



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:24 PM UTC

PDB ID : 2P5O / pdb_00002p5o
Title : Crystal structure of RB69 GP43 in complex with DNA containing an abasic site analog
Authors : Hogg, M.; Wallace, S.S.; Doublié, 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

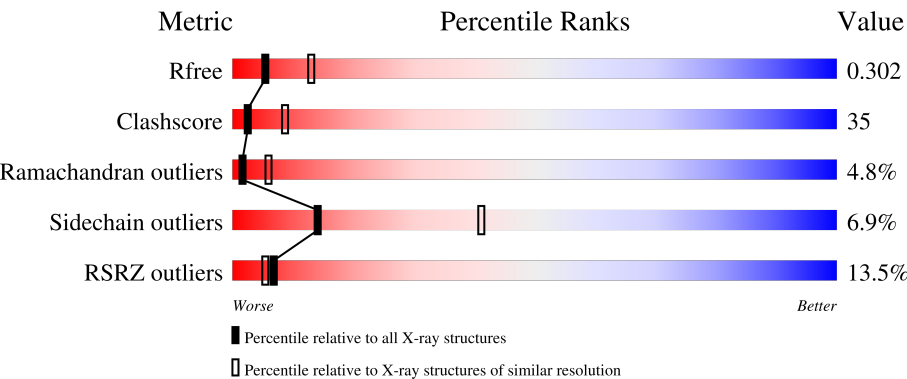
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	18	
1	G	18	
1	I	18	
1	K	18	
2	F	15	

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Mol	Chain	Length	Quality of chain
2	H	15	47% 40% 60%
2	J	15	20% 33% 67%
2	L	15	33% 7% 47% 47%
3	A	903	3% 53% 36% 5% 5%
3	B	903	12% 37% 41% 7% 15%
3	C	903	3% 48% 40% 7% 6%
3	D	903	26% 28% 38% 8% 26%

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 mutation	UNP Q38087
A	256	MSE	MET	modified residue	UNP Q38087
A	327	ALA	ASP	engineered mutation	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 mutation	UNP Q38087
B	256	MSE	MET	modified residue	UNP Q38087
B	327	ALA	ASP	engineered mutation	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 mutation	UNP Q38087
C	256	MSE	MET	modified residue	UNP Q38087
C	327	ALA	ASP	engineered mutation	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 mutation	UNP Q38087
D	256	MSE	MET	modified residue	UNP Q38087
D	327	ALA	ASP	engineered mutation	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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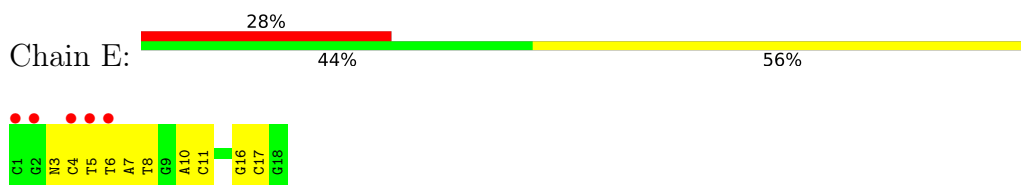
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	6	Total 6	O 6	0	0
4	A	139	Total 139	O 139	0	0
4	B	106	Total 106	O 106	0	0
4	C	147	Total 147	O 147	0	0
4	D	46	Total 46	O 46	0	0

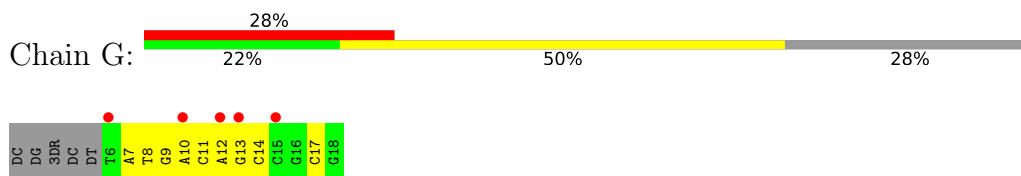
3 Residue-property plots [i](#)

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

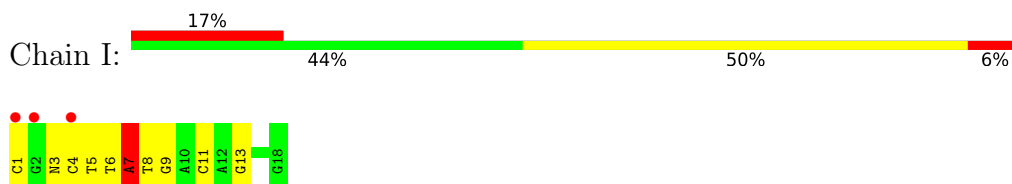
- Molecule 1: Template DNA



- Molecule 1: Template DNA



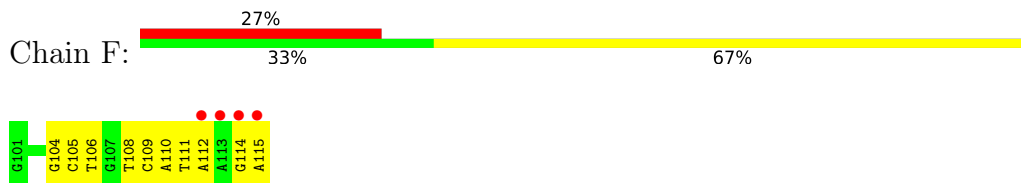
- Molecule 1: Template DNA



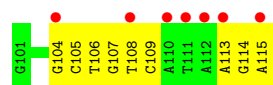
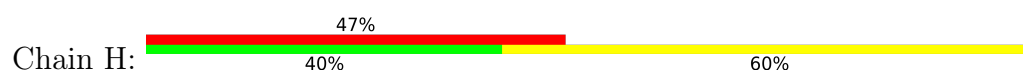
- Molecule 1: Template DNA



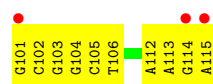
- Molecule 2: Primer DNA



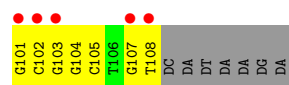
- Molecule 2: Primer DNA



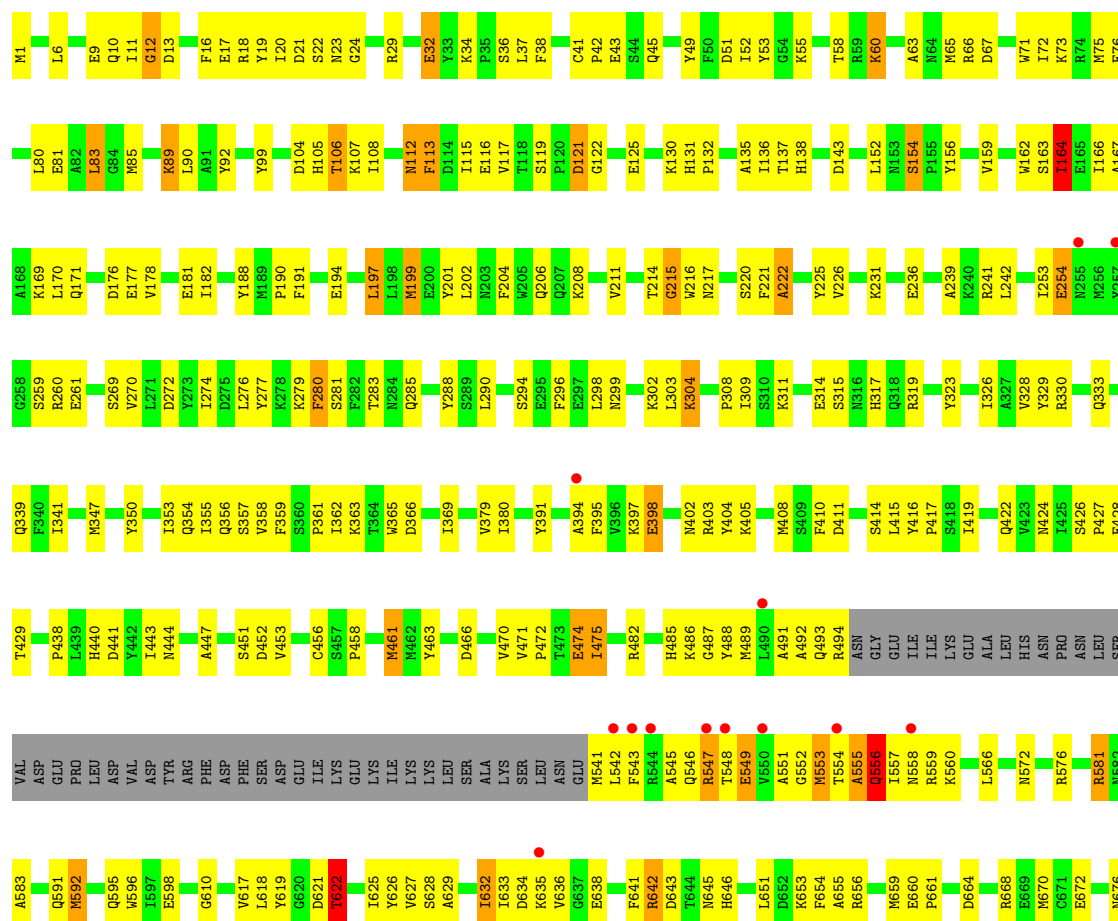
• Molecule 2: Primer DNA

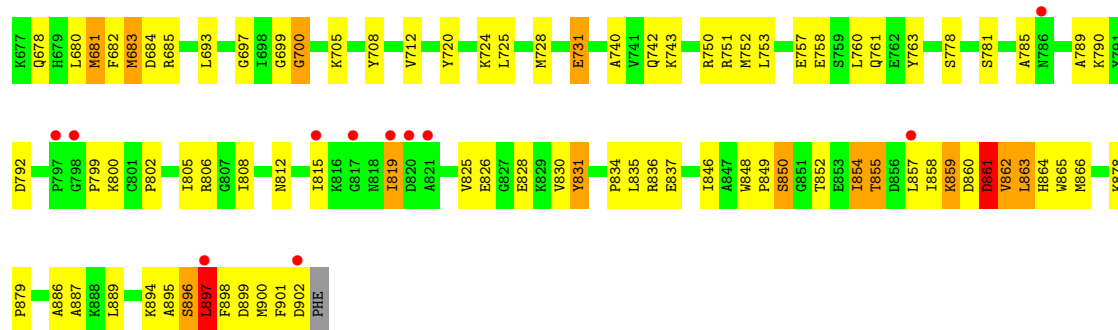


• Molecule 2: Primer DNA

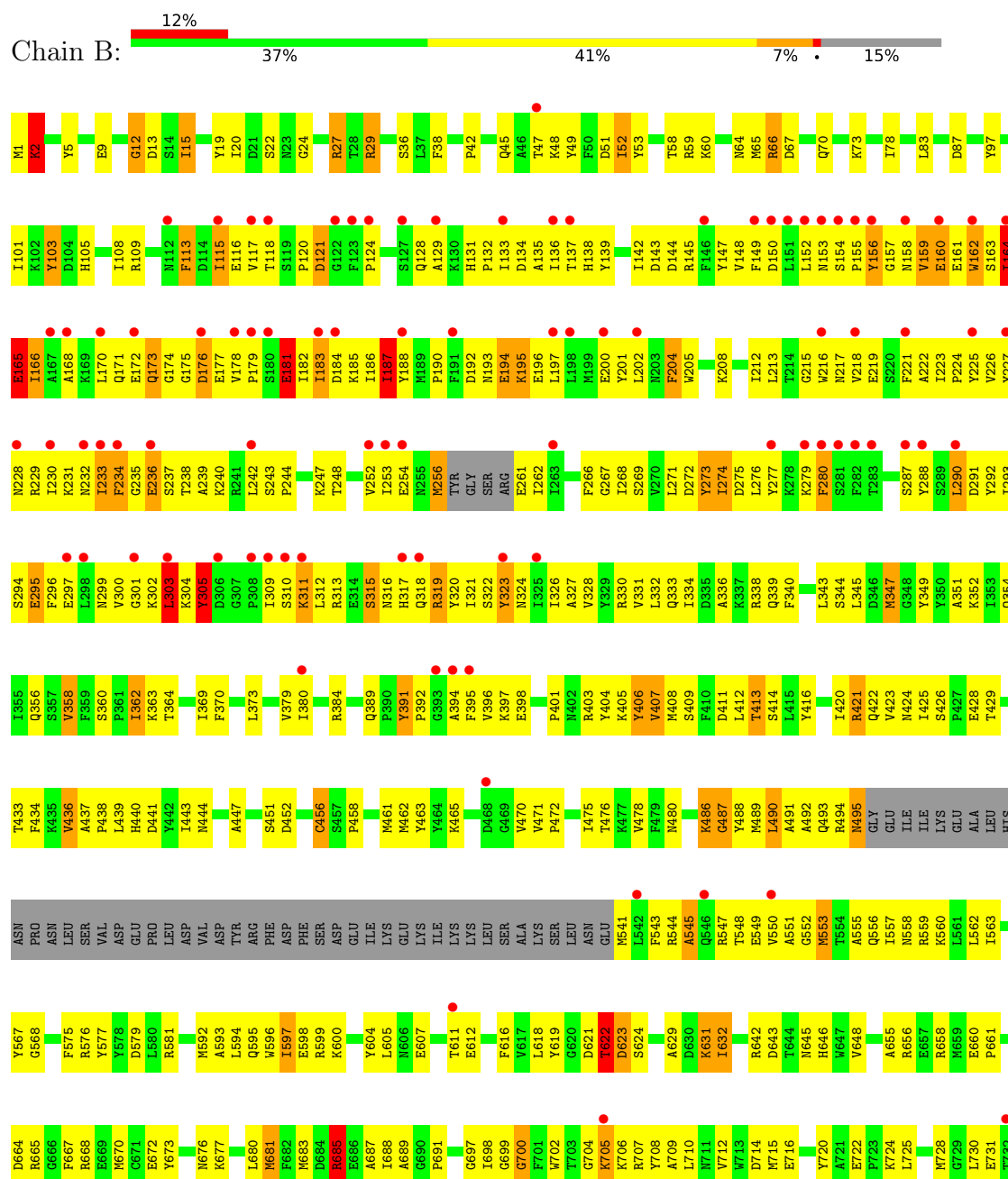


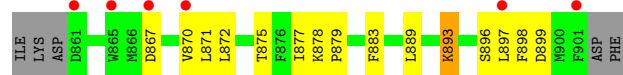
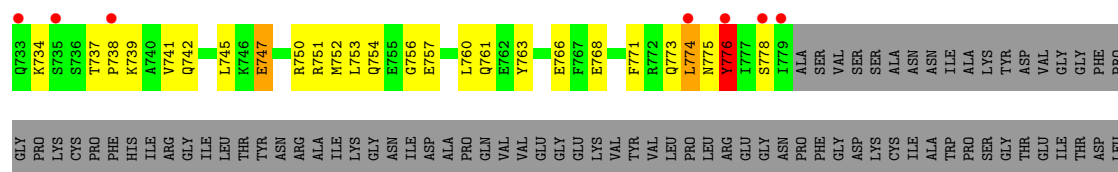
• Molecule 3: DNA polymerase



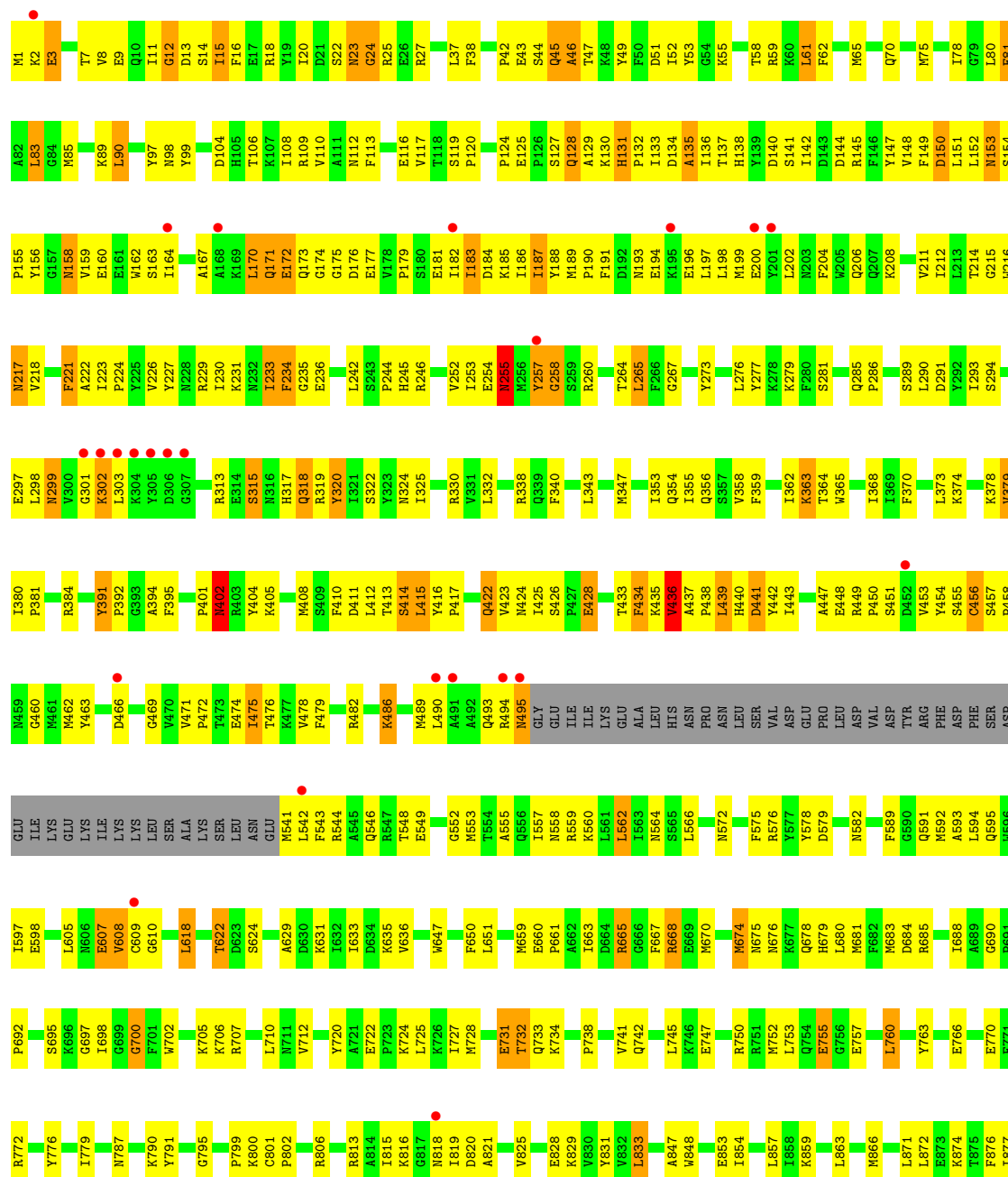


• Molecule 3: DNA polymerase



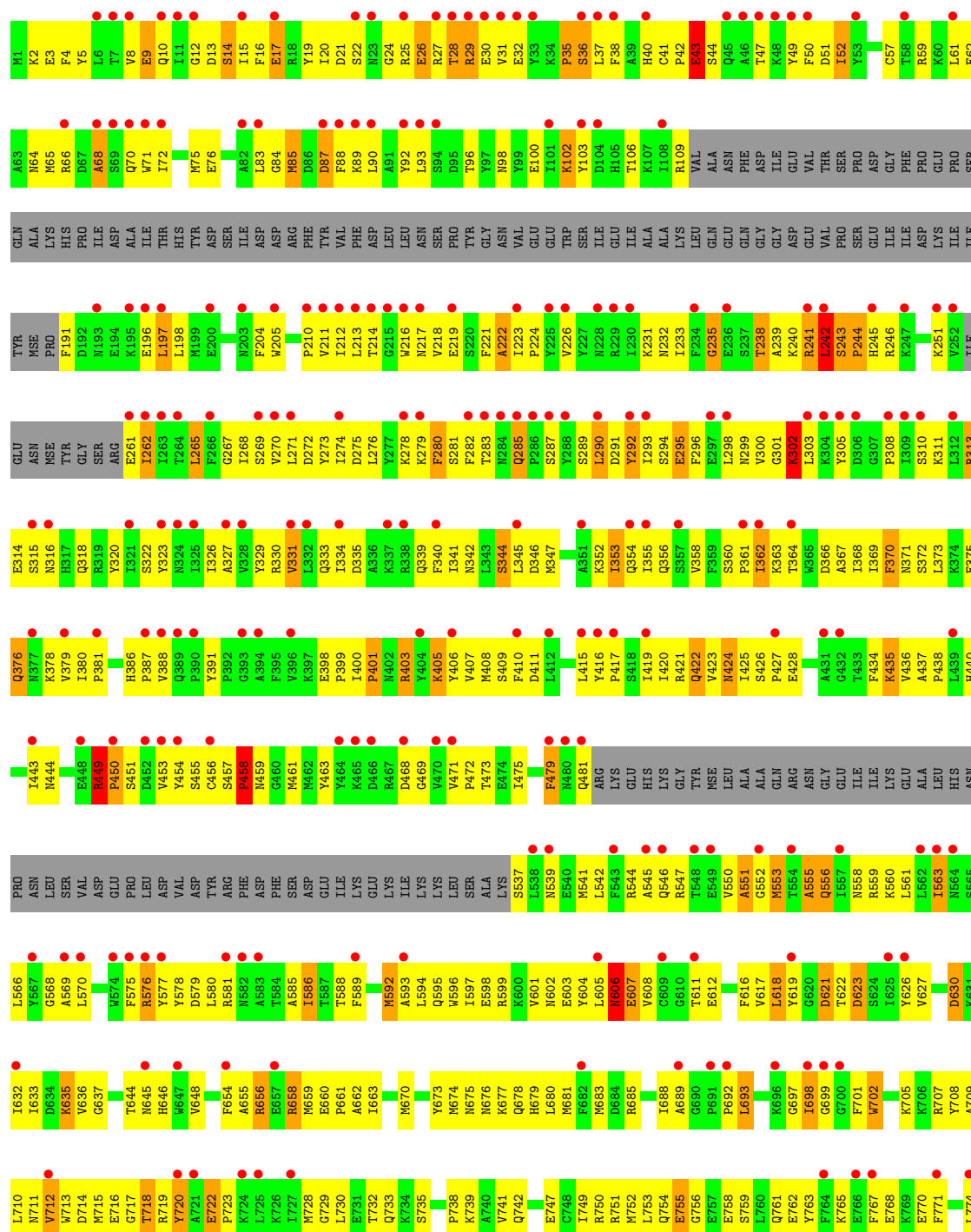
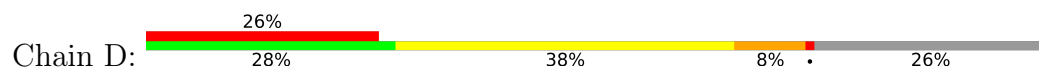


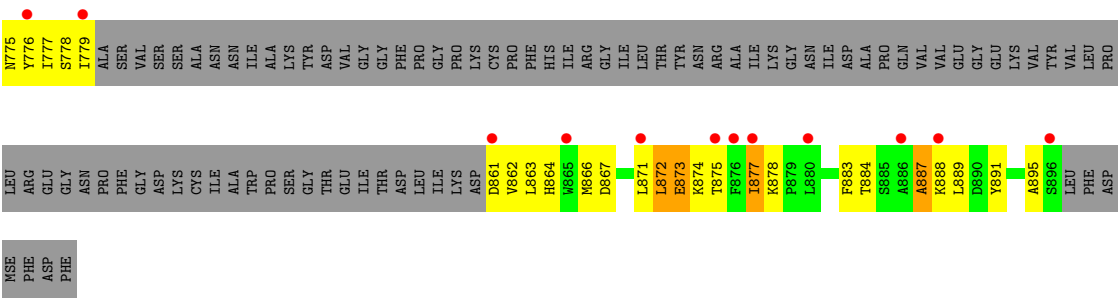
• Molecule 3: DNA polymerase





● 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 44.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.9 (44.00-2.80) 92.1 (44.00-2.80)	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	Depositor
R, R_{free}	0.245 , 0.290 0.263 , 0.302	Depositor DCC
R_{free} test set	24426 reflections (9.67%)	wwPDB-VP
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 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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	0.30	0/384	0.61	0/588
1	G	0.31	0/296	0.72	0/455
1	I	0.39	0/384	0.83	2/588 (0.3%)
1	K	0.30	0/203	0.55	0/311
2	F	0.28	0/346	0.58	0/533
2	H	0.27	0/346	0.59	0/533
2	J	0.33	0/346	0.67	0/533
2	L	0.26	0/182	0.54	0/280
3	A	0.57	0/7090	1.05	32/9555 (0.3%)
3	B	0.50	0/6376	0.97	23/8593 (0.3%)
3	C	0.54	0/7045	1.01	28/9502 (0.3%)
3	D	0.39	0/5028	0.92	19/6831 (0.3%)
All	All	0.50	0/28026	0.96	104/38302 (0.3%)

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

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

There are no bond length outliers.

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	819	ILE	N-CA-C	-9.92	103.38	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	87	ASP	N-CA-C	-8.81	101.79	112.54
3	B	486	LYS	N-CA-C	-8.64	102.66	113.55
3	A	456	CYS	N-CA-C	8.26	122.55	109.50
3	A	211	VAL	N-CA-C	-8.12	103.96	111.67
3	C	211	VAL	N-CA-C	-7.82	105.56	111.90
3	D	457	SER	CA-C-N	7.68	129.44	119.84
3	D	457	SER	C-N-CA	7.68	129.44	119.84
3	A	555	ALA	N-CA-C	-7.53	102.74	112.23
3	A	862	VAL	N-CA-C	-7.42	103.62	110.82
3	C	242	LEU	N-CA-C	-7.37	104.17	113.01
3	B	877	ILE	N-CA-C	7.27	117.36	110.53
3	B	632	ILE	N-CA-C	-7.27	103.77	110.82
3	C	755	GLU	N-CA-C	-7.25	98.89	109.18
3	B	323	TYR	N-CA-C	-6.96	103.62	111.14
3	C	476	THR	N-CA-C	-6.90	103.75	111.28
3	B	487	GLY	N-CA-C	-6.87	106.77	114.40
3	D	428	GLU	N-CA-C	6.76	121.39	113.20
3	C	881	GLU	N-CA-C	-6.60	103.19	111.11
3	D	376	GLN	N-CA-C	-6.47	105.25	113.02
3	B	294	SER	N-CA-C	-6.43	104.32	111.71
3	A	700	GLY	N-CA-C	-6.37	101.96	111.19
3	D	68	ALA	N-CA-C	-6.34	105.03	112.89
3	B	545	ALA	N-CA-C	-6.27	106.59	114.56
3	A	831	TYR	N-CA-C	-6.25	101.24	110.48
3	C	436	VAL	N-CA-C	6.22	117.26	108.36
3	C	859	LYS	N-CA-C	6.20	118.04	111.28
3	D	313	ARG	N-CA-C	-6.15	105.81	113.55
3	C	171	GLN	N-CA-C	6.13	118.89	111.40
3	D	607	GLU	N-CA-C	-6.12	105.64	113.23
3	A	453	VAL	N-CA-C	6.11	116.82	111.56
3	A	119	SER	CA-C-N	6.10	125.65	119.19
3	A	119	SER	C-N-CA	6.10	125.65	119.19
3	B	354	GLN	N-CA-C	-6.06	101.44	110.23
3	B	648	VAL	N-CA-C	-6.00	104.66	110.42
3	C	665	ARG	N-CA-C	-6.00	105.04	112.90
3	C	486	LYS	N-CA-C	-5.94	104.80	111.28
3	A	474	GLU	N-CA-C	5.92	117.73	111.28
3	B	156	TYR	N-CA-C	-5.92	105.25	112.88
3	B	358	VAL	N-CA-C	-5.91	104.29	112.50
3	A	73	LYS	N-CA-C	-5.89	104.93	111.36
3	C	755	GLU	CA-C-N	-5.87	115.23	122.75
3	C	755	GLU	C-N-CA	-5.87	115.23	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	712	VAL	N-CA-C	5.86	117.02	108.58
3	A	164	ILE	CB-CA-C	-5.82	104.40	112.02
3	C	379	VAL	N-CA-C	5.81	116.23	107.75
3	C	150	ASP	N-CA-C	5.76	118.11	108.96
3	C	712	VAL	N-CA-C	5.73	116.84	108.58
3	A	215	GLY	N-CA-C	-5.72	102.26	110.38
3	A	222	ALA	N-CA-C	5.71	117.18	111.07
3	A	556	GLN	N-CA-C	-5.69	105.08	111.28
3	B	456	CYS	N-CA-C	5.68	118.51	109.81
3	A	354	GLN	N-CA-C	-5.66	101.48	109.96
3	C	456	CYS	N-CA-C	5.65	118.46	109.81
3	B	452	ASP	N-CA-C	-5.65	105.07	112.41
3	C	434	PHE	N-CA-C	5.64	115.83	107.88
3	B	756	GLY	N-CA-C	5.63	118.61	111.85
3	D	310	SER	N-CA-C	-5.62	106.39	113.20
3	A	830	VAL	N-CA-C	5.62	116.83	108.46
3	D	546	GLN	N-CA-C	-5.60	106.58	113.41
3	D	238	THR	N-CA-C	-5.57	106.32	113.01
3	C	108	ILE	N-CA-C	5.56	115.57	108.12
3	C	877	ILE	N-CA-C	5.53	115.62	110.42
3	C	543	PHE	N-CA-C	-5.48	105.47	111.82
3	A	878	LYS	CA-C-N	-5.47	113.26	119.28
3	A	878	LYS	C-N-CA	-5.47	113.26	119.28
3	C	598	GLU	N-CA-C	-5.44	105.25	111.07
1	I	7	DA	N9-C1'-C2'	-5.39	105.42	113.50
3	B	700	GLY	N-CA-C	-5.37	101.74	110.55
3	B	656	ARG	N-CA-C	5.36	116.92	111.14
3	A	850	SER	N-CA-C	5.29	117.52	110.53
3	A	113	PHE	N-CA-C	5.28	117.09	109.07
3	B	685	ARG	N-CA-C	-5.27	102.11	109.96
3	A	452	ASP	N-CA-C	-5.26	106.80	114.12
3	B	194	GLU	N-CA-C	-5.26	106.92	113.55
3	A	276	LEU	N-CA-C	-5.25	105.45	111.07
3	A	861	ASP	N-CA-C	-5.25	105.62	112.23
3	D	545	ALA	N-CA-C	-5.24	106.66	113.16
3	C	806	ARG	N-CA-C	-5.22	105.67	111.36
3	A	451	SER	N-CA-C	5.20	116.04	108.14
3	D	17	GLU	N-CA-C	5.19	115.23	108.07
3	D	400	ILE	CA-C-N	5.17	126.30	119.84
3	D	400	ILE	C-N-CA	5.17	126.30	119.84
3	C	221	PHE	N-CA-C	5.14	119.01	112.12
3	C	700	GLY	N-CA-C	-5.14	102.76	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	389	GLN	CA-C-N	5.13	125.53	119.99
3	B	389	GLN	C-N-CA	5.13	125.53	119.99
3	A	49	TYR	N-CA-C	5.13	117.60	109.24
3	C	668	ARG	N-CA-C	-5.12	105.60	111.07
3	A	742	GLN	N-CA-C	-5.11	105.84	111.71
3	D	398	GLU	CA-C-N	5.11	125.01	119.85
3	D	398	GLU	C-N-CA	5.11	125.01	119.85
3	C	635	LYS	N-CA-C	-5.10	105.64	111.14
3	C	286	PRO	N-CA-C	-5.09	106.78	113.65
3	B	553	MSE	N-CA-C	-5.08	105.92	111.82
1	I	7	DA	C5'-C4'-O4'	-5.05	101.83	109.40
3	D	449	ARG	CA-C-N	5.05	126.15	119.84
3	D	449	ARG	C-N-CA	5.05	126.15	119.84
3	A	125	GLU	CA-C-N	5.04	124.83	119.28
3	A	125	GLU	C-N-CA	5.04	124.83	119.28
3	C	546	GLN	N-CA-C	-5.04	105.70	111.14
3	A	398	GLU	N-CA-C	-5.04	101.96	109.42
3	B	551	ALA	N-CA-C	-5.04	107.10	113.20
3	B	204	PHE	N-CA-C	-5.01	106.33	112.90

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	328	0
3	B	6245	0	6024	515	0
3	C	6895	0	6710	406	0
3	D	4934	0	4297	454	0
4	A	139	0	0	17	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	1810	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 35.

All (1810) 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
2:H:105:DC:H2''	2:H:106:DT:H5'	1.40	1.02
3:A:395:PHE:HB2	3:A:591:GLN:HG3	1.41	1.02
3:B:218:VAL:HG13	3:B:222:ALA:HB3	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	3:B:362:ILE:H	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:HB2	3:A:60:LYS:NZ	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:HD12	3:B:187:ILE:H	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
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:194:GLU:C	3:B:196:GLU:H	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:541:MSE:HG3	3:B:544:ARG:HE	1.43	0.84
1:K:13:DG:H1	2:L:105:DC:N4	1.76	0.84
3:B:405:LYS:HA	3:B:699:GLY:HA3	1.60	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:60:LYS:HB2	3:A:60:LYS:HZ2	1.43	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
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:A:424:ASN:O	3:A:429:THR:HG21	1.82	0.79
3:B:233:ILE:H	3:B:233:ILE:HD12	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
1:G:12:DA:H61	2:H:106:DT:H3	1.29	0.79
3:B:700:GLY:HA2	3:B:753:LEU:HD22	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:DT:H2''	1:E:7:DA:H5'	1.64	0.78
3:D:611:THR:HG22	3:D:612:GLU:H	1.46	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
2:L:108:DT:H3'	4:L:246:HOH:O	1.83	0.78
3:B:115:ILE:HD11	3:B:222:ALA:HA	1.66	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: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:HG	3:D:619:TYR:H	1.51	0.76
3:D:618:LEU:HD23	3:D:618:LEU:H	1.49	0.76
3:D:109:ARG:HE	3:D:211:VAL:HG23	1.51	0.76
2:L:107:DG:C1'	2:L:108:DT:H71	2.14	0.76
3:A:656:ARG:HA	3:A:660:GLU:HG3	1.68	0.76
3:B:154:SER:C	3:B:156:TYR:H	1.93	0.76
3:B:439:LEU:O	3:B:443:ILE:HG13	1.84	0.76
3:B:192:ASP:O	3:B:193:ASN:HB3	1.84	0.76
3:C:112:ASN:HB3	3:C:214:THR:CG2	2.15	0.76
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
1:K:11:DC:H4'	4:K:346:HOH:O	1.87	0.75
3:C:489:MSE:HG3	4:C:1020: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	3:C:668:ARG:HG3	1.53	0.74
2:F:114:DG:C2'	2:F:115:DA:H5''	2.15	0.74
3:B:274:ILE:HG23	3:B:275:ASP:OD1	1.87	0.74
3:C:70:GLN:NE2	3:C:70:GLN:HA	2.02	0.74
2:J:104:DG:C2'	2:J:105:DC:H5''	2.17	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
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:N	3:B:305:TYR:HD2	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
3:C:818:ASN:HD22	3:C:819:ILE:N	1.85	0.73
3:D:239:ALA:C	3:D:241:ARG:H	1.96	0.72
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
1:I:7:DA:H2'	1:I:8:DT:C6	2.24	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
3:B:15:ILE:HG13	3:B:65:MSE:HE1	1.72	0.72
2:H:108:DT:C2'	2:H:109:DC:H5''	2.20	0.72
3:B:159:VAL:HG22	3:B:160:GLU:H	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:825:VAL:HB	3:A:828:GLU:HG3	1.70	0.72
3:D:759:SER:C	3:D:761:GLN:H	1.95	0.71
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: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:C:727:ILE:O	3:C:728:MSE:HE2	1.91	0.70
3:C:818:ASN:HD22	3:C:818:ASN:C	1.97	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:B:300:VAL:HG12	3:B:301:GLY:N	2.06	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
3:C:302:LYS:HZ2	3:C:302:LYS:HB3	1.58	0.69
3:D:212:ILE:O	3:D:212:ILE:HG22	1.90	0.69
3:B:734:LYS:NZ	3:B:734:LYS:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:DT:H2''	1:E:7:DA:C5'	2.24	0.69
3:B:441:ASP:HB3	3:B:447:ALA:HB2	1.74	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
2:J:112:DA:H2''	2:J:113:DA:C8	2.29	0.68
3:C:254:GLU:HA	3:C:258:GLY:HA2	1.76	0.68
1:I:8:DT:OP1	3:C:705:LYS:HB2	1.94	0.68
3:C:549:GLU:HG2	4:C:1020:HOH:O	1.93	0.68
3:D:576:ARG:HB3	3:D:576:ARG:NH1	2.07	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:42:PRO:C	3:D:44:SER:H	2.02	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:42:PRO:HG2	3:C:45:GLN:HG3	1.76	0.67
3:C:128:GLN:HA	3:C:128:GLN:HE21	1.58	0.67
1:E:10:DA:H2''	1:E:11:DC:C5'	2.23	0.67
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
3:A:208:LYS:HE3	4:A:912:HOH:O	1.94	0.67
3:D:83:LEU:H	3:D:83:LEU:HD12	1.60	0.67
3:A:898:PHE:C	3:A:900:MSE:H	2.02	0.67
3:B:187:ILE:H	3:B:187:ILE:CD1	2.07	0.67
3:D:611:THR:HG22	3:D:612:GLU:N	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:13:DG:H2"	1:K:14:DC:OP2	1.95	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
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:HA	3:A:116:GLU:OE2	1.96	0.66
3:B:187:ILE:HD12	3:B:187:ILE:N	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
1:K:13:DG:H22	2:L:105:DC:N4	1.95	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
3:D:593:ALA:HA	3:D:670:MSE:SE	2.47	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:42:PRO:HG2	3:B:45:GLN:HG2	1.78	0.65
3:B:303:LEU:HD23	3:B:326:ILE:HG13	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:362:ILE:HD11	3:A:572:ASN:CG	2.22	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:B:273:TYR:O	3:B:274:ILE:C	2.39	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:HA	3:C:70:GLN:HE21	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:C:255:ASN:C	3:C:257:TYR:H	2.06	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:150:ASP:OD1	3:B:321:ILE:HG12	1.97	0.64
3:B:290:LEU:C	4:B:1000:HOH:O	2.40	0.64
3:B:295:GLU:HG2	3:B:300:VAL:O	1.97	0.64
3:C:230:ILE:HG23	3:C:234:PHE:HD2	1.63	0.64
2:J:104:DG:H2''	2:J:105:DC:C5'	2.28	0.64
3:B:297:GLU:HB2	4:B:983:HOH:O	1.96	0.64
3:D:85:MSE:CE	3:D:90:LEU:HB2	2.27	0.64
3:D:411:ASP:HB2	3:D:623:ASP:O	1.96	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
2:F:108:DT:H5''	4:A:1020:HOH:O	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
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: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
3:A:121:ASP:OD2	3:A:121:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:656:ARG:O	3:D:660:GLU:HB2	1.98	0.63
1:E:16:DG:H2''	1:E:17:DC:C5'	2.18	0.63
3:A:181:GLU:N	3:A:181:GLU:OE1	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:3:3DR:H4'1	3:A:572:ASN:HD22	1.64	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
3:A:11:ILE:HD12	3:A:16:PHE:CD1	2.33	0.63
3:B:52:ILE:HG22	3:B:53:TYR:CE1	2.33	0.63
3:B:183:ILE:HD13	3:B:183:ILE:N	2.13	0.63
3:C:61:LEU:HD23	3:C:62:PHE:H	1.63	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
2:H:106:DT:H2''	2:H:107:DG:C8	2.33	0.63
3:B:268:ILE:HG22	3:B:269:SER:N	2.13	0.63
3:D:85:MSE:HG3	3:D:370:PHE:CE1	2.34	0.63
3:B:687:ALA:CB	3:B:715:MSE:HE1	2.21	0.62
1:I:6:DT:H2''	1:I:7:DA:H5''	1.79	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
3:B:216:TRP:N	3:B:218:VAL:HG23	2.15	0.62
3:A:32:GLU:H	3:A:32:GLU:CD	2.07	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
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:158:ASN:O	3:B:159:VAL:HB	1.99	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
2:H:113:DA:OP1	3:B:288:TYR:HB2	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:897:LEU:HD12	3:A:897:LEU:N	2.02	0.61
3:B:631:LYS:NZ	3:B:631:LYS:HB2	2.15	0.61
3:D:40:HIS:HA	3:D:57:CYS:HB3	1.81	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
2:H:104:DG:H2''	2:H:105:DC:O5'	2.01	0.61
3:A:428:GLU:N	3:A:428:GLU:OE2	2.33	0.61
3:A:632:ILE:HD12	3:A:632:ILE:N	2.15	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
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: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:411:ASP:O	3:B:683:MSE:HA	2.00	0.61
3:B:412:LEU:CD1	3:B:623:ASP:HA	2.25	0.61
3:D:232:ASN:HB2	4:D:949:HOH:O	1.99	0.61
3:B:188:TYR:CZ	3:B:190:PRO:HB3	2.36	0.61
2:J:112:DA:H5'	3:C:734:LYS:HG2	1.82	0.61
3:C:416:TYR:HB2	3:C:417:PRO:HD3	1.81	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:HG2	3:B:319:ARG:HH11	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
3:A:541:MSE:C	3:A:543:PHE:H	2.08	0.60
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:C:171:GLN:C	3:C:173:GLN:H	2.09	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
2:L:102:DC:H2''	2:L:103:DG:C8	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:THR:C	3:C:265:LEU:HD23	2.26	0.60
3:D:43:GLU:CD	3:D:43:GLU:H	2.09	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:D:36:SER:C	3:D:37:LEU:HD12	2.27	0.60
3:A:75:MSE:HE3	3:A:80:LEU:HB2	1.84	0.60
3:A:545:ALA:O	3:A:549:GLU:HB2	2.01	0.60
3:B:105:HIS:HA	3:B:108:ILE:HD12	1.83	0.60
3:B:137:THR:HG1	3:B:328:VAL:HG21	1.66	0.60
3:B:182:ILE:HD13	3:B:185:LYS:HD2	1.84	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:D:453:VAL:HG23	3:D:454:TYR:N	2.02	0.60
1:K:13:DG:H22	2:L:105:DC:H42	1.49	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
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
2:J:102:DC:H4'	2:J:102:DC:OP1	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:313:ARG:C	3:C:315:SER:H	2.09	0.59
3:D:28:THR:O	3:D:29:ARG:HB3	2.02	0.59
3:A:199:MSE:CE	3:A:202:LEU:HD23	2.31	0.59
3:B:428:GLU:OE1	3:B:470:VAL:N	2.28	0.59
3:D:52:ILE:HD11	3:D:381:PRO:CD	2.32	0.59
3:D:274:ILE:HG23	3:D:275:ASP:OD1	2.02	0.59
3:D:775:ASN:OD1	3:D:777:ILE:HG12	2.02	0.59
3:D:592:MSE:HG2	3:D:593:ALA:N	2.16	0.59
3:D:862:VAL:C	3:D:864:HIS:H	2.08	0.59
3:A:83:LEU:HB3	3:A:379:VAL:CG1	2.33	0.59
3:C:158:ASN:HD22	3:C:158:ASN:C	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:83:LEU:HD12	3:D:83:LEU:N	2.16	0.59
1:K:13:DG:N2	2:L:105:DC:H42	2.00	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
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
1:K:11:DC:OP1	3:D:874:LYS:HE3	2.03	0.59
3:A:422:GLN:O	3:A:676:ASN:HB3	2.02	0.59
3:B:321:ILE:HD12	3:B:321:ILE:N	2.18	0.59
3:B:734:LYS:HB3	3:B:734:LYS:HZ3	1.67	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
2:F:109:DC:H2''	2:F:110:DA:C5'	2.28	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
3:D:85:MSE:CE	3:D:87:ASP:H	2.16	0.59
3:D:274:ILE:HG23	3:D:275:ASP:H	1.68	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
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:D:459:ASN:CG	3:D:585:ALA:HA	2.28	0.58
2:L:103:DG:H2''	2:L:104:DG:C8	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:301:GLY:C	3:B:303:LEU:H	2.11	0.58
3:B:331:VAL:HA	3:B:334:ILE:CD1	2.27	0.58
2:J:105:DC:H2'	2:J:106:DT:H71	1.85	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
3:C:426:SER:HB3	3:C:428:GLU:OE2	2.04	0.58
1:E:4:DC:H2''	1:E:5:DT:C7	2.34	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: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:O	3:C:183:ILE:HD13	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:37:LEU:HD12	3:D:37:LEU:N	2.18	0.57
3:D:42:PRO:C	3:D:44:SER:N	2.62	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:862:VAL:C	3:D:864:HIS:N	2.62	0.57
2:L:107:DG:C8	2:L:108:DT:H73	2.40	0.57
3:A:461:MSE:N	3:A:461:MSE:HE2	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:A:298:LEU:O	3:A:299:ASN:HB2	2.03	0.57
3:B:233:ILE:H	3:B:233:ILE:CD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:561:LEU:H	3:D:561:LEU:HD12	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
1:G:11:DC:H2"	1:G:12:DA:OP2	2.04	0.57
3:B:52:ILE:HG22	3:B:53:TYR:CD1	2.40	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: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:C:154:SER:C	3:C:156:TYR:H	2.11	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
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:87:ASP:OD1	3:B:363:LYS:HE3	2.05	0.57
3:B:223:ILE:HB	3:B:224:PRO:HD3	1.86	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:D:83:LEU:HB3	3:D:380:ILE:O	2.05	0.57
3:B:194:GLU:C	3:B:196:GLU:N	2.53	0.56
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:A:43:GLU:CD	3:A:43:GLU:N	2.64	0.56
3:A:60:LYS:HB2	3:A:60:LYS:HZ3	1.70	0.56
3:A:89:LYS:HB2	3:A:89:LYS:NZ	2.20	0.56
3:A:799:PRO:O	3:A:800:LYS:HB2	2.04	0.56
3:C:791:TYR:CD2	3:C:801:CYS:HA	2.40	0.56
3:D:550:VAL:HG23	3:D:550:VAL:O	2.04	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:108:DT:H2''	2:F:109:DC:H5''	1.88	0.56
3:B:47:THR:OG1	3:B:48:LYS:N	2.38	0.56
3:B:356:GLN:C	3:B:358:VAL:H	2.12	0.56
3:C:607:GLU:O	3:C:610:GLY:N	2.37	0.56
3:D:423:VAL:HG22	3:D:676:ASN:ND2	2.20	0.56
3:D:597:ILE:O	3:D:601:VAL:HG23	2.06	0.56
3:D:705:LYS:C	3:D:707:ARG:H	2.12	0.56
3:D:863:LEU:H	3:D:863:LEU:HD12	1.70	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:861:ASP:O	3:A:865:TRP:HD1	1.88	0.56
3:B:159:VAL:HG21	3:B:317:HIS:CB	2.36	0.56
3:B:171:GLN:NE2	3:B:174:GLY:HA2	2.20	0.56
3:B:181:GLU:HG2	3:B:181:GLU:O	2.06	0.56
3:C:11:ILE:HB	3:C:16:PHE:HE1	1.70	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:759:SER:C	3:D:761:GLN:N	2.64	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:402:ASN:HA	3:C:886:ALA:O	2.06	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:D:386:HIS:HB3	3:D:387:PRO:HD2	1.87	0.56
3:D:749:ILE:HD11	3:D:883:PHE:CE1	2.41	0.56
2:F:104:DG:H2''	2:F:105:DC:H5'	1.88	0.56
3:A:37:LEU:HD21	3:A:72:ILE:HD11	1.87	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	3:D:561:LEU:N	2.20	0.55
2:F:110:DA:C8	2:F:111:DT:C7	2.89	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:61:LEU:N	3:D:61:LEU:HD12	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
1:E:3:3DR:H2"	1:E:4:DC:H5"	1.88	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
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
1:K:15:DC:H2"	1:K:16:DG:N7	2.21	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:25:ARG:HG2	3:C:27:ARG:NH2	2.22	0.55
3:C:164:ILE:HB	3:C:183:ILE:HD11	1.88	0.55
3:D:469:GLY:C	3:D:472:PRO:HD2	2.32	0.55
3:D:738:PRO:HG2	3:D:741:VAL:CG2	2.37	0.55
3:B:171:GLN:C	3:B:173:GLN:H	2.14	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:396:VAL:O	3:B:705:LYS:NZ	2.40	0.55
3:B:425:ILE:HG12	3:B:463:TYR:CZ	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:CD2	3:A:280:PHE:N	2.73	0.55
3:B:66:ARG:NH1	3:B:66:ARG:HB2	2.21	0.55
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:D:330:ARG:O	3:D:334:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:304:LYS:O	3:A:319:ARG:HD3	2.07	0.55
3:A:862:VAL:C	3:A:864:HIS:H	2.14	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:455:SER:OG	3:C:676:ASN:HA	2.07	0.55
3:C:489:MSE:HB2	3:C:552:GLY:HA3	1.89	0.55
3:D:92:TYR:CE2	3:D:96:THR:HG21	2.40	0.55
3:D:239:ALA:C	3:D:241:ARG:N	2.64	0.55
3:D:407:VAL:HG11	3:D:710:LEU:HD22	1.87	0.55
3:C:469:GLY:C	3:C:472:PRO:HD2	2.32	0.55
3:D:218:VAL:HA	3:D:222:ALA:CB	2.36	0.55
3:D:717:GLY:O	3:D:718:THR:C	2.48	0.55
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:H	3:B:83:LEU:HD12	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:A:112:ASN:HD22	3:A:112:ASN:C	2.14	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: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
3:A:36:SER:O	3:A:37:LEU:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:789:ALA:HA	3:A:792:ASP:HB2	1.90	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:C:818:ASN:C	3:C:818:ASN:ND2	2.58	0.54
3:D:434:PHE:CE1	3:D:456:CYS:HB3	2.42	0.54
3:B:185:LYS:HG3	3:B:185:LYS:O	2.08	0.53
3:D:732:THR:HG22	3:D:733:GLN:N	2.23	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:A:89:LYS:HB2	3:A:89:LYS:HZ2	1.73	0.53
3:B:108:ILE:HD13	3:B:345:LEU:HD21	1.91	0.53
2:F:105:DC:H2''	2:F:106:DT:C6	2.43	0.53
3:A:83:LEU:HB3	3:A:379:VAL:HG12	1.90	0.53
3:A:231:LYS:HG3	3:A:236:GLU:HA	1.90	0.53
3:B:137:THR:HG23	3:B:324:ASN:OD1	2.09	0.53
3:B:177:GLU:C	3:B:179:PRO:HD3	2.33	0.53
3:C:607:GLU:O	3:C:609:CYS:N	2.40	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
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:137:THR:HG23	3:B:324:ASN:CG	2.34	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
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:C:776:TYR:OH	3:C:853:GLU:OE1	2.26	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:176:ASP:OD2	3:B:319:ARG:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:84:GLY:C	3:D:380:ILE:HD11	2.34	0.53
3:D:560:LYS:HA	3:D:563:ILE:HG13	1.90	0.53
3:C:187:ILE:O	3:C:187:ILE:HG22	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
1:I:4:DC:H2"	1:I:5:DT:OP2	2.09	0.52
3:A:461:MSE:HE2	3:A:461:MSE:CA	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
3:D:327:ALA:C	3:D:329:TYR:N	2.64	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:143:ASP:O	3:B:144:ASP:C	2.52	0.52
3:B:218:VAL:HA	4:B:929:HOH:O	2.08	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:HB3	3:D:576:ARG:HH11	1.72	0.52
1:G:12:DA:N6	2:H:106:DT:H3	2.03	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
3:B:422:GLN:HE21	3:B:676:ASN:ND2	2.06	0.52
3:B:622:THR:O	3:B:623:ASP:CB	2.57	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:C:128:GLN:HE21	3:C:128:GLN:CA	2.22	0.52
3:D:373:LEU:C	3:D:375:GLU:H	2.16	0.52
3:D:380:ILE:HB	3:D:576:ARG:NH1	2.24	0.52
1:I:3:3DR:H1'2	4:C:1010:HOH:O	2.10	0.52
3:A:898:PHE:C	3:A:900:MSE:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:776:TYR:HB2	3:C:866:MSE:HE1	1.91	0.52
2:L:107:DG:N9	2:L:108:DT:C7	2.72	0.52
3:A:176:ASP:HA	3:A:319:ARG:HH21	1.75	0.52
3:A:895:ALA:O	3:A:896:SER:C	2.52	0.52
3:B:271:LEU:CD1	3:B:356:GLN:HA	2.40	0.52
3:B:276:LEU:O	3:B:280:PHE:HD2	1.93	0.52
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
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:53:TYR:CE2	3:C:428:GLU:HA	2.44	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:720:TYR:CD2	3:C:724:LYS:HG3	2.45	0.52
3:B:52:ILE:CG1	3:B:470:VAL:HG21	2.39	0.51
3:B:52:ILE:HG23	3:B:428:GLU:HB3	1.92	0.51
3:B:396:VAL:HG13	3:B:396:VAL:O	2.11	0.51
3:B:646:HIS:HD2	4:B:977:HOH:O	1.93	0.51
3:C:83:LEU:HB3	3:C:379:VAL:CG1	2.40	0.51
3:C:188:TYR:CD2	3:C:190:PRO:HD3	2.45	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:475:ILE:HD11	3:B:563:ILE:HG12	1.92	0.51
3:B:543:PHE:C	3:B:545:ALA:H	2.19	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:302:LYS:HZ2	3:C:302:LYS:CB	2.24	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:D:542:LEU:C	3:D:544:ARG:H	2.18	0.51
3:B:145:ARG:HB3	3:B:187:ILE:HD13	1.91	0.51
3:B:771:PHE:CD2	3:B:872:LEU:HD13	2.45	0.51
3:C:37:LEU:C	3:C:38:PHE:CD1	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:NH1	3:A:656:ARG:HB3	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:318:GLN:C	3:C:318:GLN:HE21	2.19	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
1:K:16:DG:H2''	1:K:17:DC:O5'	2.11	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
3:B:157:GLY:C	3:B:313:ARG:HH12	2.19	0.51
3:B:316:ASN:C	3:B:318:GLN:H	2.17	0.51
3:C:12:GLY:C	3:C:14:SER:H	2.18	0.51
3:A:491:ALA:C	3:A:493:GLN:H	2.19	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:HD12	3:D:863:LEU:N	2.26	0.51
3:B:406:TYR:N	4:B:923:HOH:O	2.44	0.51
3:C:413:THR:O	3:C:414:SER:C	2.54	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:C:457:SER:C	3:C:674:MSE:HE2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	3:C:170:LEU:HD12	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:D:320:TYR:C	3:D:322:SER:H	2.19	0.50
2:L:107:DG:C8	2:L:108:DT:C7	2.95	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
3:D:692:PRO:O	3:D:693:LEU:C	2.54	0.50
3:B:175:GLY:HA3	4:B:976:HOH:O	2.10	0.50
3:B:893:LYS:HE2	3:B:893:LYS:HA	1.93	0.50
3:D:872:LEU:O	3:D:874:LYS:N	2.37	0.50
1:K:15:DC:H2''	1:K:16:DG:C8	2.46	0.50
3:A:37:LEU:C	3:A:38:PHE:CD1	2.90	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:486:LYS:C	3:B:488:TYR:N	2.68	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:B:300:VAL:CG1	3:B:301:GLY:N	2.74	0.50
3:D:320:TYR:C	3:D:322:SER:N	2.67	0.50
3:A:130:LYS:HG3	3:A:131:HIS:CE1	2.46	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:B:631:LYS:HB2	3:B:631:LYS:HZ2	1.76	0.50
3:C:25:ARG:HG2	3:C:27:ARG:CZ	2.41	0.50
3:C:112:ASN:CB	3:C:214:THR:HG23	2.33	0.50
3:D:323:TYR:HB2	4:D:938:HOH:O	2.11	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: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:401:PRO:HA	3:B:702:TRP:O	2.12	0.50
3:B:541:MSE:HG2	3:B:544:ARG:HD2	1.93	0.50
3:A:581:ARG:CG	3:A:581:ARG:NH1	2.71	0.50
3:A:708:TYR:CZ	3:A:728:MSE:HG3	2.47	0.50
3:B:658:ARG:C	3:B:661:PRO:HD2	2.37	0.50
3:D:223:ILE:O	3:D:226:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C	3:A:861:ASP:H	2.18	0.49
3:B:272:ASP:CG	3:B:274:ILE:HG22	2.36	0.49
3:C:848:TRP:CE3	3:C:854:ILE:HD12	2.47	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:D:537:SER:C	3:D:539:ASN:H	2.19	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
3:B:593:ALA:O	3:B:597:ILE:HG13	2.12	0.49
3:C:411:ASP:CG	3:C:624:SER:HB3	2.37	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: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:O	3:A:541:MSE:SE	2.81	0.49
3:C:1:MSE:HG2	3:C:24:GLY:H	1.78	0.49
3:C:158:ASN:ND2	3:C:159:VAL:N	2.51	0.49
3:D:21:ASP:HB2	3:D:25:ARG:C	2.37	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:H	3:B:391:TYR:HD2	1.61	0.49
3:B:398:GLU:OE2	3:B:705:LYS:HE2	2.12	0.49
3:B:421:ARG:HD3	3:B:475:ILE:HG23	1.93	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:C:448:GLU:O	3:C:449:ARG:C	2.56	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:408:MSE:CE	3:B:688:ILE:HG12	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:181:GLU:OE1	3:C:181:GLU:N	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:H	3:D:863:LEU:CD1	2.25	0.49
3:D:864:HIS:C	3:D:866:MSE:H	2.19	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:N	3:B:147:TYR:CD1	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:A:556:GLN:C	3:A:556:GLN:NE2	2.71	0.49
3:B:413:THR:O	3:B:414:SER:C	2.56	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
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:A:357:SER:C	3:A:359:PHE:N	2.70	0.49
3:A:556:GLN:HE21	3:A:556:GLN:C	2.20	0.49
3:A:596:TRP:CE2	3:A:670:MSE:HB2	2.48	0.49
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:45:GLN:O	3:C:46:ALA:C	2.56	0.49
3:C:290:LEU:HD13	3:C:290:LEU:C	2.38	0.49
3:C:405:LYS:NZ	4:C:904:HOH:O	2.46	0.49
3:C:727:ILE:C	3:C:728:MSE:HE2	2.37	0.49
3:C:795:GLY:O	3:C:813:ARG:HD3	2.12	0.49
3:D:10:GLN:CB	3:D:65:MSE:HE1	2.43	0.49
3:D:72:ILE:O	3:D:76:GLU:HG3	2.13	0.49
3:D:85:MSE:CA	3:D:380:ILE:HD11	2.43	0.49
3:D:422:GLN:HG2	3:D:678:GLN:O	2.13	0.49
3:D:872:LEU:C	3:D:874:LYS:H	2.20	0.49
3:D:597:ILE:CD1	3:D:663:ILE:HG23	2.42	0.48
3:A:83:LEU:CD2	3:A:83:LEU:N	2.76	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:443:ILE:C	3:A:444:ASN:HD22	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:230:ILE:HD12	3:B:242:LEU:HD11	1.94	0.48
3:C:319:ARG:O	3:C:320:TYR:C	2.55	0.48
3:D:29:ARG:C	3:D:31:VAL:H	2.21	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: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
1:G:14:DC:H42	2:H:104:DG:H1	1.61	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
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:331:VAL:HG23	3:B:332:LEU:N	2.27	0.48
3:B:776:TYR:CD1	3:B:776:TYR:N	2.81	0.48
3:D:89:LYS:O	3:D:93:LEU:HG	2.14	0.48
3:D:261:GLU:O	3:D:262:ILE:C	2.56	0.48
1:E:3:3DR:OP1	3:A:361:PRO:HD2	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:C:897:LEU:HD23	3:C:897:LEU:C	2.38	0.48
3:D:87:ASP:O	3:D:88:PHE:HB2	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:423:VAL:HB	3:C:425:ILE:HG13	1.95	0.48
3:D:434:PHE:CE2	3:D:450:PRO:HB3	2.48	0.48
3:D:713:TRP:O	3:D:714:ASP:HB3	2.12	0.48
1:G:12:DA:C2'	1:G:13:DG:C5'	2.82	0.48
3:B:1:MSE:O	3:B:1:MSE:HG2	2.13	0.48
3:C:110:VAL:HG13	3:C:212:ILE:HB	1.95	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:D:241:ARG:O	3:D:243:SER:N	2.46	0.48
3:D:617:VAL:HG23	3:D:617:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:DG:H2''	1:G:10:DA:OP2	2.14	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:N	3:B:234:PHE:CD1	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
3:B:66:ARG:HG3	3:B:67:ASP:N	2.29	0.48
3:B:622:THR:O	3:B:623:ASP:OD1	2.32	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: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: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:44:SER:C	3:C:46:ALA:H	2.22	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
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:5:TYR:HA	3:D:19:TYR:HA	1.96	0.47
3:D:458:PRO:HG3	3:D:592:MSE:SE	2.64	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:C:12:GLY:C	3:C:14:SER:N	2.72	0.47
3:C:138:HIS:C	3:C:138:HIS:CD2	2.92	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:339:GLN:NE2	3:A:339:GLN:HA	2.29	0.47
3:B:165:GLU:O	3:B:166:ILE:C	2.57	0.47
3:B:229:ARG:NH1	3:B:233:ILE:HD11	2.28	0.47
3:C:170:LEU:HB2	4:C:1033:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:298:LEU:O	3:C:299:ASN:HB2	2.12	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: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:C:159:VAL:HG11	3:C:317:HIS:CG	2.49	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:255:ASN:C	3:C:257:TYR:N	2.73	0.47
3:D:619:TYR:CD1	3:D:619:TYR:C	2.92	0.47
3:B:19:TYR:HE1	3:B:29:ARG:HG2	1.79	0.47
3:B:212:ILE:HG22	3:B:212:ILE:O	2.14	0.47
3:B:405:LYS:HG3	3:B:691:PRO:HD3	1.97	0.47
3:B:471:VAL:N	3:B:472:PRO:HD2	2.29	0.47
3:B:893:LYS:HA	3:B:893:LYS:CE	2.45	0.47
3:C:83:LEU:HD22	3:C:83:LEU:N	2.30	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: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:B:443:ILE:HD13	3:B:595:GLN:CB	2.45	0.47
3:D:42:PRO:O	3:D:44:SER:N	2.48	0.47
3:D:92:TYR:C	3:D:92:TYR:CD2	2.93	0.47
3:D:302:LYS:O	3:D:326:ILE:HG21	2.14	0.47
3:D:862:VAL:O	3:D:864:HIS:N	2.48	0.47
1:I:1:DC:H4'	3:C:255:ASN:OD1	2.14	0.47
1:K:18:DG:O6	3:A:380:ILE:HG12	2.14	0.47
3:A:206:GLN:NE2	3:A:241:ARG:O	2.37	0.47
3:A:303:LEU:HB3	3:A:323:TYR:HD1	1.80	0.47
3:A:339:GLN:HA	3:A:339:GLN:HE21	1.80	0.47
3:A:347:MSE:HE2	3:A:558:ASN:OD1	2.14	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:290:LEU:HD13	3:B:302:LYS:HE3	1.97	0.47
3:B:604:TYR:O	3:B:607:GLU:HB3	2.15	0.47
3:B:702:TRP:CZ3	3:B:710:LEU:HD21	2.49	0.47
3:B:730:LEU:N	3:B:730:LEU:HD23	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:482:ARG:CZ	3:C:560:LYS:HD3	2.44	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:61:LEU:C	3:D:62:PHE:CD1	2.93	0.47
3:D:210:PRO:HD2	3:D:242:LEU:HD21	1.97	0.47
3:D:415:LEU:CD2	3:D:622:THR:HG23	2.41	0.47
3:D:422:GLN:CD	3:D:681:MSE:HE2	2.40	0.47
3:D:605:LEU:HD21	3:D:654:PHE:HE1	1.79	0.47
3:D:621:ASP:O	3:D:622:THR:C	2.57	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: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:N	3:D:635:LYS:HE3	2.29	0.47
2:J:112:DA:C5'	3:C:734:LYS:HG2	2.45	0.47
3:A:83:LEU:HD22	3:A:83:LEU:N	2.30	0.47
3:A:825:VAL:HB	3:A:828:GLU:CG	2.40	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:150:ASP:C	3:C:150:ASP:OD2	2.57	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
3:D:302:LYS:C	3:D:303:LEU:HD12	2.40	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:546:GLN:O	3:A:547:ARG:C	2.57	0.47
3:A:740:ALA:HB2	3:A:778:SER:HB2	1.96	0.47
3:B:216:TRP:H	3:B:218:VAL:HG23	1.80	0.47
3:C:70:GLN:HE21	3:C:70:GLN:CA	2.25	0.47
3:C:593:ALA:CB	3:C:681:MSE:CE	2.92	0.47
3:D:313:ARG:O	3:D:313:ARG:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:316:ASN:C	3:B:318:GLN:N	2.71	0.46
3:B:396:VAL:HG13	3:B:705:LYS:HZ1	1.76	0.46
3:C:130:LYS:C	3:C:131:HIS:ND1	2.73	0.46
3:A:92:TYR:C	3:A:92:TYR:CD1	2.93	0.46
3:B:116:GLU:HB3	3:B:320:TYR:OH	2.15	0.46
3:B:288:TYR:HD1	3:B:293:ILE:HD11	1.79	0.46
3:B:356:GLN:C	3:B:358:VAL:N	2.73	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:319:ARG:O	3:C:322:SER:N	2.47	0.46
3:C:436:VAL:HG23	3:C:436:VAL:O	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:H	2.23	0.46
3:C:173:GLN:CG	3:C:174:GLY:H	2.27	0.46
3:C:880:LEU:O	3:C:881:GLU:C	2.58	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:D:644:THR:C	3:D:646:HIS:H	2.23	0.46
3:A:329:TYR:CE2	3:A:333:GLN:NE2	2.83	0.46
3:A:485:HIS:C	3:A:487:GLY:H	2.23	0.46
3:B:437:ALA:HB1	3:B:438:PRO:CD	2.46	0.46
3:B:773:GLN:O	3:B:774:LEU:C	2.58	0.46
3:C:104:ASP:OD2	3:C:106:THR:HB	2.15	0.46
3:D:102:LYS:CD	3:D:103:TYR:H	2.26	0.46
3:D:539:ASN:C	3:D:541:MSE:H	2.23	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:B:103:TYR:H	3:B:103:TYR:HD1	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: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:A:854:ILE:O	3:A:855:THR:C	2.58	0.46
3:C:8:VAL:C	3:C:9:GLU:HG2	2.41	0.46
3:D:98:ASN:O	3:D:352:LYS:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:233:ILE:N	4:D:935:HOH:O	2.49	0.46
3:D:576:ARG:HH11	3:D:576:ARG:CB	2.29	0.46
3:D:765:LYS:C	3:D:767:PHE:H	2.23	0.46
3:D:444:ASN:HA	3:D:599:ARG:NE	2.31	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:610:GLY:HA2	4:A:1037:HOH:O	2.16	0.46
3:A:621:ASP:C	3:A:622:THR:HG23	2.40	0.46
3:A:855:THR:C	3:A:857:LEU:H	2.22	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:2:LYS:O	3:C:3:GLU:HB3	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:OE1	3:C:285:GLN:HA	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:353:ILE:HB	4:C:925:HOH:O	2.15	0.46
3:D:37:LEU:C	3:D:38:PHE:CD1	2.94	0.46
3:D:692:PRO:HG3	3:D:713:TRP:HZ2	1.81	0.46
3:D:756:GLY:C	3:D:758:GLU:H	2.23	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:B:567:TYR:O	3:B:568:GLY:C	2.59	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
1:K:16:DG:H2''	1:K:17:DC:C6	2.50	0.46
3:A:411:ASP:O	3:A:683:MSE:HA	2.16	0.46
3:B:53:TYR:CD1	3:B:53:TYR:N	2.84	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:C:685:ARG:NH1	3:C:688:ILE:HG13	2.31	0.46
3:D:3:GLU:HG2	3:D:22:SER:HA	1.98	0.46
3:D:216:TRP:CD1	3:D:290:LEU:HB2	2.50	0.46
1:I:8:DT:H2''	1:I:9:DG:H8	1.81	0.45
3:A:858:ILE:O	3:A:859:LYS:O	2.33	0.45
3:B:183:ILE:H	3:B:183:ILE:CD1	2.26	0.45
3:C:144:ASP:OD2	3:C:185:LYS:HD3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:176:ASP:OD1	3:C:318:GLN:NE2	2.49	0.45
3:C:245:HIS:O	3:C:246:ARG:C	2.59	0.45
3:C:697:GLY:HA2	3:C:755:GLU:O	2.15	0.45
3:D:4:PHE:H	3:D:20:ILE:HB	1.81	0.45
3:D:109:ARG:O	3:D:109:ARG:HD2	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:A:71:TRP:O	3:A:75:MSE:HB2	2.16	0.45
3:A:112:ASN:C	3:A:112:ASN:ND2	2.74	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:83:LEU:H	3:C:83:LEU:CD2	2.30	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: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:344:SER:O	3:B:345:LEU:C	2.59	0.45
3:B:490:LEU:O	3:B:491:ALA:C	2.59	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:9:GLU:HA	3:A:89:LYS:HD3	1.98	0.45
3:A:20:ILE:HG23	3:A:24:GLY:HA2	1.97	0.45
3:A:162:TRP:CH2	3:A:164:ILE:HG23	2.51	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: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:397:LYS:HE2	3:B:598:GLU:OE1	2.17	0.45
3:B:458:PRO:HG3	3:B:592:MSE:SE	2.66	0.45
3:C:136:ILE:HB	3:C:149:PHE:HB2	1.98	0.45
3:C:373:LEU:O	3:C:374:LYS:C	2.60	0.45
3:C:395:PHE:HB2	3:C:591:GLN:HG2	1.97	0.45
3:C:416:TYR:N	3:C:416:TYR:CD2	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
1:G:12:DA:H2"	1:G:13:DG:H5"	1.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:21:ASP:C	3:A:23:ASN:H	2.24	0.45
3:A:391:TYR:CZ	3:A:583:ALA:HB1	2.51	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
3:B:775:ASN:HB3	4:B:982:HOH:O	2.16	0.45
3:C:186:ILE:C	3:C:187:ILE:HG13	2.42	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
2:L:107:DG:H2'	2:L:108:DT:H71	1.85	0.45
3:A:19:TYR:CE1	3:A:29:ARG:HG2	2.52	0.45
3:C:437:ALA:O	3:C:438:PRO:C	2.58	0.45
3:C:437:ALA:O	3:C:442:TYR:HE2	1.99	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
3:D:437:ALA:O	3:D:438:PRO:C	2.59	0.45
4:E:366:HOH:O	3:A:806:ARG:HD2	2.16	0.45
3:A:408:MSE:CE	3:A:685:ARG:HD2	2.46	0.45
3:A:859:LYS:C	3:A:861:ASP:N	2.74	0.45
3:B:200:GLU:O	3:B:201:TYR:C	2.60	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:83:LEU:HD12	3:B:83:LEU:N	2.32	0.45
3:B:256:MSE:SE	3:B:256:MSE:C	3.10	0.45
3:B:489:MSE:SE	3:B:553:MSE:SE	3.34	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:273:TYR:O	3:D:274:ILE:C	2.60	0.45
3:D:597:ILE:CG1	3:D:683:MSE:HE1	2.47	0.45
1:K:15:DC:N4	2:L:102:DC:N4	2.65	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:C:578:TYR:CD1	3:C:578:TYR:C	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:47:THR:C	3:D:49:TYR:H	2.25	0.45
3:D:705:LYS:C	3:D:707:ARG:N	2.75	0.45
3:A:634:ASP:C	3:A:636:VAL:N	2.72	0.45
3:A:653:LYS:O	3:A:654:PHE:C	2.60	0.45
3:A:697:GLY:HA3	3:A:753:LEU:O	2.16	0.45
3:A:834:PRO:O	3:A:866:MSE:HA	2.17	0.45
3:A:854:ILE:CG1	3:A:859:LYS:HB2	2.46	0.45
3:B:227:TYR:CE1	3:B:239:ALA:HB1	2.52	0.45
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:A:366:ASP:CG	3:A:576:ARG:HH11	2.25	0.44
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
1:I:8:DT:H2"	1:I:9:DG:C8	2.52	0.44
3:A:681:MSE:HE2	3:A:681:MSE:HA	1.99	0.44
3:B:548:THR:O	3:B:548:THR:HG22	2.17	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
3:D:877:ILE:O	3:D:878:LYS:C	2.60	0.44
3:B:324:ASN:C	3:B:324:ASN:HD22	2.26	0.44
3:B:394:ALA:HB1	3:B:622:THR:CB	2.41	0.44
3:B:421:ARG:HB3	3:B:680:LEU:CD1	2.46	0.44
3:C:97:TYR:C	3:C:99:TYR:H	2.26	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:D:35:PRO:HG3	3:D:65:MSE:HA	2.00	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:692:PRO:HG3	3:D:713:TRP:CZ2	2.52	0.44
3:A:369:ILE:HG12	3:A:474:GLU:HG3	1.98	0.44
3:B:2:LYS:HD3	3:B:2:LYS:HA	1.87	0.44
3:B:154:SER:C	3:B:156:TYR:N	2.61	0.44
3:B:544:ARG:HH11	3:B:544:ARG:HB2	1.82	0.44
3:B:775:ASN:O	3:B:776:TYR:C	2.61	0.44
3:C:11:ILE:HB	3:C:16:PHE:CE1	2.51	0.44
3:C:51:ASP:C	3:C:51:ASP:OD1	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:296:PHE:C	3:A:296:PHE:CD2	2.95	0.44
3:A:805:ILE:O	3:A:808:ILE:HB	2.17	0.44
3:B:279:LYS:O	3:B:279:LYS:HG2	2.17	0.44
3:B:321:ILE:N	3:B:321:ILE:CD1	2.80	0.44
3:B:433:THR:HG23	3:B:433:THR:O	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
3:C:289:SER:O	3:C:290:LEU:C	2.61	0.44
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:OE1	3:B:116:GLU:HA	2.17	0.44
3:B:276:LEU:O	3:B:280:PHE:CD2	2.71	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:362:ILE:HD11	3:C:572:ASN:CG	2.42	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:553:MSE:C	3:A:555:ALA:H	2.26	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:A:486:LYS:O	3:A:486:LYS:HG2	2.18	0.44
3:A:547:ARG:HG3	3:A:548:THR:HG23	2.00	0.44
3:B:145:ARG:HH11	3:B:145:ARG:HG3	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:HA	3:C:206:GLN:HE21	1.83	0.44
3:C:731:GLU:CD	3:C:731:GLU:H	2.25	0.44
3:D:50:PHE:O	3:D:379:VAL:HG23	2.17	0.44
3:D:362:ILE:O	3:D:363:LYS:C	2.60	0.44
3:D:578:TYR:CD1	3:D:579:ASP:N	2.86	0.44
3:A:408:MSE:CE	3:A:655:ALA:HB2	2.40	0.44
3:A:471:VAL:N	3:A:472:PRO:HD2	2.32	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:313:ARG:HD2	3:D:313:ARG:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:368:ILE:O	3:D:369:ILE:C	2.60	0.44
3:D:581:ARG:CG	3:D:581:ARG:NH1	2.78	0.44
3:D:622:THR:O	3:D:623:ASP:OD1	2.36	0.44
1:E:7:DA:H2''	1:E:8:DT:OP2	2.18	0.43
3:A:398:GLU:OE1	3:A:705:LYS:HE3	2.18	0.43
3:A:642:ARG:HE	3:A:646:HIS:CE1	2.36	0.43
3:A:752:MSE:CG	3:A:760:LEU:HD22	2.48	0.43
3:A:896:SER:C	3:A:898:PHE:H	2.26	0.43
3:B:243:SER:O	3:B:244:PRO:C	2.60	0.43
3:C:55:LYS:N	3:C:55:LYS:HD2	2.32	0.43
3:C:127:SER:O	3:C:128:GLN:NE2	2.51	0.43
3:C:313:ARG:C	3:C:315:SER:N	2.75	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
2:H:115:DA:H5'	3:B:221:PHE:CE2	2.53	0.43
1:I:7:DA:H2''	1:I:8:DT:O5'	2.19	0.43
3:A:83:LEU:CD2	3:A:83:LEU:H	2.29	0.43
3:B:322:SER:O	3:B:326:ILE:HG12	2.18	0.43
3:B:488:TYR:C	3:B:490:LEU:N	2.74	0.43
3:C:700:GLY:HA2	3:C:753:LEU:HD21	1.96	0.43
3:D:32:GLU:H	3:D:32:GLU:CD	2.25	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
3:A:164:ILE:HG12	4:A:913:HOH:O	2.19	0.43
3:B:135:ALA:C	3:B:136:ILE:HD12	2.43	0.43
3:B:171:GLN:C	3:B:173:GLN:N	2.76	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:D:43:GLU:CD	3:D:43:GLU:N	2.75	0.43
2:F:108:DT:H1'	2:F:109:DC:H5''	1.99	0.43
3:B:135:ALA:HB1	3:B:324:ASN:OD1	2.18	0.43
3:B:324:ASN:C	3:B:324:ASN:ND2	2.76	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
3:D:244:PRO:C	3:D:246:ARG:N	2.74	0.43
3:D:715:MSE:O	3:D:716:GLU:C	2.61	0.43
2:F:111:DT:C2'	2:F:112:DA:H5''	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:DA:O3'	3:B:117:VAL:HG22	2.19	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
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:HG3	3:C:313:ARG:NH1	2.34	0.43
3:C:863:LEU:CA	3:C:866:MSE:HE3	2.33	0.43
3:D:196:GLU:C	3:D:198:LEU:H	2.25	0.43
3:D:212:ILE:O	3:D:212:ILE:CG2	2.62	0.43
3:D:212:ILE:HD11	3:D:345:LEU:HD21	2.01	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
3:D:861:ASP:C	3:D:861:ASP:OD2	2.60	0.43
3:A:36:SER:HA	3:A:60:LYS:O	2.17	0.43
3:A:154:SER:C	3:A:156:TYR:N	2.74	0.43
3:A:162:TRP:HB3	3:A:188:TYR:CZ	2.53	0.43
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:73:LYS:HA	4:B:986:HOH:O	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: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:O	3:B:871:LEU:HD12	2.18	0.43
3:C:15:ILE:HG13	3:C:65:MSE:HE1	2.01	0.43
3:C:49:TYR:CE1	3:C:59:ARG:HB2	2.54	0.43
3:C:426:SER:CB	3:C:428:GLU:OE2	2.66	0.43
3:C:542:LEU:N	3:C:542:LEU:HD12	2.34	0.43
3:C:706:LYS:C	3:C:707:ARG:HG2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:87:ASP:C	3:D:89:LYS:H	2.27	0.43
3:D:205:TRP:HA	4:D:936:HOH:O	2.19	0.43
2:J:112:DA:H2"	2:J:113:DA:H8	1.77	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:182:ILE:C	3:C:182:ILE:HD12	2.43	0.43
3:C:233:ILE:HG22	3:C:234:PHE:CD1	2.54	0.43
3:C:493:GLN:O	3:C:494:ARG:C	2.61	0.43
3:C:668:ARG:NH1	3:C:668:ARG:CG	2.78	0.43
3:D:292:TYR:O	3:D:293:ILE:C	2.62	0.43
3:D:556:GLN:N	4:D:918:HOH:O	2.52	0.43
3:D:563:ILE:HG13	3:D:563:ILE:H	1.48	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:C:154:SER:C	3:C:156:TYR:N	2.73	0.43
3:C:815:ILE:O	3:C:815:ILE:HG22	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:A:858:ILE:C	3:A:859:LYS:O	2.61	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
3:D:711:ASN:O	3:D:712:VAL:C	2.62	0.43
3:D:770:GLU:O	3:D:774:LEU:HB2	2.19	0.43
2:J:102:DC:H2"	2:J:103:DG:C8	2.55	0.42
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:221:PHE:C	3:B:224:PRO:HD2	2.43	0.42
3:B:351:ALA:O	3:B:352:LYS:HB2	2.18	0.42
3:B:398:GLU:OE2	3:B:398:GLU:HA	2.19	0.42
3:B:557:ILE:O	3:B:560:LYS:HB3	2.19	0.42
3:C:83:LEU:HB3	3:C:379:VAL:HG12	2.01	0.42
3:C:380:ILE:CG2	3:C:576:ARG:HD3	2.43	0.42
3:C:541:MSE:O	3:C:544:ARG:HG3	2.19	0.42
3:C:760:LEU:CD2	3:C:760:LEU:C	2.92	0.42
3:C:818:ASN:CG	3:C:857:LEU:HD11	2.44	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:A:51:ASP:HB2	4:A:919:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	3:D:406:TYR:N	2.86	0.42
3:D:888:LYS:O	3:D:888:LYS:HG3	2.19	0.42
2:F:105:DC:C2'	2:F:106:DT:H71	2.49	0.42
3:A:214:THR:OG1	3:A:215:GLY:N	2.50	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:N	3:B:391:TYR:CD2	2.88	0.42
3:D:290:LEU:C	3:D:293:ILE:HG22	2.42	0.42
3:D:660:GLU:O	3:D:661:PRO:C	2.62	0.42
3:A:651:LEU:HD23	3:A:651:LEU:HA	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:416:TYR:O	3:C:417:PRO:C	2.63	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:64:ASN:O	3:D:68:ALA:N	2.52	0.42
3:D:327:ALA:C	3:D:329:TYR:H	2.26	0.42
3:A:6:LEU:CD2	3:A:108:ILE:HG12	2.49	0.42
3:C:7:THR:OG1	3:C:18:ARG:HD3	2.19	0.42
3:C:302:LYS:CB	3:C:302:LYS:NZ	2.82	0.42
3:C:486:LYS:O	3:C:490:LEU:HG	2.20	0.42
3:D:14:SER:O	3:D:16:PHE:N	2.52	0.42
3:D:311:LYS:C	3:D:313:ARG:H	2.27	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: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:275:ASP:O	3:B:276:LEU:C	2.61	0.42
3:B:465:LYS:O	3:B:677:LYS:HE3	2.19	0.42
3:C:8:VAL:O	3:C:9:GLU:HG2	2.19	0.42
3:C:290:LEU:HD13	3:C:290:LEU:O	2.19	0.42
3:C:394:ALA:HB1	3:C:622:THR:HA	2.01	0.42
3:C:450:PRO:O	3:C:451:SER:HB2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:578:TYR:CD1	3:D:578:TYR:C	2.97	0.42
3:D:606:ASN:O	3:D:611:THR:N	2.53	0.42
3:D:658:ARG:C	3:D:661:PRO:HD2	2.45	0.42
3:D:738:PRO:O	3:D:739:LYS:C	2.62	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:301:GLY:C	3:B:303:LEU:N	2.78	0.42
3:B:720:TYR:CZ	3:B:724:LYS:HD2	2.54	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:51:ASP:HB2	3:D:52:ILE:HD12	2.02	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:616:PHE:O	3:D:627:VAL:HA	2.20	0.42
1:I:13:DG:H5'	3:C:800:LYS:HG2	2.00	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:B:739:LYS:O	3:B:742:GLN:HB2	2.20	0.42
3:C:90:LEU:HD11	3:C:353:ILE:HG22	2.02	0.42
3:C:104:ASP:C	3:C:106:THR:N	2.76	0.42
3:C:772:ARG:HH11	3:C:772:ARG:HG3	1.83	0.42
2:L:101:DG:C3'	2:L:102:DC:H5''	2.47	0.42
3:A:105:HIS:ND1	3:A:106:THR:N	2.67	0.42
3:A:138:HIS:C	3:A:138:HIS:CD2	2.97	0.42
3:B:136:ILE:O	3:B:148:VAL:HA	2.20	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:216:TRP:CZ2	3:B:293:ILE:HD12	2.55	0.42
3:B:326:ILE:O	3:B:327:ALA:C	2.62	0.42
3:C:414:SER:O	3:C:415:LEU:C	2.63	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:434:PHE:O	3:D:435:LYS:C	2.62	0.42
3:D:776:TYR:CD1	3:D:777:ILE:N	2.88	0.42
3:A:309:ILE:HB	4:A:917:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:443:ILE:C	3:A:444:ASN:ND2	2.78	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: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:C:55:LYS:N	3:C:55:LYS:CD	2.83	0.42
3:C:253:ILE:HB	3:C:260:ARG:HB2	2.02	0.42
3:A:410:PHE:CD2	3:A:685:ARG:HA	2.55	0.41
3:A:708:TYR:CD2	3:A:708:TYR:C	2.98	0.41
3:A:848:TRP:CE2	3:A:854:ILE:HG22	2.54	0.41
3:B:52:ILE:HD11	3:B:373:LEU:HD21	2.01	0.41
3:B:186:ILE:O	3:B:187:ILE:C	2.63	0.41
3:B:304:LYS:C	3:B:305:TYR:CD2	2.98	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:896:SER:HG	3:B:898:PHE:HD2	1.67	0.41
3:C:85:MSE:HB2	3:C:370:PHE:CE2	2.56	0.41
3:C:163:SER:HB3	3:C:318:GLN:OE1	2.20	0.41
3:C:412:LEU:CD2	3:C:683:MSE:HB2	2.50	0.41
3:C:495:ASN:N	3:C:495:ASN:ND2	2.54	0.41
3:D:278:LYS:C	3:D:280:PHE:H	2.28	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:A:197:LEU:C	3:A:197:LEU:CD1	2.93	0.41
3:A:757:GLU:HB2	3:A:889:LEU:HD22	2.02	0.41
3:A:802:PRO:HG2	3:A:805:ILE:HD12	2.02	0.41
3:B:36:SER:HA	3:B:60:LYS:O	2.20	0.41
3:B:231:LYS:CB	4:B:915:HOH:O	2.68	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
3:D:285:GLN:N	3:D:285:GLN:OE1	2.53	0.41
3:A:32:GLU:CD	3:A:32:GLU:N	2.76	0.41
3:A:163:SER:HA	4:A:913:HOH:O	2.19	0.41
3:A:326:ILE:HD13	3:A:326:ILE:HA	1.90	0.41
3:B:51:ASP:OD1	3:B:51:ASP:C	2.63	0.41
3:B:70:GLN:HA	3:B:70:GLN:OE1	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:PHE:C	3:C:224:PRO:HD2	2.44	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:410:PHE:CD2	3:D:685:ARG:HA	2.55	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:A:115:ILE:HA	3:A:115:ILE:HD13	1.82	0.41
3:A:757:GLU:O	3:A:761:GLN:HG3	2.20	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
1:I:4:DC:H2"	1:I:5:DT:H71	2.03	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:HG	3:B:594:LEU:O	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:HG2	3:C:59:ARG:HH11	1.85	0.41
3:C:593:ALA:HA	3:C:670:MSE:SE	2.70	0.41
3:A:261:GLU:O	3:A:261:GLU:HG3	2.19	0.41
3:A:656:ARG:CB	3:A:656:ARG:HH11	2.33	0.41
3:A:837:GLU:OE1	3:A:837:GLU:HA	2.20	0.41
3:B:42:PRO:CG	3:B:45:GLN:HG2	2.49	0.41
3:B:149:PHE:HB3	3:B:197:LEU:CG	2.51	0.41
3:B:702:TRP:CD1	3:B:708:TYR:HB3	2.56	0.41
3:B:899:ASP:OD2	3:B:899:ASP:N	2.53	0.41
3:D:289:SER:O	3:D:290:LEU:C	2.63	0.41
3:D:293:ILE:CG2	3:D:294:SER:N	2.83	0.41
3:D:719:ARG:O	3:D:720:TYR:C	2.62	0.41
1:E:4:DC:N3	2:F:114:DG:O6	2.53	0.41
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:A:855:THR:C	3:A:857:LEU:N	2.78	0.41
3:B:121:ASP:OD2	3:B:121:ASP:N	2.54	0.41
3:B:143:ASP:OD2	3:B:208:LYS:CE	2.69	0.41
3:B:202:LEU:O	3:B:205:TRP:HB3	2.20	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:C:605:LEU:HD23	3:C:605:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:201:TYR:O	3:A:204:PHE:HB3	2.21	0.41
3:A:350:TYR:CD2	3:A:350:TYR:C	2.98	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:C:276:LEU:HD23	3:C:276:LEU:HA	1.93	0.41
3:D:85:MSE:HE1	3:D:87:ASP:N	2.36	0.41
3:D:85:MSE:CE	3:D:87:ASP:N	2.83	0.41
3:D:597:ILE:HG12	3:D:683:MSE:HE1	2.03	0.41
3:D:776:TYR:C	3:D:778:SER:N	2.77	0.41
1:G:8:DT:H2''	1:G:9:DG:OP2	2.20	0.41
2:H:108:DT:H2''	2:H:109:DC:H5'	1.98	0.41
3:A:6:LEU:HB2	3:A:18:ARG:O	2.21	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:A:365:TRP:CD2	3:A:566:LEU:HD13	2.56	0.41
3:A:862:VAL:C	3:A:864:HIS:N	2.76	0.41
3:B:5:TYR:HB3	3:B:97:TYR:CE2	2.56	0.41
3:B:178:VAL:HB	4:B:991:HOH:O	2.21	0.41
3:B:231:LYS:O	3:B:232:ASN:C	2.64	0.41
3:B:236:GLU:C	3:B:238:THR:H	2.29	0.41
3:B:304:LYS:C	3:B:305:TYR:HD2	2.29	0.41
3:B:407:VAL:HG11	3:B:710:LEU:HD22	2.02	0.41
3:B:438:PRO:HD2	3:B:441:ASP:CG	2.44	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
3:C:482:ARG:NH2	3:C:560:LYS:HD3	2.36	0.41
3:C:659:MSE:O	3:C:660:GLU:C	2.64	0.41
3:C:815:ILE:HG23	3:C:821:ALA:HB3	2.03	0.41
3:D:8:VAL:O	3:D:354:GLN:NE2	2.54	0.41
3:D:92:TYR:C	3:D:92:TYR:HD2	2.28	0.41
3:D:216:TRP:HH2	3:D:293:ILE:HG12	1.85	0.41
3:D:344:SER:O	3:D:345:LEU:C	2.64	0.41
3:D:426:SER:O	3:D:427:PRO:C	2.64	0.41
3:D:750:ARG:O	3:D:751:ARG:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:581:ARG:HG3	3:A:581:ARG:NH1	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:C:89:LYS:HZ2	3:C:354:GLN:HE22	1.64	0.41
3:C:330:ARG:HD3	3:C:330:ARG:HA	1.74	0.41
3:D:468:ASP:HB3	3:D:473:THR:OG1	2.21	0.41
3:D:539:ASN:C	3:D:541:MSE:N	2.77	0.41
3:D:655:ALA:CA	3:D:659:MSE:HB2	2.41	0.41
2:F:104:DG:H2''	2:F:105:DC:C5'	2.51	0.40
3:A:414:SER:O	3:A:415:LEU:C	2.64	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:704:GLY:O	3:B:705:LYS:C	2.65	0.40
3:C:140:ASP:OD1	3:C:142:ILE:N	2.53	0.40
3:C:589:PHE:C	3:C:589:PHE:CD1	2.98	0.40
3:D:28:THR:O	3:D:29:ARG:CB	2.68	0.40
3:D:294:SER:C	3:D:296:PHE:N	2.77	0.40
3:D:697:GLY:HA3	3:D:756:GLY:HA2	2.03	0.40
2:J:105:DC:H2'	2:J:106:DT:C7	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:164:ILE:O	3:B:165:GLU:C	2.64	0.40
3:B:178:VAL:O	3:B:178:VAL:HG23	2.21	0.40
3:C:254:GLU:CD	3:C:258:GLY:HA3	2.46	0.40
3:C:779:ILE:O	3:C:871:LEU:HD21	2.20	0.40
3:D:37:LEU:HD22	3:D:71:TRP:CZ3	2.55	0.40
3:D:373:LEU:N	3:D:373:LEU:CD1	2.84	0.40
3:D:630:ASP:O	3:D:633:ILE:HG22	2.21	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:863:LEU:HD12	3:A:866:MSE:CE	2.51	0.40
3:B:73:LYS:HG3	4:B:986:HOH:O	2.20	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
3:B:715:MSE:O	3:B:716:GLU:HB2	2.21	0.40
3:C:206:GLN:HA	3:C:206:GLN:NE2	2.36	0.40
3:C:720:TYR:CG	3:C:724:LYS:HG3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:85:MSE:HE1	3:D:87:ASP:H	1.85	0.40
3:D:318:GLN:C	3:D:320:TYR:H	2.30	0.40
3:D:644:THR:CG2	3:D:692:PRO:HA	2.52	0.40
3:D:767:PHE:O	3:D:768:GLU:C	2.64	0.40
3:A:167:ALA:O	3:A:177:GLU:N	2.54	0.40
3:B:27:ARG:HH11	3:B:27:ARG:HG3	1.86	0.40
3:B:113:PHE:CE1	3:B:213:LEU:HD11	2.57	0.40
3:B:340:PHE:O	3:B:343:LEU:HB3	2.20	0.40
3:B:364:THR:HG21	3:B:562:LEU:HD21	2.03	0.40
3:B:426:SER:O	3:B:429:THR:OG1	2.36	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:B:878:LYS:O	3:B:879:PRO:C	2.63	0.40
3:C:104:ASP:CG	3:C:106:THR:HB	2.46	0.40
3:C:124:PRO:O	3:C:125:GLU:C	2.63	0.40
3:C:170:LEU:CD1	3:C:170:LEU:N	2.84	0.40
3:C:384:ARG:HH11	3:C:384:ARG:HG2	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:104:ASP:O	3:A:105:HIS:C	2.63	0.40
3:A:621:ASP:C	3:A:622:THR:CG2	2.93	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: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:C:235:GLY:O	3:C:236:GLU:C	2.62	0.40
3:C:607:GLU:O	3:C:608:VAL:C	2.64	0.40
3:D:42:PRO:HG2	3:D:44:SER:HB2	2.04	0.40
3:D:205:TRP:N	4:D:946:HOH:O	2.55	0.40
3:D:577:TYR:CD1	3:D:577:TYR:N	2.90	0.40
3:D:756:GLY:C	3:D:758:GLU:N	2.79	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%)	6	22
3	B	763/903 (84%)	621 (81%)	110 (14%)	32 (4%)	2	7
3	C	849/903 (94%)	745 (88%)	74 (9%)	30 (4%)	3	10
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	6

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	700 (94%)	45 (6%)	17	47
3	B	663/775 (86%)	608 (92%)	55 (8%)	10	32
3	C	737/775 (95%)	692 (94%)	45 (6%)	17	46
3	D	453/775 (58%)	419 (92%)	34 (8%)	12	37
All	All	2598/3100 (84%)	2419 (93%)	179 (7%)	14	41

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	MSE
3	A	22	SER
3	A	32	GLU
3	A	34	LYS
3	A	58	THR
3	A	60	LYS
3	A	66	ARG
3	A	83	LEU
3	A	89	LYS
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

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Mol	Chain	Res	Type
3	A	254	GLU
3	A	304	LYS
3	A	461	MSE
3	A	466	ASP
3	A	475	ILE
3	A	549	GLU
3	A	553	MSE
3	A	556	GLN
3	A	581	ARG
3	A	592	MSE
3	A	622	THR
3	A	632	ILE
3	A	633	ILE
3	A	635	LYS
3	A	645	ASN
3	A	672	GLU
3	A	681	MSE
3	A	683	MSE
3	A	731	GLU
3	A	743	LYS
3	A	758	GLU
3	A	781	SER
3	A	819	ILE
3	A	854	ILE
3	A	855	THR
3	A	861	ASP
3	A	897	LEU
3	B	2	LYS
3	B	15	ILE
3	B	22	SER
3	B	27	ARG
3	B	29	ARG
3	B	52	ILE
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	160	GLU

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Mol	Chain	Res	Type
3	B	164	ILE
3	B	165	GLU
3	B	181	GLU
3	B	183	ILE
3	B	184	ASP
3	B	187	ILE
3	B	233	ILE
3	B	234	PHE
3	B	252	VAL
3	B	256	MSE
3	B	290	LEU
3	B	295	GLU
3	B	303	LEU
3	B	305	TYR
3	B	311	LYS
3	B	319	ARG
3	B	347	MSE
3	B	362	ILE
3	B	391	TYR
3	B	407	VAL
3	B	413	THR
3	B	421	ARG
3	B	436	VAL
3	B	493	GLN
3	B	495	ASN
3	B	597	ILE
3	B	618	LEU
3	B	622	THR
3	B	623	ASP
3	B	631	LYS
3	B	643	ASP
3	B	645	ASN
3	B	672	GLU
3	B	681	MSE
3	B	685	ARG
3	B	722	GLU
3	B	747	GLU
3	B	768	GLU
3	B	776	TYR
3	B	893	LYS
3	C	15	ILE
3	C	23	ASN

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Mol	Chain	Res	Type
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	131	HIS
3	C	153	ASN
3	C	158	ASN
3	C	183	ILE
3	C	194	GLU
3	C	217	ASN
3	C	255	ASN
3	C	257	TYR
3	C	265	LEU
3	C	291	ASP
3	C	299	ASN
3	C	302	LYS
3	C	318	GLN
3	C	363	LYS
3	C	391	TYR
3	C	402	ASN
3	C	422	GLN
3	C	428	GLU
3	C	436	VAL
3	C	439	LEU
3	C	440	HIS
3	C	441	ASP
3	C	475	ILE
3	C	479	PHE
3	C	495	ASN
3	C	548	THR
3	C	562	LEU
3	C	597	ILE
3	C	618	LEU
3	C	674	MSE
3	C	731	GLU
3	C	732	THR
3	C	760	LEU
3	C	799	PRO
3	C	829	LYS

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Mol	Chain	Res	Type
3	C	833	LEU
3	D	9	GLU
3	D	17	GLU
3	D	43	GLU
3	D	52	ILE
3	D	70	GLN
3	D	85	MSE
3	D	102	LYS
3	D	197	LEU
3	D	204	PHE
3	D	242	LEU
3	D	265	LEU
3	D	285	GLN
3	D	292	TYR
3	D	302	LYS
3	D	305	TYR
3	D	331	VAL
3	D	346	ASP
3	D	362	ILE
3	D	403	ARG
3	D	422	GLN
3	D	449	ARG
3	D	458	PRO
3	D	479	PHE
3	D	556	GLN
3	D	563	ILE
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	40	HIS
3	A	98	ASN
3	A	112	ASN

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Mol	Chain	Res	Type
3	A	153	ASN
3	A	255	ASN
3	A	339	GLN
3	A	354	GLN
3	A	356	GLN
3	A	376	GLN
3	A	422	GLN
3	A	444	ASN
3	A	481	GLN
3	A	493	GLN
3	A	556	GLN
3	A	564	ASN
3	A	591	GLN
3	A	645	ASN
3	A	773	GLN
3	B	10	GLN
3	B	23	ASN
3	B	45	GLN
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	354	GLN
3	B	386	HIS
3	B	389	GLN
3	B	424	ASN
3	B	444	ASN
3	B	481	GLN
3	B	493	GLN
3	B	495	ASN
3	B	556	GLN
3	B	595	GLN
3	B	645	ASN
3	B	646	HIS
3	B	676	ASN
3	B	733	GLN
3	B	742	GLN
3	C	23	ASN
3	C	45	GLN

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Mol	Chain	Res	Type
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	232	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	377	ASN
3	C	402	ASN
3	C	422	GLN
3	C	424	ASN
3	C	485	HIS
3	C	495	ASN
3	C	546	GLN
3	C	556	GLN
3	C	564	ASN
3	C	582	ASN
3	C	679	HIS
3	C	818	ASN
3	D	70	GLN
3	D	333	GLN
3	D	342	ASN
3	D	354	GLN
3	D	606	ASN
3	D	675	ASN
3	D	676	ASN
3	D	679	HIS
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	0.33	0	7,14,17	0.83	0
1	3DR	I	3	1	8,11,12	0.31	0	7,14,17	0.87	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	-	1/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	3	3DR	O4'-C4'-C5'-O5'

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	E	17/18 (94%)	1.10	5 (29%) 1 1	57, 95, 121, 134	0
1	G	13/18 (72%)	1.71	5 (38%) 1 0	48, 103, 143, 144	0
1	I	17/18 (94%)	0.14	3 (17%) 4 3	27, 43, 112, 123	0
1	K	9/18 (50%)	1.72	5 (55%) 0 0	38, 140, 155, 159	0
2	F	15/15 (100%)	1.41	4 (26%) 1 1	77, 104, 136, 140	0
2	H	15/15 (100%)	1.80	7 (46%) 0 0	75, 118, 131, 139	0
2	J	15/15 (100%)	0.59	3 (20%) 3 2	28, 57, 97, 114	0
2	L	8/15 (53%)	2.11	5 (62%) 0 0	144, 148, 149, 149	0
3	A	831/903 (92%)	0.15	24 (2%) 53 43	16, 40, 83, 133	0
3	B	746/903 (82%)	0.80	104 (13%) 6 5	19, 57, 112, 140	0
3	C	829/903 (91%)	0.29	25 (3%) 52 42	18, 46, 86, 119	0
3	D	650/903 (71%)	1.77	238 (36%) 1 0	78, 102, 134, 142	0
All	All	3165/3744 (84%)	0.71	428 (13%) 7 5	16, 56, 123, 159	0

All (428) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	896	SER	6.9
3	B	779	ILE	6.2
3	D	90	LEU	5.7
3	D	216	TRP	5.5
3	D	569	ALA	5.2
3	D	242	LEU	5.2
3	D	450	PRO	5.0
2	J	115	DA	4.7
3	B	290	LEU	4.6
3	D	48	LYS	4.5
3	B	122	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
3	A	543	PHE	4.4
3	B	901	PHE	4.4
3	D	309	ILE	4.4
3	B	252	VAL	4.4
3	D	17	GLU	4.3
3	D	340	PHE	4.3
3	D	465	LYS	4.3
3	C	542	LEU	4.3
3	D	308	PRO	4.1
3	B	137	THR	4.1
3	D	46	ALA	4.1
3	B	160	GLU	4.0
3	B	198	LEU	4.0
3	A	902	ASP	3.9
3	D	410	PHE	3.9
3	D	252	VAL	3.9
3	B	155	PRO	3.9
3	B	179	PRO	3.8
3	B	151	LEU	3.8
3	B	162	TRP	3.8
3	D	30	GLU	3.8
3	D	328	VAL	3.8
3	B	288	TYR	3.8
3	D	577	TYR	3.8
2	L	101	DG	3.7
3	D	727	ILE	3.7
3	A	490	LEU	3.7
3	D	278	LYS	3.7
3	D	619	TYR	3.7
3	B	253	ILE	3.6
3	D	8	VAL	3.6
3	D	212	ILE	3.6
3	D	7	THR	3.6
3	B	158	ASN	3.6
3	D	284	ASN	3.5
3	D	466	ASP	3.5
3	B	733	GLN	3.5
3	D	28	THR	3.5
3	B	234	PHE	3.5
3	C	898	PHE	3.5
3	D	861	ASP	3.5
2	F	115	DA	3.5

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Mol	Chain	Res	Type	RSRZ
3	D	327	ALA	3.5
3	D	448	GLU	3.4
3	D	390	PRO	3.4
3	D	876	PHE	3.4
3	D	316	ASN	3.4
3	D	625	ILE	3.4
3	B	308	PRO	3.4
3	B	164	ILE	3.4
3	B	230	ILE	3.4
3	D	611	THR	3.4
3	B	197	LEU	3.3
3	D	282	PHE	3.3
3	A	542	LEU	3.3
3	B	149	PHE	3.3
3	B	191	PHE	3.3
2	F	113	DA	3.3
3	A	817	GLY	3.3
3	D	103	TYR	3.3
3	A	394	ALA	3.3
3	D	23	ASN	3.2
3	D	193	ASN	3.2
3	D	394	ALA	3.2
3	D	354	GLN	3.2
3	D	104	ASP	3.2
3	D	223	ILE	3.2
3	D	271	LEU	3.2
3	D	293	ILE	3.2
3	D	38	PHE	3.1
3	B	870	VAL	3.1
3	D	548	THR	3.1
3	D	290	LEU	3.1
3	D	298	LEU	3.1
3	C	491	ALA	3.1
3	B	393	GLY	3.1
3	D	415	LEU	3.1
3	D	538	LEU	3.1
3	D	647	TRP	3.1
3	D	31	VAL	3.1
3	B	282	PHE	3.1
3	D	33	TYR	3.1
3	D	234	PHE	3.1
1	G	6	DT	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	558	ASN	3.1
3	D	108	ILE	3.1
3	B	124	PRO	3.1
3	D	557	ILE	3.0
3	D	563	ILE	3.0
3	D	453	VAL	3.0
3	D	377	ASN	3.0
3	D	645	ASN	3.0
3	B	183	ILE	3.0
3	D	431	ALA	3.0
3	D	626	TYR	3.0
3	C	303	LEU	3.0
3	D	357	SER	3.0
3	D	32	GLU	3.0
2	H	115	DA	3.0
3	B	167	ALA	3.0
3	D	88	PHE	3.0
3	D	388	VAL	3.0
3	B	865	TRP	3.0
3	D	195	LYS	3.0
3	D	29	ARG	3.0
3	D	605	LEU	3.0
1	E	4	DC	3.0
3	D	771	PHE	3.0
3	B	152	LEU	2.9
3	D	219	GLU	2.9
3	D	101	ILE	2.9
3	B	298	LEU	2.9
3	D	432	GLY	2.9
3	D	305	TYR	2.9
3	B	150	ASP	2.9
3	D	315	SER	2.9
3	B	395	PHE	2.9
3	B	133	ILE	2.9
3	B	897	LEU	2.9
3	D	6	LEU	2.9
3	D	197	LEU	2.9
3	B	188	TYR	2.9
3	D	92	TYR	2.9
3	D	288	TYR	2.9
3	D	696	LYS	2.9
3	D	203	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
3	B	123	PHE	2.9
3	B	280	PHE	2.9
3	A	857	LEU	2.9
3	D	443	ILE	2.9
3	D	297	GLU	2.8
3	A	821	ALA	2.8
3	D	779	ILE	2.8
3	D	70	GLN	2.8
2	H	111	DT	2.8
1	I	1	DC	2.8
3	D	470	VAL	2.8
3	D	50	PHE	2.8
3	A	786	ASN	2.8
3	A	819	ILE	2.8
3	D	875	THR	2.8
3	D	724	LYS	2.8
3	D	303	LEU	2.8
3	D	355	ILE	2.8
3	D	270	VAL	2.8
3	D	396	VAL	2.8
3	D	471	VAL	2.8
3	B	146	PHE	2.8
3	D	274	ILE	2.8
3	D	89	LYS	2.8
3	B	546	GLN	2.7
3	C	257	TYR	2.7
3	D	337	LYS	2.7
3	D	87	ASP	2.7
3	D	283	THR	2.7
3	D	94	SER	2.7
3	D	15	ILE	2.7
3	B	227	TYR	2.7
3	D	228	ASN	2.7
3	A	548	THR	2.7
3	D	554	THR	2.7
3	B	154	SER	2.7
3	D	287	SER	2.7
3	A	550	VAL	2.7
3	B	309	ILE	2.7
3	D	82	ALA	2.7
3	A	257	TYR	2.7
3	D	49	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	12	GLY	2.7
3	B	200	GLU	2.7
3	D	261	GLU	2.7
3	B	394	ALA	2.7
3	D	285	GLN	2.7
3	D	481	GLN	2.7
3	D	712	VAL	2.7
3	B	287	SER	2.7
3	A	255	ASN	2.6
1	K	10	DA	2.6
3	C	182	ILE	2.6
3	D	47	THR	2.6
3	D	83	LEU	2.6
3	D	200	GLU	2.6
3	D	331	VAL	2.6
3	D	332	LEU	2.6
3	D	774	LEU	2.6
3	D	698	ILE	2.6
3	D	766	GLU	2.6
2	H	113	DA	2.6
3	D	406	TYR	2.6
3	D	361	PRO	2.6
3	D	439	LEU	2.6
3	B	232	ASN	2.6
3	D	69	SER	2.6
3	D	865	TRP	2.6
3	D	304	LYS	2.6
3	D	214	THR	2.6
3	D	45	GLN	2.6
3	D	72	ILE	2.5
3	D	226	VAL	2.5
3	D	279	LYS	2.5
2	H	108	DT	2.5
3	D	210	PRO	2.5
3	C	307	GLY	2.5
3	B	115	ILE	2.5
3	B	233	ILE	2.5
1	E	2	DG	2.5
3	B	277	TYR	2.5
3	B	776	TYR	2.5
3	B	47	THR	2.5
3	D	389	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	168	ALA	2.5
3	B	735	SER	2.5
3	D	310	SER	2.5
3	B	774	LEU	2.5
3	D	871	LEU	2.5
3	D	880	LEU	2.5
3	D	574	TRP	2.5
3	D	225	TYR	2.5
3	D	292	TYR	2.5
3	D	776	TYR	2.5
3	D	10	GLN	2.5
3	D	264	THR	2.5
3	D	61	LEU	2.5
1	I	4	DC	2.5
3	D	419	ILE	2.5
3	B	117	VAL	2.5
1	E	5	DT	2.5
3	D	720	TYR	2.5
3	D	58	THR	2.5
3	D	593	ALA	2.5
3	B	317	HIS	2.5
3	B	112	ASN	2.5
3	A	815	ILE	2.4
3	D	215	GLY	2.4
3	B	127	SER	2.4
3	A	544	ARG	2.4
3	D	581	ARG	2.4
3	D	351	ALA	2.4
3	D	40	HIS	2.4
3	B	228	ASN	2.4
1	K	12	DA	2.4
3	B	242	LEU	2.4
3	D	312	LEU	2.4
1	G	13	DG	2.4
3	A	797	PRO	2.4
3	D	334	ILE	2.4
3	D	362	ILE	2.4
3	D	381	PRO	2.4
3	D	211	VAL	2.4
3	B	778	SER	2.4
3	D	251	LYS	2.4
3	D	654	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	657	GLU	2.4
3	B	118	THR	2.4
3	A	798	GLY	2.4
3	C	306	ASP	2.4
3	C	452	ASP	2.4
1	K	13	DG	2.4
3	D	36	SER	2.4
3	C	201	TYR	2.4
3	D	321	ILE	2.4
3	C	495	ASN	2.4
3	B	184	ASP	2.4
3	B	867	ASP	2.4
3	C	466	ASP	2.4
3	D	66	ARG	2.4
3	B	254	GLU	2.4
3	B	156	TYR	2.4
3	D	286	PRO	2.4
3	D	247	LYS	2.3
3	D	721	ALA	2.3
2	H	112	DA	2.3
3	B	216	TRP	2.3
3	A	554	THR	2.3
3	D	345	LEU	2.3
3	D	387	PRO	2.3
3	B	178	VAL	2.3
3	D	539	ASN	2.3
3	D	236	GLU	2.3
3	D	545	ALA	2.3
3	B	136	ILE	2.3
3	C	164	ILE	2.3
3	D	416	TYR	2.3
3	D	632	ILE	2.3
3	D	241	ARG	2.3
3	D	379	VAL	2.3
2	L	102	DC	2.3
3	D	479	PHE	2.3
3	D	575	PHE	2.3
3	D	682	PHE	2.3
3	B	380	ILE	2.3
1	G	10	DA	2.3
3	C	818	ASN	2.3
3	D	266	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	196	GLU	2.3
3	A	820	ASP	2.3
3	D	11	ILE	2.3
3	D	269	SER	2.3
3	B	323	TYR	2.3
3	B	153	ASN	2.2
3	B	311	LYS	2.2
3	D	546	GLN	2.2
2	L	103	DG	2.2
2	L	108	DT	2.2
3	D	68	ALA	2.2
3	B	202	LEU	2.2
2	H	110	DA	2.2
3	D	325	ILE	2.2
3	B	306	ASP	2.2
2	H	104	DG	2.2
3	B	283	THR	2.2
3	D	323	TYR	2.2
3	D	767	PHE	2.2
3	D	888	LYS	2.2
3	D	549	GLU	2.2
3	D	564	ASN	2.2
3	A	547	ARG	2.2
3	B	176	ASP	2.2
3	B	861	ASP	2.2
3	D	71	TRP	2.2
3	B	310	SER	2.2
3	D	393	GLY	2.2
3	D	404	TYR	2.2
3	B	170	LEU	2.2
3	C	490	LEU	2.2
3	B	168	ALA	2.2
3	D	583	ALA	2.2
3	B	325	ILE	2.2
3	D	229	ARG	2.2
3	D	217	ASN	2.2
3	B	550	VAL	2.2
3	D	692	PRO	2.2
1	E	6	DT	2.2
3	C	301	GLY	2.2
3	D	454	TYR	2.2
3	D	456	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	412	LEU	2.2
3	B	263	ILE	2.1
3	D	25	ARG	2.1
3	D	338	ARG	2.1
3	D	877	ILE	2.1
3	D	417	PRO	2.1
3	B	468	ASP	2.1
3	D	306	ASP	2.1
3	B	279	LYS	2.1
3	B	732	THR	2.1
3	D	552	GLY	2.1
3	D	699	GLY	2.1
3	B	221	PHE	2.1
3	B	542	LEU	2.1
3	D	93	LEU	2.1
3	D	764	PHE	2.1
3	B	180	SER	2.1
3	D	886	ALA	2.1
1	K	14	DC	2.1
2	J	114	DG	2.1
3	D	480	ASN	2.1
3	B	738	PRO	2.1
3	D	691	PRO	2.1
3	C	195	LYS	2.1
3	B	301	GLY	2.1
3	D	213	LEU	2.1
3	D	53	TYR	2.1
3	D	609	CYS	2.1
1	G	12	DA	2.1
1	E	1	DC	2.1
3	A	635	LYS	2.1
3	D	582	ASN	2.1
2	J	101	DG	2.1
2	L	107	DG	2.1
3	A	897	LEU	2.1
3	D	700	GLY	2.1
3	D	543	PHE	2.1
3	C	305	TYR	2.1
3	D	230	ILE	2.1
3	B	281	SER	2.1
3	D	22	SER	2.1
3	B	318	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	218	VAL	2.1
3	D	37	LEU	2.1
1	I	2	DG	2.1
2	F	114	DG	2.1
3	B	611	THR	2.1
3	C	494	ARG	2.1
3	D	27	ARG	2.1
3	D	364	THR	2.1
3	D	576	ARG	2.1
3	B	172	GLU	2.1
3	C	200	GLU	2.1
3	D	567	TYR	2.1
3	C	304	LYS	2.0
3	D	427	PRO	2.0
2	F	112	DA	2.0
3	B	303	LEU	2.0
3	D	324	ASN	2.0
1	G	15	DC	2.0
1	K	15	DC	2.0
3	D	589	PHE	2.0
3	D	452	ASP	2.0
3	D	689	ALA	2.0
3	B	236	GLU	2.0
3	B	705	LYS	2.0
3	C	2	LYS	2.0
3	C	302	LYS	2.0
3	D	245	HIS	2.0
3	C	609	CYS	2.0
3	D	562	LEU	2.0
3	D	570	LEU	2.0
3	D	725	LEU	2.0
3	D	262	ILE	2.0
3	D	263	ILE	2.0
3	B	129	ALA	2.0
3	B	297	GLU	2.0
3	D	468	ASP	2.0
3	D	205	TRP	2.0
3	B	225	TYR	2.0
3	D	464	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	3DR	E	3	11/12	0.79	0.24	117,125,130,133	0
1	3DR	I	3	11/12	0.89	0.18	101,102,103,103	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.