



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:27 am GMT

PDB ID : 2P5O
Title : Crystal structure of RB69 GP43 in complex with DNA containing an abasic site analog
Authors : Hogg, M.; Wallace, S.S.; Doublie, S.
Deposited on : 2007-03-15
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

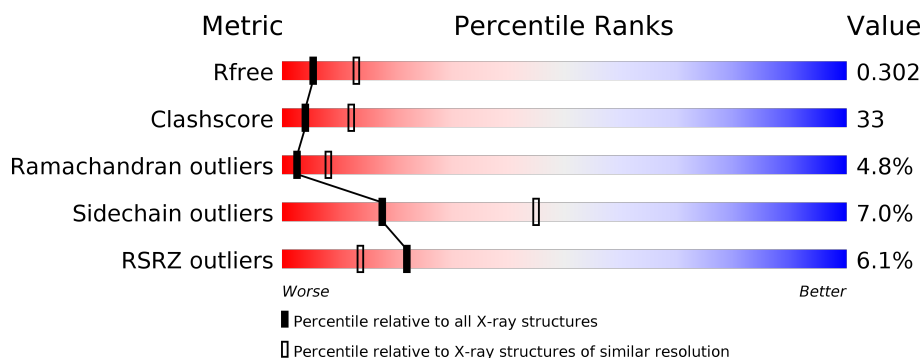
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	E	18	<div> <div>6%</div> <div>44%</div> <div>56%</div> </div>
1	G	18	<div> <div>6%</div> <div>17%</div> <div>56%</div> <div>28%</div> </div>
1	I	18	<div> <div>44%</div> <div>50%</div> <div>6%</div> </div>
1	K	18	<div> <div>28%</div> <div>6%</div> <div>44%</div> <div>50%</div> </div>
2	F	15	<div> <div>7%</div> <div>33%</div> <div>67%</div> </div>
2	H	15	<div> <div>27%</div> <div>40%</div> <div>60%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	15	<div><div></div><div>7%</div><div>33%</div><div>67%</div></div>
2	L	15	<div><div></div><div>7%</div><div>47%</div><div>47%</div><div></div></div>
3	A	903	<div><div></div><div>%</div><div>56%</div><div>35%</div><div>5%</div></div>
3	B	903	<div><div></div><div>5%</div><div>39%</div><div>40%</div><div>5%</div><div>15%</div></div>
3	C	903	<div><div></div><div>%</div><div>51%</div><div>38%</div><div>6%</div><div>6%</div></div>
3	D	903	<div><div></div><div>12%</div><div>30%</div><div>37%</div><div>7%</div><div>26%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	G	13	Total	C	N	O	P	0	0	0
			264	126	51	75	12			
1	I	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	K	9	Total	C	N	O	P	0	0	0
			181	86	37	50	8			

- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	H	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	J	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	L	8	Total	C	N	O	P	0	0	0
			163	78	30	48	7			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	856	Total	C	N	O	S	Se	0	0	0
			6941	4460	1154	1295	8	24			
3	B	771	Total	C	N	O	S	Se	0	0	0
			6245	4013	1034	1167	6	25			
3	C	853	Total	C	N	O	S	Se	0	0	0
			6895	4430	1143	1290	8	24			
3	D	671	Total	C	N	O	S	Se	0	0	0
			4934	3144	818	948	6	18			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	MODIFIED RESIDUE	UNP Q38087
A	65	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	75	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	85	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	189	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	199	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	222	ALA	ASP	ENGINEERED	UNP Q38087
A	256	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	327	ALA	ASP	ENGINEERED	UNP Q38087
A	347	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	408	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	461	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	462	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	489	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	541	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	553	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	592	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	659	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	670	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	674	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	681	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	683	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	715	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	728	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	752	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	866	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	900	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	1	MSE	-	MODIFIED RESIDUE	UNP Q38087
B	65	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	75	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	85	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	189	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	199	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	222	ALA	ASP	ENGINEERED	UNP Q38087
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B	327	ALA	ASP	ENGINEERED	UNP Q38087
B	347	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	408	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	461	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	462	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	489	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	541	MSE	MET	MODIFIED RESIDUE	UNP Q38087

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Chain	Residue	Modelled	Actual	Comment	Reference
B	553	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	592	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	659	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	670	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	674	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	681	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	683	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	715	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	728	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	752	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	866	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	900	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	1	MSE	-	MODIFIED RESIDUE	UNP Q38087
C	65	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	75	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	85	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	189	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	199	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	222	ALA	ASP	ENGINEERED	UNP Q38087
C	256	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	327	ALA	ASP	ENGINEERED	UNP Q38087
C	347	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	408	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	461	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	462	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	489	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	541	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	553	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	592	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	659	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	670	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	674	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	681	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	683	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	715	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	728	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	752	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	866	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	900	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	1	MSE	-	MODIFIED RESIDUE	UNP Q38087
D	65	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	75	MSE	MET	MODIFIED RESIDUE	UNP Q38087

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Chain	Residue	Modelled	Actual	Comment	Reference
D	85	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	189	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	199	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	222	ALA	ASP	ENGINEERED	UNP Q38087
D	256	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	327	ALA	ASP	ENGINEERED	UNP Q38087
D	347	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	408	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	461	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	462	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	489	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	541	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	553	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	592	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	659	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	670	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	674	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	681	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	683	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	715	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	728	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	752	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	866	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	900	MSE	MET	MODIFIED RESIDUE	UNP Q38087

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	3	Total O 3 3	0	0
4	F	5	Total O 5 5	0	0
4	G	7	Total O 7 7	0	0
4	H	2	Total O 2 2	0	0
4	I	17	Total O 17 17	0	0
4	J	9	Total O 9 9	0	0
4	K	8	Total O 8 8	0	0

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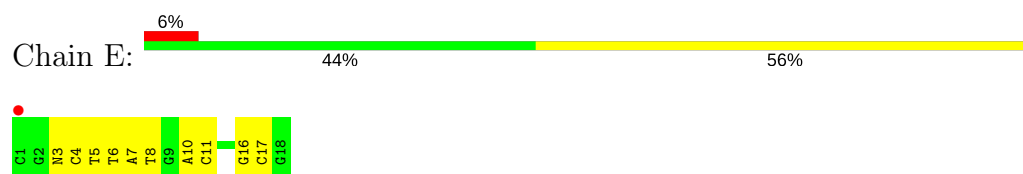
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	6	Total 6	O 6	0	0
4	A	139	Total 139	O 139	0	0
4	B	106	Total 106	O 106	0	0
4	C	147	Total 147	O 147	0	0
4	D	46	Total 46	O 46	0	0

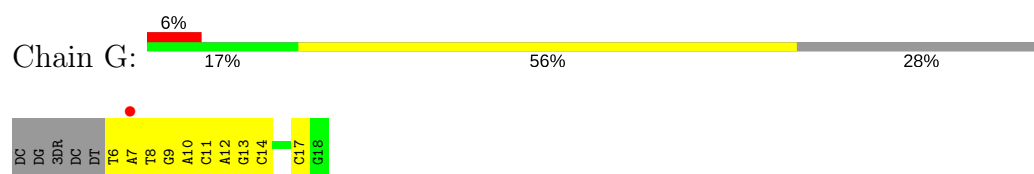
3 Residue-property plots [i](#)

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

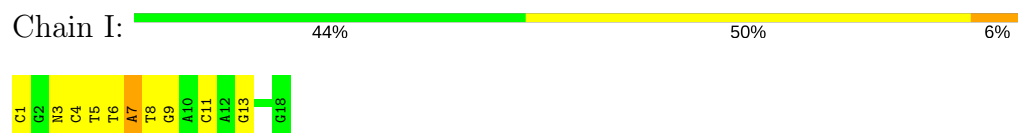
- Molecule 1: Template DNA



- Molecule 1: Template DNA



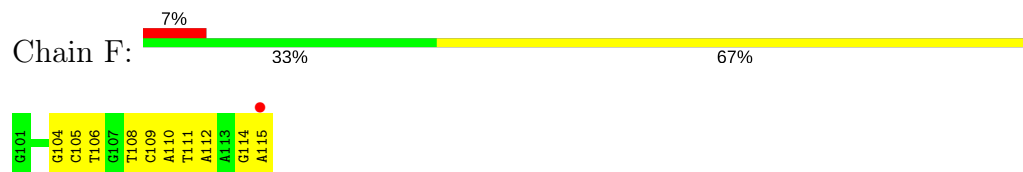
- Molecule 1: Template DNA



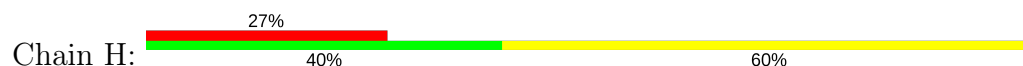
- Molecule 1: Template DNA

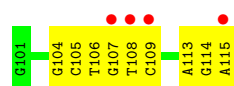


- Molecule 2: Primer DNA

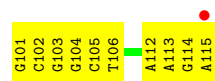


- Molecule 2: Primer DNA

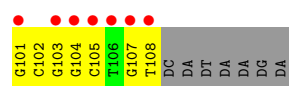




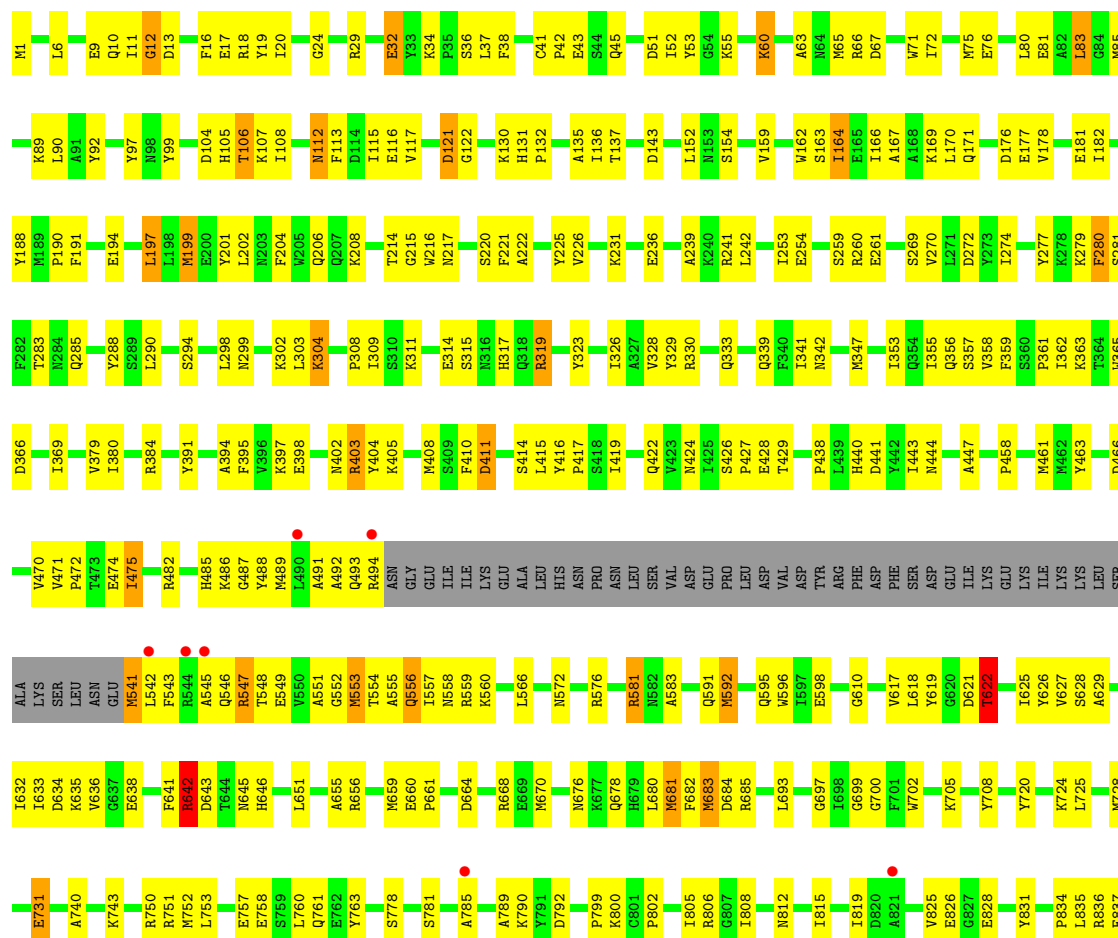
• Molecule 2: Primer DNA

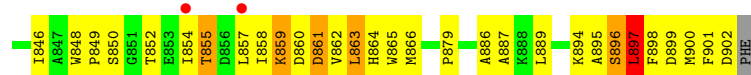


• Molecule 2: Primer DNA

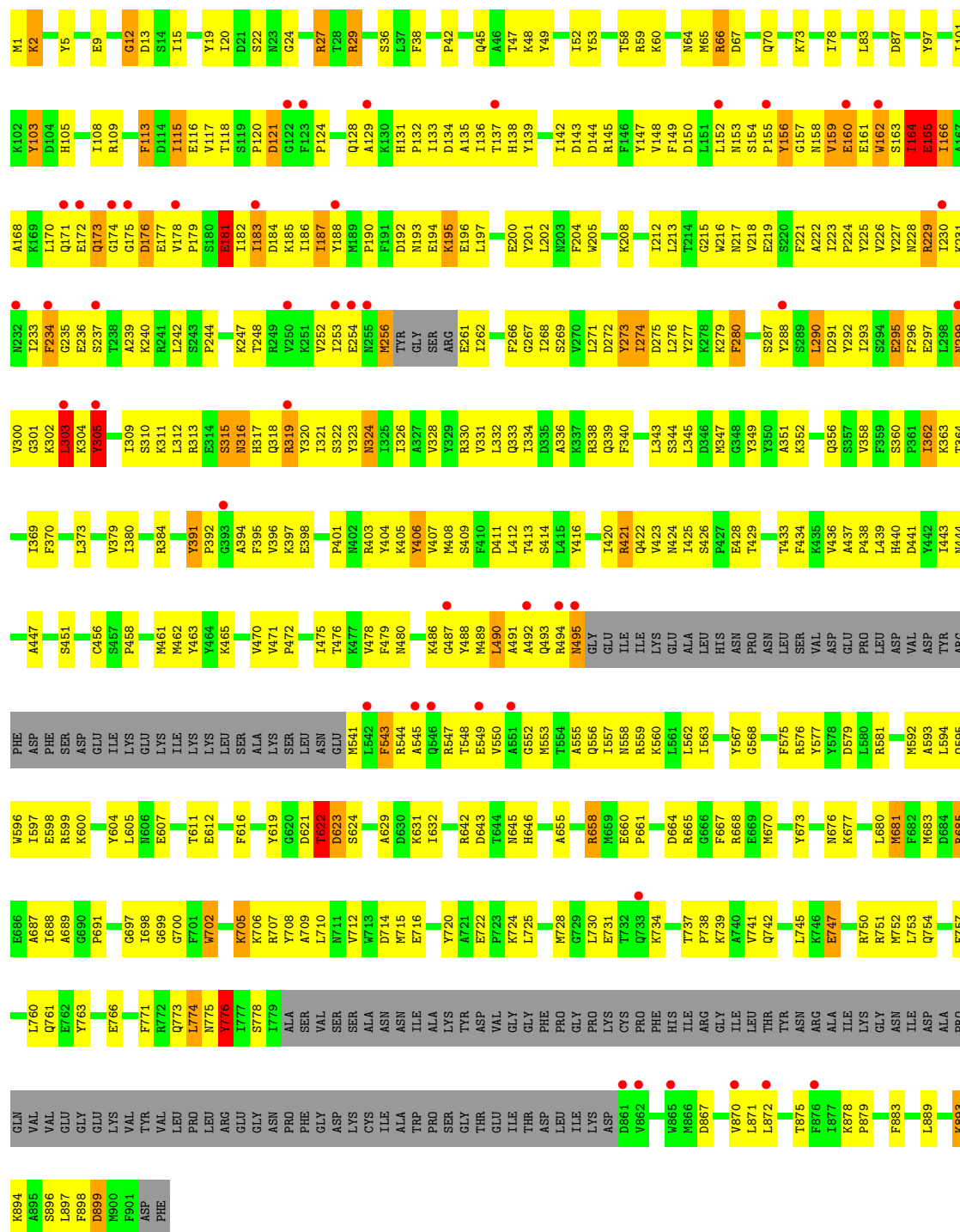


• Molecule 3: DNA polymerase

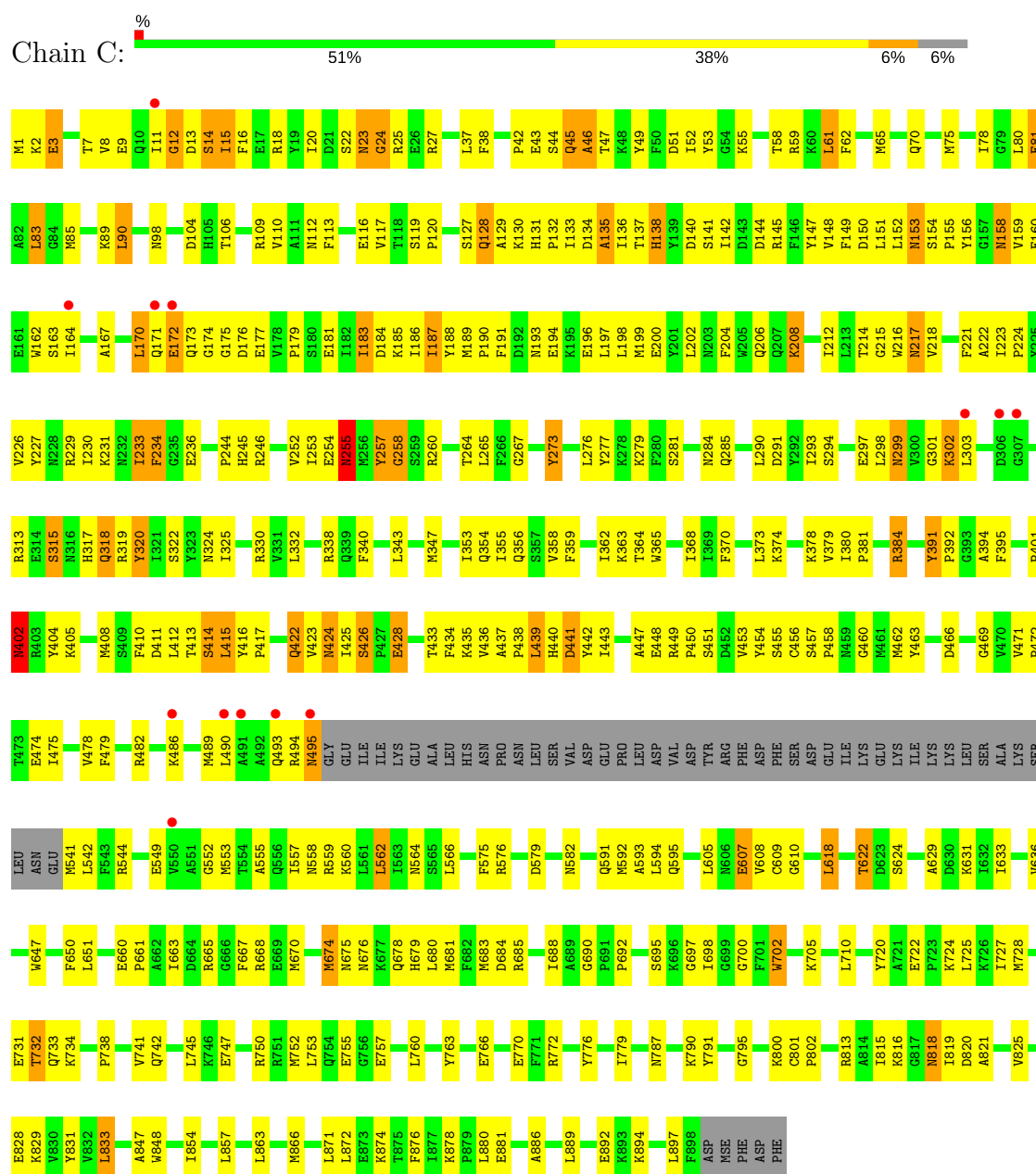




• Molecule 3: DNA polymerase



• Molecule 3: DNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.02Å 123.21Å 165.62Å 90.00° 95.82° 90.00°	Depositor
Resolution (Å)	44.00 – 2.80 44.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.9 (44.00-2.80) 95.8 (44.11-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.290 0.263 , 0.302	Depositor DCC
R_{free} test set	12094 reflections (9.67%)	DCC
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	27752	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.36	0/384	0.68	0/588
1	G	0.40	0/296	0.91	1/455 (0.2%)
1	I	0.55	0/384	0.78	0/588
1	K	0.37	0/203	0.66	0/311
2	F	0.31	0/346	0.67	0/533
2	H	0.33	0/346	0.68	0/533
2	J	0.43	0/346	0.73	0/533
2	L	0.26	0/182	0.63	0/280
3	A	0.49	0/7090	0.69	0/9555
3	B	0.42	0/6376	0.63	0/8593
3	C	0.46	0/7045	0.66	0/9502
3	D	0.33	0/5028	0.55	0/6831
All	All	0.43	0/28026	0.65	1/38302 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	I	0	1
3	B	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6	DT	C6-C5-C7	-5.18	119.79	122.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	273	TYR	Sidechain
1	G	17	DC	Sidechain
1	I	7	DA	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	355	0	200	18	0
1	G	264	0	147	12	0
1	I	355	0	200	13	0
1	K	181	0	101	15	0
2	F	308	0	170	20	0
2	H	308	0	170	18	0
2	J	308	0	170	13	0
2	L	163	0	92	24	0
3	A	6941	0	6787	309	0
3	B	6245	0	6024	495	0
3	C	6895	0	6710	380	0
3	D	4934	0	4297	420	0
4	A	139	0	0	18	0
4	B	106	0	0	24	0
4	C	147	0	0	16	0
4	D	46	0	0	9	0
4	E	3	0	0	1	0
4	F	5	0	0	0	0
4	G	7	0	0	0	0
4	H	2	0	0	0	0
4	I	17	0	0	0	0
4	J	9	0	0	0	0
4	K	8	0	0	1	0
4	L	6	0	0	2	0
All	All	27752	0	25068	1711	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 33.

All (1711) 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)
2:L:107:DG:C2'	2:L:108:DT:H71	1.77	1.14
1:G:12:DA:H2''	1:G:13:DG:H5'	1.30	1.14
3:D:14:SER:HA	3:D:32:GLU:HA	1.32	1.11
3:B:164:ILE:HD12	3:B:164:ILE:H	1.10	1.10
1:E:16:DG:H2''	1:E:17:DC:H5'	1.27	1.09
3:A:897:LEU:H	3:A:897:LEU:HD12	1.17	1.09
3:C:825:VAL:HB	3:C:828:GLU:HG3	1.32	1.08
2:L:101:DG:H2''	2:L:102:DC:H5''	1.32	1.07
3:D:52:ILE:H	3:D:52:ILE:HD12	1.10	1.07
3:D:453:VAL:HG23	3:D:454:TYR:H	1.21	1.03
3:B:687:ALA:HB2	3:B:715:MSE:HE1	1.36	1.03
3:A:395:PHE:HB2	3:A:591:GLN:HG3	1.41	1.02
2:H:105:DC:H2''	2:H:106:DT:H5'	1.40	1.02
3:B:218:VAL:HG13	3:B:222:ALA:HB3	1.41	1.02
3:B:412:LEU:HD12	3:B:623:ASP:HA	1.38	1.00
2:F:114:DG:H2''	2:F:115:DA:H5''	1.43	1.00
3:D:298:LEU:HB3	3:D:300:VAL:HG13	1.45	0.98
3:D:302:LYS:HD2	3:D:303:LEU:H	1.25	0.98
3:C:863:LEU:HA	3:C:866:MSE:HE3	1.45	0.97
2:L:107:DG:H2''	2:L:108:DT:H71	1.44	0.97
3:C:422:GLN:HG2	3:C:678:GLN:O	1.65	0.97
3:A:863:LEU:HA	3:A:866:MSE:HE3	1.46	0.96
3:B:362:ILE:H	3:B:362:ILE:HD13	1.27	0.96
3:D:191:PHE:HD1	3:D:197:LEU:HA	1.29	0.94
3:A:581:ARG:HH11	3:A:581:ARG:HG3	1.33	0.93
1:G:12:DA:H2''	1:G:13:DG:C5'	1.98	0.93
2:H:105:DC:H2'	2:H:106:DT:H71	1.50	0.93
3:A:410:PHE:HB2	3:A:683:MSE:HE3	1.51	0.92
3:A:489:MSE:SE	3:A:553:MSE:HG3	2.20	0.92
3:A:60:LYS:NZ	3:A:60:LYS:HB2	1.85	0.92
3:A:625:ILE:HD11	3:A:683:MSE:HE1	1.49	0.91
3:B:331:VAL:HA	3:B:334:ILE:HD12	1.50	0.91
3:A:308:PRO:HG2	3:A:311:LYS:HB2	1.53	0.90
3:C:112:ASN:HB3	3:C:214:THR:HG23	1.50	0.90
2:F:109:DC:H2''	2:F:110:DA:H5'	1.53	0.90
2:J:104:DG:H2''	2:J:105:DC:H5''	1.53	0.90
3:D:218:VAL:HG13	3:D:222:ALA:HB3	1.54	0.89
3:B:187:ILE:H	3:B:187:ILE:HD12	1.38	0.88
3:A:199:MSE:HE1	3:A:202:LEU:HD23	1.55	0.88
3:D:273:TYR:HA	3:D:276:LEU:HD13	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:752:MSE:HE2	3:D:889:LEU:HD22	1.52	0.88
1:E:10:DA:H2''	1:E:11:DC:H5''	1.56	0.88
3:A:270:VAL:HB	4:A:1042:HOH:O	1.75	0.87
3:B:261:GLU:HG2	3:B:262:ILE:H	1.39	0.87
3:C:158:ASN:HD22	3:C:159:VAL:N	1.73	0.86
3:B:408:MSE:HE3	3:B:688:ILE:HG12	1.56	0.86
3:C:216:TRP:O	3:C:217:ASN:HB2	1.74	0.86
3:B:121:ASP:HB2	4:B:1002:HOH:O	1.75	0.86
3:B:491:ALA:O	3:B:495:ASN:HB2	1.75	0.85
3:C:424:ASN:HD21	3:C:469:GLY:H	1.21	0.85
3:D:458:PRO:HB2	3:D:588:THR:HG22	1.59	0.85
3:A:854:ILE:HD11	3:A:859:LYS:HA	1.58	0.85
3:A:836:ARG:HH12	3:A:865:TRP:HA	1.40	0.85
3:D:602:ASN:HD22	3:D:617:VAL:HG22	1.40	0.85
3:A:116:GLU:HB2	3:A:135:ALA:HB3	1.57	0.84
3:D:52:ILE:H	3:D:52:ILE:CD1	1.87	0.84
3:B:734:LYS:HB2	3:B:737:THR:HG22	1.58	0.84
3:B:438:PRO:HD2	3:B:441:ASP:OD1	1.78	0.84
3:B:734:LYS:HB3	3:B:734:LYS:HZ3	1.43	0.84
3:B:541:MSE:HG3	3:B:544:ARG:HE	1.43	0.84
3:B:405:LYS:HA	3:B:699:GLY:HA3	1.60	0.84
1:K:13:DG:H1	2:L:105:DC:N4	1.76	0.84
3:B:143:ASP:O	3:B:145:ARG:HG2	1.78	0.83
3:C:633:ILE:HD11	3:C:651:LEU:HD11	1.60	0.83
3:D:85:MSE:N	3:D:380:ILE:HD11	1.93	0.83
2:H:108:DT:H2''	2:H:109:DC:H5''	1.61	0.83
3:A:115:ILE:CD1	3:A:136:ILE:HG12	2.09	0.83
3:C:732:THR:HG23	3:C:733:GLN:OE1	1.80	0.82
3:D:85:MSE:HE1	3:D:87:ASP:HB3	1.61	0.82
3:B:451:SER:HB2	3:B:462:MSE:HE1	1.60	0.82
3:B:486:LYS:HB2	3:B:556:GLN:NE2	1.94	0.82
3:B:541:MSE:HA	3:B:544:ARG:HG2	1.62	0.82
3:A:408:MSE:HE1	3:A:655:ALA:HB2	1.59	0.82
3:D:471:VAL:HB	3:D:472:PRO:HD3	1.60	0.82
3:B:176:ASP:HA	3:B:319:ARG:HE	1.46	0.81
3:D:654:PHE:O	3:D:658:ARG:HB3	1.80	0.81
3:D:415:LEU:HD23	3:D:622:THR:HG23	1.63	0.81
3:D:655:ALA:HA	3:D:659:MSE:HB2	1.60	0.81
3:D:605:LEU:HD13	3:D:632:ILE:HD11	1.61	0.80
3:D:722:GLU:HG3	3:D:723:PRO:HD2	1.63	0.80
2:L:101:DG:C2'	2:L:102:DC:H5''	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:461:MSE:HE2	3:B:461:MSE:HA	1.63	0.80
3:D:71:TRP:HE1	3:D:75:MSE:HE3	1.45	0.80
3:C:825:VAL:HB	3:C:828:GLU:CG	2.12	0.80
3:B:27:ARG:NH1	4:B:950:HOH:O	2.15	0.79
3:C:1:MSE:HA	3:C:1:MSE:HE3	1.63	0.79
3:B:164:ILE:H	3:B:164:ILE:CD1	1.87	0.79
3:B:194:GLU:C	3:B:196:GLU:H	1.84	0.79
3:A:424:ASN:O	3:A:429:THR:HG21	1.82	0.79
3:B:233:ILE:HD12	3:B:233:ILE:H	1.47	0.79
3:B:629:ALA:HA	3:B:632:ILE:HD13	1.65	0.79
3:D:469:GLY:HA3	3:D:472:PRO:HD2	1.64	0.79
3:B:700:GLY:HA2	3:B:753:LEU:HD22	1.63	0.79
1:G:12:DA:H61	2:H:106:DT:H3	1.29	0.79
3:A:115:ILE:HD12	3:A:136:ILE:HG12	1.65	0.79
3:C:116:GLU:HB2	3:C:135:ALA:HB3	1.65	0.79
3:D:611:THR:HG22	3:D:612:GLU:H	1.46	0.78
1:E:6:DT:H2''	1:E:7:DA:H5'	1.64	0.78
3:B:305:TYR:OH	3:B:309:ILE:HB	1.83	0.78
3:B:182:ILE:HG22	3:B:186:ILE:HD11	1.65	0.78
3:B:115:ILE:HD11	3:B:222:ALA:HA	1.66	0.78
2:L:108:DT:H3'	4:L:246:HOH:O	1.83	0.78
3:B:244:PRO:HG2	3:B:267:GLY:HA3	1.66	0.78
3:D:272:ASP:OD1	3:D:274:ILE:HG22	1.84	0.78
3:B:215:GLY:HA3	3:B:218:VAL:HG21	1.65	0.78
3:B:594:LEU:HD13	3:B:623:ASP:H	1.49	0.77
3:C:435:LYS:HA	4:C:1036:HOH:O	1.83	0.77
3:C:818:ASN:OD1	3:C:857:LEU:HD11	1.84	0.77
3:D:52:ILE:HD12	3:D:52:ILE:N	1.95	0.77
3:A:60:LYS:HZ2	3:A:60:LYS:HB2	1.45	0.77
3:C:592:MSE:HE3	3:C:670:MSE:SE	2.35	0.77
3:A:825:VAL:HG12	3:A:826:GLU:H	1.48	0.77
1:K:13:DG:H1	2:L:105:DC:H42	1.32	0.76
3:B:395:PHE:HD2	3:B:594:LEU:HD23	1.50	0.76
3:D:618:LEU:HD23	3:D:618:LEU:H	1.49	0.76
3:D:618:LEU:HG	3:D:619:TYR:H	1.51	0.76
3:D:109:ARG:HE	3:D:211:VAL:HG23	1.51	0.76
3:A:656:ARG:HA	3:A:660:GLU:HG3	1.68	0.76
3:B:192:ASP:O	3:B:193:ASN:HB3	1.84	0.76
2:L:107:DG:C1'	2:L:108:DT:H71	2.14	0.76
3:B:439:LEU:O	3:B:443:ILE:HG13	1.84	0.76
3:C:112:ASN:HB3	3:C:214:THR:CG2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:DT:H2''	2:H:109:DC:C5'	2.16	0.76
3:B:261:GLU:HG2	3:B:262:ILE:N	2.00	0.75
3:B:288:TYR:HA	3:B:293:ILE:HD11	1.68	0.75
3:B:487:GLY:HA2	3:B:490:LEU:HD12	1.69	0.75
3:D:481:GLN:HB3	3:D:559:ARG:HH11	1.51	0.75
2:J:114:DG:H2''	2:J:115:DA:OP2	1.83	0.75
3:C:863:LEU:HA	3:C:866:MSE:CE	2.15	0.75
3:C:489:MSE:HG3	4:C:1020:HOH:O	1.87	0.75
1:K:11:DC:H4'	4:K:346:HOH:O	1.87	0.75
3:B:394:ALA:HB1	3:B:622:THR:HB	1.69	0.75
3:C:1:MSE:HB3	3:C:22:SER:O	1.87	0.75
3:D:568:GLY:HA3	4:D:906:HOH:O	1.87	0.75
3:A:314:GLU:HG3	3:A:315:SER:H	1.52	0.74
3:B:486:LYS:HB2	3:B:556:GLN:HE22	1.50	0.74
3:C:495:ASN:HD22	3:C:495:ASN:N	1.83	0.74
3:A:277:TYR:O	3:A:281:SER:HB3	1.87	0.74
3:B:182:ILE:O	3:B:186:ILE:HG13	1.87	0.74
3:C:380:ILE:HG23	3:C:576:ARG:HD3	1.67	0.74
3:B:396:VAL:HG13	3:B:705:LYS:NZ	2.03	0.74
3:C:489:MSE:O	3:C:493:GLN:HG3	1.87	0.74
3:C:668:ARG:HG3	3:C:668:ARG:HH11	1.53	0.74
3:B:274:ILE:HG23	3:B:275:ASP:OD1	1.87	0.74
2:F:114:DG:C2'	2:F:115:DA:H5''	2.15	0.74
3:C:70:GLN:NE2	3:C:70:GLN:HA	2.02	0.74
3:B:752:MSE:HG2	3:B:760:LEU:HD22	1.70	0.74
3:C:422:GLN:HE21	3:C:680:LEU:H	1.35	0.74
2:J:104:DG:C2'	2:J:105:DC:H5''	2.17	0.74
3:B:118:THR:HG23	3:B:134:ASP:OD2	1.88	0.74
3:A:815:ILE:HD12	3:A:857:LEU:HD23	1.69	0.73
3:B:129:ALA:CB	3:B:229:ARG:HG2	2.18	0.73
3:C:660:GLU:HB3	3:C:661:PRO:HD3	1.69	0.73
3:C:738:PRO:HG2	3:C:741:VAL:CG2	2.18	0.73
3:B:330:ARG:O	3:B:334:ILE:HG13	1.87	0.73
3:B:305:TYR:HD2	3:B:305:TYR:N	1.85	0.73
3:C:412:LEU:HG	3:C:683:MSE:HE3	1.71	0.73
3:B:129:ALA:HB3	3:B:229:ARG:HG2	1.69	0.73
3:D:597:ILE:HD11	3:D:663:ILE:HG23	1.70	0.73
3:B:757:GLU:HB2	3:B:889:LEU:HD22	1.68	0.73
3:D:323:TYR:HA	3:D:326:ILE:CG1	2.18	0.73
3:A:394:ALA:HB1	3:A:622:THR:HB	1.71	0.73
3:B:164:ILE:HD12	3:B:164:ILE:N	1.95	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:818:ASN:HD22	3:C:819:ILE:N	1.85	0.73
3:A:81:GLU:HG2	3:A:83:LEU:HD22	1.72	0.72
3:B:42:PRO:HD2	3:B:45:GLN:HE21	1.54	0.72
3:C:254:GLU:HA	3:C:258:GLY:CA	2.19	0.72
3:A:859:LYS:HG2	3:A:860:ASP:H	1.54	0.72
3:D:712:VAL:HG12	3:D:714:ASP:H	1.53	0.72
3:D:581:ARG:HG2	3:D:581:ARG:HH11	1.53	0.72
3:D:733:GLN:HA	3:D:742:GLN:NE2	2.04	0.72
1:I:7:DA:H2'	1:I:8:DT:C6	2.24	0.72
3:B:15:ILE:HG13	3:B:65:MSE:HE1	1.72	0.72
3:B:159:VAL:HG22	3:B:160:GLU:H	1.55	0.72
2:H:108:DT:C2'	2:H:109:DC:H5''	2.20	0.72
3:A:220:SER:HB3	3:A:260:ARG:HH11	1.54	0.72
3:A:859:LYS:HG2	3:A:860:ASP:N	2.05	0.72
3:A:825:VAL:HB	3:A:828:GLU:HG3	1.70	0.72
3:D:40:HIS:NE2	3:D:83:LEU:HD21	2.06	0.71
3:D:602:ASN:ND2	3:D:617:VAL:HG22	2.06	0.71
3:A:492:ALA:O	3:A:549:GLU:HG3	1.91	0.71
3:A:581:ARG:HH11	3:A:581:ARG:CG	2.03	0.71
3:C:290:LEU:HD13	3:C:294:SER:HB2	1.72	0.71
3:B:154:SER:C	3:B:156:TYR:H	1.93	0.71
3:B:305:TYR:N	3:B:305:TYR:CD2	2.58	0.71
3:D:92:TYR:HE2	3:D:96:THR:HG21	1.54	0.71
1:E:6:DT:H1'	1:E:7:DA:H5''	1.73	0.71
3:D:290:LEU:O	3:D:293:ILE:HG22	1.91	0.71
3:B:240:LYS:HG2	3:B:248:THR:HG22	1.73	0.71
3:D:89:LYS:HE2	3:D:354:GLN:HE22	1.54	0.70
3:B:316:ASN:HD21	3:B:318:GLN:HB3	1.56	0.70
3:C:441:ASP:HB3	3:C:447:ALA:HB2	1.72	0.70
3:A:902:ASP:HA	4:A:1021:HOH:O	1.91	0.70
3:B:300:VAL:HG12	3:B:301:GLY:N	2.06	0.70
3:C:727:ILE:O	3:C:728:MSE:HE2	1.91	0.70
3:B:700:GLY:HA2	3:B:753:LEU:CD2	2.20	0.70
3:A:429:THR:HG22	3:A:463:TYR:HB3	1.72	0.70
3:B:217:ASN:HA	3:B:274:ILE:HG21	1.73	0.70
3:B:541:MSE:CG	3:B:544:ARG:HE	2.03	0.70
3:A:901:PHE:O	3:A:902:ASP:HB2	1.92	0.70
3:D:604:TYR:HE1	3:D:659:MSE:HA	1.57	0.69
3:D:547:ARG:O	3:D:550:VAL:HG22	1.92	0.69
3:A:700:GLY:HA2	3:A:753:LEU:HD22	1.74	0.69
3:D:14:SER:HA	3:D:32:GLU:CA	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:212:ILE:HG22	3:D:212:ILE:O	1.90	0.69
3:D:453:VAL:HG23	3:D:454:TYR:N	2.02	0.69
3:B:734:LYS:HB3	3:B:734:LYS:NZ	2.07	0.69
3:D:71:TRP:NE1	3:D:75:MSE:HE3	2.07	0.69
3:A:825:VAL:HG12	3:A:826:GLU:N	2.06	0.69
3:B:444:ASN:HA	3:B:599:ARG:HH11	1.57	0.69
2:F:104:DG:H1'	2:F:105:DC:H5''	1.75	0.69
3:A:415:LEU:O	3:A:419:ILE:HG13	1.92	0.69
3:A:848:TRP:HB2	3:A:849:PRO:HD2	1.73	0.69
3:C:404:TYR:CE1	3:C:618:LEU:HD13	2.28	0.69
3:B:137:THR:OG1	3:B:328:VAL:HG21	1.92	0.69
3:D:235:GLY:HA3	3:D:238:THR:HB	1.74	0.69
3:D:663:ILE:HD13	3:D:683:MSE:HE3	1.75	0.69
3:B:441:ASP:HB3	3:B:447:ALA:HB2	1.74	0.69
1:E:6:DT:H2''	1:E:7:DA:C5'	2.24	0.69
3:B:347:MSE:HG2	3:B:358:VAL:HG23	1.74	0.68
3:D:85:MSE:HE1	3:D:87:ASP:CB	2.23	0.68
3:A:660:GLU:HB2	3:A:661:PRO:HD3	1.75	0.68
3:A:897:LEU:H	3:A:897:LEU:CD1	1.94	0.68
3:B:183:ILE:HD13	3:B:183:ILE:H	1.58	0.68
3:D:776:TYR:CE1	3:D:777:ILE:HG23	2.27	0.68
3:A:85:MSE:HE1	3:A:366:ASP:OD2	1.92	0.68
3:D:361:PRO:HB2	3:D:569:ALA:HB2	1.75	0.68
3:C:89:LYS:NZ	3:C:354:GLN:HE22	1.92	0.68
3:A:231:LYS:HD3	4:A:943:HOH:O	1.93	0.68
3:C:112:ASN:HD21	3:C:332:LEU:HD21	1.57	0.68
3:C:159:VAL:HG11	3:C:317:HIS:HB3	1.75	0.68
3:C:555:ALA:O	3:C:559:ARG:HG2	1.93	0.68
3:D:421:ARG:NH1	3:D:680:LEU:HD13	2.09	0.68
3:C:254:GLU:HA	3:C:258:GLY:HA2	1.76	0.68
3:D:239:ALA:C	3:D:241:ARG:H	1.96	0.68
2:J:112:DA:H2''	2:J:113:DA:C8	2.29	0.68
3:C:549:GLU:HG2	4:C:1020:HOH:O	1.93	0.68
3:D:576:ARG:NH1	3:D:576:ARG:HB3	2.07	0.68
1:I:8:DT:OP1	3:C:705:LYS:HB2	1.94	0.68
3:A:836:ARG:NH1	3:A:865:TRP:HA	2.08	0.68
3:B:300:VAL:HG12	3:B:301:GLY:H	1.59	0.68
3:D:415:LEU:O	3:D:419:ILE:HG12	1.94	0.68
3:B:451:SER:HB2	3:B:462:MSE:CE	2.23	0.67
3:C:128:GLN:HA	3:C:128:GLN:HE21	1.58	0.67
3:C:42:PRO:HG2	3:C:45:GLN:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:422:GLN:HG3	3:A:678:GLN:O	1.94	0.67
3:B:421:ARG:HD2	3:B:476:THR:OG1	1.94	0.67
1:E:10:DA:H2''	1:E:11:DC:C5'	2.23	0.67
3:A:208:LYS:HE3	4:A:912:HOH:O	1.94	0.67
3:D:83:LEU:HD12	3:D:83:LEU:H	1.60	0.67
3:B:187:ILE:CD1	3:B:187:ILE:H	2.07	0.67
3:D:611:THR:HG22	3:D:612:GLU:N	2.10	0.67
3:D:759:SER:C	3:D:761:GLN:H	1.95	0.67
3:B:182:ILE:H	3:B:183:ILE:HD13	1.60	0.67
3:B:757:GLU:O	3:B:761:GLN:HG3	1.95	0.67
3:B:218:VAL:HG12	3:B:223:ILE:HG13	1.77	0.67
3:B:261:GLU:CG	3:B:262:ILE:H	2.02	0.67
3:A:664:ASP:O	3:A:668:ARG:HG3	1.94	0.67
3:C:173:GLN:HG2	4:C:1033:HOH:O	1.94	0.67
3:D:52:ILE:HD11	3:D:381:PRO:HD3	1.76	0.67
3:A:42:PRO:HD2	3:A:45:GLN:HG3	1.75	0.67
3:B:115:ILE:HG22	3:B:136:ILE:HG13	1.76	0.67
3:B:194:GLU:O	3:B:196:GLU:N	2.28	0.67
1:K:13:DG:H2''	1:K:14:DC:OP2	1.95	0.67
3:B:611:THR:O	3:B:612:GLU:HG3	1.95	0.66
3:D:323:TYR:HA	3:D:326:ILE:HG13	1.76	0.66
3:C:81:GLU:HG3	3:C:384:ARG:NH2	2.10	0.66
3:A:116:GLU:OE2	3:A:116:GLU:HA	1.96	0.66
3:B:187:ILE:N	3:B:187:ILE:HD12	2.09	0.66
3:D:685:ARG:HD2	3:D:688:ILE:HD11	1.77	0.66
3:B:117:VAL:HG21	3:B:124:PRO:HG3	1.76	0.66
3:D:689:ALA:HB2	3:D:712:VAL:HA	1.76	0.66
3:C:458:PRO:HG3	3:C:592:MSE:SE	2.46	0.66
3:D:302:LYS:CD	3:D:303:LEU:H	2.06	0.66
3:B:159:VAL:HG22	3:B:160:GLU:N	2.11	0.66
3:B:752:MSE:CG	3:B:760:LEU:HD22	2.26	0.66
3:C:12:GLY:O	3:C:14:SER:N	2.29	0.66
3:D:102:LYS:HD3	3:D:103:TYR:H	1.61	0.66
3:B:9:GLU:HG2	3:B:266:PHE:CD2	2.30	0.66
3:B:396:VAL:HG11	4:B:941:HOH:O	1.96	0.66
3:A:272:ASP:OD1	3:A:274:ILE:HG22	1.97	0.65
3:C:148:VAL:HG21	3:C:325:ILE:HD11	1.78	0.65
3:C:818:ASN:C	3:C:818:ASN:HD22	1.97	0.65
3:D:231:LYS:HA	3:D:239:ALA:HB2	1.78	0.65
3:D:322:SER:O	3:D:326:ILE:HG12	1.96	0.65
3:D:405:LYS:HE2	3:D:406:TYR:HE1	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:593:ALA:HA	3:D:670:MSE:SE	2.47	0.65
1:K:13:DG:H22	2:L:105:DC:N4	1.95	0.65
3:B:233:ILE:HD12	3:B:233:ILE:N	2.10	0.65
3:B:396:VAL:HG13	3:B:705:LYS:HZ2	1.61	0.65
3:D:331:VAL:HA	3:D:334:ILE:HD12	1.77	0.65
3:A:166:ILE:HA	3:A:169:LYS:HE2	1.78	0.65
3:A:90:LEU:HD11	3:A:363:LYS:HD2	1.78	0.65
3:B:159:VAL:HG21	3:B:317:HIS:CG	2.30	0.65
3:B:597:ILE:HD12	3:B:598:GLU:N	2.11	0.65
3:D:416:TYR:HB2	3:D:417:PRO:HD3	1.79	0.65
3:B:303:LEU:HD23	3:B:326:ILE:HG13	1.77	0.65
3:B:42:PRO:HG2	3:B:45:GLN:HG2	1.78	0.65
3:B:456:CYS:SG	3:B:462:MSE:HE2	2.36	0.65
3:D:420:ILE:HD11	3:D:586:ILE:HD11	1.77	0.65
3:C:110:VAL:H	3:C:141:SER:HB3	1.62	0.65
3:C:373:LEU:HB3	3:C:378:LYS:HB2	1.78	0.65
3:C:818:ASN:ND2	3:C:820:ASP:H	1.95	0.65
3:D:702:TRP:CZ3	3:D:710:LEU:HD21	2.32	0.65
3:B:179:PRO:O	3:B:183:ILE:HG23	1.97	0.64
3:B:287:SER:HB3	3:B:292:TYR:HD2	1.63	0.64
3:C:70:GLN:HE21	3:C:70:GLN:HA	1.61	0.64
1:E:10:DA:C2'	1:E:11:DC:H5''	2.25	0.64
2:L:102:DC:H2''	2:L:103:DG:N7	2.12	0.64
3:B:133:ILE:HG12	3:B:225:TYR:HE2	1.61	0.64
3:C:191:PHE:CZ	3:C:200:GLU:HG2	2.32	0.64
3:B:231:LYS:HA	3:B:235:GLY:HA2	1.78	0.64
3:B:268:ILE:HG22	3:B:269:SER:N	2.13	0.64
3:D:714:ASP:HB2	3:D:717:GLY:O	1.96	0.64
3:B:64:ASN:OD1	3:B:66:ARG:HG3	1.98	0.64
3:B:295:GLU:HG2	3:B:300:VAL:O	1.97	0.64
3:B:150:ASP:OD1	3:B:321:ILE:HG12	1.97	0.64
3:C:230:ILE:HG23	3:C:234:PHE:HD2	1.63	0.64
3:B:297:GLU:HB2	4:B:983:HOH:O	1.96	0.64
3:D:411:ASP:HB2	3:D:623:ASP:O	1.96	0.64
3:D:85:MSE:CE	3:D:90:LEU:HB2	2.27	0.64
2:J:104:DG:H2''	2:J:105:DC:C5'	2.28	0.64
3:A:410:PHE:CB	3:A:683:MSE:HE3	2.25	0.64
3:C:109:ARG:HD3	4:C:964:HOH:O	1.98	0.64
3:D:369:ILE:O	3:D:373:LEU:HD13	1.97	0.64
3:A:202:LEU:O	3:A:206:GLN:HG2	1.98	0.64
3:B:27:ARG:HG2	4:B:904:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:108:DT:H5''	4:A:1020:HOH:O	1.97	0.64
3:A:685:ARG:HD3	4:A:970:HOH:O	1.97	0.63
3:B:310:SER:O	3:B:311:LYS:HD2	1.98	0.63
3:C:301:GLY:O	3:C:302:LYS:HG2	1.98	0.63
3:D:376:GLN:HB2	3:D:378:LYS:HG2	1.81	0.63
2:F:108:DT:H2''	2:F:109:DC:C5'	2.28	0.63
2:L:107:DG:H2''	2:L:108:DT:C7	2.24	0.63
3:A:121:ASP:N	3:A:121:ASP:OD2	2.25	0.63
3:B:166:ILE:HB	4:B:949:HOH:O	1.97	0.63
3:C:173:GLN:HG3	3:C:174:GLY:N	2.14	0.63
3:C:684:ASP:HB3	4:C:934:HOH:O	1.98	0.63
3:D:656:ARG:O	3:D:660:GLU:HB2	1.98	0.63
3:A:181:GLU:OE1	3:A:181:GLU:N	2.31	0.63
3:A:643:ASP:HA	3:A:693:LEU:HD23	1.79	0.63
3:D:738:PRO:HG2	3:D:741:VAL:HG23	1.80	0.63
1:E:16:DG:H2''	1:E:17:DC:C5'	2.18	0.63
3:B:492:ALA:HB1	3:B:549:GLU:HB3	1.81	0.63
3:C:700:GLY:HA2	3:C:753:LEU:CD2	2.29	0.63
1:E:3:3DR:H4'1	3:A:572:ASN:HD22	1.64	0.63
3:A:11:ILE:HD12	3:A:16:PHE:CD1	2.33	0.63
3:B:183:ILE:HD13	3:B:183:ILE:N	2.13	0.63
3:B:52:ILE:HG22	3:B:53:TYR:CE1	2.33	0.63
3:C:61:LEU:HD23	3:C:62:PHE:H	1.63	0.63
3:D:42:PRO:C	3:D:44:SER:H	2.02	0.63
3:C:401:PRO:O	3:C:402:ASN:HB2	1.98	0.63
3:D:679:HIS:O	3:D:680:LEU:HD23	1.98	0.63
3:D:85:MSE:HG3	3:D:370:PHE:CE1	2.34	0.63
2:H:106:DT:H2''	2:H:107:DG:C8	2.33	0.63
3:A:898:PHE:C	3:A:900:MSE:H	2.02	0.62
3:B:687:ALA:CB	3:B:715:MSE:HE1	2.21	0.62
3:B:316:ASN:ND2	3:B:318:GLN:HB3	2.14	0.62
3:B:416:TYR:O	3:B:420:ILE:HG13	1.99	0.62
1:I:6:DT:H2''	1:I:7:DA:H5''	1.79	0.62
3:B:216:TRP:N	3:B:218:VAL:HG23	2.15	0.62
3:A:489:MSE:HB2	4:A:1010:HOH:O	1.97	0.62
3:B:305:TYR:HD1	3:B:312:LEU:HD13	1.65	0.62
3:B:422:GLN:HE21	3:B:676:ASN:HD22	1.45	0.62
3:B:660:GLU:HB2	3:B:661:PRO:HD3	1.79	0.62
3:D:403:ARG:HB2	3:D:698:ILE:HG21	1.81	0.62
3:D:422:GLN:O	3:D:676:ASN:HB3	1.98	0.62
3:B:158:ASN:O	3:B:159:VAL:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:DG:C2'	1:E:17:DC:H5'	2.17	0.62
2:H:105:DC:H2''	2:H:106:DT:C5'	2.23	0.62
3:B:194:GLU:C	3:B:196:GLU:N	2.53	0.62
3:A:216:TRP:O	3:A:217:ASN:HB2	1.99	0.62
3:D:362:ILE:HG22	3:D:575:PHE:HD1	1.65	0.62
3:D:458:PRO:HB2	3:D:588:THR:CG2	2.29	0.62
3:B:115:ILE:HA	3:B:135:ALA:O	1.99	0.62
3:C:147:TYR:HB3	3:C:149:PHE:HE1	1.64	0.62
3:D:109:ARG:O	3:D:211:VAL:HB	2.00	0.62
2:H:113:DA:OP1	3:B:288:TYR:HB2	1.99	0.62
3:B:331:VAL:HG23	3:B:332:LEU:HD12	1.81	0.61
3:C:167:ALA:HA	3:C:176:ASP:HB2	1.82	0.61
3:A:897:LEU:N	3:A:897:LEU:HD12	2.02	0.61
3:B:631:LYS:NZ	3:B:631:LYS:HB2	2.15	0.61
3:D:330:ARG:O	3:D:333:GLN:HB2	2.00	0.61
3:D:399:PRO:O	3:D:401:PRO:HD3	2.00	0.61
3:D:40:HIS:HA	3:D:57:CYS:HB3	1.81	0.61
3:A:428:GLU:OE2	3:A:428:GLU:N	2.33	0.61
3:A:632:ILE:HD12	3:A:632:ILE:N	2.15	0.61
2:H:104:DG:H2''	2:H:105:DC:O5'	2.01	0.61
3:C:463:TYR:OH	3:C:582:ASN:ND2	2.34	0.61
3:C:474:GLU:O	3:C:478:VAL:HG23	2.00	0.61
3:A:397:LYS:HD3	3:A:619:TYR:HA	1.81	0.61
3:B:193:ASN:ND2	3:B:194:GLU:H	1.98	0.61
3:B:412:LEU:CD1	3:B:623:ASP:HA	2.25	0.61
3:B:411:ASP:O	3:B:683:MSE:HA	2.00	0.61
3:D:232:ASN:HB2	4:D:949:HOH:O	1.99	0.61
2:H:113:DA:H2''	2:H:114:DG:OP2	2.00	0.61
2:L:107:DG:N9	2:L:108:DT:H71	2.15	0.61
3:B:188:TYR:CZ	3:B:190:PRO:HB3	2.36	0.61
3:C:416:TYR:HB2	3:C:417:PRO:HD3	1.81	0.61
2:J:112:DA:H5'	3:C:734:LYS:HG2	1.82	0.61
3:D:409:SER:HB3	3:D:626:TYR:CD2	2.36	0.61
3:D:362:ILE:HG22	3:D:575:PHE:CD1	2.36	0.61
3:D:603:GLU:O	3:D:607:GLU:HG2	1.99	0.61
3:A:32:GLU:OE1	3:A:32:GLU:N	2.21	0.61
3:B:319:ARG:HH11	3:B:319:ARG:HG2	1.66	0.61
3:C:752:MSE:HE3	3:C:889:LEU:HD12	1.83	0.61
3:A:314:GLU:HG3	3:A:315:SER:N	2.15	0.61
3:A:458:PRO:HG3	3:A:592:MSE:SE	2.51	0.61
3:D:29:ARG:O	3:D:29:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:229:ARG:HH11	3:B:233:ILE:HD11	1.66	0.60
3:B:291:ASP:O	3:B:295:GLU:HB2	2.00	0.60
3:D:323:TYR:HA	3:D:326:ILE:HG12	1.82	0.60
3:A:429:THR:CG2	3:A:463:TYR:HB3	2.31	0.60
3:B:193:ASN:HD22	3:B:194:GLU:H	1.49	0.60
3:B:395:PHE:CD2	3:B:594:LEU:HD23	2.33	0.60
3:D:35:PRO:HG2	3:D:62:PHE:HB2	1.83	0.60
3:A:541:MSE:O	3:A:543:PHE:N	2.32	0.60
3:D:85:MSE:HE2	3:D:90:LEU:HB2	1.82	0.60
3:C:302:LYS:HB3	3:C:302:LYS:HZ2	1.66	0.60
2:L:102:DC:H2''	2:L:103:DG:C8	2.37	0.60
3:A:362:ILE:HD11	3:A:572:ASN:CG	2.22	0.60
3:B:384:ARG:HH11	3:B:384:ARG:HG3	1.67	0.60
3:D:14:SER:CA	3:D:32:GLU:HA	2.18	0.60
3:A:545:ALA:O	3:A:549:GLU:HB2	2.01	0.60
3:A:75:MSE:HE3	3:A:80:LEU:HB2	1.84	0.60
3:B:105:HIS:HA	3:B:108:ILE:HD12	1.83	0.60
3:B:182:ILE:HD13	3:B:185:LYS:HD2	1.84	0.60
3:B:273:TYR:O	3:B:274:ILE:C	2.39	0.60
3:B:137:THR:HG1	3:B:328:VAL:HG21	1.66	0.60
3:B:867:ASP:OD1	3:B:870:VAL:HG23	2.01	0.60
3:C:153:ASN:ND2	3:C:158:ASN:HB2	2.16	0.60
3:A:835:LEU:HD11	3:A:846:ILE:HB	1.84	0.60
3:B:222:ALA:O	3:B:226:VAL:HG23	2.02	0.60
3:C:191:PHE:HZ	3:C:200:GLU:HG2	1.64	0.60
3:C:434:PHE:CE2	3:C:460:GLY:HA2	2.37	0.60
3:D:420:ILE:HG22	3:D:472:PRO:HG3	1.83	0.60
1:K:13:DG:H22	2:L:105:DC:H42	1.49	0.60
3:D:551:ALA:HA	3:D:555:ALA:HB3	1.84	0.60
3:B:219:GLU:HG2	3:B:262:ILE:HD11	1.84	0.59
3:B:751:ARG:NH1	3:B:763:TYR:HB2	2.17	0.59
3:C:112:ASN:HD21	3:C:332:LEU:CD2	2.15	0.59
3:C:593:ALA:HB1	3:C:681:MSE:CE	2.32	0.59
3:D:28:THR:O	3:D:29:ARG:HB3	2.02	0.59
3:A:428:GLU:OE1	3:A:470:VAL:HG23	2.02	0.59
3:B:154:SER:O	3:B:156:TYR:N	2.35	0.59
3:B:486:LYS:CB	3:B:556:GLN:HE22	2.14	0.59
3:C:255:ASN:C	3:C:257:TYR:H	2.06	0.59
2:J:102:DC:H4'	2:J:102:DC:OP1	2.02	0.59
3:A:199:MSE:CE	3:A:202:LEU:HD23	2.31	0.59
3:B:290:LEU:C	4:B:1000:HOH:O	2.40	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:428:GLU:OE1	3:B:470:VAL:N	2.28	0.59
3:D:274:ILE:HG23	3:D:275:ASP:OD1	2.02	0.59
3:D:52:ILE:HD11	3:D:381:PRO:CD	2.32	0.59
3:D:775:ASN:OD1	3:D:777:ILE:HG12	2.02	0.59
3:A:60:LYS:HZ3	3:A:60:LYS:HB2	1.67	0.59
3:D:592:MSE:HG2	3:D:593:ALA:N	2.16	0.59
3:A:83:LEU:HB3	3:A:379:VAL:CG1	2.33	0.59
3:C:222:ALA:O	3:C:226:VAL:HG23	2.03	0.59
3:C:254:GLU:HA	3:C:258:GLY:HA3	1.83	0.59
3:D:83:LEU:HD12	3:D:83:LEU:N	2.16	0.59
3:A:41:CYS:HB2	3:A:42:PRO:HD2	1.83	0.59
3:A:625:ILE:HD11	3:A:683:MSE:CE	2.27	0.59
3:D:663:ILE:HG21	3:D:683:MSE:HE2	1.85	0.59
1:K:13:DG:N2	2:L:105:DC:H42	2.00	0.59
3:A:132:PRO:HD2	4:A:909:HOH:O	2.02	0.59
3:A:176:ASP:HA	3:A:319:ARG:NH2	2.18	0.59
3:A:404:TYR:CD1	3:A:618:LEU:HD22	2.38	0.59
3:C:439:LEU:O	3:C:443:ILE:HG13	2.03	0.59
3:C:863:LEU:HD12	3:C:866:MSE:CE	2.32	0.59
3:D:342:ASN:HB2	4:D:934:HOH:O	2.02	0.59
3:D:469:GLY:CA	3:D:472:PRO:HD2	2.30	0.59
3:A:422:GLN:O	3:A:676:ASN:HB3	2.02	0.59
3:B:321:ILE:N	3:B:321:ILE:HD12	2.18	0.59
3:C:475:ILE:HG23	3:C:566:LEU:HD22	1.84	0.59
3:D:191:PHE:CD1	3:D:197:LEU:HA	2.22	0.59
3:D:449:ARG:HH21	3:D:675:ASN:HD22	1.51	0.59
3:D:555:ALA:O	3:D:558:ASN:HB3	2.03	0.59
3:D:556:GLN:HG3	4:D:918:HOH:O	2.01	0.59
1:K:11:DC:OP1	3:D:874:LYS:HE3	2.03	0.59
3:A:641:PHE:HA	3:A:646:HIS:ND1	2.18	0.59
3:D:887:ALA:O	3:D:889:LEU:HD12	2.01	0.59
2:F:109:DC:H2''	2:F:110:DA:C5'	2.28	0.59
3:D:274:ILE:HG23	3:D:275:ASP:H	1.68	0.59
3:D:85:MSE:CE	3:D:87:ASP:H	2.16	0.59
3:A:547:ARG:HH22	3:A:551:ALA:CB	2.15	0.58
3:A:720:TYR:CE2	3:A:724:LYS:HD2	2.38	0.58
3:B:219:GLU:HG2	3:B:262:ILE:CD1	2.33	0.58
3:A:260:ARG:HG2	3:A:261:GLU:N	2.18	0.58
3:B:113:PHE:HE1	3:B:218:VAL:HG11	1.68	0.58
3:B:360:SER:OG	3:B:362:ILE:HG12	2.02	0.58
3:B:380:ILE:HG23	3:B:576:ARG:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:896:SER:HG	3:B:898:PHE:HD2	1.50	0.58
3:D:475:ILE:HD13	3:D:566:LEU:HD22	1.85	0.58
3:D:750:ARG:HG2	3:D:754:GLN:CG	2.33	0.58
3:D:218:VAL:CG1	3:D:222:ALA:HB3	2.31	0.58
3:A:355:ILE:O	3:A:358:VAL:HG12	2.04	0.58
3:A:785:ALA:HB2	3:A:808:ILE:HD11	1.86	0.58
3:B:202:LEU:HD21	3:B:242:LEU:HG	1.85	0.58
3:B:331:VAL:HA	3:B:334:ILE:CD1	2.27	0.58
2:L:103:DG:H2''	2:L:104:DG:C8	2.38	0.58
3:B:272:ASP:OD2	3:B:274:ILE:HG22	2.02	0.58
3:B:404:TYR:HA	4:B:974:HOH:O	2.01	0.58
3:B:761:GLN:OE1	3:B:893:LYS:HE2	2.03	0.58
3:C:137:THR:OG1	3:C:324:ASN:ND2	2.37	0.58
3:D:216:TRP:HA	3:D:272:ASP:OD1	2.03	0.58
2:J:105:DC:H2'	2:J:106:DT:H71	1.85	0.58
3:C:426:SER:HB3	3:C:428:GLU:OE2	2.04	0.58
3:C:20:ILE:HA	3:C:25:ARG:O	2.04	0.58
3:D:41:CYS:H	3:D:57:CYS:HA	1.67	0.58
1:E:4:DC:H2''	1:E:5:DT:C7	2.34	0.58
1:I:11:DC:OP1	3:C:874:LYS:HD3	2.04	0.58
3:D:594:LEU:O	3:D:597:ILE:HG22	2.04	0.58
3:B:276:LEU:O	3:B:280:PHE:HB2	2.04	0.58
3:D:420:ILE:HD11	3:D:586:ILE:CD1	2.33	0.58
3:B:193:ASN:ND2	3:B:194:GLU:N	2.52	0.57
3:C:183:ILE:HD13	3:C:183:ILE:O	2.03	0.57
3:C:186:ILE:HG22	3:C:187:ILE:N	2.19	0.57
3:D:38:PHE:HB2	3:D:379:VAL:HG11	1.85	0.57
3:A:543:PHE:O	3:A:547:ARG:HB2	2.04	0.57
3:B:397:LYS:HD3	3:B:619:TYR:HA	1.86	0.57
3:C:766:GLU:O	3:C:770:GLU:HG2	2.04	0.57
3:D:222:ALA:O	3:D:226:VAL:HG13	2.04	0.57
3:D:295:GLU:HA	3:D:299:ASN:H	1.68	0.57
3:D:37:LEU:N	3:D:37:LEU:HD12	2.18	0.57
3:A:461:MSE:HE2	3:A:461:MSE:N	2.19	0.57
3:B:699:GLY:HA3	4:B:923:HOH:O	2.04	0.57
3:C:11:ILE:HD12	3:C:16:PHE:CE1	2.39	0.57
3:C:140:ASP:OD1	3:C:142:ILE:HB	2.04	0.57
3:C:186:ILE:O	3:C:187:ILE:HG13	2.04	0.57
3:D:550:VAL:O	3:D:550:VAL:HG23	2.04	0.57
2:L:107:DG:C8	2:L:108:DT:H73	2.40	0.57
3:A:298:LEU:O	3:A:299:ASN:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:233:ILE:CD1	3:B:233:ILE:H	2.14	0.57
3:D:366:ASP:OD1	3:D:576:ARG:HD3	2.05	0.57
3:B:145:ARG:HH11	3:B:187:ILE:HD11	1.69	0.57
3:B:221:PHE:HB3	4:B:929:HOH:O	2.03	0.57
3:B:597:ILE:HD12	3:B:598:GLU:H	1.69	0.57
3:D:268:ILE:HG22	3:D:269:SER:N	2.20	0.57
3:D:561:LEU:HD12	3:D:561:LEU:H	1.69	0.57
3:B:555:ALA:O	3:B:559:ARG:HD3	2.04	0.57
3:A:63:ALA:HB3	3:A:67:ASP:OD1	2.05	0.57
3:B:218:VAL:HG13	3:B:222:ALA:CB	2.26	0.57
3:D:596:TRP:CE2	3:D:670:MSE:HB2	2.39	0.57
3:B:162:TRP:HB3	3:B:188:TYR:CZ	2.40	0.57
3:B:472:PRO:O	3:B:475:ILE:HG22	2.04	0.57
3:B:52:ILE:HG22	3:B:53:TYR:CD1	2.40	0.57
3:B:552:GLY:O	3:B:556:GLN:HG3	2.04	0.57
3:B:730:LEU:HB3	3:B:883:PHE:CE1	2.40	0.57
3:C:149:PHE:HB3	3:C:197:LEU:HD21	1.87	0.57
3:D:274:ILE:HG23	3:D:275:ASP:N	2.20	0.57
3:D:295:GLU:HA	3:D:299:ASN:N	2.19	0.57
1:G:11:DC:H2''	1:G:12:DA:OP2	2.04	0.57
3:A:162:TRP:HB3	3:A:188:TYR:CE1	2.39	0.57
3:C:159:VAL:HG11	3:C:317:HIS:CB	2.35	0.57
3:C:698:ILE:HG12	3:C:752:MSE:O	2.04	0.57
3:C:787:ASN:HB3	3:C:790:LYS:HB3	1.85	0.57
3:D:459:ASN:OD1	3:D:585:ALA:HA	2.05	0.57
3:A:239:ALA:O	3:A:242:LEU:HB2	2.05	0.57
3:A:680:LEU:HA	3:A:682:PHE:CZ	2.40	0.57
3:B:223:ILE:HB	3:B:224:PRO:HD3	1.86	0.57
3:B:87:ASP:OD1	3:B:363:LYS:HE3	2.05	0.57
3:C:193:ASN:HB3	3:C:196:GLU:HB2	1.86	0.57
3:C:422:GLN:HG3	3:C:680:LEU:HB2	1.87	0.57
3:C:818:ASN:ND2	3:C:818:ASN:C	2.58	0.57
3:D:83:LEU:HB3	3:D:380:ILE:O	2.05	0.57
3:A:548:THR:O	3:A:552:GLY:N	2.30	0.56
3:A:815:ILE:CD1	3:A:857:LEU:HD23	2.34	0.56
3:C:833:LEU:HD22	3:C:848:TRP:CH2	2.40	0.56
3:D:697:GLY:HA3	3:D:755:GLU:O	2.04	0.56
2:H:115:DA:H3'	3:B:116:GLU:OE1	2.04	0.56
3:C:791:TYR:CD2	3:C:801:CYS:HA	2.40	0.56
3:A:799:PRO:O	3:A:800:LYS:HB2	2.04	0.56
3:A:89:LYS:HB2	3:A:89:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:274:ILE:HG23	3:B:275:ASP:H	1.70	0.56
3:C:51:ASP:HB2	4:C:917:HOH:O	2.04	0.56
3:C:700:GLY:HA2	3:C:753:LEU:HD22	1.86	0.56
3:C:75:MSE:CE	3:C:80:LEU:HB3	2.36	0.56
3:B:47:THR:OG1	3:B:48:LYS:N	2.38	0.56
3:C:607:GLU:O	3:C:610:GLY:N	2.37	0.56
3:D:597:ILE:O	3:D:601:VAL:HG23	2.06	0.56
3:D:423:VAL:HG22	3:D:676:ASN:ND2	2.20	0.56
3:D:863:LEU:HD12	3:D:863:LEU:H	1.70	0.56
2:F:108:DT:H2''	2:F:109:DC:H5''	1.88	0.56
3:A:191:PHE:CD1	3:A:197:LEU:HD22	2.41	0.56
3:A:475:ILE:HD13	3:A:566:LEU:HD23	1.86	0.56
3:A:541:MSE:C	3:A:543:PHE:H	2.08	0.56
3:A:861:ASP:O	3:A:865:TRP:HD1	1.88	0.56
3:B:171:GLN:NE2	3:B:174:GLY:HA2	2.20	0.56
3:B:181:GLU:O	3:B:181:GLU:HG2	2.06	0.56
3:B:159:VAL:HG21	3:B:317:HIS:CB	2.36	0.56
3:C:11:ILE:HB	3:C:16:PHE:HE1	1.70	0.56
3:C:171:GLN:C	3:C:173:GLN:H	2.09	0.56
3:C:264:THR:C	3:C:265:LEU:HD23	2.26	0.56
3:D:85:MSE:HG3	3:D:370:PHE:CD1	2.40	0.56
3:A:24:GLY:O	3:A:107:LYS:HD2	2.06	0.56
3:A:280:PHE:HZ	3:A:358:VAL:HG22	1.70	0.56
3:D:43:GLU:CD	3:D:43:GLU:H	2.09	0.56
3:D:873:GLU:HA	3:D:877:ILE:CB	2.35	0.56
3:B:120:PRO:HG2	3:B:121:ASP:OD2	2.05	0.56
3:C:405:LYS:O	3:C:690:GLY:HA2	2.06	0.56
3:C:878:LYS:HB3	3:C:878:LYS:NZ	2.21	0.56
3:C:402:ASN:HA	3:C:886:ALA:O	2.06	0.56
3:D:386:HIS:HB3	3:D:387:PRO:HD2	1.87	0.56
3:D:862:VAL:C	3:D:864:HIS:H	2.08	0.56
3:D:749:ILE:HD11	3:D:883:PHE:CE1	2.41	0.56
3:A:152:LEU:HD11	3:A:190:PRO:HB2	1.88	0.56
3:A:283:THR:O	3:A:285:GLN:HG2	2.06	0.56
3:A:37:LEU:HD21	3:A:72:ILE:HD11	1.87	0.56
3:B:228:ASN:HA	4:B:915:HOH:O	2.07	0.56
3:B:380:ILE:HG23	3:B:576:ARG:CD	2.36	0.56
3:C:347:MSE:HB2	3:C:558:ASN:ND2	2.20	0.56
3:D:380:ILE:HD12	3:D:576:ARG:CZ	2.36	0.56
3:D:560:LYS:HA	3:D:563:ILE:CD1	2.35	0.56
3:D:604:TYR:O	3:D:608:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:104:DG:H2''	2:F:105:DC:H5'	1.88	0.56
3:A:214:THR:HG21	3:A:341:ILE:HD11	1.88	0.55
3:A:414:SER:O	3:A:417:PRO:HD2	2.06	0.55
3:B:407:VAL:HG13	3:B:689:ALA:HB3	1.86	0.55
3:C:223:ILE:HB	3:C:224:PRO:HD3	1.88	0.55
3:D:244:PRO:HG2	3:D:267:GLY:HA3	1.88	0.55
3:D:408:MSE:O	3:D:627:VAL:HG22	2.06	0.55
3:C:279:LYS:HD2	3:C:359:PHE:HD2	1.70	0.55
3:D:298:LEU:HD11	3:D:333:GLN:HB2	1.87	0.55
3:D:561:LEU:N	3:D:561:LEU:HD12	2.20	0.55
3:C:120:PRO:HD2	3:C:131:HIS:CD2	2.42	0.55
3:C:355:ILE:O	3:C:358:VAL:HG13	2.06	0.55
3:D:36:SER:C	3:D:37:LEU:HD12	2.27	0.55
3:D:61:LEU:HD12	3:D:61:LEU:N	2.22	0.55
3:D:410:PHE:HB3	3:D:683:MSE:HG2	1.87	0.55
3:D:761:GLN:HG3	3:D:891:TYR:O	2.07	0.55
2:F:110:DA:C8	2:F:111:DT:C7	2.89	0.55
3:B:138:HIS:ND1	3:B:204:PHE:HE2	2.05	0.55
3:C:134:ASP:O	3:C:135:ALA:HB2	2.05	0.55
3:C:193:ASN:HB3	3:C:196:GLU:CB	2.37	0.55
3:C:455:SER:HA	3:C:675:ASN:O	2.07	0.55
1:E:3:3DR:H2''	1:E:4:DC:H5''	1.88	0.55
3:B:741:VAL:HG11	3:B:875:THR:HB	1.89	0.55
3:B:897:LEU:CD2	3:D:636:VAL:HB	2.36	0.55
3:C:364:THR:O	3:C:368:ILE:HG13	2.06	0.55
3:A:112:ASN:HD22	3:A:113:PHE:N	2.04	0.55
3:B:20:ILE:CG2	3:B:24:GLY:HA2	2.37	0.55
3:B:159:VAL:HG21	3:B:317:HIS:HB2	1.87	0.55
3:C:164:ILE:HB	3:C:183:ILE:HD11	1.88	0.55
3:C:25:ARG:HG2	3:C:27:ARG:NH2	2.22	0.55
3:D:738:PRO:HG2	3:D:741:VAL:CG2	2.37	0.55
1:K:15:DC:H2''	1:K:16:DG:N7	2.21	0.55
3:B:305:TYR:CD1	3:B:312:LEU:HD13	2.41	0.55
3:B:362:ILE:H	3:B:362:ILE:CD1	1.99	0.55
3:B:425:ILE:HG12	3:B:463:TYR:CZ	2.40	0.55
3:B:396:VAL:O	3:B:705:LYS:NZ	2.40	0.55
3:C:411:ASP:HB3	4:C:936:HOH:O	2.06	0.55
3:C:661:PRO:O	3:C:665:ARG:HB2	2.06	0.55
3:D:581:ARG:HH11	3:D:581:ARG:CG	2.20	0.55
3:A:280:PHE:N	3:A:280:PHE:CD2	2.73	0.55
3:B:66:ARG:HB2	3:B:66:ARG:NH1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:SER:HA	3:C:131:HIS:HD2	1.72	0.55
3:C:215:GLY:O	3:C:273:TYR:HB2	2.07	0.55
3:C:313:ARG:C	3:C:315:SER:H	2.09	0.55
3:D:330:ARG:O	3:D:334:ILE:HG13	2.07	0.55
3:A:304:LYS:O	3:A:319:ARG:HD3	2.07	0.55
3:B:486:LYS:CB	3:B:556:GLN:NE2	2.69	0.55
3:B:661:PRO:O	3:B:665:ARG:HG3	2.05	0.55
3:C:133:ILE:HD12	3:C:198:LEU:HD21	1.89	0.55
3:C:170:LEU:HA	3:C:177:GLU:HG2	1.87	0.55
3:C:489:MSE:HB2	3:C:552:GLY:HA3	1.89	0.55
3:C:455:SER:OG	3:C:676:ASN:HA	2.07	0.55
3:D:407:VAL:HG11	3:D:710:LEU:HD22	1.87	0.55
3:D:92:TYR:CE2	3:D:96:THR:HG21	2.40	0.55
3:D:218:VAL:HA	3:D:222:ALA:CB	2.36	0.55
3:C:158:ASN:HD22	3:C:158:ASN:C	2.10	0.54
3:B:268:ILE:CG2	3:B:269:SER:N	2.70	0.54
3:D:381:PRO:O	3:D:576:ARG:NH2	2.40	0.54
3:A:859:LYS:O	3:A:861:ASP:N	2.34	0.54
3:B:83:LEU:HD12	3:B:83:LEU:H	1.72	0.54
3:C:52:ILE:HD12	3:C:428:GLU:HG2	1.90	0.54
3:C:633:ILE:HD11	3:C:651:LEU:CD1	2.36	0.54
3:C:647:TRP:CE3	3:C:651:LEU:HD12	2.43	0.54
3:B:171:GLN:HE22	3:B:174:GLY:HA2	1.70	0.54
3:B:486:LYS:O	3:B:490:LEU:HG	2.08	0.54
3:B:658:ARG:O	3:B:661:PRO:HD2	2.08	0.54
3:C:725:LEU:HD11	3:C:750:ARG:HB2	1.89	0.54
3:C:848:TRP:CD2	3:C:854:ILE:HD12	2.42	0.54
3:D:455:SER:HA	3:D:675:ASN:O	2.06	0.54
3:D:561:LEU:H	3:D:561:LEU:CD1	2.20	0.54
3:D:589:PHE:CE2	3:D:674:MSE:HG3	2.43	0.54
3:B:594:LEU:HD13	3:B:623:ASP:N	2.21	0.54
3:D:362:ILE:HG13	3:D:363:LYS:H	1.72	0.54
3:B:328:VAL:O	3:B:331:VAL:HG22	2.08	0.54
3:B:621:ASP:OD1	3:B:706:LYS:HE2	2.08	0.54
3:A:812:ASN:O	3:A:815:ILE:HG22	2.08	0.54
3:B:154:SER:C	3:B:156:TYR:N	2.61	0.54
3:B:287:SER:HB3	3:B:292:TYR:CD2	2.43	0.54
3:B:391:TYR:HB2	3:B:392:PRO:HD2	1.90	0.54
3:C:204:PHE:CE1	3:C:208:LYS:HD3	2.43	0.54
3:C:422:GLN:NE2	3:C:680:LEU:H	2.03	0.54
3:D:426:SER:HB3	3:D:472:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:36:SER:O	3:A:37:LEU:HD12	2.08	0.54
3:A:789:ALA:HA	3:A:792:ASP:HB2	1.90	0.54
3:B:185:LYS:O	3:B:185:LYS:HG3	2.08	0.54
3:C:23:ASN:O	3:C:25:ARG:N	2.41	0.54
3:C:636:VAL:HG21	3:C:650:PHE:CZ	2.43	0.54
3:D:360:SER:OG	3:D:362:ILE:HG13	2.08	0.54
3:B:247:LYS:O	3:B:266:PHE:HB2	2.07	0.54
3:B:313:ARG:O	3:B:313:ARG:HD3	2.07	0.54
3:C:159:VAL:HG12	3:C:160:GLU:N	2.21	0.54
3:D:434:PHE:CE1	3:D:456:CYS:HB3	2.42	0.54
3:D:459:ASN:CG	3:D:585:ALA:HA	2.28	0.54
3:B:301:GLY:C	3:B:303:LEU:H	2.11	0.53
3:D:732:THR:HG22	3:D:733:GLN:N	2.23	0.53
3:D:862:VAL:C	3:D:864:HIS:N	2.62	0.53
3:A:137:THR:HG22	3:A:328:VAL:HG21	1.89	0.53
3:A:443:ILE:HD13	3:A:595:GLN:CB	2.38	0.53
3:C:722:GLU:HB3	4:C:1005:HOH:O	2.08	0.53
3:D:273:TYR:CA	3:D:276:LEU:HD13	2.33	0.53
3:B:108:ILE:HD13	3:B:345:LEU:HD21	1.91	0.53
3:A:231:LYS:HG3	3:A:236:GLU:HA	1.90	0.53
3:A:83:LEU:HB3	3:A:379:VAL:HG12	1.90	0.53
3:B:137:THR:HG23	3:B:324:ASN:OD1	2.09	0.53
3:C:607:GLU:O	3:C:609:CYS:N	2.40	0.53
2:F:105:DC:H2''	2:F:106:DT:C6	2.43	0.53
3:B:423:VAL:HB	3:B:425:ILE:HG13	1.90	0.53
3:C:631:LYS:HG2	4:C:957:HOH:O	2.08	0.53
3:D:62:PHE:CD2	3:D:68:ALA:HA	2.43	0.53
3:B:370:PHE:HA	3:B:380:ILE:HD11	1.90	0.53
3:B:698:ILE:HG13	3:B:753:LEU:HD23	1.91	0.53
3:B:725:LEU:HD22	3:B:753:LEU:HD12	1.90	0.53
3:C:20:ILE:CG2	3:C:24:GLY:HA2	2.39	0.53
3:C:404:TYR:CD1	3:C:618:LEU:HD13	2.43	0.53
3:D:750:ARG:HG2	3:D:754:GLN:HG3	1.90	0.53
1:E:4:DC:H2''	1:E:5:DT:C5	2.44	0.53
1:I:7:DA:H4'	1:I:8:DT:OP1	2.09	0.53
3:B:274:ILE:HG23	3:B:275:ASP:N	2.24	0.53
3:C:265:LEU:HD23	3:C:265:LEU:N	2.23	0.53
3:A:353:ILE:HD12	3:A:357:SER:HB2	1.90	0.53
3:B:133:ILE:HG12	3:B:225:TYR:CE2	2.43	0.53
3:B:216:TRP:CH2	3:B:293:ILE:HD12	2.44	0.53
3:B:305:TYR:CE1	3:B:312:LEU:HD22	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:176:ASP:OD2	3:B:319:ARG:HD2	2.09	0.53
3:B:312:LEU:HD23	3:B:320:TYR:HD1	1.74	0.53
3:C:117:VAL:HG22	3:C:133:ILE:HA	1.91	0.53
3:D:42:PRO:C	3:D:44:SER:N	2.62	0.53
3:D:560:LYS:HA	3:D:563:ILE:HG13	1.90	0.53
3:C:187:ILE:HG22	3:C:187:ILE:O	2.09	0.53
3:D:688:ILE:HB	3:D:714:ASP:OD1	2.08	0.53
3:D:871:LEU:O	3:D:875:THR:HG22	2.09	0.53
3:B:697:GLY:HA3	3:B:753:LEU:O	2.09	0.53
3:D:218:VAL:HA	3:D:222:ALA:HB3	1.89	0.53
3:A:461:MSE:CA	3:A:461:MSE:HE2	2.38	0.52
3:B:226:VAL:O	3:B:230:ILE:HG13	2.09	0.52
3:C:81:GLU:HG3	3:C:384:ARG:HH21	1.71	0.52
1:I:4:DC:H2"	1:I:5:DT:OP2	2.09	0.52
3:A:52:ILE:HG13	3:A:53:TYR:CD1	2.43	0.52
3:A:405:LYS:HA	3:A:699:GLY:HA3	1.92	0.52
3:B:218:VAL:HA	4:B:929:HOH:O	2.08	0.52
3:C:154:SER:C	3:C:156:TYR:H	2.11	0.52
3:C:692:PRO:HD2	3:C:695:SER:OG	2.09	0.52
3:D:699:GLY:O	3:D:753:LEU:HD13	2.09	0.52
3:A:269:SER:OG	3:A:356:GLN:NE2	2.42	0.52
3:A:395:PHE:HA	4:A:918:HOH:O	2.09	0.52
3:C:727:ILE:HG21	3:C:732:THR:HG21	1.90	0.52
3:D:218:VAL:HG13	3:D:222:ALA:CB	2.34	0.52
3:D:576:ARG:HH11	3:D:576:ARG:HB3	1.72	0.52
3:B:253:ILE:HG12	3:B:254:GLU:N	2.24	0.52
3:B:664:ASP:O	3:B:668:ARG:HG3	2.09	0.52
1:G:12:DA:N6	2:H:106:DT:H3	2.03	0.52
3:B:622:THR:O	3:B:623:ASP:CB	2.57	0.52
3:B:422:GLN:HE21	3:B:676:ASN:ND2	2.06	0.52
3:C:128:GLN:HE21	3:C:128:GLN:CA	2.22	0.52
3:C:38:PHE:HB2	3:C:83:LEU:HB2	1.90	0.52
3:C:75:MSE:HE3	3:C:80:LEU:HB3	1.90	0.52
3:D:380:ILE:HB	3:D:576:ARG:NH1	2.24	0.52
3:B:405:LYS:HG2	3:B:406:TYR:CD2	2.45	0.52
3:B:763:TYR:HA	3:B:766:GLU:HB3	1.91	0.52
3:C:776:TYR:HB2	3:C:866:MSE:HE1	1.91	0.52
1:I:3:3DR:H1'2	4:C:1010:HOH:O	2.10	0.52
3:A:176:ASP:HA	3:A:319:ARG:HH21	1.75	0.52
3:B:276:LEU:O	3:B:280:PHE:HD2	1.93	0.52
3:B:271:LEU:CD1	3:B:356:GLN:HA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:GLN:CG	3:C:174:GLY:N	2.73	0.52
3:C:458:PRO:N	3:C:674:MSE:HE2	2.24	0.52
3:D:291:ASP:HB3	3:D:302:LYS:HG2	1.91	0.52
2:L:107:DG:N9	2:L:108:DT:C7	2.72	0.52
3:A:43:GLU:CD	3:A:43:GLU:N	2.64	0.52
3:A:854:ILE:HG13	3:A:859:LYS:HB2	1.92	0.52
3:B:38:PHE:CE2	3:B:59:ARG:HB2	2.44	0.52
3:B:543:PHE:HB3	4:B:948:HOH:O	2.09	0.52
3:C:11:ILE:HD12	3:C:16:PHE:CD1	2.44	0.52
3:B:192:ASP:O	3:B:193:ASN:CB	2.52	0.52
3:C:110:VAL:HB	3:C:141:SER:HB2	1.91	0.52
3:C:391:TYR:HB2	3:C:392:PRO:HD2	1.92	0.52
3:C:53:TYR:CE2	3:C:428:GLU:HA	2.44	0.52
3:C:720:TYR:CD2	3:C:724:LYS:HG3	2.45	0.52
3:B:396:VAL:HG13	3:B:396:VAL:O	2.11	0.51
3:B:52:ILE:HG23	3:B:428:GLU:HB3	1.92	0.51
3:B:52:ILE:CG1	3:B:470:VAL:HG21	2.39	0.51
3:B:646:HIS:HD2	4:B:977:HOH:O	1.93	0.51
3:C:188:TYR:CD2	3:C:190:PRO:HD3	2.45	0.51
3:C:83:LEU:HB3	3:C:379:VAL:CG1	2.40	0.51
3:D:13:ASP:OD1	3:D:64:ASN:HA	2.11	0.51
3:D:733:GLN:HA	3:D:742:GLN:HE22	1.75	0.51
3:B:171:GLN:C	3:B:173:GLN:H	2.14	0.51
3:B:475:ILE:HD11	3:B:563:ILE:HG12	1.92	0.51
3:C:170:LEU:CD1	3:C:170:LEU:H	2.24	0.51
3:C:172:GLU:HG2	4:C:1033:HOH:O	2.09	0.51
3:C:493:GLN:HG2	3:C:549:GLU:OE2	2.09	0.51
3:D:9:GLU:HA	3:D:89:LYS:HE3	1.92	0.51
3:B:145:ARG:HB3	3:B:187:ILE:HD13	1.91	0.51
3:B:356:GLN:C	3:B:358:VAL:H	2.12	0.51
3:B:771:PHE:CD2	3:B:872:LEU:HD13	2.45	0.51
3:C:147:TYR:HB3	3:C:149:PHE:CE1	2.45	0.51
3:C:170:LEU:HD12	3:C:170:LEU:N	2.25	0.51
3:C:738:PRO:HG2	3:C:741:VAL:HG21	1.92	0.51
3:D:419:ILE:HD12	3:D:589:PHE:CD1	2.45	0.51
3:D:455:SER:OG	3:D:676:ASN:HA	2.10	0.51
3:D:606:ASN:ND2	3:D:611:THR:HB	2.25	0.51
3:D:705:LYS:C	3:D:707:ARG:H	2.12	0.51
3:A:854:ILE:HG13	3:A:854:ILE:O	2.09	0.51
3:B:261:GLU:CG	3:B:262:ILE:N	2.68	0.51
3:C:290:LEU:O	3:C:294:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:495:ASN:ND2	3:C:495:ASN:N	2.54	0.51
3:C:362:ILE:HG23	3:C:575:PHE:HD1	1.75	0.51
3:C:757:GLU:N	4:C:950:HOH:O	2.42	0.51
3:A:403:ARG:HD2	3:A:887:ALA:O	2.10	0.51
3:A:493:GLN:HG3	3:A:494:ARG:NH1	2.25	0.51
3:A:656:ARG:HB3	3:A:656:ARG:NH1	2.25	0.51
3:A:789:ALA:HA	3:A:792:ASP:CB	2.40	0.51
3:B:186:ILE:O	3:B:186:ILE:HG22	2.09	0.51
3:C:833:LEU:HD22	3:C:848:TRP:HH2	1.75	0.51
3:D:380:ILE:HB	3:D:576:ARG:HH12	1.76	0.51
3:D:405:LYS:HE2	3:D:406:TYR:CE1	2.43	0.51
3:D:702:TRP:CE2	3:D:708:TYR:HB3	2.46	0.51
3:D:759:SER:C	3:D:761:GLN:N	2.64	0.51
3:B:117:VAL:HG11	3:B:225:TYR:CE2	2.45	0.51
3:B:117:VAL:CG2	3:B:124:PRO:HG3	2.41	0.51
3:C:52:ILE:HD12	3:C:428:GLU:CG	2.41	0.51
1:K:16:DG:H2''	1:K:17:DC:O5'	2.11	0.51
3:B:183:ILE:HA	3:B:186:ILE:HD12	1.92	0.51
3:C:354:GLN:HB3	3:C:356:GLN:OE1	2.11	0.51
3:D:270:VAL:O	3:D:271:LEU:HD23	2.11	0.51
3:D:425:ILE:HG23	3:D:463:TYR:CE2	2.46	0.51
3:D:863:LEU:N	3:D:863:LEU:HD12	2.26	0.51
3:B:406:TYR:N	4:B:923:HOH:O	2.44	0.51
3:C:422:GLN:O	3:C:676:ASN:HB3	2.10	0.51
3:C:425:ILE:HG23	3:C:463:TYR:CE2	2.46	0.51
3:D:216:TRP:CH2	3:D:293:ILE:HG12	2.46	0.51
3:A:104:ASP:OD2	3:A:106:THR:HB	2.10	0.51
3:B:117:VAL:HG11	3:B:225:TYR:CZ	2.46	0.51
3:B:409:SER:OG	3:B:687:ALA:N	2.33	0.51
3:B:734:LYS:HB2	3:B:737:THR:CG2	2.34	0.51
3:C:3:GLU:HG3	3:C:20:ILE:O	2.11	0.51
3:B:143:ASP:OD2	3:B:208:LYS:HE2	2.12	0.50
3:B:490:LEU:HD22	3:B:494:ARG:HH12	1.76	0.50
3:C:170:LEU:HD12	3:C:170:LEU:H	1.76	0.50
3:C:475:ILE:CG2	3:C:566:LEU:HD22	2.41	0.50
3:D:191:PHE:HB2	3:D:197:LEU:HG	1.92	0.50
3:B:391:TYR:HB2	3:B:392:PRO:CD	2.41	0.50
3:D:326:ILE:O	3:D:329:TYR:HB3	2.11	0.50
2:L:107:DG:C8	2:L:108:DT:C7	2.95	0.50
3:B:175:GLY:HA3	4:B:976:HOH:O	2.10	0.50
3:B:893:LYS:HA	3:B:893:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:469:GLY:C	3:D:472:PRO:HD2	2.32	0.50
3:D:872:LEU:O	3:D:874:LYS:N	2.37	0.50
3:A:402:ASN:HA	3:A:886:ALA:O	2.12	0.50
3:B:20:ILE:HG22	3:B:24:GLY:HA2	1.93	0.50
3:B:362:ILE:HD13	3:B:362:ILE:N	2.11	0.50
3:B:547:ARG:O	3:B:550:VAL:HG22	2.11	0.50
3:B:750:ARG:HG2	3:B:754:GLN:OE1	2.12	0.50
3:D:713:TRP:O	3:D:714:ASP:HB3	2.12	0.50
1:K:15:DC:H2''	1:K:16:DG:C8	2.46	0.50
3:B:300:VAL:CG1	3:B:301:GLY:N	2.74	0.50
3:A:130:LYS:HG3	3:A:131:HIS:CE1	2.46	0.50
3:A:862:VAL:C	3:A:864:HIS:H	2.14	0.50
3:B:131:HIS:HB3	3:B:132:PRO:HD2	1.93	0.50
3:B:193:ASN:ND2	3:B:195:LYS:H	2.10	0.50
3:B:472:PRO:HA	3:B:475:ILE:HG22	1.92	0.50
3:C:112:ASN:CB	3:C:214:THR:HG23	2.33	0.50
3:C:25:ARG:HG2	3:C:27:ARG:CZ	2.41	0.50
3:D:323:TYR:HB2	4:D:938:HOH:O	2.11	0.50
3:B:136:ILE:HD12	3:B:136:ILE:N	2.27	0.50
3:B:316:ASN:OD1	3:B:319:ARG:HB2	2.11	0.50
3:B:541:MSE:HG2	3:B:544:ARG:HD2	1.93	0.50
3:B:401:PRO:HA	3:B:702:TRP:O	2.12	0.50
3:C:469:GLY:C	3:C:472:PRO:HD2	2.32	0.50
3:D:717:GLY:O	3:D:718:THR:C	2.48	0.50
2:F:108:DT:H2''	2:F:109:DC:H5'	1.94	0.50
1:G:12:DA:C2'	1:G:13:DG:H5'	2.21	0.50
3:A:581:ARG:NH1	3:A:581:ARG:CG	2.71	0.50
3:A:708:TYR:CZ	3:A:728:MSE:HG3	2.47	0.50
3:D:223:ILE:O	3:D:226:VAL:HG22	2.12	0.50
3:D:659:MSE:O	3:D:662:ALA:HB3	2.12	0.50
3:A:556:GLN:HE21	3:A:557:ILE:N	2.10	0.50
3:C:285:GLN:HG3	3:C:293:ILE:CD1	2.41	0.50
3:C:848:TRP:CE3	3:C:854:ILE:HD12	2.47	0.49
2:F:111:DT:H2''	2:F:112:DA:H5''	1.93	0.49
1:K:10:DA:H2''	1:K:11:DC:O5'	2.12	0.49
3:A:859:LYS:CG	3:A:860:ASP:N	2.74	0.49
3:B:221:PHE:O	3:B:224:PRO:HD2	2.12	0.49
3:B:667:PHE:CE1	3:B:681:MSE:HG2	2.47	0.49
3:D:440:HIS:HA	3:D:443:ILE:HD11	1.94	0.49
3:A:408:MSE:HE1	3:A:655:ALA:CB	2.38	0.49
3:B:545:ALA:HB3	4:B:988:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:593:ALA:O	3:B:597:ILE:HG13	2.12	0.49
3:C:553:MSE:O	3:C:557:ILE:HG12	2.12	0.49
3:D:707:ARG:HA	3:D:729:GLY:HA3	1.94	0.49
3:A:112:ASN:C	3:A:112:ASN:HD22	2.14	0.49
3:A:20:ILE:CG2	3:A:24:GLY:HA2	2.43	0.49
3:A:216:TRP:HZ2	3:A:288:TYR:O	1.96	0.49
3:A:294:SER:OG	3:A:330:ARG:HD2	2.12	0.49
3:A:395:PHE:CB	3:A:591:GLN:HG3	2.29	0.49
3:B:707:ARG:HA	3:B:728:MSE:O	2.12	0.49
3:C:433:THR:N	3:C:462:MSE:HE2	2.27	0.49
3:A:541:MSE:SE	3:A:541:MSE:O	2.81	0.49
3:C:158:ASN:ND2	3:C:159:VAL:N	2.51	0.49
3:C:1:MSE:HG2	3:C:24:GLY:H	1.78	0.49
3:A:859:LYS:CG	3:A:860:ASP:H	2.22	0.49
3:B:19:TYR:CE1	3:B:29:ARG:HG2	2.48	0.49
3:B:391:TYR:HD2	3:B:391:TYR:H	1.61	0.49
3:B:421:ARG:HD3	3:B:475:ILE:HG23	1.93	0.49
3:B:398:GLU:OE2	3:B:705:LYS:HE2	2.12	0.49
3:B:878:LYS:HB2	3:B:879:PRO:CD	2.42	0.49
3:C:425:ILE:HA	3:C:463:TYR:CD2	2.47	0.49
3:D:19:TYR:O	3:D:26:GLU:HA	2.13	0.49
3:D:287:SER:HB3	3:D:292:TYR:HE2	1.77	0.49
3:A:426:SER:OG	3:A:427:PRO:HD2	2.13	0.49
3:B:412:LEU:HD12	3:B:623:ASP:CA	2.25	0.49
3:B:575:PHE:CE2	3:B:577:TYR:HB2	2.47	0.49
3:B:408:MSE:CE	3:B:688:ILE:HG12	2.36	0.49
3:C:181:GLU:N	3:C:181:GLU:OE1	2.37	0.49
3:C:471:VAL:HB	3:C:472:PRO:HD3	1.93	0.49
3:C:647:TRP:CZ3	3:C:651:LEU:HD12	2.48	0.49
3:C:668:ARG:HG3	3:C:668:ARG:NH1	2.25	0.49
3:D:863:LEU:CD1	3:D:863:LEU:H	2.25	0.49
3:A:10:GLN:HG3	3:A:65:MSE:SE	2.63	0.49
3:A:178:VAL:HG13	3:A:182:ILE:HD11	1.95	0.49
3:B:147:TYR:CD1	3:B:147:TYR:N	2.81	0.49
3:C:412:LEU:HD13	3:C:415:LEU:HD13	1.94	0.49
3:A:277:TYR:O	3:A:281:SER:CB	2.60	0.49
3:B:331:VAL:HG23	3:B:332:LEU:N	2.27	0.49
3:C:408:MSE:HE2	3:C:629:ALA:HB2	1.95	0.49
3:C:738:PRO:HG2	3:C:741:VAL:HB	1.95	0.49
3:D:298:LEU:HB3	3:D:300:VAL:CG1	2.30	0.49
3:A:596:TRP:CE2	3:A:670:MSE:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:618:LEU:HG	3:A:626:TYR:O	2.13	0.49
3:B:347:MSE:HE3	3:B:358:VAL:HG22	1.94	0.49
3:B:596:TRP:CE2	3:B:670:MSE:HB2	2.47	0.49
3:C:405:LYS:NZ	4:C:904:HOH:O	2.46	0.49
3:C:795:GLY:O	3:C:813:ARG:HD3	2.12	0.49
3:D:85:MSE:CA	3:D:380:ILE:HD11	2.43	0.49
3:D:10:GLN:CB	3:D:65:MSE:HE1	2.43	0.49
3:D:422:GLN:HG2	3:D:678:GLN:O	2.13	0.49
3:D:72:ILE:O	3:D:76:GLU:HG3	2.13	0.49
2:L:104:DG:N2	4:L:318:HOH:O	2.38	0.49
2:L:107:DG:C2'	2:L:108:DT:C7	2.69	0.49
3:D:597:ILE:CD1	3:D:663:ILE:HG23	2.42	0.48
3:A:422:GLN:HE21	3:A:680:LEU:H	1.60	0.48
3:A:441:ASP:HB3	3:A:447:ALA:HB2	1.94	0.48
3:A:83:LEU:CD2	3:A:83:LEU:N	2.76	0.48
3:B:177:GLU:C	3:B:179:PRO:HD3	2.33	0.48
3:B:230:ILE:HD12	3:B:242:LEU:HD11	1.94	0.48
3:D:102:LYS:HA	3:D:102:LYS:NZ	2.28	0.48
3:D:298:LEU:HD11	3:D:333:GLN:CB	2.44	0.48
3:D:373:LEU:C	3:D:375:GLU:H	2.16	0.48
3:D:450:PRO:HB2	3:D:456:CYS:SG	2.53	0.48
3:D:604:TYR:CE1	3:D:659:MSE:HA	2.42	0.48
3:D:663:ILE:CG2	3:D:683:MSE:HE2	2.43	0.48
3:B:129:ALA:HB1	3:B:229:ARG:HG2	1.92	0.48
3:B:405:LYS:HA	3:B:699:GLY:CA	2.38	0.48
3:B:553:MSE:O	3:B:557:ILE:HG12	2.13	0.48
3:C:290:LEU:O	3:C:294:SER:CB	2.61	0.48
3:D:459:ASN:ND2	3:D:461:MSE:HG2	2.29	0.48
1:G:14:DC:H42	2:H:104:DG:H1	1.61	0.48
3:A:253:ILE:HD12	3:A:260:ARG:NH2	2.29	0.48
3:A:422:GLN:NE2	3:A:680:LEU:H	2.11	0.48
3:B:159:VAL:HG11	3:B:317:HIS:CE1	2.48	0.48
3:B:137:THR:HG23	3:B:324:ASN:CG	2.34	0.48
3:B:776:TYR:N	3:B:776:TYR:CD1	2.81	0.48
3:D:239:ALA:C	3:D:241:ARG:N	2.64	0.48
3:D:89:LYS:O	3:D:93:LEU:HG	2.14	0.48
3:A:725:LEU:HD11	3:A:750:ARG:HB2	1.96	0.48
3:A:785:ALA:CB	3:A:808:ILE:HD11	2.44	0.48
3:B:681:MSE:HE2	3:B:681:MSE:HA	1.94	0.48
3:C:254:GLU:OE1	3:C:258:GLY:HA3	2.13	0.48
3:D:87:ASP:O	3:D:88:PHE:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:3DR:OP1	3:A:361:PRO:HD2	2.14	0.48
3:B:133:ILE:HG13	3:B:229:ARG:HG3	1.95	0.48
3:B:215:GLY:HA3	3:B:218:VAL:CG2	2.41	0.48
3:B:594:LEU:HA	3:B:597:ILE:HD11	1.95	0.48
3:C:298:LEU:O	3:C:299:ASN:HB2	2.12	0.48
3:C:423:VAL:HB	3:C:425:ILE:HG13	1.95	0.48
3:D:84:GLY:C	3:D:380:ILE:HD11	2.34	0.48
3:D:434:PHE:CE2	3:D:450:PRO:HB3	2.48	0.48
3:B:1:MSE:HG2	3:B:1:MSE:O	2.13	0.48
3:C:147:TYR:CB	3:C:149:PHE:HE1	2.27	0.48
3:C:151:LEU:O	3:C:313:ARG:NH2	2.38	0.48
3:C:110:VAL:HG13	3:C:212:ILE:HB	1.95	0.48
3:D:241:ARG:O	3:D:243:SER:N	2.46	0.48
3:D:617:VAL:O	3:D:617:VAL:HG23	2.14	0.48
1:G:12:DA:C2'	1:G:13:DG:C5'	2.82	0.48
3:A:254:GLU:HA	3:A:259:SER:HA	1.96	0.48
3:A:280:PHE:CZ	3:A:358:VAL:HG22	2.49	0.48
3:B:234:PHE:CD1	3:B:234:PHE:N	2.78	0.48
3:B:421:ARG:HB3	3:B:680:LEU:HD13	1.96	0.48
3:D:20:ILE:N	3:D:20:ILE:HD12	2.29	0.48
3:D:301:GLY:O	3:D:303:LEU:N	2.47	0.48
3:D:578:TYR:OH	3:D:580:LEU:HB2	2.14	0.48
3:D:779:ILE:HD12	3:D:871:LEU:HD23	1.95	0.48
1:G:9:DG:H2''	1:G:10:DA:OP2	2.14	0.48
3:B:622:THR:O	3:B:623:ASP:OD1	2.32	0.48
3:B:66:ARG:HG3	3:B:67:ASP:N	2.29	0.48
3:C:434:PHE:CE1	3:C:456:CYS:HB3	2.49	0.48
3:C:593:ALA:HB1	3:C:681:MSE:HE3	1.96	0.48
3:C:872:LEU:HD12	3:C:876:PHE:HB3	1.95	0.48
3:D:327:ALA:C	3:D:329:TYR:N	2.64	0.48
3:A:850:SER:O	3:A:852:THR:HG23	2.13	0.48
3:B:113:PHE:CE1	3:B:218:VAL:HG11	2.48	0.48
3:B:143:ASP:O	3:B:144:ASP:C	2.52	0.48
3:B:295:GLU:O	3:B:299:ASN:HA	2.13	0.48
3:B:425:ILE:HA	3:B:463:TYR:CD2	2.48	0.48
3:C:343:LEU:HG	3:C:558:ASN:OD1	2.13	0.48
3:C:579:ASP:HB3	3:C:582:ASN:HB2	1.96	0.48
3:D:352:LYS:HD2	3:D:371:ASN:OD1	2.13	0.48
3:D:453:VAL:CG2	3:D:454:TYR:H	2.03	0.48
3:D:481:GLN:HB3	3:D:559:ARG:NH1	2.25	0.48
3:A:555:ALA:O	3:A:559:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:212:ILE:O	3:B:212:ILE:HG22	2.14	0.47
3:B:47:THR:HG23	3:B:49:TYR:H	1.79	0.47
3:B:687:ALA:HB2	3:B:715:MSE:CE	2.26	0.47
3:D:458:PRO:HG3	3:D:592:MSE:SE	2.64	0.47
3:D:5:TYR:HA	3:D:19:TYR:HA	1.96	0.47
3:D:722:GLU:CG	3:D:723:PRO:HD2	2.40	0.47
3:A:17:GLU:OE1	3:A:29:ARG:NH1	2.47	0.47
3:B:176:ASP:HA	3:B:319:ARG:NE	2.23	0.47
3:B:338:ARG:O	3:B:339:GLN:HB2	2.14	0.47
3:D:570:LEU:HD12	3:D:570:LEU:O	2.13	0.47
3:D:595:GLN:HA	3:D:598:GLU:HG2	1.96	0.47
3:A:208:LYS:NZ	4:A:925:HOH:O	2.46	0.47
3:A:339:GLN:NE2	3:A:339:GLN:HA	2.29	0.47
3:B:229:ARG:NH1	3:B:233:ILE:HD11	2.28	0.47
3:B:316:ASN:C	3:B:318:GLN:H	2.17	0.47
3:C:170:LEU:HB2	4:C:1033:HOH:O	2.14	0.47
3:C:738:PRO:HG2	3:C:741:VAL:CB	2.43	0.47
3:D:90:LEU:CD2	3:D:353:ILE:HA	2.44	0.47
3:D:732:THR:HG22	3:D:733:GLN:H	1.78	0.47
3:C:186:ILE:HG22	3:C:187:ILE:H	1.79	0.47
3:C:199:MSE:HG2	3:C:234:PHE:CZ	2.49	0.47
3:C:159:VAL:HG11	3:C:317:HIS:CG	2.49	0.47
3:C:45:GLN:O	3:C:47:THR:HG23	2.14	0.47
3:C:61:LEU:HD23	3:C:62:PHE:N	2.28	0.47
3:C:78:ILE:HG13	3:C:80:LEU:HD23	1.97	0.47
3:B:19:TYR:HE1	3:B:29:ARG:HG2	1.79	0.47
3:B:471:VAL:N	3:B:472:PRO:HD2	2.29	0.47
3:B:405:LYS:HG3	3:B:691:PRO:HD3	1.97	0.47
3:B:893:LYS:HA	3:B:893:LYS:CE	2.45	0.47
3:C:277:TYR:O	3:C:281:SER:HB3	2.14	0.47
3:C:560:LYS:HE3	3:C:564:ASN:HD21	1.78	0.47
3:C:83:LEU:N	3:C:83:LEU:HD22	2.30	0.47
3:D:449:ARG:HD2	3:D:673:TYR:O	2.15	0.47
3:D:758:GLU:O	3:D:762:GLU:CB	2.63	0.47
3:A:725:LEU:HD22	3:A:753:LEU:HD12	1.95	0.47
3:A:895:ALA:O	3:A:896:SER:C	2.52	0.47
3:B:443:ILE:HD13	3:B:595:GLN:CB	2.45	0.47
3:D:302:LYS:O	3:D:326:ILE:HG21	2.14	0.47
3:D:42:PRO:O	3:D:44:SER:N	2.48	0.47
3:D:862:VAL:O	3:D:864:HIS:N	2.48	0.47
3:A:206:GLN:NE2	3:A:241:ARG:O	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:339:GLN:HE21	3:A:339:GLN:HA	1.80	0.47
3:A:443:ILE:HD13	3:A:595:GLN:HB2	1.96	0.47
3:B:139:TYR:CE2	3:B:332:LEU:HD21	2.49	0.47
3:B:231:LYS:HA	3:B:235:GLY:CA	2.42	0.47
3:B:604:TYR:O	3:B:607:GLU:HB3	2.15	0.47
3:B:730:LEU:HD23	3:B:730:LEU:N	2.30	0.47
3:C:482:ARG:CZ	3:C:560:LYS:HD3	2.44	0.47
3:D:210:PRO:HD2	3:D:242:LEU:HD21	1.97	0.47
3:D:605:LEU:HD21	3:D:654:PHE:HE1	1.79	0.47
1:K:18:DG:O6	3:A:380:ILE:HG12	2.14	0.47
3:A:303:LEU:HB3	3:A:323:TYR:HD1	1.80	0.47
3:A:347:MSE:HE2	3:A:558:ASN:OD1	2.14	0.47
3:B:290:LEU:HD13	3:B:302:LYS:HE3	1.97	0.47
3:B:702:TRP:CZ3	3:B:710:LEU:HD21	2.49	0.47
3:C:233:ILE:HG22	3:C:234:PHE:N	2.28	0.47
3:C:424:ASN:HD21	3:C:469:GLY:N	2.03	0.47
3:C:633:ILE:CD1	3:C:651:LEU:HD11	2.39	0.47
3:D:13:ASP:HA	3:D:65:MSE:HB3	1.97	0.47
3:D:415:LEU:CD2	3:D:622:THR:HG23	2.41	0.47
1:I:1:DC:H4'	3:C:255:ASN:OD1	2.14	0.47
3:A:553:MSE:O	3:A:556:GLN:HB3	2.15	0.47
3:A:751:ARG:NE	3:A:763:TYR:HB2	2.30	0.47
3:B:145:ARG:HB2	3:B:147:TYR:CE1	2.49	0.47
3:B:154:SER:O	3:B:157:GLY:N	2.42	0.47
3:C:129:ALA:O	3:C:229:ARG:NH1	2.48	0.47
3:C:313:ARG:HH11	3:C:313:ARG:HG3	1.79	0.47
3:D:558:ASN:HA	3:D:561:LEU:HD13	1.96	0.47
3:D:635:LYS:HE3	3:D:635:LYS:N	2.29	0.47
2:F:108:DT:C2'	2:F:109:DC:H5''	2.44	0.47
2:H:115:DA:H4'	3:B:117:VAL:HG22	1.97	0.47
3:A:825:VAL:HB	3:A:828:GLU:CG	2.40	0.47
3:A:83:LEU:HD22	3:A:83:LEU:N	2.30	0.47
3:B:145:ARG:HD3	3:B:185:LYS:HB2	1.95	0.47
3:B:599:ARG:NH2	3:B:600:LYS:HE2	2.30	0.47
3:C:189:MSE:O	3:C:191:PHE:CE1	2.68	0.47
3:C:298:LEU:O	3:C:299:ASN:CB	2.63	0.47
2:J:112:DA:C5'	3:C:734:LYS:HG2	2.45	0.47
3:D:542:LEU:C	3:D:544:ARG:H	2.18	0.47
3:A:366:ASP:OD1	3:A:576:ARG:HD2	2.14	0.47
3:A:488:TYR:O	3:A:492:ALA:N	2.47	0.47
3:A:740:ALA:HB2	3:A:778:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:216:TRP:H	3:B:218:VAL:HG23	1.80	0.47
3:B:543:PHE:C	3:B:545:ALA:H	2.19	0.47
3:C:37:LEU:C	3:C:38:PHE:CD1	2.88	0.47
3:C:593:ALA:CB	3:C:681:MSE:CE	2.92	0.47
3:C:70:GLN:HE21	3:C:70:GLN:CA	2.25	0.47
3:D:313:ARG:HD2	3:D:313:ARG:O	2.15	0.47
3:B:15:ILE:HG13	3:B:65:MSE:CE	2.42	0.46
3:B:221:PHE:O	3:B:225:TYR:HB2	2.15	0.46
3:B:273:TYR:O	3:B:276:LEU:N	2.48	0.46
3:B:396:VAL:HG13	3:B:705:LYS:HZ1	1.76	0.46
3:B:288:TYR:HD1	3:B:293:ILE:HD11	1.79	0.46
3:B:116:GLU:HB3	3:B:320:TYR:OH	2.15	0.46
3:B:411:ASP:OD2	3:B:624:SER:HB2	2.16	0.46
3:B:423:VAL:O	3:B:424:ASN:HB3	2.15	0.46
3:B:434:PHE:HB3	3:B:462:MSE:HE3	1.97	0.46
3:B:747:GLU:O	3:B:751:ARG:HG3	2.15	0.46
3:C:318:GLN:C	3:C:318:GLN:HE21	2.19	0.46
3:C:319:ARG:O	3:C:322:SER:N	2.47	0.46
3:C:436:VAL:O	3:C:436:VAL:HG23	2.14	0.46
3:C:738:PRO:O	3:C:742:GLN:HG3	2.16	0.46
3:D:417:PRO:O	3:D:421:ARG:HG3	2.16	0.46
3:B:186:ILE:O	3:B:188:TYR:N	2.48	0.46
3:B:486:LYS:C	3:B:488:TYR:N	2.68	0.46
3:C:173:GLN:CG	3:C:174:GLY:H	2.27	0.46
3:D:244:PRO:HG2	3:D:245:HIS:H	1.81	0.46
3:D:293:ILE:HG23	3:D:294:SER:N	2.29	0.46
3:D:605:LEU:HD21	3:D:654:PHE:CE1	2.50	0.46
3:A:329:TYR:CE2	3:A:333:GLN:NE2	2.83	0.46
3:B:157:GLY:C	3:B:313:ARG:HH12	2.19	0.46
3:B:437:ALA:HB1	3:B:438:PRO:CD	2.46	0.46
3:C:104:ASP:OD2	3:C:106:THR:HB	2.15	0.46
3:C:12:GLY:C	3:C:14:SER:H	2.18	0.46
3:D:102:LYS:CD	3:D:103:TYR:H	2.26	0.46
3:A:309:ILE:N	4:A:917:HOH:O	2.44	0.46
3:A:438:PRO:HB2	3:A:440:HIS:CE1	2.51	0.46
3:A:491:ALA:C	3:A:493:GLN:H	2.19	0.46
3:B:103:TYR:HD1	3:B:103:TYR:H	1.61	0.46
3:B:300:VAL:CG1	3:B:301:GLY:H	2.25	0.46
3:B:451:SER:CB	3:B:462:MSE:CE	2.93	0.46
3:C:424:ASN:HD22	3:C:472:PRO:HG2	1.81	0.46
3:C:457:SER:C	3:C:674:MSE:HE2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:102:LYS:HZ2	3:D:102:LYS:HA	1.80	0.46
3:D:449:ARG:HA	3:D:450:PRO:HD2	1.72	0.46
3:D:451:SER:HB3	3:D:456:CYS:SG	2.54	0.46
3:C:413:THR:O	3:C:414:SER:C	2.54	0.46
3:D:233:ILE:N	4:D:935:HOH:O	2.49	0.46
3:D:98:ASN:O	3:D:352:LYS:HE2	2.16	0.46
3:D:576:ARG:CB	3:D:576:ARG:HH11	2.29	0.46
3:D:320:TYR:C	3:D:322:SER:N	2.67	0.46
3:D:444:ASN:HA	3:D:599:ARG:NE	2.31	0.46
3:A:610:GLY:HA2	4:A:1037:HOH:O	2.16	0.46
3:B:149:PHE:O	3:B:197:LEU:HD21	2.15	0.46
3:B:436:VAL:HG22	3:B:437:ALA:O	2.16	0.46
3:C:11:ILE:O	3:C:12:GLY:O	2.34	0.46
3:C:154:SER:O	3:C:156:TYR:N	2.49	0.46
3:C:285:GLN:HA	3:C:285:GLN:OE1	2.15	0.46
3:C:290:LEU:HD11	3:C:330:ARG:HB3	1.96	0.46
3:C:297:GLU:OE1	3:C:338:ARG:NH2	2.46	0.46
3:C:2:LYS:O	3:C:3:GLU:HB3	2.16	0.46
3:C:353:ILE:HB	4:C:925:HOH:O	2.15	0.46
3:D:692:PRO:HG3	3:D:713:TRP:HZ2	1.81	0.46
1:G:7:DA:H1'	1:G:8:DT:O5'	2.15	0.46
2:J:101:DG:H2''	2:J:102:DC:O5'	2.16	0.46
3:A:720:TYR:CZ	3:A:724:LYS:HD2	2.51	0.46
3:B:52:ILE:HG13	3:B:470:VAL:HG21	1.98	0.46
3:C:171:GLN:O	3:C:173:GLN:N	2.48	0.46
3:C:273:TYR:OH	3:C:340:PHE:HB2	2.16	0.46
3:C:410:PHE:CD2	3:C:685:ARG:HA	2.51	0.46
3:C:747:GLU:HB3	3:C:763:TYR:CE1	2.50	0.46
3:D:367:ALA:O	3:D:370:PHE:HB3	2.16	0.46
3:D:692:PRO:O	3:D:693:LEU:C	2.54	0.46
3:A:411:ASP:O	3:A:683:MSE:HA	2.16	0.46
3:B:109:ARG:CZ	3:B:142:ILE:HD12	2.46	0.46
3:B:171:GLN:O	3:B:173:GLN:N	2.49	0.46
3:B:53:TYR:CD1	3:B:53:TYR:N	2.84	0.46
3:C:685:ARG:NH1	3:C:688:ILE:HG13	2.31	0.46
3:D:216:TRP:CD1	3:D:290:LEU:HB2	2.50	0.46
3:D:3:GLU:HG2	3:D:22:SER:HA	1.98	0.46
1:K:16:DG:H2''	1:K:17:DC:C6	2.50	0.46
3:A:37:LEU:C	3:A:38:PHE:CD1	2.90	0.45
3:A:858:ILE:O	3:A:859:LYS:O	2.33	0.45
3:B:183:ILE:CD1	3:B:183:ILE:H	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:ASP:OD2	3:C:185:LYS:HD3	2.15	0.45
3:C:176:ASP:OD1	3:C:318:GLN:NE2	2.49	0.45
3:C:697:GLY:HA2	3:C:755:GLU:O	2.15	0.45
3:D:109:ARG:HD2	3:D:109:ARG:O	2.15	0.45
3:D:210:PRO:CG	3:D:242:LEU:HD21	2.46	0.45
3:D:291:ASP:OD2	3:D:303:LEU:HD13	2.15	0.45
3:D:4:PHE:H	3:D:20:ILE:HB	1.81	0.45
1:I:8:DT:H2''	1:I:9:DG:H8	1.81	0.45
3:A:71:TRP:O	3:A:75:MSE:HB2	2.16	0.45
3:B:201:TYR:O	3:B:205:TRP:N	2.48	0.45
3:B:405:LYS:HG3	3:B:691:PRO:CD	2.46	0.45
3:C:365:TRP:HZ2	3:C:562:LEU:O	1.99	0.45
3:C:443:ILE:HG21	3:C:595:GLN:HB3	1.99	0.45
3:C:776:TYR:CB	3:C:866:MSE:HE1	2.46	0.45
3:C:83:LEU:H	3:C:83:LEU:CD2	2.30	0.45
3:D:327:ALA:HA	3:D:330:ARG:HD3	1.98	0.45
3:A:217:ASN:HA	3:A:272:ASP:OD2	2.17	0.45
3:B:592:MSE:HE3	3:B:670:MSE:SE	2.65	0.45
3:C:412:LEU:HD23	3:C:683:MSE:HB2	1.98	0.45
3:D:212:ILE:O	3:D:214:THR:N	2.49	0.45
3:A:162:TRP:CH2	3:A:164:ILE:HG23	2.51	0.45
3:A:20:ILE:HG23	3:A:24:GLY:HA2	1.97	0.45
3:A:547:ARG:CZ	3:A:547:ARG:O	2.64	0.45
3:A:655:ALA:O	3:A:660:GLU:HG2	2.16	0.45
3:A:9:GLU:HA	3:A:89:LYS:HD3	1.98	0.45
3:B:116:GLU:HB2	3:B:135:ALA:H	1.81	0.45
3:B:231:LYS:O	3:B:235:GLY:N	2.49	0.45
3:B:458:PRO:HG3	3:B:592:MSE:SE	2.66	0.45
3:B:397:LYS:HE2	3:B:598:GLU:OE1	2.17	0.45
3:C:136:ILE:HB	3:C:149:PHE:HB2	1.98	0.45
3:C:395:PHE:HB2	3:C:591:GLN:HG2	1.97	0.45
3:C:416:TYR:CD2	3:C:416:TYR:N	2.82	0.45
3:C:818:ASN:HD21	3:C:820:ASP:H	1.64	0.45
3:D:13:ASP:HB2	3:D:66:ARG:CB	2.46	0.45
3:D:210:PRO:CD	3:D:242:LEU:HD21	2.46	0.45
3:D:273:TYR:CZ	3:D:340:PHE:HB2	2.52	0.45
3:D:335:ASP:O	3:D:339:GLN:N	2.43	0.45
3:A:391:TYR:CZ	3:A:583:ALA:HB1	2.51	0.45
3:B:272:ASP:CG	3:B:274:ILE:HG22	2.36	0.45
3:B:369:ILE:HG22	3:B:373:LEU:HD12	1.99	0.45
3:B:403:ARG:HH21	3:B:889:LEU:HG	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:658:ARG:C	3:B:661:PRO:HD2	2.37	0.45
3:B:775:ASN:HB3	4:B:982:HOH:O	2.16	0.45
3:D:218:VAL:CA	3:D:222:ALA:HB3	2.46	0.45
3:D:243:SER:HA	3:D:268:ILE:HD11	1.98	0.45
3:D:617:VAL:HG12	3:D:627:VAL:HG12	1.97	0.45
3:D:660:GLU:OE2	3:D:663:ILE:HD12	2.16	0.45
3:D:714:ASP:HB3	3:D:719:ARG:HD3	1.99	0.45
1:G:12:DA:H2''	1:G:13:DG:H5''	1.92	0.45
3:A:19:TYR:CE1	3:A:29:ARG:HG2	2.52	0.45
3:C:437:ALA:O	3:C:442:TYR:HE2	1.99	0.45
3:C:411:ASP:CG	3:C:624:SER:HB3	2.37	0.45
3:C:791:TYR:CE2	3:C:802:PRO:HD3	2.52	0.45
3:D:380:ILE:HD12	3:D:576:ARG:NH2	2.32	0.45
2:L:107:DG:H2'	2:L:108:DT:H71	1.85	0.45
3:A:408:MSE:CE	3:A:685:ARG:HD2	2.46	0.45
3:A:556:GLN:C	3:A:556:GLN:HE21	2.20	0.45
4:E:366:HOH:O	3:A:806:ARG:HD2	2.16	0.45
3:A:859:LYS:C	3:A:861:ASP:H	2.18	0.45
3:C:660:GLU:O	3:C:663:ILE:HB	2.16	0.45
3:D:581:ARG:HG2	3:D:581:ARG:NH1	2.29	0.45
3:D:771:PHE:CE1	3:D:779:ILE:HG21	2.51	0.45
3:A:752:MSE:HG3	3:A:760:LEU:HD22	1.98	0.45
3:B:489:MSE:SE	3:B:553:MSE:SE	3.34	0.45
3:B:83:LEU:N	3:B:83:LEU:HD12	2.32	0.45
3:C:131:HIS:HB3	3:C:132:PRO:HD2	1.99	0.45
3:C:202:LEU:O	3:C:206:GLN:HG2	2.16	0.45
3:C:347:MSE:CA	3:C:558:ASN:ND2	2.80	0.45
3:D:21:ASP:HB2	3:D:25:ARG:C	2.37	0.45
3:D:537:SER:C	3:D:539:ASN:H	2.19	0.45
3:D:597:ILE:CG1	3:D:683:MSE:HE1	2.47	0.45
3:A:222:ALA:O	3:A:226:VAL:HG23	2.17	0.45
3:A:547:ARG:HH22	3:A:551:ALA:HB2	1.82	0.45
3:B:302:LYS:O	3:B:302:LYS:HG2	2.16	0.45
3:C:204:PHE:CD1	3:C:208:LYS:HD3	2.52	0.45
3:C:218:VAL:HA	3:C:222:ALA:HB3	1.98	0.45
3:D:320:TYR:C	3:D:322:SER:H	2.19	0.45
1:K:15:DC:N4	2:L:102:DC:N4	2.65	0.45
3:A:697:GLY:HA3	3:A:753:LEU:O	2.16	0.45
3:A:854:ILE:CG1	3:A:859:LYS:HB2	2.46	0.45
3:A:834:PRO:O	3:A:866:MSE:HA	2.17	0.45
3:B:227:TYR:CE1	3:B:239:ALA:HB1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:896:SER:OG	3:B:898:PHE:HD2	2.00	0.45
3:D:243:SER:OG	3:D:246:ARG:HA	2.16	0.45
3:D:453:VAL:CG2	3:D:454:TYR:N	2.72	0.45
3:B:78:ILE:HA	3:B:78:ILE:HD12	1.85	0.44
3:D:268:ILE:HG22	3:D:269:SER:H	1.80	0.44
3:D:459:ASN:HD21	3:D:585:ALA:HB2	1.81	0.44
3:D:701:PHE:HE1	3:D:749:ILE:HG23	1.81	0.44
3:D:747:GLU:HG2	3:D:763:TYR:CE2	2.52	0.44
3:D:770:GLU:O	3:D:774:LEU:HD22	2.17	0.44
3:A:681:MSE:HA	3:A:681:MSE:HE2	1.99	0.44
3:B:548:THR:O	3:B:548:THR:HG22	2.17	0.44
3:C:897:LEU:HD23	3:C:897:LEU:C	2.38	0.44
3:C:90:LEU:HD21	3:C:363:LYS:HE3	1.98	0.44
3:D:219:GLU:HB2	3:D:272:ASP:HB2	1.99	0.44
3:D:709:ALA:O	3:D:710:LEU:HD23	2.18	0.44
1:I:8:DT:H2"	1:I:9:DG:C8	2.52	0.44
3:B:394:ALA:HB1	3:B:622:THR:CB	2.41	0.44
3:B:631:LYS:HZ2	3:B:631:LYS:HB2	1.82	0.44
3:B:421:ARG:HB3	3:B:680:LEU:CD1	2.46	0.44
3:C:144:ASP:OD2	3:C:144:ASP:O	2.36	0.44
3:C:231:LYS:HG3	3:C:236:GLU:HA	2.00	0.44
3:C:448:GLU:O	3:C:449:ARG:C	2.56	0.44
3:D:217:ASN:O	3:D:221:PHE:HB3	2.18	0.44
3:D:323:TYR:CA	3:D:326:ILE:HG12	2.48	0.44
3:D:35:PRO:HG3	3:D:65:MSE:HA	2.00	0.44
3:D:692:PRO:HG3	3:D:713:TRP:CZ2	2.52	0.44
3:D:864:HIS:C	3:D:866:MSE:H	2.19	0.44
3:A:369:ILE:HG12	3:A:474:GLU:HG3	1.98	0.44
3:B:2:LYS:HA	3:B:2:LYS:HD3	1.87	0.44
3:B:544:ARG:HH11	3:B:544:ARG:HB2	1.82	0.44
3:C:11:ILE:HB	3:C:16:PHE:CE1	2.51	0.44
3:C:152:LEU:HD11	3:C:190:PRO:HB2	1.99	0.44
3:C:347:MSE:HE1	3:C:558:ASN:O	2.18	0.44
3:C:395:PHE:HD2	3:C:594:LEU:HD23	1.83	0.44
3:A:357:SER:C	3:A:359:PHE:N	2.70	0.44
3:A:805:ILE:O	3:A:808:ILE:HB	2.17	0.44
3:B:279:LYS:HG2	3:B:279:LYS:O	2.17	0.44
3:B:321:ILE:CD1	3:B:321:ILE:N	2.80	0.44
3:B:433:THR:O	3:B:433:THR:HG23	2.17	0.44
3:C:1:MSE:HA	3:C:1:MSE:CE	2.42	0.44
3:C:252:VAL:HA	3:C:260:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:64:ASN:O	3:D:68:ALA:HB2	2.18	0.44
3:A:72:ILE:O	3:A:76:GLU:HG3	2.18	0.44
3:B:116:GLU:HA	3:B:116:GLU:OE1	2.17	0.44
3:B:276:LEU:O	3:B:280:PHE:CD2	2.71	0.44
3:B:316:ASN:C	3:B:318:GLN:N	2.71	0.44
3:B:413:THR:O	3:B:414:SER:C	2.56	0.44
3:B:440:HIS:CE1	3:B:444:ASN:HD21	2.36	0.44
3:B:681:MSE:HA	3:B:681:MSE:CE	2.46	0.44
3:C:221:PHE:O	3:C:224:PRO:HD2	2.17	0.44
3:C:290:LEU:C	3:C:290:LEU:HD13	2.38	0.44
3:C:45:GLN:O	3:C:46:ALA:C	2.56	0.44
3:C:727:ILE:C	3:C:728:MSE:HE2	2.37	0.44
3:D:606:ASN:HD22	3:D:611:THR:HB	1.81	0.44
3:A:52:ILE:O	3:A:428:GLU:HG3	2.18	0.44
3:A:556:GLN:C	3:A:556:GLN:NE2	2.71	0.44
3:A:790:LYS:HB2	4:A:991:HOH:O	2.17	0.44
3:C:173:GLN:HG3	3:C:174:GLY:H	1.80	0.44
3:C:255:ASN:O	3:C:257:TYR:N	2.49	0.44
3:C:319:ARG:O	3:C:320:TYR:C	2.55	0.44
3:A:443:ILE:C	3:A:444:ASN:HD22	2.20	0.44
3:A:486:LYS:HG2	3:A:486:LYS:O	2.18	0.44
3:A:547:ARG:HG3	3:A:548:THR:HG23	2.00	0.44
3:B:145:ARG:HG3	3:B:145:ARG:HH11	1.83	0.44
3:B:319:ARG:O	3:B:323:TYR:HB2	2.18	0.44
3:B:685:ARG:NH2	3:B:714:ASP:OD1	2.47	0.44
3:C:202:LEU:HD23	3:C:202:LEU:HA	1.76	0.44
3:C:206:GLN:HE21	3:C:206:GLN:HA	1.83	0.44
3:D:29:ARG:C	3:D:31:VAL:H	2.21	0.44
3:D:50:PHE:O	3:D:379:VAL:HG23	2.17	0.44
3:D:578:TYR:CD1	3:D:579:ASP:N	2.86	0.44
3:A:471:VAL:N	3:A:472:PRO:HD2	2.32	0.44
3:A:408:MSE:CE	3:A:655:ALA:HB2	2.40	0.44
3:C:660:GLU:CB	3:C:661:PRO:HD3	2.45	0.44
3:D:251:LYS:O	3:D:261:GLU:O	2.36	0.44
3:D:581:ARG:NH1	3:D:581:ARG:CG	2.78	0.44
3:D:622:THR:O	3:D:623:ASP:OD1	2.36	0.44
3:A:642:ARG:HE	3:A:646:HIS:CE1	2.36	0.43
3:A:398:GLU:OE1	3:A:705:LYS:HE3	2.18	0.43
3:A:752:MSE:CG	3:A:760:LEU:HD22	2.48	0.43
3:C:127:SER:O	3:C:128:GLN:NE2	2.51	0.43
3:C:55:LYS:N	3:C:55:LYS:HD2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:GLU:O	3:D:262:ILE:C	2.56	0.43
3:D:372:SER:O	3:D:376:GLN:HG3	2.18	0.43
3:D:458:PRO:CG	3:D:592:MSE:SE	3.16	0.43
3:D:611:THR:CG2	3:D:612:GLU:N	2.79	0.43
3:D:759:SER:O	3:D:763:TYR:HB3	2.17	0.43
1:E:7:DA:H2''	1:E:8:DT:OP2	2.18	0.43
3:A:83:LEU:H	3:A:83:LEU:CD2	2.29	0.43
2:H:115:DA:H5'	3:B:221:PHE:CE2	2.53	0.43
3:B:322:SER:O	3:B:326:ILE:HG12	2.18	0.43
3:C:700:GLY:HA2	3:C:753:LEU:HD21	1.96	0.43
3:D:327:ALA:O	3:D:330:ARG:N	2.52	0.43
3:D:552:GLY:O	3:D:553:MSE:HG2	2.18	0.43
1:I:7:DA:H2''	1:I:8:DT:O5'	2.19	0.43
3:A:164:ILE:HG12	4:A:913:HOH:O	2.19	0.43
3:B:745:LEU:HD22	3:B:883:PHE:HE2	1.83	0.43
3:C:113:PHE:HB2	3:C:137:THR:O	2.18	0.43
3:C:651:LEU:HD23	3:C:651:LEU:HA	1.85	0.43
3:A:214:THR:OG1	3:A:215:GLY:N	2.50	0.43
3:B:135:ALA:HB1	3:B:324:ASN:OD1	2.18	0.43
3:C:404:TYR:CZ	3:C:618:LEU:HD13	2.53	0.43
3:D:52:ILE:CD1	3:D:381:PRO:HD3	2.45	0.43
3:D:71:TRP:O	3:D:75:MSE:HG2	2.18	0.43
2:F:108:DT:H1'	2:F:109:DC:H5''	1.99	0.43
3:A:482:ARG:HH22	3:A:560:LYS:HD2	1.83	0.43
3:A:731:GLU:HG3	3:A:879:PRO:CB	2.48	0.43
2:H:115:DA:O3'	3:B:117:VAL:HG22	2.19	0.43
3:B:161:GLU:HB3	4:B:945:HOH:O	2.17	0.43
3:B:235:GLY:HA2	3:B:239:ALA:HB2	2.00	0.43
3:B:655:ALA:O	3:B:660:GLU:HG2	2.18	0.43
3:C:313:ARG:NH1	3:C:313:ARG:HG3	2.34	0.43
3:C:863:LEU:CA	3:C:866:MSE:HE3	2.33	0.43
3:D:212:ILE:HD11	3:D:345:LEU:HD21	2.01	0.43
3:D:212:ILE:CG2	3:D:212:ILE:O	2.62	0.43
3:D:216:TRP:O	3:D:217:ASN:CB	2.66	0.43
3:D:618:LEU:HD23	3:D:626:TYR:O	2.18	0.43
3:D:644:THR:O	3:D:648:VAL:HG23	2.18	0.43
3:D:698:ILE:O	3:D:753:LEU:HA	2.18	0.43
3:D:767:PHE:CD2	3:D:770:GLU:HB2	2.54	0.43
2:F:111:DT:C2'	2:F:112:DA:H5''	2.49	0.43
3:A:162:TRP:HB3	3:A:188:TYR:CZ	2.53	0.43
3:A:36:SER:HA	3:A:60:LYS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:641:PHE:HD1	3:A:646:HIS:CG	2.37	0.43
3:A:799:PRO:O	3:A:800:LYS:CB	2.66	0.43
3:B:12:GLY:O	3:B:13:ASP:HB2	2.19	0.43
3:B:162:TRP:HB3	3:B:188:TYR:OH	2.19	0.43
3:B:202:LEU:O	3:B:205:TRP:N	2.52	0.43
3:B:486:LYS:O	3:B:490:LEU:N	2.50	0.43
3:B:73:LYS:HA	4:B:986:HOH:O	2.19	0.43
3:C:162:TRP:HB3	3:C:188:TYR:CZ	2.53	0.43
3:C:422:GLN:CG	3:C:678:GLN:O	2.51	0.43
3:C:702:TRP:CZ3	3:C:710:LEU:HD21	2.54	0.43
3:A:11:ILE:O	3:A:12:GLY:O	2.36	0.43
3:A:170:LEU:HA	3:A:177:GLU:HG2	2.01	0.43
3:B:159:VAL:CG2	3:B:160:GLU:H	2.28	0.43
3:B:303:LEU:HD12	3:B:304:LYS:O	2.18	0.43
3:B:304:LYS:CG	3:B:305:TYR:H	2.31	0.43
3:B:871:LEU:HD12	3:B:871:LEU:O	2.18	0.43
3:C:15:ILE:HG13	3:C:65:MSE:HE1	2.01	0.43
3:C:426:SER:CB	3:C:428:GLU:OE2	2.66	0.43
3:C:44:SER:C	3:C:46:ALA:H	2.22	0.43
3:C:542:LEU:N	3:C:542:LEU:HD12	2.34	0.43
3:C:49:TYR:CE1	3:C:59:ARG:HB2	2.54	0.43
3:D:205:TRP:HA	4:D:936:HOH:O	2.19	0.43
3:A:825:VAL:CG1	3:A:826:GLU:H	2.23	0.43
3:A:825:VAL:CG1	3:A:826:GLU:N	2.77	0.43
3:B:159:VAL:CG2	3:B:160:GLU:N	2.81	0.43
3:C:233:ILE:HG22	3:C:234:PHE:CD1	2.54	0.43
3:C:668:ARG:CG	3:C:668:ARG:NH1	2.78	0.43
3:D:556:GLN:N	4:D:918:HOH:O	2.52	0.43
3:D:563:ILE:H	3:D:563:ILE:HG13	1.48	0.43
2:J:112:DA:H2"	2:J:113:DA:H8	1.77	0.43
3:B:101:ILE:HG21	3:B:349:TYR:CD1	2.54	0.43
3:B:425:ILE:HG23	3:B:463:TYR:CE2	2.53	0.43
3:B:70:GLN:OE1	3:B:70:GLN:HA	2.19	0.43
3:C:138:HIS:CD2	3:C:138:HIS:C	2.92	0.43
3:C:12:GLY:C	3:C:14:SER:N	2.72	0.43
3:C:815:ILE:HG22	3:C:815:ILE:O	2.18	0.43
3:D:265:LEU:HD12	3:D:265:LEU:O	2.19	0.43
3:D:551:ALA:HA	3:D:555:ALA:CB	2.48	0.43
3:C:244:PRO:HG2	3:C:267:GLY:HA3	2.00	0.43
3:C:380:ILE:HA	3:C:381:PRO:HD3	1.85	0.43
3:D:244:PRO:CG	3:D:267:GLY:HA3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:770:GLU:O	3:D:774:LEU:HB2	2.19	0.43
3:A:55:LYS:HB3	4:A:977:HOH:O	2.18	0.42
3:A:83:LEU:HB3	3:A:379:VAL:HG11	2.01	0.42
3:B:165:GLU:O	3:B:166:ILE:C	2.57	0.42
3:B:351:ALA:O	3:B:352:LYS:HB2	2.18	0.42
3:B:398:GLU:HA	3:B:398:GLU:OE2	2.19	0.42
3:B:557:ILE:O	3:B:560:LYS:HB3	2.19	0.42
3:C:541:MSE:O	3:C:544:ARG:HG3	2.19	0.42
3:C:380:ILE:CG2	3:C:576:ARG:HD3	2.43	0.42
3:C:83:LEU:HB3	3:C:379:VAL:HG12	2.01	0.42
3:D:219:GLU:CB	3:D:272:ASP:HB2	2.48	0.42
3:D:242:LEU:O	3:D:265:LEU:HD22	2.18	0.42
3:D:434:PHE:CD2	3:D:450:PRO:HB3	2.53	0.42
3:D:619:TYR:C	3:D:619:TYR:CD1	2.92	0.42
2:J:102:DC:H2''	2:J:103:DG:C8	2.55	0.42
3:A:51:ASP:HB2	4:A:919:HOH:O	2.18	0.42
3:B:170:LEU:HG	3:B:171:GLN:N	2.34	0.42
3:C:434:PHE:HE1	3:C:456:CYS:HB3	1.83	0.42
3:C:660:GLU:HB3	3:C:661:PRO:CD	2.43	0.42
3:D:406:TYR:N	3:D:406:TYR:CD1	2.86	0.42
3:D:888:LYS:HG3	3:D:888:LYS:O	2.19	0.42
3:A:860:ASP:O	3:A:864:HIS:HB2	2.19	0.42
3:B:188:TYR:CG	3:B:190:PRO:HD3	2.54	0.42
3:B:297:GLU:HA	3:B:297:GLU:OE2	2.19	0.42
3:B:391:TYR:CD2	3:B:391:TYR:N	2.88	0.42
2:F:105:DC:C2'	2:F:106:DT:H71	2.49	0.42
3:A:651:LEU:HA	3:A:651:LEU:HD23	1.84	0.42
3:B:149:PHE:HB3	3:B:197:LEU:HG	2.00	0.42
3:B:176:ASP:OD2	3:B:318:GLN:HG3	2.18	0.42
3:C:189:MSE:HE1	3:C:200:GLU:OE1	2.19	0.42
3:C:453:VAL:HG23	3:C:454:TYR:N	2.35	0.42
3:C:892:GLU:O	3:C:894:LYS:HE2	2.19	0.42
3:D:422:GLN:CD	3:D:681:MSE:HE2	2.40	0.42
3:D:61:LEU:C	3:D:62:PHE:CD1	2.93	0.42
3:D:64:ASN:O	3:D:68:ALA:N	2.52	0.42
3:D:92:TYR:CD2	3:D:92:TYR:C	2.93	0.42
3:A:6:LEU:CD2	3:A:108:ILE:HG12	2.49	0.42
3:A:898:PHE:C	3:A:900:MSE:N	2.68	0.42
3:C:302:LYS:NZ	3:C:302:LYS:CB	2.82	0.42
3:C:486:LYS:O	3:C:490:LEU:HG	2.20	0.42
3:C:7:THR:OG1	3:C:18:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:14:SER:O	3:D:16:PHE:N	2.52	0.42
3:D:326:ILE:HG23	3:D:330:ARG:NH1	2.34	0.42
3:D:426:SER:HB2	3:D:471:VAL:HG23	2.02	0.42
3:D:621:ASP:O	3:D:622:THR:C	2.57	0.42
3:A:221:PHE:O	3:A:225:TYR:HB2	2.19	0.42
3:A:405:LYS:HE2	3:A:638:GLU:OE2	2.20	0.42
3:A:629:ALA:HA	3:A:632:ILE:HD13	2.00	0.42
3:B:465:LYS:O	3:B:677:LYS:HE3	2.19	0.42
3:C:290:LEU:HD13	3:C:290:LEU:O	2.19	0.42
3:C:450:PRO:O	3:C:451:SER:HB2	2.20	0.42
3:C:394:ALA:HB1	3:C:622:THR:HA	2.01	0.42
3:C:8:VAL:O	3:C:9:GLU:HG2	2.19	0.42
3:D:222:ALA:O	3:D:226:VAL:HG22	2.19	0.42
3:D:355:ILE:HB	3:D:356:GLN:OE1	2.19	0.42
3:D:606:ASN:O	3:D:611:THR:N	2.53	0.42
3:D:884:THR:HB	3:D:889:LEU:O	2.20	0.42
3:A:410:PHE:HA	3:A:684:ASP:O	2.19	0.42
3:A:632:ILE:N	3:A:632:ILE:CD1	2.83	0.42
3:A:659:MSE:HE2	3:A:659:MSE:HB3	1.97	0.42
3:B:228:ASN:O	3:B:231:LYS:N	2.53	0.42
3:B:720:TYR:CZ	3:B:724:LYS:HD2	2.54	0.42
3:C:150:ASP:OD2	3:C:150:ASP:C	2.57	0.42
3:C:145:ARG:HB3	3:C:187:ILE:HD12	2.01	0.42
3:C:831:TYR:O	3:C:847:ALA:HA	2.20	0.42
3:D:212:ILE:CD1	3:D:345:LEU:HD21	2.50	0.42
3:D:281:SER:O	3:D:283:THR:N	2.53	0.42
3:D:347:MSE:HB2	3:D:358:VAL:HG12	2.01	0.42
3:D:51:ASP:HB2	3:D:52:ILE:HD12	2.02	0.42
3:D:539:ASN:C	3:D:541:MSE:H	2.23	0.42
3:D:616:PHE:O	3:D:627:VAL:HA	2.20	0.42
3:A:159:VAL:HG21	3:A:317:HIS:CD2	2.54	0.42
3:A:489:MSE:HG3	3:A:553:MSE:HB2	2.02	0.42
3:A:546:GLN:O	3:A:547:ARG:C	2.57	0.42
3:B:739:LYS:O	3:B:742:GLN:HB2	2.20	0.42
3:C:772:ARG:HG3	3:C:772:ARG:HH11	1.83	0.42
3:C:90:LEU:HD11	3:C:353:ILE:HG22	2.02	0.42
1:I:13:DG:H5'	3:C:800:LYS:HG2	2.00	0.42
3:A:105:HIS:ND1	3:A:106:THR:N	2.67	0.42
3:B:137:THR:OG1	3:B:328:VAL:CG2	2.66	0.42
3:B:139:TYR:HA	3:B:145:ARG:O	2.19	0.42
3:B:136:ILE:O	3:B:148:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:216:TRP:CZ2	3:B:293:ILE:HD12	2.55	0.42
3:C:667:PHE:HB3	3:C:679:HIS:HE1	1.84	0.42
3:D:244:PRO:HD2	3:D:268:ILE:HG13	2.02	0.42
3:D:273:TYR:HE2	3:D:341:ILE:HG13	1.85	0.42
3:D:408:MSE:HG3	3:D:688:ILE:HG12	2.00	0.42
3:D:776:TYR:CD1	3:D:777:ILE:N	2.88	0.42
2:L:101:DG:C3'	2:L:102:DC:H5''	2.47	0.42
3:A:309:ILE:HB	4:A:917:HOH:O	2.19	0.42
3:A:482:ARG:NH2	3:A:560:LYS:HD2	2.34	0.42
3:A:642:ARG:N	3:A:646:HIS:ND1	2.62	0.42
3:A:92:TYR:CD1	3:A:92:TYR:C	2.93	0.42
3:B:356:GLN:C	3:B:358:VAL:N	2.73	0.42
3:B:709:ALA:O	3:B:710:LEU:HD23	2.19	0.42
3:B:878:LYS:HB2	3:B:879:PRO:HD2	2.02	0.42
3:B:899:ASP:N	3:B:899:ASP:OD2	2.53	0.42
3:C:253:ILE:HB	3:C:260:ARG:HB2	2.02	0.42
3:C:55:LYS:N	3:C:55:LYS:CD	2.83	0.42
3:A:410:PHE:CD2	3:A:685:ARG:HA	2.55	0.41
3:A:848:TRP:CE2	3:A:854:ILE:HG22	2.54	0.41
3:B:315:SER:OG	3:B:316:ASN:N	2.52	0.41
3:B:441:ASP:CB	3:B:447:ALA:HB2	2.48	0.41
3:B:52:ILE:HD11	3:B:373:LEU:HD21	2.01	0.41
3:B:773:GLN:O	3:B:774:LEU:C	2.58	0.41
3:C:130:LYS:C	3:C:131:HIS:ND1	2.73	0.41
3:C:163:SER:HB3	3:C:318:GLN:OE1	2.20	0.41
3:C:85:MSE:HB2	3:C:370:PHE:CE2	2.56	0.41
3:C:412:LEU:CD2	3:C:683:MSE:HB2	2.50	0.41
3:D:463:TYR:N	3:D:463:TYR:CD1	2.88	0.41
3:D:578:TYR:CG	3:D:579:ASP:N	2.88	0.41
3:D:644:THR:C	3:D:646:HIS:H	2.23	0.41
3:A:112:ASN:C	3:A:112:ASN:ND2	2.74	0.41
3:A:485:HIS:C	3:A:487:GLY:H	2.23	0.41
3:A:802:PRO:HG2	3:A:805:ILE:HD12	2.02	0.41
3:A:757:GLU:HB2	3:A:889:LEU:HD22	2.02	0.41
3:B:231:LYS:CB	4:B:915:HOH:O	2.68	0.41
3:B:36:SER:HA	3:B:60:LYS:O	2.20	0.41
3:B:486:LYS:C	3:B:488:TYR:H	2.23	0.41
3:B:605:LEU:HD12	3:B:616:PHE:HB3	2.01	0.41
3:B:878:LYS:CB	3:B:879:PRO:CD	2.98	0.41
3:C:725:LEU:HD23	3:C:725:LEU:HA	1.80	0.41
3:C:745:LEU:HA	3:C:745:LEU:HD23	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:880:LEU:O	3:C:881:GLU:C	2.58	0.41
3:D:285:GLN:N	3:D:285:GLN:OE1	2.53	0.41
3:D:302:LYS:C	3:D:303:LEU:HD12	2.40	0.41
3:A:163:SER:HA	4:A:913:HOH:O	2.19	0.41
3:A:326:ILE:HA	3:A:326:ILE:HD13	1.90	0.41
3:B:175:GLY:O	3:B:176:ASP:O	2.39	0.41
3:B:622:THR:O	3:B:623:ASP:HB3	2.19	0.41
3:C:183:ILE:CG2	3:C:184:ASP:N	2.84	0.41
3:C:391:TYR:N	3:C:391:TYR:CD1	2.88	0.41
3:D:294:SER:HB2	3:D:298:LEU:HD12	2.02	0.41
3:D:434:PHE:O	3:D:436:VAL:N	2.52	0.41
3:D:479:PHE:CE2	3:D:563:ILE:HG21	2.55	0.41
3:D:635:LYS:HE3	3:D:635:LYS:CA	2.49	0.41
3:D:410:PHE:CD2	3:D:685:ARG:HA	2.55	0.41
3:D:765:LYS:C	3:D:767:PHE:H	2.23	0.41
3:A:115:ILE:HD13	3:A:115:ILE:HA	1.82	0.41
3:A:757:GLU:O	3:A:761:GLN:HG3	2.20	0.41
3:A:854:ILE:O	3:A:855:THR:C	2.58	0.41
3:A:855:THR:C	3:A:857:LEU:H	2.22	0.41
3:B:116:GLU:HB3	3:B:320:TYR:CZ	2.55	0.41
3:D:59:ARG:HH12	3:D:61:LEU:HG	1.85	0.41
3:D:756:GLY:C	3:D:758:GLU:H	2.23	0.41
3:A:290:LEU:O	3:A:294:SER:HB2	2.21	0.41
3:B:304:LYS:HG2	3:B:305:TYR:H	1.85	0.41
3:B:494:ARG:O	3:B:495:ASN:ND2	2.54	0.41
3:B:594:LEU:O	3:B:594:LEU:HG	2.20	0.41
3:B:689:ALA:HB2	3:B:712:VAL:HG22	2.03	0.41
3:B:747:GLU:OE1	3:B:747:GLU:HA	2.20	0.41
3:C:59:ARG:HH11	3:C:59:ARG:HG2	1.85	0.41
3:C:593:ALA:HA	3:C:670:MSE:SE	2.70	0.41
3:C:8:VAL:C	3:C:9:GLU:HG2	2.41	0.41
1:I:4:DC:H2"	1:I:5:DT:H71	2.03	0.41
3:A:261:GLU:HG3	3:A:261:GLU:O	2.19	0.41
3:A:621:ASP:C	3:A:622:THR:HG23	2.40	0.41
3:A:656:ARG:HH11	3:A:656:ARG:CB	2.33	0.41
3:A:837:GLU:OE1	3:A:837:GLU:HA	2.20	0.41
3:B:149:PHE:HB3	3:B:197:LEU:CG	2.51	0.41
3:B:42:PRO:CG	3:B:45:GLN:HG2	2.49	0.41
3:B:702:TRP:CD1	3:B:708:TYR:HB3	2.56	0.41
3:D:293:ILE:CG2	3:D:294:SER:N	2.83	0.41
3:D:37:LEU:C	3:D:38:PHE:CD1	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:LYS:HE2	3:A:323:TYR:CZ	2.55	0.41
3:A:358:VAL:HG22	3:A:358:VAL:O	2.21	0.41
3:A:625:ILE:CD1	3:A:683:MSE:HE1	2.35	0.41
3:B:121:ASP:OD2	3:B:121:ASP:N	2.54	0.41
3:B:202:LEU:O	3:B:205:TRP:HB3	2.20	0.41
3:B:143:ASP:OD2	3:B:208:LYS:CE	2.69	0.41
3:B:221:PHE:CE1	3:B:225:TYR:CD1	3.09	0.41
3:B:277:TYR:CD1	3:B:340:PHE:HE2	2.38	0.41
3:B:567:TYR:O	3:B:568:GLY:C	2.59	0.41
3:C:302:LYS:HZ3	3:C:302:LYS:HA	1.85	0.41
3:C:605:LEU:HA	3:C:605:LEU:HD23	1.93	0.41
3:D:294:SER:O	3:D:296:PHE:N	2.53	0.41
3:D:423:VAL:O	3:D:424:ASN:HB3	2.19	0.41
3:D:560:LYS:HA	3:D:563:ILE:CG1	2.50	0.41
3:D:872:LEU:C	3:D:874:LYS:H	2.20	0.41
1:E:4:DC:N3	2:F:114:DG:O6	2.53	0.41
3:A:17:GLU:OE2	3:A:97:TYR:OH	2.28	0.41
3:A:201:TYR:O	3:A:204:PHE:HB3	2.21	0.41
3:A:598:GLU:HG3	3:A:617:VAL:HB	2.02	0.41
3:A:898:PHE:O	3:A:900:MSE:N	2.53	0.41
3:B:333:GLN:O	3:B:336:ALA:HB3	2.20	0.41
3:B:715:MSE:O	3:B:716:GLU:HB2	2.21	0.41
3:C:276:LEU:HD23	3:C:276:LEU:HA	1.93	0.41
3:D:597:ILE:HG12	3:D:683:MSE:HE1	2.03	0.41
3:D:85:MSE:CE	3:D:87:ASP:N	2.83	0.41
3:D:85:MSE:HE1	3:D:87:ASP:N	2.36	0.41
1:E:4:DC:H2''	1:E:5:DT:H71	2.03	0.41
1:E:6:DT:C2'	1:E:7:DA:C5'	2.96	0.41
2:F:110:DA:C8	2:F:111:DT:H71	2.55	0.41
3:A:365:TRP:CD2	3:A:566:LEU:HD13	2.56	0.41
3:A:6:LEU:HB2	3:A:18:ARG:O	2.21	0.41
3:B:178:VAL:HB	4:B:991:HOH:O	2.21	0.41
3:B:5:TYR:HB3	3:B:97:TYR:CE2	2.56	0.41
3:C:245:HIS:O	3:C:246:ARG:C	2.59	0.41
3:C:482:ARG:NH2	3:C:560:LYS:HD3	2.36	0.41
1:G:8:DT:H2''	1:G:9:DG:OP2	2.20	0.41
3:A:117:VAL:HG13	3:A:132:PRO:O	2.21	0.41
3:A:304:LYS:HA	3:A:304:LYS:HE3	2.03	0.41
3:B:407:VAL:HG11	3:B:710:LEU:HD22	2.02	0.41
3:B:642:ARG:HB2	3:B:646:HIS:CG	2.56	0.41
3:C:362:ILE:HG23	3:C:575:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:815:ILE:HG23	3:C:821:ALA:HB3	2.03	0.41
3:D:216:TRP:HH2	3:D:293:ILE:HG12	1.85	0.41
3:D:8:VAL:O	3:D:354:GLN:NE2	2.54	0.41
2:H:108:DT:H2''	2:H:109:DC:H5'	1.98	0.41
3:A:581:ARG:NH1	3:A:581:ARG:HG3	2.14	0.41
3:B:279:LYS:O	3:B:280:PHE:CG	2.74	0.41
3:B:476:THR:HG22	3:B:480:ASN:ND2	2.36	0.41
3:B:490:LEU:O	3:B:491:ALA:C	2.59	0.41
3:C:330:ARG:HD3	3:C:330:ARG:HA	1.74	0.41
3:C:89:LYS:HZ2	3:C:354:GLN:HE22	1.64	0.41
3:D:468:ASP:HB3	3:D:473:THR:OG1	2.21	0.41
3:D:655:ALA:CA	3:D:659:MSE:HB2	2.41	0.41
3:B:344:SER:O	3:B:345:LEU:C	2.59	0.40
3:B:443:ILE:HD13	3:B:595:GLN:HB2	2.03	0.40
3:B:478:VAL:HG13	3:B:559:ARG:HG3	2.04	0.40
3:B:622:THR:O	3:B:622:THR:HG23	2.22	0.40
3:B:893:LYS:HZ3	3:B:894:LYS:H	1.69	0.40
3:C:140:ASP:OD1	3:C:142:ILE:N	2.53	0.40
3:C:373:LEU:O	3:C:374:LYS:C	2.60	0.40
3:D:28:THR:O	3:D:29:ARG:CB	2.68	0.40
3:D:697:GLY:HA3	3:D:756:GLY:HA2	2.03	0.40
2:F:104:DG:H2''	2:F:105:DC:C5'	2.51	0.40
3:A:121:ASP:HB2	3:A:122:GLY:H	1.73	0.40
3:A:269:SER:CB	3:A:356:GLN:HE21	2.35	0.40
3:A:394:ALA:CB	3:A:622:THR:HB	2.44	0.40
3:B:178:VAL:HG23	3:B:178:VAL:O	2.21	0.40
3:C:154:SER:C	3:C:156:TYR:N	2.73	0.40
3:C:779:ILE:O	3:C:871:LEU:HD21	2.20	0.40
3:D:373:LEU:CD1	3:D:373:LEU:N	2.84	0.40
3:D:437:ALA:O	3:D:438:PRO:C	2.59	0.40
3:D:630:ASP:O	3:D:633:ILE:HG22	2.21	0.40
3:D:37:LEU:HD22	3:D:71:TRP:CZ3	2.55	0.40
2:J:105:DC:H2'	2:J:106:DT:C7	2.51	0.40
3:A:132:PRO:HB3	3:A:194:GLU:OE2	2.21	0.40
3:A:416:TYR:HB2	3:A:417:PRO:HD3	2.02	0.40
3:A:627:VAL:HG12	3:A:628:SER:N	2.37	0.40
3:A:634:ASP:C	3:A:636:VAL:N	2.72	0.40
3:A:863:LEU:HD12	3:A:866:MSE:CE	2.51	0.40
3:B:188:TYR:CD1	3:B:190:PRO:HD3	2.56	0.40
3:B:292:TYR:O	3:B:296:PHE:N	2.51	0.40
3:B:343:LEU:HD12	3:B:558:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:73:LYS:HG3	4:B:986:HOH:O	2.20	0.40
3:C:206:GLN:NE2	3:C:206:GLN:HA	2.36	0.40
3:C:437:ALA:O	3:C:438:PRO:C	2.58	0.40
3:C:720:TYR:CG	3:C:724:LYS:HG3	2.57	0.40
3:D:644:THR:CG2	3:D:692:PRO:HA	2.52	0.40
3:D:85:MSE:HE1	3:D:87:ASP:H	1.85	0.40
3:A:167:ALA:O	3:A:177:GLU:N	2.54	0.40
3:A:859:LYS:C	3:A:861:ASP:N	2.74	0.40
3:B:113:PHE:CE1	3:B:213:LEU:HD11	2.57	0.40
3:B:200:GLU:O	3:B:201:TYR:C	2.60	0.40
3:B:27:ARG:HG3	3:B:27:ARG:HH11	1.86	0.40
3:B:340:PHE:O	3:B:343:LEU:HB3	2.20	0.40
3:B:426:SER:O	3:B:429:THR:OG1	2.36	0.40
3:B:364:THR:HG21	3:B:562:LEU:HD21	2.03	0.40
3:B:579:ASP:OD1	3:B:581:ARG:HB2	2.21	0.40
3:B:670:MSE:O	3:B:673:TYR:HB3	2.21	0.40
3:B:738:PRO:HD2	3:B:875:THR:HG21	2.03	0.40
3:C:170:LEU:CD1	3:C:170:LEU:N	2.84	0.40
3:C:384:ARG:HG2	3:C:384:ARG:HH11	1.86	0.40
3:D:302:LYS:HD2	3:D:303:LEU:N	2.10	0.40
3:D:697:GLY:O	3:D:698:ILE:O	2.40	0.40
3:A:831:TYR:HD2	3:A:848:TRP:NE1	2.20	0.40
3:B:225:TYR:O	3:B:229:ARG:HB2	2.22	0.40
3:B:256:MSE:C	3:B:256:MSE:SE	3.10	0.40
3:B:268:ILE:CG2	3:B:269:SER:H	2.34	0.40
3:B:302:LYS:O	3:B:303:LEU:CB	2.69	0.40
3:B:379:VAL:O	4:B:934:HOH:O	2.22	0.40
3:D:205:TRP:N	4:D:946:HOH:O	2.55	0.40
3:D:273:TYR:O	3:D:274:ILE:C	2.60	0.40
3:D:42:PRO:HG2	3:D:44:SER:HB2	2.04	0.40
3:D:577:TYR:CD1	3:D:577:TYR:N	2.90	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	
3	A	852/903 (94%)	760 (89%)	76 (9%)	16 (2%)	9	30
3	B	763/903 (84%)	621 (81%)	110 (14%)	32 (4%)	3	10
3	C	849/903 (94%)	745 (88%)	74 (9%)	30 (4%)	4	14
3	D	661/903 (73%)	433 (66%)	155 (23%)	73 (11%)	0	1
All	All	3125/3612 (86%)	2559 (82%)	415 (13%)	151 (5%)	2	8

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	12	GLY
3	A	542	LEU
3	A	859	LYS
3	A	894	LYS
3	B	164	ILE
3	B	176	ASP
3	B	195	LYS
3	B	236	GLU
3	B	305	TYR
3	B	622	THR
3	B	705	LYS
3	B	776	TYR
3	C	13	ASP
3	C	24	GLY
3	C	172	GLU
3	C	608	VAL
3	D	14	SER
3	D	28	THR
3	D	29	ARG
3	D	213	LEU
3	D	302	LYS
3	D	314	GLU
3	D	637	GLY
3	D	656	ARG
3	D	698	ILE
3	D	718	THR
3	A	280	PHE
3	A	547	ARG
3	A	622	THR
3	A	642	ARG

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Mol	Chain	Res	Type
3	B	12	GLY
3	B	153	ASN
3	B	159	VAL
3	B	162	TRP
3	B	165	GLU
3	B	168	ALA
3	B	172	GLU
3	B	315	SER
3	B	406	TYR
3	C	12	GLY
3	C	255	ASN
3	C	258	GLY
3	C	622	THR
3	C	816	LYS
3	D	2	LYS
3	D	12	GLY
3	D	15	ILE
3	D	26	GLU
3	D	235	GLY
3	D	242	LEU
3	D	244	PRO
3	D	262	ILE
3	D	282	PHE
3	D	315	SER
3	D	388	VAL
3	D	458	PRO
3	D	551	ALA
3	D	555	ALA
3	D	606	ASN
3	D	658	ARG
3	D	712	VAL
3	D	720	TYR
3	D	730	LEU
3	D	755	GLU
3	D	873	GLU
3	A	279	LYS
3	A	896	SER
3	B	181	GLU
3	B	187	ILE
3	B	237	SER
3	B	274	ILE
3	B	490	LEU

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Mol	Chain	Res	Type
3	B	731	GLU
3	C	45	GLN
3	C	46	ALA
3	C	135	ALA
3	C	179	PRO
3	C	234	PHE
3	C	315	SER
3	C	402	ASN
3	C	414	SER
3	C	415	LEU
3	C	466	ASP
3	C	607	GLU
3	D	30	GLU
3	D	43	GLU
3	D	222	ALA
3	D	241	ARG
3	D	290	LEU
3	D	295	GLU
3	D	370	PHE
3	D	405	LYS
3	D	728	MSE
3	D	735	SER
3	D	887	ALA
3	D	895	ALA
3	A	13	ASP
3	A	99	TYR
3	A	554	THR
3	A	899	ASP
3	B	155	PRO
3	B	163	SER
3	B	173	GLN
3	B	280	PHE
3	B	303	LEU
3	B	774	LEU
3	C	3	GLU
3	C	170	LEU
3	C	175	GLY
3	C	187	ILE
3	C	227	TYR
3	C	320	TYR
3	D	36	SER
3	D	100	GLU

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Mol	Chain	Res	Type
3	D	106	THR
3	D	240	LYS
3	D	280	PHE
3	D	308	PRO
3	D	364	THR
3	D	553	MSE
3	D	576	ARG
3	D	630	ASP
3	D	645	ASN
3	D	693	LEU
3	D	867	ASP
3	A	897	LEU
3	B	2	LYS
3	B	778	SER
3	C	98	ASN
3	C	303	LEU
3	D	27	ARG
3	D	35	PRO
3	D	243	SER
3	D	279	LYS
3	D	344	SER
3	D	391	TYR
3	D	435	LYS
3	D	872	LEU
3	A	863	LEU
3	C	155	PRO
3	D	224	PRO
3	D	316	ASN
3	D	424	ASN
3	C	233	ILE
3	D	353	ILE
3	D	401	PRO
3	B	166	ILE
3	D	586	ILE
3	D	450	PRO
3	D	877	ILE
3	D	24	GLY

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	745/775 (96%)	701 (94%)	44 (6%)	23	54
3	B	663/775 (86%)	613 (92%)	50 (8%)	16	41
3	C	737/775 (95%)	689 (94%)	48 (6%)	20	49
3	D	453/775 (58%)	413 (91%)	40 (9%)	12	33
All	All	2598/3100 (84%)	2416 (93%)	182 (7%)	18	45

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	MSE
3	A	32	GLU
3	A	34	LYS
3	A	60	LYS
3	A	66	ARG
3	A	83	LEU
3	A	106	THR
3	A	112	ASN
3	A	121	ASP
3	A	143	ASP
3	A	154	SER
3	A	164	ILE
3	A	171	GLN
3	A	197	LEU
3	A	199	MSE
3	A	304	LYS
3	A	319	ARG
3	A	342	ASN
3	A	384	ARG
3	A	403	ARG
3	A	411	ASP
3	A	466	ASP
3	A	475	ILE
3	A	541	MSE
3	A	553	MSE
3	A	556	GLN
3	A	581	ARG
3	A	592	MSE

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Mol	Chain	Res	Type
3	A	622	THR
3	A	633	ILE
3	A	635	LYS
3	A	642	ARG
3	A	645	ASN
3	A	681	MSE
3	A	683	MSE
3	A	702	TRP
3	A	731	GLU
3	A	743	LYS
3	A	758	GLU
3	A	781	SER
3	A	819	ILE
3	A	855	THR
3	A	861	ASP
3	A	897	LEU
3	B	22	SER
3	B	27	ARG
3	B	29	ARG
3	B	58	THR
3	B	66	ARG
3	B	103	TYR
3	B	113	PHE
3	B	115	ILE
3	B	121	ASP
3	B	128	GLN
3	B	152	LEU
3	B	156	TYR
3	B	160	GLU
3	B	164	ILE
3	B	165	GLU
3	B	181	GLU
3	B	183	ILE
3	B	184	ASP
3	B	229	ARG
3	B	234	PHE
3	B	252	VAL
3	B	256	MSE
3	B	290	LEU
3	B	295	GLU
3	B	299	ASN
3	B	303	LEU

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Mol	Chain	Res	Type
3	B	305	TYR
3	B	316	ASN
3	B	319	ARG
3	B	324	ASN
3	B	362	ILE
3	B	391	TYR
3	B	421	ARG
3	B	479	PHE
3	B	493	GLN
3	B	495	ASN
3	B	543	PHE
3	B	622	THR
3	B	623	ASP
3	B	643	ASP
3	B	645	ASN
3	B	658	ARG
3	B	681	MSE
3	B	685	ARG
3	B	702	TRP
3	B	722	GLU
3	B	747	GLU
3	B	776	TYR
3	B	893	LYS
3	B	899	ASP
3	C	14	SER
3	C	15	ILE
3	C	23	ASN
3	C	43	GLU
3	C	58	THR
3	C	61	LEU
3	C	81	GLU
3	C	83	LEU
3	C	90	LEU
3	C	128	GLN
3	C	138	HIS
3	C	153	ASN
3	C	158	ASN
3	C	183	ILE
3	C	194	GLU
3	C	208	LYS
3	C	217	ASN
3	C	255	ASN

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Mol	Chain	Res	Type
3	C	257	TYR
3	C	273	TYR
3	C	284	ASN
3	C	291	ASP
3	C	299	ASN
3	C	302	LYS
3	C	318	GLN
3	C	384	ARG
3	C	391	TYR
3	C	402	ASN
3	C	422	GLN
3	C	424	ASN
3	C	426	SER
3	C	428	GLU
3	C	439	LEU
3	C	440	HIS
3	C	441	ASP
3	C	479	PHE
3	C	494	ARG
3	C	495	ASN
3	C	562	LEU
3	C	618	LEU
3	C	674	MSE
3	C	702	TRP
3	C	731	GLU
3	C	732	THR
3	C	760	LEU
3	C	818	ASN
3	C	829	LYS
3	C	833	LEU
3	D	9	GLU
3	D	17	GLU
3	D	43	GLU
3	D	52	ILE
3	D	64	ASN
3	D	70	GLN
3	D	85	MSE
3	D	86	ASP
3	D	92	TYR
3	D	102	LYS
3	D	197	LEU
3	D	204	PHE

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Mol	Chain	Res	Type
3	D	242	LEU
3	D	273	TYR
3	D	285	GLN
3	D	292	TYR
3	D	302	LYS
3	D	305	TYR
3	D	346	ASP
3	D	354	GLN
3	D	403	ARG
3	D	422	GLN
3	D	441	ASP
3	D	449	ARG
3	D	458	PRO
3	D	479	PHE
3	D	556	GLN
3	D	563	ILE
3	D	574	TRP
3	D	592	MSE
3	D	606	ASN
3	D	618	LEU
3	D	621	ASP
3	D	623	ASP
3	D	635	LYS
3	D	677	LYS
3	D	702	TRP
3	D	722	GLU
3	D	728	MSE
3	D	768	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	112	ASN
3	A	171	GLN
3	A	339	GLN
3	A	356	GLN
3	A	422	GLN
3	A	444	ASN
3	A	493	GLN
3	A	564	ASN
3	A	645	ASN
3	A	773	GLN

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Mol	Chain	Res	Type
3	A	864	HIS
3	B	10	GLN
3	B	23	ASN
3	B	45	GLN
3	B	153	ASN
3	B	158	ASN
3	B	193	ASN
3	B	217	ASN
3	B	299	ASN
3	B	316	ASN
3	B	317	HIS
3	B	318	GLN
3	B	376	GLN
3	B	389	GLN
3	B	424	ASN
3	B	444	ASN
3	B	480	ASN
3	B	493	GLN
3	B	495	ASN
3	B	556	GLN
3	B	676	ASN
3	B	733	GLN
3	B	742	GLN
3	C	10	GLN
3	C	45	GLN
3	C	70	GLN
3	C	112	ASN
3	C	128	GLN
3	C	153	ASN
3	C	158	ASN
3	C	206	GLN
3	C	217	ASN
3	C	255	ASN
3	C	284	ASN
3	C	318	GLN
3	C	324	ASN
3	C	354	GLN
3	C	376	GLN
3	C	402	ASN
3	C	422	GLN
3	C	424	ASN
3	C	495	ASN

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Mol	Chain	Res	Type
3	C	546	GLN
3	C	556	GLN
3	C	564	ASN
3	C	582	ASN
3	C	595	GLN
3	C	679	HIS
3	C	818	ASN
3	D	70	GLN
3	D	333	GLN
3	D	354	GLN
3	D	606	ASN
3	D	675	ASN
3	D	733	GLN
3	D	742	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	3DR	E	3	1	8,11,12	0.40	0	8,14,17	0.71	0
1	3DR	I	3	1	8,11,12	0.48	0	8,14,17	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	3DR	E	3	1	-	0/3/15/16	0/1/1/1
1	3DR	I	3	1	-	0/3/15/16	0/1/1/1

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	3	3DR	3	0
1	I	3	3DR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	17/18 (94%)	0.56	1 (5%) 23 15	57, 95, 121, 134	0
1	G	13/18 (72%)	1.28	1 (7%) 14 8	48, 103, 143, 144	0
1	I	17/18 (94%)	-0.13	0 100 100	27, 43, 112, 123	0
1	K	9/18 (50%)	1.83	5 (55%) 0 0	38, 140, 155, 159	0
2	F	15/15 (100%)	0.72	1 (6%) 19 11	77, 104, 136, 140	0
2	H	15/15 (100%)	1.30	4 (26%) 1 0	75, 118, 131, 139	0
2	J	15/15 (100%)	0.10	1 (6%) 19 11	28, 57, 97, 114	0
2	L	8/15 (53%)	2.63	7 (87%) 0 0	144, 148, 149, 149	0
3	A	831/903 (92%)	-0.06	9 (1%) 80 74	16, 40, 83, 133	0
3	B	746/903 (82%)	0.28	45 (6%) 23 14	19, 57, 112, 140	0
3	C	829/903 (91%)	0.00	13 (1%) 72 65	18, 46, 86, 119	0
3	D	650/903 (71%)	0.89	106 (16%) 2 1	78, 102, 134, 142	0
All	All	3165/3744 (84%)	0.26	193 (6%) 22 14	16, 56, 123, 159	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	450	PRO	7.4
3	D	309	ILE	6.1
3	D	394	ALA	5.9
3	D	216	TRP	5.7
3	B	254	GLU	5.5
3	D	283	THR	5.3
3	D	239	ALA	4.9
3	D	875	THR	4.8
3	D	308	PRO	4.7
3	D	66	ARG	4.6
3	B	160	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
3	D	315	SER	4.5
3	D	876	PHE	4.5
3	B	546	GLN	4.5
3	D	432	GLY	4.5
3	D	771	PHE	4.4
3	D	546	GLN	4.4
3	A	490	LEU	4.2
3	D	864	HIS	4.2
3	D	306	ASP	4.1
3	D	310	SER	4.1
3	D	390	PRO	4.1
3	C	495	ASN	4.1
3	D	48	LYS	4.1
1	K	12	DA	4.0
3	D	327	ALA	4.0
3	B	545	ALA	4.0
3	D	865	TRP	3.9
3	D	203	ASN	3.9
3	B	542	LEU	3.9
3	D	50	PHE	3.8
3	D	284	ASN	3.8
3	D	545	ALA	3.7
3	B	255	ASN	3.6
3	D	305	TYR	3.6
3	B	865	TRP	3.5
2	L	103	DG	3.5
3	D	70	GLN	3.5
3	D	46	ALA	3.5
3	D	229	ARG	3.4
3	C	491	ALA	3.4
3	D	103	TYR	3.4
3	D	282	PHE	3.3
2	H	108	DT	3.3
3	B	305	TYR	3.3
3	D	215	GLY	3.3
1	K	11	DC	3.3
3	D	696	LYS	3.3
2	F	115	DA	3.2
3	C	303	LEU	3.2
3	D	448	GLU	3.2
3	B	175	GLY	3.2
3	D	298	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	886	ALA	3.2
3	B	122	GLY	3.2
3	D	325	ILE	3.1
1	K	13	DG	3.1
3	D	265	LEU	3.1
3	D	248	THR	3.1
3	B	551	ALA	3.1
2	L	106	DT	3.1
3	D	228	ASN	3.1
3	B	174	GLY	3.0
3	C	490	LEU	3.0
3	B	171	GLN	3.0
3	B	178	VAL	3.0
3	D	436	VAL	3.0
3	D	90	LEU	2.9
3	D	7	THR	2.9
3	D	869	THR	2.9
3	B	733	GLN	2.9
3	D	779	ILE	2.9
3	D	225	TYR	2.9
3	B	862	VAL	2.9
2	J	115	DA	2.9
3	D	17	GLU	2.9
3	D	337	LYS	2.9
3	C	164	ILE	2.9
3	D	293	ILE	2.8
2	L	108	DT	2.8
3	A	821	ALA	2.8
3	D	303	LEU	2.8
3	C	171	GLN	2.8
3	B	393	GLY	2.8
3	D	776	TYR	2.8
3	D	569	ALA	2.8
3	C	306	ASP	2.8
3	D	619	TYR	2.8
3	A	544	ARG	2.7
3	A	545	ALA	2.7
3	D	15	ILE	2.7
3	C	493	GLN	2.7
3	D	242	LEU	2.7
3	B	253	ILE	2.7
3	D	8	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	B	137	THR	2.7
3	C	486	LYS	2.7
3	B	230	ILE	2.6
2	L	105	DC	2.6
3	D	40	HIS	2.6
3	D	557	ILE	2.6
2	L	104	DG	2.6
3	D	297	GLU	2.6
3	D	64	ASN	2.6
3	B	250	VAL	2.6
3	B	492	ALA	2.6
3	B	129	ALA	2.5
3	B	155	PRO	2.5
3	D	323	TYR	2.5
3	D	868	TYR	2.5
3	B	172	GLU	2.5
3	B	303	LEU	2.5
3	D	563	ILE	2.5
3	D	61	LEU	2.5
3	D	227	TYR	2.5
3	D	442	TYR	2.5
2	H	107	DG	2.5
1	K	14	DC	2.5
2	H	115	DA	2.5
3	A	542	LEU	2.5
2	L	107	DG	2.4
3	D	45	GLN	2.4
3	D	340	PHE	2.4
3	D	465	LYS	2.4
3	D	872	LEU	2.4
3	D	410	PHE	2.4
3	D	479	PHE	2.4
3	B	232	ASN	2.4
3	D	338	ARG	2.4
3	D	654	PHE	2.4
3	B	162	TRP	2.4
3	D	334	ILE	2.4
3	B	487	GLY	2.3
3	B	152	LEU	2.3
2	H	109	DC	2.3
3	A	857	LEU	2.3
3	B	288	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
3	B	237	SER	2.3
3	B	870	VAL	2.3
3	D	277	TYR	2.3
3	D	415	LEU	2.3
3	B	123	PHE	2.3
3	B	876	PHE	2.3
3	D	431	ALA	2.3
3	A	854	ILE	2.3
3	D	625	ILE	2.3
3	D	191	PHE	2.3
3	D	231	LYS	2.2
3	D	240	LYS	2.2
3	D	316	ASN	2.2
3	D	47	THR	2.2
3	D	867	ASP	2.2
3	B	183	ILE	2.2
3	D	196	GLU	2.2
1	E	1	DC	2.2
3	B	299	ASN	2.2
3	D	312	LEU	2.2
3	C	550	VAL	2.2
3	B	234	PHE	2.2
3	B	861	ASP	2.2
3	D	83	LEU	2.2
3	D	870	VAL	2.2
3	D	764	PHE	2.1
3	C	172	GLU	2.1
3	B	872	LEU	2.1
3	D	205	TRP	2.1
3	B	188	TYR	2.1
3	D	767	PHE	2.1
3	D	890	ASP	2.1
3	B	495	ASN	2.1
3	D	217	ASN	2.1
3	D	328	VAL	2.1
3	D	605	LEU	2.1
3	A	785	ALA	2.1
3	B	319	ARG	2.1
1	G	7	DA	2.1
3	C	307	GLY	2.1
3	D	317	HIS	2.1
2	L	101	DG	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	241	ARG	2.1
3	A	494	ARG	2.0
3	C	11	ILE	2.0
3	D	192	ASP	2.0
3	D	212	ILE	2.0
3	B	549	GLU	2.0
3	D	32	GLU	2.0
3	B	494	ARG	2.0
3	D	552	GLY	2.0
3	D	456	CYS	2.0
3	D	774	LEU	2.0
3	D	650	PHE	2.0
1	K	10	DA	2.0
3	D	38	PHE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
1	3DR	E	3	11/12	0.78	0.38	-	117,125,130,133	0
1	3DR	I	3	11/12	0.89	0.25	-	101,102,103,103	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.