEU	3.6
3	B	503	LEU	3.6
3	C	302	LYS	3.6
3	D	63	ALA	3.6
3	A	788	ILE	3.6
3	C	174	GLY	3.5
3	D	198	LEU	3.5
3	B	158	ASN	3.5
1	E	2	DG	3.5
3	B	183	ILE	3.5
3	D	530	ILE	3.5
3	D	138	HIS	3.5
3	A	250	VAL	3.5
3	D	824	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
3	D	518	TYR	3.5
3	B	136	ILE	3.5
3	D	157	GLY	3.5
3	D	293	ILE	3.5
3	B	149	PHE	3.5
3	D	202	LEU	3.5
3	B	488	TYR	3.5
3	D	156	TYR	3.5
3	D	577	TYR	3.5
3	D	863	LEU	3.5
3	D	78	ILE	3.4
3	B	508	LEU	3.4
3	D	28	THR	3.4
3	B	322	SER	3.4
3	D	774	LEU	3.4
3	D	146	PHE	3.4
3	B	321	ILE	3.3
3	D	811	TYR	3.3
3	D	155	PRO	3.3
3	B	313	ARG	3.3
3	D	62	PHE	3.3
3	A	550	VAL	3.3
3	B	127	SER	3.3
3	D	795	GLY	3.3
3	C	508	LEU	3.3
3	B	262	ILE	3.3
3	D	187	ILE	3.3
3	D	286	PRO	3.3
3	D	548	THR	3.3
3	B	156	TYR	3.3
3	B	129	ALA	3.3
3	D	832	VAL	3.3
3	B	186	ILE	3.3
3	B	308	PRO	3.3
3	B	234	PHE	3.3
3	B	520	PHE	3.3
3	D	71	TRP	3.3
3	B	492	ALA	3.2
3	D	847	ALA	3.2
3	B	153	ASN	3.2
3	B	263	ILE	3.2
3	B	159	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
3	B	516	VAL	3.2
3	D	80	LEU	3.2
3	A	822	PRO	3.2
3	A	489	MET	3.2
3	B	485	HIS	3.2
3	C	897	LEU	3.2
3	D	223	ILE	3.2
3	D	499	ILE	3.2
3	D	58	THR	3.2
3	B	502	ALA	3.1
3	D	31	VAL	3.1
3	D	159	VAL	3.1
3	B	325	ILE	3.1
3	D	525	GLU	3.1
3	D	783	SER	3.1
3	D	300	VAL	3.1
3	D	213	LEU	3.1
3	D	162	TRP	3.1
3	D	611	THR	3.1
3	B	315	SER	3.1
3	D	520	PHE	3.1
3	A	518	TYR	3.1
3	D	194	GLU	3.1
3	D	118	THR	3.1
3	D	129	ALA	3.1
3	D	15	ILE	3.0
3	B	124	PRO	3.0
3	B	303	LEU	3.0
3	B	518	TYR	3.0
3	D	831	TYR	3.0
3	B	334	ILE	3.0
3	B	819	ILE	3.0
3	B	548	THR	3.0
3	C	304	LYS	3.0
3	D	178	VAL	3.0
3	B	166	ILE	3.0
3	D	102	LYS	3.0
3	D	64	ASN	3.0
3	A	282	PHE	3.0
3	D	802	PRO	3.0
3	A	490	LEU	3.0
3	A	819	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	142	ILE	3.0
3	B	323	TYR	3.0
3	B	865	TRP	3.0
3	C	252	VAL	2.9
3	A	498	ILE	2.9
3	D	133	ILE	2.9
3	D	38	PHE	2.9
3	C	514	LEU	2.9
3	D	6	LEU	2.9
3	D	263	ILE	2.9
3	D	33	TYR	2.9
3	C	46	ALA	2.9
3	C	151	LEU	2.9
3	D	290	LEU	2.9
3	B	252	VAL	2.9
2	J	115	DA	2.9
3	A	508	LEU	2.9
3	B	318	GLN	2.9
3	D	265	LEU	2.9
3	D	871	LEU	2.9
3	B	824	VAL	2.9
3	B	314	GLU	2.9
3	A	548	THR	2.9
3	B	164	ILE	2.9
3	D	136	ILE	2.9
3	D	868	TYR	2.8
3	D	538	LEU	2.8
3	B	555	ALA	2.8
3	D	88	PHE	2.8
3	D	379	VAL	2.8
3	B	47	THR	2.8
3	D	245	HIS	2.8
3	D	776	TYR	2.8
3	D	280	PHE	2.8
3	B	130	LYS	2.8
3	D	848	TRP	2.8
3	D	253	GLY	2.8
3	D	170	LEU	2.8
3	D	570	LEU	2.8
3	A	545	ALA	2.8
3	D	191	PHE	2.8
3	D	148	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	226	VAL	2.8
3	D	539	ASN	2.8
3	B	157	GLY	2.8
3	B	294	SER	2.8
3	D	807	GLY	2.8
3	D	506	PRO	2.8
3	D	412	LEU	2.8
3	A	520	PHE	2.8
3	D	771	PHE	2.8
3	D	830	VAL	2.8
3	B	112	ASN	2.7
3	B	526	ILE	2.7
3	D	205	TRP	2.7
3	D	215	GLY	2.7
3	D	523	SER	2.7
3	A	492	ALA	2.7
3	B	545	ALA	2.7
3	C	320	TYR	2.7
3	D	166	ILE	2.7
3	D	309	ILE	2.7
3	D	729	GLY	2.7
3	B	152	LEU	2.7
3	B	514	LEU	2.7
3	B	191	PHE	2.7
3	B	284	ASN	2.7
3	B	116	GLU	2.7
3	D	456	CYS	2.7
3	B	288	TYR	2.7
3	D	188	TYR	2.7
3	D	391	TYR	2.7
3	B	505	ASN	2.7
3	D	134	ASP	2.7
3	D	115	ILE	2.7
3	B	506	PRO	2.7
3	A	1	MET	2.7
3	D	541	MET	2.7
3	D	801	CYS	2.7
3	D	298	LEU	2.7
3	A	522	PHE	2.6
3	D	201	TYR	2.6
3	D	529	LYS	2.6
3	D	186	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	557	ILE	2.6
3	B	310	SER	2.6
3	D	760	LEU	2.6
3	B	531	LYS	2.6
3	D	313	ARG	2.6
3	A	252	VAL	2.6
3	B	226	VAL	2.6
3	B	264	THR	2.6
3	D	798	GLY	2.6
3	B	815	ILE	2.6
3	D	504	HIS	2.6
3	B	213	LEU	2.6
3	D	151	LEU	2.6
3	D	2	LYS	2.6
3	D	543	PHE	2.6
3	B	292	TYR	2.6
3	C	300	VAL	2.6
3	D	793	VAL	2.6
3	D	20	ILE	2.6
3	D	52	ILE	2.6
3	D	334	ILE	2.6
3	D	536	LYS	2.6
3	D	829	LYS	2.6
3	C	168	ALA	2.6
3	D	517	ASP	2.6
3	D	489	MET	2.6
3	A	543	PHE	2.6
3	C	898	PHE	2.6
3	D	390	PRO	2.6
3	D	575	PHE	2.6
3	D	110	VAL	2.6
3	A	526	ILE	2.6
3	B	530	ILE	2.6
3	C	530	ILE	2.6
3	D	11	ILE	2.6
3	D	164	ILE	2.6
3	D	323	TYR	2.6
2	F	101	DG	2.5
3	D	242	LEU	2.5
3	B	336	ALA	2.5
2	H	115	DA	2.5
3	A	300	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	36	SER	2.5
3	D	782	VAL	2.5
3	D	380	ILE	2.5
3	D	197	LEU	2.5
3	D	82	ALA	2.5
3	B	278	LYS	2.5
3	B	302	LYS	2.5
3	D	794	GLY	2.5
3	B	864	HIS	2.5
3	D	804	HIS	2.5
3	A	499	ILE	2.5
3	B	341	ILE	2.5
3	D	805	ILE	2.5
3	D	819	ILE	2.5
3	A	514	LEU	2.5
3	B	861	ASP	2.5
3	D	317	HIS	2.5
3	B	901	PHE	2.5
3	D	204	PHE	2.5
3	B	227	TYR	2.5
3	B	271	LEU	2.5
3	B	290	LEU	2.5
3	D	621	ASP	2.5
3	D	131	HIS	2.5
3	D	132	PRO	2.5
3	B	283	THR	2.4
3	D	841	PHE	2.4
3	B	298	LEU	2.4
3	B	343	LEU	2.4
3	A	527	LYS	2.4
1	I	2	DG	2.4
3	B	114	ASP	2.4
2	F	115	DA	2.4
3	C	496	GLY	2.4
3	B	357	SER	2.4
3	B	510	VAL	2.4
3	D	788	ILE	2.4
1	K	2	DG	2.4
3	A	551	ALA	2.4
3	D	111	ALA	2.4
3	B	499	ILE	2.4
3	B	543	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	266	PHE	2.4
3	D	862	VAL	2.4
3	A	848	TRP	2.4
3	B	319	ARG	2.4
3	B	307	GLY	2.4
3	D	814	ALA	2.4
3	A	283	THR	2.4
3	B	536	LYS	2.4
3	A	541	MET	2.4
3	C	522	PHE	2.4
3	D	312	LEU	2.4
3	D	730	LEU	2.4
3	B	188	TYR	2.3
3	D	488	TYR	2.3
3	D	822	PRO	2.3
3	D	840	PRO	2.3
3	A	817	GLY	2.3
3	A	555	ALA	2.3
3	D	304	LYS	2.3
3	B	554	THR	2.3
3	D	855	THR	2.3
3	B	220	SER	2.3
3	A	516	VAL	2.3
3	B	557	ILE	2.3
3	B	862	VAL	2.3
3	C	250	VAL	2.3
3	D	270	VAL	2.3
3	B	242	LEU	2.3
3	D	93	LEU	2.3
3	D	889	LEU	2.3
3	D	116	GLU	2.3
3	B	306	ASP	2.3
2	J	114	DG	2.3
3	B	155	PRO	2.3
3	B	329	TYR	2.3
3	D	849	PRO	2.3
3	A	496	GLY	2.3
3	B	496	GLY	2.3
3	B	239	ALA	2.3
3	D	780	ALA	2.3
3	D	785	ALA	2.3
3	B	214	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	154	SER	2.3
3	B	296	PHE	2.3
3	C	503	LEU	2.3
3	D	845	CYS	2.3
3	B	552	GLY	2.3
3	C	301	GLY	2.3
3	D	827	GLY	2.3
3	A	789	ALA	2.3
3	C	535	ALA	2.3
3	D	659	MET	2.3
3	C	309	ILE	2.3
3	D	321	ILE	2.3
3	D	632	ILE	2.3
3	D	50	PHE	2.3
3	D	470	VAL	2.3
3	D	898	PHE	2.3
3	B	490	LEU	2.3
3	B	863	LEU	2.3
3	C	175	GLY	2.3
3	B	523	SER	2.3
3	A	698	ILE	2.3
3	B	133	ILE	2.3
3	D	218	VAL	2.3
3	D	490	LEU	2.2
3	D	192	ASP	2.2
3	D	748	CYS	2.2
3	D	120	PRO	2.2
3	D	24	GLY	2.2
3	A	776	TYR	2.2
3	D	305	TYR	2.2
3	D	545	ALA	2.2
3	D	310	SER	2.2
3	D	315	SER	2.2
3	B	527	LYS	2.2
3	D	83	LEU	2.2
3	B	280	PHE	2.2
3	D	507	ASN	2.2
3	D	683	MET	2.2
3	B	167	ALA	2.2
3	B	247	LYS	2.2
3	B	535	ALA	2.2
3	D	137	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	583	ALA	2.2
3	D	784	SER	2.2
3	D	698	ILE	2.2
3	D	815	ILE	2.2
3	A	303	LEU	2.2
3	D	423	VAL	2.2
3	A	903	PHE	2.2
3	B	359	PHE	2.2
3	D	149	PHE	2.2
3	D	395	PHE	2.2
3	C	899	ASP	2.2
3	B	120	PRO	2.2
3	D	866	MET	2.2
3	B	206	GLN	2.2
3	D	173	GLN	2.2
3	D	247	LYS	2.2
3	B	551	ALA	2.2
3	D	735	SER	2.2
3	D	92	TYR	2.2
3	A	805	ILE	2.2
3	D	475	ILE	2.2
3	D	388	VAL	2.2
3	D	531	LYS	2.2
3	C	610	GLY	2.2
3	D	285	GLN	2.2
3	D	57	CYS	2.2
1	G	2	DG	2.2
2	H	114	DG	2.2
3	D	237	SER	2.2
3	D	551	ALA	2.2
3	B	519	ARG	2.1
3	B	162	TRP	2.1
3	D	271	LEU	2.1
3	D	508	LEU	2.1
3	B	189	MET	2.1
3	A	830	VAL	2.1
3	B	250	VAL	2.1
3	C	159	VAL	2.1
3	A	536	LYS	2.1
3	D	172	GLU	2.1
3	D	179	PRO	2.1
3	D	458	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	699	GLY	2.1
3	B	847	ALA	2.1
3	D	7	THR	2.1
3	A	811	TYR	2.1
3	D	273	TYR	2.1
3	A	101	ILE	2.1
3	D	430	ILE	2.1
3	D	857	LEU	2.1
3	B	160	GLU	2.1
3	B	275	ASP	2.1
3	B	820	ASP	2.1
3	D	67	ASP	2.1
3	B	132	PRO	2.1
3	C	178	VAL	2.1
3	C	506	PRO	2.1
3	D	39	ALA	2.1
3	D	821	ALA	2.1
2	L	101	DG	2.1
3	B	529	LYS	2.1
3	C	1	MET	2.1
3	A	497	GLU	2.1
3	A	525	GLU	2.1
3	D	152	LEU	2.1
3	D	225	TYR	2.1
3	D	786	ASN	2.1
1	G	1	DC	2.1
3	D	870	VAL	2.1
3	D	544	ARG	2.1
3	A	523	SER	2.1
3	B	281	SER	2.1
3	D	264	THR	2.1
3	B	111	ALA	2.1
3	D	32	GLU	2.1
3	D	40	HIS	2.1
3	D	415	LEU	2.1
3	D	503	LEU	2.1
3	B	299	ASN	2.1
3	D	284	ASN	2.1
3	D	325	ILE	2.1
3	A	506	PRO	2.1
3	C	156	TYR	2.1
3	D	392	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	510	VAL	2.1
3	B	798	GLY	2.1
3	D	221	PHE	2.1
3	B	216	TRP	2.1
3	D	216	TRP	2.1
3	D	865	TRP	2.1
3	A	279	LYS	2.0
3	B	279	LYS	2.0
3	D	238	THR	2.0
3	D	622	THR	2.0
3	D	728	MET	2.0
3	B	194	GLU	2.0
3	B	324	ASN	2.0
3	B	511	ASP	2.0
3	D	524	ASP	2.0
3	B	858	ILE	2.0
3	D	108	ILE	2.0
3	D	274	ILE	2.0
3	D	190	PRO	2.0
3	D	463	TYR	2.0
3	A	519	ARG	2.0
3	D	145	ARG	2.0
3	B	528	GLU	2.0
3	D	44	SER	2.0
3	B	346	ASP	2.0
3	A	858	ILE	2.0
3	D	777	ILE	2.0

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

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	3DR	K	3	11/12	0.51	0.16	165,167,169,169	0
1	3DR	E	3	11/12	0.58	0.16	138,143,147,147	0
1	3DR	G	3	11/12	0.75	0.13	132,137,146,147	0
1	3DR	I	3	11/12	0.79	0.16	102,105,111,112	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.