



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:00 AM UTC

PDB ID : 3RMB / pdb_00003rmb
Title : Crystal Structure of a replicative DNA polymerase bound to DNA containing
Thymine Glycol
Authors : Aller, P.; Duclos, S.; Wallace, S.S.; Doublié, S.
Deposited on : 2011-04-20
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:

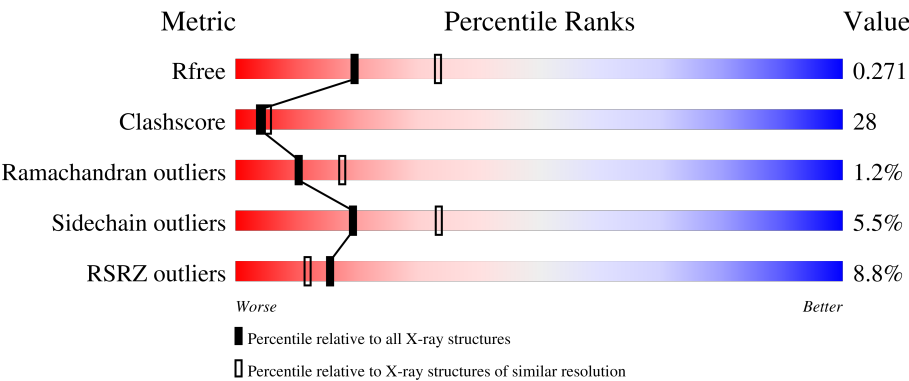
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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	A	906	10% 50% 43% 6%
1	B	906	7% 56% 40%
1	C	906	2% 59% 37%
1	D	906	17% 47% 48% 5%
2	E	18	17% 11% 83% 6%

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Mol	Chain	Length	Quality of chain
2	G	18	22%72%6%
2	I	18	39%44%17%
2	K	18	17%39%56%6%
3	F	14	21%21%79%
3	H	14	14%86%
3	J	14	29%64%7%
3	L	14	14%7%93%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32166 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	4	0	0
			7342	4715	1220	1374	33			
1	B	903	Total	C	N	O	S	0	0	0
			7294	4686	1209	1366	33			
1	C	900	Total	C	N	O	S	0	0	0
			7332	4706	1220	1373	33			
1	D	897	Total	C	N	O	S	0	0	0
			7097	4558	1163	1344	32			

There are 20 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
A	904	HIS	-	expression tag	UNP Q38087
A	905	HIS	-	expression tag	UNP Q38087
A	906	HIS	-	expression tag	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
B	904	HIS	-	expression tag	UNP Q38087
B	905	HIS	-	expression tag	UNP Q38087
B	906	HIS	-	expression tag	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
C	904	HIS	-	expression tag	UNP Q38087
C	905	HIS	-	expression tag	UNP Q38087
C	906	HIS	-	expression tag	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087
D	904	HIS	-	expression tag	UNP Q38087
D	905	HIS	-	expression tag	UNP Q38087
D	906	HIS	-	expression tag	UNP Q38087

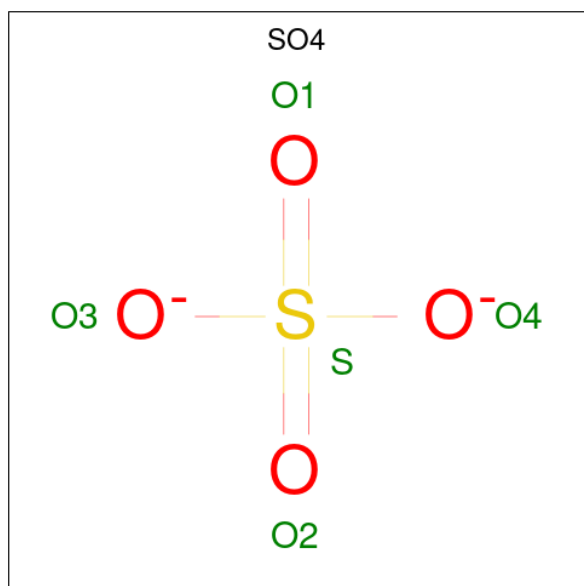
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*CP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			
2	G	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			
2	I	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			
2	K	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			
3	H	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			
3	J	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			
3	L	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		

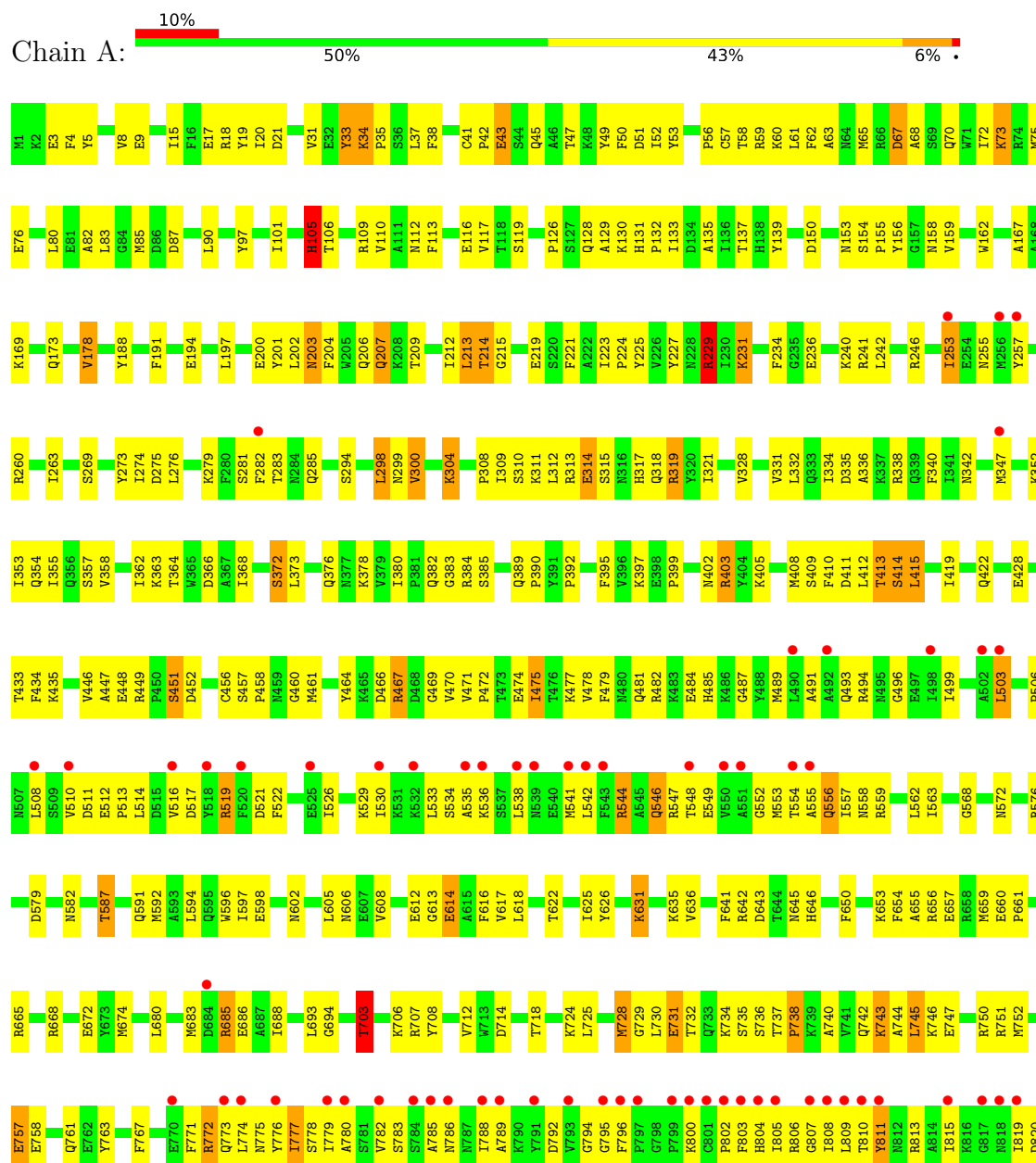
- Molecule 5 is water.

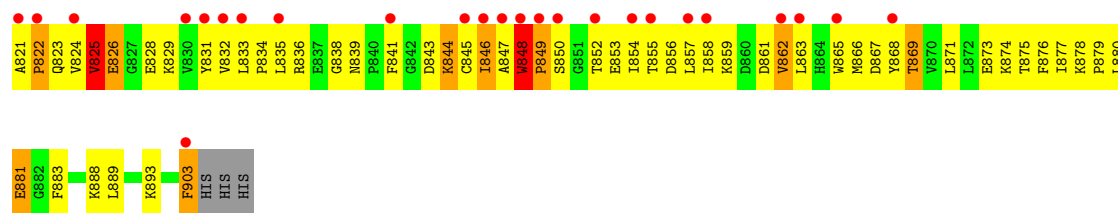
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	111	Total	O		0	0
			111	111			
5	B	129	Total	O		0	0
			129	129			
5	C	178	Total	O		0	0
			178	178			
5	D	33	Total	O		0	0
			33	33			
5	E	5	Total	O		0	0
			5	5			
5	F	4	Total	O		0	0
			4	4			
5	G	11	Total	O		0	0
			11	11			
5	H	4	Total	O		0	0
			4	4			
5	I	13	Total	O		0	0
			13	13			
5	J	7	Total	O		0	0
			7	7			
5	K	3	Total	O		0	0
			3	3			
5	L	2	Total	O		0	0
			2	2			

3 Residue-property plots

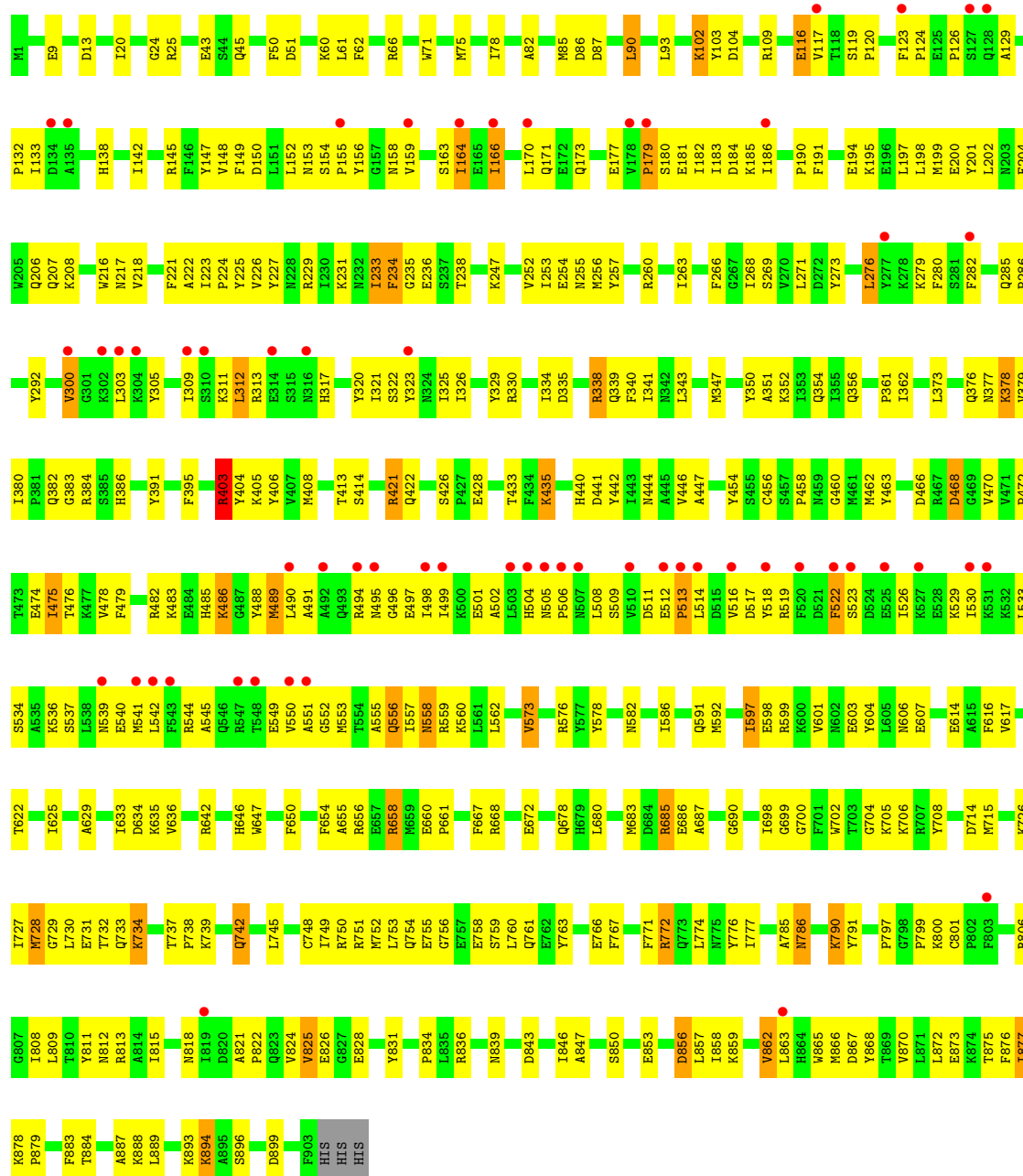
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA polymerase

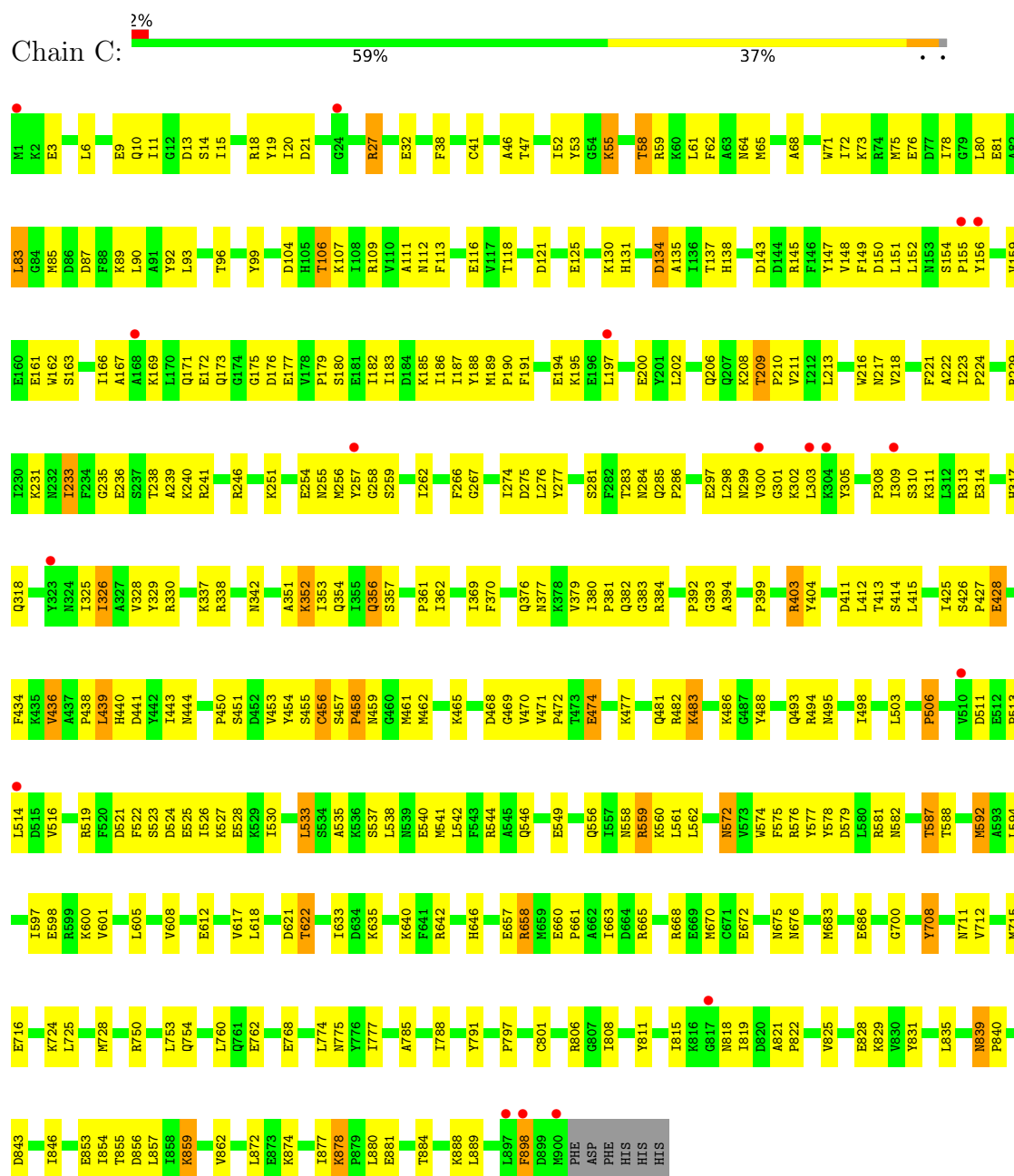




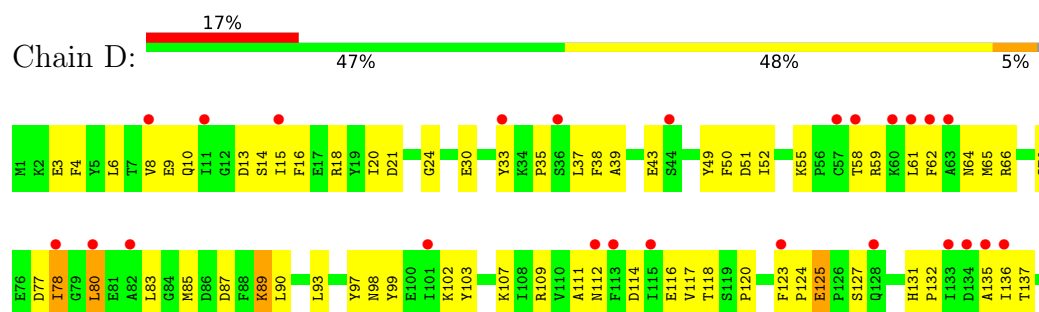
• Molecule 1: DNA polymerase

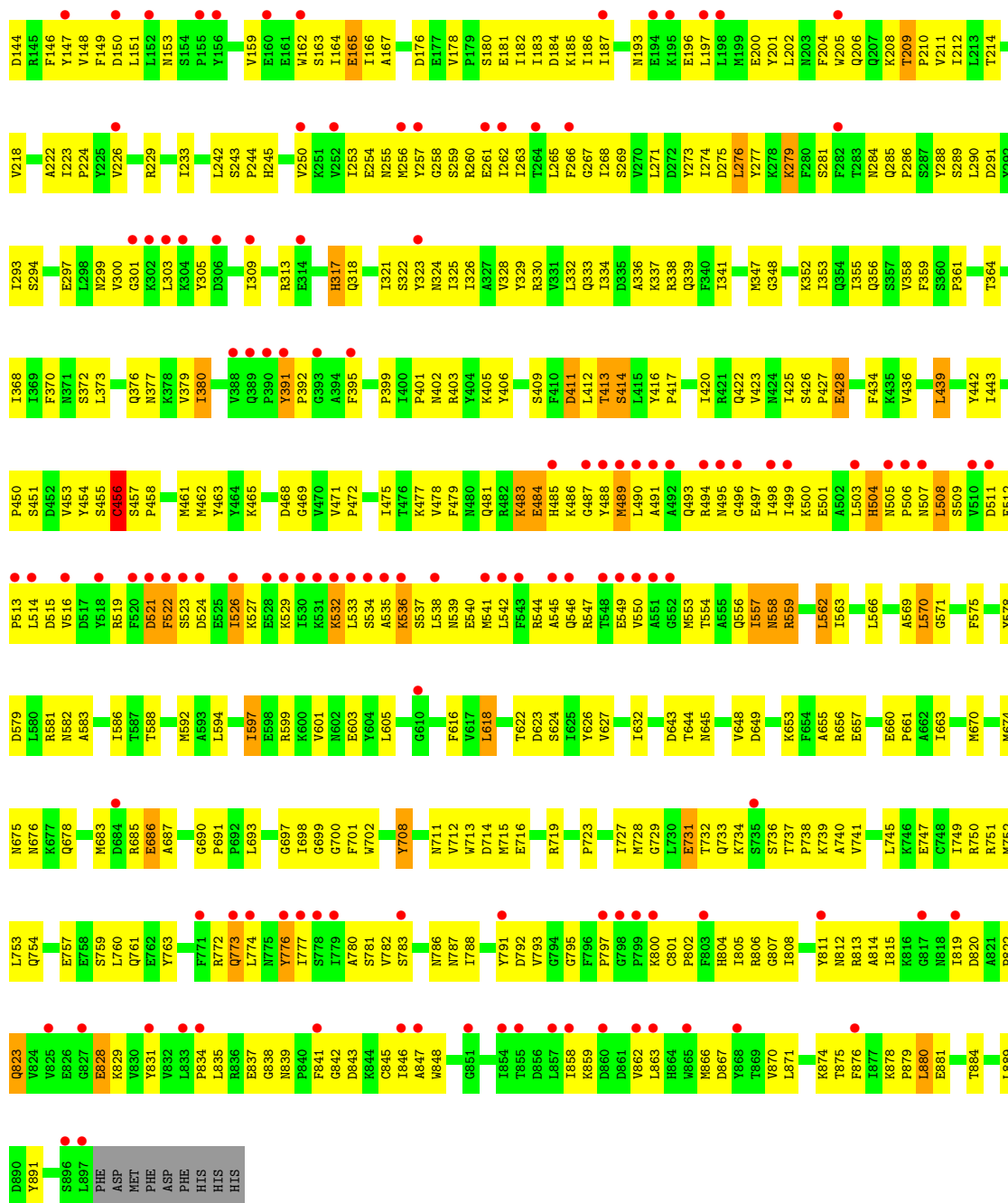


• Molecule 1: DNA polymerase

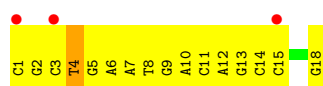


• Molecule 1: DNA polymerase

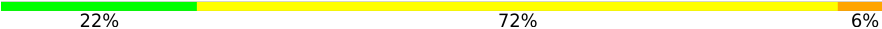


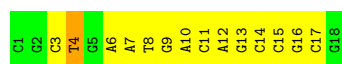


● Molecule 2: DNA (5'-D(*CP*GP*CP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C
P*GP*CP*G)-3')



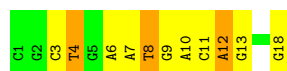
● Molecule 2: DNA (5'-D(*CP*GP*CP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C
P*GP*CP*G)-3')

Chain G:  22% 72% 6%



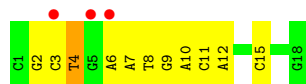
- Molecule 2: DNA (5'-D(*CP*GP*CP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C
P*GP*CP*G)-3')

Chain I:  39% 44% 17%

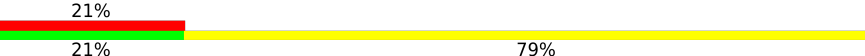


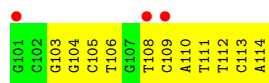
- Molecule 2: DNA (5'-D(*CP*GP*CP*(CTG)P*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*C
P*GP*CP*G)-3')

Chain K:  17% 39% 56% 6%



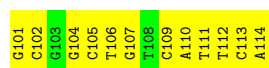
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain F:  21% 21% 79%



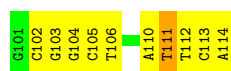
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain H:  14% 86%

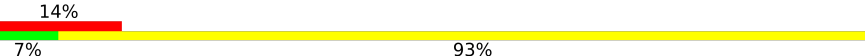


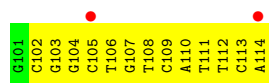
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3')

Chain J:  29% 64% 7%



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

Chain L:  14% 7% 93%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.53Å 123.44Å 164.29Å 90.00° 96.84° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-2.65) 93.8 (50.00-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.276 0.218 , 0.271	Depositor DCC
R_{free} test set	26586 reflections (9.14%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32166	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: SO4, 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	A	0.48	0/7523	0.97	27/10175 (0.3%)
1	B	0.47	0/7475	0.93	24/10121 (0.2%)
1	C	0.50	0/7511	0.96	21/10154 (0.2%)
1	D	0.39	0/7275	0.92	25/9887 (0.3%)
2	E	0.30	0/389	0.66	0/596
2	G	0.35	0/389	0.70	0/596
2	I	0.41	0/389	0.88	3/596 (0.5%)
2	K	0.28	0/389	0.51	0/596
3	F	0.28	0/312	0.63	0/478
3	H	0.31	0/312	0.73	0/478
3	J	0.37	0/312	0.84	1/478 (0.2%)
3	L	0.25	0/312	0.58	0/478
All	All	0.45	0/32588	0.92	101/44633 (0.2%)

There are no bond length outliers.

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	THR	CA-C-N	9.08	128.84	119.76
1	C	209	THR	C-N-CA	9.08	128.84	119.76
1	D	489	MET	N-CA-C	-8.46	102.97	113.38
1	D	540	GLU	N-CA-C	-8.23	103.25	113.38
1	B	786	ASN	N-CA-C	7.86	123.19	112.90
1	C	831	TYR	N-CA-C	-7.74	100.10	110.55
1	D	712	VAL	N-CA-C	7.52	118.82	108.89
1	B	862	VAL	N-CA-C	-7.50	103.63	111.58
1	A	703	THR	N-CA-C	-7.44	103.82	113.12
1	C	436	VAL	N-CA-C	7.25	118.57	107.99
1	D	507	ASN	N-CA-C	-7.10	99.04	108.34
1	A	456	CYS	N-CA-C	7.00	120.91	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ALA	N-CA-C	-6.89	104.84	113.18
1	D	838	GLY	N-CA-C	-6.75	105.44	114.95
1	A	18	ARG	N-CA-C	-6.70	98.81	109.59
1	B	540	GLU	N-CA-C	-6.65	106.12	114.56
1	D	532	LYS	N-CA-C	6.50	118.45	111.36
1	B	486	LYS	N-CA-C	-6.44	104.18	111.07
1	A	67	ASP	N-CA-C	-6.41	104.21	111.07
1	C	256	MET	N-CA-C	-6.32	104.39	111.28
1	D	242	LEU	N-CA-C	-6.32	105.53	113.18
1	C	859	LYS	N-CA-C	6.32	118.73	111.02
1	B	233	ILE	N-CA-C	6.27	116.45	110.74
1	B	403	ARG	N-CA-C	-6.25	100.38	110.32
1	A	635	LYS	N-CA-C	-6.20	104.44	111.14
1	B	598	GLU	N-CA-C	-6.16	104.48	111.07
1	A	848	TRP	N-CA-C	6.14	113.66	108.13
1	D	276	LEU	N-CA-C	-6.10	104.18	111.69
1	A	113	PHE	N-CA-C	6.09	118.96	109.52
1	A	596	TRP	N-CA-C	-6.09	104.57	111.14
1	B	338	ARG	N-CA-C	6.07	119.15	111.69
2	I	8	DT	C5'-C4'-C3'	-6.01	105.89	114.90
1	D	380	ILE	CA-C-N	5.97	125.94	120.03
1	D	380	ILE	C-N-CA	5.97	125.94	120.03
1	D	708	TYR	N-CA-C	5.97	116.30	107.88
1	B	729	GLY	N-CA-C	5.96	122.99	115.42
1	D	547	ARG	N-CA-C	-5.95	105.98	113.18
1	C	712	VAL	N-CA-C	5.94	117.14	108.58
1	D	436	VAL	N-CA-C	5.94	116.73	109.30
1	B	456	CYS	N-CA-C	5.83	118.73	109.81
1	A	794	GLY	N-CA-C	-5.78	104.89	114.48
1	B	825	VAL	N-CA-C	5.76	117.30	108.71
1	C	21	ASP	N-CA-C	5.76	118.78	109.79
1	A	415	LEU	N-CA-C	5.64	120.61	111.37
1	B	839	ASN	CA-C-N	5.63	125.34	119.82
1	B	839	ASN	C-N-CA	5.63	125.34	119.82
1	B	276	LEU	N-CA-C	-5.63	104.77	111.69
1	A	757	GLU	N-CA-C	5.59	117.37	111.28
1	B	756	GLY	N-CA-C	5.57	118.04	111.63
2	I	12	DA	C5'-C4'-C3'	-5.55	106.57	114.90
1	A	405	LYS	N-CA-C	5.55	117.02	110.97
1	A	469	GLY	N-CA-C	5.55	118.31	111.93
1	A	811	TYR	N-CA-C	-5.54	105.31	112.68
1	D	508	LEU	N-CA-C	5.54	117.92	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	808	ILE	N-CA-C	-5.49	105.37	110.53
1	B	442	TYR	N-CA-C	-5.48	105.73	112.90
1	A	403	ARG	N-CA-C	-5.47	102.39	110.48
1	C	708	TYR	N-CA-C	5.42	116.52	108.60
1	A	178	VAL	CA-C-N	5.41	125.42	119.90
1	A	178	VAL	C-N-CA	5.41	125.42	119.90
1	B	391	TYR	CA-C-N	5.41	126.60	119.84
1	B	391	TYR	C-N-CA	5.41	126.60	119.84
1	D	102	LYS	N-CA-C	-5.40	100.59	109.40
1	B	790	LYS	N-CA-C	5.38	116.84	110.97
1	B	354	GLN	N-CA-C	-5.37	103.05	110.35
1	C	233	ILE	N-CA-C	-5.34	108.07	113.20
1	C	403	ARG	N-CA-C	-5.34	101.83	110.32
1	C	665	ARG	N-CA-C	-5.33	105.37	111.07
1	A	214	THR	N-CA-C	5.32	116.36	108.86
1	B	383	GLY	N-CA-C	-5.31	104.31	111.54
1	C	134	ASP	N-CA-C	5.31	118.78	112.72
1	D	773	GLN	N-CA-C	-5.30	108.07	114.75
3	J	111	DT	C5'-C4'-O4'	-5.27	101.50	109.40
1	B	343	LEU	N-CA-C	-5.26	105.46	111.14
1	C	878	LYS	CA-C-N	-5.25	114.25	119.56
1	C	878	LYS	C-N-CA	-5.25	114.25	119.56
1	A	820	ASP	N-CA-C	-5.23	106.92	113.72
1	A	519	ARG	N-CA-C	-5.20	105.61	111.28
2	I	18	DG	C2'-C3'-O3'	-5.17	103.74	111.50
1	A	33	TYR	N-CA-C	5.17	117.97	110.42
1	A	685	ARG	N-CA-C	-5.16	102.64	110.28
1	B	656	ARG	N-CA-C	5.15	116.97	111.36
1	D	456	CYS	N-CA-C	5.15	117.98	109.85
1	D	165	GLU	N-CA-C	-5.14	105.59	111.14
1	D	820	ASP	N-CA-C	-5.10	107.06	113.28
1	A	803	PHE	N-CA-C	5.09	117.73	111.82
1	C	839	ASN	CA-C-N	5.08	126.19	119.84
1	C	839	ASN	C-N-CA	5.08	126.19	119.84
1	D	89	LYS	N-CA-C	-5.08	105.64	111.07
1	A	229	ARG	N-CA-C	-5.07	105.64	111.07
1	C	456	CYS	N-CA-C	5.07	117.00	109.69
1	D	209	THR	CA-C-N	5.07	124.83	119.76
1	D	209	THR	C-N-CA	5.07	124.83	119.76
1	A	838	GLY	N-CA-C	-5.07	107.82	115.32
1	D	504	HIS	N-CA-C	-5.05	107.29	113.50
1	C	853	GLU	N-CA-C	-5.05	102.30	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	457	SER	CA-C-N	5.04	125.31	119.47
1	D	457	SER	C-N-CA	5.04	125.31	119.47
1	C	877	ILE	N-CA-C	5.02	115.74	110.62
1	A	355	ILE	N-CA-C	5.02	115.63	110.36
1	B	877	ILE	N-CA-C	5.02	115.17	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7342	0	7193	421	0
1	B	7294	0	7096	399	0
1	C	7332	0	7212	306	0
1	D	7097	0	6752	425	0
2	E	369	0	204	29	0
2	G	369	0	204	31	0
2	I	369	0	204	20	0
2	K	369	0	204	19	0
3	F	280	0	154	25	0
3	H	280	0	154	22	0
3	J	280	0	154	19	0
3	L	280	0	154	14	0
4	C	5	0	0	0	0
5	A	111	0	0	14	0
5	B	129	0	0	11	0
5	C	178	0	0	16	0
5	D	33	0	0	3	0
5	E	5	0	0	0	0
5	F	4	0	0	3	0
5	G	11	0	0	0	0
5	H	4	0	0	1	0
5	I	13	0	0	0	0
5	J	7	0	0	0	0
5	K	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	2	0	0	0	0
All	All	32166	0	29685	1710	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 28.

All (1710) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:686:GLU:HG3	1:D:715:MET:HE1	1.22	1.18
3:L:104:DG:H2''	3:L:105:DC:H5''	1.19	1.14
1:B:309:ILE:HA	1:B:312:LEU:HB2	1.31	1.11
3:J:104:DG:H2''	3:J:105:DC:H5''	1.22	1.11
2:K:10:DA:H2''	2:K:11:DC:H5''	1.20	1.08
1:B:85:MET:HE2	1:B:87:ASP:H	1.12	1.08
1:D:514:LEU:HD21	1:D:532:LYS:HG3	1.33	1.06
1:D:442:TYR:HB3	1:D:592:MET:HE3	1.36	1.03
1:A:833:LEU:HD21	1:A:866:MET:HB2	1.40	1.03
3:J:104:DG:C2'	3:J:105:DC:H5''	1.88	1.02
1:D:495:ASN:HD21	1:D:521:ASP:HA	1.21	1.00
1:A:408:MET:HE1	1:A:655:ALA:HB2	1.39	1.00
1:A:806:ARG:HH11	1:A:844:LYS:HE3	1.26	1.00
1:D:541:MET:HA	1:D:544:ARG:HD3	1.44	0.98
1:C:482:ARG:NH1	1:C:556:GLN:HE21	1.60	0.97
1:C:41:CYS:HB3	1:C:58:THR:HG22	1.43	0.97
1:A:384:ARG:HD3	1:A:385:SER:H	1.27	0.96
1:C:392:PRO:O	1:C:587:THR:HG21	1.65	0.96
1:A:153:ASN:ND2	1:A:158:ASN:HD22	1.62	0.96
1:B:171:GLN:HE21	1:B:177:GLU:HG2	1.31	0.95
1:C:855:THR:HG22	1:C:857:LEU:H	1.31	0.95
1:D:509:SER:HB3	1:D:532:LYS:O	1.66	0.95
1:A:72:ILE:O	1:A:76:GLU:HG3	1.66	0.95
1:A:785:ALA:HB1	1:A:788:ILE:HD11	1.48	0.95
2:E:14:DC:H2''	2:E:15:DC:H5'	1.50	0.94
1:B:164:ILE:HD13	1:B:164:ILE:H	1.30	0.94
3:L:104:DG:C2'	3:L:105:DC:H5''	1.98	0.94
1:B:347:MET:HE1	1:B:562:LEU:HD11	1.48	0.93
2:K:10:DA:C2'	2:K:11:DC:H5''	1.97	0.93
1:D:80:LEU:H	1:D:80:LEU:HD22	1.36	0.91
1:B:642:ARG:H	1:B:646:HIS:HD2	1.07	0.91
1:B:863:LEU:HA	1:B:866:MET:HE3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:SER:HB3	1:C:318:GLN:HE22	1.31	0.91
3:F:103:DG:H2''	3:F:104:DG:H5'	1.51	0.90
1:D:511:ASP:HA	1:D:533:LEU:HD11	1.53	0.90
2:K:8:DT:H2''	2:K:9:DG:H5'	1.52	0.90
2:I:10:DA:H2''	2:I:11:DC:H5'	1.54	0.89
1:A:153:ASN:HD22	1:A:158:ASN:HD22	0.91	0.89
1:D:811:TYR:OH	1:D:822:PRO:HG2	1.73	0.88
1:B:82:ALA:H	1:B:382:GLN:HE21	1.22	0.87
3:J:110:DA:H2''	3:J:111:DT:H5'	1.57	0.87
1:A:347:MET:HB2	1:A:558:ASN:HD21	1.38	0.87
1:B:642:ARG:H	1:B:646:HIS:CD2	1.93	0.87
1:B:303:LEU:HD12	1:B:323:TYR:HA	1.56	0.86
1:A:835:LEU:HD23	1:A:866:MET:HA	1.58	0.86
1:A:153:ASN:HD22	1:A:158:ASN:ND2	1.74	0.86
1:C:572:ASN:ND2	1:C:574:TRP:H	1.71	0.86
1:C:152:LEU:HD11	1:C:190:PRO:HB2	1.57	0.85
1:C:482:ARG:NH1	1:C:560:LYS:HB2	1.91	0.85
1:D:516:VAL:HG11	1:D:522:PHE:HE1	1.41	0.85
1:C:572:ASN:HD22	1:C:574:TRP:H	1.22	0.85
1:B:166:ILE:HD12	1:B:166:ILE:H	1.38	0.85
2:K:10:DA:H2''	2:K:11:DC:C5'	2.06	0.85
1:C:303:LEU:HG	1:C:326:ILE:HD12	1.57	0.85
1:C:660:GLU:HB2	1:C:661:PRO:HD3	1.59	0.84
1:A:451:SER:HB2	5:A:921:HOH:O	1.77	0.84
1:D:532:LYS:HA	1:D:532:LYS:HE2	1.57	0.84
1:D:542:LEU:HD11	1:D:546:GLN:NE2	1.92	0.83
1:A:384:ARG:HD3	1:A:385:SER:N	1.94	0.83
3:F:110:DA:H2''	3:F:111:DT:H5'	1.58	0.83
1:D:514:LEU:H	1:D:544:ARG:HH22	1.22	0.83
1:D:163:SER:HB3	1:D:318:GLN:HE22	1.43	0.83
1:A:788:ILE:HD12	1:A:826:GLU:HB2	1.61	0.83
1:B:825:VAL:HB	1:B:828:GLU:HG3	1.60	0.83
3:J:112:DT:H2''	3:J:113:DC:H5''	1.59	0.82
2:E:8:DT:H2'	2:E:9:DG:C8	2.15	0.82
1:A:805:ILE:HA	1:A:808:ILE:HD12	1.61	0.82
1:B:482:ARG:NH2	1:B:560:LYS:HD2	1.95	0.82
1:B:85:MET:HE2	1:B:87:ASP:N	1.93	0.82
1:D:535:ALA:HB1	1:D:539:ASN:ND2	1.94	0.82
1:A:506:PRO:HB2	1:A:535:ALA:HB2	1.61	0.81
2:G:4:CTG:H6	2:G:4:CTG:H5'	1.62	0.81
1:D:738:PRO:HB3	1:D:780:ALA:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HA	1:A:73:LYS:HE3	1.61	0.81
1:D:493:GLN:HA	1:D:549:GLU:CD	2.05	0.81
1:D:493:GLN:HA	1:D:549:GLU:OE1	1.81	0.80
1:A:822:PRO:HD2	1:A:855:THR:HB	1.63	0.80
1:D:686:GLU:HG3	1:D:715:MET:CE	2.08	0.80
1:A:776:TYR:OH	1:A:853:GLU:HG3	1.82	0.80
1:C:308:PRO:HG2	1:C:311:LYS:HG2	1.64	0.80
1:A:738:PRO:HB3	1:A:779:ILE:O	1.81	0.80
3:J:105:DC:H2'	3:J:106:DT:H71	1.63	0.79
3:H:113:DC:H2''	3:H:114:DA:H5''	1.64	0.79
1:A:112:ASN:HB2	5:A:928:HOH:O	1.82	0.79
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.65	0.79
1:A:34:LYS:HG3	1:A:62:PHE:O	1.82	0.79
1:A:825:VAL:HG23	1:A:828:GLU:HG3	1.63	0.78
1:B:119:SER:HB2	1:B:124:PRO:HG3	1.64	0.78
1:A:631:LYS:HZ2	1:A:631:LYS:H	1.30	0.78
1:A:783:SER:HA	3:F:111:DT:OP1	1.83	0.78
1:D:336:ALA:HA	1:D:339:GLN:HE21	1.48	0.78
1:C:10:GLN:HG3	1:C:65:MET:HE1	1.63	0.78
1:D:255:ASN:ND2	1:D:256:MET:H	1.82	0.77
1:A:224:PRO:HA	1:A:263:ILE:HD12	1.63	0.77
1:C:542:LEU:O	1:C:546:GLN:HG3	1.83	0.77
1:A:482:ARG:HE	1:A:556:GLN:NE2	1.82	0.77
1:D:495:ASN:ND2	1:D:521:ASP:HA	1.98	0.77
1:A:734:LYS:HG2	1:A:736:SER:OG	1.85	0.77
1:B:818:ASN:HD21	1:B:857:LEU:CD1	1.98	0.77
1:B:82:ALA:H	1:B:382:GLN:NE2	1.83	0.77
1:D:286:PRO:O	1:D:829:LYS:HD2	1.84	0.76
2:E:10:DA:H2''	2:E:11:DC:C5'	2.15	0.76
1:C:167:ALA:HA	1:C:176:ASP:HB2	1.67	0.76
1:C:711:ASN:HD21	1:C:754:GLN:HE21	1.30	0.76
1:A:642:ARG:H	1:A:646:HIS:HD2	1.33	0.76
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.20	0.76
1:D:303:LEU:HG	1:D:326:ILE:HD12	1.67	0.76
1:A:736:SER:HA	1:A:782:VAL:HB	1.67	0.76
1:A:776:TYR:HB2	1:A:866:MET:HE1	1.67	0.76
1:C:482:ARG:HH12	1:C:556:GLN:HE21	1.30	0.76
1:D:109:ARG:HB3	1:D:211:VAL:HG23	1.67	0.76
2:G:8:DT:H2'	2:G:9:DG:C8	2.21	0.76
1:B:109:ARG:HH21	1:B:208:LYS:HG2	1.51	0.75
1:A:712:VAL:HG22	1:A:724:LYS:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:797:PRO:HG3	1:C:806:ARG:NH1	2.02	0.75
1:D:180:SER:O	1:D:183:ILE:HG22	1.85	0.75
1:D:260:ARG:HG2	1:D:261:GLU:N	2.01	0.75
1:B:117:VAL:HG22	1:B:133:ILE:HA	1.68	0.75
1:C:73:LYS:NZ	1:C:73:LYS:HB3	2.02	0.75
1:D:8:VAL:HG11	1:D:93:LEU:HD11	1.66	0.75
1:D:66:ARG:O	1:D:70:GLN:HG2	1.87	0.75
2:G:4:CTG:O6	2:G:4:CTG:H2'	1.86	0.75
1:D:426:SER:HB2	1:D:472:PRO:HD3	1.68	0.75
1:A:241:ARG:HH11	1:A:241:ARG:HG3	1.52	0.74
1:B:896:SER:HB2	1:B:899:ASP:OD1	1.87	0.74
3:J:112:DT:H2''	3:J:113:DC:C5'	2.16	0.74
1:B:229:ARG:O	1:B:233:ILE:HD13	1.86	0.74
1:A:194:GLU:OE1	1:A:229:ARG:HD2	1.88	0.74
1:D:391:TYR:HB2	1:D:392:PRO:HD2	1.69	0.74
1:C:231:LYS:HG3	1:C:236:GLU:HA	1.69	0.74
1:C:241:ARG:HG2	1:C:246:ARG:NE	2.03	0.74
1:D:514:LEU:CD2	1:D:532:LYS:HG3	2.13	0.74
1:B:164:ILE:HD13	1:B:164:ILE:N	2.02	0.74
3:J:104:DG:H2''	3:J:105:DC:C5'	2.10	0.73
1:C:236:GLU:HG2	1:C:240:LYS:HD2	1.71	0.73
2:E:6:DA:H2''	2:E:7:DA:H5'	1.70	0.73
3:L:113:DC:H2''	3:L:114:DA:O4'	1.87	0.73
1:D:223:ILE:HB	1:D:224:PRO:HD3	1.69	0.73
2:E:10:DA:H2''	2:E:11:DC:H5''	1.69	0.73
1:A:555:ALA:HB1	1:A:559:ARG:HH12	1.53	0.73
1:A:642:ARG:H	1:A:646:HIS:CD2	2.07	0.73
1:B:403:ARG:HB3	1:B:403:ARG:HH11	1.53	0.73
1:C:159:VAL:HG21	1:C:317:HIS:CD2	2.24	0.73
1:D:736:SER:HA	1:D:782:VAL:HB	1.69	0.72
1:A:110:VAL:HG22	1:A:212:ILE:HB	1.71	0.72
1:B:771:PHE:CE2	1:B:872:LEU:HB2	2.24	0.72
1:A:489:MET:HE1	1:A:553:MET:SD	2.29	0.72
2:I:6:DA:H2''	2:I:7:DA:H5'	1.71	0.72
1:D:118:THR:OG1	1:D:313:ARG:HG3	1.89	0.72
1:B:728:MET:HG3	3:H:113:DC:H5'	1.72	0.72
3:J:104:DG:C3'	3:J:105:DC:H5''	2.19	0.72
1:A:15:ILE:HG12	1:A:65:MET:HE1	1.71	0.72
1:B:164:ILE:H	1:B:164:ILE:CD1	2.02	0.72
3:F:110:DA:H2''	3:F:111:DT:C5'	2.19	0.72
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ALA:HA	1:B:494:ARG:HG2	1.71	0.71
1:D:738:PRO:HG2	1:D:741:VAL:HB	1.72	0.71
1:A:231:LYS:HG3	1:A:236:GLU:HA	1.70	0.71
2:G:11:DC:H2''	2:G:12:DA:H5'	1.71	0.71
3:H:110:DA:H2''	3:H:111:DT:H5'	1.72	0.71
1:A:778:SER:O	1:A:779:ILE:HD13	1.89	0.71
1:D:364:THR:O	1:D:368:ILE:HG13	1.90	0.71
1:A:642:ARG:HB2	1:A:642:ARG:NH1	2.06	0.71
1:C:38:PHE:CE2	1:C:59:ARG:HG3	2.25	0.71
1:D:137:THR:HB	1:D:328:VAL:HG21	1.72	0.71
1:D:490:LEU:HD23	5:D:939:HOH:O	1.90	0.71
1:B:606:ASN:HD21	1:B:614:GLU:H	1.37	0.70
1:D:660:GLU:HB2	1:D:661:PRO:HD3	1.72	0.70
1:B:505:ASN:N	1:B:506:PRO:HD3	2.05	0.70
1:B:303:LEU:HG	1:B:326:ILE:HG13	1.73	0.70
1:D:109:ARG:HD2	1:D:209:THR:O	1.92	0.70
1:A:308:PRO:HG2	1:A:311:LYS:HG2	1.74	0.70
1:B:815:ILE:O	1:B:818:ASN:HB2	1.91	0.70
1:A:806:ARG:HH11	1:A:844:LYS:CE	2.03	0.70
1:C:104:ASP:OD2	1:C:106:THR:HB	1.92	0.70
1:A:449:ARG:HH12	1:A:452:ASP:HB3	1.57	0.70
2:G:6:DA:H2''	2:G:7:DA:C5'	2.22	0.70
1:D:291:ASP:OD1	1:D:301:GLY:HA3	1.92	0.70
1:D:111:ALA:HB3	1:D:210:PRO:HB3	1.72	0.69
2:E:13:DG:H2''	2:E:14:DC:C5'	2.22	0.69
1:D:811:TYR:HH	1:D:822:PRO:HG2	1.56	0.69
3:F:104:DG:H5''	5:F:256:HOH:O	1.91	0.69
2:I:10:DA:H2''	2:I:11:DC:C5'	2.23	0.69
1:D:109:ARG:CZ	1:D:142:ILE:HD12	2.22	0.69
1:D:841:PHE:CZ	1:D:862:VAL:HG22	2.28	0.69
3:F:113:DC:H5	5:F:475:HOH:O	1.76	0.69
1:A:412:LEU:HG	1:A:683:MET:HG2	1.73	0.69
1:B:403:ARG:HH11	1:B:403:ARG:CB	2.06	0.69
2:K:11:DC:H2''	2:K:12:DA:H5'	1.75	0.69
1:D:80:LEU:H	1:D:80:LEU:CD2	2.06	0.69
2:G:10:DA:H2''	2:G:11:DC:O5'	1.90	0.69
1:B:133:ILE:HD12	1:B:198:LEU:HD21	1.75	0.69
1:A:236:GLU:HG2	1:A:240:LYS:HE2	1.74	0.68
1:D:87:ASP:CG	1:D:90:LEU:HD13	2.18	0.68
1:A:422:GLN:NE2	1:A:680:LEU:H	1.90	0.68
1:A:780:ALA:HB3	1:A:831:TYR:HD1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:PRO:HD3	5:C:959:HOH:O	1.93	0.68
1:A:376:GLN:HE21	1:A:378:LYS:HD2	1.58	0.68
1:B:732:THR:HG23	1:B:733:GLN:NE2	2.08	0.68
1:B:750:ARG:HH11	1:B:754:GLN:NE2	1.90	0.68
1:C:302:LYS:HB3	5:C:1077:HOH:O	1.92	0.68
1:C:62:PHE:CE2	1:C:68:ALA:HA	2.28	0.68
1:C:202:LEU:O	1:C:206:GLN:HG2	1.93	0.68
1:D:542:LEU:HD11	1:D:546:GLN:HE21	1.57	0.68
1:A:708:TYR:CZ	1:A:728:MET:HG3	2.28	0.68
1:D:579:ASP:HB3	1:D:582:ASN:HB2	1.74	0.68
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.74	0.68
1:C:403:ARG:NH2	1:C:889:LEU:HD23	2.08	0.68
1:C:41:CYS:HB3	1:C:58:THR:CG2	2.22	0.68
2:K:15:DC:H2'	5:K:269:HOH:O	1.93	0.68
1:D:336:ALA:HA	1:D:339:GLN:NE2	2.08	0.68
1:A:514:LEU:H	1:A:541:MET:CE	2.07	0.68
1:D:51:ASP:HB2	5:D:910:HOH:O	1.94	0.68
1:D:731:GLU:HA	1:D:734:LYS:CG	2.24	0.68
1:B:745:LEU:O	1:B:749:ILE:HG13	1.94	0.67
1:B:893:LYS:C	1:B:894:LYS:HG3	2.18	0.67
1:C:711:ASN:ND2	1:C:754:GLN:HE21	1.91	0.67
2:I:4:CTG:O6	2:I:4:CTG:H2'	1.93	0.67
1:A:511:ASP:OD2	1:A:533:LEU:HA	1.95	0.67
1:D:288:TYR:HA	1:D:293:ILE:HD11	1.75	0.67
1:C:218:VAL:HG22	1:C:223:ILE:HG13	1.75	0.67
1:D:715:MET:HE3	1:D:716:GLU:HG3	1.77	0.67
1:A:392:PRO:O	1:A:587:THR:HG21	1.95	0.67
1:A:514:LEU:HG	1:A:526:ILE:HG23	1.76	0.67
1:C:686:GLU:HG3	1:C:715:MET:CE	2.25	0.67
1:D:534:SER:O	1:D:538:LEU:HD13	1.93	0.67
1:B:145:ARG:HD3	1:B:185:LYS:O	1.94	0.67
1:D:284:ASN:HD22	1:D:285:GLN:N	1.93	0.66
3:J:110:DA:H1'	3:J:111:DT:H5''	1.78	0.66
1:D:373:LEU:HD12	1:D:380:ILE:HG22	1.76	0.66
1:A:824:VAL:O	1:A:825:VAL:HG13	1.95	0.66
1:B:506:PRO:HB3	1:B:536:LYS:HG2	1.78	0.66
1:A:362:ILE:HD11	1:A:572:ASN:HD22	1.60	0.66
1:C:482:ARG:HH12	1:C:556:GLN:NE2	1.93	0.66
1:D:546:GLN:O	1:D:550:VAL:HG23	1.95	0.66
2:E:6:DA:H2''	2:E:7:DA:C5'	2.24	0.66
1:D:116:GLU:HB2	1:D:135:ALA:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.76	0.66
1:D:148:VAL:HG21	1:D:325:ILE:HD11	1.77	0.66
1:D:858:ILE:O	1:D:862:VAL:HG23	1.94	0.66
1:B:512:GLU:O	1:B:514:LEU:HD22	1.96	0.66
3:F:110:DA:H1'	3:F:111:DT:H5''	1.78	0.66
1:A:568:GLY:HA3	2:E:3:DC:O2	1.95	0.66
1:B:85:MET:CE	1:B:87:ASP:H	1.99	0.66
1:B:894:LYS:HB2	1:B:894:LYS:NZ	2.10	0.66
1:C:482:ARG:CZ	1:C:556:GLN:HE21	2.08	0.66
1:C:818:ASN:HD22	1:C:821:ALA:HB2	1.61	0.66
1:A:693:LEU:HD12	1:A:694:GLY:N	2.11	0.65
1:D:514:LEU:HD21	1:D:532:LYS:CG	2.18	0.65
1:B:732:THR:HG23	1:B:733:GLN:HE21	1.59	0.65
1:D:546:GLN:HG2	1:D:549:GLU:OE1	1.96	0.65
3:F:104:DG:H2''	3:F:105:DC:O5'	1.96	0.65
3:H:110:DA:H2''	3:H:111:DT:C5'	2.25	0.65
1:B:482:ARG:CZ	1:B:560:LYS:HD2	2.25	0.65
1:C:9:GLU:OE2	1:C:266:PHE:HA	1.96	0.65
1:C:524:ASP:HA	1:C:527:LYS:HE2	1.77	0.65
1:A:514:LEU:HD11	1:A:529:LYS:NZ	2.11	0.65
1:B:386:HIS:HB2	1:B:573:VAL:CG2	2.27	0.65
1:C:194:GLU:HB3	5:C:969:HOH:O	1.94	0.65
1:C:439:LEU:HD12	1:C:443:ILE:HD11	1.77	0.65
1:B:875:THR:O	1:B:879:PRO:HG3	1.97	0.65
1:C:19:TYR:CE1	1:C:27:ARG:HB2	2.32	0.65
1:C:301:GLY:O	1:C:330:ARG:NH1	2.30	0.65
1:D:505:ASN:N	1:D:506:PRO:HD3	2.11	0.65
1:A:785:ALA:CB	1:A:788:ILE:HD11	2.26	0.65
1:A:255:ASN:ND2	1:A:257:TYR:HD1	1.94	0.65
1:A:482:ARG:HE	1:A:556:GLN:HE22	1.45	0.65
1:C:216:TRP:O	1:C:217:ASN:HB2	1.97	0.65
1:D:515:ASP:O	1:D:516:VAL:HG23	1.97	0.64
2:G:16:DG:H2''	2:G:17:DC:C5'	2.27	0.64
2:K:2:DG:H3'	2:K:3:DC:C5'	2.26	0.64
1:D:38:PHE:HB2	1:D:83:LEU:HB2	1.77	0.64
1:D:535:ALA:HB1	1:D:539:ASN:HD21	1.61	0.64
2:G:6:DA:H2''	2:G:7:DA:H5'	1.79	0.64
1:B:534:SER:OG	1:B:537:SER:HB2	1.98	0.64
1:B:790:LYS:HE3	1:B:791:TYR:CE1	2.32	0.64
1:C:881:GLU:HA	1:C:884:THR:OG1	1.98	0.64
1:D:326:ILE:O	1:D:330:ARG:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:TRP:CD1	1:B:708:TYR:HB3	2.33	0.64
2:E:13:DG:H2''	2:E:14:DC:H5'	1.78	0.64
1:C:412:LEU:HG	1:C:683:MET:HE3	1.77	0.64
1:A:347:MET:HG2	1:A:358:VAL:HG23	1.79	0.64
1:A:395:PHE:HB2	1:A:591:GLN:HG2	1.78	0.64
1:A:643:ASP:HA	1:A:693:LEU:HD23	1.79	0.64
1:D:504:HIS:C	1:D:506:PRO:HD3	2.22	0.64
1:A:708:TYR:CE2	1:A:728:MET:HG3	2.33	0.64
1:C:822:PRO:HD2	1:C:855:THR:OG1	1.98	0.64
1:C:27:ARG:HA	1:C:27:ARG:HE	1.62	0.64
2:E:11:DC:H2''	2:E:12:DA:H5'	1.79	0.64
3:H:112:DT:H6	3:H:112:DT:H5'	1.63	0.64
1:A:734:LYS:HB3	1:A:737:THR:OG1	1.98	0.63
1:D:182:ILE:O	1:D:186:ILE:HG13	1.98	0.63
1:B:386:HIS:HB2	1:B:573:VAL:HG22	1.79	0.63
1:D:491:ALA:O	1:D:495:ASN:ND2	2.31	0.63
1:D:837:GLU:OE1	1:D:837:GLU:HA	1.98	0.63
1:A:119:SER:HB2	1:A:131:HIS:CD2	2.32	0.63
1:B:512:GLU:N	1:B:513:PRO:HD3	2.14	0.63
1:A:60:LYS:HE3	5:A:966:HOH:O	1.98	0.63
1:A:602:ASN:HD21	1:A:617:VAL:H	1.46	0.63
1:B:486:LYS:HA	1:B:556:GLN:NE2	2.14	0.63
1:C:303:LEU:CG	1:C:326:ILE:HD12	2.28	0.63
3:J:110:DA:H2''	3:J:111:DT:C5'	2.27	0.63
1:A:203:ASN:O	1:A:207:GLN:HG2	1.98	0.63
1:A:362:ILE:CD1	1:A:572:ASN:HD22	2.10	0.63
1:A:554:THR:O	1:A:558:ASN:HB2	1.99	0.63
1:D:114:ASP:HB3	1:D:328:VAL:HG22	1.79	0.63
1:D:503:LEU:HD23	1:D:503:LEU:O	1.99	0.63
1:A:556:GLN:OE1	1:A:557:ILE:HG13	1.99	0.63
1:A:693:LEU:HD12	1:A:694:GLY:H	1.63	0.63
1:B:440:HIS:HB3	5:B:1007:HOH:O	1.98	0.63
1:A:221:PHE:O	1:A:224:PRO:HD2	1.99	0.62
1:A:641:PHE:HA	1:A:646:HIS:CD2	2.33	0.62
1:C:154:SER:C	1:C:156:TYR:H	2.05	0.62
1:C:686:GLU:OE1	1:C:716:GLU:HG2	1.99	0.62
1:D:478:VAL:HG13	1:D:559:ARG:HG3	1.80	0.62
1:A:68:ALA:O	1:A:72:ILE:HG13	1.98	0.62
1:B:494:ARG:HG3	1:B:495:ASN:N	2.14	0.62
1:A:744:ALA:HB2	1:A:767:PHE:CE2	2.34	0.62
1:D:255:ASN:HD22	1:D:256:MET:H	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:PHE:H	1:B:522:PHE:HD1	1.46	0.62
1:A:347:MET:HA	1:A:347:MET:HE3	1.82	0.62
1:B:403:ARG:NH1	1:B:887:ALA:O	2.33	0.62
1:C:298:LEU:O	1:C:299:ASN:HB2	1.98	0.62
1:D:144:ASP:O	1:D:185:LYS:HD3	2.00	0.62
1:D:422:GLN:HG3	1:D:678:GLN:O	2.00	0.62
1:A:362:ILE:HG12	1:A:572:ASN:ND2	2.15	0.62
1:D:61:LEU:HD23	1:D:62:PHE:N	2.15	0.62
1:D:805:ILE:HA	1:D:808:ILE:HD12	1.81	0.62
1:A:33:TYR:HB3	1:A:65:MET:HE2	1.81	0.62
1:B:727:ILE:HB	1:B:733:GLN:NE2	2.14	0.62
1:A:485:HIS:C	1:A:487:GLY:H	2.06	0.62
1:A:785:ALA:HB1	1:A:788:ILE:CD1	2.28	0.62
1:B:408:MET:HE1	1:B:655:ALA:HB2	1.82	0.62
1:B:166:ILE:H	1:B:166:ILE:CD1	2.12	0.62
1:B:752:MET:HG2	1:B:760:LEU:HD22	1.80	0.62
1:A:854:ILE:CD1	1:A:862:VAL:HG21	2.30	0.61
1:B:85:MET:HE3	1:B:86:ASP:N	2.15	0.61
1:B:489:MET:HE2	1:B:553:MET:SD	2.40	0.61
1:C:597:ILE:HD11	1:C:663:ILE:HG23	1.80	0.61
1:D:361:PRO:HD2	2:K:3:DC:O5'	2.00	0.61
1:A:707:ARG:NH2	1:A:731:GLU:OE1	2.34	0.61
1:C:148:VAL:HG21	1:C:325:ILE:HD11	1.82	0.61
3:F:108:DT:H2''	3:F:109:DC:O5'	2.01	0.61
1:A:642:ARG:HB2	1:A:642:ARG:HH11	1.65	0.61
1:B:166:ILE:HD12	1:B:166:ILE:N	2.13	0.61
1:C:46:ALA:O	1:C:47:THR:HG23	2.00	0.61
2:E:7:DA:H2'	2:E:8:DT:H72	1.82	0.61
1:D:412:LEU:HB2	1:D:623:ASP:HB2	1.83	0.61
1:D:511:ASP:HA	1:D:533:LEU:CD1	2.30	0.61
1:A:631:LYS:H	1:A:631:LYS:NZ	1.97	0.61
1:A:855:THR:HG23	1:A:858:ILE:HG12	1.83	0.61
1:B:818:ASN:HD21	1:B:857:LEU:HD12	1.66	0.61
2:E:18:DG:OP1	2:E:18:DG:H3'	2.01	0.61
1:C:231:LYS:HG3	1:C:236:GLU:CA	2.31	0.61
1:D:554:THR:O	1:D:558:ASN:HB2	2.01	0.61
1:B:749:ILE:O	1:B:753:LEU:HG	2.01	0.60
1:B:498:ILE:N	1:B:498:ILE:HD12	2.16	0.60
1:C:471:VAL:HB	1:C:472:PRO:HD3	1.83	0.60
1:B:109:ARG:NH2	1:B:208:LYS:HG2	2.16	0.60
1:B:668:ARG:O	1:B:672:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LYS:HG3	1:C:131:HIS:CE1	2.37	0.60
1:D:731:GLU:HA	1:D:734:LYS:HG2	1.82	0.60
1:D:804:HIS:O	1:D:808:ILE:HG13	2.02	0.60
1:A:685:ARG:NH2	1:A:714:ASP:OD2	2.34	0.60
1:B:821:ALA:HB1	1:B:822:PRO:HD2	1.82	0.60
3:F:113:DC:H2''	3:F:114:DA:H5''	1.83	0.60
1:B:182:ILE:O	1:B:186:ILE:HG13	2.02	0.60
1:B:777:ILE:CD1	1:B:853:GLU:HG2	2.32	0.60
1:C:149:PHE:O	1:C:197:LEU:HD11	2.00	0.60
1:D:328:VAL:O	1:D:332:LEU:HD13	2.01	0.60
1:D:757:GLU:O	1:D:761:GLN:HG3	2.01	0.60
1:A:478:VAL:HG13	1:A:559:ARG:HD2	1.84	0.60
1:C:180:SER:O	1:C:183:ILE:HG22	2.02	0.60
1:A:153:ASN:HB3	1:A:158:ASN:ND2	2.16	0.60
1:A:809:LEU:C	1:A:811:TYR:H	2.10	0.60
1:D:645:ASN:ND2	1:D:719:ARG:HH11	1.98	0.60
1:D:788:ILE:O	1:D:792:ASP:HB2	2.02	0.60
2:E:10:DA:C2'	2:E:11:DC:H5''	2.32	0.60
1:A:844:LYS:H	1:A:844:LYS:HD2	1.66	0.60
1:B:163:SER:HB3	1:B:166:ILE:HD13	1.83	0.60
1:B:179:PRO:HG2	1:B:329:TYR:CD2	2.36	0.60
1:B:233:ILE:HD12	1:B:233:ILE:N	2.17	0.60
1:B:408:MET:HE2	1:B:685:ARG:HD3	1.83	0.60
1:C:182:ILE:O	1:C:186:ILE:HG13	2.02	0.60
1:C:223:ILE:HB	1:C:224:PRO:HD3	1.84	0.60
1:C:455:SER:OG	1:C:676:ASN:HA	2.02	0.60
1:D:150:ASP:OD1	1:D:321:ILE:HD11	2.02	0.60
1:B:706:LYS:HD3	3:H:113:DC:H1'	1.83	0.59
1:B:808:ILE:HD13	1:B:824:VAL:HG11	1.82	0.59
1:B:858:ILE:O	1:B:862:VAL:HG23	2.01	0.59
1:C:109:ARG:HD2	1:C:209:THR:O	2.01	0.59
1:C:284:ASN:HD22	1:C:285:GLN:N	2.01	0.59
1:D:218:VAL:HA	1:D:222:ALA:HB3	1.84	0.59
1:A:255:ASN:HD22	1:A:257:TYR:HD1	1.49	0.59
1:B:403:ARG:HH22	1:B:889:LEU:HD21	1.66	0.59
1:C:130:LYS:HG3	1:C:131:HIS:ND1	2.17	0.59
2:I:10:DA:H1'	2:I:11:DC:H5''	1.84	0.59
1:B:508:LEU:HG	1:B:509:SER:H	1.67	0.59
1:A:771:PHE:HA	1:A:774:LEU:HD12	1.83	0.59
1:B:777:ILE:HD11	1:B:853:GLU:HG2	1.84	0.59
1:D:284:ASN:HD22	1:D:284:ASN:C	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:TYR:O	1:A:352:LYS:HE2	2.02	0.59
1:D:218:VAL:HG22	1:D:223:ILE:HG13	1.83	0.59
3:F:105:DC:H2''	3:F:106:DT:O5'	2.02	0.59
2:I:8:DT:H2'	2:I:9:DG:C8	2.36	0.59
1:A:641:PHE:HA	1:A:646:HIS:HD2	1.67	0.59
1:B:599:ARG:HG2	1:B:599:ARG:HH11	1.67	0.59
1:D:347:MET:HE2	1:D:558:ASN:HD21	1.67	0.59
2:E:10:DA:H2''	2:E:11:DC:H5'	1.84	0.59
1:C:482:ARG:NH1	1:C:556:GLN:NE2	2.41	0.59
1:D:305:TYR:OH	1:D:309:ILE:HG12	2.02	0.59
2:E:2:DG:H3'	2:E:3:DC:C5'	2.32	0.59
3:J:102:DC:H2''	3:J:103:DG:OP2	2.01	0.59
1:C:461:MET:SD	1:C:581:ARG:HD2	2.43	0.59
1:B:878:LYS:HD3	1:B:878:LYS:C	2.27	0.59
1:D:71:TRP:O	1:D:75:MET:HG2	2.03	0.59
1:D:197:LEU:O	1:D:197:LEU:HD23	2.03	0.59
1:D:797:PRO:HG3	1:D:806:ARG:HH11	1.68	0.59
1:C:38:PHE:CZ	1:C:59:ARG:HG3	2.38	0.58
1:C:285:GLN:HE21	1:C:286:PRO:CD	2.15	0.58
1:C:658:ARG:NH1	5:C:978:HOH:O	2.35	0.58
1:D:807:GLY:HA2	1:D:845:CYS:O	2.03	0.58
1:D:862:VAL:O	1:D:866:MET:HB3	2.03	0.58
1:B:504:HIS:C	1:B:506:PRO:HD3	2.28	0.58
1:B:786:ASN:O	1:B:826:GLU:OE1	2.22	0.58
1:C:657:GLU:C	1:C:658:ARG:HD2	2.29	0.58
1:C:818:ASN:ND2	1:C:857:LEU:HD11	2.19	0.58
1:A:876:PHE:O	1:A:879:PRO:HG2	2.03	0.58
1:D:80:LEU:HD22	1:D:80:LEU:N	2.14	0.58
1:D:495:ASN:HD21	1:D:521:ASP:CA	2.08	0.58
1:D:760:LEU:HD23	1:D:760:LEU:C	2.29	0.58
3:H:105:DC:H2'	3:H:106:DT:H71	1.83	0.58
3:J:113:DC:H5'	3:J:113:DC:H6	1.68	0.58
1:A:778:SER:C	1:A:779:ILE:HD13	2.28	0.58
1:B:71:TRP:HE1	1:B:75:MET:HE3	1.68	0.58
1:B:728:MET:HA	1:B:728:MET:HE3	1.86	0.58
1:C:572:ASN:HD22	1:C:574:TRP:N	1.98	0.58
1:D:509:SER:CB	1:D:532:LYS:O	2.48	0.58
2:I:7:DA:C2'	2:I:8:DT:H72	2.33	0.58
1:A:169:LYS:HE2	1:A:173:GLN:HB3	1.85	0.58
1:A:433:THR:HG22	1:A:461:MET:HE1	1.86	0.58
1:C:587:THR:HG22	1:C:588:THR:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:GLU:OE2	1:D:337:LYS:HE3	2.03	0.58
1:B:894:LYS:HB2	1:B:894:LYS:HZ3	1.67	0.58
2:I:6:DA:H2''	2:I:7:DA:C5'	2.33	0.58
1:D:605:LEU:HD22	1:D:632:ILE:HD11	1.86	0.58
2:E:4:CTG:H2''	2:E:5:DG:OP2	2.04	0.58
1:A:470:VAL:O	1:A:474:GLU:HG2	2.04	0.58
1:C:686:GLU:HG3	1:C:715:MET:HE3	1.84	0.57
1:C:818:ASN:ND2	1:C:821:ALA:HB2	2.18	0.57
1:D:159:VAL:HB	1:D:317:HIS:CD2	2.39	0.57
1:D:529:LYS:HB3	1:D:532:LYS:HD2	1.86	0.57
1:D:700:GLY:N	1:D:753:LEU:HD22	2.19	0.57
1:D:884:THR:HG21	1:D:891:TYR:HD1	1.69	0.57
1:A:285:GLN:HA	1:A:285:GLN:HE21	1.68	0.57
1:B:231:LYS:CG	1:B:236:GLU:HA	2.34	0.57
1:C:85:MET:HA	1:C:380:ILE:HD11	1.85	0.57
1:C:297:GLU:OE1	1:C:338:ARG:NH1	2.37	0.57
1:C:392:PRO:C	1:C:587:THR:HG21	2.28	0.57
1:B:772:ARG:HG2	1:B:772:ARG:HH11	1.68	0.57
1:D:416:TYR:HB2	1:D:417:PRO:HD3	1.86	0.57
1:D:458:PRO:HB2	1:D:588:THR:HG22	1.85	0.57
1:A:129:ALA:HA	1:A:225:TYR:CE1	2.40	0.57
1:A:819:ILE:HG13	1:A:823:GLN:OE1	2.05	0.57
1:A:873:GLU:OE2	1:A:877:ILE:HD12	2.04	0.57
1:C:477:LYS:HG2	1:C:481:GLN:NE2	2.20	0.57
1:C:503:LEU:HD21	1:C:538:LEU:HB2	1.86	0.57
1:C:658:ARG:HH11	1:C:658:ARG:HG3	1.70	0.57
1:D:653:LYS:HE3	1:D:657:GLU:OE1	2.05	0.57
1:B:60:LYS:HE3	1:B:62:PHE:CE2	2.40	0.57
1:B:71:TRP:NE1	1:B:75:MET:HE3	2.18	0.57
1:B:751:ARG:HH11	1:B:759:SER:HB3	1.69	0.57
1:C:83:LEU:HD22	1:C:83:LEU:N	2.19	0.57
1:A:51:ASP:HB2	5:A:915:HOH:O	2.05	0.57
1:A:112:ASN:HD21	1:A:331:VAL:CG1	2.18	0.57
1:A:338:ARG:HB3	1:A:340:PHE:CE1	2.39	0.57
1:D:253:ILE:HD11	1:D:262:ILE:HD13	1.87	0.57
1:D:751:ARG:NH1	1:D:763:TYR:HB2	2.20	0.57
1:A:732:THR:CG2	1:A:745:LEU:HB3	2.35	0.57
1:B:120:PRO:HG2	1:B:156:TYR:CE2	2.40	0.57
1:C:835:LEU:HD11	1:C:846:ILE:HB	1.85	0.57
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.86	0.57
1:A:506:PRO:HB2	1:A:535:ALA:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:747:GLU:O	1:D:751:ARG:HG3	2.05	0.57
1:A:542:LEU:O	1:A:546:GLN:HG2	2.05	0.57
1:A:777:ILE:HD11	1:A:848:TRP:HZ2	1.70	0.57
1:A:806:ARG:HD3	1:A:844:LYS:HE3	1.87	0.57
1:B:309:ILE:CA	1:B:312:LEU:HB2	2.20	0.57
1:B:811:TYR:OH	1:B:822:PRO:HG2	2.04	0.57
1:A:213:LEU:HD13	1:A:223:ILE:HD11	1.85	0.57
1:A:227:TYR:CD2	1:A:263:ILE:HD13	2.40	0.57
1:A:598:GLU:HG3	1:A:617:VAL:HG11	1.85	0.57
1:A:362:ILE:CG1	1:A:572:ASN:HD22	2.19	0.56
1:D:83:LEU:HB3	1:D:379:VAL:HG12	1.86	0.56
2:E:7:DA:C2'	2:E:8:DT:H72	2.35	0.56
1:A:85:MET:HE1	1:A:366:ASP:OD2	2.05	0.56
1:A:139:TYR:CD2	1:A:332:LEU:HD21	2.40	0.56
1:A:231:LYS:HG3	1:A:236:GLU:CA	2.35	0.56
1:A:808:ILE:O	1:A:811:TYR:HB3	2.04	0.56
1:A:839:ASN:HD22	1:A:841:PHE:HB2	1.70	0.56
1:D:186:ILE:HG22	1:D:187:ILE:N	2.20	0.56
1:D:469:GLY:C	1:D:472:PRO:HD2	2.30	0.56
3:H:113:DC:C2'	3:H:114:DA:H5''	2.35	0.56
1:A:499:ILE:HB	1:A:542:LEU:HD13	1.87	0.56
1:B:421:ARG:HG2	1:B:421:ARG:HH11	1.70	0.56
1:C:81:GLU:HG2	1:C:83:LEU:HD22	1.87	0.56
1:C:162:TRP:HB3	1:C:188:TYR:CE1	2.41	0.56
1:C:855:THR:HG22	1:C:857:LEU:N	2.13	0.56
1:D:162:TRP:CD1	1:D:321:ILE:HB	2.40	0.56
1:D:786:ASN:O	1:D:787:ASN:HB2	2.05	0.56
2:G:16:DG:H2''	2:G:17:DC:H5''	1.87	0.56
2:I:8:DT:H6	2:I:8:DT:H5''	1.70	0.56
1:A:732:THR:HG22	1:A:745:LEU:HB3	1.86	0.56
1:C:130:LYS:HE3	1:C:131:HIS:HE1	1.71	0.56
1:C:285:GLN:HE21	1:C:286:PRO:HD2	1.70	0.56
1:C:768:GLU:HG2	1:C:872:LEU:HD21	1.88	0.56
1:D:713:TRP:CZ3	1:D:723:PRO:HD3	2.40	0.56
1:C:55:LYS:N	1:C:55:LYS:HD2	2.18	0.56
1:D:39:ALA:O	1:D:58:THR:HG22	2.05	0.56
1:D:202:LEU:O	1:D:205:TRP:HB3	2.06	0.56
1:D:795:GLY:O	1:D:813:ARG:NH1	2.38	0.56
1:B:271:LEU:HB3	1:B:276:LEU:HD11	1.87	0.56
1:B:486:LYS:HA	1:B:556:GLN:HE22	1.70	0.56
1:D:303:LEU:CG	1:D:326:ILE:HD12	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ALA:HB1	1:A:559:ARG:NH1	2.20	0.56
1:B:498:ILE:HD12	1:B:498:ILE:H	1.69	0.56
1:B:818:ASN:HD21	1:B:857:LEU:HD13	1.70	0.56
1:D:3:GLU:HB2	1:D:20:ILE:O	2.06	0.56
1:D:348:GLY:O	1:D:352:LYS:N	2.38	0.56
1:D:597:ILE:O	1:D:601:VAL:HG23	2.03	0.56
1:A:643:ASP:HB2	5:A:923:HOH:O	2.05	0.56
1:A:811:TYR:HE1	1:A:858:ILE:HD11	1.69	0.56
1:B:446:VAL:HG22	1:B:446:VAL:O	2.06	0.56
1:B:458:PRO:HG3	1:B:592:MET:SD	2.46	0.56
1:B:523:SER:O	1:B:526:ILE:HG12	2.06	0.56
1:C:238:THR:O	1:C:241:ARG:HB2	2.06	0.56
1:C:524:ASP:HA	1:C:527:LYS:CE	2.35	0.56
1:D:347:MET:HE1	1:D:562:LEU:HD22	1.87	0.56
1:D:402:ASN:OD1	1:D:403:ARG:N	2.32	0.56
1:D:412:LEU:HD12	1:D:623:ASP:HA	1.87	0.56
1:D:686:GLU:OE1	1:D:686:GLU:HA	2.05	0.56
1:B:494:ARG:NH1	1:B:495:ASN:HB2	2.21	0.56
1:B:808:ILE:HG22	1:B:812:ASN:ND2	2.20	0.56
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.88	0.55
1:A:643:ASP:CA	1:A:693:LEU:HD23	2.36	0.55
1:C:143:ASP:OD2	1:C:208:LYS:NZ	2.39	0.55
1:D:715:MET:HE3	1:D:716:GLU:CG	2.36	0.55
1:A:34:LYS:HD2	1:A:63:ALA:O	2.07	0.55
1:A:49:TYR:CE1	1:A:59:ARG:HD3	2.40	0.55
1:B:767:PHE:HE1	1:B:774:LEU:HD11	1.72	0.55
1:C:254:GLU:HA	1:C:259:SER:HA	1.87	0.55
1:D:359:PHE:O	1:D:361:PRO:HD3	2.07	0.55
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.88	0.55
1:D:644:THR:O	1:D:648:VAL:HG23	2.07	0.55
1:A:241:ARG:NH1	5:A:985:HOH:O	2.38	0.55
1:A:397:LYS:O	1:A:399:PRO:HD3	2.06	0.55
1:A:503:LEU:N	1:A:503:LEU:HD23	2.20	0.55
1:A:555:ALA:O	1:A:559:ARG:HG2	2.06	0.55
1:A:656:ARG:HA	1:A:660:GLU:HG3	1.87	0.55
1:B:406:TYR:HB3	1:B:629:ALA:HB3	1.89	0.55
1:C:6:LEU:HB2	1:C:18:ARG:O	2.06	0.55
2:G:15:DC:H6	2:G:15:DC:H5'	1.70	0.55
1:B:745:LEU:HD22	1:B:883:PHE:HE2	1.71	0.55
1:C:118:THR:HG23	1:C:310:SER:O	2.07	0.55
1:C:351:ALA:O	1:C:352:LYS:HB2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ARG:HB3	1:A:340:PHE:CD1	2.42	0.55
1:D:212:ILE:HD13	1:D:269:SER:HB2	1.87	0.55
1:D:486:LYS:O	1:D:490:LEU:HD13	2.06	0.55
1:D:512:GLU:CB	1:D:513:PRO:HA	2.37	0.55
3:H:104:DG:H1'	3:H:105:DC:H5''	1.89	0.55
3:J:113:DC:H5'	3:J:113:DC:C6	2.41	0.55
1:A:212:ILE:HD13	1:A:269:SER:HB2	1.88	0.55
1:A:536:LYS:C	1:A:536:LYS:HD3	2.31	0.55
1:B:494:ARG:HG3	1:B:494:ARG:HH11	1.71	0.55
1:C:600:LYS:HD2	5:C:921:HOH:O	2.06	0.55
1:D:411:ASP:HB2	1:D:686:GLU:OE2	2.05	0.55
1:D:489:MET:SD	1:D:553:MET:HA	2.46	0.55
3:F:109:DC:H2''	3:F:110:DA:C5'	2.37	0.55
1:A:810:THR:HG21	1:A:845:CYS:O	2.06	0.55
1:B:541:MET:O	1:B:544:ARG:HB2	2.06	0.55
1:B:748:CYS:O	1:B:752:MET:HG3	2.06	0.55
1:C:686:GLU:OE1	1:C:716:GLU:CG	2.55	0.55
1:A:433:THR:HG22	1:A:461:MET:CE	2.37	0.55
1:A:517:ASP:OD1	1:A:519:ARG:HD3	2.07	0.55
1:B:485:HIS:HA	1:B:488:TYR:CD2	2.42	0.55
1:B:825:VAL:CB	1:B:828:GLU:HG3	2.34	0.55
1:B:846:ILE:HD11	1:B:858:ILE:HD12	1.88	0.55
2:K:6:DA:H2''	2:K:7:DA:O5'	2.07	0.55
1:A:162:TRP:HB3	1:A:188:TYR:CE1	2.41	0.55
1:C:825:VAL:HB	1:C:828:GLU:CD	2.32	0.55
1:A:668:ARG:O	1:A:672:GLU:HG3	2.06	0.55
1:A:775:ASN:HB3	1:A:778:SER:OG	2.07	0.55
1:B:361:PRO:HD2	2:G:3:DC:H5''	1.89	0.55
1:B:405:LYS:HA	1:B:698:ILE:O	2.07	0.55
1:B:732:THR:CG2	1:B:733:GLN:HE21	2.20	0.55
1:C:495:ASN:HB3	1:C:522:PHE:CE2	2.42	0.55
1:D:752:MET:HG2	1:D:760:LEU:HD12	1.89	0.55
1:C:73:LYS:HB3	1:C:73:LYS:HZ3	1.72	0.54
2:I:7:DA:H2''	2:I:8:DT:OP2	2.07	0.54
1:A:116:GLU:HB2	1:A:135:ALA:HB3	1.89	0.54
1:A:730:LEU:HD22	1:A:883:PHE:CE1	2.42	0.54
1:B:117:VAL:HG21	1:B:225:TYR:CE2	2.43	0.54
1:B:197:LEU:HD23	1:B:197:LEU:C	2.32	0.54
1:B:222:ALA:O	1:B:226:VAL:HG23	2.07	0.54
1:B:604:TYR:O	1:B:607:GLU:HB3	2.07	0.54
3:L:105:DC:H2'	3:L:106:DT:H72	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASP:OD1	1:A:686:GLU:HG3	2.07	0.54
1:B:255:ASN:HD21	1:B:257:TYR:HD1	1.54	0.54
2:G:14:DC:H2''	2:G:15:DC:H5''	1.89	0.54
2:I:12:DA:H5''	2:I:12:DA:H8	1.73	0.54
3:J:105:DC:H2'	3:J:106:DT:C7	2.35	0.54
1:A:703:THR:HG21	1:A:707:ARG:HH11	1.72	0.54
1:D:6:LEU:HB2	1:D:18:ARG:O	2.07	0.54
1:D:541:MET:CA	1:D:544:ARG:HD3	2.30	0.54
1:B:148:VAL:HG21	1:B:325:ILE:HD11	1.90	0.54
1:C:111:ALA:CB	1:C:210:PRO:HB3	2.38	0.54
3:H:104:DG:C2'	3:H:105:DC:H5''	2.38	0.54
1:A:75:MET:HE3	1:A:80:LEU:O	2.07	0.54
1:A:449:ARG:NH1	1:A:452:ASP:HB3	2.20	0.54
1:A:499:ILE:HD11	1:A:522:PHE:CZ	2.43	0.54
1:B:268:ILE:HG22	1:B:269:SER:N	2.23	0.54
1:B:351:ALA:O	1:B:352:LYS:HB2	2.07	0.54
1:C:393:GLY:O	1:C:587:THR:HG23	2.06	0.54
1:D:109:ARG:HD3	1:D:208:LYS:O	2.07	0.54
1:A:109:ARG:HD2	1:A:209:THR:O	2.08	0.54
1:A:253:ILE:C	1:A:253:ILE:HD12	2.33	0.54
1:A:850:SER:O	1:A:852:THR:HG23	2.08	0.54
1:C:112:ASN:HB2	5:C:1035:HOH:O	2.07	0.54
1:D:541:MET:O	1:D:544:ARG:N	2.38	0.54
2:G:16:DG:H2''	2:G:17:DC:H5'	1.90	0.54
3:H:104:DG:H2''	3:H:105:DC:C5'	2.38	0.54
3:L:113:DC:H2'	3:L:114:DA:C8	2.42	0.54
1:B:421:ARG:HD2	1:B:476:THR:OG1	2.08	0.54
1:B:685:ARG:HG2	1:B:685:ARG:HH11	1.72	0.54
1:C:162:TRP:HB3	1:C:188:TYR:CZ	2.43	0.54
1:D:347:MET:SD	1:D:562:LEU:HD21	2.47	0.54
1:B:218:VAL:HA	1:B:222:ALA:HB3	1.90	0.54
1:B:322:SER:O	1:B:326:ILE:HG12	2.08	0.54
1:B:330:ARG:O	1:B:334:ILE:HG13	2.08	0.54
1:B:422:GLN:HG3	1:B:678:GLN:O	2.08	0.54
1:C:660:GLU:CB	1:C:661:PRO:HD3	2.35	0.54
1:D:9:GLU:CG	1:D:267:GLY:H	2.21	0.54
1:B:9:GLU:HG2	1:B:266:PHE:HD2	1.73	0.53
1:B:152:LEU:HD11	1:B:190:PRO:HB2	1.90	0.53
1:B:221:PHE:C	1:B:224:PRO:HD2	2.33	0.53
1:C:150:ASP:OD1	1:C:151:LEU:N	2.41	0.53
1:C:239:ALA:C	1:C:241:ARG:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLU:OE1	1:A:97:TYR:OH	2.20	0.53
1:A:362:ILE:HG12	1:A:572:ASN:HD22	1.74	0.53
1:A:642:ARG:HH11	1:A:642:ARG:CB	2.21	0.53
1:B:13:ASP:CG	1:B:66:ARG:HE	2.15	0.53
1:B:475:ILE:C	1:B:475:ILE:HD13	2.33	0.53
1:B:776:TYR:HB2	1:B:866:MET:HE1	1.90	0.53
1:C:506:PRO:HB3	1:C:535:ALA:HB2	1.90	0.53
1:D:731:GLU:HA	1:D:734:LYS:HG3	1.90	0.53
1:A:353:ILE:HB	5:A:973:HOH:O	2.08	0.53
1:A:800:LYS:O	1:A:802:PRO:HD3	2.09	0.53
1:B:317:HIS:O	1:B:320:TYR:HB3	2.08	0.53
1:B:597:ILE:O	1:B:601:VAL:HG23	2.08	0.53
1:C:169:LYS:O	1:C:175:GLY:HA3	2.08	0.53
1:C:440:HIS:CE1	1:C:444:ASN:HD22	2.26	0.53
2:E:13:DG:H1	3:F:105:DC:H42	1.55	0.53
1:B:472:PRO:O	1:B:475:ILE:HG22	2.08	0.53
1:C:411:ASP:HB2	1:C:686:GLU:OE2	2.07	0.53
1:A:774:LEU:HB3	5:A:1004:HOH:O	2.08	0.53
1:D:546:GLN:O	1:D:549:GLU:HG2	2.09	0.53
2:E:13:DG:H2''	2:E:14:DC:H5''	1.89	0.53
1:A:449:ARG:HH12	1:A:452:ASP:CB	2.21	0.53
1:A:867:ASP:O	1:A:871:LEU:HB2	2.08	0.53
1:D:423:VAL:HB	1:D:425:ILE:HG13	1.91	0.53
1:A:496:GLY:HA2	1:A:542:LEU:HD11	1.91	0.53
1:A:530:ILE:HA	1:A:533:LEU:HD12	1.90	0.53
1:B:170:LEU:N	1:B:170:LEU:HD12	2.23	0.53
1:C:516:VAL:HG11	1:C:526:ILE:HD13	1.90	0.53
1:D:209:THR:HG21	1:D:244:PRO:HB3	1.91	0.53
1:D:485:HIS:HA	1:D:488:TYR:HB2	1.91	0.53
1:B:60:LYS:HE3	1:B:62:PHE:CZ	2.43	0.53
1:B:285:GLN:HG3	1:B:292:TYR:HE2	1.74	0.53
1:C:254:GLU:HG3	1:C:258:GLY:O	2.09	0.53
1:C:579:ASP:HB3	1:C:582:ASN:HB2	1.90	0.53
1:D:812:ASN:O	1:D:815:ILE:HG12	2.08	0.53
3:L:108:DT:H2''	3:L:109:DC:O5'	2.09	0.53
1:A:481:GLN:O	1:A:484:GLU:HB3	2.09	0.53
1:A:734:LYS:HG2	1:A:736:SER:HG	1.74	0.53
1:B:599:ARG:O	1:B:603:GLU:HG3	2.09	0.53
1:C:283:THR:HG23	5:C:961:HOH:O	2.08	0.53
1:D:74:ARG:HA	1:D:77:ASP:OD2	2.09	0.53
1:D:114:ASP:HB3	1:D:328:VAL:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:656:ARG:HA	1:D:660:GLU:HG2	1.91	0.53
1:A:833:LEU:CD2	1:A:866:MET:HB2	2.27	0.53
1:B:191:PHE:CZ	1:B:200:GLU:HG2	2.44	0.53
1:B:529:LYS:O	1:B:533:LEU:HD22	2.08	0.52
1:C:605:LEU:HA	1:C:608:VAL:HG22	1.92	0.52
1:D:426:SER:OG	1:D:427:PRO:HD2	2.09	0.52
1:D:738:PRO:HG2	1:D:741:VAL:CB	2.38	0.52
1:A:304:LYS:HA	1:A:304:LYS:HE3	1.91	0.52
1:A:779:ILE:HG21	1:A:871:LEU:HG	1.90	0.52
1:A:806:ARG:CD	1:A:844:LYS:HE3	2.39	0.52
1:C:83:LEU:HB3	1:C:379:VAL:HG12	1.90	0.52
1:C:297:GLU:O	1:C:337:LYS:HE2	2.09	0.52
1:D:38:PHE:CZ	1:D:59:ARG:HG3	2.44	0.52
1:A:129:ALA:HA	1:A:225:TYR:CZ	2.45	0.52
1:B:85:MET:HE3	1:B:85:MET:HA	1.91	0.52
1:B:475:ILE:HD13	1:B:475:ILE:O	2.09	0.52
1:B:654:PHE:O	1:B:658:ARG:HB2	2.10	0.52
2:G:6:DA:H2''	2:G:7:DA:H5''	1.91	0.52
3:H:104:DG:H2''	3:H:105:DC:H5''	1.91	0.52
1:A:49:TYR:O	1:A:57:CYS:N	2.40	0.52
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.44	0.52
1:B:685:ARG:NH2	1:B:714:ASP:OD1	2.41	0.52
1:B:727:ILE:HG21	1:B:732:THR:HG21	1.92	0.52
1:C:514:LEU:HB3	1:C:541:MET:CE	2.39	0.52
1:D:286:PRO:HG2	1:D:739:LYS:NZ	2.24	0.52
1:D:516:VAL:HG11	1:D:522:PHE:CE1	2.33	0.52
1:D:592:MET:SD	1:D:670:MET:HE3	2.50	0.52
1:D:745:LEU:O	1:D:749:ILE:HG13	2.10	0.52
3:F:108:DT:H4'	5:F:137:HOH:O	2.08	0.52
2:I:7:DA:H2'	2:I:8:DT:H72	1.91	0.52
1:B:253:ILE:HD12	1:B:254:GLU:H	1.75	0.52
1:C:785:ALA:HB1	1:C:788:ILE:HD11	1.91	0.52
1:D:123:PHE:CD1	1:D:124:PRO:HD2	2.44	0.52
1:D:734:LYS:HB2	1:D:737:THR:OG1	2.09	0.52
3:H:101:DG:H2''	3:H:102:DC:OP2	2.08	0.52
1:B:197:LEU:HD23	1:B:198:LEU:N	2.25	0.52
1:B:752:MET:HE3	1:B:889:LEU:HD12	1.91	0.52
1:D:52:ILE:HB	1:D:428:GLU:HG2	1.92	0.52
1:D:757:GLU:HB2	1:D:889:LEU:HD22	1.91	0.52
1:D:277:TYR:O	1:D:281:SER:HB2	2.09	0.52
1:D:536:LYS:O	1:D:536:LYS:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:SER:O	1:A:298:LEU:HD12	2.09	0.52
1:B:320:TYR:O	1:B:323:TYR:HB3	2.09	0.52
1:B:599:ARG:HG2	1:B:599:ARG:NH1	2.24	0.52
1:D:750:ARG:HG3	1:D:754:GLN:NE2	2.24	0.52
1:A:8:VAL:C	1:A:9:GLU:HG2	2.35	0.52
1:A:52:ILE:HG13	1:A:53:TYR:CD1	2.45	0.52
1:A:112:ASN:HD21	1:A:331:VAL:HG11	1.74	0.52
1:D:204:PHE:CE1	1:D:208:LYS:HG3	2.45	0.52
1:D:254:GLU:HG3	1:D:259:SER:HB2	1.92	0.52
1:A:877:ILE:O	1:A:878:LYS:C	2.51	0.52
1:B:799:PRO:O	1:B:800:LYS:HB2	2.10	0.52
1:C:477:LYS:HG2	1:C:481:GLN:HE21	1.74	0.52
1:D:519:ARG:HH11	1:D:519:ARG:HG3	1.75	0.52
1:B:486:LYS:O	1:B:490:LEU:HB2	2.10	0.51
1:B:884:THR:HB	1:B:889:LEU:O	2.10	0.51
1:D:496:GLY:HA2	1:D:545:ALA:CB	2.41	0.51
1:B:300:VAL:O	1:B:300:VAL:HG13	2.11	0.51
1:C:233:ILE:O	1:C:233:ILE:HG22	2.10	0.51
1:D:218:VAL:HG23	1:D:222:ALA:HB3	1.92	0.51
1:D:699:GLY:C	1:D:753:LEU:HD22	2.35	0.51
1:D:807:GLY:C	1:D:847:ALA:H	2.17	0.51
1:A:61:LEU:HD23	1:A:61:LEU:C	2.36	0.51
1:A:214:THR:OG1	1:A:215:GLY:N	2.42	0.51
1:B:9:GLU:HG3	5:B:928:HOH:O	2.10	0.51
1:C:138:HIS:C	1:C:138:HIS:CD2	2.88	0.51
1:C:241:ARG:HA	1:C:246:ARG:HD3	1.92	0.51
1:D:112:ASN:ND2	1:D:214:THR:HG23	2.26	0.51
1:D:125:GLU:HG3	1:D:127:SER:H	1.75	0.51
1:D:255:ASN:ND2	1:D:256:MET:N	2.55	0.51
1:D:451:SER:HB3	1:D:456:CYS:SG	2.50	0.51
1:A:362:ILE:HB	2:E:3:DC:OP1	2.10	0.51
1:B:247:LYS:HE3	1:B:266:PHE:CZ	2.45	0.51
1:B:303:LEU:HD12	1:B:323:TYR:CA	2.35	0.51
1:C:283:THR:HG21	5:C:1042:HOH:O	2.10	0.51
1:B:706:LYS:HE2	3:H:113:DC:O2	2.11	0.51
1:C:176:ASP:O	1:C:303:LEU:HD21	2.10	0.51
1:C:362:ILE:HG23	1:C:575:PHE:HD1	1.75	0.51
1:D:399:PRO:O	1:D:401:PRO:HD3	2.10	0.51
1:D:411:ASP:O	1:D:683:MET:HA	2.10	0.51
1:D:461:MET:CE	1:D:581:ARG:HD2	2.40	0.51
1:D:557:ILE:HG22	1:D:558:ASN:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:ASN:HB2	5:A:972:HOH:O	2.11	0.51
1:D:884:THR:HG21	1:D:891:TYR:CD1	2.45	0.51
1:A:743:LYS:O	1:A:746:LYS:HB3	2.11	0.51
1:B:180:SER:O	1:B:183:ILE:HG22	2.11	0.51
1:D:18:ARG:NH2	1:D:211:VAL:HA	2.26	0.51
1:D:255:ASN:O	1:D:256:MET:C	2.52	0.51
1:D:260:ARG:HG2	1:D:261:GLU:H	1.74	0.51
3:L:108:DT:H2''	3:L:109:DC:C5'	2.41	0.51
1:A:771:PHE:O	1:A:774:LEU:HB2	2.11	0.51
1:D:52:ILE:HD12	1:D:428:GLU:HG3	1.93	0.51
1:D:616:PHE:HB3	1:D:627:VAL:HG13	1.93	0.51
1:D:835:LEU:HB3	1:D:839:ASN:ND2	2.25	0.51
1:A:35:PRO:HG3	1:A:65:MET:HA	1.93	0.51
1:A:241:ARG:HG3	1:A:241:ARG:NH1	2.23	0.51
1:A:544:ARG:NH1	1:A:544:ARG:HG3	2.26	0.51
1:D:111:ALA:CB	1:D:210:PRO:HB3	2.38	0.51
1:D:406:TYR:CE2	1:D:691:PRO:HD2	2.46	0.51
1:D:500:LYS:O	1:D:503:LEU:HB3	2.11	0.51
1:A:21:ASP:OD2	1:A:21:ASP:C	2.54	0.51
1:A:819:ILE:HG12	1:A:819:ILE:O	2.11	0.51
1:B:312:LEU:HD13	1:B:312:LEU:O	2.11	0.51
1:B:557:ILE:HG22	5:B:945:HOH:O	2.09	0.51
1:C:154:SER:C	1:C:156:TYR:N	2.68	0.51
2:I:6:DA:H1'	2:I:7:DA:H5''	1.93	0.51
1:C:121:ASP:HA	1:C:819:ILE:HG12	1.91	0.50
1:C:284:ASN:HD22	1:C:284:ASN:C	2.19	0.50
1:D:685:ARG:HD2	1:D:685:ARG:C	2.36	0.50
1:D:738:PRO:HG2	1:D:741:VAL:CG2	2.41	0.50
1:A:514:LEU:HG	1:A:526:ILE:HD12	1.93	0.50
1:B:102:LYS:HD3	1:B:103:TYR:N	2.26	0.50
1:B:202:LEU:O	1:B:206:GLN:HG2	2.11	0.50
1:B:421:ARG:HB3	1:B:680:LEU:HD12	1.92	0.50
1:B:485:HIS:CD2	1:B:555:ALA:HB1	2.46	0.50
1:B:785:ALA:HB2	1:B:808:ILE:HD11	1.93	0.50
1:B:884:THR:O	1:B:888:LYS:N	2.44	0.50
1:C:370:PHE:C	1:C:370:PHE:CD2	2.88	0.50
1:D:834:PRO:HG3	1:D:871:LEU:HB2	1.93	0.50
2:G:16:DG:C2'	2:G:17:DC:H5''	2.41	0.50
1:A:833:LEU:HD23	1:A:834:PRO:O	2.12	0.50
1:B:179:PRO:HB2	1:B:182:ILE:HG12	1.93	0.50
1:C:381:PRO:HG3	5:C:1070:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:LEU:HD11	1:A:750:ARG:HB2	1.93	0.50
1:A:855:THR:C	1:A:857:LEU:H	2.19	0.50
1:B:25:ARG:HG2	1:B:25:ARG:HH11	1.75	0.50
1:B:231:LYS:HG2	1:B:236:GLU:HA	1.93	0.50
1:B:377:ASN:HD22	1:B:377:ASN:N	2.09	0.50
1:D:222:ALA:O	1:D:226:VAL:HG23	2.12	0.50
1:D:416:TYR:O	1:D:420:ILE:HG13	2.12	0.50
1:A:654:PHE:CD1	1:A:659:MET:HE2	2.47	0.50
1:D:275:ASP:O	1:D:279:LYS:HB2	2.12	0.50
1:D:413:THR:O	1:D:414:SER:C	2.53	0.50
1:A:310:SER:C	1:A:311:LYS:HD3	2.36	0.50
1:B:435:LYS:HD3	1:B:435:LYS:H	1.76	0.50
1:C:254:GLU:HG3	1:C:259:SER:HB2	1.92	0.50
1:D:146:PHE:CE1	1:D:182:ILE:HB	2.47	0.50
1:A:485:HIS:C	1:A:487:GLY:N	2.67	0.50
1:B:170:LEU:HD12	1:B:170:LEU:H	1.77	0.50
1:D:97:TYR:O	1:D:99:TYR:N	2.45	0.50
1:D:483:LYS:NZ	1:D:483:LYS:HB3	2.27	0.50
1:A:447:ALA:O	1:A:448:GLU:C	2.55	0.50
1:A:795:GLY:C	1:A:809:LEU:HD13	2.36	0.50
1:B:494:ARG:HG3	1:B:495:ASN:H	1.76	0.50
1:B:614:GLU:HB3	1:B:616:PHE:CE1	2.46	0.50
1:D:793:VAL:C	1:D:795:GLY:H	2.20	0.50
2:G:3:DC:H2"	2:G:4:CTG:OP2	2.12	0.50
1:A:63:ALA:HB3	1:A:67:ASP:OD1	2.11	0.50
1:A:213:LEU:CD1	1:A:223:ILE:HD11	2.42	0.50
1:B:194:GLU:O	1:B:197:LEU:N	2.45	0.50
1:C:92:TYR:CD1	1:C:92:TYR:C	2.90	0.50
1:C:176:ASP:O	1:C:177:GLU:HB2	2.10	0.50
1:C:530:ILE:O	1:C:533:LEU:HB2	2.12	0.50
1:D:454:TYR:HB2	1:D:462:MET:HG2	1.93	0.50
1:A:780:ALA:HB3	1:A:831:TYR:CD1	2.41	0.49
1:B:403:ARG:HH22	1:B:889:LEU:CD2	2.25	0.49
1:B:433:THR:O	1:B:462:MET:HE2	2.11	0.49
1:C:171:GLN:C	1:C:173:GLN:H	2.20	0.49
1:C:394:ALA:HB1	1:C:622:THR:HA	1.94	0.49
1:D:461:MET:HE3	1:D:581:ARG:HD2	1.93	0.49
1:B:51:ASP:C	1:B:51:ASP:OD1	2.54	0.49
1:B:129:ALA:HA	1:B:225:TYR:CE1	2.48	0.49
1:C:403:ARG:NH2	1:C:889:LEU:CD2	2.74	0.49
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:GLU:HG3	1:D:267:GLY:H	1.77	0.49
1:D:20:ILE:HD13	1:D:107:LYS:CB	2.42	0.49
1:D:355:ILE:O	1:D:358:VAL:HG13	2.12	0.49
2:G:6:DA:H1'	2:G:7:DA:H5''	1.94	0.49
1:A:34:LYS:HG2	1:A:61:LEU:HD21	1.94	0.49
1:A:73:LYS:HE3	1:A:73:LYS:CA	2.38	0.49
1:A:809:LEU:C	1:A:811:TYR:N	2.70	0.49
1:C:38:PHE:HB2	1:C:83:LEU:HB2	1.93	0.49
1:C:412:LEU:HD13	1:C:415:LEU:HD13	1.94	0.49
1:D:330:ARG:O	1:D:334:ILE:HG13	2.13	0.49
1:A:197:LEU:HD23	1:A:197:LEU:C	2.37	0.49
1:B:413:THR:O	1:B:414:SER:C	2.54	0.49
1:B:444:ASN:HA	1:B:599:ARG:HE	1.77	0.49
1:C:78:ILE:CD1	1:C:80:LEU:HD23	2.42	0.49
1:C:145:ARG:HD3	1:C:185:LYS:O	2.12	0.49
1:C:221:PHE:O	1:C:224:PRO:HD2	2.12	0.49
1:B:421:ARG:HB3	1:B:680:LEU:CD1	2.41	0.49
1:B:808:ILE:HG22	1:B:812:ASN:HD21	1.77	0.49
1:C:382:GLN:HG2	1:C:383:GLY:N	2.26	0.49
1:C:668:ARG:NH1	1:C:668:ARG:HG2	2.28	0.49
1:D:313:ARG:O	1:D:317:HIS:ND1	2.36	0.49
1:D:700:GLY:HA2	1:D:753:LEU:HD22	1.95	0.49
1:A:376:GLN:HE21	1:A:378:LYS:CD	2.24	0.49
1:B:428:GLU:OE1	1:B:470:VAL:HG23	2.12	0.49
1:D:487:GLY:HA2	1:D:490:LEU:HB2	1.94	0.49
1:D:776:TYR:HE1	1:D:848:TRP:CZ2	2.31	0.49
3:L:102:DC:H2''	3:L:103:DG:OP2	2.13	0.49
1:B:498:ILE:O	1:B:498:ILE:HG22	2.11	0.49
2:E:14:DC:H2''	2:E:15:DC:C5'	2.33	0.49
2:K:10:DA:C3'	2:K:11:DC:H5''	2.41	0.49
1:A:804:HIS:O	1:A:808:ILE:HG13	2.13	0.49
1:B:395:PHE:HB2	1:B:591:GLN:HG2	1.94	0.49
1:B:699:GLY:O	1:B:753:LEU:HD22	2.12	0.49
1:C:621:ASP:OD1	3:J:114:DA:H5'	2.13	0.49
1:D:149:PHE:HB3	1:D:197:LEU:HD21	1.95	0.49
3:F:108:DT:H1'	3:F:109:DC:H5'	1.94	0.49
1:A:49:TYR:CE1	1:A:59:ARG:HB2	2.47	0.49
1:A:446:VAL:O	1:A:446:VAL:HG23	2.13	0.49
1:B:405:LYS:N	5:B:918:HOH:O	2.44	0.49
1:B:582:ASN:O	1:B:586:ILE:HG13	2.13	0.49
1:C:285:GLN:HE21	1:C:285:GLN:HA	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:GLN:HA	1:C:285:GLN:NE2	2.28	0.49
1:D:89:LYS:O	1:D:93:LEU:HD13	2.12	0.49
1:D:117:VAL:HG13	1:D:132:PRO:O	2.13	0.49
3:H:109:DC:H2''	3:H:110:DA:H5'	1.95	0.49
3:H:110:DA:H1'	3:H:111:DT:H5''	1.93	0.49
1:A:298:LEU:HD12	1:A:298:LEU:N	2.28	0.48
1:A:544:ARG:HG3	1:A:544:ARG:HH11	1.77	0.48
1:A:731:GLU:H	1:A:731:GLU:CD	2.19	0.48
1:B:496:GLY:O	1:B:542:LEU:HD11	2.13	0.48
1:B:499:ILE:O	1:B:542:LEU:HD22	2.12	0.48
1:C:361:PRO:HD2	2:I:3:DC:H5''	1.95	0.48
1:D:645:ASN:HD21	1:D:719:ARG:HH11	1.61	0.48
1:A:514:LEU:H	1:A:541:MET:HE2	1.78	0.48
1:B:85:MET:HA	1:B:380:ILE:HD11	1.95	0.48
2:G:6:DA:C2'	2:G:7:DA:H5''	2.43	0.48
1:A:5:TYR:HE1	1:A:101:ILE:HD13	1.77	0.48
1:A:87:ASP:OD1	1:A:90:LEU:HG	2.13	0.48
1:B:150:ASP:OD1	1:B:321:ILE:HD11	2.13	0.48
1:B:154:SER:C	1:B:156:TYR:H	2.21	0.48
1:B:530:ILE:HA	1:B:533:LEU:HB2	1.95	0.48
1:B:867:ASP:CG	1:B:870:VAL:HB	2.39	0.48
1:C:516:VAL:HG21	1:C:522:PHE:HE1	1.78	0.48
1:D:439:LEU:HD12	1:D:443:ILE:HD11	1.95	0.48
1:A:276:LEU:HG	1:A:340:PHE:HB3	1.95	0.48
1:C:154:SER:O	1:C:156:TYR:N	2.46	0.48
1:D:805:ILE:HD13	1:D:808:ILE:HD12	1.96	0.48
2:G:12:DA:H2''	2:G:13:DG:O5'	2.13	0.48
1:A:738:PRO:O	1:A:742:GLN:HB2	2.14	0.48
1:B:435:LYS:CD	1:B:435:LYS:N	2.76	0.48
1:B:634:ASP:C	1:B:636:VAL:N	2.71	0.48
1:C:342:ASN:HB2	5:C:919:HOH:O	2.12	0.48
1:C:646:HIS:HB3	5:C:1043:HOH:O	2.13	0.48
1:D:146:PHE:N	1:D:146:PHE:CD1	2.82	0.48
1:D:347:MET:HE2	1:D:558:ASN:ND2	2.27	0.48
1:D:594:LEU:O	1:D:597:ILE:HG22	2.12	0.48
1:A:313:ARG:NH1	5:A:979:HOH:O	2.34	0.48
1:B:231:LYS:HG3	1:B:236:GLU:HA	1.95	0.48
1:B:234:PHE:CD1	1:B:234:PHE:N	2.81	0.48
1:B:482:ARG:HH22	1:B:560:LYS:HD2	1.76	0.48
1:B:698:ILE:HD13	1:B:889:LEU:HD11	1.94	0.48
1:C:189:MET:O	1:C:191:PHE:CE1	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:PHE:CE2	1:D:103:TYR:HB2	2.48	0.48
1:D:841:PHE:CE2	1:D:862:VAL:HG22	2.48	0.48
2:I:10:DA:C2'	2:I:11:DC:C5'	2.90	0.48
1:A:642:ARG:N	1:A:646:HIS:HD2	2.06	0.48
1:B:472:PRO:HA	1:B:475:ILE:HG22	1.94	0.48
1:C:516:VAL:HG21	1:C:522:PHE:CE1	2.48	0.48
1:C:791:TYR:CD2	1:C:801:CYS:HA	2.49	0.48
1:D:324:ASN:C	1:D:324:ASN:HD22	2.19	0.48
1:D:605:LEU:CD2	1:D:632:ILE:HD11	2.43	0.48
2:E:13:DG:H1	3:F:105:DC:N4	2.12	0.48
2:I:12:DA:H2''	2:I:13:DG:C5'	2.44	0.48
1:A:744:ALA:O	1:A:745:LEU:C	2.56	0.48
1:C:81:GLU:HB2	1:C:384:ARG:NH2	2.29	0.48
1:D:409:SER:HB3	1:D:626:TYR:CD2	2.48	0.48
1:A:49:TYR:HB2	1:A:57:CYS:O	2.13	0.48
1:A:605:LEU:HA	1:A:608:VAL:HG22	1.96	0.48
1:B:285:GLN:HG3	1:B:292:TYR:CE2	2.49	0.48
1:B:497:GLU:CG	1:B:498:ILE:HD12	2.44	0.48
1:C:668:ARG:HG2	1:C:668:ARG:HH11	1.79	0.48
1:D:597:ILE:HD11	1:D:663:ILE:HG23	1.95	0.48
1:D:806:ARG:HD2	1:D:843:ASP:OD1	2.14	0.48
3:F:110:DA:C2'	3:F:111:DT:C5'	2.91	0.48
1:A:373:LEU:HD12	1:A:380:ILE:HG22	1.95	0.48
1:A:613:GLY:O	1:A:614:GLU:C	2.56	0.48
1:A:734:LYS:C	1:A:736:SER:N	2.71	0.48
1:A:821:ALA:O	1:A:822:PRO:C	2.57	0.48
1:B:9:GLU:CG	1:B:266:PHE:HD2	2.27	0.48
1:B:772:ARG:NH2	1:B:868:TYR:HB2	2.29	0.48
1:C:104:ASP:OD1	1:C:107:LYS:HE2	2.14	0.48
1:C:231:LYS:HG2	1:C:231:LYS:O	2.14	0.48
1:C:285:GLN:HE21	1:C:285:GLN:CA	2.25	0.48
1:A:43:GLU:HA	1:A:56:PRO:HG3	1.95	0.47
1:A:771:PHE:CD1	1:A:774:LEU:HD12	2.48	0.47
1:B:647:TRP:O	1:B:650:PHE:HB3	2.14	0.47
1:B:831:TYR:O	1:B:847:ALA:HA	2.13	0.47
1:C:209:THR:HA	1:C:210:PRO:HD3	1.59	0.47
1:D:254:GLU:HG3	1:D:258:GLY:O	2.14	0.47
1:D:491:ALA:HB1	1:D:521:ASP:N	2.29	0.47
2:G:11:DC:H2''	2:G:12:DA:C5'	2.42	0.47
1:B:831:TYR:CD2	1:B:850:SER:HA	2.49	0.47
1:B:867:ASP:OD1	1:B:870:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:TYR:CD2	1:C:190:PRO:HD3	2.49	0.47
1:D:9:GLU:OE2	1:D:266:PHE:HA	2.15	0.47
1:D:411:ASP:CG	1:D:624:SER:HB3	2.39	0.47
1:D:526:ILE:HG13	1:D:526:ILE:O	2.13	0.47
1:D:880:LEU:HD22	1:D:884:THR:HG23	1.96	0.47
1:B:177:GLU:HG3	1:B:177:GLU:O	2.13	0.47
1:C:73:LYS:HB3	1:C:73:LYS:HZ2	1.79	0.47
1:C:137:THR:HB	1:C:328:VAL:HG21	1.95	0.47
1:D:859:LYS:O	1:D:863:LEU:HD13	2.14	0.47
3:F:103:DG:C2'	3:F:104:DG:H5'	2.34	0.47
1:A:274:ILE:HG23	1:A:275:ASP:N	2.29	0.47
1:A:735:SER:OG	3:F:112:DT:OP1	2.33	0.47
1:B:218:VAL:O	1:B:223:ILE:HG13	2.14	0.47
1:B:384:ARG:HH11	1:B:384:ARG:HG3	1.79	0.47
1:B:512:GLU:N	1:B:513:PRO:CD	2.76	0.47
1:B:791:TYR:CD2	1:B:801:CYS:HA	2.50	0.47
1:D:85:MET:HA	1:D:380:ILE:HD11	1.96	0.47
1:D:514:LEU:N	1:D:514:LEU:HD12	2.29	0.47
1:A:364:THR:O	1:A:368:ILE:HG13	2.15	0.47
1:A:428:GLU:OE1	1:A:470:VAL:HG23	2.15	0.47
1:A:779:ILE:HG21	1:A:871:LEU:CD2	2.45	0.47
1:B:132:PRO:HA	1:B:194:GLU:OE1	2.14	0.47
1:B:494:ARG:HG3	1:B:494:ARG:NH1	2.29	0.47
1:B:811:TYR:O	1:B:815:ILE:HG12	2.15	0.47
1:D:361:PRO:HD2	2:K:3:DC:P	2.54	0.47
1:D:514:LEU:HD13	1:D:541:MET:HE1	1.96	0.47
1:A:392:PRO:C	1:A:587:THR:HG21	2.40	0.47
1:A:471:VAL:HB	1:A:472:PRO:CD	2.44	0.47
1:A:489:MET:SD	1:A:553:MET:HG2	2.55	0.47
1:A:491:ALA:C	1:A:493:GLN:H	2.21	0.47
1:A:594:LEU:HD11	1:A:625:ILE:HG23	1.97	0.47
1:A:714:ASP:OD1	1:A:718:THR:N	2.48	0.47
1:B:109:ARG:NH1	1:B:142:ILE:HD12	2.29	0.47
1:B:183:ILE:HG23	1:B:184:ASP:OD1	2.15	0.47
1:B:508:LEU:HG	1:B:509:SER:N	2.28	0.47
1:B:846:ILE:CD1	1:B:858:ILE:HD12	2.45	0.47
1:C:240:LYS:O	1:C:246:ARG:HA	2.15	0.47
1:C:724:LYS:HE2	5:C:975:HOH:O	2.13	0.47
1:D:273:TYR:HA	1:D:276:LEU:HB2	1.97	0.47
1:D:284:ASN:C	1:D:284:ASN:ND2	2.73	0.47
1:D:700:GLY:CA	1:D:753:LEU:HD22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:DA:H2'	2:G:8:DT:H72	1.97	0.47
1:A:52:ILE:HD12	1:A:428:GLU:HB3	1.96	0.47
1:A:274:ILE:CG2	1:A:275:ASP:N	2.78	0.47
1:A:731:GLU:HA	1:A:734:LYS:HB2	1.96	0.47
1:A:772:ARG:O	1:A:774:LEU:N	2.48	0.47
1:C:403:ARG:HH22	1:C:889:LEU:HD23	1.80	0.47
2:G:14:DC:C2'	2:G:15:DC:H5''	2.45	0.47
1:A:415:LEU:O	1:A:419:ILE:HG13	2.15	0.47
1:A:494:ARG:NH2	1:A:521:ASP:HB3	2.29	0.47
1:B:338:ARG:O	1:B:339:GLN:HB2	2.15	0.47
1:B:491:ALA:HB3	1:B:518:TYR:O	2.15	0.47
1:B:534:SER:CB	1:B:537:SER:HB2	2.45	0.47
1:B:876:PHE:O	1:B:879:PRO:HG2	2.15	0.47
1:D:97:TYR:O	1:D:352:LYS:NZ	2.36	0.47
1:D:183:ILE:HG23	1:D:184:ASP:N	2.30	0.47
1:D:265:LEU:CB	1:D:268:ILE:HD12	2.45	0.47
1:D:791:TYR:CD2	1:D:801:CYS:HA	2.50	0.47
1:A:433:THR:HA	1:A:460:GLY:O	2.14	0.47
1:A:606:ASN:ND2	1:A:613:GLY:N	2.63	0.47
1:A:736:SER:HB2	1:A:782:VAL:O	2.14	0.47
1:A:836:ARG:HG3	1:A:865:TRP:O	2.14	0.47
1:B:421:ARG:HD3	1:B:475:ILE:HD12	1.97	0.47
1:B:468:ASP:OD2	1:B:468:ASP:N	2.42	0.47
1:B:489:MET:HB3	1:B:552:GLY:HA3	1.97	0.47
1:C:15:ILE:CD1	1:C:92:TYR:HB2	2.45	0.47
1:C:440:HIS:CE1	1:C:444:ASN:ND2	2.83	0.47
1:D:516:VAL:HG21	1:D:522:PHE:HZ	1.80	0.47
1:A:499:ILE:O	1:A:542:LEU:HD22	2.14	0.46
1:B:199:MET:HA	1:B:199:MET:HE3	1.95	0.46
1:B:227:TYR:CD2	1:B:263:ILE:HD13	2.50	0.46
1:B:376:GLN:NE2	1:B:378:LYS:NZ	2.62	0.46
1:B:421:ARG:HG2	1:B:421:ARG:NH1	2.30	0.46
1:B:739:LYS:HE2	1:B:739:LYS:HA	1.97	0.46
1:B:797:PRO:HG3	1:B:806:ARG:NH1	2.29	0.46
1:C:118:THR:OG1	1:C:313:ARG:HG3	2.15	0.46
1:C:376:GLN:O	1:C:377:ASN:HB2	2.15	0.46
1:C:839:ASN:HB2	1:C:840:PRO:HD2	1.97	0.46
3:F:109:DC:H2''	3:F:110:DA:H5'	1.97	0.46
1:A:221:PHE:C	1:A:224:PRO:HD2	2.39	0.46
1:A:514:LEU:HG	1:A:526:ILE:CG2	2.43	0.46
1:A:559:ARG:HG2	1:A:559:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:856:ASP:HA	1:B:859:LYS:HB2	1.97	0.46
1:C:83:LEU:HB3	1:C:379:VAL:CG1	2.44	0.46
1:D:143:ASP:O	1:D:144:ASP:HB3	2.16	0.46
1:D:503:LEU:HA	1:D:506:PRO:HG3	1.98	0.46
2:E:4:CTG:O6	2:E:4:CTG:H2'	2.13	0.46
1:A:132:PRO:HD2	5:A:1001:HOH:O	2.15	0.46
1:A:659:MET:O	1:A:660:GLU:C	2.59	0.46
1:A:661:PRO:O	1:A:665:ARG:HG3	2.16	0.46
1:B:408:MET:HE1	1:B:655:ALA:CB	2.44	0.46
1:B:502:ALA:HB3	1:B:539:ASN:OD1	2.15	0.46
1:B:597:ILE:HD13	1:B:667:PHE:CZ	2.50	0.46
1:B:809:LEU:O	1:B:813:ARG:HB2	2.15	0.46
1:C:284:ASN:HD21	1:C:829:LYS:NZ	2.14	0.46
1:C:455:SER:HA	1:C:675:ASN:O	2.16	0.46
1:C:558:ASN:HD22	1:C:558:ASN:HA	1.58	0.46
1:D:336:ALA:CA	1:D:339:GLN:HE21	2.23	0.46
1:D:353:ILE:HB	5:D:937:HOH:O	2.15	0.46
1:A:4:PHE:O	1:A:19:TYR:HB2	2.14	0.46
1:A:362:ILE:HG22	1:A:363:LYS:N	2.30	0.46
1:A:472:PRO:HA	1:A:475:ILE:HG13	1.96	0.46
1:B:878:LYS:HB3	1:B:879:PRO:CD	2.45	0.46
1:C:152:LEU:CD1	1:C:190:PRO:HB2	2.36	0.46
1:D:206:GLN:NE2	1:D:206:GLN:HA	2.31	0.46
1:D:208:LYS:O	1:D:209:THR:C	2.58	0.46
1:D:253:ILE:HD11	1:D:262:ILE:CD1	2.45	0.46
1:A:106:THR:HG22	1:A:106:THR:O	2.15	0.46
1:A:354:GLN:O	1:A:357:SER:HB2	2.15	0.46
1:A:546:GLN:HG3	1:A:547:ARG:N	2.31	0.46
1:B:468:ASP:HB3	5:B:1000:HOH:O	2.14	0.46
1:C:61:LEU:HD23	1:C:62:PHE:N	2.30	0.46
1:C:197:LEU:HD23	1:C:197:LEU:C	2.40	0.46
1:D:453:VAL:HG23	1:D:454:TYR:CD2	2.50	0.46
1:D:498:ILE:HA	1:D:501:GLU:HB3	1.96	0.46
1:D:760:LEU:C	1:D:760:LEU:CD2	2.88	0.46
3:J:112:DT:H2''	3:J:113:DC:H5'	1.97	0.46
1:A:467:ARG:HG3	1:A:467:ARG:HH11	1.81	0.46
1:B:164:ILE:HB	1:B:183:ILE:HD11	1.97	0.46
1:B:395:PHE:HB2	1:B:591:GLN:HE21	1.81	0.46
1:B:478:VAL:HG13	1:B:559:ARG:HG3	1.98	0.46
1:B:485:HIS:O	1:B:489:MET:HG3	2.16	0.46
1:B:750:ARG:HH11	1:B:754:GLN:HE22	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ILE:HB	1:C:428:GLU:HG2	1.97	0.46
1:C:235:GLY:O	1:C:236:GLU:C	2.57	0.46
1:C:598:GLU:HG3	1:C:617:VAL:HG11	1.97	0.46
1:D:13:ASP:HB3	1:D:64:ASN:HB2	1.97	0.46
1:D:243:SER:C	1:D:245:HIS:H	2.24	0.46
1:A:636:VAL:HG21	1:A:650:PHE:CZ	2.50	0.46
1:A:747:GLU:OE2	1:A:747:GLU:HA	2.16	0.46
1:B:273:TYR:HA	1:B:276:LEU:HB2	1.97	0.46
1:B:395:PHE:CB	1:B:591:GLN:HG2	2.45	0.46
1:B:406:TYR:CD2	1:B:633:ILE:HG13	2.51	0.46
3:J:110:DA:C2'	3:J:111:DT:C5'	2.94	0.46
1:C:163:SER:HB3	1:C:318:GLN:NE2	2.15	0.46
1:C:354:GLN:HB3	1:C:356:GLN:OE1	2.16	0.46
1:C:436:VAL:O	1:C:436:VAL:HG13	2.16	0.46
1:D:83:LEU:HB3	1:D:379:VAL:CG1	2.46	0.46
1:D:83:LEU:H	1:D:83:LEU:HD22	1.81	0.46
1:D:167:ALA:HA	1:D:176:ASP:HB2	1.97	0.46
1:D:209:THR:HA	1:D:210:PRO:HD3	1.81	0.46
1:D:289:SER:O	1:D:290:LEU:C	2.58	0.46
1:D:592:MET:HE1	1:D:674:MET:HE3	1.98	0.46
1:A:219:GLU:O	1:A:219:GLU:HG2	2.16	0.46
1:A:294:SER:HA	1:A:334:ILE:HD11	1.98	0.46
1:A:811:TYR:O	1:A:815:ILE:HG12	2.16	0.46
1:B:149:PHE:N	1:B:149:PHE:CD1	2.84	0.46
1:B:678:GLN:HG2	1:B:680:LEU:HG	1.98	0.46
1:D:303:LEU:HD12	1:D:323:TYR:HA	1.97	0.46
1:D:496:GLY:HA2	1:D:545:ALA:HB3	1.97	0.46
1:D:697:GLY:HA3	1:D:753:LEU:O	2.16	0.46
1:A:37:LEU:C	1:A:38:PHE:CD1	2.94	0.46
1:A:499:ILE:HD11	1:A:522:PHE:HZ	1.80	0.46
1:A:685:ARG:NH1	1:A:688:ILE:HG13	2.30	0.46
1:B:179:PRO:HG2	1:B:329:TYR:CE2	2.51	0.46
1:B:776:TYR:CE1	1:B:777:ILE:HG13	2.50	0.46
1:C:173:GLN:HE21	1:C:173:GLN:HB2	1.58	0.46
1:C:305:TYR:OH	1:C:309:ILE:CG1	2.63	0.46
1:D:132:PRO:HB3	1:D:229:ARG:NH2	2.31	0.46
1:D:481:GLN:CB	1:D:559:ARG:HD3	2.45	0.46
1:D:881:GLU:HA	1:D:884:THR:OG1	2.15	0.46
2:K:8:DT:C2'	2:K:9:DG:H5'	2.36	0.46
1:A:162:TRP:CD1	1:A:321:ILE:HB	2.51	0.45
1:A:903:PHE:C	1:A:903:PHE:CD1	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:MET:HE3	1:B:86:ASP:H	1.82	0.45
1:B:555:ALA:O	1:B:559:ARG:HD3	2.16	0.45
1:B:617:VAL:HB	5:B:973:HOH:O	2.16	0.45
1:A:534:SER:O	1:A:538:LEU:HG	2.15	0.45
1:A:761:GLN:OE1	1:A:893:LYS:CG	2.64	0.45
1:B:233:ILE:N	1:B:233:ILE:CD1	2.78	0.45
1:B:435:LYS:H	1:B:435:LYS:CD	2.29	0.45
1:B:545:ALA:O	1:B:549:GLU:HB2	2.17	0.45
1:B:739:LYS:HE2	1:B:742:GLN:HE22	1.82	0.45
1:D:578:TYR:CD1	1:D:578:TYR:C	2.93	0.45
2:K:9:DG:H2''	2:K:10:DA:C8	2.51	0.45
1:B:634:ASP:O	1:B:636:VAL:N	2.49	0.45
1:D:163:SER:HB3	1:D:318:GLN:NE2	2.21	0.45
1:D:516:VAL:HG21	1:D:522:PHE:CZ	2.52	0.45
2:G:12:DA:H1'	2:G:13:DG:H5'	1.99	0.45
1:A:15:ILE:HG12	1:A:65:MET:CE	2.44	0.45
1:A:413:THR:O	1:A:414:SER:C	2.59	0.45
1:A:491:ALA:HA	1:A:494:ARG:HE	1.81	0.45
1:A:514:LEU:HD11	1:A:529:LYS:CE	2.46	0.45
1:A:612:GLU:OE1	1:A:612:GLU:HA	2.15	0.45
1:A:744:ALA:O	1:A:747:GLU:N	2.50	0.45
1:A:776:TYR:CE1	1:A:863:LEU:HD11	2.51	0.45
1:B:894:LYS:HZ2	1:B:894:LYS:C	2.23	0.45
1:C:38:PHE:HB2	1:C:379:VAL:HG11	1.98	0.45
1:D:286:PRO:C	1:D:829:LYS:HD2	2.42	0.45
1:D:420:ILE:HG12	1:D:586:ILE:HD11	1.98	0.45
2:K:7:DA:H2''	2:K:8:DT:C6	2.52	0.45
1:A:602:ASN:ND2	1:A:616:PHE:H	2.15	0.45
1:A:779:ILE:HG21	1:A:871:LEU:CG	2.47	0.45
1:B:506:PRO:HB3	1:B:536:LYS:CG	2.44	0.45
1:C:453:VAL:HG23	1:C:454:TYR:CG	2.52	0.45
1:D:727:ILE:O	1:D:728:MET:HE2	2.17	0.45
2:E:12:DA:H2''	2:E:13:DG:O5'	2.17	0.45
1:A:592:MET:HE1	1:A:674:MET:HG3	1.98	0.45
1:A:795:GLY:O	1:A:809:LEU:HD13	2.16	0.45
1:B:386:HIS:O	1:B:573:VAL:HG21	2.17	0.45
1:B:634:ASP:C	1:B:636:VAL:H	2.25	0.45
1:B:685:ARG:HH11	1:B:685:ARG:CG	2.29	0.45
1:C:9:GLU:HG3	1:C:267:GLY:H	1.81	0.45
1:C:9:GLU:HG3	1:C:267:GLY:N	2.32	0.45
1:D:329:TYR:O	1:D:333:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:LYS:O	1:D:690:GLY:HA2	2.17	0.45
1:A:314:GLU:HG2	1:A:315:SER:N	2.31	0.45
1:A:653:LYS:HD2	1:A:653:LYS:C	2.42	0.45
1:B:516:VAL:HG12	1:B:517:ASP:N	2.32	0.45
1:B:541:MET:HG3	1:B:544:ARG:HD3	1.99	0.45
1:D:750:ARG:HG2	1:D:750:ARG:HH11	1.81	0.45
2:K:4:CTG:O6	2:K:4:CTG:H2'	2.17	0.45
1:A:730:LEU:HD22	1:A:883:PHE:HE1	1.82	0.45
1:A:731:GLU:OE1	1:A:731:GLU:N	2.48	0.45
1:B:508:LEU:CG	1:B:509:SER:H	2.30	0.45
1:B:687:ALA:HB2	1:B:715:MET:HE1	1.98	0.45
1:C:451:SER:HB3	1:C:456:CYS:SG	2.57	0.45
1:C:898:PHE:CD2	1:C:898:PHE:N	2.83	0.45
1:D:750:ARG:HG2	1:D:750:ARG:NH1	2.32	0.45
1:D:842:GLY:O	1:D:843:ASP:HB2	2.16	0.45
2:E:5:DG:H2''	2:E:6:DA:O5'	2.16	0.45
1:B:145:ARG:HB2	1:B:147:TYR:CE1	2.51	0.45
1:B:529:LYS:O	1:B:533:LEU:HB2	2.17	0.45
1:B:700:GLY:HA2	1:B:753:LEU:HD22	1.99	0.45
1:C:20:ILE:HD13	1:C:107:LYS:CB	2.47	0.45
1:C:134:ASP:O	1:C:135:ALA:HB2	2.17	0.45
1:C:194:GLU:O	1:C:195:LYS:C	2.60	0.45
1:C:305:TYR:OH	1:C:309:ILE:HG12	2.16	0.45
1:C:362:ILE:HD12	1:C:575:PHE:HB2	1.99	0.45
1:C:700:GLY:HA2	1:C:753:LEU:HD22	1.99	0.45
3:L:111:DT:H4'	3:L:111:DT:OP1	2.16	0.45
1:A:126:PRO:C	1:A:128:GLN:H	2.25	0.45
1:A:734:LYS:C	1:A:736:SER:H	2.24	0.45
1:A:761:GLN:OE1	1:A:893:LYS:HG2	2.17	0.45
1:C:89:LYS:HE3	1:C:354:GLN:NE2	2.32	0.45
1:C:197:LEU:HD23	1:C:197:LEU:O	2.17	0.45
1:D:698:ILE:HG13	1:D:753:LEU:HD23	1.99	0.45
1:D:813:ARG:HG3	1:D:813:ARG:HH11	1.81	0.45
2:I:7:DA:H2''	2:I:8:DT:C7	2.47	0.45
1:A:167:ALA:HB1	1:A:178:VAL:HG21	1.99	0.44
1:A:279:LYS:O	1:A:279:LYS:HG2	2.16	0.44
1:B:116:GLU:OE1	1:B:116:GLU:HA	2.16	0.44
1:C:71:TRP:CZ2	1:C:75:MET:HE2	2.52	0.44
1:C:254:GLU:OE2	1:C:259:SER:HB2	2.18	0.44
1:C:277:TYR:O	1:C:281:SER:CB	2.65	0.44
1:D:140:ASP:OD1	1:D:142:ILE:HB	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:LEU:O	1:D:494:ARG:NE	2.50	0.44
1:D:655:ALA:O	1:D:660:GLU:HG2	2.16	0.44
1:D:713:TRP:HZ3	1:D:723:PRO:HD3	1.82	0.44
1:D:751:ARG:HD3	1:D:759:SER:OG	2.16	0.44
1:A:83:LEU:N	1:A:83:LEU:HD12	2.31	0.44
1:A:347:MET:HG2	1:A:358:VAL:CG2	2.45	0.44
1:A:347:MET:HE1	1:A:562:LEU:HD11	1.98	0.44
1:A:778:SER:HB2	5:A:1004:HOH:O	2.16	0.44
1:A:846:ILE:HG23	1:A:846:ILE:O	2.18	0.44
1:A:854:ILE:HG23	1:A:859:LYS:HB2	1.99	0.44
1:A:854:ILE:HD11	1:A:858:ILE:HG13	1.99	0.44
1:C:83:LEU:HD22	1:C:83:LEU:H	1.82	0.44
1:D:475:ILE:HD13	1:D:566:LEU:HD22	1.98	0.44
1:D:814:ALA:HB1	1:D:841:PHE:HE1	1.83	0.44
1:A:299:ASN:O	1:A:300:VAL:HB	2.16	0.44
1:A:740:ALA:HB3	1:A:778:SER:O	2.17	0.44
1:A:832:VAL:O	1:A:833:LEU:HB2	2.16	0.44
1:A:878:LYS:N	1:A:879:PRO:HD2	2.33	0.44
1:B:126:PRO:HG2	5:B:986:HOH:O	2.17	0.44
1:B:408:MET:CE	1:B:685:ARG:HD3	2.45	0.44
1:B:597:ILE:HD12	1:B:683:MET:HE1	1.99	0.44
1:B:606:ASN:OD1	1:B:616:PHE:HE1	2.00	0.44
1:C:111:ALA:HB3	1:C:210:PRO:HB3	1.98	0.44
1:C:854:ILE:CD1	1:C:862:VAL:HG21	2.47	0.44
1:D:370:PHE:C	1:D:370:PHE:CD2	2.94	0.44
1:D:402:ASN:CG	1:D:403:ARG:H	2.24	0.44
1:A:592:MET:HE1	1:A:674:MET:CG	2.48	0.44
1:B:194:GLU:CD	1:B:229:ARG:HH21	2.24	0.44
1:C:285:GLN:NE2	1:C:286:PRO:HD2	2.33	0.44
1:C:537:SER:O	1:C:541:MET:HG3	2.15	0.44
1:D:135:ALA:O	1:D:136:ILE:HG13	2.17	0.44
1:D:149:PHE:CE2	1:D:201:TYR:HA	2.52	0.44
1:D:265:LEU:HB3	1:D:268:ILE:HD12	2.00	0.44
1:A:240:LYS:O	1:A:246:ARG:HA	2.17	0.44
1:A:514:LEU:HD23	1:A:541:MET:HE1	1.99	0.44
1:A:530:ILE:HA	1:A:533:LEU:CD1	2.47	0.44
1:A:594:LEU:HD11	1:A:625:ILE:CG2	2.47	0.44
1:A:775:ASN:N	5:A:1004:HOH:O	2.50	0.44
1:B:252:VAL:HG23	1:B:252:VAL:O	2.17	0.44
1:B:489:MET:HE2	1:B:553:MET:HE1	1.99	0.44
1:C:708:TYR:CZ	1:C:728:MET:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:LEU:HD13	1:D:443:ILE:HG13	1.99	0.44
1:D:465:LYS:NZ	1:D:675:ASN:ND2	2.65	0.44
1:A:285:GLN:HA	1:A:285:GLN:NE2	2.32	0.44
1:B:25:ARG:HG2	1:B:25:ARG:NH1	2.33	0.44
1:B:181:GLU:CD	1:B:181:GLU:H	2.25	0.44
1:B:499:ILE:HD13	1:B:530:ILE:HD12	1.99	0.44
1:C:305:TYR:CZ	1:C:309:ILE:HG12	2.53	0.44
1:C:439:LEU:HD12	1:C:443:ILE:CD1	2.45	0.44
1:C:594:LEU:O	1:C:597:ILE:HG22	2.17	0.44
1:A:194:GLU:CD	1:A:229:ARG:HH11	2.26	0.44
1:A:231:LYS:NZ	1:A:231:LYS:HB3	2.32	0.44
1:A:514:LEU:HD11	1:A:529:LYS:HZ1	1.80	0.44
1:A:772:ARG:HG3	1:A:868:TYR:CD2	2.52	0.44
1:B:50:PHE:O	1:B:378:LYS:HA	2.18	0.44
1:B:154:SER:HB2	1:B:155:PRO:HD2	1.98	0.44
1:B:894:LYS:NZ	1:B:894:LYS:CB	2.77	0.44
1:D:434:PHE:CE2	1:D:450:PRO:HB3	2.53	0.44
1:B:282:PHE:HB2	5:B:940:HOH:O	2.16	0.44
1:B:305:TYR:OH	1:B:309:ILE:HG22	2.18	0.44
1:C:495:ASN:O	1:C:498:ILE:HB	2.17	0.44
1:D:484:GLU:C	1:D:486:LYS:H	2.26	0.44
1:D:578:TYR:CD1	1:D:579:ASP:N	2.86	0.44
1:A:411:ASP:O	1:A:683:MET:HA	2.18	0.44
1:C:13:ASP:HB3	1:C:64:ASN:HB2	1.99	0.44
1:C:239:ALA:C	1:C:241:ARG:N	2.76	0.44
1:C:494:ARG:HH21	1:C:521:ASP:CG	2.25	0.44
1:C:642:ARG:HH21	1:C:642:ARG:HG3	1.82	0.44
1:D:731:GLU:C	1:D:734:LYS:HG2	2.43	0.44
2:E:6:DA:H1'	2:E:7:DA:H5''	1.99	0.44
1:A:37:LEU:HD11	1:A:72:ILE:HD11	2.00	0.43
1:A:464:TYR:HB3	1:A:467:ARG:HG2	2.00	0.43
1:A:499:ILE:O	1:A:499:ILE:HG22	2.18	0.43
1:A:751:ARG:NE	1:A:763:TYR:HB2	2.32	0.43
1:A:835:LEU:N	1:A:844:LYS:O	2.34	0.43
1:B:404:TYR:HA	5:B:918:HOH:O	2.18	0.43
1:B:444:ASN:HA	1:B:599:ARG:NE	2.33	0.43
1:B:730:LEU:HD13	1:B:883:PHE:CE1	2.53	0.43
1:B:761:GLN:OE1	1:B:893:LYS:HE3	2.18	0.43
1:C:404:TYR:HA	5:C:992:HOH:O	2.18	0.43
1:C:578:TYR:CD1	1:C:578:TYR:C	2.96	0.43
1:D:50:PHE:HA	1:D:55:LYS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ILE:HD12	1:D:318:GLN:NE2	2.33	0.43
1:D:479:PHE:CD1	1:D:563:ILE:HD13	2.53	0.43
1:D:511:ASP:CG	1:D:512:GLU:H	2.26	0.43
1:D:686:GLU:OE1	1:D:716:GLU:HG2	2.18	0.43
1:D:698:ILE:HG12	1:D:752:MET:O	2.18	0.43
3:F:105:DC:H2''	3:F:106:DT:C5'	2.47	0.43
1:A:831:TYR:O	1:A:847:ALA:HA	2.18	0.43
1:C:167:ALA:CA	1:C:176:ASP:HB2	2.43	0.43
1:C:274:ILE:HG23	1:C:275:ASP:N	2.33	0.43
1:C:514:LEU:HD21	1:C:526:ILE:HG23	2.00	0.43
1:C:633:ILE:HD13	1:C:633:ILE:HA	1.91	0.43
1:D:322:SER:O	1:D:326:ILE:HG13	2.17	0.43
1:D:570:LEU:HD23	1:D:575:PHE:CE2	2.53	0.43
1:D:686:GLU:HB3	1:D:687:ALA:H	1.66	0.43
1:D:781:SER:O	1:D:831:TYR:HA	2.19	0.43
3:L:104:DG:C3'	3:L:105:DC:H5''	2.49	0.43
1:A:105:HIS:ND1	1:A:106:THR:N	2.65	0.43
1:B:255:ASN:ND2	1:B:257:TYR:HD1	2.16	0.43
1:B:271:LEU:HD11	1:B:356:GLN:HA	2.00	0.43
1:B:362:ILE:HG12	2:G:3:DC:OP1	2.18	0.43
1:B:742:GLN:HE21	1:B:742:GLN:HB2	1.62	0.43
1:C:83:LEU:H	1:C:83:LEU:CD2	2.31	0.43
1:C:523:SER:OG	1:C:526:ILE:HG13	2.18	0.43
1:D:569:ALA:C	1:D:571:GLY:H	2.26	0.43
1:A:862:VAL:HG12	1:A:863:LEU:HD12	2.00	0.43
1:B:216:TRP:O	1:B:217:ASN:HB2	2.18	0.43
1:B:286:PRO:HG2	1:B:292:TYR:CZ	2.54	0.43
1:B:558:ASN:HD22	1:B:558:ASN:HA	1.51	0.43
1:B:686:GLU:HG3	1:B:715:MET:SD	2.58	0.43
1:C:53:TYR:CE1	1:C:428:GLU:HA	2.53	0.43
1:C:425:ILE:O	1:C:426:SER:HB2	2.18	0.43
1:D:74:ARG:O	1:D:75:MET:C	2.60	0.43
1:D:165:GLU:H	1:D:165:GLU:CD	2.26	0.43
1:D:376:GLN:O	1:D:377:ASN:HB2	2.18	0.43
1:D:599:ARG:O	1:D:603:GLU:HG3	2.18	0.43
1:D:751:ARG:CZ	1:D:763:TYR:HB2	2.48	0.43
1:D:878:LYS:N	1:D:879:PRO:HD2	2.33	0.43
3:H:107:DG:H4'	5:H:358:HOH:O	2.19	0.43
1:A:410:PHE:CD1	1:A:410:PHE:N	2.86	0.43
1:A:737:THR:O	1:A:738:PRO:C	2.62	0.43
1:A:792:ASP:OD2	1:A:792:ASP:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:MET:HE3	1:B:85:MET:CA	2.48	0.43
1:B:170:LEU:H	1:B:170:LEU:CD1	2.32	0.43
1:B:433:THR:HA	1:B:460:GLY:O	2.18	0.43
1:B:454:TYR:HB3	1:B:463:TYR:O	2.18	0.43
1:B:470:VAL:O	1:B:474:GLU:HG2	2.18	0.43
1:B:750:ARG:HG2	1:B:754:GLN:NE2	2.34	0.43
1:C:20:ILE:HD13	1:C:107:LYS:HB2	2.00	0.43
1:C:206:GLN:HA	1:C:206:GLN:NE2	2.33	0.43
1:C:277:TYR:O	1:C:281:SER:HB3	2.19	0.43
1:D:20:ILE:CG2	1:D:24:GLY:HA2	2.48	0.43
1:D:255:ASN:HD22	1:D:256:MET:N	2.14	0.43
2:E:1:DC:H2'	2:E:2:DG:C5	2.54	0.43
1:A:836:ARG:HG3	1:A:836:ARG:HH11	1.82	0.43
1:A:903:PHE:C	1:A:903:PHE:HD1	2.26	0.43
1:B:87:ASP:OD1	1:B:90:LEU:HD22	2.19	0.43
1:B:706:LYS:HD3	3:H:113:DC:C1'	2.49	0.43
5:B:1014:HOH:O	2:G:6:DA:H5'	2.19	0.43
1:C:481:GLN:HB3	1:C:559:ARG:HH11	1.83	0.43
1:C:559:ARG:HA	1:C:559:ARG:HD3	1.90	0.43
1:D:135:ALA:C	1:D:136:ILE:HG13	2.43	0.43
1:D:180:SER:HA	1:D:183:ILE:HB	2.01	0.43
1:A:304:LYS:O	1:A:319:ARG:HD3	2.18	0.43
1:A:544:ARG:HB3	1:A:547:ARG:NH2	2.32	0.43
1:A:854:ILE:HD13	1:A:859:LYS:HA	2.01	0.43
1:B:104:ASP:OD2	1:B:104:ASP:C	2.59	0.43
1:B:441:ASP:HB3	1:B:447:ALA:HB2	2.00	0.43
1:B:811:TYR:HB2	1:B:847:ALA:O	2.18	0.43
1:C:145:ARG:HB2	1:C:147:TYR:CE1	2.54	0.43
1:C:362:ILE:HG23	1:C:575:PHE:CD1	2.54	0.43
1:D:391:TYR:HD1	1:D:391:TYR:H	1.66	0.43
1:D:519:ARG:HG3	1:D:519:ARG:NH1	2.33	0.43
2:E:4:CTG:O5'	2:E:4:CTG:H6	2.19	0.43
1:A:129:ALA:HB1	1:A:229:ARG:HG2	2.01	0.43
1:A:203:ASN:HD22	1:A:203:ASN:HA	1.57	0.43
1:A:579:ASP:HB3	1:A:582:ASN:HB2	2.01	0.43
1:B:491:ALA:HA	1:B:494:ARG:CG	2.45	0.43
1:B:497:GLU:HG2	1:B:498:ILE:HD12	1.99	0.43
1:C:540:GLU:O	1:C:544:ARG:HG3	2.19	0.43
1:D:37:LEU:HD12	1:D:71:TRP:CE3	2.54	0.43
1:D:395:PHE:HD2	1:D:594:LEU:HD23	1.84	0.43
1:D:569:ALA:C	1:D:571:GLY:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:12:DA:H2''	2:I:13:DG:H5'	2.00	0.43
1:A:31:VAL:HG12	1:A:33:TYR:N	2.34	0.43
1:B:312:LEU:HD12	1:B:320:TYR:HB2	1.99	0.43
1:B:625:ILE:HG12	1:B:683:MET:CE	2.49	0.43
1:B:704:GLY:O	1:B:705:LYS:C	2.62	0.43
1:B:727:ILE:HG21	1:B:732:THR:CG2	2.48	0.43
1:C:3:GLU:O	1:C:99:TYR:OH	2.36	0.43
1:D:187:ILE:O	1:D:187:ILE:HG22	2.19	0.43
1:D:206:GLN:HA	1:D:206:GLN:HE21	1.84	0.43
1:D:569:ALA:O	1:D:571:GLY:N	2.52	0.43
3:F:109:DC:H1'	3:F:110:DA:H5''	2.01	0.43
1:A:298:LEU:HD11	1:A:334:ILE:HG12	1.99	0.43
1:A:854:ILE:HG23	1:A:859:LYS:CB	2.49	0.43
1:A:854:ILE:CG1	1:A:858:ILE:HG13	2.49	0.43
1:C:62:PHE:CD2	1:C:68:ALA:HA	2.54	0.43
1:C:83:LEU:N	1:C:83:LEU:CD2	2.82	0.43
1:C:111:ALA:HB2	1:C:210:PRO:HB3	2.00	0.43
1:C:163:SER:CB	1:C:166:ILE:HD12	2.49	0.43
1:C:465:LYS:NZ	1:C:675:ASN:ND2	2.66	0.43
1:C:775:ASN:OD1	1:C:777:ILE:N	2.50	0.43
1:D:731:GLU:CA	1:D:734:LYS:HG2	2.48	0.43
1:A:137:THR:HB	1:A:328:VAL:HG21	2.00	0.42
1:A:281:SER:O	1:A:282:PHE:C	2.62	0.42
1:A:653:LYS:HD3	1:A:657:GLU:OE1	2.18	0.42
1:A:706:LYS:HE3	3:F:113:DC:H1'	2.01	0.42
1:B:195:LYS:O	1:B:199:MET:HB2	2.18	0.42
1:B:499:ILE:HB	1:B:542:LEU:HD13	2.01	0.42
1:B:658:ARG:HH11	1:B:658:ARG:HG3	1.84	0.42
1:C:182:ILE:HG21	1:C:329:TYR:CD1	2.54	0.42
1:C:506:PRO:CG	1:C:535:ALA:HB2	2.49	0.42
1:D:15:ILE:HD12	1:D:33:TYR:HB2	2.01	0.42
2:G:11:DC:H2''	2:G:12:DA:C8	2.54	0.42
1:A:874:LYS:HG3	1:A:875:THR:HG23	2.01	0.42
1:B:494:ARG:HH12	1:B:495:ASN:HB2	1.83	0.42
1:B:751:ARG:NE	1:B:763:TYR:HB2	2.34	0.42
1:D:426:SER:HB2	1:D:472:PRO:CD	2.45	0.42
1:A:139:TYR:CE2	1:A:332:LEU:HD21	2.54	0.42
1:A:260:ARG:HG2	1:A:260:ARG:HH11	1.85	0.42
1:A:546:GLN:HE21	1:A:546:GLN:HB2	1.61	0.42
1:A:776:TYR:CD1	1:A:863:LEU:HD11	2.54	0.42
1:B:123:PHE:HA	1:B:124:PRO:HD3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:HIS:CD2	1:B:138:HIS:C	2.98	0.42
1:B:517:ASP:OD1	1:B:519:ARG:HB2	2.20	0.42
1:C:267:GLY:HA2	5:C:1018:HOH:O	2.18	0.42
1:D:10:GLN:HG3	1:D:65:MET:HE1	2.01	0.42
1:D:78:ILE:O	1:D:78:ILE:HG13	2.19	0.42
1:D:330:ARG:HD3	1:D:330:ARG:HA	1.85	0.42
2:K:3:DC:H2''	2:K:4:CTG:H72	2.00	0.42
1:A:428:GLU:OE2	1:A:428:GLU:N	2.43	0.42
1:A:508:LEU:HD22	1:A:508:LEU:N	2.33	0.42
1:A:562:LEU:O	1:A:563:ILE:C	2.63	0.42
1:A:745:LEU:HD12	1:A:745:LEU:HA	1.83	0.42
1:A:752:MET:HG2	1:A:889:LEU:HD13	2.02	0.42
1:C:725:LEU:HD11	1:C:750:ARG:HB2	1.99	0.42
1:D:167:ALA:O	1:D:178:VAL:HB	2.20	0.42
1:D:297:GLU:OE1	1:D:338:ARG:NH1	2.52	0.42
1:D:556:GLN:C	1:D:556:GLN:CD	2.88	0.42
1:D:685:ARG:NH1	1:D:714:ASP:OD2	2.49	0.42
1:D:685:ARG:NH2	1:D:714:ASP:OD2	2.50	0.42
1:D:708:TYR:CZ	1:D:728:MET:HG3	2.54	0.42
1:D:819:ILE:HG13	1:D:819:ILE:O	2.19	0.42
1:A:796:PHE:CE1	1:A:813:ARG:HD3	2.55	0.42
1:B:326:ILE:O	1:B:330:ARG:HG2	2.19	0.42
1:C:298:LEU:O	1:C:299:ASN:CB	2.66	0.42
1:C:369:ILE:HG12	1:C:474:GLU:HG2	2.02	0.42
1:C:438:PRO:HD2	1:C:441:ASP:OD2	2.19	0.42
1:D:512:GLU:CB	1:D:537:SER:HB2	2.50	0.42
1:D:823:GLN:HE21	1:D:823:GLN:HB3	1.60	0.42
1:A:844:LYS:HD2	1:A:844:LYS:N	2.31	0.42
1:B:119:SER:CB	1:B:124:PRO:HG3	2.42	0.42
1:B:625:ILE:HG12	1:B:683:MET:HE2	2.00	0.42
1:C:163:SER:OG	1:C:166:ILE:HG13	2.19	0.42
1:C:186:ILE:HG22	1:C:187:ILE:N	2.35	0.42
1:D:197:LEU:HD23	1:D:197:LEU:C	2.44	0.42
1:D:361:PRO:HD2	2:K:3:DC:OP1	2.19	0.42
1:D:740:ALA:HB1	1:D:774:LEU:HD13	2.02	0.42
2:I:12:DA:H2'	2:I:13:DG:C8	2.54	0.42
1:A:868:TYR:O	1:A:869:THR:C	2.62	0.42
1:C:465:LYS:NZ	1:C:675:ASN:HD21	2.17	0.42
1:C:469:GLY:C	1:C:472:PRO:HD2	2.44	0.42
1:C:888:LYS:NZ	5:C:1016:HOH:O	2.53	0.42
1:D:700:GLY:HA2	1:D:753:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:HB2	1:A:20:ILE:O	2.20	0.42
1:A:41:CYS:HB3	1:A:58:THR:HG22	2.01	0.42
1:A:234:PHE:CD1	1:A:234:PHE:N	2.87	0.42
1:A:510:VAL:O	1:A:510:VAL:HG23	2.18	0.42
1:A:514:LEU:CG	1:A:529:LYS:HE3	2.49	0.42
1:A:714:ASP:OD1	1:A:718:THR:C	2.63	0.42
1:A:776:TYR:CZ	1:A:777:ILE:HG13	2.54	0.42
1:B:285:GLN:NE2	1:B:286:PRO:HD2	2.35	0.42
1:B:347:MET:HE1	1:B:350:TYR:HD2	1.85	0.42
1:B:699:GLY:C	1:B:753:LEU:HD22	2.45	0.42
1:B:834:PRO:O	1:B:866:MET:HA	2.19	0.42
1:C:457:SER:O	1:C:459:ASN:N	2.52	0.42
1:C:528:GLU:HA	1:C:528:GLU:OE2	2.19	0.42
1:C:592:MET:HE2	1:C:670:MET:SD	2.59	0.42
1:C:597:ILE:O	1:C:601:VAL:HG23	2.19	0.42
1:D:880:LEU:HD22	1:D:884:THR:CG2	2.50	0.42
1:A:309:ILE:HD12	1:A:312:LEU:HD23	2.01	0.42
1:A:606:ASN:HD21	1:A:613:GLY:N	2.17	0.42
1:B:9:GLU:HG2	1:B:266:PHE:CD2	2.53	0.42
1:B:273:TYR:OH	1:B:340:PHE:HB2	2.20	0.42
1:C:411:ASP:O	1:C:683:MET:HA	2.20	0.42
1:C:458:PRO:CG	1:C:592:MET:SD	3.08	0.42
1:C:811:TYR:CE2	1:C:815:ILE:HD13	2.55	0.42
1:D:181:GLU:CD	1:D:181:GLU:H	2.28	0.42
1:D:434:PHE:HE1	1:D:461:MET:O	2.03	0.42
1:D:461:MET:HB3	1:D:463:TYR:CE1	2.54	0.42
1:D:475:ILE:HD13	1:D:566:LEU:CD2	2.50	0.42
1:D:566:LEU:HD12	1:D:566:LEU:O	2.20	0.42
1:A:191:PHE:CZ	1:A:200:GLU:HG2	2.55	0.42
1:A:422:GLN:HE21	1:A:422:GLN:HB2	1.70	0.42
1:A:434:PHE:HD1	1:A:435:LYS:O	2.03	0.42
1:A:489:MET:SD	1:A:553:MET:N	2.92	0.42
1:A:514:LEU:H	1:A:541:MET:HE3	1.82	0.42
1:A:779:ILE:HG21	1:A:871:LEU:HD21	2.02	0.42
1:B:126:PRO:HB2	1:B:224:PRO:HB2	2.02	0.42
1:B:224:PRO:HA	1:B:263:ILE:HD12	2.01	0.42
1:B:489:MET:SD	1:B:490:LEU:N	2.93	0.42
1:C:218:VAL:HA	1:C:222:ALA:HB3	2.01	0.42
1:C:283:THR:HG23	1:C:283:THR:O	2.20	0.42
1:C:413:THR:O	1:C:414:SER:C	2.63	0.42
1:D:250:VAL:HG22	1:D:263:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:LEU:CD1	1:D:326:ILE:HD12	2.49	0.42
1:D:800:LYS:O	1:D:802:PRO:HD3	2.20	0.42
3:J:110:DA:H1'	3:J:111:DT:C5'	2.49	0.42
2:K:11:DC:H2''	2:K:12:DA:C5'	2.48	0.42
1:A:202:LEU:O	1:A:206:GLN:HG2	2.20	0.41
1:A:556:GLN:HG3	1:A:557:ILE:H	1.85	0.41
1:A:789:ALA:HA	1:A:792:ASP:OD1	2.20	0.41
1:B:82:ALA:N	1:B:382:GLN:HE21	2.02	0.41
1:B:147:TYR:CD1	1:B:147:TYR:N	2.89	0.41
1:B:501:GLU:HG3	1:B:501:GLU:O	2.19	0.41
1:C:96:THR:O	1:C:96:THR:HG22	2.20	0.41
1:C:251:LYS:HB3	1:C:262:ILE:HG13	2.01	0.41
1:C:482:ARG:O	1:C:486:LYS:HB2	2.19	0.41
1:D:132:PRO:HA	1:D:229:ARG:CZ	2.50	0.41
1:D:271:LEU:HD21	1:D:356:GLN:HA	2.01	0.41
1:D:782:VAL:HG12	1:D:783:SER:N	2.33	0.41
1:D:804:HIS:NE2	3:L:110:DA:OP1	2.49	0.41
3:H:112:DT:H5'	3:H:112:DT:C6	2.50	0.41
1:A:382:GLN:O	1:A:383:GLY:C	2.60	0.41
1:B:132:PRO:HB3	1:B:194:GLU:OE2	2.20	0.41
1:B:201:TYR:O	1:B:204:PHE:HB3	2.20	0.41
1:B:309:ILE:C	1:B:311:LYS:N	2.76	0.41
1:C:14:SER:HB2	1:C:32:GLU:OE1	2.20	0.41
1:C:258:GLY:N	5:C:987:HOH:O	2.53	0.41
1:D:49:TYR:CD1	1:D:49:TYR:N	2.88	0.41
1:D:523:SER:HB2	1:D:527:LYS:HA	2.02	0.41
1:D:583:ALA:O	1:D:586:ILE:HB	2.21	0.41
1:D:687:ALA:HB2	1:D:715:MET:SD	2.60	0.41
1:A:865:TRP:O	1:A:866:MET:C	2.62	0.41
1:B:202:LEU:HD21	1:B:238:THR:O	2.19	0.41
1:B:326:ILE:HG23	1:B:330:ARG:CZ	2.51	0.41
1:B:335:ASP:OD2	1:B:341:ILE:HG12	2.20	0.41
1:B:726:LYS:NZ	5:B:970:HOH:O	2.54	0.41
1:C:493:GLN:HB2	1:C:549:GLU:OE2	2.20	0.41
1:D:273:TYR:CE2	1:D:341:ILE:HG13	2.56	0.41
1:D:741:VAL:HG11	1:D:875:THR:O	2.20	0.41
2:G:13:DG:H1'	2:G:14:DC:H5'	2.02	0.41
3:H:105:DC:H2''	3:H:106:DT:O5'	2.21	0.41
1:A:626:TYR:N	1:A:626:TYR:CD1	2.89	0.41
1:A:776:TYR:OH	1:A:854:ILE:HG22	2.20	0.41
1:B:170:LEU:O	1:B:173:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:TYR:CD1	1:B:578:TYR:C	2.99	0.41
1:B:771:PHE:HE2	1:B:872:LEU:HB2	1.80	0.41
1:C:10:GLN:HG3	1:C:65:MET:CE	2.43	0.41
1:D:193:ASN:ND2	1:D:196:GLU:H	2.18	0.41
3:F:109:DC:H2"	3:F:110:DA:H5"	2.01	0.41
1:A:294:SER:O	1:A:298:LEU:CD1	2.69	0.41
1:A:402:ASN:OD1	1:A:403:ARG:N	2.54	0.41
1:A:489:MET:HG3	1:A:552:GLY:HA3	2.03	0.41
1:B:75:MET:HA	1:B:78:ILE:HG22	2.03	0.41
1:B:85:MET:HE1	1:B:576:ARG:NH2	2.36	0.41
1:B:153:ASN:OD1	1:B:158:ASN:HB3	2.20	0.41
1:B:373:LEU:HD12	1:B:380:ILE:HG22	2.03	0.41
1:B:405:LYS:O	1:B:690:GLY:HA2	2.20	0.41
1:B:544:ARG:HH21	1:B:544:ARG:HG2	1.85	0.41
1:B:836:ARG:HG3	1:B:865:TRP:O	2.20	0.41
1:C:131:HIS:C	1:C:229:ARG:CZ	2.94	0.41
1:C:660:GLU:HB2	1:C:661:PRO:CD	2.41	0.41
1:D:201:TYR:O	1:D:204:PHE:HB3	2.20	0.41
1:D:373:LEU:CD1	1:D:380:ILE:HG22	2.48	0.41
1:D:727:ILE:HB	1:D:733:GLN:OE1	2.19	0.41
1:D:757:GLU:CB	1:D:889:LEU:HD22	2.51	0.41
1:D:876:PHE:O	1:D:880:LEU:HB2	2.21	0.41
1:A:50:PHE:CD2	1:A:56:PRO:HA	2.55	0.41
1:A:491:ALA:C	1:A:493:GLN:N	2.77	0.41
1:B:207:GLN:O	1:B:208:LYS:HG3	2.21	0.41
1:B:216:TRP:H	1:B:218:VAL:HG23	1.86	0.41
1:B:235:GLY:O	1:B:236:GLU:C	2.64	0.41
1:B:279:LYS:HE3	1:B:280:PHE:CE2	2.55	0.41
1:B:309:ILE:C	1:B:311:LYS:H	2.28	0.41
1:B:557:ILE:HD13	1:B:557:ILE:HA	1.87	0.41
1:C:414:SER:O	1:C:415:LEU:C	2.61	0.41
1:C:811:TYR:OH	1:C:822:PRO:HG2	2.21	0.41
1:D:151:LEU:HD11	1:D:153:ASN:O	2.21	0.41
1:D:391:TYR:N	1:D:391:TYR:CD1	2.89	0.41
1:D:499:ILE:HG13	1:D:545:ALA:HB3	2.01	0.41
1:A:548:THR:O	1:A:549:GLU:C	2.63	0.41
1:A:833:LEU:HD23	1:A:833:LEU:C	2.46	0.41
1:B:260:ARG:HG2	1:B:260:ARG:HH11	1.86	0.41
1:B:268:ILE:CG2	1:B:269:SER:N	2.82	0.41
1:B:426:SER:HB2	1:B:472:PRO:HD2	2.03	0.41
1:B:873:GLU:HA	1:B:877:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:HD23	1:C:62:PHE:O	2.20	0.41
1:C:72:ILE:O	1:C:76:GLU:HG3	2.21	0.41
1:C:150:ASP:OD2	1:C:317:HIS:CE1	2.73	0.41
1:C:369:ILE:HG21	1:C:577:TYR:CZ	2.55	0.41
1:C:428:GLU:H	1:C:428:GLU:HG3	1.66	0.41
1:C:434:PHE:CE2	1:C:450:PRO:HB3	2.56	0.41
1:C:658:ARG:NH1	1:C:658:ARG:HG3	2.34	0.41
1:D:83:LEU:HD22	1:D:83:LEU:N	2.35	0.41
1:D:274:ILE:CG2	1:D:275:ASP:N	2.84	0.41
1:D:453:VAL:HG23	1:D:454:TYR:CG	2.56	0.41
1:D:471:VAL:N	1:D:472:PRO:CD	2.84	0.41
2:G:8:DT:C2'	2:G:9:DG:C8	2.98	0.41
3:L:107:DG:H2''	3:L:108:DT:O5'	2.20	0.41
3:L:111:DT:H2'	3:L:112:DT:C7	2.51	0.41
1:A:458:PRO:HG3	1:A:592:MET:SD	2.60	0.41
1:A:777:ILE:O	1:A:777:ILE:CG2	2.67	0.41
1:C:353:ILE:HD12	1:C:357:SER:CB	2.51	0.41
1:C:483:LYS:HB2	1:C:483:LYS:NZ	2.36	0.41
1:D:9:GLU:HG3	1:D:267:GLY:N	2.35	0.41
1:D:75:MET:O	1:D:80:LEU:HB2	2.21	0.41
1:D:147:TYR:CE2	1:D:187:ILE:HD12	2.56	0.41
1:D:163:SER:OG	1:D:166:ILE:HG13	2.21	0.41
1:D:454:TYR:CB	1:D:462:MET:HG2	2.50	0.41
1:D:618:LEU:HD11	1:D:702:TRP:CZ3	2.56	0.41
1:D:727:ILE:HG21	1:D:732:THR:OG1	2.20	0.41
2:G:3:DC:H6	2:G:3:DC:H2'	1.59	0.41
3:H:104:DG:C1'	3:H:105:DC:H5''	2.51	0.41
3:J:105:DC:H2''	3:J:106:DT:C6	2.56	0.41
1:A:82:ALA:O	1:A:382:GLN:HB2	2.21	0.41
1:A:150:ASP:OD1	1:A:317:HIS:CE1	2.74	0.41
1:A:273:TYR:CE1	1:A:335:ASP:HB2	2.56	0.41
1:A:389:GLN:HA	1:A:390:PRO:HD3	1.84	0.41
1:A:457:SER:HA	1:A:458:PRO:HD3	1.93	0.41
1:A:806:ARG:HG3	1:A:843:ASP:OD1	2.21	0.41
1:B:253:ILE:HD12	1:B:254:GLU:N	2.35	0.41
1:B:313:ARG:HD2	1:B:320:TYR:CE2	2.56	0.41
1:B:377:ASN:N	1:B:377:ASN:ND2	2.69	0.41
1:B:466:ASP:C	1:B:466:ASP:OD2	2.63	0.41
1:C:113:PHE:CE1	1:C:213:LEU:HD11	2.55	0.41
1:C:125:GLU:OE1	1:C:125:GLU:HA	2.21	0.41
1:C:189:MET:O	1:C:191:PHE:CD1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:TYR:HB2	1:C:462:MET:HG2	2.03	0.41
1:C:488:TYR:CD2	1:C:519:ARG:HD2	2.56	0.41
1:C:854:ILE:HG23	1:C:859:LYS:HB2	2.02	0.41
1:D:16:PHE:CE2	1:D:30:GLU:HG3	2.55	0.41
1:D:120:PRO:HD2	1:D:131:HIS:CD2	2.56	0.41
1:D:164:ILE:HD11	1:D:183:ILE:O	2.21	0.41
1:D:412:LEU:HG	1:D:683:MET:HE3	2.03	0.41
1:D:846:ILE:O	1:D:846:ILE:HG23	2.21	0.41
3:L:113:DC:H2'	3:L:114:DA:H8	1.84	0.41
1:A:154:SER:C	1:A:156:TYR:N	2.77	0.41
1:A:512:GLU:HA	1:A:513:PRO:HD3	1.98	0.41
1:A:839:ASN:ND2	1:A:841:PHE:HB2	2.35	0.41
1:A:880:LEU:O	1:A:881:GLU:C	2.62	0.41
1:B:20:ILE:CG2	1:B:24:GLY:HA2	2.50	0.41
1:B:403:ARG:NH2	1:B:889:LEU:HD21	2.35	0.41
1:B:660:GLU:HB2	1:B:661:PRO:HD3	2.02	0.41
1:B:728:MET:HE3	3:H:113:DC:OP1	2.20	0.41
1:D:233:ILE:O	1:D:233:ILE:HG22	2.21	0.41
1:D:294:SER:HB3	1:D:300:VAL:O	2.21	0.41
1:D:494:ARG:O	1:D:497:GLU:HB3	2.21	0.41
1:D:499:ILE:HG13	1:D:545:ALA:CB	2.50	0.41
1:D:772:ARG:O	1:D:773:GLN:NE2	2.54	0.41
3:F:113:DC:C2'	3:F:114:DA:H5''	2.51	0.41
2:I:12:DA:H5''	2:I:12:DA:C8	2.52	0.41
2:K:2:DG:H3'	2:K:3:DC:H5'	2.01	0.41
1:A:281:SER:HA	5:A:943:HOH:O	2.21	0.40
1:A:654:PHE:HD1	1:A:659:MET:HE2	1.85	0.40
1:A:757:GLU:HB2	1:A:889:LEU:HD22	2.03	0.40
1:B:155:PRO:HG2	1:B:156:TYR:CE1	2.56	0.40
1:B:592:MET:HE2	1:B:592:MET:HB3	1.99	0.40
1:B:685:ARG:CG	1:B:685:ARG:NH1	2.83	0.40
1:C:206:GLN:HA	1:C:206:GLN:HE21	1.86	0.40
1:C:635:LYS:HA	1:C:635:LYS:HD2	1.82	0.40
1:C:774:LEU:O	1:C:775:ASN:C	2.64	0.40
1:D:186:ILE:CG2	1:D:187:ILE:N	2.83	0.40
1:D:273:TYR:HE2	1:D:341:ILE:HG13	1.86	0.40
1:D:455:SER:OG	1:D:676:ASN:HA	2.21	0.40
1:D:739:LYS:O	1:D:740:ALA:C	2.64	0.40
1:D:867:ASP:HB3	1:D:870:VAL:HB	2.03	0.40
1:A:45:GLN:O	1:A:47:THR:HG23	2.21	0.40
1:A:807:GLY:HA2	1:A:810:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:GLU:HA	1:B:734:LYS:HG2	2.02	0.40
1:C:87:ASP:OD2	1:C:90:LEU:HD13	2.20	0.40
1:D:541:MET:HA	1:D:544:ARG:CD	2.33	0.40
1:D:643:ASP:HA	1:D:693:LEU:HD23	2.04	0.40
2:E:7:DA:C2'	2:E:8:DT:C7	2.99	0.40
2:G:15:DC:H2''	2:G:16:DG:O5'	2.22	0.40
1:A:257:TYR:CD2	1:A:786:ASN:HB3	2.57	0.40
1:A:372:SER:OG	1:A:477:LYS:NZ	2.38	0.40
1:A:516:VAL:HB	1:A:526:ILE:HG13	2.03	0.40
1:A:829:LYS:O	1:A:850:SER:HB3	2.21	0.40
1:B:326:ILE:HG23	1:B:330:ARG:NH1	2.36	0.40
1:B:550:VAL:O	1:B:551:ALA:C	2.64	0.40
1:B:737:THR:HA	1:B:738:PRO:HD3	1.96	0.40
1:C:18:ARG:NH2	1:C:211:VAL:HA	2.37	0.40
1:C:658:ARG:HD2	1:C:658:ARG:N	2.35	0.40
1:C:658:ARG:N	1:C:658:ARG:CD	2.83	0.40
1:D:62:PHE:HE2	1:D:71:TRP:HB2	1.86	0.40
1:D:143:ASP:O	1:D:144:ASP:CB	2.69	0.40
1:D:218:VAL:CG2	1:D:223:ILE:HG13	2.51	0.40
1:D:757:GLU:CG	1:D:889:LEU:HD22	2.52	0.40
1:A:201:TYR:O	1:A:204:PHE:HB3	2.21	0.40
1:B:273:TYR:HA	1:B:276:LEU:HD12	2.03	0.40
1:C:750:ARG:HG2	1:C:750:ARG:NH1	2.37	0.40
1:D:289:SER:O	1:D:293:ILE:HG12	2.22	0.40
1:D:512:GLU:CB	1:D:513:PRO:CA	2.99	0.40
1:D:701:PHE:CD1	1:D:701:PHE:C	2.99	0.40
1:D:828:GLU:HB3	1:D:829:LYS:H	1.79	0.40
1:A:117:VAL:HG22	1:A:133:ILE:HA	2.03	0.40
1:A:409:SER:O	1:A:686:GLU:HB2	2.21	0.40
1:A:703:THR:HG21	1:A:707:ARG:NH1	2.36	0.40
1:A:807:GLY:O	1:A:810:THR:HG22	2.21	0.40
1:B:221:PHE:O	1:B:224:PRO:HD2	2.21	0.40
1:B:755:GLU:HB3	1:B:759:SER:OG	2.22	0.40
1:B:811:TYR:CE2	1:B:815:ILE:HD13	2.56	0.40
1:D:481:GLN:HB3	1:D:559:ARG:HH11	1.85	0.40
1:D:597:ILE:HA	1:D:597:ILE:HD12	1.70	0.40
1:D:711:ASN:HD21	1:D:723:PRO:HB2	1.87	0.40
2:G:11:DC:H2''	2:G:12:DA:H8	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	901/906 (99%)	781 (87%)	105 (12%)	15 (2%)	7	12
1	B	901/906 (99%)	816 (91%)	79 (9%)	6 (1%)	18	30
1	C	898/906 (99%)	818 (91%)	68 (8%)	12 (1%)	9	16
1	D	895/906 (99%)	769 (86%)	115 (13%)	11 (1%)	10	17
All	All	3595/3624 (99%)	3184 (89%)	367 (10%)	44 (1%)	10	17

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	524	ASP
1	A	300	VAL
1	A	773	GLN
1	A	825	VAL
1	A	856	ASP
1	C	161	GLU
1	C	300	VAL
1	D	21	ASP
1	D	35	PRO
1	D	729	GLY
1	A	105	HIS
1	B	256	MET
1	B	635	LYS
1	C	172	GLU
1	C	352	LYS
1	C	458	PRO
1	C	622	THR
1	D	80	LEU
1	D	98	ASN
1	A	283	THR
1	A	614	GLU
1	A	738	PRO

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Mol	Chain	Res	Type
1	A	849	PRO
1	B	622	THR
1	C	179	PRO
1	C	506	PRO
1	D	570	LEU
1	D	622	THR
1	A	414	SER
1	A	622	THR
1	A	869	THR
1	C	576	ARG
1	D	414	SER
1	B	179	PRO
1	C	155	PRO
1	A	846	ILE
1	A	729	GLY
1	B	300	VAL
1	B	513	PRO
1	C	470	VAL
1	C	513	PRO
1	D	78	ILE
1	D	526	ILE
1	A	822	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	792/803 (99%)	740 (93%)	52 (7%)	15	26
1	B	780/803 (97%)	742 (95%)	38 (5%)	22	38
1	C	794/803 (99%)	752 (95%)	42 (5%)	20	35
1	D	743/803 (92%)	705 (95%)	38 (5%)	21	36
All	All	3109/3212 (97%)	2939 (94%)	170 (6%)	19	33

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	43	GLU
1	A	70	GLN
1	A	73	LYS
1	A	105	HIS
1	A	130	LYS
1	A	203	ASN
1	A	207	GLN
1	A	213	LEU
1	A	229	ARG
1	A	231	LYS
1	A	242	LEU
1	A	253	ILE
1	A	298	LEU
1	A	304	LYS
1	A	314	GLU
1	A	318	GLN
1	A	319	ARG
1	A	342	ASN
1	A	372	SER
1	A	413	THR
1	A	451	SER
1	A	466	ASP
1	A	467	ARG
1	A	475	ILE
1	A	479	PHE
1	A	503	LEU
1	A	544	ARG
1	A	546	GLN
1	A	556	GLN
1	A	587	THR
1	A	597	ILE
1	A	618	LEU
1	A	631	LYS
1	A	703	THR
1	A	728	MET
1	A	731	GLU
1	A	743	LYS
1	A	745	LEU
1	A	758	GLU
1	A	772	ARG
1	A	777	ILE
1	A	825	VAL

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Mol	Chain	Res	Type
1	A	826	GLU
1	A	844	LYS
1	A	848	TRP
1	A	849	PRO
1	A	861	ASP
1	A	862	VAL
1	A	881	GLU
1	A	888	LYS
1	A	903	PHE
1	B	43	GLU
1	B	45	GLN
1	B	61	LEU
1	B	90	LEU
1	B	93	LEU
1	B	102	LYS
1	B	116	GLU
1	B	164	ILE
1	B	166	ILE
1	B	234	PHE
1	B	312	LEU
1	B	378	LYS
1	B	379	VAL
1	B	403	ARG
1	B	421	ARG
1	B	435	LYS
1	B	468	ASP
1	B	475	ILE
1	B	479	PHE
1	B	483	LYS
1	B	489	MET
1	B	511	ASP
1	B	522	PHE
1	B	556	GLN
1	B	558	ASN
1	B	573	VAL
1	B	597	ILE
1	B	658	ARG
1	B	685	ARG
1	B	728	MET
1	B	734	LYS
1	B	742	GLN
1	B	758	GLU

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Mol	Chain	Res	Type
1	B	766	GLU
1	B	772	ARG
1	B	843	ASP
1	B	856	ASP
1	B	894	LYS
1	C	11	ILE
1	C	27	ARG
1	C	55	LYS
1	C	58	THR
1	C	83	LEU
1	C	93	LEU
1	C	106	THR
1	C	200	GLU
1	C	255	ASN
1	C	257	TYR
1	C	276	LEU
1	C	314	GLU
1	C	326	ILE
1	C	356	GLN
1	C	399	PRO
1	C	428	GLU
1	C	439	LEU
1	C	468	ASP
1	C	474	GLU
1	C	483	LYS
1	C	511	ASP
1	C	525	GLU
1	C	533	LEU
1	C	559	ARG
1	C	561	LEU
1	C	562	LEU
1	C	572	ASN
1	C	587	THR
1	C	592	MET
1	C	612	GLU
1	C	618	LEU
1	C	640	LYS
1	C	658	ARG
1	C	672	GLU
1	C	760	LEU
1	C	762	GLU
1	C	843	ASP

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Mol	Chain	Res	Type
1	C	856	ASP
1	C	874	LYS
1	C	878	LYS
1	C	880	LEU
1	C	898	PHE
1	D	14	SER
1	D	43	GLU
1	D	125	GLU
1	D	200	GLU
1	D	257	TYR
1	D	279	LYS
1	D	299	ASN
1	D	317	HIS
1	D	372	SER
1	D	391	TYR
1	D	411	ASP
1	D	413	THR
1	D	428	GLU
1	D	439	LEU
1	D	456	CYS
1	D	468	ASP
1	D	477	LYS
1	D	483	LYS
1	D	484	GLU
1	D	508	LEU
1	D	521	ASP
1	D	522	PHE
1	D	536	LYS
1	D	557	ILE
1	D	558	ASN
1	D	559	ARG
1	D	562	LEU
1	D	597	ILE
1	D	618	LEU
1	D	649	ASP
1	D	686	GLU
1	D	731	GLU
1	D	776	TYR
1	D	777	ILE
1	D	823	GLN
1	D	828	GLU
1	D	874	LYS

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Mol	Chain	Res	Type
1	D	880	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	40	HIS
1	A	64	ASN
1	A	70	GLN
1	A	98	ASN
1	A	112	ASN
1	A	153	ASN
1	A	203	ASN
1	A	207	GLN
1	A	228	ASN
1	A	284	ASN
1	A	285	GLN
1	A	333	GLN
1	A	371	ASN
1	A	376	GLN
1	A	377	ASN
1	A	386	HIS
1	A	389	GLN
1	A	422	GLN
1	A	504	HIS
1	A	505	ASN
1	A	546	GLN
1	A	556	GLN
1	A	558	ASN
1	A	572	ASN
1	A	602	ASN
1	A	606	ASN
1	A	646	HIS
1	A	678	GLN
1	A	742	GLN
1	A	775	ASN
1	A	864	HIS
1	B	40	HIS
1	B	70	GLN
1	B	171	GLN
1	B	206	GLN
1	B	207	GLN

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Mol	Chain	Res	Type
1	B	255	ASN
1	B	284	ASN
1	B	285	GLN
1	B	318	GLN
1	B	333	GLN
1	B	354	GLN
1	B	376	GLN
1	B	377	ASN
1	B	382	GLN
1	B	386	HIS
1	B	389	GLN
1	B	440	HIS
1	B	444	ASN
1	B	495	ASN
1	B	558	ASN
1	B	591	GLN
1	B	595	GLN
1	B	606	ASN
1	B	646	HIS
1	B	733	GLN
1	B	742	GLN
1	B	754	GLN
1	B	775	ASN
1	B	812	ASN
1	B	818	ASN
1	B	823	GLN
1	C	10	GLN
1	C	45	GLN
1	C	112	ASN
1	C	128	GLN
1	C	173	GLN
1	C	206	GLN
1	C	207	GLN
1	C	232	ASN
1	C	245	HIS
1	C	255	ASN
1	C	284	ASN
1	C	285	GLN
1	C	318	GLN
1	C	444	ASN
1	C	539	ASN
1	C	556	GLN

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Mol	Chain	Res	Type
1	C	558	ASN
1	C	572	ASN
1	C	675	ASN
1	C	678	GLN
1	C	711	ASN
1	C	864	HIS
1	D	10	GLN
1	D	158	ASN
1	D	206	GLN
1	D	207	GLN
1	D	228	ASN
1	D	245	HIS
1	D	255	ASN
1	D	284	ASN
1	D	285	GLN
1	D	318	GLN
1	D	339	GLN
1	D	440	HIS
1	D	444	ASN
1	D	480	ASN
1	D	495	ASN
1	D	505	ASN
1	D	507	ASN
1	D	539	ASN
1	D	546	GLN
1	D	556	GLN
1	D	558	ASN
1	D	572	ASN
1	D	645	ASN
1	D	675	ASN
1	D	678	GLN
1	D	711	ASN
1	D	742	GLN
1	D	754	GLN
1	D	761	GLN
1	D	773	GLN
1	D	787	ASN
1	D	818	ASN
1	D	823	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
2	CTG	K	4	3,2	18,23,24	0.79	1 (5%)	21,35,38	0.75	1 (4%)
2	CTG	E	4	3,2	18,23,24	0.74	0	21,35,38	1.06	2 (9%)
2	CTG	G	4	3,2	18,23,24	0.71	0	21,35,38	0.96	1 (4%)
2	CTG	I	4	3,2	18,23,24	0.71	0	21,35,38	1.01	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
2	CTG	K	4	3,2	-	2/7/45/46	0/2/2/2
2	CTG	E	4	3,2	-	2/7/45/46	0/2/2/2
2	CTG	G	4	3,2	-	1/7/45/46	0/2/2/2
2	CTG	I	4	3,2	-	0/7/45/46	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	4	CTG	C1'-N1	2.14	1.48	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	CTG	C2'-C1'-N1	-3.09	111.41	115.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4	CTG	C2'-C1'-N1	-2.83	111.76	115.59
2	I	4	CTG	C2'-C1'-N1	-2.74	111.88	115.59
2	I	4	CTG	N3-C2-N1	-2.44	114.23	116.78
2	E	4	CTG	N3-C2-N1	-2.29	114.39	116.78
2	K	4	CTG	N3-C2-N1	-2.17	114.52	116.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	4	CTG	C2'-C1'-N1-C6
2	K	4	CTG	O4'-C1'-N1-C6
2	G	4	CTG	O4'-C4'-C5'-O5'
2	E	4	CTG	C2'-C1'-N1-C6
2	E	4	CTG	O4'-C1'-N1-C6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	4	CTG	2	0
2	E	4	CTG	3	0
2	G	4	CTG	3	0
2	I	4	CTG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
4	SO4	C	907	-	4,4,4	0.38	0	6,6,6	0.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	903/906 (99%)	0.43	89 (9%)	13	10	24, 53, 143, 162	1 (0%)
1	B	903/906 (99%)	0.33	60 (6%)	24	18	20, 59, 157, 172	0
1	C	900/906 (99%)	-0.00	18 (2%)	65	59	17, 47, 89, 109	0
1	D	897/906 (99%)	1.11	151 (16%)	4	3	48, 98, 134, 169	0
2	E	17/18 (94%)	1.22	3 (17%)	4	3	70, 88, 124, 132	0
2	G	17/18 (94%)	0.19	0	100	100	45, 57, 79, 92	0
2	I	17/18 (94%)	-0.26	0	100	100	32, 38, 85, 94	0
2	K	17/18 (94%)	1.36	3 (17%)	4	3	59, 126, 147, 151	0
3	F	14/14 (100%)	1.43	3 (21%)	2	1	85, 117, 130, 134	0
3	H	14/14 (100%)	0.43	0	100	100	53, 70, 83, 85	0
3	J	14/14 (100%)	-0.15	0	100	100	30, 45, 93, 99	0
3	L	14/14 (100%)	1.30	2 (14%)	6	5	120, 131, 135, 136	0
All	All	3727/3752 (99%)	0.47	329 (8%)	15	12	17, 62, 132, 172	1 (0%)

All (329) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	817	GLY	7.3
1	A	848	TRP	6.2
1	D	526	ILE	6.1
1	D	530	ILE	5.8
1	A	811	TYR	5.4
1	B	503	LEU	4.9
1	A	846	ILE	4.9
1	D	522	PHE	4.9
1	D	535	ALA	4.8
1	A	847	ALA	4.8
1	D	800	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	863	LEU	4.7
1	D	490	LEU	4.6
1	C	303	LEU	4.5
1	D	115	ILE	4.5
1	A	256	MET	4.4
1	D	799	PRO	4.4
1	D	868	TYR	4.4
1	A	815	ILE	4.3
1	B	522	PHE	4.3
1	A	824	VAL	4.3
1	A	831	TYR	4.2
1	B	499	ILE	4.2
1	A	780	ALA	4.0
1	D	198	LEU	4.0
1	D	302	LYS	4.0
1	D	514	LEU	3.9
1	D	61	LEU	3.9
1	D	847	ALA	3.9
1	A	510	VAL	3.8
1	D	771	PHE	3.7
1	A	548	THR	3.7
1	B	505	ASN	3.7
1	D	846	ILE	3.7
1	B	310	SER	3.7
1	A	841	PHE	3.7
1	B	542	LEU	3.6
1	B	548	THR	3.6
1	D	897	LEU	3.6
1	D	858	ILE	3.6
1	A	855	THR	3.6
1	D	135	ALA	3.6
1	D	524	ASP	3.5
1	A	857	LEU	3.5
1	D	80	LEU	3.5
1	A	785	ALA	3.5
1	A	779	ILE	3.5
1	A	554	THR	3.5
1	D	498	ILE	3.5
1	D	523	SER	3.5
1	B	166	ILE	3.4
1	D	133	ILE	3.4
1	D	531	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	535	ALA	3.4
1	B	303	LEU	3.4
1	C	514	LEU	3.4
2	K	5	DG	3.4
1	A	863	LEU	3.4
1	D	303	LEU	3.4
1	B	179	PRO	3.4
1	D	528	GLU	3.4
1	D	833	LEU	3.4
1	D	78	ILE	3.4
1	D	390	PRO	3.4
1	A	789	ALA	3.3
1	D	491	ALA	3.3
1	A	520	PHE	3.3
1	D	521	ASP	3.3
1	A	862	VAL	3.3
1	D	545	ALA	3.3
1	A	550	VAL	3.3
1	D	551	ALA	3.3
1	A	516	VAL	3.3
1	D	252	VAL	3.3
1	A	833	LEU	3.2
1	A	492	ALA	3.2
1	D	155	PRO	3.2
1	D	194	GLU	3.2
1	A	795	GLY	3.2
1	B	510	VAL	3.2
1	D	499	ILE	3.2
1	A	786	ASN	3.2
1	A	791	TYR	3.2
1	A	503	LEU	3.2
1	D	496	GLY	3.2
1	A	808	ILE	3.2
1	D	819	ILE	3.2
1	D	854	ILE	3.2
1	D	543	PHE	3.2
1	B	490	LEU	3.1
1	A	849	PRO	3.1
1	A	821	ALA	3.1
1	A	508	LEU	3.1
1	A	807	GLY	3.1
1	A	832	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	510	VAL	3.1
1	D	520	PHE	3.1
1	D	550	VAL	3.1
1	B	323	TYR	3.1
1	B	495	ASN	3.1
1	A	822	PRO	3.1
2	E	3	DC	3.1
1	D	304	LYS	3.1
1	D	518	TYR	3.0
1	B	513	PRO	3.0
1	D	855	THR	3.0
1	B	520	PHE	3.0
1	A	776	TYR	3.0
1	D	485	HIS	3.0
1	A	854	ILE	3.0
1	D	205	TRP	3.0
1	A	801	CYS	3.0
1	B	504	HIS	3.0
1	A	788	ILE	3.0
1	D	489	MET	3.0
1	D	777	ILE	3.0
1	A	830	VAL	3.0
1	A	809	LEU	3.0
1	D	256	MET	3.0
1	B	498	ILE	3.0
1	D	389	GLN	2.9
1	B	507	ASN	2.9
1	C	900	MET	2.9
1	B	516	VAL	2.9
1	A	773	GLN	2.9
1	D	33	TYR	2.9
1	D	134	ASP	2.9
1	A	502	ALA	2.9
1	D	538	LEU	2.9
1	D	534	SER	2.9
1	C	156	TYR	2.9
1	B	282	PHE	2.9
1	D	803	PHE	2.9
1	B	127	SER	2.9
1	B	186	ILE	2.9
1	C	323	TYR	2.9
1	A	799	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	494	ARG	2.8
1	A	784	SER	2.8
1	B	309	ILE	2.8
1	D	309	ILE	2.8
1	A	797	PRO	2.8
1	D	128	GLN	2.8
1	A	800	LYS	2.8
3	F	101	DG	2.8
1	D	825	VAL	2.8
1	D	314	GLU	2.8
1	D	162	TRP	2.8
1	B	863	LEU	2.8
1	D	487	GLY	2.8
1	D	552	GLY	2.8
1	A	802	PRO	2.8
1	D	505	ASN	2.8
1	B	541	MET	2.8
1	D	113	PHE	2.8
1	A	253	ILE	2.7
1	B	530	ILE	2.7
1	D	152	LEU	2.7
1	A	803	PHE	2.7
1	D	323	TYR	2.7
1	A	770	GLU	2.7
1	A	793	VAL	2.7
1	D	82	ALA	2.7
1	B	803	PHE	2.7
1	D	488	TYR	2.7
1	D	776	TYR	2.7
1	D	811	TYR	2.7
2	K	3	DC	2.7
1	B	170	LEU	2.7
1	B	514	LEU	2.7
1	D	735	SER	2.7
1	D	257	TYR	2.7
1	D	15	ILE	2.7
1	D	57	CYS	2.7
1	A	539	ASN	2.7
1	D	841	PHE	2.7
1	D	391	TYR	2.6
1	B	527	LYS	2.6
1	D	266	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	805	ILE	2.6
1	A	868	TYR	2.6
1	D	533	LEU	2.6
1	B	531	LYS	2.6
1	A	555	ALA	2.6
1	C	898	PHE	2.6
1	D	506	PRO	2.6
1	A	490	LEU	2.6
1	D	529	LYS	2.6
1	A	852	THR	2.6
2	K	6	DA	2.6
1	A	819	ILE	2.6
1	A	774	LEU	2.6
1	B	277	TYR	2.6
1	B	135	ALA	2.6
1	B	300	VAL	2.6
1	D	63	ALA	2.6
1	B	523	SER	2.5
1	C	304	LYS	2.5
1	C	24	GLY	2.5
1	D	851	GLY	2.5
1	D	834	PRO	2.5
1	D	862	VAL	2.5
1	A	835	LEU	2.5
1	D	542	LEU	2.5
1	A	257	TYR	2.5
1	D	147	TYR	2.5
1	D	160	GLU	2.5
1	B	178	VAL	2.5
1	C	168	ALA	2.5
1	B	302	LYS	2.5
1	D	101	ILE	2.5
1	D	546	GLN	2.5
1	D	548	THR	2.4
1	D	779	ILE	2.4
1	D	306	ASP	2.4
1	D	250	VAL	2.4
1	D	503	LEU	2.4
1	D	857	LEU	2.4
1	A	543	PHE	2.4
1	A	530	ILE	2.4
1	C	197	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	525	GLU	2.4
1	D	150	ASP	2.4
1	B	304	LYS	2.4
1	D	393	GLY	2.4
1	B	123	PHE	2.4
3	F	109	DC	2.4
1	A	518	TYR	2.3
1	B	164	ILE	2.3
1	D	262	ILE	2.3
1	D	507	ASN	2.3
1	D	44	SER	2.3
1	B	155	PRO	2.3
3	L	114	DA	2.3
1	B	494	ARG	2.3
1	D	8	VAL	2.3
1	D	388	VAL	2.3
1	B	314	GLU	2.3
1	B	134	ASP	2.3
1	C	300	VAL	2.3
1	D	860	ASP	2.3
1	A	538	LEU	2.3
1	A	845	CYS	2.3
1	B	492	ALA	2.3
1	B	551	ALA	2.3
1	D	783	SER	2.3
1	D	610	GLY	2.3
1	A	782	VAL	2.3
1	B	550	VAL	2.3
1	D	123	PHE	2.3
1	B	819	ILE	2.2
1	C	309	ILE	2.2
1	A	536	LYS	2.2
1	D	549	GLU	2.2
1	D	112	ASN	2.2
1	D	495	ASN	2.2
1	B	547	ARG	2.2
1	D	511	ASP	2.2
1	A	865	TRP	2.2
1	D	195	LYS	2.2
1	D	395	PHE	2.2
1	D	831	TYR	2.2
1	D	36	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	897	LEU	2.2
1	D	865	TRP	2.2
1	C	1	MET	2.2
1	D	541	MET	2.2
1	A	818	ASN	2.2
1	C	257	TYR	2.2
1	A	684	ASP	2.2
1	D	60	LYS	2.2
1	D	778	SER	2.2
1	A	498	ILE	2.2
1	B	543	PHE	2.2
1	D	62	PHE	2.2
1	B	316	ASN	2.2
1	B	128	GLN	2.2
1	C	817	GLY	2.2
1	D	798	GLY	2.2
1	D	516	VAL	2.2
1	D	896	SER	2.2
1	D	261	GLU	2.1
1	A	347	MET	2.1
1	D	301	GLY	2.1
3	F	108	DT	2.1
1	A	850	SER	2.1
1	A	858	ILE	2.1
1	B	159	VAL	2.1
1	C	510	VAL	2.1
1	D	187	ILE	2.1
1	A	796	PHE	2.1
2	E	15	DC	2.1
3	L	105	DC	2.1
1	D	58	THR	2.1
1	B	506	PRO	2.1
1	D	817	GLY	2.1
1	B	117	VAL	2.1
1	D	136	ILE	2.1
1	D	282	PHE	2.1
1	B	512	GLU	2.1
1	A	810	THR	2.1
1	A	532	LYS	2.1
1	D	536	LYS	2.1
1	D	773	GLN	2.1
1	D	197	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	539	ASN	2.1
1	A	804	HIS	2.1
1	D	827	GLY	2.1
1	D	11	ILE	2.1
1	D	684	ASP	2.1
1	D	876	PHE	2.1
1	C	155	PRO	2.1
1	D	797	PRO	2.1
2	E	1	DC	2.1
1	A	541	MET	2.1
1	A	282	PHE	2.1
1	D	492	ALA	2.0
1	D	532	LYS	2.0
1	D	513	PRO	2.0
1	B	518	TYR	2.0
1	D	156	TYR	2.0
1	D	791	TYR	2.0
1	A	903	PHE	2.0
1	B	525	GLU	2.0
1	A	551	ALA	2.0
1	D	264	THR	2.0
1	A	542	LEU	2.0
1	D	774	LEU	2.0
1	D	226	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
2	CTG	K	4	22/23	0.51	0.17	144,145,151,152	0
2	CTG	E	4	22/23	0.87	0.15	102,103,106,107	0
2	CTG	G	4	22/23	0.91	0.11	65,69,71,71	0
2	CTG	I	4	22/23	0.97	0.07	44,50,54,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($\text{\AA}^2$)	Q<0.9
4	SO4	C	907	5/5	0.92	0.10	89,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.