



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2021 – 01:13 PM EDT

PDB ID : 3KIE
Title : Crystal structure of adeno-associated virus serotype 3B
Authors : Lerch, T.F.; Xie, Q.; Chapman, M.S.
Deposited on : 2009-11-01
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

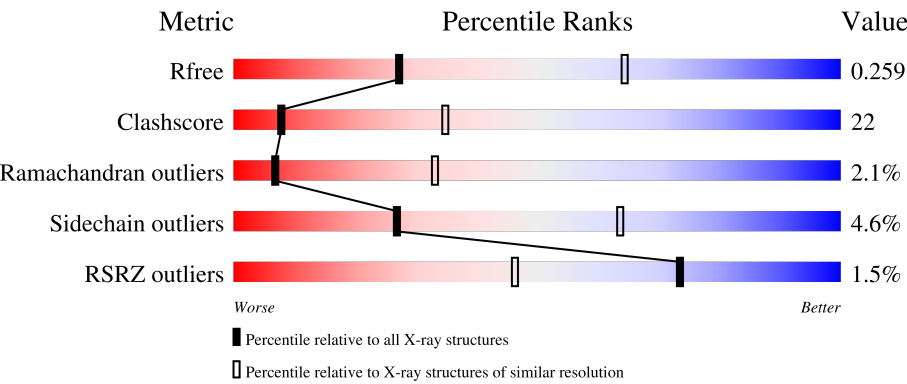
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.17.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	736	<div><div>%</div><div><div></div><div>38%</div><div>29%</div><div>.</div><div>29%</div></div></div>
1	B	736	<div><div>%</div><div><div></div><div>41%</div><div>27%</div><div>.</div><div>29%</div></div></div>
1	C	736	<div><div>%</div><div><div></div><div>39%</div><div>29%</div><div>.</div><div>29%</div></div></div>
1	D	736	<div><div>%</div><div><div></div><div>39%</div><div>29%</div><div>.</div><div>29%</div></div></div>
1	E	736	<div><div>%</div><div><div></div><div>40%</div><div>29%</div><div>.</div><div>29%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	736	
1	G	736	
1	H	736	
1	I	736	
1	J	736	
1	K	736	
1	L	736	
1	M	736	
1	N	736	
1	O	736	
1	P	736	
1	Q	736	
1	R	736	
1	S	736	
1	T	736	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	D5M	G	999	-	-	-	X
2	D5M	L	999	-	-	-	X
2	D5M	S	999	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 83520 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 Capsid protein VP1.

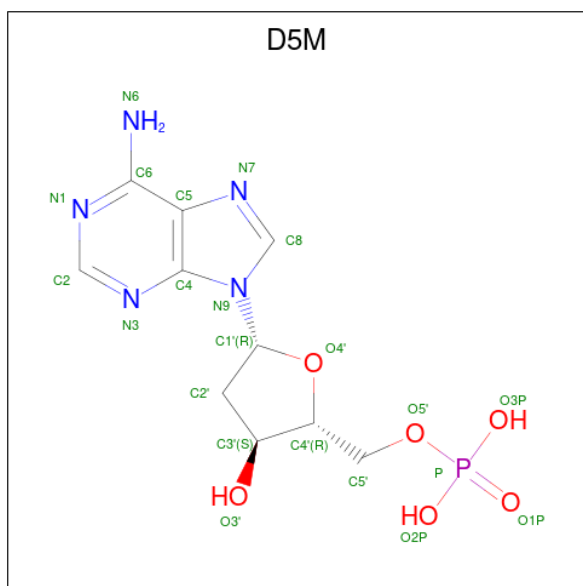
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	B	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	C	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	D	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	E	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	F	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	G	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	H	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	I	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	J	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	K	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	L	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	M	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	N	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	O	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	P	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	R	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	S	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	T	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: C₁₀H₁₄N₅O₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	E	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	G	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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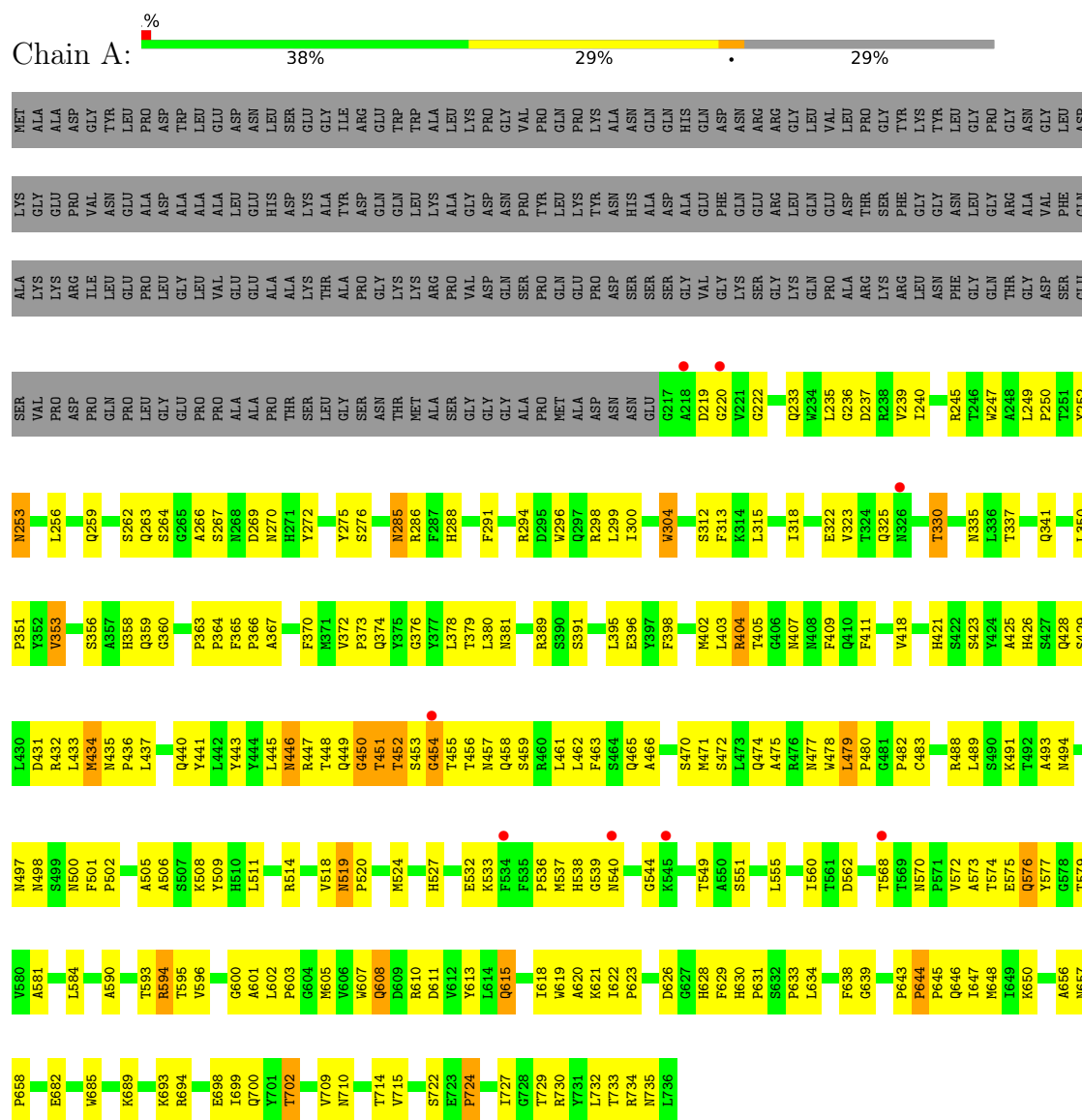
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	I	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	J	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	K	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	L	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	M	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	N	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	O	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	P	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	Q	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	R	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	S	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	T	1	Total 22	C 10	N 5	O 6	P 1	0	0

3 Residue-property plots

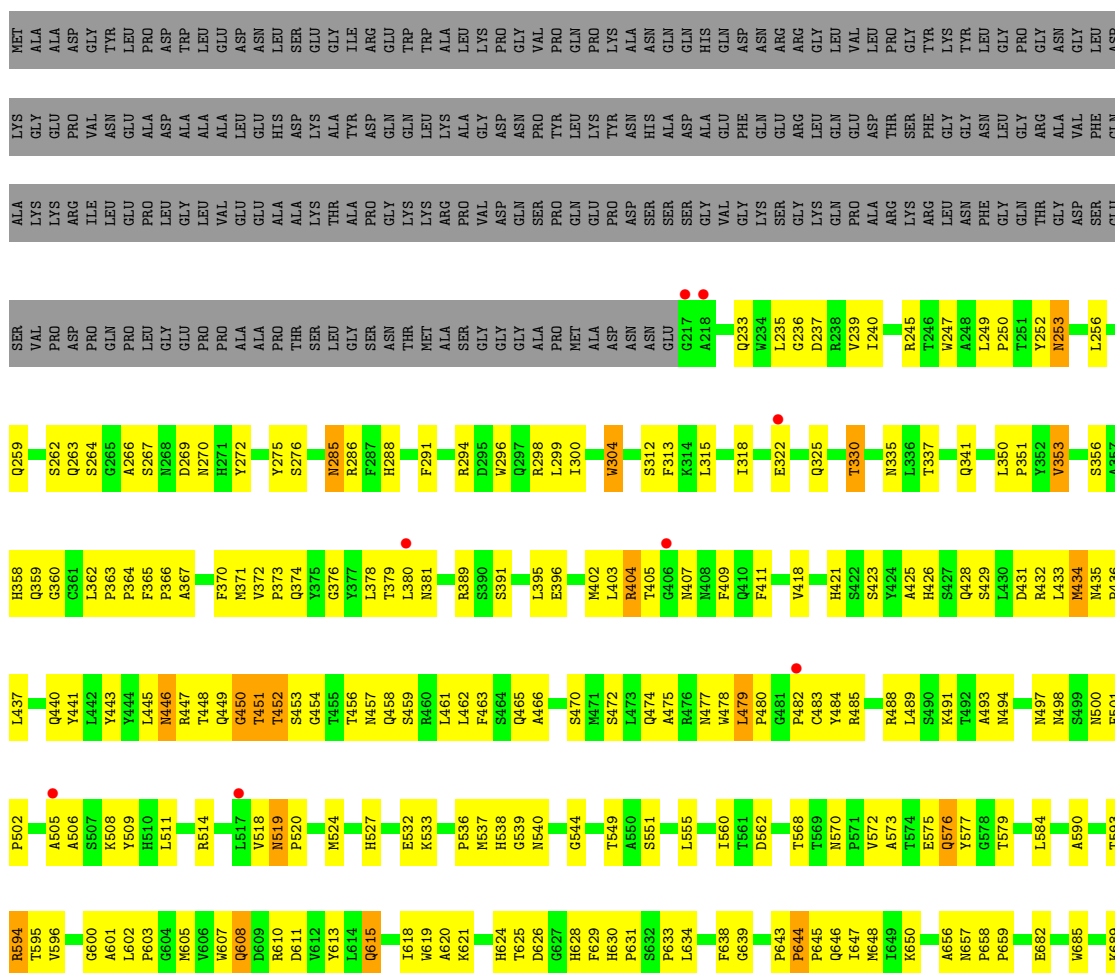
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

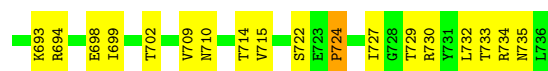
• Molecule 1: Capsid protein VP1



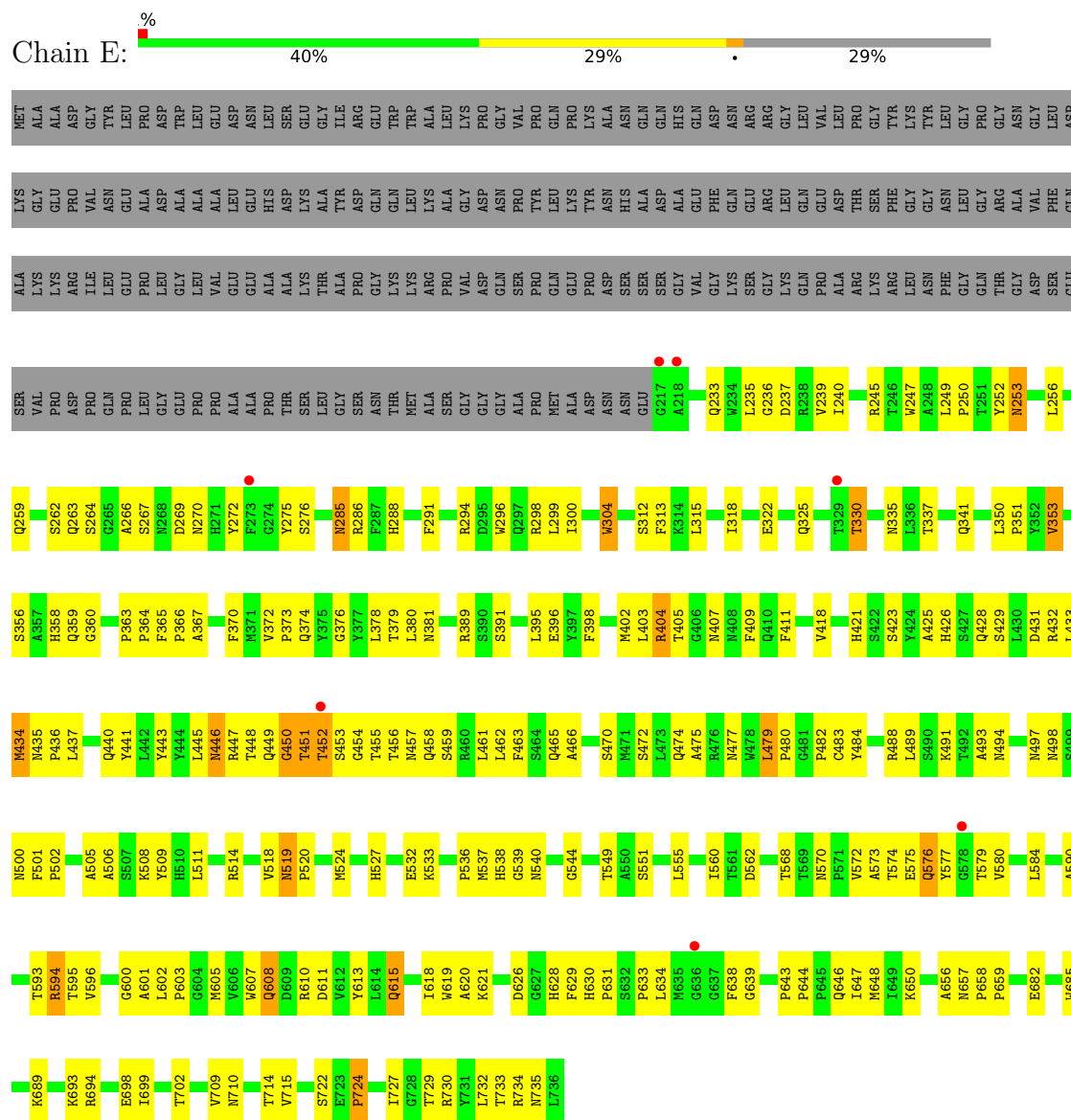
• Molecule 1: Capsid protein VP1



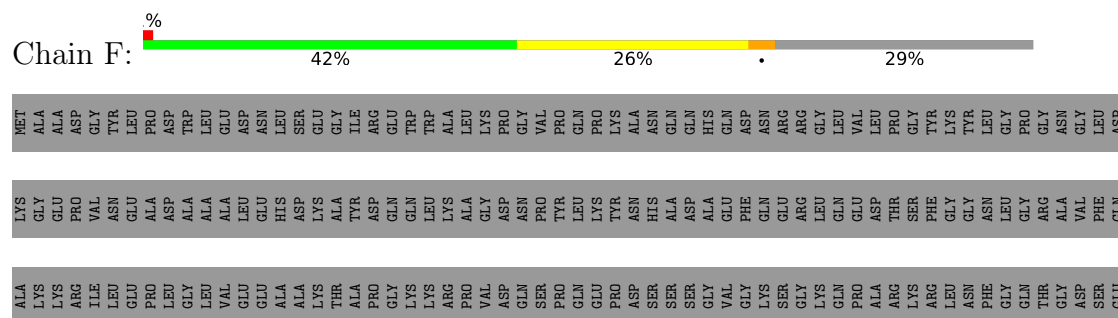


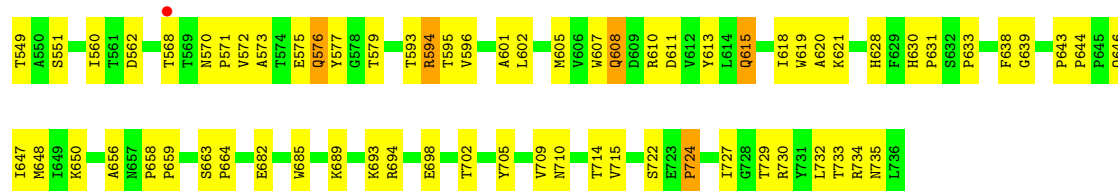


• Molecule 1: Capsid protein VP1

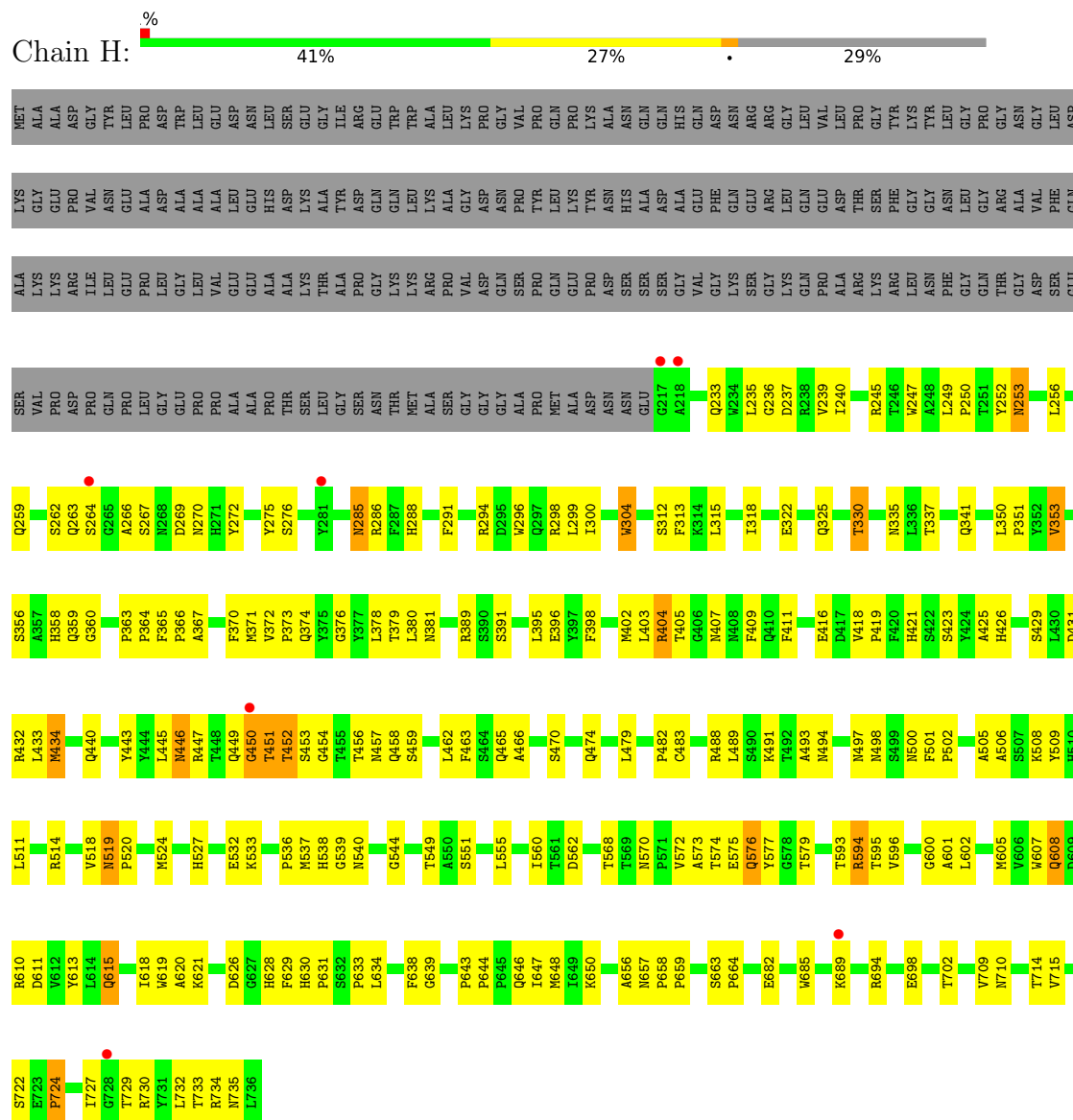


• Molecule 1: Capsid protein VP1

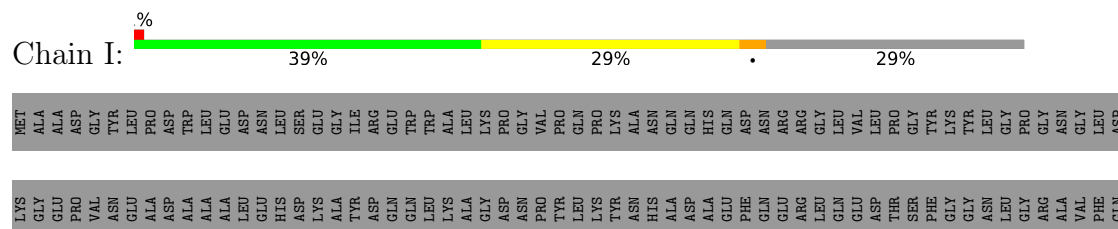


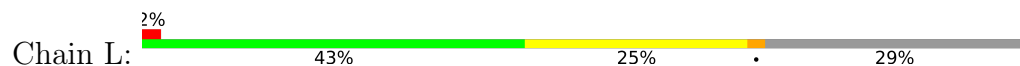


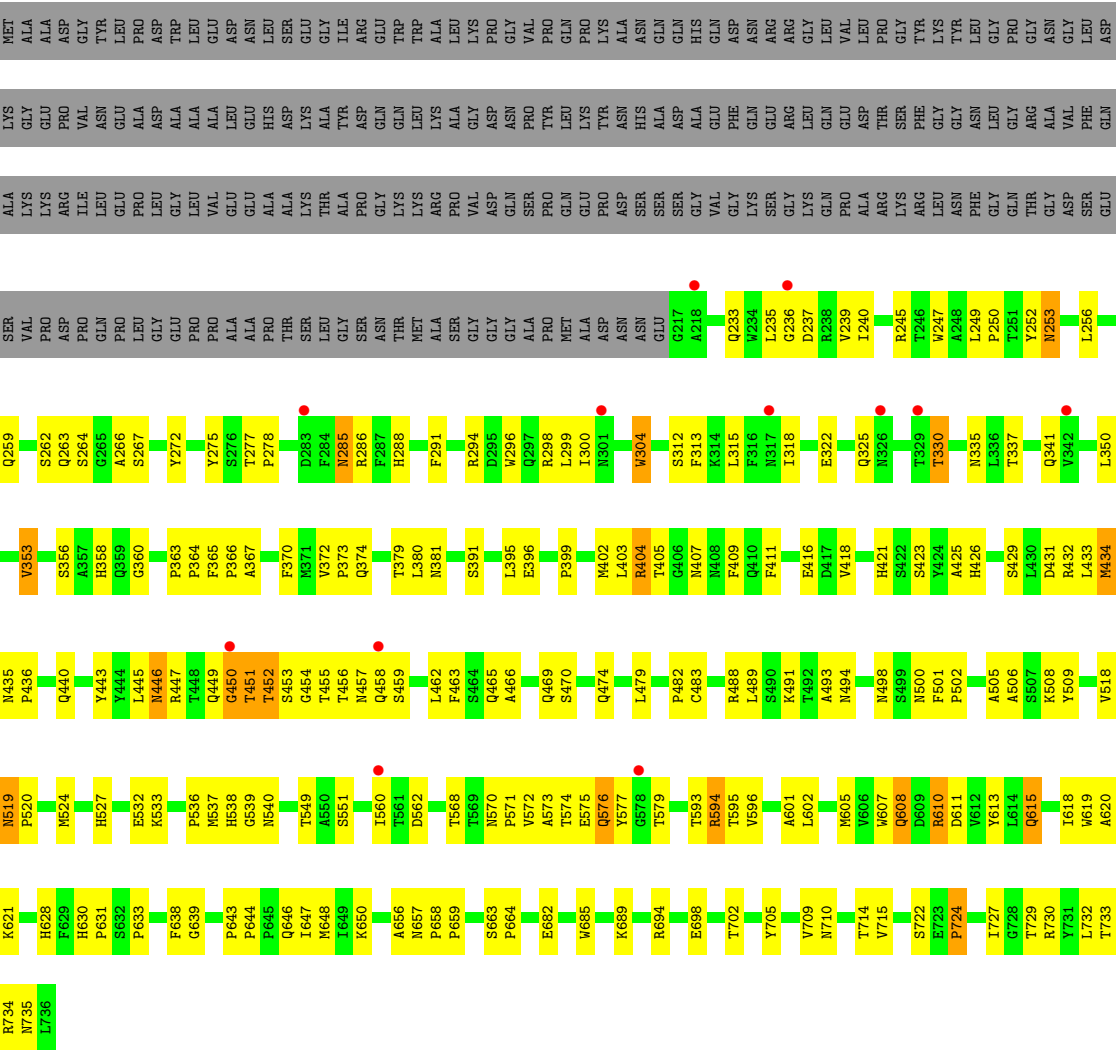
• Molecule 1: Capsid protein VP1



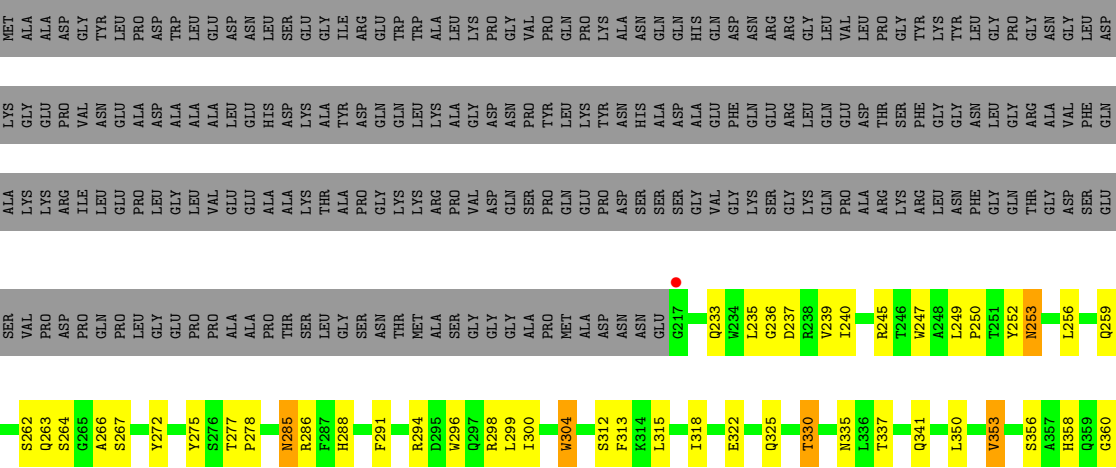
• Molecule 1: Capsid protein VP1

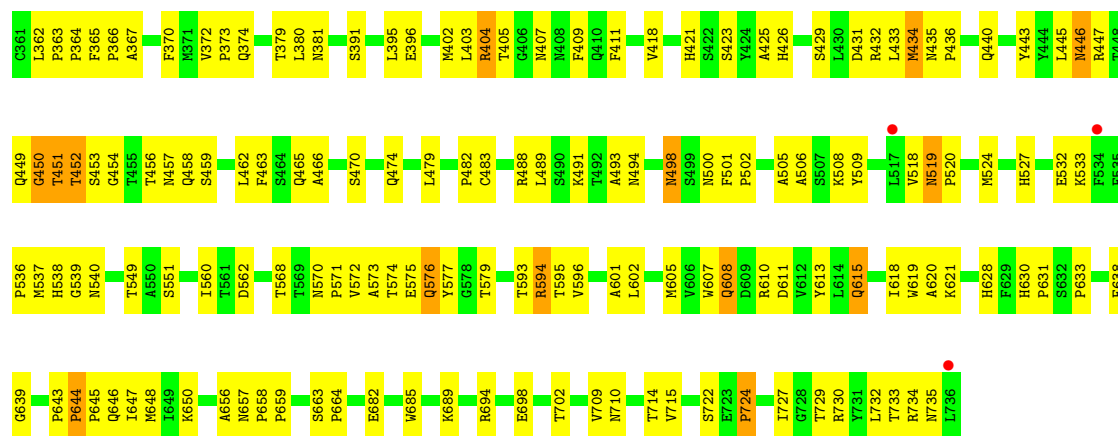




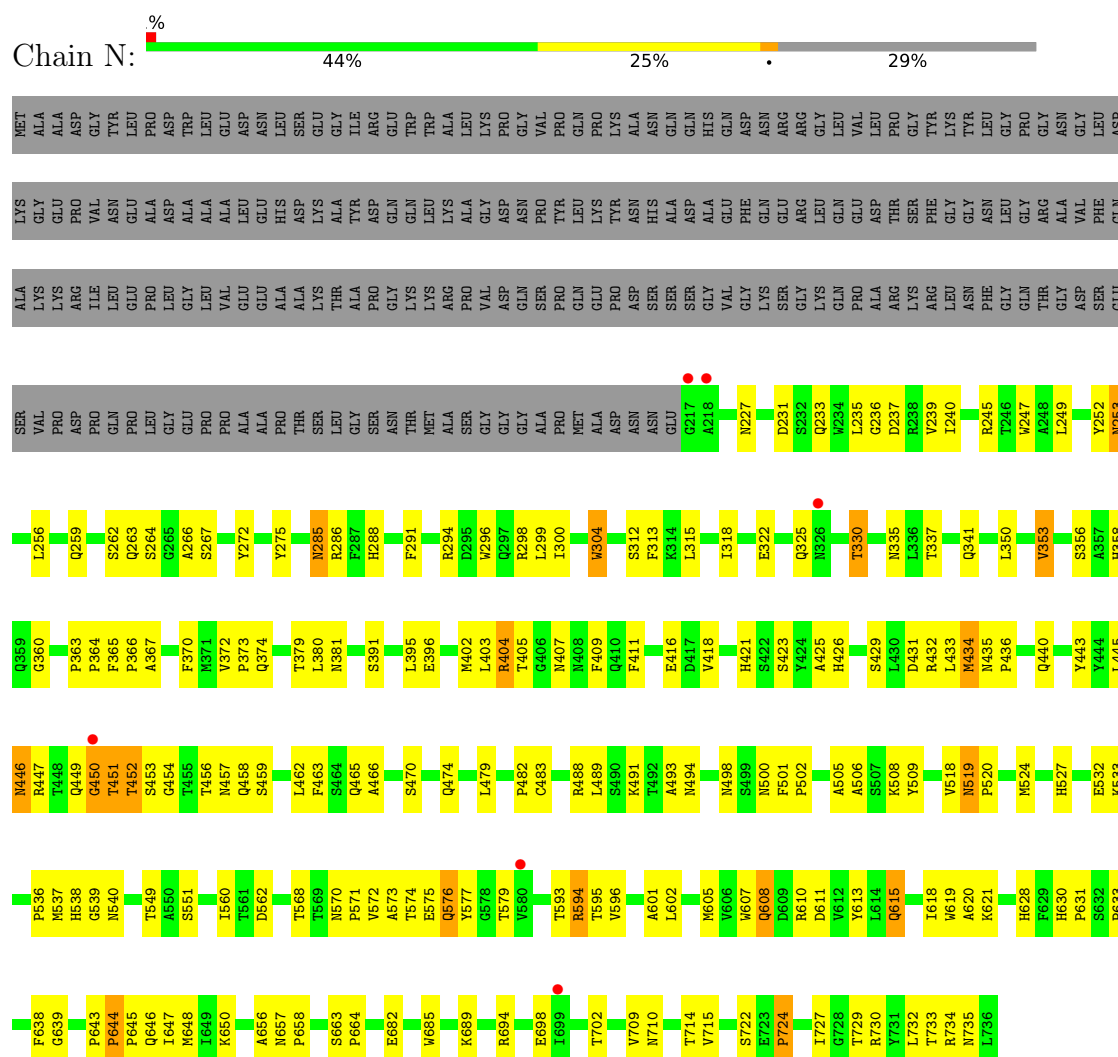


● Molecule 1: Capsid protein VP1



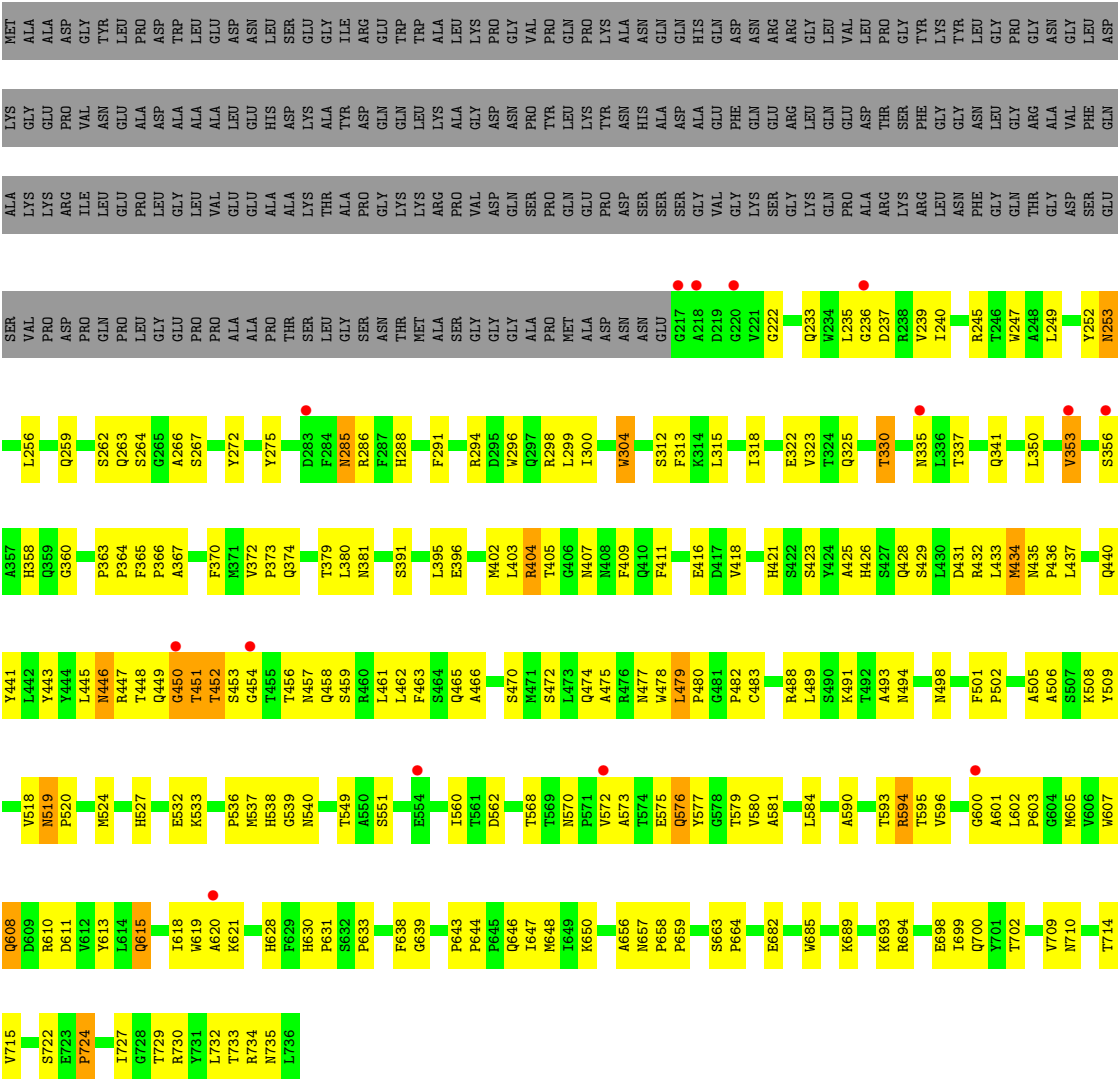


• Molecule 1: Capsid protein VP1

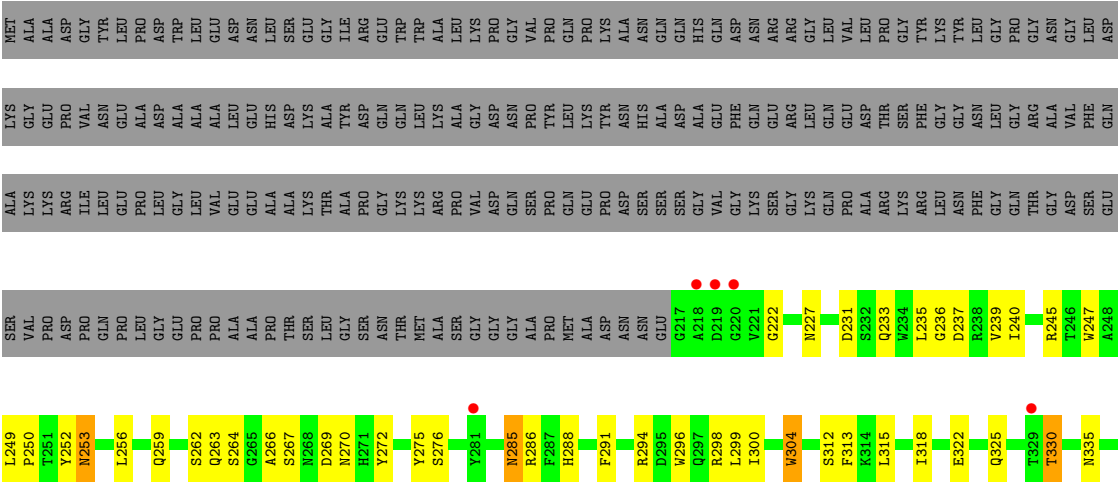


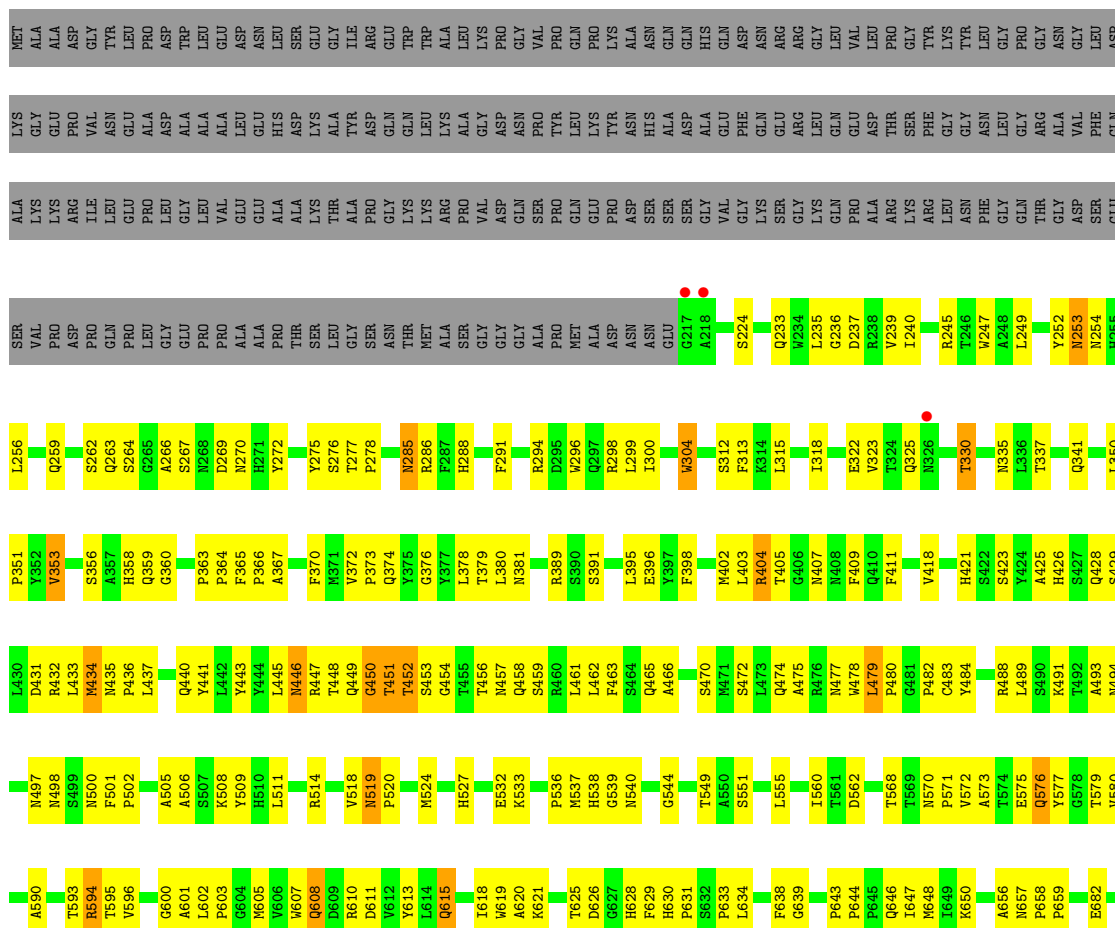
• Molecule 1: Capsid protein VP1





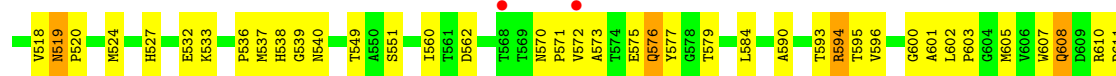
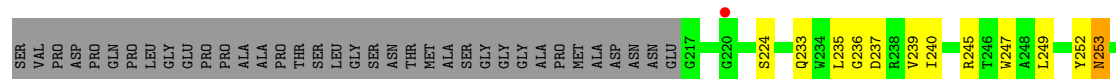
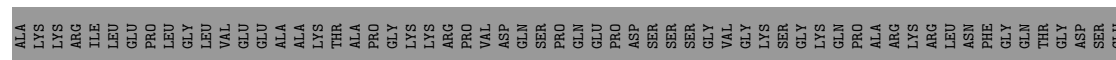
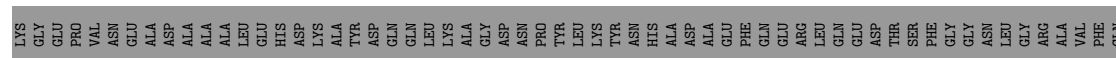
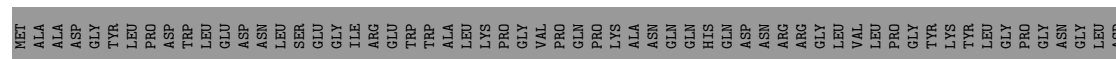
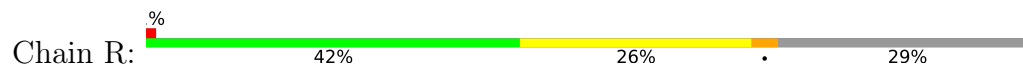
• Molecule 1: Capsid protein VP1



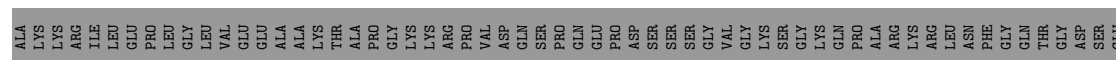
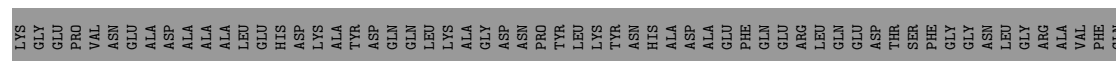
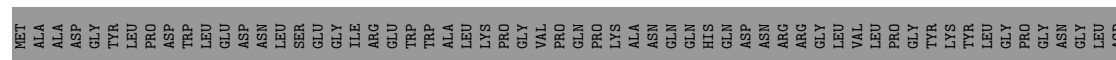
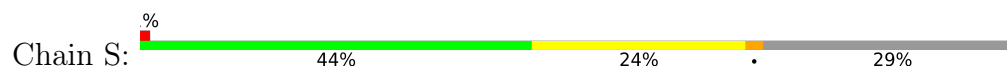


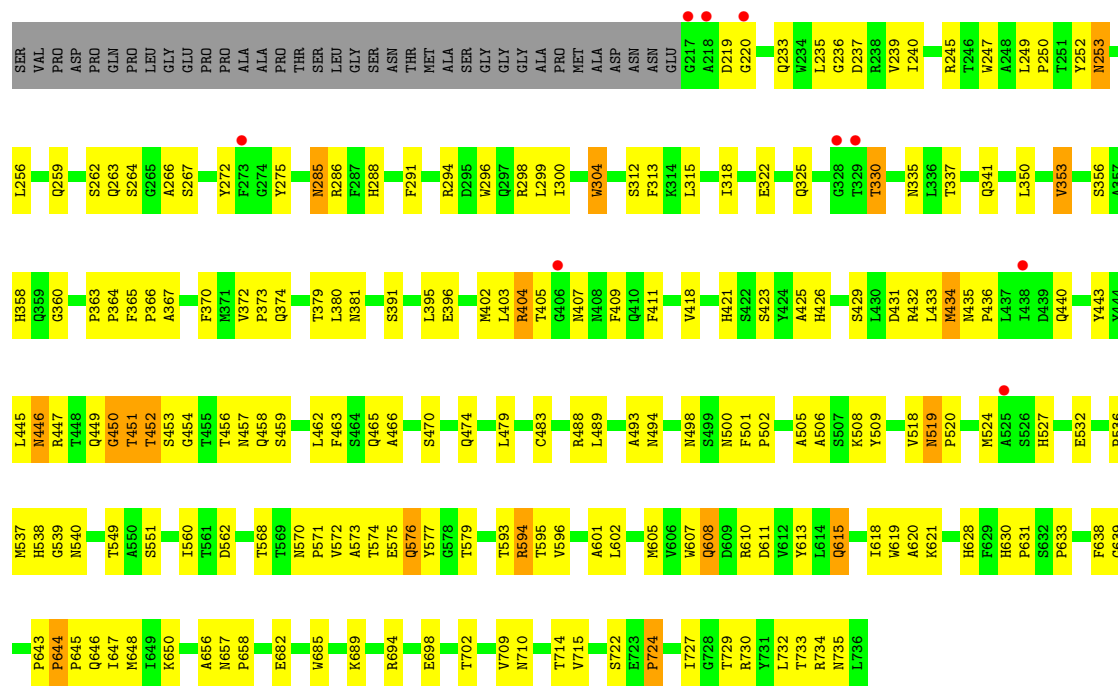


● Molecule 1: Capsid protein VP1

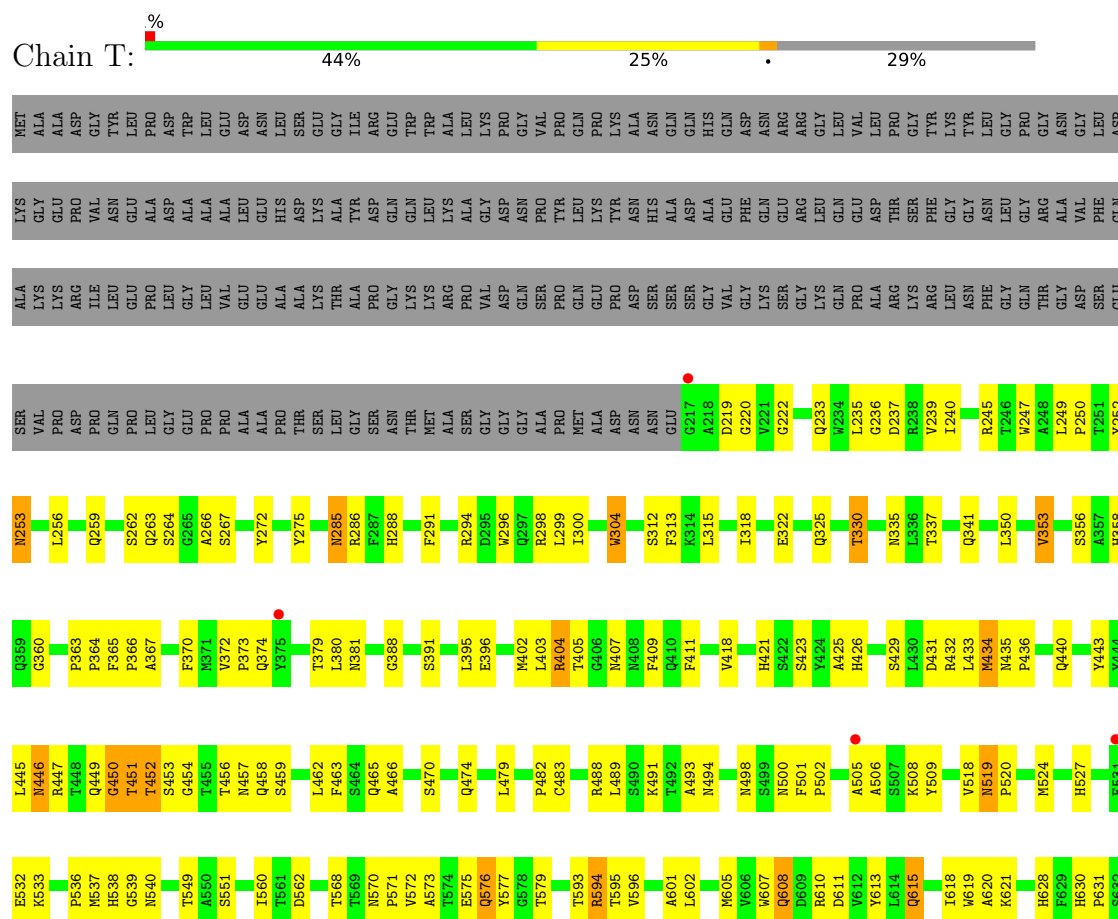


● Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	257.77Å 257.77Å 607.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	13.93 – 3.00 44.10 – 3.00	Depositor EDS
% Data completeness (in resolution range)	10.9 (13.93-3.00) 21.6 (44.10-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.231 , 0.262 0.231 , 0.259	Depositor DCC
R_{free} test set	1582 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.040 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.037 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.058 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.029 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.056 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.037 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.079 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.172 for h,-h-k,-l	Depositor
Outliers	0 of 65132 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	83520	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.68% 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: D5M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.24	0/4282	0.41	0/5843
1	B	0.24	0/4282	0.41	0/5843
1	C	0.24	0/4282	0.42	0/5843
1	D	0.24	0/4282	0.41	0/5843
1	E	0.24	0/4282	0.41	0/5843
1	F	0.24	0/4282	0.41	0/5843
1	G	0.24	0/4282	0.41	0/5843
1	H	0.24	0/4282	0.41	0/5843
1	I	0.24	0/4282	0.41	0/5843
1	J	0.24	0/4282	0.42	0/5843
1	K	0.24	0/4282	0.41	0/5843
1	L	0.24	0/4282	0.41	0/5843
1	M	0.24	0/4282	0.41	0/5843
1	N	0.24	0/4282	0.41	0/5843
1	O	0.24	0/4282	0.41	0/5843
1	P	0.24	0/4282	0.41	0/5843
1	Q	0.24	0/4282	0.41	0/5843
1	R	0.24	0/4282	0.41	0/5843
1	S	0.24	0/4282	0.41	0/5843
1	T	0.24	0/4282	0.41	0/5843
All	All	0.24	0/85640	0.41	0/116860

There are no bond length outliers.

There are no bond angle outliers.

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	4154	0	3899	250	5
1	B	4154	0	3899	212	5
1	C	4154	0	3899	256	17
1	D	4154	0	3899	254	0
1	E	4154	0	3899	242	4
1	F	4154	0	3899	206	0
1	G	4154	0	3899	162	3
1	H	4154	0	3899	209	0
1	I	4154	0	3899	247	0
1	J	4154	0	3899	201	0
1	K	4154	0	3899	200	1
1	L	4154	0	3899	170	22
1	M	4154	0	3899	166	0
1	N	4154	0	3899	162	3
1	O	4154	0	3899	200	0
1	P	4154	0	3899	207	7
1	Q	4154	0	3899	250	1
1	R	4154	0	3899	205	0
1	S	4154	0	3899	156	0
1	T	4154	0	3899	160	0
2	A	22	0	12	3	0
2	B	22	0	12	3	0
2	C	22	0	12	3	0
2	D	22	0	12	3	0
2	E	22	0	12	3	0
2	F	22	0	12	3	0
2	G	22	0	12	3	0
2	H	22	0	12	3	0
2	I	22	0	12	3	0
2	J	22	0	12	3	0
2	K	22	0	12	3	0
2	L	22	0	12	3	0
2	M	22	0	12	3	0
2	N	22	0	12	3	0
2	O	22	0	12	3	0
2	P	22	0	12	3	0
2	Q	22	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	22	0	12	3	0
2	S	22	0	12	3	0
2	T	22	0	12	3	0
All	All	83520	0	78220	3500	34

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 22.

All (3500) 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:E:519:ASN:HB3	1:E:520:PRO:HD3	1.51	0.93
1:I:519:ASN:HB3	1:I:520:PRO:HD3	1.51	0.93
1:F:479:LEU:HD22	1:P:634:LEU:HD11	1.52	0.92
1:L:519:ASN:HB3	1:L:520:PRO:HD3	1.51	0.92
1:K:519:ASN:HB3	1:K:520:PRO:HD3	1.51	0.92
1:G:519:ASN:HB3	1:G:520:PRO:HD3	1.51	0.92
1:D:519:ASN:HB3	1:D:520:PRO:HD3	1.51	0.92
1:N:519:ASN:HB3	1:N:520:PRO:HD3	1.51	0.92
1:B:519:ASN:HB3	1:B:520:PRO:HD3	1.51	0.91
1:J:519:ASN:HB3	1:J:520:PRO:HD3	1.51	0.91
1:F:519:ASN:HB3	1:F:520:PRO:HD3	1.51	0.91
1:P:519:ASN:HB3	1:P:520:PRO:HD3	1.51	0.91
1:S:519:ASN:HB3	1:S:520:PRO:HD3	1.51	0.91
1:Q:519:ASN:HB3	1:Q:520:PRO:HD3	1.51	0.91
1:A:519:ASN:HB3	1:A:520:PRO:HD3	1.51	0.91
1:O:519:ASN:HB3	1:O:520:PRO:HD3	1.52	0.91
1:C:519:ASN:HB3	1:C:520:PRO:HD3	1.51	0.91
1:R:519:ASN:HB3	1:R:520:PRO:HD3	1.52	0.90
1:H:519:ASN:HB3	1:H:520:PRO:HD3	1.51	0.90
1:M:519:ASN:HB3	1:M:520:PRO:HD3	1.51	0.90
1:T:519:ASN:HB3	1:T:520:PRO:HD3	1.51	0.89
1:K:379:THR:HG21	1:K:391:SER:H	1.40	0.87
1:O:379:THR:HG21	1:O:391:SER:H	1.40	0.87
1:F:379:THR:HG21	1:F:391:SER:H	1.40	0.87
1:Q:379:THR:HG21	1:Q:391:SER:H	1.40	0.87
1:G:379:THR:HG21	1:G:391:SER:H	1.40	0.87
1:J:634:LEU:HD11	1:O:479:LEU:HD22	1.56	0.86
1:B:379:THR:HG21	1:B:391:SER:H	1.40	0.86
1:C:379:THR:HG21	1:C:391:SER:H	1.40	0.86
1:L:379:THR:HG21	1:L:391:SER:H	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:466:ALA:HB1	1:N:474:GLN:HG2	1.58	0.86
1:E:379:THR:HG21	1:E:391:SER:H	1.40	0.86
1:M:379:THR:HG21	1:M:391:SER:H	1.40	0.86
1:S:466:ALA:HB1	1:S:474:GLN:HG2	1.58	0.86
1:H:466:ALA:HB1	1:H:474:GLN:HG2	1.58	0.86
1:O:466:ALA:HB1	1:O:474:GLN:HG2	1.58	0.86
1:D:379:THR:HG21	1:D:391:SER:H	1.40	0.86
1:I:466:ALA:HB1	1:I:474:GLN:HG2	1.58	0.86
1:E:479:LEU:HD22	1:Q:634:LEU:HD11	1.58	0.85
1:A:379:THR:HG21	1:A:391:SER:H	1.40	0.85
1:L:466:ALA:HB1	1:L:474:GLN:HG2	1.58	0.85
1:P:379:THR:HG21	1:P:391:SER:H	1.40	0.85
1:H:379:THR:HG21	1:H:391:SER:H	1.40	0.85
1:T:379:THR:HG21	1:T:391:SER:H	1.40	0.85
1:E:466:ALA:HB1	1:E:474:GLN:HG2	1.58	0.85
1:P:466:ALA:HB1	1:P:474:GLN:HG2	1.58	0.85
1:R:466:ALA:HB1	1:R:474:GLN:HG2	1.58	0.85
1:T:466:ALA:HB1	1:T:474:GLN:HG2	1.58	0.85
1:A:466:ALA:HB1	1:A:474:GLN:HG2	1.58	0.85
1:A:634:LEU:HD11	1:D:479:LEU:HD22	1.59	0.85
1:J:466:ALA:HB1	1:J:474:GLN:HG2	1.58	0.85
1:B:466:ALA:HB1	1:B:474:GLN:HG2	1.58	0.85
1:C:437:LEU:HD13	1:D:376:GLY:HA3	1.57	0.85
1:I:379:THR:HG21	1:I:391:SER:H	1.40	0.85
1:Q:466:ALA:HB1	1:Q:474:GLN:HG2	1.58	0.84
1:A:300:ILE:HD12	1:A:729:THR:HA	1.60	0.84
1:R:379:THR:HG21	1:R:391:SER:H	1.40	0.84
1:C:300:ILE:HD12	1:C:729:THR:HA	1.60	0.84
1:K:466:ALA:HB1	1:K:474:GLN:HG2	1.58	0.84
1:G:466:ALA:HB1	1:G:474:GLN:HG2	1.58	0.84
1:N:379:THR:HG21	1:N:391:SER:H	1.40	0.84
1:D:466:ALA:HB1	1:D:474:GLN:HG2	1.58	0.83
1:S:300:ILE:HD12	1:S:729:THR:HA	1.60	0.83
1:E:300:ILE:HD12	1:E:729:THR:HA	1.60	0.83
1:G:300:ILE:HD12	1:G:729:THR:HA	1.60	0.83
1:I:634:LEU:HD11	1:Q:479:LEU:HD22	1.60	0.83
1:J:379:THR:HG21	1:J:391:SER:H	1.40	0.83
1:S:379:THR:HG21	1:S:391:SER:H	1.40	0.83
1:L:304:TRP:HZ3	1:L:732:LEU:HB3	1.44	0.83
1:T:300:ILE:HD12	1:T:729:THR:HA	1.60	0.83
1:T:304:TRP:HZ3	1:T:732:LEU:HB3	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:466:ALA:HB1	1:M:474:GLN:HG2	1.58	0.83
1:C:466:ALA:HB1	1:C:474:GLN:HG2	1.58	0.83
1:H:300:ILE:HD12	1:H:729:THR:HA	1.60	0.83
1:O:304:TRP:HZ3	1:O:732:LEU:HB3	1.44	0.83
1:A:639:GLY:H	2:A:999:D5M:HN62	1.27	0.83
1:C:304:TRP:HZ3	1:C:732:LEU:HB3	1.44	0.83
1:I:304:TRP:HZ3	1:I:732:LEU:HB3	1.44	0.83
1:M:304:TRP:HZ3	1:M:732:LEU:HB3	1.44	0.83
1:N:639:GLY:H	2:N:999:D5M:HN62	1.27	0.83
1:Q:300:ILE:HD12	1:Q:729:THR:HA	1.60	0.83
1:D:304:TRP:HZ3	1:D:732:LEU:HB3	1.44	0.82
1:N:304:TRP:HZ3	1:N:732:LEU:HB3	1.44	0.82
1:S:304:TRP:HZ3	1:S:732:LEU:HB3	1.44	0.82
1:B:304:TRP:HZ3	1:B:732:LEU:HB3	1.44	0.82
1:F:300:ILE:HD12	1:F:729:THR:HA	1.60	0.82
1:F:466:ALA:HB1	1:F:474:GLN:HG2	1.58	0.82
1:K:304:TRP:HZ3	1:K:732:LEU:HB3	1.44	0.82
1:H:304:TRP:HZ3	1:H:732:LEU:HB3	1.44	0.82
1:N:294:ARG:HE	1:N:298:ARG:HE	1.27	0.82
1:O:300:ILE:HD12	1:O:729:THR:HA	1.60	0.82
1:S:294:ARG:HE	1:S:298:ARG:HE	1.27	0.82
1:C:639:GLY:H	2:C:999:D5M:HN62	1.28	0.82
1:I:294:ARG:HE	1:I:298:ARG:HE	1.27	0.82
1:J:300:ILE:HD12	1:J:729:THR:HA	1.60	0.82
1:M:294:ARG:HE	1:M:298:ARG:HE	1.27	0.82
1:M:300:ILE:HD12	1:M:729:THR:HA	1.60	0.82
1:R:300:ILE:HD12	1:R:729:THR:HA	1.60	0.82
1:T:294:ARG:HE	1:T:298:ARG:HE	1.27	0.82
1:R:304:TRP:HZ3	1:R:732:LEU:HB3	1.44	0.82
1:R:639:GLY:H	2:R:999:D5M:HN62	1.27	0.82
1:E:294:ARG:HE	1:E:298:ARG:HE	1.28	0.82
1:A:479:LEU:HD22	1:C:634:LEU:HD11	1.62	0.82
1:D:294:ARG:HE	1:D:298:ARG:HE	1.27	0.82
1:H:294:ARG:HE	1:H:298:ARG:HE	1.27	0.82
1:I:300:ILE:HD12	1:I:729:THR:HA	1.60	0.82
1:I:639:GLY:H	2:I:999:D5M:HN62	1.27	0.82
1:K:634:LEU:HD11	1:R:479:LEU:HD22	1.61	0.82
1:P:300:ILE:HD12	1:P:729:THR:HA	1.60	0.82
1:B:479:LEU:HD22	1:H:634:LEU:HD11	1.62	0.82
1:F:304:TRP:HZ3	1:F:732:LEU:HB3	1.44	0.82
1:Q:639:GLY:H	2:Q:999:D5M:HN62	1.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ILE:HD12	1:B:729:THR:HA	1.60	0.81
1:L:294:ARG:HE	1:L:298:ARG:HE	1.27	0.81
1:R:294:ARG:HE	1:R:298:ARG:HE	1.27	0.81
1:E:304:TRP:HZ3	1:E:732:LEU:HB3	1.44	0.81
1:K:300:ILE:HD12	1:K:729:THR:HA	1.60	0.81
1:Q:304:TRP:HZ3	1:Q:732:LEU:HB3	1.44	0.81
1:B:639:GLY:H	2:B:999:D5M:HN62	1.27	0.81
1:D:639:GLY:H	2:D:999:D5M:HN62	1.27	0.81
1:T:639:GLY:H	2:T:999:D5M:HN62	1.27	0.81
1:A:304:TRP:HZ3	1:A:732:LEU:HB3	1.44	0.81
1:N:300:ILE:HD12	1:N:729:THR:HA	1.60	0.81
1:D:300:ILE:HD12	1:D:729:THR:HA	1.60	0.81
1:P:294:ARG:HE	1:P:298:ARG:HE	1.27	0.81
1:J:294:ARG:HE	1:J:298:ARG:HE	1.27	0.81
1:B:421:HIS:NE2	1:B:729:THR:HG21	1.96	0.81
1:C:421:HIS:NE2	1:C:729:THR:HG21	1.96	0.81
1:P:304:TRP:HZ3	1:P:732:LEU:HB3	1.44	0.81
1:J:639:GLY:H	2:J:999:D5M:HN62	1.27	0.81
1:E:634:LEU:HD11	1:I:479:LEU:HD22	1.62	0.80
1:F:590:ALA:HA	1:P:497:ASN:ND2	1.95	0.80
1:N:421:HIS:NE2	1:N:729:THR:HG21	1.97	0.80
1:G:304:TRP:HZ3	1:G:732:LEU:HB3	1.44	0.80
1:A:421:HIS:NE2	1:A:729:THR:HG21	1.97	0.80
1:F:421:HIS:NE2	1:F:729:THR:HG21	1.97	0.80
1:L:300:ILE:HD12	1:L:729:THR:HA	1.60	0.80
1:K:294:ARG:HE	1:K:298:ARG:HE	1.27	0.80
1:P:421:HIS:NE2	1:P:729:THR:HG21	1.96	0.80
1:S:639:GLY:H	2:S:999:D5M:HN62	1.27	0.80
1:G:639:GLY:H	2:G:999:D5M:HN62	1.27	0.80
1:K:639:GLY:H	2:K:999:D5M:HN62	1.28	0.80
1:L:421:HIS:NE2	1:L:729:THR:HG21	1.96	0.80
1:O:421:HIS:NE2	1:O:729:THR:HG21	1.97	0.80
1:G:294:ARG:HE	1:G:298:ARG:HE	1.27	0.80
1:J:304:TRP:HZ3	1:J:732:LEU:HB3	1.44	0.80
1:O:294:ARG:HE	1:O:298:ARG:HE	1.27	0.80
1:B:294:ARG:HE	1:B:298:ARG:HE	1.27	0.80
1:F:294:ARG:HE	1:F:298:ARG:HE	1.27	0.80
1:G:421:HIS:NE2	1:G:729:THR:HG21	1.97	0.80
1:O:639:GLY:H	2:O:999:D5M:HN62	1.27	0.80
1:H:639:GLY:H	2:H:999:D5M:HN62	1.27	0.80
1:M:421:HIS:NE2	1:M:729:THR:HG21	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:HE	1:A:298:ARG:HE	1.27	0.80
1:C:479:LEU:HD22	1:D:634:LEU:HD11	1.63	0.80
1:E:421:HIS:NE2	1:E:729:THR:HG21	1.96	0.80
1:I:421:HIS:NE2	1:I:729:THR:HG21	1.97	0.80
1:J:421:HIS:NE2	1:J:729:THR:HG21	1.97	0.80
1:C:294:ARG:HE	1:C:298:ARG:HE	1.27	0.79
1:F:441:TYR:HB3	1:P:359:GLN:HG2	1.64	0.79
1:E:639:GLY:H	2:E:999:D5M:HN62	1.28	0.79
1:F:639:GLY:H	2:F:999:D5M:HN62	1.27	0.79
1:M:639:GLY:H	2:M:999:D5M:HN62	1.27	0.79
1:K:421:HIS:NE2	1:K:729:THR:HG21	1.96	0.79
1:D:421:HIS:NE2	1:D:729:THR:HG21	1.97	0.79
1:Q:421:HIS:NE2	1:Q:729:THR:HG21	1.97	0.79
1:A:437:LEU:HD13	1:C:376:GLY:HA3	1.64	0.79
1:T:421:HIS:NE2	1:T:729:THR:HG21	1.97	0.79
1:Q:294:ARG:HE	1:Q:298:ARG:HE	1.27	0.79
1:R:421:HIS:NE2	1:R:729:THR:HG21	1.96	0.79
1:S:421:HIS:NE2	1:S:729:THR:HG21	1.97	0.79
1:G:524:MET:HE2	1:G:573:ALA:HA	1.66	0.78
1:H:421:HIS:NE2	1:H:729:THR:HG21	1.97	0.78
1:P:639:GLY:H	2:P:999:D5M:HN62	1.27	0.78
1:M:524:MET:HE2	1:M:573:ALA:HA	1.66	0.78
1:B:366:PRO:HB2	1:C:396:GLU:HB2	1.67	0.77
1:E:376:GLY:HA3	1:I:437:LEU:HD13	1.65	0.77
1:I:376:GLY:HA3	1:Q:437:LEU:HD13	1.64	0.77
1:K:376:GLY:HA3	1:R:437:LEU:HD13	1.65	0.77
1:M:501:PHE:N	1:M:502:PRO:HD3	2.00	0.77
1:D:501:PHE:N	1:D:502:PRO:HD3	2.00	0.77
1:G:501:PHE:N	1:G:502:PRO:HD3	2.00	0.77
1:B:501:PHE:N	1:B:502:PRO:HD3	2.00	0.77
1:C:501:PHE:N	1:C:502:PRO:HD3	2.00	0.77
1:D:524:MET:HE2	1:D:573:ALA:HA	1.66	0.77
1:L:639:GLY:H	2:L:999:D5M:HN62	1.27	0.77
1:R:501:PHE:N	1:R:502:PRO:HD3	2.00	0.77
1:S:501:PHE:N	1:S:502:PRO:HD3	2.00	0.77
1:C:603:PRO:HA	1:D:629:PHE:HD2	1.47	0.77
1:E:501:PHE:N	1:E:502:PRO:HD3	2.00	0.77
1:J:501:PHE:N	1:J:502:PRO:HD3	2.00	0.77
1:N:501:PHE:N	1:N:502:PRO:HD3	2.00	0.77
1:T:501:PHE:N	1:T:502:PRO:HD3	2.00	0.77
1:R:524:MET:HE2	1:R:573:ALA:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:MET:HE2	1:B:573:ALA:HA	1.65	0.76
1:H:501:PHE:N	1:H:502:PRO:HD3	2.00	0.76
1:K:396:GLU:HB2	1:Q:366:PRO:HB2	1.67	0.76
1:K:524:MET:HE2	1:K:573:ALA:HA	1.67	0.76
1:M:285:ASN:HD21	1:M:619:TRP:H	1.33	0.76
1:C:285:ASN:HD21	1:C:619:TRP:H	1.33	0.76
1:G:285:ASN:HD21	1:G:619:TRP:H	1.34	0.76
1:A:524:MET:HE2	1:A:573:ALA:HA	1.66	0.76
1:I:501:PHE:N	1:I:502:PRO:HD3	2.00	0.76
1:K:501:PHE:N	1:K:502:PRO:HD3	2.00	0.76
1:O:285:ASN:HD21	1:O:619:TRP:H	1.34	0.76
1:E:441:TYR:HB3	1:Q:359:GLN:HG2	1.67	0.76
1:T:285:ASN:HD21	1:T:619:TRP:H	1.33	0.76
1:D:285:ASN:HD21	1:D:619:TRP:H	1.33	0.76
1:F:501:PHE:N	1:F:502:PRO:HD3	2.00	0.76
1:L:501:PHE:N	1:L:502:PRO:HD3	2.00	0.76
1:O:501:PHE:N	1:O:502:PRO:HD3	2.00	0.76
1:Q:501:PHE:N	1:Q:502:PRO:HD3	2.00	0.76
1:H:524:MET:HE2	1:H:573:ALA:HA	1.66	0.76
1:O:524:MET:HE2	1:O:573:ALA:HA	1.68	0.76
1:B:285:ASN:HD21	1:B:619:TRP:H	1.33	0.75
1:C:446:ASN:H	1:C:446:ASN:HD22	1.35	0.75
1:P:501:PHE:N	1:P:502:PRO:HD3	2.00	0.75
1:T:524:MET:HE2	1:T:573:ALA:HA	1.66	0.75
1:A:501:PHE:N	1:A:502:PRO:HD3	2.00	0.75
1:I:524:MET:HE2	1:I:573:ALA:HA	1.66	0.75
1:S:285:ASN:HD21	1:S:619:TRP:H	1.33	0.75
1:I:285:ASN:HD21	1:I:619:TRP:H	1.33	0.75
1:K:285:ASN:HD21	1:K:619:TRP:H	1.33	0.75
1:N:446:ASN:H	1:N:446:ASN:HD22	1.35	0.75
1:R:446:ASN:HD22	1:R:446:ASN:H	1.35	0.75
1:G:446:ASN:HD22	1:G:446:ASN:H	1.35	0.75
1:I:446:ASN:HD22	1:I:446:ASN:H	1.35	0.75
1:S:524:MET:HE2	1:S:573:ALA:HA	1.68	0.75
1:F:461:LEU:HD12	1:P:555:LEU:HD22	1.69	0.75
1:A:511:LEU:HD21	1:D:480:PRO:HB3	1.68	0.74
1:B:480:PRO:HB3	1:H:511:LEU:HD21	1.67	0.74
1:C:366:PRO:HB2	1:J:396:GLU:HB2	1.69	0.74
1:P:446:ASN:H	1:P:446:ASN:HD22	1.35	0.74
1:P:524:MET:HE2	1:P:573:ALA:HA	1.68	0.74
1:Q:285:ASN:HD21	1:Q:619:TRP:H	1.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:LEU:HD13	1:P:376:GLY:HA3	1.70	0.74
1:J:524:MET:HE2	1:J:573:ALA:HA	1.67	0.74
1:L:285:ASN:HD21	1:L:619:TRP:H	1.33	0.74
1:E:524:MET:HE2	1:E:573:ALA:HA	1.68	0.74
1:F:285:ASN:HD21	1:F:619:TRP:H	1.33	0.74
1:R:449:GLN:HG3	1:R:450:GLY:N	2.03	0.74
1:A:446:ASN:HD22	1:A:446:ASN:H	1.35	0.74
1:H:446:ASN:H	1:H:446:ASN:HD22	1.35	0.74
1:K:446:ASN:H	1:K:446:ASN:HD22	1.35	0.74
1:L:446:ASN:HD22	1:L:446:ASN:H	1.35	0.74
1:Q:446:ASN:H	1:Q:446:ASN:HD22	1.35	0.74
1:T:446:ASN:HD22	1:T:446:ASN:H	1.35	0.74
1:A:245:ARG:NE	1:A:366:PRO:HA	2.03	0.74
1:B:446:ASN:HD22	1:B:446:ASN:H	1.35	0.74
1:E:285:ASN:HD21	1:E:619:TRP:H	1.33	0.74
1:D:449:GLN:HG3	1:D:450:GLY:N	2.03	0.74
1:E:449:GLN:HG3	1:E:450:GLY:N	2.03	0.74
1:F:480:PRO:HB3	1:P:511:LEU:HD21	1.70	0.74
1:J:376:GLY:HA3	1:O:437:LEU:HD13	1.68	0.74
1:M:245:ARG:NE	1:M:366:PRO:HA	2.03	0.74
1:K:359:GLN:HG2	1:R:441:TYR:HB3	1.68	0.74
1:C:449:GLN:HG3	1:C:450:GLY:N	2.03	0.74
1:G:245:ARG:NE	1:G:366:PRO:HA	2.03	0.74
1:J:449:GLN:HG3	1:J:450:GLY:N	2.03	0.74
1:A:359:GLN:HG2	1:D:441:TYR:HB3	1.69	0.74
1:B:245:ARG:NE	1:B:366:PRO:HA	2.03	0.74
1:C:245:ARG:NE	1:C:366:PRO:HA	2.03	0.74
1:I:396:GLU:HB2	1:R:366:PRO:HB2	1.70	0.74
1:N:245:ARG:NE	1:N:366:PRO:HA	2.03	0.74
1:P:285:ASN:HD21	1:P:619:TRP:H	1.33	0.74
1:Q:245:ARG:NE	1:Q:366:PRO:HA	2.03	0.74
1:S:449:GLN:HG3	1:S:450:GLY:N	2.03	0.74
1:T:449:GLN:HG3	1:T:450:GLY:N	2.03	0.74
1:A:285:ASN:HD21	1:A:619:TRP:H	1.33	0.73
1:A:366:PRO:HB2	1:H:396:GLU:HB2	1.70	0.73
1:O:245:ARG:NE	1:O:366:PRO:HA	2.03	0.73
1:P:245:ARG:NE	1:P:366:PRO:HA	2.03	0.73
1:A:449:GLN:HG3	1:A:450:GLY:N	2.03	0.73
1:F:245:ARG:NE	1:F:366:PRO:HA	2.03	0.73
1:G:449:GLN:HG3	1:G:450:GLY:N	2.03	0.73
1:K:449:GLN:HG3	1:K:450:GLY:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:245:ARG:NE	1:L:366:PRO:HA	2.03	0.73
1:N:285:ASN:HD21	1:N:619:TRP:H	1.33	0.73
1:R:245:ARG:NE	1:R:366:PRO:HA	2.03	0.73
1:E:245:ARG:NE	1:E:366:PRO:HA	2.03	0.73
1:J:245:ARG:NE	1:J:366:PRO:HA	2.03	0.73
1:N:524:MET:HE2	1:N:573:ALA:HA	1.69	0.73
1:P:449:GLN:HG3	1:P:450:GLY:N	2.03	0.73
1:F:446:ASN:H	1:F:446:ASN:HD22	1.35	0.73
1:I:245:ARG:NE	1:I:366:PRO:HA	2.03	0.73
1:J:285:ASN:HD21	1:J:619:TRP:H	1.33	0.73
1:Q:449:GLN:HG3	1:Q:450:GLY:N	2.03	0.73
1:E:396:GLU:HB2	1:F:366:PRO:HB2	1.71	0.73
1:H:285:ASN:HD21	1:H:619:TRP:H	1.34	0.73
1:I:366:PRO:HB2	1:P:396:GLU:HB2	1.70	0.73
1:E:359:GLN:HG2	1:I:441:TYR:HB3	1.71	0.73
1:L:524:MET:HE2	1:L:573:ALA:HA	1.69	0.73
1:M:449:GLN:HG3	1:M:450:GLY:N	2.03	0.73
1:T:245:ARG:NE	1:T:366:PRO:HA	2.03	0.73
1:M:446:ASN:H	1:M:446:ASN:HD22	1.35	0.73
1:D:245:ARG:NE	1:D:366:PRO:HA	2.03	0.73
1:K:245:ARG:NE	1:K:366:PRO:HA	2.03	0.73
1:C:524:MET:HE2	1:C:573:ALA:HA	1.71	0.72
1:J:366:PRO:HB2	1:M:396:GLU:HB2	1.70	0.72
1:O:449:GLN:HG3	1:O:450:GLY:N	2.03	0.72
1:B:449:GLN:HG3	1:B:450:GLY:N	2.03	0.72
1:H:245:ARG:NE	1:H:366:PRO:HA	2.03	0.72
1:N:449:GLN:HG3	1:N:450:GLY:N	2.03	0.72
1:R:285:ASN:HD21	1:R:619:TRP:H	1.33	0.72
1:S:549:THR:HG22	1:S:551:SER:H	1.55	0.72
1:I:359:GLN:HG2	1:Q:441:TYR:HB3	1.71	0.72
1:I:710:ASN:HD22	1:P:259:GLN:HE22	1.36	0.72
1:N:353:VAL:H	1:N:646:GLN:NE2	1.88	0.72
1:S:245:ARG:NE	1:S:366:PRO:HA	2.03	0.72
1:M:549:THR:HG22	1:M:551:SER:H	1.55	0.72
1:G:353:VAL:H	1:G:646:GLN:NE2	1.88	0.72
1:J:549:THR:HG22	1:J:551:SER:H	1.55	0.72
1:A:353:VAL:H	1:A:646:GLN:NE2	1.88	0.72
1:E:511:LEU:HD21	1:I:480:PRO:HB3	1.71	0.72
1:F:449:GLN:HG3	1:F:450:GLY:N	2.03	0.72
1:I:500:ASN:HA	1:Q:448:THR:OG1	1.89	0.72
1:O:446:ASN:HD22	1:O:446:ASN:H	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:353:VAL:H	1:S:646:GLN:NE2	1.88	0.72
1:H:549:THR:HG22	1:H:551:SER:H	1.55	0.72
1:T:353:VAL:H	1:T:646:GLN:NE2	1.88	0.72
1:B:549:THR:HG22	1:B:551:SER:H	1.55	0.71
1:C:608:GLN:HA	1:D:626:ASP:HB2	1.71	0.71
1:D:353:VAL:H	1:D:646:GLN:NE2	1.88	0.71
1:D:446:ASN:HD22	1:D:446:ASN:H	1.35	0.71
1:E:353:VAL:H	1:E:646:GLN:NE2	1.88	0.71
1:E:629:PHE:HD2	1:I:603:PRO:HA	1.54	0.71
1:H:449:GLN:HG3	1:H:450:GLY:N	2.03	0.71
1:L:449:GLN:HG3	1:L:450:GLY:N	2.03	0.71
1:R:549:THR:HG22	1:R:551:SER:H	1.55	0.71
1:A:549:THR:HG22	1:A:551:SER:H	1.55	0.71
1:B:441:TYR:HB3	1:H:359:GLN:HG2	1.72	0.71
1:F:600:GLY:HA3	1:P:600:GLY:HA3	1.70	0.71
1:P:353:VAL:H	1:P:646:GLN:NE2	1.88	0.71
1:I:449:GLN:HG3	1:I:450:GLY:N	2.03	0.71
1:K:549:THR:HG22	1:K:551:SER:H	1.55	0.71
1:E:446:ASN:H	1:E:446:ASN:HD22	1.35	0.71
1:H:353:VAL:H	1:H:646:GLN:NE2	1.88	0.71
1:P:549:THR:HG22	1:P:551:SER:H	1.55	0.71
1:J:446:ASN:HD22	1:J:446:ASN:H	1.35	0.71
1:K:500:ASN:HA	1:R:448:THR:OG1	1.90	0.71
1:N:549:THR:HG22	1:N:551:SER:H	1.55	0.71
1:Q:549:THR:HG22	1:Q:551:SER:H	1.55	0.71
1:A:376:GLY:HA3	1:D:437:LEU:HD13	1.73	0.71
1:E:437:LEU:HD13	1:Q:376:GLY:HA3	1.71	0.71
1:E:448:THR:OG1	1:Q:500:ASN:HA	1.90	0.71
1:O:549:THR:HG22	1:O:551:SER:H	1.55	0.71
1:C:353:VAL:H	1:C:646:GLN:NE2	1.88	0.71
1:Q:353:VAL:H	1:Q:646:GLN:NE2	1.88	0.71
1:F:549:THR:HG22	1:F:551:SER:H	1.55	0.71
1:I:549:THR:HG22	1:I:551:SER:H	1.55	0.71
1:E:549:THR:HG22	1:E:551:SER:H	1.55	0.71
1:K:353:VAL:H	1:K:646:GLN:NE2	1.88	0.71
1:B:437:LEU:HD13	1:H:376:GLY:HA3	1.73	0.71
1:C:436:PRO:HG3	1:D:378:LEU:HG	1.72	0.71
1:J:353:VAL:H	1:J:646:GLN:NE2	1.88	0.71
1:R:353:VAL:H	1:R:646:GLN:NE2	1.88	0.71
1:L:353:VAL:H	1:L:646:GLN:NE2	1.88	0.70
1:B:353:VAL:H	1:B:646:GLN:NE2	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLU:HB2	1:N:366:PRO:HB2	1.72	0.70
1:F:353:VAL:H	1:F:646:GLN:NE2	1.88	0.70
1:F:524:MET:HE2	1:F:573:ALA:HA	1.71	0.70
1:L:366:PRO:HB2	1:T:396:GLU:HB2	1.71	0.70
1:C:549:THR:HG22	1:C:551:SER:H	1.55	0.70
1:G:396:GLU:HB2	1:H:366:PRO:HB2	1.72	0.70
1:K:378:LEU:HG	1:R:436:PRO:HG3	1.73	0.70
1:A:699:ILE:HD11	1:C:389:ARG:HE	1.57	0.70
1:E:480:PRO:HB3	1:Q:511:LEU:HD21	1.72	0.70
1:F:611:ASP:OD1	1:F:729:THR:HG22	1.92	0.70
1:K:353:VAL:H	1:K:646:GLN:HE22	1.40	0.70
1:S:446:ASN:H	1:S:446:ASN:HD22	1.35	0.70
1:I:353:VAL:H	1:I:646:GLN:NE2	1.88	0.70
1:H:353:VAL:H	1:H:646:GLN:HE22	1.40	0.70
1:J:359:GLN:HG2	1:O:441:TYR:HB3	1.73	0.70
1:O:353:VAL:H	1:O:646:GLN:NE2	1.88	0.70
1:O:396:GLU:HB2	1:S:366:PRO:HB2	1.74	0.70
1:T:549:THR:HG22	1:T:551:SER:H	1.55	0.70
1:T:611:ASP:OD1	1:T:729:THR:HG22	1.92	0.70
1:E:611:ASP:OD1	1:E:729:THR:HG22	1.92	0.70
1:L:549:THR:HG22	1:L:551:SER:H	1.55	0.70
1:L:611:ASP:OD1	1:L:729:THR:HG22	1.92	0.70
1:P:611:ASP:OD1	1:P:729:THR:HG22	1.92	0.70
1:A:611:ASP:OD1	1:A:729:THR:HG22	1.92	0.70
1:C:611:ASP:OD1	1:C:729:THR:HG22	1.92	0.70
1:A:500:ASN:HA	1:D:448:THR:OG1	1.91	0.69
1:A:603:PRO:HA	1:C:629:PHE:HD2	1.55	0.69
1:C:353:VAL:H	1:C:646:GLN:HE22	1.40	0.69
1:D:549:THR:HG22	1:D:551:SER:H	1.55	0.69
1:J:611:ASP:OD1	1:J:729:THR:HG22	1.92	0.69
1:M:353:VAL:H	1:M:646:GLN:NE2	1.88	0.69
1:O:611:ASP:OD1	1:O:729:THR:HG22	1.92	0.69
1:G:549:THR:HG22	1:G:551:SER:H	1.55	0.69
1:G:611:ASP:OD1	1:G:729:THR:HG22	1.92	0.69
1:H:611:ASP:OD1	1:H:729:THR:HG22	1.92	0.69
1:K:611:ASP:OD1	1:K:729:THR:HG22	1.92	0.69
1:L:396:GLU:HB2	1:P:366:PRO:HB2	1.74	0.69
1:Q:611:ASP:OD1	1:Q:729:THR:HG22	1.92	0.69
1:D:519:ASN:CB	1:D:520:PRO:HD3	2.23	0.69
1:N:611:ASP:OD1	1:N:729:THR:HG22	1.92	0.69
1:I:579:THR:HG23	1:I:593:THR:HG23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:579:THR:HG23	1:J:593:THR:HG23	1.75	0.69
1:A:353:VAL:H	1:A:646:GLN:HE22	1.40	0.69
1:B:603:PRO:HA	1:H:629:PHE:HD2	1.58	0.69
1:B:710:ASN:HD22	1:C:259:GLN:HE22	1.40	0.69
1:F:699:ILE:HD11	1:P:389:ARG:HE	1.58	0.69
1:G:353:VAL:H	1:G:646:GLN:HE22	1.40	0.69
1:H:519:ASN:CB	1:H:520:PRO:HD3	2.23	0.69
1:I:611:ASP:OD1	1:I:729:THR:HG22	1.92	0.69
1:K:579:THR:HG23	1:K:593:THR:HG23	1.75	0.69
1:M:611:ASP:OD1	1:M:729:THR:HG22	1.92	0.69
1:S:519:ASN:CB	1:S:520:PRO:HD3	2.23	0.69
1:S:611:ASP:OD1	1:S:729:THR:HG22	1.92	0.69
1:A:600:GLY:HA3	1:C:600:GLY:HA3	1.75	0.69
1:B:611:ASP:OD1	1:B:729:THR:HG22	1.92	0.69
1:C:441:TYR:HB3	1:D:359:GLN:HG2	1.75	0.69
1:Q:519:ASN:CB	1:Q:520:PRO:HD3	2.23	0.69
1:R:579:THR:HG23	1:R:593:THR:HG23	1.75	0.69
1:A:456:THR:O	1:A:456:THR:HG22	1.93	0.69
1:D:579:THR:HG23	1:D:593:THR:HG23	1.75	0.69
1:D:611:ASP:OD1	1:D:729:THR:HG22	1.92	0.69
1:J:629:PHE:HD2	1:O:603:PRO:HA	1.59	0.69
1:N:519:ASN:CB	1:N:520:PRO:HD3	2.23	0.69
1:Q:353:VAL:H	1:Q:646:GLN:HE22	1.40	0.69
1:T:519:ASN:CB	1:T:520:PRO:HD3	2.23	0.69
1:E:353:VAL:H	1:E:646:GLN:HE22	1.40	0.68
1:K:519:ASN:CB	1:K:520:PRO:HD3	2.23	0.68
1:A:579:THR:HG23	1:A:593:THR:HG23	1.75	0.68
1:B:353:VAL:H	1:B:646:GLN:HE22	1.40	0.68
1:I:440:GLN:HB2	1:I:466:ALA:HB3	1.75	0.68
1:P:519:ASN:CB	1:P:520:PRO:HD3	2.23	0.68
1:F:440:GLN:HB2	1:F:466:ALA:HB3	1.76	0.68
1:F:463:PHE:HE2	1:P:555:LEU:HA	1.58	0.68
1:J:353:VAL:H	1:J:646:GLN:HE22	1.40	0.68
1:J:440:GLN:HB2	1:J:466:ALA:HB3	1.76	0.68
1:M:366:PRO:HB2	1:N:396:GLU:HB2	1.73	0.68
1:M:519:ASN:CB	1:M:520:PRO:HD3	2.23	0.68
1:T:579:THR:HG23	1:T:593:THR:HG23	1.75	0.68
1:A:436:PRO:HG3	1:C:378:LEU:HG	1.74	0.68
1:A:440:GLN:HB2	1:A:466:ALA:HB3	1.76	0.68
1:E:579:THR:HG23	1:E:593:THR:HG23	1.75	0.68
1:E:603:PRO:HA	1:Q:629:PHE:HD2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:440:GLN:HB2	1:K:466:ALA:HB3	1.76	0.68
1:M:579:THR:HG23	1:M:593:THR:HG23	1.75	0.68
1:K:511:LEU:HD21	1:R:480:PRO:HB3	1.75	0.68
1:H:285:ASN:ND2	1:H:618:ILE:H	1.92	0.68
1:L:353:VAL:H	1:L:646:GLN:HE22	1.40	0.68
1:S:579:THR:HG23	1:S:593:THR:HG23	1.75	0.68
1:G:519:ASN:CB	1:G:520:PRO:HD3	2.23	0.68
1:K:629:PHE:HD2	1:R:603:PRO:HA	1.58	0.68
1:L:285:ASN:ND2	1:L:618:ILE:H	1.92	0.68
1:O:353:VAL:H	1:O:646:GLN:HE22	1.40	0.68
1:Q:579:THR:HG23	1:Q:593:THR:HG23	1.75	0.68
1:R:611:ASP:OD1	1:R:729:THR:HG22	1.92	0.68
1:E:440:GLN:HB2	1:E:466:ALA:HB3	1.76	0.68
1:I:519:ASN:CB	1:I:520:PRO:HD3	2.23	0.68
1:O:579:THR:HG23	1:O:593:THR:HG23	1.75	0.68
1:R:519:ASN:CB	1:R:520:PRO:HD3	2.23	0.68
1:F:353:VAL:H	1:F:646:GLN:HE22	1.40	0.68
1:F:396:GLU:HB2	1:G:366:PRO:HB2	1.76	0.68
1:B:519:ASN:CB	1:B:520:PRO:HD3	2.23	0.68
1:C:579:THR:HG23	1:C:593:THR:HG23	1.75	0.68
1:D:285:ASN:ND2	1:D:618:ILE:H	1.92	0.68
1:F:285:ASN:ND2	1:F:618:ILE:H	1.92	0.68
1:L:440:GLN:HB2	1:L:466:ALA:HB3	1.76	0.68
1:O:519:ASN:CB	1:O:520:PRO:HD3	2.23	0.68
1:S:285:ASN:ND2	1:S:618:ILE:H	1.92	0.68
1:T:440:GLN:HB2	1:T:466:ALA:HB3	1.76	0.68
1:C:285:ASN:ND2	1:C:618:ILE:H	1.92	0.67
1:D:440:GLN:HB2	1:D:466:ALA:HB3	1.76	0.67
1:S:353:VAL:H	1:S:646:GLN:HE22	1.40	0.67
1:G:579:THR:HG23	1:G:593:THR:HG23	1.75	0.67
1:I:511:LEU:HD21	1:Q:480:PRO:HB3	1.75	0.67
1:R:353:VAL:H	1:R:646:GLN:HE22	1.40	0.67
1:G:440:GLN:HB2	1:G:466:ALA:HB3	1.76	0.67
1:N:353:VAL:H	1:N:646:GLN:HE22	1.40	0.67
1:O:440:GLN:HB2	1:O:466:ALA:HB3	1.76	0.67
1:Q:325:GLN:HG3	1:Q:330:THR:HG22	1.77	0.67
1:H:440:GLN:HB2	1:H:466:ALA:HB3	1.76	0.67
1:I:353:VAL:H	1:I:646:GLN:HE22	1.40	0.67
1:S:325:GLN:HG3	1:S:330:THR:HG22	1.77	0.67
1:T:285:ASN:ND2	1:T:618:ILE:H	1.92	0.67
1:I:629:PHE:HD2	1:Q:603:PRO:HA	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:325:GLN:HG3	1:K:330:THR:HG22	1.77	0.67
1:P:579:THR:HG23	1:P:593:THR:HG23	1.75	0.67
1:S:440:GLN:HB2	1:S:466:ALA:HB3	1.76	0.67
1:M:353:VAL:H	1:M:646:GLN:HE22	1.40	0.67
1:P:325:GLN:HG3	1:P:330:THR:HG22	1.77	0.67
1:T:325:GLN:HG3	1:T:330:THR:HG22	1.77	0.67
1:D:353:VAL:H	1:D:646:GLN:HE22	1.40	0.67
1:E:325:GLN:HG3	1:E:330:THR:HG22	1.77	0.67
1:H:579:THR:HG23	1:H:593:THR:HG23	1.75	0.67
1:F:584:LEU:HB3	1:P:488:ARG:NH2	2.09	0.67
1:K:285:ASN:ND2	1:K:618:ILE:H	1.92	0.67
1:B:579:THR:HG23	1:B:593:THR:HG23	1.75	0.67
1:B:714:THR:HG21	1:C:275:TYR:OH	1.94	0.67
1:C:519:ASN:CB	1:C:520:PRO:HD3	2.23	0.67
1:J:325:GLN:HG3	1:J:330:THR:HG22	1.77	0.67
1:M:325:GLN:HG3	1:M:330:THR:HG22	1.77	0.67
1:R:285:ASN:ND2	1:R:618:ILE:H	1.92	0.67
1:A:396:GLU:HB2	1:E:366:PRO:HB2	1.77	0.67
1:D:366:PRO:HB2	1:Q:396:GLU:HB2	1.75	0.67
1:F:579:THR:HG23	1:F:593:THR:HG23	1.75	0.67
1:O:285:ASN:ND2	1:O:618:ILE:H	1.92	0.67
1:P:285:ASN:ND2	1:P:618:ILE:H	1.92	0.67
1:A:285:ASN:ND2	1:A:618:ILE:H	1.92	0.66
1:A:325:GLN:HG3	1:A:330:THR:HG22	1.77	0.66
1:B:285:ASN:ND2	1:B:618:ILE:H	1.92	0.66
1:B:440:GLN:HB2	1:B:466:ALA:HB3	1.76	0.66
1:N:579:THR:HG23	1:N:593:THR:HG23	1.75	0.66
1:Q:440:GLN:HB2	1:Q:466:ALA:HB3	1.76	0.66
1:B:448:THR:OG1	1:H:500:ASN:HA	1.94	0.66
1:P:353:VAL:H	1:P:646:GLN:HE22	1.40	0.66
1:R:288:HIS:CE1	1:R:364:PRO:HG3	2.30	0.66
1:R:440:GLN:HB2	1:R:466:ALA:HB3	1.76	0.66
1:G:285:ASN:ND2	1:G:618:ILE:H	1.92	0.66
1:L:325:GLN:HG3	1:L:330:THR:HG22	1.77	0.66
1:Q:285:ASN:ND2	1:Q:618:ILE:H	1.92	0.66
1:R:325:GLN:HG3	1:R:330:THR:HG22	1.77	0.66
1:C:440:GLN:HB2	1:C:466:ALA:HB3	1.76	0.66
1:E:285:ASN:ND2	1:E:618:ILE:H	1.92	0.66
1:H:325:GLN:HG3	1:H:330:THR:HG22	1.77	0.66
1:L:519:ASN:CB	1:L:520:PRO:HD3	2.23	0.66
1:L:579:THR:HG23	1:L:593:THR:HG23	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:ASN:ND2	1:M:618:ILE:H	1.92	0.66
1:E:519:ASN:CB	1:E:520:PRO:HD3	2.23	0.66
1:F:325:GLN:HG3	1:F:330:THR:HG22	1.77	0.66
1:G:325:GLN:HG3	1:G:330:THR:HG22	1.77	0.66
1:I:378:LEU:HG	1:Q:436:PRO:HG3	1.77	0.66
1:J:602:LEU:H	1:J:605:MET:HE2	1.60	0.66
1:K:366:PRO:HB2	1:S:396:GLU:HB2	1.78	0.66
1:K:626:ASP:HB2	1:R:608:GLN:HA	1.78	0.66
1:P:440:GLN:HB2	1:P:466:ALA:HB3	1.76	0.66
1:T:353:VAL:H	1:T:646:GLN:HE22	1.40	0.66
1:C:325:GLN:HG3	1:C:330:THR:HG22	1.77	0.66
1:D:396:GLU:HB2	1:O:366:PRO:HB2	1.78	0.66
1:F:456:THR:O	1:F:456:THR:HG22	1.96	0.66
1:N:288:HIS:CE1	1:N:364:PRO:HG3	2.31	0.66
1:D:456:THR:O	1:D:456:THR:HG22	1.96	0.66
1:K:626:ASP:H	1:R:608:GLN:NE2	1.94	0.66
1:N:285:ASN:ND2	1:N:618:ILE:H	1.93	0.66
1:N:440:GLN:HB2	1:N:466:ALA:HB3	1.76	0.66
1:O:288:HIS:CE1	1:O:364:PRO:HG3	2.31	0.66
1:Q:456:THR:O	1:Q:456:THR:HG22	1.96	0.66
1:S:602:LEU:H	1:S:605:MET:HE2	1.60	0.66
1:B:325:GLN:HG3	1:B:330:THR:HG22	1.77	0.66
1:B:456:THR:HG22	1:B:456:THR:O	1.96	0.66
1:D:288:HIS:CE1	1:D:364:PRO:HG3	2.31	0.66
1:I:626:ASP:HB2	1:Q:608:GLN:HA	1.78	0.66
1:J:285:ASN:ND2	1:J:618:ILE:H	1.92	0.66
1:J:288:HIS:CE1	1:J:364:PRO:HG3	2.31	0.66
1:J:456:THR:HG22	1:J:456:THR:O	1.96	0.66
1:J:511:LEU:HD21	1:O:480:PRO:HB3	1.77	0.66
1:N:325:GLN:HG3	1:N:330:THR:HG22	1.78	0.66
1:P:288:HIS:CE1	1:P:364:PRO:HG3	2.31	0.66
1:T:456:THR:O	1:T:456:THR:HG22	1.96	0.66
1:F:288:HIS:CE1	1:F:364:PRO:HG3	2.31	0.66
1:G:288:HIS:CE1	1:G:364:PRO:HG3	2.31	0.66
1:H:456:THR:HG22	1:H:456:THR:O	1.96	0.66
1:L:710:ASN:HD22	1:T:259:GLN:HE22	1.42	0.66
1:S:288:HIS:CE1	1:S:364:PRO:HG3	2.31	0.66
1:T:315:LEU:HB2	1:T:409:PHE:HB3	1.78	0.66
1:B:288:HIS:CE1	1:B:364:PRO:HG3	2.31	0.66
1:E:378:LEU:HG	1:I:436:PRO:HG3	1.77	0.66
1:E:500:ASN:HA	1:I:448:THR:OG1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:285:ASN:ND2	1:I:618:ILE:H	1.92	0.66
1:I:325:GLN:HG3	1:I:330:THR:HG22	1.77	0.66
1:M:288:HIS:CE1	1:M:364:PRO:HG3	2.31	0.66
1:O:456:THR:O	1:O:456:THR:HG22	1.96	0.66
1:Q:288:HIS:CE1	1:Q:364:PRO:HG3	2.31	0.66
1:D:315:LEU:HB2	1:D:409:PHE:HB3	1.78	0.65
1:F:519:ASN:CB	1:F:520:PRO:HD3	2.23	0.65
1:H:288:HIS:CE1	1:H:364:PRO:HG3	2.31	0.65
1:K:288:HIS:CE1	1:K:364:PRO:HG3	2.31	0.65
1:L:315:LEU:HB2	1:L:409:PHE:HB3	1.78	0.65
1:M:440:GLN:HB2	1:M:466:ALA:HB3	1.76	0.65
1:Q:524:MET:HE2	1:Q:573:ALA:HA	1.77	0.65
1:S:315:LEU:HB2	1:S:409:PHE:HB3	1.78	0.65
1:T:288:HIS:CE1	1:T:364:PRO:HG3	2.31	0.65
1:A:288:HIS:CE1	1:A:364:PRO:HG3	2.31	0.65
1:A:608:GLN:NE2	1:C:626:ASP:H	1.93	0.65
1:E:288:HIS:CE1	1:E:364:PRO:HG3	2.31	0.65
1:I:315:LEU:HB2	1:I:409:PHE:HB3	1.78	0.65
1:O:315:LEU:HB2	1:O:409:PHE:HB3	1.78	0.65
1:C:608:GLN:NE2	1:D:626:ASP:H	1.94	0.65
1:N:602:LEU:H	1:N:605:MET:HE2	1.60	0.65
1:P:602:LEU:H	1:P:605:MET:HE2	1.62	0.65
1:F:441:TYR:HA	1:P:359:GLN:HE21	1.61	0.65
1:I:286:ARG:HH12	1:I:615:GLN:HB2	1.62	0.65
1:I:288:HIS:CE1	1:I:364:PRO:HG3	2.31	0.65
1:M:315:LEU:HB2	1:M:409:PHE:HB3	1.78	0.65
1:P:315:LEU:HB2	1:P:409:PHE:HB3	1.78	0.65
1:H:286:ARG:HH12	1:H:615:GLN:HB2	1.62	0.65
1:J:389:ARG:HE	1:O:699:ILE:HD11	1.61	0.65
1:K:600:GLY:HA3	1:R:600:GLY:HA3	1.79	0.65
1:L:288:HIS:CE1	1:L:364:PRO:HG3	2.31	0.65
1:M:456:THR:HG22	1:M:456:THR:O	1.96	0.65
1:N:286:ARG:HH12	1:N:615:GLN:HB2	1.62	0.65
1:R:449:GLN:HG3	1:R:450:GLY:H	1.62	0.65
1:S:456:THR:O	1:S:456:THR:HG22	1.96	0.65
1:A:286:ARG:HH12	1:A:615:GLN:HB2	1.62	0.65
1:C:288:HIS:CE1	1:C:364:PRO:HG3	2.31	0.65
1:H:602:LEU:H	1:H:605:MET:HE2	1.61	0.65
1:P:456:THR:HG22	1:P:456:THR:O	1.96	0.65
1:R:315:LEU:HB2	1:R:409:PHE:HB3	1.78	0.65
1:C:602:LEU:H	1:C:605:MET:HE2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:449:GLN:HG3	1:J:450:GLY:H	1.62	0.65
1:M:286:ARG:HH12	1:M:615:GLN:HB2	1.62	0.65
1:T:449:GLN:HG3	1:T:450:GLY:H	1.62	0.65
1:E:602:LEU:H	1:E:605:MET:HE2	1.62	0.65
1:J:519:ASN:CB	1:J:520:PRO:HD3	2.23	0.65
1:B:449:GLN:HG3	1:B:450:GLY:H	1.62	0.65
1:H:449:GLN:HG3	1:H:450:GLY:H	1.62	0.65
1:L:456:THR:O	1:L:456:THR:HG22	1.95	0.65
1:Q:449:GLN:HG3	1:Q:450:GLY:H	1.62	0.65
1:A:710:ASN:HD22	1:H:259:GLN:HE22	1.45	0.65
1:B:286:ARG:HH12	1:B:615:GLN:HB2	1.62	0.65
1:B:315:LEU:HB2	1:B:409:PHE:HB3	1.78	0.65
1:E:527:HIS:HE1	1:E:562:ASP:OD2	1.80	0.65
1:I:602:LEU:H	1:I:605:MET:HE2	1.61	0.65
1:K:527:HIS:HE1	1:K:562:ASP:OD2	1.80	0.65
1:O:325:GLN:HG3	1:O:330:THR:HG22	1.77	0.65
1:A:441:TYR:HB3	1:C:359:GLN:HG2	1.78	0.64
1:A:480:PRO:HB3	1:C:511:LEU:HD21	1.78	0.64
1:A:519:ASN:CB	1:A:520:PRO:HD3	2.23	0.64
1:C:286:ARG:HH12	1:C:615:GLN:HB2	1.62	0.64
1:F:602:LEU:H	1:F:605:MET:HE2	1.62	0.64
1:G:263:GLN:HB3	1:G:266:ALA:CB	2.27	0.64
1:I:456:THR:O	1:I:456:THR:HG22	1.96	0.64
1:K:456:THR:O	1:K:456:THR:HG22	1.96	0.64
1:K:514:ARG:HD3	1:R:432:ARG:NH2	2.12	0.64
1:L:337:THR:HG22	1:P:405:THR:HG21	1.80	0.64
1:N:263:GLN:HB3	1:N:266:ALA:CB	2.28	0.64
1:P:527:HIS:HE1	1:P:562:ASP:OD2	1.81	0.64
1:R:396:GLU:HB2	1:T:366:PRO:HB2	1.79	0.64
1:E:286:ARG:HH12	1:E:615:GLN:HB2	1.62	0.64
1:J:263:GLN:HB3	1:J:266:ALA:CB	2.28	0.64
1:J:600:GLY:HA3	1:O:600:GLY:HA3	1.77	0.64
1:L:286:ARG:HH12	1:L:615:GLN:HB2	1.62	0.64
1:N:315:LEU:HB2	1:N:409:PHE:HB3	1.78	0.64
1:O:263:GLN:HB3	1:O:266:ALA:CB	2.28	0.64
1:R:456:THR:HG22	1:R:456:THR:O	1.96	0.64
1:A:315:LEU:HB2	1:A:409:PHE:HB3	1.78	0.64
1:F:286:ARG:HH12	1:F:615:GLN:HB2	1.62	0.64
1:F:315:LEU:HB2	1:F:409:PHE:HB3	1.78	0.64
1:H:527:HIS:HE1	1:H:562:ASP:OD2	1.81	0.64
1:K:602:LEU:H	1:K:605:MET:HE2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:449:GLN:HG3	1:P:450:GLY:H	1.62	0.64
1:S:449:GLN:HG3	1:S:450:GLY:H	1.62	0.64
1:T:263:GLN:HB3	1:T:266:ALA:CB	2.28	0.64
1:D:325:GLN:HG3	1:D:330:THR:HG22	1.77	0.64
1:H:263:GLN:HB3	1:H:266:ALA:CB	2.28	0.64
1:H:315:LEU:HB2	1:H:409:PHE:HB3	1.78	0.64
1:I:502:PRO:HG3	1:Q:448:THR:HG23	1.79	0.64
1:I:626:ASP:H	1:Q:608:GLN:NE2	1.95	0.64
1:J:286:ARG:HH12	1:J:615:GLN:HB2	1.62	0.64
1:O:449:GLN:HG3	1:O:450:GLY:H	1.62	0.64
1:A:446:ASN:O	1:C:502:PRO:HG2	1.98	0.64
1:B:259:GLN:HE22	1:N:710:ASN:HD22	1.44	0.64
1:C:315:LEU:HB2	1:C:409:PHE:HB3	1.78	0.64
1:I:527:HIS:HE1	1:I:562:ASP:OD2	1.80	0.64
1:N:449:GLN:HG3	1:N:450:GLY:H	1.62	0.64
1:Q:483:CYS:HB2	1:Q:524:MET:HE1	1.80	0.64
1:S:286:ARG:HH12	1:S:615:GLN:HB2	1.62	0.64
1:E:263:GLN:HB3	1:E:266:ALA:CB	2.28	0.64
1:F:449:GLN:HG3	1:F:450:GLY:H	1.62	0.64
1:G:315:LEU:HB2	1:G:409:PHE:HB3	1.78	0.64
1:I:714:THR:HG21	1:P:275:TYR:OH	1.97	0.64
1:K:315:LEU:HB2	1:K:409:PHE:HB3	1.78	0.64
1:M:263:GLN:HB3	1:M:266:ALA:CB	2.28	0.64
1:M:527:HIS:HE1	1:M:562:ASP:OD2	1.81	0.64
1:N:527:HIS:HE1	1:N:562:ASP:OD2	1.81	0.64
1:O:527:HIS:HE1	1:O:562:ASP:OD2	1.81	0.64
1:P:286:ARG:HH12	1:P:615:GLN:HB2	1.62	0.64
1:A:458:GLN:HG2	1:A:459:SER:H	1.63	0.64
1:C:456:THR:O	1:C:456:THR:HG22	1.96	0.64
1:D:263:GLN:HB3	1:D:266:ALA:CB	2.28	0.64
1:D:286:ARG:HH12	1:D:615:GLN:HB2	1.62	0.64
1:E:315:LEU:HB2	1:E:409:PHE:HB3	1.78	0.64
1:G:456:THR:O	1:G:456:THR:HG22	1.96	0.64
1:L:458:GLN:HG2	1:L:459:SER:H	1.63	0.64
1:N:456:THR:O	1:N:456:THR:HG22	1.96	0.64
1:P:263:GLN:HB3	1:P:266:ALA:CB	2.28	0.64
1:Q:263:GLN:HB3	1:Q:266:ALA:CB	2.28	0.64
1:Q:527:HIS:HE1	1:Q:562:ASP:OD2	1.81	0.64
1:S:263:GLN:HB3	1:S:266:ALA:CB	2.28	0.64
1:T:527:HIS:HE1	1:T:562:ASP:OD2	1.81	0.64
1:A:389:ARG:HE	1:D:699:ILE:HD11	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ALA:HA	1:C:519:ASN:HD22	1.62	0.64
1:B:263:GLN:HB3	1:B:266:ALA:CB	2.28	0.64
1:B:527:HIS:HE1	1:B:562:ASP:OD2	1.81	0.64
1:C:449:GLN:HG3	1:C:450:GLY:H	1.62	0.64
1:D:527:HIS:HE1	1:D:562:ASP:OD2	1.81	0.64
1:I:263:GLN:HB3	1:I:266:ALA:CB	2.28	0.64
1:J:315:LEU:HB2	1:J:409:PHE:HB3	1.78	0.64
1:N:379:THR:HG22	1:N:380:LEU:H	1.63	0.64
1:Q:315:LEU:HB2	1:Q:409:PHE:HB3	1.78	0.64
1:T:379:THR:HG22	1:T:380:LEU:H	1.63	0.64
1:A:527:HIS:HE1	1:A:562:ASP:OD2	1.81	0.64
1:C:263:GLN:HB3	1:C:266:ALA:CB	2.28	0.64
1:G:286:ARG:HH12	1:G:615:GLN:HB2	1.62	0.64
1:J:378:LEU:HG	1:O:436:PRO:HG3	1.80	0.64
1:K:263:GLN:HB3	1:K:266:ALA:CB	2.28	0.64
1:R:263:GLN:HB3	1:R:266:ALA:CB	2.28	0.64
1:R:527:HIS:HE1	1:R:562:ASP:OD2	1.81	0.64
1:E:259:GLN:HE22	1:F:710:ASN:HD22	1.45	0.64
1:E:456:THR:HG22	1:E:456:THR:O	1.96	0.64
1:L:356:SER:HB2	1:L:358:HIS:CD2	2.33	0.64
1:M:458:GLN:HG2	1:M:459:SER:H	1.63	0.64
1:N:458:GLN:HG2	1:N:459:SER:H	1.63	0.64
1:Q:379:THR:HG22	1:Q:380:LEU:H	1.63	0.64
1:S:527:HIS:HE1	1:S:562:ASP:OD2	1.80	0.64
1:T:458:GLN:HG2	1:T:459:SER:H	1.63	0.64
1:C:312:SER:HB2	1:C:682:GLU:HB3	1.81	0.63
1:D:356:SER:HB2	1:D:358:HIS:CD2	2.33	0.63
1:D:449:GLN:HG3	1:D:450:GLY:H	1.62	0.63
1:I:449:GLN:HG3	1:I:450:GLY:H	1.62	0.63
1:J:312:SER:HB2	1:J:682:GLU:HB3	1.81	0.63
1:K:286:ARG:HH12	1:K:615:GLN:HB2	1.62	0.63
1:K:449:GLN:HG3	1:K:450:GLY:H	1.62	0.63
1:M:356:SER:HB2	1:M:358:HIS:CD2	2.33	0.63
1:N:356:SER:HB2	1:N:358:HIS:CD2	2.33	0.63
1:R:286:ARG:HH12	1:R:615:GLN:HB2	1.62	0.63
1:C:356:SER:HB2	1:C:358:HIS:CD2	2.33	0.63
1:E:356:SER:HB2	1:E:358:HIS:CD2	2.33	0.63
1:F:263:GLN:HB3	1:F:266:ALA:CB	2.28	0.63
1:K:259:GLN:HE22	1:Q:710:ASN:HD22	1.45	0.63
1:O:356:SER:HB2	1:O:358:HIS:CD2	2.33	0.63
1:O:379:THR:HG22	1:O:380:LEU:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:379:THR:HG22	1:R:380:LEU:H	1.63	0.63
1:B:312:SER:HB2	1:B:682:GLU:HB3	1.80	0.63
1:B:356:SER:HB2	1:B:358:HIS:CD2	2.33	0.63
1:L:263:GLN:HB3	1:L:266:ALA:CB	2.28	0.63
1:S:296:TRP:O	1:S:300:ILE:HG12	1.99	0.63
1:S:620:ALA:HB3	1:S:633:PRO:HG3	1.81	0.63
1:T:286:ARG:HH12	1:T:615:GLN:HB2	1.62	0.63
1:A:296:TRP:O	1:A:300:ILE:HG12	1.99	0.63
1:A:449:GLN:HG3	1:A:450:GLY:H	1.62	0.63
1:B:379:THR:HG22	1:B:380:LEU:H	1.63	0.63
1:D:379:THR:HG22	1:D:380:LEU:H	1.63	0.63
1:F:527:HIS:HE1	1:F:562:ASP:OD2	1.81	0.63
1:F:590:ALA:HA	1:P:497:ASN:HD22	1.64	0.63
1:J:356:SER:HB2	1:J:358:HIS:CD2	2.34	0.63
1:K:458:GLN:HG2	1:K:459:SER:H	1.63	0.63
1:O:286:ARG:HH12	1:O:615:GLN:HB2	1.62	0.63
1:O:312:SER:HB2	1:O:682:GLU:HB3	1.81	0.63
1:Q:458:GLN:HG2	1:Q:459:SER:H	1.63	0.63
1:R:458:GLN:HG2	1:R:459:SER:H	1.63	0.63
1:E:296:TRP:O	1:E:300:ILE:HG12	1.99	0.63
1:G:356:SER:HB2	1:G:358:HIS:CD2	2.33	0.63
1:J:527:HIS:HE1	1:J:562:ASP:OD2	1.81	0.63
1:M:449:GLN:HG3	1:M:450:GLY:H	1.62	0.63
1:A:312:SER:HB2	1:A:682:GLU:HB3	1.81	0.63
1:D:458:GLN:HG2	1:D:459:SER:H	1.63	0.63
1:G:312:SER:HB2	1:G:682:GLU:HB3	1.80	0.63
1:G:458:GLN:HG2	1:G:459:SER:H	1.63	0.63
1:J:620:ALA:HB3	1:J:633:PRO:HG3	1.81	0.63
1:K:356:SER:HB2	1:K:358:HIS:CD2	2.34	0.63
1:M:536:PRO:HB2	1:M:539:GLY:HA3	1.81	0.63
1:O:602:LEU:H	1:O:605:MET:HE2	1.63	0.63
1:Q:602:LEU:H	1:Q:605:MET:HE2	1.64	0.63
1:Q:620:ALA:HB3	1:Q:633:PRO:HG3	1.81	0.63
1:R:536:PRO:HB2	1:R:539:GLY:HA3	1.81	0.63
1:I:356:SER:HB2	1:I:358:HIS:CD2	2.33	0.63
1:I:379:THR:HG22	1:I:380:LEU:H	1.63	0.63
1:I:620:ALA:HB3	1:I:633:PRO:HG3	1.81	0.63
1:M:296:TRP:O	1:M:300:ILE:HG12	1.99	0.63
1:M:379:THR:HG22	1:M:380:LEU:H	1.63	0.63
1:N:296:TRP:O	1:N:300:ILE:HG12	1.99	0.63
1:Q:286:ARG:HH12	1:Q:615:GLN:HB2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:296:TRP:O	1:Q:300:ILE:HG12	1.99	0.63
1:S:379:THR:HG22	1:S:380:LEU:H	1.63	0.63
1:A:379:THR:HG22	1:A:380:LEU:H	1.63	0.63
1:A:600:GLY:HA3	1:D:600:GLY:HA3	1.81	0.63
1:B:436:PRO:HG3	1:H:378:LEU:HG	1.80	0.63
1:F:379:THR:HG22	1:F:380:LEU:H	1.63	0.63
1:G:379:THR:HG22	1:G:380:LEU:H	1.63	0.63
1:G:527:HIS:HE1	1:G:562:ASP:OD2	1.81	0.63
1:H:458:GLN:HG2	1:H:459:SER:H	1.63	0.63
1:H:536:PRO:HB2	1:H:539:GLY:HA3	1.81	0.63
1:I:296:TRP:O	1:I:300:ILE:HG12	1.99	0.63
1:I:312:SER:HB2	1:I:682:GLU:HB3	1.81	0.63
1:K:536:PRO:HB2	1:K:539:GLY:HA3	1.81	0.63
1:O:458:GLN:HG2	1:O:459:SER:H	1.63	0.63
1:P:620:ALA:HB3	1:P:633:PRO:HG3	1.81	0.63
1:R:620:ALA:HB3	1:R:633:PRO:HG3	1.81	0.63
1:A:629:PHE:HD2	1:D:603:PRO:HA	1.62	0.63
1:B:699:ILE:HD11	1:H:389:ARG:HE	1.64	0.63
1:E:341:GLN:HG2	1:E:402:MET:HG2	1.81	0.63
1:F:458:GLN:HG2	1:F:459:SER:H	1.63	0.63
1:H:296:TRP:O	1:H:300:ILE:HG12	1.99	0.63
1:H:379:THR:HG22	1:H:380:LEU:H	1.63	0.63
1:I:536:PRO:HB2	1:I:539:GLY:HA3	1.81	0.63
1:K:396:GLU:HG3	1:Q:367:ALA:HB2	1.81	0.63
1:L:379:THR:HG22	1:L:380:LEU:H	1.63	0.63
1:L:527:HIS:HE1	1:L:562:ASP:OD2	1.81	0.63
1:L:620:ALA:HB3	1:L:633:PRO:HG3	1.81	0.63
1:M:602:LEU:H	1:M:605:MET:HE2	1.62	0.63
1:O:296:TRP:O	1:O:300:ILE:HG12	1.99	0.63
1:P:356:SER:HB2	1:P:358:HIS:CD2	2.34	0.63
1:R:356:SER:HB2	1:R:358:HIS:CD2	2.33	0.63
1:S:312:SER:HB2	1:S:682:GLU:HB3	1.80	0.63
1:S:356:SER:HB2	1:S:358:HIS:CD2	2.33	0.63
1:B:536:PRO:HB2	1:B:539:GLY:HA3	1.81	0.62
1:C:341:GLN:HG2	1:C:402:MET:HG2	1.81	0.62
1:C:458:GLN:HG2	1:C:459:SER:H	1.63	0.62
1:D:602:LEU:H	1:D:605:MET:HE2	1.64	0.62
1:E:536:PRO:HB2	1:E:539:GLY:HA3	1.81	0.62
1:F:350:LEU:HD11	1:F:395:LEU:HG	1.81	0.62
1:F:356:SER:HB2	1:F:358:HIS:CD2	2.33	0.62
1:G:296:TRP:O	1:G:300:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:341:GLN:HG2	1:H:402:MET:HG2	1.81	0.62
1:H:356:SER:HB2	1:H:358:HIS:CD2	2.33	0.62
1:M:440:GLN:NE2	1:M:474:GLN:HB3	2.14	0.62
1:N:341:GLN:HG2	1:N:402:MET:HG2	1.82	0.62
1:P:379:THR:HG22	1:P:380:LEU:H	1.63	0.62
1:S:536:PRO:HB2	1:S:539:GLY:HA3	1.81	0.62
1:T:356:SER:HB2	1:T:358:HIS:CD2	2.34	0.62
1:A:356:SER:HB2	1:A:358:HIS:CD2	2.34	0.62
1:A:378:LEU:HG	1:D:436:PRO:HG3	1.81	0.62
1:B:458:GLN:HG2	1:B:459:SER:H	1.63	0.62
1:C:350:LEU:HD11	1:C:395:LEU:HG	1.81	0.62
1:C:527:HIS:HE1	1:C:562:ASP:OD2	1.81	0.62
1:G:449:GLN:HG3	1:G:450:GLY:H	1.62	0.62
1:G:536:PRO:HB2	1:G:539:GLY:HA3	1.81	0.62
1:J:296:TRP:O	1:J:300:ILE:HG12	1.99	0.62
1:K:440:GLN:NE2	1:K:474:GLN:HB3	2.14	0.62
1:L:440:GLN:NE2	1:L:474:GLN:HB3	2.15	0.62
1:N:440:GLN:NE2	1:N:474:GLN:HB3	2.14	0.62
1:P:350:LEU:HD11	1:P:395:LEU:HG	1.81	0.62
1:S:341:GLN:HG2	1:S:402:MET:HG2	1.81	0.62
1:T:341:GLN:HG2	1:T:402:MET:HG2	1.81	0.62
1:T:620:ALA:HB3	1:T:633:PRO:HG3	1.81	0.62
1:A:263:GLN:HB3	1:A:266:ALA:CB	2.28	0.62
1:A:590:ALA:HA	1:C:497:ASN:ND2	2.14	0.62
1:C:620:ALA:HB3	1:C:633:PRO:HG3	1.81	0.62
1:E:620:ALA:HB3	1:E:633:PRO:HG3	1.81	0.62
1:I:440:GLN:NE2	1:I:474:GLN:HB3	2.15	0.62
1:K:710:ASN:HD22	1:S:259:GLN:HE22	1.46	0.62
1:L:536:PRO:HB2	1:L:539:GLY:HA3	1.81	0.62
1:M:312:SER:HB2	1:M:682:GLU:HB3	1.81	0.62
1:P:341:GLN:HG2	1:P:402:MET:HG2	1.82	0.62
1:T:296:TRP:O	1:T:300:ILE:HG12	1.99	0.62
1:A:440:GLN:NE2	1:A:474:GLN:HB3	2.15	0.62
1:D:620:ALA:HB3	1:D:633:PRO:HG3	1.81	0.62
1:F:536:PRO:HB2	1:F:539:GLY:HA3	1.81	0.62
1:J:458:GLN:HG2	1:J:459:SER:H	1.63	0.62
1:J:536:PRO:HB2	1:J:539:GLY:HA3	1.81	0.62
1:K:379:THR:HG22	1:K:380:LEU:H	1.63	0.62
1:K:620:ALA:HB3	1:K:633:PRO:HG3	1.81	0.62
1:L:296:TRP:O	1:L:300:ILE:HG12	1.99	0.62
1:T:602:LEU:H	1:T:605:MET:HE2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLN:HG2	1:A:402:MET:HG2	1.82	0.62
1:B:602:LEU:H	1:B:605:MET:HE2	1.63	0.62
1:E:449:GLN:HG3	1:E:450:GLY:H	1.62	0.62
1:E:458:GLN:HG2	1:E:459:SER:H	1.63	0.62
1:F:440:GLN:NE2	1:F:474:GLN:HB3	2.14	0.62
1:G:341:GLN:HG2	1:G:402:MET:HG2	1.81	0.62
1:G:440:GLN:NE2	1:G:474:GLN:HB3	2.15	0.62
1:G:620:ALA:HB3	1:G:633:PRO:HG3	1.81	0.62
1:H:312:SER:HB2	1:H:682:GLU:HB3	1.81	0.62
1:H:350:LEU:HD11	1:H:395:LEU:HG	1.82	0.62
1:I:350:LEU:HD11	1:I:395:LEU:HG	1.81	0.62
1:N:536:PRO:HB2	1:N:539:GLY:HA3	1.81	0.62
1:O:350:LEU:HD11	1:O:395:LEU:HG	1.81	0.62
1:P:440:GLN:NE2	1:P:474:GLN:HB3	2.15	0.62
1:Q:356:SER:HB2	1:Q:358:HIS:CD2	2.34	0.62
1:A:497:ASN:ND2	1:D:590:ALA:HA	2.14	0.62
1:A:536:PRO:HB2	1:A:539:GLY:HA3	1.81	0.62
1:B:440:GLN:NE2	1:B:474:GLN:HB3	2.15	0.62
1:B:446:ASN:O	1:H:502:PRO:HG2	2.00	0.62
1:C:379:THR:HG22	1:C:380:LEU:H	1.63	0.62
1:C:446:ASN:O	1:D:502:PRO:HG2	1.99	0.62
1:E:312:SER:HB2	1:E:682:GLU:HB3	1.81	0.62
1:E:350:LEU:HD11	1:E:395:LEU:HG	1.82	0.62
1:E:448:THR:HG23	1:Q:502:PRO:HG3	1.81	0.62
1:J:555:LEU:HD22	1:O:461:LEU:HD12	1.81	0.62
1:K:341:GLN:HG2	1:K:402:MET:HG2	1.81	0.62
1:K:389:ARG:HE	1:R:699:ILE:HD11	1.64	0.62
1:L:341:GLN:HG2	1:L:402:MET:HG2	1.81	0.62
1:Q:350:LEU:HD11	1:Q:395:LEU:HG	1.81	0.62
1:B:341:GLN:HG2	1:B:402:MET:HG2	1.81	0.62
1:B:350:LEU:HD11	1:B:395:LEU:HG	1.81	0.62
1:E:626:ASP:HB2	1:I:608:GLN:HA	1.82	0.62
1:G:602:LEU:H	1:G:605:MET:HE2	1.64	0.62
1:H:620:ALA:HB3	1:H:633:PRO:HG3	1.81	0.62
1:J:350:LEU:HD11	1:J:395:LEU:HG	1.81	0.62
1:J:710:ASN:HD22	1:M:259:GLN:HE22	1.47	0.62
1:K:350:LEU:HD11	1:K:395:LEU:HG	1.82	0.62
1:L:449:GLN:HG3	1:L:450:GLY:H	1.62	0.62
1:T:312:SER:HB2	1:T:682:GLU:HB3	1.81	0.62
1:E:608:GLN:HA	1:Q:626:ASP:HB2	1.81	0.62
1:F:296:TRP:O	1:F:300:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:458:GLN:HG2	1:I:459:SER:H	1.63	0.62
1:J:497:ASN:ND2	1:O:590:ALA:HA	2.15	0.62
1:K:312:SER:HB2	1:K:682:GLU:HB3	1.81	0.62
1:M:620:ALA:HB3	1:M:633:PRO:HG3	1.81	0.62
1:P:312:SER:HB2	1:P:682:GLU:HB3	1.81	0.62
1:A:259:GLN:HE22	1:E:710:ASN:HD22	1.46	0.62
1:C:296:TRP:O	1:C:300:ILE:HG12	1.99	0.62
1:D:350:LEU:HD11	1:D:395:LEU:HG	1.81	0.62
1:D:710:ASN:HD22	1:Q:259:GLN:HE22	1.46	0.62
1:E:440:GLN:NE2	1:E:474:GLN:HB3	2.15	0.62
1:J:440:GLN:NE2	1:J:474:GLN:HB3	2.15	0.62
1:N:312:SER:HB2	1:N:682:GLU:HB3	1.80	0.62
1:N:350:LEU:HD11	1:N:395:LEU:HG	1.82	0.62
1:O:620:ALA:HB3	1:O:633:PRO:HG3	1.81	0.62
1:Q:312:SER:HB2	1:Q:682:GLU:HB3	1.80	0.62
1:Q:341:GLN:HG2	1:Q:402:MET:HG2	1.82	0.62
1:Q:536:PRO:HB2	1:Q:539:GLY:HA3	1.81	0.62
1:R:296:TRP:O	1:R:300:ILE:HG12	1.99	0.62
1:S:440:GLN:NE2	1:S:474:GLN:HB3	2.15	0.62
1:T:536:PRO:HB2	1:T:539:GLY:HA3	1.81	0.62
1:C:432:ARG:NH2	1:D:514:ARG:HD3	2.15	0.62
1:M:350:LEU:HD11	1:M:395:LEU:HG	1.82	0.62
1:O:440:GLN:NE2	1:O:474:GLN:HB3	2.14	0.62
1:O:536:PRO:HB2	1:O:539:GLY:HA3	1.81	0.62
1:R:312:SER:HB2	1:R:682:GLU:HB3	1.80	0.62
1:D:312:SER:HB2	1:D:682:GLU:HB3	1.81	0.61
1:D:440:GLN:NE2	1:D:474:GLN:HB3	2.15	0.61
1:G:350:LEU:HD11	1:G:395:LEU:HG	1.81	0.61
1:J:379:THR:HG22	1:J:380:LEU:H	1.63	0.61
1:L:312:SER:HB2	1:L:682:GLU:HB3	1.81	0.61
1:P:296:TRP:O	1:P:300:ILE:HG12	1.99	0.61
1:A:432:ARG:NH2	1:C:514:ARG:HD3	2.15	0.61
1:A:461:LEU:HD12	1:C:555:LEU:HD22	1.82	0.61
1:C:480:PRO:HB3	1:D:511:LEU:HD21	1.82	0.61
1:D:296:TRP:O	1:D:300:ILE:HG12	1.99	0.61
1:I:341:GLN:HG2	1:I:402:MET:HG2	1.81	0.61
1:J:626:ASP:HB2	1:O:608:GLN:HA	1.82	0.61
1:L:350:LEU:HD11	1:L:395:LEU:HG	1.82	0.61
1:P:458:GLN:HG2	1:P:459:SER:H	1.63	0.61
1:S:350:LEU:HD11	1:S:395:LEU:HG	1.81	0.61
1:S:458:GLN:HG2	1:S:459:SER:H	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:PRO:HB2	1:D:539:GLY:HA3	1.81	0.61
1:E:379:THR:HG22	1:E:380:LEU:H	1.63	0.61
1:K:296:TRP:O	1:K:300:ILE:HG12	1.99	0.61
1:R:341:GLN:HG2	1:R:402:MET:HG2	1.81	0.61
1:R:602:LEU:H	1:R:605:MET:HE2	1.65	0.61
1:A:620:ALA:HB3	1:A:633:PRO:HG3	1.81	0.61
1:B:296:TRP:O	1:B:300:ILE:HG12	1.99	0.61
1:E:436:PRO:HG3	1:Q:378:LEU:HG	1.81	0.61
1:E:441:TYR:HA	1:Q:359:GLN:HE21	1.65	0.61
1:J:360:GLY:HA3	1:J:373:PRO:HG3	1.83	0.61
1:J:626:ASP:H	1:O:608:GLN:NE2	1.98	0.61
1:Q:440:GLN:NE2	1:Q:474:GLN:HB3	2.15	0.61
1:R:350:LEU:HD11	1:R:395:LEU:HG	1.82	0.61
1:F:312:SER:HB2	1:F:682:GLU:HB3	1.81	0.61
1:N:620:ALA:HB3	1:N:633:PRO:HG3	1.81	0.61
1:S:360:GLY:HA3	1:S:373:PRO:HG3	1.83	0.61
1:T:350:LEU:HD11	1:T:395:LEU:HG	1.81	0.61
1:A:350:LEU:HD11	1:A:395:LEU:HG	1.81	0.61
1:B:620:ALA:HB3	1:B:633:PRO:HG3	1.81	0.61
1:H:440:GLN:NE2	1:H:474:GLN:HB3	2.15	0.61
1:M:341:GLN:HG2	1:M:402:MET:HG2	1.81	0.61
1:C:536:PRO:HB2	1:C:539:GLY:HA3	1.81	0.61
1:F:360:GLY:HA3	1:F:373:PRO:HG3	1.83	0.61
1:F:479:LEU:CD2	1:P:634:LEU:HD11	2.30	0.61
1:G:451:THR:HG22	1:G:452:THR:H	1.66	0.61
1:J:341:GLN:HG2	1:J:402:MET:HG2	1.81	0.61
1:J:519:ASN:HD22	1:O:475:ALA:HA	1.66	0.61
1:O:341:GLN:HG2	1:O:402:MET:HG2	1.82	0.61
1:P:536:PRO:HB2	1:P:539:GLY:HA3	1.81	0.61
1:C:710:ASN:HD22	1:J:259:GLN:HE22	1.48	0.61
1:D:341:GLN:HG2	1:D:402:MET:HG2	1.81	0.61
1:I:389:ARG:HE	1:Q:699:ILE:HD11	1.66	0.61
1:L:360:GLY:HA3	1:L:373:PRO:HG3	1.83	0.61
1:L:602:LEU:H	1:L:605:MET:HE2	1.65	0.61
1:R:440:GLN:NE2	1:R:474:GLN:HB3	2.15	0.61
1:A:360:GLY:HA3	1:A:373:PRO:HG3	1.83	0.61
1:A:602:LEU:H	1:A:605:MET:HE2	1.65	0.61
1:F:620:ALA:HB3	1:F:633:PRO:HG3	1.81	0.61
1:O:451:THR:HG22	1:O:452:THR:H	1.66	0.61
1:F:341:GLN:HG2	1:F:402:MET:HG2	1.81	0.61
1:I:360:GLY:HA3	1:I:373:PRO:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:502:PRO:HG3	1:R:448:THR:HG23	1.81	0.61
1:L:451:THR:HG22	1:L:452:THR:H	1.66	0.61
1:Q:451:THR:HG22	1:Q:452:THR:H	1.66	0.61
1:R:360:GLY:HA3	1:R:373:PRO:HG3	1.83	0.61
1:T:440:GLN:NE2	1:T:474:GLN:HB3	2.15	0.61
1:F:436:PRO:HG3	1:P:378:LEU:HG	1.83	0.60
1:H:451:THR:HG22	1:H:452:THR:H	1.66	0.60
1:I:600:GLY:HA3	1:Q:600:GLY:HA3	1.83	0.60
1:P:446:ASN:HD22	1:P:446:ASN:N	1.99	0.60
1:A:608:GLN:HA	1:C:626:ASP:HB2	1.82	0.60
1:E:360:GLY:HA3	1:E:373:PRO:HG3	1.83	0.60
1:G:259:GLN:HE22	1:H:710:ASN:HD22	1.47	0.60
1:I:259:GLN:HE22	1:R:710:ASN:HD22	1.47	0.60
1:L:337:THR:CG2	1:P:405:THR:HG21	2.31	0.60
1:O:259:GLN:HE22	1:S:710:ASN:HD22	1.48	0.60
1:F:356:SER:HB2	1:F:358:HIS:HD2	1.67	0.60
1:H:360:GLY:HA3	1:H:373:PRO:HG3	1.83	0.60
1:J:451:THR:HG22	1:J:452:THR:H	1.66	0.60
1:P:360:GLY:HA3	1:P:373:PRO:HG3	1.83	0.60
1:A:451:THR:HG22	1:A:452:THR:H	1.66	0.60
1:B:451:THR:HG22	1:B:452:THR:H	1.66	0.60
1:C:440:GLN:NE2	1:C:474:GLN:HB3	2.15	0.60
1:E:502:PRO:HG3	1:I:448:THR:HG23	1.83	0.60
1:G:356:SER:HB2	1:G:358:HIS:HD2	1.67	0.60
1:H:356:SER:HB2	1:H:358:HIS:HD2	1.67	0.60
1:N:446:ASN:HD22	1:N:446:ASN:N	2.00	0.60
1:F:540:ASN:HD21	1:F:560:ILE:HG22	1.67	0.60
1:C:360:GLY:HA3	1:C:373:PRO:HG3	1.83	0.60
1:E:451:THR:HG22	1:E:452:THR:H	1.67	0.60
1:G:540:ASN:HD21	1:G:560:ILE:HG22	1.67	0.60
1:L:540:ASN:HD21	1:L:560:ILE:HG22	1.67	0.60
1:R:356:SER:HB2	1:R:358:HIS:HD2	1.67	0.60
1:T:356:SER:HB2	1:T:358:HIS:HD2	1.67	0.60
1:T:451:THR:HG22	1:T:452:THR:H	1.66	0.60
1:B:360:GLY:HA3	1:B:373:PRO:HG3	1.83	0.60
1:C:451:THR:HG22	1:C:452:THR:H	1.66	0.60
1:E:540:ASN:HD21	1:E:560:ILE:HG22	1.67	0.60
1:K:275:TYR:OH	1:Q:714:THR:HG21	2.01	0.60
1:M:540:ASN:HD21	1:M:560:ILE:HG22	1.67	0.60
1:S:451:THR:HG22	1:S:452:THR:H	1.66	0.60
1:B:446:ASN:HD22	1:B:446:ASN:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:SER:HB2	1:D:358:HIS:HD2	1.67	0.60
1:J:356:SER:HB2	1:J:358:HIS:HD2	1.67	0.60
1:K:451:THR:HG22	1:K:452:THR:H	1.66	0.60
1:R:451:THR:HG22	1:R:452:THR:H	1.66	0.60
1:A:714:THR:HG21	1:H:275:TYR:OH	2.02	0.60
1:D:360:GLY:HA3	1:D:373:PRO:HG3	1.83	0.60
1:E:514:ARG:HD3	1:I:432:ARG:NH2	2.17	0.60
1:F:603:PRO:HA	1:P:629:PHE:HD2	1.67	0.60
1:I:356:SER:HB2	1:I:358:HIS:HD2	1.67	0.60
1:I:451:THR:HG22	1:I:452:THR:H	1.66	0.60
1:I:540:ASN:HD21	1:I:560:ILE:HG22	1.67	0.60
1:J:446:ASN:HD22	1:J:446:ASN:N	2.00	0.60
1:K:360:GLY:HA3	1:K:373:PRO:HG3	1.83	0.60
1:M:360:GLY:HA3	1:M:373:PRO:HG3	1.83	0.60
1:M:446:ASN:HD22	1:M:446:ASN:N	1.99	0.60
1:M:710:ASN:HD22	1:N:259:GLN:HE22	1.48	0.60
1:O:360:GLY:HA3	1:O:373:PRO:HG3	1.83	0.60
1:T:540:ASN:HD21	1:T:560:ILE:HG22	1.67	0.60
1:H:446:ASN:HD22	1:H:446:ASN:N	2.00	0.59
1:A:356:SER:HB2	1:A:358:HIS:HD2	1.67	0.59
1:A:359:GLN:HE21	1:D:441:TYR:HA	1.66	0.59
1:C:540:ASN:HD21	1:C:560:ILE:HG22	1.67	0.59
1:E:446:ASN:O	1:Q:502:PRO:HG2	2.02	0.59
1:G:360:GLY:HA3	1:G:373:PRO:HG3	1.83	0.59
1:M:451:THR:HG22	1:M:452:THR:H	1.66	0.59
1:Q:360:GLY:HA3	1:Q:373:PRO:HG3	1.83	0.59
1:N:360:GLY:HA3	1:N:373:PRO:HG3	1.83	0.59
1:N:451:THR:HG22	1:N:452:THR:H	1.66	0.59
1:O:577:TYR:HB3	1:O:596:VAL:HG13	1.85	0.59
1:B:356:SER:HB2	1:B:358:HIS:HD2	1.67	0.59
1:E:472:SER:HB3	1:Q:269:ASP:O	2.02	0.59
1:K:356:SER:HB2	1:K:358:HIS:HD2	1.67	0.59
1:K:540:ASN:HD21	1:K:560:ILE:HG22	1.67	0.59
1:Q:356:SER:HB2	1:Q:358:HIS:HD2	1.67	0.59
1:T:360:GLY:HA3	1:T:373:PRO:HG3	1.83	0.59
1:B:590:ALA:HA	1:H:497:ASN:ND2	2.17	0.59
1:B:600:GLY:HA3	1:H:600:GLY:HA3	1.84	0.59
1:D:451:THR:HG22	1:D:452:THR:H	1.66	0.59
1:D:540:ASN:HD21	1:D:560:ILE:HG22	1.67	0.59
1:D:577:TYR:HB3	1:D:596:VAL:HG13	1.85	0.59
1:E:389:ARG:HE	1:I:699:ILE:HD11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:600:GLY:HA3	1:Q:600:GLY:HA3	1.84	0.59
1:F:395:LEU:HD23	1:F:648:MET:HG2	1.84	0.59
1:H:395:LEU:HD23	1:H:648:MET:HG2	1.85	0.59
1:I:514:ARG:HD3	1:Q:432:ARG:NH2	2.18	0.59
1:P:356:SER:HB2	1:P:358:HIS:HD2	1.67	0.59
1:P:451:THR:HG22	1:P:452:THR:H	1.66	0.59
1:A:577:TYR:HB3	1:A:596:VAL:HG13	1.85	0.59
1:E:577:TYR:HB3	1:E:596:VAL:HG13	1.85	0.59
1:F:451:THR:HG22	1:F:452:THR:H	1.66	0.59
1:R:540:ASN:HD21	1:R:560:ILE:HG22	1.67	0.59
1:S:356:SER:HB2	1:S:358:HIS:HD2	1.67	0.59
1:S:577:TYR:HB3	1:S:596:VAL:HG13	1.85	0.59
1:B:540:ASN:HD21	1:B:560:ILE:HG22	1.67	0.59
1:E:432:ARG:NH2	1:Q:514:ARG:HD3	2.18	0.59
1:F:475:ALA:HA	1:P:519:ASN:HD22	1.68	0.59
1:J:395:LEU:HD23	1:J:648:MET:HG2	1.85	0.59
1:L:356:SER:HB2	1:L:358:HIS:HD2	1.67	0.59
1:S:540:ASN:HD21	1:S:560:ILE:HG22	1.67	0.59
1:A:322:GLU:HG2	1:A:335:ASN:HB2	1.85	0.59
1:A:395:LEU:HD23	1:A:648:MET:HG2	1.85	0.59
1:A:435:ASN:HB3	1:C:358:HIS:CE1	2.37	0.59
1:A:502:PRO:HG2	1:D:446:ASN:O	2.03	0.59
1:A:540:ASN:HD21	1:A:560:ILE:HG22	1.67	0.59
1:B:432:ARG:NH2	1:H:514:ARG:HD3	2.17	0.59
1:C:699:ILE:HD11	1:D:389:ARG:HE	1.68	0.59
1:F:577:TYR:HB3	1:F:596:VAL:HG13	1.85	0.59
1:H:540:ASN:HD21	1:H:560:ILE:HG22	1.67	0.59
1:K:359:GLN:HE21	1:R:441:TYR:HA	1.67	0.59
1:M:577:TYR:HB3	1:M:596:VAL:HG13	1.85	0.59
1:O:395:LEU:HD23	1:O:648:MET:HG2	1.85	0.59
1:Q:446:ASN:HD22	1:Q:446:ASN:N	2.00	0.59
1:R:577:TYR:HB3	1:R:596:VAL:HG13	1.85	0.59
1:A:502:PRO:HG3	1:D:448:THR:HG23	1.85	0.59
1:C:428:GLN:NE2	1:D:351:PRO:HB3	2.18	0.59
1:F:259:GLN:HE22	1:G:710:ASN:HD22	1.51	0.59
1:K:395:LEU:HD23	1:K:648:MET:HG2	1.85	0.59
1:N:540:ASN:HD21	1:N:560:ILE:HG22	1.67	0.59
1:A:514:ARG:HD3	1:D:432:ARG:NH2	2.18	0.59
1:B:577:TYR:HB3	1:B:596:VAL:HG13	1.85	0.59
1:C:461:LEU:HD12	1:D:555:LEU:HD22	1.85	0.59
1:G:395:LEU:HD23	1:G:648:MET:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:577:TYR:HB3	1:G:596:VAL:HG13	1.85	0.59
1:J:634:LEU:HD11	1:O:479:LEU:CD2	2.32	0.59
1:K:502:PRO:HG2	1:R:446:ASN:O	2.02	0.59
1:N:322:GLU:HG2	1:N:335:ASN:HB2	1.85	0.59
1:R:395:LEU:HD23	1:R:648:MET:HG2	1.85	0.59
1:A:270:ASN:ND2	1:D:472:SER:H	2.01	0.58
1:C:577:TYR:HB3	1:C:596:VAL:HG13	1.85	0.58
1:E:356:SER:HB2	1:E:358:HIS:HD2	1.67	0.58
1:K:446:ASN:HD22	1:K:446:ASN:N	1.99	0.58
1:N:395:LEU:HD23	1:N:648:MET:HG2	1.85	0.58
1:S:322:GLU:HG2	1:S:335:ASN:HB2	1.85	0.58
1:T:577:TYR:HB3	1:T:596:VAL:HG13	1.85	0.58
1:E:608:GLN:NE2	1:Q:626:ASP:H	2.01	0.58
1:E:626:ASP:H	1:I:608:GLN:NE2	2.00	0.58
1:I:395:LEU:HD23	1:I:648:MET:HG2	1.85	0.58
1:K:577:TYR:HB3	1:K:596:VAL:HG13	1.85	0.58
1:O:322:GLU:HG2	1:O:335:ASN:HB2	1.85	0.58
1:Q:577:TYR:HB3	1:Q:596:VAL:HG13	1.84	0.58
1:A:443:TYR:CE2	1:C:544:GLY:HA3	2.38	0.58
1:C:356:SER:HB2	1:C:358:HIS:HD2	1.67	0.58
1:E:322:GLU:HG2	1:E:335:ASN:HB2	1.85	0.58
1:I:322:GLU:HG2	1:I:335:ASN:HB2	1.85	0.58
1:I:577:TYR:HB3	1:I:596:VAL:HG13	1.85	0.58
1:J:540:ASN:HD21	1:J:560:ILE:HG22	1.67	0.58
1:F:322:GLU:HG2	1:F:335:ASN:HB2	1.85	0.58
1:G:322:GLU:HG2	1:G:335:ASN:HB2	1.85	0.58
1:H:577:TYR:HB3	1:H:596:VAL:HG13	1.85	0.58
1:I:446:ASN:HD22	1:I:446:ASN:N	2.00	0.58
1:K:259:GLN:HE22	1:Q:710:ASN:ND2	2.01	0.58
1:P:577:TYR:HB3	1:P:596:VAL:HG13	1.85	0.58
1:D:322:GLU:HG2	1:D:335:ASN:HB2	1.85	0.58
1:H:322:GLU:HG2	1:H:335:ASN:HB2	1.85	0.58
1:L:322:GLU:HG2	1:L:335:ASN:HB2	1.85	0.58
1:M:322:GLU:HG2	1:M:335:ASN:HB2	1.85	0.58
1:M:395:LEU:HD23	1:M:648:MET:HG2	1.85	0.58
1:O:540:ASN:HD21	1:O:560:ILE:HG22	1.67	0.58
1:A:269:ASP:O	1:D:472:SER:HB3	2.04	0.58
1:A:477:ASN:HA	1:C:634:LEU:HB2	1.83	0.58
1:B:322:GLU:HG2	1:B:335:ASN:HB2	1.85	0.58
1:E:395:LEU:HD23	1:E:648:MET:HG2	1.85	0.58
1:G:446:ASN:HD22	1:G:446:ASN:N	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:356:SER:HB2	1:M:358:HIS:HD2	1.67	0.58
1:I:710:ASN:ND2	1:P:259:GLN:HE22	2.02	0.58
1:J:502:PRO:HG2	1:O:446:ASN:O	2.02	0.58
1:J:577:TYR:HB3	1:J:596:VAL:HG13	1.85	0.58
1:P:322:GLU:HG2	1:P:335:ASN:HB2	1.85	0.58
1:P:395:LEU:HD23	1:P:648:MET:HG2	1.85	0.58
1:C:600:GLY:HA3	1:D:600:GLY:HA3	1.85	0.58
1:E:502:PRO:HG2	1:I:446:ASN:O	2.03	0.58
1:E:699:ILE:HD11	1:Q:389:ARG:HE	1.68	0.58
1:I:359:GLN:HE21	1:Q:441:TYR:HA	1.68	0.58
1:J:501:PHE:HB2	1:J:505:ALA:HB3	1.86	0.58
1:O:356:SER:HB2	1:O:358:HIS:HD2	1.67	0.58
1:P:540:ASN:HD21	1:P:560:ILE:HG22	1.67	0.58
1:R:501:PHE:HB2	1:R:505:ALA:HB3	1.86	0.58
1:B:472:SER:H	1:H:270:ASN:ND2	2.02	0.58
1:D:395:LEU:HD23	1:D:648:MET:HG2	1.85	0.58
1:J:322:GLU:HG2	1:J:335:ASN:HB2	1.85	0.58
1:K:322:GLU:HG2	1:K:335:ASN:HB2	1.85	0.58
1:Q:322:GLU:HG2	1:Q:335:ASN:HB2	1.85	0.58
1:Q:540:ASN:HD21	1:Q:560:ILE:HG22	1.67	0.58
1:C:479:LEU:CD2	1:D:634:LEU:HD11	2.34	0.58
1:I:269:ASP:O	1:Q:472:SER:HB3	2.04	0.58
1:J:544:GLY:HA3	1:O:443:TYR:CE2	2.39	0.58
1:K:269:ASP:O	1:R:472:SER:HB3	2.04	0.58
1:L:395:LEU:HD23	1:L:648:MET:HG2	1.85	0.58
1:Q:395:LEU:HD23	1:Q:648:MET:HG2	1.85	0.58
1:C:395:LEU:HD23	1:C:648:MET:HG2	1.85	0.57
1:C:475:ALA:HA	1:D:519:ASN:HD22	1.69	0.57
1:D:446:ASN:HD22	1:D:446:ASN:N	2.00	0.57
1:I:502:PRO:HG2	1:Q:446:ASN:O	2.04	0.57
1:N:356:SER:HB2	1:N:358:HIS:HD2	1.67	0.57
1:E:501:PHE:HB2	1:E:505:ALA:HB3	1.86	0.57
1:F:501:PHE:HB2	1:F:505:ALA:HB3	1.86	0.57
1:K:501:PHE:HB2	1:K:505:ALA:HB3	1.86	0.57
1:B:441:TYR:HA	1:H:359:GLN:HE21	1.70	0.57
1:N:509:TYR:HD2	1:N:518:VAL:HG22	1.69	0.57
1:P:501:PHE:HB2	1:P:505:ALA:HB3	1.86	0.57
1:Q:501:PHE:HB2	1:Q:505:ALA:HB3	1.86	0.57
1:S:395:LEU:HD23	1:S:648:MET:HG2	1.85	0.57
1:P:509:TYR:HD2	1:P:518:VAL:HG22	1.70	0.57
1:S:501:PHE:HB2	1:S:505:ALA:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:501:PHE:HB2	1:M:505:ALA:HB3	1.86	0.57
1:R:322:GLU:HG2	1:R:335:ASN:HB2	1.85	0.57
1:C:322:GLU:HG2	1:C:335:ASN:HB2	1.85	0.57
1:B:395:LEU:HD23	1:B:648:MET:HG2	1.85	0.57
1:H:501:PHE:HB2	1:H:505:ALA:HB3	1.86	0.57
1:I:509:TYR:HD2	1:I:518:VAL:HG22	1.70	0.57
1:J:555:LEU:HA	1:O:463:PHE:HE2	1.69	0.57
1:L:577:TYR:HB3	1:L:596:VAL:HG13	1.85	0.57
1:M:509:TYR:HD2	1:M:518:VAL:HG22	1.69	0.57
1:O:446:ASN:HD22	1:O:446:ASN:N	1.99	0.57
1:O:501:PHE:HB2	1:O:505:ALA:HB3	1.86	0.57
1:R:509:TYR:HD2	1:R:518:VAL:HG22	1.70	0.57
1:A:626:ASP:H	1:D:608:GLN:NE2	2.02	0.57
1:D:509:TYR:HD2	1:D:518:VAL:HG22	1.70	0.57
1:E:359:GLN:HE21	1:I:441:TYR:HA	1.69	0.57
1:E:509:TYR:HD2	1:E:518:VAL:HG22	1.70	0.57
1:G:501:PHE:HB2	1:G:505:ALA:HB3	1.86	0.57
1:J:304:TRP:CE3	1:J:304:TRP:HA	2.40	0.57
1:K:304:TRP:HA	1:K:304:TRP:CE3	2.40	0.57
1:L:509:TYR:HD2	1:L:518:VAL:HG22	1.70	0.57
1:C:509:TYR:HD2	1:C:518:VAL:HG22	1.70	0.57
1:R:259:GLN:HE22	1:T:710:ASN:HD22	1.52	0.57
1:B:304:TRP:CE3	1:B:304:TRP:HA	2.40	0.57
1:C:304:TRP:HA	1:C:304:TRP:CE3	2.40	0.57
1:E:269:ASP:O	1:I:472:SER:HB3	2.04	0.57
1:E:600:GLY:HA3	1:I:600:GLY:HA3	1.86	0.57
1:H:509:TYR:HD2	1:H:518:VAL:HG22	1.70	0.57
1:N:577:TYR:HB3	1:N:596:VAL:HG13	1.85	0.57
1:R:446:ASN:HD22	1:R:446:ASN:N	1.99	0.57
1:T:322:GLU:HG2	1:T:335:ASN:HB2	1.85	0.57
1:G:304:TRP:CE3	1:G:304:TRP:HA	2.40	0.56
1:J:509:TYR:HD2	1:J:518:VAL:HG22	1.70	0.56
1:L:501:PHE:HB2	1:L:505:ALA:HB3	1.86	0.56
1:N:501:PHE:HB2	1:N:505:ALA:HB3	1.86	0.56
1:S:446:ASN:HD22	1:S:446:ASN:N	2.00	0.56
1:T:395:LEU:HD23	1:T:648:MET:HG2	1.85	0.56
1:B:472:SER:HB3	1:H:269:ASP:O	2.04	0.56
1:B:475:ALA:HA	1:H:519:ASN:HD22	1.70	0.56
1:B:710:ASN:ND2	1:C:259:GLN:HE22	2.02	0.56
1:J:500:ASN:HA	1:O:448:THR:OG1	2.05	0.56
1:T:509:TYR:HD2	1:T:518:VAL:HG22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:PHE:HB2	1:A:505:ALA:HB3	1.86	0.56
1:B:435:ASN:HB3	1:H:358:HIS:CE1	2.40	0.56
1:B:501:PHE:HB2	1:B:505:ALA:HB3	1.86	0.56
1:D:405:THR:HG21	1:Q:337:THR:HG22	1.87	0.56
1:D:501:PHE:HB2	1:D:505:ALA:HB3	1.86	0.56
1:E:472:SER:H	1:Q:270:ASN:ND2	2.03	0.56
1:F:509:TYR:HD2	1:F:518:VAL:HG22	1.70	0.56
1:F:608:GLN:NE2	1:P:626:ASP:H	2.03	0.56
1:H:304:TRP:HA	1:H:304:TRP:CE3	2.40	0.56
1:I:501:PHE:HB2	1:I:505:ALA:HB3	1.86	0.56
1:J:514:ARG:HD3	1:O:432:ARG:NH2	2.20	0.56
1:S:509:TYR:HD2	1:S:518:VAL:HG22	1.70	0.56
1:A:509:TYR:HD2	1:A:518:VAL:HG22	1.70	0.56
1:N:304:TRP:HA	1:N:304:TRP:CE3	2.40	0.56
1:A:519:ASN:HD22	1:D:475:ALA:HA	1.70	0.56
1:B:448:THR:HG23	1:H:502:PRO:HG3	1.87	0.56
1:B:509:TYR:HD2	1:B:518:VAL:HG22	1.70	0.56
1:G:509:TYR:HD2	1:G:518:VAL:HG22	1.70	0.56
1:I:275:TYR:OH	1:R:714:THR:HG21	2.06	0.56
1:I:304:TRP:HA	1:I:304:TRP:CE3	2.40	0.56
1:M:304:TRP:HA	1:M:304:TRP:CE3	2.40	0.56
1:T:501:PHE:HB2	1:T:505:ALA:HB3	1.86	0.56
1:C:501:PHE:HB2	1:C:505:ALA:HB3	1.86	0.56
1:F:446:ASN:HD22	1:F:446:ASN:N	2.00	0.56
1:R:263:GLN:HB3	1:R:266:ALA:HB2	1.88	0.56
1:I:351:PRO:HB3	1:Q:428:GLN:NE2	2.21	0.56
1:R:304:TRP:CE3	1:R:304:TRP:HA	2.40	0.56
1:S:304:TRP:HA	1:S:304:TRP:CE3	2.40	0.56
1:A:626:ASP:HB2	1:D:608:GLN:HA	1.88	0.56
1:H:263:GLN:HB3	1:H:266:ALA:HB2	1.88	0.56
1:I:519:ASN:HD22	1:Q:475:ALA:HA	1.71	0.56
1:J:359:GLN:HE21	1:O:441:TYR:HA	1.70	0.56
1:B:608:GLN:NE2	1:H:626:ASP:H	2.04	0.56
1:E:263:GLN:HB3	1:E:266:ALA:HB2	1.88	0.56
1:E:304:TRP:HA	1:E:304:TRP:CE3	2.40	0.56
1:F:304:TRP:HA	1:F:304:TRP:CE3	2.40	0.56
1:R:570:ASN:HD21	1:R:607:TRP:HB2	1.71	0.56
1:A:304:TRP:HA	1:A:304:TRP:CE3	2.40	0.56
1:A:463:PHE:HE2	1:C:555:LEU:HA	1.70	0.56
1:A:584:LEU:HB3	1:C:488:ARG:NH2	2.20	0.56
1:E:628:HIS:HB2	1:E:631:PRO:HG3	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:722:SER:O	1:G:724:PRO:HD3	2.06	0.56
1:I:722:SER:O	1:I:724:PRO:HD3	2.06	0.56
1:L:722:SER:O	1:L:724:PRO:HD3	2.06	0.56
1:O:722:SER:O	1:O:724:PRO:HD3	2.06	0.56
1:P:304:TRP:HA	1:P:304:TRP:CE3	2.40	0.56
1:A:358:HIS:CE1	1:D:435:ASN:HB3	2.41	0.55
1:E:722:SER:O	1:E:724:PRO:HD3	2.06	0.55
1:F:722:SER:O	1:F:724:PRO:HD3	2.07	0.55
1:J:263:GLN:HB3	1:J:266:ALA:HB2	1.88	0.55
1:J:628:HIS:HB2	1:J:631:PRO:HG3	1.89	0.55
1:K:263:GLN:HB3	1:K:266:ALA:HB2	1.88	0.55
1:N:628:HIS:HB2	1:N:631:PRO:HG3	1.89	0.55
1:O:304:TRP:CE3	1:O:304:TRP:HA	2.40	0.55
1:A:570:ASN:HD21	1:A:607:TRP:HB2	1.71	0.55
1:A:722:SER:O	1:A:724:PRO:HD3	2.07	0.55
1:J:714:THR:HG21	1:M:275:TYR:OH	2.06	0.55
1:K:509:TYR:HD2	1:K:518:VAL:HG22	1.70	0.55
1:L:570:ASN:HD21	1:L:607:TRP:HB2	1.72	0.55
1:M:263:GLN:HB3	1:M:266:ALA:HB2	1.88	0.55
1:O:628:HIS:HB2	1:O:631:PRO:HG3	1.89	0.55
1:A:448:THR:OG1	1:C:500:ASN:HA	2.07	0.55
1:B:628:HIS:HB2	1:B:631:PRO:HG3	1.89	0.55
1:B:722:SER:O	1:B:724:PRO:HD3	2.06	0.55
1:D:722:SER:O	1:D:724:PRO:HD3	2.07	0.55
1:E:428:GLN:NE2	1:Q:351:PRO:HB3	2.22	0.55
1:E:570:ASN:HD21	1:E:607:TRP:HB2	1.72	0.55
1:L:304:TRP:HA	1:L:304:TRP:CE3	2.40	0.55
1:Q:509:TYR:HD2	1:Q:518:VAL:HG22	1.70	0.55
1:K:628:HIS:HB2	1:K:631:PRO:HG3	1.89	0.55
1:K:634:LEU:HB2	1:R:477:ASN:HA	1.89	0.55
1:N:263:GLN:HB3	1:N:266:ALA:HB2	1.88	0.55
1:O:570:ASN:HD21	1:O:607:TRP:HB2	1.72	0.55
1:S:722:SER:O	1:S:724:PRO:HD3	2.06	0.55
1:T:304:TRP:HA	1:T:304:TRP:CE3	2.40	0.55
1:B:263:GLN:HB3	1:B:266:ALA:HB2	1.88	0.55
1:E:497:ASN:ND2	1:I:590:ALA:HA	2.21	0.55
1:F:448:THR:OG1	1:P:500:ASN:HA	2.06	0.55
1:J:570:ASN:HD21	1:J:607:TRP:HB2	1.72	0.55
1:O:509:TYR:HD2	1:O:518:VAL:HG22	1.70	0.55
1:Q:263:GLN:HB3	1:Q:266:ALA:HB2	1.88	0.55
1:Q:304:TRP:HA	1:Q:304:TRP:CE3	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:570:ASN:HD21	1:Q:607:TRP:HB2	1.72	0.55
1:S:628:HIS:HB2	1:S:631:PRO:HG3	1.89	0.55
1:D:570:ASN:HD21	1:D:607:TRP:HB2	1.71	0.55
1:F:437:LEU:HD21	1:P:276:SER:OG	2.07	0.55
1:G:263:GLN:HB3	1:G:266:ALA:HB2	1.88	0.55
1:H:570:ASN:HD21	1:H:607:TRP:HB2	1.72	0.55
1:K:519:ASN:HD22	1:R:475:ALA:HA	1.71	0.55
1:K:722:SER:O	1:K:724:PRO:HD3	2.06	0.55
1:L:628:HIS:HB2	1:L:631:PRO:HG3	1.89	0.55
1:Q:628:HIS:HB2	1:Q:631:PRO:HG3	1.89	0.55
1:R:722:SER:O	1:R:724:PRO:HD3	2.07	0.55
1:S:404:ARG:H	1:S:407:ASN:ND2	2.05	0.55
1:C:628:HIS:HB2	1:C:631:PRO:HG3	1.89	0.55
1:D:263:GLN:HB3	1:D:266:ALA:HB2	1.88	0.55
1:F:263:GLN:HB3	1:F:266:ALA:HB2	1.88	0.55
1:H:628:HIS:HB2	1:H:631:PRO:HG3	1.89	0.55
1:M:628:HIS:HB2	1:M:631:PRO:HG3	1.88	0.55
1:T:404:ARG:H	1:T:407:ASN:ND2	2.05	0.55
1:D:304:TRP:HA	1:D:304:TRP:CE3	2.40	0.55
1:J:722:SER:O	1:J:724:PRO:HD3	2.06	0.55
1:Q:722:SER:O	1:Q:724:PRO:HD3	2.06	0.55
1:B:405:THR:HG22	1:C:404:ARG:NH2	2.22	0.55
1:C:379:THR:HG22	1:C:380:LEU:N	2.22	0.55
1:C:446:ASN:HD22	1:C:446:ASN:N	1.99	0.55
1:F:628:HIS:HB2	1:F:631:PRO:HG3	1.88	0.55
1:K:404:ARG:H	1:K:407:ASN:ND2	2.05	0.55
1:P:404:ARG:H	1:P:407:ASN:ND2	2.05	0.55
1:P:628:HIS:HB2	1:P:631:PRO:HG3	1.88	0.55
1:R:628:HIS:HB2	1:R:631:PRO:HG3	1.89	0.55
1:T:379:THR:HG22	1:T:380:LEU:N	2.22	0.55
1:F:443:TYR:CE2	1:P:544:GLY:HA3	2.41	0.55
1:G:628:HIS:HB2	1:G:631:PRO:HG3	1.89	0.55
1:I:263:GLN:HB3	1:I:266:ALA:HB2	1.88	0.55
1:N:722:SER:O	1:N:724:PRO:HD3	2.06	0.55
1:C:448:THR:HG23	1:D:502:PRO:HG3	1.88	0.54
1:D:404:ARG:H	1:D:407:ASN:ND2	2.06	0.54
1:K:378:LEU:CD2	1:R:436:PRO:HG3	2.37	0.54
1:L:263:GLN:HB3	1:L:266:ALA:HB2	1.88	0.54
1:M:722:SER:O	1:M:724:PRO:HD3	2.06	0.54
1:N:379:THR:HG22	1:N:380:LEU:N	2.22	0.54
1:O:263:GLN:HB3	1:O:266:ALA:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:404:ARG:H	1:R:407:ASN:ND2	2.05	0.54
1:A:404:ARG:H	1:A:407:ASN:ND2	2.06	0.54
1:B:404:ARG:H	1:B:407:ASN:ND2	2.05	0.54
1:B:477:ASN:HA	1:H:634:LEU:HB2	1.88	0.54
1:E:404:ARG:H	1:E:407:ASN:ND2	2.05	0.54
1:F:431:ASP:O	1:F:434:MET:HE3	2.07	0.54
1:K:570:ASN:HD21	1:K:607:TRP:HB2	1.71	0.54
1:O:404:ARG:H	1:O:407:ASN:ND2	2.05	0.54
1:T:570:ASN:HD21	1:T:607:TRP:HB2	1.71	0.54
1:I:379:THR:HG22	1:I:380:LEU:N	2.22	0.54
1:Q:379:THR:HG22	1:Q:380:LEU:N	2.22	0.54
1:S:379:THR:HG22	1:S:380:LEU:N	2.22	0.54
1:B:275:TYR:OH	1:N:714:THR:HG21	2.07	0.54
1:C:404:ARG:H	1:C:407:ASN:ND2	2.05	0.54
1:C:443:TYR:CE2	1:D:544:GLY:HA3	2.42	0.54
1:E:275:TYR:OH	1:F:714:THR:HG21	2.07	0.54
1:F:379:THR:HG22	1:F:380:LEU:N	2.22	0.54
1:F:472:SER:H	1:P:270:ASN:ND2	2.05	0.54
1:I:628:HIS:HB2	1:I:631:PRO:HG3	1.89	0.54
1:J:358:HIS:CE1	1:O:435:ASN:HB3	2.42	0.54
1:J:488:ARG:NH2	1:O:584:LEU:HB3	2.22	0.54
1:K:497:ASN:ND2	1:R:590:ALA:HA	2.22	0.54
1:P:263:GLN:HB3	1:P:266:ALA:HB2	1.88	0.54
1:S:263:GLN:HB3	1:S:266:ALA:HB2	1.88	0.54
1:T:263:GLN:HB3	1:T:266:ALA:HB2	1.88	0.54
1:T:431:ASP:O	1:T:434:MET:HE3	2.08	0.54
1:G:570:ASN:HD21	1:G:607:TRP:HB2	1.72	0.54
1:I:570:ASN:HD21	1:I:607:TRP:HB2	1.72	0.54
1:N:431:ASP:O	1:N:434:MET:HE3	2.08	0.54
1:O:379:THR:HG22	1:O:380:LEU:N	2.22	0.54
1:R:379:THR:HG22	1:R:380:LEU:N	2.22	0.54
1:S:570:ASN:HD21	1:S:607:TRP:HB2	1.72	0.54
1:A:628:HIS:HB2	1:A:631:PRO:HG3	1.88	0.54
1:C:722:SER:O	1:C:724:PRO:HD3	2.06	0.54
1:N:570:ASN:HD21	1:N:607:TRP:HB2	1.71	0.54
1:P:722:SER:O	1:P:724:PRO:HD3	2.06	0.54
1:R:263:GLN:HB3	1:R:266:ALA:HB3	1.90	0.54
1:A:263:GLN:HB3	1:A:266:ALA:HB2	1.88	0.54
1:E:379:THR:HG22	1:E:380:LEU:N	2.22	0.54
1:H:722:SER:O	1:H:724:PRO:HD3	2.06	0.54
1:N:263:GLN:HB3	1:N:266:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:404:ARG:H	1:Q:407:ASN:ND2	2.05	0.54
1:B:323:VAL:HG11	1:C:657:ASN:ND2	2.23	0.54
1:F:421:HIS:CD2	1:F:729:THR:HG21	2.43	0.54
1:K:358:HIS:CE1	1:R:435:ASN:HB3	2.43	0.54
1:B:421:HIS:CD2	1:B:729:THR:HG21	2.43	0.54
1:F:294:ARG:NE	1:F:298:ARG:HE	2.04	0.54
1:H:379:THR:HG22	1:H:380:LEU:N	2.22	0.54
1:M:379:THR:HG22	1:M:380:LEU:N	2.22	0.54
1:M:570:ASN:HD21	1:M:607:TRP:HB2	1.72	0.54
1:P:379:THR:HG22	1:P:380:LEU:N	2.23	0.54
1:Q:421:HIS:CD2	1:Q:729:THR:HG21	2.43	0.54
1:R:421:HIS:CD2	1:R:729:THR:HG21	2.43	0.54
1:T:628:HIS:HB2	1:T:631:PRO:HG3	1.89	0.54
1:T:722:SER:O	1:T:724:PRO:HD3	2.07	0.54
1:B:379:THR:HG22	1:B:380:LEU:N	2.22	0.54
1:C:570:ASN:HD21	1:C:607:TRP:HB2	1.72	0.54
1:E:351:PRO:HB3	1:I:428:GLN:NE2	2.23	0.54
1:E:437:LEU:HD21	1:Q:276:SER:OG	2.08	0.54
1:F:570:ASN:HD21	1:F:607:TRP:HB2	1.71	0.54
1:G:404:ARG:H	1:G:407:ASN:ND2	2.05	0.54
1:H:404:ARG:H	1:H:407:ASN:ND2	2.06	0.54
1:I:358:HIS:CE1	1:Q:435:ASN:HB3	2.43	0.54
1:J:404:ARG:H	1:J:407:ASN:ND2	2.05	0.54
1:L:259:GLN:HE22	1:P:710:ASN:HD22	1.56	0.54
1:L:379:THR:HG22	1:L:380:LEU:N	2.22	0.54
1:C:263:GLN:HB3	1:C:266:ALA:HB2	1.88	0.53
1:C:294:ARG:NE	1:C:298:ARG:HE	2.04	0.53
1:E:480:PRO:HG3	1:Q:511:LEU:HD11	1.90	0.53
1:I:270:ASN:ND2	1:Q:472:SER:H	2.06	0.53
1:J:379:THR:HG22	1:J:380:LEU:N	2.22	0.53
1:K:270:ASN:ND2	1:R:472:SER:H	2.05	0.53
1:L:421:HIS:CD2	1:L:729:THR:HG21	2.43	0.53
1:L:482:PRO:HD3	1:L:605:MET:HE3	1.90	0.53
1:N:404:ARG:H	1:N:407:ASN:ND2	2.05	0.53
1:P:263:GLN:HB3	1:P:266:ALA:HB3	1.90	0.53
1:R:482:PRO:HD3	1:R:605:MET:HE3	1.90	0.53
1:T:447:ARG:HB2	1:T:462:LEU:HB2	1.91	0.53
1:A:447:ARG:HB2	1:A:462:LEU:HB2	1.91	0.53
1:G:379:THR:HG22	1:G:380:LEU:N	2.22	0.53
1:K:421:HIS:CD2	1:K:729:THR:HG21	2.43	0.53
1:M:404:ARG:H	1:M:407:ASN:ND2	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:506:ALA:HB1	1:N:538:HIS:HE1	1.74	0.53
1:O:447:ARG:HB2	1:O:462:LEU:HB2	1.91	0.53
1:Q:431:ASP:O	1:Q:434:MET:HE3	2.08	0.53
1:A:555:LEU:HA	1:D:463:PHE:HE2	1.74	0.53
1:D:379:THR:HG22	1:D:380:LEU:N	2.22	0.53
1:D:540:ASN:HD21	1:D:560:ILE:CG2	2.22	0.53
1:D:628:HIS:HB2	1:D:631:PRO:HG3	1.89	0.53
1:F:463:PHE:CE2	1:P:555:LEU:HA	2.42	0.53
1:I:634:LEU:HB2	1:Q:477:ASN:HA	1.90	0.53
1:J:447:ARG:HB2	1:J:462:LEU:HB2	1.91	0.53
1:L:447:ARG:HB2	1:L:462:LEU:HB2	1.90	0.53
1:A:421:HIS:CD2	1:A:729:THR:HG21	2.43	0.53
1:B:294:ARG:NE	1:B:298:ARG:HE	2.03	0.53
1:C:540:ASN:HD21	1:C:560:ILE:CG2	2.22	0.53
1:D:447:ARG:HB2	1:D:462:LEU:HB2	1.91	0.53
1:E:421:HIS:CD2	1:E:729:THR:HG21	2.43	0.53
1:E:519:ASN:HD22	1:I:475:ALA:HA	1.72	0.53
1:F:404:ARG:H	1:F:407:ASN:ND2	2.05	0.53
1:G:506:ALA:HB1	1:G:538:HIS:HE1	1.74	0.53
1:G:540:ASN:HD21	1:G:560:ILE:CG2	2.22	0.53
1:M:540:ASN:HD21	1:M:560:ILE:CG2	2.22	0.53
1:N:421:HIS:CD2	1:N:729:THR:HG21	2.43	0.53
1:N:540:ASN:HD21	1:N:560:ILE:CG2	2.22	0.53
1:P:570:ASN:HD21	1:P:607:TRP:HB2	1.72	0.53
1:S:263:GLN:HB3	1:S:266:ALA:HB3	1.90	0.53
1:S:447:ARG:HB2	1:S:462:LEU:HB2	1.91	0.53
1:B:263:GLN:HB3	1:B:266:ALA:HB3	1.90	0.53
1:D:405:THR:HG21	1:Q:337:THR:CG2	2.39	0.53
1:E:270:ASN:ND2	1:I:472:SER:H	2.06	0.53
1:E:447:ARG:HB2	1:E:462:LEU:HB2	1.91	0.53
1:E:479:LEU:CD2	1:Q:634:LEU:HD11	2.33	0.53
1:E:506:ALA:HB1	1:E:538:HIS:HE1	1.74	0.53
1:H:263:GLN:HB3	1:H:266:ALA:HB3	1.90	0.53
1:H:421:HIS:CD2	1:H:729:THR:HG21	2.43	0.53
1:I:497:ASN:ND2	1:Q:590:ALA:HA	2.23	0.53
1:M:506:ALA:HB1	1:M:538:HIS:HE1	1.74	0.53
1:O:263:GLN:HB3	1:O:266:ALA:HB3	1.90	0.53
1:P:421:HIS:CD2	1:P:729:THR:HG21	2.43	0.53
1:S:506:ALA:HB1	1:S:538:HIS:HE1	1.74	0.53
1:A:634:LEU:HB2	1:D:477:ASN:HA	1.90	0.53
1:B:540:ASN:HD21	1:B:560:ILE:CG2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:263:GLN:HB3	1:J:266:ALA:HB3	1.90	0.53
1:K:447:ARG:HB2	1:K:462:LEU:HB2	1.90	0.53
1:L:446:ASN:HD22	1:L:446:ASN:N	2.00	0.53
1:L:506:ALA:HB1	1:L:538:HIS:HE1	1.74	0.53
1:L:540:ASN:HD21	1:L:560:ILE:CG2	2.22	0.53
1:N:294:ARG:NE	1:N:298:ARG:HE	2.03	0.53
1:O:421:HIS:CD2	1:O:729:THR:HG21	2.43	0.53
1:Q:506:ALA:HB1	1:Q:538:HIS:HE1	1.74	0.53
1:B:570:ASN:HD21	1:B:607:TRP:HB2	1.72	0.53
1:B:608:GLN:HA	1:H:626:ASP:HB2	1.89	0.53
1:C:263:GLN:HB3	1:C:266:ALA:HB3	1.90	0.53
1:E:263:GLN:HB3	1:E:266:ALA:HB3	1.90	0.53
1:F:483:CYS:HB2	1:F:524:MET:HE1	1.91	0.53
1:H:540:ASN:HD21	1:H:560:ILE:CG2	2.22	0.53
1:I:263:GLN:HB3	1:I:266:ALA:HB3	1.90	0.53
1:K:379:THR:HG22	1:K:380:LEU:N	2.22	0.53
1:L:263:GLN:HB3	1:L:266:ALA:HB3	1.91	0.53
1:M:421:HIS:CD2	1:M:729:THR:HG21	2.43	0.53
1:O:245:ARG:HE	1:O:366:PRO:HA	1.74	0.53
1:Q:294:ARG:NE	1:Q:298:ARG:HE	2.04	0.53
1:Q:447:ARG:HB2	1:Q:462:LEU:HB2	1.91	0.53
1:C:447:ARG:HB2	1:C:462:LEU:HB2	1.91	0.53
1:D:259:GLN:HE22	1:O:710:ASN:HD22	1.56	0.53
1:D:421:HIS:CD2	1:D:729:THR:HG21	2.43	0.53
1:E:358:HIS:CE1	1:I:435:ASN:HB3	2.44	0.53
1:E:446:ASN:HD22	1:E:446:ASN:N	1.99	0.53
1:G:263:GLN:HB3	1:G:266:ALA:HB3	1.90	0.53
1:G:447:ARG:HB2	1:G:462:LEU:HB2	1.91	0.53
1:I:404:ARG:H	1:I:407:ASN:ND2	2.05	0.53
1:I:447:ARG:HB2	1:I:462:LEU:HB2	1.91	0.53
1:J:634:LEU:HB2	1:O:477:ASN:HA	1.91	0.53
1:K:506:ALA:HB1	1:K:538:HIS:HE1	1.74	0.53
1:L:275:TYR:OH	1:P:714:THR:HG21	2.09	0.53
1:L:601:ALA:HA	1:L:605:MET:HE1	1.91	0.53
1:M:263:GLN:HB3	1:M:266:ALA:HB3	1.90	0.53
1:T:506:ALA:HB1	1:T:538:HIS:HE1	1.74	0.53
1:A:294:ARG:NE	1:A:298:ARG:HE	2.04	0.53
1:A:446:ASN:HD22	1:A:446:ASN:N	2.00	0.53
1:B:245:ARG:HE	1:B:366:PRO:HA	1.74	0.53
1:C:421:HIS:CD2	1:C:729:THR:HG21	2.43	0.53
1:C:506:ALA:HB1	1:C:538:HIS:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:475:ALA:HA	1:Q:519:ASN:HD22	1.73	0.53
1:F:263:GLN:HB3	1:F:266:ALA:HB3	1.90	0.53
1:Q:263:GLN:HB3	1:Q:266:ALA:HB3	1.90	0.53
1:S:421:HIS:CD2	1:S:729:THR:HG21	2.43	0.53
1:A:482:PRO:HD3	1:A:605:MET:HE3	1.91	0.53
1:C:603:PRO:HA	1:D:629:PHE:CD2	2.37	0.53
1:F:432:ARG:NH2	1:P:514:ARG:HD3	2.24	0.53
1:F:506:ALA:HB1	1:F:538:HIS:HE1	1.74	0.53
1:I:245:ARG:HE	1:I:366:PRO:HA	1.74	0.53
1:L:245:ARG:HE	1:L:366:PRO:HA	1.74	0.53
1:D:263:GLN:HB3	1:D:266:ALA:HB3	1.90	0.52
1:E:435:ASN:HB3	1:Q:358:HIS:CE1	2.45	0.52
1:G:482:PRO:HD3	1:G:605:MET:HE3	1.91	0.52
1:J:540:ASN:HD21	1:J:560:ILE:CG2	2.22	0.52
1:M:714:THR:HG21	1:N:275:TYR:OH	2.09	0.52
1:N:447:ARG:HB2	1:N:462:LEU:HB2	1.91	0.52
1:T:421:HIS:CD2	1:T:729:THR:HG21	2.43	0.52
1:T:540:ASN:HD21	1:T:560:ILE:CG2	2.22	0.52
1:B:436:PRO:HG3	1:H:378:LEU:CD2	2.39	0.52
1:C:448:THR:OG1	1:D:500:ASN:HA	2.09	0.52
1:F:540:ASN:HD21	1:F:560:ILE:CG2	2.22	0.52
1:G:294:ARG:NE	1:G:298:ARG:HE	2.04	0.52
1:G:421:HIS:CD2	1:G:729:THR:HG21	2.43	0.52
1:L:404:ARG:H	1:L:407:ASN:ND2	2.05	0.52
1:R:506:ALA:HB1	1:R:538:HIS:HE1	1.74	0.52
1:B:447:ARG:HB2	1:B:462:LEU:HB2	1.91	0.52
1:C:714:THR:HG21	1:J:275:TYR:OH	2.09	0.52
1:F:448:THR:HG23	1:P:502:PRO:HG3	1.92	0.52
1:K:325:GLN:HG3	1:K:330:THR:CG2	2.40	0.52
1:A:318:ILE:O	1:A:405:THR:HG23	2.10	0.52
1:E:501:PHE:N	1:E:502:PRO:CD	2.72	0.52
1:E:511:LEU:HD11	1:I:480:PRO:HG3	1.92	0.52
1:E:540:ASN:HD21	1:E:560:ILE:CG2	2.22	0.52
1:H:714:THR:HG22	1:H:715:VAL:N	2.25	0.52
1:I:318:ILE:O	1:I:405:THR:HG23	2.10	0.52
1:J:421:HIS:CD2	1:J:729:THR:HG21	2.43	0.52
1:P:447:ARG:HB2	1:P:462:LEU:HB2	1.91	0.52
1:Q:318:ILE:O	1:Q:405:THR:HG23	2.10	0.52
1:R:318:ILE:O	1:R:405:THR:HG23	2.10	0.52
1:S:318:ILE:O	1:S:405:THR:HG23	2.10	0.52
1:S:714:THR:HG22	1:S:715:VAL:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:263:GLN:HB3	1:T:266:ALA:HB3	1.90	0.52
1:T:294:ARG:NE	1:T:298:ARG:HE	2.04	0.52
1:A:263:GLN:HB3	1:A:266:ALA:HB3	1.90	0.52
1:A:379:THR:HG22	1:A:380:LEU:N	2.22	0.52
1:C:477:ASN:HA	1:D:634:LEU:HB2	1.91	0.52
1:C:483:CYS:HB2	1:C:524:MET:HE1	1.91	0.52
1:C:714:THR:HG22	1:C:715:VAL:N	2.25	0.52
1:F:447:ARG:HB2	1:F:462:LEU:HB2	1.91	0.52
1:G:325:GLN:HG3	1:G:330:THR:CG2	2.40	0.52
1:J:351:PRO:HB3	1:O:428:GLN:NE2	2.23	0.52
1:K:263:GLN:HB3	1:K:266:ALA:HB3	1.90	0.52
1:M:245:ARG:HE	1:M:366:PRO:HA	1.74	0.52
1:Q:540:ASN:HD21	1:Q:560:ILE:CG2	2.22	0.52
1:R:294:ARG:NE	1:R:298:ARG:HE	2.04	0.52
1:R:423:SER:HA	1:R:729:THR:HG23	1.92	0.52
1:R:540:ASN:HD21	1:R:560:ILE:CG2	2.22	0.52
1:S:501:PHE:N	1:S:502:PRO:CD	2.72	0.52
1:S:621:LYS:HB2	1:S:643:PRO:HG2	1.92	0.52
1:A:378:LEU:CD2	1:D:436:PRO:HG3	2.40	0.52
1:A:540:ASN:HD21	1:A:560:ILE:CG2	2.22	0.52
1:E:555:LEU:HD22	1:I:461:LEU:HD12	1.92	0.52
1:E:621:LYS:HB2	1:E:643:PRO:HG2	1.92	0.52
1:F:318:ILE:O	1:F:405:THR:HG23	2.10	0.52
1:H:318:ILE:O	1:H:405:THR:HG23	2.10	0.52
1:K:714:THR:HG22	1:K:715:VAL:N	2.25	0.52
1:L:423:SER:HA	1:L:729:THR:HG23	1.92	0.52
1:N:318:ILE:O	1:N:405:THR:HG23	2.10	0.52
1:O:506:ALA:HB1	1:O:538:HIS:HE1	1.74	0.52
1:O:540:ASN:HD21	1:O:560:ILE:CG2	2.22	0.52
1:O:714:THR:HG22	1:O:715:VAL:N	2.25	0.52
1:Q:621:LYS:HB2	1:Q:643:PRO:HG2	1.92	0.52
1:S:540:ASN:HD21	1:S:560:ILE:CG2	2.22	0.52
1:B:318:ILE:O	1:B:405:THR:HG23	2.10	0.52
1:D:318:ILE:O	1:D:405:THR:HG23	2.10	0.52
1:D:506:ALA:HB1	1:D:538:HIS:HE1	1.74	0.52
1:E:431:ASP:O	1:E:434:MET:HE3	2.09	0.52
1:G:245:ARG:HE	1:G:366:PRO:HA	1.74	0.52
1:I:501:PHE:N	1:I:502:PRO:CD	2.72	0.52
1:J:621:LYS:HB2	1:J:643:PRO:HG2	1.92	0.52
1:K:540:ASN:HD21	1:K:560:ILE:CG2	2.22	0.52
1:M:621:LYS:HB2	1:M:643:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:325:GLN:HG3	1:N:330:THR:CG2	2.40	0.52
1:Q:325:GLN:HG3	1:Q:330:THR:CG2	2.40	0.52
1:T:501:PHE:N	1:T:502:PRO:CD	2.72	0.52
1:A:506:ALA:HB1	1:A:538:HIS:HE1	1.74	0.52
1:A:555:LEU:HD22	1:D:461:LEU:HD12	1.92	0.52
1:E:714:THR:HG22	1:E:715:VAL:N	2.25	0.52
1:G:318:ILE:O	1:G:405:THR:HG23	2.10	0.52
1:G:431:ASP:O	1:G:434:MET:HE3	2.10	0.52
1:H:447:ARG:HB2	1:H:462:LEU:HB2	1.91	0.52
1:H:621:LYS:HB2	1:H:643:PRO:HG2	1.92	0.52
1:I:421:HIS:CD2	1:I:729:THR:HG21	2.43	0.52
1:I:634:LEU:HD11	1:Q:479:LEU:CD2	2.35	0.52
1:K:431:ASP:O	1:K:434:MET:HE3	2.10	0.52
1:A:418:VAL:HG21	1:A:638:PHE:HB3	1.92	0.52
1:B:506:ALA:HB1	1:B:538:HIS:HE1	1.74	0.52
1:D:423:SER:HA	1:D:729:THR:HG23	1.92	0.52
1:D:431:ASP:O	1:D:434:MET:HE3	2.10	0.52
1:G:418:VAL:HG21	1:G:638:PHE:HB3	1.92	0.52
1:I:431:ASP:O	1:I:434:MET:HE3	2.10	0.52
1:J:318:ILE:O	1:J:405:THR:HG23	2.10	0.52
1:J:423:SER:HA	1:J:729:THR:HG23	1.92	0.52
1:K:318:ILE:O	1:K:405:THR:HG23	2.10	0.52
1:R:245:ARG:HE	1:R:366:PRO:HA	1.74	0.52
1:S:245:ARG:HE	1:S:366:PRO:HA	1.74	0.52
1:T:325:GLN:HG3	1:T:330:THR:CG2	2.40	0.52
1:A:276:SER:OG	1:D:437:LEU:HD21	2.10	0.52
1:C:418:VAL:HG21	1:C:638:PHE:HB3	1.92	0.52
1:C:423:SER:HA	1:C:729:THR:HG23	1.92	0.52
1:C:431:ASP:O	1:C:434:MET:HE3	2.10	0.52
1:D:621:LYS:HB2	1:D:643:PRO:HG2	1.92	0.52
1:E:259:GLN:HE22	1:F:710:ASN:ND2	2.08	0.52
1:F:621:LYS:HB2	1:F:643:PRO:HG2	1.92	0.52
1:G:423:SER:HA	1:G:729:THR:HG23	1.92	0.52
1:J:502:PRO:HG3	1:O:448:THR:HG23	1.91	0.52
1:O:501:PHE:N	1:O:502:PRO:CD	2.72	0.52
1:P:506:ALA:HB1	1:P:538:HIS:HE1	1.74	0.52
1:R:325:GLN:HG3	1:R:330:THR:CG2	2.40	0.52
1:S:694:ARG:CZ	1:S:698:GLU:HG2	2.40	0.52
1:T:318:ILE:O	1:T:405:THR:HG23	2.10	0.52
1:A:634:LEU:HD11	1:D:479:LEU:CD2	2.36	0.51
1:D:482:PRO:HD3	1:D:605:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:590:ALA:HA	1:Q:497:ASN:ND2	2.25	0.51
1:F:325:GLN:HG3	1:F:330:THR:CG2	2.40	0.51
1:F:472:SER:HB3	1:P:269:ASP:O	2.09	0.51
1:G:621:LYS:HB2	1:G:643:PRO:HG2	1.92	0.51
1:I:396:GLU:HG3	1:R:367:ALA:HB2	1.92	0.51
1:J:431:ASP:O	1:J:434:MET:HE3	2.10	0.51
1:L:431:ASP:O	1:L:434:MET:HE3	2.11	0.51
1:M:418:VAL:HG21	1:M:638:PHE:HB3	1.92	0.51
1:N:714:THR:HG22	1:N:715:VAL:N	2.25	0.51
1:P:418:VAL:HG21	1:P:638:PHE:HB3	1.92	0.51
1:P:540:ASN:HD21	1:P:560:ILE:CG2	2.22	0.51
1:Q:482:PRO:HD3	1:Q:605:MET:HE3	1.92	0.51
1:Q:714:THR:HG22	1:Q:715:VAL:N	2.25	0.51
1:R:714:THR:HG22	1:R:715:VAL:N	2.25	0.51
1:A:501:PHE:N	1:A:502:PRO:CD	2.72	0.51
1:B:423:SER:HA	1:B:729:THR:HG23	1.92	0.51
1:B:694:ARG:CZ	1:B:698:GLU:HG2	2.41	0.51
1:C:621:LYS:HB2	1:C:643:PRO:HG2	1.92	0.51
1:D:275:TYR:OH	1:O:714:THR:HG21	2.10	0.51
1:I:540:ASN:HD21	1:I:560:ILE:CG2	2.22	0.51
1:L:325:GLN:HG3	1:L:330:THR:CG2	2.40	0.51
1:L:714:THR:HG22	1:L:715:VAL:N	2.25	0.51
1:M:325:GLN:HG3	1:M:330:THR:CG2	2.40	0.51
1:M:431:ASP:O	1:M:434:MET:HE3	2.10	0.51
1:N:245:ARG:HE	1:N:366:PRO:HA	1.74	0.51
1:N:418:VAL:HG21	1:N:638:PHE:HB3	1.93	0.51
1:T:482:PRO:HD3	1:T:605:MET:HE3	1.92	0.51
1:A:436:PRO:HG3	1:C:378:LEU:CG	2.40	0.51
1:C:436:PRO:HG3	1:D:378:LEU:CG	2.40	0.51
1:E:694:ARG:CZ	1:E:698:GLU:HG2	2.40	0.51
1:F:714:THR:HG22	1:F:715:VAL:N	2.25	0.51
1:J:506:ALA:HB1	1:J:538:HIS:HE1	1.74	0.51
1:K:657:ASN:ND2	1:Q:323:VAL:HG11	2.25	0.51
1:L:694:ARG:CZ	1:L:698:GLU:HG2	2.41	0.51
1:O:423:SER:HA	1:O:729:THR:HG23	1.92	0.51
1:O:694:ARG:CZ	1:O:698:GLU:HG2	2.41	0.51
1:Q:418:VAL:HG21	1:Q:638:PHE:HB3	1.92	0.51
1:R:418:VAL:HG21	1:R:638:PHE:HB3	1.92	0.51
1:S:325:GLN:HG3	1:S:330:THR:CG2	2.40	0.51
1:T:694:ARG:CZ	1:T:698:GLU:HG2	2.41	0.51
1:C:325:GLN:HG3	1:C:330:THR:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:714:THR:HG22	1:D:715:VAL:N	2.25	0.51
1:G:601:ALA:HA	1:G:605:MET:HE1	1.93	0.51
1:H:325:GLN:HG3	1:H:330:THR:CG2	2.40	0.51
1:H:423:SER:HA	1:H:729:THR:HG23	1.92	0.51
1:H:431:ASP:O	1:H:434:MET:HE3	2.10	0.51
1:H:506:ALA:HB1	1:H:538:HIS:HE1	1.74	0.51
1:I:621:LYS:HB2	1:I:643:PRO:HG2	1.92	0.51
1:M:447:ARG:HB2	1:M:462:LEU:HB2	1.91	0.51
1:N:694:ARG:CZ	1:N:698:GLU:HG2	2.41	0.51
1:P:694:ARG:CZ	1:P:698:GLU:HG2	2.41	0.51
1:R:447:ARG:HB2	1:R:462:LEU:HB2	1.91	0.51
1:T:423:SER:HA	1:T:729:THR:HG23	1.92	0.51
1:T:446:ASN:HD22	1:T:446:ASN:N	2.00	0.51
1:C:694:ARG:CZ	1:C:698:GLU:HG2	2.41	0.51
1:E:634:LEU:HB2	1:I:477:ASN:HA	1.90	0.51
1:I:418:VAL:HG21	1:I:638:PHE:HB3	1.92	0.51
1:I:506:ALA:HB1	1:I:538:HIS:HE1	1.74	0.51
1:M:423:SER:HA	1:M:729:THR:HG23	1.92	0.51
1:Q:423:SER:HA	1:Q:729:THR:HG23	1.92	0.51
1:R:431:ASP:O	1:R:434:MET:HE3	2.10	0.51
1:R:601:ALA:HA	1:R:605:MET:HE1	1.91	0.51
1:S:294:ARG:NE	1:S:298:ARG:HE	2.04	0.51
1:T:714:THR:HG22	1:T:715:VAL:N	2.25	0.51
1:B:714:THR:HG22	1:B:715:VAL:N	2.25	0.51
1:D:304:TRP:HA	1:D:304:TRP:HE3	1.76	0.51
1:E:436:PRO:HG3	1:Q:378:LEU:CD2	2.41	0.51
1:H:508:LYS:HA	1:H:518:VAL:HG23	1.93	0.51
1:I:325:GLN:HG3	1:I:330:THR:CG2	2.40	0.51
1:I:423:SER:HA	1:I:729:THR:HG23	1.92	0.51
1:J:694:ARG:CZ	1:J:698:GLU:HG2	2.41	0.51
1:M:405:THR:HG21	1:N:337:THR:HG22	1.92	0.51
1:O:431:ASP:O	1:O:434:MET:HE3	2.10	0.51
1:P:325:GLN:HG3	1:P:330:THR:CG2	2.40	0.51
1:R:621:LYS:HB2	1:R:643:PRO:HG2	1.92	0.51
1:B:501:PHE:N	1:B:502:PRO:CD	2.72	0.51
1:D:325:GLN:HG3	1:D:330:THR:CG2	2.40	0.51
1:F:694:ARG:CZ	1:F:698:GLU:HG2	2.40	0.51
1:G:508:LYS:HA	1:G:518:VAL:HG23	1.93	0.51
1:I:714:THR:HG22	1:I:715:VAL:N	2.25	0.51
1:K:304:TRP:HA	1:K:304:TRP:HE3	1.76	0.51
1:L:418:VAL:HG21	1:L:638:PHE:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:245:ARG:HE	1:P:366:PRO:HA	1.74	0.51
1:R:694:ARG:CZ	1:R:698:GLU:HG2	2.41	0.51
1:A:423:SER:HA	1:A:729:THR:HG23	1.92	0.51
1:G:694:ARG:CZ	1:G:698:GLU:HG2	2.41	0.51
1:I:259:GLN:HE22	1:R:710:ASN:ND2	2.09	0.51
1:K:245:ARG:HE	1:K:366:PRO:HA	1.74	0.51
1:K:351:PRO:HB3	1:R:428:GLN:NE2	2.25	0.51
1:K:710:ASN:ND2	1:S:259:GLN:HE22	2.09	0.51
1:L:318:ILE:O	1:L:405:THR:HG23	2.10	0.51
1:L:501:PHE:N	1:L:502:PRO:CD	2.72	0.51
1:M:508:LYS:HA	1:M:518:VAL:HG23	1.93	0.51
1:O:318:ILE:O	1:O:405:THR:HG23	2.10	0.51
1:P:304:TRP:HA	1:P:304:TRP:HE3	1.76	0.51
1:R:304:TRP:HA	1:R:304:TRP:HE3	1.76	0.51
1:R:501:PHE:N	1:R:502:PRO:CD	2.72	0.51
1:T:304:TRP:HA	1:T:304:TRP:HE3	1.76	0.51
1:A:714:THR:HG22	1:A:715:VAL:N	2.25	0.51
1:C:245:ARG:HE	1:C:366:PRO:HA	1.74	0.51
1:C:435:ASN:HB3	1:D:358:HIS:CE1	2.45	0.51
1:E:318:ILE:O	1:E:405:THR:HG23	2.10	0.51
1:E:378:LEU:CD2	1:I:436:PRO:HG3	2.41	0.51
1:F:508:LYS:HA	1:F:518:VAL:HG23	1.93	0.51
1:G:337:THR:HG22	1:H:405:THR:HG21	1.92	0.51
1:H:245:ARG:HE	1:H:366:PRO:HA	1.74	0.51
1:M:714:THR:HG22	1:M:715:VAL:N	2.25	0.51
1:Q:694:ARG:CZ	1:Q:698:GLU:HG2	2.41	0.51
1:A:694:ARG:CZ	1:A:698:GLU:HG2	2.41	0.51
1:F:245:ARG:HE	1:F:366:PRO:HA	1.74	0.51
1:F:304:TRP:HA	1:F:304:TRP:HE3	1.76	0.51
1:F:418:VAL:HG21	1:F:638:PHE:HB3	1.93	0.51
1:F:630:HIS:CE1	2:F:999:D5M:H8	2.46	0.51
1:J:418:VAL:HG21	1:J:638:PHE:HB3	1.92	0.51
1:J:714:THR:HG22	1:J:715:VAL:N	2.25	0.51
1:K:276:SER:OG	1:R:437:LEU:HD21	2.10	0.51
1:L:621:LYS:HB2	1:L:643:PRO:HG2	1.92	0.51
1:L:710:ASN:ND2	1:T:259:GLN:HE22	2.08	0.51
1:O:325:GLN:HG3	1:O:330:THR:CG2	2.40	0.51
1:Q:501:PHE:N	1:Q:502:PRO:CD	2.72	0.51
1:S:508:LYS:HA	1:S:518:VAL:HG23	1.93	0.51
1:A:325:GLN:HG3	1:A:330:THR:CG2	2.40	0.50
1:A:441:TYR:HA	1:C:359:GLN:HE21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:LYS:HA	1:A:518:VAL:HG23	1.93	0.50
1:A:621:LYS:HB2	1:A:643:PRO:HG2	1.92	0.50
1:A:630:HIS:CE1	2:A:999:D5M:H8	2.46	0.50
1:B:431:ASP:O	1:B:434:MET:HE3	2.10	0.50
1:B:443:TYR:CE2	1:H:544:GLY:HA3	2.46	0.50
1:D:418:VAL:HG21	1:D:638:PHE:HB3	1.92	0.50
1:D:694:ARG:CZ	1:D:698:GLU:HG2	2.40	0.50
1:E:276:SER:OG	1:I:437:LEU:HD21	2.12	0.50
1:E:294:ARG:NE	1:E:298:ARG:HE	2.04	0.50
1:G:714:THR:HG22	1:G:715:VAL:N	2.25	0.50
1:K:630:HIS:CE1	2:K:999:D5M:H8	2.47	0.50
1:M:318:ILE:O	1:M:405:THR:HG23	2.10	0.50
1:N:508:LYS:HA	1:N:518:VAL:HG23	1.93	0.50
1:N:621:LYS:HB2	1:N:643:PRO:HG2	1.92	0.50
1:P:318:ILE:O	1:P:405:THR:HG23	2.10	0.50
1:P:508:LYS:HA	1:P:518:VAL:HG23	1.93	0.50
1:S:423:SER:HA	1:S:729:THR:HG23	1.92	0.50
1:A:405:THR:HG21	1:H:337:THR:HG22	1.93	0.50
1:C:480:PRO:HG3	1:D:511:LEU:HD11	1.93	0.50
1:C:580:VAL:HG22	1:D:484:TYR:CZ	2.47	0.50
1:E:304:TRP:HA	1:E:304:TRP:HE3	1.76	0.50
1:E:325:GLN:HG3	1:E:330:THR:CG2	2.40	0.50
1:I:694:ARG:CZ	1:I:698:GLU:HG2	2.41	0.50
1:J:501:PHE:N	1:J:502:PRO:CD	2.72	0.50
1:M:304:TRP:HA	1:M:304:TRP:HE3	1.76	0.50
1:M:694:ARG:CZ	1:M:698:GLU:HG2	2.41	0.50
1:P:621:LYS:HB2	1:P:643:PRO:HG2	1.92	0.50
1:Q:304:TRP:HA	1:Q:304:TRP:HE3	1.76	0.50
1:T:418:VAL:HG21	1:T:638:PHE:HB3	1.92	0.50
1:A:479:LEU:CD2	1:C:634:LEU:HD11	2.38	0.50
1:D:501:PHE:N	1:D:502:PRO:CD	2.72	0.50
1:H:418:VAL:HG21	1:H:638:PHE:HB3	1.92	0.50
1:K:621:LYS:HB2	1:K:643:PRO:HG2	1.92	0.50
1:M:501:PHE:N	1:M:502:PRO:CD	2.72	0.50
1:O:275:TYR:OH	1:S:714:THR:HG21	2.11	0.50
1:O:304:TRP:HA	1:O:304:TRP:HE3	1.76	0.50
1:O:621:LYS:HB2	1:O:643:PRO:HG2	1.92	0.50
1:P:630:HIS:CE1	2:P:999:D5M:H8	2.46	0.50
1:Q:508:LYS:HA	1:Q:518:VAL:HG23	1.93	0.50
1:A:247:TRP:HB3	1:A:370:PHE:CZ	2.47	0.50
1:A:304:TRP:HA	1:A:304:TRP:HE3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ALA:HA	1:A:605:MET:HE1	1.93	0.50
1:C:318:ILE:O	1:C:405:THR:HG23	2.10	0.50
1:E:423:SER:HA	1:E:729:THR:HG23	1.92	0.50
1:G:304:TRP:HA	1:G:304:TRP:HE3	1.76	0.50
1:H:694:ARG:CZ	1:H:698:GLU:HG2	2.41	0.50
1:I:511:LEU:HD11	1:Q:480:PRO:HG3	1.92	0.50
1:J:325:GLN:HG3	1:J:330:THR:CG2	2.40	0.50
1:K:378:LEU:CG	1:R:436:PRO:HG3	2.38	0.50
1:K:423:SER:HA	1:K:729:THR:HG23	1.92	0.50
1:K:694:ARG:CZ	1:K:698:GLU:HG2	2.41	0.50
1:L:304:TRP:HA	1:L:304:TRP:HE3	1.76	0.50
1:S:304:TRP:HA	1:S:304:TRP:HE3	1.76	0.50
1:S:418:VAL:HG21	1:S:638:PHE:HB3	1.92	0.50
1:B:621:LYS:HB2	1:B:643:PRO:HG2	1.92	0.50
1:B:630:HIS:CE1	2:B:999:D5M:H8	2.46	0.50
1:C:501:PHE:N	1:C:502:PRO:CD	2.72	0.50
1:I:630:HIS:CE1	2:I:999:D5M:H8	2.47	0.50
1:J:405:THR:HG21	1:M:337:THR:HG22	1.94	0.50
1:C:441:TYR:HA	1:D:359:GLN:HE21	1.76	0.50
1:F:435:ASN:HB3	1:P:358:HIS:CE1	2.46	0.50
1:K:247:TRP:HB3	1:K:370:PHE:CZ	2.47	0.50
1:L:247:TRP:HB3	1:L:370:PHE:CZ	2.47	0.50
1:N:423:SER:HA	1:N:729:THR:HG23	1.92	0.50
1:N:501:PHE:N	1:N:502:PRO:CD	2.72	0.50
1:O:418:VAL:HG21	1:O:638:PHE:HB3	1.92	0.50
1:P:714:THR:HG22	1:P:715:VAL:N	2.25	0.50
1:C:630:HIS:CE1	2:C:999:D5M:H8	2.47	0.50
1:E:245:ARG:HE	1:E:366:PRO:HA	1.74	0.50
1:F:423:SER:HA	1:F:729:THR:HG23	1.92	0.50
1:G:630:HIS:CE1	2:G:999:D5M:H8	2.46	0.50
1:J:247:TRP:HB3	1:J:370:PHE:CZ	2.47	0.50
1:J:508:LYS:HA	1:J:518:VAL:HG23	1.93	0.50
1:L:426:HIS:HA	1:L:734:ARG:O	2.12	0.50
1:M:630:HIS:CE1	2:M:999:D5M:H8	2.46	0.50
1:O:630:HIS:CE1	2:O:999:D5M:H8	2.46	0.50
1:Q:235:LEU:C	1:Q:237:ASP:H	2.15	0.50
1:R:630:HIS:CE1	2:R:999:D5M:H8	2.47	0.50
1:T:247:TRP:HB3	1:T:370:PHE:CZ	2.47	0.50
1:A:245:ARG:HE	1:A:366:PRO:HA	1.74	0.50
1:B:235:LEU:C	1:B:237:ASP:H	2.15	0.50
1:B:482:PRO:HD3	1:B:605:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LEU:C	1:C:237:ASP:H	2.15	0.50
1:E:630:HIS:CE1	2:E:999:D5M:H8	2.47	0.50
1:L:630:HIS:CE1	2:L:999:D5M:H8	2.46	0.50
1:N:630:HIS:CE1	2:N:999:D5M:H8	2.46	0.50
1:Q:630:HIS:CE1	2:Q:999:D5M:H8	2.47	0.50
1:R:508:LYS:HA	1:R:518:VAL:HG23	1.93	0.50
1:S:235:LEU:C	1:S:237:ASP:H	2.16	0.50
1:S:630:HIS:CE1	2:S:999:D5M:H8	2.46	0.50
1:T:630:HIS:CE1	2:T:999:D5M:H8	2.47	0.50
1:C:304:TRP:HA	1:C:304:TRP:HE3	1.76	0.50
1:C:367:ALA:HB2	1:J:396:GLU:HG3	1.94	0.50
1:E:426:HIS:HA	1:E:734:ARG:O	2.12	0.50
1:E:477:ASN:HA	1:Q:634:LEU:HB2	1.94	0.50
1:F:235:LEU:C	1:F:237:ASP:H	2.16	0.50
1:F:426:HIS:HA	1:F:734:ARG:O	2.12	0.50
1:F:477:ASN:HA	1:P:634:LEU:HB2	1.94	0.50
1:J:235:LEU:C	1:J:237:ASP:H	2.15	0.50
1:N:235:LEU:C	1:N:237:ASP:H	2.15	0.50
1:Q:245:ARG:HE	1:Q:366:PRO:HA	1.74	0.50
1:S:247:TRP:HB3	1:S:370:PHE:CZ	2.47	0.50
1:S:426:HIS:HA	1:S:734:ARG:O	2.12	0.50
1:T:508:LYS:HA	1:T:518:VAL:HG23	1.93	0.50
1:A:235:LEU:C	1:A:237:ASP:H	2.16	0.49
1:B:418:VAL:HG21	1:B:638:PHE:HB3	1.92	0.49
1:B:463:PHE:HE2	1:H:555:LEU:HA	1.76	0.49
1:C:508:LYS:HA	1:C:518:VAL:HG23	1.93	0.49
1:C:710:ASN:ND2	1:J:259:GLN:HE22	2.10	0.49
1:F:247:TRP:HB3	1:F:370:PHE:CZ	2.47	0.49
1:G:247:TRP:HB3	1:G:370:PHE:CZ	2.47	0.49
1:I:508:LYS:HA	1:I:518:VAL:HG23	1.93	0.49
1:J:245:ARG:HE	1:J:366:PRO:HA	1.74	0.49
1:J:426:HIS:HA	1:J:734:ARG:O	2.12	0.49
1:J:630:HIS:CE1	2:J:999:D5M:H8	2.46	0.49
1:K:508:LYS:HA	1:K:518:VAL:HG23	1.93	0.49
1:S:431:ASP:O	1:S:434:MET:HE3	2.11	0.49
1:T:621:LYS:HB2	1:T:643:PRO:HG2	1.92	0.49
1:A:478:TRP:N	1:C:634:LEU:HD12	2.27	0.49
1:B:247:TRP:HB3	1:B:370:PHE:CZ	2.47	0.49
1:B:259:GLN:HE22	1:N:710:ASN:ND2	2.09	0.49
1:J:304:TRP:HA	1:J:304:TRP:HE3	1.76	0.49
1:N:426:HIS:HA	1:N:734:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:247:TRP:HB3	1:O:370:PHE:CZ	2.47	0.49
1:P:294:ARG:NE	1:P:298:ARG:HE	2.03	0.49
1:Q:247:TRP:HB3	1:Q:370:PHE:CZ	2.47	0.49
1:C:247:TRP:HB3	1:C:370:PHE:CZ	2.47	0.49
1:H:630:HIS:CE1	2:H:999:D5M:H8	2.47	0.49
1:K:418:VAL:HG21	1:K:638:PHE:HB3	1.92	0.49
1:K:714:THR:HG21	1:S:275:TYR:OH	2.12	0.49
1:M:247:TRP:HB3	1:M:370:PHE:CZ	2.47	0.49
1:N:304:TRP:HA	1:N:304:TRP:HE3	1.76	0.49
1:P:423:SER:HA	1:P:729:THR:HG23	1.92	0.49
1:Q:426:HIS:HA	1:Q:734:ARG:O	2.12	0.49
1:Q:601:ALA:HA	1:Q:605:MET:HE1	1.94	0.49
1:A:436:PRO:HG3	1:C:378:LEU:CD2	2.43	0.49
1:B:337:THR:HG22	1:N:405:THR:HG21	1.95	0.49
1:B:508:LYS:HA	1:B:518:VAL:HG23	1.93	0.49
1:D:247:TRP:HB3	1:D:370:PHE:CZ	2.47	0.49
1:D:630:HIS:CE1	2:D:999:D5M:H8	2.47	0.49
1:E:418:VAL:HG21	1:E:638:PHE:HB3	1.92	0.49
1:E:555:LEU:HA	1:I:463:PHE:HE2	1.77	0.49
1:K:572:VAL:HB	1:K:575:GLU:HB2	1.95	0.49
1:L:572:VAL:HB	1:L:575:GLU:HB2	1.95	0.49
1:M:235:LEU:C	1:M:237:ASP:H	2.15	0.49
1:O:426:HIS:HA	1:O:734:ARG:O	2.12	0.49
1:O:508:LYS:HA	1:O:518:VAL:HG23	1.93	0.49
1:P:239:VAL:HG13	1:P:685:TRP:HB2	1.95	0.49
1:P:431:ASP:O	1:P:434:MET:HE3	2.10	0.49
1:A:572:VAL:HB	1:A:575:GLU:HB2	1.95	0.49
1:A:710:ASN:ND2	1:H:259:GLN:HE22	2.09	0.49
1:D:508:LYS:HA	1:D:518:VAL:HG23	1.93	0.49
1:D:710:ASN:ND2	1:Q:259:GLN:HE22	2.11	0.49
1:E:378:LEU:CG	1:I:436:PRO:HG3	2.43	0.49
1:G:239:VAL:HG13	1:G:685:TRP:HB2	1.95	0.49
1:K:235:LEU:C	1:K:237:ASP:H	2.15	0.49
1:K:404:ARG:NH2	1:Q:405:THR:HG22	2.28	0.49
1:K:426:HIS:HA	1:K:734:ARG:O	2.12	0.49
1:K:501:PHE:N	1:K:502:PRO:CD	2.72	0.49
1:L:508:LYS:HA	1:L:518:VAL:HG23	1.93	0.49
1:O:235:LEU:C	1:O:237:ASP:H	2.15	0.49
1:R:239:VAL:HG13	1:R:685:TRP:HB2	1.95	0.49
1:B:426:HIS:HA	1:B:734:ARG:O	2.13	0.49
1:B:461:LEU:HD12	1:H:555:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:VAL:HB	1:C:575:GLU:HB2	1.95	0.49
1:D:426:HIS:HA	1:D:734:ARG:O	2.12	0.49
1:E:508:LYS:HA	1:E:518:VAL:HG23	1.93	0.49
1:E:544:GLY:HA3	1:I:443:TYR:CE2	2.47	0.49
1:G:235:LEU:C	1:G:237:ASP:H	2.15	0.49
1:K:239:VAL:HG13	1:K:685:TRP:HB2	1.95	0.49
1:P:235:LEU:C	1:P:237:ASP:H	2.16	0.49
1:P:247:TRP:HB3	1:P:370:PHE:CZ	2.47	0.49
1:P:501:PHE:N	1:P:502:PRO:CD	2.72	0.49
1:R:572:VAL:HB	1:R:575:GLU:HB2	1.95	0.49
1:A:448:THR:HG23	1:C:502:PRO:HG3	1.95	0.49
1:B:325:GLN:HG3	1:B:330:THR:CG2	2.40	0.49
1:B:437:LEU:HD21	1:H:276:SER:OG	2.12	0.49
1:B:475:ALA:CB	1:H:519:ASN:HD22	2.25	0.49
1:B:480:PRO:HG3	1:H:511:LEU:HD11	1.95	0.49
1:B:572:VAL:HB	1:B:575:GLU:HB2	1.95	0.49
1:F:428:GLN:NE2	1:P:351:PRO:HB3	2.28	0.49
1:H:294:ARG:NE	1:H:298:ARG:HE	2.04	0.49
1:I:247:TRP:HB3	1:I:370:PHE:CZ	2.47	0.49
1:I:544:GLY:HA3	1:Q:443:TYR:CE2	2.48	0.49
1:J:710:ASN:ND2	1:M:259:GLN:HE22	2.10	0.49
1:K:555:LEU:HD22	1:R:461:LEU:HD12	1.95	0.49
1:N:247:TRP:HB3	1:N:370:PHE:CZ	2.47	0.49
1:O:572:VAL:HB	1:O:575:GLU:HB2	1.95	0.49
1:T:572:VAL:HB	1:T:575:GLU:HB2	1.95	0.49
1:A:544:GLY:HA3	1:D:443:TYR:CE2	2.47	0.49
1:E:693:LYS:HG3	1:Q:398:PHE:CZ	2.48	0.49
1:G:426:HIS:HA	1:G:734:ARG:O	2.12	0.49
1:H:235:LEU:C	1:H:237:ASP:H	2.15	0.49
1:H:247:TRP:HB3	1:H:370:PHE:CZ	2.47	0.49
1:M:426:HIS:HA	1:M:734:ARG:O	2.12	0.49
1:E:235:LEU:C	1:E:237:ASP:H	2.15	0.49
1:F:436:PRO:HG3	1:P:378:LEU:CD2	2.43	0.49
1:F:446:ASN:O	1:P:502:PRO:HG2	2.12	0.49
1:F:608:GLN:HA	1:P:626:ASP:HB2	1.93	0.49
1:F:699:ILE:HD11	1:P:389:ARG:NE	2.25	0.49
1:H:304:TRP:HA	1:H:304:TRP:HE3	1.76	0.49
1:B:436:PRO:HG3	1:H:378:LEU:CG	2.43	0.49
1:D:601:ALA:HA	1:D:605:MET:HE1	1.94	0.49
1:E:247:TRP:HB3	1:E:370:PHE:CZ	2.47	0.49
1:E:519:ASN:HB3	1:E:520:PRO:CD	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:441:TYR:CD2	1:P:286:ARG:NH2	2.81	0.49
1:I:572:VAL:HB	1:I:575:GLU:HB2	1.95	0.49
1:L:714:THR:HG21	1:T:275:TYR:OH	2.12	0.49
1:N:239:VAL:HG13	1:N:685:TRP:HB2	1.95	0.49
1:Q:239:VAL:HG13	1:Q:685:TRP:HB2	1.95	0.49
1:R:235:LEU:C	1:R:237:ASP:H	2.15	0.49
1:R:247:TRP:HB3	1:R:370:PHE:CZ	2.47	0.49
1:A:511:LEU:HD11	1:D:480:PRO:HG3	1.95	0.48
1:E:572:VAL:HB	1:E:575:GLU:HB2	1.95	0.48
1:J:572:VAL:HB	1:J:575:GLU:HB2	1.95	0.48
1:T:601:ALA:HA	1:T:605:MET:HE1	1.94	0.48
1:A:426:HIS:HA	1:A:734:ARG:O	2.12	0.48
1:A:475:ALA:CB	1:C:519:ASN:HD22	2.26	0.48
1:A:699:ILE:HD11	1:C:389:ARG:NE	2.28	0.48
1:H:239:VAL:HG13	1:H:685:TRP:HB2	1.95	0.48
1:I:239:VAL:HG13	1:I:685:TRP:HB2	1.95	0.48
1:I:426:HIS:HA	1:I:734:ARG:O	2.13	0.48
1:L:483:CYS:HB2	1:L:524:MET:HE1	1.95	0.48
1:M:572:VAL:HB	1:M:575:GLU:HB2	1.95	0.48
1:T:245:ARG:HE	1:T:366:PRO:HA	1.74	0.48
1:A:239:VAL:HG13	1:A:685:TRP:HB2	1.95	0.48
1:C:426:HIS:HA	1:C:734:ARG:O	2.12	0.48
1:D:572:VAL:HB	1:D:575:GLU:HB2	1.95	0.48
1:H:572:VAL:HB	1:H:575:GLU:HB2	1.95	0.48
1:I:235:LEU:C	1:I:237:ASP:H	2.15	0.48
1:I:304:TRP:HA	1:I:304:TRP:HE3	1.76	0.48
1:J:269:ASP:O	1:O:472:SER:HB3	2.12	0.48
1:J:270:ASN:ND2	1:O:472:SER:H	2.11	0.48
1:L:235:LEU:C	1:L:237:ASP:H	2.15	0.48
1:R:275:TYR:OH	1:T:714:THR:HG21	2.12	0.48
1:T:235:LEU:C	1:T:237:ASP:H	2.15	0.48
1:A:431:ASP:O	1:A:434:MET:HE3	2.13	0.48
1:C:405:THR:HG21	1:J:337:THR:HG22	1.95	0.48
1:F:501:PHE:N	1:F:502:PRO:CD	2.72	0.48
1:F:584:LEU:HD13	1:P:488:ARG:CZ	2.44	0.48
1:G:501:PHE:N	1:G:502:PRO:CD	2.72	0.48
1:L:239:VAL:HG13	1:L:685:TRP:HB2	1.95	0.48
1:M:239:VAL:HG13	1:M:685:TRP:HB2	1.95	0.48
1:P:426:HIS:HA	1:P:734:ARG:O	2.12	0.48
1:A:519:ASN:HD22	1:D:475:ALA:CB	2.27	0.48
1:D:235:LEU:C	1:D:237:ASP:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:SER:OG	1:Q:437:LEU:HD21	2.13	0.48
1:O:482:PRO:HD3	1:O:605:MET:HE3	1.95	0.48
1:Q:572:VAL:HB	1:Q:575:GLU:HB2	1.95	0.48
1:R:426:HIS:HA	1:R:734:ARG:O	2.13	0.48
1:A:275:TYR:OH	1:E:714:THR:HG21	2.13	0.48
1:B:601:ALA:HA	1:B:605:MET:HE1	1.96	0.48
1:C:239:VAL:HG13	1:C:685:TRP:HB2	1.95	0.48
1:D:245:ARG:HE	1:D:366:PRO:HA	1.74	0.48
1:E:634:LEU:HD11	1:I:479:LEU:CD2	2.36	0.48
1:H:426:HIS:HA	1:H:734:ARG:O	2.12	0.48
1:P:572:VAL:HB	1:P:575:GLU:HB2	1.95	0.48
1:C:463:PHE:HE2	1:D:555:LEU:HA	1.79	0.48
1:I:378:LEU:CD2	1:Q:436:PRO:HG3	2.44	0.48
1:K:382:ASN:CG	1:Q:707:LYS:HD3	2.34	0.48
1:K:634:LEU:HD11	1:R:479:LEU:CD2	2.37	0.48
1:P:252:TYR:CE2	1:P:374:GLN:HB2	2.49	0.48
1:T:239:VAL:HG13	1:T:685:TRP:HB2	1.95	0.48
1:B:252:TYR:CE2	1:B:374:GLN:HB2	2.49	0.48
1:D:239:VAL:HG13	1:D:685:TRP:HB2	1.95	0.48
1:F:437:LEU:HD23	1:P:374:GLN:NE2	2.29	0.48
1:G:259:GLN:HE22	1:H:710:ASN:ND2	2.12	0.48
1:I:252:TYR:CE2	1:I:374:GLN:HB2	2.49	0.48
1:I:555:LEU:HD22	1:Q:461:LEU:HD12	1.96	0.48
1:N:572:VAL:HB	1:N:575:GLU:HB2	1.95	0.48
1:A:458:GLN:HG2	1:A:459:SER:N	2.29	0.48
1:F:239:VAL:HG13	1:F:685:TRP:HB2	1.95	0.48
1:G:572:VAL:HB	1:G:575:GLU:HB2	1.95	0.48
1:H:252:TYR:CE2	1:H:374:GLN:HB2	2.49	0.48
1:H:458:GLN:HG2	1:H:459:SER:N	2.29	0.48
1:I:405:THR:HG22	1:P:404:ARG:NH2	2.29	0.48
1:J:252:TYR:CE2	1:J:374:GLN:HB2	2.49	0.48
1:K:458:GLN:HG2	1:K:459:SER:N	2.29	0.48
1:O:337:THR:HG22	1:S:405:THR:HG21	1.96	0.48
1:T:426:HIS:HA	1:T:734:ARG:O	2.12	0.48
1:B:239:VAL:HG13	1:B:685:TRP:HB2	1.95	0.48
1:C:472:SER:HB3	1:D:269:ASP:O	2.13	0.48
1:D:294:ARG:NE	1:D:298:ARG:HE	2.04	0.48
1:E:458:GLN:HG2	1:E:459:SER:N	2.29	0.48
1:I:323:VAL:HG11	1:P:657:ASN:ND2	2.29	0.48
1:L:252:TYR:CE2	1:L:374:GLN:HB2	2.49	0.48
1:S:239:VAL:HG13	1:S:685:TRP:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TYR:CE2	1:A:374:GLN:HB2	2.49	0.47
1:F:252:TYR:CE2	1:F:374:GLN:HB2	2.49	0.47
1:G:458:GLN:HG2	1:G:459:SER:N	2.29	0.47
1:H:501:PHE:N	1:H:502:PRO:CD	2.72	0.47
1:K:294:ARG:NE	1:K:298:ARG:HE	2.04	0.47
1:M:252:TYR:CE2	1:M:374:GLN:HB2	2.49	0.47
1:C:252:TYR:CE2	1:C:374:GLN:HB2	2.49	0.47
1:I:555:LEU:HA	1:Q:463:PHE:HE2	1.79	0.47
1:S:572:VAL:HB	1:S:575:GLU:HB2	1.95	0.47
1:A:351:PRO:HB3	1:D:428:GLN:NE2	2.28	0.47
1:B:446:ASN:C	1:H:502:PRO:HG2	2.35	0.47
1:B:479:LEU:CD2	1:H:634:LEU:HD11	2.39	0.47
1:C:436:PRO:HG3	1:D:378:LEU:CD2	2.44	0.47
1:E:252:TYR:CE2	1:E:374:GLN:HB2	2.49	0.47
1:F:572:VAL:HB	1:F:575:GLU:HB2	1.95	0.47
1:N:240:ILE:HD12	1:N:240:ILE:N	2.30	0.47
1:Q:379:THR:CG2	1:Q:391:SER:H	2.21	0.47
1:R:519:ASN:HB3	1:R:520:PRO:CD	2.36	0.47
1:T:304:TRP:CZ3	1:T:732:LEU:HB3	2.36	0.47
1:D:519:ASN:HB3	1:D:520:PRO:CD	2.36	0.47
1:G:252:TYR:CE2	1:G:374:GLN:HB2	2.49	0.47
1:H:240:ILE:N	1:H:240:ILE:HD12	2.30	0.47
1:N:483:CYS:HB2	1:N:524:MET:HE1	1.97	0.47
1:O:240:ILE:HD12	1:O:240:ILE:N	2.29	0.47
1:Q:702:THR:CB	1:R:700:GLN:H	2.25	0.47
1:R:252:TYR:CE2	1:R:374:GLN:HB2	2.49	0.47
1:A:472:SER:H	1:C:270:ASN:ND2	2.13	0.47
1:E:239:VAL:HG13	1:E:685:TRP:HB2	1.95	0.47
1:E:240:ILE:N	1:E:240:ILE:HD12	2.30	0.47
1:F:482:PRO:HD3	1:F:605:MET:HE3	1.97	0.47
1:I:240:ILE:HD12	1:I:240:ILE:N	2.30	0.47
1:J:374:GLN:NE2	1:O:437:LEU:HD23	2.29	0.47
1:K:511:LEU:HD11	1:R:480:PRO:HG3	1.96	0.47
1:J:276:SER:OG	1:O:437:LEU:HD21	2.15	0.47
1:L:734:ARG:HG2	1:L:735:ASN:N	2.30	0.47
1:N:458:GLN:HG2	1:N:459:SER:N	2.29	0.47
1:O:239:VAL:HG13	1:O:685:TRP:HB2	1.95	0.47
1:S:252:TYR:CE2	1:S:374:GLN:HB2	2.49	0.47
1:T:252:TYR:CE2	1:T:374:GLN:HB2	2.49	0.47
1:A:428:GLN:NE2	1:C:351:PRO:HB3	2.28	0.47
1:B:240:ILE:N	1:B:240:ILE:HD12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:TRP:HA	1:B:304:TRP:HE3	1.76	0.47
1:C:482:PRO:HD3	1:C:605:MET:HE3	1.97	0.47
1:C:519:ASN:HB3	1:C:520:PRO:CD	2.36	0.47
1:D:657:ASN:HA	1:D:658:PRO:HD3	1.71	0.47
1:E:463:PHE:HE2	1:Q:555:LEU:HA	1.79	0.47
1:E:482:PRO:HD3	1:E:605:MET:HE3	1.97	0.47
1:F:240:ILE:HD12	1:F:240:ILE:N	2.30	0.47
1:F:470:SER:O	1:F:474:GLN:HG3	2.15	0.47
1:J:286:ARG:NH2	1:O:441:TYR:CD2	2.82	0.47
1:K:502:PRO:HG2	1:R:446:ASN:C	2.35	0.47
1:M:240:ILE:N	1:M:240:ILE:HD12	2.30	0.47
1:N:252:TYR:CE2	1:N:374:GLN:HB2	2.49	0.47
1:O:294:ARG:NE	1:O:298:ARG:HE	2.04	0.47
1:O:657:ASN:HA	1:O:658:PRO:HD3	1.71	0.47
1:P:644:PRO:HA	1:P:645:PRO:HD2	1.79	0.47
1:Q:252:TYR:CE2	1:Q:374:GLN:HB2	2.49	0.47
1:Q:734:ARG:HG2	1:Q:735:ASN:N	2.30	0.47
1:R:470:SER:O	1:R:474:GLN:HG3	2.15	0.47
1:A:240:ILE:HD12	1:A:240:ILE:N	2.30	0.47
1:A:488:ARG:NH2	1:D:584:LEU:HB3	2.29	0.47
1:B:657:ASN:HA	1:B:658:PRO:HD3	1.70	0.47
1:G:734:ARG:HG2	1:G:735:ASN:N	2.30	0.47
1:I:734:ARG:HG2	1:I:735:ASN:N	2.30	0.47
1:K:252:TYR:CE2	1:K:374:GLN:HB2	2.49	0.47
1:O:734:ARG:HG2	1:O:735:ASN:N	2.30	0.47
1:P:304:TRP:CZ3	1:P:732:LEU:HB3	2.36	0.47
1:S:458:GLN:HG2	1:S:459:SER:N	2.29	0.47
1:A:472:SER:HB3	1:C:269:ASP:O	2.15	0.47
1:B:428:GLN:NE2	1:H:351:PRO:HB3	2.29	0.47
1:D:252:TYR:CE2	1:D:374:GLN:HB2	2.49	0.47
1:E:446:ASN:C	1:Q:502:PRO:HG2	2.35	0.47
1:G:240:ILE:HD12	1:G:240:ILE:N	2.30	0.47
1:J:239:VAL:HG13	1:J:685:TRP:HB2	1.95	0.47
1:M:644:PRO:HA	1:M:645:PRO:HD2	1.79	0.47
1:N:253:ASN:HB3	1:N:256:LEU:O	2.15	0.47
1:N:734:ARG:HG2	1:N:735:ASN:N	2.30	0.47
1:Q:519:ASN:CB	1:Q:520:PRO:CD	2.93	0.47
1:A:253:ASN:HB3	1:A:256:LEU:O	2.15	0.47
1:A:378:LEU:CG	1:D:436:PRO:HG3	2.44	0.47
1:C:590:ALA:HA	1:D:497:ASN:ND2	2.30	0.47
1:D:714:THR:HG21	1:Q:275:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:658:PRO:HA	1:F:659:PRO:HD3	1.78	0.47
1:I:458:GLN:HG2	1:I:459:SER:N	2.29	0.47
1:M:294:ARG:NE	1:M:298:ARG:HE	2.04	0.47
1:O:483:CYS:HB2	1:O:524:MET:HE1	1.97	0.47
1:Q:245:ARG:NH1	1:Q:363:PRO:O	2.48	0.47
1:A:475:ALA:CA	1:C:519:ASN:HD22	2.27	0.46
1:E:734:ARG:HG2	1:E:735:ASN:N	2.30	0.46
1:F:451:THR:O	1:F:453:SER:N	2.49	0.46
1:H:470:SER:O	1:H:474:GLN:HG3	2.15	0.46
1:K:240:ILE:HD12	1:K:240:ILE:N	2.30	0.46
1:K:470:SER:O	1:K:474:GLN:HG3	2.15	0.46
1:N:245:ARG:NH1	1:N:363:PRO:O	2.49	0.46
1:O:252:TYR:CE2	1:O:374:GLN:HB2	2.49	0.46
1:A:398:PHE:CZ	1:D:693:LYS:HG3	2.51	0.46
1:D:519:ASN:CB	1:D:520:PRO:CD	2.93	0.46
1:E:396:GLU:HG3	1:F:367:ALA:HB2	1.97	0.46
1:E:437:LEU:HD23	1:Q:374:GLN:NE2	2.30	0.46
1:E:451:THR:O	1:E:453:SER:N	2.49	0.46
1:E:461:LEU:HD12	1:Q:555:LEU:HD22	1.96	0.46
1:H:734:ARG:HG2	1:H:735:ASN:N	2.30	0.46
1:I:245:ARG:NH1	1:I:363:PRO:O	2.49	0.46
1:I:294:ARG:NE	1:I:298:ARG:HE	2.04	0.46
1:I:378:LEU:CG	1:Q:436:PRO:HG3	2.44	0.46
1:J:240:ILE:N	1:J:240:ILE:HD12	2.30	0.46
1:J:378:LEU:CD2	1:O:436:PRO:HG3	2.46	0.46
1:K:253:ASN:HB3	1:K:256:LEU:O	2.15	0.46
1:K:519:ASN:HD22	1:R:475:ALA:CB	2.28	0.46
1:K:734:ARG:HG2	1:K:735:ASN:N	2.30	0.46
1:Q:470:SER:O	1:Q:474:GLN:HG3	2.15	0.46
1:R:304:TRP:CZ3	1:R:732:LEU:HB3	2.36	0.46
1:S:734:ARG:HG2	1:S:735:ASN:N	2.30	0.46
1:T:240:ILE:HD12	1:T:240:ILE:N	2.30	0.46
1:A:304:TRP:CZ3	1:A:732:LEU:HB3	2.36	0.46
1:C:240:ILE:HD12	1:C:240:ILE:N	2.30	0.46
1:C:449:GLN:HG2	1:D:500:ASN:N	2.30	0.46
1:C:458:GLN:HG2	1:C:459:SER:N	2.29	0.46
1:D:245:ARG:NH1	1:D:363:PRO:O	2.49	0.46
1:D:734:ARG:HG2	1:D:735:ASN:N	2.30	0.46
1:E:443:TYR:CE2	1:Q:544:GLY:HA3	2.50	0.46
1:E:449:GLN:HG2	1:Q:500:ASN:N	2.29	0.46
1:E:470:SER:O	1:E:474:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:337:THR:HG22	1:G:405:THR:HG21	1.97	0.46
1:F:734:ARG:HG2	1:F:735:ASN:N	2.30	0.46
1:G:451:THR:O	1:G:453:SER:N	2.49	0.46
1:G:470:SER:O	1:G:474:GLN:HG3	2.15	0.46
1:M:470:SER:O	1:M:474:GLN:HG3	2.15	0.46
1:O:304:TRP:CZ3	1:O:732:LEU:HB3	2.36	0.46
1:R:451:THR:O	1:R:453:SER:N	2.49	0.46
1:R:734:ARG:HG2	1:R:735:ASN:N	2.30	0.46
1:S:240:ILE:N	1:S:240:ILE:HD12	2.30	0.46
1:A:590:ALA:HA	1:C:497:ASN:HD22	1.79	0.46
1:A:630:HIS:NE2	2:A:999:D5M:H8	2.31	0.46
1:B:734:ARG:HG2	1:B:735:ASN:N	2.30	0.46
1:C:734:ARG:HG2	1:C:735:ASN:N	2.30	0.46
1:E:253:ASN:HB3	1:E:256:LEU:O	2.16	0.46
1:E:435:ASN:HA	1:E:436:PRO:HD3	1.83	0.46
1:L:658:PRO:HB2	1:P:250:PRO:HG3	1.97	0.46
1:M:405:THR:HG21	1:N:337:THR:CG2	2.45	0.46
1:R:245:ARG:NH1	1:R:363:PRO:O	2.49	0.46
1:R:253:ASN:HB3	1:R:256:LEU:O	2.16	0.46
1:S:470:SER:O	1:S:474:GLN:HG3	2.15	0.46
1:T:245:ARG:NH1	1:T:363:PRO:O	2.49	0.46
1:T:253:ASN:HB3	1:T:256:LEU:O	2.15	0.46
1:T:470:SER:O	1:T:474:GLN:HG3	2.15	0.46
1:A:657:ASN:HA	1:A:658:PRO:HD3	1.70	0.46
1:A:734:ARG:HG2	1:A:735:ASN:N	2.30	0.46
1:B:519:ASN:HB3	1:B:520:PRO:CD	2.36	0.46
1:F:630:HIS:NE2	2:F:999:D5M:H8	2.31	0.46
1:I:500:ASN:N	1:Q:449:GLN:HG2	2.30	0.46
1:I:519:ASN:HB3	1:I:520:PRO:CD	2.36	0.46
1:I:625:THR:HA	1:Q:608:GLN:HE22	1.81	0.46
1:J:734:ARG:HG2	1:J:735:ASN:N	2.30	0.46
1:K:379:THR:CG2	1:K:391:SER:H	2.21	0.46
1:L:240:ILE:HD12	1:L:240:ILE:N	2.30	0.46
1:L:365:PHE:HA	1:L:366:PRO:HD3	1.82	0.46
1:L:458:GLN:HG2	1:L:459:SER:N	2.29	0.46
1:O:253:ASN:HB3	1:O:256:LEU:O	2.16	0.46
1:O:470:SER:O	1:O:474:GLN:HG3	2.15	0.46
1:P:240:ILE:N	1:P:240:ILE:HD12	2.30	0.46
1:Q:702:THR:HB	1:R:700:GLN:H	1.81	0.46
1:T:734:ARG:HG2	1:T:735:ASN:N	2.30	0.46
1:A:405:THR:HG22	1:H:404:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ASN:HB3	1:B:256:LEU:O	2.15	0.46
1:B:367:ALA:HB2	1:C:396:GLU:HG3	1.98	0.46
1:B:458:GLN:HG2	1:B:459:SER:N	2.29	0.46
1:C:470:SER:O	1:C:474:GLN:HG3	2.16	0.46
1:D:470:SER:O	1:D:474:GLN:HG3	2.15	0.46
1:H:253:ASN:HB3	1:H:256:LEU:O	2.15	0.46
1:I:451:THR:O	1:I:453:SER:N	2.49	0.46
1:J:511:LEU:HD11	1:O:480:PRO:HG3	1.97	0.46
1:L:253:ASN:HB3	1:L:256:LEU:O	2.15	0.46
1:L:294:ARG:NE	1:L:298:ARG:HE	2.04	0.46
1:L:405:THR:HG21	1:T:337:THR:HG22	1.97	0.46
1:L:470:SER:O	1:L:474:GLN:HG3	2.15	0.46
1:M:451:THR:O	1:M:453:SER:N	2.49	0.46
1:O:245:ARG:NH1	1:O:363:PRO:O	2.49	0.46
1:O:458:GLN:HG2	1:O:459:SER:N	2.29	0.46
1:P:245:ARG:NH1	1:P:363:PRO:O	2.49	0.46
1:P:458:GLN:HG2	1:P:459:SER:N	2.29	0.46
1:R:240:ILE:N	1:R:240:ILE:HD12	2.30	0.46
1:A:451:THR:O	1:A:453:SER:N	2.49	0.46
1:A:603:PRO:HA	1:C:629:PHE:CD2	2.43	0.46
1:B:470:SER:O	1:B:474:GLN:HG3	2.15	0.46
1:E:714:THR:HG22	1:E:715:VAL:O	2.16	0.46
1:G:253:ASN:HB3	1:G:256:LEU:O	2.16	0.46
1:G:275:TYR:OH	1:H:714:THR:HG21	2.15	0.46
1:I:286:ARG:HD3	1:I:288:HIS:NE2	2.31	0.46
1:J:458:GLN:HG2	1:J:459:SER:N	2.29	0.46
1:K:555:LEU:HA	1:R:463:PHE:HE2	1.79	0.46
1:L:714:THR:HG22	1:L:715:VAL:O	2.16	0.46
1:O:451:THR:O	1:O:453:SER:N	2.49	0.46
1:O:630:HIS:NE2	2:O:999:D5M:H8	2.31	0.46
1:O:714:THR:HG22	1:O:715:VAL:O	2.16	0.46
1:P:253:ASN:HB3	1:P:256:LEU:O	2.16	0.46
1:Q:519:ASN:HB3	1:Q:520:PRO:CD	2.36	0.46
1:S:451:THR:O	1:S:453:SER:N	2.49	0.46
1:T:630:HIS:NE2	2:T:999:D5M:H8	2.31	0.46
1:A:236:GLY:O	1:A:689:LYS:HE3	2.16	0.46
1:B:714:THR:HG22	1:B:715:VAL:O	2.16	0.46
1:C:245:ARG:NH1	1:C:363:PRO:O	2.49	0.46
1:D:250:PRO:HG3	1:Q:658:PRO:HB2	1.97	0.46
1:E:630:HIS:NE2	2:E:999:D5M:H8	2.31	0.46
1:G:714:THR:HG22	1:G:715:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:358:HIS:CE1	1:O:435:ASN:H	2.33	0.46
1:J:398:PHE:CZ	1:O:693:LYS:HG3	2.51	0.46
1:O:286:ARG:HD3	1:O:288:HIS:NE2	2.31	0.46
1:P:630:HIS:NE2	2:P:999:D5M:H8	2.31	0.46
1:Q:304:TRP:CZ3	1:Q:732:LEU:HB3	2.36	0.46
1:R:570:ASN:HA	1:R:571:PRO:HD3	1.85	0.46
1:S:630:HIS:NE2	2:S:999:D5M:H8	2.31	0.46
1:A:245:ARG:NH1	1:A:363:PRO:O	2.49	0.46
1:B:224:SER:H	1:C:407:ASN:HD21	1.64	0.46
1:B:478:TRP:N	1:H:634:LEU:HD12	2.31	0.46
1:B:630:HIS:NE2	2:B:999:D5M:H8	2.31	0.46
1:D:253:ASN:HB3	1:D:256:LEU:O	2.15	0.46
1:D:435:ASN:HA	1:D:436:PRO:HD3	1.83	0.46
1:D:451:THR:O	1:D:453:SER:N	2.49	0.46
1:E:236:GLY:O	1:E:689:LYS:HE3	2.16	0.46
1:E:245:ARG:NH1	1:E:363:PRO:O	2.49	0.46
1:F:733:THR:HG21	1:P:389:ARG:O	2.16	0.46
1:H:451:THR:O	1:H:453:SER:N	2.49	0.46
1:I:253:ASN:HB3	1:I:256:LEU:O	2.16	0.46
1:I:519:ASN:HD22	1:Q:475:ALA:CB	2.29	0.46
1:K:286:ARG:HD3	1:K:288:HIS:NE2	2.31	0.46
1:N:470:SER:O	1:N:474:GLN:HG3	2.15	0.46
1:P:734:ARG:HG2	1:P:735:ASN:N	2.30	0.46
1:Q:451:THR:O	1:Q:453:SER:N	2.49	0.46
1:S:519:ASN:CB	1:S:520:PRO:CD	2.93	0.46
1:A:337:THR:HG22	1:E:405:THR:HG21	1.98	0.46
1:B:519:ASN:CB	1:B:520:PRO:CD	2.93	0.46
1:C:286:ARG:HD3	1:C:288:HIS:NE2	2.31	0.46
1:D:630:HIS:NE2	2:D:999:D5M:H8	2.31	0.46
1:F:236:GLY:O	1:F:689:LYS:HE3	2.16	0.46
1:H:714:THR:HG22	1:H:715:VAL:O	2.16	0.46
1:J:294:ARG:NE	1:J:298:ARG:HE	2.04	0.46
1:K:500:ASN:N	1:R:449:GLN:HG2	2.30	0.46
1:L:286:ARG:HD3	1:L:288:HIS:NE2	2.31	0.46
1:L:304:TRP:CZ3	1:L:732:LEU:HB3	2.36	0.46
1:L:367:ALA:HB2	1:T:396:GLU:HG3	1.98	0.46
1:L:451:THR:O	1:L:453:SER:N	2.49	0.46
1:M:253:ASN:HB3	1:M:256:LEU:O	2.16	0.46
1:M:286:ARG:HD3	1:M:288:HIS:NE2	2.31	0.46
1:M:630:HIS:NE2	2:M:999:D5M:H8	2.31	0.46
1:O:601:ALA:HA	1:O:605:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:714:THR:HG22	1:P:715:VAL:O	2.16	0.46
1:Q:253:ASN:HB3	1:Q:256:LEU:O	2.15	0.46
1:R:236:GLY:O	1:R:689:LYS:HE3	2.16	0.46
1:R:714:THR:HG22	1:R:715:VAL:O	2.16	0.46
1:S:253:ASN:HB3	1:S:256:LEU:O	2.15	0.46
1:T:286:ARG:HD3	1:T:288:HIS:NE2	2.31	0.46
1:T:458:GLN:HG2	1:T:459:SER:N	2.29	0.46
1:A:286:ARG:HD3	1:A:288:HIS:NE2	2.31	0.45
1:A:644:PRO:HA	1:A:645:PRO:HD2	1.79	0.45
1:B:286:ARG:HD3	1:B:288:HIS:NE2	2.31	0.45
1:B:365:PHE:HA	1:B:366:PRO:HD3	1.82	0.45
1:C:436:PRO:HD2	1:D:376:GLY:C	2.36	0.45
1:C:584:LEU:HB3	1:D:488:ARG:NH2	2.31	0.45
1:C:601:ALA:HA	1:C:605:MET:HE1	1.98	0.45
1:D:240:ILE:HD12	1:D:240:ILE:N	2.30	0.45
1:G:236:GLY:O	1:G:689:LYS:HE3	2.16	0.45
1:G:396:GLU:HG3	1:H:367:ALA:HB2	1.98	0.45
1:G:630:HIS:NE2	2:G:999:D5M:H8	2.31	0.45
1:H:245:ARG:NH1	1:H:363:PRO:O	2.49	0.45
1:I:470:SER:O	1:I:474:GLN:HG3	2.15	0.45
1:J:253:ASN:HB3	1:J:256:LEU:O	2.15	0.45
1:K:451:THR:O	1:K:453:SER:N	2.49	0.45
1:K:544:GLY:HA3	1:R:443:TYR:CE2	2.51	0.45
1:P:286:ARG:HD3	1:P:288:HIS:NE2	2.31	0.45
1:P:483:CYS:HB2	1:P:524:MET:HE1	1.98	0.45
1:Q:240:ILE:HD12	1:Q:240:ILE:N	2.30	0.45
1:R:630:HIS:NE2	2:R:999:D5M:H8	2.31	0.45
1:S:286:ARG:HD3	1:S:288:HIS:NE2	2.31	0.45
1:T:451:THR:O	1:T:453:SER:N	2.49	0.45
1:A:470:SER:O	1:A:474:GLN:HG3	2.15	0.45
1:B:245:ARG:NH1	1:B:363:PRO:O	2.49	0.45
1:C:451:THR:O	1:C:453:SER:N	2.48	0.45
1:G:286:ARG:HD3	1:G:288:HIS:NE2	2.31	0.45
1:J:497:ASN:HD22	1:O:590:ALA:HA	1.81	0.45
1:M:734:ARG:HG2	1:M:735:ASN:N	2.30	0.45
1:N:286:ARG:HD3	1:N:288:HIS:NE2	2.31	0.45
1:N:403:LEU:HA	1:N:407:ASN:HD22	1.82	0.45
1:N:451:THR:O	1:N:453:SER:N	2.49	0.45
1:N:630:HIS:NE2	2:N:999:D5M:H8	2.31	0.45
1:O:236:GLY:O	1:O:689:LYS:HE3	2.16	0.45
1:S:245:ARG:NH1	1:S:363:PRO:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:365:PHE:HA	1:S:366:PRO:HD3	1.82	0.45
1:A:323:VAL:HG11	1:H:657:ASN:ND2	2.32	0.45
1:B:584:LEU:HB3	1:H:488:ARG:NH2	2.31	0.45
1:D:458:GLN:HG2	1:D:459:SER:N	2.29	0.45
1:E:425:ALA:O	1:E:733:THR:HA	2.17	0.45
1:F:245:ARG:NH1	1:F:363:PRO:O	2.49	0.45
1:G:570:ASN:HA	1:G:571:PRO:HD3	1.85	0.45
1:I:379:THR:CG2	1:I:391:SER:H	2.21	0.45
1:J:378:LEU:CG	1:O:436:PRO:HG3	2.46	0.45
1:J:714:THR:HG22	1:J:715:VAL:O	2.16	0.45
1:K:367:ALA:HB2	1:S:396:GLU:HG3	1.97	0.45
1:L:245:ARG:NH1	1:L:363:PRO:O	2.49	0.45
1:L:404:ARG:HG2	1:P:222:GLY:HA2	1.98	0.45
1:L:570:ASN:HA	1:L:571:PRO:HD3	1.85	0.45
1:M:236:GLY:O	1:M:689:LYS:HE3	2.16	0.45
1:M:435:ASN:HA	1:M:436:PRO:HD3	1.83	0.45
1:N:714:THR:HG22	1:N:715:VAL:O	2.16	0.45
1:P:451:THR:O	1:P:453:SER:N	2.49	0.45
1:Q:714:THR:HG22	1:Q:715:VAL:O	2.16	0.45
1:S:236:GLY:O	1:S:689:LYS:HE3	2.17	0.45
1:T:519:ASN:CB	1:T:520:PRO:CD	2.93	0.45
1:E:519:ASN:CB	1:E:520:PRO:CD	2.93	0.45
1:F:425:ALA:O	1:F:733:THR:HA	2.17	0.45
1:F:644:PRO:HA	1:F:645:PRO:HD2	1.79	0.45
1:H:286:ARG:HD3	1:H:288:HIS:NE2	2.31	0.45
1:I:374:GLN:NE2	1:Q:437:LEU:HD23	2.31	0.45
1:I:398:PHE:CZ	1:Q:693:LYS:HG3	2.52	0.45
1:I:403:LEU:HA	1:I:407:ASN:HD22	1.82	0.45
1:I:630:HIS:NE2	2:I:999:D5M:H8	2.31	0.45
1:J:403:LEU:HA	1:J:407:ASN:HD22	1.82	0.45
1:J:451:THR:O	1:J:453:SER:N	2.49	0.45
1:L:425:ALA:O	1:L:733:THR:HA	2.17	0.45
1:M:425:ALA:O	1:M:733:THR:HA	2.17	0.45
1:M:519:ASN:CB	1:M:520:PRO:CD	2.93	0.45
1:P:470:SER:O	1:P:474:GLN:HG3	2.15	0.45
1:A:403:LEU:HA	1:A:407:ASN:HD22	1.82	0.45
1:B:451:THR:O	1:B:453:SER:N	2.49	0.45
1:B:483:CYS:HB2	1:B:524:MET:CE	2.47	0.45
1:F:702:THR:HB	1:I:700:GLN:H	1.81	0.45
1:G:425:ALA:O	1:G:733:THR:HA	2.17	0.45
1:H:236:GLY:O	1:H:689:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:272:TYR:HA	1:I:381:ASN:ND2	2.32	0.45
1:I:425:ALA:O	1:I:733:THR:HA	2.17	0.45
1:K:657:ASN:HA	1:K:658:PRO:HD3	1.70	0.45
1:M:483:CYS:HB2	1:M:524:MET:CE	2.47	0.45
1:M:570:ASN:HA	1:M:571:PRO:HD3	1.85	0.45
1:M:710:ASN:ND2	1:N:259:GLN:HE22	2.13	0.45
1:O:425:ALA:O	1:O:733:THR:HA	2.17	0.45
1:P:482:PRO:HD3	1:P:605:MET:HE3	1.98	0.45
1:Q:236:GLY:O	1:Q:689:LYS:HE3	2.17	0.45
1:R:286:ARG:HD3	1:R:288:HIS:NE2	2.31	0.45
1:R:403:LEU:HA	1:R:407:ASN:HD22	1.82	0.45
1:A:483:CYS:HB2	1:A:524:MET:CE	2.47	0.45
1:C:253:ASN:HB3	1:C:256:LEU:O	2.15	0.45
1:C:437:LEU:HD21	1:D:276:SER:OG	2.16	0.45
1:C:483:CYS:HB2	1:C:524:MET:CE	2.47	0.45
1:C:714:THR:HG22	1:C:715:VAL:O	2.16	0.45
1:F:403:LEU:HA	1:F:407:ASN:HD22	1.82	0.45
1:F:601:ALA:HA	1:F:605:MET:HE1	1.98	0.45
1:F:714:THR:HG22	1:F:715:VAL:O	2.16	0.45
1:G:403:LEU:HA	1:G:407:ASN:HD22	1.82	0.45
1:G:483:CYS:HB2	1:G:524:MET:CE	2.47	0.45
1:H:272:TYR:HA	1:H:381:ASN:ND2	2.32	0.45
1:I:508:LYS:HG3	1:Q:579:THR:HB	1.99	0.45
1:I:714:THR:HG22	1:I:715:VAL:O	2.16	0.45
1:K:403:LEU:HA	1:K:407:ASN:HD22	1.82	0.45
1:K:488:ARG:NH2	1:R:584:LEU:HB3	2.32	0.45
1:M:658:PRO:HA	1:M:659:PRO:HD3	1.78	0.45
1:P:519:ASN:CB	1:P:520:PRO:CD	2.93	0.45
1:T:435:ASN:HA	1:T:436:PRO:HD3	1.83	0.45
1:D:483:CYS:HB2	1:D:524:MET:CE	2.47	0.45
1:E:272:TYR:HA	1:E:381:ASN:ND2	2.32	0.45
1:E:601:ALA:HA	1:E:605:MET:HE1	1.98	0.45
1:F:519:ASN:CB	1:F:520:PRO:CD	2.93	0.45
1:H:403:LEU:HA	1:H:407:ASN:HD22	1.82	0.45
1:J:470:SER:O	1:J:474:GLN:HG3	2.15	0.45
1:L:236:GLY:O	1:L:689:LYS:HE3	2.16	0.45
1:M:245:ARG:NH1	1:M:363:PRO:O	2.49	0.45
1:M:403:LEU:HA	1:M:407:ASN:HD22	1.82	0.45
1:M:714:THR:HG22	1:M:715:VAL:O	2.16	0.45
1:P:658:PRO:HA	1:P:659:PRO:HD3	1.78	0.45
1:S:483:CYS:HB2	1:S:524:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:483:CYS:HB2	1:T:524:MET:CE	2.47	0.45
1:A:374:GLN:NE2	1:D:437:LEU:HD23	2.32	0.45
1:A:634:LEU:HD12	1:D:478:TRP:N	2.31	0.45
1:A:702:THR:CB	1:B:700:GLN:H	2.30	0.45
1:B:236:GLY:O	1:B:689:LYS:HE3	2.16	0.45
1:C:304:TRP:CZ3	1:C:732:LEU:HB3	2.36	0.45
1:C:425:ALA:O	1:C:733:THR:HA	2.17	0.45
1:F:396:GLU:HG3	1:G:367:ALA:HB2	1.98	0.45
1:G:245:ARG:NH1	1:G:363:PRO:O	2.49	0.45
1:H:483:CYS:HB2	1:H:524:MET:CE	2.47	0.45
1:J:236:GLY:O	1:J:689:LYS:HE3	2.17	0.45
1:J:425:ALA:O	1:J:733:THR:HA	2.17	0.45
1:J:630:HIS:NE2	2:J:999:D5M:H8	2.31	0.45
1:K:236:GLY:O	1:K:689:LYS:HE3	2.17	0.45
1:K:425:ALA:O	1:K:733:THR:HA	2.17	0.45
1:K:435:ASN:HA	1:K:436:PRO:HD3	1.83	0.45
1:N:519:ASN:HB3	1:N:520:PRO:CD	2.36	0.45
1:O:272:TYR:HA	1:O:381:ASN:ND2	2.32	0.45
1:O:379:THR:CG2	1:O:391:SER:H	2.21	0.45
1:Q:403:LEU:HA	1:Q:407:ASN:HD22	1.82	0.45
1:T:249:LEU:HA	1:T:250:PRO:HD3	1.81	0.45
1:A:714:THR:HG22	1:A:715:VAL:O	2.16	0.45
1:B:222:GLY:HA2	1:C:404:ARG:HG2	1.98	0.45
1:C:236:GLY:O	1:C:689:LYS:HE3	2.16	0.45
1:E:436:PRO:HG3	1:Q:378:LEU:CG	2.46	0.45
1:E:483:CYS:HB2	1:E:524:MET:CE	2.47	0.45
1:H:630:HIS:NE2	2:H:999:D5M:H8	2.31	0.45
1:I:483:CYS:HB2	1:I:524:MET:CE	2.47	0.45
1:I:488:ARG:C	1:I:489:LEU:HD12	2.38	0.45
1:J:245:ARG:NH1	1:J:363:PRO:O	2.49	0.45
1:J:483:CYS:HB2	1:J:524:MET:CE	2.47	0.45
1:N:657:ASN:HA	1:N:658:PRO:HD3	1.71	0.45
1:P:236:GLY:O	1:P:689:LYS:HE3	2.16	0.45
1:P:519:ASN:HB3	1:P:520:PRO:CD	2.36	0.45
1:Q:630:HIS:NE2	2:Q:999:D5M:H8	2.31	0.45
1:R:372:VAL:HA	1:R:373:PRO:HD3	1.87	0.45
1:S:249:LEU:HA	1:S:250:PRO:HD3	1.81	0.45
1:S:272:TYR:HA	1:S:381:ASN:ND2	2.32	0.45
1:A:441:TYR:CD2	1:C:286:ARG:NH2	2.85	0.45
1:B:693:LYS:HG3	1:H:398:PHE:CZ	2.51	0.45
1:C:436:PRO:HD2	1:D:376:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:TYR:HA	1:D:381:ASN:ND2	2.32	0.45
1:D:286:ARG:HD3	1:D:288:HIS:NE2	2.31	0.45
1:F:253:ASN:HB3	1:F:256:LEU:O	2.15	0.45
1:I:236:GLY:O	1:I:689:LYS:HE3	2.17	0.45
1:J:625:THR:HA	1:O:608:GLN:HE22	1.82	0.45
1:K:608:GLN:HA	1:K:608:GLN:HE21	1.82	0.45
1:K:634:LEU:HD12	1:R:478:TRP:N	2.32	0.45
1:L:402:MET:H	1:P:227:ASN:ND2	2.15	0.45
1:N:272:TYR:HA	1:N:381:ASN:ND2	2.32	0.45
1:P:483:CYS:HB2	1:P:524:MET:CE	2.47	0.45
1:Q:488:ARG:C	1:Q:489:LEU:HD12	2.37	0.45
1:R:483:CYS:HB2	1:R:524:MET:CE	2.47	0.45
1:R:608:GLN:HA	1:R:608:GLN:HE21	1.82	0.45
1:S:608:GLN:HA	1:S:608:GLN:HE21	1.82	0.45
1:S:644:PRO:HA	1:S:645:PRO:HD2	1.79	0.45
1:T:236:GLY:O	1:T:689:LYS:HE3	2.16	0.45
1:T:425:ALA:O	1:T:733:THR:HA	2.17	0.45
1:T:714:THR:HG22	1:T:715:VAL:O	2.16	0.45
1:A:405:THR:HG21	1:H:337:THR:CG2	2.47	0.44
1:A:581:ALA:O	1:C:485:ARG:HD3	2.16	0.44
1:B:249:LEU:HA	1:B:250:PRO:HD3	1.81	0.44
1:B:337:THR:CG2	1:N:405:THR:HG21	2.47	0.44
1:C:272:TYR:HA	1:C:381:ASN:ND2	2.32	0.44
1:D:236:GLY:O	1:D:689:LYS:HE3	2.17	0.44
1:D:488:ARG:C	1:D:489:LEU:HD12	2.38	0.44
1:D:714:THR:HG22	1:D:715:VAL:O	2.16	0.44
1:E:379:THR:CG2	1:E:391:SER:H	2.21	0.44
1:E:403:LEU:HA	1:E:407:ASN:HD22	1.82	0.44
1:E:475:ALA:CB	1:Q:519:ASN:HD22	2.30	0.44
1:H:425:ALA:O	1:H:733:THR:HA	2.17	0.44
1:J:286:ARG:HD3	1:J:288:HIS:NE2	2.32	0.44
1:K:245:ARG:NH1	1:K:363:PRO:O	2.49	0.44
1:K:630:HIS:NE2	2:K:999:D5M:H8	2.31	0.44
1:L:483:CYS:HB2	1:L:524:MET:CE	2.47	0.44
1:M:608:GLN:HA	1:M:608:GLN:HE21	1.82	0.44
1:N:416:GLU:H	1:N:416:GLU:HG2	1.60	0.44
1:N:425:ALA:O	1:N:733:THR:HA	2.17	0.44
1:N:483:CYS:HB2	1:N:524:MET:CE	2.47	0.44
1:Q:286:ARG:HD3	1:Q:288:HIS:NE2	2.31	0.44
1:Q:425:ALA:O	1:Q:733:THR:HA	2.17	0.44
1:S:291:PHE:CE2	1:S:299:LEU:HD12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:304:TRP:CZ3	1:S:732:LEU:HB3	2.36	0.44
1:S:483:CYS:HB2	1:S:524:MET:CE	2.47	0.44
1:S:488:ARG:C	1:S:489:LEU:HD12	2.38	0.44
1:S:714:THR:HG22	1:S:715:VAL:O	2.16	0.44
1:T:403:LEU:HA	1:T:407:ASN:HD22	1.82	0.44
1:A:272:TYR:HA	1:A:381:ASN:ND2	2.32	0.44
1:C:488:ARG:C	1:C:489:LEU:HD12	2.38	0.44
1:C:630:HIS:NE2	2:C:999:D5M:H8	2.31	0.44
1:D:403:LEU:HA	1:D:407:ASN:HD22	1.82	0.44
1:D:425:ALA:O	1:D:733:THR:HA	2.17	0.44
1:D:658:PRO:HA	1:D:659:PRO:HD3	1.78	0.44
1:E:286:ARG:HD3	1:E:288:HIS:NE2	2.31	0.44
1:F:272:TYR:HA	1:F:381:ASN:ND2	2.32	0.44
1:F:435:ASN:H	1:P:358:HIS:CE1	2.34	0.44
1:F:700:GLN:H	1:I:702:THR:HB	1.81	0.44
1:G:272:TYR:HA	1:G:381:ASN:ND2	2.32	0.44
1:G:658:PRO:HB2	1:H:250:PRO:HG3	1.99	0.44
1:I:657:ASN:HA	1:I:658:PRO:HD3	1.71	0.44
1:J:488:ARG:C	1:J:489:LEU:HD12	2.37	0.44
1:K:714:THR:HG22	1:K:715:VAL:O	2.16	0.44
1:L:630:HIS:NE2	2:L:999:D5M:H8	2.31	0.44
1:M:601:ALA:HA	1:M:605:MET:HE1	2.00	0.44
1:N:236:GLY:O	1:N:689:LYS:HE3	2.17	0.44
1:B:272:TYR:HA	1:B:381:ASN:ND2	2.32	0.44
1:B:291:PHE:CE2	1:B:299:LEU:HD12	2.53	0.44
1:B:435:ASN:H	1:H:358:HIS:CE1	2.35	0.44
1:F:478:TRP:N	1:P:634:LEU:HD12	2.32	0.44
1:G:488:ARG:C	1:G:489:LEU:HD12	2.38	0.44
1:K:272:TYR:HA	1:K:381:ASN:ND2	2.32	0.44
1:N:488:ARG:C	1:N:489:LEU:HD12	2.38	0.44
1:P:488:ARG:C	1:P:489:LEU:HD12	2.38	0.44
1:P:663:SER:HA	1:P:664:PRO:HD3	1.84	0.44
1:Q:570:ASN:HA	1:Q:571:PRO:HD3	1.85	0.44
1:R:644:PRO:HA	1:R:645:PRO:HD2	1.79	0.44
1:S:425:ALA:O	1:S:733:THR:HA	2.17	0.44
1:C:435:ASN:HB2	1:D:353:VAL:HG22	1.98	0.44
1:C:608:GLN:HA	1:C:608:GLN:HE21	1.82	0.44
1:D:608:GLN:HA	1:D:608:GLN:HE21	1.82	0.44
1:D:657:ASN:ND2	1:O:323:VAL:HG11	2.32	0.44
1:E:304:TRP:CZ3	1:E:732:LEU:HB3	2.36	0.44
1:E:488:ARG:C	1:E:489:LEU:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:519:ASN:HD22	1:I:475:ALA:CB	2.30	0.44
1:E:608:GLN:HE22	1:Q:625:THR:HA	1.82	0.44
1:F:286:ARG:HD3	1:F:288:HIS:NE2	2.31	0.44
1:F:488:ARG:C	1:F:489:LEU:HD12	2.38	0.44
1:G:291:PHE:CE2	1:G:299:LEU:HD12	2.53	0.44
1:H:488:ARG:C	1:H:489:LEU:HD12	2.38	0.44
1:K:488:ARG:C	1:K:489:LEU:HD12	2.37	0.44
1:L:272:TYR:HA	1:L:381:ASN:ND2	2.32	0.44
1:L:663:SER:HA	1:L:664:PRO:HD3	1.84	0.44
1:M:272:TYR:HA	1:M:381:ASN:ND2	2.32	0.44
1:M:488:ARG:C	1:M:489:LEU:HD12	2.38	0.44
1:N:644:PRO:HA	1:N:645:PRO:HD2	1.79	0.44
1:O:488:ARG:C	1:O:489:LEU:HD12	2.38	0.44
1:P:272:TYR:HA	1:P:381:ASN:ND2	2.32	0.44
1:P:403:LEU:HA	1:P:407:ASN:HD22	1.82	0.44
1:R:272:TYR:HA	1:R:381:ASN:ND2	2.32	0.44
1:S:403:LEU:HA	1:S:407:ASN:HD22	1.82	0.44
1:T:272:TYR:HA	1:T:381:ASN:ND2	2.32	0.44
1:T:488:ARG:C	1:T:489:LEU:HD12	2.38	0.44
1:A:358:HIS:CE1	1:D:435:ASN:H	2.35	0.44
1:F:427:SER:O	1:P:380:LEU:N	2.50	0.44
1:F:700:GLN:H	1:I:702:THR:CB	2.30	0.44
1:H:657:ASN:HA	1:H:658:PRO:HD3	1.71	0.44
1:I:502:PRO:HG2	1:Q:446:ASN:C	2.37	0.44
1:J:291:PHE:CE2	1:J:299:LEU:HD12	2.53	0.44
1:K:483:CYS:HB2	1:K:524:MET:CE	2.47	0.44
1:L:291:PHE:CE2	1:L:299:LEU:HD12	2.53	0.44
1:M:482:PRO:HD3	1:M:605:MET:HE3	1.98	0.44
1:N:291:PHE:CE2	1:N:299:LEU:HD12	2.53	0.44
1:O:291:PHE:CE2	1:O:299:LEU:HD12	2.53	0.44
1:O:429:SER:HB3	1:O:432:ARG:HB2	2.00	0.44
1:O:608:GLN:HA	1:O:608:GLN:HE21	1.83	0.44
1:Q:252:TYR:CD2	1:Q:374:GLN:HB2	2.53	0.44
1:Q:291:PHE:CE2	1:Q:299:LEU:HD12	2.53	0.44
1:R:488:ARG:C	1:R:489:LEU:HD12	2.38	0.44
1:S:252:TYR:CD2	1:S:374:GLN:HB2	2.53	0.44
1:S:613:TYR:HA	1:S:727:ILE:O	2.18	0.44
1:T:608:GLN:HE21	1:T:608:GLN:HA	1.82	0.44
1:A:222:GLY:HA2	1:H:404:ARG:HG2	2.00	0.44
1:A:435:ASN:H	1:C:358:HIS:CE1	2.35	0.44
1:A:488:ARG:C	1:A:489:LEU:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:SER:HB3	1:E:432:ARG:HB2	2.00	0.44
1:E:508:LYS:HG3	1:I:579:THR:HB	2.00	0.44
1:F:291:PHE:CE2	1:F:299:LEU:HD12	2.53	0.44
1:F:458:GLN:HG2	1:F:459:SER:N	2.30	0.44
1:G:252:TYR:CD2	1:G:374:GLN:HB2	2.53	0.44
1:G:519:ASN:HB3	1:G:520:PRO:CD	2.36	0.44
1:H:608:GLN:HA	1:H:608:GLN:HE21	1.83	0.44
1:I:222:GLY:HA2	1:P:404:ARG:HG2	1.98	0.44
1:J:272:TYR:HA	1:J:381:ASN:ND2	2.32	0.44
1:J:613:TYR:HA	1:J:727:ILE:O	2.18	0.44
1:K:291:PHE:CE2	1:K:299:LEU:HD12	2.53	0.44
1:L:403:LEU:HA	1:L:407:ASN:HD22	1.82	0.44
1:L:519:ASN:HB3	1:L:520:PRO:CD	2.36	0.44
1:L:657:ASN:HA	1:L:658:PRO:HD3	1.71	0.44
1:M:291:PHE:CE2	1:M:299:LEU:HD12	2.53	0.44
1:N:663:SER:HA	1:N:664:PRO:HD3	1.84	0.44
1:P:291:PHE:CE2	1:P:299:LEU:HD12	2.53	0.44
1:P:425:ALA:O	1:P:733:THR:HA	2.17	0.44
1:Q:608:GLN:HA	1:Q:608:GLN:HE21	1.82	0.44
1:Q:701:TYR:O	1:R:700:GLN:HG3	2.18	0.44
1:R:337:THR:HG22	1:T:405:THR:HG21	1.98	0.44
1:R:714:THR:CG2	1:R:715:VAL:N	2.81	0.44
1:T:613:TYR:HA	1:T:727:ILE:O	2.18	0.44
1:B:608:GLN:HA	1:B:608:GLN:HE21	1.82	0.44
1:B:613:TYR:HA	1:B:727:ILE:O	2.18	0.44
1:C:252:TYR:CD2	1:C:374:GLN:HB2	2.53	0.44
1:C:441:TYR:CD2	1:D:286:ARG:NH2	2.85	0.44
1:D:404:ARG:HG2	1:O:222:GLY:HA2	1.98	0.44
1:E:374:GLN:NE2	1:I:437:LEU:HD23	2.32	0.44
1:I:291:PHE:CE2	1:I:299:LEU:HD12	2.53	0.44
1:N:608:GLN:HA	1:N:608:GLN:HE21	1.82	0.44
1:Q:272:TYR:HA	1:Q:381:ASN:ND2	2.32	0.44
1:Q:657:ASN:HA	1:Q:658:PRO:HD3	1.71	0.44
1:R:291:PHE:CE2	1:R:299:LEU:HD12	2.53	0.44
1:R:429:SER:HB3	1:R:432:ARG:HB2	2.00	0.44
1:A:425:ALA:O	1:A:733:THR:HA	2.17	0.44
1:A:502:PRO:HG2	1:D:446:ASN:C	2.37	0.44
1:B:403:LEU:HA	1:B:407:ASN:HD22	1.82	0.44
1:B:733:THR:HG21	1:H:389:ARG:O	2.18	0.44
1:E:291:PHE:CE2	1:E:299:LEU:HD12	2.53	0.44
1:F:613:TYR:HA	1:F:727:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:663:SER:HA	1:H:664:PRO:HD3	1.84	0.44
1:H:714:THR:CG2	1:H:715:VAL:N	2.81	0.44
1:I:657:ASN:ND2	1:R:323:VAL:HG11	2.33	0.44
1:K:304:TRP:CZ3	1:K:732:LEU:HB3	2.36	0.44
1:K:644:PRO:HA	1:K:645:PRO:HD2	1.79	0.44
1:O:483:CYS:HB2	1:O:524:MET:CE	2.47	0.44
1:P:252:TYR:CD2	1:P:374:GLN:HB2	2.53	0.44
1:P:429:SER:HB3	1:P:432:ARG:HB2	2.00	0.44
1:R:252:TYR:CD2	1:R:374:GLN:HB2	2.53	0.44
1:S:657:ASN:HA	1:S:658:PRO:HD3	1.70	0.44
1:A:252:TYR:CD2	1:A:374:GLN:HB2	2.53	0.44
1:B:437:LEU:HD23	1:H:374:GLN:NE2	2.33	0.44
1:B:488:ARG:C	1:B:489:LEU:HD12	2.37	0.44
1:C:582:ASN:HA	1:D:485:ARG:HD3	1.99	0.44
1:D:337:THR:HG22	1:O:405:THR:HG21	1.98	0.44
1:D:429:SER:HB3	1:D:432:ARG:HB2	2.00	0.44
1:E:337:THR:HG22	1:F:405:THR:HG21	1.99	0.44
1:E:500:ASN:N	1:I:449:GLN:HG2	2.33	0.44
1:F:252:TYR:CD2	1:F:374:GLN:HB2	2.53	0.44
1:F:429:SER:HB3	1:F:432:ARG:HB2	2.00	0.44
1:F:483:CYS:HB2	1:F:524:MET:CE	2.47	0.44
1:F:608:GLN:HA	1:F:608:GLN:HE21	1.82	0.44
1:I:252:TYR:CD2	1:I:374:GLN:HB2	2.53	0.44
1:I:404:ARG:NH2	1:R:405:THR:HG22	2.32	0.44
1:I:608:GLN:HA	1:I:608:GLN:HE21	1.82	0.44
1:J:608:GLN:HE21	1:J:608:GLN:HA	1.82	0.44
1:M:252:TYR:CD2	1:M:374:GLN:HB2	2.53	0.44
1:M:458:GLN:HG2	1:M:459:SER:N	2.29	0.44
1:O:613:TYR:HA	1:O:727:ILE:O	2.18	0.44
1:P:613:TYR:HA	1:P:727:ILE:O	2.18	0.44
1:Q:458:GLN:HG2	1:Q:459:SER:N	2.29	0.44
1:R:379:THR:CG2	1:R:391:SER:H	2.21	0.44
1:S:379:THR:CG2	1:S:391:SER:H	2.21	0.44
1:T:291:PHE:CE2	1:T:299:LEU:HD12	2.53	0.44
1:D:613:TYR:HA	1:D:727:ILE:O	2.18	0.43
1:E:249:LEU:HA	1:E:250:PRO:HD3	1.81	0.43
1:E:608:GLN:HA	1:E:608:GLN:HE21	1.82	0.43
1:E:613:TYR:HA	1:E:727:ILE:O	2.18	0.43
1:F:436:PRO:HG3	1:P:378:LEU:CG	2.47	0.43
1:F:578:GLY:HA3	1:P:508:LYS:O	2.17	0.43
1:F:702:THR:CB	1:I:700:GLN:H	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:714:THR:CG2	1:F:715:VAL:N	2.81	0.43
1:I:429:SER:HB3	1:I:432:ARG:HB2	2.00	0.43
1:I:482:PRO:HD3	1:I:605:MET:HE3	2.00	0.43
1:M:714:THR:CG2	1:M:715:VAL:N	2.81	0.43
1:N:252:TYR:CD2	1:N:374:GLN:HB2	2.53	0.43
1:N:613:TYR:HA	1:N:727:ILE:O	2.18	0.43
1:O:259:GLN:HE22	1:S:710:ASN:ND2	2.15	0.43
1:Q:524:MET:CE	1:Q:573:ALA:HA	2.47	0.43
1:R:613:TYR:HA	1:R:727:ILE:O	2.18	0.43
1:A:608:GLN:HA	1:A:608:GLN:HE21	1.82	0.43
1:A:634:LEU:HD12	1:D:477:ASN:C	2.39	0.43
1:D:252:TYR:CD2	1:D:374:GLN:HB2	2.53	0.43
1:E:286:ARG:NH1	1:E:288:HIS:NE2	2.67	0.43
1:E:658:PRO:HA	1:E:659:PRO:HD3	1.78	0.43
1:J:405:THR:HG21	1:M:337:THR:CG2	2.48	0.43
1:J:429:SER:HB3	1:J:432:ARG:HB2	2.00	0.43
1:K:663:SER:HA	1:K:664:PRO:HD3	1.84	0.43
1:L:399:PRO:HD3	1:P:231:ASP:HB2	2.00	0.43
1:M:286:ARG:NH1	1:M:288:HIS:NE2	2.66	0.43
1:Q:483:CYS:HB2	1:Q:524:MET:CE	2.47	0.43
1:R:425:ALA:O	1:R:733:THR:HA	2.17	0.43
1:T:657:ASN:HA	1:T:658:PRO:HD3	1.70	0.43
1:C:608:GLN:HE22	1:D:625:THR:HA	1.84	0.43
1:D:291:PHE:CE2	1:D:299:LEU:HD12	2.53	0.43
1:E:579:THR:HB	1:Q:508:LYS:HG3	1.99	0.43
1:H:429:SER:HB3	1:H:432:ARG:HB2	2.00	0.43
1:I:337:THR:HG22	1:R:405:THR:HG21	2.01	0.43
1:J:252:TYR:CD2	1:J:374:GLN:HB2	2.53	0.43
1:K:613:TYR:HA	1:K:727:ILE:O	2.18	0.43
1:L:249:LEU:HA	1:L:250:PRO:HD3	1.81	0.43
1:L:445:LEU:HD12	1:L:463:PHE:CE1	2.54	0.43
1:M:613:TYR:HA	1:M:727:ILE:O	2.18	0.43
1:M:663:SER:HA	1:M:664:PRO:HD3	1.84	0.43
1:N:570:ASN:HA	1:N:571:PRO:HD3	1.85	0.43
1:O:403:LEU:HA	1:O:407:ASN:HD22	1.82	0.43
1:P:445:LEU:HD12	1:P:463:PHE:CE1	2.54	0.43
1:Q:613:TYR:HA	1:Q:727:ILE:O	2.18	0.43
1:Q:714:THR:CG2	1:Q:715:VAL:N	2.81	0.43
1:S:429:SER:HB3	1:S:432:ARG:HB2	2.00	0.43
1:S:519:ASN:HB3	1:S:520:PRO:CD	2.36	0.43
1:A:613:TYR:HA	1:A:727:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ALA:O	1:B:733:THR:HA	2.17	0.43
1:B:477:ASN:C	1:H:634:LEU:HD12	2.38	0.43
1:C:291:PHE:CE2	1:C:299:LEU:HD12	2.53	0.43
1:E:249:LEU:HD13	1:E:372:VAL:HB	2.01	0.43
1:E:252:TYR:CD2	1:E:374:GLN:HB2	2.53	0.43
1:E:483:CYS:HB2	1:E:524:MET:HE1	1.98	0.43
1:F:445:LEU:HD12	1:F:463:PHE:CE1	2.54	0.43
1:G:519:ASN:CB	1:G:520:PRO:CD	2.93	0.43
1:G:658:PRO:HA	1:G:659:PRO:HD3	1.78	0.43
1:H:291:PHE:CE2	1:H:299:LEU:HD12	2.53	0.43
1:H:613:TYR:HA	1:H:727:ILE:O	2.18	0.43
1:I:277:THR:HA	1:I:278:PRO:HD3	1.87	0.43
1:J:519:ASN:HD22	1:O:475:ALA:CB	2.31	0.43
1:J:714:THR:CG2	1:J:715:VAL:N	2.81	0.43
1:K:286:ARG:NH1	1:K:288:HIS:NE2	2.67	0.43
1:L:250:PRO:HG3	1:T:658:PRO:HB2	2.01	0.43
1:L:252:TYR:CD2	1:L:374:GLN:HB2	2.53	0.43
1:M:657:ASN:HA	1:M:658:PRO:HD3	1.70	0.43
1:T:365:PHE:CE2	1:T:367:ALA:HB3	2.54	0.43
1:T:714:THR:CG2	1:T:715:VAL:N	2.81	0.43
1:B:714:THR:CG2	1:B:715:VAL:N	2.81	0.43
1:C:403:LEU:HA	1:C:407:ASN:HD22	1.82	0.43
1:C:445:LEU:HD12	1:C:463:PHE:CE1	2.54	0.43
1:D:286:ARG:NH1	1:D:288:HIS:NE2	2.67	0.43
1:E:580:VAL:HG22	1:Q:484:TYR:CZ	2.53	0.43
1:F:388:GLY:HA3	1:G:705:TYR:HA	2.00	0.43
1:F:480:PRO:HG3	1:P:511:LEU:HD11	2.00	0.43
1:F:584:LEU:HD13	1:P:488:ARG:NH1	2.33	0.43
1:H:416:GLU:H	1:H:416:GLU:HG2	1.59	0.43
1:I:613:TYR:HA	1:I:727:ILE:O	2.18	0.43
1:I:714:THR:CG2	1:I:715:VAL:N	2.81	0.43
1:J:634:LEU:HD12	1:O:478:TRP:N	2.33	0.43
1:K:714:THR:CG2	1:K:715:VAL:N	2.81	0.43
1:L:429:SER:HB3	1:L:432:ARG:HB2	2.00	0.43
1:L:608:GLN:CA	1:L:608:GLN:HE21	2.32	0.43
1:L:613:TYR:HA	1:L:727:ILE:O	2.18	0.43
1:M:365:PHE:CE2	1:M:367:ALA:HB3	2.54	0.43
1:N:286:ARG:NH1	1:N:288:HIS:NE2	2.67	0.43
1:R:445:LEU:HD12	1:R:463:PHE:CE1	2.54	0.43
1:T:445:LEU:HD12	1:T:463:PHE:CE1	2.54	0.43
1:A:389:ARG:NE	1:D:699:ILE:HD11	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:TYR:CZ	1:A:465:GLN:HB2	2.54	0.43
1:B:252:TYR:CD2	1:B:374:GLN:HB2	2.53	0.43
1:C:249:LEU:HD13	1:C:372:VAL:HB	2.01	0.43
1:E:502:PRO:HG2	1:I:446:ASN:C	2.38	0.43
1:G:443:TYR:CZ	1:G:465:GLN:HB2	2.54	0.43
1:G:608:GLN:HE21	1:G:608:GLN:HA	1.82	0.43
1:G:613:TYR:HA	1:G:727:ILE:O	2.18	0.43
1:G:714:THR:CG2	1:G:715:VAL:N	2.81	0.43
1:H:249:LEU:HD13	1:H:372:VAL:HB	2.01	0.43
1:H:445:LEU:HD12	1:H:463:PHE:CE1	2.54	0.43
1:I:365:PHE:CE2	1:I:367:ALA:HB3	2.54	0.43
1:K:608:GLN:HE21	1:K:608:GLN:CA	2.32	0.43
1:L:249:LEU:HD13	1:L:372:VAL:HB	2.00	0.43
1:L:488:ARG:C	1:L:489:LEU:HD12	2.38	0.43
1:M:250:PRO:HG3	1:N:658:PRO:HB2	2.01	0.43
1:M:429:SER:HB3	1:M:432:ARG:HB2	2.00	0.43
1:M:519:ASN:HB3	1:M:520:PRO:CD	2.36	0.43
1:O:252:TYR:CD2	1:O:374:GLN:HB2	2.53	0.43
1:O:443:TYR:CZ	1:O:465:GLN:HB2	2.54	0.43
1:Q:443:TYR:CZ	1:Q:465:GLN:HB2	2.54	0.43
1:Q:445:LEU:HD12	1:Q:463:PHE:CE1	2.54	0.43
1:R:286:ARG:NH1	1:R:288:HIS:NE2	2.67	0.43
1:S:286:ARG:NH1	1:S:288:HIS:NE2	2.67	0.43
1:S:445:LEU:HD12	1:S:463:PHE:CE1	2.54	0.43
1:A:291:PHE:CE2	1:A:299:LEU:HD12	2.53	0.43
1:A:337:THR:CG2	1:E:405:THR:HG21	2.49	0.43
1:A:429:SER:HB3	1:A:432:ARG:HB2	2.00	0.43
1:B:429:SER:HB3	1:B:432:ARG:HB2	2.00	0.43
1:C:429:SER:HB3	1:C:432:ARG:HB2	2.00	0.43
1:D:714:THR:CG2	1:D:715:VAL:N	2.81	0.43
1:G:519:ASN:HA	1:G:538:HIS:CD2	2.54	0.43
1:H:482:PRO:HD3	1:H:605:MET:HE3	1.99	0.43
1:K:252:TYR:CD2	1:K:374:GLN:HB2	2.53	0.43
1:K:407:ASN:HD21	1:Q:224:SER:H	1.66	0.43
1:K:519:ASN:HB3	1:K:520:PRO:CD	2.36	0.43
1:L:608:GLN:HE21	1:L:608:GLN:HA	1.82	0.43
1:M:445:LEU:HD12	1:M:463:PHE:CE1	2.54	0.43
1:P:249:LEU:HD13	1:P:372:VAL:HB	2.01	0.43
1:P:286:ARG:NH1	1:P:288:HIS:NE2	2.67	0.43
1:P:443:TYR:CZ	1:P:465:GLN:HB2	2.54	0.43
1:Q:286:ARG:NH1	1:Q:288:HIS:NE2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:365:PHE:CE2	1:Q:367:ALA:HB3	2.54	0.43
1:S:608:GLN:HE21	1:S:608:GLN:CA	2.32	0.43
1:T:443:TYR:CZ	1:T:465:GLN:HB2	2.54	0.43
1:B:286:ARG:NH1	1:B:288:HIS:NE2	2.67	0.43
1:C:519:ASN:HA	1:C:538:HIS:CD2	2.54	0.43
1:E:735:ASN:ND2	1:Q:351:PRO:HG3	2.34	0.43
1:F:443:TYR:CZ	1:F:465:GLN:HB2	2.53	0.43
1:H:286:ARG:NH1	1:H:288:HIS:NE2	2.67	0.43
1:H:576:GLN:NE2	1:H:595:THR:HG23	2.34	0.43
1:J:555:LEU:HA	1:O:463:PHE:CE2	2.52	0.43
1:L:435:ASN:HA	1:L:436:PRO:HD3	1.83	0.43
1:L:519:ASN:HA	1:L:538:HIS:CD2	2.54	0.43
1:M:443:TYR:CZ	1:M:465:GLN:HB2	2.54	0.43
1:P:714:THR:CG2	1:P:715:VAL:N	2.81	0.43
1:Q:249:LEU:HD13	1:Q:372:VAL:HB	2.01	0.43
1:Q:608:GLN:HE21	1:Q:608:GLN:CA	2.32	0.43
1:R:249:LEU:HD13	1:R:372:VAL:HB	2.01	0.43
1:T:576:GLN:NE2	1:T:595:THR:HG23	2.34	0.43
1:A:477:ASN:C	1:C:634:LEU:HD12	2.39	0.43
1:A:576:GLN:NE2	1:A:595:THR:HG23	2.34	0.43
1:A:714:THR:CG2	1:A:715:VAL:N	2.81	0.43
1:C:608:GLN:HE21	1:C:608:GLN:CA	2.32	0.43
1:E:500:ASN:C	1:E:502:PRO:HD3	2.39	0.43
1:E:714:THR:CG2	1:E:715:VAL:N	2.81	0.43
1:F:286:ARG:NH1	1:F:288:HIS:NE2	2.67	0.43
1:J:367:ALA:HB2	1:M:396:GLU:HG3	2.00	0.43
1:J:576:GLN:NE2	1:J:595:THR:HG23	2.34	0.43
1:K:365:PHE:CE2	1:K:367:ALA:HB3	2.54	0.43
1:K:405:THR:HG21	1:S:337:THR:HG22	2.01	0.43
1:K:443:TYR:CZ	1:K:465:GLN:HB2	2.54	0.43
1:K:445:LEU:HD12	1:K:463:PHE:CE1	2.54	0.43
1:L:714:THR:CG2	1:L:715:VAL:N	2.81	0.43
1:M:647:ILE:HD12	1:M:647:ILE:N	2.34	0.43
1:N:443:TYR:CZ	1:N:465:GLN:HB2	2.54	0.43
1:O:365:PHE:CE2	1:O:367:ALA:HB3	2.54	0.43
1:P:452:THR:O	1:P:457:ASN:ND2	2.52	0.43
1:P:608:GLN:HA	1:P:608:GLN:HE21	1.82	0.43
1:Q:372:VAL:HA	1:Q:373:PRO:HD3	1.87	0.43
1:R:443:TYR:CZ	1:R:465:GLN:HB2	2.54	0.43
1:R:458:GLN:HG2	1:R:459:SER:N	2.29	0.43
1:R:576:GLN:NE2	1:R:595:THR:HG23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:296:TRP:CD1	1:S:727:ILE:HG21	2.54	0.43
1:S:570:ASN:HA	1:S:571:PRO:HD3	1.85	0.43
1:T:252:TYR:CD2	1:T:374:GLN:HB2	2.53	0.43
1:B:519:ASN:HA	1:B:538:HIS:CD2	2.54	0.43
1:C:365:PHE:CE2	1:C:367:ALA:HB3	2.54	0.43
1:D:445:LEU:HD12	1:D:463:PHE:CE1	2.54	0.43
1:E:396:GLU:CB	1:F:366:PRO:HB2	2.46	0.43
1:E:443:TYR:CZ	1:E:465:GLN:HB2	2.54	0.43
1:E:519:ASN:HA	1:E:538:HIS:CD2	2.54	0.43
1:F:365:PHE:CE2	1:F:367:ALA:HB3	2.54	0.43
1:F:576:GLN:NE2	1:F:595:THR:HG23	2.34	0.43
1:G:286:ARG:NH1	1:G:288:HIS:NE2	2.67	0.43
1:G:304:TRP:CZ3	1:G:732:LEU:HB3	2.36	0.43
1:H:500:ASN:C	1:H:502:PRO:HD3	2.39	0.43
1:H:601:ALA:HA	1:H:605:MET:HE1	2.01	0.43
1:I:358:HIS:CE1	1:Q:435:ASN:H	2.37	0.43
1:I:445:LEU:HD12	1:I:463:PHE:CE1	2.54	0.43
1:I:519:ASN:HA	1:I:538:HIS:CD2	2.54	0.43
1:I:532:GLU:OE2	1:I:562:ASP:OD2	2.37	0.43
1:J:304:TRP:CZ3	1:J:732:LEU:HB3	2.36	0.43
1:J:372:VAL:HA	1:J:373:PRO:HD3	1.87	0.43
1:J:611:ASP:OD1	1:J:730:ARG:HG3	2.19	0.43
1:K:576:GLN:NE2	1:K:595:THR:HG23	2.34	0.43
1:N:379:THR:CG2	1:N:391:SER:H	2.21	0.43
1:N:429:SER:HB3	1:N:432:ARG:HB2	2.00	0.43
1:N:714:THR:CG2	1:N:715:VAL:N	2.81	0.43
1:O:445:LEU:HD12	1:O:463:PHE:CE1	2.54	0.43
1:O:663:SER:HA	1:O:664:PRO:HD3	1.84	0.43
1:O:714:THR:CG2	1:O:715:VAL:N	2.81	0.43
1:P:365:PHE:CE2	1:P:367:ALA:HB3	2.54	0.43
1:P:519:ASN:HA	1:P:538:HIS:CD2	2.54	0.43
1:P:608:GLN:HE21	1:P:608:GLN:CA	2.31	0.43
1:Q:435:ASN:HA	1:Q:436:PRO:HD3	1.83	0.43
1:R:365:PHE:CE2	1:R:367:ALA:HB3	2.54	0.43
1:R:611:ASP:OD1	1:R:730:ARG:HG3	2.19	0.43
1:S:249:LEU:HD13	1:S:372:VAL:HB	2.00	0.43
1:T:608:GLN:HE21	1:T:608:GLN:CA	2.32	0.43
1:T:658:PRO:HA	1:T:659:PRO:HD3	1.78	0.43
1:A:249:LEU:HD13	1:A:372:VAL:HB	2.01	0.42
1:A:365:PHE:CE2	1:A:367:ALA:HB3	2.54	0.42
1:B:304:TRP:CZ3	1:B:732:LEU:HB3	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:GLN:HE21	1:B:608:GLN:CA	2.32	0.42
1:C:249:LEU:HA	1:C:250:PRO:HD3	1.81	0.42
1:C:443:TYR:CZ	1:C:465:GLN:HB2	2.54	0.42
1:D:500:ASN:C	1:D:502:PRO:HD3	2.39	0.42
1:D:576:GLN:NE2	1:D:595:THR:HG23	2.34	0.42
1:G:576:GLN:NE2	1:G:595:THR:HG23	2.34	0.42
1:H:443:TYR:CZ	1:H:465:GLN:HB2	2.54	0.42
1:H:519:ASN:CB	1:H:520:PRO:CD	2.93	0.42
1:H:532:GLU:OE2	1:H:562:ASP:OD2	2.37	0.42
1:I:296:TRP:CD1	1:I:727:ILE:HG21	2.54	0.42
1:I:647:ILE:N	1:I:647:ILE:HD12	2.34	0.42
1:J:249:LEU:HD13	1:J:372:VAL:HB	2.01	0.42
1:J:500:ASN:C	1:J:502:PRO:HD3	2.39	0.42
1:J:532:GLU:OE2	1:J:562:ASP:OD2	2.37	0.42
1:J:570:ASN:HA	1:J:571:PRO:HD3	1.85	0.42
1:M:576:GLN:NE2	1:M:595:THR:HG23	2.34	0.42
1:O:608:GLN:HE21	1:O:608:GLN:CA	2.32	0.42
1:P:500:ASN:C	1:P:502:PRO:HD3	2.39	0.42
1:S:443:TYR:CZ	1:S:465:GLN:HB2	2.54	0.42
1:S:519:ASN:HA	1:S:538:HIS:CD2	2.54	0.42
1:T:611:ASP:OD1	1:T:730:ARG:HG3	2.19	0.42
1:A:286:ARG:NH1	1:A:288:HIS:NE2	2.66	0.42
1:A:463:PHE:CE2	1:C:555:LEU:HA	2.52	0.42
1:A:519:ASN:HA	1:A:538:HIS:CD2	2.54	0.42
1:B:249:LEU:HD13	1:B:372:VAL:HB	2.01	0.42
1:B:603:PRO:HA	1:H:629:PHE:CD2	2.47	0.42
1:C:581:ALA:O	1:D:485:ARG:HD3	2.19	0.42
1:C:603:PRO:CA	1:D:629:PHE:HD2	2.24	0.42
1:D:647:ILE:HD12	1:D:647:ILE:N	2.34	0.42
1:E:296:TRP:CD1	1:E:727:ILE:HG21	2.54	0.42
1:E:365:PHE:CE2	1:E:367:ALA:HB3	2.54	0.42
1:E:576:GLN:NE2	1:E:595:THR:HG23	2.34	0.42
1:F:519:ASN:HA	1:F:538:HIS:CD2	2.54	0.42
1:F:579:THR:HB	1:P:508:LYS:HG3	2.00	0.42
1:G:249:LEU:HD13	1:G:372:VAL:HB	2.01	0.42
1:G:365:PHE:CE2	1:G:367:ALA:HB3	2.54	0.42
1:G:647:ILE:HD12	1:G:647:ILE:N	2.34	0.42
1:H:304:TRP:CZ3	1:H:732:LEU:HB3	2.36	0.42
1:K:482:PRO:HD3	1:K:605:MET:HE3	2.01	0.42
1:L:405:THR:O	1:P:222:GLY:O	2.38	0.42
1:L:500:ASN:C	1:L:502:PRO:HD3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:262:SER:HA	1:M:272:TYR:CE2	2.55	0.42
1:M:296:TRP:CD1	1:M:727:ILE:HG21	2.55	0.42
1:O:296:TRP:CD1	1:O:727:ILE:HG21	2.55	0.42
1:Q:262:SER:HA	1:Q:272:TYR:CE2	2.54	0.42
1:Q:576:GLN:NE2	1:Q:595:THR:HG23	2.34	0.42
1:R:296:TRP:CD1	1:R:727:ILE:HG21	2.54	0.42
1:R:500:ASN:C	1:R:502:PRO:HD3	2.39	0.42
1:R:519:ASN:HA	1:R:538:HIS:CD2	2.54	0.42
1:R:532:GLU:OE2	1:R:562:ASP:OD2	2.37	0.42
1:R:647:ILE:HD12	1:R:647:ILE:N	2.34	0.42
1:S:435:ASN:HA	1:S:436:PRO:HD3	1.83	0.42
1:S:714:THR:CG2	1:S:715:VAL:N	2.81	0.42
1:C:532:GLU:OE2	1:C:562:ASP:OD2	2.37	0.42
1:C:613:TYR:HA	1:C:727:ILE:O	2.18	0.42
1:D:532:GLU:OE2	1:D:562:ASP:OD2	2.37	0.42
1:F:446:ASN:HD21	1:P:552:ASN:ND2	2.17	0.42
1:F:532:GLU:OE2	1:F:562:ASP:OD2	2.37	0.42
1:F:579:THR:HB	1:P:508:LYS:CG	2.49	0.42
1:F:608:GLN:HE21	1:F:608:GLN:CA	2.32	0.42
1:G:500:ASN:C	1:G:502:PRO:HD3	2.39	0.42
1:H:252:TYR:CD2	1:H:374:GLN:HB2	2.53	0.42
1:H:519:ASN:HA	1:H:538:HIS:CD2	2.54	0.42
1:I:443:TYR:CZ	1:I:465:GLN:HB2	2.54	0.42
1:J:443:TYR:CZ	1:J:465:GLN:HB2	2.54	0.42
1:J:445:LEU:HD12	1:J:463:PHE:CE1	2.54	0.42
1:J:484:TYR:CZ	1:O:580:VAL:HG22	2.54	0.42
1:L:379:THR:CG2	1:L:391:SER:H	2.21	0.42
1:L:576:GLN:NE2	1:L:595:THR:HG23	2.34	0.42
1:M:249:LEU:HD13	1:M:372:VAL:HB	2.00	0.42
1:M:519:ASN:HA	1:M:538:HIS:CD2	2.54	0.42
1:N:296:TRP:CD1	1:N:727:ILE:HG21	2.55	0.42
1:N:576:GLN:NE2	1:N:595:THR:HG23	2.34	0.42
1:O:519:ASN:HA	1:O:538:HIS:CD2	2.54	0.42
1:O:576:GLN:NE2	1:O:595:THR:HG23	2.34	0.42
1:P:601:ALA:HA	1:P:605:MET:HE1	2.00	0.42
1:S:500:ASN:C	1:S:502:PRO:HD3	2.39	0.42
1:S:532:GLU:OE2	1:S:562:ASP:OD2	2.38	0.42
1:T:249:LEU:HD13	1:T:372:VAL:HB	2.01	0.42
1:T:429:SER:HB3	1:T:432:ARG:HB2	2.00	0.42
1:T:647:ILE:N	1:T:647:ILE:HD12	2.34	0.42
1:A:296:TRP:CD1	1:A:727:ILE:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:LEU:HD12	1:A:463:PHE:CE1	2.54	0.42
1:B:435:ASN:HA	1:B:436:PRO:HD3	1.83	0.42
1:B:445:LEU:HD12	1:B:463:PHE:CE1	2.54	0.42
1:C:286:ARG:NH1	1:C:288:HIS:NE2	2.67	0.42
1:C:435:ASN:HA	1:C:436:PRO:HD3	1.83	0.42
1:D:304:TRP:CZ3	1:D:732:LEU:HB3	2.36	0.42
1:D:519:ASN:HA	1:D:538:HIS:CD2	2.54	0.42
1:D:608:GLN:HE21	1:D:608:GLN:CA	2.31	0.42
1:E:299:LEU:HD23	1:E:299:LEU:C	2.40	0.42
1:E:435:ASN:H	1:Q:358:HIS:CE1	2.37	0.42
1:E:445:LEU:HD12	1:E:463:PHE:CE1	2.54	0.42
1:E:608:GLN:HE21	1:E:608:GLN:CA	2.32	0.42
1:E:611:ASP:OD1	1:E:730:ARG:HG3	2.20	0.42
1:F:249:LEU:HD13	1:F:372:VAL:HB	2.01	0.42
1:G:296:TRP:CD1	1:G:727:ILE:HG21	2.54	0.42
1:G:608:GLN:HE21	1:G:608:GLN:CA	2.31	0.42
1:H:365:PHE:CE2	1:H:367:ALA:HB3	2.54	0.42
1:I:452:THR:O	1:I:457:ASN:ND2	2.53	0.42
1:I:601:ALA:HA	1:I:605:MET:HE1	2.01	0.42
1:I:634:LEU:HD12	1:Q:478:TRP:N	2.34	0.42
1:L:262:SER:HA	1:L:272:TYR:CE2	2.55	0.42
1:L:286:ARG:NH1	1:L:288:HIS:NE2	2.67	0.42
1:L:365:PHE:CE2	1:L:367:ALA:HB3	2.54	0.42
1:L:452:THR:O	1:L:457:ASN:ND2	2.53	0.42
1:L:611:ASP:OD1	1:L:730:ARG:HG3	2.19	0.42
1:M:379:THR:CG2	1:M:391:SER:H	2.21	0.42
1:M:532:GLU:OE2	1:M:562:ASP:OD2	2.37	0.42
1:N:445:LEU:HD12	1:N:463:PHE:CE1	2.54	0.42
1:O:299:LEU:HD23	1:O:299:LEU:C	2.40	0.42
1:R:277:THR:HA	1:R:278:PRO:HD3	1.87	0.42
1:A:601:ALA:HB3	1:C:601:ALA:HB3	2.02	0.42
1:B:299:LEU:C	1:B:299:LEU:HD23	2.40	0.42
1:B:647:ILE:HD12	1:B:647:ILE:N	2.34	0.42
1:D:262:SER:HA	1:D:272:TYR:CE2	2.55	0.42
1:E:488:ARG:NH2	1:I:584:LEU:HB3	2.34	0.42
1:F:500:ASN:C	1:F:502:PRO:HD3	2.39	0.42
1:G:445:LEU:HD12	1:G:463:PHE:CE1	2.54	0.42
1:J:262:SER:HA	1:J:272:TYR:CE2	2.55	0.42
1:J:296:TRP:CD1	1:J:727:ILE:HG21	2.54	0.42
1:K:296:TRP:CD1	1:K:727:ILE:HG21	2.54	0.42
1:K:429:SER:HB3	1:K:432:ARG:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:611:ASP:OD1	1:K:730:ARG:HG3	2.20	0.42
1:L:443:TYR:CZ	1:L:465:GLN:HB2	2.54	0.42
1:M:304:TRP:CZ3	1:M:732:LEU:HB3	2.36	0.42
1:M:452:THR:O	1:M:457:ASN:ND2	2.53	0.42
1:O:249:LEU:HD13	1:O:372:VAL:HB	2.01	0.42
1:O:262:SER:HA	1:O:272:TYR:CE2	2.55	0.42
1:O:286:ARG:NH1	1:O:288:HIS:NE2	2.67	0.42
1:Q:296:TRP:CD1	1:Q:727:ILE:HG21	2.54	0.42
1:Q:500:ASN:C	1:Q:502:PRO:HD3	2.39	0.42
1:R:404:ARG:HG2	1:T:222:GLY:HA2	2.01	0.42
1:S:365:PHE:CE2	1:S:367:ALA:HB3	2.54	0.42
1:S:611:ASP:OD1	1:S:730:ARG:HG3	2.19	0.42
1:T:286:ARG:NH1	1:T:288:HIS:NE2	2.67	0.42
1:T:296:TRP:CD1	1:T:727:ILE:HG21	2.54	0.42
1:B:611:ASP:OD1	1:B:730:ARG:HG3	2.19	0.42
1:C:227:ASN:HD22	1:C:227:ASN:HA	1.67	0.42
1:C:647:ILE:N	1:C:647:ILE:HD12	2.34	0.42
1:D:249:LEU:HD13	1:D:372:VAL:HB	2.01	0.42
1:G:313:PHE:HB3	1:G:411:PHE:HB3	2.02	0.42
1:G:537:MET:O	1:G:538:HIS:CG	2.73	0.42
1:I:286:ARG:NH1	1:I:288:HIS:NE2	2.67	0.42
1:I:537:MET:O	1:I:538:HIS:CG	2.73	0.42
1:J:608:GLN:HE21	1:J:608:GLN:CA	2.32	0.42
1:K:500:ASN:C	1:K:502:PRO:HD3	2.39	0.42
1:L:532:GLU:OE2	1:L:562:ASP:OD2	2.38	0.42
1:M:611:ASP:OD1	1:M:730:ARG:HG3	2.19	0.42
1:N:365:PHE:CE2	1:N:367:ALA:HB3	2.54	0.42
1:N:532:GLU:OE2	1:N:562:ASP:OD2	2.37	0.42
1:N:537:MET:O	1:N:538:HIS:CG	2.73	0.42
1:P:647:ILE:HD12	1:P:647:ILE:N	2.34	0.42
1:T:452:THR:O	1:T:457:ASN:ND2	2.53	0.42
1:A:608:GLN:HE21	1:A:608:GLN:CA	2.32	0.42
1:A:611:ASP:OD1	1:A:730:ARG:HG3	2.20	0.42
1:B:262:SER:HA	1:B:272:TYR:CE2	2.55	0.42
1:B:296:TRP:CD1	1:B:727:ILE:HG21	2.54	0.42
1:B:365:PHE:CE2	1:B:367:ALA:HB3	2.54	0.42
1:B:658:PRO:HA	1:B:659:PRO:HD3	1.78	0.42
1:C:296:TRP:CD1	1:C:727:ILE:HG21	2.55	0.42
1:C:537:MET:O	1:C:538:HIS:CG	2.73	0.42
1:E:262:SER:HA	1:E:272:TYR:CE2	2.55	0.42
1:E:537:MET:O	1:E:538:HIS:CG	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:SER:HA	1:G:272:TYR:CE2	2.54	0.42
1:H:452:THR:O	1:H:457:ASN:ND2	2.53	0.42
1:H:611:ASP:OD1	1:H:730:ARG:HG3	2.19	0.42
1:H:647:ILE:HD12	1:H:647:ILE:N	2.34	0.42
1:I:262:SER:HA	1:I:272:TYR:CE2	2.55	0.42
1:I:299:LEU:HD23	1:I:299:LEU:C	2.40	0.42
1:J:313:PHE:HB3	1:J:411:PHE:HB3	2.02	0.42
1:J:323:VAL:HG11	1:M:657:ASN:ND2	2.35	0.42
1:J:647:ILE:HD12	1:J:647:ILE:N	2.34	0.42
1:K:519:ASN:CB	1:K:520:PRO:CD	2.93	0.42
1:K:519:ASN:HA	1:K:538:HIS:CD2	2.54	0.42
1:K:532:GLU:OE2	1:K:562:ASP:OD2	2.37	0.42
1:K:625:THR:HA	1:R:608:GLN:HE22	1.84	0.42
1:L:537:MET:O	1:L:538:HIS:CG	2.73	0.42
1:M:537:MET:O	1:M:538:HIS:CG	2.73	0.42
1:R:299:LEU:C	1:R:299:LEU:HD23	2.40	0.42
1:A:259:GLN:HE22	1:E:710:ASN:ND2	2.13	0.42
1:B:313:PHE:HB3	1:B:411:PHE:HB3	2.02	0.42
1:B:576:GLN:NE2	1:B:595:THR:HG23	2.34	0.42
1:C:262:SER:HA	1:C:272:TYR:CE2	2.55	0.42
1:C:299:LEU:HD23	1:C:299:LEU:C	2.40	0.42
1:C:437:LEU:HD23	1:D:374:GLN:NE2	2.34	0.42
1:C:500:ASN:C	1:C:502:PRO:HD3	2.39	0.42
1:D:296:TRP:CD1	1:D:727:ILE:HG21	2.54	0.42
1:D:299:LEU:HD23	1:D:299:LEU:C	2.40	0.42
1:D:404:ARG:NH2	1:O:405:THR:HG22	2.34	0.42
1:D:611:ASP:OD1	1:D:730:ARG:HG3	2.19	0.42
1:J:365:PHE:CE2	1:J:367:ALA:HB3	2.54	0.42
1:J:379:THR:CG2	1:J:391:SER:H	2.21	0.42
1:K:249:LEU:HD13	1:K:372:VAL:HB	2.01	0.42
1:K:396:GLU:CB	1:Q:366:PRO:HB2	2.45	0.42
1:K:570:ASN:HA	1:K:571:PRO:HD3	1.85	0.42
1:M:313:PHE:HB3	1:M:411:PHE:HB3	2.02	0.42
1:M:458:GLN:CD	1:M:458:GLN:H	2.23	0.42
1:N:249:LEU:HD13	1:N:372:VAL:HB	2.01	0.42
1:N:519:ASN:HA	1:N:538:HIS:CD2	2.54	0.42
1:N:611:ASP:OD1	1:N:730:ARG:HG3	2.19	0.42
1:P:296:TRP:CD1	1:P:727:ILE:HG21	2.55	0.42
1:Q:299:LEU:HD23	1:Q:299:LEU:C	2.40	0.42
1:Q:532:GLU:OE2	1:Q:562:ASP:OD2	2.38	0.42
1:Q:647:ILE:N	1:Q:647:ILE:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:483:CYS:HB2	1:R:524:MET:HE1	2.01	0.42
1:S:262:SER:HA	1:S:272:TYR:CE2	2.55	0.42
1:S:647:ILE:N	1:S:647:ILE:HD12	2.35	0.42
1:T:219:ASP:HB3	1:T:220:GLY:H	1.76	0.42
1:A:555:LEU:HA	1:D:463:PHE:CE2	2.55	0.42
1:B:644:PRO:HA	1:B:645:PRO:HD2	1.79	0.42
1:C:452:THR:O	1:C:457:ASN:ND2	2.53	0.42
1:C:714:THR:CG2	1:C:715:VAL:N	2.81	0.42
1:D:443:TYR:CZ	1:D:465:GLN:HB2	2.54	0.42
1:D:452:THR:O	1:D:457:ASN:ND2	2.53	0.42
1:E:398:PHE:CZ	1:I:693:LYS:HG3	2.55	0.42
1:F:262:SER:HA	1:F:272:TYR:CE2	2.55	0.42
1:H:262:SER:HA	1:H:272:TYR:CE2	2.54	0.42
1:H:296:TRP:CD1	1:H:727:ILE:HG21	2.55	0.42
1:I:458:GLN:H	1:I:458:GLN:CD	2.23	0.42
1:J:299:LEU:C	1:J:299:LEU:HD23	2.40	0.42
1:J:405:THR:HG22	1:M:404:ARG:NH2	2.35	0.42
1:J:519:ASN:HA	1:J:538:HIS:CD2	2.54	0.42
1:J:537:MET:O	1:J:538:HIS:CG	2.73	0.42
1:L:313:PHE:HB3	1:L:411:PHE:HB3	2.02	0.42
1:N:458:GLN:CD	1:N:458:GLN:H	2.24	0.42
1:O:313:PHE:HB3	1:O:411:PHE:HB3	2.02	0.42
1:O:337:THR:CG2	1:S:405:THR:HG21	2.50	0.42
1:P:458:GLN:CD	1:P:458:GLN:H	2.24	0.42
1:Q:429:SER:HB3	1:Q:432:ARG:HB2	2.00	0.42
1:Q:611:ASP:OD1	1:Q:730:ARG:HG3	2.19	0.42
1:R:262:SER:HA	1:R:272:TYR:CE2	2.55	0.42
1:R:337:THR:CG2	1:T:405:THR:HG21	2.49	0.42
1:R:537:MET:O	1:R:538:HIS:CG	2.73	0.42
1:S:299:LEU:HD23	1:S:299:LEU:C	2.40	0.42
1:A:313:PHE:HB3	1:A:411:PHE:HB3	2.02	0.42
1:A:647:ILE:N	1:A:647:ILE:HD12	2.34	0.42
1:A:700:GLN:H	1:B:702:THR:CB	2.33	0.42
1:B:458:GLN:CD	1:B:458:GLN:H	2.24	0.42
1:B:500:ASN:C	1:B:502:PRO:HD3	2.39	0.42
1:D:337:THR:CG2	1:O:405:THR:HG21	2.50	0.42
1:E:647:ILE:HD12	1:E:647:ILE:N	2.34	0.42
1:F:299:LEU:HD23	1:F:299:LEU:C	2.40	0.42
1:F:735:ASN:ND2	1:P:351:PRO:HG3	2.35	0.42
1:G:396:GLU:CB	1:H:366:PRO:HB2	2.44	0.42
1:G:429:SER:HB3	1:G:432:ARG:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:491:LYS:HG3	1:G:533:LYS:O	2.20	0.42
1:G:532:GLU:OE2	1:G:562:ASP:OD2	2.37	0.42
1:H:458:GLN:CD	1:H:458:GLN:H	2.24	0.42
1:I:376:GLY:C	1:Q:436:PRO:HD2	2.41	0.42
1:I:658:PRO:HA	1:I:659:PRO:HD3	1.78	0.42
1:J:435:ASN:HA	1:J:436:PRO:HD3	1.83	0.42
1:J:452:THR:O	1:J:457:ASN:ND2	2.53	0.42
1:K:491:LYS:HG3	1:K:533:LYS:O	2.20	0.42
1:M:299:LEU:HD23	1:M:299:LEU:C	2.40	0.42
1:P:262:SER:HA	1:P:272:TYR:CE2	2.55	0.42
1:P:576:GLN:NE2	1:P:595:THR:HG23	2.34	0.42
1:P:601:ALA:HA	1:P:605:MET:CE	2.50	0.42
1:P:611:ASP:OD1	1:P:730:ARG:HG3	2.20	0.42
1:S:219:ASP:HB3	1:S:220:GLY:H	1.76	0.42
1:S:576:GLN:NE2	1:S:595:THR:HG23	2.34	0.42
1:T:313:PHE:HB3	1:T:411:PHE:HB3	2.02	0.42
1:A:601:ALA:HA	1:A:605:MET:CE	2.50	0.41
1:B:452:THR:O	1:B:457:ASN:ND2	2.53	0.41
1:C:313:PHE:HB3	1:C:411:PHE:HB3	2.02	0.41
1:C:611:ASP:OD1	1:C:730:ARG:HG3	2.19	0.41
1:D:362:LEU:HA	1:D:363:PRO:HD3	1.96	0.41
1:D:371:MET:CE	1:Q:659:PRO:HD2	2.50	0.41
1:E:458:GLN:CD	1:E:458:GLN:H	2.24	0.41
1:E:532:GLU:OE2	1:E:562:ASP:OD2	2.37	0.41
1:F:296:TRP:CD1	1:F:727:ILE:HG21	2.54	0.41
1:F:452:THR:O	1:F:457:ASN:ND2	2.53	0.41
1:F:537:MET:O	1:F:538:HIS:CG	2.73	0.41
1:G:452:THR:O	1:G:457:ASN:ND2	2.53	0.41
1:J:286:ARG:NH1	1:J:288:HIS:NE2	2.67	0.41
1:K:262:SER:HA	1:K:272:TYR:CE2	2.55	0.41
1:M:491:LYS:HG3	1:M:533:LYS:O	2.20	0.41
1:N:299:LEU:HD23	1:N:299:LEU:C	2.40	0.41
1:N:647:ILE:N	1:N:647:ILE:HD12	2.34	0.41
1:O:452:THR:O	1:O:457:ASN:ND2	2.53	0.41
1:O:532:GLU:OE2	1:O:562:ASP:OD2	2.38	0.41
1:O:647:ILE:HD12	1:O:647:ILE:N	2.34	0.41
1:O:658:PRO:HA	1:O:659:PRO:HD3	1.78	0.41
1:P:532:GLU:OE2	1:P:562:ASP:OD2	2.38	0.41
1:Q:519:ASN:HA	1:Q:538:HIS:CD2	2.54	0.41
1:Q:537:MET:O	1:Q:538:HIS:CG	2.73	0.41
1:R:601:ALA:HA	1:R:605:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:SER:HA	1:A:272:TYR:CE2	2.55	0.41
1:A:537:MET:O	1:A:538:HIS:CG	2.73	0.41
1:B:405:THR:HG21	1:C:337:THR:HG22	2.02	0.41
1:B:532:GLU:OE2	1:B:562:ASP:OD2	2.38	0.41
1:B:735:ASN:ND2	1:H:351:PRO:HG3	2.34	0.41
1:D:537:MET:O	1:D:538:HIS:CG	2.73	0.41
1:G:372:VAL:HA	1:G:373:PRO:HD3	1.87	0.41
1:I:491:LYS:HG3	1:I:533:LYS:O	2.21	0.41
1:I:601:ALA:HA	1:I:605:MET:CE	2.50	0.41
1:I:608:GLN:HE21	1:I:608:GLN:CA	2.32	0.41
1:J:485:ARG:HD3	1:O:581:ALA:O	2.20	0.41
1:O:491:LYS:HG3	1:O:533:LYS:O	2.20	0.41
1:P:435:ASN:HA	1:P:436:PRO:HD3	1.83	0.41
1:Q:452:THR:O	1:Q:457:ASN:ND2	2.53	0.41
1:R:449:GLN:HA	1:R:459:SER:HA	2.02	0.41
1:S:452:THR:O	1:S:457:ASN:ND2	2.53	0.41
1:S:601:ALA:HA	1:S:605:MET:CE	2.50	0.41
1:T:262:SER:HA	1:T:272:TYR:CE2	2.55	0.41
1:T:519:ASN:HA	1:T:538:HIS:CD2	2.54	0.41
1:T:537:MET:O	1:T:538:HIS:CG	2.73	0.41
1:A:491:LYS:HG3	1:A:533:LYS:O	2.20	0.41
1:A:508:LYS:HG3	1:D:579:THR:HB	2.01	0.41
1:C:405:THR:HG22	1:J:404:ARG:NH2	2.35	0.41
1:C:472:SER:H	1:D:270:ASN:ND2	2.18	0.41
1:C:576:GLN:NE2	1:C:595:THR:HG23	2.34	0.41
1:C:608:GLN:NE2	1:D:626:ASP:N	2.66	0.41
1:D:365:PHE:CE2	1:D:367:ALA:HB3	2.54	0.41
1:E:452:THR:O	1:E:457:ASN:ND2	2.53	0.41
1:E:491:LYS:HG3	1:E:533:LYS:O	2.20	0.41
1:E:601:ALA:HA	1:E:605:MET:CE	2.50	0.41
1:F:259:GLN:HE22	1:G:710:ASN:ND2	2.16	0.41
1:F:458:GLN:CD	1:F:458:GLN:H	2.24	0.41
1:F:611:ASP:OD1	1:F:730:ARG:HG3	2.19	0.41
1:H:299:LEU:HD23	1:H:299:LEU:C	2.40	0.41
1:H:379:THR:CG2	1:H:391:SER:H	2.21	0.41
1:H:608:GLN:HE21	1:H:608:GLN:CA	2.32	0.41
1:I:249:LEU:HD13	1:I:372:VAL:HB	2.01	0.41
1:I:500:ASN:C	1:I:502:PRO:HD3	2.39	0.41
1:I:611:ASP:OD1	1:I:730:ARG:HG3	2.19	0.41
1:J:458:GLN:H	1:J:458:GLN:CD	2.23	0.41
1:J:601:ALA:HA	1:J:605:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:299:LEU:HD23	1:K:299:LEU:C	2.40	0.41
1:K:537:MET:O	1:K:538:HIS:CG	2.73	0.41
1:L:299:LEU:HD23	1:L:299:LEU:C	2.40	0.41
1:M:365:PHE:HA	1:M:366:PRO:HD3	1.82	0.41
1:M:429:SER:HA	1:M:568:THR:HB	2.02	0.41
1:M:608:GLN:HE21	1:M:608:GLN:CA	2.32	0.41
1:N:608:GLN:HE21	1:N:608:GLN:CA	2.32	0.41
1:O:537:MET:O	1:O:538:HIS:CG	2.73	0.41
1:Q:313:PHE:HB3	1:Q:411:PHE:HB3	2.02	0.41
1:S:449:GLN:HA	1:S:459:SER:HA	2.03	0.41
1:S:537:MET:O	1:S:538:HIS:CG	2.73	0.41
1:T:532:GLU:OE2	1:T:562:ASP:OD2	2.38	0.41
1:A:299:LEU:HD23	1:A:299:LEU:C	2.40	0.41
1:A:437:LEU:HD21	1:C:276:SER:OG	2.19	0.41
1:A:519:ASN:HB3	1:A:520:PRO:CD	2.36	0.41
1:A:532:GLU:OE2	1:A:562:ASP:OD2	2.37	0.41
1:B:399:PRO:HD3	1:N:231:ASP:HB2	2.03	0.41
1:B:443:TYR:CZ	1:B:465:GLN:HB2	2.54	0.41
1:B:491:LYS:HG3	1:B:533:LYS:O	2.21	0.41
1:B:594:ARG:HD3	1:B:594:ARG:C	2.41	0.41
1:C:519:ASN:CB	1:C:520:PRO:CD	2.93	0.41
1:D:491:LYS:HG3	1:D:533:LYS:O	2.21	0.41
1:E:313:PHE:HB3	1:E:411:PHE:HB3	2.02	0.41
1:E:634:LEU:HD12	1:I:478:TRP:N	2.35	0.41
1:F:275:TYR:OH	1:G:714:THR:HG21	2.20	0.41
1:F:396:GLU:CB	1:G:366:PRO:HB2	2.47	0.41
1:F:449:GLN:HA	1:F:459:SER:HA	2.02	0.41
1:G:594:ARG:C	1:G:594:ARG:HD3	2.41	0.41
1:G:601:ALA:HA	1:G:605:MET:CE	2.50	0.41
1:G:611:ASP:OD1	1:G:730:ARG:HG3	2.19	0.41
1:G:663:SER:HA	1:G:664:PRO:HD3	1.84	0.41
1:H:491:LYS:HG3	1:H:533:LYS:O	2.21	0.41
1:I:594:ARG:C	1:I:594:ARG:HD3	2.41	0.41
1:J:657:ASN:HA	1:J:658:PRO:HD3	1.71	0.41
1:K:647:ILE:N	1:K:647:ILE:HD12	2.34	0.41
1:N:262:SER:HA	1:N:272:TYR:CE2	2.55	0.41
1:P:537:MET:O	1:P:538:HIS:CG	2.73	0.41
1:Q:702:THR:HB	1:R:700:GLN:HB2	2.03	0.41
1:R:458:GLN:H	1:R:458:GLN:CD	2.24	0.41
1:T:299:LEU:HD23	1:T:299:LEU:C	2.40	0.41
1:T:500:ASN:C	1:T:502:PRO:HD3	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:594:ARG:C	1:T:594:ARG:HD3	2.41	0.41
1:A:351:PRO:HG3	1:D:735:ASN:ND2	2.34	0.41
1:A:372:VAL:HA	1:A:373:PRO:HD3	1.87	0.41
1:A:458:GLN:CD	1:A:458:GLN:H	2.24	0.41
1:C:366:PRO:HB2	1:J:396:GLU:CB	2.44	0.41
1:C:458:GLN:CD	1:C:458:GLN:H	2.24	0.41
1:C:602:LEU:HB2	1:C:605:MET:HG3	2.03	0.41
1:D:365:PHE:HA	1:D:366:PRO:HD3	1.82	0.41
1:D:429:SER:HA	1:D:568:THR:HB	2.02	0.41
1:E:594:ARG:C	1:E:594:ARG:HD3	2.41	0.41
1:G:458:GLN:H	1:G:458:GLN:CD	2.24	0.41
1:J:449:GLN:HA	1:J:459:SER:HA	2.03	0.41
1:K:452:THR:O	1:K:457:ASN:ND2	2.53	0.41
1:L:416:GLU:H	1:L:416:GLU:HG2	1.59	0.41
1:L:501:PHE:HB2	1:L:505:ALA:CB	2.51	0.41
1:L:647:ILE:HD12	1:L:647:ILE:N	2.34	0.41
1:M:449:GLN:HA	1:M:459:SER:HA	2.03	0.41
1:O:602:LEU:HB2	1:O:605:MET:HG3	2.03	0.41
1:P:299:LEU:HD23	1:P:299:LEU:C	2.40	0.41
1:P:313:PHE:HB3	1:P:411:PHE:HB3	2.02	0.41
1:A:250:PRO:HG3	1:H:658:PRO:HB2	2.03	0.41
1:A:446:ASN:C	1:C:502:PRO:HG2	2.40	0.41
1:A:702:THR:HB	1:B:700:GLN:H	1.84	0.41
1:B:449:GLN:HA	1:B:459:SER:HA	2.03	0.41
1:B:537:MET:O	1:B:538:HIS:CG	2.73	0.41
1:C:449:GLN:HA	1:C:459:SER:HA	2.03	0.41
1:D:372:VAL:HA	1:D:373:PRO:HD3	1.87	0.41
1:D:602:LEU:HB2	1:D:605:MET:HG3	2.03	0.41
1:F:594:ARG:C	1:F:594:ARG:HD3	2.41	0.41
1:F:647:ILE:N	1:F:647:ILE:HD12	2.34	0.41
1:G:299:LEU:C	1:G:299:LEU:HD23	2.40	0.41
1:G:337:THR:CG2	1:H:405:THR:HG21	2.50	0.41
1:G:429:SER:HA	1:G:568:THR:HB	2.02	0.41
1:H:313:PHE:HB3	1:H:411:PHE:HB3	2.02	0.41
1:I:576:GLN:NE2	1:I:595:THR:HG23	2.34	0.41
1:J:389:ARG:NE	1:O:699:ILE:HD11	2.32	0.41
1:L:491:LYS:HG3	1:L:533:LYS:O	2.21	0.41
1:L:594:ARG:HD3	1:L:594:ARG:C	2.41	0.41
1:M:372:VAL:HA	1:M:373:PRO:HD3	1.87	0.41
1:M:500:ASN:C	1:M:502:PRO:HD3	2.39	0.41
1:N:435:ASN:HA	1:N:436:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:452:THR:O	1:N:457:ASN:ND2	2.53	0.41
1:O:611:ASP:OD1	1:O:730:ARG:HG3	2.19	0.41
1:R:491:LYS:HG3	1:R:533:LYS:O	2.20	0.41
1:S:429:SER:HA	1:S:568:THR:HB	2.02	0.41
1:A:429:SER:HA	1:A:568:THR:HB	2.02	0.41
1:A:434:MET:HE2	1:A:471:MET:HG3	2.02	0.41
1:A:500:ASN:C	1:A:502:PRO:HD3	2.39	0.41
1:A:501:PHE:HB2	1:A:505:ALA:CB	2.51	0.41
1:A:519:ASN:HD22	1:D:475:ALA:CA	2.33	0.41
1:B:396:GLU:CB	1:N:366:PRO:HB2	2.47	0.41
1:C:429:SER:HA	1:C:568:THR:HB	2.02	0.41
1:E:429:SER:HA	1:E:568:THR:HB	2.02	0.41
1:E:511:LEU:HD21	1:I:480:PRO:CB	2.47	0.41
1:E:629:PHE:CD2	1:I:603:PRO:HA	2.44	0.41
1:G:443:TYR:CE1	1:G:465:GLN:HB2	2.56	0.41
1:H:601:ALA:HA	1:H:605:MET:CE	2.50	0.41
1:I:443:TYR:CE1	1:I:465:GLN:HB2	2.56	0.41
1:K:313:PHE:HB3	1:K:411:PHE:HB3	2.02	0.41
1:K:594:ARG:HD3	1:K:594:ARG:C	2.41	0.41
1:L:429:SER:HA	1:L:568:THR:HB	2.02	0.41
1:L:601:ALA:HA	1:L:605:MET:CE	2.50	0.41
1:O:429:SER:HA	1:O:568:THR:HB	2.02	0.41
1:O:594:ARG:C	1:O:594:ARG:HD3	2.41	0.41
1:P:594:ARG:HD3	1:P:594:ARG:C	2.41	0.41
1:T:429:SER:HA	1:T:568:THR:HB	2.02	0.41
1:T:458:GLN:H	1:T:458:GLN:CD	2.24	0.41
1:T:602:LEU:HB2	1:T:605:MET:HG3	2.03	0.41
1:B:429:SER:HA	1:B:568:THR:HB	2.02	0.41
1:B:449:GLN:HG2	1:H:500:ASN:N	2.36	0.41
1:C:224:SER:H	1:J:407:ASN:HD21	1.69	0.41
1:C:498:ASN:HD22	1:C:498:ASN:HA	1.69	0.41
1:C:594:ARG:C	1:C:594:ARG:HD3	2.41	0.41
1:C:601:ALA:HA	1:C:605:MET:CE	2.51	0.41
1:C:702:THR:CB	1:O:700:GLN:H	2.33	0.41
1:D:449:GLN:HA	1:D:459:SER:HA	2.02	0.41
1:D:458:GLN:H	1:D:458:GLN:CD	2.24	0.41
1:D:594:ARG:C	1:D:594:ARG:HD3	2.41	0.41
1:F:435:ASN:HA	1:F:436:PRO:HD3	1.83	0.41
1:F:491:LYS:HG3	1:F:533:LYS:O	2.21	0.41
1:H:418:VAL:HA	1:H:419:PRO:HD3	1.96	0.41
1:H:519:ASN:HB3	1:H:520:PRO:CD	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:658:PRO:HA	1:H:659:PRO:HD3	1.78	0.41
1:J:429:SER:HA	1:J:568:THR:HB	2.02	0.41
1:J:483:CYS:HB2	1:J:524:MET:HE1	2.03	0.41
1:K:429:SER:HA	1:K:568:THR:HB	2.02	0.41
1:K:443:TYR:CE1	1:K:465:GLN:HB2	2.56	0.41
1:L:277:THR:HA	1:L:278:PRO:HD3	1.87	0.41
1:L:296:TRP:CD1	1:L:727:ILE:HG21	2.54	0.41
1:L:443:TYR:CE1	1:L:465:GLN:HB2	2.56	0.41
1:N:313:PHE:HB3	1:N:411:PHE:HB3	2.02	0.41
1:N:491:LYS:HG3	1:N:533:LYS:O	2.21	0.41
1:Q:277:THR:HA	1:Q:278:PRO:HD3	1.87	0.41
1:Q:449:GLN:HA	1:Q:459:SER:HA	2.02	0.41
1:Q:594:ARG:C	1:Q:594:ARG:HD3	2.41	0.41
1:Q:601:ALA:HA	1:Q:605:MET:CE	2.50	0.41
1:R:313:PHE:HB3	1:R:411:PHE:HB3	2.02	0.41
1:R:452:THR:O	1:R:457:ASN:ND2	2.53	0.41
1:S:443:TYR:CE1	1:S:465:GLN:HB2	2.56	0.41
1:T:601:ALA:HA	1:T:605:MET:CE	2.50	0.41
1:A:452:THR:O	1:A:457:ASN:ND2	2.53	0.41
1:B:372:VAL:HA	1:B:373:PRO:HD3	1.87	0.41
1:B:601:ALA:HA	1:B:605:MET:CE	2.50	0.41
1:C:446:ASN:C	1:D:502:PRO:HG2	2.41	0.41
1:C:491:LYS:HG3	1:C:533:LYS:O	2.21	0.41
1:C:524:MET:CE	1:C:573:ALA:HA	2.47	0.41
1:D:313:PHE:HB3	1:D:411:PHE:HB3	2.02	0.41
1:D:601:ALA:HA	1:D:605:MET:CE	2.50	0.41
1:F:443:TYR:CE1	1:F:465:GLN:HB2	2.56	0.41
1:F:601:ALA:HA	1:F:605:MET:CE	2.50	0.41
1:F:602:LEU:HB2	1:F:605:MET:HG3	2.03	0.41
1:H:429:SER:HA	1:H:568:THR:HB	2.02	0.41
1:H:443:TYR:CE1	1:H:465:GLN:HB2	2.56	0.41
1:H:537:MET:O	1:H:538:HIS:CG	2.73	0.41
1:H:594:ARG:HD3	1:H:594:ARG:C	2.41	0.41
1:I:484:TYR:CZ	1:Q:580:VAL:HG22	2.55	0.41
1:I:501:PHE:HB2	1:I:505:ALA:CB	2.51	0.41
1:J:379:THR:HG21	1:J:391:SER:N	2.22	0.41
1:K:277:THR:HA	1:K:278:PRO:HD3	1.87	0.41
1:K:634:LEU:HD12	1:R:477:ASN:C	2.41	0.41
1:L:404:ARG:NH2	1:P:405:THR:HG22	2.35	0.41
1:L:705:TYR:HA	1:T:388:GLY:HA3	2.03	0.41
1:M:362:LEU:HA	1:M:363:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:443:TYR:CE1	1:M:465:GLN:HB2	2.56	0.41
1:M:488:ARG:HB2	1:M:574:THR:HB	2.03	0.41
1:M:594:ARG:C	1:M:594:ARG:HD3	2.41	0.41
1:M:601:ALA:HA	1:M:605:MET:CE	2.50	0.41
1:N:304:TRP:CZ3	1:N:732:LEU:HB3	2.36	0.41
1:O:396:GLU:CB	1:S:366:PRO:HB2	2.49	0.41
1:O:601:ALA:HA	1:O:605:MET:CE	2.50	0.41
1:P:449:GLN:HA	1:P:459:SER:HA	2.03	0.41
1:P:602:LEU:HB2	1:P:605:MET:HG3	2.03	0.41
1:P:652:THR:HA	1:P:653:PRO:HD3	1.94	0.41
1:R:594:ARG:HD3	1:R:594:ARG:C	2.41	0.41
1:R:608:GLN:HE21	1:R:608:GLN:CA	2.32	0.41
1:S:313:PHE:HB3	1:S:411:PHE:HB3	2.02	0.41
1:S:488:ARG:HB2	1:S:574:THR:HB	2.03	0.41
1:T:443:TYR:CE1	1:T:465:GLN:HB2	2.56	0.41
1:T:449:GLN:HA	1:T:459:SER:HA	2.03	0.41
1:T:491:LYS:HG3	1:T:533:LYS:O	2.20	0.41
1:B:699:ILE:HD11	1:H:389:ARG:NE	2.33	0.41
1:C:591:PRO:HB2	1:D:505:ALA:HB1	2.03	0.41
1:D:259:GLN:HE22	1:O:710:ASN:ND2	2.19	0.41
1:E:488:ARG:HB2	1:E:574:THR:HB	2.03	0.41
1:F:304:TRP:CZ3	1:F:732:LEU:HB3	2.36	0.41
1:G:449:GLN:HA	1:G:459:SER:HA	2.02	0.41
1:G:693:LYS:HA	1:G:693:LYS:HD2	1.90	0.41
1:I:313:PHE:HB3	1:I:411:PHE:HB3	2.02	0.41
1:J:501:PHE:HB2	1:J:505:ALA:CB	2.51	0.41
1:K:449:GLN:HA	1:K:459:SER:HA	2.03	0.41
1:K:601:ALA:HA	1:K:605:MET:HE1	2.03	0.41
1:K:602:LEU:HB2	1:K:605:MET:HG3	2.03	0.41
1:L:519:ASN:CB	1:L:520:PRO:CD	2.93	0.41
1:N:372:VAL:HA	1:N:373:PRO:HD3	1.87	0.41
1:N:429:SER:HA	1:N:568:THR:HB	2.02	0.41
1:N:488:ARG:HB2	1:N:574:THR:HB	2.03	0.41
1:N:506:ALA:O	1:N:508:LYS:HG2	2.21	0.41
1:N:594:ARG:C	1:N:594:ARG:HD3	2.41	0.41
1:P:443:TYR:CE1	1:P:465:GLN:HB2	2.56	0.41
1:Q:458:GLN:CD	1:Q:458:GLN:H	2.24	0.41
1:A:602:LEU:HB2	1:A:605:MET:HG3	2.03	0.40
1:B:693:LYS:HA	1:B:693:LYS:HD2	1.90	0.40
1:D:443:TYR:CE1	1:D:465:GLN:HB2	2.56	0.40
1:D:644:PRO:HA	1:D:645:PRO:HD2	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:698:GLU:OE1	1:H:732:LEU:HA	2.21	0.40
1:I:304:TRP:CZ3	1:I:732:LEU:HB3	2.36	0.40
1:I:407:ASN:HD21	1:R:224:SER:H	1.69	0.40
1:I:449:GLN:HA	1:I:459:SER:HA	2.03	0.40
1:I:488:ARG:HB2	1:I:574:THR:HB	2.03	0.40
1:J:443:TYR:CE1	1:J:465:GLN:HB2	2.56	0.40
1:K:365:PHE:HA	1:K:366:PRO:HD3	1.82	0.40
1:L:458:GLN:CD	1:L:458:GLN:H	2.23	0.40
1:L:658:PRO:HA	1:L:659:PRO:HD3	1.78	0.40
1:N:698:GLU:OE1	1:N:732:LEU:HA	2.22	0.40
1:O:416:GLU:H	1:O:416:GLU:HG2	1.60	0.40
1:Q:443:TYR:CE1	1:Q:465:GLN:HB2	2.56	0.40
1:R:259:GLN:HE22	1:T:710:ASN:ND2	2.18	0.40
1:R:443:TYR:CE1	1:R:465:GLN:HB2	2.56	0.40
1:S:506:ALA:O	1:S:508:LYS:HG2	2.22	0.40
1:T:644:PRO:HA	1:T:645:PRO:HD2	1.79	0.40
1:B:498:ASN:HD22	1:B:498:ASN:HA	1.69	0.40
1:C:426:HIS:HE1	1:D:624:HIS:O	2.04	0.40
1:E:506:ALA:O	1:E:508:LYS:HG2	2.21	0.40
1:E:698:GLU:OE1	1:E:732:LEU:HA	2.22	0.40
1:F:429:SER:HA	1:F:568:THR:HB	2.02	0.40
1:G:506:ALA:O	1:G:508:LYS:HG2	2.22	0.40
1:I:372:VAL:HA	1:I:373:PRO:HD3	1.87	0.40
1:I:429:SER:HA	1:I:568:THR:HB	2.02	0.40
1:J:594:ARG:C	1:J:594:ARG:HD3	2.41	0.40
1:K:249:LEU:HA	1:K:250:PRO:HD3	1.81	0.40
1:M:277:THR:HA	1:M:278:PRO:HD3	1.86	0.40
1:M:501:PHE:HB2	1:M:505:ALA:CB	2.51	0.40
1:M:602:LEU:HB2	1:M:605:MET:HG3	2.03	0.40
1:N:601:ALA:HA	1:N:605:MET:CE	2.50	0.40
1:Q:491:LYS:HG3	1:Q:533:LYS:O	2.20	0.40
1:Q:698:GLU:OE1	1:Q:732:LEU:HA	2.22	0.40
1:R:657:ASN:HA	1:R:658:PRO:HD3	1.70	0.40
1:S:458:GLN:CD	1:S:458:GLN:H	2.23	0.40
1:T:698:GLU:OE1	1:T:732:LEU:HA	2.21	0.40
1:A:389:ARG:O	1:D:733:THR:HG21	2.20	0.40
1:A:693:LYS:HA	1:A:693:LYS:HD2	1.90	0.40
1:B:475:ALA:CA	1:H:519:ASN:HD22	2.32	0.40
1:B:570:ASN:HA	1:B:571:PRO:HD3	1.85	0.40
1:C:418:VAL:HA	1:C:419:PRO:HD3	1.96	0.40
1:E:484:TYR:CZ	1:I:580:VAL:HG22	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:602:LEU:HB2	1:E:605:MET:HG3	2.03	0.40
1:E:657:ASN:HA	1:E:658:PRO:HD3	1.70	0.40
1:F:365:PHE:HA	1:F:366:PRO:HD3	1.82	0.40
1:G:615:GLN:HE21	1:G:615:GLN:HB3	1.75	0.40
1:G:698:GLU:OE1	1:G:732:LEU:HA	2.22	0.40
1:I:500:ASN:HA	1:Q:448:THR:HG1	1.85	0.40
1:J:491:LYS:HG3	1:J:533:LYS:O	2.21	0.40
1:K:374:GLN:NE2	1:R:437:LEU:HD23	2.37	0.40
1:K:483:CYS:HB2	1:K:524:MET:HE1	2.03	0.40
1:L:610:ARG:HB3	1:L:611:ASP:H	1.72	0.40
1:L:698:GLU:OE1	1:L:732:LEU:HA	2.22	0.40
1:M:498:ASN:HD22	1:M:498:ASN:HA	1.69	0.40
1:N:449:GLN:HA	1:N:459:SER:HA	2.02	0.40
1:O:506:ALA:O	1:O:508:LYS:HG2	2.22	0.40
1:P:693:LYS:HD2	1:P:693:LYS:HA	1.90	0.40
1:Q:700:GLN:H	1:R:702:THR:HB	1.86	0.40
1:R:698:GLU:OE1	1:R:732:LEU:HA	2.22	0.40
1:T:570:ASN:HA	1:T:571:PRO:HD3	1.85	0.40
1:A:443:TYR:CE1	1:A:465:GLN:HB2	2.56	0.40
1:A:449:GLN:HA	1:A:459:SER:HA	2.03	0.40
1:A:488:ARG:HB2	1:A:574:THR:HB	2.03	0.40
1:A:594:ARG:C	1:A:594:ARG:HD3	2.41	0.40
1:B:443:TYR:CE1	1:B:465:GLN:HB2	2.56	0.40
1:B:480:PRO:CB	1:H:511:LEU:HD21	2.45	0.40
1:B:602:LEU:HB2	1:B:605:MET:HG3	2.03	0.40
1:C:405:THR:HG21	1:J:337:THR:CG2	2.52	0.40
1:C:475:ALA:CB	1:D:519:ASN:HD22	2.34	0.40
1:C:652:THR:HA	1:C:653:PRO:HD3	1.94	0.40
1:D:396:GLU:HG3	1:O:367:ALA:HB2	2.03	0.40
1:E:286:ARG:NH2	1:I:441:TYR:CD2	2.90	0.40
1:E:443:TYR:CE1	1:E:465:GLN:HB2	2.56	0.40
1:E:584:LEU:HB3	1:Q:488:ARG:NH2	2.36	0.40
1:F:506:ALA:O	1:F:508:LYS:HG2	2.22	0.40
1:H:379:THR:HG21	1:H:391:SER:N	2.22	0.40
1:H:488:ARG:HB2	1:H:574:THR:HB	2.03	0.40
1:K:501:PHE:HB2	1:K:505:ALA:CB	2.51	0.40
1:L:506:ALA:O	1:L:508:LYS:HG2	2.22	0.40
1:N:227:ASN:HD22	1:N:227:ASN:HA	1.67	0.40
1:N:443:TYR:CE1	1:N:465:GLN:HB2	2.56	0.40
1:O:443:TYR:CE1	1:O:465:GLN:HB2	2.56	0.40
1:O:519:ASN:CB	1:O:520:PRO:CD	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:429:SER:HA	1:P:568:THR:HB	2.02	0.40
1:S:594:ARG:HD3	1:S:594:ARG:C	2.41	0.40
1:T:365:PHE:HA	1:T:366:PRO:HD3	1.82	0.40
1:T:506:ALA:O	1:T:508:LYS:HG2	2.22	0.40
1:A:219:ASP:HB3	1:A:220:GLY:H	1.76	0.40
1:A:622:ILE:HA	1:A:623:PRO:HD3	1.97	0.40
1:C:657:ASN:HA	1:C:658:PRO:HD3	1.70	0.40
1:D:698:GLU:OE1	1:D:732:LEU:HA	2.21	0.40
1:E:576:GLN:HE21	1:E:576:GLN:HB2	1.67	0.40
1:E:693:LYS:HA	1:E:693:LYS:HD2	1.90	0.40
1:G:501:PHE:HB2	1:G:505:ALA:CB	2.51	0.40
1:G:659:PRO:HD2	1:H:371:MET:CE	2.51	0.40
1:H:506:ALA:O	1:H:508:LYS:HG2	2.22	0.40
1:I:498:ASN:HD22	1:I:498:ASN:HA	1.69	0.40
1:I:630:HIS:O	1:I:632:SER:N	2.53	0.40
1:K:508:LYS:HG3	1:R:579:THR:HB	2.03	0.40
1:L:488:ARG:HB2	1:L:574:THR:HB	2.03	0.40
1:L:602:LEU:HB2	1:L:605:MET:HG3	2.03	0.40
1:N:482:PRO:HD3	1:N:605:MET:HE3	2.03	0.40
1:N:500:ASN:C	1:N:502:PRO:HD3	2.39	0.40
1:N:519:ASN:CB	1:N:520:PRO:CD	2.93	0.40
1:Q:429:SER:HA	1:Q:568:THR:HB	2.02	0.40
1:R:379:THR:HG21	1:R:391:SER:N	2.22	0.40
1:R:451:THR:HG21	1:R:460:ARG:CZ	2.52	0.40
1:R:506:ALA:O	1:R:508:LYS:HG2	2.22	0.40
1:R:519:ASN:CB	1:R:520:PRO:CD	2.93	0.40

All (34) 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:B:657:ASN:OD1	1:P:455:THR:OG1[5_445]	1.30	0.90
1:E:456:THR:OG1	1:K:469:GLN:O[3_445]	1.45	0.75
1:C:267:SER:C	1:L:455:THR:CG2[4_445]	1.62	0.58
1:B:657:ASN:CG	1:P:455:THR:OG1[5_445]	1.65	0.55
1:C:267:SER:O	1:L:456:THR:OG1[4_445]	1.65	0.55
1:A:455:THR:OG1	1:L:469:GLN:CA[4_445]	1.77	0.43
1:A:456:THR:CG2	1:L:263:GLN:CG[6_445]	1.83	0.37
1:C:267:SER:OG	1:L:455:THR:CB[4_445]	1.87	0.33
1:B:455:THR:OG1	1:Q:254:ASN:OD1[3_545]	1.90	0.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:SER:CA	1:L:455:THR:C[4_445]	1.91	0.29
1:C:268:ASN:N	1:L:456:THR:N[4_445]	1.93	0.27
1:B:657:ASN:ND2	1:P:455:THR:OG1[5_445]	1.94	0.26
1:C:268:ASN:N	1:L:455:THR:CG2[4_445]	1.95	0.25
1:N:330:THR:CG2	1:P:452:THR:O[5_445]	1.95	0.25
1:E:455:THR:OG1	1:G:272:TYR:CE2[2_445]	1.96	0.24
1:C:267:SER:CA	1:L:455:THR:O[4_445]	1.99	0.21
1:C:267:SER:N	1:L:456:THR:CB[4_445]	2.01	0.19
1:C:268:ASN:N	1:L:455:THR:CA[4_445]	2.02	0.18
1:C:270:ASN:N	1:L:455:THR:OG1[4_445]	2.02	0.18
1:E:452:THR:OG1	1:G:263:GLN:NE2[2_445]	2.05	0.15
1:C:267:SER:C	1:L:456:THR:OG1[4_445]	2.09	0.11
1:C:267:SER:CB	1:L:455:THR:CB[4_445]	2.10	0.10
1:N:330:THR:OG1	1:P:453:SER:O[5_445]	2.10	0.10
1:N:330:THR:OG1	1:P:453:SER:C[5_445]	2.10	0.10
1:A:454:GLY:O	1:L:469:GLN:O[4_445]	2.11	0.09
1:C:267:SER:O	1:L:455:THR:CG2[4_445]	2.13	0.07
1:E:455:THR:OG1	1:G:272:TYR:CD2[2_445]	2.13	0.07
1:A:455:THR:OG1	1:L:469:GLN:N[4_445]	2.14	0.06
1:C:267:SER:C	1:L:456:THR:N[4_445]	2.15	0.05
1:C:268:ASN:N	1:L:455:THR:C[4_445]	2.16	0.04
1:C:265:GLY:C	1:L:456:THR:CG2[4_445]	2.17	0.03
1:A:455:THR:N	1:L:469:GLN:CB[4_445]	2.18	0.02
1:B:657:ASN:OD1	1:P:455:THR:CB[5_445]	2.19	0.01
1:C:267:SER:CB	1:L:455:THR:CG2[4_445]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	B	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	D	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	E	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	F	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	G	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	H	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	I	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	J	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	K	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	L	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	M	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	N	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	O	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	P	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	Q	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	R	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	S	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
1	T	518/736 (70%)	456 (88%)	51 (10%)	11 (2%)	7	33
All	All	10360/14720 (70%)	9120 (88%)	1020 (10%)	220 (2%)	7	33

All (220) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	450	GLY
1	A	610	ARG
1	A	656	ALA
1	A	709	VAL
1	B	450	GLY
1	B	610	ARG
1	B	656	ALA
1	B	709	VAL
1	C	450	GLY
1	C	610	ARG
1	C	656	ALA
1	C	709	VAL
1	D	450	GLY

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Mol	Chain	Res	Type
1	D	610	ARG
1	D	656	ALA
1	D	709	VAL
1	E	450	GLY
1	E	610	ARG
1	E	656	ALA
1	E	709	VAL
1	F	450	GLY
1	F	610	ARG
1	F	656	ALA
1	F	709	VAL
1	G	450	GLY
1	G	610	ARG
1	G	656	ALA
1	G	709	VAL
1	H	450	GLY
1	H	610	ARG
1	H	656	ALA
1	H	709	VAL
1	I	450	GLY
1	I	610	ARG
1	I	656	ALA
1	I	709	VAL
1	J	450	GLY
1	J	610	ARG
1	J	656	ALA
1	J	709	VAL
1	K	450	GLY
1	K	610	ARG
1	K	656	ALA
1	K	709	VAL
1	L	450	GLY
1	L	610	ARG
1	L	656	ALA
1	L	709	VAL
1	M	450	GLY
1	M	610	ARG
1	M	656	ALA
1	M	709	VAL
1	N	450	GLY
1	N	610	ARG
1	N	656	ALA

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Mol	Chain	Res	Type
1	N	709	VAL
1	O	450	GLY
1	O	610	ARG
1	O	656	ALA
1	O	709	VAL
1	P	450	GLY
1	P	610	ARG
1	P	656	ALA
1	P	709	VAL
1	Q	450	GLY
1	Q	610	ARG
1	Q	656	ALA
1	Q	709	VAL
1	R	450	GLY
1	R	610	ARG
1	R	656	ALA
1	R	709	VAL
1	S	450	GLY
1	S	610	ARG
1	S	656	ALA
1	S	709	VAL
1	T	450	GLY
1	T	610	ARG
1	T	656	ALA
1	T	709	VAL
1	A	264	SER
1	A	452	THR
1	B	264	SER
1	B	452	THR
1	C	264	SER
1	C	452	THR
1	D	264	SER
1	D	452	THR
1	E	264	SER
1	E	452	THR
1	F	264	SER
1	F	452	THR
1	G	264	SER
1	G	452	THR
1	H	264	SER
1	H	452	THR
1	I	264	SER

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Mol	Chain	Res	Type
1	I	452	THR
1	J	264	SER
1	J	452	THR
1	K	264	SER
1	K	452	THR
1	L	264	SER
1	L	452	THR
1	M	264	SER
1	M	452	THR
1	N	264	SER
1	N	452	THR
1	O	264	SER
1	O	452	THR
1	P	264	SER
1	P	452	THR
1	Q	264	SER
1	Q	452	THR
1	R	264	SER
1	R	452	THR
1	S	264	SER
1	S	452	THR
1	T	264	SER
1	T	452	THR
1	A	454	GLY
1	B	454	GLY
1	C	454	GLY
1	D	454	GLY
1	E	454	GLY
1	F	454	GLY
1	G	454	GLY
1	H	454	GLY
1	I	454	GLY
1	J	454	GLY
1	K	454	GLY
1	L	454	GLY
1	M	454	GLY
1	N	454	GLY
1	O	454	GLY
1	P	454	GLY
1	Q	454	GLY
1	R	454	GLY
1	S	454	GLY

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Mol	Chain	Res	Type
1	T	454	GLY
1	A	493	ALA
1	B	493	ALA
1	C	493	ALA
1	D	493	ALA
1	E	493	ALA
1	F	493	ALA
1	G	493	ALA
1	H	493	ALA
1	I	493	ALA
1	J	493	ALA
1	K	493	ALA
1	L	493	ALA
1	M	493	ALA
1	N	493	ALA
1	O	493	ALA
1	P	493	ALA
1	Q	493	ALA
1	R	493	ALA
1	S	493	ALA
1	T	493	ALA
1	A	519	ASN
1	A	724	PRO
1	B	519	ASN
1	B	724	PRO
1	C	519	ASN
1	C	724	PRO
1	D	519	ASN
1	D	724	PRO
1	E	519	ASN
1	E	724	PRO
1	F	519	ASN
1	F	724	PRO
1	G	519	ASN
1	G	724	PRO
1	H	519	ASN
1	H	724	PRO
1	I	519	ASN
1	I	724	PRO
1	J	519	ASN
1	J	724	PRO
1	K	519	ASN

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Mol	Chain	Res	Type
1	K	724	PRO
1	L	519	ASN
1	L	724	PRO
1	M	519	ASN
1	M	724	PRO
1	N	519	ASN
1	N	724	PRO
1	O	519	ASN
1	O	724	PRO
1	P	519	ASN
1	P	724	PRO
1	Q	519	ASN
1	Q	724	PRO
1	R	519	ASN
1	R	724	PRO
1	S	519	ASN
1	S	724	PRO
1	T	519	ASN
1	T	724	PRO
1	A	644	PRO
1	B	644	PRO
1	C	644	PRO
1	D	644	PRO
1	E	644	PRO
1	F	644	PRO
1	G	644	PRO
1	H	644	PRO
1	I	644	PRO
1	J	644	PRO
1	K	644	PRO
1	L	644	PRO
1	M	644	PRO
1	N	644	PRO
1	O	644	PRO
1	P	644	PRO
1	Q	644	PRO
1	R	644	PRO
1	S	644	PRO
1	T	644	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	B	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	C	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	D	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	E	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	F	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	G	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	H	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	I	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	J	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	K	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	L	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	M	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	N	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	O	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	P	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	Q	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	R	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	S	459/627 (73%)	438 (95%)	21 (5%)	27	64
1	T	459/627 (73%)	438 (95%)	21 (5%)	27	64
All	All	9180/12540 (73%)	8760 (95%)	420 (5%)	27	64

All (420) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	253	ASN
1	A	267	SER

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Mol	Chain	Res	Type
1	A	285	ASN
1	A	304	TRP
1	A	330	THR
1	A	353	VAL
1	A	404	ARG
1	A	433	LEU
1	A	434	MET
1	A	446	ASN
1	A	451	THR
1	A	479	LEU
1	A	494	ASN
1	A	498	ASN
1	A	576	GLN
1	A	594	ARG
1	A	608	GLN
1	A	615	GLN
1	A	650	LYS
1	A	702	THR
1	B	233	GLN
1	B	253	ASN
1	B	267	SER
1	B	285	ASN
1	B	304	TRP
1	B	330	THR
1	B	353	VAL
1	B	404	ARG
1	B	433	LEU
1	B	434	MET
1	B	446	ASN
1	B	451	THR
1	B	479	LEU
1	B	494	ASN
1	B	498	ASN
1	B	576	GLN
1	B	594	ARG
1	B	608	GLN
1	B	615	GLN
1	B	650	LYS
1	B	702	THR
1	C	233	GLN
1	C	253	ASN
1	C	267	SER

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Mol	Chain	Res	Type
1	C	285	ASN
1	C	304	TRP
1	C	330	THR
1	C	353	VAL
1	C	404	ARG
1	C	433	LEU
1	C	434	MET
1	C	446	ASN
1	C	451	THR
1	C	479	LEU
1	C	494	ASN
1	C	498	ASN
1	C	576	GLN
1	C	594	ARG
1	C	608	GLN
1	C	615	GLN
1	C	650	LYS
1	C	702	THR
1	D	233	GLN
1	D	253	ASN
1	D	267	SER
1	D	285	ASN
1	D	304	TRP
1	D	330	THR
1	D	353	VAL
1	D	404	ARG
1	D	433	LEU
1	D	434	MET
1	D	446	ASN
1	D	451	THR
1	D	479	LEU
1	D	494	ASN
1	D	498	ASN
1	D	576	GLN
1	D	594	ARG
1	D	608	GLN
1	D	615	GLN
1	D	650	LYS
1	D	702	THR
1	E	233	GLN
1	E	253	ASN
1	E	267	SER

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Mol	Chain	Res	Type
1	E	285	ASN
1	E	304	TRP
1	E	330	THR
1	E	353	VAL
1	E	404	ARG
1	E	433	LEU
1	E	434	MET
1	E	446	ASN
1	E	451	THR
1	E	479	LEU
1	E	494	ASN
1	E	498	ASN
1	E	576	GLN
1	E	594	ARG
1	E	608	GLN
1	E	615	GLN
1	E	650	LYS
1	E	702	THR
1	F	233	GLN
1	F	253	ASN
1	F	267	SER
1	F	285	ASN
1	F	304	TRP
1	F	330	THR
1	F	353	VAL
1	F	404	ARG
1	F	433	LEU
1	F	434	MET
1	F	446	ASN
1	F	451	THR
1	F	479	LEU
1	F	494	ASN
1	F	498	ASN
1	F	576	GLN
1	F	594	ARG
1	F	608	GLN
1	F	615	GLN
1	F	650	LYS
1	F	702	THR
1	G	233	GLN
1	G	253	ASN
1	G	267	SER

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Mol	Chain	Res	Type
1	G	285	ASN
1	G	304	TRP
1	G	330	THR
1	G	353	VAL
1	G	404	ARG
1	G	433	LEU
1	G	434	MET
1	G	446	ASN
1	G	451	THR
1	G	479	LEU
1	G	494	ASN
1	G	498	ASN
1	G	576	GLN
1	G	594	ARG
1	G	608	GLN
1	G	615	GLN
1	G	650	LYS
1	G	702	THR
1	H	233	GLN
1	H	253	ASN
1	H	267	SER
1	H	285	ASN
1	H	304	TRP
1	H	330	THR
1	H	353	VAL
1	H	404	ARG
1	H	433	LEU
1	H	434	MET
1	H	446	ASN
1	H	451	THR
1	H	479	LEU
1	H	494	ASN
1	H	498	ASN
1	H	576	GLN
1	H	594	ARG
1	H	608	GLN
1	H	615	GLN
1	H	650	LYS
1	H	702	THR
1	I	233	GLN
1	I	253	ASN
1	I	267	SER

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Mol	Chain	Res	Type
1	I	285	ASN
1	I	304	TRP
1	I	330	THR
1	I	353	VAL
1	I	404	ARG
1	I	433	LEU
1	I	434	MET
1	I	446	ASN
1	I	451	THR
1	I	479	LEU
1	I	494	ASN
1	I	498	ASN
1	I	576	GLN
1	I	594	ARG
1	I	608	GLN
1	I	615	GLN
1	I	650	LYS
1	I	702	THR
1	J	233	GLN
1	J	253	ASN
1	J	267	SER
1	J	285	ASN
1	J	304	TRP
1	J	330	THR
1	J	353	VAL
1	J	404	ARG
1	J	433	LEU
1	J	434	MET
1	J	446	ASN
1	J	451	THR
1	J	479	LEU
1	J	494	ASN
1	J	498	ASN
1	J	576	GLN
1	J	594	ARG
1	J	608	GLN
1	J	615	GLN
1	J	650	LYS
1	J	702	THR
1	K	233	GLN
1	K	253	ASN
1	K	267	SER

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Mol	Chain	Res	Type
1	K	285	ASN
1	K	304	TRP
1	K	330	THR
1	K	353	VAL
1	K	404	ARG
1	K	433	LEU
1	K	434	MET
1	K	446	ASN
1	K	451	THR
1	K	479	LEU
1	K	494	ASN
1	K	498	ASN
1	K	576	GLN
1	K	594	ARG
1	K	608	GLN
1	K	615	GLN
1	K	650	LYS
1	K	702	THR
1	L	233	GLN
1	L	253	ASN
1	L	267	SER
1	L	285	ASN
1	L	304	TRP
1	L	330	THR
1	L	353	VAL
1	L	404	ARG
1	L	433	LEU
1	L	434	MET
1	L	446	ASN
1	L	451	THR
1	L	479	LEU
1	L	494	ASN
1	L	498	ASN
1	L	576	GLN
1	L	594	ARG
1	L	608	GLN
1	L	615	GLN
1	L	650	LYS
1	L	702	THR
1	M	233	GLN
1	M	253	ASN
1	M	267	SER

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Mol	Chain	Res	Type
1	M	285	ASN
1	M	304	TRP
1	M	330	THR
1	M	353	VAL
1	M	404	ARG
1	M	433	LEU
1	M	434	MET
1	M	446	ASN
1	M	451	THR
1	M	479	LEU
1	M	494	ASN
1	M	498	ASN
1	M	576	GLN
1	M	594	ARG
1	M	608	GLN
1	M	615	GLN
1	M	650	LYS
1	M	702	THR
1	N	233	GLN
1	N	253	ASN
1	N	267	SER
1	N	285	ASN
1	N	304	TRP
1	N	330	THR
1	N	353	VAL
1	N	404	ARG
1	N	433	LEU
1	N	434	MET
1	N	446	ASN
1	N	451	THR
1	N	479	LEU
1	N	494	ASN
1	N	498	ASN
1	N	576	GLN
1	N	594	ARG
1	N	608	GLN
1	N	615	GLN
1	N	650	LYS
1	N	702	THR
1	O	233	GLN
1	O	253	ASN
1	O	267	SER

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Mol	Chain	Res	Type
1	O	285	ASN
1	O	304	TRP
1	O	330	THR
1	O	353	VAL
1	O	404	ARG
1	O	433	LEU
1	O	434	MET
1	O	446	ASN
1	O	451	THR
1	O	479	LEU
1	O	494	ASN
1	O	498	ASN
1	O	576	GLN
1	O	594	ARG
1	O	608	GLN
1	O	615	GLN
1	O	650	LYS
1	O	702	THR
1	P	233	GLN
1	P	253	ASN
1	P	267	SER
1	P	285	ASN
1	P	304	TRP
1	P	330	THR
1	P	353	VAL
1	P	404	ARG
1	P	433	LEU
1	P	434	MET
1	P	446	ASN
1	P	451	THR
1	P	479	LEU
1	P	494	ASN
1	P	498	ASN
1	P	576	GLN
1	P	594	ARG
1	P	608	GLN
1	P	615	GLN
1	P	650	LYS
1	P	702	THR
1	Q	233	GLN
1	Q	253	ASN
1	Q	267	SER

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Mol	Chain	Res	Type
1	Q	285	ASN
1	Q	304	TRP
1	Q	330	THR
1	Q	353	VAL
1	Q	404	ARG
1	Q	433	LEU
1	Q	434	MET
1	Q	446	ASN
1	Q	451	THR
1	Q	479	LEU
1	Q	494	ASN
1	Q	498	ASN
1	Q	576	GLN
1	Q	594	ARG
1	Q	608	GLN
1	Q	615	GLN
1	Q	650	LYS
1	Q	702	THR
1	R	233	GLN
1	R	253	ASN
1	R	267	SER
1	R	285	ASN
1	R	304	TRP
1	R	330	THR
1	R	353	VAL
1	R	404	ARG
1	R	433	LEU
1	R	434	MET
1	R	446	ASN
1	R	451	THR
1	R	479	LEU
1	R	494	ASN
1	R	498	ASN
1	R	576	GLN
1	R	594	ARG
1	R	608	GLN
1	R	615	GLN
1	R	650	LYS
1	R	702	THR
1	S	233	GLN
1	S	253	ASN
1	S	267	SER

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Mol	Chain	Res	Type
1	S	285	ASN
1	S	304	TRP
1	S	330	THR
1	S	353	VAL
1	S	404	ARG
1	S	433	LEU
1	S	434	MET
1	S	446	ASN
1	S	451	THR
1	S	479	LEU
1	S	494	ASN
1	S	498	ASN
1	S	576	GLN
1	S	594	ARG
1	S	608	GLN
1	S	615	GLN
1	S	650	LYS
1	S	702	THR
1	T	233	GLN
1	T	253	ASN
1	T	267	SER
1	T	285	ASN
1	T	304	TRP
1	T	330	THR
1	T	353	VAL
1	T	404	ARG
1	T	433	LEU
1	T	434	MET
1	T	446	ASN
1	T	451	THR
1	T	479	LEU
1	T	494	ASN
1	T	498	ASN
1	T	576	GLN
1	T	594	ARG
1	T	608	GLN
1	T	615	GLN
1	T	650	LYS
1	T	702	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (477) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	233	GLN
1	A	268	ASN
1	A	270	ASN
1	A	285	ASN
1	A	349	GLN
1	A	359	GLN
1	A	374	GLN
1	A	407	ASN
1	A	410	GLN
1	A	426	HIS
1	A	428	GLN
1	A	446	ASN
1	A	457	ASN
1	A	494	ASN
1	A	498	ASN
1	A	510	HIS
1	A	519	ASN
1	A	538	HIS
1	A	540	ASN
1	A	552	ASN
1	A	576	GLN
1	A	608	GLN
1	A	646	GLN
1	A	657	ASN
1	A	704	ASN
1	A	710	ASN
1	B	227	ASN
1	B	233	GLN
1	B	268	ASN
1	B	285	ASN
1	B	358	HIS
1	B	374	GLN
1	B	407	ASN
1	B	410	GLN
1	B	426	HIS
1	B	428	GLN
1	B	446	ASN
1	B	457	ASN
1	B	494	ASN
1	B	498	ASN
1	B	510	HIS
1	B	538	HIS

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Mol	Chain	Res	Type
1	B	540	ASN
1	B	576	GLN
1	B	608	GLN
1	B	646	GLN
1	B	657	ASN
1	B	704	ASN
1	B	710	ASN
1	C	227	ASN
1	C	233	GLN
1	C	268	ASN
1	C	270	ASN
1	C	285	ASN
1	C	374	GLN
1	C	407	ASN
1	C	410	GLN
1	C	426	HIS
1	C	428	GLN
1	C	446	ASN
1	C	457	ASN
1	C	494	ASN
1	C	498	ASN
1	C	510	HIS
1	C	519	ASN
1	C	538	HIS
1	C	540	ASN
1	C	552	ASN
1	C	576	GLN
1	C	608	GLN
1	C	646	GLN
1	C	657	ASN
1	C	704	ASN
1	C	710	ASN
1	D	227	ASN
1	D	233	GLN
1	D	268	ASN
1	D	270	ASN
1	D	285	ASN
1	D	374	GLN
1	D	407	ASN
1	D	410	GLN
1	D	426	HIS
1	D	428	GLN

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Mol	Chain	Res	Type
1	D	446	ASN
1	D	457	ASN
1	D	494	ASN
1	D	498	ASN
1	D	510	HIS
1	D	519	ASN
1	D	538	HIS
1	D	540	ASN
1	D	552	ASN
1	D	576	GLN
1	D	608	GLN
1	D	624	HIS
1	D	646	GLN
1	D	657	ASN
1	D	704	ASN
1	D	710	ASN
1	E	227	ASN
1	E	233	GLN
1	E	270	ASN
1	E	285	ASN
1	E	349	GLN
1	E	359	GLN
1	E	374	GLN
1	E	407	ASN
1	E	410	GLN
1	E	426	HIS
1	E	428	GLN
1	E	446	ASN
1	E	457	ASN
1	E	494	ASN
1	E	498	ASN
1	E	510	HIS
1	E	519	ASN
1	E	538	HIS
1	E	540	ASN
1	E	552	ASN
1	E	576	GLN
1	E	608	GLN
1	E	646	GLN
1	E	657	ASN
1	E	704	ASN
1	E	710	ASN

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Mol	Chain	Res	Type
1	F	227	ASN
1	F	233	GLN
1	F	268	ASN
1	F	285	ASN
1	F	358	HIS
1	F	374	GLN
1	F	407	ASN
1	F	410	GLN
1	F	426	HIS
1	F	428	GLN
1	F	446	ASN
1	F	457	ASN
1	F	494	ASN
1	F	498	ASN
1	F	510	HIS
1	F	538	HIS
1	F	540	ASN
1	F	576	GLN
1	F	608	GLN
1	F	646	GLN
1	F	657	ASN
1	F	704	ASN
1	F	710	ASN
1	G	227	ASN
1	G	233	GLN
1	G	285	ASN
1	G	358	HIS
1	G	374	GLN
1	G	407	ASN
1	G	410	GLN
1	G	446	ASN
1	G	457	ASN
1	G	465	GLN
1	G	494	ASN
1	G	498	ASN
1	G	510	HIS
1	G	538	HIS
1	G	540	ASN
1	G	576	GLN
1	G	608	GLN
1	G	646	GLN
1	G	657	ASN

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Mol	Chain	Res	Type
1	G	704	ASN
1	G	710	ASN
1	H	227	ASN
1	H	233	GLN
1	H	268	ASN
1	H	270	ASN
1	H	285	ASN
1	H	349	GLN
1	H	374	GLN
1	H	407	ASN
1	H	410	GLN
1	H	446	ASN
1	H	457	ASN
1	H	465	GLN
1	H	494	ASN
1	H	498	ASN
1	H	510	HIS
1	H	519	ASN
1	H	538	HIS
1	H	540	ASN
1	H	552	ASN
1	H	576	GLN
1	H	608	GLN
1	H	624	HIS
1	H	646	GLN
1	H	657	ASN
1	H	704	ASN
1	H	710	ASN
1	I	227	ASN
1	I	233	GLN
1	I	270	ASN
1	I	285	ASN
1	I	349	GLN
1	I	359	GLN
1	I	374	GLN
1	I	407	ASN
1	I	410	GLN
1	I	426	HIS
1	I	428	GLN
1	I	446	ASN
1	I	457	ASN
1	I	494	ASN

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Mol	Chain	Res	Type
1	I	498	ASN
1	I	510	HIS
1	I	519	ASN
1	I	538	HIS
1	I	540	ASN
1	I	552	ASN
1	I	576	GLN
1	I	608	GLN
1	I	624	HIS
1	I	646	GLN
1	I	657	ASN
1	I	704	ASN
1	I	710	ASN
1	J	227	ASN
1	J	233	GLN
1	J	268	ASN
1	J	270	ASN
1	J	285	ASN
1	J	349	GLN
1	J	359	GLN
1	J	374	GLN
1	J	407	ASN
1	J	410	GLN
1	J	446	ASN
1	J	457	ASN
1	J	465	GLN
1	J	494	ASN
1	J	498	ASN
1	J	510	HIS
1	J	519	ASN
1	J	538	HIS
1	J	540	ASN
1	J	552	ASN
1	J	576	GLN
1	J	608	GLN
1	J	646	GLN
1	J	657	ASN
1	J	704	ASN
1	J	710	ASN
1	K	227	ASN
1	K	233	GLN
1	K	270	ASN

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Mol	Chain	Res	Type
1	K	285	ASN
1	K	349	GLN
1	K	359	GLN
1	K	374	GLN
1	K	407	ASN
1	K	410	GLN
1	K	446	ASN
1	K	457	ASN
1	K	465	GLN
1	K	494	ASN
1	K	498	ASN
1	K	510	HIS
1	K	519	ASN
1	K	538	HIS
1	K	540	ASN
1	K	552	ASN
1	K	576	GLN
1	K	608	GLN
1	K	624	HIS
1	K	646	GLN
1	K	657	ASN
1	K	704	ASN
1	K	710	ASN
1	L	227	ASN
1	L	233	GLN
1	L	285	ASN
1	L	358	HIS
1	L	374	GLN
1	L	407	ASN
1	L	410	GLN
1	L	446	ASN
1	L	457	ASN
1	L	465	GLN
1	L	494	ASN
1	L	498	ASN
1	L	510	HIS
1	L	538	HIS
1	L	540	ASN
1	L	576	GLN
1	L	608	GLN
1	L	646	GLN
1	L	657	ASN

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Mol	Chain	Res	Type
1	L	704	ASN
1	L	710	ASN
1	M	227	ASN
1	M	233	GLN
1	M	285	ASN
1	M	358	HIS
1	M	374	GLN
1	M	407	ASN
1	M	410	GLN
1	M	446	ASN
1	M	457	ASN
1	M	465	GLN
1	M	494	ASN
1	M	498	ASN
1	M	510	HIS
1	M	538	HIS
1	M	540	ASN
1	M	576	GLN
1	M	608	GLN
1	M	646	GLN
1	M	657	ASN
1	M	704	ASN
1	M	710	ASN
1	N	227	ASN
1	N	233	GLN
1	N	285	ASN
1	N	358	HIS
1	N	374	GLN
1	N	407	ASN
1	N	410	GLN
1	N	446	ASN
1	N	457	ASN
1	N	465	GLN
1	N	494	ASN
1	N	498	ASN
1	N	510	HIS
1	N	538	HIS
1	N	540	ASN
1	N	576	GLN
1	N	608	GLN
1	N	646	GLN
1	N	657	ASN

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Mol	Chain	Res	Type
1	N	704	ASN
1	N	710	ASN
1	O	227	ASN
1	O	233	GLN
1	O	285	ASN
1	O	358	HIS
1	O	374	GLN
1	O	407	ASN
1	O	410	GLN
1	O	426	HIS
1	O	428	GLN
1	O	446	ASN
1	O	457	ASN
1	O	494	ASN
1	O	498	ASN
1	O	510	HIS
1	O	538	HIS
1	O	540	ASN
1	O	576	GLN
1	O	608	GLN
1	O	646	GLN
1	O	657	ASN
1	O	704	ASN
1	O	710	ASN
1	P	227	ASN
1	P	233	GLN
1	P	270	ASN
1	P	285	ASN
1	P	349	GLN
1	P	359	GLN
1	P	374	GLN
1	P	407	ASN
1	P	410	GLN
1	P	446	ASN
1	P	457	ASN
1	P	465	GLN
1	P	494	ASN
1	P	498	ASN
1	P	510	HIS
1	P	519	ASN
1	P	538	HIS
1	P	540	ASN

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Mol	Chain	Res	Type
1	P	552	ASN
1	P	576	GLN
1	P	608	GLN
1	P	624	HIS
1	P	646	GLN
1	P	657	ASN
1	P	704	ASN
1	P	710	ASN
1	Q	227	ASN
1	Q	233	GLN
1	Q	270	ASN
1	Q	285	ASN
1	Q	349	GLN
1	Q	359	GLN
1	Q	374	GLN
1	Q	407	ASN
1	Q	410	GLN
1	Q	426	HIS
1	Q	428	GLN
1	Q	446	ASN
1	Q	457	ASN
1	Q	494	ASN
1	Q	498	ASN
1	Q	510	HIS
1	Q	519	ASN
1	Q	538	HIS
1	Q	540	ASN
1	Q	552	ASN
1	Q	576	GLN
1	Q	608	GLN
1	Q	646	GLN
1	Q	704	ASN
1	Q	710	ASN
1	R	227	ASN
1	R	233	GLN
1	R	285	ASN
1	R	358	HIS
1	R	374	GLN
1	R	407	ASN
1	R	410	GLN
1	R	426	HIS
1	R	428	GLN

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Mol	Chain	Res	Type
1	R	446	ASN
1	R	457	ASN
1	R	494	ASN
1	R	498	ASN
1	R	510	HIS
1	R	538	HIS
1	R	540	ASN
1	R	576	GLN
1	R	608	GLN
1	R	646	GLN
1	R	657	ASN
1	R	704	ASN
1	R	710	ASN
1	S	227	ASN
1	S	233	GLN
1	S	268	ASN
1	S	285	ASN
1	S	358	HIS
1	S	374	GLN
1	S	407	ASN
1	S	410	GLN
1	S	446	ASN
1	S	457	ASN
1	S	465	GLN
1	S	494	ASN
1	S	498	ASN
1	S	510	HIS
1	S	538	HIS
1	S	540	ASN
1	S	576	GLN
1	S	608	GLN
1	S	646	GLN
1	S	657	ASN
1	S	704	ASN
1	S	710	ASN
1	T	227	ASN
1	T	233	GLN
1	T	285	ASN
1	T	358	HIS
1	T	374	GLN
1	T	407	ASN
1	T	410	GLN

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Mol	Chain	Res	Type
1	T	446	ASN
1	T	457	ASN
1	T	465	GLN
1	T	494	ASN
1	T	498	ASN
1	T	510	HIS
1	T	538	HIS
1	T	540	ASN
1	T	576	GLN
1	T	608	GLN
1	T	646	GLN
1	T	657	ASN
1	T	704	ASN
1	T	710	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	D5M	J	999	-	22,24,24	0.93	2 (9%)	24,36,36	1.16	2 (8%)
2	D5M	Q	999	-	22,24,24	0.92	2 (9%)	24,36,36	1.16	2 (8%)
2	D5M	K	999	-	22,24,24	0.92	2 (9%)	24,36,36	1.16	2 (8%)
2	D5M	N	999	-	22,24,24	0.94	2 (9%)	24,36,36	1.16	2 (8%)
2	D5M	D	999	-	22,24,24	0.93	2 (9%)	24,36,36	1.15	2 (8%)
2	D5M	R	999	-	22,24,24	0.93	2 (9%)	24,36,36	1.16	2 (8%)
2	D5M	I	999	-	22,24,24	0.92	1 (4%)	24,36,36	1.16	2 (8%)
2	D5M	L	999	-	22,24,24	0.92	1 (4%)	24,36,36	1.15	2 (8%)
2	D5M	O	999	-	22,24,24	0.92	2 (9%)	24,36,36	1.16	2 (8%)
2	D5M	G	999	-	22,24,24	0.93	2 (9%)	24,36,36	1.15	2 (8%)
2	D5M	B	999	-	22,24,24	0.92	1 (4%)	24,36,36	1.16	2 (8%)
2	D5M	H	999	-	22,24,24	0.92	2 (9%)	24,36,36	1.16	2 (8%)
2	D5M	F	999	-	22,24,24	0.92	2 (9%)	24,36,36	1.16	2 (8%)
2	D5M	C	999	-	22,24,24	0.92	1 (4%)	24,36,36	1.17	2 (8%)
2	D5M	M	999	-	22,24,24	0.93	2 (9%)	24,36,36	1.15	2 (8%)
2	D5M	S	999	-	22,24,24	0.92	2 (9%)	24,36,36	1.16	2 (8%)
2	D5M	A	999	-	22,24,24	0.93	2 (9%)	24,36,36	1.16	2 (8%)
2	D5M	T	999	-	22,24,24	0.93	2 (9%)	24,36,36	1.15	2 (8%)
2	D5M	P	999	-	22,24,24	0.92	2 (9%)	24,36,36	1.15	2 (8%)
2	D5M	E	999	-	22,24,24	0.93	2 (9%)	24,36,36	1.16	2 (8%)

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	D5M	J	999	-	-	0/6/22/22	0/3/3/3
2	D5M	Q	999	-	-	0/6/22/22	0/3/3/3
2	D5M	K	999	-	-	0/6/22/22	0/3/3/3
2	D5M	N	999	-	-	0/6/22/22	0/3/3/3
2	D5M	D	999	-	-	0/6/22/22	0/3/3/3
2	D5M	R	999	-	-	0/6/22/22	0/3/3/3
2	D5M	I	999	-	-	0/6/22/22	0/3/3/3
2	D5M	L	999	-	-	0/6/22/22	0/3/3/3
2	D5M	O	999	-	-	0/6/22/22	0/3/3/3
2	D5M	G	999	-	-	0/6/22/22	0/3/3/3
2	D5M	B	999	-	-	0/6/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	H	999	-	-	0/6/22/22	0/3/3/3
2	D5M	F	999	-	-	0/6/22/22	0/3/3/3
2	D5M	C	999	-	-	0/6/22/22	0/3/3/3
2	D5M	M	999	-	-	0/6/22/22	0/3/3/3
2	D5M	S	999	-	-	0/6/22/22	0/3/3/3
2	D5M	A	999	-	-	0/6/22/22	0/3/3/3
2	D5M	T	999	-	-	0/6/22/22	0/3/3/3
2	D5M	P	999	-	-	0/6/22/22	0/3/3/3
2	D5M	E	999	-	-	0/6/22/22	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	999	D5M	C5-C4	2.62	1.47	1.40
2	A	999	D5M	C5-C4	2.62	1.47	1.40
2	E	999	D5M	C5-C4	2.61	1.47	1.40
2	T	999	D5M	C5-C4	2.61	1.47	1.40
2	G	999	D5M	C5-C4	2.60	1.47	1.40
2	F	999	D5M	C5-C4	2.60	1.47	1.40
2	D	999	D5M	C5-C4	2.60	1.47	1.40
2	L	999	D5M	C5-C4	2.60	1.47	1.40
2	M	999	D5M	C5-C4	2.60	1.47	1.40
2	J	999	D5M	C5-C4	2.59	1.47	1.40
2	O	999	D5M	C5-C4	2.59	1.47	1.40
2	R	999	D5M	C5-C4	2.59	1.47	1.40
2	S	999	D5M	C5-C4	2.59	1.47	1.40
2	N	999	D5M	C5-C4	2.59	1.47	1.40
2	C	999	D5M	C5-C4	2.59	1.47	1.40
2	H	999	D5M	C5-C4	2.59	1.47	1.40
2	Q	999	D5M	C5-C4	2.58	1.47	1.40
2	P	999	D5M	C5-C4	2.58	1.47	1.40
2	B	999	D5M	C5-C4	2.57	1.47	1.40
2	K	999	D5M	C5-C4	2.56	1.47	1.40
2	N	999	D5M	C2-N3	2.09	1.35	1.32
2	G	999	D5M	C2-N3	2.07	1.35	1.32
2	D	999	D5M	C2-N3	2.07	1.35	1.32
2	J	999	D5M	C2-N3	2.04	1.35	1.32
2	M	999	D5M	C2-N3	2.03	1.35	1.32
2	R	999	D5M	C2-N3	2.03	1.35	1.32
2	O	999	D5M	C2-N3	2.02	1.35	1.32
2	H	999	D5M	C2-N3	2.02	1.35	1.32
2	A	999	D5M	C2-N3	2.02	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	999	D5M	C2-N3	2.02	1.35	1.32
2	P	999	D5M	C2-N3	2.02	1.35	1.32
2	K	999	D5M	C2-N3	2.02	1.35	1.32
2	E	999	D5M	C2-N3	2.01	1.35	1.32
2	S	999	D5M	C2-N3	2.01	1.35	1.32
2	F	999	D5M	C2-N3	2.00	1.35	1.32
2	Q	999	D5M	C2-N3	2.00	1.35	1.32

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	999	D5M	N3-C2-N1	-2.82	124.27	128.68
2	H	999	D5M	N3-C2-N1	-2.82	124.27	128.68
2	B	999	D5M	N3-C2-N1	-2.82	124.28	128.68
2	Q	999	D5M	N3-C2-N1	-2.81	124.29	128.68
2	N	999	D5M	N3-C2-N1	-2.81	124.29	128.68
2	J	999	D5M	N3-C2-N1	-2.81	124.29	128.68
2	F	999	D5M	N3-C2-N1	-2.80	124.30	128.68
2	O	999	D5M	N3-C2-N1	-2.80	124.30	128.68
2	R	999	D5M	N3-C2-N1	-2.80	124.30	128.68
2	C	999	D5M	N3-C2-N1	-2.80	124.30	128.68
2	E	999	D5M	N3-C2-N1	-2.80	124.31	128.68
2	T	999	D5M	N3-C2-N1	-2.79	124.31	128.68
2	I	999	D5M	N3-C2-N1	-2.79	124.31	128.68
2	P	999	D5M	N3-C2-N1	-2.79	124.33	128.68
2	A	999	D5M	N3-C2-N1	-2.78	124.33	128.68
2	L	999	D5M	N3-C2-N1	-2.78	124.34	128.68
2	G	999	D5M	N3-C2-N1	-2.76	124.36	128.68
2	M	999	D5M	N3-C2-N1	-2.76	124.36	128.68
2	D	999	D5M	N3-C2-N1	-2.75	124.37	128.68
2	S	999	D5M	N3-C2-N1	-2.74	124.40	128.68
2	C	999	D5M	C4-C5-N7	-2.65	106.64	109.40
2	D	999	D5M	C4-C5-N7	-2.64	106.64	109.40
2	Q	999	D5M	C4-C5-N7	-2.63	106.66	109.40
2	N	999	D5M	C4-C5-N7	-2.63	106.66	109.40
2	H	999	D5M	C4-C5-N7	-2.63	106.66	109.40
2	S	999	D5M	C4-C5-N7	-2.62	106.67	109.40
2	F	999	D5M	C4-C5-N7	-2.62	106.67	109.40
2	O	999	D5M	C4-C5-N7	-2.62	106.67	109.40
2	E	999	D5M	C4-C5-N7	-2.61	106.68	109.40
2	R	999	D5M	C4-C5-N7	-2.60	106.69	109.40
2	A	999	D5M	C4-C5-N7	-2.60	106.69	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	999	D5M	C4-C5-N7	-2.60	106.69	109.40
2	G	999	D5M	C4-C5-N7	-2.59	106.70	109.40
2	K	999	D5M	C4-C5-N7	-2.59	106.70	109.40
2	J	999	D5M	C4-C5-N7	-2.58	106.70	109.40
2	I	999	D5M	C4-C5-N7	-2.58	106.71	109.40
2	B	999	D5M	C4-C5-N7	-2.58	106.71	109.40
2	M	999	D5M	C4-C5-N7	-2.58	106.72	109.40
2	L	999	D5M	C4-C5-N7	-2.57	106.72	109.40
2	P	999	D5M	C4-C5-N7	-2.52	106.78	109.40

There are no chirality outliers.

There are no torsion outliers.

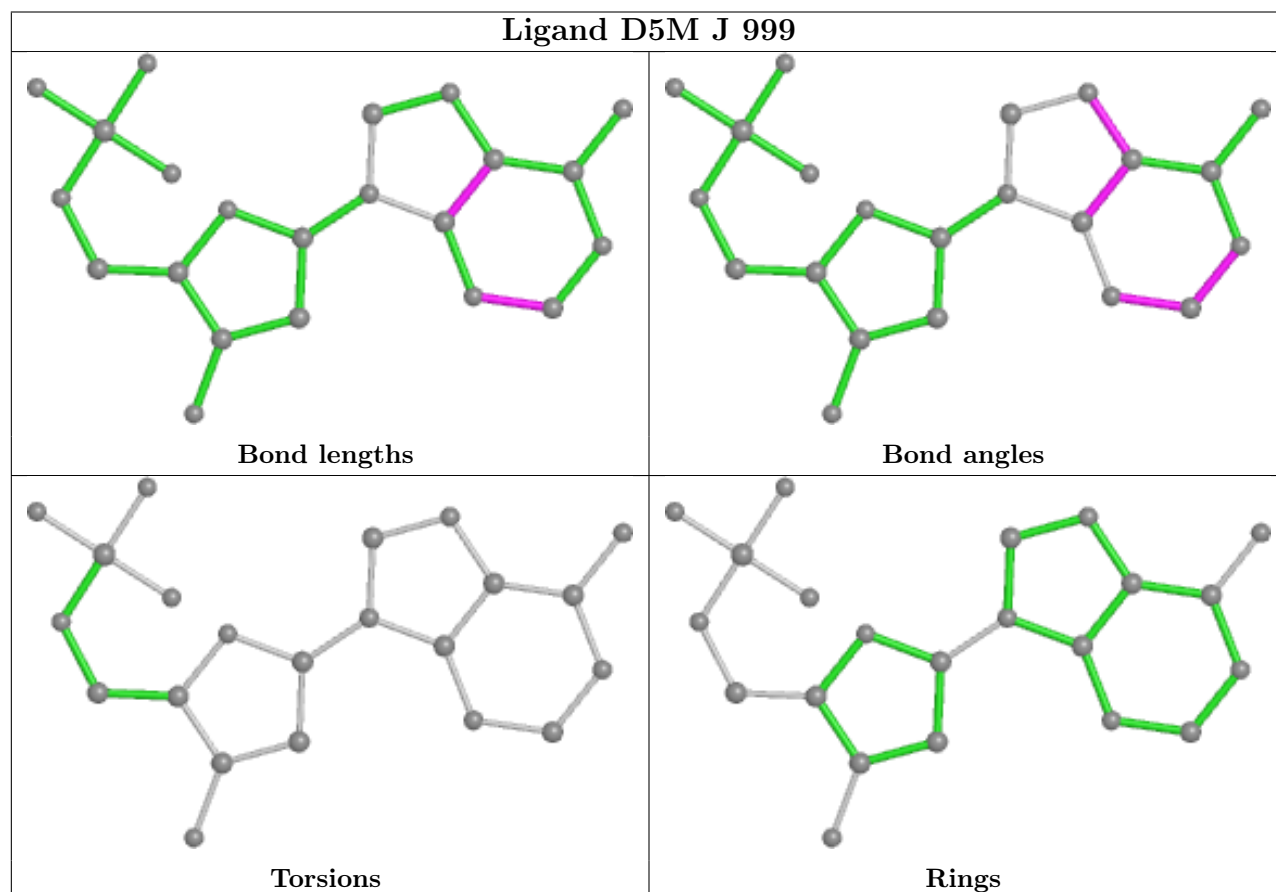
There are no ring outliers.

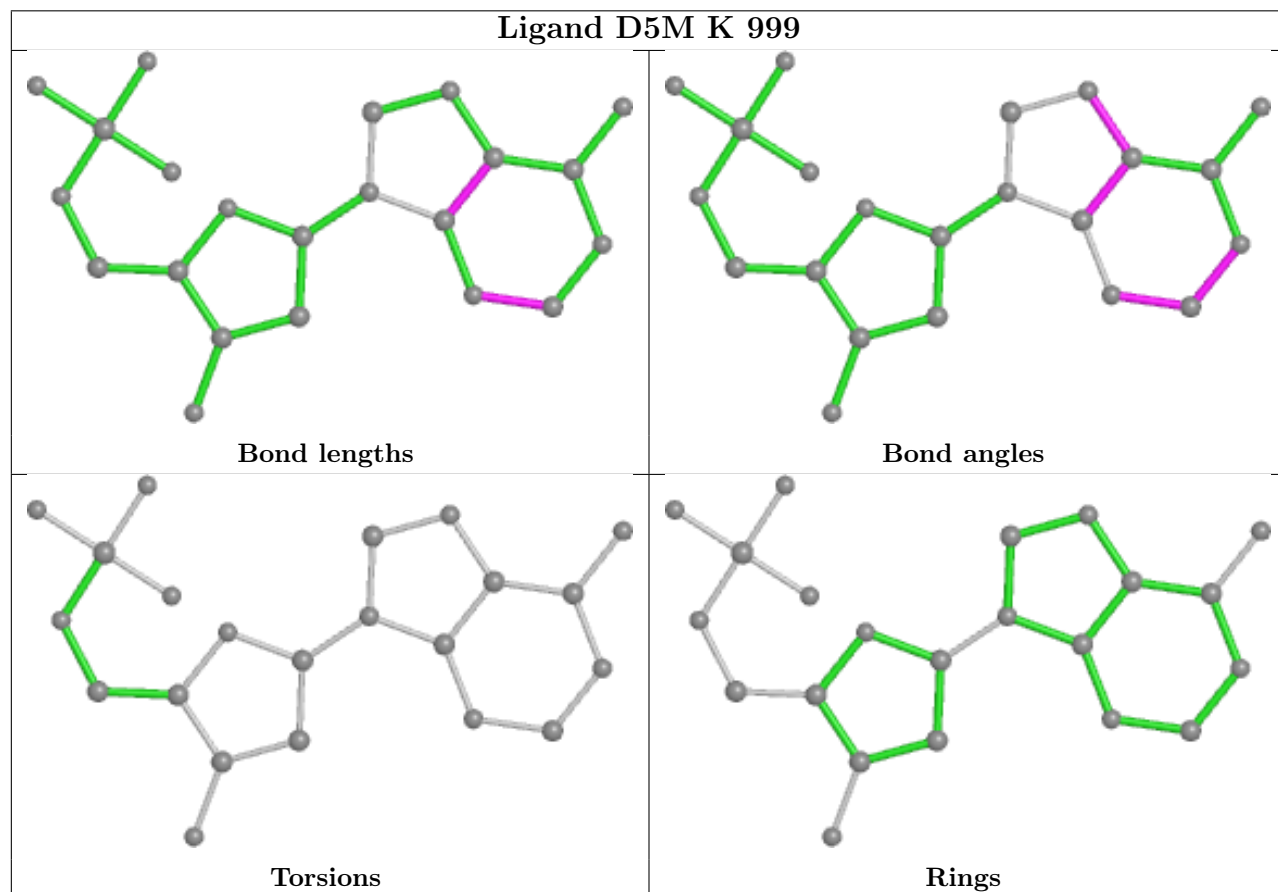
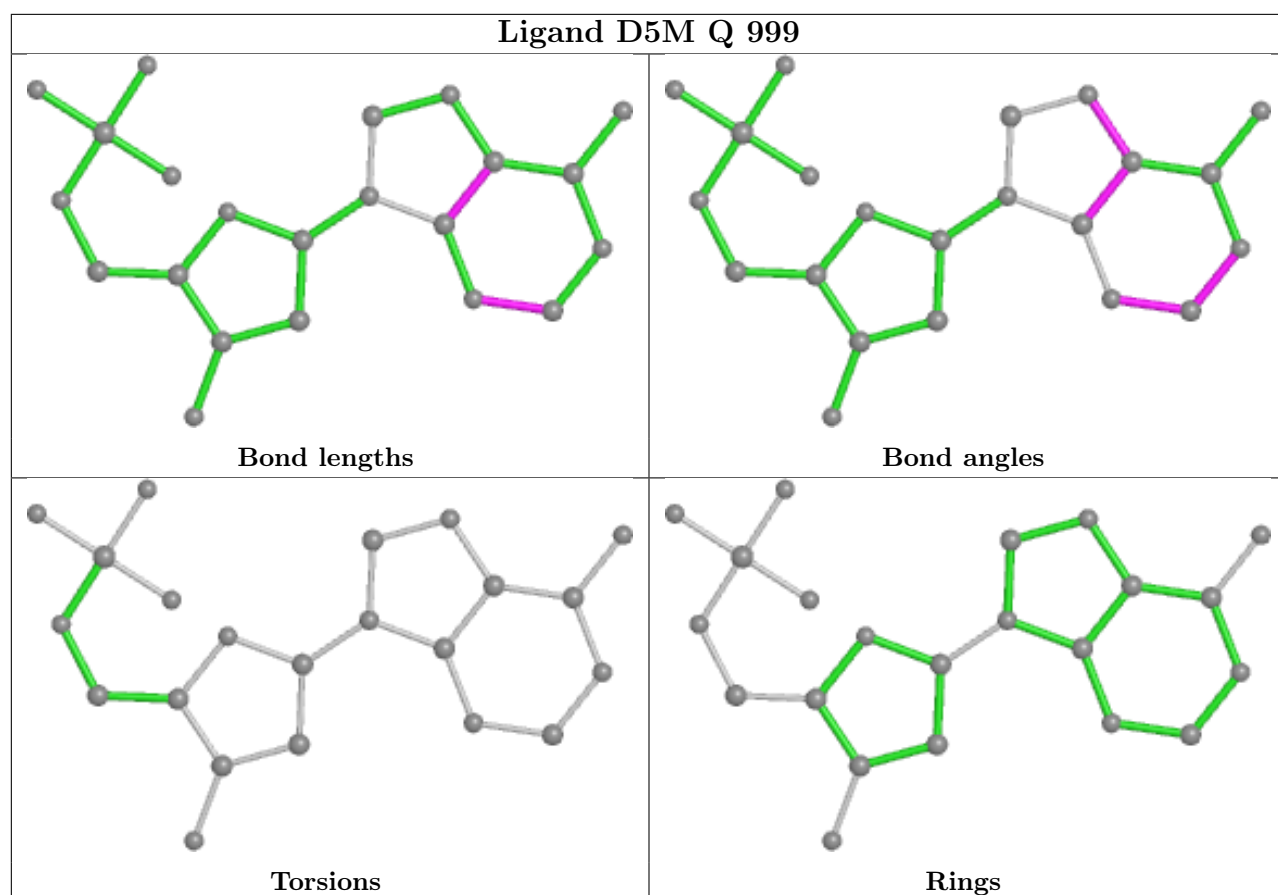
20 monomers are involved in 60 short contacts:

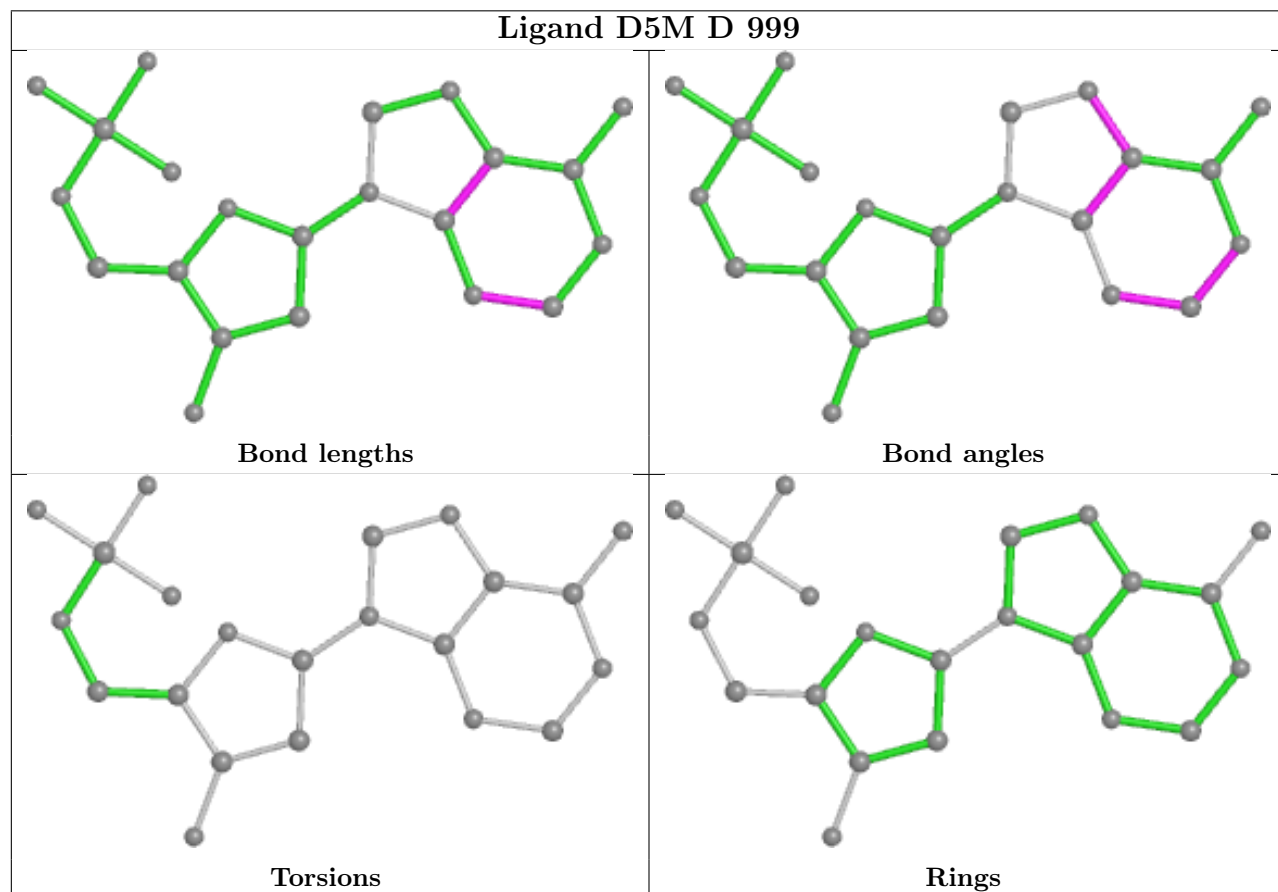
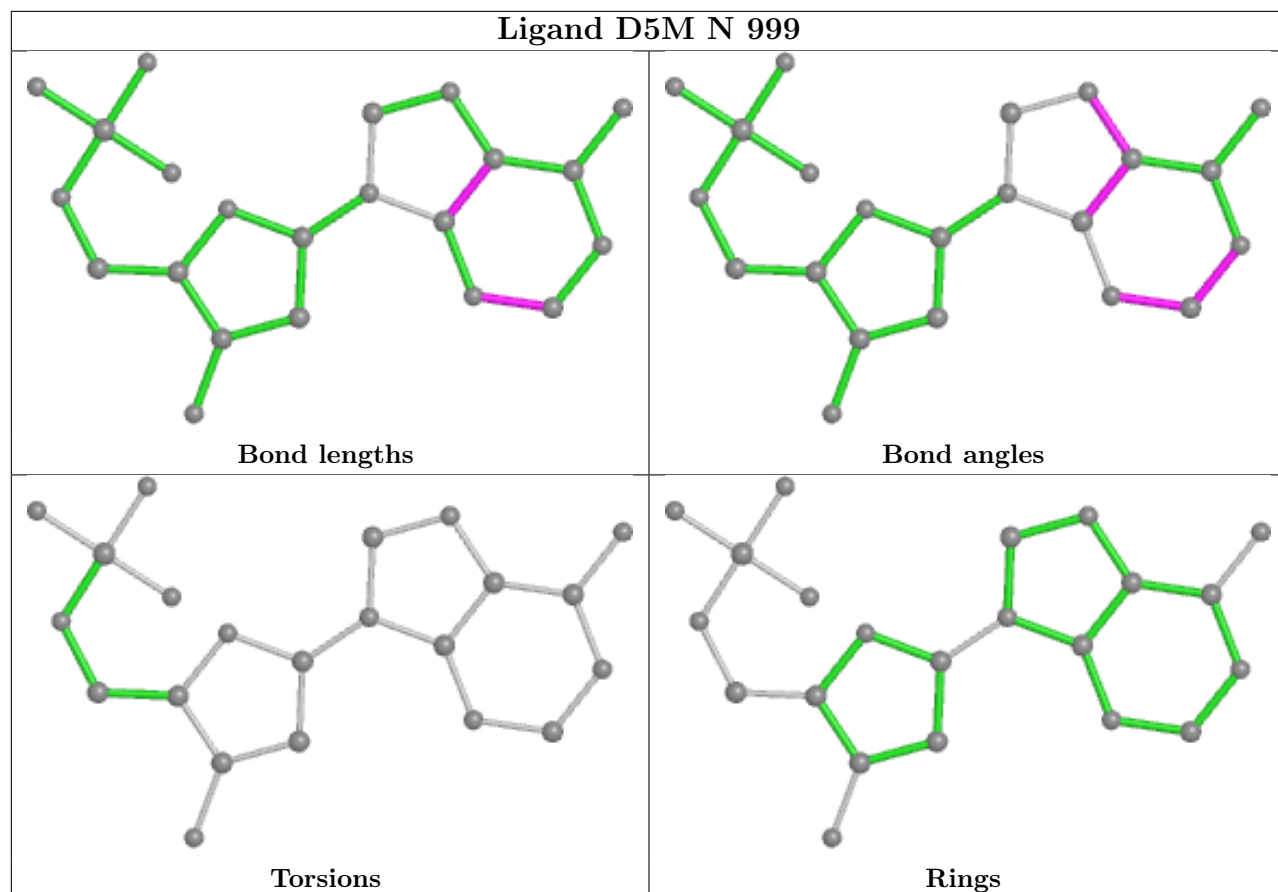
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	999	D5M	3	0
2	Q	999	D5M	3	0
2	K	999	D5M	3	0
2	N	999	D5M	3	0
2	D	999	D5M	3	0
2	R	999	D5M	3	0
2	I	999	D5M	3	0
2	L	999	D5M	3	0
2	O	999	D5M	3	0
2	G	999	D5M	3	0
2	B	999	D5M	3	0
2	H	999	D5M	3	0
2	F	999	D5M	3	0
2	C	999	D5M	3	0
2	M	999	D5M	3	0
2	S	999	D5M	3	0
2	A	999	D5M	3	0
2	T	999	D5M	3	0
2	P	999	D5M	3	0
2	E	999	D5M	3	0

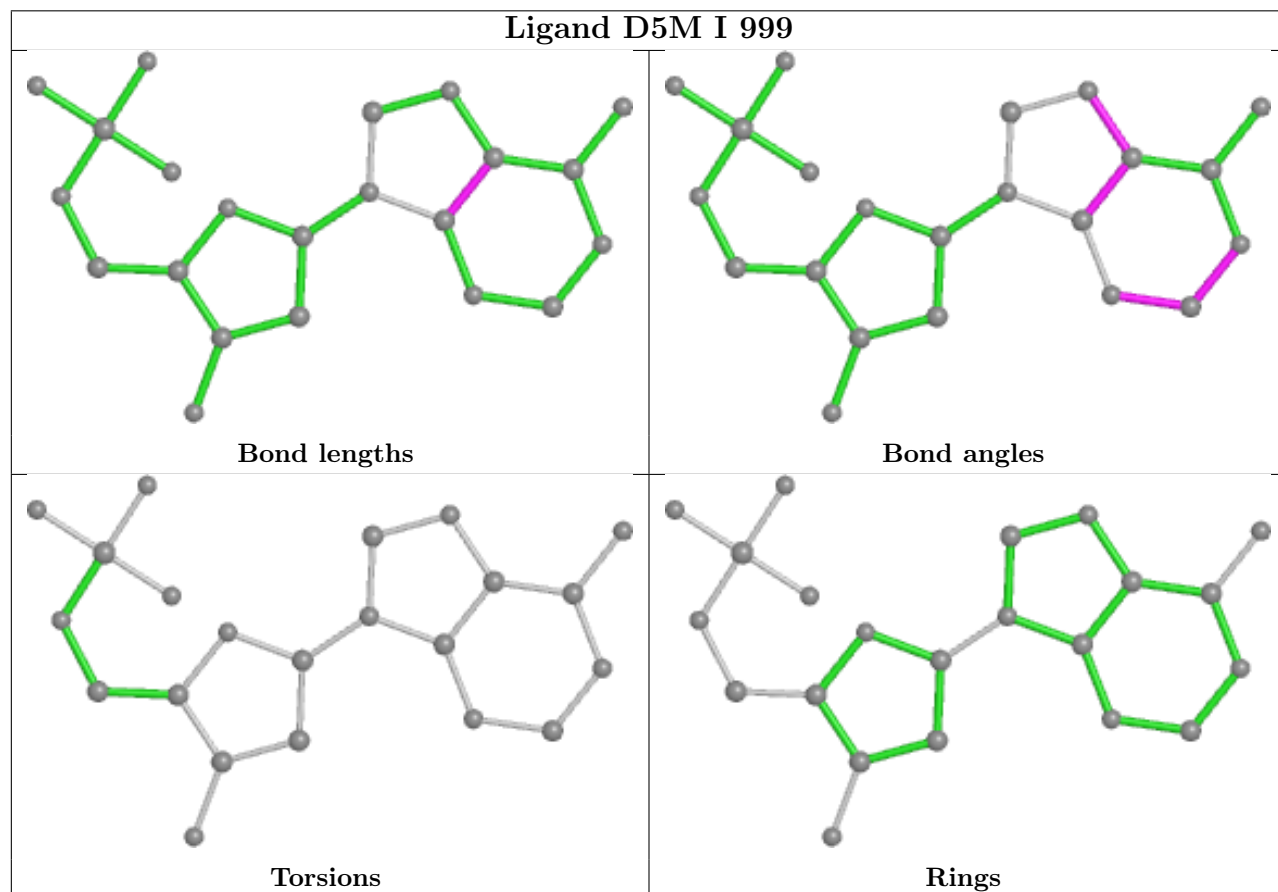
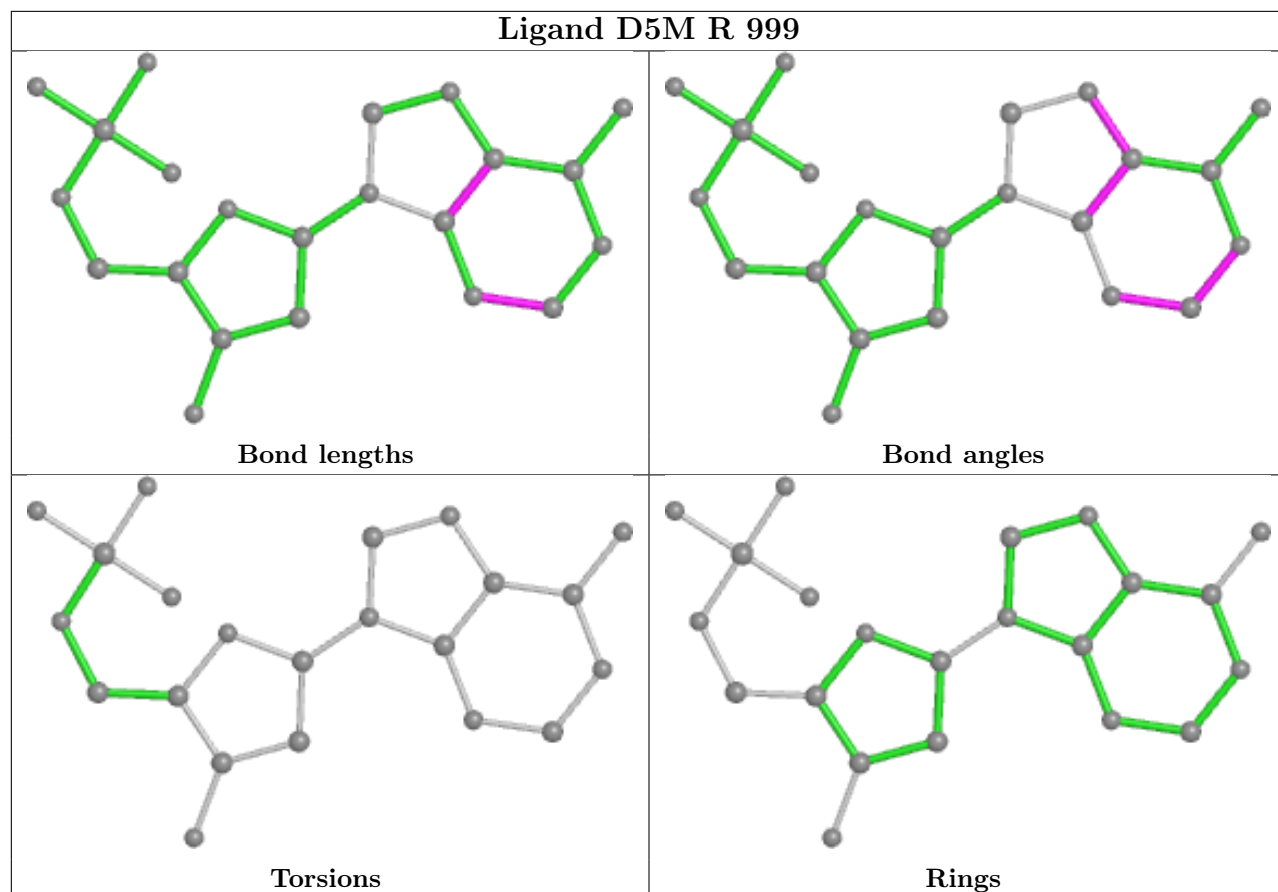
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

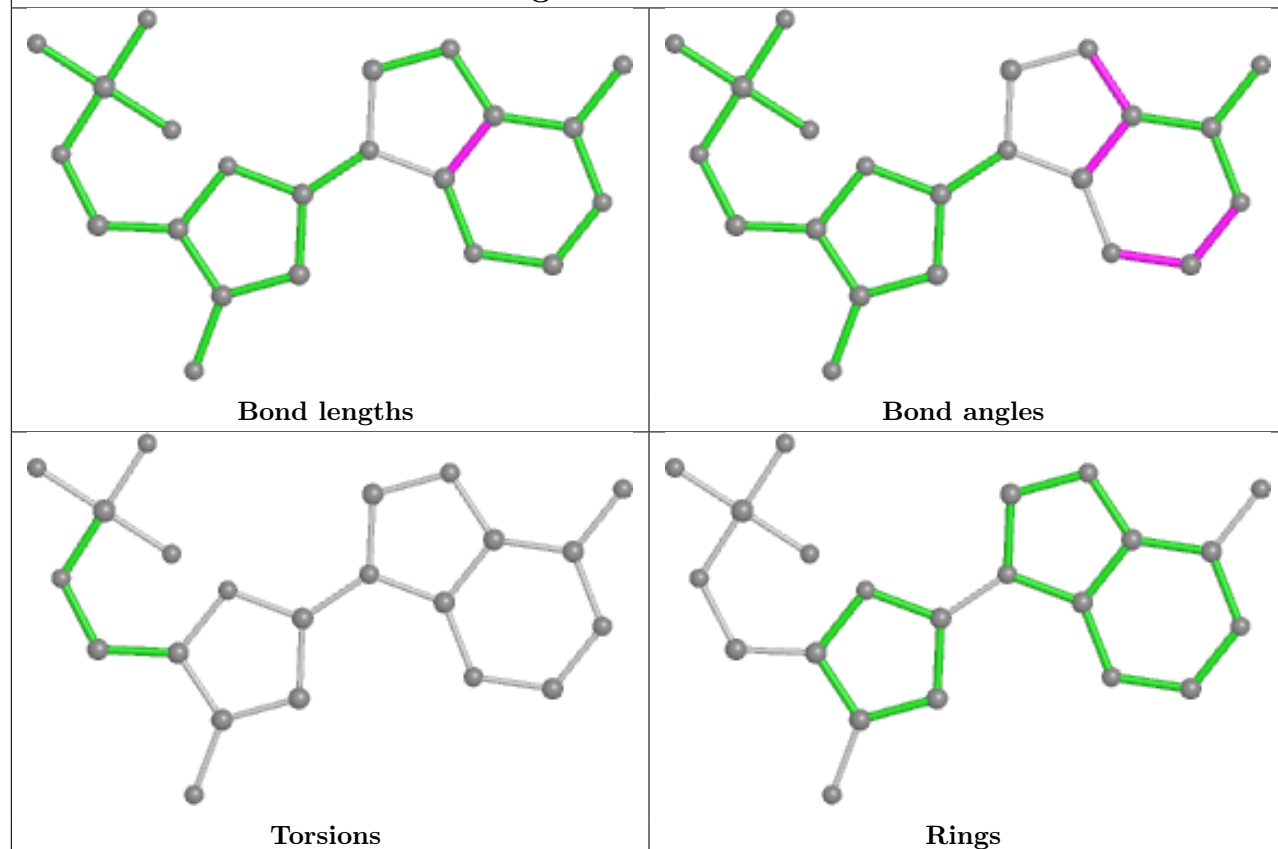




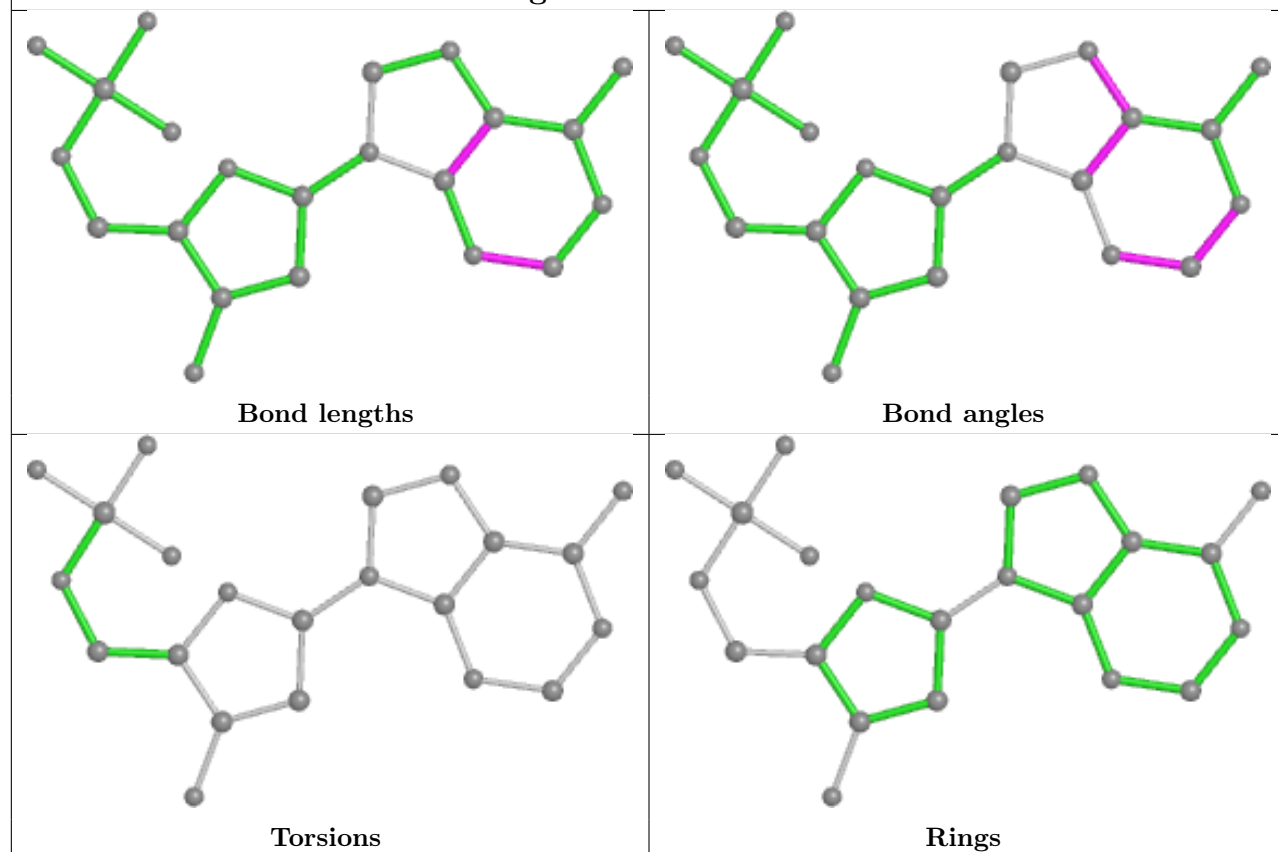


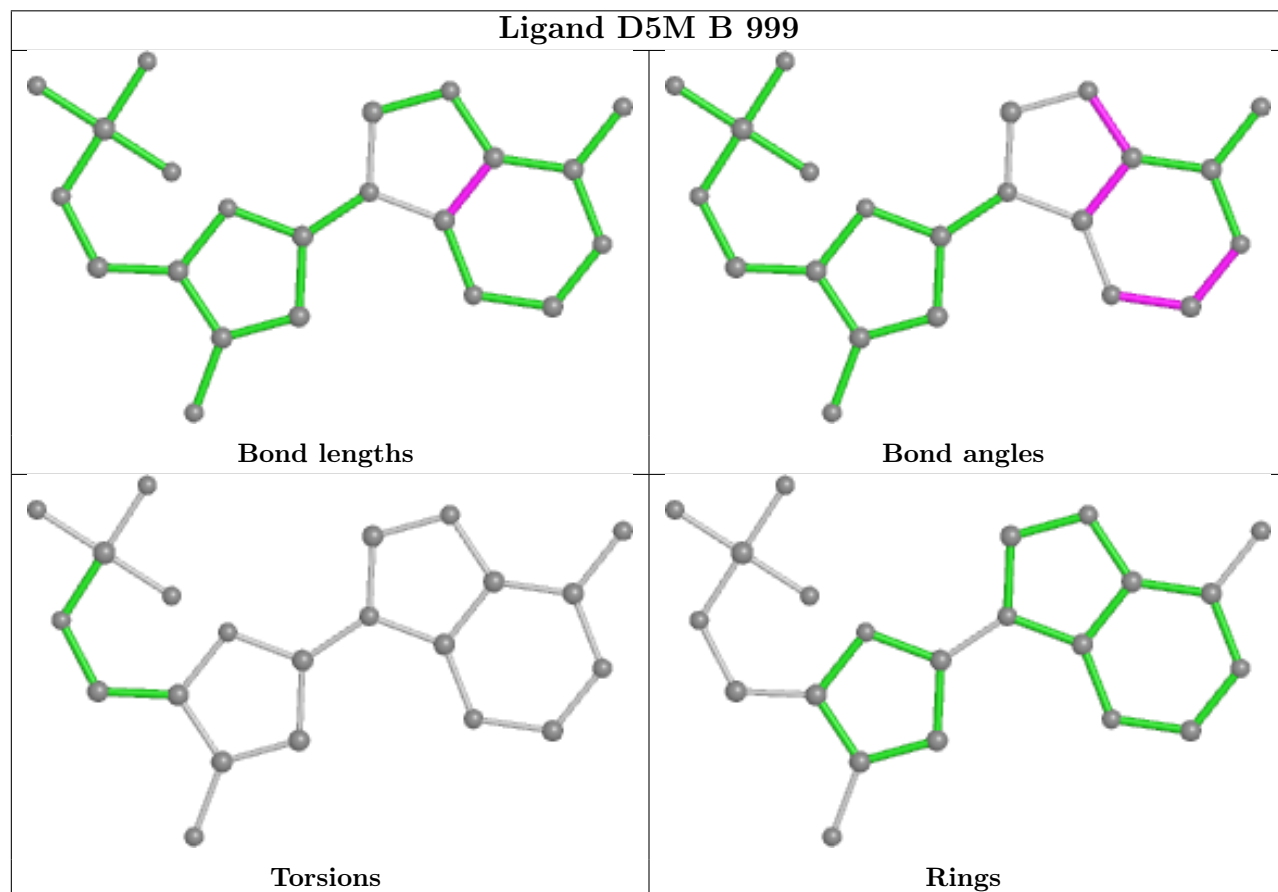
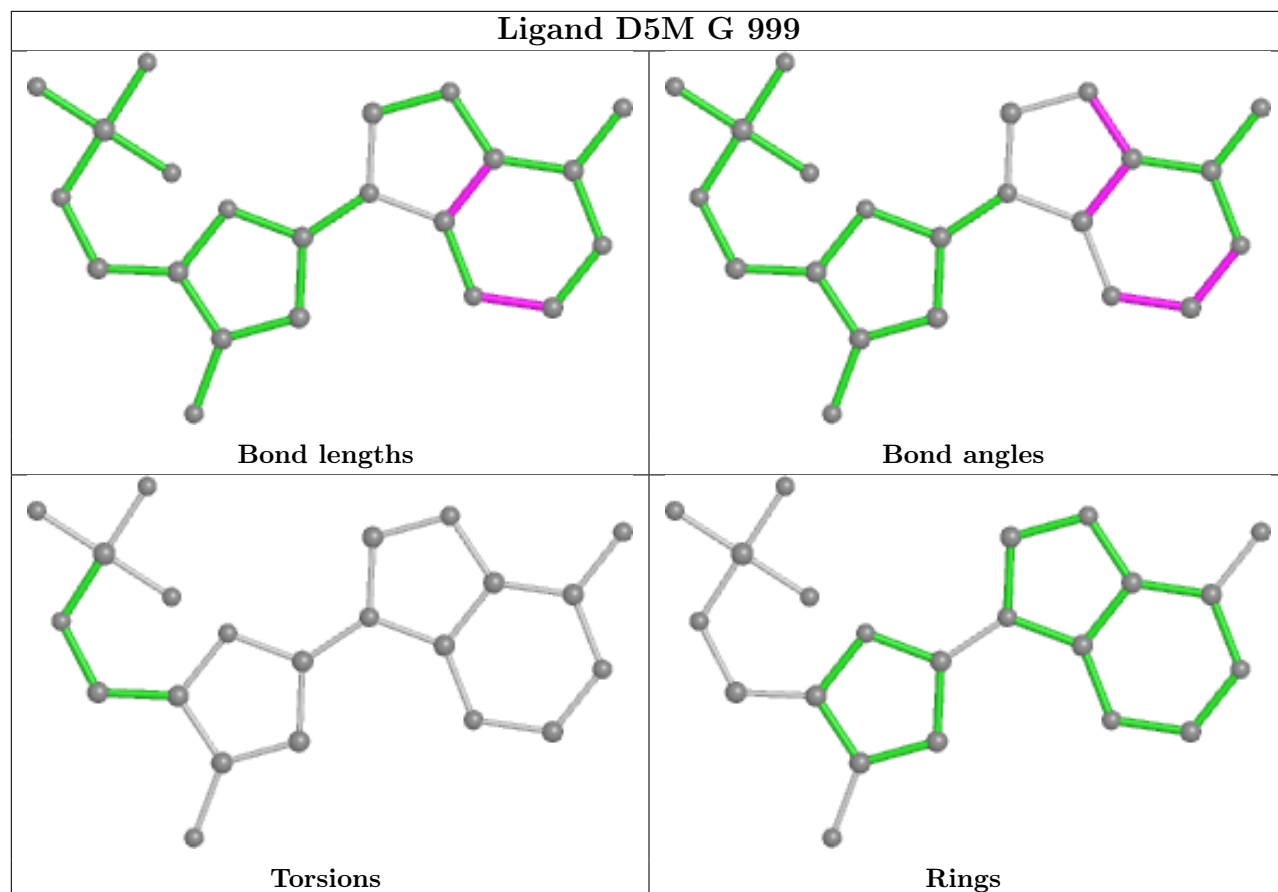


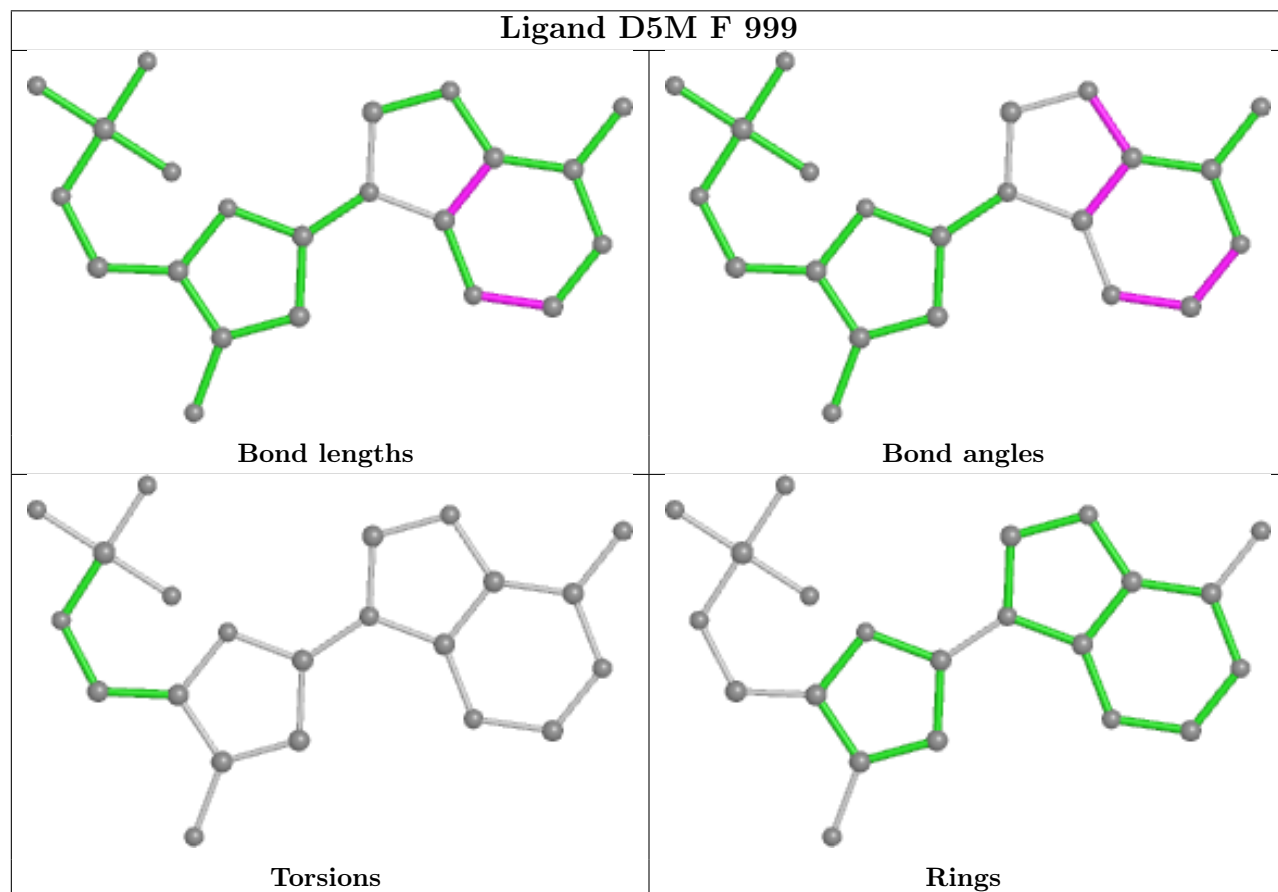
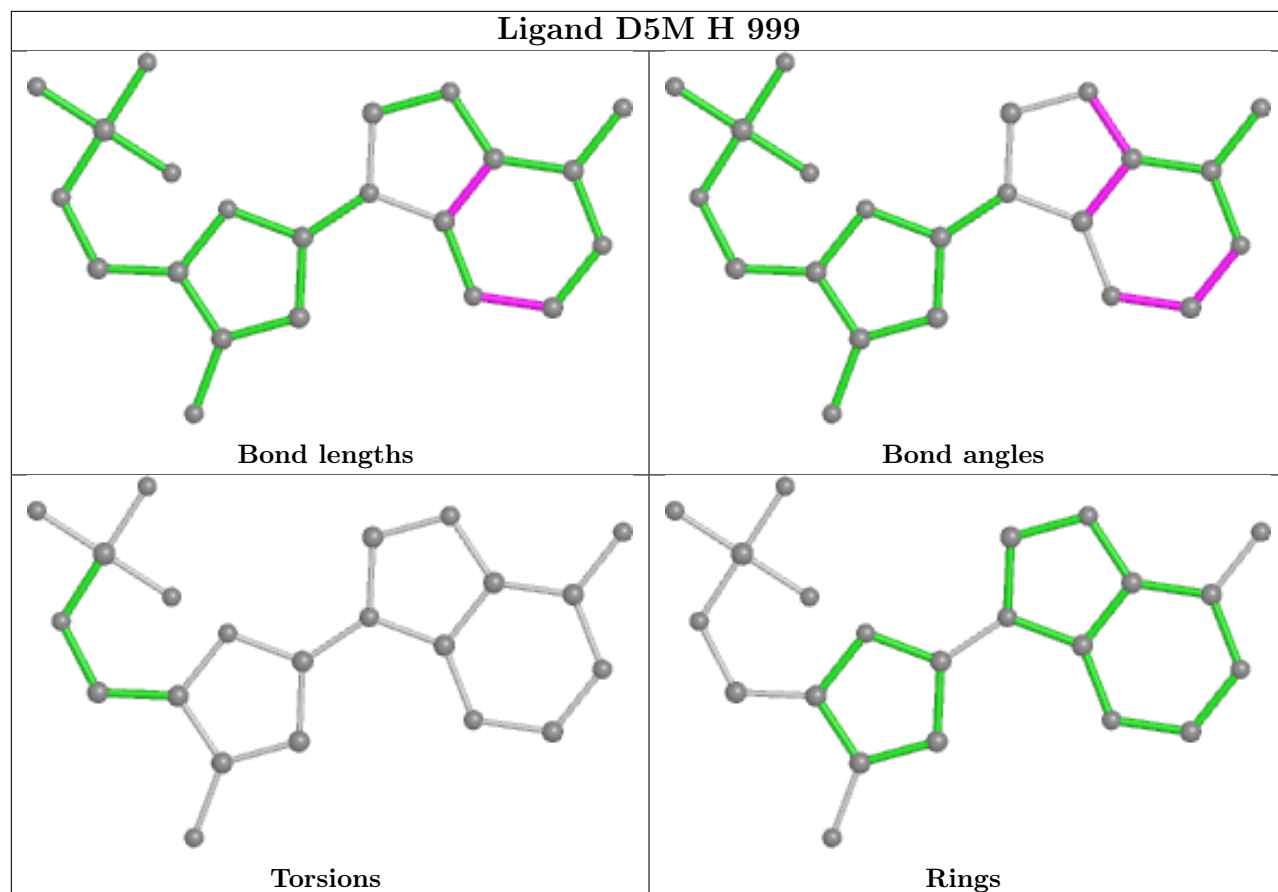
Ligand D5M L 999

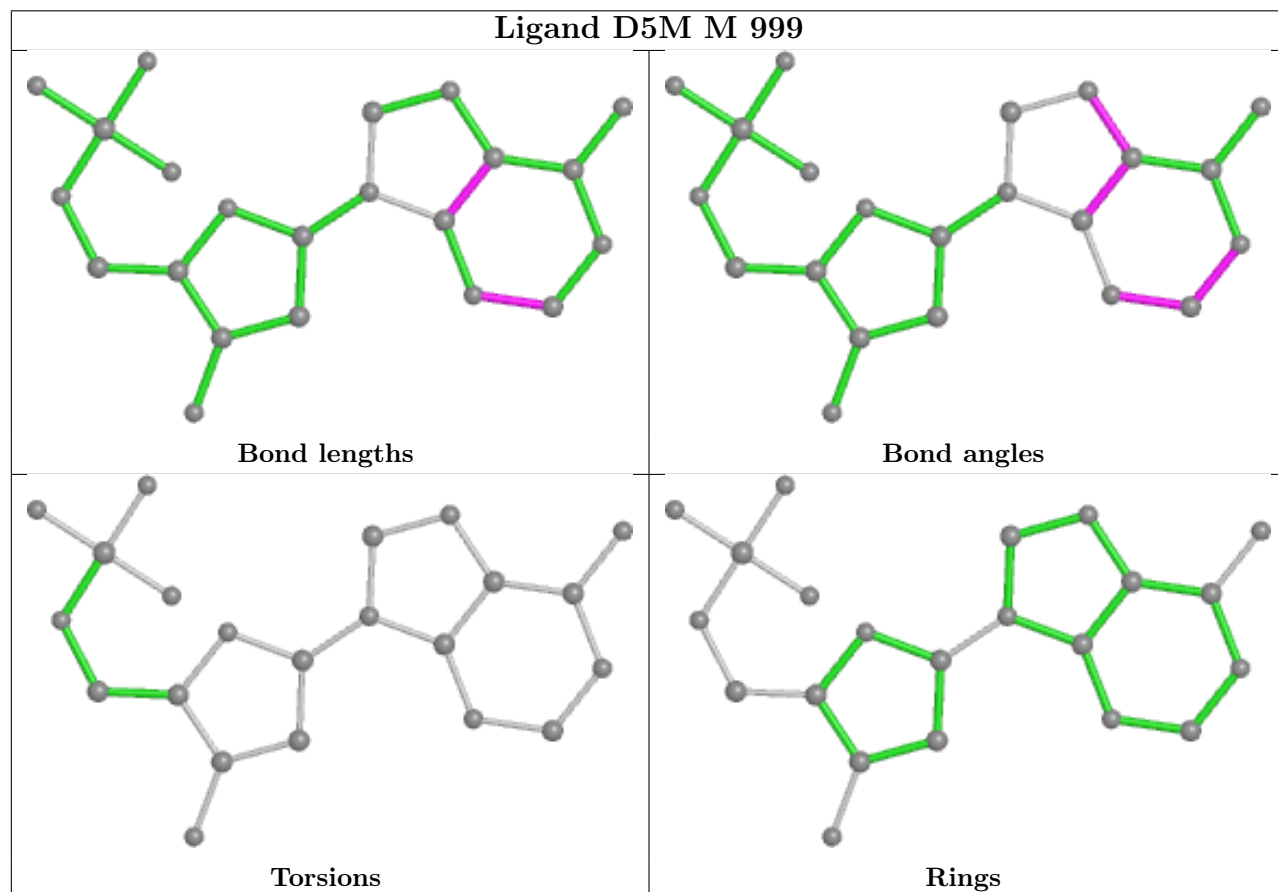
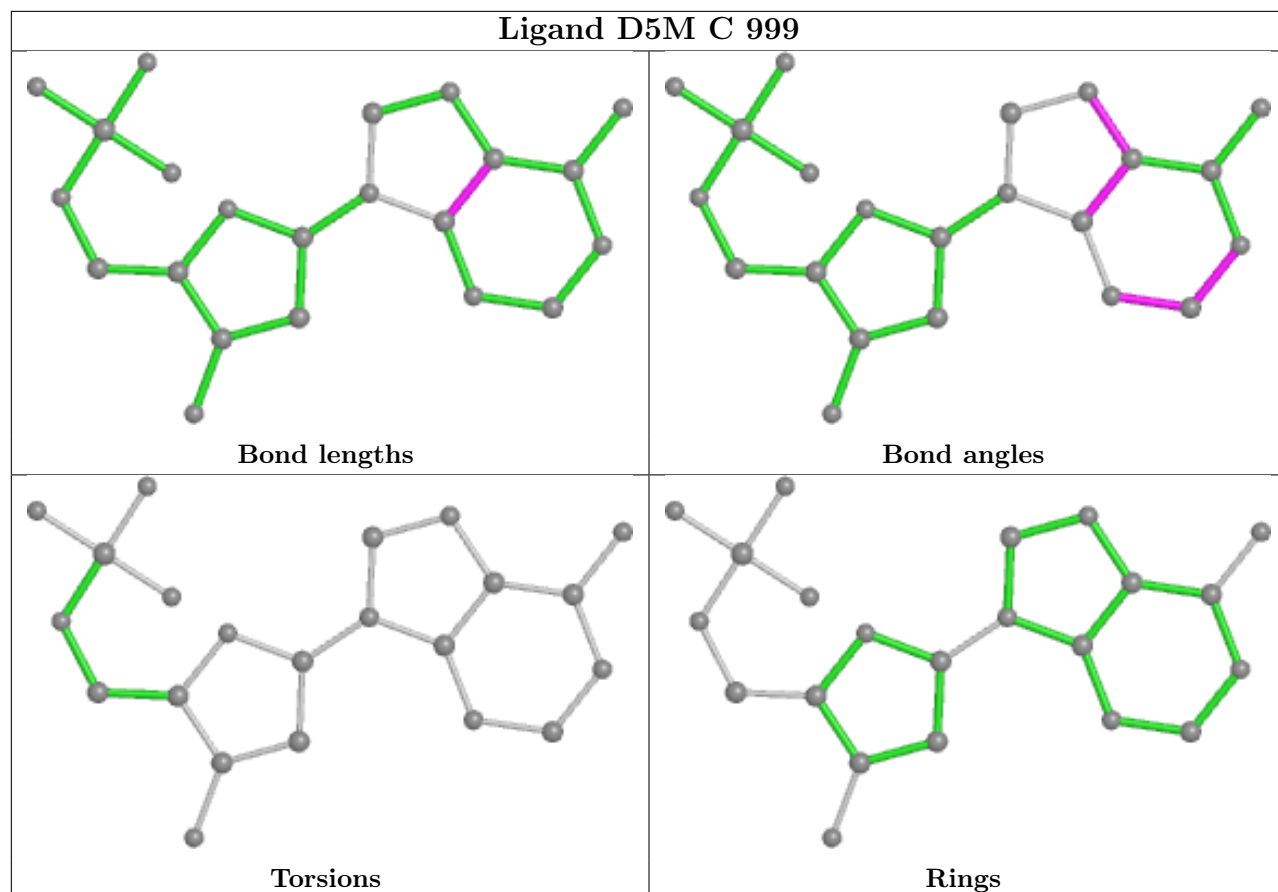


Ligand D5M O 999

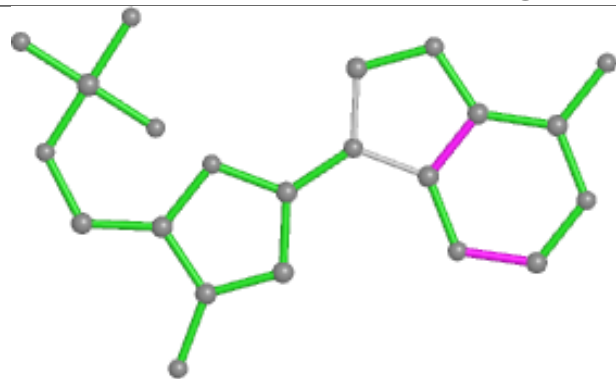




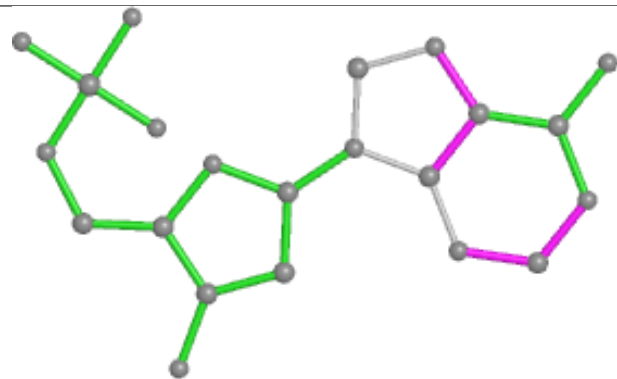




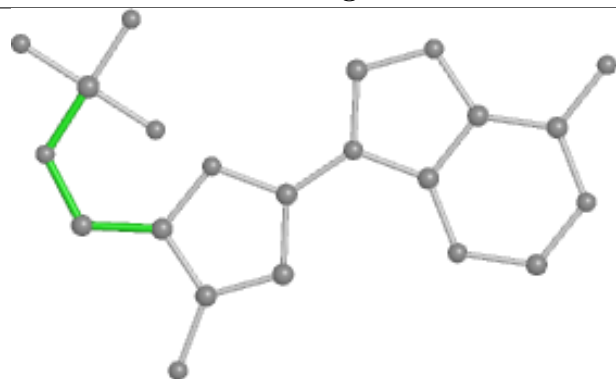
Ligand D5M S 999



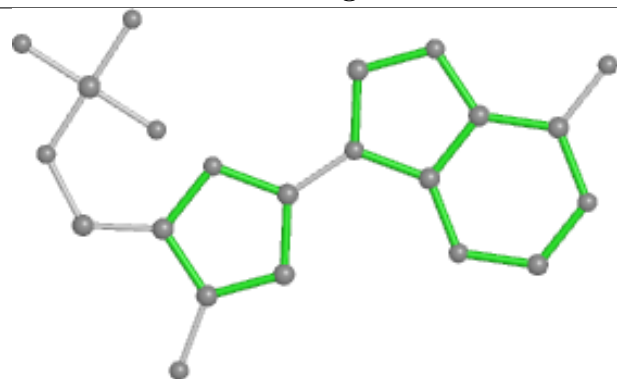
Bond lengths



Bond angles

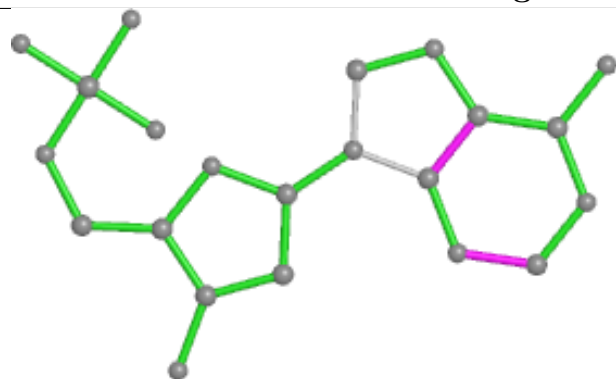


Torsions

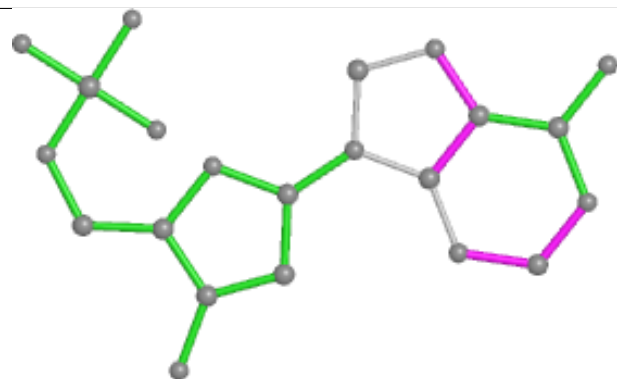


Rings

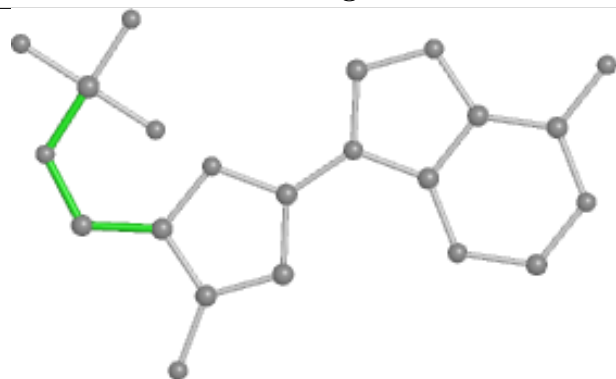
Ligand D5M A 999



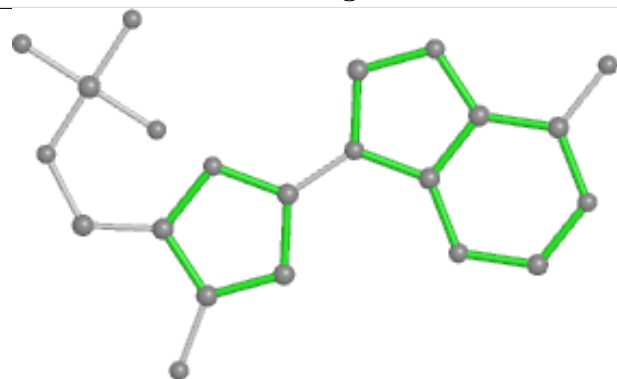
Bond lengths



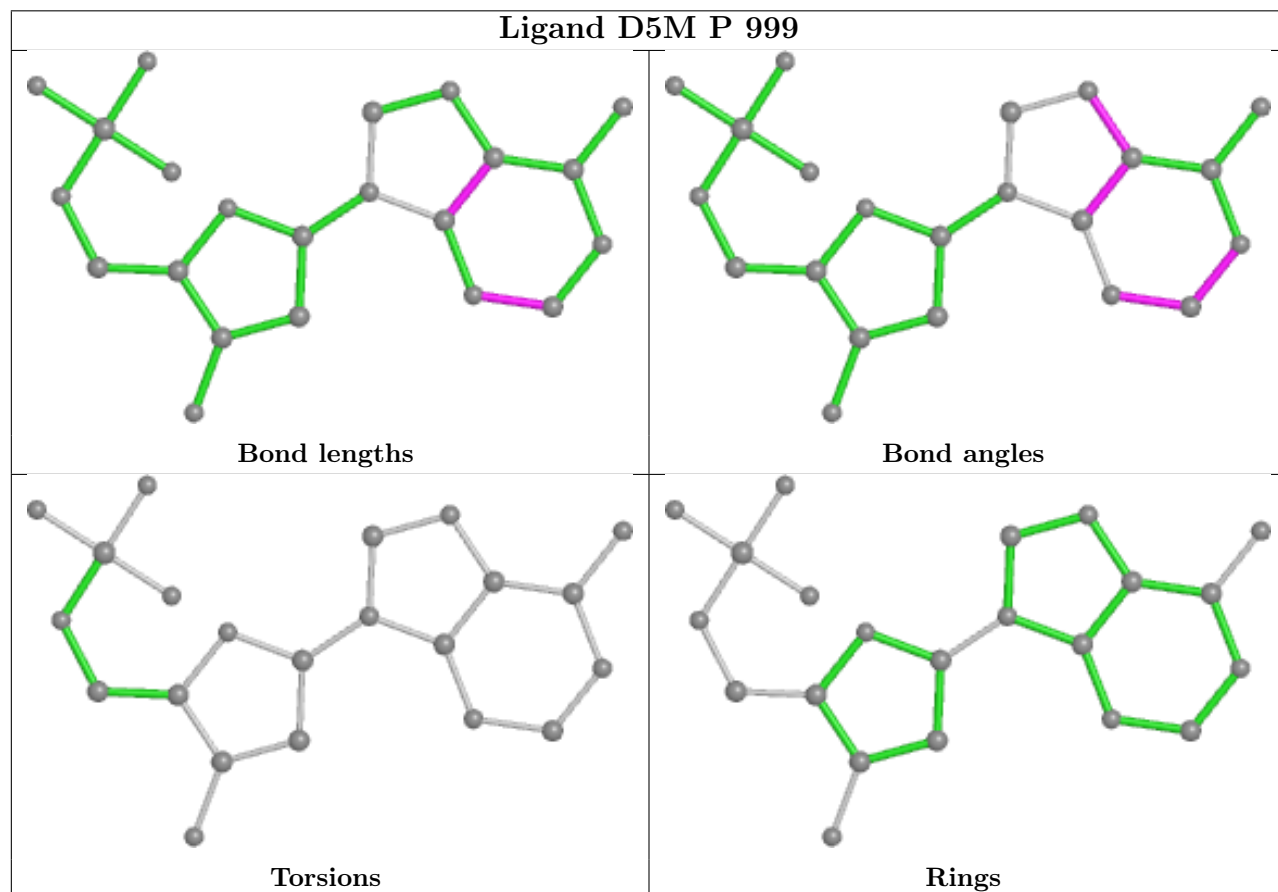
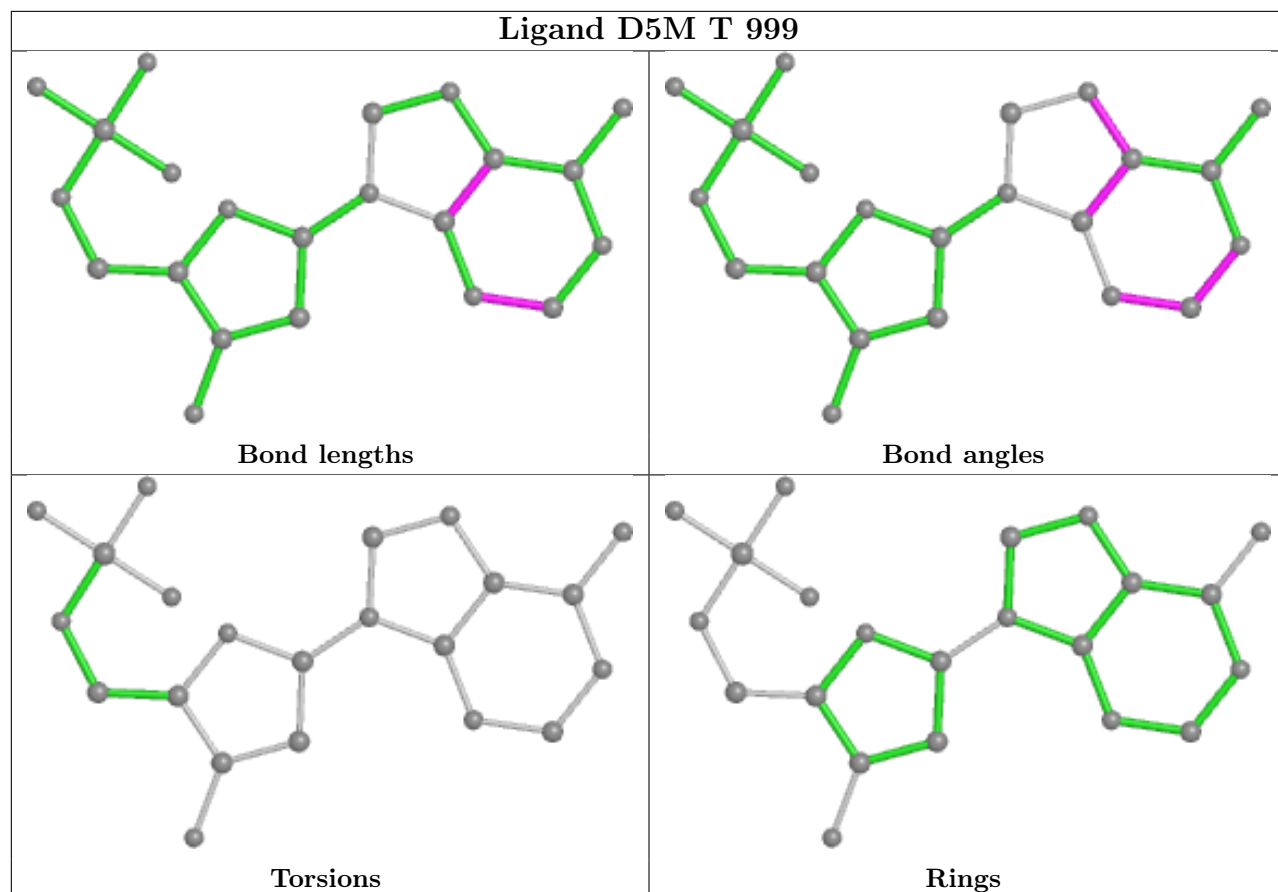
Bond angles

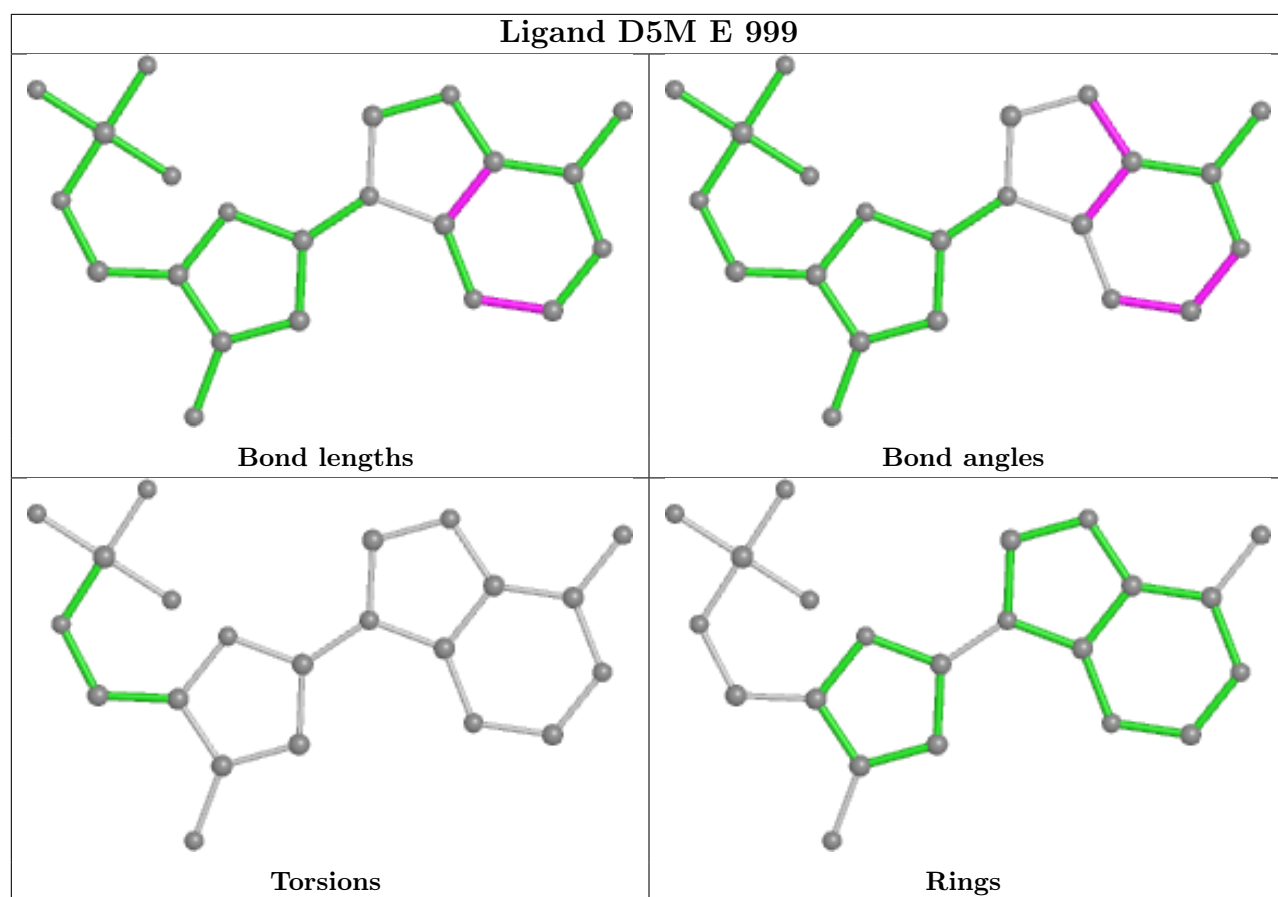


Torsions



Rings





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	520/736 (70%)	0.11	8 (1%) 73 46	76, 102, 141, 181	0
1	B	520/736 (70%)	0.12	9 (1%) 70 41	76, 103, 141, 181	0
1	C	520/736 (70%)	0.15	10 (1%) 66 37	76, 102, 141, 181	0
1	D	520/736 (70%)	0.13	8 (1%) 73 46	76, 102, 141, 181	0
1	E	520/736 (70%)	0.15	7 (1%) 77 51	76, 102, 141, 181	0
1	F	520/736 (70%)	0.12	7 (1%) 77 51	76, 102, 141, 181	0
1	G	520/736 (70%)	0.13	8 (1%) 73 46	76, 102, 141, 181	0
1	H	520/736 (70%)	0.12	7 (1%) 77 51	76, 102, 141, 181	0
1	I	520/736 (70%)	0.10	6 (1%) 79 54	76, 102, 141, 181	0
1	J	520/736 (70%)	0.12	5 (0%) 82 59	76, 103, 141, 181	0
1	K	520/736 (70%)	0.15	9 (1%) 70 41	76, 102, 141, 181	0
1	L	520/736 (70%)	0.14	12 (2%) 60 31	76, 102, 141, 181	0
1	M	520/736 (70%)	0.08	4 (0%) 86 65	76, 103, 141, 181	0
1	N	520/736 (70%)	0.11	6 (1%) 79 54	76, 103, 141, 181	0
1	O	520/736 (70%)	0.13	14 (2%) 54 26	76, 102, 141, 181	0
1	P	520/736 (70%)	0.12	9 (1%) 70 41	76, 103, 141, 181	0
1	Q	520/736 (70%)	0.12	4 (0%) 86 65	76, 102, 141, 181	0
1	R	520/736 (70%)	0.13	6 (1%) 79 54	76, 103, 141, 181	0
1	S	520/736 (70%)	0.15	9 (1%) 70 41	76, 102, 141, 181	0
1	T	520/736 (70%)	0.12	5 (0%) 82 59	76, 103, 141, 181	0
All	All	10400/14720 (70%)	0.13	153 (1%) 73 46	76, 103, 141, 181	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	217	GLY	7.2
1	S	329	THR	6.0
1	S	218	ALA	5.7
1	C	326	ASN	5.5
1	P	220	GLY	5.4
1	F	326	ASN	5.2
1	N	217	GLY	5.0
1	H	217	GLY	4.8
1	O	218	ALA	4.8
1	N	218	ALA	4.7
1	D	218	ALA	4.7
1	D	217	GLY	4.6
1	B	219	ASP	4.4
1	O	454	GLY	4.3
1	G	218	ALA	4.3
1	L	218	ALA	4.3
1	E	329	THR	4.2
1	L	450	GLY	3.9
1	D	406	GLY	3.9
1	O	217	GLY	3.8
1	D	505	ALA	3.8
1	N	326	ASN	3.8
1	K	217	GLY	3.7
1	L	301	ASN	3.7
1	I	219	ASP	3.7
1	A	454	GLY	3.6
1	E	218	ALA	3.6
1	C	217	GLY	3.6
1	R	322	GLU	3.5
1	L	236	GLY	3.5
1	O	600	GLY	3.4
1	G	217	GLY	3.3
1	A	326	ASN	3.2
1	J	456	THR	3.2
1	E	273	PHE	3.2
1	S	328	GLY	3.1
1	B	506	ALA	3.1
1	C	406	GLY	3.1
1	K	706	ASN	3.0
1	I	220	GLY	3.0
1	P	428	GLN	3.0
1	P	329	THR	3.0
1	Q	326	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	P	219	ASP	3.0
1	F	329	THR	3.0
1	S	217	GLY	2.9
1	L	458	GLN	2.9
1	G	456	THR	2.9
1	P	648	MET	2.9
1	J	333	ALA	2.9
1	L	329	THR	2.9
1	S	406	GLY	2.8
1	D	380	LEU	2.8
1	H	281	TYR	2.8
1	K	731	TYR	2.8
1	J	641	LYS	2.7
1	M	217	GLY	2.7
1	B	460	ARG	2.7
1	O	450	GLY	2.7
1	H	728	GLY	2.7
1	H	450	GLY	2.7
1	R	456	THR	2.6
1	C	300	ILE	2.6
1	C	572	VAL	2.6
1	O	236	GLY	2.6
1	B	719	GLY	2.6
1	R	220	GLY	2.6
1	I	428	GLN	2.5
1	C	220	GLY	2.5
1	H	264	SER	2.5
1	F	554	GLU	2.5
1	J	470	SER	2.5
1	M	517	LEU	2.5
1	B	456	THR	2.5
1	B	531	GLU	2.4
1	K	470	SER	2.4
1	O	572	VAL	2.4
1	C	573	ALA	2.4
1	O	335	ASN	2.4
1	G	236	GLY	2.4
1	Q	736	LEU	2.4
1	S	220	GLY	2.4
1	P	568	THR	2.4
1	T	217	GLY	2.4
1	C	273	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	534	PHE	2.4
1	G	356	SER	2.4
1	I	236	GLY	2.4
1	D	322	GLU	2.4
1	T	531	GLU	2.4
1	M	736	LEU	2.4
1	G	568	THR	2.4
1	S	273	PHE	2.3
1	C	429	SER	2.3
1	G	380	LEU	2.3
1	L	560	ILE	2.3
1	K	534	PHE	2.3
1	E	452	THR	2.3
1	H	689	LYS	2.3
1	I	732	LEU	2.3
1	N	699	ILE	2.3
1	Q	217	GLY	2.3
1	L	283	ASP	2.3
1	R	329	THR	2.3
1	L	326	ASN	2.3
1	Q	218	ALA	2.3
1	K	516	SER	2.3
1	E	636	GLY	2.3
1	A	540	ASN	2.3
1	K	636	GLY	2.3
1	O	554	GLU	2.3
1	A	218	ALA	2.2
1	D	482	PRO	2.2
1	O	220	GLY	2.2
1	T	505	ALA	2.2
1	A	568	THR	2.2
1	R	568	THR	2.2
1	C	506	ALA	2.2
1	B	329	THR	2.2
1	O	620	ALA	2.2
1	F	736	LEU	2.2
1	A	534	PHE	2.2
1	F	568	THR	2.2
1	A	220	GLY	2.2
1	B	220	GLY	2.2
1	O	353	VAL	2.2
1	K	385	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	317	ASN	2.1
1	L	578	GLY	2.1
1	F	381	ASN	2.1
1	H	218	ALA	2.1
1	A	545	LYS	2.1
1	R	572	VAL	2.1
1	P	281	TYR	2.1
1	T	704	ASN	2.1
1	N	450	GLY	2.1
1	T	375	TYR	2.1
1	E	578	GLY	2.1
1	P	735	ASN	2.1
1	J	363	PRO	2.1
1	P	218	ALA	2.1
1	O	283	ASP	2.1
1	S	438	ILE	2.1
1	K	445	LEU	2.1
1	F	248	ALA	2.0
1	O	356	SER	2.0
1	G	387	VAL	2.0
1	B	675	SER	2.0
1	N	580	VAL	2.0
1	I	736	LEU	2.0
1	S	525	ALA	2.0
1	D	517	LEU	2.0
1	L	342	VAL	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

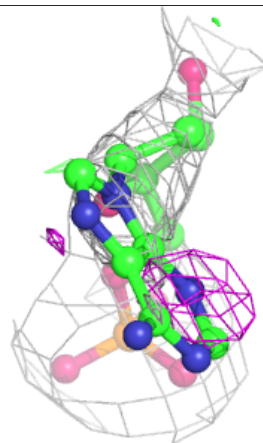
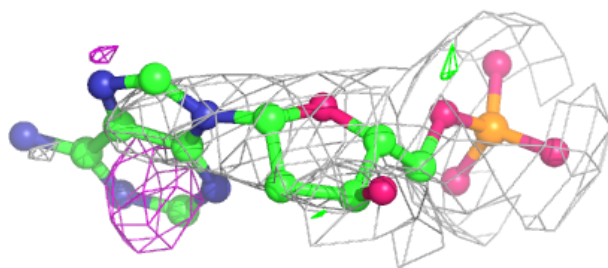
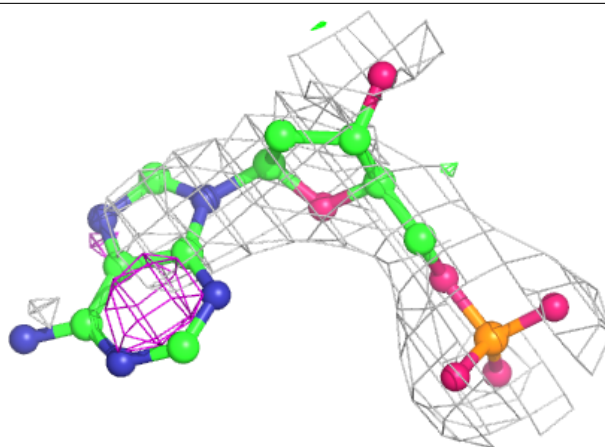
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	D5M	S	999	22/22	0.70	0.48	97,97,97,97	22
2	D5M	L	999	22/22	0.71	0.40	97,97,97,97	22
2	D5M	G	999	22/22	0.72	0.42	97,97,97,97	22
2	D5M	P	999	22/22	0.73	0.34	97,97,97,97	22
2	D5M	D	999	22/22	0.75	0.39	97,97,97,97	22
2	D5M	A	999	22/22	0.76	0.29	97,97,97,97	22
2	D5M	F	999	22/22	0.78	0.37	97,97,97,97	22
2	D5M	R	999	22/22	0.79	0.40	97,97,97,97	22
2	D5M	B	999	22/22	0.80	0.38	97,97,97,97	22
2	D5M	I	999	22/22	0.80	0.30	97,97,97,97	22
2	D5M	Q	999	22/22	0.80	0.29	97,97,97,97	22
2	D5M	J	999	22/22	0.80	0.37	97,97,97,97	22
2	D5M	K	999	22/22	0.80	0.38	97,97,97,97	22
2	D5M	H	999	22/22	0.81	0.34	97,97,97,97	22
2	D5M	N	999	22/22	0.81	0.33	97,97,97,97	22
2	D5M	M	999	22/22	0.83	0.30	97,97,97,97	22
2	D5M	C	999	22/22	0.84	0.40	97,97,97,97	22
2	D5M	O	999	22/22	0.85	0.31	97,97,97,97	22
2	D5M	E	999	22/22	0.87	0.27	97,97,97,97	22
2	D5M	T	999	22/22	0.89	0.29	97,97,97,97	22

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.

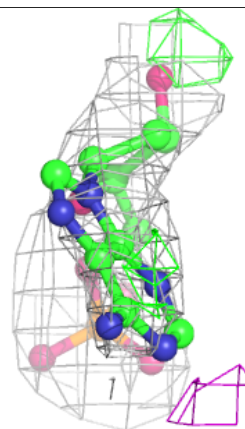
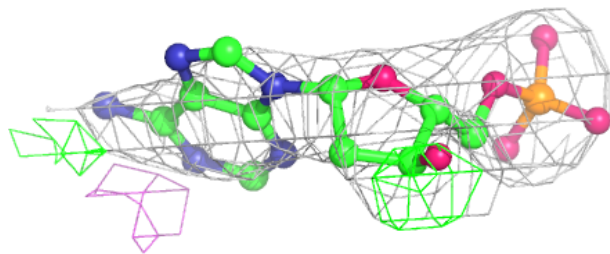
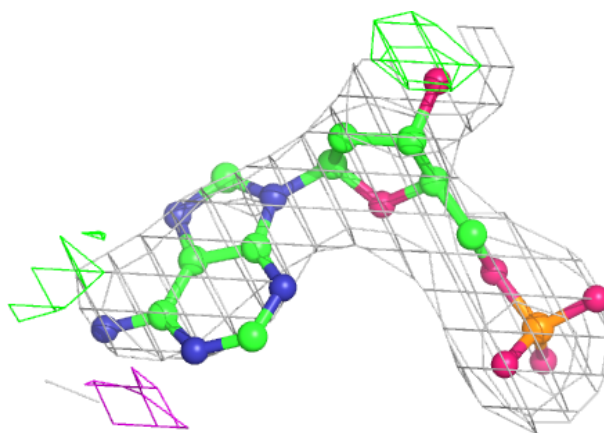
Electron density around D5M S 999:

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



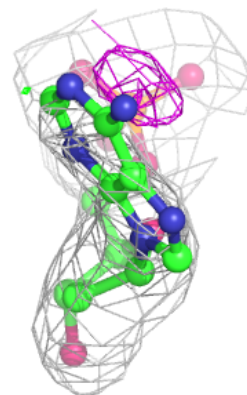
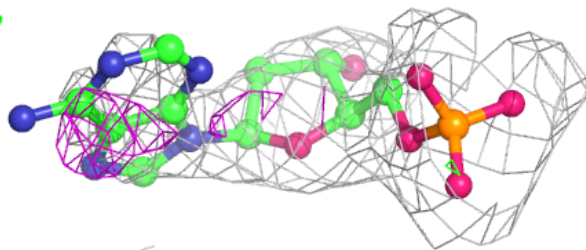
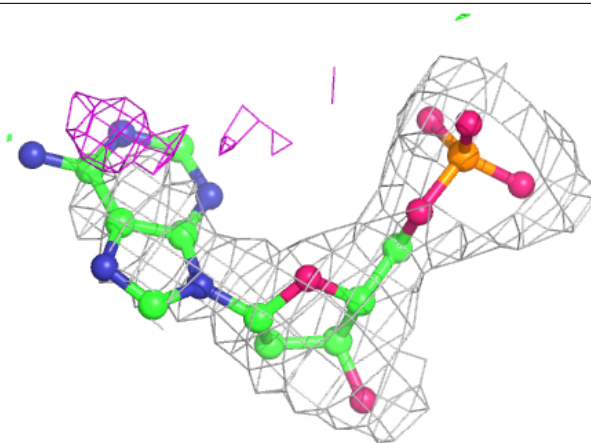
Electron density around D5M L 999:

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



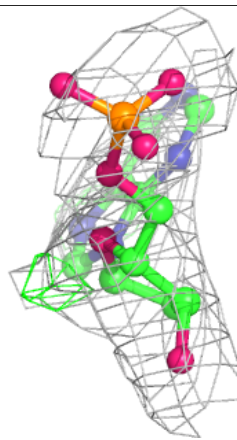
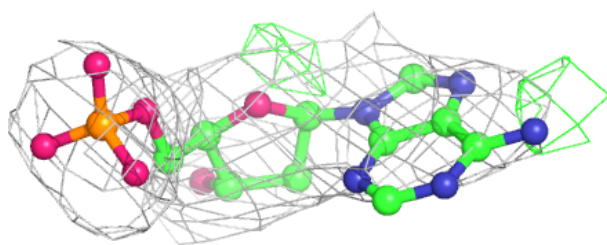
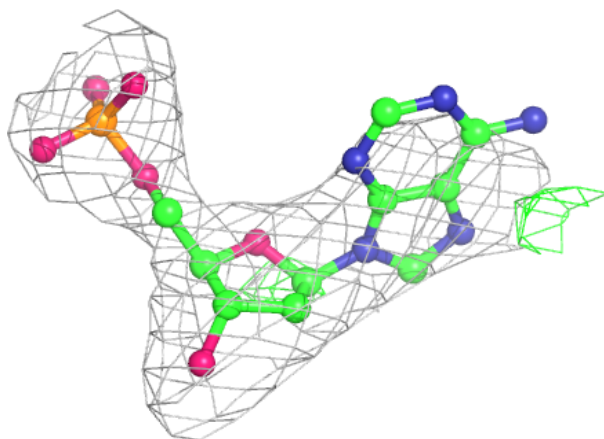
Electron density around D5M G 999:

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



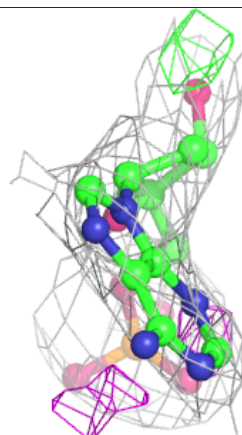
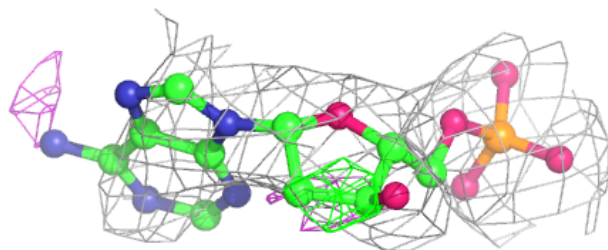
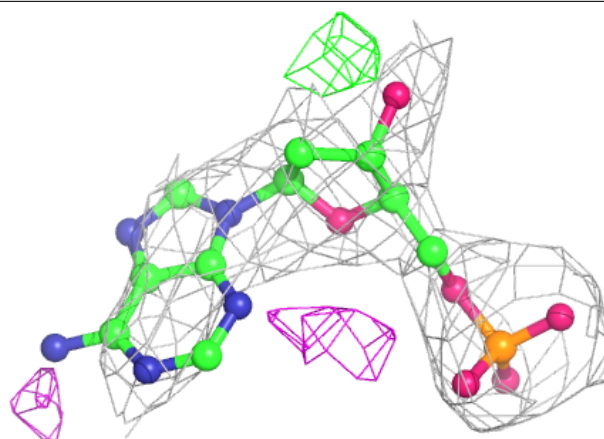
Electron density around D5M P 999:

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



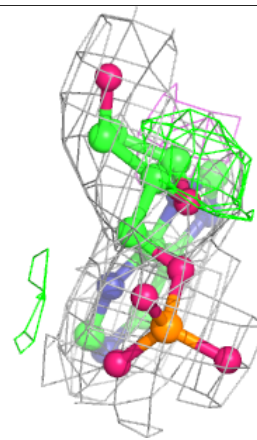
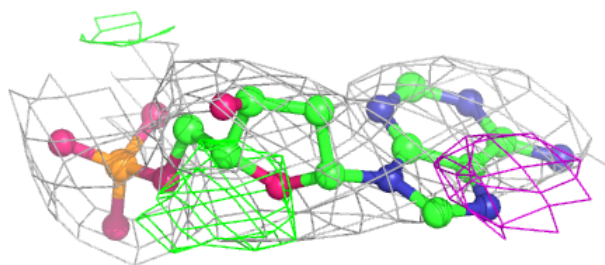
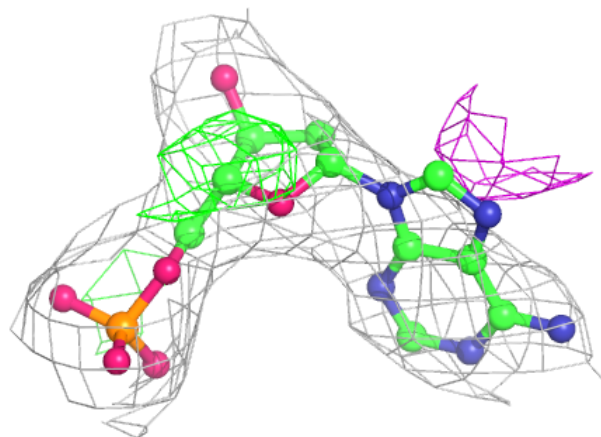
Electron density around D5M D 999:

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



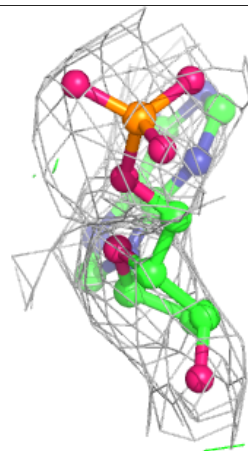
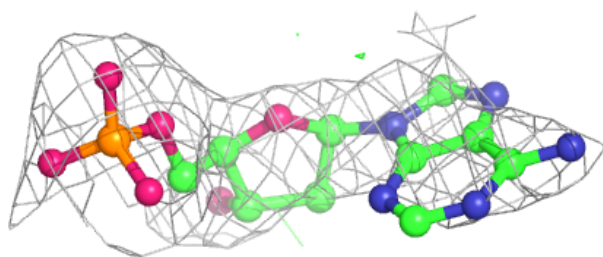
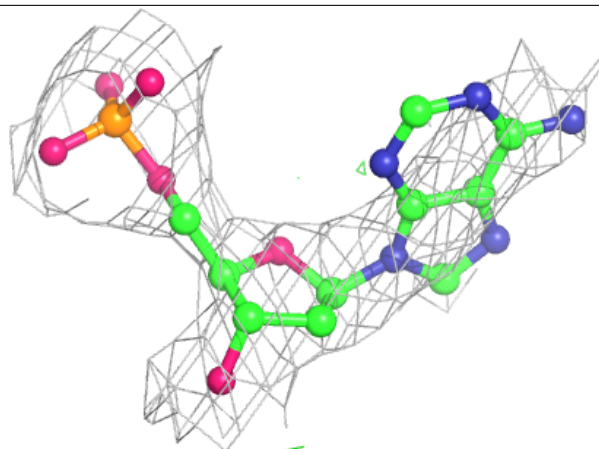
Electron density around D5M A 999:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

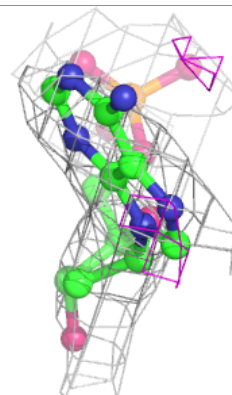
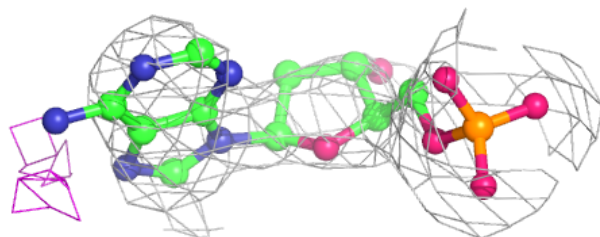
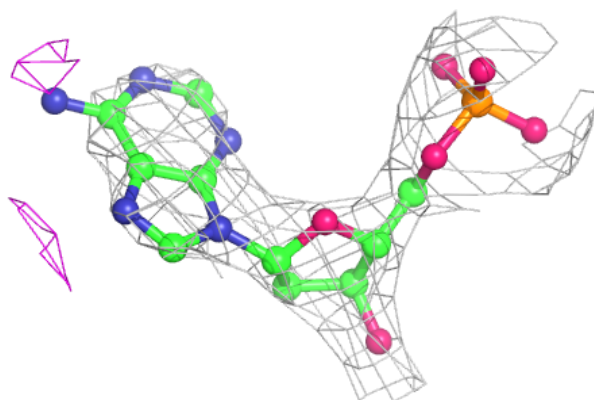


Electron density around D5M F 999:

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

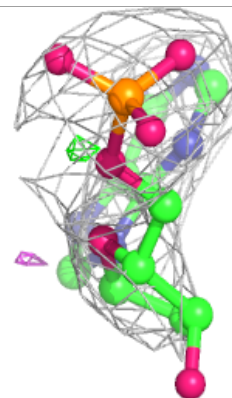
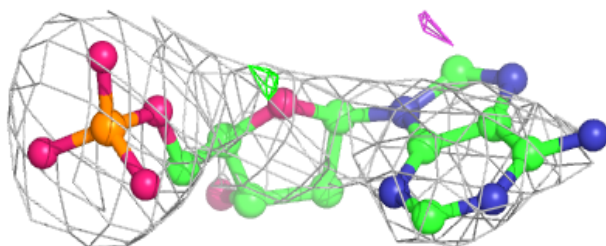
**Electron density around D5M R 999:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

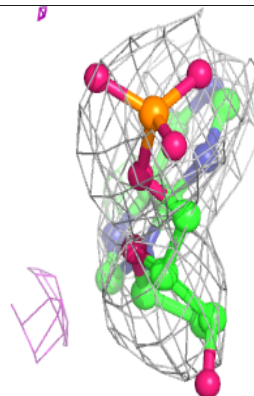
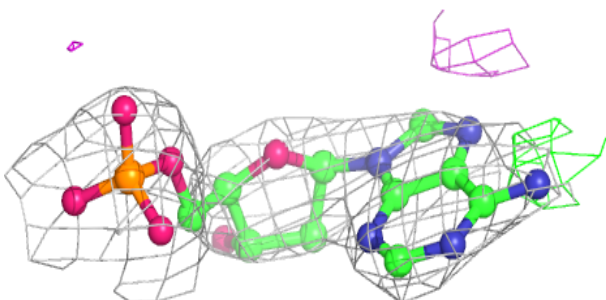
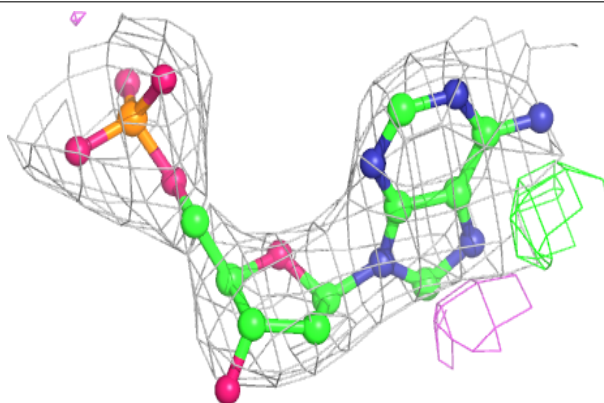


Electron density around D5M B 999:

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

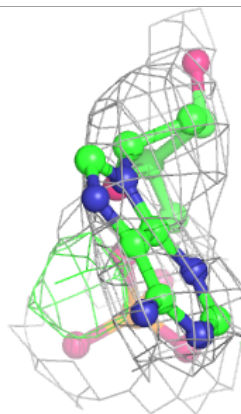
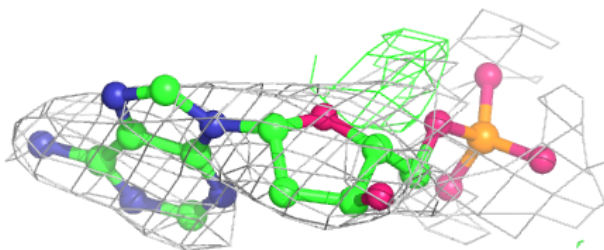
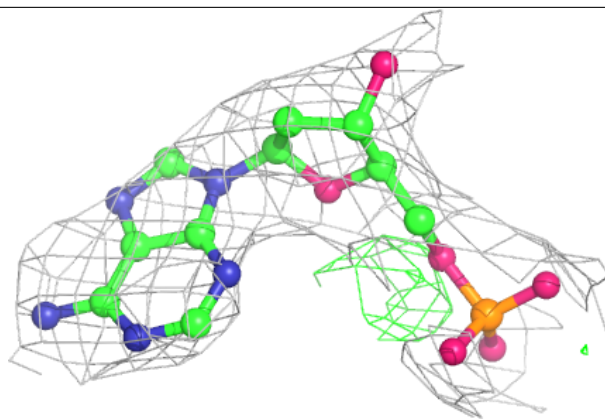
**Electron density around D5M I 999:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



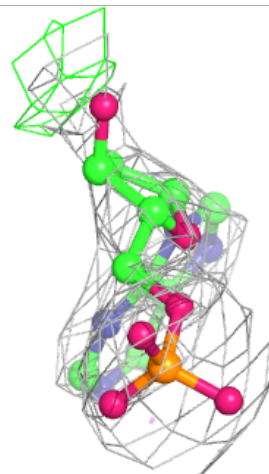
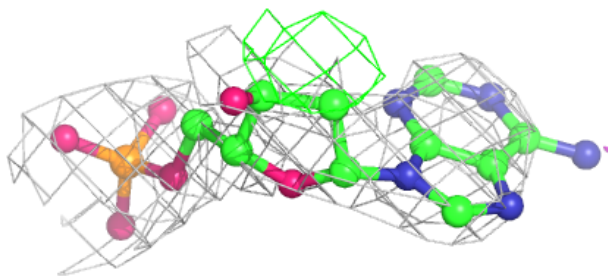
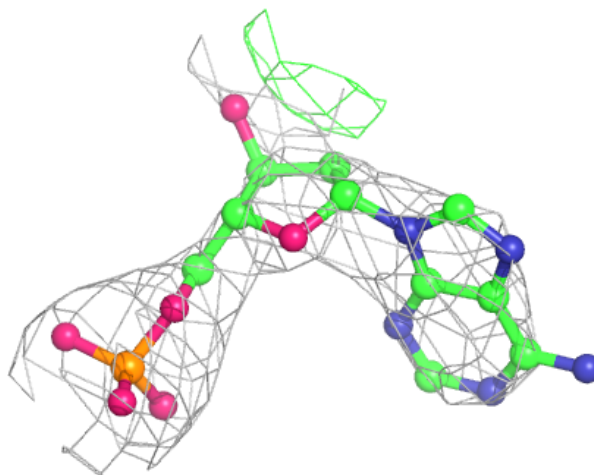
Electron density around D5M Q 999:

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



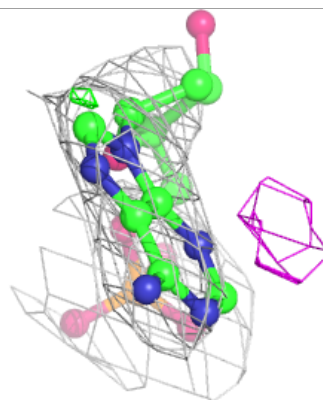
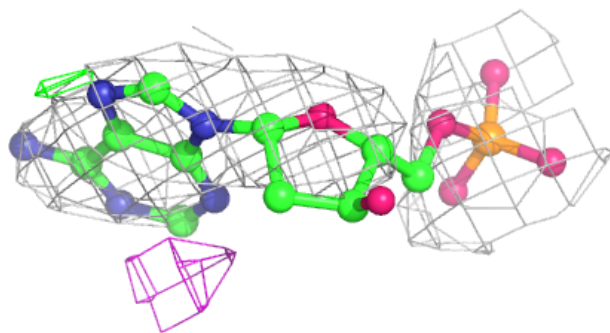
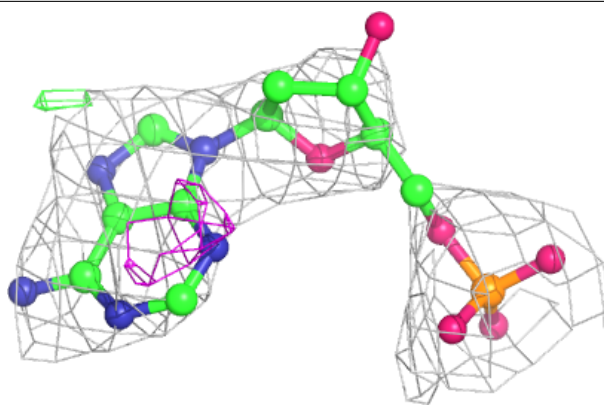
Electron density around D5M J 999:

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



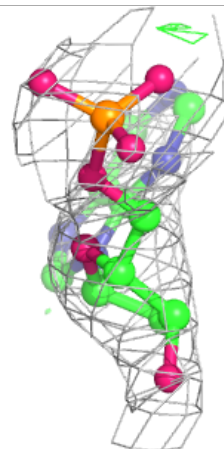
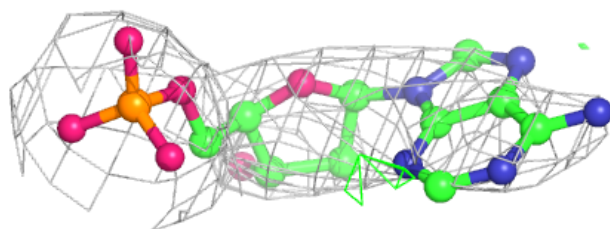
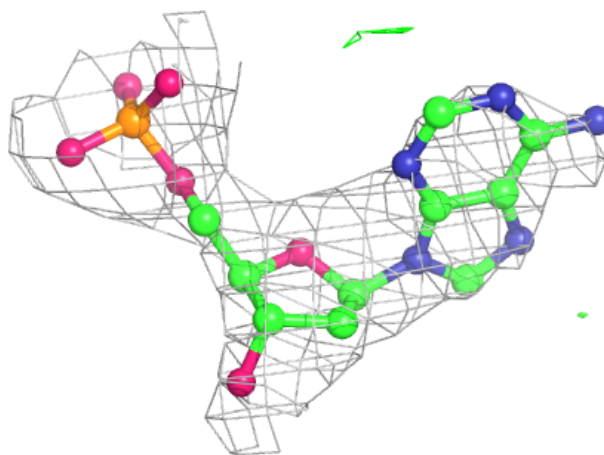
Electron density around D5M K 999:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



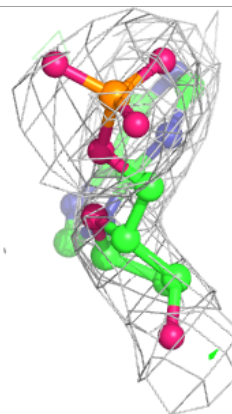
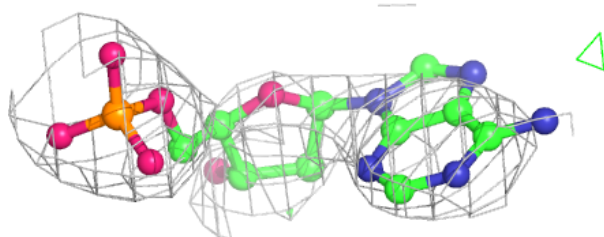
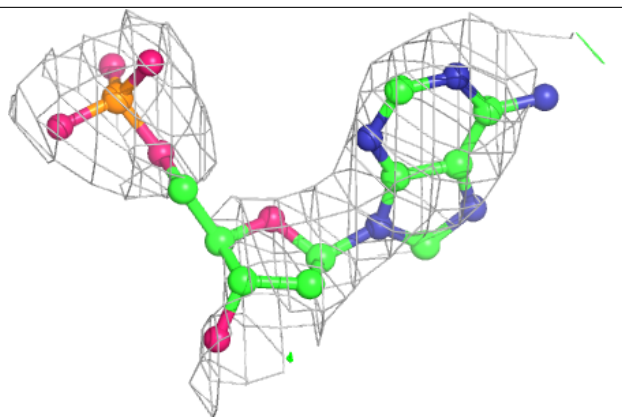
Electron density around D5M H 999:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

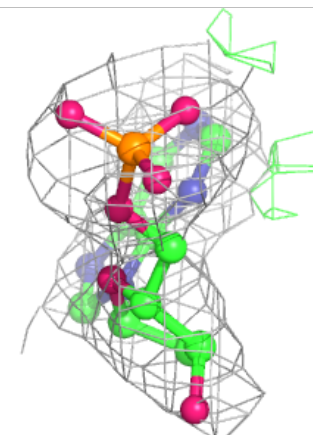
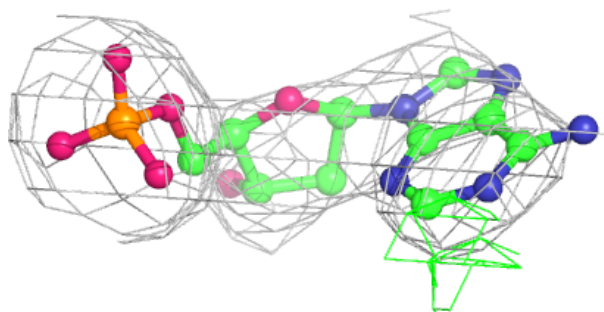
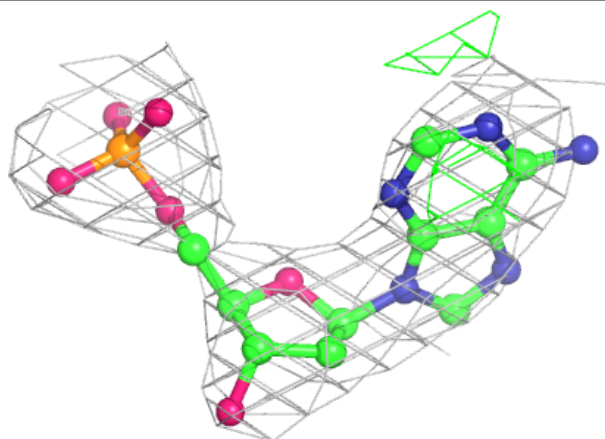


Electron density around D5M N 999:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

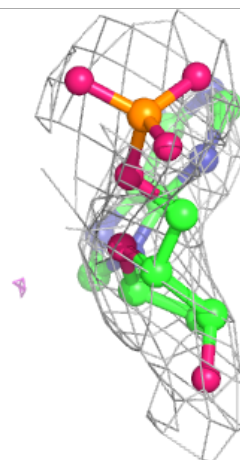
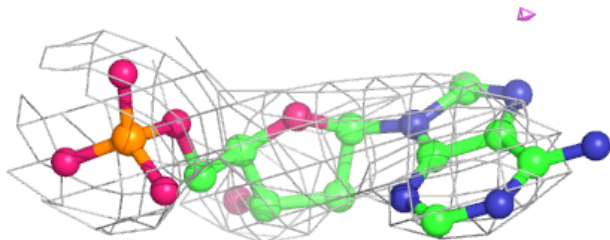
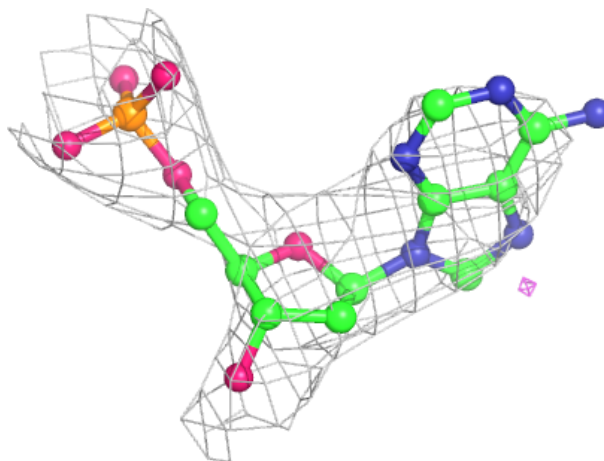
**Electron density around D5M M 999:**

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



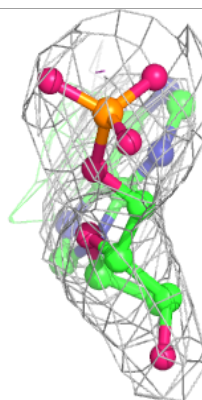
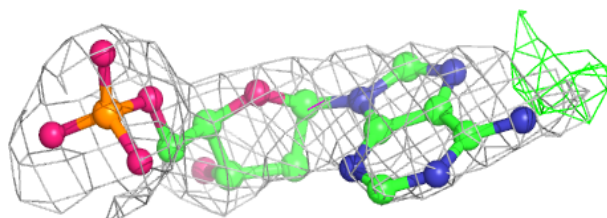
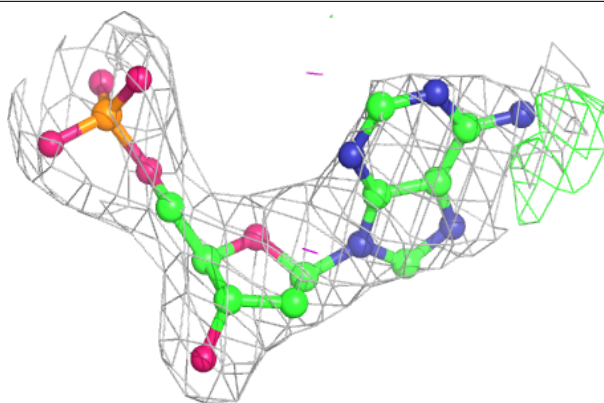
Electron density around D5M C 999:

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

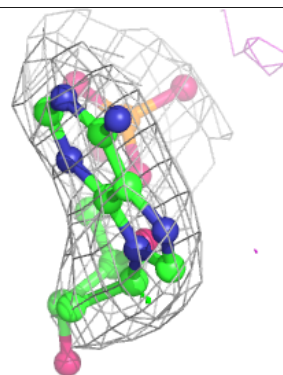
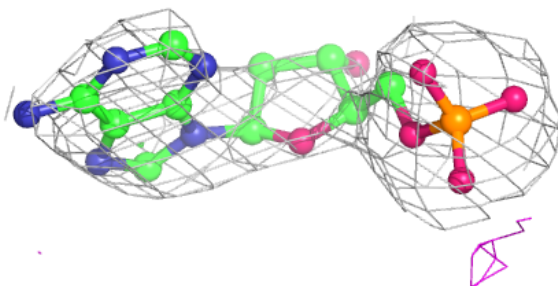
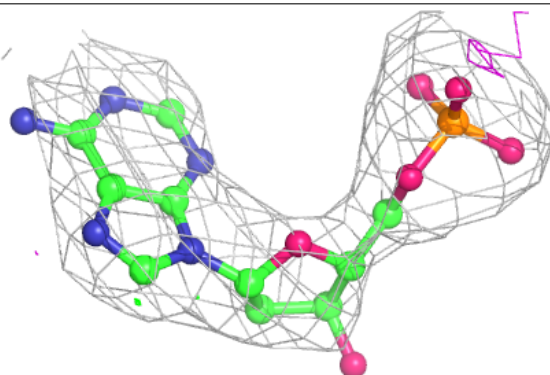


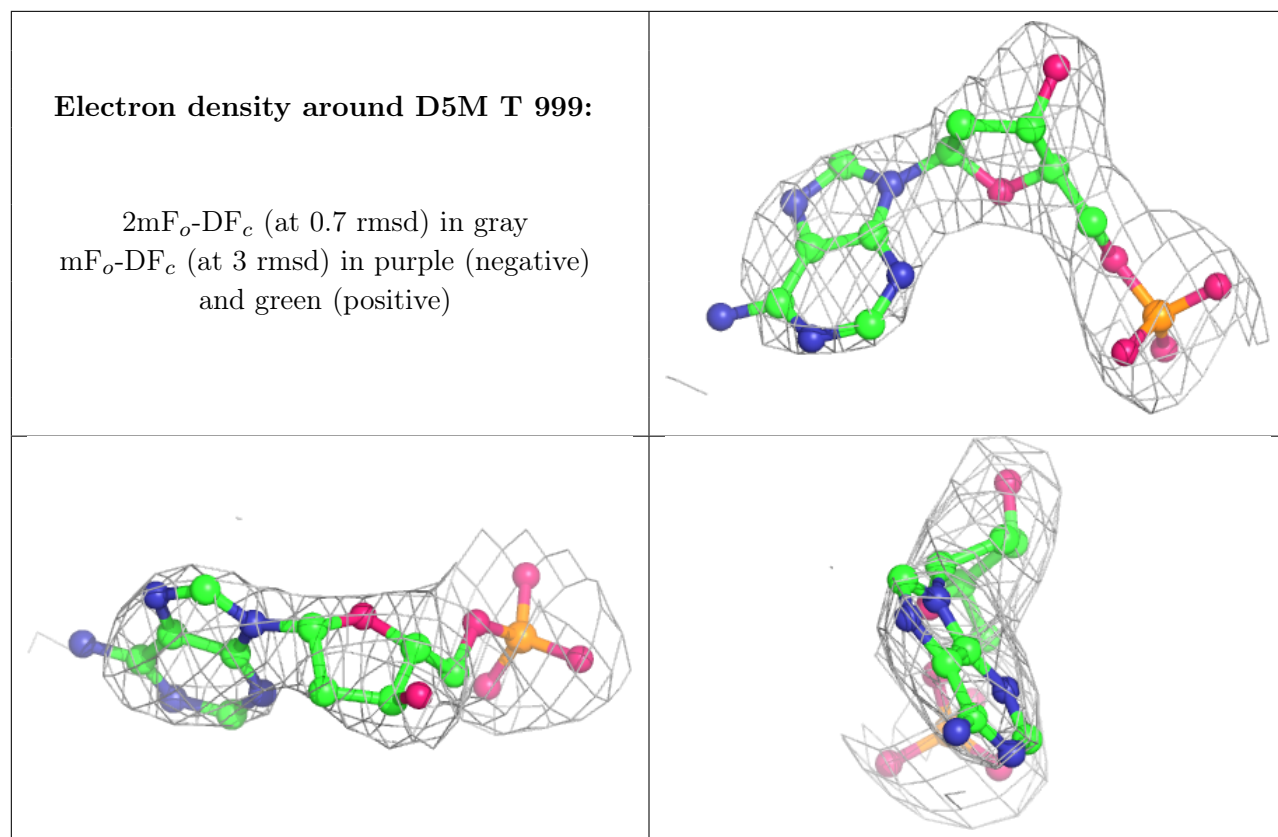
Electron density around D5M O 999:

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

**Electron density around D5M E 999:**

$2mF_o - DF_c$ (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.