



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:50 AM UTC

PDB ID : 3HQQ / pdb_00003hqq
Title : Crystal structure of Leishmania mexicana pyruvate kinase (LmPYK) in complex with Fructose 2,6 biphosphate
Authors : Morgan, H.P.; Walkinshaw, M.D.
Deposited on : 2009-06-08
Resolution : 5.07 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

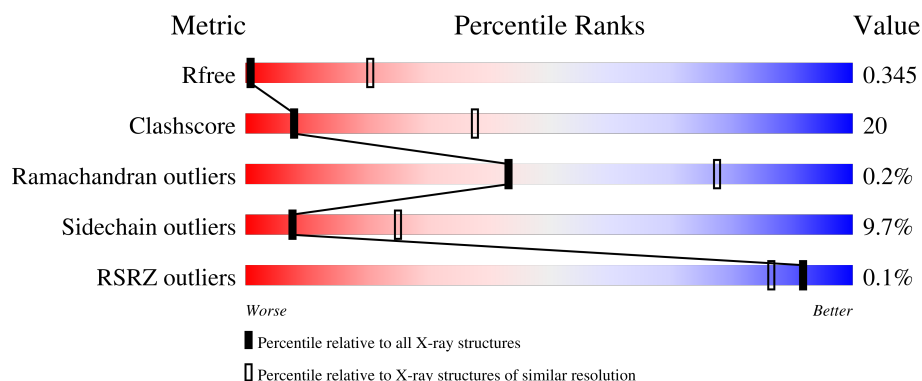
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.07 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	1020 (6.16-3.98)
Clashscore	190562	1053 (6.16-4.00)
Ramachandran outliers	187476	1022 (6.22-3.92)
Sidechain outliers	187428	1139 (6.22-3.90)
RSRZ outliers	180081	1015 (6.16-3.98)

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

Mol	Chain	Length	Quality of chain
1	A	499	64% 28% 7%
1	B	499	65% 27% 7%
1	C	499	63% 30% 7%
1	D	499	64% 29% 6%
1	E	499	64% 29% 6%

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Mol	Chain	Length	Quality of chain
1	F	499	 65%29%6%
1	G	499	 65%28%7%
1	H	499	 63%30%7%
1	I	499	 64%28%7%
1	J	499	 65%28%7% .
1	K	499	 64%29%6% .
1	L	499	 64%28%7% .
1	M	499	 63%29%7%
1	N	499	 64%28%7% .
1	O	499	 63%29%7%
1	P	499	 64%28%7%
1	Q	499	 63%29%7% .
1	R	499	 65%28%7% .
1	S	499	 64%28%7% .
1	T	499	 64%28%7%
1	U	499	 63%30%7%
1	V	499	 64%28%7% .
1	W	499	 64%29%6%
1	X	499	 65%29%6% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 91656 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	B	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	C	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	D	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	E	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	F	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	G	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	H	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	I	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	J	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	K	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	L	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	M	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	N	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	O	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	P	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	R	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	S	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	T	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	U	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	V	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	W	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	X	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	SER	GLY	SEE REMARK 999	UNP Q27686
A	389	TYR	SER	SEE REMARK 999	UNP Q27686
A	404	ARG	ALA	SEE REMARK 999	UNP Q27686
A	405	SER	GLY	SEE REMARK 999	UNP Q27686
B	382	SER	GLY	SEE REMARK 999	UNP Q27686
B	389	TYR	SER	SEE REMARK 999	UNP Q27686
B	404	ARG	ALA	SEE REMARK 999	UNP Q27686
B	405	SER	GLY	SEE REMARK 999	UNP Q27686
C	382	SER	GLY	SEE REMARK 999	UNP Q27686
C	389	TYR	SER	SEE REMARK 999	UNP Q27686
C	404	ARG	ALA	SEE REMARK 999	UNP Q27686
C	405	SER	GLY	SEE REMARK 999	UNP Q27686
D	382	SER	GLY	SEE REMARK 999	UNP Q27686
D	389	TYR	SER	SEE REMARK 999	UNP Q27686
D	404	ARG	ALA	SEE REMARK 999	UNP Q27686
D	405	SER	GLY	SEE REMARK 999	UNP Q27686
E	382	SER	GLY	SEE REMARK 999	UNP Q27686
E	389	TYR	SER	SEE REMARK 999	UNP Q27686
E	404	ARG	ALA	SEE REMARK 999	UNP Q27686
E	405	SER	GLY	SEE REMARK 999	UNP Q27686
F	382	SER	GLY	SEE REMARK 999	UNP Q27686
F	389	TYR	SER	SEE REMARK 999	UNP Q27686
F	404	ARG	ALA	SEE REMARK 999	UNP Q27686

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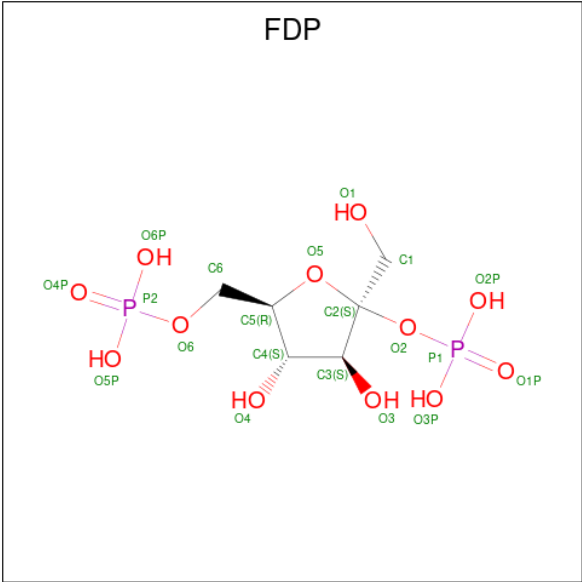
Chain	Residue	Modelled	Actual	Comment	Reference
F	405	SER	GLY	SEE REMARK 999	UNP Q27686
G	382	SER	GLY	SEE REMARK 999	UNP Q27686
G	389	TYR	SER	SEE REMARK 999	UNP Q27686
G	404	ARG	ALA	SEE REMARK 999	UNP Q27686
G	405	SER	GLY	SEE REMARK 999	UNP Q27686
H	382	SER	GLY	SEE REMARK 999	UNP Q27686
H	389	TYR	SER	SEE REMARK 999	UNP Q27686
H	404	ARG	ALA	SEE REMARK 999	UNP Q27686
H	405	SER	GLY	SEE REMARK 999	UNP Q27686
I	382	SER	GLY	SEE REMARK 999	UNP Q27686
I	389	TYR	SER	SEE REMARK 999	UNP Q27686
I	404	ARG	ALA	SEE REMARK 999	UNP Q27686
I	405	SER	GLY	SEE REMARK 999	UNP Q27686
J	382	SER	GLY	SEE REMARK 999	UNP Q27686
J	389	TYR	SER	SEE REMARK 999	UNP Q27686
J	404	ARG	ALA	SEE REMARK 999	UNP Q27686
J	405	SER	GLY	SEE REMARK 999	UNP Q27686
K	382	SER	GLY	SEE REMARK 999	UNP Q27686
K	389	TYR	SER	SEE REMARK 999	UNP Q27686
K	404	ARG	ALA	SEE REMARK 999	UNP Q27686
K	405	SER	GLY	SEE REMARK 999	UNP Q27686
L	382	SER	GLY	SEE REMARK 999	UNP Q27686
L	389	TYR	SER	SEE REMARK 999	UNP Q27686
L	404	ARG	ALA	SEE REMARK 999	UNP Q27686
L	405	SER	GLY	SEE REMARK 999	UNP Q27686
M	382	SER	GLY	SEE REMARK 999	UNP Q27686
M	389	TYR	SER	SEE REMARK 999	UNP Q27686
M	404	ARG	ALA	SEE REMARK 999	UNP Q27686
M	405	SER	GLY	SEE REMARK 999	UNP Q27686
N	382	SER	GLY	SEE REMARK 999	UNP Q27686
N	389	TYR	SER	SEE REMARK 999	UNP Q27686
N	404	ARG	ALA	SEE REMARK 999	UNP Q27686
N	405	SER	GLY	SEE REMARK 999	UNP Q27686
O	382	SER	GLY	SEE REMARK 999	UNP Q27686
O	389	TYR	SER	SEE REMARK 999	UNP Q27686
O	404	ARG	ALA	SEE REMARK 999	UNP Q27686
O	405	SER	GLY	SEE REMARK 999	UNP Q27686
P	382	SER	GLY	SEE REMARK 999	UNP Q27686
P	389	TYR	SER	SEE REMARK 999	UNP Q27686
P	404	ARG	ALA	SEE REMARK 999	UNP Q27686
P	405	SER	GLY	SEE REMARK 999	UNP Q27686
Q	382	SER	GLY	SEE REMARK 999	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	389	TYR	SER	SEE REMARK 999	UNP Q27686
Q	404	ARG	ALA	SEE REMARK 999	UNP Q27686
Q	405	SER	GLY	SEE REMARK 999	UNP Q27686
R	382	SER	GLY	SEE REMARK 999	UNP Q27686
R	389	TYR	SER	SEE REMARK 999	UNP Q27686
R	404	ARG	ALA	SEE REMARK 999	UNP Q27686
R	405	SER	GLY	SEE REMARK 999	UNP Q27686
S	382	SER	GLY	SEE REMARK 999	UNP Q27686
S	389	TYR	SER	SEE REMARK 999	UNP Q27686
S	404	ARG	ALA	SEE REMARK 999	UNP Q27686
S	405	SER	GLY	SEE REMARK 999	UNP Q27686
T	382	SER	GLY	SEE REMARK 999	UNP Q27686
T	389	TYR	SER	SEE REMARK 999	UNP Q27686
T	404	ARG	ALA	SEE REMARK 999	UNP Q27686
T	405	SER	GLY	SEE REMARK 999	UNP Q27686
U	382	SER	GLY	SEE REMARK 999	UNP Q27686
U	389	TYR	SER	SEE REMARK 999	UNP Q27686
U	404	ARG	ALA	SEE REMARK 999	UNP Q27686
U	405	SER	GLY	SEE REMARK 999	UNP Q27686
V	382	SER	GLY	SEE REMARK 999	UNP Q27686
V	389	TYR	SER	SEE REMARK 999	UNP Q27686
V	404	ARG	ALA	SEE REMARK 999	UNP Q27686
V	405	SER	GLY	SEE REMARK 999	UNP Q27686
W	382	SER	GLY	SEE REMARK 999	UNP Q27686
W	389	TYR	SER	SEE REMARK 999	UNP Q27686
W	404	ARG	ALA	SEE REMARK 999	UNP Q27686
W	405	SER	GLY	SEE REMARK 999	UNP Q27686
X	382	SER	GLY	SEE REMARK 999	UNP Q27686
X	389	TYR	SER	SEE REMARK 999	UNP Q27686
X	404	ARG	ALA	SEE REMARK 999	UNP Q27686
X	405	SER	GLY	SEE REMARK 999	UNP Q27686

- Molecule 2 is 2,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FDP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
2	H	1	Total	C	O	P	0	0
			20	6	12	2		
2	I	1	Total	C	O	P	0	0
			20	6	12	2		
2	J	1	Total	C	O	P	0	0
			20	6	12	2		
2	K	1	Total	C	O	P	0	0
			20	6	12	2		
2	L	1	Total	C	O	P	0	0
			20	6	12	2		
2	M	1	Total	C	O	P	0	0
			20	6	12	2		
2	N	1	Total	C	O	P	0	0
			20	6	12	2		

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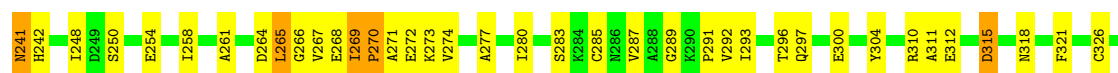
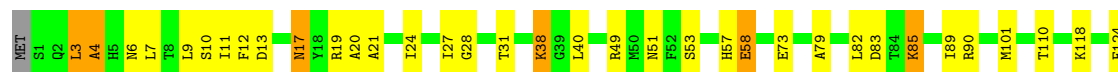
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total 20	C 6	O 12	P 2	0	0
2	P	1	Total 20	C 6	O 12	P 2	0	0
2	Q	1	Total 20	C 6	O 12	P 2	0	0
2	R	1	Total 20	C 6	O 12	P 2	0	0
2	S	1	Total 20	C 6	O 12	P 2	0	0
2	T	1	Total 20	C 6	O 12	P 2	0	0
2	U	1	Total 20	C 6	O 12	P 2	0	0
2	V	1	Total 20	C 6	O 12	P 2	0	0
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2	X	1	Total 20	C 6	O 12	P 2	0	0



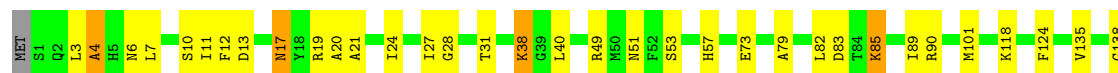
• Molecule 1: Pyruvate kinase

Chain C: 63% 30% 7%



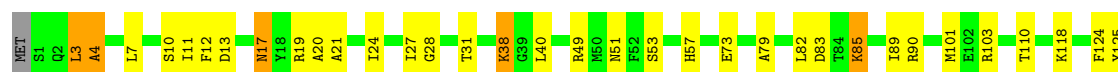
• Molecule 1: Pyruvate kinase

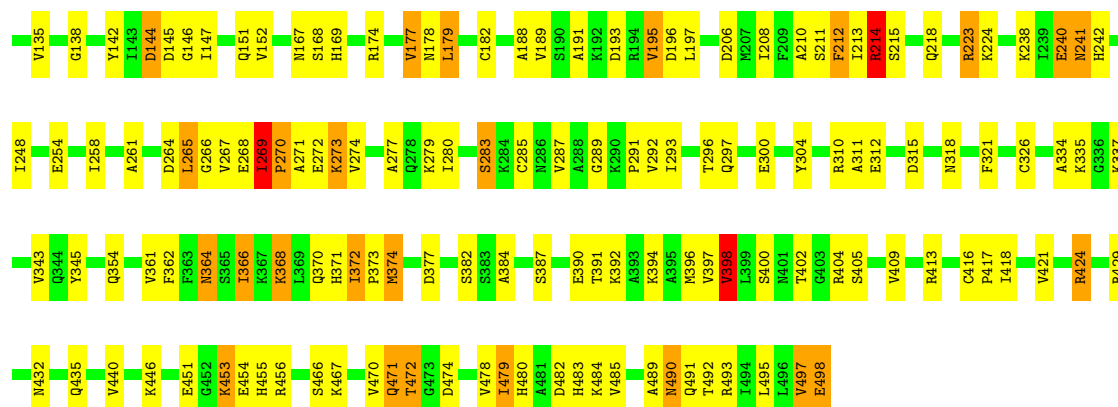
Chain D: 64% 29% 6%



• Molecule 1: Pyruvate kinase

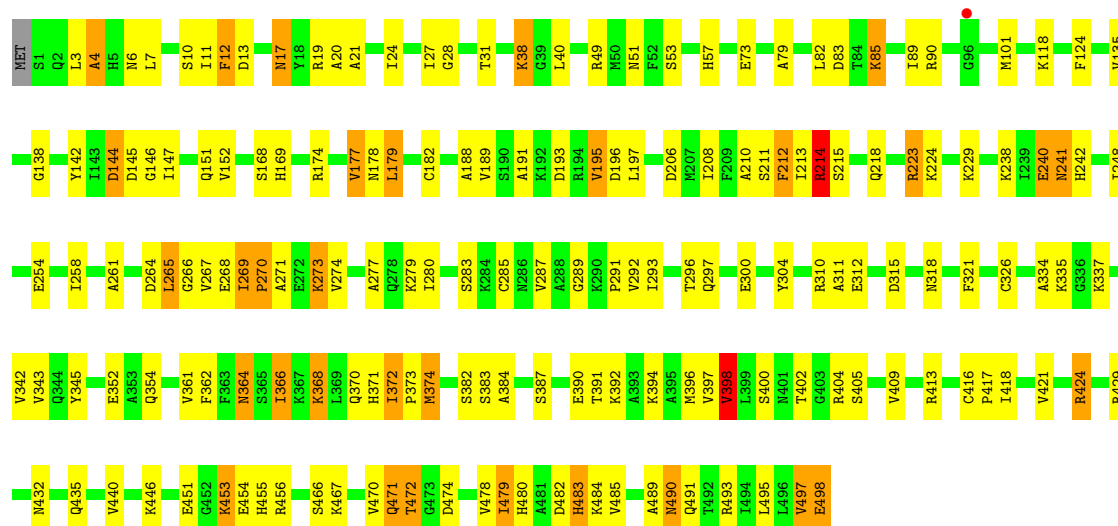
Chain E: 64% 29% 6%





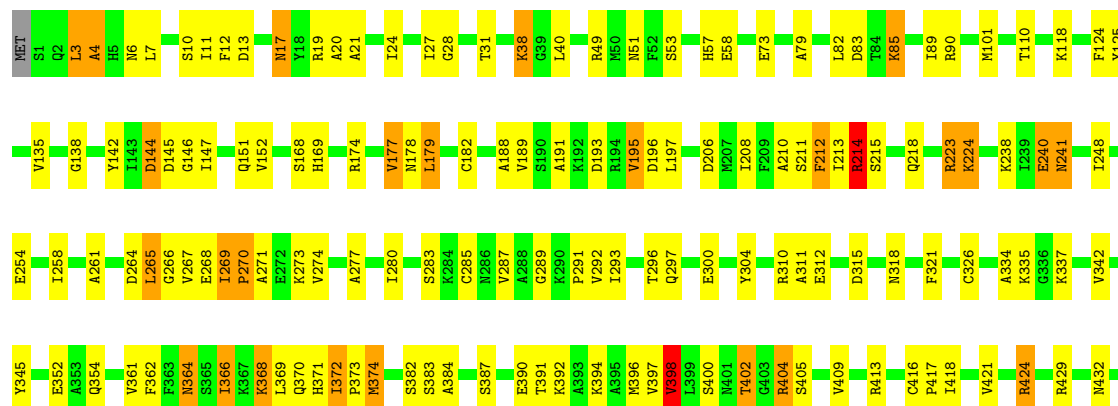
• Molecule 1: Pyruvate kinase

Chain F: 65% 29% 6%



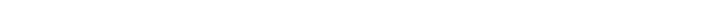
• Molecule 1: Pyruvate kinase

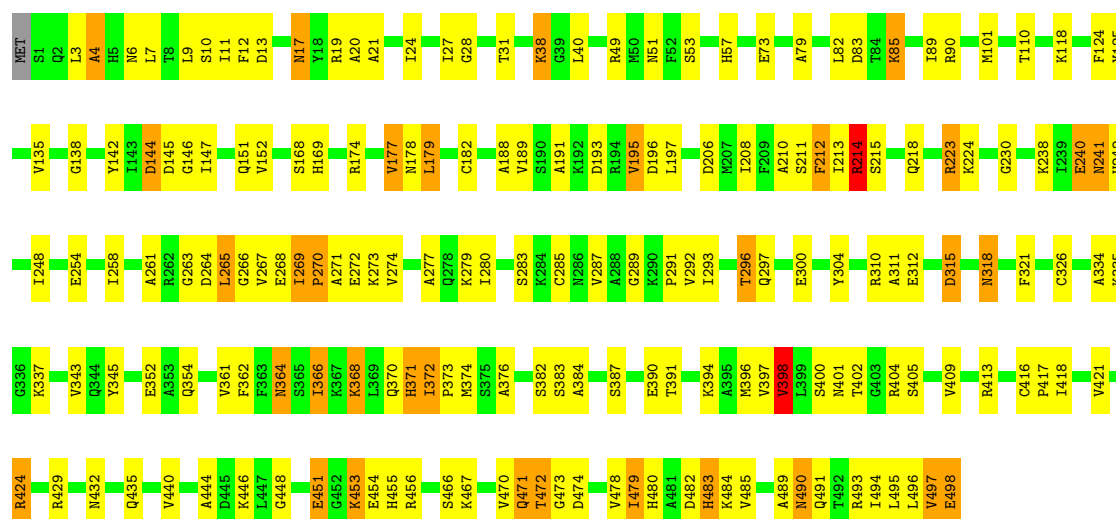
Chain G: 65% 28% 7%



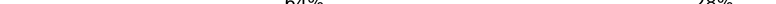


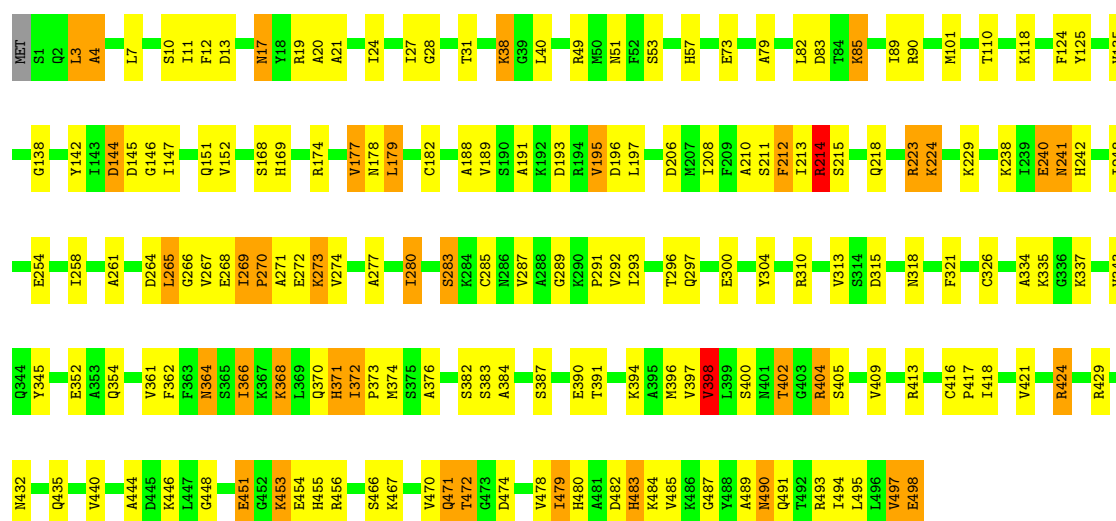
- Molecule 1: Pyruvate kinase

Chain H:  63% 30% 7%



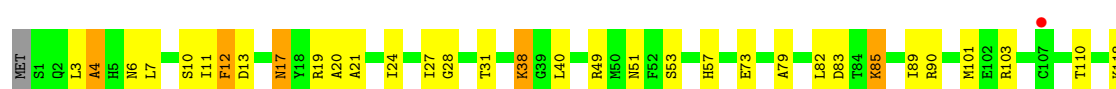
- Molecule 1: Pyruvate kinase

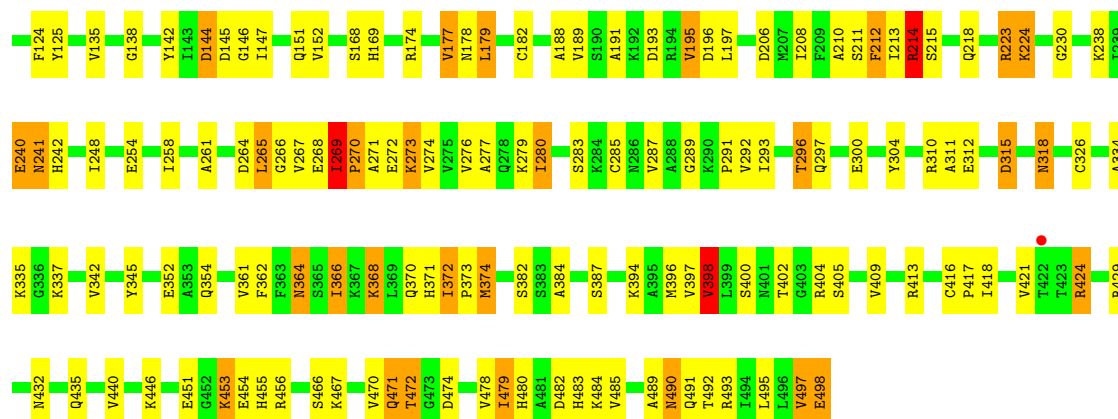
Chain I:  64% 28% 7%



- Molecule 1: Pyruvate kinase

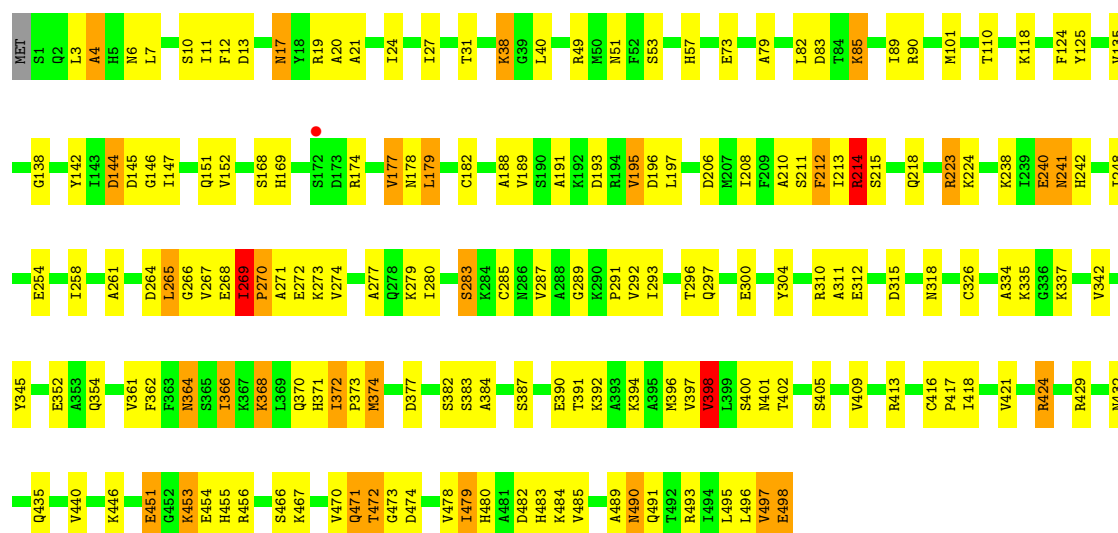
Chain J: 65% 28% 7%





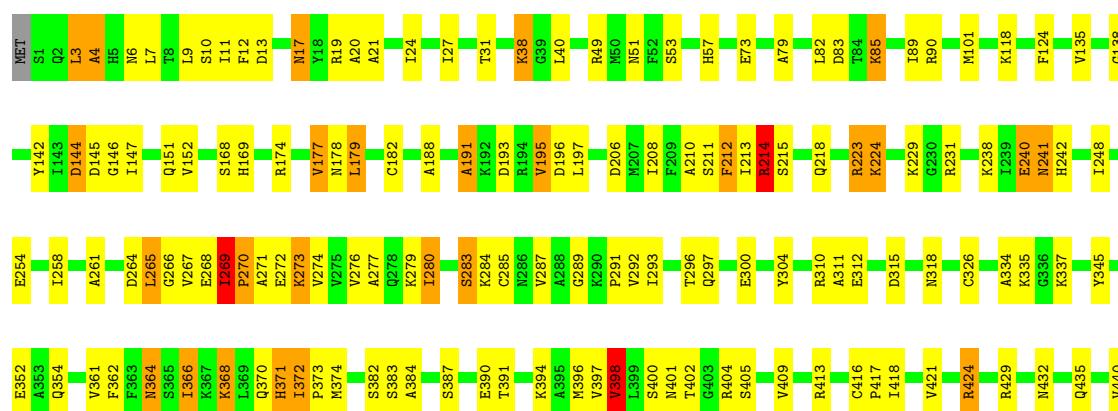
• Molecule 1: Pyruvate kinase

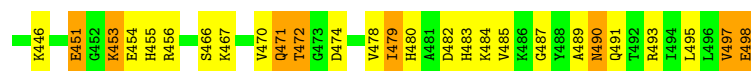
Chain K: 64% 29% 6%



• Molecule 1: Pyruvate kinase

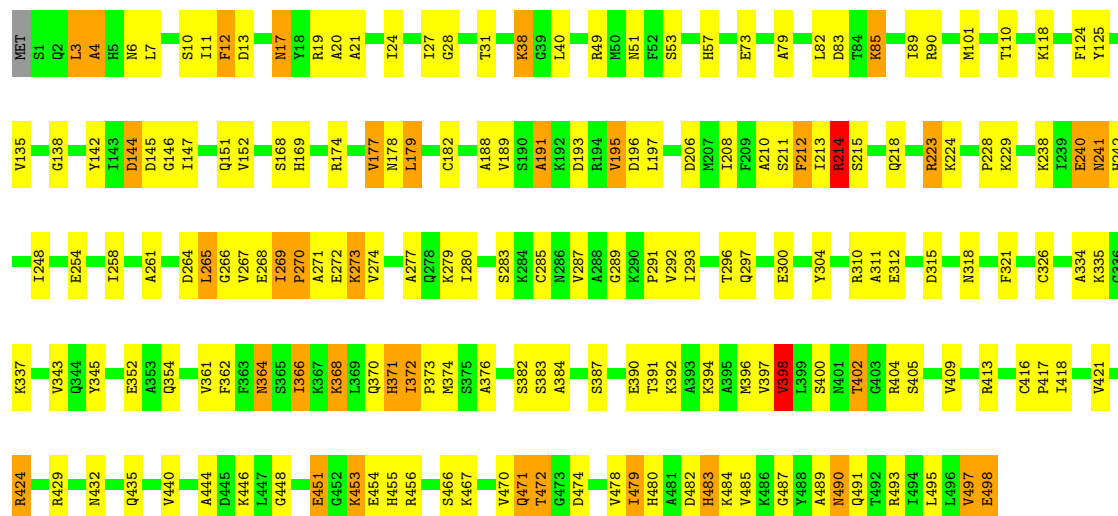
Chain L: 64% 28% 7%





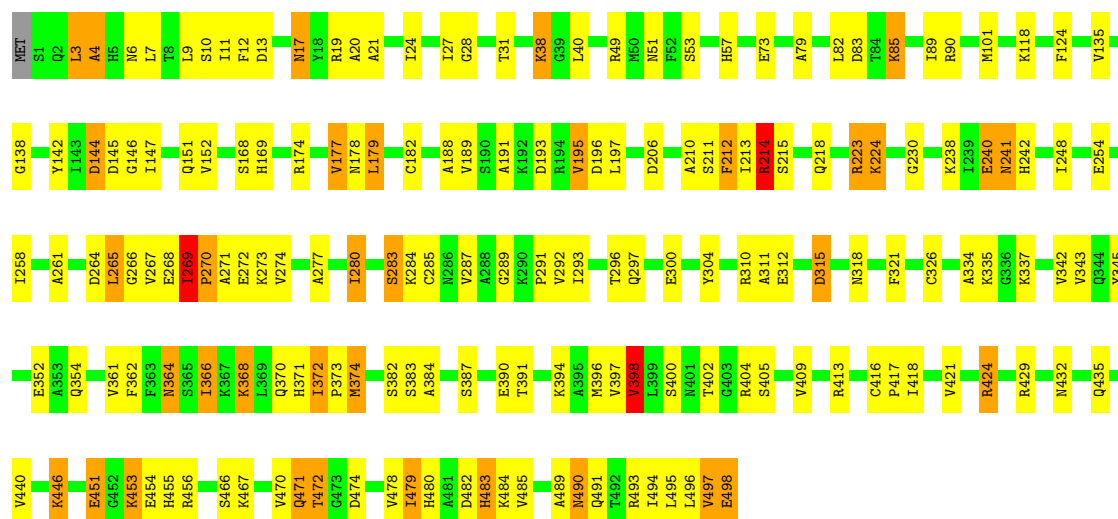
• Molecule 1: Pyruvate kinase

Chain M: 63% 29% 7%



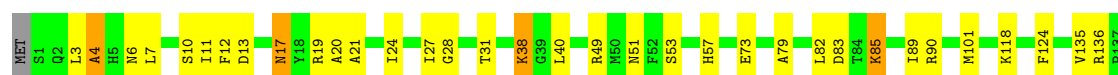
• Molecule 1: Pyruvate kinase

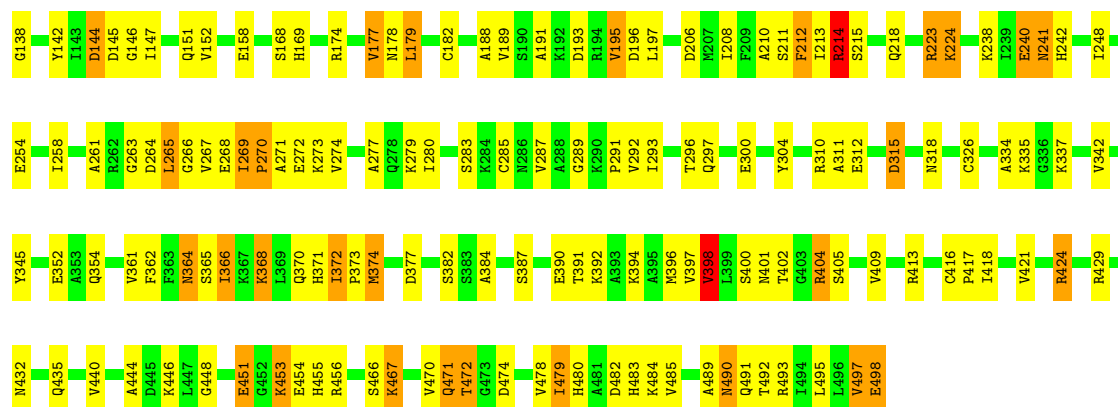
Chain N: 64% 28% 7%



• Molecule 1: Pyruvate kinase

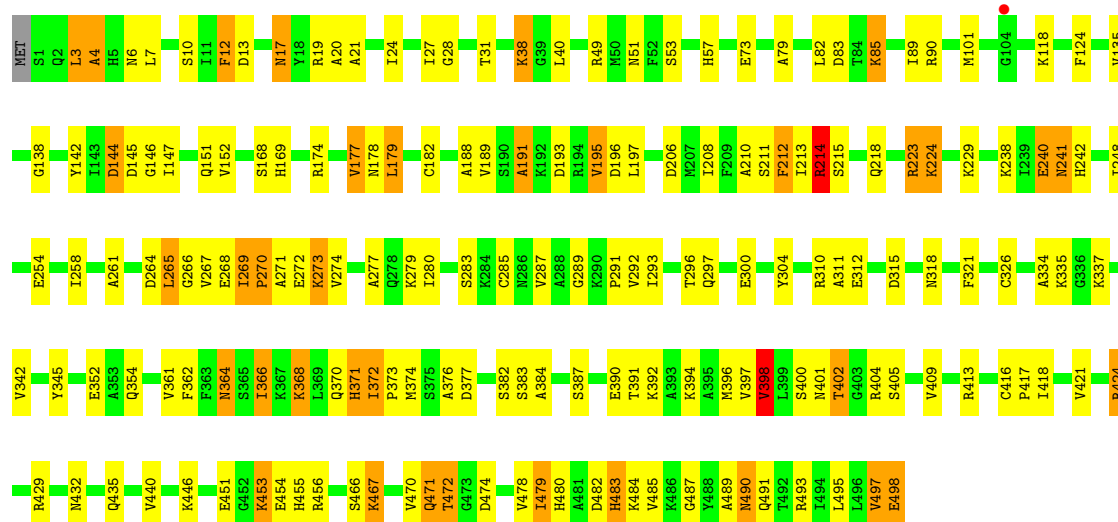
Chain O: 63% 29% 7%





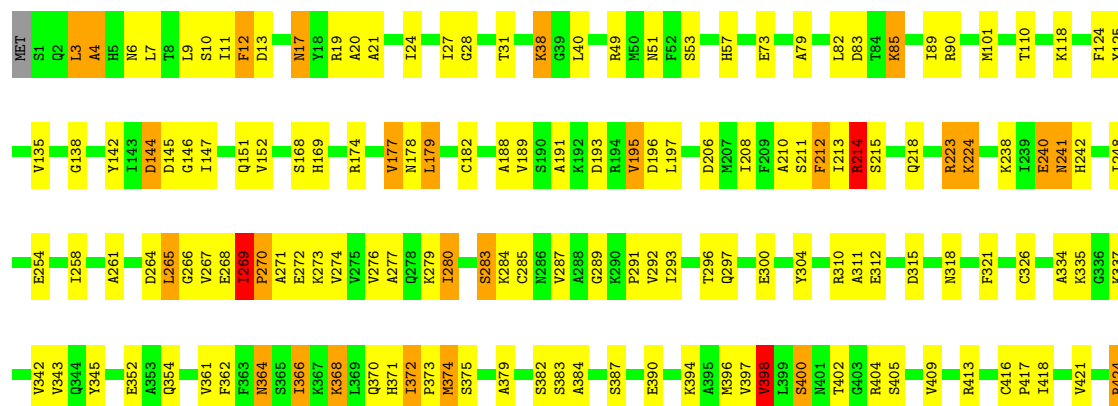
• Molecule 1: Pyruvate kinase

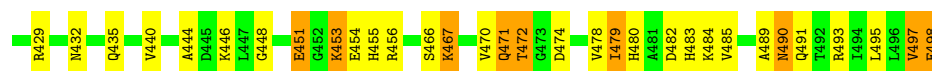
Chain P: 64% 28% 7%



• Molecule 1: Pyruvate kinase

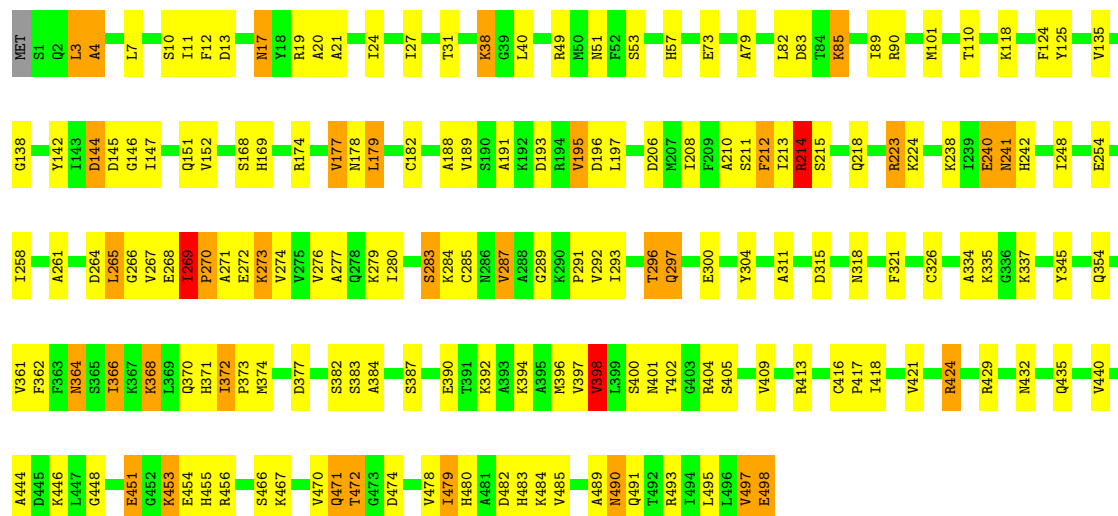
Chain Q: 63% 29% 7%





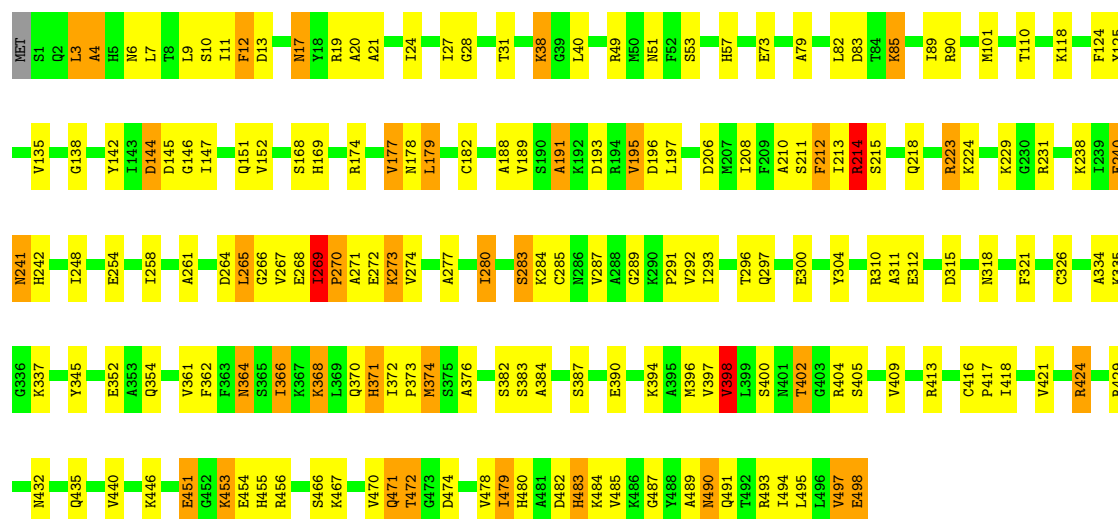
• Molecule 1: Pyruvate kinase

Chain R: 65% 28% 7%



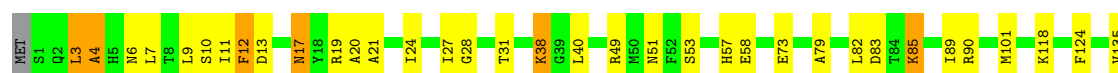
• Molecule 1: Pyruvate kinase

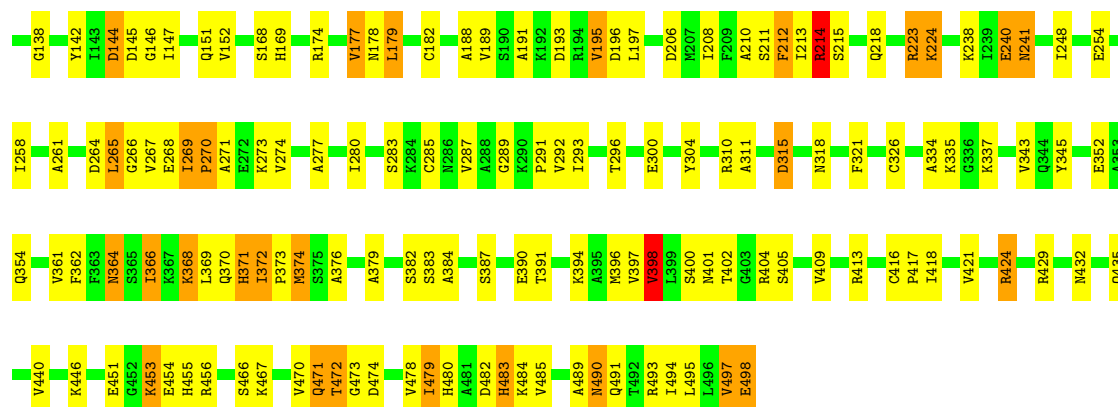
Chain S: 64% 28% 7%



• Molecule 1: Pyruvate kinase

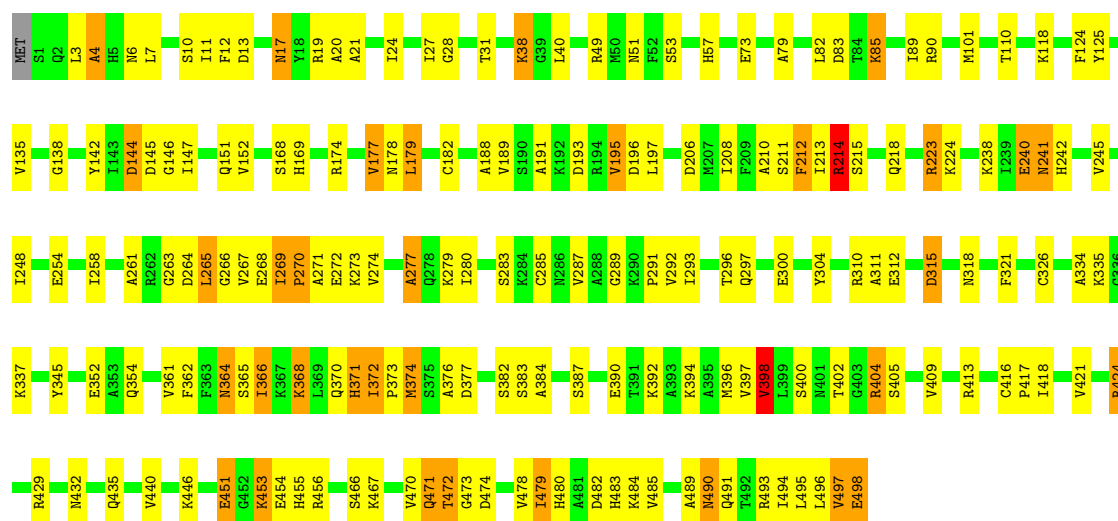
Chain T: 64% 28% 7%





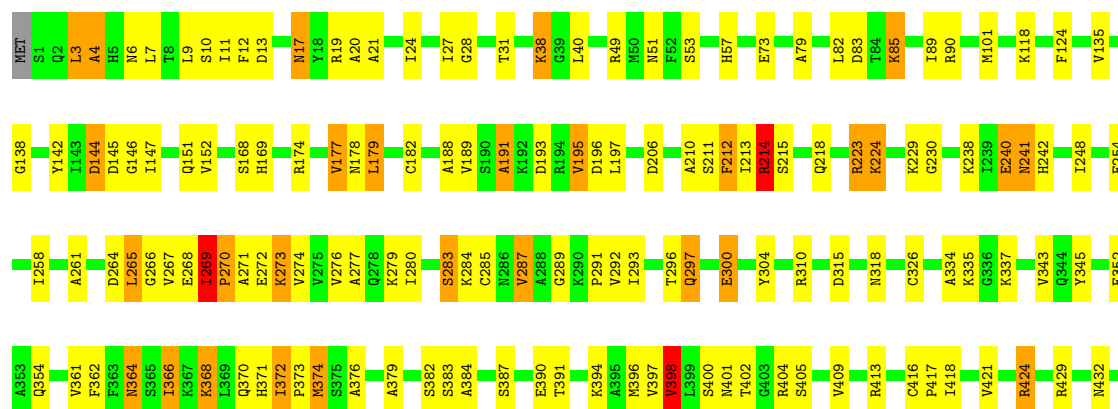
• Molecule 1: Pyruvate kinase

Chain U: 63% 30% 7%



• Molecule 1: Pyruvate kinase

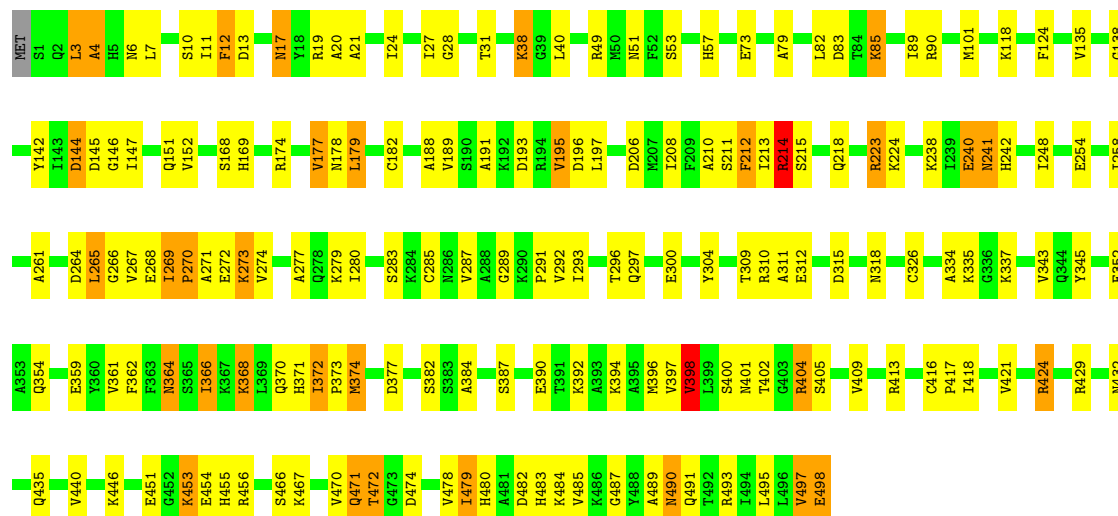
Chain V: 64% 28% 7%





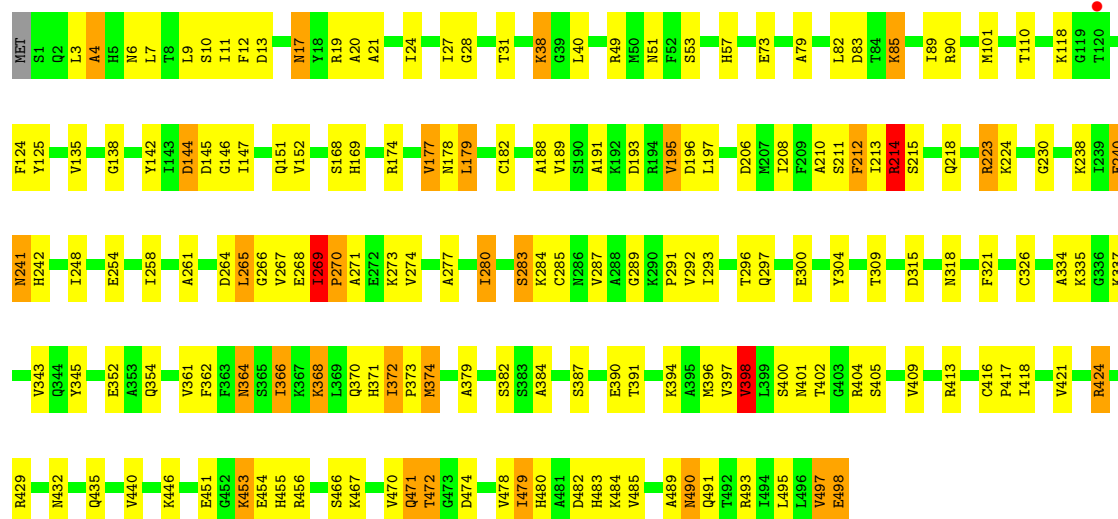
• Molecule 1: Pyruvate kinase

Chain W: 64% 29% 6%



• Molecule 1: Pyruvate kinase

Chain X: 65% 29% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	243.84Å 254.69Å 892.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 5.07 39.81 – 5.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.81-5.07) 86.3 (39.81-5.07)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 5.09Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.353 , 0.357 0.343 , 0.345	Depositor DCC
R_{free} test set	5652 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.118 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	91656	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: FDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.87	47/3856 (1.2%)	1.26	33/5220 (0.6%)
1	B	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	C	1.87	46/3856 (1.2%)	1.26	32/5220 (0.6%)
1	D	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	E	1.88	45/3856 (1.2%)	1.26	33/5220 (0.6%)
1	F	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	G	1.88	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	H	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	I	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	J	1.87	45/3856 (1.2%)	1.26	33/5220 (0.6%)
1	K	1.87	45/3856 (1.2%)	1.26	31/5220 (0.6%)
1	L	1.87	43/3856 (1.1%)	1.26	30/5220 (0.6%)
1	M	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	N	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	O	1.87	44/3856 (1.1%)	1.26	33/5220 (0.6%)
1	P	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	Q	1.87	47/3856 (1.2%)	1.26	33/5220 (0.6%)
1	R	1.87	43/3856 (1.1%)	1.26	30/5220 (0.6%)
1	S	1.87	45/3856 (1.2%)	1.26	33/5220 (0.6%)
1	T	1.87	45/3856 (1.2%)	1.26	34/5220 (0.7%)
1	U	1.87	44/3856 (1.1%)	1.26	33/5220 (0.6%)
1	V	1.87	43/3856 (1.1%)	1.26	32/5220 (0.6%)
1	W	1.88	45/3856 (1.2%)	1.26	33/5220 (0.6%)
1	X	1.87	46/3856 (1.2%)	1.26	34/5220 (0.7%)
All	All	1.87	1087/92544 (1.2%)	1.26	784/125280 (0.6%)

All (1087) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	413	ARG	C-O	-7.01	1.20	1.23
1	L	413	ARG	C-O	-6.87	1.20	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	413	ARG	C-O	-6.86	1.20	1.23
1	S	413	ARG	C-O	-6.86	1.20	1.23
1	E	413	ARG	C-O	-6.85	1.20	1.23
1	U	413	ARG	C-O	-6.84	1.20	1.23
1	N	413	ARG	C-O	-6.83	1.20	1.23
1	C	413	ARG	C-O	-6.80	1.20	1.23
1	J	413	ARG	C-O	-6.78	1.20	1.23
1	Q	413	ARG	C-O	-6.78	1.20	1.23
1	F	413	ARG	C-O	-6.78	1.20	1.23
1	I	85	LYS	C-O	-6.78	1.16	1.24
1	B	85	LYS	C-O	-6.77	1.16	1.24
1	I	413	ARG	C-O	-6.77	1.20	1.23
1	G	413	ARG	C-O	-6.75	1.20	1.23
1	D	413	ARG	C-O	-6.75	1.20	1.23
1	X	413	ARG	C-O	-6.73	1.20	1.23
1	C	85	LYS	C-O	-6.73	1.16	1.24
1	W	413	ARG	C-O	-6.71	1.20	1.23
1	H	85	LYS	C-O	-6.70	1.16	1.24
1	O	85	LYS	C-O	-6.70	1.16	1.24
1	J	85	LYS	C-O	-6.69	1.16	1.24
1	H	413	ARG	C-O	-6.68	1.20	1.23
1	N	85	LYS	C-O	-6.68	1.16	1.24
1	V	413	ARG	C-O	-6.68	1.20	1.23
1	D	85	LYS	C-O	-6.67	1.16	1.24
1	W	85	LYS	C-O	-6.67	1.16	1.24
1	S	85	LYS	C-O	-6.67	1.16	1.24
1	A	85	LYS	C-O	-6.67	1.16	1.24
1	L	85	LYS	C-O	-6.66	1.16	1.24
1	V	85	LYS	C-O	-6.66	1.16	1.24
1	O	413	ARG	C-O	-6.66	1.20	1.23
1	T	85	LYS	C-O	-6.65	1.16	1.24
1	F	85	LYS	C-O	-6.65	1.16	1.24
1	R	413	ARG	C-O	-6.65	1.20	1.23
1	P	85	LYS	C-O	-6.65	1.16	1.24
1	R	85	LYS	C-O	-6.65	1.16	1.24
1	P	413	ARG	C-O	-6.64	1.20	1.23
1	U	85	LYS	C-O	-6.64	1.16	1.24
1	Q	85	LYS	C-O	-6.64	1.16	1.24
1	X	85	LYS	C-O	-6.63	1.16	1.24
1	G	85	LYS	C-O	-6.63	1.16	1.24
1	M	85	LYS	C-O	-6.63	1.16	1.24
1	E	85	LYS	C-O	-6.62	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	413	ARG	C-O	-6.62	1.20	1.23
1	K	85	LYS	C-O	-6.61	1.16	1.24
1	E	416	CYS	C-O	-6.60	1.18	1.24
1	K	413	ARG	C-O	-6.59	1.20	1.23
1	U	416	CYS	C-O	-6.59	1.18	1.24
1	T	416	CYS	C-O	-6.57	1.18	1.24
1	W	416	CYS	C-O	-6.56	1.18	1.24
1	C	416	CYS	C-O	-6.52	1.18	1.24
1	M	416	CYS	C-O	-6.52	1.18	1.24
1	Q	416	CYS	C-O	-6.52	1.18	1.24
1	X	416	CYS	C-O	-6.52	1.18	1.24
1	B	416	CYS	C-O	-6.51	1.18	1.24
1	O	416	CYS	C-O	-6.51	1.18	1.24
1	I	416	CYS	C-O	-6.51	1.18	1.24
1	D	416	CYS	C-O	-6.51	1.18	1.24
1	K	416	CYS	C-O	-6.50	1.18	1.24
1	L	416	CYS	C-O	-6.50	1.18	1.24
1	V	416	CYS	C-O	-6.50	1.18	1.24
1	F	416	CYS	C-O	-6.47	1.18	1.24
1	H	416	CYS	C-O	-6.46	1.18	1.24
1	R	416	CYS	C-O	-6.46	1.18	1.24
1	N	416	CYS	C-O	-6.46	1.18	1.24
1	A	416	CYS	C-O	-6.46	1.18	1.24
1	J	416	CYS	C-O	-6.44	1.18	1.24
1	A	413	ARG	C-O	-6.42	1.21	1.23
1	P	416	CYS	C-O	-6.40	1.18	1.24
1	G	416	CYS	C-O	-6.39	1.18	1.24
1	S	416	CYS	C-O	-6.37	1.18	1.24
1	P	354	GLN	C-O	-6.29	1.16	1.24
1	S	354	GLN	C-O	-6.29	1.16	1.24
1	X	354	GLN	C-O	-6.28	1.16	1.24
1	O	354	GLN	C-O	-6.28	1.16	1.24
1	C	354	GLN	C-O	-6.28	1.16	1.24
1	N	354	GLN	C-O	-6.28	1.16	1.24
1	U	354	GLN	C-O	-6.27	1.16	1.24
1	J	354	GLN	C-O	-6.26	1.16	1.24
1	F	354	GLN	C-O	-6.26	1.16	1.24
1	A	354	GLN	C-O	-6.26	1.16	1.24
1	W	354	GLN	C-O	-6.26	1.16	1.24
1	B	354	GLN	C-O	-6.25	1.16	1.24
1	C	285	CYS	C-O	-6.24	1.16	1.24
1	R	354	GLN	C-O	-6.24	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	354	GLN	C-O	-6.24	1.16	1.24
1	Q	354	GLN	C-O	-6.23	1.16	1.24
1	K	354	GLN	C-O	-6.23	1.16	1.24
1	V	354	GLN	C-O	-6.23	1.16	1.24
1	Q	285	CYS	C-O	-6.23	1.16	1.24
1	K	285	CYS	C-O	-6.22	1.16	1.24
1	T	285	CYS	C-O	-6.22	1.16	1.24
1	G	285	CYS	C-O	-6.22	1.16	1.24
1	B	285	CYS	C-O	-6.22	1.16	1.24
1	G	354	GLN	C-O	-6.21	1.16	1.24
1	M	354	GLN	C-O	-6.21	1.16	1.24
1	J	285	CYS	C-O	-6.21	1.16	1.24
1	A	285	CYS	C-O	-6.21	1.16	1.24
1	D	354	GLN	C-O	-6.21	1.16	1.24
1	X	285	CYS	C-O	-6.19	1.16	1.24
1	R	285	CYS	C-O	-6.18	1.16	1.24
1	N	285	CYS	C-O	-6.17	1.16	1.24
1	V	285	CYS	C-O	-6.16	1.16	1.24
1	E	354	GLN	C-O	-6.16	1.17	1.24
1	T	354	GLN	C-O	-6.16	1.17	1.24
1	W	285	CYS	C-O	-6.16	1.16	1.24
1	I	354	GLN	C-O	-6.16	1.17	1.24
1	L	354	GLN	C-O	-6.16	1.17	1.24
1	P	285	CYS	C-O	-6.15	1.16	1.24
1	S	210	ALA	CA-CB	-6.15	1.45	1.53
1	L	285	CYS	C-O	-6.15	1.16	1.24
1	O	210	ALA	CA-CB	-6.14	1.45	1.53
1	T	210	ALA	CA-CB	-6.14	1.45	1.53
1	S	285	CYS	C-O	-6.12	1.16	1.24
1	F	285	CYS	C-O	-6.12	1.16	1.24
1	G	210	ALA	CA-CB	-6.12	1.45	1.53
1	W	210	ALA	CA-CB	-6.12	1.45	1.53
1	B	210	ALA	CA-CB	-6.11	1.45	1.53
1	P	210	ALA	CA-CB	-6.11	1.45	1.53
1	U	285	CYS	C-O	-6.11	1.16	1.24
1	D	285	CYS	C-O	-6.11	1.16	1.24
1	O	285	CYS	C-O	-6.11	1.16	1.24
1	G	418	ILE	C-O	-6.10	1.17	1.24
1	H	285	CYS	C-O	-6.10	1.16	1.24
1	U	269	ILE	CA-C	-6.10	1.46	1.52
1	D	210	ALA	CA-CB	-6.10	1.45	1.53
1	Q	210	ALA	CA-CB	-6.10	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	210	ALA	CA-CB	-6.09	1.45	1.53
1	K	210	ALA	CA-CB	-6.09	1.45	1.53
1	E	285	CYS	C-O	-6.08	1.16	1.24
1	M	285	CYS	C-O	-6.08	1.16	1.24
1	T	418	ILE	C-O	-6.08	1.17	1.24
1	E	210	ALA	CA-CB	-6.08	1.45	1.53
1	I	285	CYS	C-O	-6.07	1.16	1.24
1	N	418	ILE	C-O	-6.07	1.17	1.24
1	U	418	ILE	C-O	-6.07	1.17	1.24
1	E	269	ILE	CA-C	-6.07	1.46	1.52
1	V	210	ALA	CA-CB	-6.06	1.45	1.53
1	G	269	ILE	CA-C	-6.06	1.46	1.52
1	N	27	ILE	C-O	-6.06	1.17	1.24
1	W	418	ILE	C-O	-6.06	1.17	1.24
1	X	418	ILE	C-O	-6.06	1.17	1.24
1	L	210	ALA	CA-CB	-6.05	1.45	1.53
1	W	269	ILE	CA-C	-6.05	1.46	1.52
1	F	269	ILE	CA-C	-6.05	1.46	1.52
1	R	269	ILE	CA-C	-6.05	1.46	1.52
1	R	27	ILE	C-O	-6.05	1.17	1.24
1	I	210	ALA	CA-CB	-6.04	1.45	1.53
1	X	210	ALA	CA-CB	-6.04	1.45	1.53
1	N	210	ALA	CA-CB	-6.04	1.45	1.53
1	B	269	ILE	CA-C	-6.04	1.46	1.52
1	C	269	ILE	CA-C	-6.04	1.46	1.52
1	F	418	ILE	C-O	-6.04	1.17	1.24
1	C	210	ALA	CA-CB	-6.04	1.45	1.53
1	O	418	ILE	C-O	-6.04	1.17	1.24
1	S	269	ILE	CA-C	-6.04	1.46	1.52
1	L	269	ILE	CA-C	-6.03	1.46	1.52
1	F	210	ALA	CA-CB	-6.03	1.45	1.53
1	M	418	ILE	C-O	-6.03	1.17	1.24
1	P	418	ILE	C-O	-6.02	1.17	1.24
1	R	418	ILE	C-O	-6.02	1.17	1.24
1	E	418	ILE	C-O	-6.02	1.17	1.24
1	J	269	ILE	CA-C	-6.02	1.46	1.52
1	D	418	ILE	C-O	-6.01	1.17	1.24
1	K	27	ILE	C-O	-6.01	1.17	1.24
1	P	27	ILE	C-O	-6.01	1.17	1.24
1	A	418	ILE	C-O	-6.01	1.17	1.24
1	H	418	ILE	C-O	-6.01	1.17	1.24
1	I	418	ILE	C-O	-6.01	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	418	ILE	C-O	-6.01	1.17	1.24
1	J	210	ALA	CA-CB	-6.01	1.45	1.53
1	A	210	ALA	CA-CB	-6.01	1.45	1.53
1	M	27	ILE	C-O	-6.01	1.17	1.24
1	H	210	ALA	CA-CB	-6.01	1.45	1.53
1	Q	27	ILE	C-O	-6.00	1.17	1.24
1	S	27	ILE	C-O	-5.99	1.17	1.24
1	N	269	ILE	CA-C	-5.99	1.46	1.52
1	K	418	ILE	C-O	-5.98	1.17	1.24
1	R	210	ALA	CA-CB	-5.98	1.45	1.53
1	J	27	ILE	C-O	-5.98	1.17	1.24
1	Q	418	ILE	C-O	-5.98	1.17	1.24
1	F	27	ILE	C-O	-5.97	1.17	1.24
1	V	418	ILE	C-O	-5.97	1.17	1.24
1	M	210	ALA	CA-CB	-5.97	1.45	1.53
1	S	418	ILE	C-O	-5.97	1.17	1.24
1	V	269	ILE	CA-C	-5.97	1.46	1.52
1	X	27	ILE	C-O	-5.97	1.17	1.24
1	E	27	ILE	C-O	-5.97	1.17	1.24
1	I	27	ILE	C-O	-5.96	1.17	1.24
1	W	27	ILE	C-O	-5.96	1.17	1.24
1	T	269	ILE	CA-C	-5.96	1.46	1.52
1	H	269	ILE	CA-C	-5.96	1.46	1.52
1	B	27	ILE	C-O	-5.96	1.17	1.24
1	B	418	ILE	C-O	-5.95	1.17	1.24
1	H	27	ILE	C-O	-5.95	1.17	1.24
1	D	269	ILE	CA-C	-5.94	1.46	1.52
1	Q	269	ILE	CA-C	-5.94	1.46	1.52
1	O	269	ILE	CA-C	-5.94	1.46	1.52
1	D	27	ILE	C-O	-5.94	1.17	1.24
1	G	27	ILE	C-O	-5.94	1.17	1.24
1	L	27	ILE	C-O	-5.93	1.17	1.24
1	W	489	ALA	CA-CB	-5.93	1.45	1.53
1	U	27	ILE	C-O	-5.93	1.17	1.24
1	T	27	ILE	C-O	-5.93	1.17	1.24
1	K	269	ILE	CA-C	-5.92	1.46	1.52
1	A	269	ILE	CA-C	-5.91	1.46	1.52
1	I	269	ILE	CA-C	-5.91	1.46	1.52
1	V	27	ILE	C-O	-5.90	1.17	1.24
1	X	269	ILE	CA-C	-5.89	1.46	1.52
1	J	418	ILE	C-O	-5.89	1.17	1.24
1	T	489	ALA	CA-CB	-5.88	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	269	ILE	CA-C	-5.88	1.46	1.52
1	P	269	ILE	CA-C	-5.88	1.46	1.52
1	C	418	ILE	C-O	-5.87	1.17	1.24
1	F	489	ALA	CA-CB	-5.87	1.45	1.53
1	O	27	ILE	C-O	-5.85	1.17	1.24
1	C	27	ILE	C-O	-5.85	1.17	1.24
1	S	489	ALA	CA-CB	-5.85	1.45	1.53
1	C	212	PHE	C-N	5.84	1.39	1.33
1	L	489	ALA	CA-CB	-5.84	1.45	1.53
1	I	489	ALA	CA-CB	-5.84	1.45	1.53
1	M	361	VAL	C-O	-5.84	1.17	1.24
1	F	212	PHE	C-N	5.84	1.39	1.33
1	A	27	ILE	C-O	-5.83	1.17	1.24
1	R	489	ALA	CA-CB	-5.83	1.45	1.53
1	H	489	ALA	CA-CB	-5.83	1.45	1.53
1	V	489	ALA	CA-CB	-5.83	1.45	1.53
1	G	489	ALA	CA-CB	-5.83	1.45	1.53
1	O	292	VAL	C-O	-5.83	1.18	1.24
1	Q	489	ALA	CA-CB	-5.82	1.45	1.53
1	D	489	ALA	CA-CB	-5.82	1.45	1.53
1	K	489	ALA	CA-CB	-5.82	1.45	1.53
1	T	292	VAL	C-O	-5.82	1.18	1.24
1	C	489	ALA	CA-CB	-5.81	1.45	1.53
1	H	292	VAL	C-O	-5.81	1.18	1.24
1	P	212	PHE	C-N	5.81	1.39	1.33
1	Q	361	VAL	C-O	-5.81	1.17	1.24
1	A	361	VAL	C-O	-5.81	1.17	1.24
1	J	489	ALA	CA-CB	-5.81	1.45	1.53
1	U	489	ALA	CA-CB	-5.81	1.45	1.53
1	E	489	ALA	CA-CB	-5.81	1.45	1.53
1	B	361	VAL	C-O	-5.80	1.17	1.24
1	M	489	ALA	CA-CB	-5.80	1.45	1.53
1	P	489	ALA	CA-CB	-5.80	1.45	1.53
1	R	212	PHE	C-N	5.80	1.39	1.33
1	G	361	VAL	C-O	-5.80	1.17	1.24
1	F	361	VAL	C-O	-5.80	1.17	1.24
1	I	361	VAL	C-O	-5.79	1.17	1.24
1	C	283	SER	C-O	-5.79	1.17	1.24
1	L	361	VAL	C-O	-5.79	1.17	1.24
1	X	292	VAL	C-O	-5.79	1.18	1.24
1	A	489	ALA	CA-CB	-5.78	1.45	1.53
1	S	212	PHE	C-N	5.78	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	212	PHE	C-N	5.78	1.39	1.33
1	W	292	VAL	C-O	-5.78	1.18	1.24
1	H	212	PHE	C-N	5.78	1.39	1.33
1	N	489	ALA	CA-CB	-5.78	1.45	1.53
1	E	292	VAL	C-O	-5.78	1.18	1.24
1	A	212	PHE	C-N	5.77	1.39	1.33
1	G	292	VAL	C-O	-5.77	1.18	1.24
1	T	361	VAL	C-O	-5.77	1.17	1.24
1	E	361	VAL	C-O	-5.77	1.17	1.24
1	X	489	ALA	CA-CB	-5.77	1.45	1.53
1	E	283	SER	C-O	-5.77	1.17	1.24
1	O	283	SER	C-O	-5.77	1.17	1.24
1	O	361	VAL	C-O	-5.77	1.17	1.24
1	I	212	PHE	C-N	5.76	1.39	1.33
1	T	212	PHE	C-N	5.76	1.39	1.33
1	H	397	VAL	C-O	-5.76	1.18	1.24
1	R	283	SER	C-O	-5.76	1.17	1.24
1	U	212	PHE	C-N	5.76	1.39	1.33
1	C	292	VAL	C-O	-5.75	1.18	1.24
1	U	283	SER	C-O	-5.75	1.17	1.24
1	O	489	ALA	CA-CB	-5.75	1.45	1.53
1	N	361	VAL	C-O	-5.75	1.17	1.24
1	P	361	VAL	C-O	-5.75	1.17	1.24
1	L	283	SER	C-O	-5.75	1.17	1.24
1	R	361	VAL	C-O	-5.74	1.17	1.24
1	W	361	VAL	C-O	-5.74	1.17	1.24
1	K	212	PHE	C-N	5.74	1.39	1.33
1	H	283	SER	C-O	-5.73	1.17	1.24
1	N	292	VAL	C-O	-5.73	1.18	1.24
1	H	361	VAL	C-O	-5.73	1.17	1.24
1	U	292	VAL	C-O	-5.73	1.18	1.24
1	J	361	VAL	C-O	-5.73	1.17	1.24
1	B	489	ALA	CA-CB	-5.72	1.45	1.53
1	Q	212	PHE	C-N	5.72	1.39	1.33
1	W	212	PHE	C-N	5.72	1.39	1.33
1	V	283	SER	C-O	-5.72	1.17	1.24
1	V	212	PHE	C-N	5.72	1.39	1.33
1	A	283	SER	C-O	-5.71	1.17	1.24
1	G	212	PHE	C-N	5.71	1.39	1.33
1	I	292	VAL	C-O	-5.71	1.18	1.24
1	R	292	VAL	C-O	-5.71	1.18	1.24
1	B	292	VAL	C-O	-5.71	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	191	ALA	C-O	-5.71	1.17	1.24
1	K	292	VAL	C-O	-5.71	1.18	1.24
1	C	361	VAL	C-O	-5.71	1.17	1.24
1	M	292	VAL	C-O	-5.71	1.18	1.24
1	S	283	SER	C-O	-5.71	1.17	1.24
1	U	361	VAL	C-O	-5.71	1.17	1.24
1	F	440	VAL	C-O	-5.71	1.18	1.24
1	W	283	SER	C-O	-5.70	1.17	1.24
1	D	292	VAL	C-O	-5.70	1.18	1.24
1	K	361	VAL	C-O	-5.70	1.17	1.24
1	J	212	PHE	C-N	5.70	1.39	1.33
1	K	283	SER	C-O	-5.70	1.17	1.24
1	X	361	VAL	C-O	-5.70	1.17	1.24
1	C	421	VAL	C-O	-5.70	1.18	1.24
1	P	292	VAL	C-O	-5.70	1.18	1.24
1	E	212	PHE	C-N	5.70	1.39	1.33
1	V	292	VAL	C-O	-5.70	1.18	1.24
1	J	283	SER	C-O	-5.69	1.17	1.24
1	X	212	PHE	C-N	5.69	1.39	1.33
1	D	283	SER	C-O	-5.69	1.17	1.24
1	I	283	SER	C-O	-5.69	1.17	1.24
1	Q	292	VAL	C-O	-5.68	1.18	1.24
1	V	397	VAL	C-O	-5.68	1.18	1.24
1	I	397	VAL	C-O	-5.68	1.18	1.24
1	O	212	PHE	C-N	5.68	1.39	1.33
1	Q	283	SER	C-O	-5.68	1.17	1.24
1	N	283	SER	C-O	-5.68	1.17	1.24
1	X	368	LYS	C-O	-5.68	1.17	1.24
1	J	292	VAL	C-O	-5.68	1.18	1.24
1	S	361	VAL	C-O	-5.67	1.17	1.24
1	T	283	SER	C-O	-5.67	1.17	1.24
1	T	440	VAL	C-O	-5.67	1.18	1.24
1	A	292	VAL	C-O	-5.67	1.18	1.24
1	S	292	VAL	C-O	-5.67	1.18	1.24
1	N	212	PHE	C-N	5.67	1.39	1.33
1	V	361	VAL	C-O	-5.67	1.17	1.24
1	N	397	VAL	C-O	-5.67	1.18	1.24
1	F	261	ALA	CA-CB	-5.67	1.45	1.52
1	F	292	VAL	C-O	-5.67	1.18	1.24
1	B	212	PHE	C-N	5.66	1.39	1.33
1	S	368	LYS	C-O	-5.66	1.17	1.24
1	B	283	SER	C-O	-5.66	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	440	VAL	C-O	-5.66	1.18	1.24
1	J	397	VAL	C-O	-5.66	1.18	1.24
1	P	283	SER	C-O	-5.66	1.17	1.24
1	S	397	VAL	C-O	-5.66	1.18	1.24
1	C	191	ALA	C-O	-5.65	1.17	1.24
1	D	212	PHE	C-N	5.65	1.39	1.33
1	W	397	VAL	C-O	-5.65	1.18	1.24
1	I	368	LYS	C-O	-5.65	1.17	1.24
1	M	191	ALA	C-O	-5.65	1.17	1.24
1	M	283	SER	C-O	-5.65	1.17	1.24
1	O	261	ALA	CA-CB	-5.65	1.45	1.52
1	A	191	ALA	C-O	-5.65	1.17	1.24
1	L	292	VAL	C-O	-5.65	1.18	1.24
1	B	397	VAL	C-O	-5.64	1.18	1.24
1	D	361	VAL	C-O	-5.64	1.17	1.24
1	G	283	SER	C-O	-5.64	1.17	1.24
1	K	271	ALA	C-O	-5.64	1.17	1.24
1	U	397	VAL	C-O	-5.64	1.18	1.24
1	T	397	VAL	C-O	-5.64	1.18	1.24
1	X	283	SER	C-O	-5.64	1.17	1.24
1	D	397	VAL	C-O	-5.64	1.18	1.24
1	F	283	SER	C-O	-5.63	1.17	1.24
1	H	271	ALA	C-O	-5.63	1.17	1.24
1	O	191	ALA	C-O	-5.63	1.17	1.24
1	D	368	LYS	C-O	-5.63	1.17	1.24
1	I	440	VAL	C-O	-5.63	1.18	1.24
1	L	421	VAL	C-O	-5.63	1.18	1.24
1	O	368	LYS	C-O	-5.63	1.17	1.24
1	V	368	LYS	C-O	-5.63	1.17	1.24
1	L	261	ALA	CA-CB	-5.63	1.45	1.52
1	M	212	PHE	C-N	5.63	1.39	1.33
1	R	397	VAL	C-O	-5.63	1.18	1.24
1	C	368	LYS	C-O	-5.63	1.17	1.24
1	G	397	VAL	C-O	-5.63	1.18	1.24
1	F	397	VAL	C-O	-5.62	1.18	1.24
1	O	421	VAL	C-O	-5.62	1.18	1.24
1	W	368	LYS	C-O	-5.62	1.17	1.24
1	A	368	LYS	C-O	-5.62	1.17	1.24
1	X	191	ALA	C-O	-5.62	1.17	1.24
1	P	440	VAL	C-O	-5.62	1.18	1.24
1	U	191	ALA	C-O	-5.62	1.17	1.24
1	B	368	LYS	C-O	-5.62	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	261	ALA	CA-CB	-5.62	1.45	1.52
1	R	191	ALA	C-O	-5.62	1.17	1.24
1	X	261	ALA	CA-CB	-5.62	1.45	1.52
1	O	397	VAL	C-O	-5.62	1.18	1.24
1	U	368	LYS	C-O	-5.61	1.17	1.24
1	D	271	ALA	C-O	-5.61	1.17	1.24
1	P	191	ALA	C-O	-5.61	1.17	1.24
1	Q	368	LYS	C-O	-5.61	1.17	1.24
1	R	368	LYS	C-O	-5.61	1.17	1.24
1	W	24	ILE	C-O	-5.61	1.18	1.24
1	E	440	VAL	C-O	-5.61	1.18	1.24
1	H	261	ALA	CA-CB	-5.61	1.45	1.52
1	K	261	ALA	CA-CB	-5.61	1.45	1.52
1	Q	397	VAL	C-O	-5.61	1.18	1.24
1	T	368	LYS	C-O	-5.61	1.17	1.24
1	J	421	VAL	C-O	-5.61	1.18	1.24
1	C	24	ILE	C-O	-5.60	1.18	1.24
1	G	368	LYS	C-O	-5.60	1.17	1.24
1	H	440	VAL	C-O	-5.60	1.18	1.24
1	J	440	VAL	C-O	-5.60	1.18	1.24
1	K	368	LYS	C-O	-5.60	1.17	1.24
1	M	271	ALA	C-O	-5.60	1.17	1.24
1	B	261	ALA	CA-CB	-5.60	1.45	1.52
1	H	421	VAL	C-O	-5.60	1.18	1.24
1	M	368	LYS	C-O	-5.60	1.17	1.24
1	G	191	ALA	C-O	-5.59	1.17	1.24
1	L	191	ALA	C-O	-5.59	1.17	1.24
1	I	191	ALA	C-O	-5.59	1.17	1.24
1	L	24	ILE	C-O	-5.59	1.18	1.24
1	Q	261	ALA	CA-CB	-5.59	1.45	1.52
1	F	24	ILE	C-O	-5.59	1.18	1.24
1	N	261	ALA	CA-CB	-5.59	1.45	1.52
1	B	440	VAL	C-O	-5.59	1.18	1.24
1	E	368	LYS	C-O	-5.59	1.17	1.24
1	J	368	LYS	C-O	-5.59	1.17	1.24
1	A	440	VAL	C-O	-5.59	1.18	1.24
1	B	421	VAL	C-O	-5.59	1.18	1.24
1	D	191	ALA	C-O	-5.59	1.17	1.24
1	R	271	ALA	C-O	-5.59	1.17	1.24
1	B	271	ALA	C-O	-5.58	1.17	1.24
1	G	440	VAL	C-O	-5.58	1.18	1.24
1	T	261	ALA	CA-CB	-5.58	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	261	ALA	CA-CB	-5.58	1.45	1.52
1	I	261	ALA	CA-CB	-5.58	1.45	1.52
1	L	368	LYS	C-O	-5.58	1.17	1.24
1	T	24	ILE	C-O	-5.58	1.18	1.24
1	S	440	VAL	C-O	-5.58	1.18	1.24
1	B	191	ALA	C-O	-5.58	1.17	1.24
1	W	191	ALA	C-O	-5.58	1.17	1.24
1	A	271	ALA	C-O	-5.58	1.17	1.24
1	X	397	VAL	C-O	-5.58	1.18	1.24
1	A	397	VAL	C-O	-5.57	1.18	1.24
1	Q	421	VAL	C-O	-5.57	1.18	1.24
1	A	261	ALA	CA-CB	-5.57	1.45	1.52
1	S	191	ALA	C-O	-5.57	1.17	1.24
1	D	261	ALA	CA-CB	-5.57	1.45	1.52
1	H	191	ALA	C-O	-5.57	1.17	1.24
1	Q	191	ALA	C-O	-5.57	1.17	1.24
1	J	261	ALA	CA-CB	-5.57	1.45	1.52
1	R	261	ALA	CA-CB	-5.57	1.45	1.52
1	W	213	ILE	C-O	-5.57	1.17	1.23
1	U	261	ALA	CA-CB	-5.57	1.45	1.52
1	C	261	ALA	CA-CB	-5.56	1.45	1.52
1	D	24	ILE	C-O	-5.56	1.18	1.24
1	O	271	ALA	C-O	-5.56	1.17	1.24
1	R	440	VAL	C-O	-5.56	1.18	1.24
1	X	440	VAL	C-O	-5.56	1.18	1.24
1	E	265	LEU	C-O	-5.56	1.17	1.24
1	Q	213	ILE	C-O	-5.56	1.17	1.23
1	V	271	ALA	C-O	-5.56	1.17	1.24
1	Q	265	LEU	C-O	-5.56	1.17	1.24
1	Q	271	ALA	C-O	-5.56	1.17	1.24
1	H	24	ILE	C-O	-5.56	1.18	1.24
1	K	397	VAL	C-O	-5.56	1.18	1.24
1	F	191	ALA	C-O	-5.55	1.17	1.24
1	F	271	ALA	C-O	-5.55	1.17	1.24
1	J	191	ALA	C-O	-5.55	1.17	1.24
1	M	397	VAL	C-O	-5.55	1.18	1.24
1	N	191	ALA	C-O	-5.55	1.17	1.24
1	P	397	VAL	C-O	-5.55	1.18	1.24
1	V	421	VAL	C-O	-5.55	1.18	1.24
1	P	265	LEU	C-O	-5.55	1.17	1.24
1	D	265	LEU	C-O	-5.55	1.17	1.24
1	G	261	ALA	CA-CB	-5.55	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	24	ILE	C-O	-5.55	1.18	1.24
1	H	368	LYS	C-O	-5.55	1.17	1.24
1	M	421	VAL	C-O	-5.55	1.18	1.24
1	N	368	LYS	C-O	-5.55	1.17	1.24
1	P	261	ALA	CA-CB	-5.55	1.45	1.52
1	V	191	ALA	C-O	-5.54	1.17	1.24
1	X	421	VAL	C-O	-5.54	1.18	1.24
1	U	440	VAL	C-O	-5.54	1.18	1.24
1	E	271	ALA	C-O	-5.54	1.17	1.24
1	F	368	LYS	C-O	-5.54	1.17	1.24
1	P	368	LYS	C-O	-5.54	1.17	1.24
1	C	397	VAL	C-O	-5.54	1.18	1.24
1	D	440	VAL	C-O	-5.54	1.18	1.24
1	O	440	VAL	C-O	-5.54	1.18	1.24
1	Q	440	VAL	C-O	-5.54	1.18	1.24
1	S	271	ALA	C-O	-5.54	1.17	1.24
1	N	271	ALA	C-O	-5.53	1.17	1.24
1	W	440	VAL	C-O	-5.53	1.18	1.24
1	C	271	ALA	C-O	-5.53	1.17	1.24
1	E	421	VAL	C-O	-5.53	1.18	1.24
1	T	271	ALA	C-O	-5.53	1.17	1.24
1	A	24	ILE	C-O	-5.53	1.18	1.24
1	V	265	LEU	C-O	-5.53	1.17	1.24
1	L	397	VAL	C-O	-5.53	1.18	1.24
1	U	271	ALA	C-O	-5.53	1.17	1.24
1	X	265	LEU	C-O	-5.53	1.17	1.24
1	B	265	LEU	C-O	-5.53	1.17	1.24
1	K	421	VAL	C-O	-5.53	1.18	1.24
1	M	440	VAL	C-O	-5.53	1.18	1.24
1	R	213	ILE	C-O	-5.53	1.17	1.23
1	S	261	ALA	CA-CB	-5.52	1.45	1.52
1	E	24	ILE	C-O	-5.52	1.18	1.24
1	W	265	LEU	C-O	-5.52	1.17	1.24
1	G	421	VAL	C-O	-5.52	1.18	1.24
1	S	421	VAL	C-O	-5.52	1.18	1.24
1	J	271	ALA	C-O	-5.52	1.17	1.24
1	R	265	LEU	C-O	-5.52	1.17	1.24
1	W	271	ALA	C-O	-5.52	1.17	1.24
1	U	213	ILE	C-O	-5.52	1.17	1.23
1	F	421	VAL	C-O	-5.51	1.18	1.24
1	K	191	ALA	C-O	-5.51	1.17	1.24
1	Q	24	ILE	C-O	-5.51	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	VAL	C-O	-5.51	1.18	1.24
1	G	265	LEU	C-O	-5.51	1.17	1.24
1	L	271	ALA	C-O	-5.51	1.17	1.24
1	S	265	LEU	C-O	-5.51	1.17	1.24
1	T	421	VAL	C-O	-5.51	1.18	1.24
1	W	421	VAL	C-O	-5.51	1.18	1.24
1	K	440	VAL	C-O	-5.51	1.18	1.24
1	O	24	ILE	C-O	-5.51	1.18	1.24
1	I	421	VAL	C-O	-5.50	1.18	1.24
1	M	24	ILE	C-O	-5.50	1.18	1.24
1	P	213	ILE	C-O	-5.50	1.17	1.23
1	V	261	ALA	CA-CB	-5.50	1.45	1.52
1	N	421	VAL	C-O	-5.50	1.18	1.24
1	E	397	VAL	C-O	-5.50	1.18	1.24
1	H	213	ILE	C-O	-5.50	1.17	1.23
1	O	265	LEU	C-O	-5.50	1.17	1.24
1	X	271	ALA	C-O	-5.50	1.17	1.24
1	L	213	ILE	C-O	-5.50	1.17	1.23
1	N	24	ILE	C-O	-5.50	1.18	1.24
1	N	440	VAL	C-O	-5.50	1.18	1.24
1	U	421	VAL	C-O	-5.50	1.18	1.24
1	V	24	ILE	C-O	-5.50	1.18	1.24
1	P	421	VAL	C-O	-5.50	1.18	1.24
1	S	24	ILE	C-O	-5.50	1.18	1.24
1	K	480	HIS	C-O	-5.49	1.19	1.24
1	V	440	VAL	C-O	-5.49	1.18	1.24
1	G	271	ALA	C-O	-5.49	1.17	1.24
1	K	24	ILE	C-O	-5.49	1.18	1.24
1	I	271	ALA	C-O	-5.49	1.17	1.24
1	R	421	VAL	C-O	-5.49	1.18	1.24
1	T	480	HIS	C-O	-5.49	1.19	1.24
1	B	24	ILE	C-O	-5.49	1.18	1.24
1	I	265	LEU	C-O	-5.49	1.17	1.24
1	C	265	LEU	C-O	-5.49	1.17	1.24
1	F	265	LEU	C-O	-5.49	1.17	1.24
1	K	265	LEU	C-O	-5.49	1.17	1.24
1	T	191	ALA	C-O	-5.48	1.17	1.24
1	D	421	VAL	C-O	-5.48	1.18	1.24
1	M	265	LEU	C-O	-5.48	1.17	1.24
1	P	24	ILE	C-O	-5.48	1.18	1.24
1	X	277	ALA	C-O	-5.48	1.17	1.24
1	M	213	ILE	C-O	-5.47	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	440	VAL	C-O	-5.47	1.18	1.24
1	J	24	ILE	C-O	-5.47	1.18	1.24
1	Q	277	ALA	C-O	-5.47	1.17	1.24
1	X	24	ILE	C-O	-5.46	1.18	1.24
1	A	265	LEU	C-O	-5.46	1.17	1.24
1	M	261	ALA	CA-CB	-5.46	1.45	1.52
1	P	480	HIS	C-O	-5.46	1.19	1.24
1	V	213	ILE	C-O	-5.46	1.17	1.23
1	E	480	HIS	C-O	-5.45	1.19	1.24
1	G	24	ILE	C-O	-5.45	1.18	1.24
1	O	213	ILE	C-O	-5.45	1.17	1.23
1	S	213	ILE	C-O	-5.45	1.17	1.23
1	P	271	ALA	C-O	-5.45	1.17	1.24
1	P	334	ALA	CA-CB	-5.45	1.44	1.53
1	R	277	ALA	C-O	-5.45	1.17	1.24
1	F	480	HIS	C-O	-5.44	1.19	1.24
1	I	213	ILE	C-O	-5.44	1.17	1.23
1	T	265	LEU	C-O	-5.44	1.17	1.24
1	V	334	ALA	CA-CB	-5.44	1.44	1.53
1	R	24	ILE	C-O	-5.44	1.18	1.24
1	W	480	HIS	C-O	-5.44	1.19	1.24
1	C	480	HIS	C-O	-5.44	1.19	1.24
1	N	213	ILE	C-O	-5.44	1.17	1.23
1	U	265	LEU	C-O	-5.44	1.17	1.24
1	L	265	LEU	C-O	-5.44	1.17	1.24
1	G	277	ALA	C-O	-5.43	1.17	1.24
1	X	274	VAL	C-O	-5.43	1.17	1.24
1	A	213	ILE	C-O	-5.43	1.17	1.23
1	I	334	ALA	CA-CB	-5.43	1.44	1.53
1	N	265	LEU	C-O	-5.43	1.17	1.24
1	E	213	ILE	C-O	-5.43	1.17	1.23
1	J	265	LEU	C-O	-5.43	1.17	1.24
1	K	213	ILE	C-O	-5.43	1.17	1.23
1	C	213	ILE	C-O	-5.43	1.17	1.23
1	U	266	GLY	C-O	-5.43	1.17	1.23
1	A	266	GLY	C-O	-5.43	1.17	1.23
1	R	334	ALA	CA-CB	-5.43	1.44	1.53
1	F	213	ILE	C-O	-5.42	1.17	1.23
1	I	480	HIS	C-O	-5.42	1.19	1.24
1	U	24	ILE	C-O	-5.42	1.18	1.24
1	N	480	HIS	C-O	-5.42	1.19	1.24
1	Q	287	VAL	C-O	-5.42	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	480	HIS	C-O	-5.42	1.19	1.24
1	B	266	GLY	C-O	-5.42	1.17	1.23
1	T	334	ALA	CA-CB	-5.42	1.44	1.53
1	D	213	ILE	C-O	-5.42	1.17	1.23
1	J	480	HIS	C-O	-5.41	1.19	1.24
1	N	274	VAL	C-O	-5.41	1.17	1.24
1	B	277	ALA	C-O	-5.41	1.17	1.24
1	J	213	ILE	C-O	-5.41	1.17	1.23
1	Q	289	GLY	C-O	-5.41	1.18	1.24
1	H	480	HIS	C-O	-5.41	1.19	1.24
1	D	334	ALA	CA-CB	-5.41	1.44	1.53
1	H	334	ALA	CA-CB	-5.41	1.44	1.53
1	I	277	ALA	C-O	-5.41	1.17	1.24
1	U	277	ALA	C-O	-5.41	1.17	1.24
1	X	334	ALA	CA-CB	-5.41	1.44	1.53
1	O	480	HIS	C-O	-5.41	1.19	1.24
1	A	277	ALA	C-O	-5.40	1.17	1.24
1	H	265	LEU	C-O	-5.40	1.17	1.24
1	L	334	ALA	CA-CB	-5.40	1.44	1.53
1	E	287	VAL	C-O	-5.40	1.17	1.24
1	Q	274	VAL	C-O	-5.40	1.17	1.24
1	V	266	GLY	C-O	-5.40	1.17	1.23
1	H	274	VAL	C-O	-5.40	1.17	1.24
1	V	417	PRO	C-O	-5.39	1.17	1.23
1	W	417	PRO	C-O	-5.39	1.17	1.23
1	G	364	ASN	C-O	-5.39	1.17	1.24
1	A	417	PRO	C-O	-5.39	1.17	1.23
1	R	274	VAL	C-O	-5.39	1.17	1.24
1	L	480	HIS	C-O	-5.39	1.19	1.24
1	K	287	VAL	C-O	-5.39	1.17	1.24
1	M	480	HIS	C-O	-5.39	1.19	1.24
1	T	266	GLY	C-O	-5.39	1.17	1.23
1	U	417	PRO	C-O	-5.39	1.17	1.23
1	G	334	ALA	CA-CB	-5.38	1.44	1.53
1	J	277	ALA	C-O	-5.38	1.17	1.24
1	M	274	VAL	C-O	-5.38	1.17	1.24
1	U	334	ALA	CA-CB	-5.38	1.44	1.53
1	E	334	ALA	CA-CB	-5.38	1.44	1.53
1	B	289	GLY	C-O	-5.38	1.18	1.24
1	K	266	GLY	C-O	-5.38	1.17	1.23
1	W	334	ALA	CA-CB	-5.38	1.44	1.53
1	C	334	ALA	CA-CB	-5.38	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	287	VAL	C-O	-5.38	1.17	1.24
1	L	289	GLY	C-O	-5.38	1.18	1.24
1	M	289	GLY	C-O	-5.38	1.18	1.24
1	N	289	GLY	C-O	-5.38	1.18	1.24
1	E	364	ASN	C-O	-5.38	1.17	1.24
1	J	266	GLY	C-O	-5.38	1.17	1.23
1	J	287	VAL	C-O	-5.38	1.17	1.24
1	D	277	ALA	C-O	-5.38	1.17	1.24
1	R	289	GLY	C-O	-5.38	1.18	1.24
1	L	277	ALA	C-O	-5.38	1.17	1.24
1	G	274	VAL	C-O	-5.37	1.17	1.24
1	P	266	GLY	C-O	-5.37	1.17	1.23
1	E	266	GLY	C-O	-5.37	1.17	1.23
1	G	213	ILE	C-O	-5.37	1.18	1.23
1	K	289	GLY	C-O	-5.37	1.18	1.24
1	S	277	ALA	C-O	-5.37	1.17	1.24
1	S	480	HIS	C-O	-5.37	1.19	1.24
1	F	334	ALA	CA-CB	-5.37	1.44	1.53
1	J	269	ILE	N-CA	-5.37	1.40	1.46
1	I	318	ASN	C-O	-5.37	1.17	1.24
1	K	277	ALA	C-O	-5.37	1.17	1.24
1	B	334	ALA	CA-CB	-5.37	1.44	1.53
1	U	480	HIS	C-O	-5.37	1.19	1.24
1	C	277	ALA	C-O	-5.36	1.17	1.24
1	D	364	ASN	C-O	-5.36	1.17	1.24
1	L	269	ILE	N-CA	-5.36	1.40	1.46
1	L	318	ASN	C-O	-5.36	1.17	1.24
1	F	266	GLY	C-O	-5.36	1.17	1.23
1	L	417	PRO	C-O	-5.36	1.17	1.23
1	O	417	PRO	C-O	-5.36	1.17	1.23
1	W	266	GLY	C-O	-5.36	1.17	1.23
1	C	266	GLY	C-O	-5.36	1.17	1.23
1	F	277	ALA	C-O	-5.36	1.17	1.24
1	F	318	ASN	C-O	-5.36	1.17	1.24
1	H	287	VAL	C-O	-5.36	1.17	1.24
1	T	364	ASN	C-O	-5.36	1.17	1.24
1	W	287	VAL	C-O	-5.36	1.17	1.24
1	R	266	GLY	C-O	-5.36	1.17	1.23
1	B	417	PRO	C-O	-5.36	1.17	1.23
1	H	289	GLY	C-O	-5.36	1.18	1.24
1	J	334	ALA	CA-CB	-5.36	1.44	1.53
1	T	289	GLY	C-O	-5.36	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	277	ALA	C-O	-5.35	1.17	1.24
1	K	291	PRO	C-O	-5.35	1.17	1.23
1	Q	334	ALA	CA-CB	-5.35	1.44	1.53
1	N	334	ALA	CA-CB	-5.35	1.44	1.53
1	X	213	ILE	C-O	-5.35	1.18	1.23
1	X	287	VAL	C-O	-5.35	1.17	1.24
1	E	274	VAL	C-O	-5.35	1.17	1.24
1	R	287	VAL	C-O	-5.35	1.17	1.24
1	D	417	PRO	C-O	-5.35	1.17	1.23
1	F	289	GLY	C-O	-5.35	1.18	1.24
1	L	266	GLY	C-O	-5.35	1.17	1.23
1	N	266	GLY	C-O	-5.35	1.17	1.23
1	O	274	VAL	C-O	-5.35	1.17	1.24
1	Q	266	GLY	C-O	-5.35	1.17	1.23
1	R	480	HIS	C-O	-5.35	1.19	1.24
1	V	277	ALA	C-O	-5.35	1.17	1.24
1	O	287	VAL	C-O	-5.35	1.17	1.24
1	B	213	ILE	C-O	-5.34	1.18	1.23
1	D	287	VAL	C-O	-5.34	1.17	1.24
1	H	266	GLY	C-O	-5.34	1.17	1.23
1	I	287	VAL	C-O	-5.34	1.17	1.24
1	S	334	ALA	CA-CB	-5.34	1.44	1.53
1	X	266	GLY	C-O	-5.34	1.17	1.23
1	T	287	VAL	C-O	-5.34	1.17	1.24
1	D	269	ILE	N-CA	-5.34	1.40	1.46
1	O	334	ALA	CA-CB	-5.34	1.45	1.53
1	S	287	VAL	C-O	-5.34	1.17	1.24
1	T	274	VAL	C-O	-5.34	1.17	1.24
1	G	291	PRO	C-O	-5.34	1.17	1.23
1	P	364	ASN	C-O	-5.34	1.17	1.24
1	T	280	ILE	C-O	-5.34	1.18	1.24
1	V	289	GLY	C-O	-5.34	1.18	1.24
1	C	318	ASN	C-O	-5.34	1.17	1.24
1	K	417	PRO	C-O	-5.34	1.17	1.23
1	E	318	ASN	C-O	-5.34	1.17	1.24
1	P	269	ILE	N-CA	-5.33	1.40	1.46
1	V	287	VAL	C-O	-5.33	1.17	1.24
1	M	277	ALA	C-O	-5.33	1.17	1.24
1	M	291	PRO	C-O	-5.33	1.17	1.23
1	S	266	GLY	C-O	-5.33	1.17	1.23
1	A	334	ALA	CA-CB	-5.33	1.45	1.53
1	B	318	ASN	C-O	-5.33	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	266	GLY	C-O	-5.33	1.17	1.23
1	M	318	ASN	C-O	-5.33	1.17	1.24
1	S	417	PRO	C-O	-5.33	1.17	1.23
1	T	213	ILE	C-O	-5.33	1.18	1.23
1	H	318	ASN	C-O	-5.33	1.17	1.24
1	J	417	PRO	C-O	-5.33	1.17	1.23
1	K	274	VAL	C-O	-5.33	1.17	1.24
1	U	269	ILE	N-CA	-5.33	1.40	1.46
1	H	417	PRO	C-O	-5.33	1.17	1.23
1	K	334	ALA	CA-CB	-5.33	1.45	1.53
1	M	334	ALA	CA-CB	-5.33	1.45	1.53
1	R	318	ASN	C-O	-5.33	1.17	1.24
1	G	318	ASN	C-O	-5.33	1.17	1.24
1	X	318	ASN	C-O	-5.33	1.17	1.24
1	C	417	PRO	C-O	-5.33	1.17	1.23
1	X	269	ILE	N-CA	-5.32	1.40	1.46
1	X	364	ASN	C-O	-5.32	1.17	1.24
1	G	289	GLY	C-O	-5.32	1.18	1.24
1	X	289	GLY	C-O	-5.32	1.18	1.24
1	C	287	VAL	C-O	-5.32	1.17	1.24
1	O	478	VAL	C-O	-5.32	1.18	1.24
1	V	274	VAL	C-O	-5.32	1.17	1.24
1	W	289	GLY	C-O	-5.32	1.18	1.24
1	E	289	GLY	C-O	-5.32	1.18	1.24
1	F	417	PRO	C-O	-5.32	1.17	1.23
1	H	280	ILE	C-O	-5.32	1.18	1.24
1	J	289	GLY	C-O	-5.32	1.18	1.24
1	N	277	ALA	C-O	-5.32	1.17	1.24
1	Q	417	PRO	C-O	-5.32	1.17	1.23
1	D	266	GLY	C-O	-5.32	1.17	1.23
1	E	417	PRO	C-O	-5.32	1.17	1.23
1	M	287	VAL	C-O	-5.32	1.17	1.24
1	P	274	VAL	C-O	-5.32	1.17	1.24
1	U	289	GLY	C-O	-5.32	1.18	1.24
1	B	480	HIS	C-O	-5.31	1.19	1.24
1	O	364	ASN	C-O	-5.31	1.18	1.24
1	S	274	VAL	C-O	-5.31	1.17	1.24
1	A	269	ILE	N-CA	-5.31	1.40	1.46
1	H	364	ASN	C-O	-5.31	1.18	1.24
1	I	274	VAL	C-O	-5.31	1.17	1.24
1	O	280	ILE	C-O	-5.31	1.18	1.24
1	W	269	ILE	N-CA	-5.31	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	274	VAL	C-O	-5.31	1.17	1.24
1	B	258	ILE	C-O	-5.31	1.18	1.24
1	G	417	PRO	C-O	-5.31	1.17	1.23
1	S	318	ASN	C-O	-5.31	1.17	1.24
1	W	277	ALA	C-O	-5.31	1.18	1.24
1	B	287	VAL	C-O	-5.31	1.17	1.24
1	O	277	ALA	C-O	-5.31	1.18	1.24
1	R	291	PRO	C-O	-5.31	1.17	1.23
1	V	318	ASN	C-O	-5.31	1.17	1.24
1	A	287	VAL	C-O	-5.31	1.17	1.24
1	I	364	ASN	C-O	-5.31	1.18	1.24
1	O	318	ASN	C-O	-5.30	1.17	1.24
1	P	277	ALA	C-O	-5.30	1.18	1.24
1	G	480	HIS	C-O	-5.30	1.19	1.24
1	M	266	GLY	C-O	-5.30	1.17	1.23
1	O	266	GLY	C-O	-5.30	1.17	1.23
1	A	291	PRO	C-O	-5.30	1.17	1.23
1	P	287	VAL	C-O	-5.30	1.17	1.24
1	P	289	GLY	C-O	-5.30	1.18	1.24
1	L	274	VAL	C-O	-5.30	1.17	1.24
1	C	269	ILE	N-CA	-5.30	1.40	1.46
1	O	291	PRO	C-O	-5.30	1.17	1.23
1	R	417	PRO	C-O	-5.30	1.17	1.23
1	D	318	ASN	C-O	-5.29	1.17	1.24
1	W	364	ASN	C-O	-5.29	1.18	1.24
1	V	364	ASN	C-O	-5.29	1.18	1.24
1	I	269	ILE	N-CA	-5.29	1.40	1.46
1	S	364	ASN	C-O	-5.29	1.18	1.24
1	U	287	VAL	C-O	-5.29	1.17	1.24
1	A	274	VAL	C-O	-5.29	1.17	1.24
1	M	280	ILE	C-O	-5.29	1.18	1.24
1	O	289	GLY	C-O	-5.29	1.18	1.24
1	D	289	GLY	C-O	-5.29	1.18	1.24
1	N	318	ASN	C-O	-5.29	1.17	1.24
1	U	274	VAL	C-O	-5.29	1.17	1.24
1	F	291	PRO	C-O	-5.29	1.17	1.23
1	J	291	PRO	C-O	-5.29	1.17	1.23
1	G	266	GLY	C-O	-5.28	1.17	1.23
1	G	287	VAL	C-O	-5.28	1.17	1.24
1	X	480	HIS	C-O	-5.28	1.19	1.24
1	A	318	ASN	C-O	-5.28	1.17	1.24
1	K	318	ASN	C-O	-5.28	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	291	PRO	C-O	-5.28	1.17	1.23
1	D	274	VAL	C-O	-5.28	1.17	1.24
1	J	274	VAL	C-O	-5.28	1.17	1.24
1	L	364	ASN	C-O	-5.28	1.18	1.24
1	N	291	PRO	C-O	-5.28	1.17	1.23
1	P	291	PRO	C-O	-5.28	1.17	1.23
1	P	318	ASN	C-O	-5.28	1.17	1.24
1	C	364	ASN	C-O	-5.28	1.18	1.24
1	Q	480	HIS	C-O	-5.28	1.19	1.24
1	F	478	VAL	C-O	-5.27	1.18	1.24
1	T	277	ALA	C-O	-5.27	1.18	1.24
1	M	417	PRO	C-O	-5.27	1.17	1.23
1	Q	280	ILE	C-O	-5.27	1.18	1.24
1	X	258	ILE	C-O	-5.27	1.18	1.24
1	B	364	ASN	C-O	-5.27	1.18	1.24
1	P	417	PRO	C-O	-5.27	1.17	1.23
1	Q	269	ILE	N-CA	-5.27	1.40	1.46
1	A	364	ASN	C-O	-5.27	1.18	1.24
1	R	258	ILE	C-O	-5.27	1.18	1.24
1	A	280	ILE	C-O	-5.27	1.18	1.24
1	R	364	ASN	C-O	-5.27	1.18	1.24
1	E	280	ILE	C-O	-5.26	1.18	1.24
1	K	280	ILE	C-O	-5.26	1.18	1.24
1	Q	258	ILE	C-O	-5.26	1.18	1.24
1	V	269	ILE	N-CA	-5.26	1.40	1.46
1	I	289	GLY	C-O	-5.26	1.18	1.24
1	A	480	HIS	C-O	-5.26	1.19	1.24
1	E	258	ILE	C-O	-5.26	1.18	1.24
1	I	258	ILE	C-O	-5.26	1.18	1.24
1	I	478	VAL	C-O	-5.26	1.18	1.24
1	O	258	ILE	C-O	-5.26	1.18	1.24
1	S	280	ILE	C-O	-5.26	1.18	1.24
1	U	258	ILE	C-O	-5.26	1.18	1.24
1	W	318	ASN	C-O	-5.26	1.17	1.24
1	B	269	ILE	N-CA	-5.26	1.40	1.46
1	I	417	PRO	C-O	-5.26	1.17	1.23
1	J	478	VAL	C-O	-5.26	1.18	1.24
1	O	269	ILE	N-CA	-5.26	1.40	1.46
1	A	478	VAL	C-O	-5.26	1.18	1.24
1	C	478	VAL	C-O	-5.25	1.18	1.24
1	J	318	ASN	C-O	-5.25	1.17	1.24
1	W	291	PRO	C-O	-5.25	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	291	PRO	C-O	-5.25	1.17	1.23
1	T	318	ASN	C-O	-5.25	1.17	1.24
1	U	280	ILE	C-O	-5.25	1.18	1.24
1	V	291	PRO	C-O	-5.25	1.17	1.23
1	A	289	GLY	C-O	-5.25	1.18	1.24
1	N	417	PRO	C-O	-5.25	1.17	1.23
1	F	287	VAL	C-O	-5.25	1.17	1.24
1	N	364	ASN	C-O	-5.25	1.18	1.24
1	A	258	ILE	C-O	-5.25	1.18	1.24
1	B	291	PRO	C-O	-5.25	1.17	1.23
1	Q	270	PRO	C-O	-5.25	1.18	1.23
1	T	269	ILE	C-O	-5.25	1.17	1.24
1	P	478	VAL	C-O	-5.24	1.18	1.24
1	T	291	PRO	C-O	-5.24	1.17	1.23
1	H	478	VAL	C-O	-5.24	1.18	1.24
1	Q	364	ASN	C-O	-5.24	1.18	1.24
1	S	289	GLY	C-O	-5.24	1.18	1.24
1	U	291	PRO	C-O	-5.24	1.17	1.23
1	I	280	ILE	C-O	-5.24	1.18	1.24
1	J	208	ILE	C-O	-5.24	1.18	1.24
1	K	269	ILE	N-CA	-5.24	1.40	1.46
1	T	478	VAL	C-O	-5.24	1.18	1.24
1	G	258	ILE	C-O	-5.24	1.18	1.24
1	J	364	ASN	C-O	-5.24	1.18	1.24
1	B	280	ILE	C-O	-5.24	1.18	1.24
1	J	258	ILE	C-O	-5.24	1.18	1.24
1	O	270	PRO	C-O	-5.24	1.18	1.23
1	P	270	PRO	C-O	-5.24	1.18	1.23
1	U	318	ASN	C-O	-5.24	1.17	1.24
1	W	478	VAL	C-O	-5.24	1.18	1.24
1	M	269	ILE	N-CA	-5.23	1.40	1.46
1	K	258	ILE	C-O	-5.23	1.18	1.24
1	U	364	ASN	C-O	-5.23	1.18	1.24
1	I	269	ILE	C-O	-5.23	1.17	1.24
1	M	364	ASN	C-O	-5.23	1.18	1.24
1	N	287	VAL	C-O	-5.23	1.18	1.24
1	C	280	ILE	C-O	-5.23	1.18	1.24
1	W	280	ILE	C-O	-5.23	1.18	1.24
1	K	364	ASN	C-O	-5.23	1.18	1.24
1	D	480	HIS	C-O	-5.22	1.19	1.24
1	F	364	ASN	C-O	-5.22	1.18	1.24
1	D	280	ILE	C-O	-5.22	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	277	ALA	C-O	-5.22	1.18	1.24
1	W	270	PRO	C-O	-5.22	1.18	1.23
1	D	291	PRO	C-O	-5.22	1.17	1.23
1	F	280	ILE	C-O	-5.22	1.18	1.24
1	N	478	VAL	C-O	-5.22	1.18	1.24
1	Q	478	VAL	C-O	-5.22	1.18	1.24
1	U	478	VAL	C-O	-5.22	1.18	1.24
1	C	291	PRO	C-O	-5.22	1.17	1.23
1	R	269	ILE	N-CA	-5.22	1.40	1.46
1	C	289	GLY	C-O	-5.22	1.18	1.24
1	E	291	PRO	C-O	-5.22	1.17	1.23
1	B	478	VAL	C-O	-5.21	1.18	1.24
1	G	478	VAL	C-O	-5.21	1.18	1.24
1	M	258	ILE	C-O	-5.21	1.18	1.24
1	P	280	ILE	C-O	-5.21	1.18	1.24
1	W	258	ILE	C-O	-5.21	1.18	1.24
1	X	417	PRO	C-O	-5.21	1.17	1.23
1	C	274	VAL	C-O	-5.21	1.17	1.24
1	S	270	PRO	C-O	-5.21	1.18	1.23
1	G	315	ASP	C-O	-5.21	1.18	1.24
1	M	478	VAL	C-O	-5.21	1.18	1.24
1	V	258	ILE	C-O	-5.21	1.19	1.24
1	F	269	ILE	N-CA	-5.21	1.40	1.46
1	Q	318	ASN	C-O	-5.21	1.17	1.24
1	T	269	ILE	N-CA	-5.21	1.40	1.46
1	K	269	ILE	C-O	-5.20	1.17	1.24
1	P	269	ILE	C-O	-5.20	1.17	1.24
1	N	269	ILE	N-CA	-5.20	1.40	1.46
1	X	291	PRO	C-O	-5.20	1.17	1.23
1	D	258	ILE	C-O	-5.20	1.19	1.24
1	G	270	PRO	C-O	-5.20	1.18	1.23
1	H	258	ILE	C-O	-5.20	1.19	1.24
1	M	270	PRO	C-O	-5.20	1.18	1.23
1	L	280	ILE	C-O	-5.20	1.18	1.24
1	L	478	VAL	C-O	-5.20	1.18	1.24
1	U	208	ILE	C-O	-5.20	1.18	1.24
1	F	274	VAL	C-O	-5.19	1.17	1.24
1	E	478	VAL	C-O	-5.19	1.18	1.24
1	B	269	ILE	C-O	-5.19	1.17	1.24
1	B	274	VAL	C-O	-5.19	1.17	1.24
1	H	291	PRO	C-O	-5.19	1.17	1.23
1	V	270	PRO	C-O	-5.19	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	269	ILE	N-CA	-5.19	1.40	1.46
1	E	315	ASP	C-O	-5.18	1.18	1.24
1	S	269	ILE	C-O	-5.18	1.17	1.24
1	T	417	PRO	C-O	-5.18	1.17	1.23
1	A	270	PRO	C-O	-5.18	1.18	1.23
1	H	269	ILE	C-O	-5.18	1.17	1.24
1	N	258	ILE	C-O	-5.18	1.19	1.24
1	E	269	ILE	N-CA	-5.18	1.40	1.46
1	C	258	ILE	C-O	-5.18	1.19	1.24
1	D	478	VAL	C-O	-5.18	1.18	1.24
1	N	315	ASP	C-O	-5.17	1.18	1.24
1	I	291	PRO	C-O	-5.17	1.17	1.23
1	R	270	PRO	C-O	-5.17	1.18	1.23
1	C	208	ILE	C-O	-5.17	1.18	1.24
1	J	280	ILE	C-O	-5.17	1.18	1.24
1	H	269	ILE	N-CA	-5.17	1.40	1.46
1	N	270	PRO	C-O	-5.17	1.18	1.23
1	A	269	ILE	C-O	-5.17	1.18	1.24
1	L	291	PRO	C-O	-5.17	1.17	1.23
1	T	258	ILE	C-O	-5.17	1.19	1.24
1	U	315	ASP	C-O	-5.17	1.18	1.24
1	X	280	ILE	C-O	-5.17	1.18	1.24
1	C	270	PRO	C-O	-5.17	1.18	1.23
1	I	270	PRO	C-O	-5.16	1.18	1.23
1	X	478	VAL	C-O	-5.16	1.18	1.24
1	E	269	ILE	C-O	-5.16	1.18	1.24
1	D	269	ILE	C-O	-5.16	1.18	1.24
1	G	269	ILE	C-O	-5.16	1.18	1.24
1	P	258	ILE	C-O	-5.16	1.18	1.24
1	C	269	ILE	C-O	-5.16	1.18	1.24
1	L	270	PRO	C-O	-5.15	1.18	1.23
1	R	315	ASP	C-O	-5.15	1.18	1.24
1	S	269	ILE	N-CA	-5.15	1.40	1.46
1	S	315	ASP	C-O	-5.15	1.18	1.24
1	W	269	ILE	C-O	-5.15	1.18	1.24
1	L	258	ILE	C-O	-5.14	1.19	1.24
1	E	270	PRO	C-O	-5.14	1.18	1.23
1	L	315	ASP	C-O	-5.14	1.18	1.24
1	S	478	VAL	C-O	-5.14	1.18	1.24
1	U	270	PRO	C-O	-5.14	1.18	1.23
1	V	269	ILE	C-O	-5.14	1.18	1.24
1	G	208	ILE	C-O	-5.14	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	478	VAL	C-O	-5.14	1.18	1.24
1	R	208	ILE	C-O	-5.13	1.18	1.24
1	F	270	PRO	C-O	-5.13	1.18	1.23
1	X	270	PRO	C-O	-5.13	1.18	1.23
1	N	280	ILE	C-O	-5.13	1.18	1.24
1	M	269	ILE	C-O	-5.13	1.18	1.24
1	H	270	PRO	C-O	-5.13	1.18	1.23
1	X	269	ILE	C-O	-5.13	1.18	1.24
1	L	269	ILE	C-O	-5.12	1.18	1.24
1	O	315	ASP	C-O	-5.12	1.18	1.24
1	T	208	ILE	C-O	-5.12	1.18	1.24
1	D	315	ASP	C-O	-5.12	1.18	1.24
1	R	269	ILE	C-O	-5.12	1.18	1.24
1	R	478	VAL	C-O	-5.12	1.18	1.24
1	A	321	PHE	C-O	-5.11	1.18	1.24
1	F	258	ILE	C-O	-5.11	1.18	1.24
1	G	280	ILE	C-O	-5.11	1.18	1.24
1	M	315	ASP	C-O	-5.11	1.18	1.24
1	J	270	PRO	C-O	-5.11	1.18	1.23
1	H	315	ASP	C-O	-5.11	1.18	1.24
1	P	208	ILE	C-O	-5.11	1.18	1.24
1	T	321	PHE	C-O	-5.11	1.18	1.24
1	X	208	ILE	C-O	-5.11	1.18	1.24
1	X	343	VAL	C-O	-5.11	1.18	1.24
1	K	270	PRO	C-O	-5.10	1.18	1.23
1	B	402	THR	C-O	-5.10	1.17	1.24
1	N	269	ILE	C-O	-5.10	1.18	1.24
1	O	208	ILE	C-O	-5.10	1.18	1.24
1	V	343	VAL	C-O	-5.10	1.18	1.24
1	U	321	PHE	C-O	-5.10	1.18	1.24
1	D	270	PRO	C-O	-5.09	1.18	1.23
1	U	269	ILE	C-O	-5.09	1.18	1.24
1	B	342	VAL	C-O	-5.09	1.18	1.24
1	O	269	ILE	C-O	-5.09	1.18	1.24
1	W	315	ASP	C-O	-5.09	1.18	1.24
1	H	321	PHE	C-O	-5.09	1.18	1.24
1	L	208	ILE	C-O	-5.09	1.18	1.24
1	C	402	THR	C-O	-5.08	1.17	1.24
1	W	208	ILE	C-O	-5.08	1.18	1.24
1	S	208	ILE	C-O	-5.08	1.18	1.24
1	H	208	ILE	C-O	-5.08	1.18	1.24
1	A	208	ILE	C-O	-5.08	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	PRO	C-O	-5.08	1.18	1.23
1	F	269	ILE	C-O	-5.08	1.18	1.24
1	I	315	ASP	C-O	-5.08	1.18	1.24
1	K	478	VAL	C-O	-5.08	1.18	1.24
1	P	315	ASP	C-O	-5.08	1.18	1.24
1	G	321	PHE	C-O	-5.07	1.18	1.24
1	J	315	ASP	C-O	-5.07	1.18	1.24
1	O	342	VAL	C-O	-5.07	1.18	1.24
1	T	270	PRO	C-O	-5.07	1.18	1.23
1	X	321	PHE	C-O	-5.07	1.18	1.24
1	I	208	ILE	C-O	-5.07	1.18	1.24
1	P	321	PHE	C-O	-5.07	1.18	1.24
1	A	342	VAL	C-O	-5.06	1.18	1.24
1	E	208	ILE	C-O	-5.06	1.18	1.24
1	J	269	ILE	C-O	-5.06	1.18	1.24
1	Q	269	ILE	C-O	-5.06	1.18	1.24
1	Q	342	VAL	C-O	-5.06	1.18	1.24
1	T	315	ASP	C-O	-5.06	1.18	1.24
1	D	208	ILE	C-O	-5.06	1.18	1.24
1	J	230	GLY	C-O	-5.06	1.19	1.24
1	K	402	THR	C-O	-5.06	1.17	1.24
1	S	258	ILE	C-O	-5.06	1.19	1.24
1	A	402	THR	C-O	-5.06	1.17	1.24
1	I	321	PHE	C-O	-5.06	1.18	1.24
1	Q	315	ASP	C-O	-5.06	1.18	1.24
1	F	315	ASP	C-O	-5.06	1.18	1.24
1	D	321	PHE	C-O	-5.05	1.18	1.24
1	B	208	ILE	C-O	-5.05	1.18	1.24
1	D	343	VAL	C-O	-5.05	1.18	1.24
1	Q	321	PHE	C-O	-5.05	1.18	1.24
1	V	230	GLY	C-O	-5.05	1.19	1.24
1	F	321	PHE	C-O	-5.05	1.18	1.24
1	N	321	PHE	C-O	-5.05	1.18	1.24
1	M	208	ILE	C-O	-5.04	1.18	1.24
1	N	342	VAL	C-O	-5.04	1.18	1.24
1	B	321	PHE	C-O	-5.04	1.18	1.24
1	M	321	PHE	C-O	-5.04	1.18	1.24
1	S	321	PHE	C-O	-5.04	1.18	1.24
1	K	208	ILE	C-O	-5.04	1.18	1.24
1	A	315	ASP	C-O	-5.04	1.18	1.24
1	E	343	VAL	C-O	-5.04	1.18	1.24
1	B	343	VAL	C-O	-5.03	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	359	GLU	C-O	-5.03	1.17	1.24
1	K	315	ASP	C-O	-5.03	1.18	1.24
1	C	315	ASP	C-O	-5.03	1.18	1.24
1	I	343	VAL	C-O	-5.03	1.18	1.24
1	M	343	VAL	C-O	-5.03	1.18	1.24
1	T	343	VAL	C-O	-5.03	1.18	1.24
1	X	315	ASP	C-O	-5.03	1.18	1.24
1	C	342	VAL	C-O	-5.03	1.18	1.24
1	X	230	GLY	C-O	-5.03	1.19	1.24
1	F	342	VAL	C-O	-5.03	1.18	1.24
1	H	343	VAL	C-O	-5.03	1.18	1.24
1	J	342	VAL	C-O	-5.03	1.18	1.24
1	P	342	VAL	C-O	-5.03	1.18	1.24
1	M	402	THR	C-O	-5.02	1.17	1.24
1	V	315	ASP	C-O	-5.02	1.18	1.24
1	Q	208	ILE	C-O	-5.02	1.18	1.24
1	F	343	VAL	C-O	-5.02	1.18	1.24
1	G	402	THR	C-O	-5.02	1.17	1.24
1	A	343	VAL	C-O	-5.02	1.18	1.24
1	Q	400	SER	C-O	-5.02	1.18	1.23
1	K	342	VAL	C-O	-5.02	1.18	1.24
1	N	343	VAL	C-O	-5.02	1.18	1.24
1	G	342	VAL	C-O	-5.02	1.18	1.24
1	N	230	GLY	C-O	-5.02	1.19	1.24
1	I	402	THR	C-O	-5.01	1.17	1.24
1	W	359	GLU	C-O	-5.01	1.17	1.24
1	C	321	PHE	C-O	-5.01	1.18	1.24
1	F	208	ILE	C-O	-5.01	1.18	1.24
1	E	321	PHE	C-O	-5.00	1.18	1.24
1	H	230	GLY	C-O	-5.00	1.19	1.24
1	P	402	THR	C-O	-5.00	1.17	1.24
1	Q	343	VAL	C-O	-5.00	1.18	1.24
1	R	321	PHE	C-O	-5.00	1.18	1.24
1	S	402	THR	C-O	-5.00	1.17	1.24
1	W	343	VAL	C-O	-5.00	1.18	1.24

All (784) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	270	PRO	O-C-N	9.28	134.24	123.10
1	K	270	PRO	O-C-N	9.26	134.21	123.10
1	P	270	PRO	O-C-N	9.23	134.18	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	270	PRO	O-C-N	9.22	134.17	123.10
1	C	270	PRO	O-C-N	9.21	134.16	123.10
1	O	270	PRO	O-C-N	9.21	134.16	123.10
1	E	270	PRO	O-C-N	9.20	134.14	123.10
1	H	270	PRO	O-C-N	9.20	134.14	123.10
1	U	270	PRO	O-C-N	9.20	134.14	123.10
1	M	270	PRO	O-C-N	9.20	134.14	123.10
1	L	270	PRO	O-C-N	9.20	134.14	123.10
1	T	270	PRO	O-C-N	9.20	134.14	123.10
1	A	270	PRO	O-C-N	9.19	134.13	123.10
1	B	270	PRO	O-C-N	9.19	134.13	123.10
1	G	270	PRO	O-C-N	9.19	134.12	123.10
1	W	270	PRO	O-C-N	9.18	134.12	123.10
1	Q	270	PRO	O-C-N	9.18	134.11	123.10
1	R	270	PRO	O-C-N	9.18	134.11	123.10
1	X	270	PRO	O-C-N	9.18	134.11	123.10
1	S	270	PRO	O-C-N	9.17	134.10	123.10
1	J	270	PRO	O-C-N	9.14	134.07	123.10
1	F	270	PRO	O-C-N	9.13	134.06	123.10
1	N	270	PRO	O-C-N	9.13	134.06	123.10
1	D	270	PRO	O-C-N	9.10	134.01	123.10
1	L	484	LYS	N-CA-C	8.71	120.55	111.14
1	N	484	LYS	N-CA-C	8.68	120.52	111.14
1	O	484	LYS	N-CA-C	8.68	120.52	111.14
1	R	484	LYS	N-CA-C	8.67	120.51	111.14
1	G	484	LYS	N-CA-C	8.67	120.50	111.14
1	D	484	LYS	N-CA-C	8.65	120.49	111.14
1	E	484	LYS	N-CA-C	8.65	120.49	111.14
1	S	484	LYS	N-CA-C	8.65	120.49	111.14
1	C	484	LYS	N-CA-C	8.65	120.48	111.14
1	J	484	LYS	N-CA-C	8.65	120.48	111.14
1	P	484	LYS	N-CA-C	8.64	120.47	111.14
1	K	484	LYS	N-CA-C	8.64	120.47	111.14
1	X	484	LYS	N-CA-C	8.64	120.47	111.14
1	F	484	LYS	N-CA-C	8.63	120.47	111.14
1	V	484	LYS	N-CA-C	8.63	120.47	111.14
1	U	484	LYS	N-CA-C	8.62	120.45	111.14
1	W	484	LYS	N-CA-C	8.61	120.44	111.14
1	M	484	LYS	N-CA-C	8.61	120.44	111.14
1	Q	484	LYS	N-CA-C	8.60	120.43	111.14
1	H	484	LYS	N-CA-C	8.60	120.42	111.14
1	T	484	LYS	N-CA-C	8.59	120.42	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	LYS	N-CA-C	8.58	120.40	111.14
1	I	484	LYS	N-CA-C	8.57	120.40	111.14
1	B	484	LYS	N-CA-C	8.57	120.39	111.14
1	W	206	ASP	N-CA-C	8.23	120.33	111.36
1	F	206	ASP	N-CA-C	8.22	120.31	111.36
1	M	206	ASP	N-CA-C	8.20	120.30	111.36
1	T	206	ASP	N-CA-C	8.20	120.29	111.36
1	B	206	ASP	N-CA-C	8.19	120.29	111.36
1	E	206	ASP	N-CA-C	8.19	120.29	111.36
1	O	206	ASP	N-CA-C	8.19	120.29	111.36
1	K	206	ASP	N-CA-C	8.19	120.28	111.36
1	P	206	ASP	N-CA-C	8.19	120.28	111.36
1	N	206	ASP	N-CA-C	8.19	120.28	111.36
1	X	206	ASP	N-CA-C	8.18	120.28	111.36
1	C	206	ASP	N-CA-C	8.18	120.28	111.36
1	U	206	ASP	N-CA-C	8.18	120.27	111.36
1	D	206	ASP	N-CA-C	8.17	120.27	111.36
1	V	206	ASP	N-CA-C	8.17	120.27	111.36
1	Q	206	ASP	N-CA-C	8.17	120.26	111.36
1	A	206	ASP	N-CA-C	8.16	120.26	111.36
1	R	206	ASP	N-CA-C	8.15	120.25	111.36
1	I	206	ASP	N-CA-C	8.15	120.25	111.36
1	J	206	ASP	N-CA-C	8.15	120.24	111.36
1	G	206	ASP	N-CA-C	8.15	120.24	111.36
1	F	212	PHE	CA-C-O	-8.14	112.39	121.84
1	S	206	ASP	N-CA-C	8.14	120.24	111.36
1	N	212	PHE	CA-C-O	-8.14	112.40	121.84
1	H	206	ASP	N-CA-C	8.12	120.21	111.36
1	S	212	PHE	CA-C-O	-8.12	112.42	121.84
1	B	212	PHE	CA-C-O	-8.11	112.43	121.84
1	L	206	ASP	N-CA-C	8.11	120.20	111.36
1	J	212	PHE	CA-C-O	-8.11	112.44	121.84
1	G	212	PHE	CA-C-O	-8.10	112.45	121.84
1	I	212	PHE	CA-C-O	-8.10	112.44	121.84
1	U	212	PHE	CA-C-O	-8.10	112.45	121.84
1	D	212	PHE	CA-C-O	-8.09	112.45	121.84
1	O	212	PHE	CA-C-O	-8.09	112.45	121.84
1	X	212	PHE	CA-C-O	-8.09	112.45	121.84
1	M	212	PHE	CA-C-O	-8.09	112.46	121.84
1	P	212	PHE	CA-C-O	-8.08	112.47	121.84
1	Q	212	PHE	CA-C-O	-8.07	112.48	121.84
1	V	212	PHE	CA-C-O	-8.07	112.48	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	212	PHE	CA-C-O	-8.07	112.48	121.84
1	H	212	PHE	CA-C-O	-8.07	112.48	121.84
1	E	212	PHE	CA-C-O	-8.06	112.49	121.84
1	L	212	PHE	CA-C-O	-8.05	112.50	121.84
1	K	212	PHE	CA-C-O	-8.05	112.50	121.84
1	T	212	PHE	CA-C-O	-8.02	112.53	121.84
1	A	212	PHE	CA-C-O	-8.02	112.53	121.84
1	R	212	PHE	CA-C-O	-8.01	112.54	121.84
1	C	212	PHE	CA-C-O	-8.01	112.55	121.84
1	I	398	VAL	CB-CA-C	-7.95	97.98	110.69
1	T	398	VAL	CB-CA-C	-7.93	98.00	110.69
1	C	398	VAL	CB-CA-C	-7.93	98.00	110.69
1	G	398	VAL	CB-CA-C	-7.92	98.01	110.69
1	B	398	VAL	CB-CA-C	-7.92	98.02	110.69
1	V	398	VAL	CB-CA-C	-7.92	98.01	110.69
1	E	398	VAL	CB-CA-C	-7.92	98.02	110.69
1	L	398	VAL	CB-CA-C	-7.92	98.03	110.69
1	W	398	VAL	CB-CA-C	-7.91	98.04	110.69
1	J	398	VAL	CB-CA-C	-7.91	98.04	110.69
1	X	398	VAL	CB-CA-C	-7.91	98.04	110.69
1	Q	398	VAL	CB-CA-C	-7.90	98.06	110.69
1	A	398	VAL	CB-CA-C	-7.89	98.06	110.69
1	F	398	VAL	CB-CA-C	-7.89	98.06	110.69
1	H	398	VAL	CB-CA-C	-7.89	98.06	110.69
1	R	398	VAL	CB-CA-C	-7.89	98.07	110.69
1	S	398	VAL	CB-CA-C	-7.88	98.08	110.69
1	M	398	VAL	CB-CA-C	-7.88	98.08	110.69
1	O	398	VAL	CB-CA-C	-7.88	98.08	110.69
1	U	398	VAL	CB-CA-C	-7.87	98.09	110.69
1	D	398	VAL	CB-CA-C	-7.87	98.09	110.69
1	K	398	VAL	CB-CA-C	-7.87	98.09	110.69
1	N	398	VAL	CB-CA-C	-7.86	98.12	110.69
1	P	398	VAL	CB-CA-C	-7.84	98.14	110.69
1	M	270	PRO	CA-C-N	7.74	130.65	120.28
1	M	270	PRO	C-N-CA	7.74	130.65	120.28
1	D	270	PRO	CA-C-N	7.72	130.63	120.28
1	D	270	PRO	C-N-CA	7.72	130.63	120.28
1	R	270	PRO	CA-C-N	7.71	130.62	120.28
1	R	270	PRO	C-N-CA	7.71	130.62	120.28
1	U	270	PRO	CA-C-N	7.71	130.61	120.28
1	U	270	PRO	C-N-CA	7.71	130.61	120.28
1	G	270	PRO	CA-C-N	7.71	130.61	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	270	PRO	C-N-CA	7.71	130.61	120.28
1	H	270	PRO	CA-C-N	7.70	130.60	120.28
1	H	270	PRO	C-N-CA	7.70	130.60	120.28
1	C	270	PRO	CA-C-N	7.70	130.60	120.28
1	C	270	PRO	C-N-CA	7.70	130.60	120.28
1	N	270	PRO	CA-C-N	7.70	130.59	120.28
1	N	270	PRO	C-N-CA	7.70	130.59	120.28
1	F	270	PRO	CA-C-N	7.69	130.59	120.28
1	F	270	PRO	C-N-CA	7.69	130.59	120.28
1	L	270	PRO	CA-C-N	7.69	130.59	120.28
1	L	270	PRO	C-N-CA	7.69	130.59	120.28
1	Q	270	PRO	CA-C-N	7.69	130.59	120.28
1	Q	270	PRO	C-N-CA	7.69	130.59	120.28
1	X	270	PRO	CA-C-N	7.69	130.58	120.28
1	X	270	PRO	C-N-CA	7.69	130.58	120.28
1	J	270	PRO	CA-C-N	7.69	130.58	120.28
1	J	270	PRO	C-N-CA	7.69	130.58	120.28
1	W	270	PRO	CA-C-N	7.69	130.58	120.28
1	W	270	PRO	C-N-CA	7.69	130.58	120.28
1	B	270	PRO	CA-C-N	7.68	130.58	120.28
1	B	270	PRO	C-N-CA	7.68	130.58	120.28
1	T	270	PRO	CA-C-N	7.68	130.57	120.28
1	T	270	PRO	C-N-CA	7.68	130.57	120.28
1	A	270	PRO	CA-C-N	7.68	130.56	120.28
1	A	270	PRO	C-N-CA	7.68	130.56	120.28
1	I	270	PRO	CA-C-N	7.68	130.57	120.28
1	I	270	PRO	C-N-CA	7.68	130.57	120.28
1	P	270	PRO	CA-C-N	7.67	130.56	120.28
1	P	270	PRO	C-N-CA	7.67	130.56	120.28
1	S	270	PRO	CA-C-N	7.67	130.56	120.28
1	S	270	PRO	C-N-CA	7.67	130.56	120.28
1	E	270	PRO	CA-C-N	7.65	130.53	120.28
1	E	270	PRO	C-N-CA	7.65	130.53	120.28
1	O	270	PRO	CA-C-N	7.64	130.52	120.28
1	O	270	PRO	C-N-CA	7.64	130.52	120.28
1	V	270	PRO	CA-C-N	7.64	130.51	120.28
1	V	270	PRO	C-N-CA	7.64	130.51	120.28
1	K	270	PRO	CA-C-N	7.60	130.47	120.28
1	K	270	PRO	C-N-CA	7.60	130.47	120.28
1	H	409	VAL	N-CA-C	7.58	118.38	110.72
1	I	409	VAL	N-CA-C	7.57	118.36	110.72
1	R	409	VAL	N-CA-C	7.56	118.36	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	409	VAL	N-CA-C	7.55	118.35	110.72
1	O	409	VAL	N-CA-C	7.55	118.35	110.72
1	A	409	VAL	N-CA-C	7.55	118.35	110.72
1	T	409	VAL	N-CA-C	7.55	118.35	110.72
1	D	409	VAL	N-CA-C	7.55	118.34	110.72
1	V	409	VAL	N-CA-C	7.55	118.34	110.72
1	S	409	VAL	N-CA-C	7.54	118.34	110.72
1	K	409	VAL	N-CA-C	7.54	118.34	110.72
1	M	409	VAL	N-CA-C	7.53	118.33	110.72
1	Q	409	VAL	N-CA-C	7.53	118.32	110.72
1	J	409	VAL	N-CA-C	7.52	118.32	110.72
1	L	409	VAL	N-CA-C	7.52	118.31	110.72
1	N	409	VAL	N-CA-C	7.52	118.32	110.72
1	F	409	VAL	N-CA-C	7.51	118.31	110.72
1	X	409	VAL	N-CA-C	7.51	118.30	110.72
1	U	409	VAL	N-CA-C	7.49	118.28	110.72
1	W	409	VAL	N-CA-C	7.48	118.28	110.72
1	P	409	VAL	N-CA-C	7.47	118.27	110.72
1	G	409	VAL	N-CA-C	7.46	118.26	110.72
1	B	409	VAL	N-CA-C	7.45	118.25	110.72
1	C	409	VAL	N-CA-C	7.41	118.20	110.72
1	C	144	ASP	N-CA-C	7.13	121.76	111.56
1	G	144	ASP	N-CA-C	7.12	121.74	111.56
1	P	144	ASP	N-CA-C	7.12	121.74	111.56
1	I	144	ASP	N-CA-C	7.11	121.73	111.56
1	R	144	ASP	N-CA-C	7.10	121.71	111.56
1	E	144	ASP	N-CA-C	7.10	121.71	111.56
1	M	144	ASP	N-CA-C	7.10	121.71	111.56
1	S	144	ASP	N-CA-C	7.09	121.70	111.56
1	A	144	ASP	N-CA-C	7.09	121.70	111.56
1	B	144	ASP	N-CA-C	7.09	121.70	111.56
1	X	144	ASP	N-CA-C	7.09	121.70	111.56
1	F	144	ASP	N-CA-C	7.09	121.70	111.56
1	Q	144	ASP	N-CA-C	7.09	121.69	111.56
1	D	144	ASP	N-CA-C	7.08	121.68	111.56
1	O	144	ASP	N-CA-C	7.08	121.68	111.56
1	V	144	ASP	N-CA-C	7.08	121.68	111.56
1	U	144	ASP	N-CA-C	7.08	121.68	111.56
1	J	144	ASP	N-CA-C	7.08	121.68	111.56
1	N	144	ASP	N-CA-C	7.08	121.68	111.56
1	K	144	ASP	N-CA-C	7.07	121.67	111.56
1	L	144	ASP	N-CA-C	7.06	121.65	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	144	ASP	N-CA-C	7.06	121.65	111.56
1	W	144	ASP	N-CA-C	7.05	121.64	111.56
1	H	144	ASP	N-CA-C	7.05	121.64	111.56
1	V	195	VAL	N-CA-C	-6.96	102.82	112.50
1	K	195	VAL	N-CA-C	-6.96	102.83	112.50
1	M	195	VAL	N-CA-C	-6.96	102.83	112.50
1	C	195	VAL	N-CA-C	-6.95	102.83	112.50
1	W	195	VAL	N-CA-C	-6.94	102.85	112.50
1	G	195	VAL	N-CA-C	-6.94	102.85	112.50
1	X	195	VAL	N-CA-C	-6.94	102.85	112.50
1	A	195	VAL	N-CA-C	-6.94	102.85	112.50
1	B	195	VAL	N-CA-C	-6.94	102.86	112.50
1	I	195	VAL	N-CA-C	-6.94	102.86	112.50
1	L	195	VAL	N-CA-C	-6.94	102.86	112.50
1	P	195	VAL	N-CA-C	-6.94	102.86	112.50
1	N	195	VAL	N-CA-C	-6.93	102.86	112.50
1	O	195	VAL	N-CA-C	-6.93	102.87	112.50
1	F	195	VAL	N-CA-C	-6.92	102.88	112.50
1	S	195	VAL	N-CA-C	-6.92	102.88	112.50
1	T	195	VAL	N-CA-C	-6.92	102.88	112.50
1	R	195	VAL	N-CA-C	-6.92	102.88	112.50
1	E	195	VAL	N-CA-C	-6.92	102.89	112.50
1	J	195	VAL	N-CA-C	-6.91	102.89	112.50
1	U	195	VAL	N-CA-C	-6.91	102.89	112.50
1	D	195	VAL	N-CA-C	-6.91	102.90	112.50
1	H	195	VAL	N-CA-C	-6.91	102.90	112.50
1	Q	195	VAL	N-CA-C	-6.90	102.91	112.50
1	D	248	ILE	N-CA-C	6.77	117.53	110.62
1	H	248	ILE	N-CA-C	6.76	117.51	110.62
1	K	248	ILE	N-CA-C	6.74	117.50	110.62
1	S	248	ILE	N-CA-C	6.74	117.49	110.62
1	F	248	ILE	N-CA-C	6.73	117.49	110.62
1	X	248	ILE	N-CA-C	6.73	117.48	110.62
1	J	248	ILE	N-CA-C	6.72	117.48	110.62
1	A	241	ASN	N-CA-C	6.72	118.34	108.86
1	U	248	ILE	N-CA-C	6.71	117.47	110.62
1	E	248	ILE	N-CA-C	6.71	117.47	110.62
1	O	248	ILE	N-CA-C	6.71	117.46	110.62
1	M	248	ILE	N-CA-C	6.71	117.46	110.62
1	G	248	ILE	N-CA-C	6.70	117.46	110.62
1	B	248	ILE	N-CA-C	6.70	117.45	110.62
1	F	241	ASN	N-CA-C	6.70	118.30	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	248	ILE	N-CA-C	6.70	117.45	110.62
1	O	241	ASN	N-CA-C	6.69	118.30	108.86
1	P	248	ILE	N-CA-C	6.69	117.45	110.62
1	C	241	ASN	N-CA-C	6.69	118.30	108.86
1	T	241	ASN	N-CA-C	6.69	118.29	108.86
1	L	248	ILE	N-CA-C	6.69	117.44	110.62
1	N	248	ILE	N-CA-C	6.69	117.44	110.62
1	I	248	ILE	N-CA-C	6.68	117.44	110.62
1	V	248	ILE	N-CA-C	6.68	117.44	110.62
1	T	248	ILE	N-CA-C	6.68	117.43	110.62
1	B	241	ASN	N-CA-C	6.67	118.27	108.86
1	D	241	ASN	N-CA-C	6.67	118.26	108.86
1	U	241	ASN	N-CA-C	6.67	118.26	108.86
1	Q	248	ILE	N-CA-C	6.66	117.41	110.62
1	A	248	ILE	N-CA-C	6.66	117.41	110.62
1	G	241	ASN	N-CA-C	6.66	118.25	108.86
1	Q	241	ASN	N-CA-C	6.65	118.24	108.86
1	R	248	ILE	N-CA-C	6.64	117.39	110.62
1	R	241	ASN	N-CA-C	6.64	118.22	108.86
1	C	248	ILE	N-CA-C	6.63	117.39	110.62
1	N	241	ASN	N-CA-C	6.63	118.21	108.86
1	K	300	GLU	N-CA-C	6.57	118.44	111.28
1	R	300	GLU	N-CA-C	6.57	118.44	111.28
1	L	300	GLU	N-CA-C	6.56	118.43	111.28
1	D	300	GLU	N-CA-C	6.56	118.43	111.28
1	E	300	GLU	N-CA-C	6.55	118.42	111.28
1	N	300	GLU	N-CA-C	6.54	118.41	111.28
1	U	300	GLU	N-CA-C	6.54	118.41	111.28
1	J	300	GLU	N-CA-C	6.54	118.41	111.28
1	Q	300	GLU	N-CA-C	6.54	118.40	111.28
1	P	300	GLU	N-CA-C	6.53	118.40	111.28
1	B	300	GLU	N-CA-C	6.53	118.40	111.28
1	G	300	GLU	N-CA-C	6.53	118.40	111.28
1	C	300	GLU	N-CA-C	6.53	118.40	111.28
1	T	300	GLU	N-CA-C	6.53	118.40	111.28
1	V	300	GLU	N-CA-C	6.53	118.39	111.28
1	F	300	GLU	N-CA-C	6.52	118.39	111.28
1	W	300	GLU	N-CA-C	6.52	118.39	111.28
1	O	300	GLU	N-CA-C	6.52	118.38	111.28
1	A	300	GLU	N-CA-C	6.50	118.37	111.28
1	X	300	GLU	N-CA-C	6.50	118.36	111.28
1	H	300	GLU	N-CA-C	6.50	118.36	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	300	GLU	N-CA-C	6.50	118.36	111.28
1	S	300	GLU	N-CA-C	6.49	118.35	111.28
1	I	300	GLU	N-CA-C	6.48	118.34	111.28
1	V	241	ASN	N-CA-C	6.47	118.37	109.18
1	E	241	ASN	N-CA-C	6.46	118.35	109.18
1	I	241	ASN	N-CA-C	6.44	118.32	109.18
1	L	241	ASN	N-CA-C	6.43	118.32	109.18
1	S	241	ASN	N-CA-C	6.43	118.31	109.18
1	H	241	ASN	N-CA-C	6.42	118.30	109.18
1	X	241	ASN	N-CA-C	6.42	118.29	109.18
1	P	241	ASN	N-CA-C	6.41	118.29	109.18
1	W	241	ASN	N-CA-C	6.41	118.29	109.18
1	J	241	ASN	N-CA-C	6.41	118.28	109.18
1	K	241	ASN	N-CA-C	6.39	118.26	109.18
1	M	241	ASN	N-CA-C	6.38	118.24	109.18
1	N	82	LEU	O-C-N	6.37	130.78	123.27
1	B	82	LEU	O-C-N	6.35	130.76	123.27
1	Q	82	LEU	O-C-N	6.34	130.76	123.27
1	P	82	LEU	O-C-N	6.34	130.75	123.27
1	X	82	LEU	O-C-N	6.33	130.75	123.27
1	E	82	LEU	O-C-N	6.32	130.73	123.27
1	O	82	LEU	O-C-N	6.32	130.73	123.27
1	G	82	LEU	O-C-N	6.32	130.73	123.27
1	I	82	LEU	O-C-N	6.32	130.72	123.27
1	V	82	LEU	O-C-N	6.31	130.72	123.27
1	M	82	LEU	O-C-N	6.31	130.71	123.27
1	K	82	LEU	O-C-N	6.30	130.70	123.27
1	S	82	LEU	O-C-N	6.30	130.70	123.27
1	U	82	LEU	O-C-N	6.29	130.70	123.27
1	C	82	LEU	O-C-N	6.28	130.68	123.27
1	F	82	LEU	O-C-N	6.28	130.68	123.27
1	A	82	LEU	O-C-N	6.28	130.68	123.27
1	T	82	LEU	O-C-N	6.28	130.68	123.27
1	L	82	LEU	O-C-N	6.27	130.67	123.27
1	J	82	LEU	O-C-N	6.27	130.67	123.27
1	R	82	LEU	O-C-N	6.27	130.66	123.27
1	W	82	LEU	O-C-N	6.26	130.66	123.27
1	H	82	LEU	O-C-N	6.24	130.63	123.27
1	M	215	SER	N-CA-C	6.23	118.54	109.07
1	D	82	LEU	O-C-N	6.22	130.62	123.27
1	D	215	SER	N-CA-C	6.22	118.53	109.07
1	K	215	SER	N-CA-C	6.21	118.52	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	215	SER	N-CA-C	6.21	118.51	109.07
1	R	215	SER	N-CA-C	6.21	118.51	109.07
1	E	215	SER	N-CA-C	6.21	118.50	109.07
1	Q	215	SER	N-CA-C	6.21	118.50	109.07
1	N	215	SER	N-CA-C	6.20	118.50	109.07
1	H	215	SER	N-CA-C	6.20	118.50	109.07
1	T	215	SER	N-CA-C	6.20	118.49	109.07
1	X	215	SER	N-CA-C	6.20	118.49	109.07
1	O	215	SER	N-CA-C	6.20	118.49	109.07
1	B	215	SER	N-CA-C	6.19	118.48	109.07
1	F	215	SER	N-CA-C	6.19	118.48	109.07
1	J	215	SER	N-CA-C	6.19	118.48	109.07
1	A	215	SER	N-CA-C	6.19	118.47	109.07
1	U	215	SER	N-CA-C	6.18	118.47	109.07
1	C	215	SER	N-CA-C	6.18	118.46	109.07
1	G	215	SER	N-CA-C	6.18	118.46	109.07
1	M	20	ALA	N-CA-C	6.18	117.81	111.14
1	V	215	SER	N-CA-C	6.18	118.46	109.07
1	P	215	SER	N-CA-C	6.17	118.45	109.07
1	L	20	ALA	N-CA-C	6.17	117.81	111.14
1	X	20	ALA	N-CA-C	6.17	117.80	111.14
1	L	215	SER	N-CA-C	6.16	118.44	109.07
1	F	20	ALA	N-CA-C	6.16	117.79	111.14
1	H	214	ARG	N-CA-C	6.16	118.96	111.82
1	W	215	SER	N-CA-C	6.15	118.42	109.07
1	S	215	SER	N-CA-C	6.15	118.42	109.07
1	W	20	ALA	N-CA-C	6.15	117.78	111.14
1	O	214	ARG	N-CA-C	6.15	118.95	111.82
1	I	214	ARG	N-CA-C	6.14	118.95	111.82
1	O	20	ALA	N-CA-C	6.14	117.77	111.14
1	A	214	ARG	N-CA-C	6.14	118.94	111.82
1	K	214	ARG	N-CA-C	6.14	118.94	111.82
1	N	20	ALA	N-CA-C	6.14	117.77	111.14
1	C	214	ARG	N-CA-C	6.14	118.94	111.82
1	E	214	ARG	N-CA-C	6.14	118.94	111.82
1	N	214	ARG	N-CA-C	6.14	118.94	111.82
1	V	20	ALA	N-CA-C	6.14	117.77	111.14
1	G	20	ALA	N-CA-C	6.13	117.76	111.14
1	F	214	ARG	N-CA-C	6.13	118.93	111.82
1	D	20	ALA	N-CA-C	6.13	117.76	111.14
1	J	20	ALA	N-CA-C	6.13	117.76	111.14
1	Q	214	ARG	N-CA-C	6.12	118.92	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ARG	N-CA-C	6.12	118.92	111.82
1	R	20	ALA	N-CA-C	6.12	117.75	111.14
1	T	20	ALA	N-CA-C	6.12	117.75	111.14
1	T	214	ARG	N-CA-C	6.12	118.92	111.82
1	V	214	ARG	N-CA-C	6.12	118.92	111.82
1	X	214	ARG	N-CA-C	6.12	118.92	111.82
1	I	20	ALA	N-CA-C	6.12	117.74	111.14
1	J	214	ARG	N-CA-C	6.12	118.91	111.82
1	R	214	ARG	N-CA-C	6.11	118.91	111.82
1	P	214	ARG	N-CA-C	6.10	118.90	111.82
1	S	214	ARG	N-CA-C	6.10	118.90	111.82
1	W	214	ARG	N-CA-C	6.10	118.90	111.82
1	D	214	ARG	N-CA-C	6.10	118.90	111.82
1	U	214	ARG	N-CA-C	6.10	118.89	111.82
1	L	214	ARG	N-CA-C	6.10	118.89	111.82
1	E	20	ALA	N-CA-C	6.10	117.72	111.14
1	M	214	ARG	N-CA-C	6.09	118.89	111.82
1	S	20	ALA	N-CA-C	6.09	117.71	111.14
1	K	20	ALA	N-CA-C	6.08	117.71	111.14
1	H	20	ALA	N-CA-C	6.07	117.70	111.14
1	G	214	ARG	N-CA-C	6.07	118.86	111.82
1	U	20	ALA	N-CA-C	6.07	117.69	111.14
1	Q	20	ALA	N-CA-C	6.04	117.67	111.14
1	C	337	LYS	N-CA-C	6.00	117.90	111.36
1	W	337	LYS	N-CA-C	5.96	117.85	111.36
1	G	337	LYS	N-CA-C	5.95	117.84	111.36
1	A	337	LYS	N-CA-C	5.95	117.84	111.36
1	X	337	LYS	N-CA-C	5.94	117.84	111.36
1	C	20	ALA	N-CA-C	5.94	117.83	111.36
1	I	337	LYS	N-CA-C	5.94	117.83	111.36
1	S	337	LYS	N-CA-C	5.94	117.83	111.36
1	P	20	ALA	N-CA-C	5.93	117.82	111.36
1	R	337	LYS	N-CA-C	5.93	117.82	111.36
1	H	337	LYS	N-CA-C	5.93	117.82	111.36
1	E	337	LYS	N-CA-C	5.92	117.82	111.36
1	B	20	ALA	N-CA-C	5.92	117.81	111.36
1	J	337	LYS	N-CA-C	5.92	117.81	111.36
1	O	337	LYS	N-CA-C	5.92	117.81	111.36
1	B	337	LYS	N-CA-C	5.92	117.81	111.36
1	M	269	ILE	N-CA-C	-5.91	96.11	108.88
1	D	337	LYS	N-CA-C	5.91	117.80	111.36
1	N	337	LYS	N-CA-C	5.91	117.80	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	269	ILE	N-CA-C	-5.90	96.13	108.88
1	V	337	LYS	N-CA-C	5.90	117.80	111.36
1	A	20	ALA	N-CA-C	5.89	117.78	111.36
1	P	337	LYS	N-CA-C	5.89	117.78	111.36
1	B	269	ILE	N-CA-C	-5.89	96.16	108.88
1	E	269	ILE	N-CA-C	-5.89	96.16	108.88
1	K	337	LYS	N-CA-C	5.89	117.78	111.36
1	N	269	ILE	N-CA-C	-5.89	96.16	108.88
1	S	269	ILE	N-CA-C	-5.89	96.16	108.88
1	T	337	LYS	N-CA-C	5.89	117.78	111.36
1	F	337	LYS	N-CA-C	5.88	117.77	111.36
1	U	337	LYS	N-CA-C	5.88	117.77	111.36
1	F	269	ILE	N-CA-C	-5.88	96.17	108.88
1	V	269	ILE	N-CA-C	-5.88	96.18	108.88
1	A	269	ILE	N-CA-C	-5.88	96.19	108.88
1	Q	269	ILE	N-CA-C	-5.88	96.19	108.88
1	U	269	ILE	N-CA-C	-5.87	96.19	108.88
1	R	269	ILE	N-CA-C	-5.87	96.20	108.88
1	L	269	ILE	N-CA-C	-5.87	96.21	108.88
1	H	269	ILE	N-CA-C	-5.87	96.21	108.88
1	I	269	ILE	N-CA-C	-5.86	96.22	108.88
1	T	269	ILE	N-CA-C	-5.86	96.22	108.88
1	O	269	ILE	N-CA-C	-5.86	96.22	108.88
1	Q	337	LYS	N-CA-C	5.86	117.75	111.36
1	K	269	ILE	N-CA-C	-5.86	96.23	108.88
1	M	337	LYS	N-CA-C	5.86	117.74	111.36
1	D	269	ILE	N-CA-C	-5.85	96.24	108.88
1	C	269	ILE	N-CA-C	-5.85	96.24	108.88
1	W	269	ILE	N-CA-C	-5.85	96.24	108.88
1	X	269	ILE	N-CA-C	-5.85	96.24	108.88
1	G	269	ILE	N-CA-C	-5.85	96.25	108.88
1	J	269	ILE	N-CA-C	-5.84	96.26	108.88
1	K	485	VAL	N-CA-C	5.82	117.08	109.58
1	G	485	VAL	N-CA-C	5.79	117.04	109.58
1	N	485	VAL	N-CA-C	5.78	117.03	109.58
1	E	485	VAL	N-CA-C	5.78	117.03	109.58
1	I	485	VAL	N-CA-C	5.76	117.02	109.58
1	R	485	VAL	N-CA-C	5.76	117.02	109.58
1	P	485	VAL	N-CA-C	5.75	116.99	109.58
1	O	485	VAL	N-CA-C	5.74	116.99	109.58
1	U	485	VAL	N-CA-C	5.74	116.98	109.58
1	L	485	VAL	N-CA-C	5.74	116.98	109.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	485	VAL	N-CA-C	5.73	116.98	109.58
1	W	485	VAL	N-CA-C	5.73	116.97	109.58
1	M	485	VAL	N-CA-C	5.72	116.96	109.58
1	T	485	VAL	N-CA-C	5.72	116.96	109.58
1	X	485	VAL	N-CA-C	5.72	116.96	109.58
1	D	485	VAL	N-CA-C	5.71	116.95	109.58
1	J	485	VAL	N-CA-C	5.71	116.94	109.58
1	S	485	VAL	N-CA-C	5.71	116.94	109.58
1	B	485	VAL	N-CA-C	5.70	116.94	109.58
1	C	485	VAL	N-CA-C	5.70	116.94	109.58
1	V	485	VAL	N-CA-C	5.70	116.93	109.58
1	H	485	VAL	N-CA-C	5.69	116.92	109.58
1	A	485	VAL	N-CA-C	5.68	116.91	109.58
1	F	485	VAL	N-CA-C	5.68	116.91	109.58
1	F	4	ALA	CA-C-N	5.66	128.13	120.38
1	F	4	ALA	C-N-CA	5.66	128.13	120.38
1	V	212	PHE	N-CA-CB	-5.65	103.34	111.70
1	D	4	ALA	CA-C-N	5.64	128.11	120.38
1	D	4	ALA	C-N-CA	5.64	128.11	120.38
1	O	212	PHE	N-CA-CB	-5.63	103.37	111.70
1	R	212	PHE	N-CA-CB	-5.62	103.38	111.70
1	H	212	PHE	N-CA-CB	-5.62	103.38	111.70
1	B	4	ALA	CA-C-N	5.62	128.07	120.38
1	B	4	ALA	C-N-CA	5.62	128.07	120.38
1	S	4	ALA	CA-C-N	5.62	128.07	120.38
1	S	4	ALA	C-N-CA	5.62	128.07	120.38
1	X	4	ALA	CA-C-N	5.62	128.07	120.38
1	X	4	ALA	C-N-CA	5.62	128.07	120.38
1	U	212	PHE	N-CA-CB	-5.61	103.39	111.70
1	W	4	ALA	CA-C-N	5.61	128.07	120.38
1	W	4	ALA	C-N-CA	5.61	128.07	120.38
1	E	4	ALA	CA-C-N	5.61	128.07	120.38
1	E	4	ALA	C-N-CA	5.61	128.07	120.38
1	O	4	ALA	CA-C-N	5.61	128.06	120.38
1	O	4	ALA	C-N-CA	5.61	128.06	120.38
1	Q	212	PHE	N-CA-CB	-5.61	103.40	111.70
1	K	212	PHE	N-CA-CB	-5.61	103.41	111.70
1	J	212	PHE	N-CA-CB	-5.60	103.41	111.70
1	T	212	PHE	N-CA-CB	-5.60	103.41	111.70
1	W	212	PHE	N-CA-CB	-5.60	103.41	111.70
1	L	4	ALA	CA-C-N	5.60	128.05	120.38
1	L	4	ALA	C-N-CA	5.60	128.05	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	212	PHE	N-CA-CB	-5.60	103.42	111.70
1	C	4	ALA	CA-C-N	5.60	128.05	120.38
1	C	4	ALA	C-N-CA	5.60	128.05	120.38
1	I	212	PHE	N-CA-CB	-5.59	103.42	111.70
1	J	4	ALA	CA-C-N	5.59	128.04	120.38
1	J	4	ALA	C-N-CA	5.59	128.04	120.38
1	V	4	ALA	CA-C-N	5.59	128.04	120.38
1	V	4	ALA	C-N-CA	5.59	128.04	120.38
1	A	212	PHE	N-CA-CB	-5.59	103.42	111.70
1	D	212	PHE	N-CA-CB	-5.59	103.43	111.70
1	G	212	PHE	N-CA-CB	-5.59	103.42	111.70
1	N	4	ALA	CA-C-N	5.59	128.04	120.38
1	N	4	ALA	C-N-CA	5.59	128.04	120.38
1	R	4	ALA	CA-C-N	5.59	128.04	120.38
1	R	4	ALA	C-N-CA	5.59	128.04	120.38
1	M	4	ALA	CA-C-N	5.59	128.03	120.38
1	M	4	ALA	C-N-CA	5.59	128.03	120.38
1	B	212	PHE	N-CA-CB	-5.59	103.43	111.70
1	E	212	PHE	N-CA-CB	-5.58	103.44	111.70
1	H	4	ALA	CA-C-N	5.58	128.03	120.38
1	H	4	ALA	C-N-CA	5.58	128.03	120.38
1	L	212	PHE	N-CA-CB	-5.58	103.44	111.70
1	P	4	ALA	CA-C-N	5.58	128.03	120.38
1	P	4	ALA	C-N-CA	5.58	128.03	120.38
1	S	212	PHE	N-CA-CB	-5.58	103.45	111.70
1	F	212	PHE	N-CA-CB	-5.57	103.45	111.70
1	G	4	ALA	CA-C-N	5.57	128.02	120.38
1	G	4	ALA	C-N-CA	5.57	128.02	120.38
1	P	212	PHE	N-CA-CB	-5.57	103.46	111.70
1	K	4	ALA	CA-C-N	5.57	128.01	120.38
1	K	4	ALA	C-N-CA	5.57	128.01	120.38
1	T	4	ALA	CA-C-N	5.57	128.01	120.38
1	T	4	ALA	C-N-CA	5.57	128.01	120.38
1	M	212	PHE	N-CA-CB	-5.57	103.46	111.70
1	A	4	ALA	CA-C-N	5.56	128.00	120.38
1	A	4	ALA	C-N-CA	5.56	128.00	120.38
1	N	212	PHE	N-CA-CB	-5.56	103.47	111.70
1	C	212	PHE	N-CA-CB	-5.56	103.47	111.70
1	Q	4	ALA	CA-C-N	5.55	127.99	120.38
1	Q	4	ALA	C-N-CA	5.55	127.99	120.38
1	U	4	ALA	CA-C-N	5.55	127.99	120.38
1	U	4	ALA	C-N-CA	5.55	127.99	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	4	ALA	CA-C-N	5.52	127.94	120.38
1	I	4	ALA	C-N-CA	5.52	127.94	120.38
1	P	280	ILE	CB-CA-C	-5.49	104.94	111.97
1	A	280	ILE	CB-CA-C	-5.48	104.96	111.97
1	K	280	ILE	CB-CA-C	-5.48	104.96	111.97
1	F	280	ILE	CB-CA-C	-5.44	105.00	111.97
1	S	280	ILE	CB-CA-C	-5.44	105.01	111.97
1	J	280	ILE	CB-CA-C	-5.44	105.01	111.97
1	G	280	ILE	CB-CA-C	-5.42	104.92	112.02
1	Q	280	ILE	CB-CA-C	-5.41	105.05	111.97
1	C	280	ILE	CB-CA-C	-5.41	104.94	112.02
1	I	470	VAL	N-CA-C	5.40	117.67	108.86
1	L	280	ILE	CB-CA-C	-5.40	104.94	112.02
1	N	280	ILE	CB-CA-C	-5.40	104.95	112.02
1	E	470	VAL	N-CA-C	5.39	117.65	108.86
1	H	470	VAL	N-CA-C	5.39	117.65	108.86
1	B	280	ILE	CB-CA-C	-5.39	104.96	112.02
1	H	280	ILE	CB-CA-C	-5.39	104.96	112.02
1	I	280	ILE	CB-CA-C	-5.39	104.96	112.02
1	E	280	ILE	CB-CA-C	-5.38	104.97	112.02
1	F	470	VAL	N-CA-C	5.38	117.63	108.86
1	O	280	ILE	CB-CA-C	-5.38	104.97	112.02
1	D	280	ILE	CB-CA-C	-5.38	104.98	112.02
1	X	280	ILE	CB-CA-C	-5.38	104.98	112.02
1	T	280	ILE	CB-CA-C	-5.37	104.98	112.02
1	Q	470	VAL	N-CA-C	5.37	117.62	108.86
1	X	470	VAL	N-CA-C	5.37	117.61	108.86
1	T	470	VAL	N-CA-C	5.37	117.61	108.86
1	J	470	VAL	N-CA-C	5.37	117.61	108.86
1	M	470	VAL	N-CA-C	5.36	117.60	108.86
1	C	470	VAL	N-CA-C	5.36	117.60	108.86
1	G	470	VAL	N-CA-C	5.36	117.60	108.86
1	K	470	VAL	N-CA-C	5.36	117.60	108.86
1	P	470	VAL	N-CA-C	5.35	117.59	108.86
1	N	470	VAL	N-CA-C	5.35	117.58	108.86
1	W	280	ILE	CB-CA-C	-5.35	105.01	112.02
1	W	470	VAL	N-CA-C	5.35	117.58	108.86
1	L	470	VAL	N-CA-C	5.35	117.58	108.86
1	R	470	VAL	N-CA-C	5.35	117.58	108.86
1	S	470	VAL	N-CA-C	5.35	117.58	108.86
1	U	280	ILE	CB-CA-C	-5.35	105.02	112.02
1	B	470	VAL	N-CA-C	5.34	117.57	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	470	VAL	N-CA-C	5.34	117.57	108.86
1	O	470	VAL	N-CA-C	5.34	117.56	108.86
1	D	470	VAL	N-CA-C	5.34	117.56	108.86
1	A	470	VAL	N-CA-C	5.33	117.56	108.86
1	A	483	HIS	N-CA-C	5.33	117.17	111.36
1	U	470	VAL	N-CA-C	5.33	117.54	108.86
1	R	483	HIS	N-CA-C	5.32	117.16	111.36
1	X	483	HIS	N-CA-C	5.32	117.16	111.36
1	B	265	LEU	CA-C-N	5.32	125.88	119.98
1	B	265	LEU	C-N-CA	5.32	125.88	119.98
1	M	280	ILE	CB-CA-C	-5.32	105.05	112.02
1	G	483	HIS	N-CA-C	5.31	117.15	111.36
1	I	483	HIS	N-CA-C	5.31	117.15	111.36
1	H	483	HIS	N-CA-C	5.30	117.14	111.36
1	J	265	LEU	CA-C-N	5.30	125.86	119.98
1	J	265	LEU	C-N-CA	5.30	125.86	119.98
1	O	265	LEU	CA-C-N	5.30	125.86	119.98
1	O	265	LEU	C-N-CA	5.30	125.86	119.98
1	D	483	HIS	N-CA-C	5.30	117.14	111.36
1	L	483	HIS	N-CA-C	5.30	117.14	111.36
1	B	483	HIS	N-CA-C	5.30	117.13	111.36
1	W	483	HIS	N-CA-C	5.29	117.13	111.36
1	I	265	LEU	CA-C-N	5.29	125.85	119.98
1	I	265	LEU	C-N-CA	5.29	125.85	119.98
1	N	265	LEU	CA-C-N	5.29	125.85	119.98
1	N	265	LEU	C-N-CA	5.29	125.85	119.98
1	P	483	HIS	N-CA-C	5.29	117.12	111.36
1	Q	265	LEU	CA-C-N	5.29	125.85	119.98
1	Q	265	LEU	C-N-CA	5.29	125.85	119.98
1	O	483	HIS	N-CA-C	5.29	117.12	111.36
1	K	483	HIS	N-CA-C	5.28	117.12	111.36
1	C	265	LEU	CA-C-N	5.28	125.84	119.98
1	C	265	LEU	C-N-CA	5.28	125.84	119.98
1	P	265	LEU	CA-C-N	5.28	125.84	119.98
1	P	265	LEU	C-N-CA	5.28	125.84	119.98
1	A	265	LEU	CA-C-N	5.27	125.83	119.98
1	A	265	LEU	C-N-CA	5.27	125.83	119.98
1	F	483	HIS	N-CA-C	5.27	117.11	111.36
1	T	265	LEU	CA-C-N	5.27	125.83	119.98
1	T	265	LEU	C-N-CA	5.27	125.83	119.98
1	M	265	LEU	CA-C-N	5.27	125.83	119.98
1	M	265	LEU	C-N-CA	5.27	125.83	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	483	HIS	N-CA-C	5.26	117.10	111.36
1	U	483	HIS	N-CA-C	5.26	117.10	111.36
1	V	483	HIS	N-CA-C	5.26	117.10	111.36
1	F	265	LEU	CA-C-N	5.26	125.82	119.98
1	F	265	LEU	C-N-CA	5.26	125.82	119.98
1	M	483	HIS	N-CA-C	5.26	117.09	111.36
1	V	265	LEU	CA-C-N	5.25	125.81	119.98
1	V	265	LEU	C-N-CA	5.25	125.81	119.98
1	C	483	HIS	N-CA-C	5.25	117.08	111.36
1	S	265	LEU	CA-C-N	5.24	125.80	119.98
1	S	265	LEU	C-N-CA	5.24	125.80	119.98
1	K	265	LEU	CA-C-N	5.24	125.80	119.98
1	K	265	LEU	C-N-CA	5.24	125.80	119.98
1	G	265	LEU	CA-C-N	5.23	125.79	119.98
1	G	265	LEU	C-N-CA	5.23	125.79	119.98
1	T	483	HIS	N-CA-C	5.23	117.06	111.36
1	L	265	LEU	CA-C-N	5.22	125.78	119.98
1	L	265	LEU	C-N-CA	5.22	125.78	119.98
1	Q	483	HIS	N-CA-C	5.22	117.05	111.36
1	H	265	LEU	CA-C-N	5.21	125.77	119.98
1	H	265	LEU	C-N-CA	5.21	125.77	119.98
1	J	483	HIS	N-CA-C	5.21	117.04	111.36
1	X	265	LEU	CA-C-N	5.21	125.77	119.98
1	X	265	LEU	C-N-CA	5.21	125.77	119.98
1	E	265	LEU	CA-C-N	5.20	125.75	119.98
1	E	265	LEU	C-N-CA	5.20	125.75	119.98
1	R	265	LEU	CA-C-N	5.19	125.74	119.98
1	R	265	LEU	C-N-CA	5.19	125.74	119.98
1	N	483	HIS	N-CA-C	5.19	117.02	111.36
1	S	483	HIS	N-CA-C	5.19	117.02	111.36
1	D	265	LEU	CA-C-N	5.18	125.73	119.98
1	D	265	LEU	C-N-CA	5.18	125.73	119.98
1	U	265	LEU	CA-C-N	5.17	125.72	119.98
1	U	265	LEU	C-N-CA	5.17	125.72	119.98
1	A	479	ILE	N-CA-C	5.16	115.41	107.77
1	W	265	LEU	CA-C-N	5.15	125.70	119.98
1	W	265	LEU	C-N-CA	5.15	125.70	119.98
1	V	455	HIS	N-CA-C	5.15	116.70	111.14
1	G	455	HIS	N-CA-C	5.15	116.70	111.14
1	H	479	ILE	N-CA-C	5.15	115.39	107.77
1	I	479	ILE	N-CA-C	5.15	115.39	107.77
1	P	479	ILE	N-CA-C	5.12	115.35	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	455	HIS	N-CA-C	5.12	116.67	111.14
1	M	479	ILE	N-CA-C	5.12	115.35	107.77
1	Q	254	GLU	N-CA-C	5.12	116.94	111.36
1	T	455	HIS	N-CA-C	5.12	116.67	111.14
1	V	479	ILE	N-CA-C	5.12	115.34	107.77
1	R	479	ILE	N-CA-C	5.11	115.34	107.77
1	X	455	HIS	N-CA-C	5.11	116.66	111.14
1	B	455	HIS	N-CA-C	5.11	116.66	111.14
1	J	479	ILE	N-CA-C	5.11	115.33	107.77
1	V	254	GLU	N-CA-C	5.11	116.93	111.36
1	N	479	ILE	N-CA-C	5.11	115.33	107.77
1	D	479	ILE	N-CA-C	5.11	115.33	107.77
1	K	479	ILE	N-CA-C	5.11	115.33	107.77
1	L	455	HIS	N-CA-C	5.11	116.66	111.14
1	H	254	GLU	N-CA-C	5.11	116.92	111.36
1	T	479	ILE	N-CA-C	5.11	115.33	107.77
1	C	479	ILE	N-CA-C	5.10	115.32	107.77
1	F	254	GLU	N-CA-C	5.10	116.92	111.36
1	R	455	HIS	N-CA-C	5.10	116.65	111.14
1	T	4	ALA	CA-C-O	5.10	125.95	120.70
1	X	479	ILE	N-CA-C	5.10	115.32	107.77
1	E	479	ILE	N-CA-C	5.10	115.32	107.77
1	I	455	HIS	N-CA-C	5.10	116.64	111.14
1	J	455	HIS	N-CA-C	5.09	116.64	111.14
1	X	4	ALA	CA-C-O	5.09	125.95	120.70
1	I	254	GLU	N-CA-C	5.09	116.91	111.36
1	L	479	ILE	N-CA-C	5.08	115.30	107.77
1	B	479	ILE	N-CA-C	5.08	115.29	107.77
1	G	479	ILE	N-CA-C	5.08	115.29	107.77
1	K	455	HIS	N-CA-C	5.08	116.63	111.14
1	U	479	ILE	N-CA-C	5.08	115.30	107.77
1	N	455	HIS	N-CA-C	5.08	116.63	111.14
1	S	28	GLY	CA-C-N	5.08	124.69	119.05
1	S	28	GLY	C-N-CA	5.08	124.69	119.05
1	Q	479	ILE	N-CA-C	5.08	115.29	107.77
1	O	254	GLU	N-CA-C	5.08	116.89	111.36
1	P	455	HIS	N-CA-C	5.08	116.62	111.14
1	S	479	ILE	N-CA-C	5.08	115.28	107.77
1	W	455	HIS	N-CA-C	5.08	116.62	111.14
1	D	254	GLU	N-CA-C	5.07	116.89	111.36
1	U	28	GLY	CA-C-N	5.07	124.68	119.05
1	U	28	GLY	C-N-CA	5.07	124.68	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	479	ILE	N-CA-C	5.07	115.27	107.77
1	E	254	GLU	N-CA-C	5.07	116.88	111.36
1	F	479	ILE	N-CA-C	5.07	115.27	107.77
1	R	254	GLU	N-CA-C	5.07	116.88	111.36
1	U	455	HIS	N-CA-C	5.07	116.61	111.14
1	W	28	GLY	CA-C-N	5.07	124.67	119.05
1	W	28	GLY	C-N-CA	5.07	124.67	119.05
1	O	455	HIS	N-CA-C	5.06	116.61	111.14
1	O	479	ILE	N-CA-C	5.06	115.26	107.77
1	N	254	GLU	N-CA-C	5.06	116.88	111.36
1	E	455	HIS	N-CA-C	5.06	116.60	111.14
1	G	28	GLY	CA-C-N	5.06	124.66	119.05
1	G	28	GLY	C-N-CA	5.06	124.66	119.05
1	Q	455	HIS	N-CA-C	5.06	116.60	111.14
1	W	254	GLU	N-CA-C	5.06	116.87	111.36
1	C	455	HIS	N-CA-C	5.05	116.60	111.14
1	F	455	HIS	N-CA-C	5.05	116.59	111.14
1	M	254	GLU	N-CA-C	5.05	116.86	111.36
1	O	28	GLY	CA-C-N	5.05	124.66	119.05
1	O	28	GLY	C-N-CA	5.05	124.66	119.05
1	Q	28	GLY	CA-C-N	5.05	124.65	119.05
1	Q	28	GLY	C-N-CA	5.05	124.65	119.05
1	S	254	GLU	N-CA-C	5.05	116.86	111.36
1	K	254	GLU	N-CA-C	5.05	116.86	111.36
1	U	254	GLU	N-CA-C	5.05	116.86	111.36
1	P	254	GLU	N-CA-C	5.04	116.86	111.36
1	A	28	GLY	CA-C-N	5.04	124.65	119.05
1	A	28	GLY	C-N-CA	5.04	124.65	119.05
1	T	254	GLU	N-CA-C	5.04	116.86	111.36
1	F	28	GLY	CA-C-N	5.04	124.64	119.05
1	F	28	GLY	C-N-CA	5.04	124.64	119.05
1	H	455	HIS	N-CA-C	5.04	116.58	111.14
1	D	455	HIS	N-CA-C	5.03	116.58	111.14
1	M	28	GLY	CA-C-N	5.03	124.64	119.05
1	M	28	GLY	C-N-CA	5.03	124.64	119.05
1	P	28	GLY	CA-C-N	5.03	124.64	119.05
1	P	28	GLY	C-N-CA	5.03	124.64	119.05
1	I	28	GLY	CA-C-N	5.03	124.63	119.05
1	I	28	GLY	C-N-CA	5.03	124.63	119.05
1	J	254	GLU	N-CA-C	5.03	116.84	111.36
1	L	254	GLU	N-CA-C	5.03	116.84	111.36
1	A	254	GLU	N-CA-C	5.03	116.84	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	GLY	CA-C-N	5.03	124.63	119.05
1	D	28	GLY	C-N-CA	5.03	124.63	119.05
1	J	28	GLY	CA-C-N	5.03	124.63	119.05
1	J	28	GLY	C-N-CA	5.03	124.63	119.05
1	N	28	GLY	CA-C-N	5.03	124.63	119.05
1	N	28	GLY	C-N-CA	5.03	124.63	119.05
1	X	254	GLU	N-CA-C	5.03	116.84	111.36
1	B	254	GLU	N-CA-C	5.03	116.84	111.36
1	G	254	GLU	N-CA-C	5.02	116.83	111.36
1	M	455	HIS	N-CA-C	5.02	116.56	111.14
1	T	28	GLY	CA-C-N	5.02	124.62	119.05
1	T	28	GLY	C-N-CA	5.02	124.62	119.05
1	C	28	GLY	CA-C-N	5.02	124.62	119.05
1	C	28	GLY	C-N-CA	5.02	124.62	119.05
1	V	28	GLY	CA-C-N	5.02	124.62	119.05
1	V	28	GLY	C-N-CA	5.02	124.62	119.05
1	X	28	GLY	CA-C-N	5.01	124.62	119.05
1	X	28	GLY	C-N-CA	5.01	124.62	119.05
1	H	28	GLY	CA-C-N	5.01	124.61	119.05
1	H	28	GLY	C-N-CA	5.01	124.61	119.05
1	B	28	GLY	CA-C-N	5.01	124.61	119.05
1	B	28	GLY	C-N-CA	5.01	124.61	119.05
1	E	28	GLY	CA-C-N	5.01	124.61	119.05
1	E	28	GLY	C-N-CA	5.01	124.61	119.05
1	A	455	HIS	N-CA-C	5.00	116.55	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3799	0	3802	144	0
1	B	3799	0	3802	168	0
1	C	3799	0	3802	213	0
1	D	3799	0	3802	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3799	0	3802	156	0
1	F	3799	0	3802	146	3
1	G	3799	0	3802	158	0
1	H	3799	0	3802	242	0
1	I	3799	0	3802	184	0
1	J	3799	0	3802	199	1
1	K	3799	0	3802	174	0
1	L	3799	0	3802	231	0
1	M	3799	0	3802	197	0
1	N	3799	0	3802	238	0
1	O	3799	0	3802	169	0
1	P	3799	0	3802	204	0
1	Q	3799	0	3802	190	0
1	R	3799	0	3802	202	0
1	S	3799	0	3802	233	0
1	T	3799	0	3802	216	1
1	U	3799	0	3802	220	0
1	V	3799	0	3802	259	0
1	W	3799	0	3802	192	3
1	X	3799	0	3802	188	0
2	A	20	0	10	4	0
2	B	20	0	10	4	0
2	C	20	0	10	4	0
2	D	20	0	10	4	0
2	E	20	0	10	4	0
2	F	20	0	10	4	0
2	G	20	0	10	4	0
2	H	20	0	10	5	0
2	I	20	0	10	5	0
2	J	20	0	10	4	0
2	K	20	0	10	5	0
2	L	20	0	10	5	0
2	M	20	0	10	4	0
2	N	20	0	10	4	0
2	O	20	0	10	5	0
2	P	20	0	10	5	0
2	Q	20	0	10	4	0
2	R	20	0	10	5	0
2	S	20	0	10	4	0
2	T	20	0	10	5	0
2	U	20	0	10	4	0
2	V	20	0	10	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	20	0	10	5	0
2	X	20	0	10	5	0
All	All	91656	0	91488	3592	4

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 20.

All (3592) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ALA:CB	1:N:446:LYS:HD3	1.49	1.42
1:C:250:SER:CB	1:N:446:LYS:HG2	1.49	1.41
1:U:242:HIS:HE1	1:W:12:PHE:CZ	1.42	1.38
1:H:12:PHE:CZ	1:J:242:HIS:HE1	1.41	1.37
1:P:487:GLY:HA2	1:V:229:LYS:CE	1.56	1.33
1:F:188:ALA:CB	1:F:218:GLN:HG3	1.62	1.30
1:M:188:ALA:CB	1:M:218:GLN:HG3	1.62	1.30
1:B:188:ALA:CB	1:B:218:GLN:HG3	1.62	1.30
1:J:188:ALA:CB	1:J:218:GLN:HG3	1.62	1.30
1:D:188:ALA:CB	1:D:218:GLN:HG3	1.62	1.29
1:K:12:PHE:CZ	1:M:242:HIS:HE1	1.49	1.29
1:G:188:ALA:CB	1:G:218:GLN:HG3	1.62	1.29
1:U:188:ALA:CB	1:U:218:GLN:HG3	1.62	1.29
1:O:188:ALA:CB	1:O:218:GLN:HG3	1.62	1.28
1:R:188:ALA:CB	1:R:218:GLN:HG3	1.62	1.28
1:C:250:SER:HB2	1:N:446:LYS:CG	1.61	1.28
1:K:188:ALA:CB	1:K:218:GLN:HG3	1.62	1.28
1:L:188:ALA:CB	1:L:218:GLN:HG3	1.62	1.28
1:V:284:LYS:HG3	1:X:7:LEU:CD2	1.60	1.28
1:N:188:ALA:CB	1:N:218:GLN:HG3	1.62	1.28
1:T:188:ALA:CB	1:T:218:GLN:HG3	1.62	1.28
1:C:188:ALA:CB	1:C:218:GLN:HG3	1.62	1.28
1:E:188:ALA:CB	1:E:218:GLN:HG3	1.62	1.28
1:U:242:HIS:CE1	1:W:12:PHE:CZ	2.20	1.28
1:V:188:ALA:CB	1:V:218:GLN:HG3	1.62	1.28
1:W:188:ALA:CB	1:W:218:GLN:HG3	1.62	1.28
1:S:188:ALA:CB	1:S:218:GLN:HG3	1.62	1.28
1:A:188:ALA:CB	1:A:218:GLN:HG3	1.62	1.27
1:I:188:ALA:CB	1:I:218:GLN:HG3	1.62	1.27
1:P:188:ALA:CB	1:P:218:GLN:HG3	1.62	1.27
1:Q:188:ALA:CB	1:Q:218:GLN:HG3	1.62	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:188:ALA:CB	1:X:218:GLN:HG3	1.62	1.27
1:H:188:ALA:CB	1:H:218:GLN:HG3	1.62	1.27
1:L:242:HIS:HE1	1:N:12:PHE:CE2	1.51	1.27
1:I:229:LYS:CE	1:M:487:GLY:HA2	1.64	1.26
1:R:280:ILE:HG12	1:T:6:ASN:O	1.35	1.23
1:L:242:HIS:CE1	1:N:12:PHE:CE2	2.28	1.21
1:R:284:LYS:HG3	1:T:7:LEU:CD2	1.69	1.21
1:K:12:PHE:CE2	1:M:242:HIS:CE1	2.28	1.20
1:U:372:ILE:HG13	1:V:390:GLU:HA	1.22	1.19
1:E:297:GLN:OE1	1:G:310:ARG:HG2	1.44	1.18
1:D:472:THR:HG22	1:D:498:GLU:HA	1.25	1.17
1:Q:472:THR:HG22	1:Q:498:GLU:HA	1.25	1.17
1:S:373:PRO:HB3	1:T:391:THR:HA	1.25	1.17
1:C:390:GLU:HA	1:P:372:ILE:HG13	1.23	1.17
1:H:310:ARG:HG2	1:J:297:GLN:CG	1.75	1.17
1:H:310:ARG:HG2	1:J:297:GLN:CB	1.73	1.17
1:I:487:GLY:CA	1:M:229:LYS:HG3	1.73	1.17
1:L:283:SER:HB3	1:N:3:LEU:CD2	1.75	1.16
1:M:472:THR:HG22	1:M:498:GLU:HA	1.25	1.16
1:T:3:LEU:HD23	1:T:3:LEU:C	1.70	1.16
1:H:12:PHE:CZ	1:J:242:HIS:CE1	2.31	1.16
1:H:371:HIS:O	1:H:374:MET:HG2	1.44	1.16
1:R:472:THR:HG22	1:R:498:GLU:HA	1.25	1.16
1:K:472:THR:HG22	1:K:498:GLU:HA	1.25	1.16
1:F:373:PRO:HA	1:G:390:GLU:O	1.40	1.15
1:I:487:GLY:HA2	1:M:229:LYS:CG	1.76	1.15
1:A:472:THR:HG22	1:A:498:GLU:HA	1.25	1.15
1:U:12:PHE:CE2	1:W:242:HIS:HE1	1.64	1.15
1:L:472:THR:HG22	1:L:498:GLU:HA	1.25	1.14
1:S:472:THR:HG22	1:S:498:GLU:HA	1.25	1.14
1:V:472:THR:HG22	1:V:498:GLU:HA	1.25	1.14
1:H:310:ARG:CG	1:J:297:GLN:HB2	1.76	1.14
1:B:12:PHE:CE2	1:C:242:HIS:HE1	1.65	1.13
1:P:487:GLY:HA2	1:V:229:LYS:CD	1.77	1.13
1:S:372:ILE:HD11	1:T:390:GLU:HG2	1.29	1.13
1:B:472:THR:HG22	1:B:498:GLU:HA	1.25	1.13
1:H:297:GLN:HB2	1:J:310:ARG:HG2	1.26	1.13
1:S:372:ILE:CG1	1:T:390:GLU:HA	1.77	1.13
1:U:242:HIS:CE1	1:W:12:PHE:CE2	2.37	1.13
1:Q:297:GLN:OE1	1:S:310:ARG:HG2	1.43	1.13
1:H:312:GLU:HA	1:J:311:ALA:CB	1.78	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:12:PHE:CZ	1:M:242:HIS:CE1	2.36	1.12
1:U:11:ILE:HB	1:W:273:LYS:CG	1.77	1.12
1:K:12:PHE:CE2	1:M:242:HIS:HE1	1.65	1.12
1:U:297:GLN:HB2	1:W:310:ARG:HG2	1.32	1.12
1:W:472:THR:HG22	1:W:498:GLU:HA	1.25	1.12
1:B:188:ALA:CB	1:B:218:GLN:CG	2.28	1.12
1:L:188:ALA:CB	1:L:218:GLN:CG	2.28	1.12
1:U:472:THR:HG22	1:U:498:GLU:HA	1.25	1.12
1:F:188:ALA:CB	1:F:218:GLN:CG	2.28	1.11
1:O:472:THR:HG22	1:O:498:GLU:HA	1.25	1.11
1:S:373:PRO:HA	1:T:390:GLU:O	1.49	1.11
1:T:188:ALA:CB	1:T:218:GLN:CG	2.28	1.11
1:C:472:THR:HG22	1:C:498:GLU:HA	1.25	1.11
1:H:188:ALA:CB	1:H:218:GLN:CG	2.28	1.11
1:M:188:ALA:CB	1:M:218:GLN:CG	2.28	1.11
1:O:188:ALA:CB	1:O:218:GLN:CG	2.28	1.11
1:S:188:ALA:CB	1:S:218:GLN:CG	2.28	1.11
1:U:11:ILE:HB	1:W:273:LYS:HG2	1.13	1.11
1:U:188:ALA:CB	1:U:218:GLN:CG	2.28	1.11
1:F:472:THR:HG22	1:F:498:GLU:HA	1.25	1.11
1:I:188:ALA:CB	1:I:218:GLN:CG	2.28	1.11
1:Q:188:ALA:CB	1:Q:218:GLN:CG	2.28	1.11
1:C:188:ALA:CB	1:C:218:GLN:CG	2.28	1.11
1:H:242:HIS:CE1	1:J:12:PHE:CE2	2.39	1.11
1:I:229:LYS:HE3	1:M:487:GLY:HA2	1.15	1.11
1:V:242:HIS:CE1	1:X:12:PHE:CE2	2.39	1.11
1:X:472:THR:HG22	1:X:498:GLU:HA	1.25	1.11
1:O:11:ILE:HB	1:P:273:LYS:HG2	1.27	1.10
1:R:371:HIS:O	1:R:374:MET:HG2	1.48	1.10
1:V:188:ALA:CB	1:V:218:GLN:CG	2.29	1.10
1:V:280:ILE:HG12	1:X:6:ASN:O	1.51	1.10
1:X:188:ALA:CB	1:X:218:GLN:CG	2.28	1.10
1:U:11:ILE:CB	1:W:273:LYS:HG2	1.81	1.10
1:W:188:ALA:CB	1:W:218:GLN:CG	2.28	1.10
1:A:188:ALA:CB	1:A:218:GLN:CG	2.28	1.10
1:A:392:LYS:HD2	1:J:373:PRO:HD3	1.34	1.10
1:J:188:ALA:CB	1:J:218:GLN:CG	2.28	1.10
1:P:487:GLY:CA	1:V:229:LYS:HE3	1.82	1.10
1:E:188:ALA:CB	1:E:218:GLN:CG	2.28	1.10
1:G:472:THR:HG22	1:G:498:GLU:HA	1.25	1.10
1:K:188:ALA:CB	1:K:218:GLN:CG	2.28	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:188:ALA:CB	1:P:218:GLN:CG	2.28	1.10
1:D:188:ALA:CB	1:D:218:GLN:CG	2.28	1.09
1:E:472:THR:HG22	1:E:498:GLU:HA	1.25	1.09
1:I:188:ALA:HB2	1:I:218:GLN:CG	1.82	1.09
1:I:472:THR:HG22	1:I:498:GLU:HA	1.25	1.09
1:N:188:ALA:CB	1:N:218:GLN:CG	2.28	1.09
1:O:12:PHE:CE2	1:P:242:HIS:HE1	1.69	1.09
1:R:188:ALA:CB	1:R:218:GLN:CG	2.28	1.09
1:S:188:ALA:HB2	1:S:218:GLN:CG	1.82	1.09
1:P:188:ALA:HB2	1:P:218:GLN:CG	1.82	1.09
1:U:312:GLU:HA	1:W:311:ALA:HB1	1.32	1.09
1:A:188:ALA:HB2	1:A:218:GLN:CG	1.83	1.09
1:G:188:ALA:CB	1:G:218:GLN:CG	2.28	1.09
1:G:188:ALA:HB2	1:G:218:GLN:CG	1.82	1.09
1:L:188:ALA:HB2	1:L:218:GLN:CG	1.83	1.09
1:M:188:ALA:HB2	1:M:218:GLN:CG	1.82	1.09
1:Q:188:ALA:HB2	1:Q:218:GLN:CG	1.82	1.09
1:S:372:ILE:HG12	1:T:390:GLU:HA	1.30	1.09
1:C:188:ALA:HB2	1:C:218:GLN:CG	1.83	1.09
1:F:390:GLU:O	1:G:373:PRO:HA	1.52	1.09
1:N:472:THR:HG22	1:N:498:GLU:HA	1.25	1.09
1:R:272:GLU:CG	1:T:352:GLU:HG2	1.80	1.09
1:D:188:ALA:HB2	1:D:218:GLN:CG	1.83	1.08
1:K:188:ALA:HB2	1:K:218:GLN:CG	1.83	1.08
1:P:472:THR:HG22	1:P:498:GLU:HA	1.25	1.08
1:R:269:ILE:HG12	1:T:11:ILE:HD12	1.29	1.08
1:E:270:PRO:HG2	1:E:273:LYS:HE2	1.35	1.08
1:R:270:PRO:HG2	1:R:273:LYS:HE2	1.36	1.08
1:V:188:ALA:HB2	1:V:218:GLN:CG	1.83	1.08
1:X:188:ALA:HB2	1:X:218:GLN:CG	1.83	1.08
1:P:371:HIS:O	1:P:374:MET:HG2	1.51	1.08
1:V:270:PRO:HG2	1:V:273:LYS:HE2	1.35	1.08
1:B:188:ALA:HB2	1:B:218:GLN:CG	1.83	1.08
1:H:188:ALA:HB2	1:H:218:GLN:CG	1.83	1.08
1:L:424:ARG:HG2	1:L:424:ARG:NH1	1.55	1.08
1:O:188:ALA:HB2	1:O:218:GLN:CG	1.82	1.08
1:C:216:ALA:HB3	1:N:446:LYS:HD3	1.28	1.08
1:F:188:ALA:HB2	1:F:218:GLN:CG	1.83	1.08
1:T:472:THR:HG22	1:T:498:GLU:HA	1.25	1.08
1:U:371:HIS:O	1:U:374:MET:HG2	1.54	1.08
1:C:424:ARG:HG2	1:C:424:ARG:NH1	1.55	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:472:THR:HG22	1:H:498:GLU:HA	1.25	1.07
1:T:188:ALA:HB2	1:T:218:GLN:CG	1.83	1.07
1:B:424:ARG:HG2	1:B:424:ARG:NH1	1.56	1.07
1:N:188:ALA:HB2	1:N:218:GLN:CG	1.83	1.07
1:L:270:PRO:HG2	1:L:273:LYS:HE2	1.35	1.07
1:U:188:ALA:HB2	1:U:218:GLN:CG	1.83	1.07
1:E:188:ALA:HB2	1:E:218:GLN:CG	1.83	1.07
1:H:242:HIS:HE1	1:J:12:PHE:CE2	1.69	1.07
1:H:496:LEU:HG	1:M:195:VAL:CG2	1.85	1.07
1:I:424:ARG:HG2	1:I:424:ARG:NH1	1.55	1.07
1:L:297:GLN:OE1	1:N:310:ARG:HG2	1.50	1.07
1:U:11:ILE:O	1:W:273:LYS:HE3	1.54	1.07
1:H:242:HIS:HE1	1:J:12:PHE:CZ	1.72	1.07
1:J:188:ALA:HB2	1:J:218:GLN:CG	1.82	1.06
1:J:472:THR:HG22	1:J:498:GLU:HA	1.25	1.06
1:T:424:ARG:HH11	1:T:424:ARG:CG	1.68	1.06
1:P:229:LYS:HG3	1:V:487:GLY:CA	1.84	1.06
1:V:284:LYS:HG3	1:X:7:LEU:HD21	1.35	1.06
1:I:270:PRO:HG2	1:I:273:LYS:HE2	1.36	1.06
1:J:296:THR:HG22	1:J:297:GLN:HG2	1.37	1.06
1:R:188:ALA:HB2	1:R:218:GLN:CG	1.83	1.06
1:C:216:ALA:HB3	1:N:446:LYS:O	1.55	1.06
1:H:496:LEU:CD2	1:M:195:VAL:HG22	1.83	1.06
1:S:424:ARG:HH11	1:S:424:ARG:CG	1.68	1.06
1:W:188:ALA:HB2	1:W:218:GLN:CG	1.83	1.06
1:B:297:GLN:OE1	1:C:310:ARG:HG2	1.55	1.06
1:B:424:ARG:HH11	1:B:424:ARG:CG	1.68	1.06
1:C:216:ALA:CB	1:N:446:LYS:CD	2.34	1.06
1:D:424:ARG:HH11	1:D:424:ARG:CG	1.68	1.06
1:H:311:ALA:CB	1:J:312:GLU:HA	1.85	1.06
1:I:229:LYS:HE3	1:M:487:GLY:CA	1.86	1.06
1:I:229:LYS:CD	1:M:487:GLY:HA2	1.86	1.06
1:I:371:HIS:O	1:I:374:MET:HG2	1.55	1.06
1:I:424:ARG:HH11	1:I:424:ARG:CG	1.68	1.06
1:U:311:ALA:HB1	1:W:312:GLU:HA	1.32	1.06
1:O:12:PHE:CZ	1:P:242:HIS:HE1	1.73	1.05
1:W:424:ARG:HG2	1:W:424:ARG:NH1	1.55	1.05
1:U:372:ILE:HG13	1:V:390:GLU:CA	1.87	1.05
1:A:424:ARG:HH11	1:A:424:ARG:CG	1.68	1.05
1:N:424:ARG:HH11	1:N:424:ARG:CG	1.69	1.05
1:C:424:ARG:HH11	1:C:424:ARG:CG	1.68	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:ARG:HG2	1:F:424:ARG:NH1	1.55	1.05
1:P:229:LYS:HG3	1:V:487:GLY:HA2	1.36	1.05
1:R:424:ARG:HG2	1:R:424:ARG:NH1	1.55	1.05
1:G:424:ARG:HH11	1:G:424:ARG:CG	1.68	1.04
1:H:312:GLU:HA	1:J:311:ALA:HB1	1.06	1.04
1:H:496:LEU:CG	1:M:195:VAL:HG22	1.85	1.04
1:O:12:PHE:CE2	1:P:242:HIS:CE1	2.45	1.04
1:U:12:PHE:HE2	1:W:242:HIS:CE1	1.75	1.04
1:L:371:HIS:O	1:L:374:MET:HG2	1.58	1.04
1:K:424:ARG:HH11	1:K:424:ARG:CG	1.68	1.04
1:V:424:ARG:HH11	1:V:424:ARG:CG	1.68	1.04
1:H:372:ILE:HG23	1:I:390:GLU:O	1.57	1.04
1:M:373:PRO:HA	1:N:390:GLU:O	1.58	1.04
1:R:284:LYS:HG3	1:T:7:LEU:HD22	1.36	1.04
1:V:372:ILE:HD11	1:V:374:MET:HE2	1.40	1.04
1:L:424:ARG:HH11	1:L:424:ARG:CG	1.68	1.04
1:M:424:ARG:HH11	1:M:424:ARG:CG	1.68	1.04
1:O:372:ILE:HD11	1:O:374:MET:HE2	1.40	1.03
1:V:242:HIS:HE1	1:X:12:PHE:CE2	1.74	1.03
1:X:424:ARG:HH11	1:X:424:ARG:CG	1.68	1.03
1:K:372:ILE:HD11	1:K:374:MET:HE2	1.40	1.03
1:O:424:ARG:HH11	1:O:424:ARG:CG	1.68	1.03
1:P:424:ARG:HH11	1:P:424:ARG:CG	1.68	1.03
1:Q:424:ARG:HH11	1:Q:424:ARG:CG	1.68	1.03
1:H:424:ARG:HH11	1:H:424:ARG:CG	1.68	1.03
1:M:372:ILE:HG13	1:N:390:GLU:HA	1.36	1.03
1:W:424:ARG:HH11	1:W:424:ARG:CG	1.68	1.03
1:J:424:ARG:HH11	1:J:424:ARG:CG	1.68	1.03
1:Q:242:HIS:CE1	1:S:12:PHE:CE2	2.47	1.03
1:S:371:HIS:O	1:S:374:MET:HG2	1.58	1.03
1:F:424:ARG:HH11	1:F:424:ARG:CG	1.69	1.02
1:U:373:PRO:HA	1:V:390:GLU:O	1.59	1.02
1:U:424:ARG:HH11	1:U:424:ARG:CG	1.68	1.02
1:R:269:ILE:HG12	1:T:11:ILE:CD1	1.89	1.02
1:V:276:VAL:HG12	1:V:280:ILE:HD11	1.36	1.02
1:C:372:ILE:HD11	1:C:374:MET:HE2	1.40	1.02
1:R:297:GLN:HG3	1:T:310:ARG:HG3	1.40	1.02
1:S:372:ILE:HG13	1:T:390:GLU:CA	1.89	1.02
1:H:372:ILE:HG13	1:I:390:GLU:HA	1.40	1.02
1:P:487:GLY:HA2	1:V:229:LYS:HE3	1.06	1.02
1:E:372:ILE:HD11	1:E:374:MET:HE2	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:310:ARG:HG2	1:J:297:GLN:HB2	1.30	1.01
1:S:372:ILE:HG13	1:T:390:GLU:O	1.59	1.01
1:W:372:ILE:HD11	1:W:374:MET:HE2	1.40	1.01
1:W:373:PRO:HB3	1:X:391:THR:HA	1.39	1.01
1:K:424:ARG:HG2	1:K:424:ARG:NH1	1.55	1.01
1:O:311:ALA:HB1	1:P:312:GLU:HA	1.41	1.01
1:G:372:ILE:HD11	1:G:374:MET:HE2	1.40	1.01
1:H:310:ARG:HG2	1:J:297:GLN:HG3	1.42	1.01
1:L:283:SER:CB	1:N:3:LEU:CD2	2.38	1.01
1:F:372:ILE:HD11	1:F:374:MET:HE2	1.40	1.01
1:J:372:ILE:HD11	1:J:374:MET:HE2	1.40	1.01
1:D:372:ILE:HD11	1:D:374:MET:HE2	1.40	1.01
1:E:242:HIS:HE1	1:G:12:PHE:CZ	1.77	1.01
1:M:371:HIS:O	1:M:374:MET:HG2	1.60	1.01
1:U:12:PHE:CE2	1:W:242:HIS:CE1	2.49	1.01
1:T:371:HIS:O	1:T:374:MET:HG2	1.61	1.00
1:V:284:LYS:CG	1:X:7:LEU:CD2	2.37	1.00
1:W:372:ILE:HG13	1:X:390:GLU:HA	1.39	1.00
1:E:424:ARG:HG2	1:E:424:ARG:NH1	1.55	1.00
1:K:496:LEU:HG	1:S:195:VAL:HG22	1.40	1.00
1:N:372:ILE:HD11	1:N:374:MET:HE2	1.40	1.00
1:X:372:ILE:HD11	1:X:374:MET:HE2	1.40	1.00
1:H:311:ALA:HB1	1:J:312:GLU:CA	1.90	1.00
1:P:195:VAL:HG22	1:U:496:LEU:HG	1.43	1.00
1:Q:283:SER:HB3	1:S:3:LEU:CD2	1.92	1.00
1:R:424:ARG:HH11	1:R:424:ARG:CG	1.68	1.00
1:E:424:ARG:HH11	1:E:424:ARG:CG	1.68	1.00
1:Q:372:ILE:HD11	1:Q:374:MET:HE2	1.40	1.00
1:A:372:ILE:HD11	1:A:374:MET:HE2	1.40	1.00
1:R:272:GLU:HG3	1:T:352:GLU:HB2	1.42	1.00
1:D:424:ARG:HG2	1:D:424:ARG:NH1	1.55	0.99
1:H:496:LEU:HG	1:M:195:VAL:HG22	1.39	0.99
1:U:372:ILE:HG23	1:V:390:GLU:O	1.62	0.99
1:H:12:PHE:CE2	1:J:242:HIS:HE1	1.80	0.99
1:I:229:LYS:HG3	1:M:487:GLY:CA	1.91	0.99
1:K:12:PHE:HE2	1:M:242:HIS:CE1	1.75	0.99
1:P:424:ARG:HG2	1:P:424:ARG:NH1	1.55	0.99
1:B:372:ILE:HD11	1:B:374:MET:HE2	1.40	0.99
1:M:424:ARG:HG2	1:M:424:ARG:NH1	1.55	0.99
1:J:424:ARG:HG2	1:J:424:ARG:NH1	1.55	0.98
1:I:229:LYS:HG3	1:M:487:GLY:HA3	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:12:PHE:HE2	1:P:242:HIS:CE1	1.81	0.98
1:V:297:GLN:HE21	1:V:300:GLU:CB	1.76	0.98
1:A:424:ARG:HG2	1:A:424:ARG:NH1	1.55	0.98
1:B:12:PHE:HE2	1:C:242:HIS:CE1	1.80	0.98
1:T:424:ARG:HG2	1:T:424:ARG:NH1	1.55	0.98
1:U:424:ARG:HG2	1:U:424:ARG:NH1	1.55	0.98
1:H:310:ARG:CB	1:J:297:GLN:HB2	1.93	0.98
1:O:312:GLU:HA	1:P:311:ALA:HB1	1.45	0.98
1:G:424:ARG:HG2	1:G:424:ARG:NH1	1.55	0.97
1:H:311:ALA:HB1	1:J:312:GLU:HA	0.98	0.97
1:K:373:PRO:HA	1:L:390:GLU:O	1.63	0.97
1:P:195:VAL:HG22	1:U:496:LEU:CD2	1.95	0.97
1:S:373:PRO:HB3	1:T:391:THR:CA	1.93	0.97
1:T:3:LEU:HD23	1:T:3:LEU:O	1.63	0.97
1:X:424:ARG:HG2	1:X:424:ARG:NH1	1.55	0.97
1:H:297:GLN:CB	1:J:310:ARG:HG2	1.94	0.97
1:K:242:HIS:CE1	1:M:12:PHE:CE2	2.53	0.97
1:S:424:ARG:HG2	1:S:424:ARG:NH1	1.55	0.97
1:C:473:GLY:HA3	1:V:191:ALA:HB1	1.46	0.97
1:L:283:SER:CB	1:N:3:LEU:HD23	1.95	0.96
1:A:3:LEU:CD2	1:I:283:SER:HB3	1.95	0.96
1:H:424:ARG:HG2	1:H:424:ARG:NH1	1.55	0.96
1:S:373:PRO:CB	1:T:391:THR:HA	1.95	0.96
1:H:472:THR:HG22	1:H:498:GLU:CA	1.96	0.96
1:C:496:LEU:HG	1:V:195:VAL:HG22	1.48	0.96
1:F:472:THR:HG22	1:F:498:GLU:CA	1.96	0.96
1:H:297:GLN:HB2	1:J:310:ARG:CG	1.94	0.96
1:V:424:ARG:HG2	1:V:424:ARG:NH1	1.56	0.96
1:B:472:THR:HG22	1:B:498:GLU:CA	1.96	0.96
1:L:472:THR:HG22	1:L:498:GLU:CA	1.96	0.96
1:Q:472:THR:HG22	1:Q:498:GLU:CA	1.96	0.96
1:V:297:GLN:NE2	1:V:300:GLU:CG	2.29	0.96
1:D:472:THR:HG22	1:D:498:GLU:CA	1.96	0.96
1:Q:424:ARG:HG2	1:Q:424:ARG:NH1	1.55	0.96
1:A:472:THR:HG22	1:A:498:GLU:CA	1.96	0.96
1:C:390:GLU:O	1:P:373:PRO:HA	1.66	0.95
1:R:472:THR:HG22	1:R:498:GLU:CA	1.96	0.95
1:B:373:PRO:HD3	1:O:392:LYS:HD2	1.45	0.95
1:F:372:ILE:HG13	1:G:390:GLU:HA	1.48	0.95
1:K:472:THR:HG22	1:K:498:GLU:CA	1.96	0.95
1:R:269:ILE:CG1	1:T:11:ILE:HD12	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:472:THR:HG22	1:S:498:GLU:CA	1.96	0.95
1:P:195:VAL:HG22	1:U:496:LEU:CG	1.95	0.95
1:S:372:ILE:HG13	1:T:390:GLU:C	1.91	0.95
1:U:472:THR:HG22	1:U:498:GLU:CA	1.96	0.95
1:V:472:THR:HG22	1:V:498:GLU:CA	1.96	0.95
1:C:472:THR:HG22	1:C:498:GLU:CA	1.96	0.95
1:V:297:GLN:NE2	1:V:300:GLU:CB	2.30	0.95
1:O:472:THR:HG22	1:O:498:GLU:CA	1.96	0.95
1:X:472:THR:HG22	1:X:498:GLU:CA	1.96	0.95
1:C:373:PRO:HA	1:P:390:GLU:O	1.66	0.94
1:G:472:THR:HG22	1:G:498:GLU:CA	1.96	0.94
1:P:472:THR:HG22	1:P:498:GLU:CA	1.96	0.94
1:W:472:THR:HG22	1:W:498:GLU:CA	1.96	0.94
1:D:12:PHE:CZ	1:F:242:HIS:HE1	1.84	0.94
1:E:472:THR:HG22	1:E:498:GLU:CA	1.96	0.94
1:N:472:THR:HG22	1:N:498:GLU:CA	1.96	0.94
1:I:472:THR:HG22	1:I:498:GLU:CA	1.96	0.94
1:M:472:THR:HG22	1:M:498:GLU:CA	1.96	0.94
1:T:472:THR:HG22	1:T:498:GLU:CA	1.96	0.94
1:F:188:ALA:HB1	1:F:218:GLN:CG	1.98	0.94
1:H:6:ASN:OD1	1:J:279:LYS:HE3	1.64	0.94
1:S:372:ILE:CG1	1:T:390:GLU:CA	2.44	0.94
1:D:12:PHE:CE2	1:F:242:HIS:CE1	2.55	0.94
1:U:188:ALA:HB1	1:U:218:GLN:CG	1.98	0.94
1:D:188:ALA:HB1	1:D:218:GLN:CG	1.98	0.93
1:Q:390:GLU:HA	1:R:372:ILE:HG13	1.45	0.93
1:W:372:ILE:HG13	1:X:390:GLU:CA	1.98	0.93
1:N:188:ALA:HB1	1:N:218:GLN:CG	1.98	0.93
1:E:242:HIS:CE1	1:G:12:PHE:CE2	2.56	0.93
1:N:424:ARG:HG2	1:N:424:ARG:NH1	1.55	0.93
1:P:487:GLY:HA3	1:V:229:LYS:HG3	1.51	0.93
1:R:276:VAL:HG12	1:R:280:ILE:HD11	1.50	0.93
1:U:373:PRO:HB3	1:V:391:THR:HA	1.51	0.93
1:B:12:PHE:CE2	1:C:242:HIS:CE1	2.56	0.93
1:D:392:LYS:HD2	1:E:373:PRO:HD3	1.51	0.93
1:J:472:THR:HG22	1:J:498:GLU:CA	1.96	0.93
1:R:370:GLN:HB3	1:R:374:MET:SD	2.08	0.93
1:E:242:HIS:HE1	1:G:12:PHE:CE2	1.86	0.93
1:I:487:GLY:HA2	1:M:229:LYS:HG3	0.93	0.93
1:W:188:ALA:HB1	1:W:218:GLN:CG	1.98	0.93
1:I:188:ALA:HB1	1:I:218:GLN:CG	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:6:ASN:OD1	1:P:279:LYS:HE3	1.68	0.93
1:O:11:ILE:HB	1:P:273:LYS:CG	1.99	0.93
1:G:188:ALA:HB1	1:G:218:GLN:CG	1.98	0.93
1:L:283:SER:OG	1:N:3:LEU:HD23	1.67	0.93
1:M:188:ALA:HB1	1:M:218:GLN:CG	1.98	0.93
1:R:272:GLU:HG3	1:T:352:GLU:CB	1.98	0.93
1:B:188:ALA:HB1	1:B:218:GLN:CG	1.98	0.93
1:H:473:GLY:HA3	1:M:191:ALA:HB1	1.51	0.93
1:K:373:PRO:HB3	1:L:391:THR:HA	1.50	0.93
1:Q:269:ILE:HG12	1:S:11:ILE:HD12	1.51	0.93
1:R:188:ALA:HB1	1:R:218:GLN:CG	1.98	0.93
1:K:188:ALA:HB1	1:K:218:GLN:CG	1.98	0.92
1:V:276:VAL:HG12	1:V:280:ILE:CD1	1.99	0.92
1:A:188:ALA:HB1	1:A:218:GLN:CG	1.98	0.92
1:O:188:ALA:HB1	1:O:218:GLN:CG	1.98	0.92
1:P:188:ALA:HB1	1:P:218:GLN:CG	1.98	0.92
1:D:12:PHE:CE2	1:F:242:HIS:HE1	1.88	0.92
1:H:242:HIS:CE1	1:J:12:PHE:CZ	2.55	0.92
1:J:188:ALA:HB1	1:J:218:GLN:CG	1.98	0.92
1:R:272:GLU:CG	1:T:352:GLU:CG	2.46	0.92
1:L:280:ILE:HG12	1:N:6:ASN:O	1.69	0.92
1:L:487:GLY:CA	1:S:229:LYS:HG3	1.99	0.92
1:H:188:ALA:HB1	1:H:218:GLN:CG	1.98	0.92
1:Q:188:ALA:HB1	1:Q:218:GLN:CG	1.98	0.91
1:F:373:PRO:HB3	1:G:391:THR:HA	1.52	0.91
1:T:3:LEU:C	1:T:3:LEU:CD2	2.42	0.91
1:V:283:SER:CB	1:X:3:LEU:HG	2.00	0.91
1:K:188:ALA:HB2	1:K:218:GLN:HG3	0.91	0.91
1:L:188:ALA:HB2	1:L:218:GLN:HG3	0.91	0.91
1:L:242:HIS:CE1	1:N:12:PHE:HE2	1.81	0.91
1:M:188:ALA:HB2	1:M:218:GLN:HG3	0.91	0.91
1:X:188:ALA:HB2	1:X:218:GLN:HG3	0.91	0.91
1:C:188:ALA:HB1	1:C:218:GLN:CG	1.98	0.91
1:I:188:ALA:HB2	1:I:218:GLN:HG3	0.91	0.91
1:L:188:ALA:HB1	1:L:218:GLN:CG	1.98	0.91
1:U:6:ASN:OD1	1:W:279:LYS:HE3	1.69	0.91
1:A:242:HIS:CE1	1:I:12:PHE:CE2	2.59	0.91
1:D:188:ALA:HB2	1:D:218:GLN:HG3	0.91	0.91
1:K:312:GLU:HA	1:M:311:ALA:HB1	1.53	0.91
1:N:371:HIS:O	1:N:374:MET:HG2	1.71	0.91
1:O:424:ARG:HG2	1:O:424:ARG:NH1	1.55	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:372:ILE:CD1	1:T:390:GLU:HG2	2.00	0.91
1:C:216:ALA:HB2	1:N:446:LYS:HD3	1.52	0.91
1:M:390:GLU:O	1:N:373:PRO:HA	1.69	0.91
1:E:188:ALA:HB1	1:E:218:GLN:CG	1.98	0.91
1:O:371:HIS:O	1:O:374:MET:HG2	1.71	0.91
1:P:487:GLY:CA	1:V:229:LYS:HG3	2.00	0.91
1:S:188:ALA:HB1	1:S:218:GLN:CG	1.98	0.91
1:X:188:ALA:HB1	1:X:218:GLN:CG	1.98	0.91
1:K:242:HIS:HE1	1:M:12:PHE:CE2	1.89	0.90
1:T:188:ALA:HB1	1:T:218:GLN:CG	1.98	0.90
1:G:371:HIS:O	1:G:374:MET:HG2	1.71	0.90
1:R:279:LYS:HB3	1:T:6:ASN:CG	1.96	0.90
1:A:188:ALA:HB2	1:A:218:GLN:HG3	0.91	0.90
1:A:371:HIS:O	1:A:374:MET:HG2	1.71	0.90
1:G:188:ALA:HB2	1:G:218:GLN:HG3	0.91	0.90
1:H:188:ALA:HB2	1:H:218:GLN:HG3	0.91	0.90
1:R:272:GLU:HG2	1:T:352:GLU:HG2	1.53	0.90
1:P:195:VAL:CG2	1:U:496:LEU:HG	2.01	0.90
1:R:273:LYS:HD3	1:T:11:ILE:O	1.69	0.90
1:I:370:GLN:HB3	1:I:374:MET:SD	2.11	0.90
1:V:297:GLN:HE21	1:V:300:GLU:HB2	1.34	0.90
1:P:487:GLY:CA	1:V:229:LYS:CD	2.50	0.90
1:R:296:THR:HG22	1:R:297:GLN:HG2	1.54	0.90
1:S:372:ILE:HG23	1:T:390:GLU:O	1.70	0.90
1:U:188:ALA:HB2	1:U:218:GLN:HG3	0.91	0.90
1:V:188:ALA:HB1	1:V:218:GLN:CG	1.98	0.90
1:I:229:LYS:CG	1:M:487:GLY:HA2	2.02	0.90
1:E:371:HIS:O	1:E:374:MET:HG2	1.71	0.90
1:K:371:HIS:O	1:K:374:MET:HG2	1.71	0.90
1:Q:188:ALA:HB2	1:Q:218:GLN:HG3	0.91	0.90
1:R:297:GLN:HG3	1:T:310:ARG:CG	2.02	0.90
1:V:188:ALA:HB2	1:V:218:GLN:HG3	0.91	0.90
1:B:371:HIS:O	1:B:374:MET:HG2	1.71	0.90
1:C:371:HIS:O	1:C:374:MET:HG2	1.71	0.90
1:H:312:GLU:CA	1:J:311:ALA:HB1	2.00	0.90
1:U:263:GLY:HA2	1:W:310:ARG:HH11	1.34	0.90
1:R:276:VAL:CG1	1:T:9:LEU:HB3	2.02	0.89
1:T:188:ALA:HB2	1:T:218:GLN:HG3	0.91	0.89
1:D:11:ILE:HB	1:F:273:LYS:HG2	1.52	0.89
1:F:188:ALA:HB2	1:F:218:GLN:HG3	0.91	0.89
1:W:373:PRO:HA	1:X:390:GLU:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:12:PHE:HZ	1:M:242:HIS:HE1	1.20	0.89
1:O:11:ILE:CB	1:P:273:LYS:HG2	2.03	0.89
1:P:144:ASP:O	1:P:145:ASP:HB2	1.73	0.89
1:R:284:LYS:CG	1:T:7:LEU:HD22	2.01	0.89
1:S:144:ASP:O	1:S:145:ASP:HB2	1.73	0.89
1:U:312:GLU:HA	1:W:311:ALA:CB	2.01	0.89
1:E:144:ASP:O	1:E:145:ASP:HB2	1.72	0.89
1:F:144:ASP:O	1:F:145:ASP:HB2	1.72	0.89
1:G:144:ASP:O	1:G:145:ASP:HB2	1.72	0.89
1:N:144:ASP:O	1:N:145:ASP:HB2	1.72	0.89
1:C:216:ALA:HB1	1:N:446:LYS:HE2	1.54	0.89
1:L:487:GLY:HA2	1:S:229:LYS:HE3	1.53	0.89
1:S:188:ALA:HB2	1:S:218:GLN:HG3	0.91	0.89
1:W:144:ASP:O	1:W:145:ASP:HB2	1.72	0.89
1:B:188:ALA:HB2	1:B:218:GLN:HG3	0.91	0.89
1:V:371:HIS:O	1:V:374:MET:HG2	1.71	0.89
1:J:188:ALA:HB2	1:J:218:GLN:HG3	0.91	0.89
1:P:188:ALA:HB2	1:P:218:GLN:HG3	0.91	0.89
1:Q:144:ASP:O	1:Q:145:ASP:HB2	1.72	0.89
1:W:188:ALA:HB2	1:W:218:GLN:HG3	0.91	0.89
1:X:371:HIS:O	1:X:374:MET:HG2	1.71	0.89
1:K:144:ASP:O	1:K:145:ASP:HB2	1.72	0.89
1:L:242:HIS:HE1	1:N:12:PHE:CZ	1.90	0.89
1:O:144:ASP:O	1:O:145:ASP:HB2	1.72	0.89
1:Q:371:HIS:O	1:Q:374:MET:HG2	1.71	0.89
1:V:284:LYS:CG	1:X:7:LEU:HD22	2.01	0.89
1:D:144:ASP:O	1:D:145:ASP:HB2	1.72	0.88
1:W:371:HIS:O	1:W:374:MET:HG2	1.71	0.88
1:E:188:ALA:HB2	1:E:218:GLN:HG3	0.91	0.88
1:Q:280:ILE:HG12	1:S:6:ASN:O	1.71	0.88
1:R:188:ALA:HB2	1:R:218:GLN:HG3	0.91	0.88
1:U:272:GLU:O	1:W:352:GLU:HG2	1.72	0.88
1:J:371:HIS:O	1:J:374:MET:HG2	1.71	0.88
1:R:297:GLN:HB2	1:T:310:ARG:HB2	1.53	0.88
1:N:188:ALA:HB2	1:N:218:GLN:HG3	0.91	0.88
1:T:144:ASP:O	1:T:145:ASP:HB2	1.72	0.88
1:P:229:LYS:CG	1:V:487:GLY:HA2	2.03	0.88
1:B:144:ASP:O	1:B:145:ASP:HB2	1.72	0.88
1:H:383:SER:HB2	1:I:383:SER:HB2	1.54	0.88
1:H:11:ILE:HB	1:J:273:LYS:HG2	1.53	0.88
1:X:144:ASP:O	1:X:145:ASP:HB2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:371:HIS:O	1:F:374:MET:HG2	1.71	0.88
1:F:373:PRO:CA	1:G:390:GLU:O	2.20	0.88
1:U:144:ASP:O	1:U:145:ASP:HB2	1.72	0.88
1:C:144:ASP:O	1:C:145:ASP:HB2	1.72	0.88
1:D:371:HIS:O	1:D:374:MET:HG2	1.71	0.88
1:J:144:ASP:O	1:J:145:ASP:HB2	1.72	0.88
1:C:390:GLU:CA	1:P:372:ILE:HG13	2.04	0.87
1:D:297:GLN:OE1	1:F:310:ARG:HG2	1.75	0.87
1:V:297:GLN:HE21	1:V:300:GLU:CG	1.87	0.87
1:B:272:GLU:HG3	1:C:352:GLU:HB2	1.55	0.87
1:H:144:ASP:O	1:H:145:ASP:HB2	1.72	0.87
1:L:144:ASP:O	1:L:145:ASP:HB2	1.72	0.87
1:Q:242:HIS:HE1	1:S:12:PHE:CE2	1.87	0.87
1:H:188:ALA:HB1	1:H:218:GLN:HG2	1.56	0.87
1:C:496:LEU:HG	1:V:195:VAL:CG2	2.05	0.87
1:I:404:ARG:NH2	1:M:228:PRO:HG2	1.89	0.87
1:L:229:LYS:HG3	1:S:487:GLY:CA	2.05	0.87
1:V:144:ASP:O	1:V:145:ASP:HB2	1.72	0.87
1:B:312:GLU:HA	1:C:311:ALA:HB1	1.56	0.87
1:C:188:ALA:HB2	1:C:218:GLN:HG3	0.91	0.87
1:G:188:ALA:HB1	1:G:218:GLN:HG2	1.56	0.87
1:O:188:ALA:HB2	1:O:218:GLN:HG3	0.91	0.87
1:R:188:ALA:HB1	1:R:218:GLN:HG2	1.56	0.87
1:R:272:GLU:HG3	1:T:352:GLU:CG	2.05	0.87
1:W:372:ILE:HG23	1:X:390:GLU:O	1.75	0.87
1:L:269:ILE:HG12	1:N:11:ILE:HD12	1.57	0.87
1:M:144:ASP:O	1:M:145:ASP:HB2	1.72	0.87
1:J:188:ALA:HB1	1:J:218:GLN:HG2	1.56	0.86
1:R:144:ASP:O	1:R:145:ASP:HB2	1.72	0.86
1:F:188:ALA:HB1	1:F:218:GLN:HG2	1.56	0.86
1:I:144:ASP:O	1:I:145:ASP:HB2	1.72	0.86
1:M:188:ALA:HB1	1:M:218:GLN:HG2	1.56	0.86
1:T:188:ALA:HB1	1:T:218:GLN:HG2	1.57	0.86
1:U:390:GLU:O	1:V:373:PRO:CB	2.22	0.86
1:K:311:ALA:HB1	1:M:312:GLU:HA	1.57	0.86
1:A:144:ASP:O	1:A:145:ASP:HB2	1.72	0.86
1:S:390:GLU:OE1	1:T:379:ALA:CB	2.23	0.86
1:U:11:ILE:CA	1:W:273:LYS:HG2	2.05	0.86
1:U:188:ALA:HB1	1:U:218:GLN:HG2	1.56	0.86
1:D:188:ALA:HB1	1:D:218:GLN:HG2	1.57	0.86
1:H:310:ARG:HB2	1:J:297:GLN:HB2	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:ALA:HB1	1:K:218:GLN:HG2	1.56	0.86
1:Q:188:ALA:HB1	1:Q:218:GLN:HG2	1.56	0.86
1:U:12:PHE:CZ	1:W:242:HIS:HE1	1.93	0.86
1:L:188:ALA:HB1	1:L:218:GLN:HG2	1.56	0.86
1:O:310:ARG:HG2	1:P:297:GLN:OE1	1.75	0.86
1:P:188:ALA:HB1	1:P:218:GLN:HG2	1.56	0.86
1:E:11:ILE:CG1	1:E:12:PHE:CE2	2.60	0.85
1:H:11:ILE:O	1:J:273:LYS:CD	2.24	0.85
1:N:188:ALA:HB1	1:N:218:GLN:HG2	1.56	0.85
1:H:12:PHE:CE2	1:J:242:HIS:CE1	2.59	0.85
1:H:370:GLN:HB3	1:H:374:MET:SD	2.16	0.85
1:V:424:ARG:HH11	1:V:424:ARG:HG2	0.74	0.85
1:A:188:ALA:HB1	1:A:218:GLN:HG2	1.56	0.85
1:E:242:HIS:CE1	1:G:12:PHE:CZ	2.64	0.85
1:H:272:GLU:O	1:J:352:GLU:HG2	1.76	0.85
1:U:310:ARG:HG2	1:W:297:GLN:OE1	1.77	0.85
1:C:188:ALA:HB1	1:C:218:GLN:HG2	1.56	0.85
1:M:383:SER:HB2	1:N:383:SER:HB2	1.59	0.85
1:M:424:ARG:HH11	1:M:424:ARG:HG2	0.74	0.85
1:O:242:HIS:HE1	1:P:12:PHE:CZ	1.94	0.85
1:K:496:LEU:CG	1:S:195:VAL:HG22	2.06	0.85
1:O:188:ALA:HB1	1:O:218:GLN:HG2	1.56	0.85
1:X:188:ALA:HB1	1:X:218:GLN:HG2	1.56	0.85
1:H:352:GLU:HG2	1:J:272:GLU:O	1.77	0.85
1:I:11:ILE:CG1	1:I:12:PHE:CE2	2.60	0.85
1:I:188:ALA:HB1	1:I:218:GLN:HG2	1.56	0.85
1:I:11:ILE:HD11	1:I:12:PHE:CE2	2.12	0.85
1:L:11:ILE:CG1	1:L:12:PHE:CE2	2.59	0.85
1:U:11:ILE:O	1:W:273:LYS:CE	2.25	0.85
1:U:372:ILE:CG1	1:V:390:GLU:HA	2.04	0.85
1:B:188:ALA:HB1	1:B:218:GLN:HG2	1.56	0.84
1:E:188:ALA:HB1	1:E:218:GLN:HG2	1.56	0.84
1:Q:272:GLU:HG3	1:S:352:GLU:HB2	1.59	0.84
1:R:11:ILE:CG1	1:R:12:PHE:CE2	2.59	0.84
1:V:11:ILE:HD11	1:V:12:PHE:CE2	2.12	0.84
1:L:11:ILE:HG13	1:L:12:PHE:CD2	2.12	0.84
1:V:188:ALA:HB1	1:V:218:GLN:HG2	1.56	0.84
1:S:483:HIS:CD2	1:T:483:HIS:NE2	2.44	0.84
1:I:11:ILE:HG13	1:I:12:PHE:CD2	2.13	0.84
1:K:390:GLU:HA	1:L:372:ILE:HG13	1.60	0.84
1:O:12:PHE:CZ	1:P:242:HIS:CE1	2.64	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:483:HIS:NE2	1:T:483:HIS:CD2	2.44	0.84
1:R:11:ILE:HD11	1:R:12:PHE:CE2	2.12	0.84
1:S:483:HIS:NE2	1:T:483:HIS:HD2	1.75	0.84
1:L:11:ILE:HD11	1:L:12:PHE:CE2	2.12	0.84
1:L:297:GLN:HB2	1:N:310:ARG:HG3	1.59	0.84
1:S:188:ALA:HB1	1:S:218:GLN:HG2	1.57	0.84
1:V:11:ILE:CG1	1:V:12:PHE:CE2	2.60	0.84
1:E:11:ILE:HD11	1:E:12:PHE:CE2	2.12	0.84
1:R:11:ILE:HG13	1:R:12:PHE:CD2	2.12	0.84
1:E:424:ARG:HG2	1:E:424:ARG:HH11	0.74	0.84
1:K:297:GLN:OE1	1:M:310:ARG:HG2	1.77	0.84
1:U:310:ARG:HG2	1:W:297:GLN:HB2	1.59	0.84
1:W:188:ALA:HB1	1:W:218:GLN:HG2	1.56	0.84
1:W:373:PRO:HB3	1:X:391:THR:CA	2.07	0.84
1:R:272:GLU:CB	1:T:352:GLU:HG2	2.08	0.83
1:U:297:GLN:HB2	1:W:310:ARG:CG	2.08	0.83
1:E:11:ILE:HG13	1:E:12:PHE:CD2	2.12	0.83
1:H:10:SER:HB3	1:H:13:ASP:OD1	1.78	0.83
1:S:10:SER:HB3	1:S:13:ASP:OD1	1.79	0.83
1:I:229:LYS:CG	1:M:487:GLY:CA	2.56	0.83
1:L:11:ILE:HD11	1:L:12:PHE:HE2	1.44	0.83
1:R:10:SER:HB3	1:R:13:ASP:OD1	1.79	0.83
1:T:10:SER:HB3	1:T:13:ASP:OD1	1.78	0.83
1:V:11:ILE:HG13	1:V:12:PHE:CD2	2.12	0.83
1:B:279:LYS:HE3	1:C:6:ASN:OD1	1.78	0.83
1:H:496:LEU:CD2	1:M:195:VAL:CG2	2.56	0.83
1:L:10:SER:HB3	1:L:13:ASP:OD1	1.78	0.83
1:C:254:GLU:HG2	1:N:446:LYS:HE2	1.60	0.83
1:G:10:SER:HB3	1:G:13:ASP:OD1	1.79	0.83
1:M:10:SER:HB3	1:M:13:ASP:OD1	1.79	0.83
1:O:10:SER:HB3	1:O:13:ASP:OD1	1.78	0.83
1:R:11:ILE:HD11	1:R:12:PHE:HE2	1.43	0.83
1:V:272:GLU:CG	1:X:352:GLU:HG2	2.09	0.83
1:A:242:HIS:NE2	1:I:12:PHE:CZ	2.47	0.83
1:E:279:LYS:HE3	1:G:6:ASN:OD1	1.76	0.83
1:H:315:ASP:HB2	1:J:311:ALA:HA	1.61	0.83
1:I:11:ILE:HD11	1:I:12:PHE:HE2	1.44	0.83
1:M:390:GLU:O	1:N:373:PRO:CB	2.27	0.83
1:A:10:SER:HB3	1:A:13:ASP:OD1	1.78	0.83
1:V:10:SER:HB3	1:V:13:ASP:OD1	1.79	0.83
1:F:10:SER:HB3	1:F:13:ASP:OD1	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:390:GLU:O	1:N:373:PRO:CA	2.26	0.83
1:N:10:SER:HB3	1:N:13:ASP:OD1	1.79	0.83
1:U:10:SER:HB3	1:U:13:ASP:OD1	1.78	0.83
1:V:3:LEU:HD23	1:X:283:SER:HB3	1.61	0.83
1:I:10:SER:HB3	1:I:13:ASP:OD1	1.79	0.83
1:J:10:SER:HB3	1:J:13:ASP:OD1	1.79	0.83
1:K:424:ARG:HH11	1:K:424:ARG:HG2	0.74	0.83
1:L:280:ILE:CG1	1:N:6:ASN:O	2.26	0.83
1:R:280:ILE:HD11	1:T:9:LEU:HB2	1.59	0.82
1:V:7:LEU:CD2	1:X:284:LYS:HG3	2.08	0.82
1:A:3:LEU:HD21	1:I:283:SER:HB3	1.61	0.82
1:E:10:SER:HB3	1:E:13:ASP:OD1	1.79	0.82
1:H:310:ARG:CG	1:J:297:GLN:CG	2.57	0.82
1:I:229:LYS:CD	1:M:487:GLY:CA	2.57	0.82
1:K:12:PHE:HZ	1:M:242:HIS:CE1	1.91	0.82
1:C:10:SER:HB3	1:C:13:ASP:OD1	1.78	0.82
1:F:390:GLU:O	1:G:373:PRO:CA	2.26	0.82
1:V:284:LYS:CG	1:X:7:LEU:HD21	2.07	0.82
1:B:10:SER:HB3	1:B:13:ASP:OD1	1.79	0.82
1:F:373:PRO:CB	1:G:391:THR:HA	2.09	0.82
1:A:453:LYS:NZ	2:A:700:FDP:O1P	2.12	0.82
1:C:453:LYS:NZ	2:C:700:FDP:O1P	2.12	0.82
1:O:424:ARG:HH11	1:O:424:ARG:HG2	0.74	0.82
1:C:496:LEU:CG	1:V:195:VAL:HG22	2.10	0.82
1:D:10:SER:HB3	1:D:13:ASP:OD1	1.79	0.82
1:H:11:ILE:CA	1:J:273:LYS:HG2	2.08	0.82
1:Q:310:ARG:HG2	1:S:297:GLN:OE1	1.80	0.82
1:F:453:LYS:NZ	2:F:700:FDP:O1P	2.13	0.82
1:I:424:ARG:HG2	1:I:424:ARG:HH11	0.74	0.82
1:V:11:ILE:HD11	1:V:12:PHE:HE2	1.44	0.82
1:W:10:SER:HB3	1:W:13:ASP:OD1	1.79	0.82
1:A:424:ARG:HH11	1:A:424:ARG:HG2	0.74	0.82
1:Q:283:SER:CB	1:S:3:LEU:CD2	2.57	0.82
1:Q:283:SER:CB	1:S:3:LEU:HD23	2.09	0.82
1:X:10:SER:HB3	1:X:13:ASP:OD1	1.78	0.82
1:B:453:LYS:NZ	2:B:700:FDP:O1P	2.13	0.81
1:E:453:LYS:NZ	2:E:700:FDP:O1P	2.13	0.81
1:K:10:SER:HB3	1:K:13:ASP:OD1	1.79	0.81
1:L:11:ILE:O	1:N:273:LYS:HE3	1.79	0.81
1:P:487:GLY:HA2	1:V:229:LYS:CG	2.09	0.81
1:R:424:ARG:HG2	1:R:424:ARG:HH11	0.74	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:LYS:NZ	2:D:700:FDP:O1P	2.13	0.81
1:H:496:LEU:CG	1:M:195:VAL:CG2	2.52	0.81
1:J:453:LYS:NZ	2:J:700:FDP:O1P	2.13	0.81
1:L:487:GLY:HA2	1:S:229:LYS:HG3	1.59	0.81
1:N:453:LYS:NZ	2:N:700:FDP:O1P	2.13	0.81
1:Q:10:SER:HB3	1:Q:13:ASP:OD1	1.78	0.81
1:C:424:ARG:HG2	1:C:424:ARG:HH11	0.74	0.81
1:Q:453:LYS:NZ	2:Q:700:FDP:O1P	2.13	0.81
1:D:12:PHE:HE2	1:F:242:HIS:CE1	1.95	0.81
1:E:11:ILE:HD11	1:E:12:PHE:HE2	1.44	0.81
1:N:446:LYS:O	1:N:446:LYS:HD2	1.81	0.81
1:S:453:LYS:NZ	2:S:700:FDP:O1P	2.13	0.81
1:P:10:SER:HB3	1:P:13:ASP:OD1	1.79	0.81
1:F:373:PRO:HB3	1:G:391:THR:CA	2.11	0.81
1:V:280:ILE:CG1	1:X:6:ASN:O	2.29	0.81
1:L:311:ALA:HB1	1:N:312:GLU:HA	1.63	0.81
1:V:12:PHE:CE2	1:X:242:HIS:CE1	2.69	0.81
1:B:373:PRO:HB3	1:O:391:THR:C	2.06	0.81
1:D:12:PHE:CZ	1:F:242:HIS:CE1	2.69	0.81
1:K:496:LEU:HG	1:S:195:VAL:CG2	2.10	0.81
1:L:229:LYS:HE3	1:S:487:GLY:HA2	1.61	0.81
1:L:487:GLY:HA2	1:S:229:LYS:CE	2.09	0.81
1:M:370:GLN:HB3	1:M:374:MET:SD	2.20	0.81
1:S:483:HIS:CD2	1:T:483:HIS:CD2	2.69	0.81
1:T:424:ARG:HH11	1:T:424:ARG:HG2	0.74	0.81
1:W:390:GLU:OE1	1:X:379:ALA:CB	2.29	0.81
1:I:453:LYS:NZ	2:I:700:FDP:O1P	2.13	0.81
1:S:424:ARG:HH11	1:S:424:ARG:HG2	0.74	0.81
1:U:390:GLU:OE1	1:V:379:ALA:CB	2.29	0.81
1:K:372:ILE:HG13	1:L:390:GLU:HA	1.61	0.81
1:H:11:ILE:HB	1:J:273:LYS:CG	2.10	0.80
1:R:453:LYS:NZ	2:R:700:FDP:O1P	2.13	0.80
1:I:270:PRO:HG2	1:I:273:LYS:CE	2.11	0.80
1:D:424:ARG:HH11	1:D:424:ARG:HG2	0.74	0.80
1:G:424:ARG:HH11	1:G:424:ARG:HG2	0.74	0.80
1:V:283:SER:OG	1:X:3:LEU:HG	1.82	0.80
1:E:270:PRO:HG2	1:E:273:LYS:CE	2.11	0.80
1:H:315:ASP:CB	1:J:311:ALA:HA	2.12	0.80
1:R:280:ILE:CG1	1:T:6:ASN:O	2.26	0.80
1:U:310:ARG:CG	1:W:297:GLN:HB2	2.11	0.80
1:V:453:LYS:NZ	2:V:700:FDP:O1P	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:453:LYS:NZ	2:W:700:FDP:O1P	2.15	0.80
1:B:269:ILE:HG12	1:C:11:ILE:HD12	1.64	0.80
1:U:372:ILE:HD11	1:U:374:MET:HE2	1.63	0.80
1:H:390:GLU:O	1:I:373:PRO:HA	1.79	0.80
1:R:270:PRO:HG2	1:R:273:LYS:CE	2.11	0.80
1:V:270:PRO:HG2	1:V:273:LYS:CE	2.11	0.80
1:X:424:ARG:HH11	1:X:424:ARG:HG2	0.74	0.80
1:U:453:LYS:NZ	2:U:700:FDP:O1P	2.13	0.80
1:X:453:LYS:NZ	2:X:700:FDP:O1P	2.15	0.80
1:H:453:LYS:NZ	2:H:700:FDP:O1P	2.15	0.79
1:K:453:LYS:NZ	2:K:700:FDP:O1P	2.15	0.79
1:O:453:LYS:NZ	2:O:700:FDP:O1P	2.14	0.79
1:N:142:TYR:HB3	1:N:146:GLY:HA2	1.65	0.79
1:U:242:HIS:NE2	1:W:12:PHE:CE2	2.49	0.79
1:B:372:ILE:HG13	1:O:390:GLU:HA	1.64	0.79
1:H:11:ILE:O	1:J:273:LYS:CG	2.30	0.79
1:H:496:LEU:HD23	1:M:195:VAL:HG22	1.64	0.79
1:L:142:TYR:HB3	1:L:146:GLY:HA2	1.65	0.79
1:L:487:GLY:HA2	1:S:229:LYS:CG	2.11	0.79
1:V:276:VAL:CG1	1:V:280:ILE:HD11	2.11	0.79
1:W:390:GLU:OE1	1:X:379:ALA:HB1	1.82	0.79
1:H:424:ARG:HH11	1:H:424:ARG:HG2	0.74	0.79
1:N:446:LYS:O	1:N:446:LYS:CD	2.30	0.79
1:O:312:GLU:HA	1:P:311:ALA:CB	2.13	0.79
1:P:370:GLN:HB3	1:P:374:MET:SD	2.22	0.79
1:P:453:LYS:NZ	2:P:700:FDP:O1P	2.15	0.79
1:G:142:TYR:HB3	1:G:146:GLY:HA2	1.65	0.79
1:L:312:GLU:HA	1:N:311:ALA:HB1	1.64	0.79
1:T:142:TYR:HB3	1:T:146:GLY:HA2	1.65	0.79
1:T:453:LYS:NZ	2:T:700:FDP:O1P	2.15	0.79
1:V:242:HIS:HE1	1:X:12:PHE:CZ	2.00	0.79
1:P:487:GLY:CA	1:V:229:LYS:CG	2.61	0.79
1:Q:280:ILE:HD11	1:S:9:LEU:HB2	1.65	0.79
1:K:142:TYR:HB3	1:K:146:GLY:HA2	1.65	0.79
1:Q:142:TYR:HB3	1:Q:146:GLY:HA2	1.65	0.79
1:H:11:ILE:O	1:J:273:LYS:HE3	1.83	0.79
1:L:12:PHE:CZ	1:N:242:HIS:CE1	2.70	0.79
1:M:453:LYS:NZ	2:M:700:FDP:O1P	2.15	0.79
1:R:3:LEU:HD13	1:T:369:LEU:HD12	1.65	0.79
1:W:142:TYR:HB3	1:W:146:GLY:HA2	1.65	0.79
1:B:424:ARG:HG2	1:B:424:ARG:HH11	0.74	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:453:LYS:NZ	2:L:700:FDP:O1P	2.15	0.79
1:R:371:HIS:O	1:R:374:MET:CG	2.30	0.79
1:V:269:ILE:HG12	1:X:11:ILE:HD12	1.64	0.79
1:A:142:TYR:HB3	1:A:146:GLY:HA2	1.65	0.78
1:B:142:TYR:HB3	1:B:146:GLY:HA2	1.65	0.78
1:H:11:ILE:CB	1:J:273:LYS:HG2	2.13	0.78
1:B:4:ALA:O	1:B:7:LEU:HB2	1.84	0.78
1:C:216:ALA:HB1	1:N:446:LYS:CE	2.13	0.78
1:H:142:TYR:HB3	1:H:146:GLY:HA2	1.64	0.78
1:L:270:PRO:HG2	1:L:273:LYS:CE	2.11	0.78
1:L:284:LYS:HG3	1:N:7:LEU:CD2	2.13	0.78
1:S:4:ALA:O	1:S:7:LEU:HB2	1.83	0.78
1:N:424:ARG:HH11	1:N:424:ARG:HG2	0.74	0.78
1:R:284:LYS:HG3	1:T:7:LEU:HD21	1.59	0.78
1:T:4:ALA:O	1:T:7:LEU:HB2	1.84	0.78
1:W:373:PRO:CB	1:X:391:THR:HA	2.12	0.78
1:D:142:TYR:HB3	1:D:146:GLY:HA2	1.65	0.78
1:K:242:HIS:HE1	1:M:12:PHE:CZ	2.01	0.78
1:L:370:GLN:HB3	1:L:374:MET:SD	2.22	0.78
1:P:4:ALA:O	1:P:7:LEU:HB2	1.84	0.78
1:W:4:ALA:O	1:W:7:LEU:HB2	1.84	0.78
1:G:453:LYS:NZ	2:G:700:FDP:O1P	2.15	0.78
1:I:4:ALA:O	1:I:7:LEU:HB2	1.84	0.78
1:J:142:TYR:HB3	1:J:146:GLY:HA2	1.65	0.78
1:N:4:ALA:O	1:N:7:LEU:HB2	1.84	0.78
1:R:142:TYR:HB3	1:R:146:GLY:HA2	1.65	0.78
1:U:142:TYR:HB3	1:U:146:GLY:HA2	1.65	0.78
1:H:373:PRO:HA	1:I:390:GLU:O	1.84	0.78
1:K:4:ALA:O	1:K:7:LEU:HB2	1.84	0.78
1:R:284:LYS:CG	1:T:7:LEU:CD2	2.56	0.78
1:C:223:ARG:HG2	1:C:223:ARG:HH11	1.49	0.78
1:F:424:ARG:HG2	1:F:424:ARG:HH11	0.74	0.78
1:L:272:GLU:CG	1:N:352:GLU:HG2	2.13	0.78
1:P:223:ARG:HG2	1:P:223:ARG:HH11	1.49	0.78
1:Q:283:SER:HB3	1:S:3:LEU:HD23	1.65	0.78
1:D:4:ALA:O	1:D:7:LEU:HB2	1.83	0.78
1:E:4:ALA:O	1:E:7:LEU:HB2	1.84	0.78
1:H:372:ILE:HG13	1:I:390:GLU:CA	2.14	0.78
1:K:390:GLU:O	1:L:373:PRO:HA	1.83	0.78
1:V:7:LEU:CD2	1:X:284:LYS:CG	2.62	0.78
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ALA:O	1:C:7:LEU:HB2	1.84	0.78
1:R:4:ALA:O	1:R:7:LEU:HB2	1.84	0.78
1:W:223:ARG:HG2	1:W:223:ARG:HH11	1.49	0.78
1:D:223:ARG:HG2	1:D:223:ARG:HH11	1.49	0.78
1:L:4:ALA:O	1:L:7:LEU:HB2	1.83	0.78
1:L:223:ARG:HG2	1:L:223:ARG:HH11	1.49	0.78
1:P:142:TYR:HB3	1:P:146:GLY:HA2	1.65	0.78
1:C:142:TYR:HB3	1:C:146:GLY:HA2	1.65	0.77
1:F:223:ARG:HG2	1:F:223:ARG:HH11	1.49	0.77
1:X:4:ALA:O	1:X:7:LEU:HB2	1.84	0.77
1:P:424:ARG:HH11	1:P:424:ARG:HG2	0.74	0.77
1:A:4:ALA:O	1:A:7:LEU:HB2	1.84	0.77
1:G:4:ALA:O	1:G:7:LEU:HB2	1.83	0.77
1:I:142:TYR:HB3	1:I:146:GLY:HA2	1.65	0.77
1:J:223:ARG:HG2	1:J:223:ARG:HH11	1.49	0.77
1:L:487:GLY:HA3	1:S:229:LYS:HG3	1.64	0.77
1:X:142:TYR:HB3	1:X:146:GLY:HA2	1.64	0.77
1:J:4:ALA:O	1:J:7:LEU:HB2	1.84	0.77
1:O:4:ALA:O	1:O:7:LEU:HB2	1.84	0.77
1:Q:424:ARG:HH11	1:Q:424:ARG:HG2	0.74	0.77
1:R:279:LYS:HE3	1:T:6:ASN:OD1	1.85	0.77
1:V:276:VAL:O	1:V:280:ILE:HD12	1.85	0.77
1:A:223:ARG:HG2	1:A:223:ARG:HH11	1.49	0.77
1:H:297:GLN:CG	1:J:310:ARG:HG2	2.15	0.77
1:V:142:TYR:HB3	1:V:146:GLY:HA2	1.65	0.77
1:B:311:ALA:HB1	1:C:312:GLU:HA	1.65	0.77
1:E:142:TYR:HB3	1:E:146:GLY:HA2	1.65	0.77
1:F:4:ALA:O	1:F:7:LEU:HB2	1.83	0.77
1:Q:223:ARG:HH11	1:Q:223:ARG:HG2	1.49	0.77
1:S:223:ARG:HG2	1:S:223:ARG:HH11	1.49	0.77
1:S:370:GLN:HB3	1:S:374:MET:SD	2.25	0.77
1:W:424:ARG:HG2	1:W:424:ARG:HH11	0.74	0.77
1:D:372:ILE:HG13	1:E:390:GLU:HA	1.67	0.77
1:F:142:TYR:HB3	1:F:146:GLY:HA2	1.65	0.77
1:H:4:ALA:O	1:H:7:LEU:HB2	1.84	0.77
1:M:4:ALA:O	1:M:7:LEU:HB2	1.84	0.77
1:M:142:TYR:HB3	1:M:146:GLY:HA2	1.65	0.77
1:O:142:TYR:HB3	1:O:146:GLY:HA2	1.65	0.77
1:Q:283:SER:OG	1:S:3:LEU:HD23	1.83	0.77
1:Q:284:LYS:HG3	1:S:7:LEU:CD2	2.15	0.77
1:T:223:ARG:HG2	1:T:223:ARG:HH11	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:223:ARG:HG2	1:U:223:ARG:HH11	1.49	0.77
1:U:4:ALA:O	1:U:7:LEU:HB2	1.84	0.77
1:V:283:SER:HB3	1:X:3:LEU:HG	1.66	0.77
1:G:223:ARG:HG2	1:G:223:ARG:HH11	1.49	0.76
1:H:223:ARG:HG2	1:H:223:ARG:HH11	1.49	0.76
1:M:214:ARG:H	1:M:218:GLN:HE22	1.33	0.76
1:Q:4:ALA:O	1:Q:7:LEU:HB2	1.84	0.76
1:S:142:TYR:HB3	1:S:146:GLY:HA2	1.64	0.76
1:V:12:PHE:CZ	1:X:242:HIS:CE1	2.72	0.76
1:V:283:SER:HB3	1:X:3:LEU:CD2	2.15	0.76
1:Q:390:GLU:O	1:R:372:ILE:HG23	1.86	0.76
1:V:214:ARG:H	1:V:218:GLN:HE22	1.33	0.76
1:A:392:LYS:CD	1:J:373:PRO:HD3	2.13	0.76
1:K:223:ARG:HG2	1:K:223:ARG:HH11	1.49	0.76
1:L:269:ILE:HG12	1:N:11:ILE:CD1	2.15	0.76
1:X:223:ARG:HG2	1:X:223:ARG:HH11	1.49	0.76
1:K:214:ARG:H	1:K:218:GLN:HE22	1.34	0.76
1:N:223:ARG:HG2	1:N:223:ARG:HH11	1.49	0.76
1:B:214:ARG:H	1:B:218:GLN:HE22	1.33	0.76
1:I:214:ARG:H	1:I:218:GLN:HE22	1.33	0.76
1:L:229:LYS:HG3	1:S:487:GLY:HA3	1.67	0.76
1:O:223:ARG:HG2	1:O:223:ARG:HH11	1.49	0.76
1:I:223:ARG:HH11	1:I:223:ARG:HG2	1.49	0.76
1:R:223:ARG:HG2	1:R:223:ARG:HH11	1.49	0.76
1:L:229:LYS:HG3	1:S:487:GLY:HA2	1.66	0.76
1:C:373:PRO:CA	1:P:390:GLU:O	2.34	0.76
1:M:223:ARG:HG2	1:M:223:ARG:HH11	1.49	0.76
1:B:12:PHE:HE2	1:C:242:HIS:HE1	0.88	0.75
1:O:11:ILE:O	1:P:273:LYS:HE3	1.85	0.75
1:U:390:GLU:O	1:V:373:PRO:HB3	1.85	0.75
1:L:283:SER:HB3	1:N:3:LEU:HD23	1.57	0.75
1:C:214:ARG:H	1:C:218:GLN:HE22	1.33	0.75
1:F:383:SER:HB2	1:G:383:SER:HB2	1.69	0.75
1:V:4:ALA:O	1:V:7:LEU:HB2	1.84	0.75
1:V:223:ARG:HG2	1:V:223:ARG:HH11	1.49	0.75
1:B:297:GLN:HB2	1:C:310:ARG:CG	2.15	0.75
1:D:373:PRO:HA	1:E:390:GLU:O	1.85	0.75
1:Q:12:PHE:HE2	1:S:242:HIS:CE1	2.05	0.75
1:S:372:ILE:HD11	1:S:374:MET:HE2	1.67	0.75
1:H:310:ARG:CG	1:J:297:GLN:CB	2.49	0.75
1:P:214:ARG:H	1:P:218:GLN:HE22	1.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:390:GLU:OE1	1:T:379:ALA:HB1	1.86	0.75
1:A:214:ARG:H	1:A:218:GLN:HE22	1.33	0.75
1:E:214:ARG:H	1:E:218:GLN:HE22	1.33	0.75
1:O:214:ARG:H	1:O:218:GLN:HE22	1.34	0.75
1:K:272:GLU:HG3	1:M:352:GLU:HB2	1.68	0.74
1:L:214:ARG:H	1:L:218:GLN:HE22	1.33	0.74
1:R:276:VAL:CG1	1:T:9:LEU:CB	2.64	0.74
1:E:223:ARG:HG2	1:E:223:ARG:HH11	1.49	0.74
1:H:297:GLN:HG3	1:J:310:ARG:HG2	1.69	0.74
1:S:491:GLN:HG3	1:T:491:GLN:HG3	1.68	0.74
1:U:242:HIS:CE1	1:W:12:PHE:HZ	2.00	0.74
1:V:280:ILE:HD11	1:X:9:LEU:HB2	1.68	0.74
1:I:195:VAL:HG22	1:N:496:LEU:HG	1.69	0.74
1:X:214:ARG:H	1:X:218:GLN:HE22	1.33	0.74
1:C:58:GLU:CD	1:E:103:ARG:HD2	2.12	0.74
1:F:390:GLU:HA	1:G:372:ILE:HG13	1.69	0.74
1:K:11:ILE:HB	1:M:273:LYS:HG2	1.68	0.74
1:L:191:ALA:HB1	1:T:473:GLY:HA3	1.69	0.74
1:P:229:LYS:HG3	1:V:487:GLY:HA3	1.69	0.74
1:T:372:ILE:HD11	1:T:374:MET:HE2	1.69	0.74
1:U:214:ARG:H	1:U:218:GLN:HE22	1.33	0.74
1:A:391:THR:C	1:J:373:PRO:HB3	2.13	0.74
1:Q:280:ILE:CG1	1:S:6:ASN:O	2.34	0.74
1:C:373:PRO:HB3	1:P:391:THR:HA	1.69	0.74
1:D:214:ARG:H	1:D:218:GLN:HE22	1.33	0.74
1:G:214:ARG:H	1:G:218:GLN:HE22	1.33	0.74
1:P:372:ILE:HD11	1:P:374:MET:HE2	1.69	0.74
1:T:214:ARG:H	1:T:218:GLN:HE22	1.33	0.74
1:V:297:GLN:NE2	1:V:300:GLU:HG2	2.02	0.74
1:I:193:ASP:HA	1:I:196:ASP:HB2	1.70	0.74
1:F:391:THR:HA	1:G:373:PRO:HB3	1.70	0.74
1:J:214:ARG:H	1:J:218:GLN:HE22	1.33	0.74
1:K:193:ASP:HA	1:K:196:ASP:HB2	1.70	0.74
1:M:193:ASP:HA	1:M:196:ASP:HB2	1.70	0.74
1:Q:12:PHE:CE2	1:S:242:HIS:HE1	2.06	0.74
1:Q:214:ARG:H	1:Q:218:GLN:HE22	1.33	0.74
1:W:193:ASP:HA	1:W:196:ASP:HB2	1.70	0.74
1:O:193:ASP:HA	1:O:196:ASP:HB2	1.70	0.74
1:R:276:VAL:HG13	1:T:9:LEU:CB	2.18	0.74
1:V:9:LEU:HB2	1:X:280:ILE:HD11	1.68	0.74
1:V:297:GLN:OE1	1:X:309:THR:HB	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:392:LYS:HD2	1:X:373:PRO:HD3	1.69	0.74
1:L:193:ASP:HA	1:L:196:ASP:HB2	1.70	0.73
1:L:283:SER:CB	1:N:3:LEU:HD21	2.17	0.73
1:S:494:ILE:HD12	1:T:376:ALA:HB1	1.68	0.73
1:H:214:ARG:H	1:H:218:GLN:HE22	1.34	0.73
1:Q:390:GLU:O	1:R:373:PRO:HA	1.88	0.73
1:S:214:ARG:H	1:S:218:GLN:HE22	1.33	0.73
1:A:179:LEU:HB3	1:A:182:CYS:HB2	1.71	0.73
1:C:383:SER:HB2	1:P:383:SER:HB2	1.70	0.73
1:E:11:ILE:CG1	1:E:12:PHE:CD2	2.71	0.73
1:F:193:ASP:HA	1:F:196:ASP:HB2	1.70	0.73
1:N:179:LEU:HB3	1:N:182:CYS:HB2	1.70	0.73
1:P:193:ASP:HA	1:P:196:ASP:HB2	1.70	0.73
1:V:310:ARG:HG2	1:X:297:GLN:OE1	1.88	0.73
1:I:11:ILE:CG1	1:I:12:PHE:CD2	2.71	0.73
1:R:11:ILE:CG1	1:R:12:PHE:CD2	2.71	0.73
1:C:216:ALA:HB3	1:N:446:LYS:CD	2.12	0.73
1:F:214:ARG:H	1:F:218:GLN:HE22	1.33	0.73
1:J:179:LEU:HB3	1:J:182:CYS:HB2	1.70	0.73
1:U:193:ASP:HA	1:U:196:ASP:HB2	1.70	0.73
1:B:373:PRO:HA	1:O:390:GLU:O	1.88	0.73
1:K:242:HIS:CE1	1:M:12:PHE:CZ	2.75	0.73
1:L:424:ARG:HG2	1:L:424:ARG:HH11	0.74	0.73
1:O:242:HIS:CE1	1:P:12:PHE:CZ	2.77	0.73
1:Q:297:GLN:OE1	1:S:310:ARG:CG	2.31	0.73
1:R:214:ARG:H	1:R:218:GLN:HE22	1.33	0.73
1:S:193:ASP:HA	1:S:196:ASP:HB2	1.70	0.73
1:V:297:GLN:HE21	1:V:300:GLU:CD	1.97	0.73
1:C:216:ALA:HB1	1:N:446:LYS:CD	2.15	0.73
1:D:179:LEU:HB3	1:D:182:CYS:HB2	1.70	0.73
1:N:214:ARG:H	1:N:218:GLN:HE22	1.33	0.73
1:Q:312:GLU:HA	1:S:311:ALA:HB1	1.70	0.73
1:V:11:ILE:CG1	1:V:12:PHE:CD2	2.71	0.73
1:W:179:LEU:HB3	1:W:182:CYS:HB2	1.70	0.73
1:C:179:LEU:HB3	1:C:182:CYS:HB2	1.70	0.73
1:D:193:ASP:HA	1:D:196:ASP:HB2	1.70	0.73
1:I:179:LEU:HB3	1:I:182:CYS:HB2	1.70	0.73
1:N:193:ASP:HA	1:N:196:ASP:HB2	1.70	0.73
1:N:446:LYS:HD2	1:N:446:LYS:C	2.14	0.73
1:C:496:LEU:CD2	1:V:195:VAL:HG22	2.19	0.73
1:T:179:LEU:HB3	1:T:182:CYS:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:179:LEU:HB3	1:U:182:CYS:HB2	1.70	0.73
1:W:214:ARG:H	1:W:218:GLN:HE22	1.33	0.73
1:O:179:LEU:HB3	1:O:182:CYS:HB2	1.71	0.73
1:T:370:GLN:HB3	1:T:374:MET:SD	2.29	0.73
1:A:193:ASP:HA	1:A:196:ASP:HB2	1.70	0.72
1:L:11:ILE:CG1	1:L:12:PHE:CD2	2.71	0.72
1:Q:193:ASP:HA	1:Q:196:ASP:HB2	1.70	0.72
1:U:424:ARG:HH11	1:U:424:ARG:HG2	0.74	0.72
1:X:179:LEU:HB3	1:X:182:CYS:HB2	1.70	0.72
1:M:390:GLU:O	1:N:373:PRO:HB3	1.87	0.72
1:Q:373:PRO:HA	1:R:390:GLU:O	1.89	0.72
1:L:229:LYS:CE	1:S:487:GLY:HA2	2.19	0.72
1:P:191:ALA:HB1	1:U:473:GLY:HA3	1.69	0.72
1:R:193:ASP:HA	1:R:196:ASP:HB2	1.70	0.72
1:U:370:GLN:HB3	1:U:374:MET:SD	2.29	0.72
1:L:487:GLY:HA2	1:S:229:LYS:CD	2.20	0.72
1:V:179:LEU:HB3	1:V:182:CYS:HB2	1.70	0.72
1:Q:179:LEU:HB3	1:Q:182:CYS:HB2	1.71	0.72
1:V:193:ASP:HA	1:V:196:ASP:HB2	1.70	0.72
1:C:193:ASP:HA	1:C:196:ASP:HB2	1.70	0.72
1:J:193:ASP:HA	1:J:196:ASP:HB2	1.70	0.72
1:Q:3:LEU:CD2	1:S:283:SER:HB3	2.20	0.72
1:Q:11:ILE:HB	1:S:273:LYS:HG2	1.72	0.72
1:R:276:VAL:HG13	1:T:9:LEU:HD13	1.71	0.72
1:S:179:LEU:HB3	1:S:182:CYS:HB2	1.70	0.72
1:U:373:PRO:CB	1:V:391:THR:HA	2.19	0.72
1:V:242:HIS:CE1	1:X:12:PHE:CZ	2.75	0.72
1:F:179:LEU:HB3	1:F:182:CYS:HB2	1.70	0.72
1:L:272:GLU:HG3	1:N:352:GLU:HB2	1.70	0.72
1:Q:373:PRO:HD3	1:R:392:LYS:HD2	1.72	0.72
1:U:373:PRO:HB3	1:V:391:THR:CA	2.19	0.72
1:A:390:GLU:HA	1:J:372:ILE:HG13	1.70	0.72
1:E:193:ASP:HA	1:E:196:ASP:HB2	1.70	0.72
1:F:491:GLN:HG3	1:G:491:GLN:HG3	1.72	0.72
1:J:424:ARG:HH11	1:J:424:ARG:HG2	0.74	0.72
1:L:179:LEU:HB3	1:L:182:CYS:HB2	1.70	0.72
1:P:179:LEU:HB3	1:P:182:CYS:HB2	1.70	0.72
1:U:372:ILE:HD11	1:V:390:GLU:HG2	1.71	0.72
1:H:11:ILE:O	1:J:273:LYS:HG2	1.90	0.72
1:M:179:LEU:HB3	1:M:182:CYS:HB2	1.70	0.72
1:R:276:VAL:HG13	1:T:9:LEU:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:315:ASP:HB2	1:W:311:ALA:HA	1.71	0.72
1:A:242:HIS:CE1	1:I:12:PHE:CZ	2.77	0.72
1:B:193:ASP:HA	1:B:196:ASP:HB2	1.70	0.72
1:V:6:ASN:O	1:X:280:ILE:HG12	1.90	0.72
1:H:193:ASP:HA	1:H:196:ASP:HB2	1.70	0.71
1:H:179:LEU:HB3	1:H:182:CYS:HB2	1.70	0.71
1:K:179:LEU:HB3	1:K:182:CYS:HB2	1.70	0.71
1:G:179:LEU:HB3	1:G:182:CYS:HB2	1.70	0.71
1:H:11:ILE:O	1:J:273:LYS:CE	2.37	0.71
1:L:372:ILE:HD11	1:L:374:MET:HE2	1.71	0.71
1:S:376:ALA:HA	1:T:494:ILE:HD12	1.71	0.71
1:K:297:GLN:HB2	1:M:310:ARG:HG2	1.71	0.71
1:R:179:LEU:HB3	1:R:182:CYS:HB2	1.70	0.71
1:A:283:SER:HB3	1:I:3:LEU:CD2	2.21	0.71
1:Q:272:GLU:CG	1:S:352:GLU:HG2	2.21	0.71
1:S:373:PRO:HB3	1:T:391:THR:C	2.16	0.71
1:I:370:GLN:CB	1:I:374:MET:SD	2.78	0.71
1:K:473:GLY:HA3	1:S:191:ALA:HB1	1.73	0.71
1:L:273:LYS:HD3	1:N:11:ILE:O	1.90	0.71
1:P:487:GLY:CA	1:V:229:LYS:CE	2.49	0.71
1:R:276:VAL:HG12	1:R:280:ILE:CD1	2.21	0.71
1:U:315:ASP:CB	1:W:311:ALA:HA	2.21	0.71
1:C:254:GLU:CG	1:N:446:LYS:HE2	2.21	0.71
1:E:179:LEU:HB3	1:E:182:CYS:HB2	1.70	0.71
1:G:193:ASP:HA	1:G:196:ASP:HB2	1.70	0.71
1:L:229:LYS:CG	1:S:487:GLY:HA2	2.20	0.71
1:O:310:ARG:HG2	1:P:297:GLN:HB2	1.72	0.71
1:X:193:ASP:HA	1:X:196:ASP:HB2	1.70	0.71
1:B:179:LEU:HB3	1:B:182:CYS:HB2	1.70	0.70
1:F:373:PRO:HB3	1:G:391:THR:C	2.16	0.70
1:L:273:LYS:CG	1:N:11:ILE:HB	2.21	0.70
1:B:297:GLN:HB2	1:C:310:ARG:HG2	1.73	0.70
1:C:270:PRO:HG2	1:C:273:LYS:CD	2.21	0.70
1:H:352:GLU:HG2	1:J:272:GLU:C	2.16	0.70
1:V:3:LEU:CD2	1:X:283:SER:HB3	2.20	0.70
1:H:311:ALA:HB3	1:J:312:GLU:HG3	1.73	0.70
1:K:496:LEU:CD2	1:S:195:VAL:HG22	2.21	0.70
1:Q:270:PRO:HG2	1:Q:273:LYS:CD	2.22	0.70
1:Q:311:ALA:HB1	1:S:312:GLU:HA	1.74	0.70
1:L:242:HIS:CE1	1:N:12:PHE:CZ	2.71	0.70
1:R:276:VAL:O	1:R:280:ILE:HG13	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:193:ASP:HA	1:T:196:ASP:HB2	1.70	0.70
1:V:7:LEU:HD22	1:X:284:LYS:HG2	1.74	0.70
1:M:491:GLN:HG3	1:N:491:GLN:HG3	1.72	0.70
1:R:370:GLN:CB	1:R:374:MET:SD	2.78	0.70
1:X:456:ARG:NH2	2:X:700:FDP:O1P	2.25	0.70
1:A:270:PRO:HG2	1:A:273:LYS:CD	2.21	0.70
1:K:390:GLU:HG2	1:L:374:MET:HE2	1.74	0.70
1:R:11:ILE:CD1	1:R:12:PHE:CE2	2.75	0.70
1:S:372:ILE:CG1	1:T:390:GLU:O	2.36	0.70
1:U:390:GLU:OE1	1:V:379:ALA:HB1	1.91	0.70
1:A:135:VAL:HG11	1:A:152:VAL:HG21	1.74	0.70
1:B:373:PRO:HD3	1:O:392:LYS:CD	2.22	0.70
1:I:11:ILE:CD1	1:I:12:PHE:CE2	2.75	0.70
1:R:280:ILE:HG23	1:T:7:LEU:HA	1.74	0.70
1:Q:38:LYS:HE3	1:Q:73:GLU:OE1	1.92	0.70
1:R:38:LYS:HE3	1:R:73:GLU:OE1	1.92	0.70
1:U:315:ASP:CG	1:W:311:ALA:HA	2.16	0.70
1:B:135:VAL:HG11	1:B:152:VAL:HG21	1.74	0.70
1:C:38:LYS:HE3	1:C:73:GLU:OE1	1.92	0.70
1:E:11:ILE:CD1	1:E:12:PHE:CE2	2.75	0.70
1:O:38:LYS:HE3	1:O:73:GLU:OE1	1.92	0.70
1:T:38:LYS:HE3	1:T:73:GLU:OE1	1.92	0.70
1:X:135:VAL:HG11	1:X:152:VAL:HG21	1.74	0.70
1:I:38:LYS:HE3	1:I:73:GLU:OE1	1.92	0.69
1:V:11:ILE:CD1	1:V:12:PHE:CE2	2.75	0.69
1:B:270:PRO:HG2	1:B:273:LYS:CD	2.22	0.69
1:E:38:LYS:HE3	1:E:73:GLU:OE1	1.92	0.69
1:F:38:LYS:HE3	1:F:73:GLU:OE1	1.92	0.69
1:L:11:ILE:CD1	1:L:12:PHE:CE2	2.75	0.69
1:M:135:VAL:HG11	1:M:152:VAL:HG21	1.74	0.69
1:D:38:LYS:HE3	1:D:73:GLU:OE1	1.92	0.69
1:D:310:ARG:HG2	1:F:297:GLN:OE1	1.92	0.69
1:K:270:PRO:HG2	1:K:273:LYS:CD	2.22	0.69
1:K:383:SER:HB2	1:L:383:SER:HB2	1.74	0.69
1:N:38:LYS:HE3	1:N:73:GLU:OE1	1.92	0.69
1:R:276:VAL:HG11	1:T:9:LEU:HB3	1.74	0.69
1:U:38:LYS:HE3	1:U:73:GLU:OE1	1.92	0.69
1:V:272:GLU:HG3	1:X:352:GLU:HB2	1.73	0.69
1:A:38:LYS:HE3	1:A:73:GLU:OE1	1.92	0.69
1:F:373:PRO:HD3	1:G:392:LYS:HD2	1.75	0.69
1:H:270:PRO:HG2	1:H:273:LYS:CD	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:456:ARG:NH2	2:H:700:FDP:O1P	2.25	0.69
1:L:38:LYS:HE3	1:L:73:GLU:OE1	1.92	0.69
1:O:297:GLN:HB2	1:P:310:ARG:HG2	1.74	0.69
1:X:38:LYS:HE3	1:X:73:GLU:OE1	1.92	0.69
1:A:3:LEU:HD23	1:I:283:SER:HB3	1.74	0.69
1:B:272:GLU:CG	1:C:352:GLU:HG2	2.23	0.69
1:D:270:PRO:HG2	1:D:273:LYS:CD	2.22	0.69
1:J:38:LYS:HE3	1:J:73:GLU:OE1	1.92	0.69
1:U:270:PRO:HG2	1:U:273:LYS:CD	2.22	0.69
1:V:135:VAL:HG11	1:V:152:VAL:HG21	1.74	0.69
1:H:12:PHE:HZ	1:J:242:HIS:CE1	2.02	0.69
1:K:272:GLU:O	1:M:352:GLU:HG2	1.92	0.69
1:M:456:ARG:NH2	2:M:700:FDP:O1P	2.25	0.69
1:U:297:GLN:CB	1:W:310:ARG:HG2	2.17	0.69
1:V:276:VAL:HG13	1:X:9:LEU:HD13	1.75	0.69
1:W:38:LYS:HE3	1:W:73:GLU:OE1	1.92	0.69
1:J:135:VAL:HG11	1:J:152:VAL:HG21	1.74	0.69
1:O:310:ARG:CG	1:P:297:GLN:HB2	2.22	0.69
1:T:135:VAL:HG11	1:T:152:VAL:HG21	1.74	0.69
1:G:135:VAL:HG11	1:G:152:VAL:HG21	1.74	0.69
1:H:38:LYS:HE3	1:H:73:GLU:OE1	1.92	0.69
1:O:135:VAL:HG11	1:O:152:VAL:HG21	1.74	0.69
1:O:270:PRO:HG2	1:O:273:LYS:CD	2.21	0.69
1:P:456:ARG:NH2	2:P:700:FDP:O1P	2.25	0.69
1:R:135:VAL:HG11	1:R:152:VAL:HG21	1.74	0.69
1:R:372:ILE:HD11	1:R:374:MET:HE2	1.75	0.69
1:S:38:LYS:HE3	1:S:73:GLU:OE1	1.92	0.69
1:W:372:ILE:HG13	1:X:390:GLU:O	1.93	0.69
1:W:456:ARG:NH2	2:W:700:FDP:O1P	2.25	0.69
1:G:38:LYS:HE3	1:G:73:GLU:OE1	1.92	0.69
1:H:11:ILE:HB	1:J:273:LYS:HB3	1.74	0.69
1:H:11:ILE:HD12	1:J:269:ILE:HG12	1.74	0.69
1:H:311:ALA:HB3	1:J:312:GLU:CG	2.23	0.69
1:M:38:LYS:HE3	1:M:73:GLU:OE1	1.92	0.69
1:P:38:LYS:HE3	1:P:73:GLU:OE1	1.92	0.69
1:V:272:GLU:HG2	1:X:352:GLU:HG2	1.73	0.69
1:G:456:ARG:NH2	2:G:700:FDP:O1P	2.25	0.69
1:N:135:VAL:HG11	1:N:152:VAL:HG21	1.74	0.69
1:O:456:ARG:NH2	2:O:700:FDP:O1P	2.25	0.69
1:V:38:LYS:HE3	1:V:73:GLU:OE1	1.92	0.69
1:E:135:VAL:HG11	1:E:152:VAL:HG21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:297:GLN:HB2	1:N:310:ARG:CG	2.24	0.68
1:S:372:ILE:CG2	1:T:390:GLU:O	2.42	0.68
1:K:38:LYS:HE3	1:K:73:GLU:OE1	1.92	0.68
1:S:135:VAL:HG11	1:S:152:VAL:HG21	1.74	0.68
1:B:273:LYS:HB3	1:C:11:ILE:HB	1.75	0.68
1:K:297:GLN:HB2	1:M:310:ARG:CG	2.23	0.68
1:P:135:VAL:HG11	1:P:152:VAL:HG21	1.74	0.68
1:B:38:LYS:HE3	1:B:73:GLU:OE1	1.92	0.68
1:L:456:ARG:NH2	2:L:700:FDP:O1P	2.25	0.68
1:Q:135:VAL:HG11	1:Q:152:VAL:HG21	1.74	0.68
1:F:392:LYS:HD2	1:G:373:PRO:HD3	1.74	0.68
1:H:135:VAL:HG11	1:H:152:VAL:HG21	1.74	0.68
1:V:242:HIS:CE1	1:X:12:PHE:HE2	2.06	0.68
1:K:456:ARG:NH2	2:K:700:FDP:O1P	2.25	0.68
1:L:11:ILE:HG13	1:L:12:PHE:CE2	2.29	0.68
1:R:372:ILE:HD12	1:R:374:MET:HG3	1.75	0.68
1:W:135:VAL:HG11	1:W:152:VAL:HG21	1.74	0.68
1:C:390:GLU:O	1:P:372:ILE:HG23	1.92	0.68
1:F:135:VAL:HG11	1:F:152:VAL:HG21	1.74	0.68
1:I:135:VAL:HG11	1:I:152:VAL:HG21	1.74	0.68
1:Q:269:ILE:HG12	1:S:11:ILE:CD1	2.22	0.68
1:S:483:HIS:HD2	1:T:483:HIS:NE2	1.90	0.68
1:K:279:LYS:HE3	1:M:6:ASN:OD1	1.94	0.68
1:U:135:VAL:HG11	1:U:152:VAL:HG21	1.74	0.68
1:U:371:HIS:CD2	1:U:373:PRO:O	2.47	0.68
1:V:11:ILE:HG13	1:V:12:PHE:CE2	2.29	0.68
1:L:135:VAL:HG11	1:L:152:VAL:HG21	1.74	0.68
1:R:297:GLN:CG	1:T:310:ARG:CG	2.71	0.68
1:V:456:ARG:NH2	2:V:700:FDP:O1P	2.25	0.68
1:B:297:GLN:OE1	1:C:310:ARG:CG	2.39	0.67
1:T:456:ARG:NH2	2:T:700:FDP:O1P	2.25	0.67
1:U:242:HIS:NE2	1:W:12:PHE:HE2	1.93	0.67
1:H:315:ASP:CG	1:J:311:ALA:HA	2.19	0.67
1:L:12:PHE:CE2	1:N:242:HIS:CE1	2.82	0.67
1:Q:12:PHE:HE2	1:S:242:HIS:HE1	1.40	0.67
1:R:296:THR:HG22	1:R:297:GLN:CG	2.25	0.67
1:A:390:GLU:O	1:J:373:PRO:HA	1.94	0.67
1:B:272:GLU:C	1:C:352:GLU:HG2	2.20	0.67
1:C:135:VAL:HG11	1:C:152:VAL:HG21	1.74	0.67
1:C:391:THR:HA	1:P:373:PRO:HB3	1.75	0.67
1:H:370:GLN:CB	1:H:374:MET:SD	2.82	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:383:SER:HB2	1:T:383:SER:HB2	1.76	0.67
1:D:135:VAL:HG11	1:D:152:VAL:HG21	1.74	0.67
1:A:371:HIS:CD2	1:A:373:PRO:O	2.48	0.67
1:D:390:GLU:O	1:E:373:PRO:HA	1.94	0.67
1:L:283:SER:HB3	1:N:3:LEU:HD21	1.71	0.67
1:W:371:HIS:CD2	1:W:373:PRO:O	2.48	0.67
1:X:371:HIS:CD2	1:X:373:PRO:O	2.48	0.67
1:B:371:HIS:CD2	1:B:373:PRO:O	2.48	0.67
1:C:371:HIS:CD2	1:C:373:PRO:O	2.48	0.67
1:K:392:LYS:HD2	1:L:373:PRO:HD3	1.77	0.67
1:L:273:LYS:HB3	1:N:11:ILE:HB	1.77	0.67
1:C:254:GLU:HG2	1:N:446:LYS:CE	2.24	0.67
1:H:263:GLY:HA2	1:J:310:ARG:HH11	1.60	0.67
1:R:11:ILE:HG13	1:R:12:PHE:CE2	2.29	0.67
1:V:283:SER:HB3	1:X:3:LEU:CG	2.25	0.67
1:D:373:PRO:HD3	1:E:392:LYS:HD2	1.76	0.67
1:J:371:HIS:CD2	1:J:373:PRO:O	2.48	0.67
1:K:135:VAL:HG11	1:K:152:VAL:HG21	1.74	0.67
1:L:280:ILE:HD11	1:N:9:LEU:HB2	1.76	0.67
1:N:371:HIS:CD2	1:N:373:PRO:O	2.48	0.66
1:U:311:ALA:CB	1:W:312:GLU:HA	2.19	0.66
1:L:272:GLU:CB	1:N:352:GLU:HG2	2.24	0.66
1:S:491:GLN:HG3	1:T:491:GLN:CG	2.24	0.66
1:V:371:HIS:CD2	1:V:373:PRO:O	2.48	0.66
1:H:53:SER:OG	1:H:85:LYS:HA	1.96	0.66
1:K:371:HIS:CD2	1:K:373:PRO:O	2.48	0.66
1:F:371:HIS:CD2	1:F:373:PRO:O	2.48	0.66
1:F:391:THR:HA	1:G:373:PRO:CB	2.25	0.66
1:H:310:ARG:CG	1:J:297:GLN:HG3	2.22	0.66
1:L:53:SER:OG	1:L:85:LYS:HA	1.96	0.66
1:U:242:HIS:HE1	1:W:12:PHE:CE2	1.85	0.66
1:G:53:SER:OG	1:G:85:LYS:HA	1.96	0.66
1:R:53:SER:OG	1:R:85:LYS:HA	1.96	0.66
1:R:279:LYS:HB3	1:T:6:ASN:OD1	1.95	0.66
1:V:3:LEU:HD23	1:X:283:SER:CB	2.26	0.66
1:V:12:PHE:CZ	1:X:242:HIS:NE2	2.63	0.66
1:D:53:SER:OG	1:D:85:LYS:HA	1.96	0.66
1:E:371:HIS:CD2	1:E:373:PRO:O	2.48	0.66
1:F:53:SER:OG	1:F:85:LYS:HA	1.96	0.66
1:L:352:GLU:HG2	1:N:272:GLU:O	1.96	0.66
1:O:12:PHE:HZ	1:P:242:HIS:HE1	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:371:HIS:CD2	1:Q:373:PRO:O	2.48	0.66
1:X:53:SER:OG	1:X:85:LYS:HA	1.96	0.66
1:D:371:HIS:CD2	1:D:373:PRO:O	2.48	0.66
1:O:371:HIS:CD2	1:O:373:PRO:O	2.48	0.66
1:C:53:SER:OG	1:C:85:LYS:HA	1.96	0.66
1:L:279:LYS:HE3	1:N:6:ASN:OD1	1.96	0.66
1:S:53:SER:OG	1:S:85:LYS:HA	1.96	0.66
1:C:391:THR:C	1:P:373:PRO:HB3	2.21	0.66
1:R:283:SER:HB3	1:T:3:LEU:HG	1.77	0.66
1:V:297:GLN:NE2	1:V:300:GLU:CD	2.53	0.66
1:A:53:SER:OG	1:A:85:LYS:HA	1.96	0.66
1:C:250:SER:HB3	1:N:446:LYS:HG2	1.71	0.66
1:E:283:SER:OG	1:G:3:LEU:HD23	1.97	0.65
1:M:53:SER:OG	1:M:85:LYS:HA	1.96	0.65
1:U:11:ILE:O	1:W:273:LYS:CD	2.45	0.65
1:B:144:ASP:O	1:B:145:ASP:CB	2.45	0.65
1:E:11:ILE:HG13	1:E:12:PHE:CE2	2.29	0.65
1:E:53:SER:OG	1:E:85:LYS:HA	1.96	0.65
1:N:53:SER:OG	1:N:85:LYS:HA	1.96	0.65
1:V:269:ILE:HG12	1:X:11:ILE:CD1	2.27	0.65
1:W:53:SER:OG	1:W:85:LYS:HA	1.96	0.65
1:A:242:HIS:HE1	1:I:12:PHE:CE2	2.10	0.65
1:B:272:GLU:O	1:C:352:GLU:HG2	1.96	0.65
1:H:352:GLU:HB2	1:J:272:GLU:HG3	1.78	0.65
1:I:53:SER:OG	1:I:85:LYS:HA	1.96	0.65
1:S:491:GLN:HG3	1:T:491:GLN:CD	2.21	0.65
1:T:53:SER:OG	1:T:85:LYS:HA	1.96	0.65
1:U:390:GLU:O	1:V:373:PRO:CA	2.44	0.65
1:A:3:LEU:CD2	1:I:283:SER:CB	2.74	0.65
1:V:144:ASP:O	1:V:145:ASP:CB	2.45	0.65
1:W:144:ASP:O	1:W:145:ASP:CB	2.45	0.65
1:E:312:GLU:HA	1:G:311:ALA:HB1	1.78	0.65
1:G:371:HIS:CD2	1:G:373:PRO:O	2.48	0.65
1:H:144:ASP:O	1:H:145:ASP:CB	2.45	0.65
1:J:53:SER:OG	1:J:85:LYS:HA	1.96	0.65
1:O:242:HIS:CE1	1:P:12:PHE:CE2	2.84	0.65
1:A:144:ASP:O	1:A:145:ASP:CB	2.45	0.65
1:I:372:ILE:HD11	1:I:374:MET:HE2	1.78	0.65
1:O:53:SER:OG	1:O:85:LYS:HA	1.96	0.65
1:R:269:ILE:CG1	1:T:11:ILE:CD1	2.65	0.65
1:E:472:THR:CG2	1:E:498:GLU:C	2.70	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:53:SER:OG	1:K:85:LYS:HA	1.96	0.65
1:N:472:THR:CG2	1:N:498:GLU:C	2.70	0.65
1:Q:144:ASP:O	1:Q:145:ASP:CB	2.45	0.65
1:Q:373:PRO:CB	1:R:390:GLU:O	2.45	0.65
1:T:472:THR:CG2	1:T:498:GLU:C	2.70	0.65
1:V:297:GLN:HE22	1:V:300:GLU:HG2	1.62	0.65
1:X:472:THR:CG2	1:X:498:GLU:C	2.70	0.65
1:A:472:THR:CG2	1:A:498:GLU:C	2.70	0.65
1:D:144:ASP:O	1:D:145:ASP:CB	2.45	0.65
1:O:311:ALA:CB	1:P:312:GLU:HA	2.23	0.65
1:P:53:SER:OG	1:P:85:LYS:HA	1.96	0.65
1:Q:53:SER:OG	1:Q:85:LYS:HA	1.96	0.65
1:U:372:ILE:CG2	1:V:390:GLU:O	2.43	0.65
1:B:53:SER:OG	1:B:85:LYS:HA	1.96	0.65
1:B:472:THR:CG2	1:B:498:GLU:C	2.70	0.65
1:G:472:THR:CG2	1:G:498:GLU:C	2.70	0.65
1:H:11:ILE:HB	1:J:273:LYS:CB	2.27	0.65
1:K:472:THR:CG2	1:K:498:GLU:C	2.70	0.65
1:M:372:ILE:HD11	1:M:374:MET:HE2	1.79	0.65
1:R:3:LEU:HD13	1:T:369:LEU:CD1	2.26	0.65
1:T:371:HIS:CD2	1:T:373:PRO:O	2.49	0.65
1:V:370:GLN:HB3	1:V:374:MET:SD	2.37	0.65
1:W:472:THR:CG2	1:W:498:GLU:C	2.70	0.65
1:F:472:THR:CG2	1:F:498:GLU:C	2.70	0.65
1:J:472:THR:CG2	1:J:498:GLU:C	2.70	0.65
1:O:472:THR:CG2	1:O:498:GLU:C	2.70	0.65
1:P:472:THR:CG2	1:P:498:GLU:C	2.70	0.65
1:R:472:THR:CG2	1:R:498:GLU:C	2.70	0.65
1:H:472:THR:CG2	1:H:498:GLU:C	2.70	0.64
1:M:472:THR:CG2	1:M:498:GLU:C	2.70	0.64
1:N:472:THR:HG22	1:N:498:GLU:C	2.22	0.64
1:Q:390:GLU:CA	1:R:372:ILE:HG13	2.24	0.64
1:U:53:SER:OG	1:U:85:LYS:HA	1.96	0.64
1:V:269:ILE:CG1	1:X:11:ILE:HD12	2.27	0.64
1:V:472:THR:CG2	1:V:498:GLU:C	2.70	0.64
1:I:472:THR:CG2	1:I:498:GLU:C	2.70	0.64
1:T:214:ARG:N	1:T:218:GLN:HE22	1.96	0.64
1:L:472:THR:CG2	1:L:498:GLU:C	2.70	0.64
1:Q:383:SER:HB2	1:R:383:SER:HB2	1.79	0.64
1:R:144:ASP:O	1:R:145:ASP:CB	2.45	0.64
1:U:472:THR:CG2	1:U:498:GLU:C	2.70	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:370:GLN:HB3	1:X:374:MET:SD	2.37	0.64
1:F:144:ASP:O	1:F:145:ASP:CB	2.45	0.64
1:G:370:GLN:HB3	1:G:374:MET:SD	2.38	0.64
1:K:370:GLN:HB3	1:K:374:MET:SD	2.37	0.64
1:L:269:ILE:CG1	1:N:11:ILE:HD12	2.27	0.64
1:O:472:THR:HG22	1:O:498:GLU:C	2.23	0.64
1:U:245:VAL:HG11	1:W:11:ILE:HD13	1.79	0.64
1:B:272:GLU:HG3	1:C:352:GLU:CB	2.26	0.64
1:F:472:THR:HG22	1:F:498:GLU:C	2.23	0.64
1:J:472:THR:HG22	1:J:498:GLU:C	2.23	0.64
1:L:310:ARG:HG2	1:N:297:GLN:HB2	1.78	0.64
1:M:214:ARG:N	1:M:218:GLN:HE22	1.96	0.64
1:M:472:THR:HG22	1:M:498:GLU:C	2.23	0.64
1:Q:370:GLN:HB3	1:Q:374:MET:SD	2.38	0.64
1:T:472:THR:HG22	1:T:498:GLU:C	2.23	0.64
1:X:214:ARG:N	1:X:218:GLN:HE22	1.96	0.64
1:B:370:GLN:HB3	1:B:374:MET:SD	2.38	0.64
1:C:214:ARG:N	1:C:218:GLN:HE22	1.96	0.64
1:D:370:GLN:HB3	1:D:374:MET:SD	2.38	0.64
1:D:472:THR:HG22	1:D:498:GLU:C	2.22	0.64
1:N:370:GLN:HB3	1:N:374:MET:SD	2.37	0.64
1:Q:272:GLU:HG3	1:S:352:GLU:CB	2.27	0.64
1:Q:373:PRO:CA	1:R:390:GLU:O	2.46	0.64
1:R:273:LYS:CD	1:T:11:ILE:O	2.42	0.64
1:U:11:ILE:HB	1:W:273:LYS:CB	2.27	0.64
1:V:53:SER:OG	1:V:85:LYS:HA	1.96	0.64
1:V:472:THR:HG22	1:V:498:GLU:C	2.23	0.64
1:W:370:GLN:HB3	1:W:374:MET:SD	2.37	0.64
1:H:472:THR:HG22	1:H:498:GLU:C	2.23	0.64
1:O:370:GLN:HB3	1:O:374:MET:SD	2.37	0.64
1:S:390:GLU:OE1	1:T:379:ALA:HB2	1.98	0.64
1:U:310:ARG:NH2	1:W:297:GLN:OE1	2.30	0.64
1:C:472:THR:CG2	1:C:498:GLU:C	2.70	0.64
1:D:472:THR:CG2	1:D:498:GLU:C	2.70	0.64
1:E:370:GLN:HB3	1:E:374:MET:SD	2.37	0.64
1:I:371:HIS:CD2	1:I:373:PRO:O	2.50	0.64
1:L:472:THR:HG22	1:L:498:GLU:C	2.22	0.64
1:Q:472:THR:HG22	1:Q:498:GLU:C	2.23	0.64
1:Q:472:THR:CG2	1:Q:498:GLU:C	2.70	0.64
1:E:144:ASP:O	1:E:145:ASP:CB	2.45	0.64
1:F:370:GLN:HB3	1:F:374:MET:SD	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:373:PRO:CA	1:L:390:GLU:O	2.42	0.64
1:K:373:PRO:CB	1:L:391:THR:HA	2.25	0.64
1:W:214:ARG:N	1:W:218:GLN:HE22	1.96	0.64
1:X:472:THR:HG22	1:X:498:GLU:C	2.23	0.64
1:A:370:GLN:HB3	1:A:374:MET:SD	2.38	0.64
1:B:214:ARG:N	1:B:218:GLN:HE22	1.96	0.64
1:C:370:GLN:HB3	1:C:374:MET:SD	2.37	0.64
1:H:214:ARG:N	1:H:218:GLN:HE22	1.96	0.64
1:J:214:ARG:N	1:J:218:GLN:HE22	1.96	0.64
1:Q:6:ASN:O	1:S:280:ILE:HG12	1.98	0.64
1:S:491:GLN:CD	1:T:491:GLN:NE2	2.56	0.64
1:U:214:ARG:N	1:U:218:GLN:HE22	1.96	0.64
1:W:472:THR:HG22	1:W:498:GLU:C	2.23	0.64
1:T:144:ASP:O	1:T:145:ASP:CB	2.45	0.63
1:E:297:GLN:OE1	1:G:310:ARG:CG	2.35	0.63
1:Q:214:ARG:N	1:Q:218:GLN:HE22	1.95	0.63
1:S:472:THR:CG2	1:S:498:GLU:C	2.70	0.63
1:A:214:ARG:N	1:A:218:GLN:HE22	1.96	0.63
1:O:11:ILE:CA	1:P:273:LYS:HG2	2.28	0.63
1:P:472:THR:HG22	1:P:498:GLU:C	2.23	0.63
1:V:214:ARG:N	1:V:218:GLN:HE22	1.96	0.63
1:A:492:THR:HG22	1:J:492:THR:HG22	1.79	0.63
1:C:472:THR:HG22	1:C:498:GLU:C	2.23	0.63
1:F:214:ARG:N	1:F:218:GLN:HE22	1.96	0.63
1:F:391:THR:CA	1:G:373:PRO:HB3	2.29	0.63
1:H:297:GLN:HB2	1:J:310:ARG:CB	2.28	0.63
1:L:311:ALA:CB	1:N:312:GLU:HA	2.28	0.63
1:U:472:THR:HG22	1:U:498:GLU:C	2.23	0.63
1:A:472:THR:HG22	1:A:498:GLU:C	2.22	0.63
1:G:214:ARG:N	1:G:218:GLN:HE22	1.96	0.63
1:I:371:HIS:O	1:I:374:MET:CG	2.41	0.63
1:I:472:THR:HG22	1:I:498:GLU:C	2.23	0.63
1:J:370:GLN:HB3	1:J:374:MET:SD	2.37	0.63
1:M:370:GLN:CB	1:M:374:MET:SD	2.86	0.63
1:P:195:VAL:CG2	1:U:496:LEU:CD2	2.73	0.63
1:R:214:ARG:N	1:R:218:GLN:HE22	1.96	0.63
1:H:11:ILE:C	1:J:273:LYS:HG2	2.23	0.63
1:L:272:GLU:CG	1:N:352:GLU:CG	2.76	0.63
1:P:214:ARG:N	1:P:218:GLN:HE22	1.96	0.63
1:D:214:ARG:N	1:D:218:GLN:HE22	1.96	0.63
1:K:214:ARG:N	1:K:218:GLN:HE22	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:472:THR:HG22	1:K:498:GLU:C	2.23	0.63
1:L:9:LEU:HB2	1:N:280:ILE:HD11	1.81	0.63
1:L:11:ILE:HD12	1:N:269:ILE:HG12	1.80	0.63
1:X:144:ASP:O	1:X:145:ASP:CB	2.45	0.63
1:O:144:ASP:O	1:O:145:ASP:CB	2.45	0.63
1:O:214:ARG:N	1:O:218:GLN:HE22	1.96	0.63
1:P:487:GLY:CA	1:V:229:LYS:HD2	2.27	0.63
1:S:472:THR:HG22	1:S:498:GLU:C	2.23	0.63
1:V:7:LEU:HD23	1:X:284:LYS:HG3	1.80	0.63
1:B:472:THR:HG22	1:B:498:GLU:C	2.22	0.62
1:L:214:ARG:N	1:L:218:GLN:HE22	1.96	0.62
1:S:214:ARG:N	1:S:218:GLN:HE22	1.96	0.62
1:E:11:ILE:CD1	1:E:12:PHE:HE2	2.12	0.62
1:I:11:ILE:HG13	1:I:12:PHE:CE2	2.29	0.62
1:I:214:ARG:N	1:I:218:GLN:HE22	1.96	0.62
1:K:456:ARG:NH1	2:K:700:FDP:O2P	2.28	0.62
1:M:373:PRO:HB3	1:N:391:THR:HA	1.80	0.62
1:P:144:ASP:O	1:P:145:ASP:CB	2.45	0.62
1:U:372:ILE:HG13	1:V:390:GLU:C	2.24	0.62
1:F:372:ILE:HD11	1:G:390:GLU:HG2	1.81	0.62
1:H:372:ILE:HD12	1:H:374:MET:HG3	1.81	0.62
1:E:472:THR:HG22	1:E:498:GLU:C	2.23	0.62
1:G:144:ASP:O	1:G:145:ASP:CB	2.45	0.62
1:K:310:ARG:HG2	1:M:297:GLN:HB2	1.80	0.62
1:R:472:THR:HG22	1:R:498:GLU:C	2.23	0.62
1:S:371:HIS:CD2	1:S:373:PRO:O	2.53	0.62
1:H:372:ILE:CG2	1:I:390:GLU:O	2.43	0.62
1:L:370:GLN:CB	1:L:374:MET:SD	2.87	0.62
1:H:273:LYS:HB3	1:J:11:ILE:HB	1.82	0.62
1:O:315:ASP:HB2	1:P:311:ALA:HA	1.82	0.62
1:P:371:HIS:CD2	1:P:373:PRO:O	2.53	0.62
1:P:456:ARG:NH1	2:P:700:FDP:O2P	2.28	0.62
1:W:372:ILE:HG13	1:X:390:GLU:C	2.24	0.62
1:L:310:ARG:HG2	1:N:297:GLN:OE1	1.99	0.62
1:L:144:ASP:O	1:L:145:ASP:CB	2.45	0.62
1:N:214:ARG:N	1:N:218:GLN:HE22	1.96	0.62
1:N:446:LYS:CD	1:N:446:LYS:C	2.72	0.62
1:R:276:VAL:CG1	1:R:280:ILE:HD11	2.27	0.62
1:D:373:PRO:HB3	1:E:391:THR:C	2.25	0.61
1:G:472:THR:HG22	1:G:498:GLU:C	2.23	0.61
1:L:242:HIS:NE2	1:N:12:PHE:HE2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:SER:OG	1:C:3:LEU:HD23	1.99	0.61
1:K:269:ILE:HG12	1:M:11:ILE:HD12	1.82	0.61
1:S:144:ASP:O	1:S:145:ASP:CB	2.45	0.61
1:L:283:SER:HB3	1:N:3:LEU:HD22	1.79	0.61
1:C:250:SER:HB2	1:N:446:LYS:HG2	0.69	0.61
1:D:492:THR:HG22	1:E:492:THR:HG22	1.83	0.61
1:H:315:ASP:HB2	1:J:311:ALA:CA	2.30	0.61
1:V:456:ARG:NH1	2:V:700:FDP:O2P	2.28	0.61
1:C:390:GLU:HA	1:P:372:ILE:CG1	2.15	0.61
1:E:214:ARG:N	1:E:218:GLN:HE22	1.96	0.61
1:F:372:ILE:CD1	1:F:374:MET:HE2	2.25	0.61
1:Q:270:PRO:HG2	1:Q:273:LYS:HE2	1.83	0.61
1:V:7:LEU:CD2	1:X:284:LYS:HG2	2.30	0.61
1:V:272:GLU:HG3	1:X:352:GLU:CB	2.30	0.61
1:H:352:GLU:CG	1:J:272:GLU:O	2.49	0.61
1:S:373:PRO:CA	1:T:390:GLU:O	2.37	0.61
1:K:372:ILE:CD1	1:K:374:MET:HE2	2.25	0.61
1:B:270:PRO:HG2	1:B:273:LYS:HE2	1.83	0.61
1:C:250:SER:CB	1:N:446:LYS:CG	2.46	0.61
1:L:11:ILE:CD1	1:L:12:PHE:HE2	2.12	0.61
1:P:370:GLN:CB	1:P:374:MET:SD	2.88	0.61
1:U:270:PRO:HG2	1:U:273:LYS:HE2	1.83	0.61
1:U:310:ARG:CZ	1:W:297:GLN:OE1	2.49	0.61
1:U:352:GLU:HG2	1:W:272:GLU:CB	2.30	0.61
1:E:11:ILE:HB	1:G:273:LYS:HG2	1.82	0.61
1:H:279:LYS:HE3	1:J:6:ASN:OD1	2.01	0.61
1:J:144:ASP:O	1:J:145:ASP:CB	2.45	0.61
1:K:373:PRO:HB3	1:L:391:THR:CA	2.26	0.61
1:O:456:ARG:NH1	2:O:700:FDP:O2P	2.28	0.61
1:R:287:VAL:HG23	1:T:3:LEU:HD11	1.83	0.61
1:M:456:ARG:NH1	2:M:700:FDP:O2P	2.28	0.61
1:T:456:ARG:NH1	2:T:700:FDP:O2P	2.28	0.61
1:X:372:ILE:CD1	1:X:374:MET:HE2	2.25	0.61
1:B:103:ARG:HD2	1:G:58:GLU:OE1	2.01	0.60
1:Q:456:ARG:NH2	2:Q:700:FDP:O1P	2.34	0.60
1:D:400:SER:HB2	1:D:405:SER:HB2	1.84	0.60
1:E:311:ALA:HB1	1:G:312:GLU:HA	1.82	0.60
1:E:372:ILE:CD1	1:E:374:MET:HE2	2.25	0.60
1:H:270:PRO:HG2	1:H:273:LYS:HE2	1.83	0.60
1:N:446:LYS:HD3	1:N:446:LYS:O	2.00	0.60
1:V:7:LEU:HD22	1:X:284:LYS:CG	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:PRO:HG2	1:D:273:LYS:HE2	1.83	0.60
1:K:272:GLU:C	1:M:352:GLU:HG2	2.26	0.60
1:N:456:ARG:NH2	2:N:700:FDP:O1P	2.34	0.60
1:O:400:SER:HB2	1:O:405:SER:HB2	1.83	0.60
1:Q:400:SER:HB2	1:Q:405:SER:HB2	1.84	0.60
1:K:270:PRO:HG2	1:K:273:LYS:HE2	1.83	0.60
1:M:400:SER:HB2	1:M:405:SER:HB2	1.83	0.60
1:O:270:PRO:HG2	1:O:273:LYS:HE2	1.83	0.60
1:B:272:GLU:CB	1:C:352:GLU:HG2	2.30	0.60
1:C:58:GLU:OE1	1:E:103:ARG:HD2	2.02	0.60
1:H:296:THR:HG22	1:H:297:GLN:HG2	1.83	0.60
1:U:372:ILE:HG13	1:V:390:GLU:O	2.01	0.60
1:U:390:GLU:O	1:V:373:PRO:HA	2.02	0.60
1:V:242:HIS:NE2	1:X:12:PHE:HE2	1.99	0.60
1:E:242:HIS:CE1	1:G:12:PHE:HE2	2.17	0.60
1:F:490:ASN:H	1:F:490:ASN:HD22	1.50	0.60
1:H:400:SER:HB2	1:H:405:SER:HB2	1.84	0.60
1:K:400:SER:HB2	1:K:405:SER:HB2	1.84	0.60
1:L:400:SER:HB2	1:L:405:SER:HB2	1.84	0.60
1:S:490:ASN:H	1:S:490:ASN:HD22	1.50	0.60
1:T:400:SER:HB2	1:T:405:SER:HB2	1.83	0.60
1:W:372:ILE:CD1	1:W:374:MET:HE2	2.25	0.60
1:A:242:HIS:NE2	1:I:12:PHE:HZ	1.99	0.60
1:A:270:PRO:HG2	1:A:273:LYS:HE2	1.83	0.60
1:D:212:PHE:CE1	1:D:241:ASN:ND2	2.70	0.60
1:E:212:PHE:CE1	1:E:241:ASN:ND2	2.70	0.60
1:G:400:SER:HB2	1:G:405:SER:HB2	1.83	0.60
1:O:490:ASN:HD22	1:O:490:ASN:H	1.50	0.60
1:W:212:PHE:CE1	1:W:241:ASN:ND2	2.70	0.60
1:L:276:VAL:CG1	1:N:9:LEU:HB3	2.31	0.60
1:U:12:PHE:CZ	1:W:242:HIS:CE1	2.84	0.60
1:U:144:ASP:O	1:U:145:ASP:CB	2.45	0.60
1:W:490:ASN:HD22	1:W:490:ASN:H	1.50	0.60
1:B:103:ARG:HB3	1:G:58:GLU:OE1	2.02	0.60
1:D:456:ARG:NH2	2:D:700:FDP:O1P	2.34	0.60
1:E:11:ILE:O	1:G:273:LYS:HE3	2.01	0.60
1:G:372:ILE:CD1	1:G:374:MET:HE2	2.25	0.60
1:H:390:GLU:O	1:I:373:PRO:CA	2.48	0.60
1:J:490:ASN:HD22	1:J:490:ASN:H	1.50	0.60
1:P:212:PHE:CE1	1:P:241:ASN:ND2	2.70	0.60
1:R:400:SER:HB2	1:R:405:SER:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:372:ILE:CG1	1:T:390:GLU:HG2	2.32	0.60
1:U:383:SER:HB2	1:V:383:SER:HB2	1.81	0.60
1:C:270:PRO:HG2	1:C:273:LYS:HE2	1.83	0.60
1:C:456:ARG:NH2	2:C:700:FDP:O1P	2.34	0.60
1:F:456:ARG:NH2	2:F:700:FDP:O1P	2.35	0.60
1:J:456:ARG:NH2	2:J:700:FDP:O1P	2.34	0.60
1:M:490:ASN:HD22	1:M:490:ASN:H	1.50	0.60
1:P:195:VAL:CG2	1:U:496:LEU:CG	2.68	0.60
1:P:400:SER:HB2	1:P:405:SER:HB2	1.83	0.60
1:R:11:ILE:CD1	1:R:12:PHE:HE2	2.12	0.60
1:R:297:GLN:CG	1:T:310:ARG:HG2	2.32	0.60
1:B:147:ILE:CG2	1:B:169:HIS:CD2	2.85	0.59
1:C:400:SER:HB2	1:C:405:SER:HB2	1.84	0.59
1:C:490:ASN:H	1:C:490:ASN:HD22	1.50	0.59
1:F:400:SER:HB2	1:F:405:SER:HB2	1.83	0.59
1:Q:3:LEU:HD23	1:S:283:SER:HB3	1.84	0.59
1:X:456:ARG:HH22	2:X:700:FDP:P1	2.25	0.59
1:A:490:ASN:HD22	1:A:490:ASN:H	1.50	0.59
1:C:212:PHE:CE1	1:C:241:ASN:ND2	2.70	0.59
1:H:147:ILE:CG2	1:H:169:HIS:CD2	2.85	0.59
1:O:147:ILE:CG2	1:O:169:HIS:CD2	2.85	0.59
1:R:272:GLU:C	1:T:352:GLU:HG2	2.27	0.59
1:R:276:VAL:HG13	1:T:9:LEU:CD1	2.32	0.59
1:U:311:ALA:HB1	1:W:312:GLU:CA	2.21	0.59
1:V:147:ILE:CG2	1:V:169:HIS:CD2	2.85	0.59
1:V:297:GLN:NE2	1:V:300:GLU:HB2	2.05	0.59
1:V:456:ARG:HH22	2:V:700:FDP:P1	2.25	0.59
1:V:490:ASN:H	1:V:490:ASN:HD22	1.50	0.59
1:X:400:SER:HB2	1:X:405:SER:HB2	1.83	0.59
1:X:456:ARG:NH1	2:X:700:FDP:O2P	2.28	0.59
1:B:400:SER:HB2	1:B:405:SER:HB2	1.83	0.59
1:C:144:ASP:O	1:C:145:ASP:CB	2.45	0.59
1:G:147:ILE:CG2	1:G:169:HIS:CD2	2.86	0.59
1:M:147:ILE:CG2	1:M:169:HIS:CD2	2.86	0.59
1:U:147:ILE:CG2	1:U:169:HIS:CD2	2.85	0.59
1:U:400:SER:HB2	1:U:405:SER:HB2	1.84	0.59
1:V:400:SER:HB2	1:V:405:SER:HB2	1.84	0.59
1:E:400:SER:HB2	1:E:405:SER:HB2	1.84	0.59
1:I:147:ILE:CG2	1:I:169:HIS:CD2	2.85	0.59
1:I:404:ARG:CZ	1:M:228:PRO:HG2	2.31	0.59
1:K:490:ASN:H	1:K:490:ASN:HD22	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:297:GLN:HB2	1:S:310:ARG:CG	2.32	0.59
1:S:456:ARG:NH2	2:S:700:FDP:O1P	2.34	0.59
1:F:212:PHE:CE1	1:F:241:ASN:ND2	2.70	0.59
1:L:371:HIS:CD2	1:L:373:PRO:O	2.55	0.59
1:P:490:ASN:H	1:P:490:ASN:HD22	1.50	0.59
1:S:383:SER:HB2	1:T:383:SER:CB	2.33	0.59
1:A:147:ILE:CG2	1:A:169:HIS:CD2	2.85	0.59
1:A:456:ARG:NH2	2:A:700:FDP:O1P	2.34	0.59
1:B:272:GLU:CG	1:C:352:GLU:CG	2.79	0.59
1:G:456:ARG:NH1	2:G:700:FDP:O2P	2.28	0.59
1:H:352:GLU:HG2	1:J:272:GLU:CB	2.32	0.59
1:I:11:ILE:CD1	1:I:12:PHE:HE2	2.12	0.59
1:K:352:GLU:HG2	1:M:272:GLU:O	2.03	0.59
1:L:490:ASN:HD22	1:L:490:ASN:H	1.50	0.59
1:Q:147:ILE:CG2	1:Q:169:HIS:CD2	2.85	0.59
1:S:147:ILE:CG2	1:S:169:HIS:CD2	2.85	0.59
1:S:370:GLN:CB	1:S:374:MET:SD	2.90	0.59
1:U:456:ARG:NH2	2:U:700:FDP:O1P	2.35	0.59
1:A:400:SER:HB2	1:A:405:SER:HB2	1.83	0.59
1:B:311:ALA:CB	1:C:312:GLU:HA	2.32	0.59
1:E:456:ARG:NH2	2:E:700:FDP:O1P	2.34	0.59
1:F:147:ILE:CG2	1:F:169:HIS:CD2	2.85	0.59
1:H:371:HIS:O	1:H:374:MET:CG	2.36	0.59
1:K:212:PHE:CE1	1:K:241:ASN:ND2	2.70	0.59
1:K:311:ALA:CB	1:M:312:GLU:HA	2.32	0.59
1:K:456:ARG:HH22	2:K:700:FDP:P1	2.26	0.59
1:L:147:ILE:CG2	1:L:169:HIS:CD2	2.86	0.59
1:L:272:GLU:HG3	1:N:352:GLU:CG	2.33	0.59
1:O:456:ARG:HH22	2:O:700:FDP:P1	2.25	0.59
1:P:147:ILE:CG2	1:P:169:HIS:CD2	2.86	0.59
1:P:456:ARG:HH22	2:P:700:FDP:P1	2.26	0.59
1:R:147:ILE:CG2	1:R:169:HIS:CD2	2.85	0.59
1:W:147:ILE:CG2	1:W:169:HIS:CD2	2.85	0.59
1:C:373:PRO:CB	1:P:390:GLU:O	2.51	0.59
1:H:383:SER:HB2	1:I:383:SER:CB	2.29	0.59
1:L:270:PRO:CG	1:L:273:LYS:HE2	2.23	0.59
1:L:273:LYS:CB	1:N:11:ILE:HB	2.33	0.59
1:O:242:HIS:HE1	1:P:12:PHE:CE2	2.20	0.59
1:S:400:SER:HB2	1:S:405:SER:HB2	1.84	0.59
1:T:490:ASN:HD22	1:T:490:ASN:H	1.50	0.59
1:B:490:ASN:HD22	1:B:490:ASN:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:456:ARG:HH22	2:G:700:FDP:P1	2.26	0.59
1:J:400:SER:HB2	1:J:405:SER:HB2	1.84	0.59
1:Q:272:GLU:C	1:S:352:GLU:HG2	2.28	0.59
1:U:212:PHE:CE1	1:U:241:ASN:ND2	2.70	0.59
1:U:365:SER:HB3	1:W:3:LEU:HD12	1.84	0.59
1:W:400:SER:HB2	1:W:405:SER:HB2	1.84	0.59
1:I:490:ASN:HD22	1:I:490:ASN:H	1.50	0.59
1:K:147:ILE:CG2	1:K:169:HIS:CD2	2.86	0.59
1:L:229:LYS:HE3	1:S:487:GLY:CA	2.33	0.59
1:L:456:ARG:NH1	2:L:700:FDP:O2P	2.29	0.59
1:M:371:HIS:CD2	1:M:373:PRO:O	2.55	0.59
1:M:456:ARG:HH22	2:M:700:FDP:P1	2.26	0.59
1:R:272:GLU:HG2	1:T:352:GLU:CG	2.21	0.59
1:U:352:GLU:HG2	1:W:272:GLU:HB2	1.85	0.59
1:V:279:LYS:HB3	1:X:6:ASN:CG	2.28	0.59
1:E:272:GLU:CG	1:G:352:GLU:HG2	2.32	0.58
1:R:490:ASN:HD22	1:R:490:ASN:H	1.50	0.58
1:E:270:PRO:CG	1:E:273:LYS:HE2	2.24	0.58
1:H:311:ALA:CB	1:J:312:GLU:CG	2.81	0.58
1:N:147:ILE:CG2	1:N:169:HIS:CD2	2.85	0.58
1:W:372:ILE:CG1	1:X:390:GLU:HA	2.23	0.58
1:E:490:ASN:H	1:E:490:ASN:HD22	1.50	0.58
1:J:147:ILE:CG2	1:J:169:HIS:CD2	2.85	0.58
1:L:487:GLY:CA	1:S:229:LYS:HE3	2.28	0.58
1:N:490:ASN:H	1:N:490:ASN:HD22	1.50	0.58
1:O:212:PHE:CE1	1:O:241:ASN:ND2	2.70	0.58
1:R:212:PHE:CE1	1:R:241:ASN:ND2	2.70	0.58
1:U:372:ILE:HD12	1:U:374:MET:CG	2.33	0.58
1:V:212:PHE:CE1	1:V:241:ASN:ND2	2.70	0.58
1:W:456:ARG:HH22	2:W:700:FDP:P1	2.26	0.58
1:K:57:HIS:HE1	1:K:195:VAL:HG12	1.69	0.58
1:L:297:GLN:HB2	1:N:310:ARG:HB2	1.84	0.58
1:L:456:ARG:HH22	2:L:700:FDP:P1	2.26	0.58
1:M:212:PHE:CE1	1:M:241:ASN:ND2	2.70	0.58
1:N:144:ASP:O	1:N:145:ASP:CB	2.45	0.58
1:Q:242:HIS:CE1	1:S:12:PHE:CZ	2.91	0.58
1:T:147:ILE:CG2	1:T:169:HIS:CD2	2.85	0.58
1:V:283:SER:O	1:X:3:LEU:HD21	2.03	0.58
1:D:490:ASN:HD22	1:D:490:ASN:H	1.50	0.58
1:E:147:ILE:CG2	1:E:169:HIS:CD2	2.85	0.58
1:H:456:ARG:NH1	2:H:700:FDP:O2P	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:212:PHE:CE1	1:I:241:ASN:ND2	2.70	0.58
1:M:57:HIS:HE1	1:M:195:VAL:HG12	1.69	0.58
1:N:400:SER:HB2	1:N:405:SER:HB2	1.84	0.58
1:T:212:PHE:CE1	1:T:241:ASN:ND2	2.70	0.58
1:X:57:HIS:HE1	1:X:195:VAL:HG12	1.69	0.58
1:B:283:SER:HB3	1:C:3:LEU:CD2	2.34	0.58
1:H:57:HIS:HE1	1:H:195:VAL:HG12	1.69	0.58
1:H:371:HIS:CD2	1:H:373:PRO:O	2.57	0.58
1:I:400:SER:HB2	1:I:405:SER:HB2	1.84	0.58
1:O:57:HIS:HE1	1:O:195:VAL:HG12	1.69	0.58
1:Q:11:ILE:HD12	1:S:269:ILE:HG12	1.85	0.58
1:Q:212:PHE:CE1	1:Q:241:ASN:ND2	2.70	0.58
1:Q:269:ILE:CG1	1:S:11:ILE:HD12	2.31	0.58
1:U:490:ASN:HD22	1:U:490:ASN:H	1.50	0.58
1:V:57:HIS:HE1	1:V:195:VAL:HG12	1.69	0.58
1:X:147:ILE:CG2	1:X:169:HIS:CD2	2.86	0.58
1:A:212:PHE:CE1	1:A:241:ASN:ND2	2.70	0.58
1:A:242:HIS:CE1	1:I:12:PHE:HE2	2.18	0.58
1:C:147:ILE:CG2	1:C:169:HIS:CD2	2.86	0.58
1:C:391:THR:HA	1:P:373:PRO:CB	2.32	0.58
1:D:11:ILE:HB	1:F:273:LYS:CG	2.31	0.58
1:J:372:ILE:CD1	1:J:374:MET:HE2	2.25	0.58
1:W:373:PRO:HB3	1:X:391:THR:C	2.28	0.58
1:B:57:HIS:HE1	1:B:195:VAL:HG12	1.69	0.58
1:B:212:PHE:CE1	1:B:241:ASN:ND2	2.70	0.58
1:D:147:ILE:CG2	1:D:169:HIS:CD2	2.85	0.58
1:F:483:HIS:CD2	1:G:483:HIS:CD2	2.92	0.58
1:H:11:ILE:HA	1:J:273:LYS:HG2	1.86	0.58
1:H:490:ASN:H	1:H:490:ASN:HD22	1.50	0.58
1:I:456:ARG:NH2	2:I:700:FDP:O1P	2.34	0.58
1:L:212:PHE:CE1	1:L:241:ASN:ND2	2.70	0.58
1:X:490:ASN:H	1:X:490:ASN:HD22	1.50	0.58
1:D:279:LYS:HE3	1:F:6:ASN:OD1	2.04	0.58
1:H:11:ILE:O	1:J:273:LYS:HD3	2.04	0.58
1:M:472:THR:HA	1:M:497:VAL:O	2.04	0.58
1:N:212:PHE:CE1	1:N:241:ASN:ND2	2.70	0.58
1:B:297:GLN:CD	1:C:310:ARG:HG2	2.26	0.58
1:C:391:THR:CA	1:P:373:PRO:HB3	2.33	0.58
1:H:456:ARG:HH22	2:H:700:FDP:P1	2.26	0.58
1:L:283:SER:OG	1:N:3:LEU:CD2	2.42	0.58
1:N:472:THR:HA	1:N:497:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:456:ARG:HH22	2:T:700:FDP:P1	2.26	0.58
1:T:472:THR:HA	1:T:497:VAL:O	2.04	0.58
1:U:310:ARG:HG2	1:W:297:GLN:CB	2.30	0.58
1:F:57:HIS:HE1	1:F:195:VAL:HG12	1.69	0.57
1:G:472:THR:HA	1:G:497:VAL:O	2.04	0.57
1:H:9:LEU:HB3	1:J:276:VAL:HG13	1.85	0.57
1:R:472:THR:HA	1:R:497:VAL:O	2.04	0.57
1:U:272:GLU:HG3	1:W:352:GLU:HB2	1.86	0.57
1:U:472:THR:HA	1:U:497:VAL:O	2.04	0.57
1:G:212:PHE:CE1	1:G:241:ASN:ND2	2.70	0.57
1:N:57:HIS:HE1	1:N:195:VAL:HG12	1.69	0.57
1:P:472:THR:HA	1:P:497:VAL:O	2.04	0.57
1:C:472:THR:HA	1:C:497:VAL:O	2.04	0.57
1:E:272:GLU:HG3	1:G:352:GLU:HB2	1.85	0.57
1:H:491:GLN:HG3	1:I:491:GLN:HG3	1.86	0.57
1:I:472:THR:HA	1:I:497:VAL:O	2.05	0.57
1:U:57:HIS:HE1	1:U:195:VAL:HG12	1.69	0.57
1:B:456:ARG:NH2	2:B:700:FDP:O1P	2.34	0.57
1:C:57:HIS:HE1	1:C:195:VAL:HG12	1.69	0.57
1:L:272:GLU:HG3	1:N:352:GLU:CB	2.33	0.57
1:L:472:THR:HA	1:L:497:VAL:O	2.04	0.57
1:Q:490:ASN:H	1:Q:490:ASN:HD22	1.50	0.57
1:R:280:ILE:CD1	1:T:9:LEU:HB2	2.32	0.57
1:A:283:SER:HB3	1:I:3:LEU:HD23	1.86	0.57
1:A:310:ARG:HG2	1:I:297:GLN:OE1	2.04	0.57
1:C:372:ILE:HG13	1:P:390:GLU:HA	1.85	0.57
1:E:57:HIS:HE1	1:E:195:VAL:HG12	1.69	0.57
1:H:212:PHE:CE1	1:H:241:ASN:ND2	2.70	0.57
1:P:57:HIS:HE1	1:P:195:VAL:HG12	1.69	0.57
1:Q:472:THR:HA	1:Q:497:VAL:O	2.05	0.57
1:S:372:ILE:HG13	1:T:390:GLU:CB	2.33	0.57
1:T:472:THR:CG2	1:T:498:GLU:HA	2.18	0.57
1:G:490:ASN:HD22	1:G:490:ASN:H	1.50	0.57
1:H:496:LEU:HD21	1:M:195:VAL:CG2	2.33	0.57
1:J:57:HIS:HE1	1:J:195:VAL:HG12	1.69	0.57
1:T:57:HIS:HE1	1:T:195:VAL:HG12	1.69	0.57
1:V:242:HIS:NE2	1:X:12:PHE:CE2	2.73	0.57
1:X:472:THR:HA	1:X:497:VAL:O	2.04	0.57
1:A:472:THR:HA	1:A:497:VAL:O	2.04	0.57
1:B:373:PRO:HB3	1:O:391:THR:O	2.03	0.57
1:B:472:THR:HA	1:B:497:VAL:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:HIS:HE1	1:D:195:VAL:HG12	1.69	0.57
1:E:472:THR:HA	1:E:497:VAL:O	2.04	0.57
1:F:472:THR:HA	1:F:497:VAL:O	2.04	0.57
1:H:242:HIS:CE1	1:J:12:PHE:HE2	2.13	0.57
1:I:57:HIS:HE1	1:I:195:VAL:HG12	1.69	0.57
1:L:6:ASN:O	1:N:280:ILE:HG12	2.04	0.57
1:L:57:HIS:HE1	1:L:195:VAL:HG12	1.69	0.57
1:Q:11:ILE:O	1:S:273:LYS:HE3	2.05	0.57
1:Q:57:HIS:HE1	1:Q:195:VAL:HG12	1.69	0.57
1:Q:372:ILE:CD1	1:Q:374:MET:HE2	2.25	0.57
1:W:472:THR:HA	1:W:497:VAL:O	2.04	0.57
1:C:373:PRO:CB	1:P:391:THR:HA	2.33	0.57
1:E:283:SER:HB3	1:G:3:LEU:CD2	2.35	0.57
1:G:57:HIS:HE1	1:G:195:VAL:HG12	1.69	0.57
1:L:280:ILE:HG13	1:N:6:ASN:O	2.03	0.57
1:R:11:ILE:HG12	1:R:12:PHE:CE2	2.40	0.57
1:R:57:HIS:HE1	1:R:195:VAL:HG12	1.69	0.57
1:S:212:PHE:CE1	1:S:241:ASN:ND2	2.70	0.57
1:H:472:THR:HA	1:H:497:VAL:O	2.04	0.57
1:L:273:LYS:CD	1:N:11:ILE:O	2.53	0.57
1:Q:12:PHE:CE2	1:S:242:HIS:CE1	2.86	0.57
1:R:273:LYS:HB3	1:T:11:ILE:HB	1.85	0.57
1:R:456:ARG:NH2	2:R:700:FDP:O1P	2.34	0.57
1:V:472:THR:HA	1:V:497:VAL:O	2.04	0.57
1:J:212:PHE:CE1	1:J:241:ASN:ND2	2.70	0.57
1:V:272:GLU:CG	1:X:352:GLU:CG	2.82	0.57
1:W:57:HIS:HE1	1:W:195:VAL:HG12	1.69	0.57
1:J:472:THR:HA	1:J:497:VAL:O	2.04	0.56
1:K:472:THR:HA	1:K:497:VAL:O	2.04	0.56
1:L:472:THR:CG2	1:L:498:GLU:HA	2.18	0.56
1:S:472:THR:HA	1:S:497:VAL:O	2.04	0.56
1:A:3:LEU:HD23	1:I:283:SER:CB	2.34	0.56
1:A:57:HIS:HE1	1:A:195:VAL:HG12	1.69	0.56
1:D:472:THR:HA	1:D:497:VAL:O	2.04	0.56
1:M:372:ILE:HG23	1:N:390:GLU:O	2.05	0.56
1:C:57:HIS:CE1	1:C:195:VAL:HG12	2.41	0.56
1:C:498:GLU:HG2	1:V:195:VAL:HG11	1.87	0.56
1:F:57:HIS:CE1	1:F:195:VAL:HG12	2.41	0.56
1:I:229:LYS:HE3	1:M:487:GLY:N	2.19	0.56
1:K:310:ARG:HG2	1:M:297:GLN:OE1	2.05	0.56
1:M:372:ILE:HD11	1:N:390:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:472:THR:HA	1:O:497:VAL:O	2.04	0.56
1:P:195:VAL:HG22	1:U:496:LEU:HD23	1.85	0.56
1:Q:272:GLU:HG2	1:S:352:GLU:HG2	1.85	0.56
1:S:493:ARG:NE	1:T:482:ASP:OD2	2.34	0.56
1:U:11:ILE:HA	1:W:273:LYS:HG2	1.85	0.56
1:U:223:ARG:HH11	1:U:223:ARG:CG	2.19	0.56
1:U:272:GLU:C	1:W:352:GLU:HG2	2.29	0.56
1:U:315:ASP:HB2	1:W:311:ALA:CA	2.34	0.56
1:X:57:HIS:CE1	1:X:195:VAL:HG12	2.41	0.56
1:X:212:PHE:CE1	1:X:241:ASN:ND2	2.70	0.56
1:G:472:THR:CG2	1:G:498:GLU:HA	2.18	0.56
1:K:491:GLN:HG3	1:L:491:GLN:HG3	1.87	0.56
1:L:352:GLU:HB2	1:N:272:GLU:HG3	1.87	0.56
1:N:57:HIS:CE1	1:N:195:VAL:HG12	2.41	0.56
1:O:57:HIS:CE1	1:O:195:VAL:HG12	2.41	0.56
1:P:223:ARG:HH11	1:P:223:ARG:CG	2.19	0.56
1:U:57:HIS:CE1	1:U:195:VAL:HG12	2.41	0.56
1:V:57:HIS:CE1	1:V:195:VAL:HG12	2.41	0.56
1:D:312:GLU:HA	1:F:311:ALA:HB1	1.87	0.56
1:E:57:HIS:CE1	1:E:195:VAL:HG12	2.41	0.56
1:G:57:HIS:CE1	1:G:195:VAL:HG12	2.41	0.56
1:L:11:ILE:HG12	1:L:12:PHE:CE2	2.40	0.56
1:S:57:HIS:HE1	1:S:195:VAL:HG12	1.69	0.56
1:A:223:ARG:HH11	1:A:223:ARG:CG	2.19	0.56
1:H:390:GLU:HA	1:I:372:ILE:HG13	1.88	0.56
1:K:57:HIS:CE1	1:K:195:VAL:HG12	2.41	0.56
1:N:372:ILE:CD1	1:N:374:MET:HE2	2.25	0.56
1:Q:57:HIS:CE1	1:Q:195:VAL:HG12	2.41	0.56
1:Q:272:GLU:CG	1:S:352:GLU:CG	2.83	0.56
1:S:57:HIS:CE1	1:S:195:VAL:HG12	2.41	0.56
1:B:57:HIS:CE1	1:B:195:VAL:HG12	2.41	0.56
1:E:273:LYS:CG	1:G:11:ILE:HB	2.36	0.56
1:L:297:GLN:OE1	1:N:310:ARG:CG	2.41	0.56
1:C:223:ARG:HH11	1:C:223:ARG:CG	2.19	0.56
1:I:57:HIS:CE1	1:I:195:VAL:HG12	2.41	0.56
1:J:57:HIS:CE1	1:J:195:VAL:HG12	2.41	0.56
1:T:57:HIS:CE1	1:T:195:VAL:HG12	2.41	0.56
1:T:370:GLN:CB	1:T:374:MET:SD	2.94	0.56
1:C:472:THR:CG2	1:C:498:GLU:HA	2.18	0.56
1:I:270:PRO:CG	1:I:273:LYS:HE2	2.24	0.56
1:R:57:HIS:CE1	1:R:195:VAL:HG12	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD21	1:I:283:SER:CB	2.34	0.56
1:B:269:ILE:HG12	1:C:11:ILE:CD1	2.35	0.56
1:L:297:GLN:CB	1:N:310:ARG:HG3	2.33	0.56
1:T:223:ARG:HH11	1:T:223:ARG:CG	2.19	0.56
1:U:372:ILE:HG23	1:V:390:GLU:C	2.29	0.56
1:U:392:LYS:HD2	1:V:373:PRO:HD3	1.87	0.56
1:X:223:ARG:HH11	1:X:223:ARG:CG	2.19	0.56
1:D:311:ALA:HB1	1:F:312:GLU:HA	1.88	0.55
1:K:144:ASP:O	1:K:145:ASP:CB	2.45	0.55
1:W:223:ARG:HH11	1:W:223:ARG:CG	2.19	0.55
1:W:456:ARG:NH1	2:W:700:FDP:O2P	2.28	0.55
1:E:223:ARG:HH11	1:E:223:ARG:CG	2.19	0.55
1:H:472:THR:CG2	1:H:498:GLU:HA	2.18	0.55
1:M:144:ASP:O	1:M:145:ASP:CB	2.45	0.55
1:U:370:GLN:CB	1:U:374:MET:SD	2.94	0.55
1:A:372:ILE:CD1	1:A:374:MET:HE2	2.25	0.55
1:D:57:HIS:CE1	1:D:195:VAL:HG12	2.41	0.55
1:H:57:HIS:CE1	1:H:195:VAL:HG12	2.41	0.55
1:I:223:ARG:HH11	1:I:223:ARG:CG	2.19	0.55
1:P:57:HIS:CE1	1:P:195:VAL:HG12	2.41	0.55
1:Q:9:LEU:HB2	1:S:280:ILE:HD11	1.88	0.55
1:W:57:HIS:CE1	1:W:195:VAL:HG12	2.41	0.55
1:B:297:GLN:HB2	1:C:310:ARG:HB2	1.87	0.55
1:D:372:ILE:CD1	1:D:374:MET:HE2	2.25	0.55
1:R:283:SER:CB	1:T:3:LEU:HG	2.36	0.55
1:D:223:ARG:HH11	1:D:223:ARG:CG	2.19	0.55
1:H:273:LYS:HG2	1:J:11:ILE:O	2.07	0.55
1:H:318:ASN:ND2	1:J:318:ASN:ND2	2.55	0.55
1:L:57:HIS:CE1	1:L:195:VAL:HG12	2.41	0.55
1:P:487:GLY:HA3	1:V:229:LYS:CG	2.27	0.55
1:U:365:SER:CB	1:W:3:LEU:HD12	2.37	0.55
1:V:11:ILE:CD1	1:V:12:PHE:HE2	2.12	0.55
1:A:57:HIS:CE1	1:A:195:VAL:HG12	2.41	0.55
1:U:373:PRO:HB3	1:V:391:THR:C	2.32	0.55
1:Q:272:GLU:O	1:S:352:GLU:HG2	2.07	0.55
1:S:372:ILE:HG12	1:T:390:GLU:CA	2.16	0.55
1:H:147:ILE:HG22	1:H:169:HIS:CD2	2.42	0.55
1:H:352:GLU:OE1	1:J:272:GLU:CG	2.54	0.55
1:M:57:HIS:CE1	1:M:195:VAL:HG12	2.41	0.55
1:O:372:ILE:CD1	1:O:374:MET:HE2	2.25	0.55
1:Q:372:ILE:HD12	1:Q:374:MET:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:147:ILE:HG22	1:U:169:HIS:CD2	2.42	0.55
1:D:53:SER:HA	1:D:85:LYS:HG3	1.89	0.55
1:D:372:ILE:HD12	1:D:374:MET:HG2	1.89	0.55
1:H:372:ILE:CG1	1:I:390:GLU:HA	2.26	0.55
1:I:147:ILE:HG22	1:I:169:HIS:CD2	2.42	0.55
1:S:390:GLU:O	1:T:373:PRO:CB	2.55	0.55
1:W:147:ILE:HG22	1:W:169:HIS:CD2	2.42	0.55
1:X:147:ILE:HG22	1:X:169:HIS:CD2	2.42	0.55
1:I:11:ILE:HG12	1:I:12:PHE:CE2	2.40	0.55
1:J:193:ASP:O	1:J:197:LEU:N	2.38	0.55
1:N:147:ILE:HG22	1:N:169:HIS:CD2	2.42	0.55
1:N:223:ARG:HH11	1:N:223:ARG:CG	2.19	0.55
1:N:372:ILE:HD12	1:N:374:MET:HG2	1.89	0.55
1:P:147:ILE:HG22	1:P:169:HIS:CD2	2.42	0.55
1:Q:242:HIS:HE1	1:S:12:PHE:CZ	2.25	0.55
1:R:147:ILE:HG22	1:R:169:HIS:CD2	2.42	0.55
1:V:372:ILE:HD12	1:V:374:MET:HG2	1.89	0.55
1:W:372:ILE:CG2	1:X:390:GLU:O	2.53	0.55
1:B:53:SER:HA	1:B:85:LYS:HG3	1.89	0.54
1:C:372:ILE:HD12	1:C:374:MET:HG2	1.89	0.54
1:D:147:ILE:HG22	1:D:169:HIS:CD2	2.42	0.54
1:D:390:GLU:HA	1:E:372:ILE:HG13	1.89	0.54
1:H:352:GLU:OE1	1:J:272:GLU:HG3	2.07	0.54
1:L:53:SER:HA	1:L:85:LYS:HG3	1.89	0.54
1:L:147:ILE:HG22	1:L:169:HIS:CD2	2.42	0.54
1:W:372:ILE:HD12	1:W:374:MET:HG2	1.89	0.54
1:H:372:ILE:HD11	1:H:374:MET:HE2	1.89	0.54
1:Q:147:ILE:HG22	1:Q:169:HIS:CD2	2.42	0.54
1:Q:223:ARG:HH11	1:Q:223:ARG:CG	2.19	0.54
1:V:147:ILE:HG22	1:V:169:HIS:CD2	2.42	0.54
1:X:49:ARG:NE	1:X:83:ASP:OD2	2.33	0.54
1:A:53:SER:HA	1:A:85:LYS:HG3	1.89	0.54
1:A:147:ILE:HG22	1:A:169:HIS:CD2	2.42	0.54
1:G:372:ILE:HD12	1:G:374:MET:HG2	1.89	0.54
1:O:147:ILE:HG22	1:O:169:HIS:CD2	2.42	0.54
1:O:372:ILE:HD12	1:O:374:MET:HG2	1.89	0.54
1:C:147:ILE:HG22	1:C:169:HIS:CD2	2.42	0.54
1:J:53:SER:HA	1:J:85:LYS:HG3	1.89	0.54
1:J:372:ILE:HD12	1:J:374:MET:HG2	1.89	0.54
1:K:53:SER:HA	1:K:85:LYS:HG3	1.89	0.54
1:K:372:ILE:HD12	1:K:374:MET:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:284:LYS:HG3	1:N:7:LEU:HD21	1.89	0.54
1:R:270:PRO:CG	1:R:273:LYS:HE2	2.23	0.54
1:R:273:LYS:HD3	1:T:11:ILE:C	2.33	0.54
1:T:147:ILE:HG22	1:T:169:HIS:CD2	2.42	0.54
1:V:272:GLU:HG3	1:X:352:GLU:CG	2.37	0.54
1:B:147:ILE:HG22	1:B:169:HIS:CD2	2.42	0.54
1:E:11:ILE:HG12	1:E:12:PHE:CE2	2.40	0.54
1:M:147:ILE:HG22	1:M:169:HIS:CD2	2.42	0.54
1:Q:11:ILE:HB	1:S:273:LYS:CG	2.37	0.54
1:R:456:ARG:NH1	2:R:700:FDP:O2P	2.34	0.54
1:V:276:VAL:O	1:V:280:ILE:CD1	2.54	0.54
1:H:9:LEU:O	1:J:280:ILE:HD11	2.07	0.54
1:K:223:ARG:HH11	1:K:223:ARG:CG	2.19	0.54
1:O:53:SER:HA	1:O:85:LYS:HG3	1.89	0.54
1:O:223:ARG:HH11	1:O:223:ARG:CG	2.19	0.54
1:S:147:ILE:HG22	1:S:169:HIS:CD2	2.42	0.54
1:T:53:SER:HA	1:T:85:LYS:HG3	1.89	0.54
1:U:53:SER:HA	1:U:85:LYS:HG3	1.89	0.54
1:V:273:LYS:HD3	1:X:11:ILE:O	2.08	0.54
1:C:373:PRO:HB3	1:P:391:THR:CA	2.38	0.54
1:F:193:ASP:O	1:F:197:LEU:N	2.38	0.54
1:H:223:ARG:HH11	1:H:223:ARG:CG	2.19	0.54
1:H:272:GLU:C	1:J:352:GLU:HG2	2.32	0.54
1:I:144:ASP:O	1:I:145:ASP:CB	2.45	0.54
1:J:147:ILE:HG22	1:J:169:HIS:CD2	2.42	0.54
1:E:472:THR:CG2	1:E:498:GLU:HA	2.18	0.54
1:F:53:SER:HA	1:F:85:LYS:HG3	1.89	0.54
1:F:147:ILE:HG22	1:F:169:HIS:CD2	2.42	0.54
1:F:223:ARG:HH11	1:F:223:ARG:CG	2.19	0.54
1:G:147:ILE:HG22	1:G:169:HIS:CD2	2.42	0.54
1:J:456:ARG:NH1	2:J:700:FDP:O2P	2.34	0.54
1:N:53:SER:HA	1:N:85:LYS:HG3	1.89	0.54
1:Q:53:SER:HA	1:Q:85:LYS:HG3	1.89	0.54
1:R:49:ARG:NE	1:R:83:ASP:OD2	2.33	0.54
1:S:53:SER:HA	1:S:85:LYS:HG3	1.89	0.54
1:V:270:PRO:CG	1:V:273:LYS:HE2	2.24	0.54
1:E:372:ILE:HD12	1:E:374:MET:HG2	1.89	0.54
1:H:270:PRO:HB2	1:H:273:LYS:HD2	1.90	0.54
1:P:53:SER:HA	1:P:85:LYS:HG3	1.89	0.54
1:Q:273:LYS:HB3	1:S:11:ILE:HB	1.88	0.54
1:Q:283:SER:CB	1:S:3:LEU:HD21	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:276:VAL:CG1	1:X:9:LEU:HB3	2.37	0.54
1:W:53:SER:HA	1:W:85:LYS:HG3	1.89	0.54
1:X:472:THR:CG2	1:X:498:GLU:HA	2.18	0.54
1:B:273:LYS:HG2	1:C:11:ILE:O	2.07	0.54
1:C:373:PRO:HB3	1:P:390:GLU:O	2.08	0.54
1:D:12:PHE:HZ	1:F:242:HIS:CE1	2.24	0.54
1:K:270:PRO:HB2	1:K:273:LYS:HD2	1.90	0.54
1:U:270:PRO:HB2	1:U:273:LYS:HD2	1.90	0.54
1:V:11:ILE:HG12	1:V:12:PHE:CE2	2.40	0.54
1:V:276:VAL:C	1:V:280:ILE:HD12	2.33	0.54
1:A:270:PRO:HG2	1:A:273:LYS:CE	2.38	0.53
1:C:270:PRO:HB2	1:C:273:LYS:HD2	1.90	0.53
1:E:53:SER:HA	1:E:85:LYS:HG3	1.89	0.53
1:E:147:ILE:HG22	1:E:169:HIS:CD2	2.42	0.53
1:H:11:ILE:CD1	1:J:269:ILE:HG12	2.38	0.53
1:I:195:VAL:HG22	1:N:496:LEU:CG	2.36	0.53
1:L:276:VAL:HG13	1:N:9:LEU:HB3	1.90	0.53
1:O:272:GLU:O	1:P:352:GLU:HG2	2.08	0.53
1:R:273:LYS:CD	1:T:11:ILE:HB	2.39	0.53
1:S:223:ARG:HH11	1:S:223:ARG:CG	2.19	0.53
1:U:297:GLN:OE1	1:W:310:ARG:NH2	2.41	0.53
1:F:391:THR:C	1:G:373:PRO:HB3	2.33	0.53
1:K:147:ILE:HG22	1:K:169:HIS:CD2	2.42	0.53
1:B:270:PRO:HB2	1:B:273:LYS:HD2	1.90	0.53
1:F:390:GLU:O	1:G:373:PRO:CB	2.56	0.53
1:I:53:SER:HA	1:I:85:LYS:HG3	1.89	0.53
1:L:229:LYS:CD	1:S:487:GLY:HA2	2.38	0.53
1:O:12:PHE:HZ	1:P:242:HIS:CE1	2.21	0.53
1:A:456:ARG:NH1	2:A:700:FDP:O2P	2.34	0.53
1:B:270:PRO:HG2	1:B:273:LYS:CE	2.38	0.53
1:F:372:ILE:HD12	1:F:374:MET:HG2	1.89	0.53
1:L:297:GLN:CB	1:N:310:ARG:HB2	2.38	0.53
1:R:472:THR:CG2	1:R:498:GLU:HA	2.18	0.53
1:U:494:ILE:HD12	1:V:376:ALA:HB1	1.89	0.53
1:B:372:ILE:CD1	1:B:374:MET:HE2	2.25	0.53
1:D:270:PRO:HG2	1:D:273:LYS:CE	2.38	0.53
1:D:391:THR:C	1:E:373:PRO:HB3	2.34	0.53
1:L:223:ARG:HH11	1:L:223:ARG:CG	2.19	0.53
1:N:472:THR:CG2	1:N:498:GLU:HA	2.18	0.53
1:F:483:HIS:NE2	1:G:483:HIS:HD2	2.07	0.53
1:G:223:ARG:HH11	1:G:223:ARG:CG	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:374:MET:HE2	1:N:390:GLU:HG2	1.90	0.53
1:Q:270:PRO:HG2	1:Q:273:LYS:CE	2.38	0.53
1:X:372:ILE:HD12	1:X:374:MET:HG2	1.89	0.53
1:C:390:GLU:HG2	1:P:374:MET:HE2	1.91	0.53
1:G:53:SER:HA	1:G:85:LYS:HG3	1.89	0.53
1:K:270:PRO:HG2	1:K:273:LYS:CE	2.38	0.53
1:L:310:ARG:CG	1:N:297:GLN:HB2	2.37	0.53
1:O:270:PRO:HB2	1:O:273:LYS:HD2	1.90	0.53
1:O:472:THR:CG2	1:O:498:GLU:HA	2.18	0.53
1:Q:270:PRO:HB2	1:Q:273:LYS:HD2	1.90	0.53
1:Q:352:GLU:HB2	1:S:272:GLU:HG3	1.89	0.53
1:R:193:ASP:O	1:R:197:LEU:N	2.38	0.53
1:R:273:LYS:CG	1:T:11:ILE:HB	2.39	0.53
1:B:372:ILE:HD12	1:B:374:MET:HG2	1.89	0.53
1:C:89:ILE:CG2	1:C:177:VAL:HG22	2.39	0.53
1:H:53:SER:HA	1:H:85:LYS:HG3	1.89	0.53
1:M:392:LYS:HD2	1:N:373:PRO:HD3	1.91	0.53
1:P:89:ILE:CG2	1:P:177:VAL:HG22	2.39	0.53
1:P:472:THR:CG2	1:P:498:GLU:HA	2.18	0.53
1:R:53:SER:HA	1:R:85:LYS:HG3	1.89	0.53
1:X:53:SER:HA	1:X:85:LYS:HG3	1.89	0.53
1:B:297:GLN:CB	1:C:310:ARG:HG2	2.38	0.53
1:D:89:ILE:CG2	1:D:177:VAL:HG22	2.39	0.53
1:K:89:ILE:CG2	1:K:177:VAL:HG22	2.39	0.53
1:L:89:ILE:CG2	1:L:177:VAL:HG22	2.39	0.53
1:N:89:ILE:CG2	1:N:177:VAL:HG22	2.39	0.53
1:O:311:ALA:HB1	1:P:312:GLU:CA	2.26	0.53
1:Q:297:GLN:CD	1:S:310:ARG:HG2	2.24	0.53
1:S:89:ILE:CG2	1:S:177:VAL:HG22	2.39	0.53
1:U:352:GLU:OE1	1:W:272:GLU:HG3	2.09	0.53
1:V:11:ILE:HG13	1:V:12:PHE:HD2	1.72	0.53
1:V:53:SER:HA	1:V:85:LYS:HG3	1.89	0.53
1:A:270:PRO:HB2	1:A:273:LYS:HD2	1.90	0.53
1:B:3:LEU:HD13	1:C:369:LEU:HD12	1.90	0.53
1:B:89:ILE:CG2	1:B:177:VAL:HG22	2.39	0.53
1:B:297:GLN:HB2	1:C:310:ARG:CB	2.39	0.53
1:C:193:ASP:O	1:C:197:LEU:N	2.38	0.53
1:F:89:ILE:CG2	1:F:177:VAL:HG22	2.39	0.53
1:H:296:THR:HG22	1:H:297:GLN:CG	2.39	0.53
1:J:240:GLU:HB3	1:J:264:ASP:HB2	1.91	0.53
1:M:240:GLU:HB3	1:M:264:ASP:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:270:PRO:O	1:R:273:LYS:HB2	2.09	0.53
1:S:372:ILE:HG23	1:T:390:GLU:C	2.33	0.53
1:T:89:ILE:CG2	1:T:177:VAL:HG22	2.39	0.53
1:U:89:ILE:CG2	1:U:177:VAL:HG22	2.39	0.53
1:U:270:PRO:HG2	1:U:273:LYS:CE	2.38	0.53
1:W:89:ILE:CG2	1:W:177:VAL:HG22	2.39	0.53
1:A:240:GLU:HB3	1:A:264:ASP:HB2	1.91	0.52
1:A:372:ILE:HD12	1:A:374:MET:HG2	1.89	0.52
1:E:270:PRO:O	1:E:273:LYS:HB2	2.09	0.52
1:I:270:PRO:O	1:I:273:LYS:HB2	2.09	0.52
1:L:272:GLU:HG2	1:N:352:GLU:HG2	1.91	0.52
1:L:276:VAL:HG13	1:N:9:LEU:CB	2.39	0.52
1:M:383:SER:HB2	1:N:383:SER:CB	2.33	0.52
1:V:372:ILE:CD1	1:V:374:MET:HE2	2.25	0.52
1:C:53:SER:HA	1:C:85:LYS:HG3	1.90	0.52
1:C:270:PRO:HG2	1:C:273:LYS:CE	2.38	0.52
1:C:390:GLU:HG2	1:P:372:ILE:HD11	1.91	0.52
1:G:89:ILE:CG2	1:G:177:VAL:HG22	2.39	0.52
1:J:89:ILE:CG2	1:J:177:VAL:HG22	2.39	0.52
1:L:273:LYS:CD	1:N:11:ILE:HB	2.39	0.52
1:M:53:SER:HA	1:M:85:LYS:HG3	1.89	0.52
1:N:193:ASP:O	1:N:197:LEU:N	2.38	0.52
1:R:297:GLN:CD	1:T:310:ARG:HG2	2.34	0.52
1:S:240:GLU:HB3	1:S:264:ASP:HB2	1.91	0.52
1:H:372:ILE:HD12	1:H:374:MET:CG	2.38	0.52
1:I:89:ILE:CG2	1:I:177:VAL:HG22	2.39	0.52
1:R:273:LYS:HG2	1:T:11:ILE:HA	1.91	0.52
1:S:372:ILE:CG1	1:T:390:GLU:CB	2.87	0.52
1:T:193:ASP:O	1:T:197:LEU:N	2.38	0.52
1:U:49:ARG:NE	1:U:83:ASP:OD2	2.33	0.52
1:W:240:GLU:HB3	1:W:264:ASP:HB2	1.91	0.52
1:X:89:ILE:CG2	1:X:177:VAL:HG22	2.39	0.52
1:H:352:GLU:HG2	1:J:272:GLU:HB2	1.92	0.52
1:K:273:LYS:HB3	1:M:11:ILE:HB	1.91	0.52
1:M:89:ILE:CG2	1:M:177:VAL:HG22	2.39	0.52
1:M:193:ASP:O	1:M:197:LEU:N	2.38	0.52
1:M:223:ARG:HH11	1:M:223:ARG:CG	2.19	0.52
1:V:240:GLU:HB3	1:V:264:ASP:HB2	1.91	0.52
1:V:270:PRO:O	1:V:273:LYS:HB2	2.09	0.52
1:X:193:ASP:O	1:X:197:LEU:N	2.38	0.52
1:B:240:GLU:HB3	1:B:264:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:GLU:HB3	1:E:264:ASP:HB2	1.91	0.52
1:H:270:PRO:HG2	1:H:273:LYS:CE	2.38	0.52
1:O:89:ILE:CG2	1:O:177:VAL:HG22	2.39	0.52
1:O:270:PRO:HG2	1:O:273:LYS:CE	2.38	0.52
1:R:89:ILE:CG2	1:R:177:VAL:HG22	2.39	0.52
1:V:287:VAL:HG23	1:X:3:LEU:CD2	2.40	0.52
1:D:12:PHE:HZ	1:F:242:HIS:HE1	1.51	0.52
1:D:270:PRO:HB2	1:D:273:LYS:HD2	1.90	0.52
1:H:391:THR:HA	1:I:373:PRO:HB3	1.91	0.52
1:J:223:ARG:HH11	1:J:223:ARG:CG	2.19	0.52
1:M:373:PRO:CB	1:N:391:THR:HA	2.39	0.52
1:O:193:ASP:O	1:O:197:LEU:N	2.38	0.52
1:O:270:PRO:HG2	1:O:273:LYS:HD2	1.92	0.52
1:P:193:ASP:O	1:P:197:LEU:N	2.38	0.52
1:Q:471:GLN:O	1:Q:497:VAL:CG2	2.58	0.52
1:S:390:GLU:O	1:T:373:PRO:HB3	2.09	0.52
1:U:240:GLU:HB3	1:U:264:ASP:HB2	1.91	0.52
1:U:471:GLN:O	1:U:497:VAL:CG2	2.58	0.52
1:V:280:ILE:HA	1:X:6:ASN:HB3	1.90	0.52
1:X:240:GLU:HB3	1:X:264:ASP:HB2	1.91	0.52
1:A:89:ILE:CG2	1:A:177:VAL:HG22	2.39	0.52
1:B:193:ASP:O	1:B:197:LEU:N	2.38	0.52
1:H:89:ILE:CG2	1:H:177:VAL:HG22	2.39	0.52
1:H:193:ASP:O	1:H:197:LEU:N	2.38	0.52
1:H:240:GLU:HB3	1:H:264:ASP:HB2	1.91	0.52
1:N:240:GLU:HB3	1:N:264:ASP:HB2	1.91	0.52
1:Q:89:ILE:CG2	1:Q:177:VAL:HG22	2.39	0.52
1:V:89:ILE:CG2	1:V:177:VAL:HG22	2.39	0.52
1:C:471:GLN:O	1:C:497:VAL:CG2	2.58	0.52
1:M:471:GLN:O	1:M:497:VAL:CG2	2.58	0.52
1:O:310:ARG:CZ	1:P:297:GLN:OE1	2.58	0.52
1:Q:270:PRO:HG2	1:Q:273:LYS:HD2	1.92	0.52
1:U:390:GLU:OE1	1:V:379:ALA:HB2	2.10	0.52
1:X:471:GLN:O	1:X:497:VAL:CG2	2.58	0.52
1:A:270:PRO:HG2	1:A:273:LYS:HD2	1.92	0.52
1:H:371:HIS:C	1:H:372:ILE:HD13	2.34	0.52
1:K:270:PRO:HG2	1:K:273:LYS:HD2	1.92	0.52
1:O:471:GLN:O	1:O:497:VAL:CG2	2.58	0.52
1:Q:373:PRO:HB3	1:R:390:GLU:O	2.09	0.52
1:S:193:ASP:O	1:S:197:LEU:N	2.38	0.52
1:W:471:GLN:O	1:W:497:VAL:CG2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:GLN:O	1:D:497:VAL:CG2	2.58	0.51
1:E:456:ARG:HH22	2:E:700:FDP:P1	2.33	0.51
1:G:240:GLU:HB3	1:G:264:ASP:HB2	1.91	0.51
1:L:193:ASP:O	1:L:197:LEU:N	2.38	0.51
1:N:471:GLN:O	1:N:497:VAL:CG2	2.58	0.51
1:B:223:ARG:HH11	1:B:223:ARG:CG	2.19	0.51
1:B:280:ILE:HG12	1:C:6:ASN:O	2.10	0.51
1:C:240:GLU:HB3	1:C:264:ASP:HB2	1.91	0.51
1:D:270:PRO:HG2	1:D:273:LYS:HD2	1.92	0.51
1:F:188:ALA:HA	1:F:218:GLN:OE1	2.11	0.51
1:L:188:ALA:HA	1:L:218:GLN:OE1	2.11	0.51
1:L:270:PRO:O	1:L:273:LYS:HB2	2.09	0.51
1:L:471:GLN:O	1:L:497:VAL:CG2	2.58	0.51
1:R:223:ARG:HH11	1:R:223:ARG:CG	2.19	0.51
1:R:240:GLU:HB3	1:R:264:ASP:HB2	1.91	0.51
1:R:471:GLN:O	1:R:497:VAL:CG2	2.58	0.51
1:B:297:GLN:OE1	1:C:310:ARG:CZ	2.58	0.51
1:E:89:ILE:CG2	1:E:177:VAL:HG22	2.39	0.51
1:F:471:GLN:O	1:F:497:VAL:CG2	2.58	0.51
1:G:471:GLN:O	1:G:497:VAL:CG2	2.58	0.51
1:H:270:PRO:HG2	1:H:273:LYS:HD2	1.92	0.51
1:H:471:GLN:O	1:H:497:VAL:CG2	2.58	0.51
1:P:240:GLU:HB3	1:P:264:ASP:HB2	1.92	0.51
1:S:372:ILE:HD11	1:T:390:GLU:CG	2.21	0.51
1:S:372:ILE:CB	1:T:390:GLU:O	2.58	0.51
1:T:471:GLN:O	1:T:497:VAL:CG2	2.58	0.51
1:V:471:GLN:O	1:V:497:VAL:CG2	2.58	0.51
1:W:188:ALA:HA	1:W:218:GLN:OE1	2.11	0.51
1:B:471:GLN:O	1:B:497:VAL:CG2	2.58	0.51
1:I:193:ASP:O	1:I:197:LEU:N	2.38	0.51
1:L:372:ILE:HD12	1:L:374:MET:CG	2.41	0.51
1:N:456:ARG:HH22	2:N:700:FDP:P1	2.34	0.51
1:P:471:GLN:O	1:P:497:VAL:CG2	2.58	0.51
1:Q:279:LYS:HE3	1:S:6:ASN:OD1	2.10	0.51
1:V:223:ARG:HH11	1:V:223:ARG:CG	2.19	0.51
1:V:352:GLU:OE1	1:X:273:LYS:NZ	2.43	0.51
1:A:188:ALA:HA	1:A:218:GLN:OE1	2.11	0.51
1:A:471:GLN:O	1:A:497:VAL:CG2	2.58	0.51
1:C:491:GLN:HG3	1:P:491:GLN:HG3	1.93	0.51
1:M:188:ALA:HA	1:M:218:GLN:OE1	2.11	0.51
1:N:456:ARG:NH1	2:N:700:FDP:O2P	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:3:LEU:HD23	1:S:283:SER:CB	2.41	0.51
1:S:471:GLN:O	1:S:497:VAL:CG2	2.58	0.51
1:T:188:ALA:HA	1:T:218:GLN:OE1	2.11	0.51
1:V:188:ALA:HA	1:V:218:GLN:OE1	2.11	0.51
1:B:103:ARG:CB	1:G:58:GLU:OE1	2.59	0.51
1:B:270:PRO:HG2	1:B:273:LYS:HD2	1.92	0.51
1:B:492:THR:HG22	1:O:492:THR:HG22	1.92	0.51
1:C:372:ILE:CD1	1:C:374:MET:HE2	2.25	0.51
1:I:188:ALA:HA	1:I:218:GLN:OE1	2.11	0.51
1:M:483:HIS:NE2	1:N:483:HIS:HD2	2.09	0.51
1:P:211:SER:HA	1:P:238:LYS:HD3	1.93	0.51
1:R:297:GLN:CB	1:T:310:ARG:HB2	2.34	0.51
1:T:240:GLU:HB3	1:T:264:ASP:HB2	1.91	0.51
1:V:11:ILE:O	1:X:273:LYS:HE3	2.10	0.51
1:B:276:VAL:HG13	1:C:9:LEU:HB3	1.93	0.51
1:C:456:ARG:NH1	2:C:700:FDP:O2P	2.34	0.51
1:F:240:GLU:HB3	1:F:264:ASP:HB2	1.91	0.51
1:I:471:GLN:O	1:I:497:VAL:CG2	2.58	0.51
1:Q:240:GLU:HB3	1:Q:264:ASP:HB2	1.91	0.51
1:W:372:ILE:CG1	1:X:390:GLU:O	2.58	0.51
1:C:211:SER:HA	1:C:238:LYS:HD3	1.93	0.51
1:D:188:ALA:HA	1:D:218:GLN:OE1	2.11	0.51
1:D:193:ASP:O	1:D:197:LEU:N	2.38	0.51
1:D:211:SER:HA	1:D:238:LYS:HD3	1.93	0.51
1:E:193:ASP:O	1:E:196:ASP:N	2.44	0.51
1:E:471:GLN:O	1:E:497:VAL:CG2	2.58	0.51
1:H:193:ASP:O	1:H:196:ASP:N	2.44	0.51
1:I:270:PRO:HD2	1:I:273:LYS:HD2	1.93	0.51
1:J:49:ARG:NE	1:J:83:ASP:OD2	2.33	0.51
1:J:193:ASP:O	1:J:196:ASP:N	2.44	0.51
1:J:471:GLN:O	1:J:497:VAL:CG2	2.58	0.51
1:K:211:SER:HA	1:K:238:LYS:HD3	1.93	0.51
1:K:240:GLU:HB3	1:K:264:ASP:HB2	1.91	0.51
1:L:49:ARG:NE	1:L:83:ASP:OD2	2.33	0.51
1:P:372:ILE:HD12	1:P:374:MET:CG	2.40	0.51
1:S:188:ALA:HA	1:S:218:GLN:OE1	2.11	0.51
1:V:49:ARG:NE	1:V:83:ASP:OD2	2.33	0.51
1:V:193:ASP:O	1:V:196:ASP:N	2.44	0.51
1:E:269:ILE:HG12	1:G:11:ILE:HD12	1.93	0.51
1:H:373:PRO:HB3	1:I:391:THR:HA	1.92	0.51
1:I:147:ILE:HG21	1:I:169:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:240:GLU:HB3	1:I:264:ASP:HB2	1.91	0.51
1:K:188:ALA:HA	1:K:218:GLN:OE1	2.11	0.51
1:M:483:HIS:CD2	1:N:483:HIS:CD2	2.98	0.51
1:Q:193:ASP:O	1:Q:196:ASP:N	2.44	0.51
1:R:456:ARG:HH22	2:R:700:FDP:P1	2.34	0.51
1:S:147:ILE:HG21	1:S:169:HIS:NE2	2.26	0.51
1:U:211:SER:HA	1:U:238:LYS:HD3	1.93	0.51
1:U:352:GLU:HG2	1:W:272:GLU:CG	2.40	0.51
1:V:270:PRO:HD2	1:V:273:LYS:HD2	1.93	0.51
1:V:284:LYS:HG2	1:X:7:LEU:HD22	1.86	0.51
1:A:193:ASP:O	1:A:196:ASP:N	2.44	0.51
1:A:193:ASP:O	1:A:197:LEU:N	2.38	0.51
1:B:270:PRO:O	1:B:273:LYS:HB2	2.11	0.51
1:B:272:GLU:HG2	1:C:352:GLU:HG2	1.93	0.51
1:C:270:PRO:O	1:C:273:LYS:HB2	2.11	0.51
1:E:456:ARG:NH1	2:E:700:FDP:O2P	2.34	0.51
1:F:483:HIS:HD2	1:G:483:HIS:NE2	2.08	0.51
1:K:270:PRO:O	1:K:273:LYS:HB2	2.11	0.51
1:L:147:ILE:HG21	1:L:169:HIS:CD2	2.46	0.51
1:M:193:ASP:O	1:M:196:ASP:N	2.44	0.51
1:O:11:ILE:O	1:P:273:LYS:CE	2.56	0.51
1:O:188:ALA:HA	1:O:218:GLN:OE1	2.11	0.51
1:O:240:GLU:HB3	1:O:264:ASP:HB2	1.91	0.51
1:Q:270:PRO:O	1:Q:273:LYS:HB2	2.11	0.51
1:Q:456:ARG:HH22	2:Q:700:FDP:P1	2.34	0.51
1:S:49:ARG:NE	1:S:83:ASP:OD2	2.33	0.51
1:S:193:ASP:O	1:S:196:ASP:N	2.44	0.51
1:V:193:ASP:O	1:V:197:LEU:N	2.38	0.51
1:W:211:SER:HA	1:W:238:LYS:HD3	1.93	0.51
1:X:193:ASP:O	1:X:196:ASP:N	2.44	0.51
1:X:211:SER:HA	1:X:238:LYS:HD3	1.93	0.51
1:B:188:ALA:HA	1:B:218:GLN:OE1	2.11	0.50
1:B:310:ARG:HG2	1:C:297:GLN:HB2	1.92	0.50
1:D:193:ASP:O	1:D:196:ASP:N	2.44	0.50
1:E:147:ILE:HG21	1:E:169:HIS:NE2	2.27	0.50
1:E:188:ALA:HA	1:E:218:GLN:OE1	2.11	0.50
1:E:283:SER:CB	1:G:3:LEU:CD2	2.89	0.50
1:K:193:ASP:O	1:K:196:ASP:N	2.44	0.50
1:K:471:GLN:O	1:K:497:VAL:CG2	2.58	0.50
1:O:147:ILE:HG21	1:O:169:HIS:NE2	2.26	0.50
1:O:270:PRO:O	1:O:273:LYS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:195:VAL:CG2	1:U:496:LEU:HD21	2.40	0.50
1:U:188:ALA:HA	1:U:218:GLN:OE1	2.11	0.50
1:U:193:ASP:O	1:U:196:ASP:N	2.44	0.50
1:V:147:ILE:HG21	1:V:169:HIS:NE2	2.26	0.50
1:W:193:ASP:O	1:W:197:LEU:N	2.38	0.50
1:A:270:PRO:O	1:A:273:LYS:HB2	2.11	0.50
1:B:193:ASP:O	1:B:196:ASP:N	2.44	0.50
1:C:147:ILE:HG21	1:C:169:HIS:NE2	2.27	0.50
1:C:456:ARG:HH22	2:C:700:FDP:P1	2.34	0.50
1:E:270:PRO:HD2	1:E:273:LYS:HD2	1.93	0.50
1:F:147:ILE:HG21	1:F:169:HIS:NE2	2.26	0.50
1:F:193:ASP:O	1:F:196:ASP:N	2.44	0.50
1:H:49:ARG:NE	1:H:83:ASP:OD2	2.33	0.50
1:H:311:ALA:HA	1:J:315:ASP:HB2	1.93	0.50
1:I:211:SER:HA	1:I:238:LYS:HD3	1.93	0.50
1:J:456:ARG:HH22	2:J:700:FDP:P1	2.34	0.50
1:J:472:THR:CG2	1:J:498:GLU:HA	2.18	0.50
1:L:193:ASP:O	1:L:196:ASP:N	2.44	0.50
1:L:240:GLU:HB3	1:L:264:ASP:HB2	1.91	0.50
1:L:270:PRO:HD2	1:L:273:LYS:HD2	1.93	0.50
1:L:297:GLN:HB2	1:N:310:ARG:CB	2.41	0.50
1:L:297:GLN:CB	1:N:310:ARG:CG	2.89	0.50
1:M:211:SER:HA	1:M:238:LYS:HD3	1.93	0.50
1:N:147:ILE:HG21	1:N:169:HIS:NE2	2.27	0.50
1:N:193:ASP:O	1:N:196:ASP:N	2.44	0.50
1:N:211:SER:HA	1:N:238:LYS:HD3	1.93	0.50
1:O:193:ASP:O	1:O:196:ASP:N	2.44	0.50
1:P:147:ILE:HG21	1:P:169:HIS:NE2	2.27	0.50
1:P:188:ALA:HA	1:P:218:GLN:OE1	2.11	0.50
1:Q:193:ASP:C	1:Q:196:ASP:H	2.20	0.50
1:R:188:ALA:HA	1:R:218:GLN:OE1	2.11	0.50
1:R:193:ASP:O	1:R:196:ASP:N	2.44	0.50
1:T:147:ILE:HG21	1:T:169:HIS:NE2	2.27	0.50
1:T:193:ASP:O	1:T:196:ASP:N	2.44	0.50
1:X:147:ILE:HG21	1:X:169:HIS:CD2	2.47	0.50
1:A:147:ILE:HG21	1:A:169:HIS:NE2	2.27	0.50
1:A:211:SER:HA	1:A:238:LYS:HD3	1.93	0.50
1:A:456:ARG:HH22	2:A:700:FDP:P1	2.33	0.50
1:B:147:ILE:HG21	1:B:169:HIS:CD2	2.46	0.50
1:D:193:ASP:C	1:D:196:ASP:H	2.20	0.50
1:D:270:PRO:O	1:D:273:LYS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:LYS:HG2	1:G:11:ILE:HB	1.92	0.50
1:F:147:ILE:HG21	1:F:169:HIS:CD2	2.46	0.50
1:H:211:SER:HA	1:H:238:LYS:HD3	1.93	0.50
1:J:188:ALA:HA	1:J:218:GLN:OE1	2.11	0.50
1:P:193:ASP:O	1:P:196:ASP:N	2.44	0.50
1:R:270:PRO:HD2	1:R:273:LYS:HD2	1.93	0.50
1:S:211:SER:HA	1:S:238:LYS:HD3	1.93	0.50
1:V:193:ASP:C	1:V:196:ASP:H	2.20	0.50
1:V:211:SER:HA	1:V:238:LYS:HD3	1.93	0.50
1:B:193:ASP:C	1:B:196:ASP:H	2.20	0.50
1:D:240:GLU:HB3	1:D:264:ASP:HB2	1.91	0.50
1:D:456:ARG:HH22	2:D:700:FDP:P1	2.34	0.50
1:H:193:ASP:C	1:H:196:ASP:H	2.20	0.50
1:I:472:THR:CG2	1:I:498:GLU:HA	2.18	0.50
1:J:193:ASP:CA	1:J:196:ASP:HB2	2.41	0.50
1:N:147:ILE:HG21	1:N:169:HIS:CD2	2.46	0.50
1:N:188:ALA:HA	1:N:218:GLN:OE1	2.11	0.50
1:Q:147:ILE:HG21	1:Q:169:HIS:NE2	2.26	0.50
1:U:147:ILE:HG21	1:U:169:HIS:CD2	2.46	0.50
1:U:270:PRO:O	1:U:273:LYS:HB2	2.11	0.50
1:V:280:ILE:CD1	1:X:9:LEU:HB2	2.40	0.50
1:W:147:ILE:HG21	1:W:169:HIS:NE2	2.26	0.50
1:W:193:ASP:O	1:W:196:ASP:N	2.44	0.50
1:X:193:ASP:C	1:X:196:ASP:H	2.20	0.50
1:B:147:ILE:HG21	1:B:169:HIS:NE2	2.27	0.50
1:B:211:SER:HA	1:B:238:LYS:HD3	1.93	0.50
1:G:188:ALA:HA	1:G:218:GLN:OE1	2.11	0.50
1:H:312:GLU:CA	1:J:311:ALA:CB	2.71	0.50
1:K:352:GLU:HB2	1:M:272:GLU:HG3	1.94	0.50
1:L:193:ASP:C	1:L:196:ASP:H	2.20	0.50
1:M:147:ILE:HG21	1:M:169:HIS:CD2	2.46	0.50
1:O:352:GLU:HG2	1:P:272:GLU:O	2.11	0.50
1:R:147:ILE:HG21	1:R:169:HIS:NE2	2.26	0.50
1:T:193:ASP:CA	1:T:196:ASP:HB2	2.42	0.50
1:U:11:ILE:O	1:W:273:LYS:CG	2.60	0.50
1:U:297:GLN:OE1	1:W:309:THR:HA	2.12	0.50
1:W:390:GLU:OE1	1:X:379:ALA:HA	2.12	0.50
1:B:456:ARG:HH22	2:B:700:FDP:P1	2.34	0.50
1:C:188:ALA:HA	1:C:218:GLN:OE1	2.11	0.50
1:D:147:ILE:HG21	1:D:169:HIS:NE2	2.26	0.50
1:E:211:SER:HA	1:E:238:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:147:ILE:HG21	1:J:169:HIS:CD2	2.46	0.50
1:J:147:ILE:HG21	1:J:169:HIS:NE2	2.26	0.50
1:K:297:GLN:OE1	1:M:310:ARG:NH2	2.45	0.50
1:K:372:ILE:HD11	1:L:390:GLU:HG2	1.93	0.50
1:L:272:GLU:C	1:N:352:GLU:HG2	2.36	0.50
1:O:147:ILE:HG21	1:O:169:HIS:CD2	2.46	0.50
1:P:193:ASP:C	1:P:196:ASP:H	2.20	0.50
1:R:211:SER:HA	1:R:238:LYS:HD3	1.93	0.50
1:T:193:ASP:C	1:T:196:ASP:H	2.20	0.50
1:U:263:GLY:HA2	1:W:310:ARG:NH1	2.16	0.50
1:A:193:ASP:C	1:A:196:ASP:H	2.20	0.50
1:B:472:THR:CG2	1:B:498:GLU:HA	2.18	0.50
1:C:193:ASP:O	1:C:196:ASP:N	2.44	0.50
1:E:193:ASP:O	1:E:197:LEU:N	2.38	0.50
1:H:188:ALA:HA	1:H:218:GLN:OE1	2.11	0.50
1:H:270:PRO:O	1:H:273:LYS:HB2	2.11	0.50
1:I:11:ILE:HG13	1:I:12:PHE:HD2	1.72	0.50
1:L:7:LEU:CD2	1:N:284:LYS:HG3	2.42	0.50
1:N:193:ASP:C	1:N:196:ASP:H	2.20	0.50
1:R:311:ALA:HB1	1:T:315:ASP:HB2	1.94	0.50
1:T:211:SER:HA	1:T:238:LYS:HD3	1.93	0.50
1:V:11:ILE:HG12	1:V:12:PHE:CD2	2.47	0.50
1:A:49:ARG:NE	1:A:83:ASP:OD2	2.33	0.50
1:G:147:ILE:HG21	1:G:169:HIS:NE2	2.27	0.50
1:G:211:SER:HA	1:G:238:LYS:HD3	1.93	0.50
1:L:211:SER:HA	1:L:238:LYS:HD3	1.93	0.50
1:P:372:ILE:HD12	1:P:374:MET:HG3	1.92	0.50
1:Q:211:SER:HA	1:Q:238:LYS:HD3	1.93	0.50
1:Q:491:GLN:HG3	1:R:491:GLN:HG3	1.93	0.50
1:S:51:ASN:HA	1:S:83:ASP:HB3	1.94	0.50
1:S:193:ASP:C	1:S:196:ASP:H	2.20	0.50
1:V:284:LYS:CE	1:X:7:LEU:HD22	2.41	0.50
1:X:188:ALA:HA	1:X:218:GLN:OE1	2.11	0.50
1:B:51:ASN:HA	1:B:83:ASP:HB3	1.94	0.50
1:C:51:ASN:HA	1:C:83:ASP:HB3	1.94	0.50
1:D:49:ARG:NE	1:D:83:ASP:OD2	2.33	0.50
1:F:193:ASP:C	1:F:196:ASP:H	2.20	0.50
1:I:193:ASP:O	1:I:196:ASP:N	2.44	0.50
1:J:193:ASP:C	1:J:196:ASP:H	2.20	0.50
1:J:211:SER:HA	1:J:238:LYS:HD3	1.93	0.50
1:K:147:ILE:HG21	1:K:169:HIS:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:272:GLU:CB	1:S:352:GLU:HG2	2.42	0.50
1:S:456:ARG:HH22	2:S:700:FDP:P1	2.34	0.50
1:V:147:ILE:HG21	1:V:169:HIS:CD2	2.46	0.50
1:W:472:THR:CG2	1:W:498:GLU:HA	2.18	0.50
1:X:147:ILE:HG21	1:X:169:HIS:NE2	2.27	0.50
1:F:211:SER:HA	1:F:238:LYS:HD3	1.93	0.49
1:I:12:PHE:CD2	1:I:12:PHE:N	2.79	0.49
1:K:147:ILE:HG21	1:K:169:HIS:CD2	2.47	0.49
1:O:193:ASP:C	1:O:196:ASP:H	2.20	0.49
1:Q:188:ALA:HA	1:Q:218:GLN:OE1	2.11	0.49
1:Q:193:ASP:CA	1:Q:196:ASP:HB2	2.42	0.49
1:T:147:ILE:HG21	1:T:169:HIS:CD2	2.47	0.49
1:U:352:GLU:HB2	1:W:272:GLU:HG3	1.94	0.49
1:C:193:ASP:C	1:C:196:ASP:H	2.20	0.49
1:D:147:ILE:HG21	1:D:169:HIS:CD2	2.46	0.49
1:F:49:ARG:NE	1:F:83:ASP:OD2	2.33	0.49
1:G:193:ASP:O	1:G:196:ASP:N	2.44	0.49
1:H:147:ILE:HG21	1:H:169:HIS:NE2	2.26	0.49
1:M:147:ILE:HG21	1:M:169:HIS:NE2	2.26	0.49
1:N:51:ASN:HA	1:N:83:ASP:HB3	1.94	0.49
1:R:147:ILE:HG21	1:R:169:HIS:CD2	2.46	0.49
1:R:193:ASP:C	1:R:196:ASP:H	2.20	0.49
1:U:193:ASP:C	1:U:196:ASP:H	2.20	0.49
1:U:383:SER:HB2	1:V:383:SER:CB	2.42	0.49
1:U:456:ARG:HH22	2:U:700:FDP:P1	2.34	0.49
1:U:456:ARG:NH1	2:U:700:FDP:O2P	2.35	0.49
1:A:51:ASN:HA	1:A:83:ASP:HB3	1.95	0.49
1:A:147:ILE:HG21	1:A:169:HIS:CD2	2.46	0.49
1:F:456:ARG:HH22	2:F:700:FDP:P1	2.34	0.49
1:G:193:ASP:C	1:G:196:ASP:H	2.20	0.49
1:H:51:ASN:HA	1:H:83:ASP:HB3	1.94	0.49
1:I:193:ASP:C	1:I:196:ASP:H	2.20	0.49
1:K:391:THR:C	1:L:373:PRO:HB3	2.37	0.49
1:O:211:SER:HA	1:O:238:LYS:HD3	1.93	0.49
1:Q:51:ASN:HA	1:Q:83:ASP:HB3	1.94	0.49
1:W:390:GLU:OE1	1:X:379:ALA:CA	2.60	0.49
1:H:147:ILE:HG21	1:H:169:HIS:CD2	2.46	0.49
1:I:49:ARG:NE	1:I:83:ASP:OD2	2.33	0.49
1:L:147:ILE:HG21	1:L:169:HIS:NE2	2.27	0.49
1:Q:471:GLN:O	1:Q:497:VAL:HG22	2.13	0.49
1:R:11:ILE:HG12	1:R:12:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:270:PRO:HG2	1:U:273:LYS:HD2	1.92	0.49
1:V:273:LYS:CD	1:X:11:ILE:HB	2.43	0.49
1:V:283:SER:HB3	1:X:3:LEU:HD23	1.93	0.49
1:W:147:ILE:HG21	1:W:169:HIS:CD2	2.46	0.49
1:X:270:PRO:O	1:X:273:LYS:HB2	2.12	0.49
1:A:391:THR:O	1:J:373:PRO:HB3	2.11	0.49
1:B:270:PRO:HD2	1:B:273:LYS:HD3	1.95	0.49
1:E:51:ASN:HA	1:E:83:ASP:HB3	1.94	0.49
1:E:193:ASP:C	1:E:196:ASP:H	2.20	0.49
1:L:12:PHE:CZ	1:N:242:HIS:NE2	2.80	0.49
1:L:51:ASN:HA	1:L:83:ASP:HB3	1.94	0.49
1:M:19:ARG:NH1	1:M:21:ALA:O	2.46	0.49
1:P:147:ILE:HG21	1:P:169:HIS:CD2	2.46	0.49
1:Q:147:ILE:HG21	1:Q:169:HIS:CD2	2.46	0.49
1:Q:284:LYS:HG3	1:S:7:LEU:HD22	1.93	0.49
1:S:147:ILE:HG21	1:S:169:HIS:CD2	2.46	0.49
1:U:471:GLN:O	1:U:497:VAL:HG22	2.13	0.49
1:A:19:ARG:NH1	1:A:21:ALA:O	2.46	0.49
1:C:471:GLN:O	1:C:497:VAL:HG22	2.13	0.49
1:E:147:ILE:HG21	1:E:169:HIS:CD2	2.46	0.49
1:G:19:ARG:NH1	1:G:21:ALA:O	2.46	0.49
1:G:147:ILE:HG21	1:G:169:HIS:CD2	2.47	0.49
1:I:229:LYS:HD2	1:M:487:GLY:CA	2.41	0.49
1:I:456:ARG:HH22	2:I:700:FDP:P1	2.34	0.49
1:J:17:ASN:C	1:J:17:ASN:HD22	2.21	0.49
1:L:284:LYS:HG3	1:N:7:LEU:HD22	1.92	0.49
1:L:487:GLY:CA	1:S:229:LYS:CG	2.76	0.49
1:M:391:THR:HA	1:N:373:PRO:HB3	1.94	0.49
1:P:17:ASN:HD22	1:P:17:ASN:C	2.21	0.49
1:Q:7:LEU:CD2	1:S:284:LYS:HG3	2.43	0.49
1:Q:193:ASP:O	1:Q:197:LEU:N	2.38	0.49
1:U:147:ILE:HG21	1:U:169:HIS:NE2	2.26	0.49
1:V:17:ASN:C	1:V:17:ASN:HD22	2.21	0.49
1:V:19:ARG:NH1	1:V:21:ALA:O	2.46	0.49
1:A:193:ASP:CA	1:A:196:ASP:HB2	2.41	0.49
1:B:471:GLN:O	1:B:497:VAL:HG22	2.13	0.49
1:C:17:ASN:C	1:C:17:ASN:HD22	2.21	0.49
1:C:147:ILE:HG21	1:C:169:HIS:CD2	2.47	0.49
1:D:17:ASN:C	1:D:17:ASN:HD22	2.21	0.49
1:F:193:ASP:CA	1:F:196:ASP:HB2	2.42	0.49
1:H:19:ARG:NH1	1:H:21:ALA:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:51:ASN:HA	1:I:83:ASP:HB3	1.94	0.49
1:I:147:ILE:HG21	1:I:169:HIS:NE2	2.26	0.49
1:L:3:LEU:CD2	1:N:283:SER:HB3	2.42	0.49
1:L:17:ASN:C	1:L:17:ASN:HD22	2.21	0.49
1:N:270:PRO:O	1:N:273:LYS:HB2	2.12	0.49
1:T:270:PRO:O	1:T:273:LYS:HB2	2.12	0.49
1:T:471:GLN:O	1:T:497:VAL:HG22	2.13	0.49
1:U:51:ASN:HA	1:U:83:ASP:HB3	1.94	0.49
1:V:482:ASP:H	1:V:490:ASN:HD21	1.61	0.49
1:A:17:ASN:C	1:A:17:ASN:HD22	2.21	0.49
1:D:51:ASN:HA	1:D:83:ASP:HB3	1.94	0.49
1:F:51:ASN:HA	1:F:83:ASP:HB3	1.95	0.49
1:G:49:ARG:NE	1:G:83:ASP:OD2	2.33	0.49
1:G:471:GLN:O	1:G:497:VAL:HG22	2.13	0.49
1:H:311:ALA:HA	1:J:315:ASP:CB	2.43	0.49
1:H:352:GLU:CB	1:J:272:GLU:HB2	2.42	0.49
1:K:51:ASN:HA	1:K:83:ASP:HB3	1.94	0.49
1:K:193:ASP:C	1:K:196:ASP:H	2.20	0.49
1:M:193:ASP:C	1:M:196:ASP:H	2.20	0.49
1:N:49:ARG:NE	1:N:83:ASP:OD2	2.33	0.49
1:O:471:GLN:O	1:O:497:VAL:HG22	2.13	0.49
1:S:471:GLN:O	1:S:497:VAL:HG22	2.13	0.49
1:U:482:ASP:H	1:U:490:ASN:HD21	1.61	0.49
1:V:51:ASN:HA	1:V:83:ASP:HB3	1.94	0.49
1:V:471:GLN:O	1:V:497:VAL:HG22	2.13	0.49
1:X:51:ASN:HA	1:X:83:ASP:HB3	1.94	0.49
1:A:270:PRO:HD2	1:A:273:LYS:HD3	1.95	0.49
1:C:216:ALA:CB	1:N:446:LYS:CE	2.81	0.49
1:E:273:LYS:HB3	1:G:11:ILE:HB	1.95	0.49
1:F:482:ASP:H	1:F:490:ASN:HD21	1.61	0.49
1:N:482:ASP:H	1:N:490:ASN:HD21	1.61	0.49
1:S:482:ASP:H	1:S:490:ASN:HD21	1.61	0.49
1:W:51:ASN:HA	1:W:83:ASP:HB3	1.95	0.49
1:W:193:ASP:C	1:W:196:ASP:H	2.20	0.49
1:A:12:PHE:CE2	1:I:242:HIS:CE1	3.00	0.49
1:B:19:ARG:NH1	1:B:21:ALA:O	2.46	0.49
1:C:19:ARG:NH1	1:C:21:ALA:O	2.46	0.49
1:F:471:GLN:O	1:F:497:VAL:HG22	2.13	0.49
1:K:17:ASN:HD22	1:K:17:ASN:C	2.21	0.49
1:K:310:ARG:CG	1:M:297:GLN:HB2	2.43	0.49
1:L:11:ILE:HG13	1:L:12:PHE:HD2	1.72	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:482:ASP:H	1:L:490:ASN:HD21	1.61	0.49
1:M:471:GLN:O	1:M:497:VAL:HG22	2.13	0.49
1:M:482:ASP:H	1:M:490:ASN:HD21	1.61	0.49
1:O:270:PRO:HD2	1:O:273:LYS:HD3	1.95	0.49
1:U:352:GLU:HG2	1:W:272:GLU:O	2.13	0.49
1:C:482:ASP:H	1:C:490:ASN:HD21	1.61	0.48
1:D:193:ASP:CA	1:D:196:ASP:HB2	2.41	0.48
1:D:482:ASP:H	1:D:490:ASN:HD21	1.61	0.48
1:G:51:ASN:HA	1:G:83:ASP:HB3	1.94	0.48
1:G:90:ARG:HD3	1:G:174:ARG:O	2.13	0.48
1:G:270:PRO:O	1:G:273:LYS:HB2	2.12	0.48
1:H:17:ASN:HD22	1:H:17:ASN:C	2.21	0.48
1:J:471:GLN:O	1:J:497:VAL:HG22	2.13	0.48
1:L:11:ILE:HG12	1:L:12:PHE:CD2	2.47	0.48
1:L:471:GLN:O	1:L:497:VAL:HG22	2.13	0.48
1:O:17:ASN:C	1:O:17:ASN:HD22	2.21	0.48
1:P:471:GLN:O	1:P:497:VAL:HG22	2.13	0.48
1:R:90:ARG:HD3	1:R:174:ARG:O	2.13	0.48
1:T:90:ARG:HD3	1:T:174:ARG:O	2.14	0.48
1:U:17:ASN:HD22	1:U:17:ASN:C	2.21	0.48
1:U:310:ARG:CB	1:W:297:GLN:HB2	2.42	0.48
1:W:482:ASP:H	1:W:490:ASN:HD21	1.61	0.48
1:B:283:SER:CB	1:C:3:LEU:CD2	2.91	0.48
1:B:297:GLN:OE1	1:C:310:ARG:NH2	2.45	0.48
1:C:270:PRO:HG2	1:C:273:LYS:HD2	1.92	0.48
1:C:270:PRO:HD2	1:C:273:LYS:HD3	1.95	0.48
1:E:17:ASN:HD22	1:E:17:ASN:C	2.21	0.48
1:H:482:ASP:H	1:H:490:ASN:HD21	1.61	0.48
1:J:90:ARG:HD3	1:J:174:ARG:O	2.13	0.48
1:K:472:THR:CG2	1:K:498:GLU:HA	2.18	0.48
1:L:90:ARG:HD3	1:L:174:ARG:O	2.13	0.48
1:L:272:GLU:HB2	1:N:352:GLU:HG2	1.94	0.48
1:L:352:GLU:HG2	1:N:272:GLU:C	2.38	0.48
1:P:89:ILE:HG21	1:P:177:VAL:HG22	1.96	0.48
1:P:90:ARG:HD3	1:P:174:ARG:O	2.14	0.48
1:R:12:PHE:CD2	1:R:12:PHE:N	2.79	0.48
1:S:90:ARG:HD3	1:S:174:ARG:O	2.13	0.48
1:V:284:LYS:HG3	1:X:7:LEU:HD23	1.80	0.48
1:A:482:ASP:H	1:A:490:ASN:HD21	1.61	0.48
1:B:272:GLU:HG3	1:C:352:GLU:CG	2.43	0.48
1:E:471:GLN:O	1:E:497:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:482:ASP:H	1:E:490:ASN:HD21	1.61	0.48
1:F:17:ASN:C	1:F:17:ASN:HD22	2.21	0.48
1:H:471:GLN:O	1:H:497:VAL:HG22	2.13	0.48
1:I:89:ILE:HG21	1:I:177:VAL:HG22	1.96	0.48
1:I:90:ARG:HD3	1:I:174:ARG:O	2.13	0.48
1:K:89:ILE:HG21	1:K:177:VAL:HG22	1.96	0.48
1:M:89:ILE:HG21	1:M:177:VAL:HG22	1.96	0.48
1:O:51:ASN:HA	1:O:83:ASP:HB3	1.94	0.48
1:O:90:ARG:HD3	1:O:174:ARG:O	2.13	0.48
1:Q:3:LEU:CD2	1:S:283:SER:CB	2.91	0.48
1:Q:17:ASN:C	1:Q:17:ASN:HD22	2.21	0.48
1:U:90:ARG:HD3	1:U:174:ARG:O	2.13	0.48
1:D:19:ARG:NH1	1:D:21:ALA:O	2.46	0.48
1:F:90:ARG:HD3	1:F:174:ARG:O	2.13	0.48
1:H:90:ARG:HD3	1:H:174:ARG:O	2.13	0.48
1:H:372:ILE:HD11	1:I:390:GLU:HG2	1.94	0.48
1:K:471:GLN:O	1:K:497:VAL:HG22	2.13	0.48
1:M:17:ASN:HD22	1:M:17:ASN:C	2.21	0.48
1:M:90:ARG:HD3	1:M:174:ARG:O	2.13	0.48
1:R:273:LYS:CB	1:T:11:ILE:HB	2.43	0.48
1:T:19:ARG:NH1	1:T:21:ALA:O	2.46	0.48
1:T:51:ASN:HA	1:T:83:ASP:HB3	1.94	0.48
1:U:11:ILE:HB	1:W:273:LYS:HB3	1.93	0.48
1:U:19:ARG:NH1	1:U:21:ALA:O	2.46	0.48
1:V:284:LYS:HE2	1:X:7:LEU:HD22	1.95	0.48
1:W:17:ASN:C	1:W:17:ASN:HD22	2.21	0.48
1:A:89:ILE:HG21	1:A:177:VAL:HG22	1.96	0.48
1:B:456:ARG:NH1	2:B:700:FDP:O2P	2.34	0.48
1:D:212:PHE:HD2	1:D:214:ARG:HH21	1.62	0.48
1:J:51:ASN:HA	1:J:83:ASP:HB3	1.94	0.48
1:Q:270:PRO:HD2	1:Q:273:LYS:HD3	1.95	0.48
1:R:272:GLU:HG2	1:T:352:GLU:CD	2.39	0.48
1:R:482:ASP:H	1:R:490:ASN:HD21	1.61	0.48
1:U:311:ALA:HB3	1:W:312:GLU:HG3	1.95	0.48
1:V:89:ILE:HG21	1:V:177:VAL:HG22	1.96	0.48
1:W:193:ASP:CA	1:W:196:ASP:HB2	2.42	0.48
1:X:90:ARG:HD3	1:X:174:ARG:O	2.13	0.48
1:A:90:ARG:HD3	1:A:174:ARG:O	2.14	0.48
1:D:242:HIS:CE1	1:F:12:PHE:CE2	3.02	0.48
1:F:472:THR:CG2	1:F:498:GLU:HA	2.18	0.48
1:H:272:GLU:HG3	1:J:352:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:483:HIS:CD2	1:I:483:HIS:CD2	3.01	0.48
1:J:19:ARG:NH1	1:J:21:ALA:O	2.46	0.48
1:L:19:ARG:NH1	1:L:21:ALA:O	2.46	0.48
1:M:51:ASN:HA	1:M:83:ASP:HB3	1.94	0.48
1:M:376:ALA:HA	1:N:494:ILE:HD12	1.96	0.48
1:Q:482:ASP:H	1:Q:490:ASN:HD21	1.61	0.48
1:S:17:ASN:HD22	1:S:17:ASN:C	2.21	0.48
1:U:297:GLN:HB3	1:W:310:ARG:H	1.77	0.48
1:W:90:ARG:HD3	1:W:174:ARG:O	2.13	0.48
1:C:390:GLU:O	1:P:372:ILE:HG13	2.14	0.48
1:E:90:ARG:HD3	1:E:174:ARG:O	2.13	0.48
1:E:212:PHE:HD2	1:E:214:ARG:HH21	1.62	0.48
1:F:89:ILE:HG21	1:F:177:VAL:HG22	1.96	0.48
1:G:193:ASP:CA	1:G:196:ASP:HB2	2.41	0.48
1:H:89:ILE:HG21	1:H:177:VAL:HG22	1.96	0.48
1:I:195:VAL:CG2	1:N:496:LEU:HG	2.43	0.48
1:Q:212:PHE:HD2	1:Q:214:ARG:HH21	1.62	0.48
1:Q:276:VAL:CG1	1:S:9:LEU:HB3	2.43	0.48
1:Q:379:ALA:CB	1:R:390:GLU:OE1	2.62	0.48
1:T:17:ASN:C	1:T:17:ASN:HD22	2.21	0.48
1:V:9:LEU:CB	1:X:280:ILE:HD11	2.42	0.48
1:V:279:LYS:HB3	1:X:6:ASN:OD1	2.13	0.48
1:W:372:ILE:HD11	1:X:390:GLU:HG2	1.96	0.48
1:B:402:THR:OG1	1:B:404:ARG:HB2	2.14	0.48
1:D:471:GLN:O	1:D:497:VAL:HG22	2.13	0.48
1:I:193:ASP:CA	1:I:196:ASP:HB2	2.41	0.48
1:K:272:GLU:CG	1:M:352:GLU:HG2	2.44	0.48
1:M:49:ARG:NE	1:M:83:ASP:OD2	2.33	0.48
1:M:373:PRO:CA	1:N:390:GLU:O	2.46	0.48
1:N:90:ARG:HD3	1:N:174:ARG:O	2.13	0.48
1:Q:193:ASP:O	1:Q:196:ASP:HB2	2.14	0.48
1:R:51:ASN:HA	1:R:83:ASP:HB3	1.94	0.48
1:S:372:ILE:CG1	1:T:390:GLU:CG	2.91	0.48
1:U:89:ILE:HG21	1:U:177:VAL:HG22	1.96	0.48
1:V:212:PHE:HD2	1:V:214:ARG:HH21	1.62	0.48
1:W:471:GLN:O	1:W:497:VAL:HG22	2.13	0.48
1:X:212:PHE:HD2	1:X:214:ARG:HH21	1.62	0.48
1:X:471:GLN:O	1:X:497:VAL:HG22	2.13	0.48
1:B:17:ASN:HD22	1:B:17:ASN:C	2.21	0.48
1:E:402:THR:OG1	1:E:404:ARG:HB2	2.14	0.48
1:F:270:PRO:O	1:F:273:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:GLU:HG2	1:G:372:ILE:HD11	1.94	0.48
1:G:193:ASP:O	1:G:196:ASP:HB2	2.14	0.48
1:I:402:THR:OG1	1:I:404:ARG:HB2	2.14	0.48
1:J:402:THR:OG1	1:J:404:ARG:HB2	2.14	0.48
1:J:482:ASP:H	1:J:490:ASN:HD21	1.61	0.48
1:M:212:PHE:HD2	1:M:214:ARG:HH21	1.62	0.48
1:O:49:ARG:NE	1:O:83:ASP:OD2	2.33	0.48
1:P:270:PRO:O	1:P:273:LYS:HB2	2.14	0.48
1:Q:311:ALA:CB	1:S:312:GLU:HA	2.43	0.48
1:T:49:ARG:NE	1:T:83:ASP:OD2	2.33	0.48
1:T:89:ILE:HG21	1:T:177:VAL:HG22	1.96	0.48
1:V:12:PHE:CD2	1:V:12:PHE:N	2.79	0.48
1:V:402:THR:OG1	1:V:404:ARG:HB2	2.14	0.48
1:X:19:ARG:NH1	1:X:21:ALA:O	2.46	0.48
1:G:212:PHE:HD2	1:G:214:ARG:HH21	1.62	0.48
1:I:471:GLN:O	1:I:497:VAL:HG22	2.13	0.48
1:J:212:PHE:HD2	1:J:214:ARG:HH21	1.62	0.48
1:K:19:ARG:NH1	1:K:21:ALA:O	2.46	0.48
1:M:193:ASP:O	1:M:196:ASP:HB2	2.14	0.48
1:N:471:GLN:O	1:N:497:VAL:HG22	2.13	0.48
1:O:193:ASP:O	1:O:196:ASP:HB2	2.14	0.48
1:P:51:ASN:HA	1:P:83:ASP:HB3	1.94	0.48
1:P:402:THR:OG1	1:P:404:ARG:HB2	2.14	0.48
1:R:19:ARG:NH1	1:R:21:ALA:O	2.46	0.48
1:S:193:ASP:O	1:S:196:ASP:HB2	2.14	0.48
1:D:270:PRO:HD2	1:D:273:LYS:HD3	1.95	0.47
1:D:402:THR:OG1	1:D:404:ARG:HB2	2.14	0.47
1:E:89:ILE:HG21	1:E:177:VAL:HG22	1.96	0.47
1:H:311:ALA:O	1:J:311:ALA:O	2.31	0.47
1:I:11:ILE:HG12	1:I:12:PHE:CD2	2.47	0.47
1:I:17:ASN:C	1:I:17:ASN:HD22	2.21	0.47
1:J:193:ASP:O	1:J:196:ASP:HB2	2.14	0.47
1:J:270:PRO:O	1:J:273:LYS:HB2	2.14	0.47
1:L:273:LYS:HG2	1:N:11:ILE:CA	2.44	0.47
1:L:279:LYS:HB3	1:N:6:ASN:CG	2.39	0.47
1:L:372:ILE:HD12	1:L:374:MET:HG3	1.96	0.47
1:N:17:ASN:C	1:N:17:ASN:HD22	2.21	0.47
1:O:89:ILE:HG21	1:O:177:VAL:HG22	1.96	0.47
1:Q:19:ARG:NH1	1:Q:21:ALA:O	2.46	0.47
1:Q:402:THR:OG1	1:Q:404:ARG:HB2	2.14	0.47
1:S:19:ARG:NH1	1:S:21:ALA:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:402:THR:OG1	1:S:404:ARG:HB2	2.14	0.47
1:V:90:ARG:HD3	1:V:174:ARG:O	2.13	0.47
1:X:89:ILE:HG21	1:X:177:VAL:HG22	1.96	0.47
1:X:193:ASP:O	1:X:196:ASP:HB2	2.14	0.47
1:X:402:THR:OG1	1:X:404:ARG:HB2	2.14	0.47
1:B:89:ILE:HG21	1:B:177:VAL:HG22	1.96	0.47
1:C:49:ARG:NE	1:C:83:ASP:OD2	2.33	0.47
1:G:17:ASN:C	1:G:17:ASN:HD22	2.21	0.47
1:N:89:ILE:HG21	1:N:177:VAL:HG22	1.95	0.47
1:R:471:GLN:O	1:R:497:VAL:HG22	2.13	0.47
1:S:384:ALA:O	1:S:387:SER:HB2	2.14	0.47
1:U:193:ASP:O	1:U:196:ASP:HB2	2.14	0.47
1:X:17:ASN:HD22	1:X:17:ASN:C	2.21	0.47
1:A:193:ASP:O	1:A:196:ASP:HB2	2.14	0.47
1:A:471:GLN:O	1:A:497:VAL:HG22	2.13	0.47
1:C:402:THR:OG1	1:C:404:ARG:HB2	2.14	0.47
1:D:472:THR:CG2	1:D:498:GLU:HA	2.18	0.47
1:K:193:ASP:CA	1:K:196:ASP:HB2	2.41	0.47
1:K:270:PRO:HD2	1:K:273:LYS:HD3	1.95	0.47
1:L:89:ILE:HG21	1:L:177:VAL:HG22	1.95	0.47
1:O:315:ASP:CB	1:P:311:ALA:HA	2.42	0.47
1:O:365:SER:CB	1:P:3:LEU:HD12	2.45	0.47
1:R:212:PHE:HD2	1:R:214:ARG:HH21	1.62	0.47
1:T:193:ASP:O	1:T:196:ASP:HB2	2.14	0.47
1:U:6:ASN:OD1	1:W:279:LYS:CE	2.51	0.47
1:C:193:ASP:O	1:C:196:ASP:HB2	2.14	0.47
1:C:390:GLU:C	1:P:372:ILE:HG13	2.39	0.47
1:D:384:ALA:O	1:D:387:SER:HB2	2.14	0.47
1:E:103:ARG:HG3	1:E:167:ASN:HA	1.97	0.47
1:H:270:PRO:HD2	1:H:273:LYS:HD3	1.95	0.47
1:I:193:ASP:O	1:I:196:ASP:HB2	2.14	0.47
1:I:482:ASP:H	1:I:490:ASN:HD21	1.61	0.47
1:P:384:ALA:O	1:P:387:SER:HB2	2.15	0.47
1:Q:49:ARG:NE	1:Q:83:ASP:OD2	2.33	0.47
1:R:11:ILE:HB	1:T:273:LYS:HG2	1.95	0.47
1:R:371:HIS:C	1:R:372:ILE:HD13	2.39	0.47
1:T:212:PHE:HD2	1:T:214:ARG:HH21	1.62	0.47
1:T:402:THR:OG1	1:T:404:ARG:HB2	2.14	0.47
1:W:19:ARG:NH1	1:W:21:ALA:O	2.46	0.47
1:X:482:ASP:H	1:X:490:ASN:HD21	1.61	0.47
1:C:90:ARG:HD3	1:C:174:ARG:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASP:CA	1:C:196:ASP:HB2	2.41	0.47
1:C:496:LEU:CG	1:V:195:VAL:CG2	2.80	0.47
1:D:456:ARG:NH1	2:D:700:FDP:O2P	2.34	0.47
1:G:482:ASP:H	1:G:490:ASN:HD21	1.61	0.47
1:H:384:ALA:O	1:H:387:SER:HB2	2.14	0.47
1:J:384:ALA:O	1:J:387:SER:HB2	2.14	0.47
1:O:19:ARG:NH1	1:O:21:ALA:O	2.46	0.47
1:O:310:ARG:NH2	1:P:297:GLN:OE1	2.47	0.47
1:Q:90:ARG:HD3	1:Q:174:ARG:O	2.14	0.47
1:R:17:ASN:C	1:R:17:ASN:HD22	2.21	0.47
1:U:6:ASN:CG	1:W:279:LYS:HE3	2.36	0.47
1:V:193:ASP:O	1:V:196:ASP:HB2	2.14	0.47
1:X:193:ASP:CA	1:X:196:ASP:HB2	2.41	0.47
1:X:384:ALA:O	1:X:387:SER:HB2	2.14	0.47
1:C:384:ALA:O	1:C:387:SER:HB2	2.14	0.47
1:D:89:ILE:HG21	1:D:177:VAL:HG22	1.96	0.47
1:D:90:ARG:HD3	1:D:174:ARG:O	2.13	0.47
1:F:193:ASP:O	1:F:196:ASP:HB2	2.14	0.47
1:K:482:ASP:H	1:K:490:ASN:HD21	1.61	0.47
1:L:384:ALA:O	1:L:387:SER:HB2	2.14	0.47
1:M:193:ASP:CA	1:M:196:ASP:HB2	2.41	0.47
1:N:193:ASP:O	1:N:196:ASP:HB2	2.14	0.47
1:N:224:LYS:HB3	1:N:224:LYS:HE3	1.81	0.47
1:O:270:PRO:CG	1:O:273:LYS:HD2	2.45	0.47
1:O:310:ARG:HG2	1:P:297:GLN:CB	2.42	0.47
1:P:19:ARG:NH1	1:P:21:ALA:O	2.46	0.47
1:P:212:PHE:HD2	1:P:214:ARG:HH21	1.62	0.47
1:S:89:ILE:HG21	1:S:177:VAL:HG22	1.96	0.47
1:U:270:PRO:HD2	1:U:273:LYS:HD3	1.95	0.47
1:C:250:SER:HB2	1:N:446:LYS:CD	2.37	0.47
1:D:193:ASP:O	1:D:196:ASP:HB2	2.14	0.47
1:F:384:ALA:O	1:F:387:SER:HB2	2.14	0.47
1:G:89:ILE:HG21	1:G:177:VAL:HG22	1.96	0.47
1:G:384:ALA:O	1:G:387:SER:HB2	2.15	0.47
1:G:402:THR:OG1	1:G:404:ARG:HB2	2.15	0.47
1:H:193:ASP:O	1:H:196:ASP:HB2	2.14	0.47
1:H:270:PRO:CG	1:H:273:LYS:HD2	2.45	0.47
1:I:384:ALA:O	1:I:387:SER:HB2	2.14	0.47
1:J:89:ILE:HG21	1:J:177:VAL:HG22	1.96	0.47
1:K:193:ASP:O	1:K:196:ASP:HB2	2.14	0.47
1:K:193:ASP:O	1:K:197:LEU:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:12:PHE:CD2	1:L:12:PHE:N	2.79	0.47
1:L:193:ASP:CA	1:L:196:ASP:HB2	2.41	0.47
1:N:402:THR:OG1	1:N:404:ARG:HB2	2.14	0.47
1:O:212:PHE:HD2	1:O:214:ARG:HH21	1.62	0.47
1:O:365:SER:HB3	1:P:3:LEU:HD12	1.95	0.47
1:O:384:ALA:O	1:O:387:SER:HB2	2.14	0.47
1:O:482:ASP:H	1:O:490:ASN:HD21	1.61	0.47
1:Q:284:LYS:CG	1:S:7:LEU:CD2	2.90	0.47
1:Q:297:GLN:HB2	1:S:310:ARG:HG2	1.95	0.47
1:S:493:ARG:HG2	1:T:482:ASP:OD2	2.15	0.47
1:U:212:PHE:HD2	1:U:214:ARG:HH21	1.62	0.47
1:U:310:ARG:HB2	1:W:297:GLN:HB2	1.97	0.47
1:U:372:ILE:HD12	1:U:374:MET:HG2	1.97	0.47
1:W:89:ILE:HG21	1:W:177:VAL:HG22	1.96	0.47
1:W:212:PHE:HD2	1:W:214:ARG:HH21	1.62	0.47
1:W:384:ALA:O	1:W:387:SER:HB2	2.14	0.47
1:B:482:ASP:H	1:B:490:ASN:HD21	1.61	0.47
1:E:384:ALA:O	1:E:387:SER:HB2	2.14	0.47
1:F:402:THR:OG1	1:F:404:ARG:HB2	2.14	0.47
1:H:11:ILE:HG13	1:H:12:PHE:HD2	1.80	0.47
1:H:242:HIS:NE2	1:J:12:PHE:HE2	2.11	0.47
1:I:212:PHE:HD2	1:I:214:ARG:HH21	1.62	0.47
1:I:456:ARG:NH1	2:I:700:FDP:O2P	2.34	0.47
1:J:224:LYS:HB3	1:J:224:LYS:HE3	1.82	0.47
1:K:90:ARG:HD3	1:K:174:ARG:O	2.13	0.47
1:M:270:PRO:O	1:M:273:LYS:HB2	2.14	0.47
1:P:49:ARG:NE	1:P:83:ASP:OD2	2.33	0.47
1:P:193:ASP:O	1:P:196:ASP:HB2	2.14	0.47
1:R:89:ILE:HG21	1:R:177:VAL:HG22	1.96	0.47
1:C:89:ILE:HG21	1:C:177:VAL:HG22	1.96	0.47
1:D:11:ILE:O	1:F:273:LYS:HE3	2.15	0.47
1:D:270:PRO:CG	1:D:273:LYS:HD2	2.45	0.47
1:E:193:ASP:O	1:E:196:ASP:HB2	2.14	0.47
1:F:212:PHE:HD2	1:F:214:ARG:HH21	1.62	0.47
1:H:193:ASP:CA	1:H:196:ASP:HB2	2.42	0.47
1:K:297:GLN:CB	1:M:310:ARG:HG2	2.44	0.47
1:N:19:ARG:NH1	1:N:21:ALA:O	2.46	0.47
1:Q:89:ILE:HG21	1:Q:177:VAL:HG22	1.96	0.47
1:U:384:ALA:O	1:U:387:SER:HB2	2.14	0.47
1:V:193:ASP:CA	1:V:196:ASP:HB2	2.41	0.47
1:V:370:GLN:CB	1:V:374:MET:SD	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PRO:CG	1:A:273:LYS:HD2	2.45	0.47
1:A:370:GLN:CB	1:A:374:MET:SD	3.03	0.47
1:B:270:PRO:CG	1:B:273:LYS:HD2	2.45	0.47
1:B:384:ALA:O	1:B:387:SER:HB2	2.14	0.47
1:D:373:PRO:HB3	1:E:391:THR:HA	1.97	0.47
1:I:19:ARG:NH1	1:I:21:ALA:O	2.46	0.47
1:L:212:PHE:HD2	1:L:214:ARG:HH21	1.62	0.47
1:L:231:ARG:HH21	1:S:231:ARG:HH21	1.62	0.47
1:L:273:LYS:HG2	1:N:11:ILE:HB	1.96	0.47
1:M:402:THR:OG1	1:M:404:ARG:HB2	2.14	0.47
1:N:384:ALA:O	1:N:387:SER:HB2	2.14	0.47
1:O:11:ILE:HB	1:P:273:LYS:CB	2.45	0.47
1:S:270:PRO:O	1:S:273:LYS:HB2	2.14	0.47
1:T:384:ALA:O	1:T:387:SER:HB2	2.14	0.47
1:W:193:ASP:O	1:W:196:ASP:HB2	2.14	0.47
1:A:283:SER:HB3	1:I:3:LEU:HD21	1.96	0.46
1:A:402:THR:OG1	1:A:404:ARG:HB2	2.14	0.46
1:B:193:ASP:O	1:B:196:ASP:HB2	2.14	0.46
1:B:193:ASP:CA	1:B:196:ASP:HB2	2.41	0.46
1:C:212:PHE:HD2	1:C:214:ARG:HH21	1.62	0.46
1:E:12:PHE:CD2	1:E:12:PHE:N	2.79	0.46
1:H:311:ALA:CB	1:J:312:GLU:HG2	2.44	0.46
1:P:482:ASP:H	1:P:490:ASN:HD21	1.61	0.46
1:U:193:ASP:CA	1:U:196:ASP:HB2	2.41	0.46
1:A:384:ALA:O	1:A:387:SER:HB2	2.14	0.46
1:B:311:ALA:HA	1:C:315:ASP:HB2	1.97	0.46
1:D:272:GLU:HG3	1:F:352:GLU:HB2	1.97	0.46
1:L:193:ASP:O	1:L:196:ASP:HB2	2.14	0.46
1:M:384:ALA:O	1:M:387:SER:HB2	2.14	0.46
1:O:424:ARG:CG	1:O:424:ARG:NH1	2.41	0.46
1:P:193:ASP:CA	1:P:196:ASP:HB2	2.42	0.46
1:Q:284:LYS:CG	1:S:7:LEU:HD22	2.46	0.46
1:T:372:ILE:HD12	1:T:374:MET:CG	2.46	0.46
1:V:384:ALA:O	1:V:387:SER:HB2	2.14	0.46
1:X:370:GLN:CB	1:X:374:MET:SD	3.03	0.46
1:A:273:LYS:NZ	1:I:352:GLU:OE1	2.48	0.46
1:A:369:LEU:CD1	1:I:3:LEU:HD13	2.45	0.46
1:C:270:PRO:CG	1:C:273:LYS:HD2	2.45	0.46
1:I:229:LYS:CG	1:M:487:GLY:HA3	2.25	0.46
1:K:372:ILE:HD12	1:K:374:MET:CG	2.46	0.46
1:Q:370:GLN:CB	1:Q:374:MET:SD	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:11:ILE:HG13	1:R:12:PHE:HD2	1.72	0.46
1:R:193:ASP:O	1:R:196:ASP:HB2	2.14	0.46
1:R:297:GLN:HE21	1:R:297:GLN:HB3	1.50	0.46
1:R:384:ALA:O	1:R:387:SER:HB2	2.15	0.46
1:W:270:PRO:O	1:W:273:LYS:HB2	2.14	0.46
1:B:276:VAL:CG1	1:C:9:LEU:HB3	2.45	0.46
1:B:370:GLN:CB	1:B:374:MET:SD	3.03	0.46
1:E:297:GLN:HB2	1:G:310:ARG:CG	2.46	0.46
1:E:370:GLN:CB	1:E:374:MET:SD	3.03	0.46
1:K:212:PHE:HD2	1:K:214:ARG:HH21	1.62	0.46
1:K:270:PRO:CG	1:K:273:LYS:HD2	2.45	0.46
1:K:384:ALA:O	1:K:387:SER:HB2	2.14	0.46
1:M:391:THR:HA	1:N:373:PRO:CB	2.45	0.46
1:O:311:ALA:HB3	1:P:312:GLU:HG3	1.97	0.46
1:P:371:HIS:C	1:P:372:ILE:HD13	2.40	0.46
1:Q:270:PRO:CG	1:Q:273:LYS:HD2	2.45	0.46
1:Q:384:ALA:O	1:Q:387:SER:HB2	2.14	0.46
1:X:372:ILE:HD12	1:X:374:MET:CG	2.46	0.46
1:B:212:PHE:HD2	1:B:214:ARG:HH21	1.62	0.46
1:E:19:ARG:NH1	1:E:21:ALA:O	2.46	0.46
1:H:372:ILE:HG13	1:I:390:GLU:O	2.15	0.46
1:J:372:ILE:HD12	1:J:374:MET:CG	2.46	0.46
1:N:193:ASP:CA	1:N:196:ASP:HB2	2.42	0.46
1:N:372:ILE:HD12	1:N:372:ILE:HA	1.73	0.46
1:O:370:GLN:CB	1:O:374:MET:SD	3.03	0.46
1:T:364:ASN:O	1:T:368:LYS:HG2	2.16	0.46
1:T:482:ASP:H	1:T:490:ASN:HD21	1.61	0.46
1:W:372:ILE:HD12	1:W:374:MET:CG	2.46	0.46
1:X:424:ARG:CG	1:X:424:ARG:NH1	2.41	0.46
1:C:391:THR:O	1:P:373:PRO:HB3	2.16	0.46
1:F:370:GLN:CB	1:F:374:MET:SD	3.03	0.46
1:L:273:LYS:HG2	1:N:11:ILE:HA	1.96	0.46
1:L:364:ASN:O	1:L:368:LYS:HG2	2.16	0.46
1:N:370:GLN:CB	1:N:374:MET:SD	3.03	0.46
1:O:297:GLN:OE1	1:P:310:ARG:NH2	2.49	0.46
1:O:402:THR:OG1	1:O:404:ARG:HB2	2.15	0.46
1:R:297:GLN:HB2	1:T:310:ARG:CB	2.36	0.46
1:U:270:PRO:CG	1:U:273:LYS:HD2	2.45	0.46
1:A:12:PHE:HE2	1:I:242:HIS:CE1	2.34	0.46
1:A:297:GLN:OE1	1:I:310:ARG:HG2	2.15	0.46
1:A:362:PHE:HD2	1:A:366:ILE:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASN:O	1:B:368:LYS:HG2	2.16	0.46
1:C:364:ASN:O	1:C:368:LYS:HG2	2.16	0.46
1:C:370:GLN:CB	1:C:374:MET:SD	3.03	0.46
1:D:370:GLN:CB	1:D:374:MET:SD	3.03	0.46
1:D:424:ARG:CG	1:D:424:ARG:NH1	2.41	0.46
1:F:19:ARG:NH1	1:F:21:ALA:O	2.46	0.46
1:F:372:ILE:HD12	1:F:374:MET:CG	2.46	0.46
1:G:372:ILE:HD12	1:G:374:MET:CG	2.46	0.46
1:H:390:GLU:O	1:I:373:PRO:CB	2.63	0.46
1:I:400:SER:OG	2:I:700:FDP:O4P	2.32	0.46
1:K:272:GLU:HG3	1:M:352:GLU:CB	2.43	0.46
1:L:276:VAL:CG1	1:N:9:LEU:CB	2.92	0.46
1:L:310:ARG:CZ	1:N:297:GLN:OE1	2.64	0.46
1:M:483:HIS:HD2	1:N:483:HIS:NE2	2.13	0.46
1:N:212:PHE:HD2	1:N:214:ARG:HH21	1.62	0.46
1:A:364:ASN:O	1:A:368:LYS:HG2	2.16	0.46
1:B:90:ARG:HD3	1:B:174:ARG:O	2.13	0.46
1:K:364:ASN:O	1:K:368:LYS:HG2	2.16	0.46
1:M:364:ASN:O	1:M:368:LYS:HG2	2.16	0.46
1:O:362:PHE:HD2	1:O:366:ILE:HD12	1.81	0.46
1:Q:472:THR:CG2	1:Q:498:GLU:HA	2.18	0.46
1:S:212:PHE:HD2	1:S:214:ARG:HH21	1.62	0.46
1:V:287:VAL:CG2	1:X:3:LEU:HD22	2.46	0.46
1:V:297:GLN:NE2	1:V:300:GLU:HB3	2.24	0.46
1:A:472:THR:CG2	1:A:498:GLU:HA	2.18	0.46
1:B:79:ALA:HB2	1:B:429:ARG:O	2.16	0.46
1:E:79:ALA:HB2	1:E:429:ARG:O	2.16	0.46
1:I:364:ASN:O	1:I:368:LYS:HG2	2.16	0.46
1:J:362:PHE:HD2	1:J:366:ILE:HD12	1.81	0.46
1:M:79:ALA:HB2	1:M:429:ARG:O	2.16	0.46
1:R:364:ASN:O	1:R:368:LYS:HG2	2.16	0.46
1:W:402:THR:OG1	1:W:404:ARG:HB2	2.16	0.46
1:A:224:LYS:HB3	1:A:224:LYS:HE3	1.82	0.46
1:C:362:PHE:HD2	1:C:366:ILE:HD12	1.81	0.46
1:E:11:ILE:HG12	1:E:12:PHE:CD2	2.47	0.46
1:H:212:PHE:HD2	1:H:214:ARG:HH21	1.62	0.46
1:Q:362:PHE:HD2	1:Q:366:ILE:HD12	1.81	0.46
1:W:370:GLN:CB	1:W:374:MET:SD	3.03	0.46
1:X:364:ASN:O	1:X:368:LYS:HG2	2.16	0.46
1:C:372:ILE:HD12	1:C:374:MET:CG	2.46	0.45
1:E:372:ILE:HD12	1:E:374:MET:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:373:PRO:CB	1:G:390:GLU:O	2.64	0.45
1:G:364:ASN:O	1:G:368:LYS:HG2	2.16	0.45
1:H:79:ALA:HB2	1:H:429:ARG:O	2.16	0.45
1:S:101:MET:HE1	1:S:124:PHE:CE1	2.52	0.45
1:S:362:PHE:HD2	1:S:366:ILE:HD12	1.81	0.45
1:S:364:ASN:O	1:S:368:LYS:HG2	2.16	0.45
1:V:79:ALA:HB2	1:V:429:ARG:O	2.16	0.45
1:A:212:PHE:HD2	1:A:214:ARG:HH21	1.62	0.45
1:A:372:ILE:HD12	1:A:374:MET:CG	2.46	0.45
1:B:224:LYS:HB3	1:B:224:LYS:HE3	1.82	0.45
1:D:101:MET:HE1	1:D:124:PHE:CE1	2.52	0.45
1:D:372:ILE:HD12	1:D:374:MET:CG	2.46	0.45
1:F:362:PHE:HD2	1:F:366:ILE:HD12	1.81	0.45
1:F:374:MET:HE2	1:G:390:GLU:HG2	1.98	0.45
1:G:370:GLN:CB	1:G:374:MET:SD	3.03	0.45
1:H:297:GLN:HG3	1:J:310:ARG:CG	2.43	0.45
1:H:352:GLU:OE1	1:J:272:GLU:HG2	2.16	0.45
1:H:364:ASN:O	1:H:368:LYS:HG2	2.16	0.45
1:H:376:ALA:HA	1:I:494:ILE:HD12	1.98	0.45
1:I:79:ALA:HB2	1:I:429:ARG:O	2.16	0.45
1:K:12:PHE:CE2	1:M:242:HIS:NE2	2.77	0.45
1:K:390:GLU:HG2	1:L:374:MET:CE	2.45	0.45
1:N:362:PHE:HD2	1:N:366:ILE:HD12	1.81	0.45
1:Q:456:ARG:NH1	2:Q:700:FDP:O2P	2.34	0.45
1:R:79:ALA:HB2	1:R:429:ARG:O	2.16	0.45
1:T:362:PHE:HD2	1:T:366:ILE:HD12	1.81	0.45
1:V:372:ILE:HD12	1:V:374:MET:CG	2.46	0.45
1:A:101:MET:HE1	1:A:124:PHE:CE1	2.52	0.45
1:C:168:SER:O	1:C:169:HIS:HB2	2.17	0.45
1:C:383:SER:CB	1:P:383:SER:HB2	2.45	0.45
1:D:364:ASN:O	1:D:368:LYS:HG2	2.16	0.45
1:E:193:ASP:CA	1:E:196:ASP:HB2	2.41	0.45
1:G:79:ALA:HB2	1:G:429:ARG:O	2.16	0.45
1:H:496:LEU:HD21	1:M:195:VAL:HG23	1.97	0.45
1:I:195:VAL:HG22	1:N:496:LEU:CD2	2.46	0.45
1:J:364:ASN:O	1:J:368:LYS:HG2	2.16	0.45
1:K:49:ARG:NE	1:K:83:ASP:OD2	2.33	0.45
1:N:79:ALA:HB2	1:N:429:ARG:O	2.16	0.45
1:N:101:MET:HE1	1:N:124:PHE:CE1	2.52	0.45
1:O:79:ALA:HB2	1:O:429:ARG:O	2.16	0.45
1:O:193:ASP:CA	1:O:196:ASP:HB2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:79:ALA:HB2	1:Q:429:ARG:O	2.16	0.45
1:Q:272:GLU:HG3	1:S:352:GLU:CG	2.45	0.45
1:S:168:SER:O	1:S:169:HIS:HB2	2.17	0.45
1:U:168:SER:O	1:U:169:HIS:HB2	2.17	0.45
1:B:280:ILE:CG1	1:C:6:ASN:O	2.64	0.45
1:G:193:ASP:O	1:G:197:LEU:N	2.38	0.45
1:J:101:MET:HE1	1:J:124:PHE:CE1	2.52	0.45
1:N:364:ASN:O	1:N:368:LYS:HG2	2.16	0.45
1:O:279:LYS:HE3	1:P:6:ASN:OD1	2.15	0.45
1:O:372:ILE:HD12	1:O:374:MET:CG	2.46	0.45
1:P:364:ASN:O	1:P:368:LYS:HG2	2.16	0.45
1:Q:372:ILE:HD12	1:Q:374:MET:CG	2.46	0.45
1:S:456:ARG:NH1	2:S:700:FDP:O2P	2.34	0.45
1:V:284:LYS:HG2	1:X:7:LEU:CD2	2.38	0.45
1:V:364:ASN:O	1:V:368:LYS:HG2	2.16	0.45
1:W:79:ALA:HB2	1:W:429:ARG:O	2.16	0.45
1:W:101:MET:HE1	1:W:124:PHE:CE1	2.52	0.45
1:D:79:ALA:HB2	1:D:429:ARG:O	2.16	0.45
1:D:272:GLU:CG	1:F:352:GLU:HG2	2.47	0.45
1:E:101:MET:HE1	1:E:124:PHE:CE1	2.52	0.45
1:F:79:ALA:HB2	1:F:429:ARG:O	2.16	0.45
1:F:101:MET:HE1	1:F:124:PHE:CE1	2.52	0.45
1:G:168:SER:O	1:G:169:HIS:HB2	2.17	0.45
1:H:311:ALA:CB	1:J:312:GLU:CA	2.72	0.45
1:J:370:GLN:CB	1:J:374:MET:SD	3.03	0.45
1:K:370:GLN:CB	1:K:374:MET:SD	3.03	0.45
1:M:101:MET:HE1	1:M:124:PHE:CE1	2.52	0.45
1:R:362:PHE:HD2	1:R:366:ILE:HD12	1.81	0.45
1:T:101:MET:HE1	1:T:124:PHE:CE1	2.52	0.45
1:U:193:ASP:O	1:U:197:LEU:N	2.38	0.45
1:A:79:ALA:HB2	1:A:429:ARG:O	2.16	0.45
1:C:494:ILE:HD12	1:P:376:ALA:HA	1.97	0.45
1:F:456:ARG:NH1	2:F:700:FDP:O2P	2.34	0.45
1:G:362:PHE:HD2	1:G:366:ILE:HD12	1.81	0.45
1:H:242:HIS:NE2	1:J:12:PHE:CE2	2.79	0.45
1:N:168:SER:O	1:N:169:HIS:HB2	2.17	0.45
1:N:372:ILE:HD12	1:N:374:MET:CG	2.46	0.45
1:O:11:ILE:O	1:P:273:LYS:CD	2.65	0.45
1:R:311:ALA:CB	1:T:315:ASP:HB2	2.46	0.45
1:U:364:ASN:O	1:U:368:LYS:HG2	2.16	0.45
1:W:362:PHE:HD2	1:W:366:ILE:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:401:ASN:N	2:X:700:FDP:O5P	2.50	0.45
1:B:168:SER:O	1:B:169:HIS:HB2	2.17	0.45
1:C:79:ALA:HB2	1:C:429:ARG:O	2.16	0.45
1:E:11:ILE:HG13	1:E:12:PHE:HD2	1.72	0.45
1:H:315:ASP:CB	1:J:311:ALA:CA	2.89	0.45
1:H:318:ASN:CG	1:J:318:ASN:ND2	2.75	0.45
1:I:168:SER:O	1:I:169:HIS:HB2	2.17	0.45
1:K:362:PHE:HD2	1:K:366:ILE:HD12	1.81	0.45
1:O:168:SER:O	1:O:169:HIS:HB2	2.17	0.45
1:A:223:ARG:HG2	1:A:223:ARG:NH1	2.25	0.45
1:C:101:MET:HE1	1:C:124:PHE:CE1	2.52	0.45
1:E:242:HIS:NE2	1:G:12:PHE:HE2	2.15	0.45
1:F:168:SER:O	1:F:169:HIS:HB2	2.17	0.45
1:J:79:ALA:HB2	1:J:429:ARG:O	2.16	0.45
1:P:362:PHE:HD2	1:P:366:ILE:HD12	1.81	0.45
1:R:101:MET:HE1	1:R:124:PHE:CE1	2.52	0.45
1:R:311:ALA:HB1	1:T:311:ALA:O	2.16	0.45
1:X:101:MET:HE1	1:X:124:PHE:CE1	2.52	0.45
1:C:178:ASN:OD1	1:C:268:GLU:OE2	2.35	0.45
1:G:101:MET:HE1	1:G:124:PHE:CE1	2.52	0.45
1:H:101:MET:HE1	1:H:124:PHE:CE1	2.52	0.45
1:H:270:PRO:CG	1:H:273:LYS:CD	2.94	0.45
1:K:101:MET:HE1	1:K:124:PHE:CE1	2.52	0.45
1:K:297:GLN:OE1	1:M:310:ARG:CZ	2.65	0.45
1:L:178:ASN:OD1	1:L:268:GLU:OE2	2.35	0.45
1:L:272:GLU:O	1:N:352:GLU:HG2	2.17	0.45
1:S:79:ALA:HB2	1:S:429:ARG:O	2.16	0.45
1:S:494:ILE:HD12	1:T:376:ALA:CB	2.44	0.45
1:U:188:ALA:CB	1:U:218:GLN:HG2	2.21	0.45
1:U:372:ILE:HD12	1:U:372:ILE:HA	1.78	0.45
1:V:9:LEU:HB2	1:X:280:ILE:CD1	2.42	0.45
1:V:273:LYS:CG	1:X:11:ILE:HB	2.47	0.45
1:W:364:ASN:O	1:W:368:LYS:HG2	2.16	0.45
1:X:178:ASN:OD1	1:X:268:GLU:OE2	2.35	0.45
1:F:364:ASN:O	1:F:368:LYS:HG2	2.16	0.45
1:F:372:ILE:HD12	1:F:372:ILE:HA	1.73	0.45
1:H:9:LEU:CB	1:J:276:VAL:HG13	2.46	0.45
1:H:372:ILE:HG23	1:I:390:GLU:C	2.37	0.45
1:O:101:MET:HE1	1:O:124:PHE:CE1	2.52	0.45
1:P:178:ASN:OD1	1:P:268:GLU:OE2	2.35	0.45
1:Q:11:ILE:CB	1:S:273:LYS:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:101:MET:HE1	1:U:124:PHE:CE1	2.52	0.45
1:V:101:MET:HE1	1:V:124:PHE:CE1	2.52	0.45
1:W:168:SER:O	1:W:169:HIS:HB2	2.17	0.45
1:B:362:PHE:HD2	1:B:366:ILE:HD12	1.81	0.44
1:D:224:LYS:HB3	1:D:224:LYS:HE3	1.82	0.44
1:E:364:ASN:O	1:E:368:LYS:HG2	2.16	0.44
1:H:311:ALA:HB3	1:J:312:GLU:HG2	1.98	0.44
1:I:178:ASN:OD1	1:I:268:GLU:OE2	2.35	0.44
1:I:362:PHE:HD2	1:I:366:ILE:HD12	1.81	0.44
1:N:178:ASN:OD1	1:N:268:GLU:OE2	2.35	0.44
1:P:487:GLY:N	1:V:229:LYS:HE3	2.29	0.44
1:Q:352:GLU:HG2	1:S:272:GLU:O	2.16	0.44
1:U:372:ILE:CG1	1:V:390:GLU:O	2.65	0.44
1:C:270:PRO:CG	1:C:273:LYS:CD	2.94	0.44
1:D:178:ASN:OD1	1:D:268:GLU:OE2	2.35	0.44
1:E:283:SER:OG	1:G:3:LEU:CD2	2.64	0.44
1:G:372:ILE:HD12	1:G:372:ILE:HA	1.73	0.44
1:H:362:PHE:HD2	1:H:366:ILE:HD12	1.81	0.44
1:M:472:THR:CG2	1:M:498:GLU:HA	2.18	0.44
1:Q:101:MET:HE1	1:Q:124:PHE:CE1	2.52	0.44
1:Q:178:ASN:OD1	1:Q:268:GLU:OE2	2.35	0.44
1:S:193:ASP:CA	1:S:196:ASP:HB2	2.42	0.44
1:T:188:ALA:CB	1:T:218:GLN:HG2	2.21	0.44
1:U:491:GLN:OE1	1:U:493:ARG:HD2	2.18	0.44
1:B:311:ALA:HA	1:C:315:ASP:CG	2.43	0.44
1:B:372:ILE:HD12	1:B:374:MET:CG	2.46	0.44
1:F:178:ASN:OD1	1:F:268:GLU:OE2	2.35	0.44
1:I:101:MET:HE1	1:I:124:PHE:CE1	2.52	0.44
1:J:491:GLN:OE1	1:J:493:ARG:HD2	2.18	0.44
1:K:491:GLN:OE1	1:K:493:ARG:HD2	2.18	0.44
1:M:483:HIS:CD2	1:N:483:HIS:NE2	2.85	0.44
1:O:178:ASN:OD1	1:O:268:GLU:OE2	2.35	0.44
1:Q:270:PRO:CG	1:Q:273:LYS:CD	2.94	0.44
1:S:376:ALA:HB1	1:T:494:ILE:HB	1.99	0.44
1:T:168:SER:O	1:T:169:HIS:HB2	2.17	0.44
1:X:79:ALA:HB2	1:X:429:ARG:O	2.16	0.44
1:X:362:PHE:HD2	1:X:366:ILE:HD12	1.81	0.44
1:B:178:ASN:OD1	1:B:268:GLU:OE2	2.35	0.44
1:K:79:ALA:HB2	1:K:429:ARG:O	2.17	0.44
1:M:168:SER:O	1:M:169:HIS:HB2	2.17	0.44
1:M:373:PRO:HB3	1:N:391:THR:CA	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:398:VAL:HG13	1:O:479:ILE:HB	2.00	0.44
1:P:101:MET:HE1	1:P:124:PHE:CE1	2.52	0.44
1:P:168:SER:O	1:P:169:HIS:HB2	2.17	0.44
1:R:284:LYS:CG	1:T:7:LEU:HD21	2.38	0.44
1:T:178:ASN:OD1	1:T:268:GLU:OE2	2.35	0.44
1:U:362:PHE:HD2	1:U:366:ILE:HD12	1.81	0.44
1:V:178:ASN:OD1	1:V:268:GLU:OE2	2.35	0.44
1:B:280:ILE:HD11	1:C:9:LEU:HB2	1.99	0.44
1:J:178:ASN:OD1	1:J:268:GLU:OE2	2.35	0.44
1:L:3:LEU:HD23	1:N:283:SER:HB3	1.98	0.44
1:L:491:GLN:OE1	1:L:493:ARG:HD2	2.18	0.44
1:M:483:HIS:NE2	1:N:483:HIS:CD2	2.86	0.44
1:N:451:GLU:H	1:N:451:GLU:HG2	1.59	0.44
1:O:6:ASN:OD1	1:P:279:LYS:CE	2.54	0.44
1:P:224:LYS:HB3	1:P:224:LYS:HE3	1.82	0.44
1:R:491:GLN:OE1	1:R:493:ARG:HD2	2.18	0.44
1:U:11:ILE:HG13	1:W:273:LYS:HD3	1.99	0.44
1:U:79:ALA:HB2	1:U:429:ARG:O	2.16	0.44
1:V:362:PHE:HD2	1:V:366:ILE:HD12	1.81	0.44
1:V:491:GLN:OE1	1:V:493:ARG:HD2	2.18	0.44
1:A:168:SER:O	1:A:169:HIS:HB2	2.17	0.44
1:A:178:ASN:OD1	1:A:268:GLU:OE2	2.35	0.44
1:B:101:MET:HE1	1:B:124:PHE:CE1	2.52	0.44
1:B:398:VAL:HG13	1:B:479:ILE:HB	2.00	0.44
1:D:491:GLN:HG3	1:E:491:GLN:HG3	1.99	0.44
1:E:491:GLN:OE1	1:E:493:ARG:HD2	2.18	0.44
1:J:168:SER:O	1:J:169:HIS:HB2	2.17	0.44
1:L:79:ALA:HB2	1:L:429:ARG:O	2.16	0.44
1:O:352:GLU:HB2	1:P:272:GLU:HG3	1.99	0.44
1:P:79:ALA:HB2	1:P:429:ARG:O	2.16	0.44
1:Q:383:SER:CB	1:R:383:SER:HB2	2.46	0.44
1:U:372:ILE:HD12	1:U:374:MET:HG3	1.99	0.44
1:V:372:ILE:HD12	1:V:372:ILE:HA	1.73	0.44
1:X:372:ILE:HD12	1:X:372:ILE:HA	1.73	0.44
1:X:491:GLN:OE1	1:X:493:ARG:HD2	2.18	0.44
1:D:362:PHE:HD2	1:D:366:ILE:HD12	1.81	0.44
1:D:398:VAL:HG13	1:D:479:ILE:HB	2.00	0.44
1:E:398:VAL:HG13	1:E:479:ILE:HB	2.00	0.44
1:H:491:GLN:OE1	1:H:493:ARG:HD2	2.18	0.44
1:K:168:SER:O	1:K:169:HIS:HB2	2.17	0.44
1:L:401:ASN:N	2:L:700:FDP:O5P	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:364:ASN:O	1:O:368:LYS:HG2	2.16	0.44
1:P:424:ARG:CG	1:P:424:ARG:NH1	2.41	0.44
1:Q:297:GLN:HB2	1:S:310:ARG:HB2	2.00	0.44
1:Q:364:ASN:O	1:Q:368:LYS:HG2	2.16	0.44
1:T:3:LEU:HD23	1:T:4:ALA:N	2.24	0.44
1:T:79:ALA:HB2	1:T:429:ARG:O	2.16	0.44
1:T:491:GLN:OE1	1:T:493:ARG:HD2	2.18	0.44
1:V:168:SER:O	1:V:169:HIS:HB2	2.17	0.44
1:W:178:ASN:OD1	1:W:268:GLU:OE2	2.35	0.44
1:W:398:VAL:HG13	1:W:479:ILE:HB	2.00	0.44
1:E:362:PHE:HD2	1:E:366:ILE:HD12	1.81	0.44
1:H:312:GLU:CG	1:J:311:ALA:HB3	2.48	0.44
1:J:398:VAL:HG13	1:J:479:ILE:HB	2.00	0.44
1:O:401:ASN:N	2:O:700:FDP:O5P	2.50	0.44
1:Q:451:GLU:H	1:Q:451:GLU:HG2	1.59	0.44
1:Q:491:GLN:OE1	1:Q:493:ARG:HD2	2.18	0.44
1:W:49:ARG:NE	1:W:83:ASP:OD2	2.33	0.44
1:X:168:SER:O	1:X:169:HIS:HB2	2.17	0.44
1:C:483:HIS:CD2	1:P:483:HIS:CD2	3.06	0.44
1:C:491:GLN:OE1	1:C:493:ARG:HD2	2.18	0.44
1:D:6:ASN:OD1	1:F:279:LYS:HE3	2.17	0.44
1:D:491:GLN:OE1	1:D:493:ARG:HD2	2.18	0.44
1:H:398:VAL:HG13	1:H:479:ILE:HB	2.00	0.44
1:K:178:ASN:OD1	1:K:268:GLU:OE2	2.35	0.44
1:L:101:MET:HE1	1:L:124:PHE:CE1	2.52	0.44
1:M:362:PHE:HD2	1:M:366:ILE:HD12	1.81	0.44
1:M:491:GLN:OE1	1:M:493:ARG:HD2	2.18	0.44
1:W:401:ASN:N	2:W:700:FDP:O5P	2.50	0.44
1:B:491:GLN:OE1	1:B:493:ARG:HD2	2.18	0.43
1:D:168:SER:O	1:D:169:HIS:HB2	2.17	0.43
1:D:242:HIS:HE1	1:F:12:PHE:CE2	2.36	0.43
1:G:178:ASN:OD1	1:G:268:GLU:OE2	2.35	0.43
1:H:178:ASN:OD1	1:H:268:GLU:OE2	2.35	0.43
1:K:270:PRO:CG	1:K:273:LYS:CD	2.94	0.43
1:R:178:ASN:OD1	1:R:268:GLU:OE2	2.35	0.43
1:R:193:ASP:CA	1:R:196:ASP:HB2	2.41	0.43
1:R:371:HIS:CD2	1:R:373:PRO:O	2.71	0.43
1:S:178:ASN:OD1	1:S:268:GLU:OE2	2.35	0.43
1:X:398:VAL:HG13	1:X:479:ILE:HB	2.00	0.43
1:A:369:LEU:HD12	1:I:3:LEU:HD13	2.00	0.43
1:E:310:ARG:HG2	1:G:297:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:398:VAL:HG13	1:G:479:ILE:HB	2.00	0.43
1:G:491:GLN:OE1	1:G:493:ARG:HD2	2.18	0.43
1:H:168:SER:O	1:H:169:HIS:HB2	2.17	0.43
1:K:372:ILE:HA	1:K:373:PRO:C	2.44	0.43
1:L:362:PHE:HD2	1:L:366:ILE:HD12	1.81	0.43
1:O:315:ASP:CG	1:P:311:ALA:HA	2.42	0.43
1:O:372:ILE:HD12	1:O:372:ILE:HA	1.73	0.43
1:R:168:SER:O	1:R:169:HIS:HB2	2.17	0.43
1:W:491:GLN:OE1	1:W:493:ARG:HD2	2.18	0.43
1:A:372:ILE:HD12	1:A:372:ILE:HA	1.73	0.43
1:A:398:VAL:HG13	1:A:479:ILE:HB	2.00	0.43
1:D:273:LYS:HG2	1:F:11:ILE:HB	1.99	0.43
1:E:311:ALA:CB	1:G:312:GLU:HA	2.47	0.43
1:M:373:PRO:HB3	1:N:391:THR:C	2.42	0.43
1:P:491:GLN:OE1	1:P:493:ARG:HD2	2.18	0.43
1:U:371:HIS:C	1:U:372:ILE:HD13	2.43	0.43
1:A:270:PRO:CG	1:A:273:LYS:CD	2.94	0.43
1:B:3:LEU:HD13	1:C:369:LEU:CD1	2.48	0.43
1:B:372:ILE:HD12	1:B:372:ILE:HA	1.73	0.43
1:C:398:VAL:HG13	1:C:479:ILE:HB	2.00	0.43
1:E:272:GLU:CB	1:G:352:GLU:HG2	2.49	0.43
1:K:11:ILE:HB	1:M:273:LYS:CG	2.43	0.43
1:M:178:ASN:OD1	1:M:268:GLU:OE2	2.35	0.43
1:N:398:VAL:HG13	1:N:479:ILE:HB	2.00	0.43
1:Q:224:LYS:HB3	1:Q:224:LYS:HE3	1.81	0.43
1:Q:398:VAL:HG13	1:Q:479:ILE:HB	2.00	0.43
1:R:402:THR:OG1	1:R:404:ARG:HB2	2.19	0.43
1:U:178:ASN:OD1	1:U:268:GLU:OE2	2.35	0.43
1:U:310:ARG:HG2	1:W:297:GLN:CD	2.42	0.43
1:A:491:GLN:OE1	1:A:493:ARG:HD2	2.18	0.43
1:B:272:GLU:O	1:C:352:GLU:CG	2.66	0.43
1:E:168:SER:O	1:E:169:HIS:HB2	2.17	0.43
1:H:371:HIS:CD2	1:H:371:HIS:C	2.95	0.43
1:I:491:GLN:OE1	1:I:493:ARG:HD2	2.18	0.43
1:L:168:SER:O	1:L:169:HIS:HB2	2.17	0.43
1:N:491:GLN:OE1	1:N:493:ARG:HD2	2.18	0.43
1:Q:168:SER:O	1:Q:169:HIS:HB2	2.17	0.43
1:R:276:VAL:CG1	1:T:9:LEU:HB2	2.45	0.43
1:V:273:LYS:HD3	1:X:11:ILE:HB	1.99	0.43
1:V:287:VAL:HG23	1:X:3:LEU:HD21	2.00	0.43
1:C:496:LEU:CD2	1:V:195:VAL:CG2	2.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:487:GLY:HA2	1:M:229:LYS:CD	2.42	0.43
1:O:451:GLU:H	1:O:451:GLU:HG2	1.59	0.43
1:O:491:GLN:OE1	1:O:493:ARG:HD2	2.18	0.43
1:R:280:ILE:HD11	1:T:9:LEU:CB	2.40	0.43
1:R:398:VAL:HG13	1:R:479:ILE:HB	2.00	0.43
1:R:424:ARG:NH1	1:R:424:ARG:CG	2.41	0.43
1:S:398:VAL:HG13	1:S:479:ILE:HB	2.00	0.43
1:E:178:ASN:OD1	1:E:268:GLU:OE2	2.35	0.43
1:F:398:VAL:HG13	1:F:479:ILE:HB	2.00	0.43
1:I:224:LYS:HB3	1:I:224:LYS:HE3	1.81	0.43
1:L:398:VAL:HG13	1:L:479:ILE:HB	2.00	0.43
1:M:398:VAL:HG13	1:M:479:ILE:HB	2.00	0.43
1:O:429:ARG:O	1:O:432:ASN:HB2	2.19	0.43
1:U:402:THR:OG1	1:U:404:ARG:HB2	2.18	0.43
1:V:287:VAL:HG23	1:X:3:LEU:HD22	2.01	0.43
1:W:372:ILE:HA	1:W:373:PRO:C	2.44	0.43
1:B:372:ILE:HA	1:B:373:PRO:C	2.44	0.43
1:F:483:HIS:CD2	1:G:483:HIS:NE2	2.86	0.43
1:F:491:GLN:OE1	1:F:493:ARG:HD2	2.18	0.43
1:G:224:LYS:HB3	1:G:224:LYS:HE3	1.82	0.43
1:G:429:ARG:O	1:G:432:ASN:HB2	2.19	0.43
1:H:401:ASN:N	2:H:700:FDP:O5P	2.50	0.43
1:K:283:SER:HB3	1:M:3:LEU:CD2	2.49	0.43
1:R:272:GLU:CG	1:T:352:GLU:CD	2.92	0.43
1:T:398:VAL:HG13	1:T:479:ILE:HB	2.00	0.43
1:T:429:ARG:O	1:T:432:ASN:HB2	2.19	0.43
1:J:429:ARG:O	1:J:432:ASN:HB2	2.19	0.43
1:L:293:ILE:HG12	1:L:326:CYS:HB2	2.01	0.43
1:S:429:ARG:O	1:S:432:ASN:HB2	2.19	0.43
1:S:491:GLN:OE1	1:S:493:ARG:HD2	2.18	0.43
1:V:424:ARG:CG	1:V:424:ARG:NH1	2.41	0.43
1:W:293:ILE:HG12	1:W:326:CYS:HB2	2.01	0.43
1:C:373:PRO:HD3	1:P:392:LYS:HD2	2.01	0.43
1:C:429:ARG:O	1:C:432:ASN:HB2	2.19	0.43
1:D:188:ALA:CB	1:D:218:GLN:HG2	2.21	0.43
1:D:429:ARG:O	1:D:432:ASN:HB2	2.19	0.43
1:H:293:ILE:HG12	1:H:326:CYS:HB2	2.01	0.43
1:K:6:ASN:OD1	1:M:279:LYS:HE3	2.18	0.43
1:L:276:VAL:HG13	1:N:9:LEU:HD13	2.01	0.43
1:O:377:ASP:OD2	1:O:377:ASP:N	2.52	0.43
1:P:293:ILE:HG12	1:P:326:CYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:242:HIS:CE1	1:T:12:PHE:CE2	3.07	0.43
1:S:451:GLU:H	1:S:451:GLU:HG2	1.59	0.43
1:V:79:ALA:HA	1:V:429:ARG:HB3	2.01	0.43
1:V:272:GLU:CB	1:X:352:GLU:HG2	2.49	0.43
1:V:293:ILE:HG12	1:V:326:CYS:HB2	2.01	0.43
1:W:362:PHE:O	1:W:366:ILE:HD12	2.19	0.43
1:W:429:ARG:O	1:W:432:ASN:HB2	2.19	0.43
1:B:79:ALA:HA	1:B:429:ARG:HB3	2.01	0.42
1:E:377:ASP:OD2	1:E:377:ASP:N	2.52	0.42
1:F:362:PHE:O	1:F:366:ILE:HD12	2.19	0.42
1:H:498:GLU:HG2	1:M:195:VAL:HG11	2.01	0.42
1:J:372:ILE:HA	1:J:373:PRO:C	2.43	0.42
1:K:398:VAL:HG13	1:K:479:ILE:HB	2.00	0.42
1:M:390:GLU:HA	1:N:372:ILE:HG13	2.01	0.42
1:P:362:PHE:O	1:P:366:ILE:HD12	2.19	0.42
1:P:429:ARG:O	1:P:432:ASN:HB2	2.19	0.42
1:Q:297:GLN:OE1	1:S:310:ARG:CZ	2.67	0.42
1:U:138:GLY:HA2	1:U:151:GLN:HE21	1.84	0.42
1:U:279:LYS:HE3	1:W:6:ASN:OD1	2.19	0.42
1:U:398:VAL:HG13	1:U:479:ILE:HB	2.00	0.42
1:X:293:ILE:HG12	1:X:326:CYS:HB2	2.01	0.42
1:A:6:ASN:O	1:I:280:ILE:HG12	2.19	0.42
1:A:429:ARG:O	1:A:432:ASN:HB2	2.19	0.42
1:E:429:ARG:O	1:E:432:ASN:HB2	2.19	0.42
1:F:212:PHE:CD2	1:F:214:ARG:NE	2.88	0.42
1:G:79:ALA:HA	1:G:429:ARG:HB3	2.02	0.42
1:H:79:ALA:HA	1:H:429:ARG:HB3	2.01	0.42
1:H:138:GLY:HA2	1:H:151:GLN:HE21	1.85	0.42
1:H:312:GLU:HG3	1:J:311:ALA:HB3	2.00	0.42
1:H:451:GLU:H	1:H:451:GLU:HG2	1.59	0.42
1:H:496:LEU:HG	1:M:195:VAL:HG21	1.89	0.42
1:K:293:ILE:HG12	1:K:326:CYS:HB2	2.01	0.42
1:K:451:GLU:H	1:K:451:GLU:HG2	1.59	0.42
1:L:362:PHE:O	1:L:366:ILE:HD12	2.19	0.42
1:M:293:ILE:HG12	1:M:326:CYS:HB2	2.01	0.42
1:O:79:ALA:HA	1:O:429:ARG:HB3	2.01	0.42
1:P:138:GLY:HA2	1:P:151:GLN:HE21	1.84	0.42
1:S:293:ILE:HG12	1:S:326:CYS:HB2	2.01	0.42
1:T:224:LYS:HB3	1:T:224:LYS:HE3	1.81	0.42
1:T:474:ASP:O	1:T:497:VAL:HG13	2.20	0.42
1:U:293:ILE:HG12	1:U:326:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:451:GLU:H	1:U:451:GLU:HG2	1.59	0.42
1:W:79:ALA:HA	1:W:429:ARG:HB3	2.01	0.42
1:C:138:GLY:HA2	1:C:151:GLN:HE21	1.85	0.42
1:C:293:ILE:HG12	1:C:326:CYS:HB2	2.01	0.42
1:H:362:PHE:O	1:H:366:ILE:HD12	2.19	0.42
1:M:491:GLN:HG3	1:N:491:GLN:CG	2.47	0.42
1:N:293:ILE:HG12	1:N:326:CYS:HB2	2.01	0.42
1:N:362:PHE:O	1:N:366:ILE:HD12	2.19	0.42
1:P:398:VAL:HG13	1:P:479:ILE:HB	2.00	0.42
1:Q:242:HIS:NE2	1:S:12:PHE:CE2	2.85	0.42
1:Q:310:ARG:HG2	1:S:297:GLN:HB2	2.00	0.42
1:T:79:ALA:HA	1:T:429:ARG:HB3	2.01	0.42
1:T:212:PHE:CD2	1:T:214:ARG:NE	2.88	0.42
1:T:472:THR:CG2	1:T:498:GLU:CA	2.84	0.42
1:V:212:PHE:CD2	1:V:214:ARG:NE	2.88	0.42
1:V:429:ARG:O	1:V:432:ASN:HB2	2.19	0.42
1:B:352:GLU:HG2	1:C:272:GLU:O	2.18	0.42
1:C:372:ILE:HA	1:C:373:PRO:C	2.44	0.42
1:C:377:ASP:OD2	1:C:377:ASP:N	2.52	0.42
1:E:49:ARG:NE	1:E:83:ASP:OD2	2.33	0.42
1:E:293:ILE:HG12	1:E:326:CYS:HB2	2.01	0.42
1:E:362:PHE:O	1:E:366:ILE:HD12	2.19	0.42
1:F:372:ILE:HA	1:F:373:PRO:C	2.44	0.42
1:F:483:HIS:NE2	1:G:483:HIS:CD2	2.86	0.42
1:G:212:PHE:CD2	1:G:214:ARG:NE	2.88	0.42
1:I:293:ILE:HG12	1:I:326:CYS:HB2	2.01	0.42
1:I:429:ARG:O	1:I:432:ASN:HB2	2.19	0.42
1:K:12:PHE:HE2	1:M:242:HIS:NE2	2.08	0.42
1:M:362:PHE:O	1:M:366:ILE:HD12	2.19	0.42
1:N:429:ARG:O	1:N:432:ASN:HB2	2.19	0.42
1:Q:276:VAL:HG13	1:S:9:LEU:HB3	2.02	0.42
1:R:429:ARG:O	1:R:432:ASN:HB2	2.19	0.42
1:S:362:PHE:O	1:S:366:ILE:HD12	2.19	0.42
1:S:474:ASP:O	1:S:497:VAL:HG13	2.20	0.42
1:T:293:ILE:HG12	1:T:326:CYS:HB2	2.01	0.42
1:U:79:ALA:HA	1:U:429:ARG:HB3	2.01	0.42
1:U:372:ILE:CD1	1:V:390:GLU:HG2	2.45	0.42
1:U:377:ASP:OD2	1:U:377:ASP:N	2.52	0.42
1:U:491:GLN:HG3	1:V:491:GLN:HG3	2.01	0.42
1:V:276:VAL:HG13	1:X:9:LEU:CD1	2.48	0.42
1:V:372:ILE:HA	1:V:373:PRO:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:398:VAL:HG13	1:V:479:ILE:HB	2.00	0.42
1:A:79:ALA:HA	1:A:429:ARG:HB3	2.01	0.42
1:A:352:GLU:HG2	1:I:272:GLU:CG	2.50	0.42
1:B:138:GLY:HA2	1:B:151:GLN:HE21	1.85	0.42
1:B:429:ARG:O	1:B:432:ASN:HB2	2.19	0.42
1:D:79:ALA:HA	1:D:429:ARG:HB3	2.01	0.42
1:D:138:GLY:HA2	1:D:151:GLN:HE21	1.85	0.42
1:F:138:GLY:HA2	1:F:151:GLN:HE21	1.84	0.42
1:H:297:GLN:HB2	1:J:310:ARG:HB2	1.99	0.42
1:H:429:ARG:O	1:H:432:ASN:HB2	2.19	0.42
1:I:398:VAL:HG13	1:I:479:ILE:HB	2.00	0.42
1:J:79:ALA:HA	1:J:429:ARG:HB3	2.01	0.42
1:K:474:ASP:O	1:K:497:VAL:HG13	2.20	0.42
1:L:474:ASP:O	1:L:497:VAL:HG13	2.20	0.42
1:N:474:ASP:O	1:N:497:VAL:HG13	2.20	0.42
1:O:212:PHE:CD2	1:O:214:ARG:NE	2.88	0.42
1:O:474:ASP:O	1:O:497:VAL:HG13	2.20	0.42
1:R:138:GLY:HA2	1:R:151:GLN:HE21	1.85	0.42
1:R:212:PHE:CD2	1:R:214:ARG:NE	2.88	0.42
1:R:377:ASP:OD2	1:R:377:ASP:N	2.52	0.42
1:U:270:PRO:CG	1:U:273:LYS:CD	2.94	0.42
1:V:224:LYS:HB3	1:V:224:LYS:HE3	1.81	0.42
1:W:138:GLY:HA2	1:W:151:GLN:HE21	1.84	0.42
1:D:270:PRO:CG	1:D:273:LYS:CD	2.94	0.42
1:G:293:ILE:HG12	1:G:326:CYS:HB2	2.01	0.42
1:H:212:PHE:CD2	1:H:214:ARG:NE	2.88	0.42
1:H:372:ILE:HA	1:H:373:PRO:C	2.43	0.42
1:J:474:ASP:O	1:J:497:VAL:HG13	2.20	0.42
1:K:312:GLU:HA	1:M:311:ALA:CB	2.35	0.42
1:K:377:ASP:OD2	1:K:377:ASP:N	2.52	0.42
1:L:79:ALA:HA	1:L:429:ARG:HB3	2.01	0.42
1:M:429:ARG:O	1:M:432:ASN:HB2	2.19	0.42
1:R:79:ALA:HA	1:R:429:ARG:HB3	2.01	0.42
1:S:79:ALA:HA	1:S:429:ARG:HB3	2.01	0.42
1:T:3:LEU:CD2	1:T:4:ALA:N	2.80	0.42
1:T:138:GLY:HA2	1:T:151:GLN:HE21	1.85	0.42
1:V:472:THR:CG2	1:V:498:GLU:HA	2.18	0.42
1:X:212:PHE:CD2	1:X:214:ARG:NE	2.88	0.42
1:F:429:ARG:O	1:F:432:ASN:HB2	2.19	0.42
1:H:424:ARG:CG	1:H:424:ARG:NH1	2.41	0.42
1:J:362:PHE:O	1:J:366:ILE:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:79:ALA:HA	1:K:429:ARG:HB3	2.02	0.42
1:K:362:PHE:O	1:K:366:ILE:HD12	2.20	0.42
1:K:372:ILE:HD12	1:K:372:ILE:HA	1.73	0.42
1:L:283:SER:CA	1:N:3:LEU:HD21	2.49	0.42
1:M:79:ALA:HA	1:M:429:ARG:HB3	2.02	0.42
1:M:424:ARG:CG	1:M:424:ARG:NH1	2.41	0.42
1:M:474:ASP:O	1:M:497:VAL:HG13	2.20	0.42
1:T:53:SER:HA	1:T:85:LYS:CG	2.50	0.42
1:V:11:ILE:HD12	1:X:269:ILE:HG12	2.02	0.42
1:X:79:ALA:HA	1:X:429:ARG:HB3	2.01	0.42
1:B:276:VAL:HG13	1:C:9:LEU:CB	2.49	0.42
1:E:3:LEU:HD13	1:G:369:LEU:HD12	2.01	0.42
1:F:474:ASP:O	1:F:497:VAL:HG13	2.20	0.42
1:J:138:GLY:HA2	1:J:151:GLN:HE21	1.85	0.42
1:L:212:PHE:CD2	1:L:214:ARG:NE	2.88	0.42
1:L:224:LYS:HB3	1:L:224:LYS:HE3	1.82	0.42
1:L:273:LYS:HD3	1:N:11:ILE:C	2.45	0.42
1:L:487:GLY:CA	1:S:229:LYS:CD	2.94	0.42
1:O:263:GLY:HA2	1:P:310:ARG:HH11	1.84	0.42
1:O:362:PHE:O	1:O:366:ILE:HD12	2.19	0.42
1:P:53:SER:HA	1:P:85:LYS:CG	2.50	0.42
1:Q:270:PRO:CB	1:Q:273:LYS:HD2	2.50	0.42
1:R:11:ILE:O	1:T:273:LYS:HE3	2.20	0.42
1:S:189:VAL:HG13	1:S:193:ASP:HB2	2.02	0.42
1:U:424:ARG:CG	1:U:424:ARG:NH1	2.41	0.42
1:U:429:ARG:O	1:U:432:ASN:HB2	2.19	0.42
1:A:189:VAL:HG13	1:A:193:ASP:HB2	2.02	0.42
1:A:293:ILE:HG12	1:A:326:CYS:HB2	2.01	0.42
1:A:371:HIS:O	1:A:374:MET:CG	2.57	0.42
1:B:293:ILE:HG12	1:B:326:CYS:HB2	2.01	0.42
1:C:53:SER:HA	1:C:85:LYS:CG	2.50	0.42
1:D:270:PRO:CB	1:D:273:LYS:HD2	2.50	0.42
1:E:138:GLY:HA2	1:E:151:GLN:HE21	1.85	0.42
1:G:362:PHE:O	1:G:366:ILE:HD12	2.19	0.42
1:I:362:PHE:O	1:I:366:ILE:HD12	2.19	0.42
1:I:372:ILE:HD12	1:I:374:MET:HG3	2.00	0.42
1:J:189:VAL:HG13	1:J:193:ASP:HB2	2.02	0.42
1:K:401:ASN:N	2:K:700:FDP:O5P	2.50	0.42
1:N:79:ALA:HA	1:N:429:ARG:HB3	2.01	0.42
1:P:474:ASP:O	1:P:497:VAL:HG13	2.20	0.42
1:Q:79:ALA:HA	1:Q:429:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:429:ARG:O	1:Q:432:ASN:HB2	2.19	0.42
1:R:272:GLU:HB2	1:T:352:GLU:HG2	1.94	0.42
1:U:362:PHE:O	1:U:366:ILE:HD12	2.19	0.42
1:W:189:VAL:HG13	1:W:193:ASP:HB2	2.02	0.42
1:W:212:PHE:CD2	1:W:214:ARG:NE	2.88	0.42
1:A:270:PRO:CB	1:A:273:LYS:HD2	2.50	0.42
1:B:362:PHE:O	1:B:366:ILE:HD12	2.19	0.42
1:B:373:PRO:HB3	1:O:391:THR:CA	2.49	0.42
1:C:474:ASP:O	1:C:497:VAL:HG13	2.20	0.42
1:D:293:ILE:HG12	1:D:326:CYS:HB2	2.01	0.42
1:E:53:SER:HA	1:E:85:LYS:CG	2.50	0.42
1:F:371:HIS:O	1:F:374:MET:CG	2.57	0.42
1:H:402:THR:OG1	1:H:404:ARG:HB2	2.20	0.42
1:M:189:VAL:HG13	1:M:193:ASP:HB2	2.02	0.42
1:O:53:SER:HA	1:O:85:LYS:CG	2.50	0.42
1:P:401:ASN:N	2:P:700:FDP:O5P	2.50	0.42
1:U:352:GLU:CG	1:W:272:GLU:CG	2.98	0.42
1:V:138:GLY:HA2	1:V:151:GLN:HE21	1.85	0.42
1:W:474:ASP:O	1:W:497:VAL:HG13	2.20	0.42
1:B:53:SER:HA	1:B:85:LYS:CG	2.50	0.41
1:B:212:PHE:CD2	1:B:214:ARG:NE	2.88	0.41
1:C:79:ALA:HA	1:C:429:ARG:HB3	2.01	0.41
1:C:212:PHE:CD2	1:C:214:ARG:NE	2.88	0.41
1:C:270:PRO:CB	1:C:273:LYS:HD2	2.50	0.41
1:D:362:PHE:O	1:D:366:ILE:HD12	2.19	0.41
1:F:293:ILE:HG12	1:F:326:CYS:HB2	2.01	0.41
1:G:53:SER:HA	1:G:85:LYS:CG	2.50	0.41
1:H:53:SER:HA	1:H:85:LYS:CG	2.50	0.41
1:L:311:ALA:HA	1:N:315:ASP:HB2	2.01	0.41
1:M:138:GLY:HA2	1:M:151:GLN:HE21	1.85	0.41
1:P:212:PHE:CD2	1:P:214:ARG:NE	2.88	0.41
1:Q:474:ASP:O	1:Q:497:VAL:HG13	2.20	0.41
1:S:138:GLY:HA2	1:S:151:GLN:HE21	1.84	0.41
1:U:11:ILE:HB	1:W:273:LYS:CD	2.42	0.41
1:U:212:PHE:CD2	1:U:214:ARG:NE	2.88	0.41
1:U:311:ALA:HB3	1:W:312:GLU:CG	2.49	0.41
1:X:362:PHE:O	1:X:366:ILE:HD12	2.19	0.41
1:D:474:ASP:O	1:D:497:VAL:HG13	2.20	0.41
1:E:272:GLU:HG3	1:G:352:GLU:CB	2.50	0.41
1:I:474:ASP:O	1:I:497:VAL:HG13	2.20	0.41
1:K:242:HIS:NE2	1:M:12:PHE:CE2	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:284:LYS:CG	1:N:7:LEU:HD22	2.50	0.41
1:L:429:ARG:O	1:L:432:ASN:HB2	2.19	0.41
1:N:372:ILE:HA	1:N:373:PRO:C	2.43	0.41
1:O:135:VAL:HG12	1:O:136:ARG:N	2.35	0.41
1:O:293:ILE:HG12	1:O:326:CYS:HB2	2.01	0.41
1:O:315:ASP:HB2	1:P:311:ALA:CA	2.48	0.41
1:P:79:ALA:HA	1:P:429:ARG:HB3	2.02	0.41
1:P:189:VAL:HG13	1:P:193:ASP:HB2	2.02	0.41
1:Q:293:ILE:HG12	1:Q:326:CYS:HB2	2.01	0.41
1:Q:362:PHE:O	1:Q:366:ILE:HD12	2.19	0.41
1:R:362:PHE:O	1:R:366:ILE:HD12	2.19	0.41
1:X:474:ASP:O	1:X:497:VAL:HG13	2.20	0.41
1:A:138:GLY:HA2	1:A:151:GLN:HE21	1.85	0.41
1:A:362:PHE:O	1:A:366:ILE:HD12	2.19	0.41
1:B:188:ALA:CB	1:B:218:GLN:HG2	2.21	0.41
1:B:270:PRO:CB	1:B:273:LYS:HD2	2.50	0.41
1:B:474:ASP:O	1:B:497:VAL:HG13	2.20	0.41
1:C:223:ARG:HG2	1:C:223:ARG:NH1	2.26	0.41
1:E:189:VAL:HG13	1:E:193:ASP:HB2	2.02	0.41
1:E:474:ASP:O	1:E:497:VAL:HG13	2.20	0.41
1:G:189:VAL:HG13	1:G:193:ASP:HB2	2.02	0.41
1:H:189:VAL:HG13	1:H:193:ASP:HB2	2.02	0.41
1:H:296:THR:O	1:J:310:ARG:HG3	2.20	0.41
1:I:53:SER:HA	1:I:85:LYS:CG	2.50	0.41
1:K:212:PHE:CD2	1:K:214:ARG:NE	2.88	0.41
1:L:53:SER:HA	1:L:85:LYS:CG	2.50	0.41
1:N:138:GLY:HA2	1:N:151:GLN:HE21	1.85	0.41
1:O:6:ASN:CG	1:P:279:LYS:HE3	2.41	0.41
1:O:270:PRO:CB	1:O:273:LYS:HD2	2.50	0.41
1:Q:212:PHE:CD2	1:Q:214:ARG:NE	2.88	0.41
1:Q:390:GLU:O	1:R:372:ILE:HG13	2.20	0.41
1:R:474:ASP:O	1:R:497:VAL:HG13	2.20	0.41
1:U:352:GLU:HG2	1:W:272:GLU:C	2.45	0.41
1:U:474:ASP:O	1:U:497:VAL:HG13	2.20	0.41
1:V:401:ASN:N	2:V:700:FDP:O5P	2.50	0.41
1:X:138:GLY:HA2	1:X:151:GLN:HE21	1.84	0.41
1:F:189:VAL:HG13	1:F:193:ASP:HB2	2.02	0.41
1:G:474:ASP:O	1:G:497:VAL:HG13	2.20	0.41
1:I:79:ALA:HA	1:I:429:ARG:HB3	2.01	0.41
1:I:212:PHE:CD2	1:I:214:ARG:NE	2.88	0.41
1:J:293:ILE:HG12	1:J:326:CYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:297:GLN:HB2	1:M:310:ARG:HB2	2.01	0.41
1:N:189:VAL:HG13	1:N:193:ASP:HB2	2.02	0.41
1:P:214:ARG:HH11	1:P:214:ARG:HG3	1.86	0.41
1:Q:467:LYS:HE2	1:Q:467:LYS:HB3	1.86	0.41
1:S:491:GLN:NE2	1:T:491:GLN:NE2	2.68	0.41
1:T:362:PHE:O	1:T:366:ILE:HD12	2.19	0.41
1:U:214:ARG:HG3	1:U:214:ARG:HH11	1.86	0.41
1:V:189:VAL:HG13	1:V:193:ASP:HB2	2.02	0.41
1:B:49:ARG:NE	1:B:83:ASP:OD2	2.33	0.41
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.86	0.41
1:C:214:ARG:HG3	1:C:214:ARG:HH11	1.86	0.41
1:C:362:PHE:O	1:C:366:ILE:HD12	2.20	0.41
1:D:372:ILE:HA	1:D:373:PRO:C	2.44	0.41
1:H:474:ASP:O	1:H:497:VAL:HG13	2.20	0.41
1:K:138:GLY:HA2	1:K:151:GLN:HE21	1.84	0.41
1:K:429:ARG:O	1:K:432:ASN:HB2	2.19	0.41
1:L:138:GLY:HA2	1:L:151:GLN:HE21	1.84	0.41
1:N:212:PHE:CD2	1:N:214:ARG:NE	2.88	0.41
1:T:424:ARG:CG	1:T:424:ARG:NH1	2.41	0.41
1:U:189:VAL:HG13	1:U:193:ASP:HB2	2.02	0.41
1:V:362:PHE:O	1:V:366:ILE:HD12	2.19	0.41
1:W:223:ARG:HG2	1:W:223:ARG:NH1	2.25	0.41
1:H:310:ARG:H	1:J:297:GLN:HB3	1.86	0.41
1:K:270:PRO:CB	1:K:273:LYS:HD2	2.50	0.41
1:L:310:ARG:NH2	1:N:297:GLN:OE1	2.53	0.41
1:P:377:ASP:OD2	1:P:377:ASP:N	2.52	0.41
1:U:311:ALA:CB	1:W:312:GLU:CG	2.99	0.41
1:V:474:ASP:O	1:V:497:VAL:HG13	2.20	0.41
1:W:53:SER:HA	1:W:85:LYS:CG	2.50	0.41
1:X:429:ARG:O	1:X:432:ASN:HB2	2.19	0.41
1:A:272:GLU:HA	1:I:313:VAL:CG1	2.51	0.41
1:B:272:GLU:CG	1:C:352:GLU:CB	2.98	0.41
1:E:79:ALA:HA	1:E:429:ARG:HB3	2.01	0.41
1:F:79:ALA:HA	1:F:429:ARG:HB3	2.01	0.41
1:F:214:ARG:HH11	1:F:214:ARG:HG3	1.86	0.41
1:F:373:PRO:HB2	1:G:391:THR:HA	1.95	0.41
1:G:138:GLY:HA2	1:G:151:GLN:HE21	1.85	0.41
1:H:270:PRO:CB	1:H:273:LYS:HD2	2.50	0.41
1:H:310:ARG:H	1:J:297:GLN:CB	2.34	0.41
1:I:138:GLY:HA2	1:I:151:GLN:HE21	1.84	0.41
1:I:451:GLU:H	1:I:451:GLU:HG2	1.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:212:PHE:CD2	1:J:214:ARG:NE	2.88	0.41
1:K:214:ARG:HG3	1:K:214:ARG:HH11	1.86	0.41
1:K:283:SER:OG	1:M:3:LEU:HD23	2.21	0.41
1:L:402:THR:OG1	1:L:404:ARG:HB2	2.20	0.41
1:O:214:ARG:HH11	1:O:214:ARG:HG3	1.86	0.41
1:P:467:LYS:HE2	1:P:467:LYS:HB3	1.87	0.41
1:U:315:ASP:CB	1:W:311:ALA:CB	2.99	0.41
1:V:53:SER:HA	1:V:85:LYS:CG	2.50	0.41
1:W:372:ILE:HG23	1:X:390:GLU:C	2.44	0.41
1:X:189:VAL:HG13	1:X:193:ASP:HB2	2.02	0.41
1:X:214:ARG:HH11	1:X:214:ARG:HG3	1.86	0.41
1:D:214:ARG:HH11	1:D:214:ARG:HG3	1.86	0.41
1:F:390:GLU:HG2	1:G:374:MET:HE2	2.03	0.41
1:G:214:ARG:HG3	1:G:214:ARG:HH11	1.86	0.41
1:I:372:ILE:CD1	1:I:374:MET:HE2	2.49	0.41
1:K:189:VAL:HG13	1:K:193:ASP:HB2	2.02	0.41
1:N:53:SER:HA	1:N:85:LYS:CG	2.50	0.41
1:O:138:GLY:HA2	1:O:151:GLN:HE21	1.84	0.41
1:O:224:LYS:HB3	1:O:224:LYS:HE3	1.82	0.41
1:Q:444:ALA:O	1:Q:448:GLY:N	2.54	0.41
1:R:279:LYS:CE	1:T:6:ASN:OD1	2.63	0.41
1:R:293:ILE:HG12	1:R:326:CYS:HB2	2.01	0.41
1:U:376:ALA:HA	1:V:494:ILE:HD12	2.03	0.41
1:A:214:ARG:HG3	1:A:214:ARG:HH11	1.86	0.41
1:A:372:ILE:HA	1:A:373:PRO:C	2.44	0.41
1:A:474:ASP:O	1:A:497:VAL:HG13	2.20	0.41
1:B:101:MET:CE	1:B:124:PHE:CE1	3.04	0.41
1:C:189:VAL:HG13	1:C:193:ASP:HB2	2.02	0.41
1:D:444:ALA:O	1:D:448:GLY:N	2.54	0.41
1:E:212:PHE:CD2	1:E:214:ARG:NE	2.88	0.41
1:E:242:HIS:CE1	1:G:12:PHE:HZ	2.34	0.41
1:E:372:ILE:HA	1:E:373:PRO:C	2.44	0.41
1:H:352:GLU:CG	1:J:272:GLU:CG	2.99	0.41
1:H:390:GLU:O	1:I:373:PRO:HB3	2.21	0.41
1:I:189:VAL:HG13	1:I:193:ASP:HB2	2.02	0.41
1:I:444:ALA:O	1:I:448:GLY:N	2.54	0.41
1:J:214:ARG:HH11	1:J:214:ARG:HG3	1.86	0.41
1:K:11:ILE:O	1:M:273:LYS:HE3	2.21	0.41
1:M:101:MET:CE	1:M:124:PHE:CE1	3.04	0.41
1:M:444:ALA:O	1:M:448:GLY:N	2.54	0.41
1:O:297:GLN:HB2	1:P:310:ARG:CG	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:312:GLU:CA	1:P:311:ALA:HB1	2.33	0.41
1:P:372:ILE:HA	1:P:373:PRO:C	2.46	0.41
1:Q:189:VAL:HG13	1:Q:193:ASP:HB2	2.02	0.41
1:Q:284:LYS:HG3	1:S:7:LEU:HD21	2.00	0.41
1:Q:310:ARG:CG	1:S:297:GLN:HB2	2.51	0.41
1:Q:374:MET:HB2	1:Q:375:SER:H	1.78	0.41
1:S:212:PHE:CD2	1:S:214:ARG:NE	2.88	0.41
1:S:214:ARG:HH11	1:S:214:ARG:HG3	1.86	0.41
1:T:189:VAL:HG13	1:T:193:ASP:HB2	2.02	0.41
1:U:101:MET:CE	1:U:124:PHE:CE1	3.04	0.41
1:V:101:MET:CE	1:V:124:PHE:CE1	3.04	0.41
1:W:377:ASP:OD2	1:W:377:ASP:N	2.52	0.41
1:W:424:ARG:NH1	1:W:424:ARG:CG	2.41	0.41
1:C:389:TYR:O	1:P:372:ILE:HG21	2.21	0.41
1:D:212:PHE:CD2	1:D:214:ARG:NE	2.88	0.41
1:E:372:ILE:HD12	1:E:372:ILE:HA	1.73	0.41
1:H:444:ALA:O	1:H:448:GLY:N	2.54	0.41
1:L:195:VAL:HG11	1:T:498:GLU:HG2	2.02	0.41
1:O:189:VAL:HG13	1:O:193:ASP:HB2	2.02	0.41
1:P:101:MET:CE	1:P:124:PHE:CE1	3.04	0.41
1:P:372:ILE:HD12	1:P:372:ILE:HA	1.80	0.41
1:S:223:ARG:HG2	1:S:223:ARG:NH1	2.26	0.41
1:S:472:THR:CG2	1:S:498:GLU:CA	2.84	0.41
1:U:277:ALA:HB2	1:W:11:ILE:HG21	2.03	0.41
1:A:53:SER:HA	1:A:85:LYS:CG	2.50	0.40
1:A:212:PHE:CD2	1:A:214:ARG:NE	2.88	0.40
1:A:444:ALA:O	1:A:448:GLY:N	2.54	0.40
1:B:110:THR:O	1:B:125:TYR:HA	2.22	0.40
1:B:189:VAL:HG13	1:B:193:ASP:HB2	2.02	0.40
1:B:270:PRO:CG	1:B:273:LYS:CD	2.94	0.40
1:H:101:MET:CE	1:H:124:PHE:CE1	3.04	0.40
1:I:101:MET:CE	1:I:124:PHE:CE1	3.04	0.40
1:K:53:SER:HA	1:K:85:LYS:CG	2.50	0.40
1:K:188:ALA:CB	1:K:218:GLN:HG2	2.21	0.40
1:L:214:ARG:HH11	1:L:214:ARG:HG3	1.86	0.40
1:L:229:LYS:CG	1:S:487:GLY:CA	2.84	0.40
1:L:451:GLU:H	1:L:451:GLU:HG2	1.59	0.40
1:N:101:MET:CE	1:N:124:PHE:CE1	3.04	0.40
1:O:444:ALA:O	1:O:448:GLY:N	2.54	0.40
1:Q:110:THR:O	1:Q:125:TYR:HA	2.22	0.40
1:Q:138:GLY:HA2	1:Q:151:GLN:HE21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:273:LYS:HG2	1:S:11:ILE:O	2.21	0.40
1:R:53:SER:HA	1:R:85:LYS:CG	2.50	0.40
1:S:372:ILE:HA	1:S:373:PRO:C	2.45	0.40
1:U:53:SER:HA	1:U:85:LYS:CG	2.50	0.40
1:W:214:ARG:HH11	1:W:214:ARG:HG3	1.86	0.40
1:A:12:PHE:CE2	1:I:242:HIS:HE1	2.38	0.40
1:A:101:MET:CE	1:A:124:PHE:CE1	3.04	0.40
1:A:110:THR:O	1:A:125:TYR:HA	2.22	0.40
1:B:451:GLU:O	1:B:453:LYS:HE2	2.21	0.40
1:C:451:GLU:O	1:C:453:LYS:HE2	2.22	0.40
1:E:110:THR:O	1:E:125:TYR:HA	2.22	0.40
1:F:188:ALA:CB	1:F:218:GLN:HG2	2.21	0.40
1:G:110:THR:O	1:G:125:TYR:HA	2.21	0.40
1:H:494:ILE:HD12	1:I:376:ALA:HB1	2.03	0.40
1:I:110:THR:O	1:I:125:TYR:HA	2.21	0.40
1:J:110:THR:O	1:J:125:TYR:HA	2.22	0.40
1:M:110:THR:O	1:M:125:TYR:HA	2.22	0.40
1:N:424:ARG:CG	1:N:424:ARG:NH1	2.41	0.40
1:O:310:ARG:CG	1:P:297:GLN:OE1	2.60	0.40
1:Q:53:SER:HA	1:Q:85:LYS:CG	2.50	0.40
1:Q:276:VAL:HG13	1:S:9:LEU:HD13	2.04	0.40
1:R:189:VAL:HG13	1:R:193:ASP:HB2	2.02	0.40
1:R:444:ALA:O	1:R:448:GLY:N	2.54	0.40
1:T:214:ARG:HG3	1:T:214:ARG:HH11	1.86	0.40
1:U:310:ARG:CG	1:W:297:GLN:OE1	2.59	0.40
1:V:482:ASP:OD1	1:V:482:ASP:C	2.65	0.40
1:X:110:THR:O	1:X:125:TYR:HA	2.22	0.40
1:A:451:GLU:O	1:A:453:LYS:HE2	2.22	0.40
1:A:482:ASP:C	1:A:482:ASP:OD1	2.65	0.40
1:B:371:HIS:O	1:B:374:MET:CG	2.57	0.40
1:C:110:THR:O	1:C:125:TYR:HA	2.21	0.40
1:C:451:GLU:H	1:C:451:GLU:HG2	1.59	0.40
1:D:189:VAL:HG13	1:D:193:ASP:HB2	2.02	0.40
1:E:214:ARG:HH11	1:E:214:ARG:HG3	1.86	0.40
1:E:482:ASP:OD1	1:E:482:ASP:C	2.65	0.40
1:H:110:THR:O	1:H:125:TYR:HA	2.22	0.40
1:I:451:GLU:O	1:I:453:LYS:HE2	2.22	0.40
1:J:372:ILE:HD12	1:J:372:ILE:HA	1.73	0.40
1:K:110:THR:O	1:K:125:TYR:HA	2.22	0.40
1:K:273:LYS:HG2	1:M:11:ILE:O	2.22	0.40
1:L:312:GLU:HG3	1:N:311:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:270:PRO:CG	1:O:273:LYS:CD	2.94	0.40
1:O:372:ILE:HA	1:O:373:PRO:C	2.44	0.40
1:O:467:LYS:HE2	1:O:467:LYS:HB3	1.86	0.40
1:Q:101:MET:CE	1:Q:124:PHE:CE1	3.04	0.40
1:Q:214:ARG:HH11	1:Q:214:ARG:HG3	1.86	0.40
1:R:110:THR:O	1:R:125:TYR:HA	2.22	0.40
1:T:401:ASN:N	2:T:700:FDP:O5P	2.50	0.40
1:V:371:HIS:O	1:V:374:MET:CG	2.57	0.40
1:W:482:ASP:OD1	1:W:482:ASP:C	2.65	0.40
1:A:467:LYS:HE2	1:A:467:LYS:HB3	1.86	0.40
1:C:372:ILE:HD12	1:C:372:ILE:HA	1.73	0.40
1:F:101:MET:CE	1:F:124:PHE:CE1	3.04	0.40
1:G:482:ASP:OD1	1:G:482:ASP:C	2.65	0.40
1:I:482:ASP:OD1	1:I:482:ASP:C	2.64	0.40
1:J:482:ASP:OD1	1:J:482:ASP:C	2.65	0.40
1:K:310:ARG:NH2	1:M:297:GLN:OE1	2.54	0.40
1:M:53:SER:HA	1:M:85:LYS:CG	2.50	0.40
1:M:451:GLU:O	1:M:453:LYS:HE2	2.22	0.40
1:R:401:ASN:N	2:R:700:FDP:O5P	2.54	0.40
1:R:451:GLU:O	1:R:453:LYS:HE2	2.22	0.40
1:S:110:THR:O	1:S:125:TYR:HA	2.22	0.40
1:U:110:THR:O	1:U:125:TYR:HA	2.22	0.40
1:B:482:ASP:HB3	1:B:491:GLN:HE21	1.87	0.40
1:H:451:GLU:O	1:H:453:LYS:HE2	2.22	0.40
1:K:297:GLN:HB2	1:M:310:ARG:CB	2.51	0.40
1:K:482:ASP:C	1:K:482:ASP:OD1	2.65	0.40
1:M:372:ILE:HD12	1:M:374:MET:HG3	2.04	0.40
1:O:101:MET:CE	1:O:124:PHE:CE1	3.04	0.40
1:Q:451:GLU:O	1:Q:453:LYS:HE2	2.22	0.40
1:R:101:MET:CE	1:R:124:PHE:CE1	3.04	0.40
1:R:372:ILE:HA	1:R:373:PRO:C	2.44	0.40
1:S:482:ASP:HB3	1:S:491:GLN:HE21	1.87	0.40
1:U:270:PRO:CB	1:U:273:LYS:HD2	2.50	0.40
1:V:214:ARG:HG3	1:V:214:ARG:HH11	1.86	0.40
1:X:371:HIS:C	1:X:372:ILE:HD13	2.47	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:103:ARG:CD	1:T:58:GLU:OE1[5_545]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:LYS:CE	1:W:487:GLY:CA[5_545]	2.08	0.12
1:F:229:LYS:CD	1:W:487:GLY:CA[5_545]	2.15	0.05
1:F:229:LYS:CG	1:W:487:GLY:CA[5_545]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	B	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	C	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	D	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	E	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	F	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	G	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	H	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	I	496/499 (99%)	485 (98%)	10 (2%)	1 (0%)	43	77
1	J	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	K	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	L	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	M	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	N	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	O	496/499 (99%)	485 (98%)	10 (2%)	1 (0%)	43	77
1	P	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	Q	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	R	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	S	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	U	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	V	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	W	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	X	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
All	All	11904/11976 (99%)	11662 (98%)	218 (2%)	24 (0%)	43	77

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	THR
1	B	296	THR
1	C	296	THR
1	D	296	THR
1	E	296	THR
1	F	296	THR
1	G	296	THR
1	H	296	THR
1	I	296	THR
1	J	296	THR
1	K	296	THR
1	L	296	THR
1	M	296	THR
1	N	296	THR
1	O	296	THR
1	P	296	THR
1	Q	296	THR
1	R	296	THR
1	S	296	THR
1	T	296	THR
1	U	296	THR
1	V	296	THR
1	W	296	THR
1	X	296	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	416/417 (100%)	377 (91%)	39 (9%)	8	26
1	B	416/417 (100%)	377 (91%)	39 (9%)	8	26
1	C	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	D	416/417 (100%)	376 (90%)	40 (10%)	8	25
1	E	416/417 (100%)	376 (90%)	40 (10%)	8	25
1	F	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	G	416/417 (100%)	376 (90%)	40 (10%)	8	25
1	H	416/417 (100%)	377 (91%)	39 (9%)	8	26
1	I	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	J	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	K	416/417 (100%)	377 (91%)	39 (9%)	8	26
1	L	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	M	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	N	416/417 (100%)	377 (91%)	39 (9%)	8	26
1	O	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	P	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	Q	416/417 (100%)	376 (90%)	40 (10%)	8	25
1	R	416/417 (100%)	376 (90%)	40 (10%)	8	25
1	S	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	T	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	U	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	V	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	W	416/417 (100%)	374 (90%)	42 (10%)	7	23
1	X	416/417 (100%)	378 (91%)	38 (9%)	9	28
All	All	9984/10008 (100%)	9017 (90%)	967 (10%)	8	25

All (967) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	17	ASN
1	A	31	THR

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Mol	Chain	Res	Type
1	A	38	LYS
1	A	40	LEU
1	A	118	LYS
1	A	177	VAL
1	A	179	LEU
1	A	214	ARG
1	A	223	ARG
1	A	224	LYS
1	A	240	GLU
1	A	265	LEU
1	A	267	VAL
1	A	269	ILE
1	A	304	TYR
1	A	335	LYS
1	A	345	TYR
1	A	366	ILE
1	A	372	ILE
1	A	374	MET
1	A	382	SER
1	A	394	LYS
1	A	396	MET
1	A	398	VAL
1	A	424	ARG
1	A	435	GLN
1	A	446	LYS
1	A	451	GLU
1	A	453	LYS
1	A	454	GLU
1	A	466	SER
1	A	467	LYS
1	A	471	GLN
1	A	472	THR
1	A	490	ASN
1	A	495	LEU
1	A	497	VAL
1	A	498	GLU
1	B	3	LEU
1	B	17	ASN
1	B	31	THR
1	B	38	LYS
1	B	40	LEU
1	B	118	LYS

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Mol	Chain	Res	Type
1	B	177	VAL
1	B	179	LEU
1	B	214	ARG
1	B	223	ARG
1	B	224	LYS
1	B	240	GLU
1	B	265	LEU
1	B	267	VAL
1	B	269	ILE
1	B	304	TYR
1	B	335	LYS
1	B	345	TYR
1	B	366	ILE
1	B	372	ILE
1	B	374	MET
1	B	382	SER
1	B	394	LYS
1	B	396	MET
1	B	398	VAL
1	B	424	ARG
1	B	435	GLN
1	B	446	LYS
1	B	451	GLU
1	B	453	LYS
1	B	454	GLU
1	B	466	SER
1	B	467	LYS
1	B	471	GLN
1	B	472	THR
1	B	490	ASN
1	B	495	LEU
1	B	497	VAL
1	B	498	GLU
1	C	3	LEU
1	C	12	PHE
1	C	17	ASN
1	C	31	THR
1	C	38	LYS
1	C	40	LEU
1	C	58	GLU
1	C	118	LYS
1	C	177	VAL

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Mol	Chain	Res	Type
1	C	179	LEU
1	C	214	ARG
1	C	223	ARG
1	C	224	LYS
1	C	240	GLU
1	C	265	LEU
1	C	267	VAL
1	C	269	ILE
1	C	304	TYR
1	C	335	LYS
1	C	345	TYR
1	C	366	ILE
1	C	372	ILE
1	C	374	MET
1	C	382	SER
1	C	394	LYS
1	C	396	MET
1	C	398	VAL
1	C	424	ARG
1	C	435	GLN
1	C	446	LYS
1	C	451	GLU
1	C	453	LYS
1	C	454	GLU
1	C	466	SER
1	C	467	LYS
1	C	471	GLN
1	C	472	THR
1	C	490	ASN
1	C	495	LEU
1	C	497	VAL
1	C	498	GLU
1	D	3	LEU
1	D	17	ASN
1	D	31	THR
1	D	38	LYS
1	D	40	LEU
1	D	118	LYS
1	D	177	VAL
1	D	179	LEU
1	D	214	ARG
1	D	223	ARG

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Mol	Chain	Res	Type
1	D	224	LYS
1	D	240	GLU
1	D	265	LEU
1	D	267	VAL
1	D	269	ILE
1	D	304	TYR
1	D	335	LYS
1	D	345	TYR
1	D	366	ILE
1	D	372	ILE
1	D	374	MET
1	D	382	SER
1	D	394	LYS
1	D	396	MET
1	D	398	VAL
1	D	404	ARG
1	D	424	ARG
1	D	435	GLN
1	D	446	LYS
1	D	451	GLU
1	D	453	LYS
1	D	454	GLU
1	D	466	SER
1	D	467	LYS
1	D	471	GLN
1	D	472	THR
1	D	490	ASN
1	D	495	LEU
1	D	497	VAL
1	D	498	GLU
1	E	3	LEU
1	E	17	ASN
1	E	31	THR
1	E	38	LYS
1	E	40	LEU
1	E	118	LYS
1	E	177	VAL
1	E	179	LEU
1	E	214	ARG
1	E	223	ARG
1	E	224	LYS
1	E	240	GLU

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Mol	Chain	Res	Type
1	E	265	LEU
1	E	267	VAL
1	E	269	ILE
1	E	273	LYS
1	E	304	TYR
1	E	335	LYS
1	E	345	TYR
1	E	366	ILE
1	E	372	ILE
1	E	374	MET
1	E	382	SER
1	E	394	LYS
1	E	396	MET
1	E	398	VAL
1	E	424	ARG
1	E	435	GLN
1	E	446	LYS
1	E	451	GLU
1	E	453	LYS
1	E	454	GLU
1	E	466	SER
1	E	467	LYS
1	E	471	GLN
1	E	472	THR
1	E	490	ASN
1	E	495	LEU
1	E	497	VAL
1	E	498	GLU
1	F	3	LEU
1	F	12	PHE
1	F	17	ASN
1	F	31	THR
1	F	38	LYS
1	F	40	LEU
1	F	118	LYS
1	F	177	VAL
1	F	179	LEU
1	F	214	ARG
1	F	223	ARG
1	F	224	LYS
1	F	240	GLU
1	F	265	LEU

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Mol	Chain	Res	Type
1	F	267	VAL
1	F	269	ILE
1	F	273	LYS
1	F	304	TYR
1	F	335	LYS
1	F	345	TYR
1	F	366	ILE
1	F	372	ILE
1	F	374	MET
1	F	382	SER
1	F	394	LYS
1	F	396	MET
1	F	398	VAL
1	F	424	ARG
1	F	435	GLN
1	F	446	LYS
1	F	451	GLU
1	F	453	LYS
1	F	454	GLU
1	F	466	SER
1	F	467	LYS
1	F	471	GLN
1	F	472	THR
1	F	490	ASN
1	F	495	LEU
1	F	497	VAL
1	F	498	GLU
1	G	3	LEU
1	G	17	ASN
1	G	31	THR
1	G	38	LYS
1	G	40	LEU
1	G	118	LYS
1	G	177	VAL
1	G	179	LEU
1	G	214	ARG
1	G	223	ARG
1	G	224	LYS
1	G	240	GLU
1	G	265	LEU
1	G	267	VAL
1	G	269	ILE

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Mol	Chain	Res	Type
1	G	304	TYR
1	G	335	LYS
1	G	345	TYR
1	G	366	ILE
1	G	372	ILE
1	G	374	MET
1	G	382	SER
1	G	394	LYS
1	G	396	MET
1	G	398	VAL
1	G	404	ARG
1	G	424	ARG
1	G	435	GLN
1	G	446	LYS
1	G	451	GLU
1	G	453	LYS
1	G	454	GLU
1	G	466	SER
1	G	467	LYS
1	G	471	GLN
1	G	472	THR
1	G	490	ASN
1	G	495	LEU
1	G	497	VAL
1	G	498	GLU
1	H	3	LEU
1	H	17	ASN
1	H	31	THR
1	H	38	LYS
1	H	40	LEU
1	H	118	LYS
1	H	177	VAL
1	H	179	LEU
1	H	214	ARG
1	H	223	ARG
1	H	224	LYS
1	H	240	GLU
1	H	265	LEU
1	H	267	VAL
1	H	269	ILE
1	H	304	TYR
1	H	335	LYS

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Mol	Chain	Res	Type
1	H	345	TYR
1	H	366	ILE
1	H	371	HIS
1	H	372	ILE
1	H	382	SER
1	H	394	LYS
1	H	396	MET
1	H	398	VAL
1	H	424	ARG
1	H	435	GLN
1	H	446	LYS
1	H	451	GLU
1	H	453	LYS
1	H	454	GLU
1	H	466	SER
1	H	467	LYS
1	H	471	GLN
1	H	472	THR
1	H	490	ASN
1	H	495	LEU
1	H	497	VAL
1	H	498	GLU
1	I	3	LEU
1	I	17	ASN
1	I	31	THR
1	I	38	LYS
1	I	40	LEU
1	I	118	LYS
1	I	177	VAL
1	I	179	LEU
1	I	214	ARG
1	I	223	ARG
1	I	224	LYS
1	I	240	GLU
1	I	265	LEU
1	I	267	VAL
1	I	269	ILE
1	I	273	LYS
1	I	304	TYR
1	I	335	LYS
1	I	345	TYR
1	I	366	ILE

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Mol	Chain	Res	Type
1	I	371	HIS
1	I	372	ILE
1	I	382	SER
1	I	394	LYS
1	I	396	MET
1	I	398	VAL
1	I	404	ARG
1	I	424	ARG
1	I	435	GLN
1	I	446	LYS
1	I	451	GLU
1	I	453	LYS
1	I	454	GLU
1	I	466	SER
1	I	467	LYS
1	I	471	GLN
1	I	472	THR
1	I	490	ASN
1	I	495	LEU
1	I	497	VAL
1	I	498	GLU
1	J	3	LEU
1	J	12	PHE
1	J	17	ASN
1	J	31	THR
1	J	38	LYS
1	J	40	LEU
1	J	118	LYS
1	J	177	VAL
1	J	179	LEU
1	J	214	ARG
1	J	223	ARG
1	J	224	LYS
1	J	240	GLU
1	J	265	LEU
1	J	267	VAL
1	J	269	ILE
1	J	273	LYS
1	J	304	TYR
1	J	335	LYS
1	J	345	TYR
1	J	366	ILE

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Mol	Chain	Res	Type
1	J	372	ILE
1	J	374	MET
1	J	382	SER
1	J	394	LYS
1	J	396	MET
1	J	398	VAL
1	J	424	ARG
1	J	435	GLN
1	J	446	LYS
1	J	451	GLU
1	J	453	LYS
1	J	454	GLU
1	J	466	SER
1	J	467	LYS
1	J	471	GLN
1	J	472	THR
1	J	490	ASN
1	J	495	LEU
1	J	497	VAL
1	J	498	GLU
1	K	3	LEU
1	K	17	ASN
1	K	31	THR
1	K	38	LYS
1	K	40	LEU
1	K	118	LYS
1	K	177	VAL
1	K	179	LEU
1	K	214	ARG
1	K	223	ARG
1	K	224	LYS
1	K	240	GLU
1	K	265	LEU
1	K	267	VAL
1	K	269	ILE
1	K	304	TYR
1	K	335	LYS
1	K	345	TYR
1	K	366	ILE
1	K	372	ILE
1	K	374	MET
1	K	382	SER

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Mol	Chain	Res	Type
1	K	394	LYS
1	K	396	MET
1	K	398	VAL
1	K	424	ARG
1	K	435	GLN
1	K	446	LYS
1	K	451	GLU
1	K	453	LYS
1	K	454	GLU
1	K	466	SER
1	K	467	LYS
1	K	471	GLN
1	K	472	THR
1	K	490	ASN
1	K	495	LEU
1	K	497	VAL
1	K	498	GLU
1	L	3	LEU
1	L	17	ASN
1	L	31	THR
1	L	38	LYS
1	L	40	LEU
1	L	118	LYS
1	L	177	VAL
1	L	179	LEU
1	L	214	ARG
1	L	223	ARG
1	L	224	LYS
1	L	240	GLU
1	L	265	LEU
1	L	267	VAL
1	L	269	ILE
1	L	273	LYS
1	L	304	TYR
1	L	335	LYS
1	L	337	LYS
1	L	345	TYR
1	L	366	ILE
1	L	371	HIS
1	L	372	ILE
1	L	382	SER
1	L	394	LYS

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Mol	Chain	Res	Type
1	L	396	MET
1	L	398	VAL
1	L	424	ARG
1	L	435	GLN
1	L	446	LYS
1	L	451	GLU
1	L	453	LYS
1	L	454	GLU
1	L	466	SER
1	L	467	LYS
1	L	471	GLN
1	L	472	THR
1	L	490	ASN
1	L	495	LEU
1	L	497	VAL
1	L	498	GLU
1	M	3	LEU
1	M	12	PHE
1	M	17	ASN
1	M	31	THR
1	M	38	LYS
1	M	40	LEU
1	M	118	LYS
1	M	177	VAL
1	M	179	LEU
1	M	214	ARG
1	M	223	ARG
1	M	224	LYS
1	M	240	GLU
1	M	265	LEU
1	M	267	VAL
1	M	269	ILE
1	M	273	LYS
1	M	304	TYR
1	M	335	LYS
1	M	345	TYR
1	M	366	ILE
1	M	371	HIS
1	M	372	ILE
1	M	382	SER
1	M	394	LYS
1	M	396	MET

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Mol	Chain	Res	Type
1	M	398	VAL
1	M	424	ARG
1	M	435	GLN
1	M	446	LYS
1	M	451	GLU
1	M	453	LYS
1	M	454	GLU
1	M	466	SER
1	M	467	LYS
1	M	471	GLN
1	M	472	THR
1	M	490	ASN
1	M	495	LEU
1	M	497	VAL
1	M	498	GLU
1	N	3	LEU
1	N	17	ASN
1	N	31	THR
1	N	38	LYS
1	N	40	LEU
1	N	118	LYS
1	N	177	VAL
1	N	179	LEU
1	N	214	ARG
1	N	223	ARG
1	N	224	LYS
1	N	240	GLU
1	N	265	LEU
1	N	267	VAL
1	N	269	ILE
1	N	304	TYR
1	N	335	LYS
1	N	345	TYR
1	N	366	ILE
1	N	372	ILE
1	N	374	MET
1	N	382	SER
1	N	394	LYS
1	N	396	MET
1	N	398	VAL
1	N	424	ARG
1	N	435	GLN

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Mol	Chain	Res	Type
1	N	446	LYS
1	N	451	GLU
1	N	453	LYS
1	N	454	GLU
1	N	466	SER
1	N	467	LYS
1	N	471	GLN
1	N	472	THR
1	N	490	ASN
1	N	495	LEU
1	N	497	VAL
1	N	498	GLU
1	O	3	LEU
1	O	17	ASN
1	O	31	THR
1	O	38	LYS
1	O	40	LEU
1	O	118	LYS
1	O	158	GLU
1	O	177	VAL
1	O	179	LEU
1	O	214	ARG
1	O	223	ARG
1	O	224	LYS
1	O	240	GLU
1	O	265	LEU
1	O	267	VAL
1	O	269	ILE
1	O	304	TYR
1	O	335	LYS
1	O	345	TYR
1	O	366	ILE
1	O	372	ILE
1	O	374	MET
1	O	382	SER
1	O	394	LYS
1	O	396	MET
1	O	398	VAL
1	O	404	ARG
1	O	424	ARG
1	O	435	GLN
1	O	446	LYS

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Mol	Chain	Res	Type
1	O	451	GLU
1	O	453	LYS
1	O	454	GLU
1	O	466	SER
1	O	467	LYS
1	O	471	GLN
1	O	472	THR
1	O	490	ASN
1	O	495	LEU
1	O	497	VAL
1	O	498	GLU
1	P	3	LEU
1	P	12	PHE
1	P	17	ASN
1	P	31	THR
1	P	38	LYS
1	P	40	LEU
1	P	118	LYS
1	P	177	VAL
1	P	179	LEU
1	P	214	ARG
1	P	223	ARG
1	P	224	LYS
1	P	240	GLU
1	P	265	LEU
1	P	267	VAL
1	P	269	ILE
1	P	273	LYS
1	P	304	TYR
1	P	335	LYS
1	P	345	TYR
1	P	366	ILE
1	P	371	HIS
1	P	372	ILE
1	P	382	SER
1	P	394	LYS
1	P	396	MET
1	P	398	VAL
1	P	424	ARG
1	P	435	GLN
1	P	446	LYS
1	P	451	GLU

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Mol	Chain	Res	Type
1	P	453	LYS
1	P	454	GLU
1	P	466	SER
1	P	467	LYS
1	P	471	GLN
1	P	472	THR
1	P	490	ASN
1	P	495	LEU
1	P	497	VAL
1	P	498	GLU
1	Q	3	LEU
1	Q	12	PHE
1	Q	17	ASN
1	Q	31	THR
1	Q	38	LYS
1	Q	40	LEU
1	Q	118	LYS
1	Q	177	VAL
1	Q	179	LEU
1	Q	214	ARG
1	Q	223	ARG
1	Q	224	LYS
1	Q	240	GLU
1	Q	265	LEU
1	Q	267	VAL
1	Q	269	ILE
1	Q	304	TYR
1	Q	335	LYS
1	Q	345	TYR
1	Q	366	ILE
1	Q	372	ILE
1	Q	374	MET
1	Q	382	SER
1	Q	394	LYS
1	Q	396	MET
1	Q	398	VAL
1	Q	424	ARG
1	Q	435	GLN
1	Q	446	LYS
1	Q	451	GLU
1	Q	453	LYS
1	Q	454	GLU

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Mol	Chain	Res	Type
1	Q	466	SER
1	Q	467	LYS
1	Q	471	GLN
1	Q	472	THR
1	Q	490	ASN
1	Q	495	LEU
1	Q	497	VAL
1	Q	498	GLU
1	R	3	LEU
1	R	17	ASN
1	R	31	THR
1	R	38	LYS
1	R	40	LEU
1	R	118	LYS
1	R	177	VAL
1	R	179	LEU
1	R	214	ARG
1	R	223	ARG
1	R	224	LYS
1	R	240	GLU
1	R	265	LEU
1	R	267	VAL
1	R	269	ILE
1	R	273	LYS
1	R	297	GLN
1	R	304	TYR
1	R	335	LYS
1	R	345	TYR
1	R	366	ILE
1	R	372	ILE
1	R	382	SER
1	R	394	LYS
1	R	396	MET
1	R	398	VAL
1	R	424	ARG
1	R	435	GLN
1	R	446	LYS
1	R	451	GLU
1	R	453	LYS
1	R	454	GLU
1	R	466	SER
1	R	467	LYS

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Mol	Chain	Res	Type
1	R	471	GLN
1	R	472	THR
1	R	490	ASN
1	R	495	LEU
1	R	497	VAL
1	R	498	GLU
1	S	3	LEU
1	S	12	PHE
1	S	17	ASN
1	S	31	THR
1	S	38	LYS
1	S	40	LEU
1	S	118	LYS
1	S	177	VAL
1	S	179	LEU
1	S	214	ARG
1	S	223	ARG
1	S	224	LYS
1	S	240	GLU
1	S	265	LEU
1	S	267	VAL
1	S	269	ILE
1	S	273	LYS
1	S	304	TYR
1	S	335	LYS
1	S	345	TYR
1	S	366	ILE
1	S	371	HIS
1	S	374	MET
1	S	382	SER
1	S	394	LYS
1	S	396	MET
1	S	398	VAL
1	S	424	ARG
1	S	435	GLN
1	S	446	LYS
1	S	451	GLU
1	S	453	LYS
1	S	454	GLU
1	S	466	SER
1	S	467	LYS
1	S	471	GLN

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Mol	Chain	Res	Type
1	S	472	THR
1	S	490	ASN
1	S	495	LEU
1	S	497	VAL
1	S	498	GLU
1	T	3	LEU
1	T	12	PHE
1	T	17	ASN
1	T	31	THR
1	T	38	LYS
1	T	40	LEU
1	T	118	LYS
1	T	177	VAL
1	T	179	LEU
1	T	214	ARG
1	T	223	ARG
1	T	224	LYS
1	T	240	GLU
1	T	265	LEU
1	T	267	VAL
1	T	269	ILE
1	T	304	TYR
1	T	335	LYS
1	T	345	TYR
1	T	366	ILE
1	T	371	HIS
1	T	372	ILE
1	T	374	MET
1	T	382	SER
1	T	394	LYS
1	T	396	MET
1	T	398	VAL
1	T	424	ARG
1	T	435	GLN
1	T	446	LYS
1	T	451	GLU
1	T	453	LYS
1	T	454	GLU
1	T	466	SER
1	T	467	LYS
1	T	471	GLN
1	T	472	THR

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Mol	Chain	Res	Type
1	T	490	ASN
1	T	495	LEU
1	T	497	VAL
1	T	498	GLU
1	U	3	LEU
1	U	17	ASN
1	U	31	THR
1	U	38	LYS
1	U	40	LEU
1	U	118	LYS
1	U	177	VAL
1	U	179	LEU
1	U	214	ARG
1	U	223	ARG
1	U	224	LYS
1	U	240	GLU
1	U	265	LEU
1	U	267	VAL
1	U	269	ILE
1	U	304	TYR
1	U	335	LYS
1	U	345	TYR
1	U	366	ILE
1	U	371	HIS
1	U	372	ILE
1	U	374	MET
1	U	382	SER
1	U	394	LYS
1	U	396	MET
1	U	398	VAL
1	U	404	ARG
1	U	424	ARG
1	U	435	GLN
1	U	446	LYS
1	U	451	GLU
1	U	453	LYS
1	U	454	GLU
1	U	466	SER
1	U	467	LYS
1	U	471	GLN
1	U	472	THR
1	U	490	ASN

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Mol	Chain	Res	Type
1	U	495	LEU
1	U	497	VAL
1	U	498	GLU
1	V	3	LEU
1	V	17	ASN
1	V	31	THR
1	V	38	LYS
1	V	40	LEU
1	V	118	LYS
1	V	177	VAL
1	V	179	LEU
1	V	214	ARG
1	V	223	ARG
1	V	224	LYS
1	V	240	GLU
1	V	265	LEU
1	V	267	VAL
1	V	269	ILE
1	V	273	LYS
1	V	297	GLN
1	V	304	TYR
1	V	335	LYS
1	V	345	TYR
1	V	366	ILE
1	V	372	ILE
1	V	374	MET
1	V	382	SER
1	V	394	LYS
1	V	396	MET
1	V	398	VAL
1	V	424	ARG
1	V	435	GLN
1	V	446	LYS
1	V	451	GLU
1	V	453	LYS
1	V	454	GLU
1	V	466	SER
1	V	467	LYS
1	V	471	GLN
1	V	472	THR
1	V	490	ASN
1	V	495	LEU

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Mol	Chain	Res	Type
1	V	497	VAL
1	V	498	GLU
1	W	3	LEU
1	W	12	PHE
1	W	17	ASN
1	W	31	THR
1	W	38	LYS
1	W	40	LEU
1	W	118	LYS
1	W	177	VAL
1	W	179	LEU
1	W	214	ARG
1	W	223	ARG
1	W	224	LYS
1	W	240	GLU
1	W	265	LEU
1	W	267	VAL
1	W	269	ILE
1	W	273	LYS
1	W	304	TYR
1	W	335	LYS
1	W	345	TYR
1	W	366	ILE
1	W	372	ILE
1	W	374	MET
1	W	382	SER
1	W	394	LYS
1	W	396	MET
1	W	398	VAL
1	W	404	ARG
1	W	424	ARG
1	W	435	GLN
1	W	446	LYS
1	W	451	GLU
1	W	453	LYS
1	W	454	GLU
1	W	466	SER
1	W	467	LYS
1	W	471	GLN
1	W	472	THR
1	W	490	ASN
1	W	495	LEU

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Mol	Chain	Res	Type
1	W	497	VAL
1	W	498	GLU
1	X	17	ASN
1	X	31	THR
1	X	38	LYS
1	X	40	LEU
1	X	118	LYS
1	X	177	VAL
1	X	179	LEU
1	X	214	ARG
1	X	223	ARG
1	X	224	LYS
1	X	240	GLU
1	X	265	LEU
1	X	267	VAL
1	X	269	ILE
1	X	304	TYR
1	X	335	LYS
1	X	345	TYR
1	X	366	ILE
1	X	372	ILE
1	X	374	MET
1	X	382	SER
1	X	394	LYS
1	X	396	MET
1	X	398	VAL
1	X	424	ARG
1	X	435	GLN
1	X	446	LYS
1	X	451	GLU
1	X	453	LYS
1	X	454	GLU
1	X	466	SER
1	X	467	LYS
1	X	471	GLN
1	X	472	THR
1	X	490	ASN
1	X	495	LEU
1	X	497	VAL
1	X	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (431) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	5	HIS
1	A	17	ASN
1	A	93	GLN
1	A	139	ASN
1	A	151	GLN
1	A	178	ASN
1	A	218	GLN
1	A	246	GLN
1	A	286	ASN
1	A	305	ASN
1	A	318	ASN
1	A	340	ASN
1	A	371	HIS
1	A	435	GLN
1	A	490	ASN
1	B	2	GLN
1	B	5	HIS
1	B	17	ASN
1	B	93	GLN
1	B	139	ASN
1	B	151	GLN
1	B	178	ASN
1	B	218	GLN
1	B	242	HIS
1	B	246	GLN
1	B	278	GLN
1	B	286	ASN
1	B	305	ASN
1	B	322	ASN
1	B	340	ASN
1	B	371	HIS
1	B	435	GLN
1	B	490	ASN
1	C	2	GLN
1	C	5	HIS
1	C	17	ASN
1	C	93	GLN
1	C	139	ASN
1	C	151	GLN
1	C	178	ASN
1	C	218	GLN
1	C	242	HIS

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Mol	Chain	Res	Type
1	C	246	GLN
1	C	286	ASN
1	C	305	ASN
1	C	340	ASN
1	C	371	HIS
1	C	435	GLN
1	C	483	HIS
1	C	490	ASN
1	D	2	GLN
1	D	5	HIS
1	D	17	ASN
1	D	93	GLN
1	D	139	ASN
1	D	151	GLN
1	D	178	ASN
1	D	218	GLN
1	D	242	HIS
1	D	246	GLN
1	D	278	GLN
1	D	286	ASN
1	D	305	ASN
1	D	322	ASN
1	D	340	ASN
1	D	371	HIS
1	D	435	GLN
1	D	483	HIS
1	D	490	ASN
1	E	2	GLN
1	E	5	HIS
1	E	17	ASN
1	E	93	GLN
1	E	139	ASN
1	E	151	GLN
1	E	178	ASN
1	E	218	GLN
1	E	242	HIS
1	E	246	GLN
1	E	278	GLN
1	E	286	ASN
1	E	305	ASN
1	E	322	ASN
1	E	340	ASN

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Mol	Chain	Res	Type
1	E	371	HIS
1	E	435	GLN
1	E	483	HIS
1	E	490	ASN
1	F	2	GLN
1	F	5	HIS
1	F	17	ASN
1	F	93	GLN
1	F	139	ASN
1	F	151	GLN
1	F	178	ASN
1	F	218	GLN
1	F	242	HIS
1	F	246	GLN
1	F	278	GLN
1	F	286	ASN
1	F	305	ASN
1	F	322	ASN
1	F	340	ASN
1	F	371	HIS
1	F	435	GLN
1	F	483	HIS
1	F	490	ASN
1	G	2	GLN
1	G	5	HIS
1	G	17	ASN
1	G	93	GLN
1	G	139	ASN
1	G	151	GLN
1	G	178	ASN
1	G	218	GLN
1	G	246	GLN
1	G	286	ASN
1	G	305	ASN
1	G	340	ASN
1	G	371	HIS
1	G	435	GLN
1	G	483	HIS
1	G	490	ASN
1	G	491	GLN
1	H	2	GLN
1	H	5	HIS

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Mol	Chain	Res	Type
1	H	17	ASN
1	H	93	GLN
1	H	139	ASN
1	H	151	GLN
1	H	178	ASN
1	H	218	GLN
1	H	242	HIS
1	H	246	GLN
1	H	286	ASN
1	H	305	ASN
1	H	318	ASN
1	H	340	ASN
1	H	371	HIS
1	H	435	GLN
1	H	483	HIS
1	H	490	ASN
1	I	2	GLN
1	I	5	HIS
1	I	17	ASN
1	I	93	GLN
1	I	139	ASN
1	I	151	GLN
1	I	178	ASN
1	I	218	GLN
1	I	242	HIS
1	I	246	GLN
1	I	286	ASN
1	I	305	ASN
1	I	318	ASN
1	I	340	ASN
1	I	371	HIS
1	I	435	GLN
1	I	483	HIS
1	I	490	ASN
1	J	2	GLN
1	J	5	HIS
1	J	17	ASN
1	J	93	GLN
1	J	139	ASN
1	J	151	GLN
1	J	178	ASN
1	J	218	GLN

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Mol	Chain	Res	Type
1	J	242	HIS
1	J	246	GLN
1	J	286	ASN
1	J	297	GLN
1	J	305	ASN
1	J	318	ASN
1	J	340	ASN
1	J	371	HIS
1	J	435	GLN
1	J	490	ASN
1	K	2	GLN
1	K	5	HIS
1	K	17	ASN
1	K	93	GLN
1	K	139	ASN
1	K	151	GLN
1	K	178	ASN
1	K	218	GLN
1	K	242	HIS
1	K	246	GLN
1	K	278	GLN
1	K	286	ASN
1	K	305	ASN
1	K	318	ASN
1	K	322	ASN
1	K	340	ASN
1	K	371	HIS
1	K	435	GLN
1	K	483	HIS
1	K	490	ASN
1	L	2	GLN
1	L	5	HIS
1	L	17	ASN
1	L	93	GLN
1	L	139	ASN
1	L	151	GLN
1	L	178	ASN
1	L	218	GLN
1	L	242	HIS
1	L	246	GLN
1	L	286	ASN
1	L	305	ASN

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Mol	Chain	Res	Type
1	L	340	ASN
1	L	371	HIS
1	L	435	GLN
1	L	483	HIS
1	L	490	ASN
1	M	2	GLN
1	M	5	HIS
1	M	17	ASN
1	M	93	GLN
1	M	139	ASN
1	M	151	GLN
1	M	178	ASN
1	M	218	GLN
1	M	242	HIS
1	M	246	GLN
1	M	286	ASN
1	M	305	ASN
1	M	340	ASN
1	M	371	HIS
1	M	435	GLN
1	M	483	HIS
1	M	490	ASN
1	N	2	GLN
1	N	5	HIS
1	N	17	ASN
1	N	93	GLN
1	N	139	ASN
1	N	151	GLN
1	N	178	ASN
1	N	218	GLN
1	N	242	HIS
1	N	246	GLN
1	N	286	ASN
1	N	305	ASN
1	N	340	ASN
1	N	371	HIS
1	N	435	GLN
1	N	483	HIS
1	N	490	ASN
1	N	491	GLN
1	O	2	GLN
1	O	5	HIS

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Mol	Chain	Res	Type
1	O	17	ASN
1	O	93	GLN
1	O	139	ASN
1	O	151	GLN
1	O	178	ASN
1	O	218	GLN
1	O	242	HIS
1	O	246	GLN
1	O	286	ASN
1	O	305	ASN
1	O	318	ASN
1	O	340	ASN
1	O	371	HIS
1	O	435	GLN
1	O	490	ASN
1	P	2	GLN
1	P	5	HIS
1	P	17	ASN
1	P	93	GLN
1	P	139	ASN
1	P	151	GLN
1	P	178	ASN
1	P	218	GLN
1	P	242	HIS
1	P	246	GLN
1	P	278	GLN
1	P	286	ASN
1	P	305	ASN
1	P	318	ASN
1	P	322	ASN
1	P	340	ASN
1	P	371	HIS
1	P	435	GLN
1	P	483	HIS
1	P	490	ASN
1	Q	2	GLN
1	Q	5	HIS
1	Q	17	ASN
1	Q	93	GLN
1	Q	139	ASN
1	Q	151	GLN
1	Q	178	ASN

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Mol	Chain	Res	Type
1	Q	218	GLN
1	Q	242	HIS
1	Q	246	GLN
1	Q	286	ASN
1	Q	305	ASN
1	Q	340	ASN
1	Q	371	HIS
1	Q	435	GLN
1	Q	483	HIS
1	Q	490	ASN
1	R	2	GLN
1	R	5	HIS
1	R	17	ASN
1	R	93	GLN
1	R	139	ASN
1	R	151	GLN
1	R	178	ASN
1	R	218	GLN
1	R	242	HIS
1	R	246	GLN
1	R	286	ASN
1	R	297	GLN
1	R	305	ASN
1	R	318	ASN
1	R	340	ASN
1	R	371	HIS
1	R	435	GLN
1	R	483	HIS
1	R	490	ASN
1	S	2	GLN
1	S	5	HIS
1	S	17	ASN
1	S	93	GLN
1	S	139	ASN
1	S	151	GLN
1	S	178	ASN
1	S	218	GLN
1	S	242	HIS
1	S	246	GLN
1	S	286	ASN
1	S	305	ASN
1	S	340	ASN

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Mol	Chain	Res	Type
1	S	371	HIS
1	S	435	GLN
1	S	490	ASN
1	T	5	HIS
1	T	17	ASN
1	T	93	GLN
1	T	139	ASN
1	T	151	GLN
1	T	178	ASN
1	T	218	GLN
1	T	246	GLN
1	T	286	ASN
1	T	305	ASN
1	T	340	ASN
1	T	371	HIS
1	T	435	GLN
1	T	483	HIS
1	T	490	ASN
1	T	491	GLN
1	U	2	GLN
1	U	5	HIS
1	U	17	ASN
1	U	93	GLN
1	U	139	ASN
1	U	151	GLN
1	U	178	ASN
1	U	218	GLN
1	U	242	HIS
1	U	246	GLN
1	U	286	ASN
1	U	305	ASN
1	U	318	ASN
1	U	340	ASN
1	U	371	HIS
1	U	435	GLN
1	U	483	HIS
1	U	490	ASN
1	V	2	GLN
1	V	5	HIS
1	V	17	ASN
1	V	93	GLN
1	V	139	ASN

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Mol	Chain	Res	Type
1	V	151	GLN
1	V	178	ASN
1	V	218	GLN
1	V	242	HIS
1	V	246	GLN
1	V	278	GLN
1	V	286	ASN
1	V	297	GLN
1	V	305	ASN
1	V	322	ASN
1	V	340	ASN
1	V	371	HIS
1	V	435	GLN
1	V	483	HIS
1	V	490	ASN
1	W	2	GLN
1	W	5	HIS
1	W	17	ASN
1	W	93	GLN
1	W	139	ASN
1	W	151	GLN
1	W	178	ASN
1	W	218	GLN
1	W	242	HIS
1	W	246	GLN
1	W	278	GLN
1	W	286	ASN
1	W	305	ASN
1	W	318	ASN
1	W	322	ASN
1	W	340	ASN
1	W	371	HIS
1	W	435	GLN
1	W	483	HIS
1	W	490	ASN
1	X	2	GLN
1	X	5	HIS
1	X	17	ASN
1	X	93	GLN
1	X	139	ASN
1	X	151	GLN
1	X	178	ASN

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Mol	Chain	Res	Type
1	X	218	GLN
1	X	242	HIS
1	X	246	GLN
1	X	286	ASN
1	X	305	ASN
1	X	340	ASN
1	X	371	HIS
1	X	435	GLN
1	X	483	HIS
1	X	490	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FDP	N	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	R	700	-	19,20,20	1.07	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	Q	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FDP	G	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	K	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	I	700	-	19,20,20	1.07	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	H	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	V	700	-	19,20,20	1.09	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	D	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	X	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	J	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	P	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	B	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	A	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	O	700	-	19,20,20	1.07	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	E	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	L	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	C	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	S	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	W	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	T	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	M	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	F	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	U	700	-	19,20,20	1.07	2 (10%)	29,32,32	1.40	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDP	N	700	-	-	1/12/34/34	0/1/1/1
2	FDP	R	700	-	-	1/12/34/34	0/1/1/1
2	FDP	Q	700	-	-	1/12/34/34	0/1/1/1
2	FDP	G	700	-	-	1/12/34/34	0/1/1/1
2	FDP	K	700	-	-	1/12/34/34	0/1/1/1
2	FDP	I	700	-	-	1/12/34/34	0/1/1/1
2	FDP	H	700	-	-	1/12/34/34	0/1/1/1
2	FDP	V	700	-	-	1/12/34/34	0/1/1/1
2	FDP	D	700	-	-	1/12/34/34	0/1/1/1
2	FDP	X	700	-	-	1/12/34/34	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDP	J	700	-	-	1/12/34/34	0/1/1/1
2	FDP	P	700	-	-	1/12/34/34	0/1/1/1
2	FDP	B	700	-	-	1/12/34/34	0/1/1/1
2	FDP	A	700	-	-	1/12/34/34	0/1/1/1
2	FDP	O	700	-	-	1/12/34/34	0/1/1/1
2	FDP	E	700	-	-	1/12/34/34	0/1/1/1
2	FDP	L	700	-	-	1/12/34/34	0/1/1/1
2	FDP	C	700	-	-	1/12/34/34	0/1/1/1
2	FDP	S	700	-	-	1/12/34/34	0/1/1/1
2	FDP	W	700	-	-	1/12/34/34	0/1/1/1
2	FDP	T	700	-	-	1/12/34/34	0/1/1/1
2	FDP	M	700	-	-	1/12/34/34	0/1/1/1
2	FDP	F	700	-	-	1/12/34/34	0/1/1/1
2	FDP	U	700	-	-	1/12/34/34	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	700	FDP	O4-C4	-2.35	1.37	1.43
2	X	700	FDP	O4-C4	-2.34	1.37	1.43
2	A	700	FDP	O4-C4	-2.34	1.37	1.43
2	W	700	FDP	O4-C4	-2.34	1.37	1.43
2	E	700	FDP	O4-C4	-2.34	1.37	1.43
2	C	700	FDP	O4-C4	-2.33	1.37	1.43
2	V	700	FDP	O4-C4	-2.33	1.37	1.43
2	M	700	FDP	O4-C4	-2.32	1.37	1.43
2	D	700	FDP	O4-C4	-2.32	1.37	1.43
2	N	700	FDP	O4-C4	-2.32	1.37	1.43
2	F	700	FDP	O4-C4	-2.32	1.37	1.43
2	L	700	FDP	O4-C4	-2.32	1.37	1.43
2	B	700	FDP	O4-C4	-2.31	1.37	1.43
2	P	700	FDP	O4-C4	-2.31	1.37	1.43
2	J	700	FDP	O4-C4	-2.31	1.37	1.43
2	I	700	FDP	O4-C4	-2.31	1.37	1.43
2	N	700	FDP	P2-O5P	-2.31	1.46	1.54
2	E	700	FDP	P2-O5P	-2.31	1.46	1.54
2	Q	700	FDP	O4-C4	-2.31	1.37	1.43
2	O	700	FDP	O4-C4	-2.30	1.37	1.43
2	H	700	FDP	P2-O5P	-2.30	1.46	1.54
2	G	700	FDP	O4-C4	-2.30	1.37	1.43
2	P	700	FDP	P2-O5P	-2.30	1.46	1.54
2	S	700	FDP	O4-C4	-2.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	700	FDP	O4-C4	-2.30	1.37	1.43
2	Q	700	FDP	P2-O5P	-2.30	1.46	1.54
2	T	700	FDP	O4-C4	-2.29	1.37	1.43
2	H	700	FDP	O4-C4	-2.29	1.37	1.43
2	T	700	FDP	P2-O5P	-2.29	1.46	1.54
2	W	700	FDP	P2-O5P	-2.29	1.46	1.54
2	R	700	FDP	O4-C4	-2.29	1.37	1.43
2	A	700	FDP	P2-O5P	-2.29	1.46	1.54
2	U	700	FDP	P2-O5P	-2.29	1.46	1.54
2	M	700	FDP	P2-O5P	-2.29	1.46	1.54
2	K	700	FDP	P2-O5P	-2.28	1.46	1.54
2	X	700	FDP	P2-O5P	-2.28	1.46	1.54
2	I	700	FDP	P2-O5P	-2.28	1.46	1.54
2	G	700	FDP	P2-O5P	-2.28	1.46	1.54
2	V	700	FDP	P2-O5P	-2.28	1.46	1.54
2	C	700	FDP	P2-O5P	-2.28	1.46	1.54
2	J	700	FDP	P2-O5P	-2.28	1.46	1.54
2	R	700	FDP	P2-O5P	-2.28	1.46	1.54
2	S	700	FDP	P2-O5P	-2.28	1.46	1.54
2	O	700	FDP	P2-O5P	-2.28	1.46	1.54
2	D	700	FDP	P2-O5P	-2.28	1.46	1.54
2	L	700	FDP	P2-O5P	-2.28	1.46	1.54
2	B	700	FDP	P2-O5P	-2.27	1.46	1.54
2	F	700	FDP	P2-O5P	-2.27	1.46	1.54

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	700	FDP	O2-C2-C3	3.29	118.53	108.28
2	E	700	FDP	O2-C2-C3	3.29	118.52	108.28
2	R	700	FDP	O2-C2-C3	3.29	118.52	108.28
2	F	700	FDP	O2-C2-C3	3.29	118.52	108.28
2	I	700	FDP	O2-C2-C3	3.28	118.51	108.28
2	J	700	FDP	O2-C2-C3	3.28	118.50	108.28
2	W	700	FDP	O2-C2-C3	3.28	118.50	108.28
2	K	700	FDP	O2-C2-C3	3.28	118.50	108.28
2	V	700	FDP	O2-C2-C3	3.28	118.50	108.28
2	C	700	FDP	O2-C2-C3	3.28	118.49	108.28
2	G	700	FDP	O2-C2-C3	3.28	118.49	108.28
2	Q	700	FDP	O2-C2-C3	3.28	118.49	108.28
2	B	700	FDP	O2-C2-C3	3.28	118.48	108.28
2	H	700	FDP	O2-C2-C3	3.27	118.48	108.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	700	FDP	O2-C2-C3	3.27	118.48	108.28
2	A	700	FDP	O2-C2-C3	3.27	118.46	108.28
2	M	700	FDP	O2-C2-C3	3.27	118.46	108.28
2	S	700	FDP	O2-C2-C3	3.27	118.46	108.28
2	X	700	FDP	O2-C2-C3	3.27	118.46	108.28
2	L	700	FDP	O2-C2-C3	3.27	118.45	108.28
2	U	700	FDP	O2-C2-C3	3.26	118.45	108.28
2	P	700	FDP	O2-C2-C3	3.26	118.44	108.28
2	N	700	FDP	O2-C2-C3	3.26	118.43	108.28
2	D	700	FDP	O2-C2-C3	3.26	118.43	108.28
2	V	700	FDP	O6-P2-O4P	3.20	115.10	106.44
2	O	700	FDP	O6-P2-O4P	3.20	115.09	106.44
2	M	700	FDP	O6-P2-O4P	3.20	115.09	106.44
2	X	700	FDP	O6-P2-O4P	3.20	115.09	106.44
2	F	700	FDP	O6-P2-O4P	3.20	115.08	106.44
2	I	700	FDP	O6-P2-O4P	3.19	115.07	106.44
2	S	700	FDP	O6-P2-O4P	3.19	115.07	106.44
2	B	700	FDP	O6-P2-O4P	3.19	115.07	106.44
2	Q	700	FDP	O6-P2-O4P	3.19	115.06	106.44
2	G	700	FDP	O6-P2-O4P	3.19	115.06	106.44
2	L	700	FDP	O6-P2-O4P	3.19	115.06	106.44
2	R	700	FDP	O6-P2-O4P	3.18	115.05	106.44
2	J	700	FDP	O6-P2-O4P	3.18	115.04	106.44
2	T	700	FDP	O6-P2-O4P	3.18	115.04	106.44
2	A	700	FDP	O6-P2-O4P	3.18	115.03	106.44
2	U	700	FDP	O6-P2-O4P	3.18	115.03	106.44
2	E	700	FDP	O6-P2-O4P	3.18	115.03	106.44
2	K	700	FDP	O6-P2-O4P	3.18	115.03	106.44
2	D	700	FDP	O6-P2-O4P	3.18	115.03	106.44
2	P	700	FDP	O6-P2-O4P	3.18	115.02	106.44
2	H	700	FDP	O6-P2-O4P	3.17	115.01	106.44
2	C	700	FDP	O6-P2-O4P	3.17	115.01	106.44
2	N	700	FDP	O6-P2-O4P	3.17	115.00	106.44
2	W	700	FDP	O6-P2-O4P	3.17	115.00	106.44
2	F	700	FDP	C6-C5-C4	-2.76	105.28	115.21
2	X	700	FDP	C6-C5-C4	-2.76	105.29	115.21
2	W	700	FDP	C6-C5-C4	-2.75	105.30	115.21
2	O	700	FDP	C6-C5-C4	-2.75	105.30	115.21
2	Q	700	FDP	C6-C5-C4	-2.75	105.31	115.21
2	R	700	FDP	C6-C5-C4	-2.75	105.31	115.21
2	U	700	FDP	C6-C5-C4	-2.75	105.32	115.21
2	C	700	FDP	C6-C5-C4	-2.75	105.32	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	FDP	C6-C5-C4	-2.75	105.32	115.21
2	B	700	FDP	C6-C5-C4	-2.75	105.32	115.21
2	T	700	FDP	C6-C5-C4	-2.75	105.32	115.21
2	N	700	FDP	C6-C5-C4	-2.75	105.32	115.21
2	K	700	FDP	C6-C5-C4	-2.75	105.33	115.21
2	A	700	FDP	C6-C5-C4	-2.75	105.33	115.21
2	J	700	FDP	C6-C5-C4	-2.75	105.33	115.21
2	I	700	FDP	C6-C5-C4	-2.74	105.33	115.21
2	P	700	FDP	C6-C5-C4	-2.74	105.34	115.21
2	G	700	FDP	C6-C5-C4	-2.74	105.34	115.21
2	M	700	FDP	C6-C5-C4	-2.74	105.34	115.21
2	E	700	FDP	C6-C5-C4	-2.74	105.35	115.21
2	S	700	FDP	C6-C5-C4	-2.74	105.35	115.21
2	L	700	FDP	C6-C5-C4	-2.74	105.36	115.21
2	H	700	FDP	C6-C5-C4	-2.73	105.38	115.21
2	V	700	FDP	C6-C5-C4	-2.73	105.38	115.21
2	R	700	FDP	O5-C2-C3	-2.26	100.88	105.42
2	A	700	FDP	O5-C2-C3	-2.25	100.89	105.42
2	O	700	FDP	O5-C2-C3	-2.25	100.90	105.42
2	L	700	FDP	O5-C2-C3	-2.25	100.90	105.42
2	P	700	FDP	O5-C2-C3	-2.25	100.91	105.42
2	B	700	FDP	O5-C2-C3	-2.24	100.91	105.42
2	Q	700	FDP	O5-C2-C3	-2.24	100.92	105.42
2	I	700	FDP	O5-C2-C3	-2.24	100.92	105.42
2	K	700	FDP	O5-C2-C3	-2.24	100.93	105.42
2	V	700	FDP	O5-C2-C3	-2.23	100.93	105.42
2	F	700	FDP	O5-C2-C3	-2.23	100.93	105.42
2	U	700	FDP	O5-C2-C3	-2.23	100.94	105.42
2	S	700	FDP	O5-C2-C3	-2.23	100.94	105.42
2	T	700	FDP	O5-C2-C3	-2.23	100.94	105.42
2	M	700	FDP	O5-C2-C3	-2.23	100.95	105.42
2	N	700	FDP	O5-C2-C3	-2.22	100.95	105.42
2	H	700	FDP	O5-C2-C3	-2.22	100.95	105.42
2	E	700	FDP	O5-C2-C3	-2.22	100.96	105.42
2	J	700	FDP	O5-C2-C3	-2.22	100.96	105.42
2	D	700	FDP	O5-C2-C3	-2.22	100.96	105.42
2	C	700	FDP	O5-C2-C3	-2.22	100.97	105.42
2	G	700	FDP	O5-C2-C3	-2.22	100.97	105.42
2	X	700	FDP	O5-C2-C3	-2.22	100.97	105.42
2	W	700	FDP	O5-C2-C3	-2.21	100.97	105.42
2	K	700	FDP	C1-C2-C3	-2.11	108.62	114.83
2	H	700	FDP	C1-C2-C3	-2.11	108.62	114.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	700	FDP	C1-C2-C3	-2.11	108.63	114.83
2	J	700	FDP	C1-C2-C3	-2.11	108.63	114.83
2	G	700	FDP	C1-C2-C3	-2.11	108.64	114.83
2	S	700	FDP	C1-C2-C3	-2.11	108.64	114.83
2	B	700	FDP	C1-C2-C3	-2.11	108.64	114.83
2	W	700	FDP	C1-C2-C3	-2.10	108.64	114.83
2	E	700	FDP	C1-C2-C3	-2.10	108.65	114.83
2	I	700	FDP	C1-C2-C3	-2.10	108.65	114.83
2	N	700	FDP	C1-C2-C3	-2.10	108.65	114.83
2	D	700	FDP	C1-C2-C3	-2.10	108.66	114.83
2	A	700	FDP	C1-C2-C3	-2.10	108.66	114.83
2	F	700	FDP	C1-C2-C3	-2.10	108.66	114.83
2	U	700	FDP	C1-C2-C3	-2.10	108.67	114.83
2	C	700	FDP	C1-C2-C3	-2.10	108.67	114.83
2	Q	700	FDP	C1-C2-C3	-2.10	108.67	114.83
2	T	700	FDP	C1-C2-C3	-2.09	108.68	114.83
2	M	700	FDP	C1-C2-C3	-2.09	108.68	114.83
2	R	700	FDP	C1-C2-C3	-2.09	108.68	114.83
2	L	700	FDP	C1-C2-C3	-2.09	108.69	114.83
2	P	700	FDP	C1-C2-C3	-2.09	108.69	114.83
2	V	700	FDP	C1-C2-C3	-2.08	108.71	114.83
2	X	700	FDP	C1-C2-C3	-2.08	108.71	114.83

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	FDP	O1-C1-C2-C3
2	B	700	FDP	O1-C1-C2-C3
2	C	700	FDP	O1-C1-C2-C3
2	D	700	FDP	O1-C1-C2-C3
2	E	700	FDP	O1-C1-C2-C3
2	F	700	FDP	O1-C1-C2-C3
2	G	700	FDP	O1-C1-C2-C3
2	H	700	FDP	O1-C1-C2-C3
2	I	700	FDP	O1-C1-C2-C3
2	J	700	FDP	O1-C1-C2-C3
2	K	700	FDP	O1-C1-C2-C3
2	L	700	FDP	O1-C1-C2-C3
2	M	700	FDP	O1-C1-C2-C3
2	N	700	FDP	O1-C1-C2-C3
2	O	700	FDP	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	P	700	FDP	O1-C1-C2-C3
2	Q	700	FDP	O1-C1-C2-C3
2	R	700	FDP	O1-C1-C2-C3
2	S	700	FDP	O1-C1-C2-C3
2	T	700	FDP	O1-C1-C2-C3
2	U	700	FDP	O1-C1-C2-C3
2	V	700	FDP	O1-C1-C2-C3
2	W	700	FDP	O1-C1-C2-C3
2	X	700	FDP	O1-C1-C2-C3

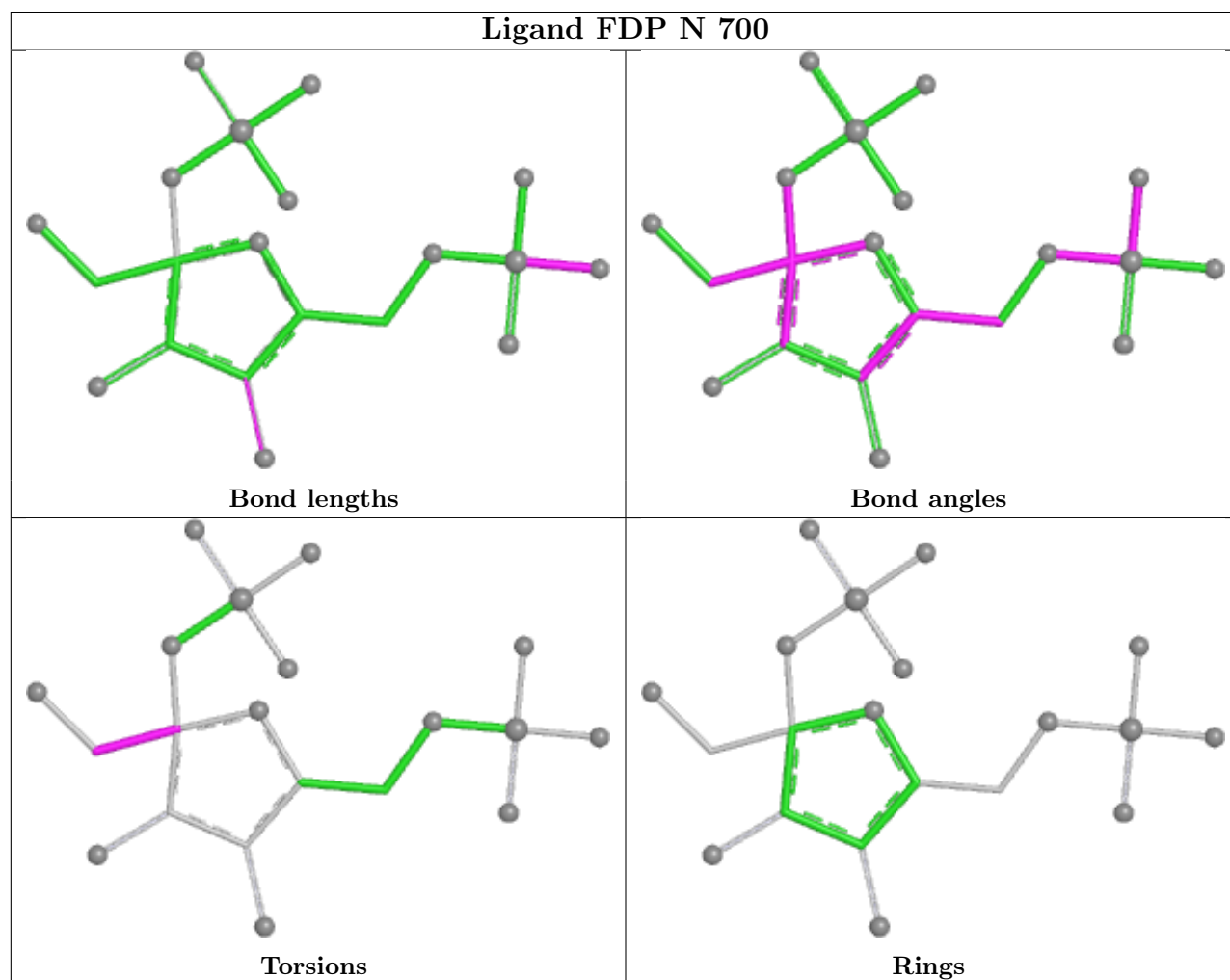
There are no ring outliers.

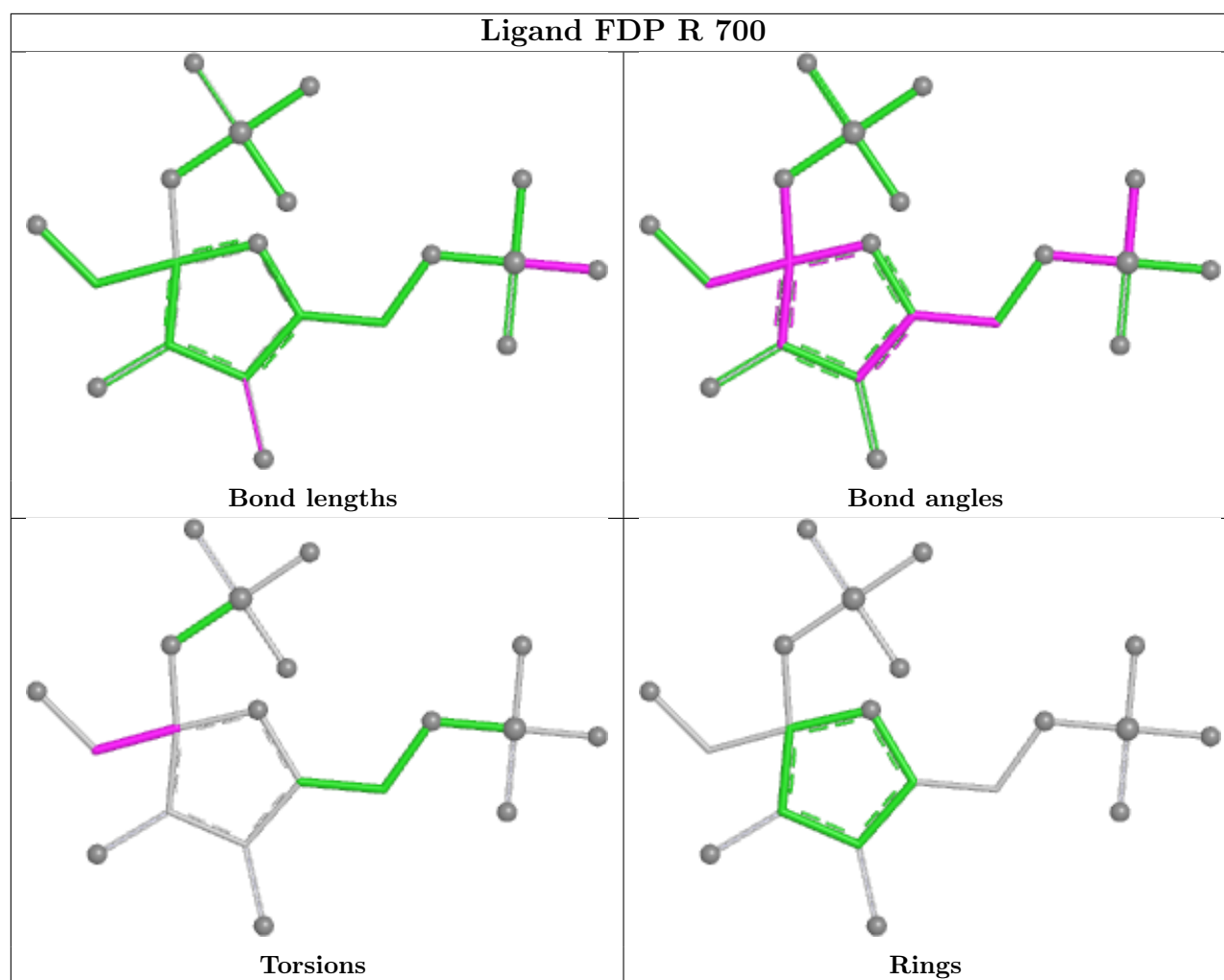
24 monomers are involved in 107 short contacts:

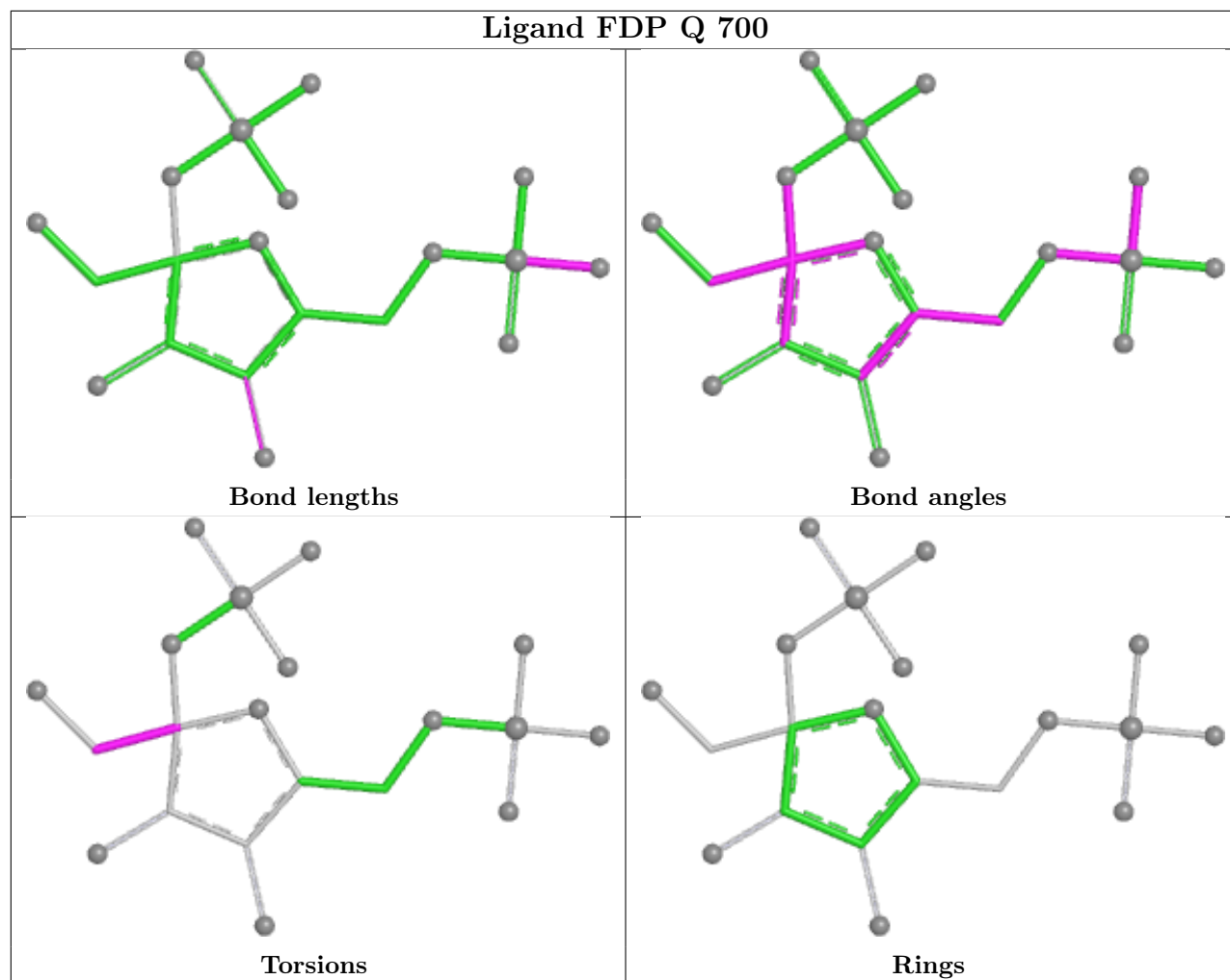
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	700	FDP	4	0
2	R	700	FDP	5	0
2	Q	700	FDP	4	0
2	G	700	FDP	4	0
2	K	700	FDP	5	0
2	I	700	FDP	5	0
2	H	700	FDP	5	0
2	V	700	FDP	5	0
2	D	700	FDP	4	0
2	X	700	FDP	5	0
2	J	700	FDP	4	0
2	P	700	FDP	5	0
2	B	700	FDP	4	0
2	A	700	FDP	4	0
2	O	700	FDP	5	0
2	E	700	FDP	4	0
2	L	700	FDP	5	0
2	C	700	FDP	4	0
2	S	700	FDP	4	0
2	W	700	FDP	5	0
2	T	700	FDP	5	0
2	M	700	FDP	4	0
2	F	700	FDP	4	0
2	U	700	FDP	4	0

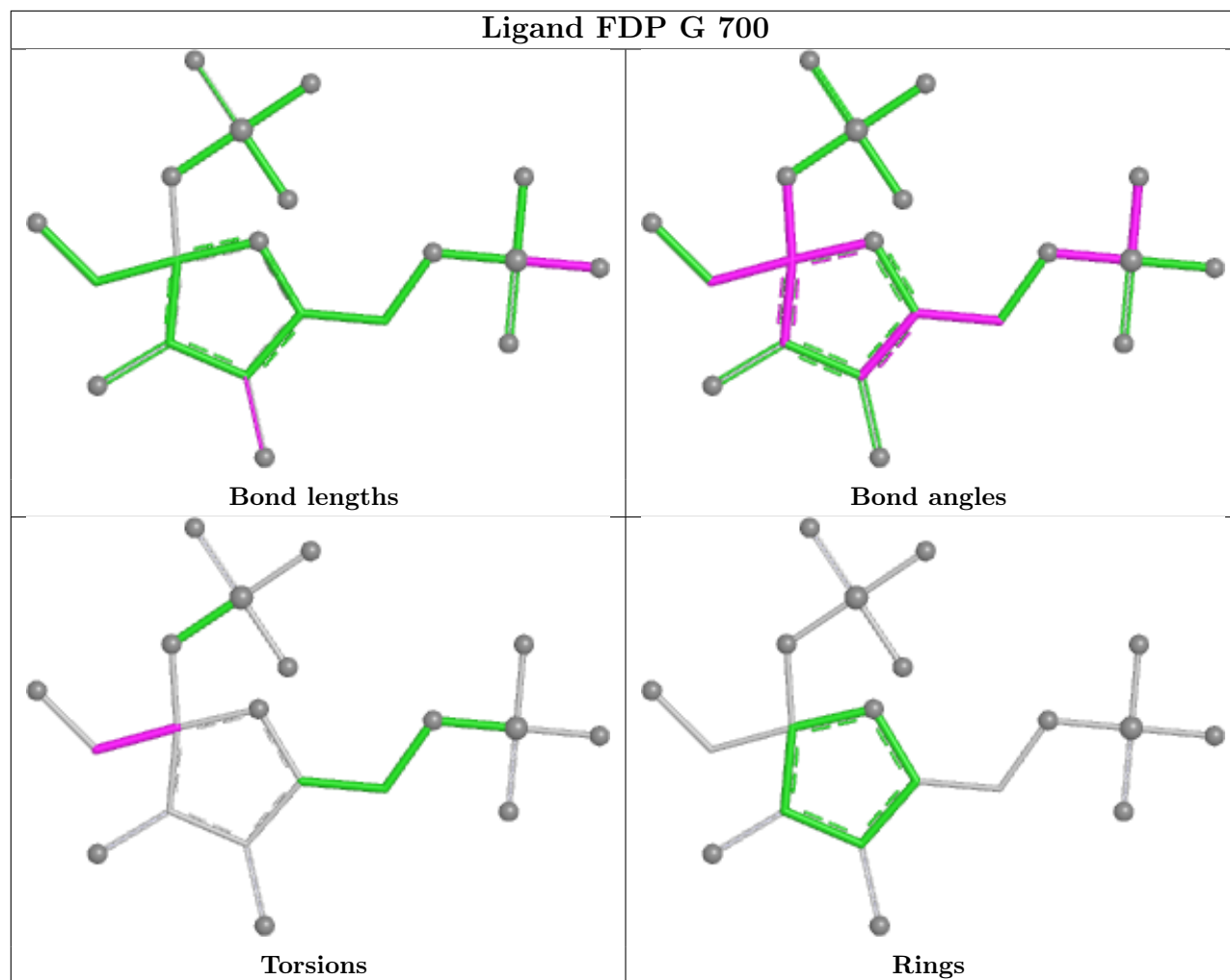
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

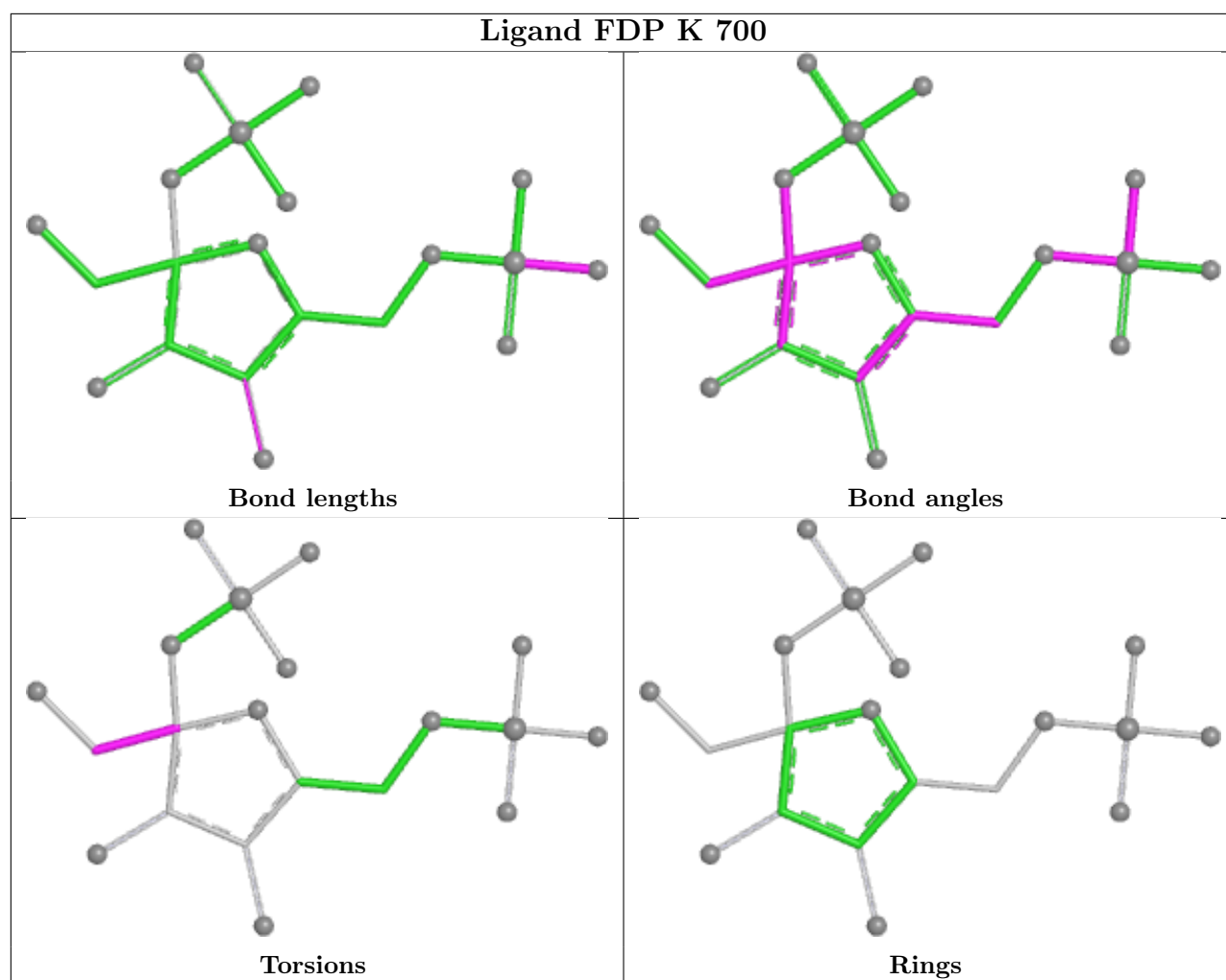
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



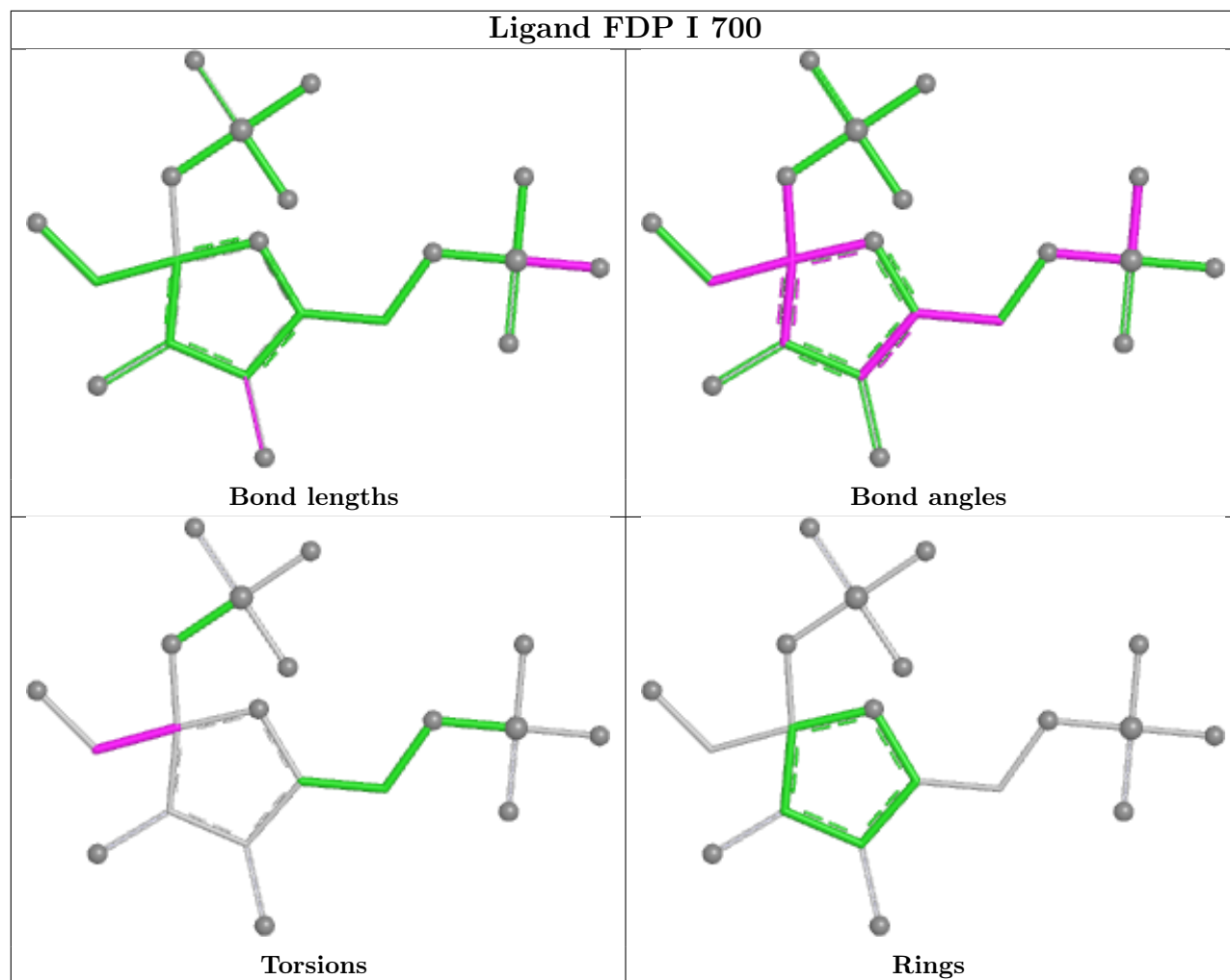


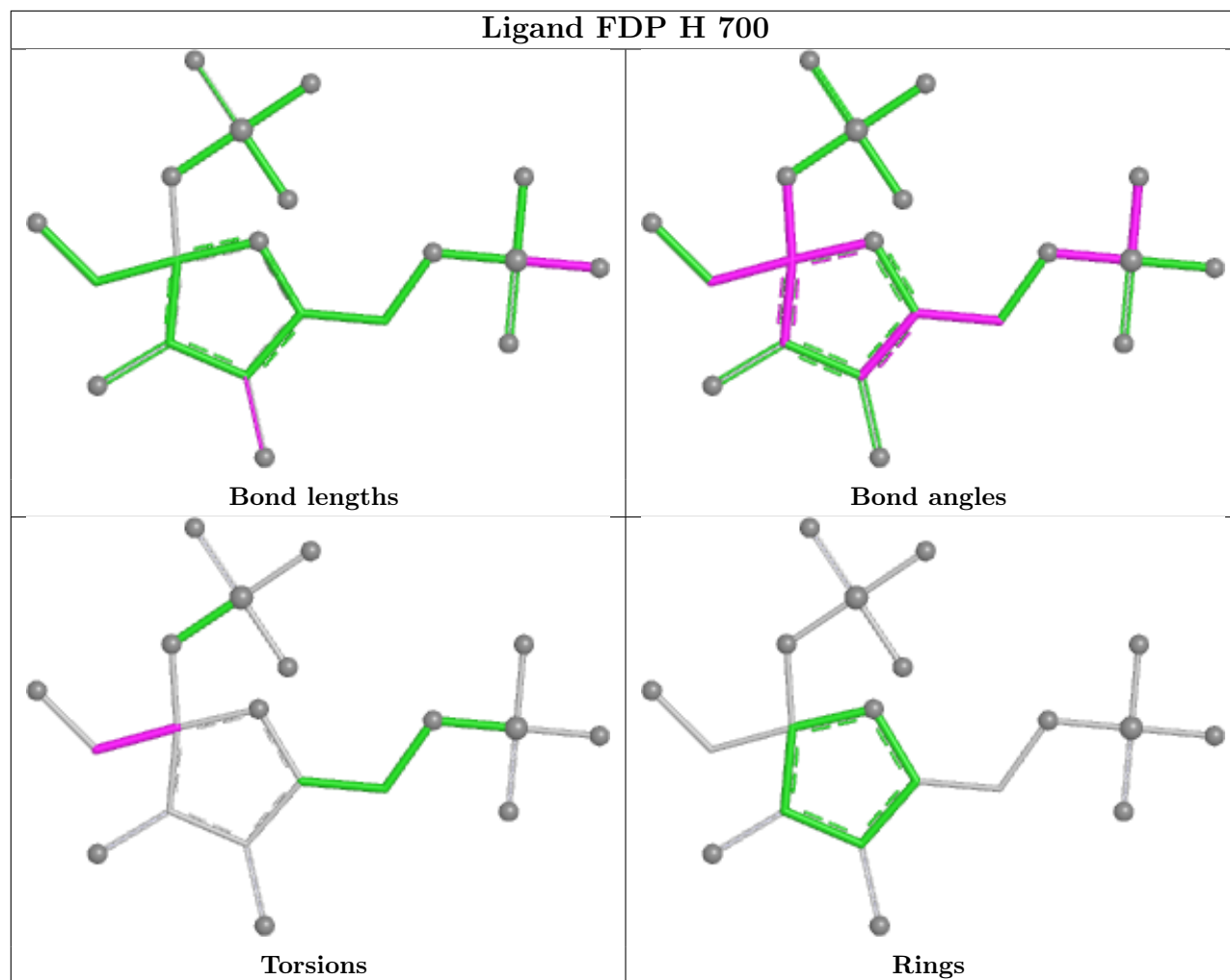


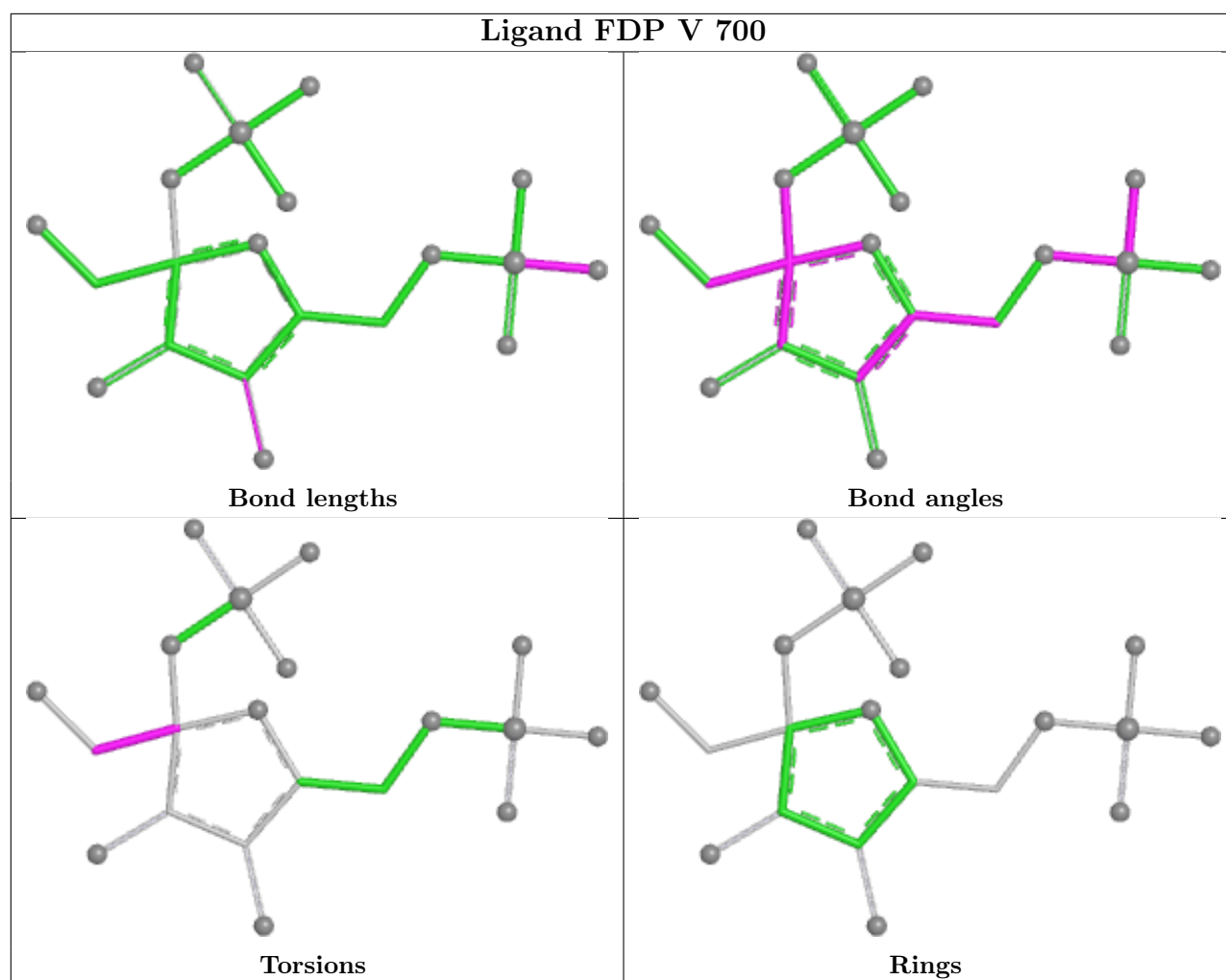


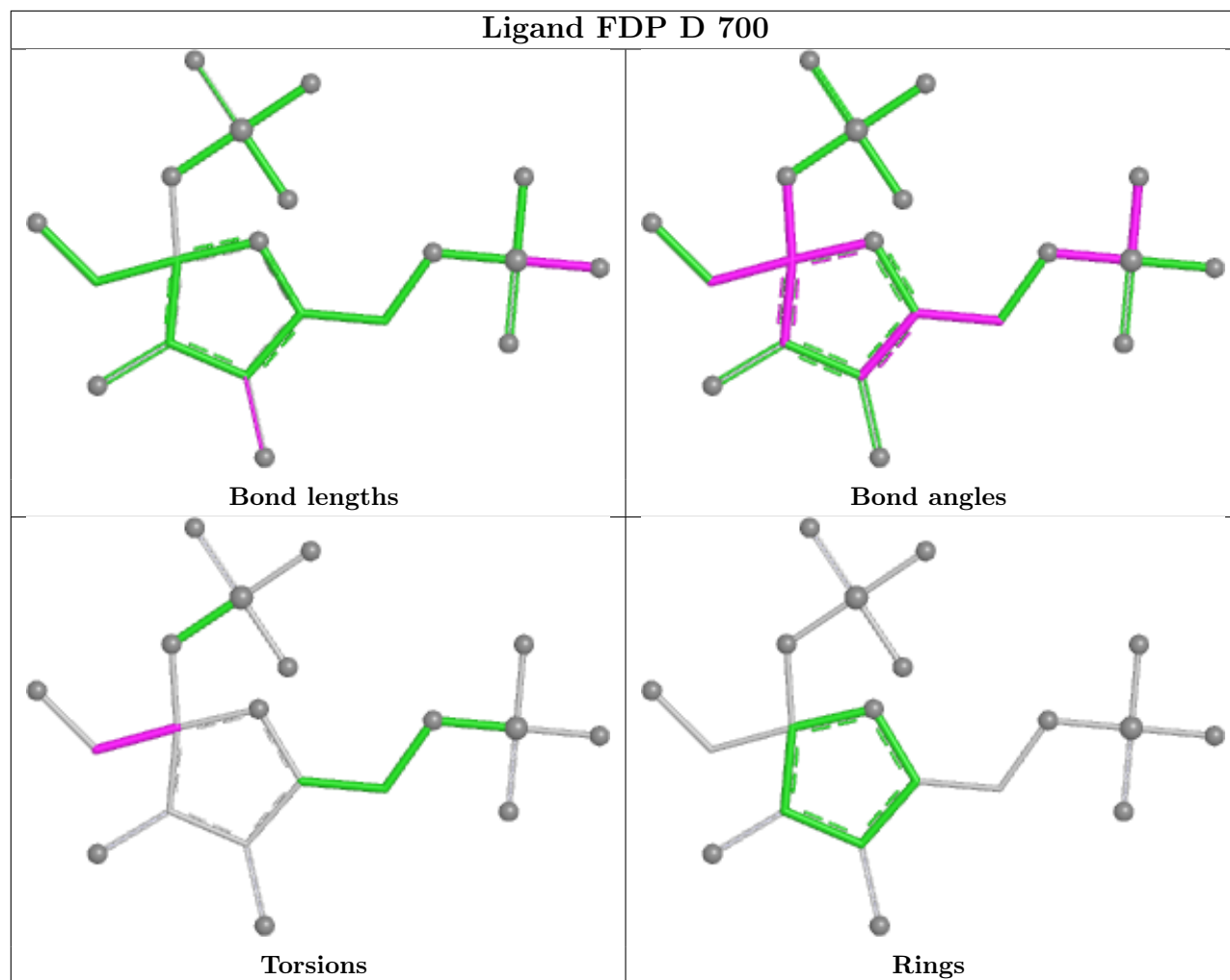


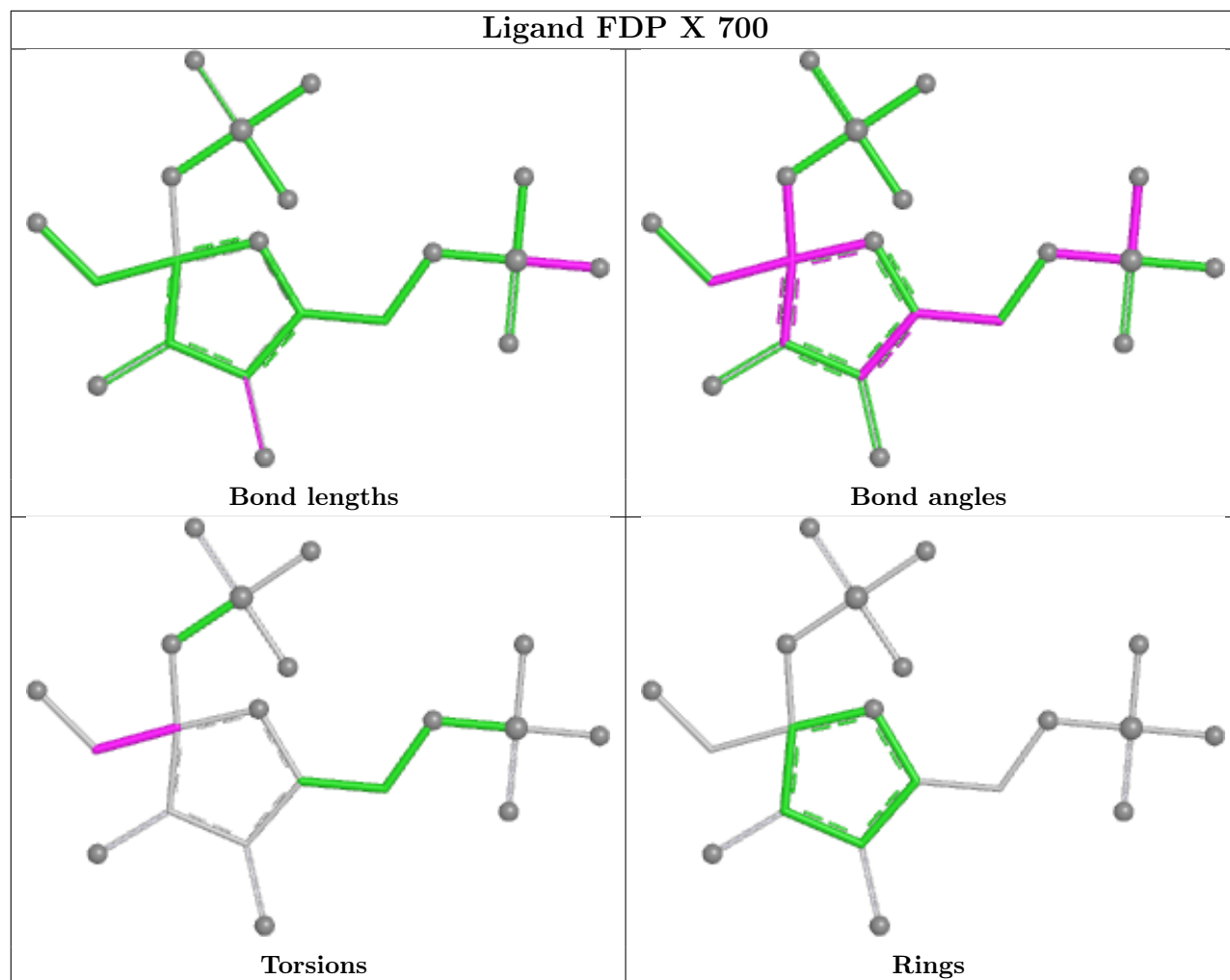
Ligand FDP I 700

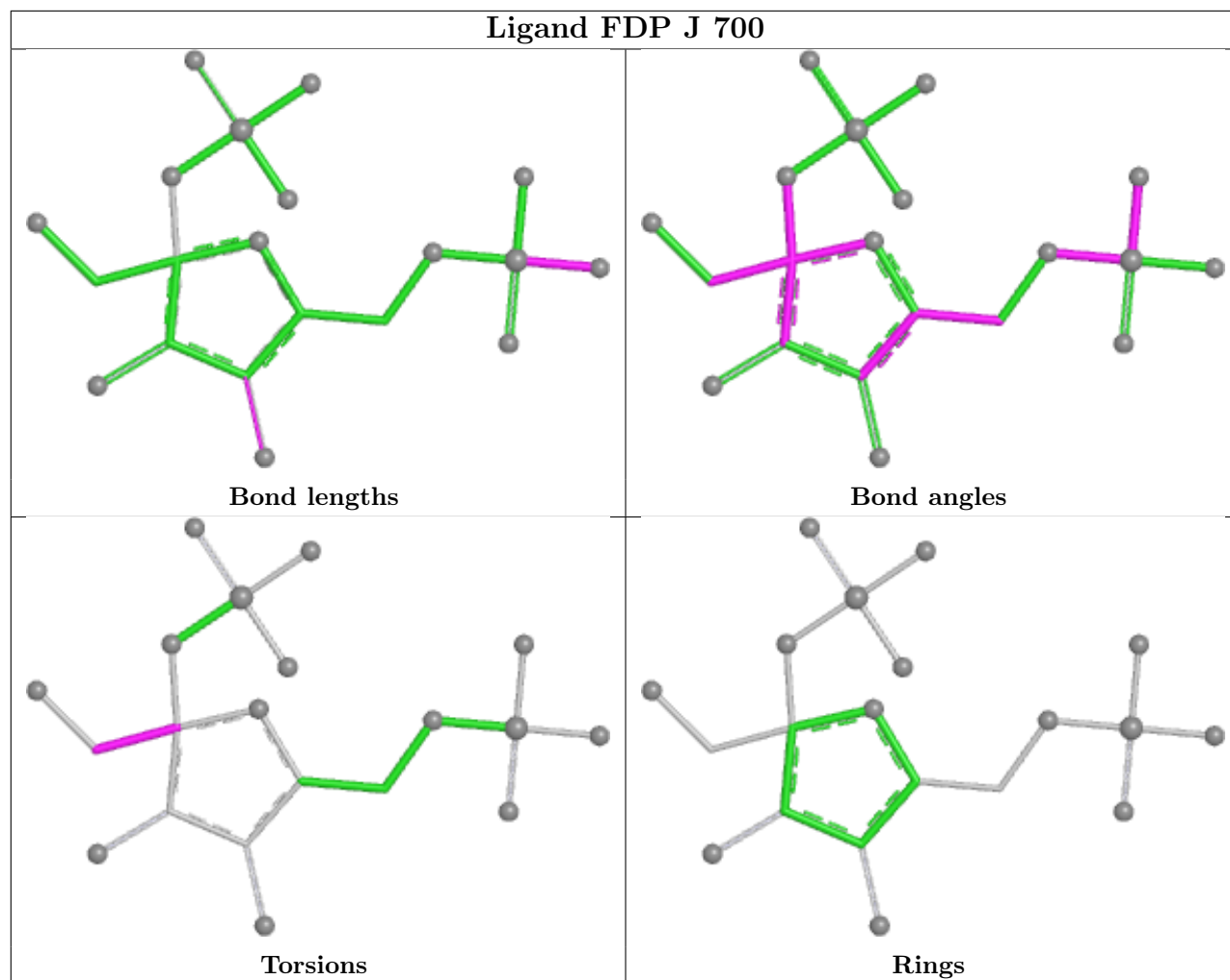




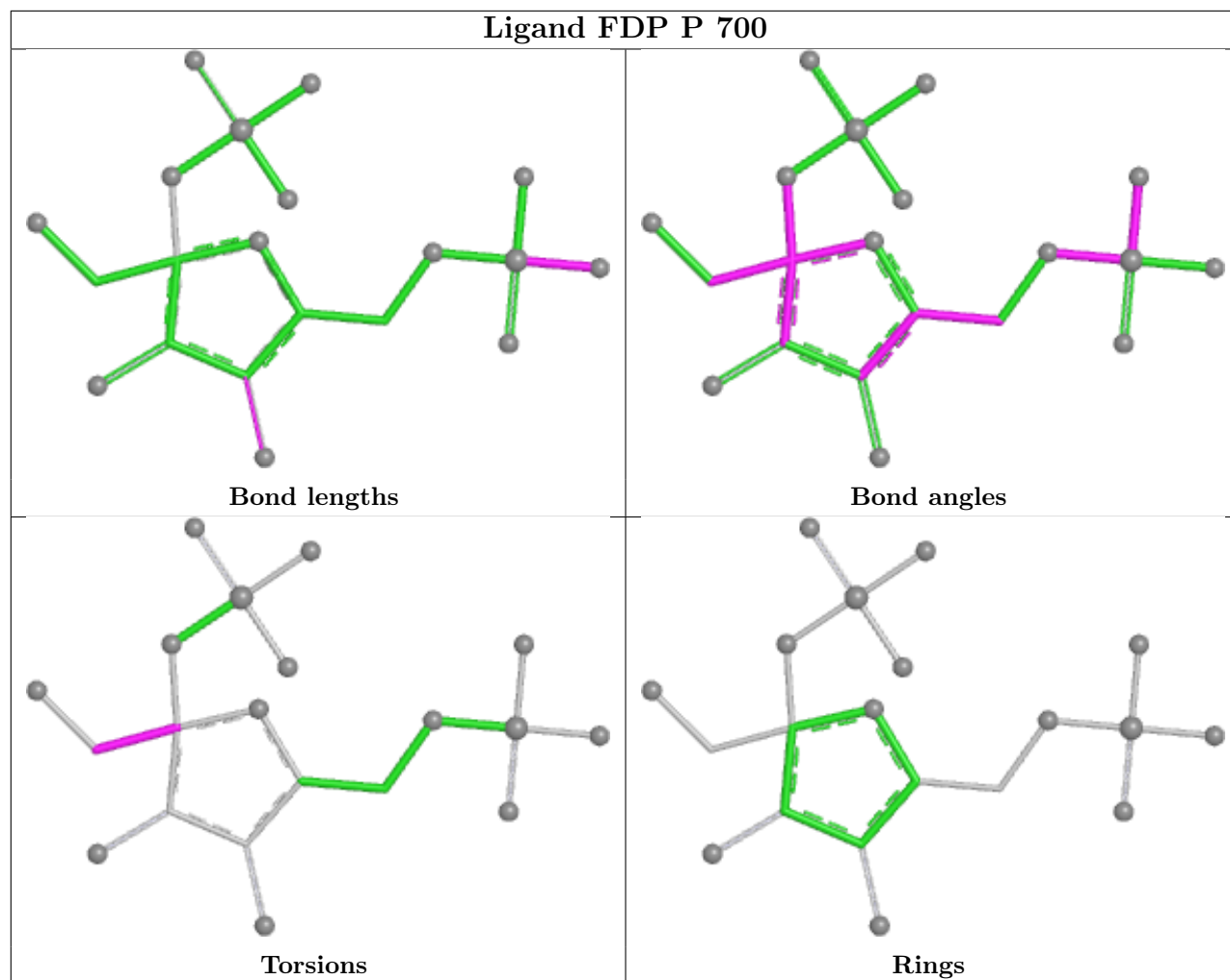


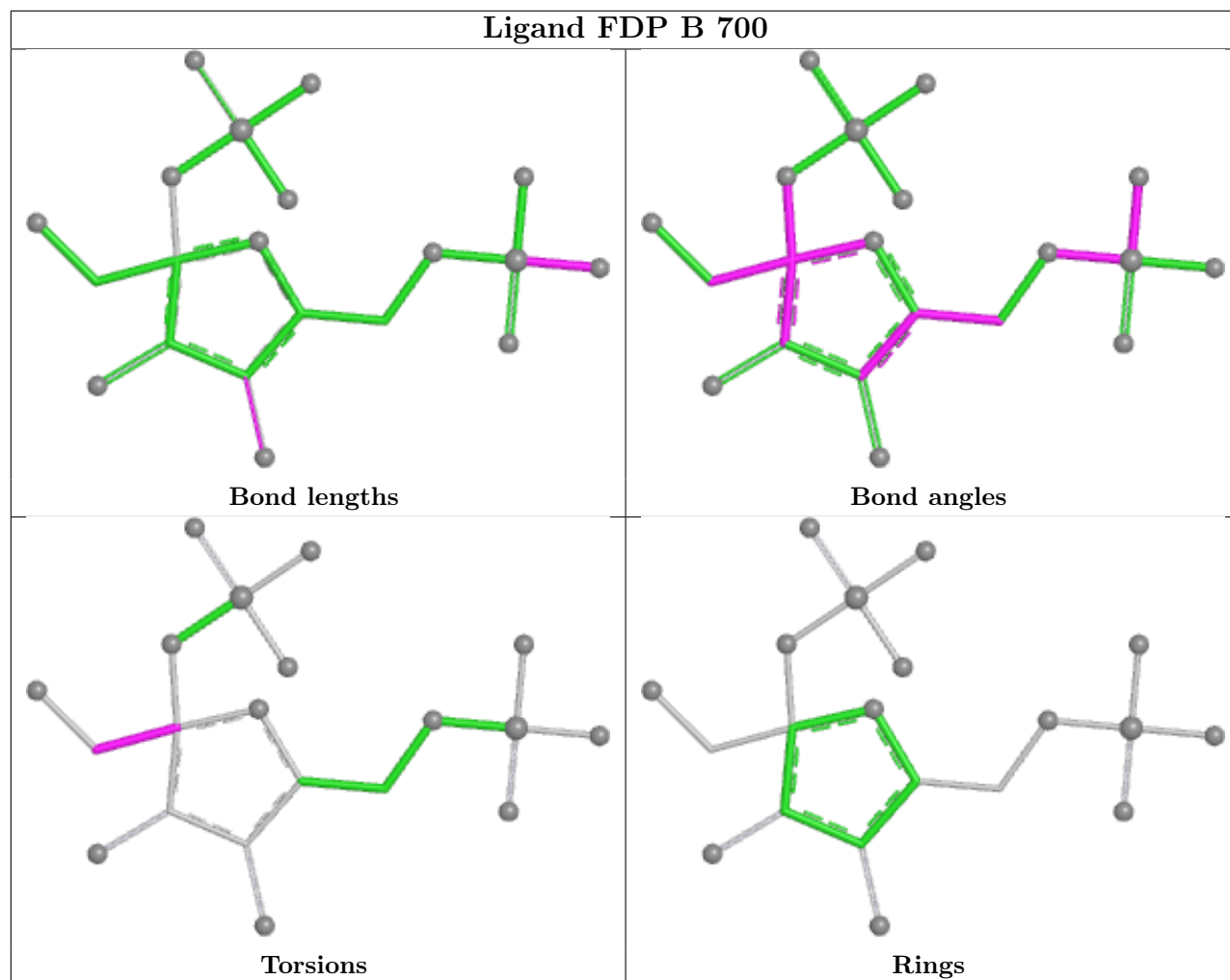


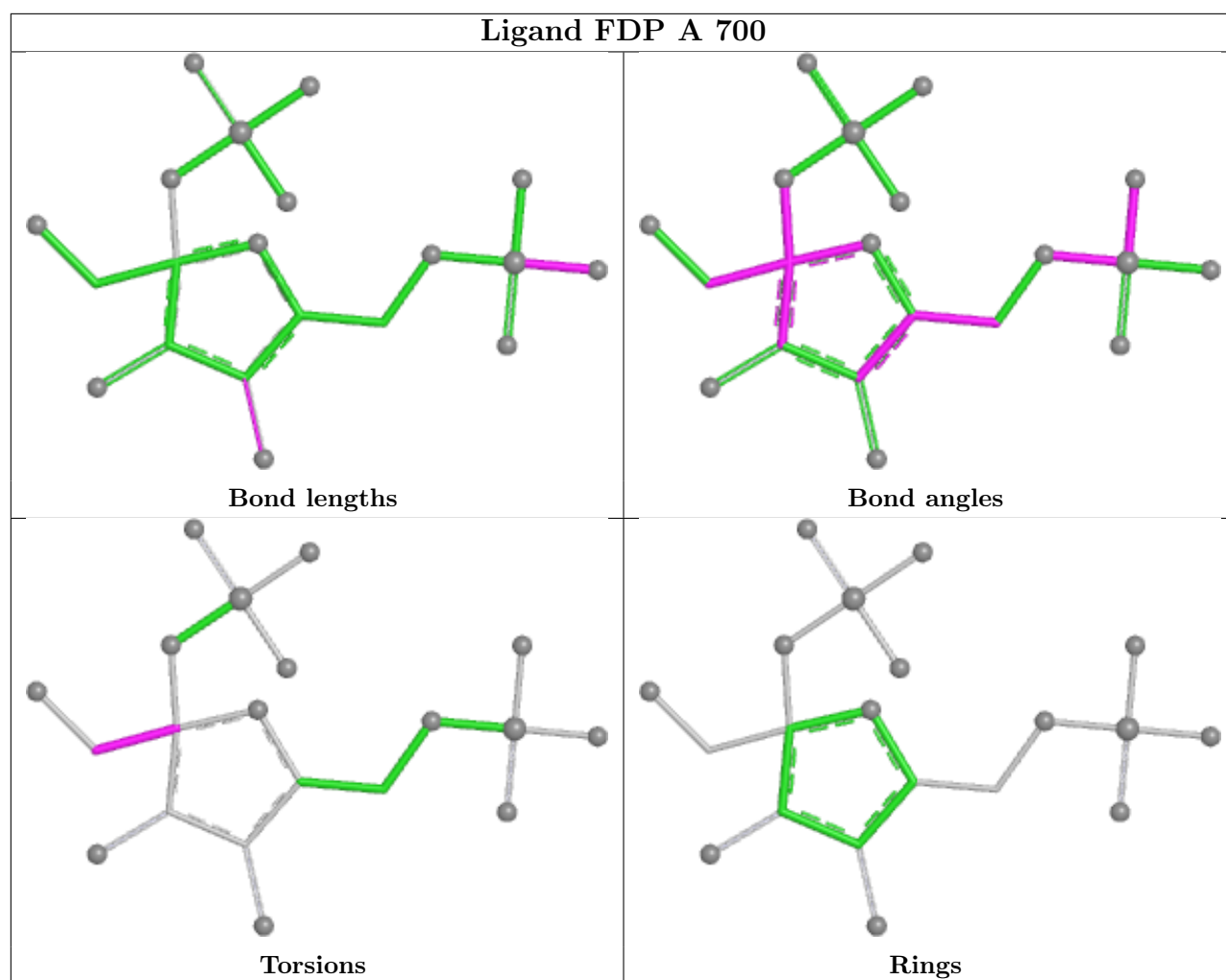


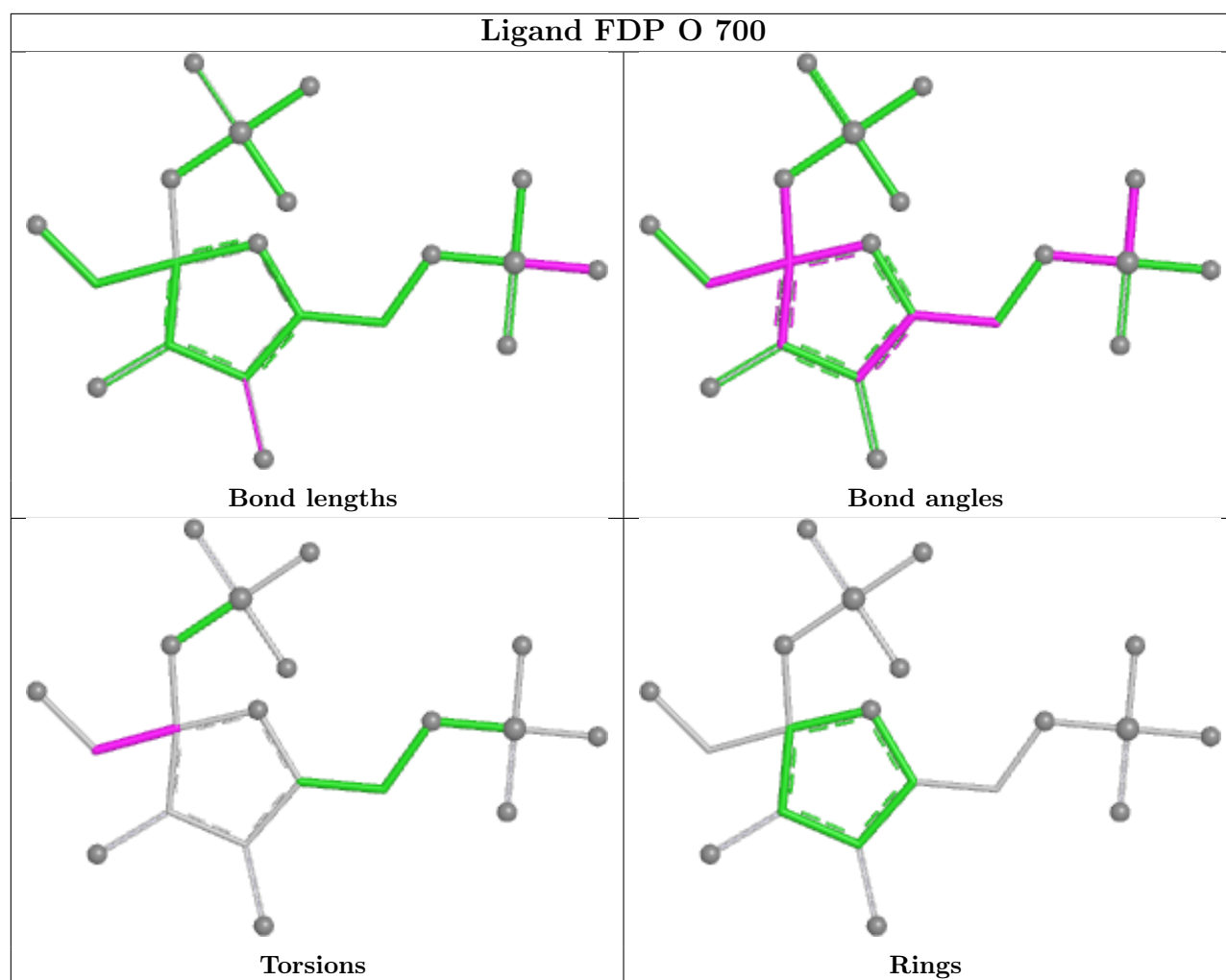


Ligand FDP P 700

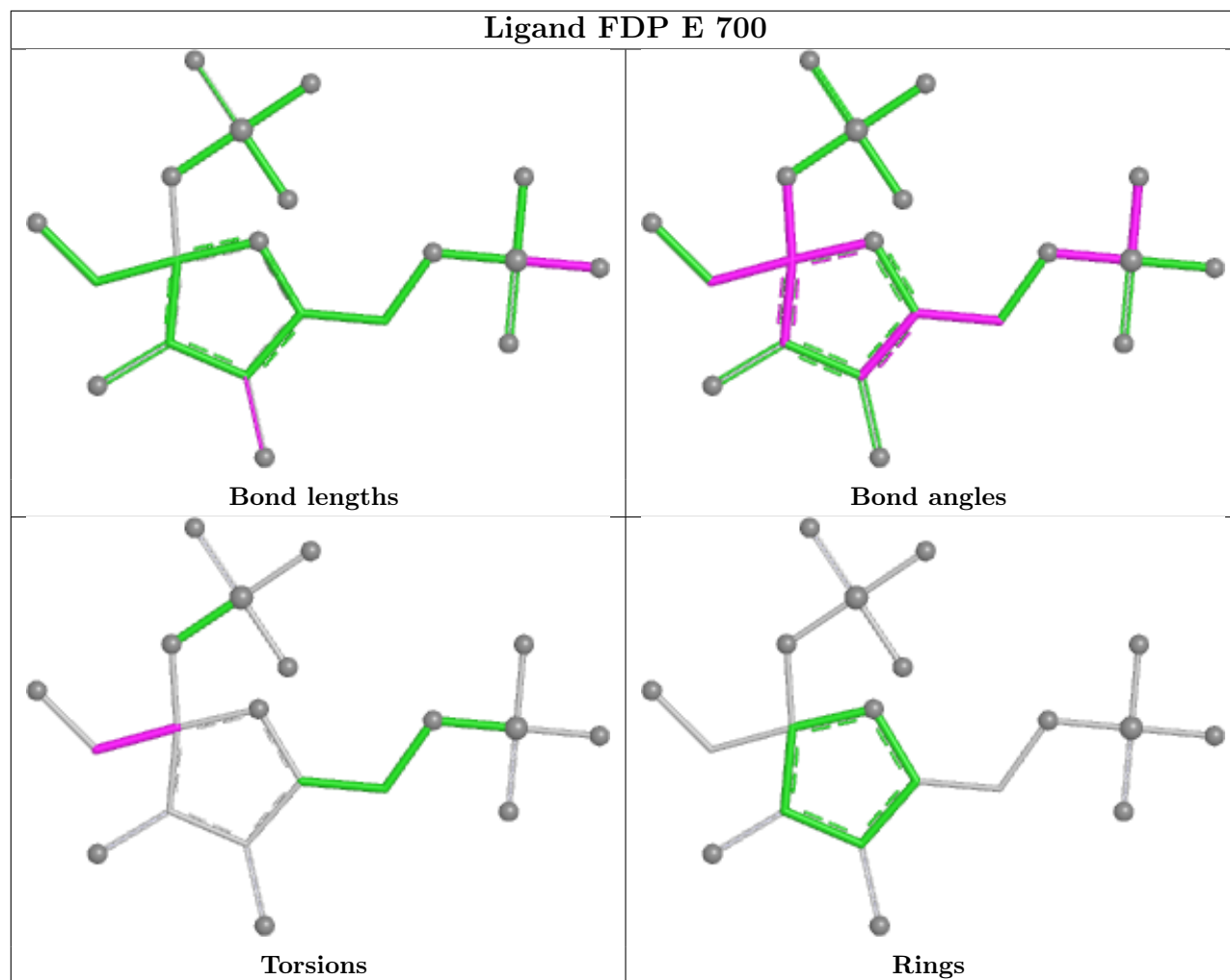




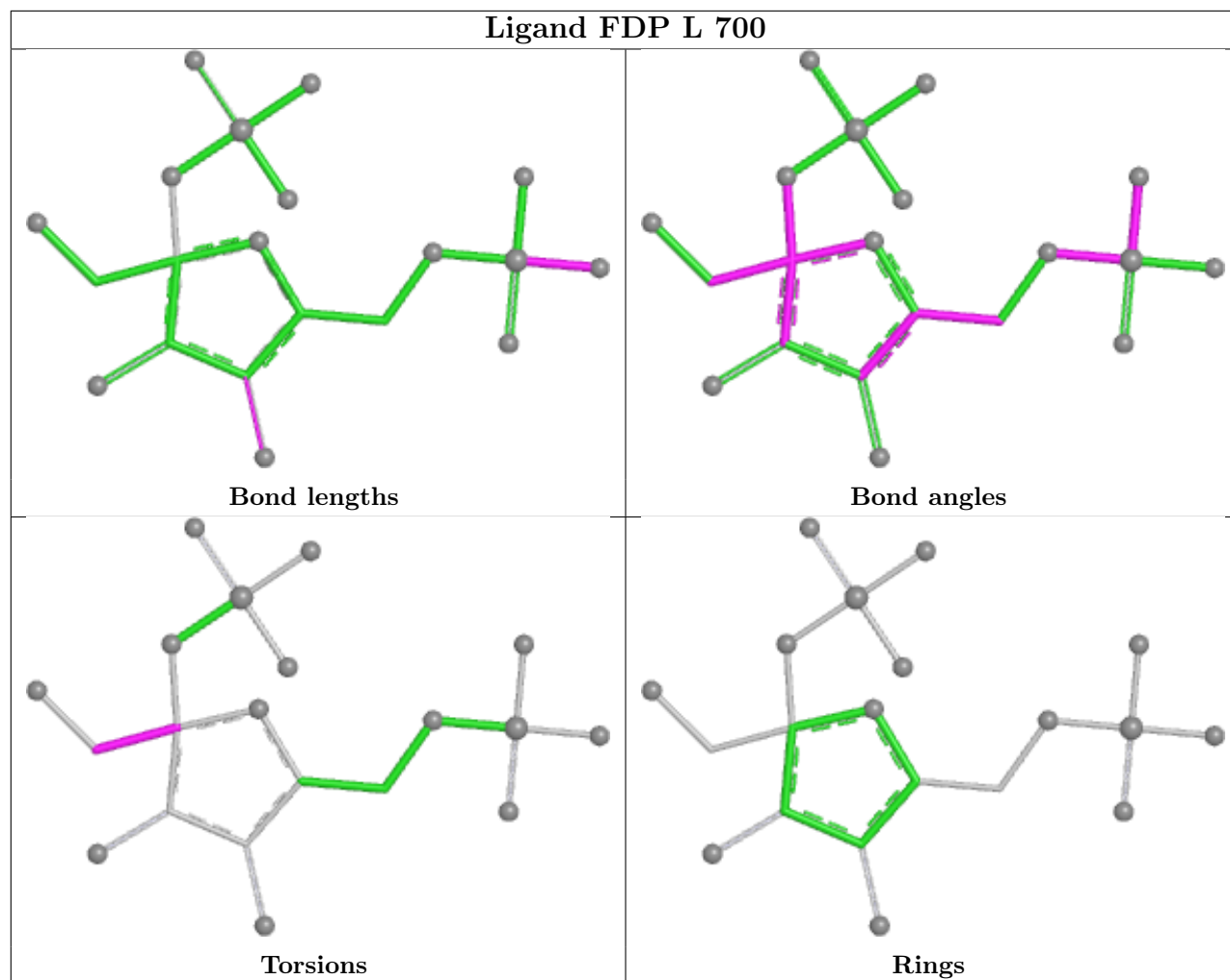


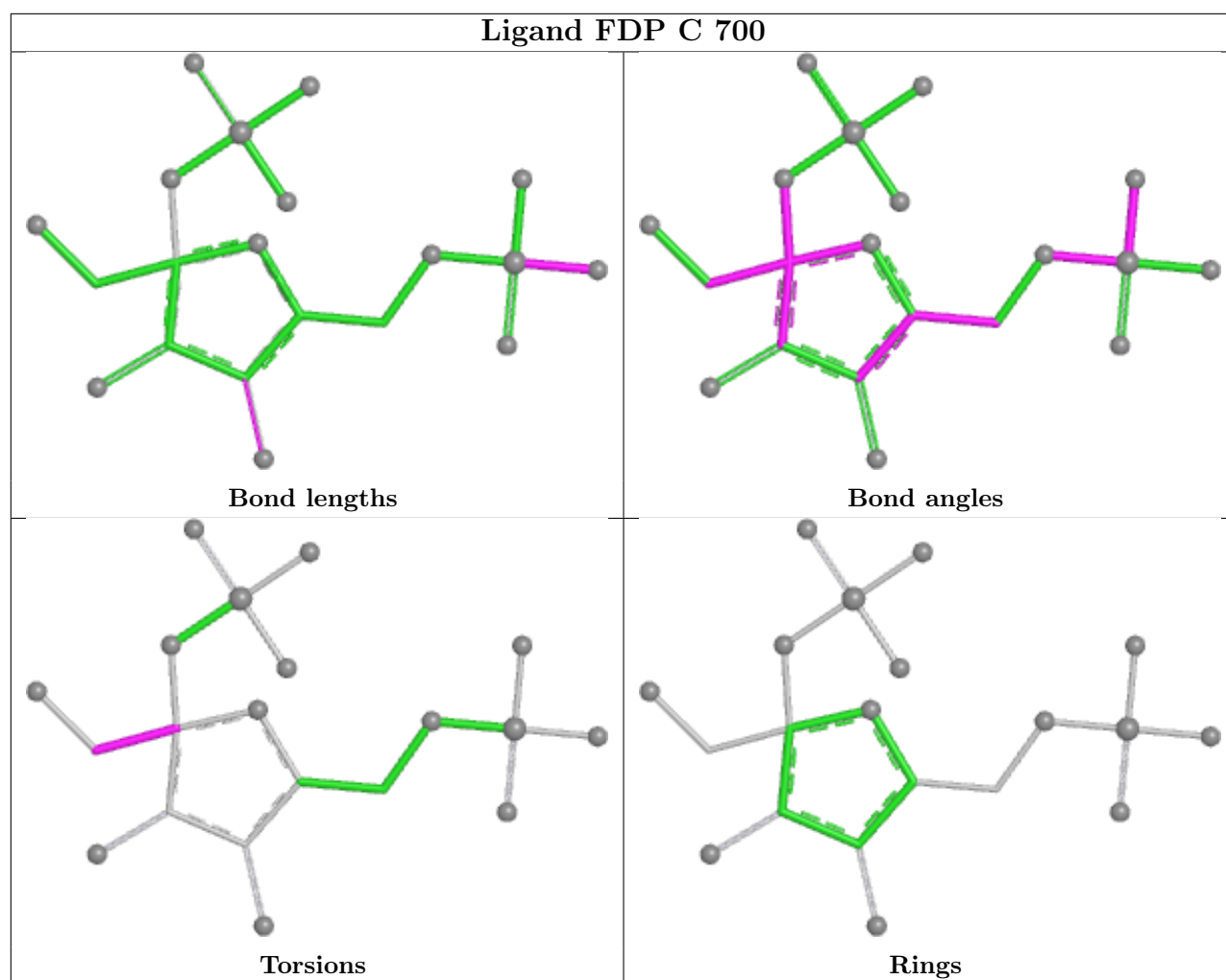


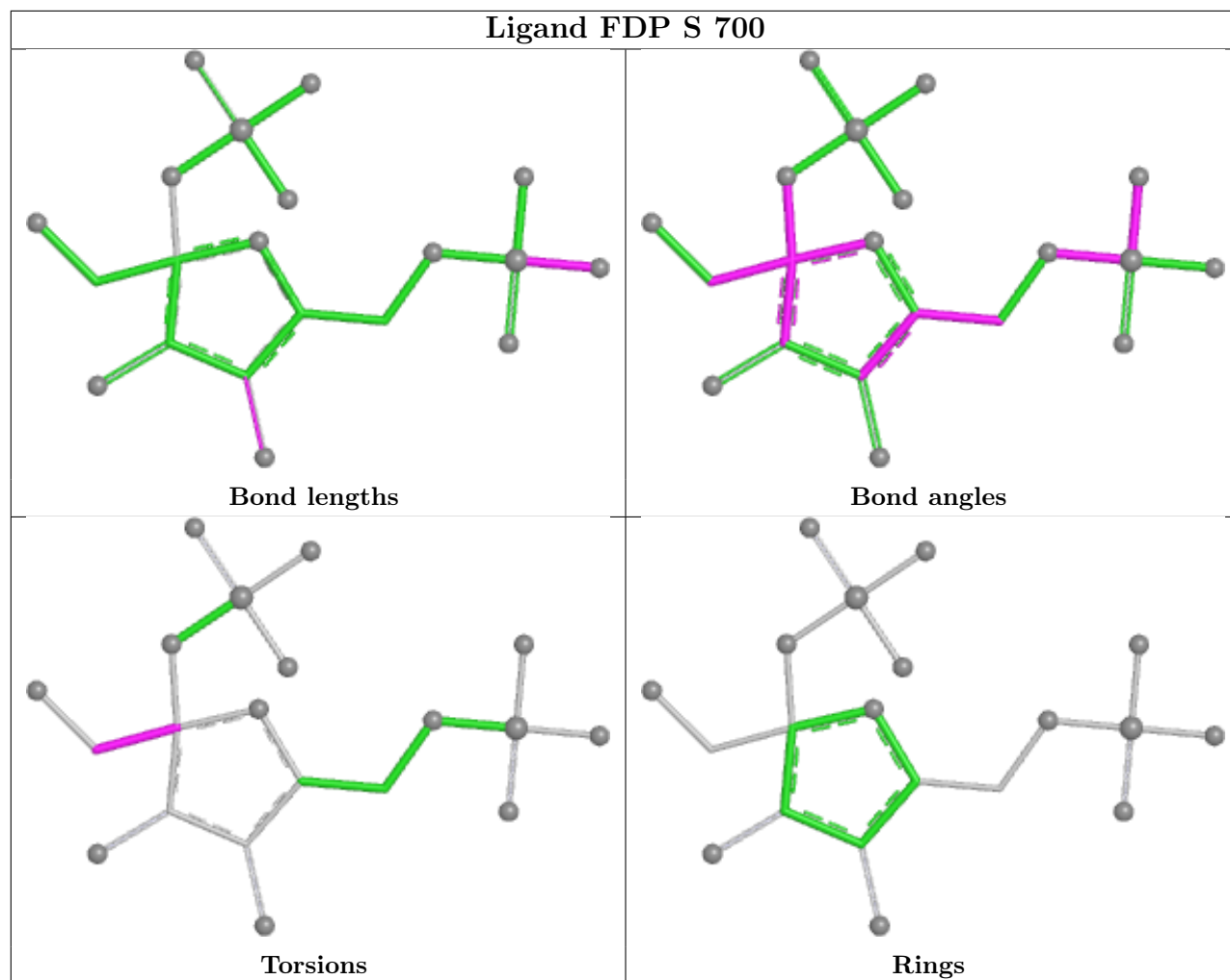
Ligand FDP E 700

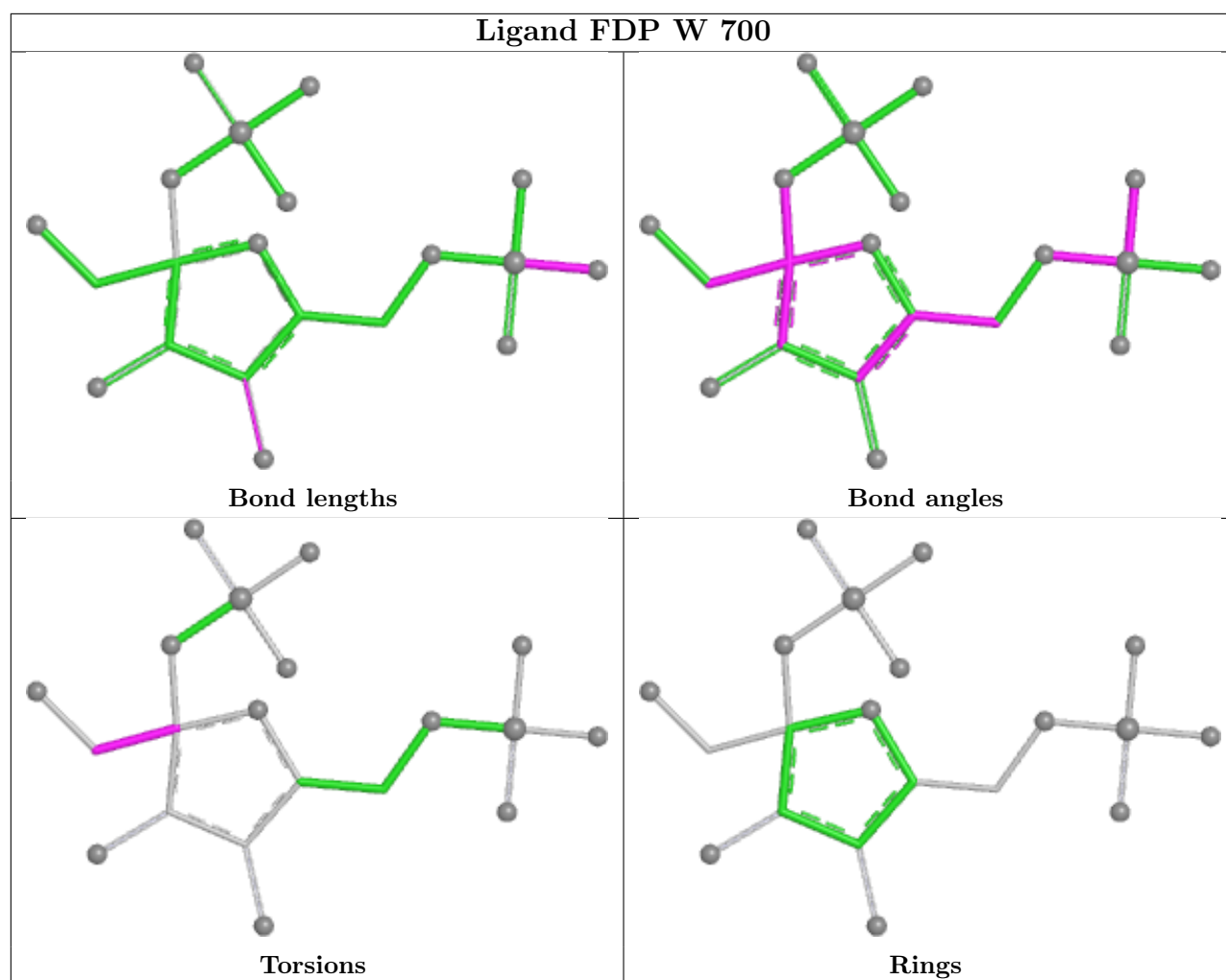


Ligand FDP L 700

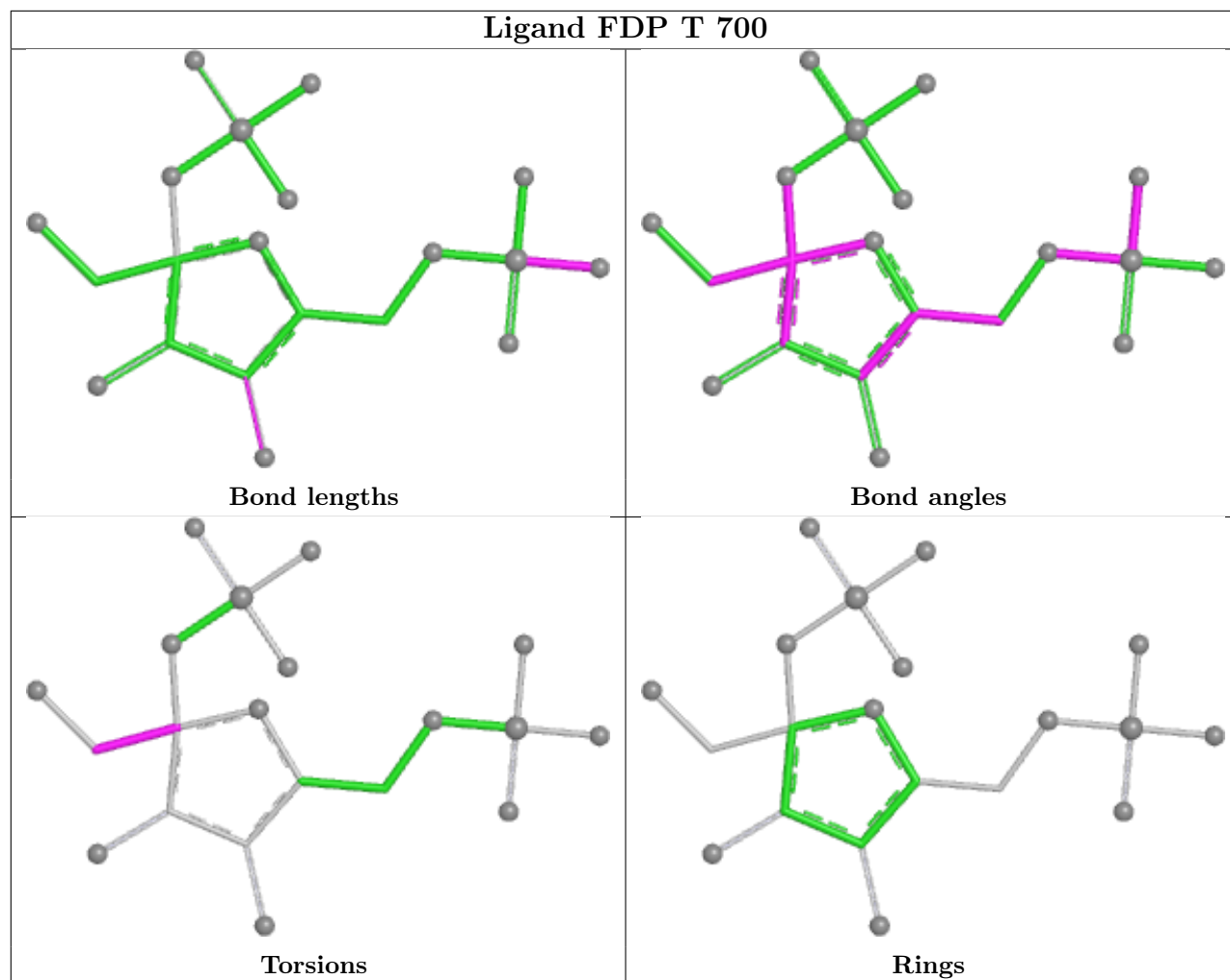


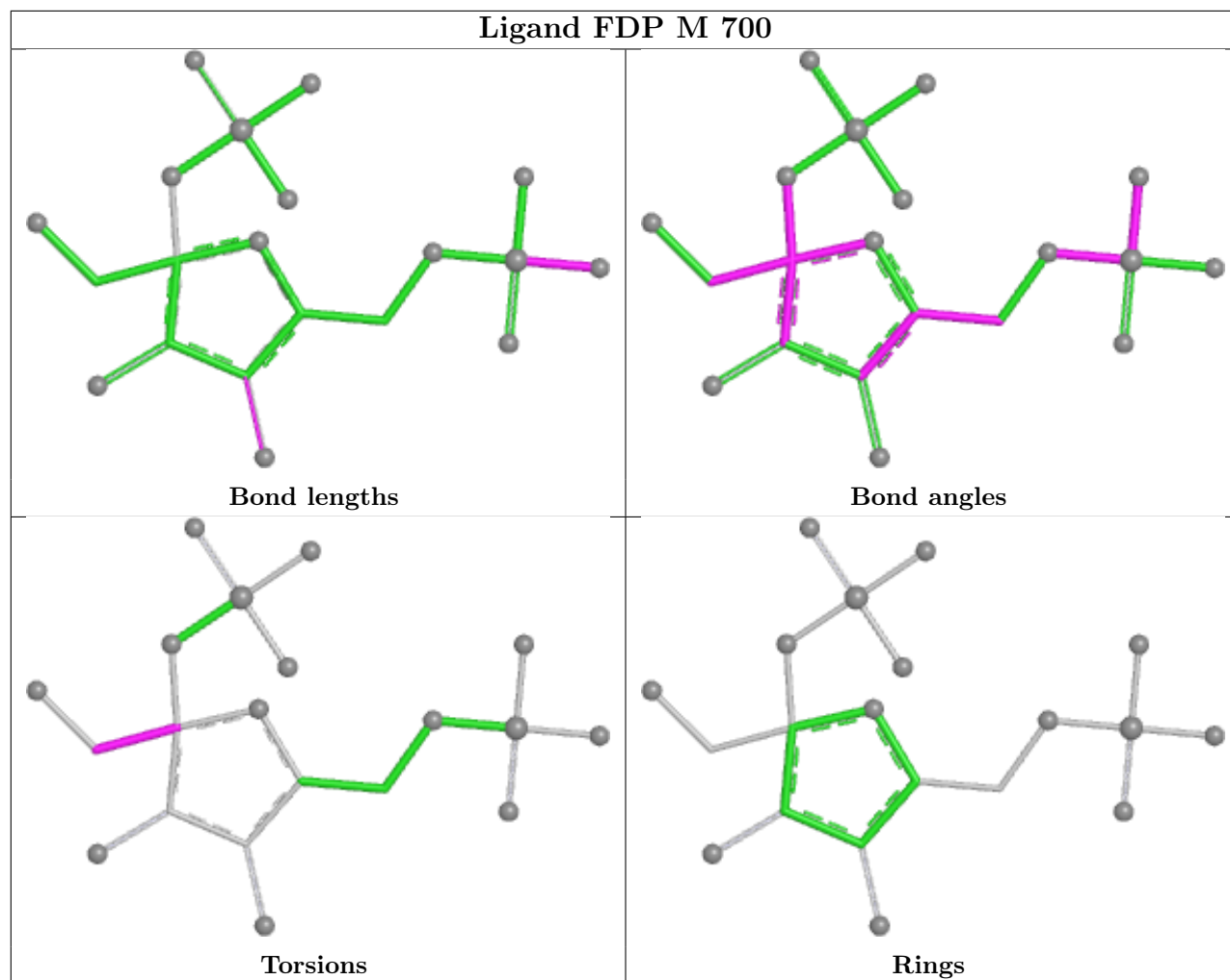




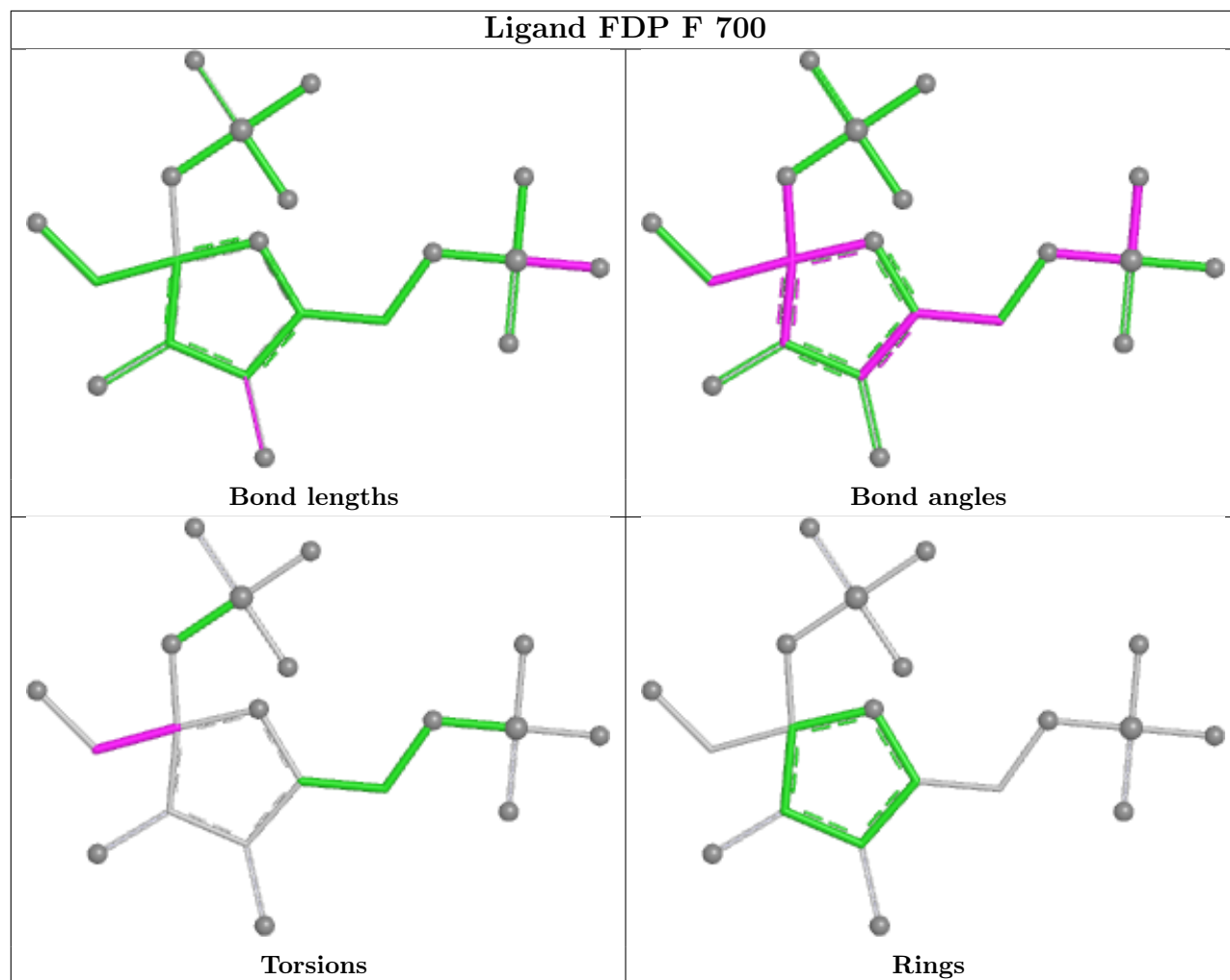


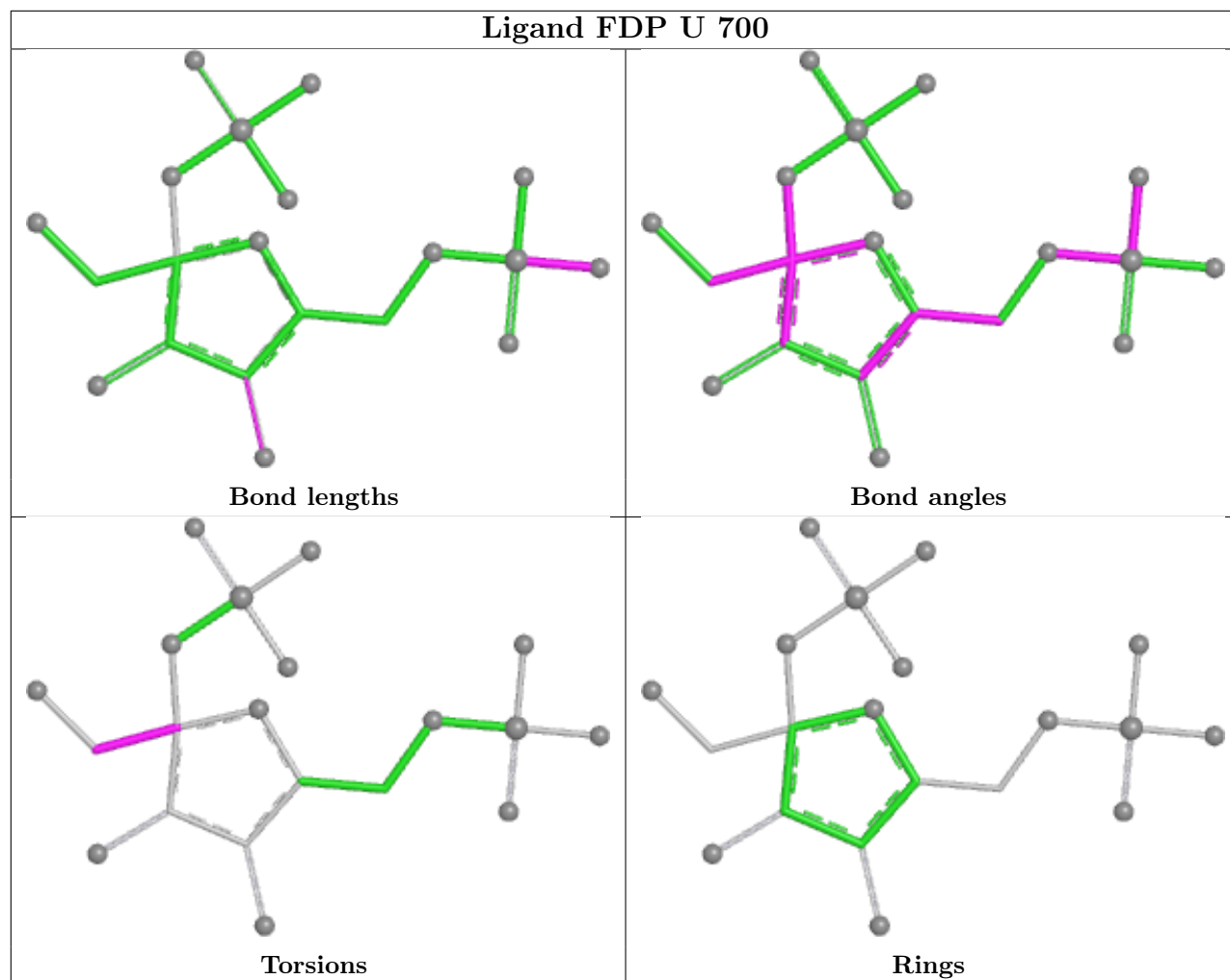
Ligand FDP T 700





Ligand FDP F 700





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	498/499 (99%)	-0.47	4 (0%) 82 69	13, 23, 36, 46	0
1	B	498/499 (99%)	-0.56	0 100 100	13, 23, 36, 46	0
1	C	498/499 (99%)	-0.63	1 (0%) 91 83	13, 23, 36, 46	0
1	D	498/499 (99%)	-0.60	0 100 100	13, 23, 36, 46	0
1	E	498/499 (99%)	-0.63	0 100 100	13, 23, 36, 46	0
1	F	498/499 (99%)	-0.63	1 (0%) 91 83	13, 23, 36, 46	0
1	G	498/499 (99%)	-0.62	0 100 100	13, 23, 36, 46	0
1	H	498/499 (99%)	-0.65	0 100 100	13, 23, 36, 46	0
1	I	498/499 (99%)	-0.60	0 100 100	13, 23, 36, 46	0
1	J	498/499 (99%)	-0.61	2 (0%) 88 77	13, 23, 36, 46	0
1	K	498/499 (99%)	-0.59	1 (0%) 91 83	13, 23, 36, 46	0
1	L	498/499 (99%)	-0.64	0 100 100	13, 23, 36, 46	0
1	M	498/499 (99%)	-0.63	0 100 100	13, 23, 36, 46	0
1	N	498/499 (99%)	-0.66	0 100 100	13, 23, 36, 46	0
1	O	498/499 (99%)	-0.53	0 100 100	13, 23, 36, 46	0
1	P	498/499 (99%)	-0.57	1 (0%) 91 83	13, 23, 36, 46	0
1	Q	498/499 (99%)	-0.63	0 100 100	13, 23, 36, 46	0
1	R	498/499 (99%)	-0.60	0 100 100	13, 23, 36, 46	0
1	S	498/499 (99%)	-0.62	0 100 100	13, 23, 36, 46	0
1	T	498/499 (99%)	-0.57	0 100 100	13, 23, 36, 46	0
1	U	498/499 (99%)	-0.65	0 100 100	13, 23, 36, 46	0
1	V	498/499 (99%)	-0.60	0 100 100	13, 23, 36, 46	0
1	W	498/499 (99%)	-0.65	0 100 100	13, 23, 36, 46	0
1	X	498/499 (99%)	-0.61	1 (0%) 91 83	13, 23, 36, 46	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	11952/11976 (99%)	-0.61	11 (0%) 92 86	13, 23, 36, 46	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	GLY	4.4
1	J	107	CYS	3.6
1	C	158	GLU	2.9
1	P	104	GLY	2.9
1	A	302	MET	2.4
1	X	120	THR	2.4
1	J	422	THR	2.4
1	A	114	ALA	2.3
1	F	96	GLY	2.3
1	K	172	SER	2.3
1	A	203	GLN	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FDP	I	700	20/20	0.97	0.07	25,32,34,35	0
2	FDP	K	700	20/20	0.97	0.09	25,32,34,35	0
2	FDP	B	700	20/20	0.98	0.07	25,32,34,35	0
2	FDP	G	700	20/20	0.98	0.08	25,32,34,35	0
2	FDP	M	700	20/20	0.98	0.06	25,32,34,35	0
2	FDP	N	700	20/20	0.98	0.06	25,32,34,35	0

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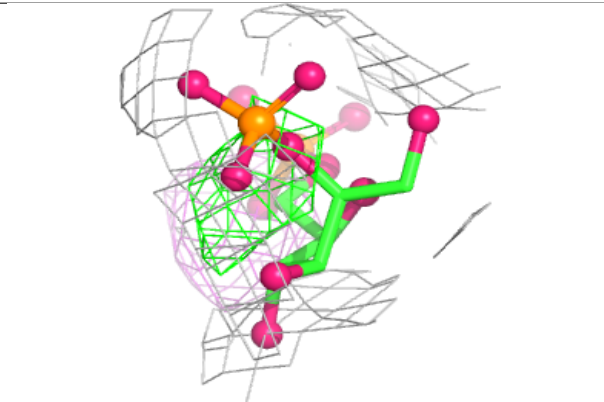
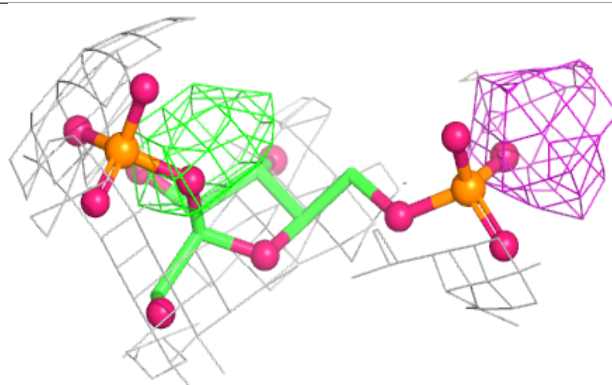
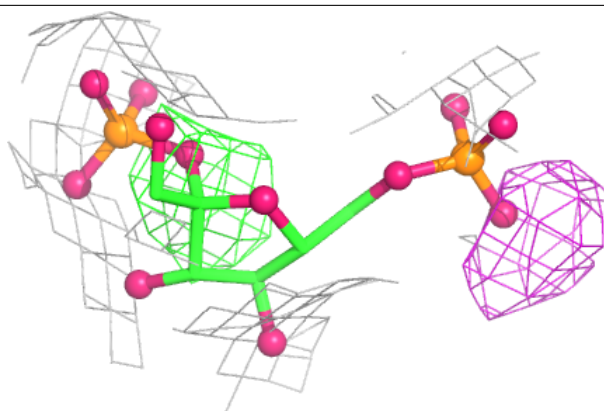
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FDP	X	700	20/20	0.98	0.07	25,32,34,35	0
2	FDP	H	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	C	700	20/20	0.99	0.07	25,32,34,35	0
2	FDP	J	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	D	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	L	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	E	700	20/20	0.99	0.07	25,32,34,35	0
2	FDP	F	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	O	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	P	700	20/20	0.99	0.06	25,32,34,35	0
2	FDP	Q	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	R	700	20/20	0.99	0.06	25,32,34,35	0
2	FDP	S	700	20/20	0.99	0.04	25,32,34,35	0
2	FDP	T	700	20/20	0.99	0.07	25,32,34,35	0
2	FDP	U	700	20/20	0.99	0.06	25,32,34,35	0
2	FDP	V	700	20/20	0.99	0.06	25,32,34,35	0
2	FDP	W	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	A	700	20/20	0.99	0.04	25,32,34,35	0

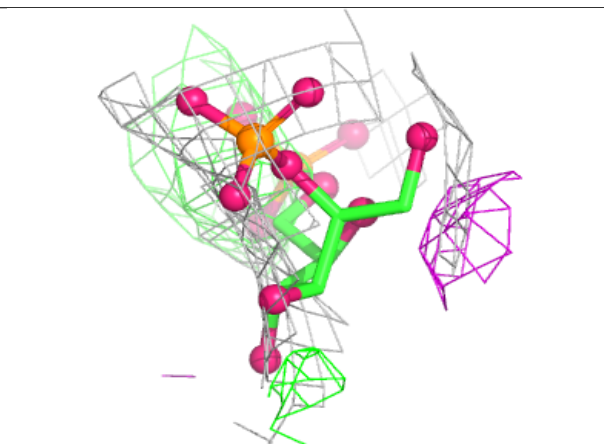
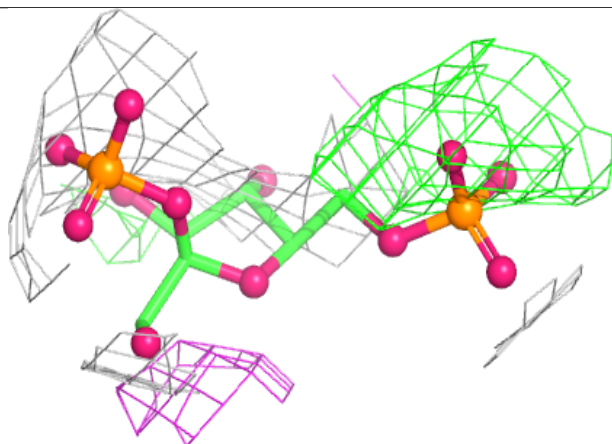
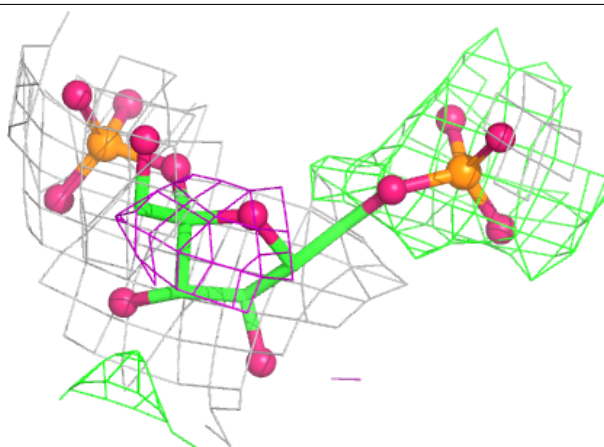
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FDP I 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

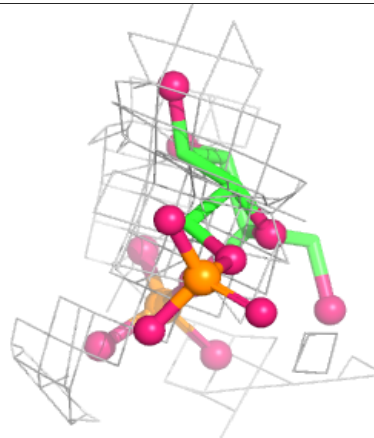
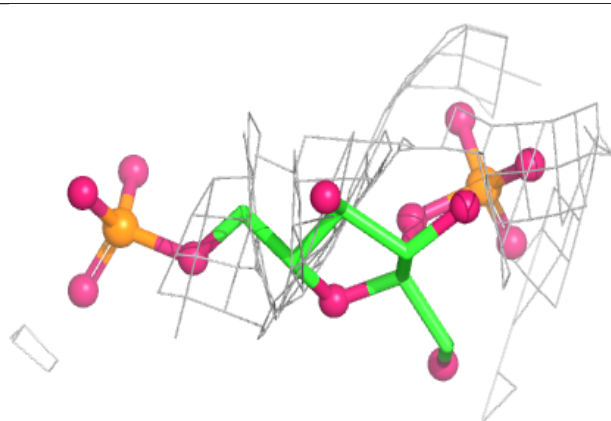
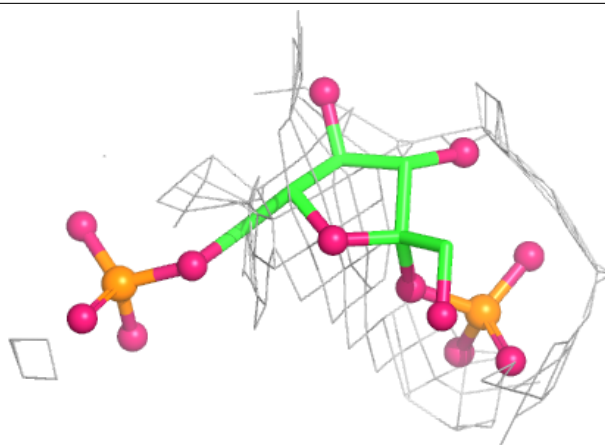
**Electron density around FDP K 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



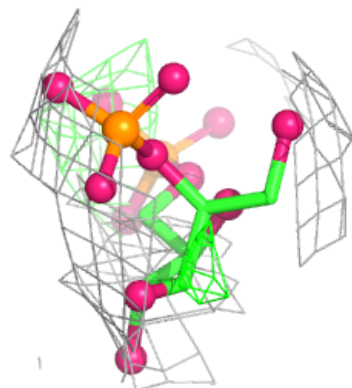
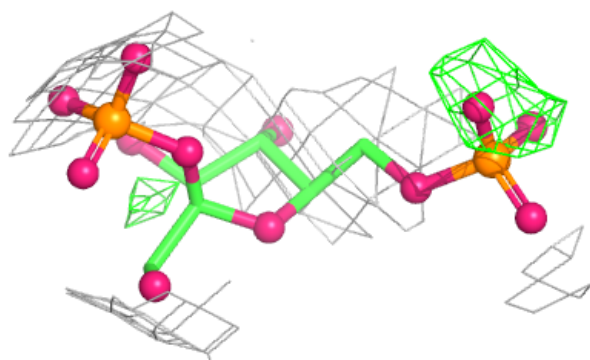
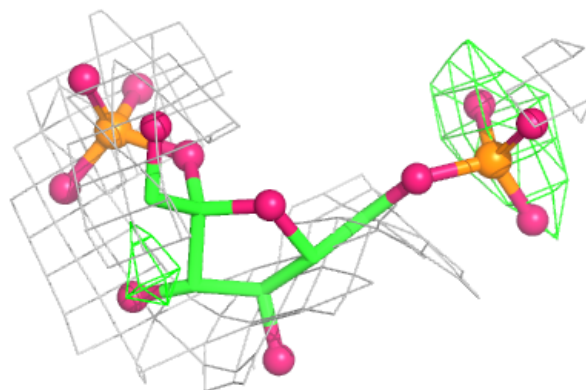
Electron density around FDP B 700:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

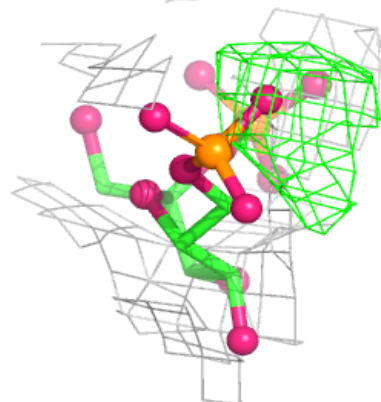
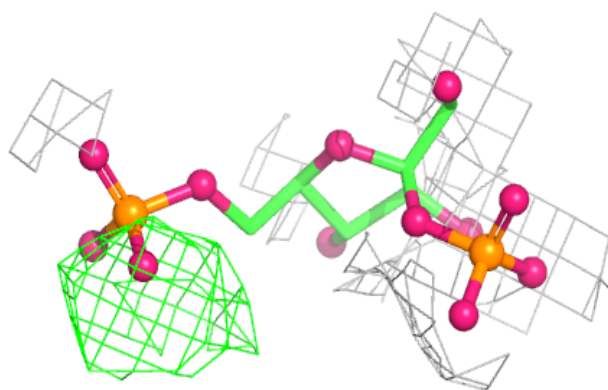
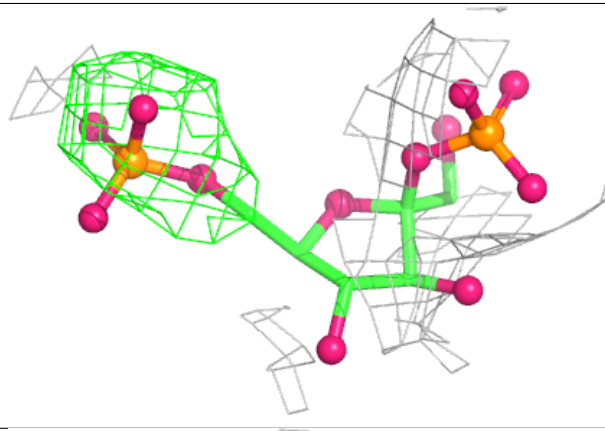


Electron density around FDP G 700:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

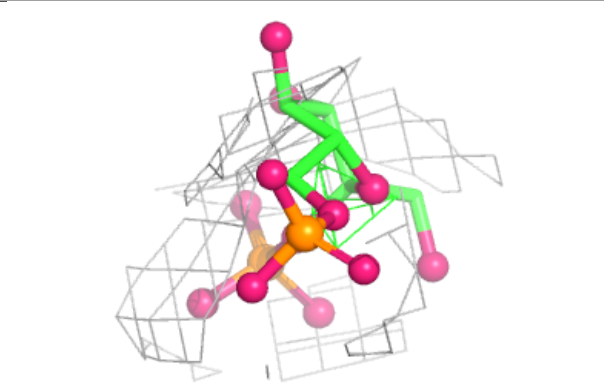
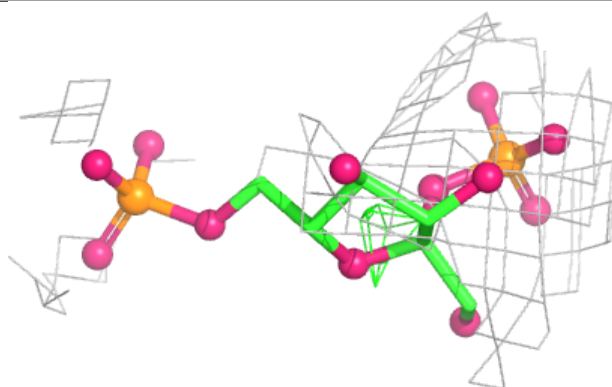
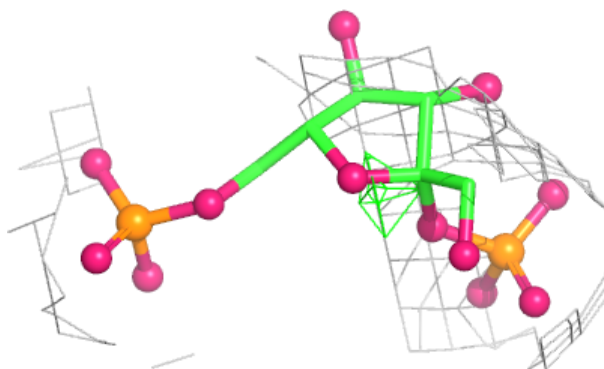
**Electron density around FDP M 700:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

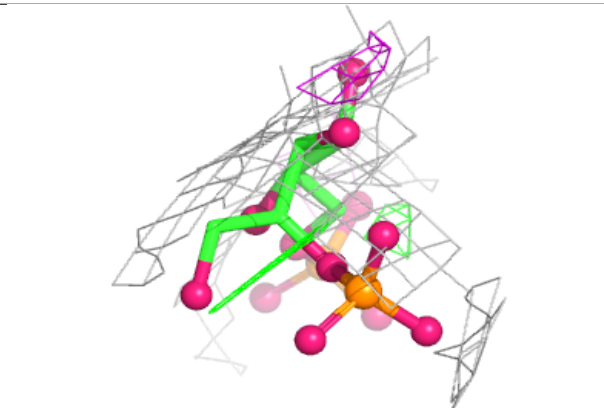
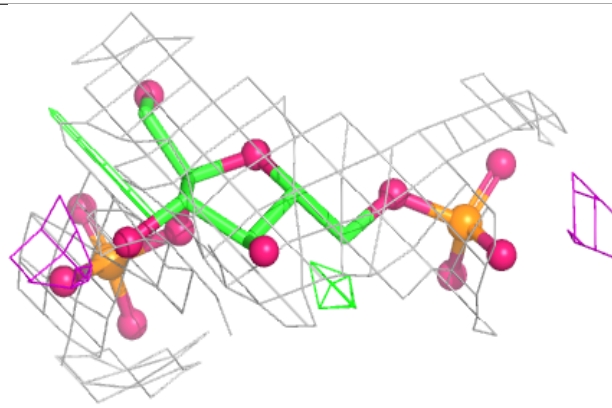
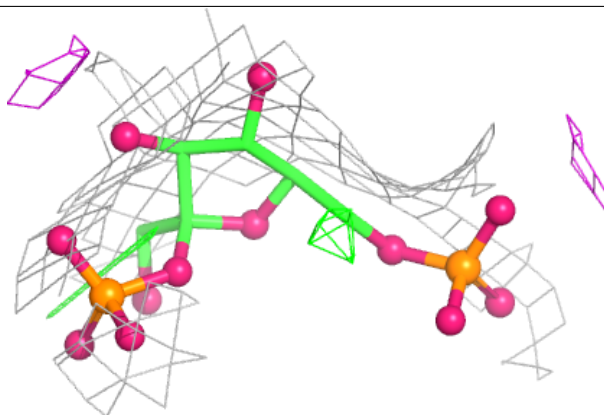


Electron density around FDP N 700:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

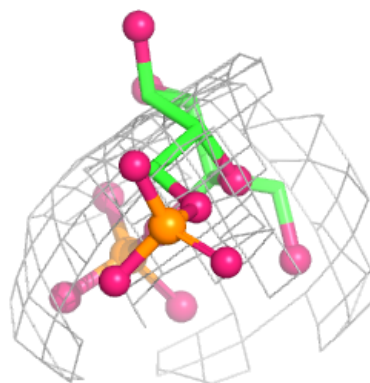
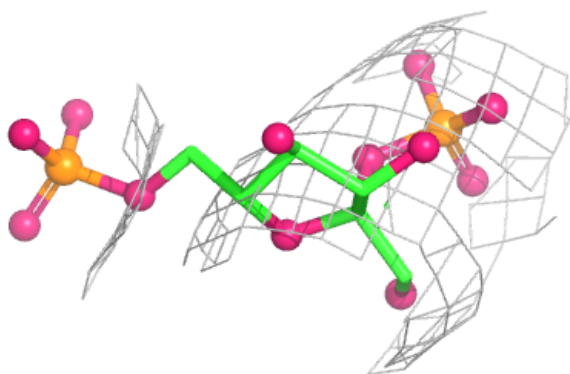
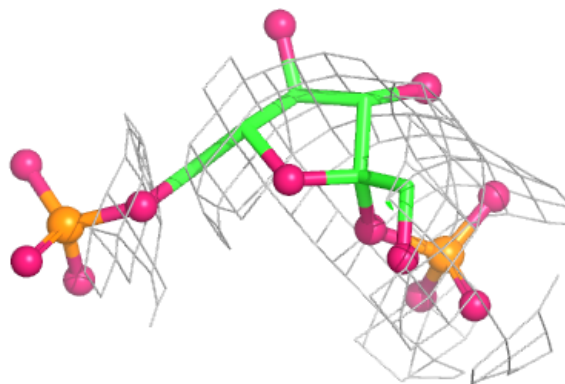
**Electron density around FDP X 700:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



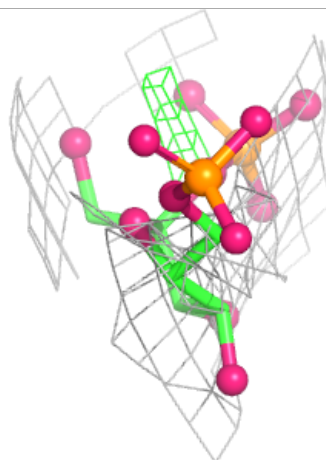
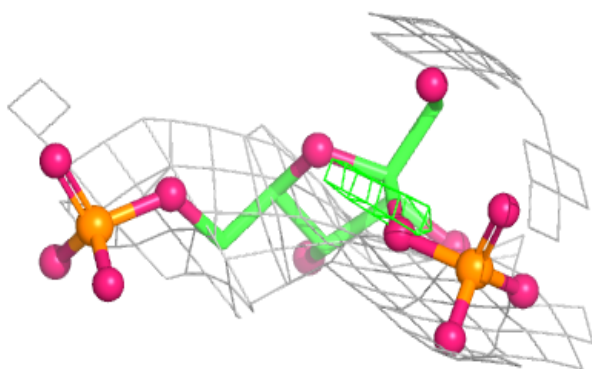
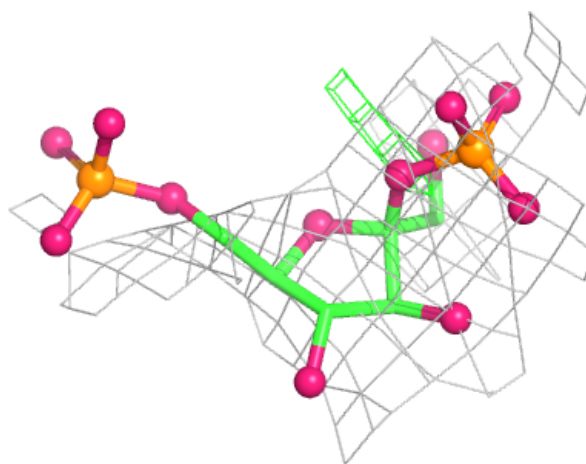
Electron density around FDP H 700:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



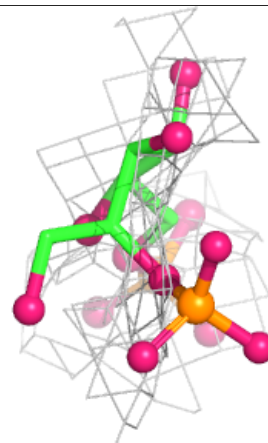
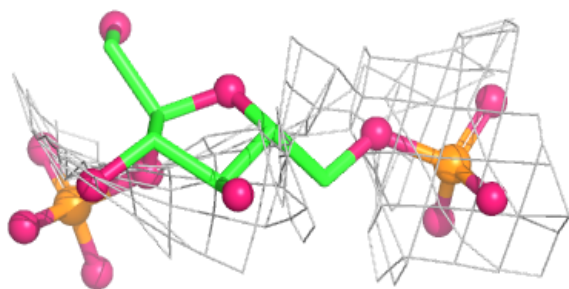
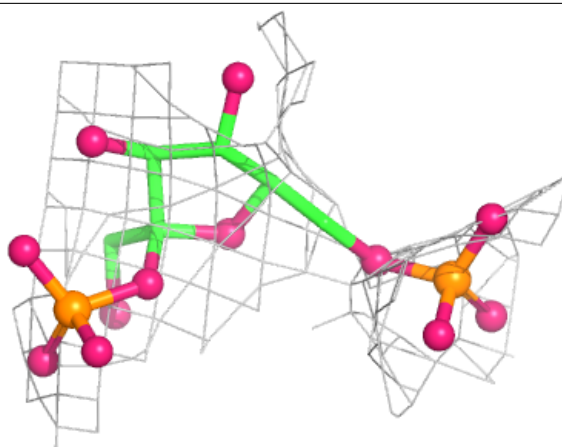
Electron density around FDP C 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



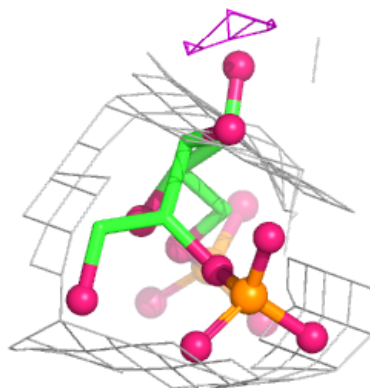
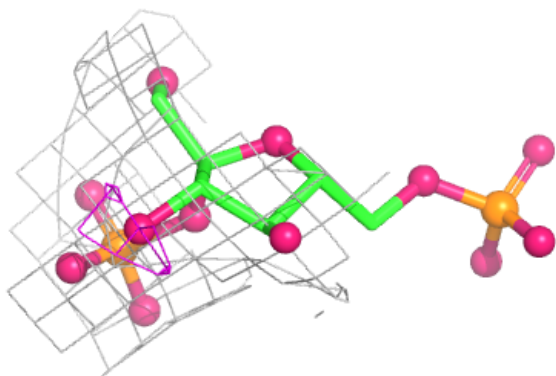
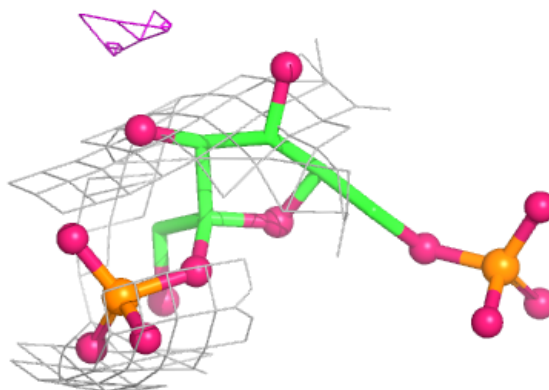
Electron density around FDP J 700:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

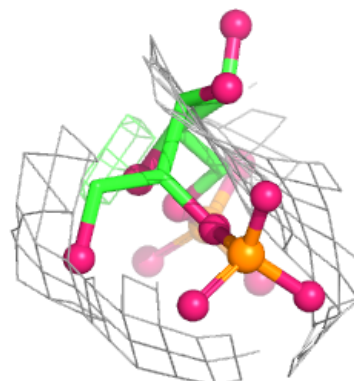
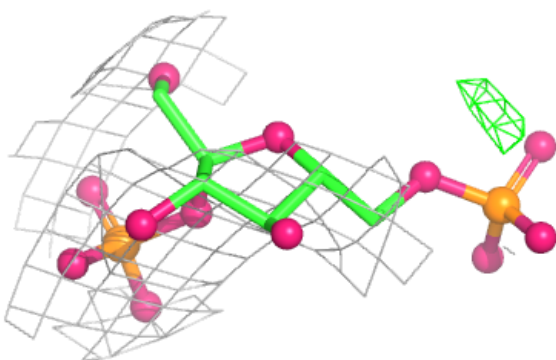
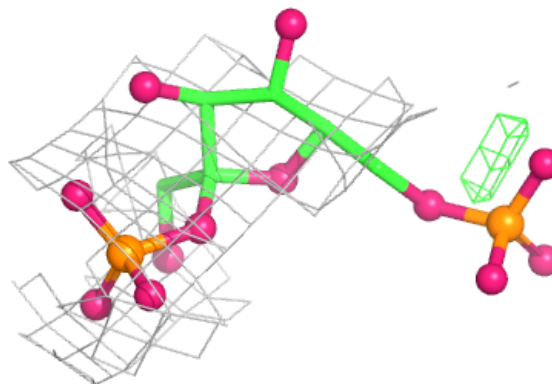


Electron density around FDP D 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

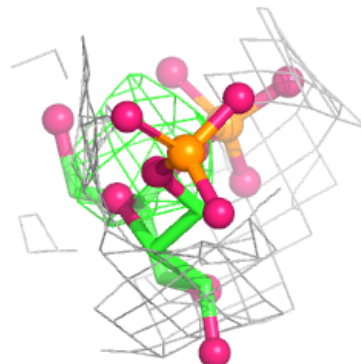
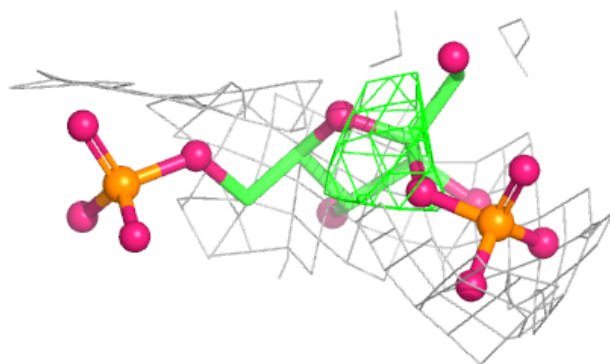
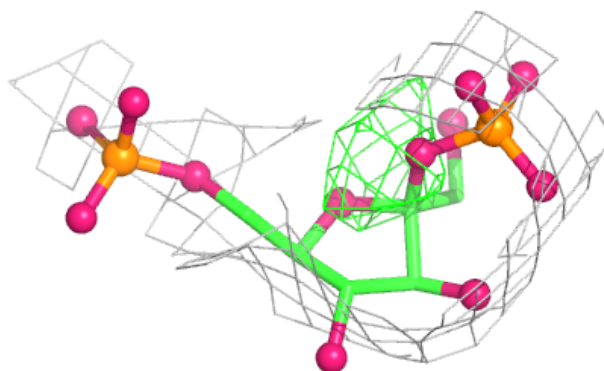
**Electron density around FDP L 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

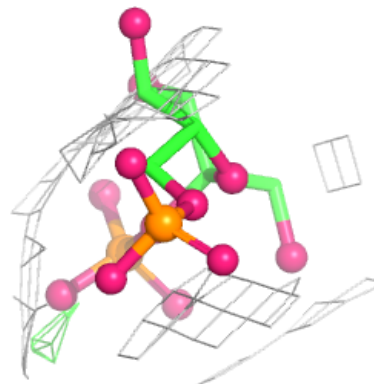
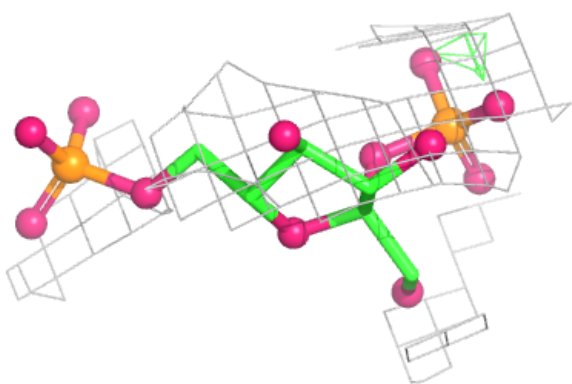
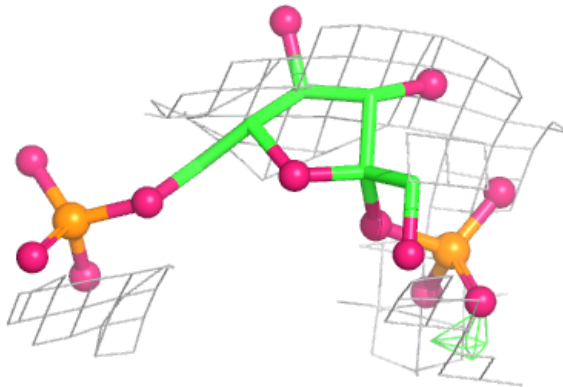


Electron density around FDP E 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

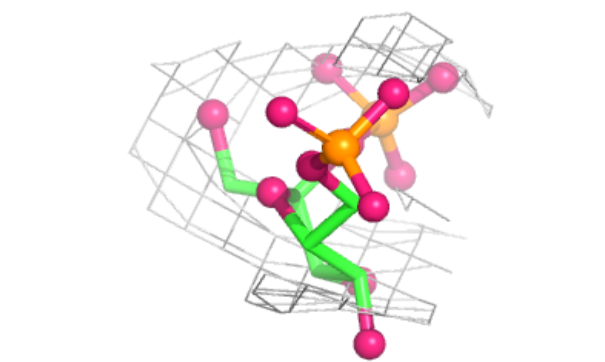
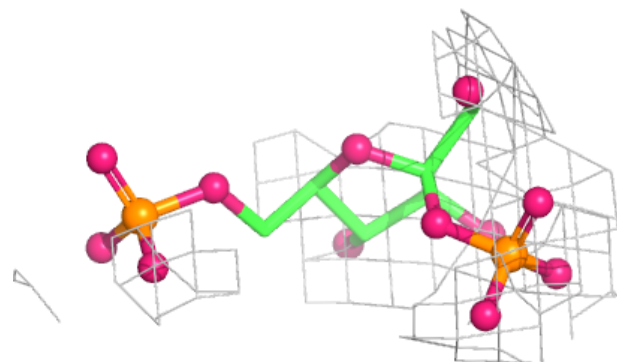
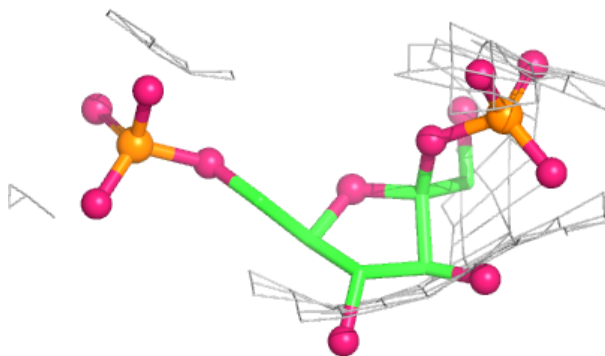
**Electron density around FDP F 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

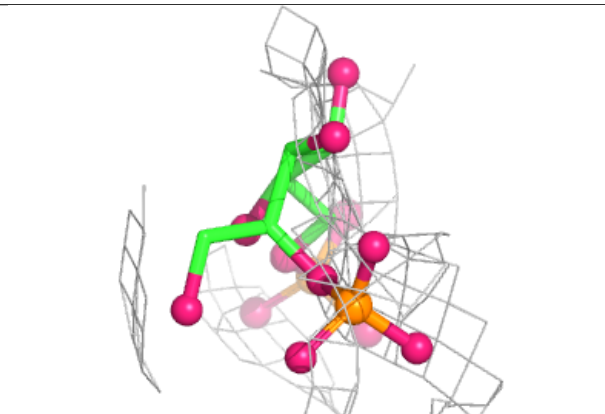
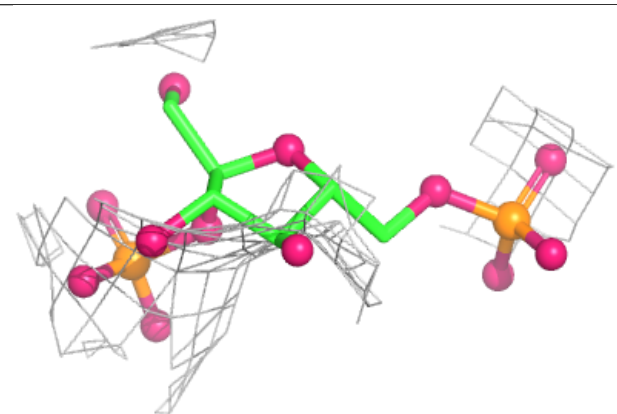
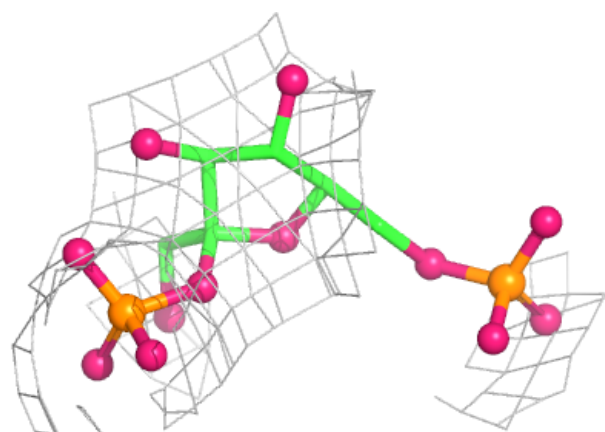


Electron density around FDP O 700:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

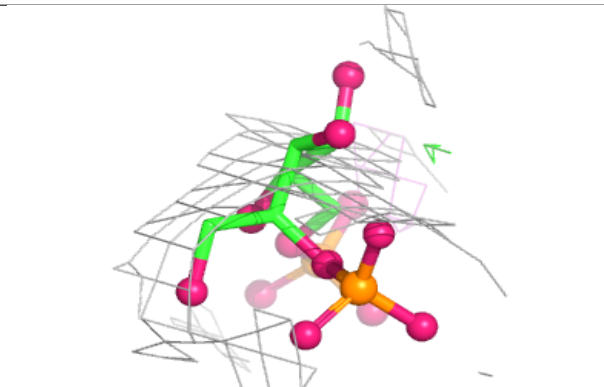
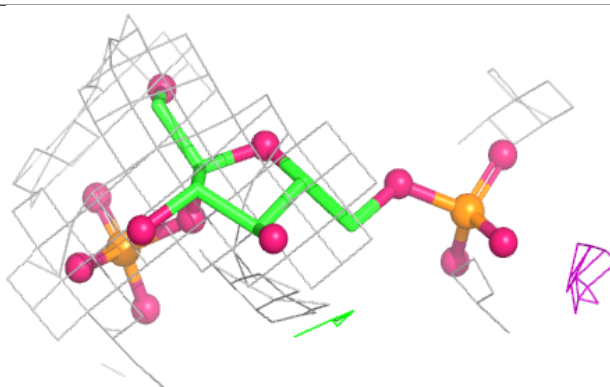
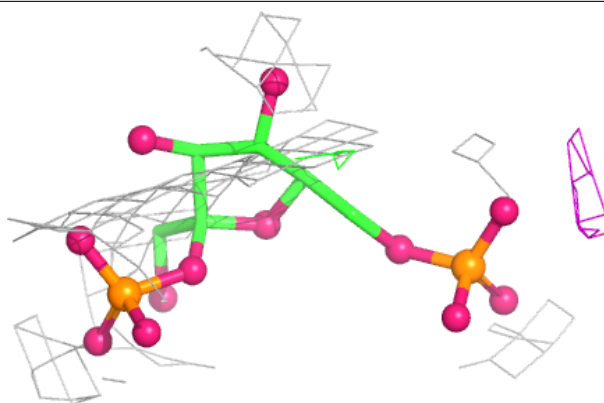
**Electron density around FDP P 700:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

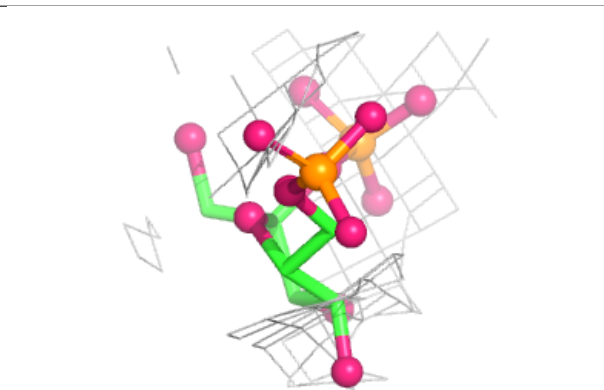
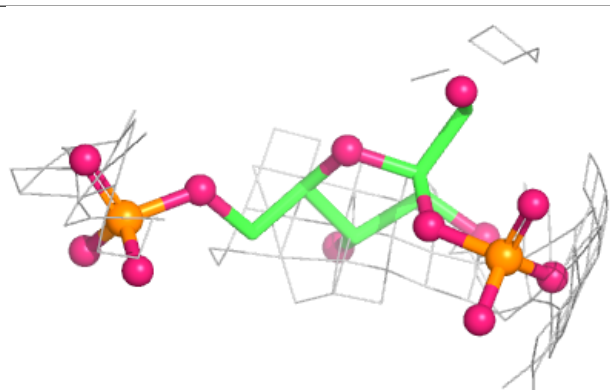
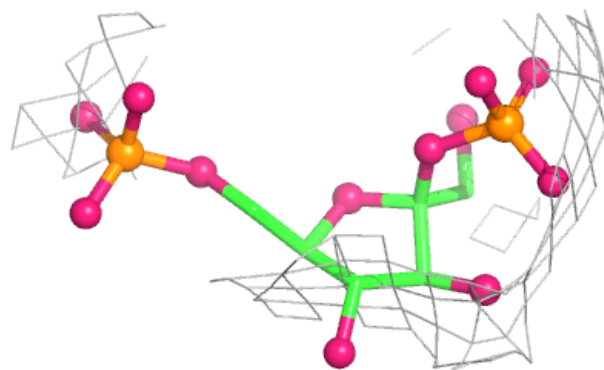


Electron density around FDP Q 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

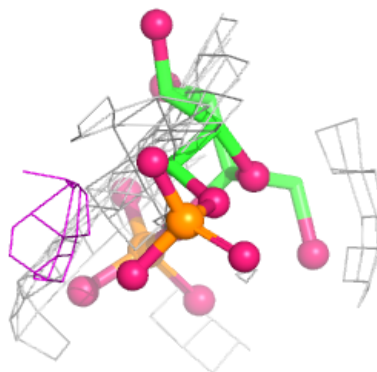
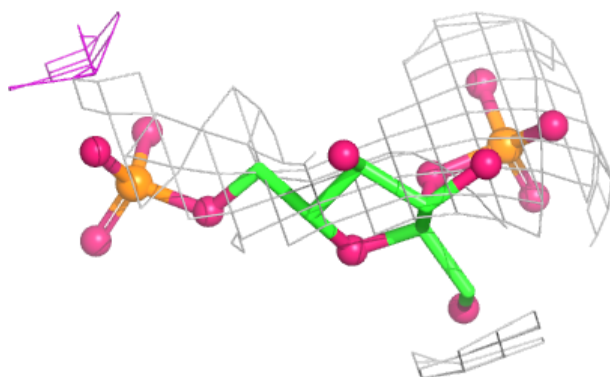
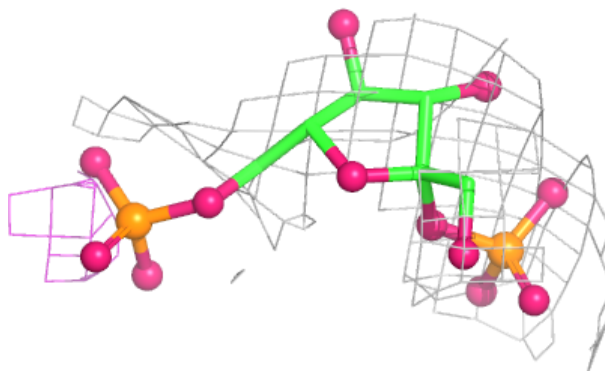
**Electron density around FDP R 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



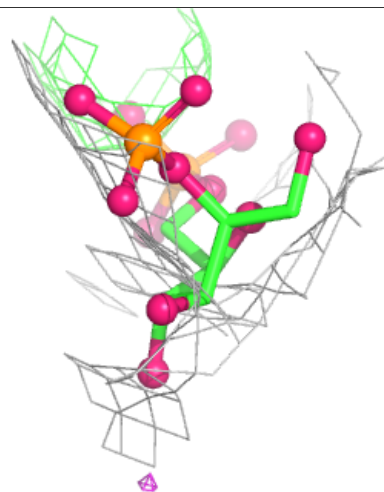
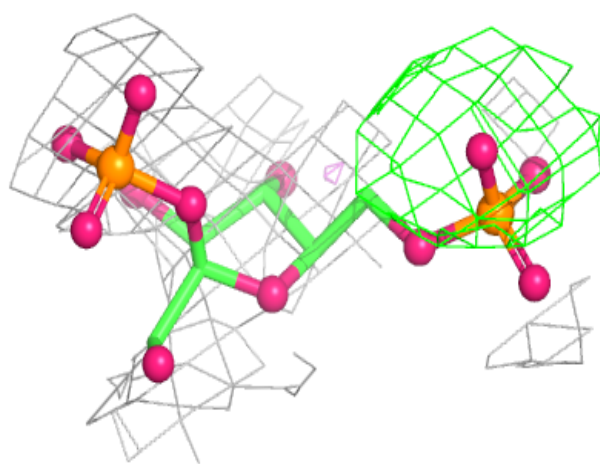
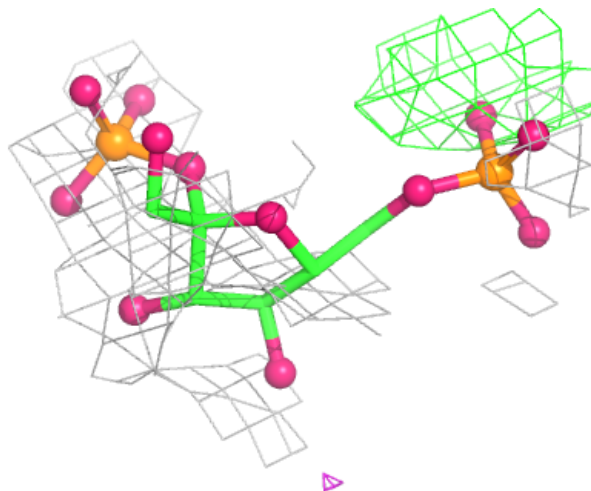
Electron density around FDP S 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



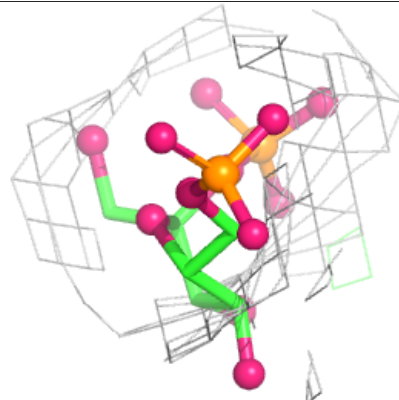
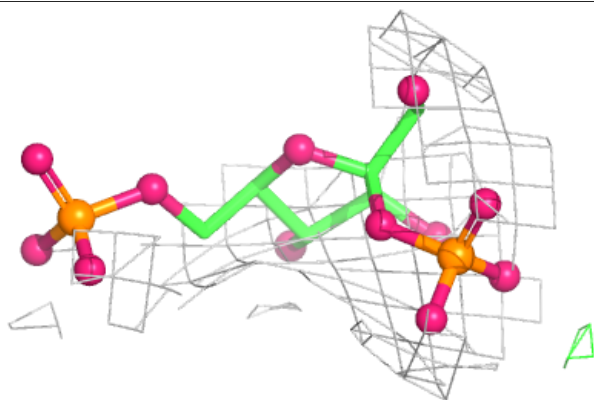
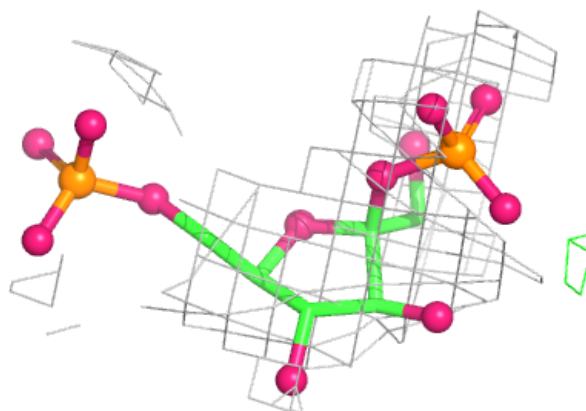
Electron density around FDP T 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

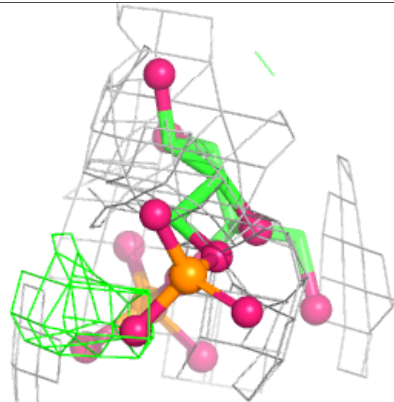
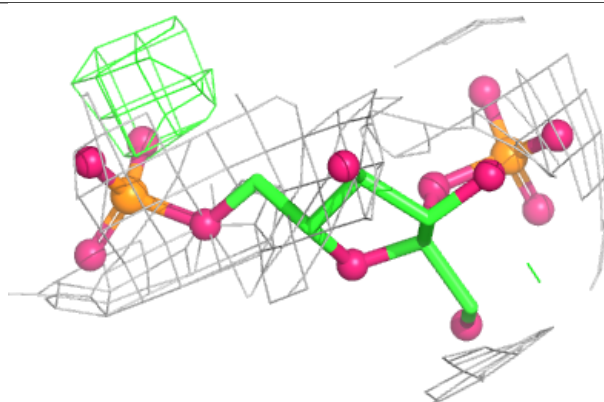
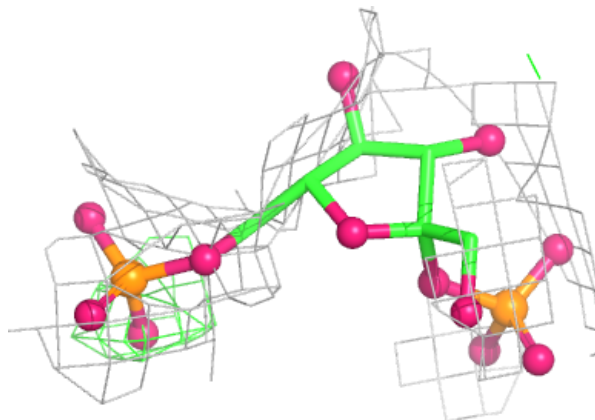


Electron density around FDP U 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

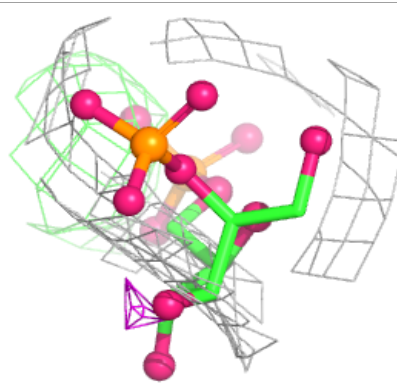
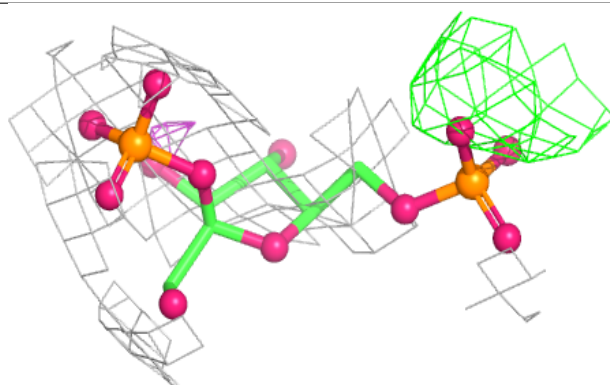
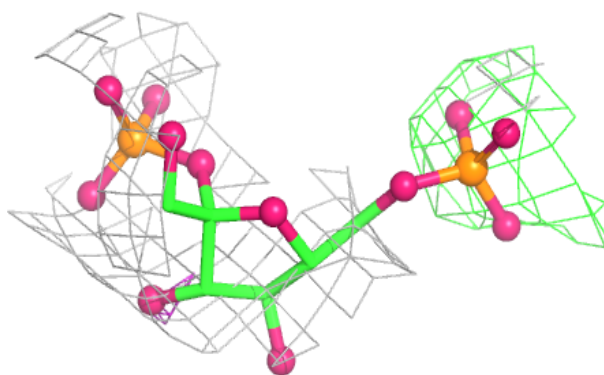
**Electron density around FDP V 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

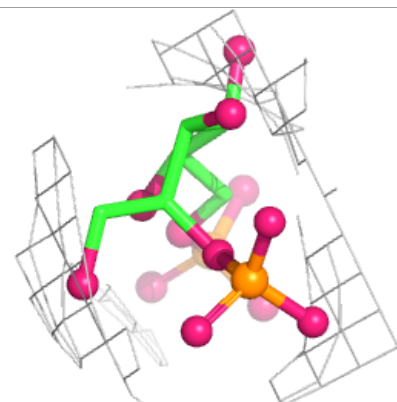
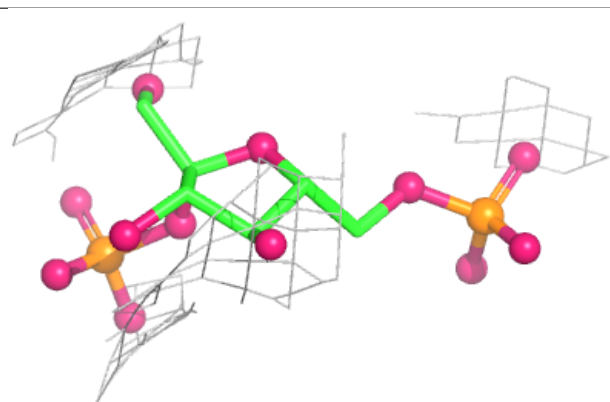
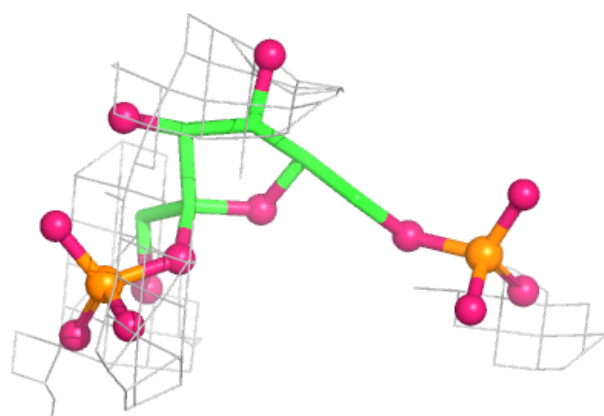


Electron density around FDP W 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FDP A 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.