



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:30 PM BST

PDB ID : 1YAJ
Title : Crystal Structure of Human Liver Carboxylesterase in complex with benzil
Authors : Fleming, C.D.; Bencharit, S.; Edwards, C.C.; Hyatt, J.L.; Morton, C.M.; Howard-Williams, E.L.; Potter, P.M.; Redinbo, M.R.
Deposited on : 2004-12-17
Resolution : 3.20 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 : 2.13.1
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) : 2.13.1

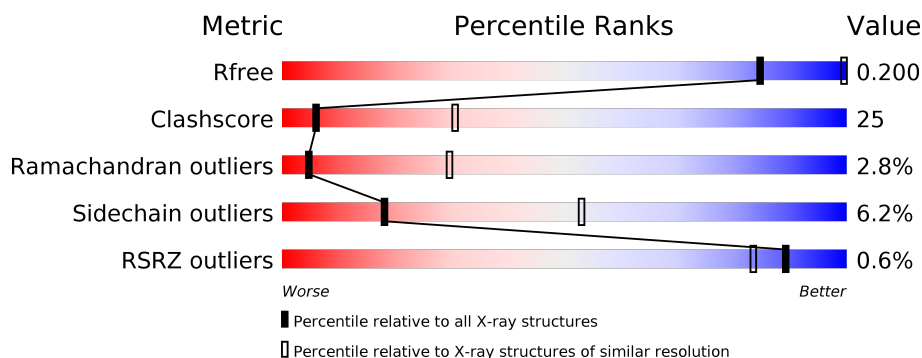
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	532	<div> <div></div> <div>52%44%.</div> </div>
1	B	532	<div> <div>%</div> <div>56%40%.</div> </div>
1	C	532	<div> <div>%</div> <div>56%40%.</div> </div>
1	D	532	<div> <div>%</div> <div>52%42%5%.</div> </div>
1	E	532	<div> <div>%</div> <div>54%42%.</div> </div>
1	F	532	<div> <div>%</div> <div>55%41%.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	532	
1	H	532	
1	I	532	
1	J	532	
1	K	532	
1	L	532	

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	NAG	A	1179	-	-	-	X
2	NAG	B	1279	X	-	-	-
2	NAG	F	2379	X	-	-	-
2	NAG	G	3179	X	-	-	-
2	NAG	J	4179	X	-	-	-
2	NAG	K	4279	X	-	-	-
3	SIA	A	1181	-	-	X	-
5	BEZ	B	12	-	-	X	-
5	BEZ	D	2385	-	X	-	-
5	BEZ	G	3386	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 50793 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 CES1 protein.

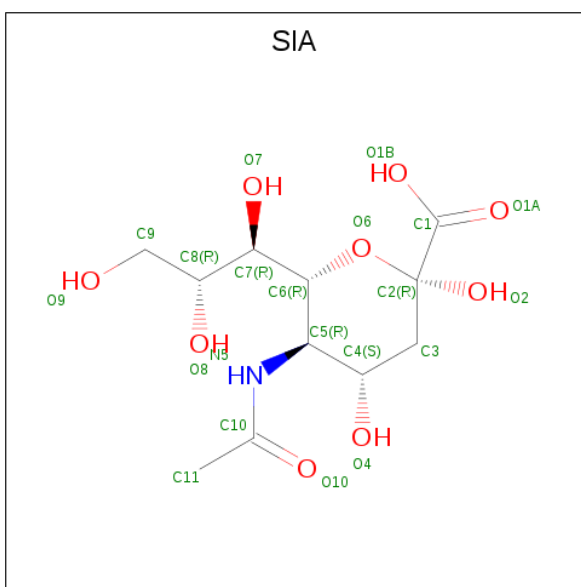
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	C	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	D	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	E	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	F	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	G	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	H	532	Total	C	N	O	S	0	0	0
			4129	2662	685	762	20			
1	I	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	J	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	K	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	L	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	D	1	Total	C	N	O	0	0
			21	11	1	9		
3	E	1	Total	C	N	O	0	0
			21	11	1	9		
3	F	1	Total	C	N	O	0	0
			21	11	1	9		
3	G	1	Total	C	N	O	0	0
			21	11	1	9		
3	H	1	Total	C	N	O	0	0
			21	11	1	9		
3	I	1	Total	C	N	O	0	0
			21	11	1	9		
3	J	1	Total	C	N	O	0	0
			21	11	1	9		
3	K	1	Total	C	N	O	0	0
			21	11	1	9		
3	L	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



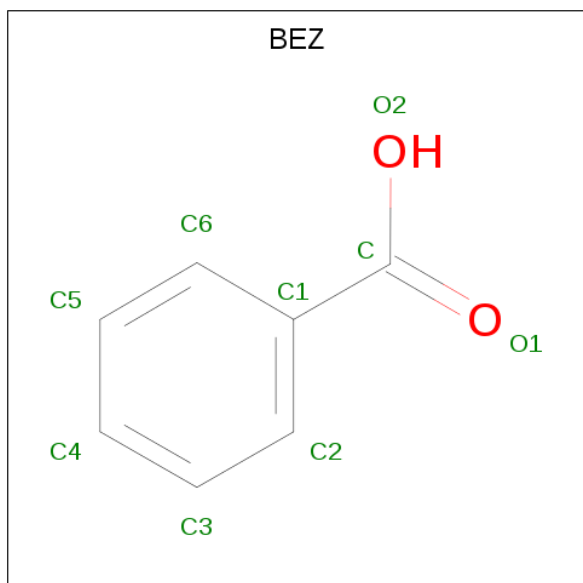
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is BENZOIC ACID (three-letter code: BEZ) (formula: C₇H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	7	2		
5	B	1	Total	C	O	0	0
			9	7	2		
5	B	1	Total	C	O	0	0
			9	7	2		
5	C	1	Total	C	O	0	0
			8	7	1		
5	C	1	Total	C	O	0	0
			9	7	2		
5	D	1	Total	C	O	0	0
			9	7	2		
5	D	1	Total	C	O	0	0
			9	7	2		
5	E	1	Total	C	O	0	0
			9	7	2		
5	E	1	Total	C	O	0	0
			9	7	2		
5	F	1	Total	C	O	0	0
			8	7	1		
5	F	1	Total	C	O	0	0
			9	7	2		
5	G	1	Total	C	O	0	0
			9	7	2		
5	G	1	Total	C	O	0	0
			9	7	2		
5	H	1	Total	C	O	0	0
			9	7	2		
5	H	1	Total	C	O	0	0
			9	7	2		
5	I	1	Total	C	O	0	0
			9	7	2		
5	I	1	Total	C	O	0	0
			9	7	2		
5	J	1	Total	C	O	0	0
			8	7	1		
5	J	1	Total	C	O	0	0
			9	7	2		
5	K	1	Total	C	O	0	0
			9	7	2		
5	K	1	Total	C	O	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			9	7	2		
5	L	1	Total	C	O	0	0
			9	7	2		

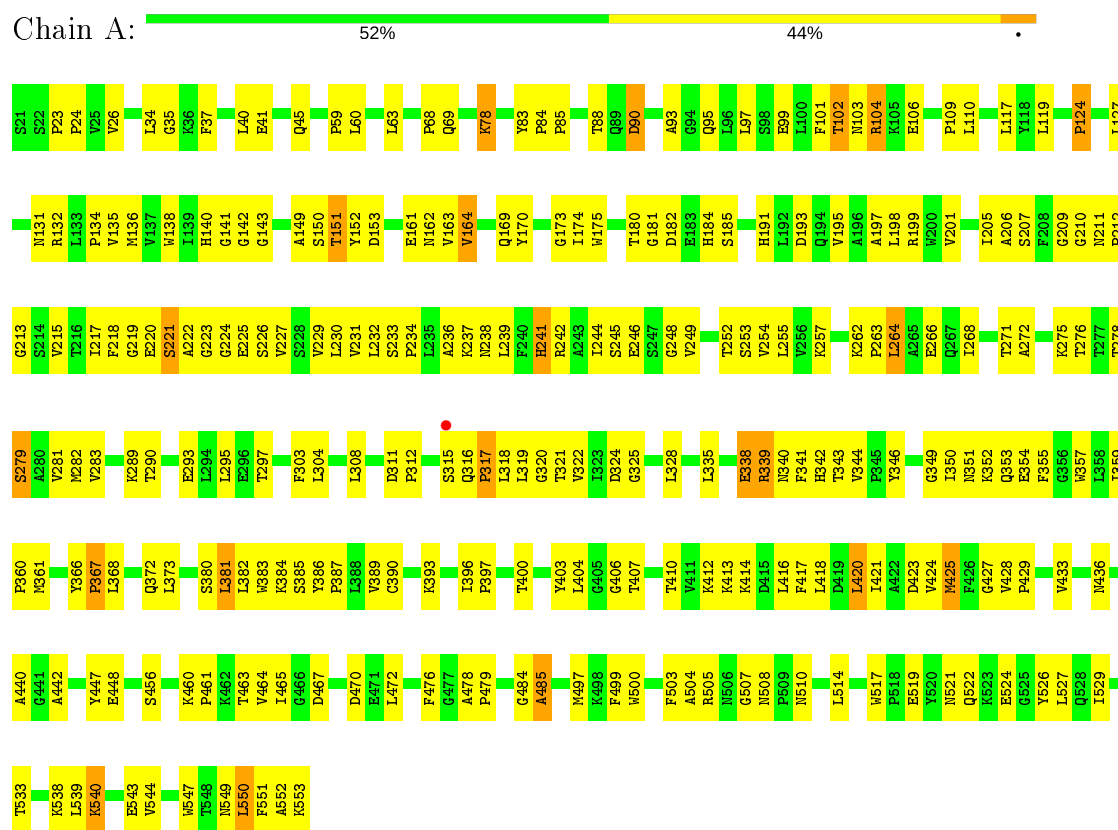
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total	O	0	0
			43	43		
6	B	30	Total	O	0	0
			30	30		
6	C	33	Total	O	0	0
			33	33		
6	D	49	Total	O	0	0
			49	49		
6	E	38	Total	O	0	0
			38	38		
6	F	42	Total	O	0	0
			42	42		
6	G	41	Total	O	0	0
			41	41		
6	H	37	Total	O	0	0
			37	37		
6	I	34	Total	O	0	0
			34	34		
6	J	38	Total	O	0	0
			38	38		
6	K	50	Total	O	0	0
			50	50		
6	L	39	Total	O	0	0
			39	39		

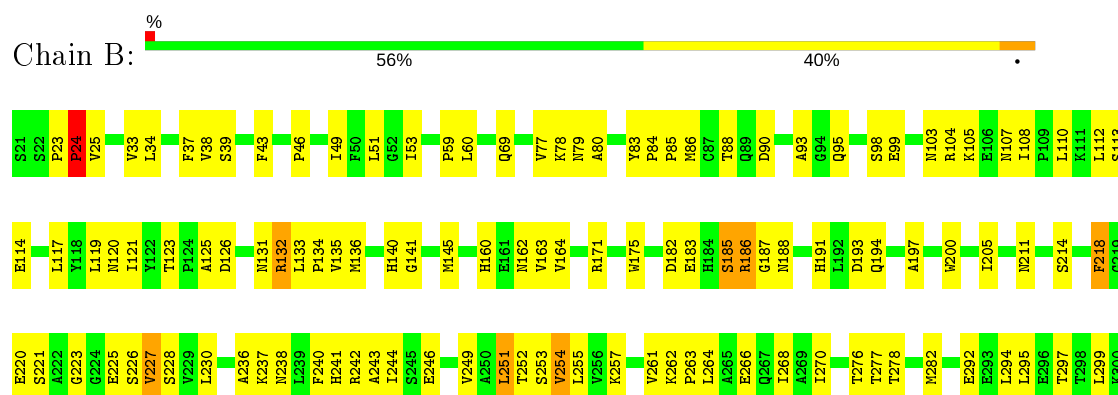
3 Residue-property plots

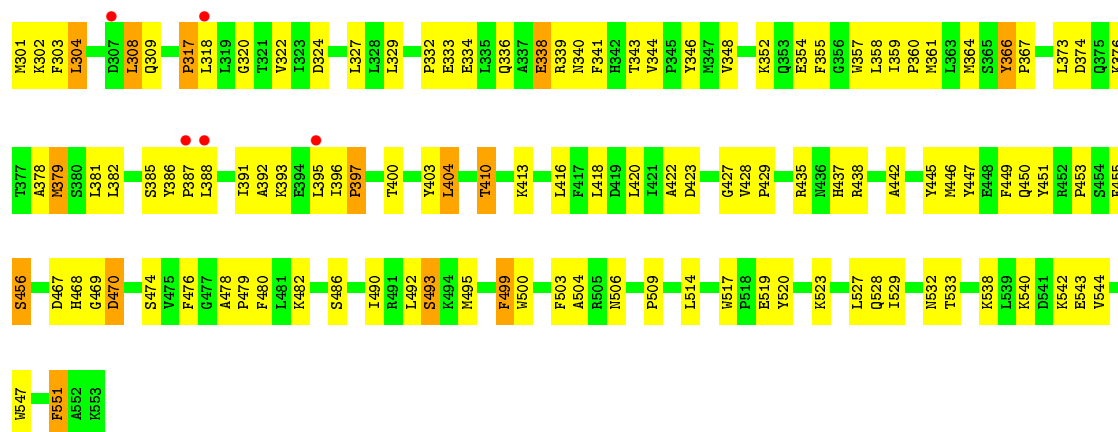
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CES1 protein

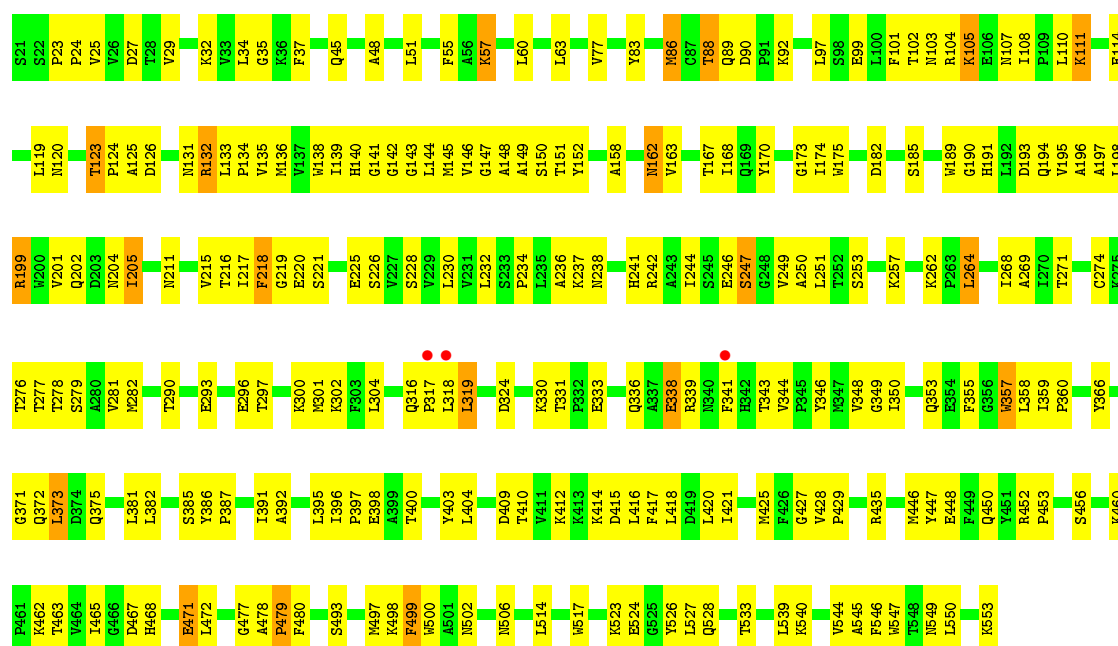


• Molecule 1: CES1 protein

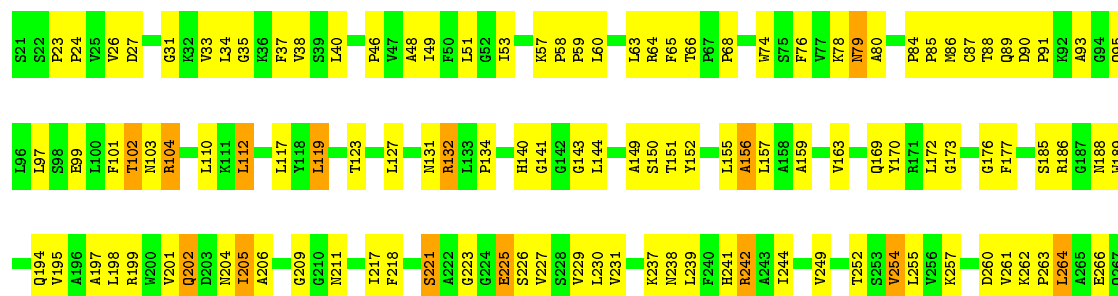


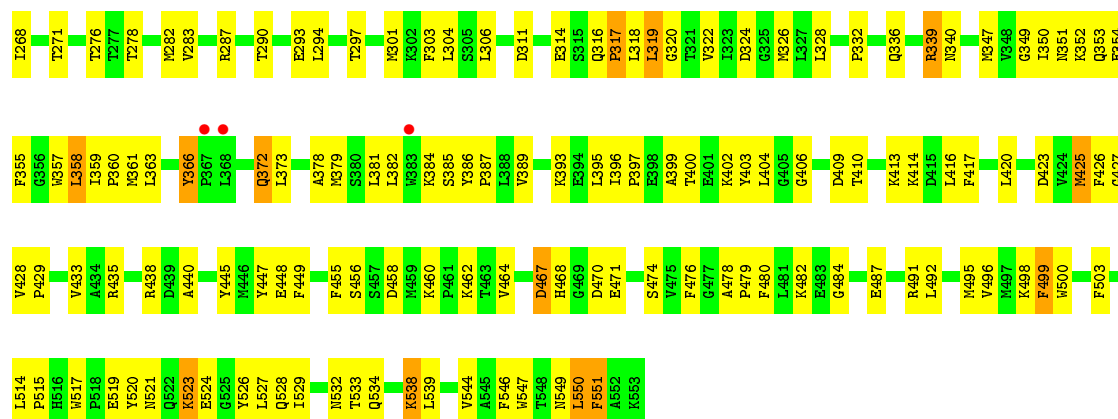


• Molecule 1: CES1 protein

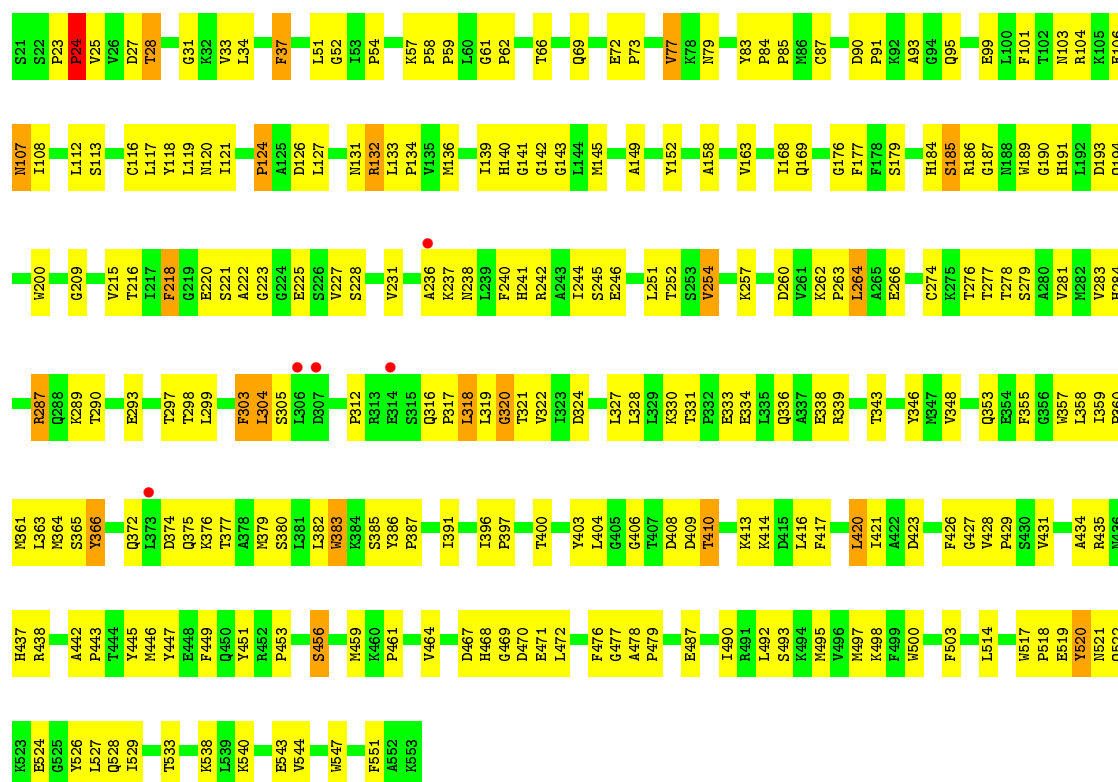


• Molecule 1: CES1 protein

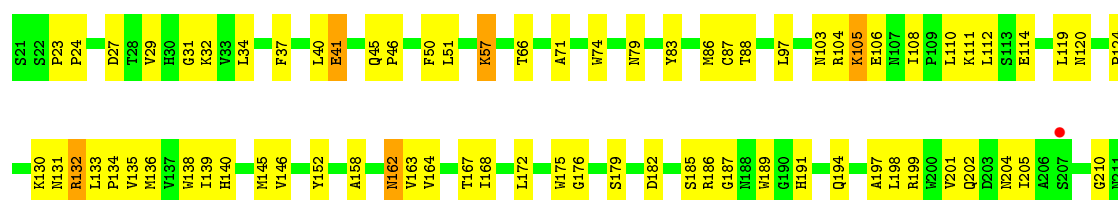


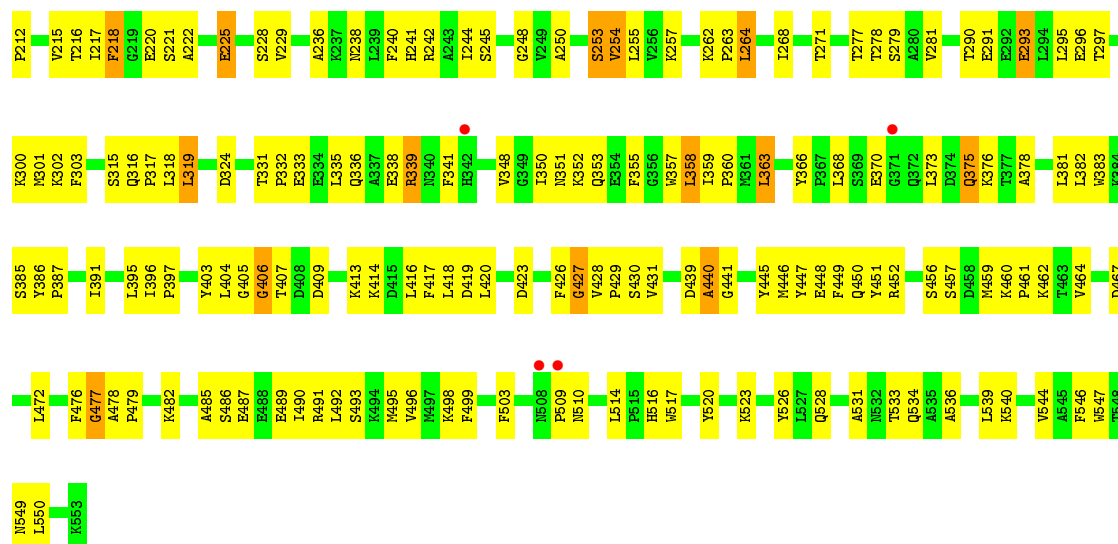


• Molecule 1: CES1 protein

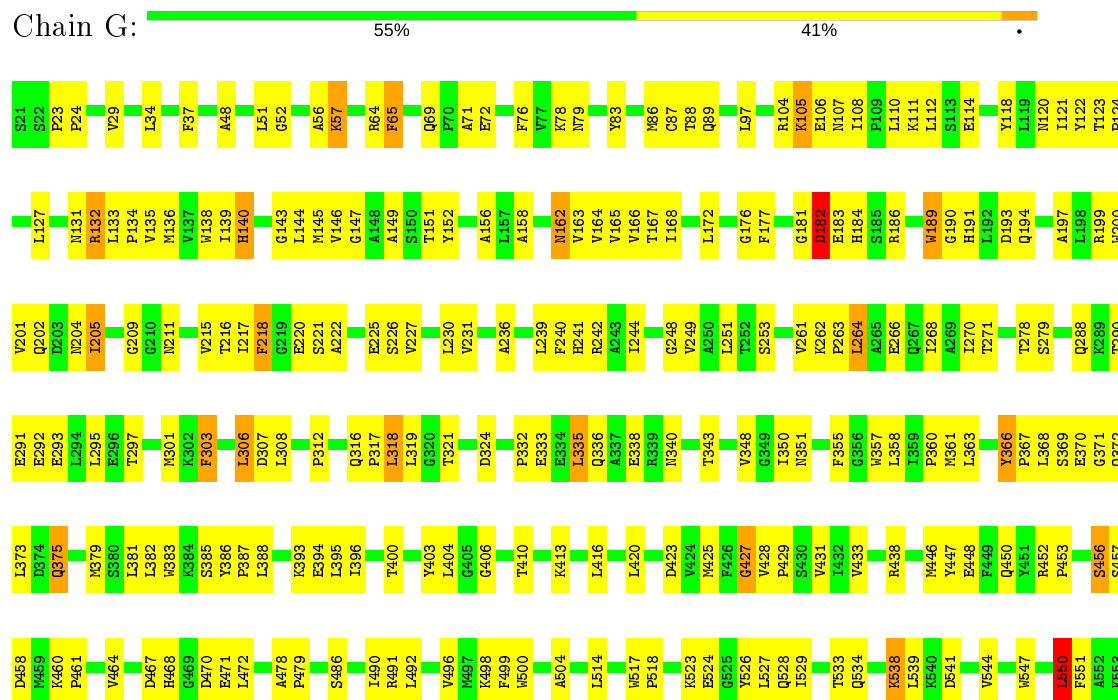


• Molecule 1: CES1 protein

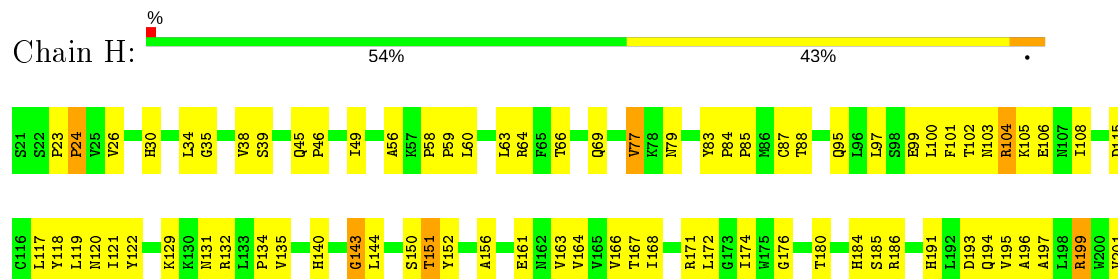


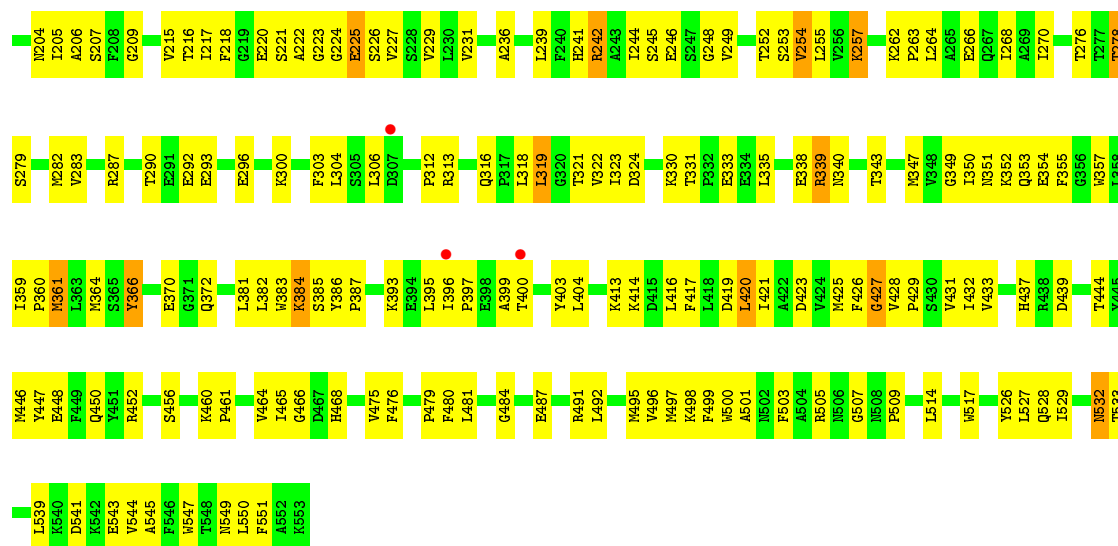


• Molecule 1: CES1 protein



• Molecule 1: CES1 protein

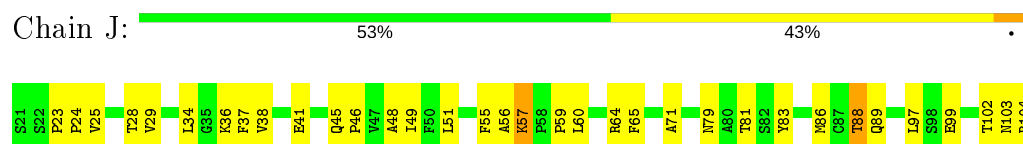


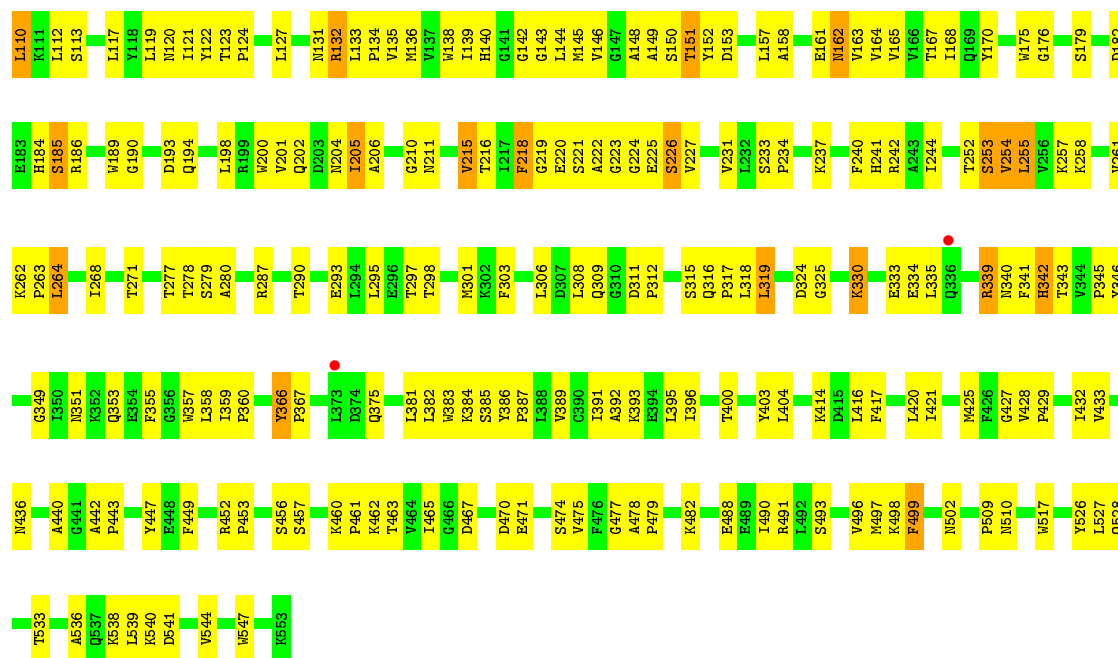


- Molecule 1: CES1 protein

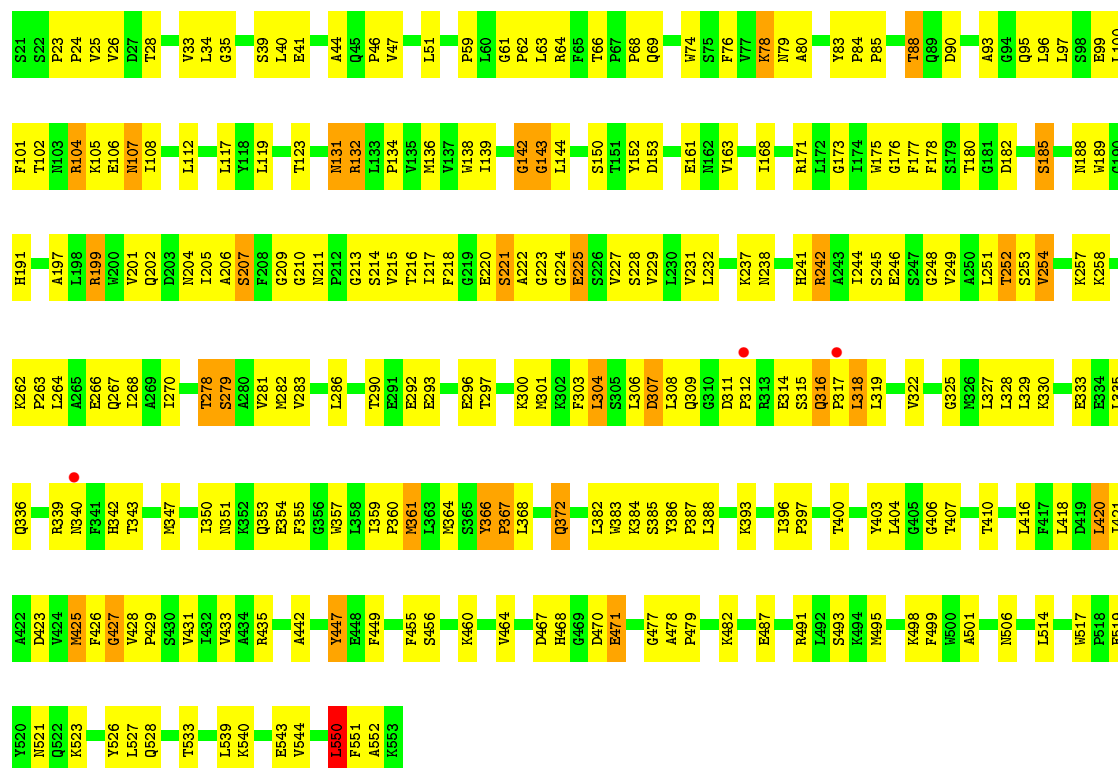


- Molecule 1: CES1 protein



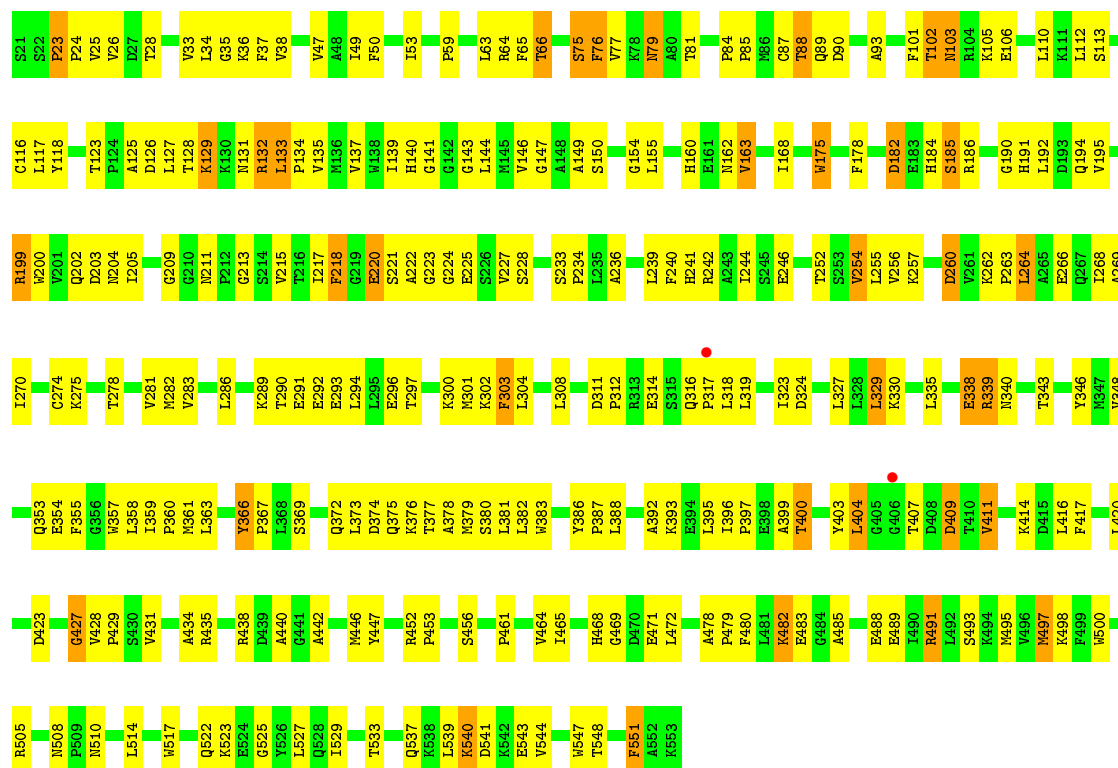


• Molecule 1: CES1 protein



• Molecule 1: CES1 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.56Å 181.49Å 202.71Å 90.12° 89.93° 89.72°	Depositor
Resolution (Å)	54.56 – 3.20 54.56 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (54.56-3.20) 95.8 (54.56-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.287 0.196 , 0.200	Depositor DCC
R_{free} test set	6249 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.388 for h,-k,-l 0.377 for -h,k,-l 0.389 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	50793	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: BEZ, SIA, NAG, SO4

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	0.64	4/4236 (0.1%)	0.70	2/5754 (0.0%)
1	B	0.62	3/4237 (0.1%)	0.66	3/5754 (0.1%)
1	C	0.62	3/4237 (0.1%)	0.66	0/5754
1	D	0.60	0/4236	0.67	1/5754 (0.0%)
1	E	0.71	6/4237 (0.1%)	0.69	4/5754 (0.1%)
1	F	0.63	3/4237 (0.1%)	0.67	2/5754 (0.0%)
1	G	0.73	10/4236 (0.2%)	0.78	9/5754 (0.2%)
1	H	0.70	2/4235 (0.0%)	0.70	1/5752 (0.0%)
1	I	0.92	12/4237 (0.3%)	0.76	13/5754 (0.2%)
1	J	0.61	3/4237 (0.1%)	0.68	2/5754 (0.0%)
1	K	0.60	4/4236 (0.1%)	0.68	1/5754 (0.0%)
1	L	0.64	4/4237 (0.1%)	0.68	3/5754 (0.1%)
All	All	0.67	54/50838 (0.1%)	0.69	41/69046 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	2
1	K	0	1
All	All	0	4

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	383	TRP	CD2-CE2	21.55	1.67	1.41
1	I	383	TRP	CE3-CZ3	20.67	1.73	1.38
1	H	77	VAL	CB-CG1	19.61	1.94	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	383	TRP	CE2-CZ2	17.00	1.68	1.39
1	E	77	VAL	CB-CG1	15.91	1.86	1.52
1	G	550	LEU	C-N	-14.79	1.00	1.34
1	I	383	TRP	CD2-CE3	13.71	1.60	1.40
1	G	550	LEU	CA-C	13.25	1.87	1.52
1	E	24	PRO	CA-C	13.18	1.79	1.52
1	I	24	PRO	CA-C	12.36	1.77	1.52
1	B	24	PRO	CA-C	11.61	1.76	1.52
1	I	383	TRP	NE1-CE2	10.82	1.51	1.37
1	F	57	LYS	CB-CG	10.76	1.81	1.52
1	E	77	VAL	CA-CB	-10.65	1.32	1.54
1	H	23	PRO	C-N	10.46	1.54	1.34
1	G	181	GLY	C-O	-10.44	1.06	1.23
1	I	383	TRP	CG-CD1	9.80	1.50	1.36
1	I	383	TRP	CG-CD2	9.54	1.59	1.43
1	G	189	TRP	CE3-CZ3	-8.92	1.23	1.38
1	A	550	LEU	CA-C	8.84	1.75	1.52
1	I	57	LYS	CB-CG	8.02	1.74	1.52
1	A	550	LEU	C-O	-7.94	1.08	1.23
1	E	23	PRO	C-N	7.82	1.49	1.34
1	G	189	TRP	CE2-CZ2	-7.60	1.26	1.39
1	L	77	VAL	CB-CG1	7.45	1.68	1.52
1	K	550	LEU	C-N	7.43	1.51	1.34
1	L	77	VAL	CB-CG2	-7.23	1.37	1.52
1	F	57	LYS	CA-CB	7.18	1.69	1.53
1	L	175	TRP	CZ3-CH2	-7.15	1.28	1.40
1	B	77	VAL	CB-CG1	6.94	1.67	1.52
1	I	24	PRO	N-CD	6.43	1.56	1.47
1	A	181	GLY	C-O	-6.42	1.13	1.23
1	L	23	PRO	C-N	6.27	1.46	1.34
1	J	57	LYS	CB-CG	6.12	1.69	1.52
1	K	74	TRP	CZ3-CH2	-6.10	1.30	1.40
1	G	57	LYS	C-O	6.07	1.34	1.23
1	C	57	LYS	CA-CB	5.87	1.66	1.53
1	C	57	LYS	CA-C	5.85	1.68	1.52
1	J	57	LYS	CA-CB	5.79	1.66	1.53
1	G	57	LYS	CA-C	5.76	1.68	1.52
1	E	383	TRP	CZ3-CH2	-5.73	1.30	1.40
1	J	57	LYS	CA-C	5.61	1.67	1.52
1	B	175	TRP	CZ3-CH2	-5.48	1.31	1.40
1	I	383	TRP	CD1-NE1	5.44	1.47	1.38
1	I	77	VAL	CA-CB	-5.36	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	ASP	CB-CG	-5.31	1.40	1.51
1	F	57	LYS	CA-C	5.25	1.66	1.52
1	G	57	LYS	CA-CB	5.18	1.65	1.53
1	G	57	LYS	CB-CG	5.16	1.66	1.52
1	C	189	TRP	CE3-CZ3	-5.15	1.29	1.38
1	E	383	TRP	CD2-CE2	-5.12	1.35	1.41
1	G	186	ARG	CG-CD	-5.07	1.39	1.51
1	K	550	LEU	CA-C	5.06	1.66	1.52
1	K	175	TRP	CZ3-CH2	-5.00	1.32	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	550	LEU	O-C-N	13.71	144.63	122.70
1	G	550	LEU	CA-C-O	-12.66	93.51	120.10
1	G	182	ASP	CB-CG-OD1	11.15	128.34	118.30
1	A	550	LEU	O-C-N	8.86	136.88	122.70
1	I	186	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	G	181	GLY	CA-C-N	8.75	136.46	117.20
1	I	383	TRP	CE2-CD2-CE3	-7.82	109.32	118.70
1	G	181	GLY	N-CA-C	-7.63	94.02	113.10
1	J	186	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	I	383	TRP	CB-CG-CD2	7.45	136.29	126.60
1	E	303	PHE	N-CA-C	7.11	130.20	111.00
1	L	303	PHE	N-CA-C	6.98	129.84	111.00
1	H	303	PHE	N-CA-C	6.75	129.22	111.00
1	I	24	PRO	CA-N-CD	-6.71	102.10	111.50
1	I	303	PHE	N-CA-C	6.58	128.78	111.00
1	D	303	PHE	N-CA-C	6.58	128.77	111.00
1	K	303	PHE	N-CA-C	6.52	128.60	111.00
1	A	303	PHE	N-CA-C	6.48	128.50	111.00
1	G	303	PHE	N-CA-C	6.37	128.19	111.00
1	G	182	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	I	24	PRO	CB-CA-C	-6.34	96.14	112.00
1	I	383	TRP	CB-CG-CD1	-6.17	118.98	127.00
1	I	383	TRP	CA-CB-CG	-6.15	102.02	113.70
1	I	186	ARG	NH1-CZ-NH2	-6.08	112.71	119.40
1	F	57	LYS	CA-CB-CG	6.04	126.69	113.40
1	F	57	LYS	CB-CA-C	6.02	122.44	110.40
1	G	181	GLY	CA-C-O	-6.00	109.81	120.60
1	B	24	PRO	CB-CA-C	-5.71	97.73	112.00
1	J	57	LYS	CB-CA-C	5.68	121.76	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	77	VAL	CA-CB-CG2	5.66	119.38	110.90
1	I	34	LEU	CB-CG-CD2	-5.65	101.40	111.00
1	G	181	GLY	O-C-N	-5.62	113.71	122.70
1	E	24	PRO	CB-CA-C	-5.53	98.18	112.00
1	I	57	LYS	CB-CA-C	5.50	121.39	110.40
1	L	303	PHE	CB-CA-C	-5.45	99.51	110.40
1	E	77	VAL	CA-CB-CG1	-5.43	102.76	110.90
1	E	24	PRO	N-CA-C	-5.39	98.08	112.10
1	I	383	TRP	NE1-CE2-CD2	-5.34	101.96	107.30
1	I	383	TRP	NE1-CE2-CZ2	-5.26	124.61	130.40
1	B	24	PRO	CA-N-CD	-5.25	104.16	111.50
1	B	24	PRO	N-CA-C	-5.01	99.06	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	550	LEU	Mainchain
1	G	550	LEU	Mainchain
1	G	57	LYS	Mainchain
1	K	550	LEU	Mainchain

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	4130	0	4131	221	0
1	B	4131	0	4130	180	0
1	C	4131	0	4130	199	0
1	D	4130	0	4130	199	0
1	E	4131	0	4131	202	0
1	F	4131	0	4130	184	0
1	G	4130	0	4129	192	0
1	H	4129	0	4131	206	0
1	I	4131	0	4131	212	0
1	J	4131	0	4129	214	0
1	K	4130	0	4130	219	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	4131	0	4131	227	0
2	A	14	0	13	0	0
2	B	14	0	13	1	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	3	0
2	G	14	0	13	1	0
2	H	14	0	13	0	0
2	I	14	0	13	0	0
2	J	14	0	13	1	0
2	K	14	0	13	2	0
2	L	14	0	13	0	0
3	A	42	0	36	13	0
3	B	21	0	18	5	0
3	D	21	0	18	8	0
3	E	21	0	18	2	0
3	F	21	0	18	1	0
3	G	21	0	18	6	0
3	H	21	0	18	1	0
3	I	21	0	18	5	0
3	J	21	0	18	5	0
3	K	21	0	18	7	0
3	L	21	0	18	7	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
4	G	10	0	0	0	0
4	H	10	0	0	0	0
4	I	10	0	0	1	0
4	J	15	0	0	0	0
4	K	10	0	0	0	0
4	L	5	0	0	0	0
5	A	18	0	10	2	0
5	B	18	0	11	6	0
5	C	17	0	10	4	0
5	D	18	0	11	3	0
5	E	18	0	10	0	0
5	F	17	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	18	0	10	1	0
5	H	18	0	10	1	0
5	I	18	0	10	1	0
5	J	17	0	10	1	0
5	K	18	0	10	0	0
5	L	18	0	10	1	0
6	A	43	0	0	11	0
6	B	30	0	0	5	0
6	C	33	0	0	5	0
6	D	49	0	0	8	0
6	E	38	0	0	16	0
6	F	42	0	0	4	0
6	G	41	0	0	8	0
6	H	37	0	0	8	0
6	I	34	0	0	9	0
6	J	38	0	0	9	0
6	K	50	0	0	11	0
6	L	39	0	0	12	0
All	All	50793	0	50057	2486	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (2486) 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)
5:B:12:BEZ:C3	5:B:12:BEZ:C2	1.76	1.62
5:B:12:BEZ:C1	5:B:12:BEZ:C2	1.78	1.59
5:B:12:BEZ:C5	5:B:12:BEZ:C6	1.74	1.58
5:B:12:BEZ:C1	5:B:12:BEZ:C6	1.78	1.57
1:B:24:PRO:C	1:B:24:PRO:CA	1.76	1.54
1:F:57:LYS:CB	1:F:57:LYS:CG	1.81	1.54
1:I:24:PRO:C	1:I:24:PRO:CA	1.77	1.53
5:B:12:BEZ:C4	5:B:12:BEZ:C3	1.85	1.53
5:D:2385:BEZ:C3	5:D:2385:BEZ:C4	1.82	1.53
5:D:2385:BEZ:C5	5:D:2385:BEZ:C4	1.81	1.51
5:B:12:BEZ:C5	5:B:12:BEZ:C4	1.84	1.51
1:E:77:VAL:CB	1:E:77:VAL:CG1	1.86	1.50
1:E:24:PRO:C	1:E:24:PRO:CA	1.79	1.50
1:A:550:LEU:C	1:A:550:LEU:CA	1.75	1.50
1:H:77:VAL:CB	1:H:77:VAL:CG1	1.94	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:550:LEU:CA	1:G:550:LEU:C	1.87	1.43
1:A:372:GLN:HB2	1:A:410:THR:HB	1.35	1.08
1:L:343:THR:HB	1:L:442:ALA:HB2	1.34	1.07
1:H:199:ARG:HH11	1:H:199:ARG:HB3	1.27	1.00
1:H:319:LEU:HD23	1:H:319:LEU:H	1.23	1.00
1:G:290:THR:OG1	1:G:293:GLU:HG3	1.62	0.99
3:A:1181:SIA:HN5	3:A:1181:SIA:H92	1.27	0.97
1:I:134:PRO:HG2	1:I:163:VAL:HG12	1.46	0.97
1:L:25:VAL:HG22	1:L:34:LEU:HD23	1.44	0.96
1:G:303:PHE:O	1:G:317:PRO:O	1.84	0.94
1:D:103:ASN:ND2	1:D:476:PHE:HB3	1.85	0.92
1:I:242:ARG:HH11	1:I:242:ARG:HG2	1.34	0.91
1:L:125:ALA:HB2	1:L:133:LEU:HD11	1.53	0.91
1:I:472:LEU:HD12	6:I:6117:HOH:O	1.71	0.91
1:F:215:VAL:H	1:F:241:HIS:HD2	1.16	0.90
3:L:1282:SIA:H92	3:L:1282:SIA:H112	1.51	0.90
1:H:216:THR:HG23	1:H:242:ARG:HB2	1.52	0.89
3:L:1282:SIA:H7	6:L:6029:HOH:O	1.72	0.89
1:D:316:GLN:NE2	1:D:317:PRO:HD2	1.86	0.89
1:E:77:VAL:CG1	1:E:77:VAL:CA	2.51	0.89
1:D:241:HIS:O	1:D:242:ARG:HG3	1.72	0.88
1:J:124:PRO:HD3	1:J:158:ALA:HB1	1.53	0.88
1:J:134:PRO:HG2	1:J:163:VAL:HG12	1.54	0.88
1:G:404:LEU:HD23	1:G:413:LYS:HB3	1.56	0.88
1:K:68:PRO:HA	6:K:6330:HOH:O	1.73	0.88
1:C:319:LEU:HD23	1:C:319:LEU:H	1.39	0.87
1:K:343:THR:HA	6:K:6389:HOH:O	1.73	0.87
1:C:202:GLN:HE22	1:C:215:VAL:HG21	1.37	0.87
1:D:359:ILE:HB	1:D:360:PRO:HD3	1.57	0.87
3:J:1082:SIA:H112	1:K:278:THR:HA	1.55	0.87
1:L:495:MET:HE3	1:L:533:THR:HG21	1.56	0.86
1:D:350:ILE:C	1:D:351:ASN:HD22	1.79	0.86
1:G:105:LYS:HE2	1:G:106:GLU:HG2	1.59	0.85
3:A:1181:SIA:N5	3:A:1181:SIA:H92	1.91	0.85
1:E:355:PHE:CE1	1:E:360:PRO:HG3	2.11	0.84
1:I:105:LYS:HG3	1:I:106:GLU:H	1.42	0.84
1:I:257:LYS:HG3	1:I:316:GLN:HE22	1.43	0.84
1:I:303:PHE:O	1:I:317:PRO:O	1.96	0.83
1:J:317:PRO:HB3	1:J:387:PRO:HB2	1.60	0.83
1:K:25:VAL:HG22	1:K:34:LEU:CD2	2.07	0.83
1:J:86:MET:HE2	1:J:110:LEU:HB2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:139:ILE:HG12	1:J:168:ILE:HD11	1.61	0.83
1:E:327:LEU:HD23	1:E:328:LEU:HG	1.61	0.83
1:G:550:LEU:CA	1:G:551:PHE:N	2.41	0.82
1:I:24:PRO:CB	1:I:24:PRO:C	2.46	0.82
1:F:357:TRP:O	1:F:360:PRO:HD2	1.79	0.82
1:C:216:THR:HG23	1:C:242:ARG:HB2	1.62	0.82
1:D:435:ARG:HB3	1:D:438:ARG:NH2	1.95	0.82
1:E:372:GLN:HB2	1:E:410:THR:HB	1.60	0.82
1:C:242:ARG:HH11	1:C:242:ARG:HG2	1.41	0.82
1:E:24:PRO:C	1:E:24:PRO:CB	2.48	0.82
1:B:24:PRO:C	1:B:24:PRO:CB	2.47	0.82
1:E:359:ILE:HB	1:E:360:PRO:HD3	1.62	0.81
1:K:495:MET:HE3	1:K:533:THR:HG21	1.61	0.81
1:B:134:PRO:HG2	1:B:163:VAL:HG12	1.63	0.81
1:K:199:ARG:HH11	1:K:199:ARG:HB3	1.44	0.81
1:L:199:ARG:HB3	1:L:199:ARG:HH11	1.45	0.81
3:A:1180:SIA:H112	1:B:278:THR:HG22	1.61	0.81
1:C:414:LYS:NZ	5:C:5014:BEZ:O2	2.12	0.81
1:D:244:ILE:HG12	1:D:347:MET:HB3	1.61	0.81
1:J:290:THR:OG1	1:J:293:GLU:HG3	1.80	0.81
1:L:382:LEU:HD23	1:L:396:ILE:HG23	1.63	0.81
1:E:495:MET:HE3	1:E:533:THR:HG21	1.62	0.81
1:J:357:TRP:O	1:J:360:PRO:HD2	1.79	0.80
1:F:131:ASN:O	1:F:132:ARG:HD2	1.81	0.80
1:K:431:VAL:HG21	1:K:540:LYS:HB2	1.63	0.80
1:E:134:PRO:HG2	1:E:163:VAL:HG12	1.64	0.79
1:D:262:LYS:NZ	2:F:2379:NAG:H82	1.97	0.79
1:A:220:GLU:HG3	1:A:472:LEU:HD21	1.64	0.79
1:C:357:TRP:O	1:C:360:PRO:HD2	1.81	0.79
1:E:141:GLY:CA	6:E:6472:HOH:O	2.30	0.79
1:A:499:PHE:CE2	1:A:514:LEU:HD22	2.18	0.79
1:E:251:LEU:HD11	1:E:336:GLN:HE22	1.48	0.79
1:C:271:THR:HG22	1:C:297:THR:HG23	1.66	0.78
1:H:335:LEU:O	1:H:338:GLU:HB3	1.83	0.78
1:K:318:LEU:H	1:K:318:LEU:HD22	1.47	0.78
1:H:359:ILE:HB	1:H:360:PRO:HD3	1.65	0.78
1:L:105:LYS:HG3	6:L:6432:HOH:O	1.82	0.78
1:B:25:VAL:HG22	1:B:34:LEU:HD23	1.66	0.78
1:F:114:GLU:HG3	1:F:291:GLU:HG3	1.65	0.78
1:A:410:THR:HA	1:A:413:LYS:HD2	1.63	0.78
1:F:134:PRO:HG2	1:F:163:VAL:HG12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:456:SER:HB3	1:F:460:LYS:HE2	1.66	0.78
1:H:119:LEU:HB3	1:H:168:ILE:HG22	1.66	0.78
1:C:277:THR:HG22	1:C:278:THR:HG23	1.66	0.77
1:E:24:PRO:HG3	1:E:37:PHE:CE1	2.20	0.77
1:H:164:VAL:HG11	1:H:205:ILE:HD11	1.66	0.77
1:G:86:MET:HE2	1:G:110:LEU:HB2	1.66	0.77
1:G:357:TRP:O	1:G:360:PRO:HD2	1.83	0.77
1:F:495:MET:HE3	1:F:533:THR:HG21	1.67	0.77
1:J:400:THR:HG23	1:J:404:LEU:HD12	1.66	0.77
1:A:223:GLY:O	1:A:227:VAL:HG23	1.84	0.77
1:G:517:TRP:CE3	1:G:527:LEU:HD23	2.20	0.77
1:D:403:TYR:O	1:D:416:LEU:HD13	1.83	0.76
1:F:528:GLN:HE21	1:F:536:ALA:HB2	1.48	0.76
1:L:87:CYS:HB3	6:L:6115:HOH:O	1.83	0.76
1:G:550:LEU:O	1:G:550:LEU:CA	2.32	0.76
1:L:200:TRP:O	1:L:204:ASN:HB2	1.85	0.76
1:L:303:PHE:O	1:L:317:PRO:O	2.02	0.76
1:H:255:LEU:HA	1:H:318:LEU:HD11	1.68	0.76
1:F:225:GLU:O	1:F:229:VAL:HG23	1.86	0.76
1:K:107:ASN:HD22	1:K:108:ILE:H	1.34	0.76
1:C:191:HIS:HA	1:C:194:GLN:OE1	1.85	0.76
1:F:105:LYS:HE2	1:F:106:GLU:HG2	1.66	0.76
1:A:241:HIS:O	1:A:242:ARG:HG3	1.85	0.76
3:D:2180:SIA:O10	3:D:2180:SIA:H92	1.85	0.76
1:F:253:SER:HA	6:F:6118:HOH:O	1.84	0.76
1:K:79:ASN:O	3:K:1182:SIA:H32	1.86	0.76
1:D:227:VAL:O	1:D:231:VAL:HG23	1.86	0.75
1:C:493:SER:O	1:C:497:MET:HG3	1.85	0.75
1:D:271:THR:HG22	1:D:297:THR:HG23	1.69	0.75
1:J:97:LEU:HD22	1:J:146:VAL:HG23	1.68	0.75
1:K:257:LYS:HA	1:K:257:LYS:HE2	1.66	0.75
1:A:103:ASN:ND2	1:A:476:PHE:HB3	2.02	0.75
1:B:495:MET:HE3	1:B:533:THR:HG21	1.68	0.75
1:C:355:PHE:CE1	1:C:360:PRO:HG3	2.22	0.75
1:K:105:LYS:HG3	1:K:106:GLU:H	1.52	0.75
1:D:95:GLN:O	1:D:99:GLU:HG3	1.86	0.74
1:A:215:VAL:H	1:A:241:HIS:CD2	2.05	0.74
1:G:266:GLU:O	1:G:270:ILE:HG13	1.87	0.74
1:J:120:ASN:HB2	1:J:167:THR:OG1	1.87	0.74
1:I:236:ALA:HB1	1:I:240:PHE:HE1	1.51	0.74
1:I:242:ARG:NH1	1:I:242:ARG:HG2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:353:GLN:NE2	1:J:465:ILE:H	1.86	0.74
1:B:527:LEU:HD11	1:B:533:THR:HG22	1.67	0.74
1:E:141:GLY:HA3	6:E:6472:HOH:O	1.86	0.74
1:G:456:SER:HB3	1:G:460:LYS:HE2	1.69	0.74
1:K:139:ILE:HG12	1:K:168:ILE:HD11	1.69	0.74
1:G:164:VAL:HG11	1:G:205:ILE:HD11	1.68	0.73
1:H:241:HIS:O	1:H:242:ARG:HG3	1.87	0.73
1:B:317:PRO:HD2	6:B:6020:HOH:O	1.86	0.73
1:L:498:LYS:HD2	1:L:514:LEU:HD21	1.70	0.73
1:A:59:PRO:HD3	1:A:117:LEU:HD12	1.69	0.73
1:B:529:ILE:HA	1:B:533:THR:HG23	1.69	0.73
1:L:453:PRO:HG2	1:L:456:SER:OG	1.88	0.73
1:B:359:ILE:HB	1:B:360:PRO:HD3	1.70	0.73
1:G:242:ARG:HG2	1:G:242:ARG:HH11	1.52	0.73
1:A:161:GLU:HG3	1:A:497:MET:O	1.89	0.73
1:A:359:ILE:HB	1:A:360:PRO:HD3	1.69	0.73
1:H:262:LYS:HE3	1:H:279:SER:OG	1.89	0.73
1:I:322:VAL:HG12	1:I:323:ILE:N	2.03	0.72
1:K:83:TYR:CD1	1:K:150:SER:HB3	2.24	0.72
1:L:236:ALA:HA	1:L:239:LEU:HD12	1.71	0.72
1:D:529:ILE:HA	1:D:533:THR:HG23	1.71	0.72
1:F:135:VAL:HG21	1:F:205:ILE:HG12	1.71	0.72
1:L:242:ARG:HG2	1:L:242:ARG:HH11	1.51	0.72
1:L:348:VAL:O	1:L:446:MET:HA	1.89	0.72
1:B:495:MET:CE	1:B:533:THR:HG21	2.20	0.72
1:L:88:THR:HG21	1:L:291:GLU:HG3	1.70	0.72
1:B:392:ALA:HB3	1:B:395:LEU:HG	1.69	0.72
1:K:428:VAL:HG13	1:K:544:VAL:HG22	1.71	0.72
1:L:89:GLN:HB2	1:L:146:VAL:HG12	1.70	0.72
1:L:128:THR:OG1	1:L:129:LYS:HE3	1.90	0.72
1:C:234:PRO:HA	1:C:341:PHE:HZ	1.55	0.72
1:H:168:ILE:HG21	1:H:197:ALA:HB1	1.70	0.72
1:C:403:TYR:O	1:C:416:LEU:HD13	1.90	0.72
1:L:367:PRO:HG2	1:L:381:LEU:HD21	1.72	0.72
1:A:90:ASP:HB3	1:A:93:ALA:HB3	1.71	0.72
1:F:86:MET:HG3	1:F:112:LEU:HD23	1.70	0.71
1:H:201:VAL:HG13	1:H:205:ILE:HB	1.71	0.71
1:L:24:PRO:HG3	1:L:37:PHE:CZ	2.25	0.71
1:K:241:HIS:O	1:K:242:ARG:HG3	1.89	0.71
1:F:526:TYR:CD2	1:F:539:LEU:HB2	2.26	0.71
1:G:403:TYR:O	1:G:416:LEU:HD13	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:PRO:HB2	1:F:34:LEU:HD21	1.70	0.71
1:K:185:SER:HB2	1:K:283:VAL:HG21	1.72	0.71
1:E:24:PRO:HG3	1:E:37:PHE:CZ	2.26	0.71
1:L:403:TYR:CD1	1:L:420:LEU:HD23	2.26	0.71
1:A:26:VAL:CG1	1:A:207:SER:HB3	2.21	0.71
1:C:199:ARG:HH11	1:C:199:ARG:HB3	1.55	0.71
1:A:550:LEU:CA	1:A:551:PHE:N	2.54	0.71
1:B:403:TYR:O	1:B:416:LEU:HD13	1.91	0.71
1:J:463:THR:HG23	6:J:6348:HOH:O	1.90	0.71
1:K:85:PRO:HD3	3:K:1182:SIA:H91	1.72	0.71
1:D:229:VAL:HG13	1:D:328:LEU:HD11	1.73	0.70
1:D:34:LEU:HB3	1:D:79:ASN:HB3	1.72	0.70
1:I:359:ILE:HB	1:I:360:PRO:HD3	1.73	0.70
1:A:550:LEU:CA	1:A:550:LEU:O	2.36	0.70
1:E:103:ASN:ND2	1:E:476:PHE:HB3	2.06	0.70
1:E:236:ALA:HB1	1:E:240:PHE:HE1	1.56	0.70
1:B:317:PRO:HG2	1:B:318:LEU:H	1.57	0.70
1:C:242:ARG:NH1	1:C:242:ARG:HG2	2.05	0.70
1:I:368:LEU:HD21	1:I:373:LEU:HD22	1.73	0.70
1:A:373:LEU:O	1:A:413:LYS:HD3	1.92	0.70
1:K:252:THR:HG22	1:K:254:VAL:HG12	1.72	0.70
1:E:103:ASN:HD22	1:E:476:PHE:HB3	1.55	0.70
1:F:105:LYS:HG3	1:F:106:GLU:H	1.56	0.70
1:K:229:VAL:HG13	1:K:328:LEU:HD11	1.74	0.70
1:A:341:PHE:HB2	6:A:6326:HOH:O	1.90	0.70
1:L:359:ILE:HB	1:L:360:PRO:HD3	1.71	0.70
1:C:86:MET:HE2	1:C:110:LEU:HD13	1.72	0.69
1:G:268:ILE:HG12	1:G:301:MET:HE2	1.75	0.69
1:D:290:THR:OG1	1:D:293:GLU:HG3	1.92	0.69
1:G:220:GLU:HG3	1:G:472:LEU:HD21	1.73	0.69
1:L:396:ILE:HB	1:L:397:PRO:HD3	1.73	0.69
1:B:24:PRO:HG3	1:B:37:PHE:CZ	2.27	0.69
3:L:1282:SIA:H92	3:L:1282:SIA:C11	2.22	0.69
1:L:372:GLN:HE21	1:L:411:VAL:HG13	1.56	0.69
1:A:339:ARG:HG2	1:A:440:ALA:HA	1.75	0.69
3:A:1181:SIA:HN5	3:A:1181:SIA:C9	2.04	0.69
1:D:59:PRO:HD3	1:D:117:LEU:HD12	1.74	0.69
1:G:134:PRO:HG2	1:G:163:VAL:HG12	1.75	0.69
1:G:215:VAL:H	1:G:241:HIS:HD2	1.41	0.69
1:K:311:ASP:HB3	1:K:314:GLU:HG3	1.73	0.69
1:L:218:PHE:CB	1:L:244:ILE:HB	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASN:HB2	1:C:167:THR:OG1	1.92	0.69
1:I:25:VAL:HG22	1:I:34:LEU:CD2	2.23	0.69
1:H:428:VAL:HB	1:H:429:PRO:HD3	1.73	0.68
1:H:60:LEU:HA	6:H:6248:HOH:O	1.92	0.68
1:J:403:TYR:O	1:J:416:LEU:HD13	1.92	0.68
1:A:262:LYS:HB3	1:A:263:PRO:HD3	1.74	0.68
1:H:217:ILE:HG13	1:H:227:VAL:HG13	1.75	0.68
1:I:278:THR:OG1	1:I:281:VAL:HG23	1.93	0.68
1:K:330:LYS:HG3	1:K:335:LEU:HG	1.73	0.68
1:L:498:LYS:HD3	6:L:6137:HOH:O	1.92	0.68
1:A:226:SER:HA	1:A:229:VAL:HG23	1.76	0.68
1:B:236:ALA:HB1	1:B:240:PHE:HE1	1.57	0.68
1:B:382:LEU:HD23	1:B:396:ILE:HG23	1.75	0.68
3:D:2180:SIA:C10	3:D:2180:SIA:H92	2.24	0.68
3:D:2180:SIA:C11	1:E:278:THR:HG22	2.24	0.68
3:G:782:SIA:H112	1:H:278:THR:HA	1.75	0.68
1:L:379:MET:CE	1:L:397:PRO:HG3	2.23	0.68
1:C:343:THR:HA	6:C:6124:HOH:O	1.92	0.68
1:H:77:VAL:CA	1:H:77:VAL:CG1	2.70	0.68
1:I:277:THR:HG22	1:I:278:THR:HG23	1.75	0.68
1:J:277:THR:HG22	1:J:278:THR:HG23	1.76	0.68
1:K:262:LYS:HB3	1:K:263:PRO:HD3	1.75	0.68
1:L:372:GLN:NE2	1:L:411:VAL:HG13	2.09	0.68
1:B:403:TYR:CD1	1:B:420:LEU:HD23	2.29	0.68
1:C:526:TYR:CD2	1:C:539:LEU:HB2	2.28	0.68
1:B:266:GLU:HG2	1:B:282:MET:HE2	1.75	0.68
1:L:423:ASP:O	1:L:428:VAL:HG23	1.94	0.68
1:K:85:PRO:HD3	3:K:1182:SIA:C9	2.24	0.68
1:J:277:THR:HG21	1:L:113:SER:HB2	1.76	0.68
1:I:322:VAL:HG12	1:I:323:ILE:H	1.58	0.67
1:L:495:MET:CE	1:L:533:THR:HG21	2.23	0.67
1:A:140:HIS:HD2	1:A:141:GLY:O	1.77	0.67
3:J:1082:SIA:H4	1:K:262:LYS:NZ	2.10	0.67
1:B:141:GLY:HA2	1:B:223:GLY:H	1.59	0.67
1:C:290:THR:OG1	1:C:293:GLU:HG3	1.94	0.67
1:D:266:GLU:HG2	1:D:282:MET:HE2	1.75	0.67
1:G:114:GLU:HG3	1:G:291:GLU:HG3	1.76	0.67
1:L:392:ALA:HB3	1:L:395:LEU:HG	1.75	0.67
1:B:223:GLY:O	1:B:227:VAL:HG23	1.93	0.67
1:I:306:LEU:HD11	1:I:387:PRO:HG2	1.77	0.67
1:K:88:THR:HA	1:K:112:LEU:HD22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:423:ASP:OD2	1:K:543:GLU:HG2	1.95	0.67
1:K:90:ASP:HB3	1:K:93:ALA:HB3	1.75	0.67
1:L:36:LYS:HB3	6:L:6146:HOH:O	1.94	0.67
1:D:396:ILE:HB	1:D:397:PRO:HD3	1.75	0.67
1:D:425:MET:HB2	1:D:426:PHE:CE1	2.30	0.67
1:D:51:LEU:O	1:D:80:ALA:HB1	1.95	0.67
1:E:117:LEU:HD21	1:E:193:ASP:OD2	1.94	0.67
1:E:403:TYR:O	1:E:416:LEU:HD13	1.95	0.67
1:H:151:THR:HG22	1:H:152:TYR:CD1	2.30	0.67
1:I:118:TYR:CE2	3:I:982:SIA:H92	2.29	0.67
1:I:403:TYR:O	1:I:416:LEU:HD13	1.95	0.67
1:K:372:GLN:HB2	1:K:410:THR:HB	1.77	0.67
3:B:1280:SIA:H113	1:C:262:LYS:NZ	2.10	0.67
1:B:78:LYS:HG3	3:B:1280:SIA:O1B	1.93	0.67
1:D:34:LEU:HD13	1:D:35:GLY:N	2.10	0.67
1:E:423:ASP:O	1:E:428:VAL:HG23	1.95	0.67
1:E:526:TYR:CE1	1:E:528:GLN:HG2	2.30	0.67
1:A:99:GLU:O	1:A:102:THR:HG22	1.94	0.67
1:H:83:TYR:CD1	1:H:150:SER:HB3	2.30	0.67
1:L:529:ILE:HA	1:L:533:THR:HG23	1.76	0.67
1:D:474:SER:HB3	1:D:496:VAL:HG21	1.76	0.66
1:H:349:GLY:HA3	1:H:447:TYR:CE1	2.30	0.66
1:K:232:LEU:HD21	1:K:336:GLN:HE21	1.60	0.66
1:D:38:VAL:HG21	1:D:49:ILE:HD12	1.76	0.66
1:E:257:LYS:HE2	1:E:264:LEU:HD12	1.75	0.66
1:A:403:TYR:O	1:A:416:LEU:HD13	1.95	0.66
1:A:529:ILE:HD12	1:A:529:ILE:N	2.10	0.66
1:C:60:LEU:CD2	1:C:114:GLU:HB3	2.26	0.66
1:E:251:LEU:HD21	1:E:333:GLU:HG3	1.76	0.66
1:G:452:ARG:HH11	1:G:452:ARG:HG2	1.61	0.66
1:I:216:THR:HG23	1:I:242:ARG:HB2	1.77	0.66
1:A:349:GLY:HA3	1:A:447:TYR:CD1	2.30	0.66
1:G:140:HIS:HE1	6:G:6042:HOH:O	1.77	0.66
1:G:97:LEU:HD22	1:G:146:VAL:HG23	1.76	0.66
1:H:353:GLN:NE2	1:H:465:ILE:H	1.94	0.66
1:K:215:VAL:H	1:K:241:HIS:HD2	1.43	0.66
1:L:106:GLU:HG2	6:L:6432:HOH:O	1.96	0.66
1:B:24:PRO:N	1:B:24:PRO:C	2.49	0.66
1:F:403:TYR:O	1:F:416:LEU:HD13	1.96	0.66
1:J:133:LEU:HD22	1:J:162:ASN:O	1.94	0.66
1:J:382:LEU:HD11	1:J:391:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:257:LYS:HE2	1:L:316:GLN:OE1	1.95	0.66
1:H:199:ARG:CB	1:H:199:ARG:HH11	2.07	0.66
1:J:339:ARG:HG3	1:J:440:ALA:HA	1.77	0.66
1:F:120:ASN:HB2	1:F:167:THR:OG1	1.95	0.66
1:J:428:VAL:HB	1:J:429:PRO:HD3	1.76	0.66
1:I:266:GLU:O	1:I:270:ILE:HG13	1.96	0.66
1:J:131:ASN:O	1:J:132:ARG:HD2	1.95	0.66
1:J:237:LYS:HE3	1:J:342:HIS:HB3	1.79	0.66
1:K:467:ASP:HB3	1:K:470:ASP:OD2	1.96	0.66
1:C:215:VAL:H	1:C:241:HIS:HD2	1.43	0.65
1:G:268:ILE:HG12	1:G:301:MET:CE	2.26	0.65
1:K:131:ASN:C	1:K:132:ARG:HD2	2.16	0.65
1:B:355:PHE:CE1	1:B:360:PRO:HG3	2.31	0.65
1:D:264:LEU:HD22	1:D:268:ILE:HD11	1.78	0.65
1:E:24:PRO:C	1:E:24:PRO:N	2.49	0.65
1:G:355:PHE:CE1	1:G:360:PRO:HG3	2.31	0.65
1:G:48:ALA:HB3	1:G:123:THR:HG23	1.78	0.65
1:I:498:LYS:HB3	1:I:514:LEU:HD11	1.77	0.65
1:E:95:GLN:O	1:E:99:GLU:HG3	1.95	0.65
1:G:191:HIS:HA	1:G:194:GLN:OE1	1.97	0.65
1:K:498:LYS:HB3	1:K:514:LEU:HD11	1.79	0.65
1:H:428:VAL:O	1:H:432:ILE:HG13	1.97	0.65
1:E:77:VAL:CG1	1:E:77:VAL:C	2.65	0.65
1:G:249:VAL:HG21	1:G:433:VAL:HG21	1.79	0.65
1:J:176:GLY:HA2	1:J:189:TRP:HB2	1.78	0.65
1:K:34:LEU:HD13	1:K:35:GLY:N	2.12	0.65
1:C:131:ASN:O	1:C:132:ARG:HD2	1.97	0.65
1:G:139:ILE:HG12	1:G:168:ILE:HD11	1.77	0.65
1:I:87:CYS:O	1:I:89:GLN:HG2	1.97	0.65
1:C:88:THR:HB	1:C:175:TRP:CZ3	2.32	0.65
1:A:529:ILE:HA	1:A:533:THR:HG23	1.78	0.64
1:A:271:THR:HG22	1:A:297:THR:HG23	1.79	0.64
1:D:140:HIS:HD2	1:D:141:GLY:O	1.80	0.64
1:G:428:VAL:HB	1:G:429:PRO:HD3	1.79	0.64
1:F:164:VAL:HG11	1:F:205:ILE:HD11	1.79	0.64
1:G:492:LEU:O	1:G:496:VAL:HG23	1.96	0.64
1:G:64:ARG:O	1:G:65:PHE:HB2	1.98	0.64
1:H:201:VAL:O	1:H:205:ILE:HG22	1.96	0.64
1:J:429:PRO:O	1:J:433:VAL:HG23	1.98	0.64
1:K:227:VAL:O	1:K:231:VAL:HG23	1.97	0.64
1:B:404:LEU:N	1:B:404:LEU:HD23	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:417:PHE:O	1:H:420:LEU:HB3	1.97	0.64
1:H:64:ARG:O	1:H:66:THR:HG23	1.98	0.64
1:A:264:LEU:HD22	1:A:268:ILE:HD11	1.79	0.64
1:I:379:MET:HA	1:I:396:ILE:HG21	1.78	0.64
1:C:86:MET:CE	1:C:110:LEU:HD13	2.27	0.64
1:D:102:THR:OG1	1:D:104:ARG:HG3	1.98	0.64
1:F:331:THR:HB	1:F:333:GLU:OE1	1.98	0.64
3:F:682:SIA:H113	3:F:682:SIA:H91	1.80	0.64
1:G:86:MET:HE2	1:G:110:LEU:HD12	1.80	0.64
1:A:349:GLY:HA3	1:A:447:TYR:CE1	2.31	0.64
1:B:145:MET:HE1	1:B:303:PHE:HD1	1.62	0.64
1:D:97:LEU:HD13	5:D:2385:BEZ:H4	1.79	0.64
1:J:140:HIS:HE1	6:J:6125:HOH:O	1.79	0.64
1:A:88:THR:HG22	1:A:295:LEU:HD13	1.79	0.64
1:C:134:PRO:HG2	1:C:163:VAL:HG12	1.80	0.64
1:C:382:LEU:HD11	1:C:391:ILE:HD12	1.78	0.64
1:D:349:GLY:HA3	1:D:447:TYR:CE1	2.33	0.64
1:K:225:GLU:O	1:K:229:VAL:HG23	1.98	0.64
1:C:135:VAL:HG21	1:C:205:ILE:HG12	1.80	0.64
1:E:339:ARG:NH2	6:E:6307:HOH:O	2.30	0.64
1:F:395:LEU:HD13	1:F:550:LEU:HG	1.79	0.64
1:I:143:GLY:H	1:I:222:ALA:HB2	1.63	0.64
1:I:24:PRO:HD2	1:I:35:GLY:O	1.98	0.64
1:J:308:LEU:HA	1:J:384:LYS:HD3	1.79	0.64
1:D:425:MET:HB2	1:D:426:PHE:CD1	2.33	0.64
1:D:524:GLU:OE2	1:D:538:LYS:HG2	1.98	0.64
1:K:215:VAL:H	1:K:241:HIS:CD2	2.16	0.64
1:K:431:VAL:O	1:K:435:ARG:HG3	1.98	0.63
1:C:132:ARG:HH11	1:C:132:ARG:HG2	1.63	0.63
1:D:445:TYR:CE1	1:D:519:GLU:HA	2.34	0.63
1:I:86:MET:HB3	1:I:148:ALA:HB2	1.79	0.63
1:A:227:VAL:O	1:A:231:VAL:HG23	1.98	0.63
1:I:283:VAL:O	1:I:287:ARG:HG3	1.98	0.63
1:A:386:TYR:N	1:A:387:PRO:HD2	2.13	0.63
1:F:216:THR:HG23	1:F:242:ARG:HB2	1.81	0.63
1:I:157:LEU:HD13	1:I:497:MET:HG2	1.81	0.63
1:B:386:TYR:N	1:B:387:PRO:HD2	2.14	0.63
1:B:474:SER:HA	1:B:493:SER:HB2	1.81	0.63
1:D:173:GLY:HA3	6:D:6075:HOH:O	1.97	0.63
1:E:477:GLY:HA3	1:E:497:MET:HE2	1.81	0.63
1:H:456:SER:HB3	1:H:460:LYS:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:149:ALA:HB2	1:L:168:ILE:O	1.98	0.63
1:K:328:LEU:HA	6:K:6425:HOH:O	1.98	0.63
1:F:215:VAL:H	1:F:241:HIS:CD2	2.07	0.63
1:H:304:LEU:HD12	1:H:364:MET:HE2	1.80	0.63
1:B:262:LYS:HB3	1:B:263:PRO:HD3	1.79	0.63
1:C:218:PHE:HB3	1:C:244:ILE:HB	1.81	0.63
1:F:133:LEU:HD22	1:F:162:ASN:O	1.98	0.63
1:G:498:LYS:HD2	1:G:514:LEU:HD21	1.81	0.63
1:I:24:PRO:C	1:I:24:PRO:N	2.52	0.63
1:J:343:THR:HB	1:J:442:ALA:HB2	1.80	0.63
1:J:386:TYR:N	1:J:387:PRO:HD2	2.14	0.63
1:A:350:ILE:C	1:A:351:ASN:HD22	2.02	0.63
1:F:439:ASP:C	1:F:441:GLY:H	2.01	0.63
1:L:400:THR:HG22	1:L:404:LEU:HD11	1.80	0.63
1:J:102:THR:HG21	1:J:107:ASN:HD22	1.64	0.62
1:J:119:LEU:HD12	1:J:119:LEU:O	1.98	0.62
1:L:23:PRO:HB2	1:L:34:LEU:HD21	1.81	0.62
1:K:107:ASN:HD22	1:K:108:ILE:N	1.96	0.62
1:K:197:ALA:O	1:K:201:VAL:HG23	1.99	0.62
1:K:264:LEU:O	1:K:268:ILE:HG13	1.99	0.62
1:K:359:ILE:HB	1:K:360:PRO:HD3	1.80	0.62
1:F:136:MET:HB3	1:F:218:PHE:CE1	2.34	0.62
1:L:190:GLY:O	1:L:194:GLN:HG3	1.99	0.62
1:L:220:GLU:HG2	1:L:221:SER:N	2.13	0.62
1:L:343:THR:HB	1:L:442:ALA:CB	2.20	0.62
1:C:385:SER:C	1:C:387:PRO:HD2	2.19	0.62
1:L:134:PRO:HG2	1:L:163:VAL:HG12	1.82	0.62
1:C:357:TRP:C	1:C:360:PRO:HD2	2.20	0.62
1:C:386:TYR:N	1:C:387:PRO:HD2	2.14	0.62
1:F:428:VAL:HG13	1:F:544:VAL:HG22	1.82	0.62
1:H:354:GLU:O	1:H:468:HIS:HB2	1.99	0.62
1:A:134:PRO:HG2	1:A:163:VAL:HG12	1.81	0.62
1:I:24:PRO:O	1:I:34:LEU:HD22	2.00	0.62
1:J:262:LYS:HB3	1:J:263:PRO:HD3	1.82	0.62
1:K:105:LYS:HG3	1:K:106:GLU:N	2.15	0.62
1:K:351:ASN:HD22	1:K:351:ASN:N	1.98	0.62
1:A:396:ILE:HB	1:A:397:PRO:HD3	1.81	0.62
1:B:403:TYR:CE1	1:B:420:LEU:HD23	2.34	0.62
1:F:242:ARG:HG2	1:F:242:ARG:HH11	1.65	0.62
2:K:4279:NAG:H81	1:L:260:ASP:HB2	1.82	0.62
1:F:386:TYR:N	1:F:387:PRO:HD2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:H	1:A:241:HIS:HD2	1.48	0.62
3:D:2180:SIA:O10	3:D:2180:SIA:C9	2.47	0.62
1:G:350:ILE:O	1:G:448:GLU:HA	2.00	0.62
1:K:244:ILE:HG12	1:K:347:MET:HB3	1.82	0.62
1:C:338:GLU:OE2	1:C:341:PHE:HB2	2.00	0.62
1:E:379:MET:CE	1:E:397:PRO:HG3	2.30	0.62
1:G:135:VAL:HG21	1:G:205:ILE:HG12	1.82	0.62
1:J:135:VAL:HG21	1:J:205:ILE:HG12	1.81	0.62
1:E:279:SER:O	1:E:283:VAL:HG23	1.99	0.61
1:H:399:ALA:HB2	1:H:550:LEU:HD21	1.82	0.61
1:H:95:GLN:O	1:H:99:GLU:HG3	2.00	0.61
1:C:48:ALA:HB3	1:C:123:THR:HG23	1.81	0.61
1:C:498:LYS:HD2	1:C:514:LEU:HD11	1.81	0.61
1:H:135:VAL:HG21	1:H:205:ILE:HG12	1.82	0.61
1:G:357:TRP:C	1:G:360:PRO:HD2	2.21	0.61
1:L:254:VAL:HG13	1:L:255:LEU:HG	1.82	0.61
1:D:399:ALA:HB2	1:D:550:LEU:HD21	1.83	0.61
1:H:223:GLY:O	1:H:227:VAL:HG23	2.01	0.61
1:K:119:LEU:HB3	1:K:168:ILE:HG22	1.82	0.61
1:K:396:ILE:HB	1:K:397:PRO:HD3	1.82	0.61
1:L:218:PHE:HB2	1:L:244:ILE:HB	1.82	0.61
1:A:232:LEU:HB3	1:A:335:LEU:HD13	1.82	0.61
1:A:420:LEU:C	1:A:420:LEU:HD13	2.20	0.61
1:C:198:LEU:O	1:C:201:VAL:HB	1.99	0.61
1:D:547:TRP:O	1:D:551:PHE:HB2	2.01	0.61
1:I:379:MET:SD	1:I:396:ILE:HG22	2.40	0.61
1:L:38:VAL:HG21	1:L:49:ILE:HD12	1.83	0.61
1:B:264:LEU:O	1:B:268:ILE:HG13	2.01	0.61
1:C:331:THR:HB	1:C:333:GLU:OE1	2.00	0.61
1:A:131:ASN:O	1:A:132:ARG:HD2	2.00	0.61
1:A:529:ILE:H	1:A:529:ILE:HD12	1.65	0.61
1:E:343:THR:HA	6:E:6126:HOH:O	2.00	0.61
1:L:547:TRP:O	1:L:551:PHE:HB2	2.01	0.61
1:D:382:LEU:HD23	1:D:396:ILE:HG23	1.82	0.61
1:E:222:ALA:N	6:E:6472:HOH:O	2.04	0.61
1:D:262:LYS:HZ1	2:F:2379:NAG:H82	1.65	0.61
1:I:257:LYS:HG3	1:I:316:GLN:NE2	2.14	0.61
1:I:427:GLY:O	1:I:431:VAL:HG23	2.01	0.61
1:K:526:TYR:CD2	1:K:539:LEU:HB2	2.36	0.61
1:B:295:LEU:O	1:B:299:LEU:HG	2.01	0.60
1:C:316:GLN:NE2	1:C:316:GLN:HA	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:LYS:O	1:G:266:GLU:HG3	2.01	0.60
1:H:216:THR:HG23	1:H:242:ARG:CB	2.26	0.60
1:D:467:ASP:CG	1:D:468:HIS:H	2.05	0.60
3:I:982:SIA:H7	6:I:6011:HOH:O	2.01	0.60
1:J:498:LYS:O	1:J:502:ASN:HB2	2.01	0.60
1:D:103:ASN:HD22	1:D:476:PHE:HB3	1.65	0.60
1:D:53:ILE:HB	1:D:119:LEU:HD12	1.83	0.60
1:E:382:LEU:HD11	1:E:391:ILE:HD12	1.83	0.60
1:F:423:ASP:HA	1:F:427:GLY:HA3	1.83	0.60
1:G:350:ILE:C	1:G:351:ASN:HD22	2.03	0.60
1:F:499:PHE:CE2	1:F:514:LEU:HB3	2.35	0.60
1:F:87:CYS:HB2	1:F:172:LEU:HD12	1.83	0.60
1:J:23:PRO:HB2	1:J:34:LEU:HD21	1.84	0.60
1:J:312:PRO:HG2	1:J:383:TRP:NE1	2.15	0.60
1:K:83:TYR:HD1	1:K:150:SER:HB3	1.66	0.60
3:L:1282:SIA:N5	3:L:1282:SIA:O9	2.33	0.60
1:L:292:GLU:O	1:L:296:GLU:HG3	2.01	0.60
1:L:64:ARG:O	1:L:65:PHE:HB2	2.02	0.60
1:E:303:PHE:O	1:E:317:PRO:O	2.20	0.60
1:F:86:MET:HE2	1:F:110:LEU:HD12	1.83	0.60
1:F:131:ASN:C	1:F:132:ARG:HD2	2.21	0.60
1:F:218:PHE:HB3	1:F:244:ILE:HB	1.84	0.60
3:I:982:SIA:H8	3:I:982:SIA:H113	1.84	0.60
1:A:197:ALA:O	1:A:201:VAL:HG23	2.01	0.60
1:G:88:THR:HG22	1:G:295:LEU:HD13	1.82	0.60
1:I:127:LEU:H	1:I:127:LEU:HD12	1.65	0.60
1:I:223:GLY:O	1:I:227:VAL:HG23	2.02	0.60
1:I:357:TRP:CZ2	1:I:361:MET:HG3	2.36	0.60
1:I:379:MET:HA	1:I:396:ILE:CG2	2.32	0.60
1:J:190:GLY:O	1:J:194:GLN:HG3	2.02	0.60
1:F:271:THR:HG22	1:F:297:THR:HG23	1.84	0.60
1:F:262:LYS:HE3	1:F:279:SER:OG	2.02	0.60
1:A:252:THR:HG22	1:A:254:VAL:HG12	1.82	0.60
1:D:276:THR:HB	1:D:282:MET:HE2	1.82	0.60
1:H:262:LYS:HB3	1:H:263:PRO:HD3	1.83	0.60
1:K:495:MET:CE	1:K:533:THR:HG21	2.31	0.60
1:A:382:LEU:HD23	1:A:396:ILE:HG23	1.84	0.60
1:E:33:VAL:HG12	1:E:34:LEU:N	2.17	0.60
1:H:420:LEU:HD13	1:H:421:ILE:N	2.17	0.60
1:I:103:ASN:HB2	1:I:478:ALA:HB2	1.83	0.60
1:I:215:VAL:H	1:I:241:HIS:HD2	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PHE:CB	1:A:244:ILE:HB	2.32	0.60
1:A:88:THR:HB	1:A:175:TRP:CZ3	2.36	0.60
1:B:140:HIS:HD2	1:B:141:GLY:O	1.85	0.60
1:E:379:MET:SD	1:E:396:ILE:HG22	2.41	0.60
1:C:527:LEU:HD11	1:C:533:THR:HG22	1.82	0.59
1:E:353:GLN:O	1:E:467:ASP:HA	2.01	0.59
1:G:382:LEU:HD23	1:G:396:ILE:HG23	1.82	0.59
1:G:479:PRO:HB3	1:G:490:ILE:HG12	1.83	0.59
1:C:316:GLN:NE2	1:C:317:PRO:HD2	2.16	0.59
1:A:255:LEU:HD23	1:A:318:LEU:HD11	1.83	0.59
1:B:133:LEU:O	1:B:211:ASN:N	2.36	0.59
1:E:242:ARG:HG2	1:E:242:ARG:HH11	1.67	0.59
1:G:107:ASN:ND2	1:G:108:ILE:H	2.00	0.59
1:H:400:THR:HG23	1:H:404:LEU:HD12	1.83	0.59
1:I:409:ASP:O	1:I:413:LYS:HG3	2.03	0.59
1:L:428:VAL:HG13	1:L:544:VAL:HG22	1.85	0.59
1:C:63:LEU:HD11	6:C:6271:HOH:O	2.02	0.59
1:G:271:THR:HG22	1:G:297:THR:HG23	1.85	0.59
1:C:398:GLU:HB3	1:C:550:LEU:HD11	1.83	0.59
1:D:46:PRO:HA	6:D:6225:HOH:O	2.03	0.59
1:I:453:PRO:HG2	1:I:456:SER:OG	2.03	0.59
1:A:279:SER:HB2	3:A:1181:SIA:H111	1.84	0.59
1:H:194:GLN:OE1	1:H:226:SER:HB3	2.03	0.59
1:B:373:LEU:O	1:B:410:THR:HG22	2.02	0.59
1:C:138:TRP:HH2	1:C:220:GLU:HB2	1.67	0.59
1:C:355:PHE:CD1	1:C:360:PRO:HG3	2.37	0.59
1:E:304:LEU:HG	1:E:305:SER:N	2.18	0.59
1:G:400:THR:HG23	1:G:404:LEU:HD13	1.84	0.59
1:G:423:ASP:HA	1:G:427:GLY:HA3	1.84	0.59
1:H:34:LEU:HB2	1:H:77:VAL:CG1	2.32	0.59
1:I:495:MET:HE3	1:I:533:THR:HG21	1.84	0.59
1:I:538:LYS:HB3	1:I:541:ASP:HB2	1.84	0.59
1:J:526:TYR:CD2	1:J:539:LEU:HB2	2.38	0.59
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.67	0.59
1:A:266:GLU:HG2	1:A:282:MET:CE	2.33	0.59
1:C:546:PHE:O	1:C:549:ASN:HB2	2.02	0.59
1:E:190:GLY:O	1:E:194:GLN:HG3	2.03	0.59
1:G:218:PHE:HB3	1:G:244:ILE:HB	1.84	0.59
1:G:78:LYS:HD3	3:G:782:SIA:H91	1.84	0.59
1:H:545:ALA:O	1:H:549:ASN:ND2	2.36	0.59
1:I:253:SER:O	1:I:255:LEU:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ALA:HA	1:A:239:LEU:HD12	1.84	0.59
1:D:264:LEU:O	1:D:268:ILE:HG13	2.03	0.59
1:H:131:ASN:O	1:H:209:GLY:HA2	2.03	0.59
1:B:134:PRO:CG	1:B:163:VAL:HG12	2.32	0.59
1:D:186:ARG:HD2	1:D:326:MET:HG3	1.85	0.59
1:H:227:VAL:O	1:H:231:VAL:HG23	2.03	0.59
1:H:352:LYS:HD2	1:H:448:GLU:OE1	2.03	0.59
1:I:461:PRO:HG2	1:I:464:VAL:HG23	1.85	0.59
1:A:226:SER:HA	1:A:229:VAL:CG2	2.32	0.58
1:C:99:GLU:HG2	1:C:107:ASN:OD1	2.02	0.58
1:C:317:PRO:HB3	1:C:387:PRO:HB2	1.85	0.58
1:D:204:ASN:O	1:D:206:ALA:N	2.36	0.58
1:J:57:LYS:HB2	1:J:71:ALA:HA	1.84	0.58
1:K:201:VAL:O	1:K:205:ILE:HG22	2.02	0.58
1:C:174:ILE:HA	1:C:319:LEU:HD11	1.85	0.58
1:C:428:VAL:HB	1:C:429:PRO:HD3	1.84	0.58
1:D:318:LEU:HD12	1:D:318:LEU:O	2.03	0.58
1:E:547:TRP:O	1:E:551:PHE:HB2	2.02	0.58
1:G:29:VAL:HG23	1:G:204:ASN:OD1	2.03	0.58
1:J:105:LYS:HG3	1:J:106:GLU:H	1.67	0.58
1:K:278:THR:O	1:K:282:MET:HG3	2.03	0.58
1:L:118:TYR:CE2	3:L:1282:SIA:H91	2.38	0.58
1:L:386:TYR:N	1:L:387:PRO:HD2	2.18	0.58
1:D:423:ASP:O	1:D:428:VAL:HG23	2.03	0.58
1:I:145:MET:HE1	1:I:303:PHE:HD1	1.68	0.58
1:K:318:LEU:N	1:K:318:LEU:HD22	2.17	0.58
1:B:357:TRP:CZ2	1:B:361:MET:HG3	2.39	0.58
1:D:34:LEU:HB3	1:D:79:ASN:HA	1.85	0.58
1:H:351:ASN:HD22	1:H:351:ASN:N	2.01	0.58
1:I:396:ILE:HB	1:I:397:PRO:HD3	1.84	0.58
1:L:59:PRO:HD3	1:L:117:LEU:HD12	1.85	0.58
1:C:241:HIS:O	1:C:242:ARG:HG2	2.03	0.58
1:I:188:ASN:HD22	1:I:324:ASP:CG	2.06	0.58
1:L:373:LEU:HD11	1:L:377:THR:HB	1.85	0.58
1:A:229:VAL:HG13	1:A:328:LEU:HD11	1.84	0.58
1:A:338:GLU:HB3	1:A:340:ASN:OD1	2.03	0.58
1:C:447:TYR:HA	1:C:527:LEU:O	2.04	0.58
1:J:218:PHE:HB3	1:J:244:ILE:HB	1.86	0.58
1:K:202:GLN:HG2	6:K:6081:HOH:O	2.02	0.58
1:K:242:ARG:HG2	1:K:242:ARG:HH11	1.69	0.58
1:L:297:THR:HA	1:L:300:LYS:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:LYS:HE2	1:F:316:GLN:HE22	1.69	0.58
1:C:359:ILE:HB	1:C:360:PRO:HD3	1.86	0.58
1:D:252:THR:HG22	1:D:254:VAL:HG12	1.86	0.58
1:H:241:HIS:C	1:H:242:ARG:HG3	2.22	0.58
1:L:262:LYS:HB3	1:L:263:PRO:HD3	1.85	0.58
1:C:350:ILE:O	1:C:448:GLU:HA	2.03	0.58
1:D:318:LEU:O	1:D:319:LEU:C	2.42	0.58
1:E:386:TYR:N	1:E:387:PRO:HD2	2.18	0.58
1:F:300:LYS:O	1:F:302:LYS:HG3	2.03	0.58
1:J:527:LEU:HD11	1:J:533:THR:HG22	1.86	0.58
1:K:343:THR:HB	1:K:442:ALA:HB2	1.86	0.58
1:E:131:ASN:O	1:E:132:ARG:HD2	2.04	0.58
1:F:332:PRO:O	1:F:336:GLN:HG2	2.04	0.58
1:I:131:ASN:O	1:I:132:ARG:HD2	2.04	0.58
1:I:311:ASP:OD1	1:I:313:ARG:HB2	2.04	0.58
1:J:306:LEU:HD22	1:J:366:TYR:CE1	2.39	0.58
1:C:29:VAL:HG23	1:C:204:ASN:OD1	2.03	0.57
1:D:221:SER:HB3	6:D:6019:HOH:O	2.04	0.57
1:J:349:GLY:HA3	1:J:447:TYR:CE1	2.39	0.57
1:L:76:PHE:H	1:L:76:PHE:HD1	1.52	0.57
3:A:1180:SIA:O10	3:A:1180:SIA:O8	2.21	0.57
1:C:359:ILE:HG12	5:C:5013:BEZ:H3	1.86	0.57
1:D:355:PHE:CE1	1:D:360:PRO:HG3	2.39	0.57
3:G:782:SIA:H7	6:G:6005:HOH:O	2.04	0.57
1:J:25:VAL:HG22	1:J:34:LEU:HD23	1.86	0.57
1:D:97:LEU:HD11	1:D:101:PHE:CE2	2.40	0.57
1:D:319:LEU:HD23	1:D:319:LEU:N	2.19	0.57
1:K:107:ASN:ND2	1:K:108:ILE:H	2.00	0.57
1:E:252:THR:HG22	1:E:254:VAL:HG12	1.86	0.57
1:K:237:LYS:O	1:K:238:ASN:HB2	2.03	0.57
1:K:253:SER:CB	1:K:258:LYS:HZ3	2.17	0.57
1:L:338:GLU:HG2	1:L:340:ASN:H	1.68	0.57
1:E:186:ARG:HB3	1:E:324:ASP:HB2	1.87	0.57
1:H:97:LEU:HA	1:H:100:LEU:HD12	1.86	0.57
1:L:126:ASP:HB3	1:L:129:LYS:CG	2.34	0.57
1:H:495:MET:HE3	1:H:533:THR:HG21	1.86	0.57
1:L:262:LYS:HE3	1:L:282:MET:CE	2.35	0.57
3:D:2180:SIA:N5	3:D:2180:SIA:H92	2.19	0.57
1:D:218:PHE:HB3	1:D:244:ILE:HB	1.86	0.57
1:D:385:SER:O	1:D:389:VAL:HG22	2.04	0.57
1:G:124:PRO:HG3	1:G:158:ALA:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:373:LEU:HD21	1:G:381:LEU:HD12	1.86	0.57
1:J:164:VAL:HG11	1:J:205:ILE:HD11	1.86	0.57
1:J:86:MET:SD	1:J:110:LEU:HD22	2.45	0.57
1:L:184:HIS:O	1:L:185:SER:HB2	2.05	0.57
1:L:367:PRO:CG	1:L:381:LEU:HD21	2.34	0.57
1:B:449:PHE:CE2	1:B:451:TYR:HB3	2.40	0.57
1:C:435:ARG:NE	1:C:524:GLU:OE1	2.38	0.57
1:C:60:LEU:HD22	1:C:114:GLU:HB3	1.86	0.57
1:F:191:HIS:HA	1:F:194:GLN:OE1	2.03	0.57
1:F:316:GLN:HE21	1:F:316:GLN:HA	1.69	0.57
1:H:56:ALA:HB3	1:H:117:LEU:HD13	1.86	0.57
1:J:491:ARG:HD2	6:J:6263:HOH:O	2.05	0.57
1:J:493:SER:O	1:J:497:MET:HG3	2.04	0.57
1:A:215:VAL:N	1:A:241:HIS:HD2	2.03	0.57
1:G:264:LEU:HD11	1:G:316:GLN:HG2	1.85	0.57
1:H:383:TRP:C	1:H:385:SER:H	2.07	0.57
1:I:251:LEU:HD13	1:I:433:VAL:HG22	1.87	0.57
1:J:231:VAL:HA	1:J:240:PHE:HZ	1.69	0.57
1:J:254:VAL:HG13	1:J:255:LEU:H	1.70	0.57
1:J:308:LEU:CA	1:J:384:LYS:HD3	2.35	0.57
1:K:185:SER:HB2	1:K:283:VAL:CG2	2.35	0.57
1:L:192:LEU:HD23	1:L:327:LEU:HD12	1.87	0.57
1:A:428:VAL:HB	1:A:429:PRO:HD3	1.87	0.57
1:B:186:ARG:HB3	1:B:324:ASP:HB2	1.86	0.57
1:B:103:ASN:ND2	1:B:476:PHE:HB3	2.20	0.57
1:D:48:ALA:HB3	1:D:123:THR:HG23	1.87	0.57
1:D:318:LEU:O	1:D:320:GLY:N	2.38	0.57
1:G:199:ARG:HH11	1:G:199:ARG:HG2	1.70	0.57
1:H:319:LEU:HD23	1:H:319:LEU:N	2.07	0.57
1:L:218:PHE:HB3	1:L:244:ILE:HB	1.86	0.57
1:B:447:TYR:HB3	1:B:517:TRP:CZ2	2.40	0.56
1:F:355:PHE:CE1	1:F:360:PRO:HG3	2.40	0.56
1:F:461:PRO:HG2	1:F:464:VAL:HG23	1.86	0.56
1:G:351:ASN:HD22	1:G:351:ASN:N	2.02	0.56
1:J:135:VAL:CG2	1:J:205:ILE:HG12	2.35	0.56
1:A:527:LEU:HD11	1:A:533:THR:HG22	1.86	0.56
1:H:215:VAL:H	1:H:241:HIS:HD2	1.53	0.56
1:J:268:ILE:HG12	1:J:301:MET:HE2	1.86	0.56
1:K:353:GLN:OE1	1:K:464:VAL:HG13	2.05	0.56
1:L:343:THR:CB	1:L:442:ALA:HB2	2.23	0.56
1:A:278:THR:OG1	1:A:281:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:SER:O	1:A:389:VAL:HG22	2.05	0.56
1:H:59:PRO:HD3	1:H:117:LEU:HD12	1.88	0.56
1:I:358:LEU:HD23	1:I:468:HIS:HB3	1.86	0.56
1:J:24:PRO:HG3	1:J:37:PHE:CZ	2.40	0.56
1:K:63:LEU:HD21	1:K:69:GLN:NE2	2.21	0.56
1:E:77:VAL:CG1	1:E:77:VAL:CG2	2.81	0.56
1:F:130:LYS:C	1:F:131:ASN:HD22	2.09	0.56
1:H:350:ILE:C	1:H:351:ASN:HD22	2.08	0.56
1:B:428:VAL:HG13	1:B:544:VAL:HA	1.87	0.56
1:C:57:LYS:HD2	1:C:63:LEU:CD1	2.36	0.56
1:E:24:PRO:O	1:E:34:LEU:HD22	2.05	0.56
1:F:428:VAL:HB	1:F:429:PRO:HD3	1.87	0.56
1:G:355:PHE:CD1	1:G:360:PRO:HG3	2.40	0.56
1:H:161:GLU:HB3	1:H:501:ALA:HB2	1.88	0.56
1:A:367:PRO:HG2	1:A:381:LEU:HD21	1.88	0.56
1:A:393:LYS:HA	1:A:396:ILE:HG12	1.87	0.56
1:B:23:PRO:HB2	1:B:34:LEU:HD21	1.86	0.56
1:E:218:PHE:CB	1:E:244:ILE:HB	2.35	0.56
1:H:382:LEU:HB2	1:H:417:PHE:HE1	1.68	0.56
1:L:24:PRO:HB3	1:L:127:LEU:HD12	1.87	0.56
1:L:469:GLY:O	1:L:472:LEU:HG	2.06	0.56
1:A:60:LEU:O	1:A:63:LEU:HB2	2.05	0.56
1:B:252:THR:HG22	1:B:254:VAL:HG12	1.88	0.56
1:E:333:GLU:CD	1:E:333:GLU:H	2.09	0.56
1:G:358:LEU:HD23	1:G:468:HIS:HB3	1.86	0.56
1:K:266:GLU:O	1:K:270:ILE:HG13	2.06	0.56
1:G:404:LEU:HD23	1:G:413:LYS:CB	2.34	0.56
1:G:446:MET:HE1	1:G:539:LEU:HD23	1.87	0.56
1:H:77:VAL:CG2	1:H:77:VAL:CG1	2.81	0.56
1:J:145:MET:HE1	1:J:303:PHE:CD1	2.41	0.56
1:C:119:LEU:HD12	1:C:119:LEU:O	2.05	0.56
1:H:161:GLU:HB3	1:H:501:ALA:CB	2.36	0.56
1:H:503:PHE:O	1:H:507:GLY:HA2	2.06	0.56
1:I:386:TYR:N	1:I:387:PRO:HD2	2.20	0.56
1:J:318:LEU:HD12	1:J:318:LEU:O	2.05	0.56
1:K:46:PRO:HA	6:K:6235:HOH:O	2.05	0.56
1:A:424:VAL:HG12	1:A:424:VAL:O	2.04	0.56
1:C:145:MET:SD	1:C:173:GLY:HA2	2.46	0.56
1:E:90:ASP:HB3	1:E:93:ALA:HB3	1.87	0.56
1:F:350:ILE:C	1:F:351:ASN:HD22	2.08	0.56
1:I:255:LEU:HD23	1:I:318:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:PRO:HG3	1:I:37:PHE:CZ	2.40	0.56
1:G:136:MET:HB3	1:G:218:PHE:CE1	2.41	0.56
1:G:527:LEU:HD11	1:G:533:THR:HG22	1.89	0.56
1:I:56:ALA:HB3	1:I:117:LEU:HD13	1.86	0.56
1:I:95:GLN:O	1:I:99:GLU:HG3	2.05	0.56
1:B:24:PRO:HG3	1:B:37:PHE:CE1	2.41	0.55
1:E:396:ILE:HB	1:E:397:PRO:HD3	1.88	0.55
1:H:172:LEU:HB2	6:H:6375:HOH:O	2.05	0.55
1:J:333:GLU:CD	1:J:333:GLU:H	2.10	0.55
1:L:403:TYR:O	1:L:416:LEU:HD13	2.06	0.55
1:A:484:GLY:O	1:A:485:ALA:C	2.45	0.55
1:B:348:VAL:O	1:B:446:MET:HA	2.06	0.55
1:E:431:VAL:O	1:E:434:ALA:HB3	2.06	0.55
3:H:882:SIA:O4	3:H:882:SIA:C10	2.55	0.55
1:A:316:GLN:NE2	1:A:317:PRO:HD2	2.21	0.55
1:F:197:ALA:O	1:F:201:VAL:HG23	2.06	0.55
1:G:428:VAL:HG13	1:G:544:VAL:HA	1.88	0.55
1:H:395:LEU:HD22	1:H:550:LEU:CD1	2.36	0.55
1:I:143:GLY:N	1:I:222:ALA:HB2	2.20	0.55
1:I:503:PHE:HD1	1:I:509:PRO:HD3	1.71	0.55
1:J:268:ILE:HG12	1:J:301:MET:CE	2.35	0.55
1:K:318:LEU:N	1:K:318:LEU:HD13	2.22	0.55
1:K:499:PHE:CZ	1:K:514:LEU:HD22	2.41	0.55
1:L:133:LEU:HD12	1:L:209:GLY:O	2.07	0.55
1:A:320:GLY:O	1:A:322:VAL:HG13	2.06	0.55
1:B:251:LEU:HD12	1:B:336:GLN:NE2	2.20	0.55
1:C:316:GLN:HA	1:C:316:GLN:HE21	1.70	0.55
3:L:1282:SIA:C7	6:L:6029:HOH:O	2.41	0.55
1:A:237:LYS:O	1:A:238:ASN:HB2	2.06	0.55
1:C:417:PHE:O	1:C:420:LEU:HB3	2.07	0.55
1:E:374:ASP:OD2	1:E:376:LYS:HB2	2.06	0.55
1:E:346:TYR:HB3	1:E:437:HIS:CD2	2.42	0.55
1:F:103:ASN:HA	1:F:482:LYS:HD2	1.88	0.55
1:F:485:ALA:HB3	6:F:6306:HOH:O	2.05	0.55
1:H:245:SER:HB3	1:H:248:GLY:O	2.06	0.55
1:K:64:ARG:O	1:K:66:THR:HG23	2.07	0.55
3:A:1181:SIA:N5	3:A:1181:SIA:C9	2.67	0.55
1:A:134:PRO:HG3	1:A:505:ARG:HG2	1.87	0.55
1:E:330:LYS:HB2	1:E:334:GLU:OE1	2.06	0.55
1:G:104:ARG:HD2	1:G:108:ILE:HG12	1.87	0.55
1:H:461:PRO:HG2	1:H:464:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:353:GLN:O	1:I:467:ASP:HA	2.06	0.55
1:K:216:THR:HG23	1:K:242:ARG:HB2	1.87	0.55
1:K:264:LEU:HD22	1:K:268:ILE:HD11	1.89	0.55
1:A:308:LEU:HD21	1:A:367:PRO:HG3	1.89	0.55
1:E:77:VAL:C	1:E:77:VAL:HG12	2.27	0.55
1:G:431:VAL:HG22	1:G:446:MET:HE1	1.89	0.55
1:J:202:GLN:HE22	1:J:215:VAL:HG21	1.72	0.55
1:J:432:ILE:HD11	1:J:544:VAL:HG13	1.87	0.55
1:K:368:LEU:HD11	1:K:418:LEU:HD21	1.88	0.55
1:C:104:ARG:HD2	1:C:108:ILE:HG12	1.89	0.55
1:C:77:VAL:O	1:C:77:VAL:HG12	2.06	0.55
1:G:318:LEU:O	1:G:318:LEU:HD12	2.06	0.55
1:I:176:GLY:HA2	1:I:189:TRP:HB2	1.88	0.55
1:I:24:PRO:HG3	1:I:37:PHE:CE1	2.42	0.55
1:B:445:TYR:CE1	1:B:519:GLU:HA	2.41	0.55
1:E:215:VAL:H	1:E:241:HIS:HD2	1.55	0.55
1:H:323:ILE:HD12	1:H:331:THR:HA	1.89	0.55
1:A:550:LEU:CB	1:A:550:LEU:C	2.70	0.55
1:B:95:GLN:HG2	1:B:99:GLU:OE2	2.07	0.55
1:D:290:THR:HG23	1:D:293:GLU:OE2	2.07	0.55
1:E:290:THR:OG1	1:E:293:GLU:HG3	2.07	0.55
1:F:316:GLN:NE2	1:F:317:PRO:HD2	2.21	0.55
1:F:324:ASP:OD2	1:F:324:ASP:N	2.40	0.55
1:F:499:PHE:CD2	1:F:514:LEU:HD13	2.42	0.55
1:H:134:PRO:HG2	1:H:163:VAL:HG12	1.89	0.55
1:K:249:VAL:HB	1:K:433:VAL:HG21	1.89	0.55
1:L:372:GLN:HE22	1:L:411:VAL:HG22	1.72	0.55
1:C:373:LEU:HD21	1:C:414:LYS:HA	1.88	0.54
1:D:358:LEU:HD23	1:D:468:HIS:HB3	1.89	0.54
1:J:330:LYS:HB2	1:J:334:GLU:OE2	2.07	0.54
1:K:232:LEU:HD21	1:K:336:GLN:NE2	2.22	0.54
1:K:215:VAL:N	1:K:241:HIS:HD2	2.06	0.54
1:K:350:ILE:C	1:K:351:ASN:HD22	2.09	0.54
1:B:338:GLU:OE2	1:B:341:PHE:HB2	2.07	0.54
1:D:351:ASN:HD22	1:D:351:ASN:N	1.96	0.54
1:E:331:THR:OG1	1:E:334:GLU:HG3	2.07	0.54
1:H:319:LEU:CD2	1:H:319:LEU:H	2.01	0.54
1:H:370:GLU:HB2	1:H:372:GLN:HG2	1.89	0.54
1:B:266:GLU:O	1:B:270:ILE:HG13	2.07	0.54
1:C:249:VAL:HG23	1:C:251:LEU:H	1.72	0.54
1:C:353:GLN:HG3	1:C:465:ILE:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:ARG:HB3	1:D:324:ASP:HB2	1.90	0.54
1:D:495:MET:HE1	1:D:533:THR:HB	1.88	0.54
1:G:268:ILE:HD11	1:G:319:LEU:HD21	1.89	0.54
1:A:339:ARG:CG	1:A:440:ALA:HA	2.37	0.54
1:A:97:LEU:HD11	1:A:101:PHE:CE2	2.42	0.54
1:E:133:LEU:HB3	1:E:134:PRO:HD2	1.88	0.54
3:D:2180:SIA:H112	1:E:278:THR:HG22	1.89	0.54
3:G:782:SIA:H4	1:H:262:LYS:NZ	2.22	0.54
1:H:431:VAL:HG22	1:H:446:MET:HE1	1.88	0.54
1:I:71:ALA:HB1	6:I:6282:HOH:O	2.07	0.54
1:K:403:TYR:O	1:K:416:LEU:HD13	2.08	0.54
1:L:428:VAL:HG13	1:L:544:VAL:HG13	1.89	0.54
1:B:86:MET:CE	1:B:110:LEU:HB2	2.37	0.54
1:F:407:THR:HG22	1:F:409:ASP:H	1.72	0.54
1:F:97:LEU:HD22	1:F:146:VAL:HG23	1.90	0.54
1:H:428:VAL:HG21	1:H:547:TRP:CD1	2.43	0.54
1:K:180:THR:HG22	1:K:282:MET:HE3	1.90	0.54
1:K:28:THR:HB	1:K:204:ASN:OD1	2.08	0.54
1:A:380:SER:O	1:A:384:LYS:HG3	2.08	0.54
1:E:251:LEU:HD11	1:E:336:GLN:NE2	2.20	0.54
1:I:338:GLU:HG2	1:I:339:ARG:N	2.22	0.54
1:K:107:ASN:ND2	1:K:108:ILE:N	2.55	0.54
1:K:306:LEU:HG	1:K:307:ASP:N	2.23	0.54
1:L:47:VAL:HG13	1:L:123:THR:O	2.08	0.54
1:A:217:ILE:HG13	1:A:227:VAL:HG13	1.88	0.54
1:A:456:SER:HB3	1:A:460:LYS:HD3	1.88	0.54
1:D:386:TYR:N	1:D:387:PRO:HD2	2.23	0.54
1:F:449:PHE:CE2	1:F:451:TYR:HB3	2.42	0.54
1:G:143:GLY:O	1:G:144:LEU:HB2	2.07	0.54
1:G:216:THR:HG23	1:G:242:ARG:HB2	1.89	0.54
1:K:47:VAL:HG13	1:K:123:THR:O	2.07	0.54
1:D:495:MET:HE2	1:D:533:THR:HG21	1.90	0.54
1:H:257:LYS:NZ	1:H:257:LYS:HA	2.22	0.54
1:H:447:TYR:C	1:H:447:TYR:CD2	2.80	0.54
1:K:171:ARG:HB3	1:K:176:GLY:CA	2.37	0.54
1:K:429:PRO:O	1:K:433:VAL:HG23	2.08	0.54
1:D:372:GLN:HB2	1:D:410:THR:C	2.28	0.54
1:J:104:ARG:O	1:J:482:LYS:HE3	2.06	0.54
1:K:131:ASN:O	1:K:132:ARG:HD2	2.07	0.54
1:K:355:PHE:CE1	1:K:360:PRO:HG3	2.43	0.54
1:L:178:PHE:CZ	1:L:286:LEU:HD12	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PHE:HB3	1:A:244:ILE:HB	1.90	0.54
3:B:1280:SIA:H113	1:C:262:LYS:HZ1	1.72	0.54
1:F:119:LEU:HD12	1:F:119:LEU:O	2.07	0.54
1:F:268:ILE:HG12	1:F:301:MET:CE	2.38	0.54
1:G:288:GLN:HG3	6:I:6384:HOH:O	2.07	0.54
1:D:262:LYS:HB3	1:D:263:PRO:HD3	1.88	0.53
1:C:89:GLN:HB2	1:C:146:VAL:HG12	1.90	0.53
1:C:24:PRO:HD2	1:C:35:GLY:O	2.08	0.53
1:C:526:TYR:CE2	1:C:539:LEU:HB2	2.43	0.53
1:E:227:VAL:O	1:E:231:VAL:HG23	2.06	0.53
1:F:385:SER:C	1:F:387:PRO:HD2	2.29	0.53
1:F:439:ASP:C	1:F:441:GLY:N	2.62	0.53
1:G:138:TRP:HH2	1:G:220:GLU:HB2	1.73	0.53
1:H:283:VAL:HG12	1:H:287:ARG:NH1	2.22	0.53
1:I:348:VAL:O	1:I:446:MET:HA	2.08	0.53
1:J:29:VAL:HG23	1:J:204:ASN:OD1	2.07	0.53
1:K:447:TYR:C	1:K:447:TYR:CD2	2.81	0.53
1:A:317:PRO:HG2	1:A:318:LEU:H	1.72	0.53
1:A:478:ALA:N	1:A:479:PRO:CD	2.71	0.53
1:B:396:ILE:HB	1:B:397:PRO:HD3	1.89	0.53
1:B:39:SER:OG	1:B:46:PRO:HB3	2.09	0.53
1:C:218:PHE:CB	1:C:244:ILE:HB	2.38	0.53
1:D:218:PHE:CB	1:D:244:ILE:HB	2.38	0.53
1:D:393:LYS:HA	1:D:396:ILE:HG12	1.91	0.53
1:G:87:CYS:O	1:G:89:GLN:HG2	2.07	0.53
1:J:339:ARG:CG	1:J:440:ALA:HA	2.39	0.53
1:C:139:ILE:HG12	1:C:168:ILE:HD11	1.91	0.53
1:C:257:LYS:HE3	1:C:316:GLN:HE22	1.72	0.53
1:E:116:CYS:O	1:E:118:TYR:N	2.40	0.53
1:E:348:VAL:O	1:E:446:MET:HA	2.08	0.53
1:H:532:ASN:ND2	1:H:532:ASN:H	2.06	0.53
1:I:527:LEU:HD23	1:I:529:ILE:HG12	1.90	0.53
1:L:199:ARG:CB	1:L:199:ARG:HH11	2.19	0.53
1:L:227:VAL:O	1:L:228:SER:C	2.46	0.53
1:A:417:PHE:O	1:A:420:LEU:HB3	2.08	0.53
1:C:344:VAL:HG12	6:C:6160:HOH:O	2.08	0.53
1:E:24:PRO:CA	1:E:25:VAL:N	2.66	0.53
1:F:41:GLU:HG3	1:F:41:GLU:O	2.09	0.53
1:H:290:THR:OG1	1:H:293:GLU:HG3	2.08	0.53
1:K:357:TRP:CZ2	1:K:361:MET:HG3	2.44	0.53
1:L:373:LEU:HD21	1:L:378:ALA:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:GLY:N	6:G:6144:HOH:O	2.42	0.53
1:H:199:ARG:NH1	1:H:199:ARG:HB3	2.09	0.53
1:I:313:ARG:HD2	1:I:386:TYR:CE2	2.43	0.53
1:I:186:ARG:HB3	1:I:324:ASP:HB2	1.91	0.53
1:J:385:SER:C	1:J:387:PRO:HD2	2.29	0.53
1:K:393:LYS:HA	1:K:396:ILE:HG12	1.91	0.53
1:A:266:GLU:HG2	1:A:282:MET:HE2	1.89	0.53
1:A:352:LYS:HD2	1:A:448:GLU:OE1	2.09	0.53
1:A:510:ASN:HD21	1:A:517:TRP:H	1.55	0.53
1:C:202:GLN:NE2	1:C:215:VAL:HG21	2.15	0.53
1:G:120:ASN:HB2	1:G:167:THR:OG1	2.08	0.53
1:I:132:ARG:HH11	1:I:132:ARG:HG2	1.74	0.53
1:K:143:GLY:O	1:K:144:LEU:HB2	2.08	0.53
1:L:264:LEU:O	1:L:268:ILE:HG13	2.09	0.53
1:A:312:PRO:O	1:A:315:SER:HB3	2.08	0.53
1:C:553:LYS:OXT	1:C:553:LYS:HD3	2.09	0.53
1:E:222:ALA:CB	6:E:6472:HOH:O	2.57	0.53
1:E:319:LEU:O	1:E:320:GLY:O	2.26	0.53
1:E:467:ASP:CG	1:E:468:HIS:H	2.12	0.53
1:F:241:HIS:C	1:F:242:ARG:HG3	2.29	0.53
1:G:241:HIS:O	1:G:242:ARG:HG2	2.09	0.53
1:H:218:PHE:CB	1:H:244:ILE:HB	2.39	0.53
1:H:501:ALA:HB1	1:H:505:ARG:NH1	2.23	0.53
1:I:498:LYS:O	1:I:502:ASN:HB2	2.09	0.53
1:J:131:ASN:C	1:J:132:ARG:HD2	2.29	0.53
1:L:379:MET:HE3	1:L:397:PRO:HG3	1.90	0.53
1:L:383:TRP:CZ3	1:L:393:LYS:HB2	2.43	0.53
1:B:59:PRO:HD3	1:B:117:LEU:HD12	1.91	0.53
1:K:477:GLY:HA2	1:K:493:SER:OG	2.09	0.53
1:A:215:VAL:N	1:A:241:HIS:CD2	2.76	0.53
1:A:34:LEU:HD13	1:A:34:LEU:C	2.29	0.53
1:B:343:THR:HB	1:B:442:ALA:HB2	1.90	0.53
1:C:111:LYS:H	1:C:111:LYS:HD2	1.74	0.53
1:D:104:ARG:O	1:D:482:LYS:HE2	2.09	0.53
1:E:453:PRO:HG3	1:E:470:ASP:OD1	2.09	0.53
1:G:164:VAL:CG1	1:G:205:ILE:HD11	2.38	0.53
1:G:64:ARG:O	1:G:65:PHE:CB	2.57	0.53
1:H:526:TYR:CD2	1:H:539:LEU:HB2	2.44	0.53
1:J:157:LEU:HD23	1:J:165:VAL:HG22	1.91	0.53
1:C:297:THR:O	1:C:301:MET:HG2	2.09	0.52
1:E:343:THR:HB	1:E:442:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:438:ARG:HD2	1:E:521:ASN:C	2.29	0.52
1:F:145:MET:HE1	1:F:303:PHE:CD1	2.45	0.52
1:C:268:ILE:HG12	1:C:301:MET:CE	2.39	0.52
1:E:478:ALA:N	1:E:479:PRO:CD	2.71	0.52
1:F:528:GLN:HE21	1:F:536:ALA:CB	2.21	0.52
1:G:217:ILE:CD1	1:G:227:VAL:HG13	2.39	0.52
1:H:63:LEU:HD21	1:H:69:GLN:HE21	1.74	0.52
1:K:132:ARG:HA	1:K:209:GLY:O	2.09	0.52
1:C:371:GLY:HA2	1:C:414:LYS:HZ2	1.75	0.52
1:D:86:MET:HE2	1:D:110:LEU:HD12	1.91	0.52
1:F:358:LEU:O	1:F:363:LEU:HD12	2.09	0.52
1:I:423:ASP:OD1	1:I:540:LYS:HD2	2.09	0.52
1:K:104:ARG:NH1	1:K:153:ASP:HB2	2.25	0.52
1:L:323:ILE:HD12	1:L:330:LYS:O	2.09	0.52
1:D:527:LEU:HD11	1:D:533:THR:HG22	1.90	0.52
1:E:526:TYR:HE1	1:E:528:GLN:HG2	1.75	0.52
1:G:386:TYR:N	1:G:387:PRO:HD2	2.24	0.52
1:H:393:LYS:HA	1:H:396:ILE:HG12	1.91	0.52
1:H:425:MET:HB2	1:H:426:PHE:CD1	2.44	0.52
1:I:435:ARG:NH1	1:I:544:VAL:HG11	2.24	0.52
1:I:499:PHE:HD2	1:I:509:PRO:HB2	1.74	0.52
1:K:393:LYS:HA	1:K:396:ILE:CG1	2.40	0.52
1:B:428:VAL:HG13	1:B:544:VAL:HG13	1.91	0.52
1:E:498:LYS:HD2	1:E:514:LEU:HD21	1.91	0.52
1:H:103:ASN:ND2	1:H:476:PHE:O	2.43	0.52
1:I:225:GLU:O	1:I:229:VAL:HG23	2.09	0.52
1:I:322:VAL:CG1	1:I:323:ILE:N	2.72	0.52
1:A:461:PRO:HG2	1:A:464:VAL:CG2	2.39	0.52
1:B:53:ILE:HD12	1:B:121:ILE:HD12	1.90	0.52
1:B:392:ALA:HB3	1:B:395:LEU:CG	2.38	0.52
1:D:467:ASP:N	1:D:470:ASP:OD2	2.41	0.52
1:E:493:SER:O	1:E:497:MET:HG3	2.10	0.52
1:H:351:ASN:HB3	1:H:466:GLY:O	2.09	0.52
1:I:190:GLY:O	1:I:194:GLN:HG3	2.09	0.52
1:A:423:ASP:OD2	1:A:543:GLU:HG2	2.09	0.52
1:B:420:LEU:CD2	1:B:547:TRP:HZ2	2.23	0.52
1:I:310:GLY:O	1:I:312:PRO:HD3	2.10	0.52
1:I:431:VAL:HG12	1:I:435:ARG:HD2	1.91	0.52
1:I:435:ARG:O	1:I:438:ARG:HB3	2.10	0.52
1:J:360:PRO:O	1:J:366:TYR:HB2	2.10	0.52
1:J:79:ASN:OD1	2:J:4179:NAG:H3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:95:GLN:O	1:K:99:GLU:HG3	2.09	0.52
1:A:328:LEU:HA	6:A:6261:HOH:O	2.08	0.52
1:B:236:ALA:HB1	1:B:240:PHE:CE1	2.42	0.52
1:D:499:PHE:CD2	1:D:514:LEU:HD13	2.44	0.52
1:G:97:LEU:HD22	1:G:146:VAL:CG2	2.40	0.52
1:H:386:TYR:N	1:H:387:PRO:HD2	2.24	0.52
1:H:396:ILE:HB	1:H:397:PRO:HD3	1.90	0.52
1:H:501:ALA:HB1	1:H:505:ARG:HH12	1.75	0.52
1:I:264:LEU:HD11	1:I:316:GLN:HG2	1.92	0.52
1:K:550:LEU:C	1:K:552:ALA:H	2.13	0.52
1:L:103:ASN:HA	1:L:482:LYS:HE2	1.92	0.52
1:L:431:VAL:O	1:L:434:ALA:HB3	2.09	0.52
1:L:75:SER:O	1:L:76:PHE:O	2.26	0.52
1:A:211:ASN:C	1:A:213:GLY:H	2.13	0.52
1:F:218:PHE:CB	1:F:244:ILE:HB	2.39	0.52
1:H:495:MET:HE3	1:H:533:THR:CB	2.39	0.52
1:L:543:GLU:O	1:L:547:TRP:HD1	1.91	0.52
1:A:317:PRO:O	1:A:318:LEU:HB3	2.09	0.52
1:A:550:LEU:C	1:A:550:LEU:N	2.57	0.52
1:B:98:SER:O	1:B:107:ASN:ND2	2.43	0.52
1:C:221:SER:HA	1:C:247:SER:O	2.09	0.52
1:D:526:TYR:CD2	1:D:539:LEU:HB2	2.45	0.52
1:E:303:PHE:CZ	1:E:319:LEU:HD21	2.45	0.52
1:G:242:ARG:HD2	1:G:504:ALA:HA	1.92	0.52
1:G:478:ALA:N	1:G:479:PRO:CD	2.72	0.52
1:C:372:GLN:O	1:C:373:LEU:HB3	2.09	0.51
1:F:138:TRP:HE3	1:F:218:PHE:CD2	2.28	0.51
1:H:264:LEU:O	1:H:268:ILE:HG13	2.10	0.51
1:H:395:LEU:HD22	1:H:550:LEU:HD12	1.92	0.51
1:J:417:PHE:O	1:J:420:LEU:HB3	2.09	0.51
1:K:306:LEU:HG	1:K:307:ASP:H	1.74	0.51
1:L:215:VAL:N	1:L:241:HIS:HD2	2.08	0.51
1:D:491:ARG:HH11	1:D:491:ARG:HG3	1.75	0.51
1:F:205:ILE:HG13	1:F:210:GLY:HA3	1.92	0.51
1:F:254:VAL:HG13	1:F:255:LEU:N	2.25	0.51
1:J:59:PRO:HD3	1:J:117:LEU:HD12	1.93	0.51
1:A:34:LEU:HD13	1:A:35:GLY:O	2.11	0.51
1:A:83:TYR:CD1	1:A:150:SER:HB3	2.46	0.51
1:B:382:LEU:HD11	1:B:391:ILE:HD12	1.93	0.51
1:G:393:LYS:C	1:G:395:LEU:H	2.14	0.51
1:G:447:TYR:HB3	1:G:517:TRP:CZ2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:526:TYR:CE2	1:H:539:LEU:HB2	2.45	0.51
1:I:345:PRO:HA	1:I:443:PRO:HB2	1.92	0.51
1:J:324:ASP:OD2	1:J:325:GLY:N	2.41	0.51
1:L:262:LYS:HE3	1:L:282:MET:HE2	1.92	0.51
1:B:255:LEU:HD23	1:B:318:LEU:HD11	1.91	0.51
1:C:403:TYR:CG	1:C:420:LEU:HD23	2.45	0.51
1:D:87:CYS:O	1:D:89:GLN:HG2	2.11	0.51
1:E:220:GLU:HA	1:E:246:GLU:O	2.11	0.51
1:F:262:LYS:HB3	1:F:263:PRO:HD3	1.92	0.51
1:G:145:MET:HE1	1:G:303:PHE:CD1	2.46	0.51
1:I:426:PHE:C	1:I:429:PRO:HD2	2.31	0.51
1:I:527:LEU:HD23	1:I:529:ILE:CG1	2.40	0.51
1:K:223:GLY:O	1:K:227:VAL:HG23	2.11	0.51
1:L:268:ILE:HD11	1:L:319:LEU:HD21	1.91	0.51
1:A:152:TYR:HB3	1:A:476:PHE:CE2	2.45	0.51
1:C:264:LEU:HG	1:C:316:GLN:HG2	1.92	0.51
1:C:290:THR:HG23	1:C:293:GLU:OE2	2.09	0.51
1:D:498:LYS:HD2	6:D:6232:HOH:O	2.10	0.51
1:E:355:PHE:CD1	1:E:360:PRO:HG3	2.44	0.51
1:F:539:LEU:HD12	1:F:540:LYS:H	1.74	0.51
1:G:221:SER:OG	5:G:3385:BEZ:H2	2.10	0.51
1:H:381:LEU:HD22	1:H:417:PHE:CE2	2.45	0.51
1:I:403:TYR:CG	1:I:420:LEU:HD23	2.45	0.51
1:K:138:TRP:O	6:K:6407:HOH:O	2.19	0.51
1:K:152:TYR:CD1	1:K:152:TYR:N	2.76	0.51
1:K:218:PHE:HB3	1:K:244:ILE:HB	1.92	0.51
1:L:110:LEU:HD11	1:L:150:SER:HB2	1.92	0.51
1:A:425:MET:O	1:A:429:PRO:HG2	2.10	0.51
1:C:262:LYS:HE3	1:C:279:SER:OG	2.10	0.51
1:C:268:ILE:HG12	1:C:301:MET:HE2	1.91	0.51
1:D:264:LEU:HD22	1:D:268:ILE:CD1	2.40	0.51
3:J:1082:SIA:H4	1:K:262:LYS:HZ3	1.74	0.51
1:J:456:SER:HB3	1:J:460:LYS:HE2	1.93	0.51
1:K:221:SER:O	1:K:224:GLY:N	2.43	0.51
1:K:25:VAL:HG22	1:K:34:LEU:HD23	1.88	0.51
1:L:290:THR:OG1	1:L:293:GLU:HG3	2.10	0.51
1:A:316:GLN:NE2	1:A:316:GLN:HA	2.25	0.51
1:B:277:THR:HG22	1:B:278:THR:HG23	1.92	0.51
1:B:364:MET:HE1	1:B:388:LEU:HD21	1.93	0.51
1:E:142:GLY:N	6:E:6472:HOH:O	2.24	0.51
1:E:445:TYR:CE1	1:E:519:GLU:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:TYR:CD2	1:E:447:TYR:C	2.84	0.51
1:G:222:ALA:CB	6:G:6473:HOH:O	2.58	0.51
1:I:281:VAL:O	1:I:284:HIS:HB3	2.11	0.51
1:J:241:HIS:C	1:J:242:ARG:HG3	2.30	0.51
1:A:26:VAL:CG2	1:A:127:LEU:HD13	2.41	0.51
1:A:184:HIS:HD2	1:A:279:SER:HB3	1.74	0.51
1:A:24:PRO:HG3	1:A:37:PHE:CZ	2.45	0.51
1:A:383:TRP:CE3	1:A:393:LYS:HB2	2.46	0.51
1:C:499:PHE:CE2	1:C:514:LEU:HB3	2.46	0.51
1:E:241:HIS:C	1:E:242:ARG:HG3	2.31	0.51
1:F:202:GLN:NE2	1:F:212:PRO:O	2.44	0.51
1:F:293:GLU:O	1:F:296:GLU:HB3	2.10	0.51
1:F:445:TYR:CZ	1:F:509:PRO:HD2	2.45	0.51
1:F:539:LEU:HD12	1:F:540:LYS:N	2.26	0.51
1:G:132:ARG:HB3	1:G:211:ASN:HB2	1.91	0.51
1:I:200:TRP:CE2	1:I:204:ASN:ND2	2.79	0.51
1:I:539:LEU:O	1:I:541:ASP:N	2.44	0.51
1:J:218:PHE:CB	1:J:244:ILE:HB	2.41	0.51
1:J:359:ILE:HB	1:J:360:PRO:HD3	1.92	0.51
1:L:215:VAL:H	1:L:241:HIS:HD2	1.59	0.51
1:B:218:PHE:CB	1:B:244:ILE:HB	2.41	0.51
1:D:339:ARG:HH12	1:D:440:ALA:HB2	1.75	0.51
1:D:526:TYR:CE2	1:D:539:LEU:HB2	2.45	0.51
1:E:101:PHE:HD2	1:E:152:TYR:HH	1.58	0.51
1:E:237:LYS:O	1:E:238:ASN:HB2	2.10	0.51
1:F:57:LYS:HB2	1:F:71:ALA:HA	1.93	0.51
1:G:86:MET:CE	1:G:110:LEU:HB2	2.40	0.51
1:H:255:LEU:HD23	1:H:318:LEU:CD1	2.41	0.51
1:I:171:ARG:HD2	1:I:175:TRP:O	2.11	0.51
1:J:218:PHE:HA	1:J:244:ILE:O	2.11	0.51
1:K:257:LYS:HB2	1:K:322:VAL:HG12	1.93	0.51
1:L:527:LEU:HD11	1:L:533:THR:HG22	1.92	0.51
1:B:25:VAL:HG22	1:B:34:LEU:CD2	2.40	0.51
1:C:198:LEU:HD21	1:C:217:ILE:CG2	2.41	0.51
1:D:260:ASP:OD2	1:D:263:PRO:HD3	2.12	0.51
1:E:317:PRO:HD2	6:E:6027:HOH:O	2.09	0.51
1:F:236:ALA:HB1	1:F:240:PHE:HE1	1.76	0.51
1:H:34:LEU:HB2	1:H:77:VAL:HG12	1.92	0.51
1:B:86:MET:HG3	1:B:112:LEU:HD23	1.94	0.50
1:D:478:ALA:N	1:D:479:PRO:CD	2.74	0.50
1:I:194:GLN:OE1	1:I:226:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:427:GLY:O	1:L:431:VAL:HG23	2.11	0.50
1:D:152:TYR:HB3	1:D:476:PHE:CE2	2.46	0.50
1:F:510:ASN:OD1	1:F:516:HIS:HA	2.12	0.50
1:F:447:TYR:HB3	1:F:517:TRP:CZ2	2.46	0.50
1:J:264:LEU:HG	1:J:316:GLN:HG2	1.93	0.50
1:J:478:ALA:N	1:J:479:PRO:CD	2.73	0.50
1:L:105:LYS:HG3	1:L:106:GLU:H	1.76	0.50
1:A:343:THR:HA	6:A:6423:HOH:O	2.11	0.50
1:B:141:GLY:HA2	1:B:223:GLY:N	2.26	0.50
1:D:255:LEU:HA	1:D:318:LEU:HD11	1.93	0.50
1:D:428:VAL:HG13	1:D:544:VAL:HA	1.93	0.50
1:D:349:GLY:HA3	1:D:447:TYR:CD1	2.47	0.50
1:G:131:ASN:HB2	1:G:209:GLY:HA2	1.93	0.50
1:H:312:PRO:HG3	1:H:384:LYS:HA	1.93	0.50
1:L:357:TRP:C	1:L:360:PRO:HD2	2.31	0.50
1:E:91:PRO:HB3	1:E:112:LEU:HD11	1.93	0.50
1:F:104:ARG:HD2	1:F:108:ILE:HG12	1.93	0.50
1:F:452:ARG:NH2	1:F:460:LYS:O	2.45	0.50
1:H:193:ASP:O	1:H:196:ALA:HB3	2.11	0.50
1:H:244:ILE:HG12	1:H:347:MET:HB3	1.93	0.50
1:I:149:ALA:HB2	1:I:168:ILE:O	2.12	0.50
1:I:491:ARG:HH11	1:I:491:ARG:HG3	1.76	0.50
1:J:88:THR:HG22	1:J:295:LEU:HD22	1.93	0.50
1:L:87:CYS:O	1:L:89:GLN:HG2	2.11	0.50
1:A:211:ASN:O	1:A:213:GLY:N	2.44	0.50
1:K:517:TRP:CE3	1:K:527:LEU:HD22	2.46	0.50
1:L:355:PHE:CE1	1:L:360:PRO:HG3	2.47	0.50
1:D:428:VAL:HB	1:D:429:PRO:HD3	1.94	0.50
1:F:221:SER:OG	1:F:222:ALA:N	2.44	0.50
1:F:333:GLU:H	1:F:333:GLU:CD	2.15	0.50
1:F:457:SER:C	1:F:459:MET:H	2.15	0.50
1:F:88:THR:HB	1:F:175:TRP:CZ3	2.47	0.50
1:J:88:THR:CG2	1:J:295:LEU:HD22	2.41	0.50
1:A:237:LYS:HE3	1:A:342:HIS:HB2	1.92	0.50
1:B:90:ASP:HB3	1:B:93:ALA:HB3	1.94	0.50
1:C:319:LEU:H	1:C:319:LEU:CD2	2.17	0.50
1:D:231:VAL:O	1:D:231:VAL:HG12	2.12	0.50
1:D:456:SER:HB3	1:D:460:LYS:HD3	1.93	0.50
1:E:260:ASP:OD2	1:E:263:PRO:HD3	2.12	0.50
1:F:220:GLU:HG3	1:F:472:LEU:HD21	1.93	0.50
1:I:301:MET:O	1:I:302:LYS:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:540:LYS:O	1:J:544:VAL:HG23	2.11	0.50
1:L:255:LEU:HD23	1:L:318:LEU:HD11	1.93	0.50
1:B:317:PRO:CD	6:B:6020:HOH:O	2.53	0.50
1:E:477:GLY:CA	1:E:497:MET:HE2	2.42	0.50
1:F:382:LEU:HD11	1:F:391:ILE:HD12	1.94	0.50
1:G:149:ALA:HB2	1:G:168:ILE:O	2.12	0.50
1:I:351:ASN:ND2	1:I:449:PHE:HB3	2.26	0.50
1:I:34:LEU:HB2	1:I:77:VAL:HG12	1.94	0.50
1:I:89:GLN:HA	6:I:6167:HOH:O	2.12	0.50
1:L:447:TYR:HB3	1:L:517:TRP:CZ2	2.47	0.50
1:A:276:THR:HG22	1:A:282:MET:HE2	1.93	0.50
1:C:293:GLU:O	1:C:296:GLU:HB2	2.12	0.50
1:D:186:ARG:HD3	1:D:324:ASP:HB2	1.94	0.50
1:E:221:SER:HB3	6:E:6472:HOH:O	2.11	0.50
1:H:355:PHE:CE1	1:H:360:PRO:HG3	2.47	0.50
1:H:49:ILE:HD13	1:H:122:TYR:HE2	1.76	0.50
1:H:87:CYS:HB3	6:H:6375:HOH:O	2.12	0.50
1:I:417:PHE:O	1:I:420:LEU:HB3	2.12	0.50
1:K:252:THR:HG22	1:K:254:VAL:CG1	2.41	0.50
1:K:267:GLN:HE22	1:K:316:GLN:HG2	1.77	0.50
1:A:88:THR:CG2	1:A:295:LEU:HD13	2.40	0.49
1:A:461:PRO:HB2	1:A:463:THR:HG22	1.94	0.49
1:B:123:THR:HB	1:B:164:VAL:HG13	1.94	0.49
1:C:143:GLY:O	1:C:144:LEU:HB2	2.11	0.49
1:D:24:PRO:HG3	1:D:37:PHE:CZ	2.46	0.49
1:D:257:LYS:HB2	1:D:322:VAL:HG12	1.94	0.49
1:D:359:ILE:HB	1:D:360:PRO:CD	2.38	0.49
1:D:521:ASN:HD21	1:D:523:LYS:HD3	1.77	0.49
1:E:177:PHE:HB3	1:E:319:LEU:O	2.12	0.49
1:I:41:GLU:OE1	1:I:41:GLU:N	2.40	0.49
1:J:295:LEU:O	1:J:298:THR:HB	2.12	0.49
1:J:357:TRP:C	1:J:360:PRO:HD2	2.33	0.49
1:J:381:LEU:HD22	1:J:417:PHE:CE2	2.47	0.49
1:L:357:TRP:O	1:L:360:PRO:HD2	2.11	0.49
1:A:503:PHE:O	1:A:507:GLY:N	2.45	0.49
1:B:447:TYR:HB3	1:B:517:TRP:HZ2	1.77	0.49
1:F:368:LEU:HD13	1:F:418:LEU:HD21	1.94	0.49
1:H:121:ILE:HG12	1:H:166:VAL:HG22	1.93	0.49
1:I:349:GLY:HA3	1:I:447:TYR:CE1	2.47	0.49
1:J:99:GLU:HA	1:J:107:ASN:ND2	2.27	0.49
1:J:241:HIS:O	1:J:345:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:379:MET:HE1	1:L:397:PRO:HG3	1.93	0.49
1:A:219:GLY:N	1:A:227:VAL:HG21	2.27	0.49
1:A:366:TYR:HD2	1:A:368:LEU:HG	1.76	0.49
1:C:392:ALA:HB3	1:C:395:LEU:HG	1.94	0.49
1:E:143:GLY:N	6:E:6469:HOH:O	2.40	0.49
1:F:257:LYS:HE2	1:F:316:GLN:NE2	2.27	0.49
1:F:546:PHE:O	1:F:549:ASN:HB2	2.13	0.49
1:F:57:LYS:CB	1:F:57:LYS:CD	2.77	0.49
1:H:129:LYS:HD2	6:H:6358:HOH:O	2.12	0.49
1:I:251:LEU:HD11	1:I:336:GLN:OE1	2.12	0.49
1:I:355:PHE:CE1	1:I:360:PRO:HG3	2.48	0.49
1:K:136:MET:HB3	1:K:218:PHE:CE1	2.48	0.49
1:K:242:ARG:CG	1:K:242:ARG:HH11	2.25	0.49
1:B:327:LEU:HD23	1:B:327:LEU:C	2.33	0.49
1:C:228:SER:O	1:C:232:LEU:HG	2.13	0.49
1:D:194:GLN:O	1:D:197:ALA:HB3	2.13	0.49
1:E:254:VAL:O	1:E:254:VAL:HG22	2.12	0.49
1:E:363:LEU:C	1:E:365:SER:H	2.15	0.49
1:H:350:ILE:O	1:H:448:GLU:HA	2.13	0.49
1:H:249:VAL:HB	1:H:433:VAL:HG21	1.93	0.49
1:I:389:VAL:HB	1:I:424:VAL:HG11	1.93	0.49
1:K:487:GLU:HG3	1:K:491:ARG:NH1	2.27	0.49
1:L:252:THR:HG22	1:L:254:VAL:HG12	1.94	0.49
1:D:59:PRO:HD3	1:D:117:LEU:CD1	2.42	0.49
1:F:254:VAL:HG13	1:F:255:LEU:H	1.77	0.49
1:G:89:GLN:OE1	1:G:146:VAL:HB	2.12	0.49
1:H:56:ALA:CB	1:H:117:LEU:HD13	2.42	0.49
1:H:413:LYS:O	1:H:416:LEU:N	2.45	0.49
1:H:339:ARG:HH22	1:H:439:ASP:HB3	1.77	0.49
1:I:262:LYS:HB3	1:I:263:PRO:HD3	1.93	0.49
1:J:355:PHE:CE1	1:J:360:PRO:HG3	2.48	0.49
1:L:215:VAL:H	1:L:241:HIS:CD2	2.31	0.49
1:B:243:ALA:C	1:B:244:ILE:HG13	2.33	0.49
1:B:423:ASP:OD1	1:B:540:LYS:HD2	2.13	0.49
1:E:236:ALA:HB1	1:E:240:PHE:CE1	2.42	0.49
1:E:428:VAL:HG13	1:E:544:VAL:HA	1.94	0.49
1:F:139:ILE:HG12	1:F:168:ILE:HD11	1.95	0.49
1:G:348:VAL:O	1:G:446:MET:HA	2.12	0.49
1:I:322:VAL:CG1	1:I:323:ILE:H	2.25	0.49
1:J:257:LYS:HE3	1:J:316:GLN:HE22	1.78	0.49
1:A:151:THR:HG22	1:A:152:TYR:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TRP:CZ2	1:A:361:MET:HG3	2.48	0.49
1:A:355:PHE:CE1	1:A:360:PRO:HG3	2.47	0.49
1:B:447:TYR:C	1:B:447:TYR:CD2	2.86	0.49
1:D:223:GLY:O	1:D:227:VAL:HG23	2.13	0.49
1:D:311:ASP:HB3	1:D:314:GLU:HG2	1.94	0.49
1:D:492:LEU:O	1:D:496:VAL:HG23	2.12	0.49
1:H:323:ILE:CD1	1:H:331:THR:HA	2.42	0.49
1:I:493:SER:O	1:I:497:MET:HE2	2.12	0.49
1:J:64:ARG:O	1:J:65:PHE:HB2	2.13	0.49
1:L:178:PHE:CD1	1:L:178:PHE:O	2.65	0.49
1:L:236:ALA:HB1	1:L:240:PHE:HE1	1.77	0.49
1:L:25:VAL:HG22	1:L:34:LEU:CD2	2.31	0.49
1:E:357:TRP:CZ2	1:E:361:MET:HG3	2.47	0.49
1:F:368:LEU:C	1:F:370:GLU:H	2.16	0.49
1:G:121:ILE:HD11	1:G:200:TRP:HZ3	1.77	0.49
1:H:351:ASN:N	1:H:351:ASN:ND2	2.60	0.49
1:J:222:ALA:O	1:J:226:SER:OG	2.31	0.49
1:J:254:VAL:HG13	1:J:255:LEU:N	2.28	0.49
1:L:24:PRO:HG3	1:L:37:PHE:CE1	2.48	0.49
1:L:64:ARG:O	1:L:65:PHE:CB	2.61	0.49
1:A:134:PRO:HD3	6:A:6314:HOH:O	2.11	0.49
1:C:527:LEU:HD11	1:C:533:THR:CG2	2.42	0.49
1:C:90:ASP:OD1	1:C:92:LYS:HG3	2.13	0.49
1:D:103:ASN:ND2	1:D:476:PHE:O	2.46	0.49
1:I:324:ASP:C	1:I:326:MET:H	2.16	0.49
1:I:431:VAL:HG21	1:I:540:LYS:HB2	1.94	0.49
1:J:393:LYS:HA	1:J:396:ILE:HG12	1.93	0.49
1:B:126:ASP:H	1:B:131:ASN:ND2	2.10	0.49
1:E:228:SER:O	1:E:231:VAL:HB	2.13	0.49
1:E:414:LYS:O	1:E:417:PHE:HB3	2.13	0.49
1:G:343:THR:HA	6:G:6372:HOH:O	2.13	0.49
1:H:115:ASP:OD2	1:H:118:TYR:OH	2.31	0.49
1:H:423:ASP:OD2	1:H:543:GLU:HG2	2.13	0.49
1:K:372:GLN:HG3	1:K:410:THR:HB	1.95	0.49
1:A:103:ASN:ND2	1:A:476:PHE:O	2.46	0.48
1:A:316:GLN:CD	1:A:317:PRO:HD2	2.33	0.48
1:A:499:PHE:CE2	1:A:514:LEU:HB3	2.48	0.48
1:B:276:THR:HB	1:B:282:MET:HE2	1.95	0.48
1:C:371:GLY:HA2	1:C:414:LYS:NZ	2.28	0.48
1:C:348:VAL:O	1:C:446:MET:HA	2.13	0.48
1:E:447:TYR:HB3	1:E:517:TRP:CZ2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:LYS:HG3	6:F:6052:HOH:O	2.12	0.48
1:I:450:GLN:NE2	6:I:6101:HOH:O	2.43	0.48
1:B:333:GLU:H	1:B:333:GLU:CD	2.16	0.48
1:B:113:SER:HB2	1:C:277:THR:HG21	1.94	0.48
1:D:176:GLY:HA2	1:D:189:TRP:HB2	1.95	0.48
1:D:283:VAL:O	1:D:287:ARG:HG3	2.13	0.48
1:F:357:TRP:C	1:F:360:PRO:HD2	2.32	0.48
1:G:121:ILE:HD11	1:G:200:TRP:CZ3	2.48	0.48
1:H:349:GLY:HA3	1:H:447:TYR:CD1	2.48	0.48
1:H:58:PRO:O	1:H:60:LEU:N	2.44	0.48
1:J:86:MET:CB	1:J:148:ALA:HB2	2.43	0.48
1:L:311:ASP:HB3	1:L:314:GLU:OE1	2.13	0.48
1:D:266:GLU:HG2	1:D:282:MET:CE	2.41	0.48
1:D:372:GLN:HG3	1:D:410:THR:HB	1.95	0.48
1:E:312:PRO:HG2	1:E:383:TRP:NE1	2.28	0.48
1:F:355:PHE:CD1	1:F:360:PRO:HG3	2.48	0.48
1:G:199:ARG:NH1	1:G:199:ARG:HG2	2.28	0.48
1:G:456:SER:CB	1:G:460:LYS:HE2	2.42	0.48
1:K:491:ARG:HH11	1:K:491:ARG:HG3	1.78	0.48
1:L:353:GLN:HE22	1:L:465:ILE:H	1.61	0.48
1:B:218:PHE:CD1	1:B:218:PHE:N	2.81	0.48
1:B:60:LEU:CD2	1:B:114:GLU:HB3	2.43	0.48
1:D:131:ASN:O	1:D:209:GLY:HA2	2.13	0.48
1:D:449:PHE:CE2	1:D:471:GLU:HA	2.49	0.48
1:F:134:PRO:CG	1:F:163:VAL:HG12	2.40	0.48
1:F:348:VAL:O	1:F:446:MET:HA	2.13	0.48
1:F:45:GLN:NE2	6:F:6068:HOH:O	2.46	0.48
1:F:486:SER:O	1:F:490:ILE:HG13	2.13	0.48
1:G:452:ARG:NH1	1:G:452:ARG:HG2	2.27	0.48
1:I:450:GLN:HB2	6:I:6101:HOH:O	2.13	0.48
1:J:467:ASP:N	1:J:470:ASP:OD2	2.44	0.48
1:K:404:LEU:H	1:K:404:LEU:HD12	1.79	0.48
1:K:540:LYS:O	1:K:544:VAL:HG23	2.13	0.48
1:L:139:ILE:O	1:L:223:GLY:HA3	2.13	0.48
1:A:351:ASN:N	1:A:354:GLU:OE2	2.46	0.48
1:B:392:ALA:HB3	1:B:395:LEU:CD1	2.44	0.48
1:B:478:ALA:N	1:B:479:PRO:CD	2.77	0.48
1:C:456:SER:HB3	1:C:460:LYS:HE2	1.94	0.48
1:D:85:PRO:HA	6:D:6246:HOH:O	2.13	0.48
1:D:91:PRO:HB3	1:D:112:LEU:HD11	1.95	0.48
1:E:254:VAL:O	1:E:318:LEU:HD11	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:86:MET:HB3	1:J:148:ALA:HB2	1.95	0.48
1:J:392:ALA:HB3	1:J:395:LEU:HD12	1.95	0.48
3:J:1082:SIA:H4	1:K:262:LYS:HZ1	1.74	0.48
1:K:427:GLY:O	1:K:431:VAL:HG23	2.13	0.48
1:K:471:GLU:N	1:K:471:GLU:OE1	2.46	0.48
1:L:160:HIS:NE2	1:L:480:PHE:CD2	2.81	0.48
1:L:199:ARG:O	1:L:202:GLN:HB2	2.13	0.48
1:C:409:ASP:OD2	1:C:412:LYS:HE2	2.13	0.48
1:D:447:TYR:HB3	1:D:517:TRP:CZ2	2.48	0.48
1:I:316:GLN:OE1	1:I:317:PRO:HD2	2.14	0.48
1:B:218:PHE:HB3	1:B:244:ILE:HB	1.96	0.48
1:C:246:GLU:HG2	1:C:447:TYR:OH	2.14	0.48
1:E:321:THR:HG22	1:E:322:VAL:N	2.28	0.48
1:E:521:ASN:HB2	1:E:522:GLN:OE1	2.14	0.48
1:J:242:ARG:HG2	1:J:242:ARG:HH11	1.78	0.48
1:K:526:TYR:CE1	1:K:539:LEU:HD13	2.49	0.48
1:G:176:GLY:O	1:G:189:TRP:HB2	2.14	0.48
1:I:447:TYR:HB3	1:I:517:TRP:CZ2	2.49	0.48
1:K:206:ALA:HA	1:K:210:GLY:O	2.14	0.48
1:L:353:GLN:NE2	1:L:465:ILE:H	2.11	0.48
1:A:264:LEU:O	1:A:268:ILE:HG13	2.14	0.48
1:A:138:TRP:CD2	1:A:476:PHE:HZ	2.32	0.48
1:A:519:GLU:O	1:A:521:ASN:N	2.42	0.48
1:C:304:LEU:HD11	5:C:5013:BEZ:H5	1.96	0.48
1:D:417:PHE:O	1:D:420:LEU:HB3	2.13	0.48
1:E:218:PHE:HB3	1:E:244:ILE:HB	1.95	0.48
1:E:527:LEU:HD23	1:E:529:ILE:CG1	2.44	0.48
1:E:527:LEU:HD23	1:E:529:ILE:HG12	1.95	0.48
1:G:107:ASN:ND2	1:G:108:ILE:N	2.62	0.48
1:G:122:TYR:HB2	1:G:165:VAL:HB	1.96	0.48
1:H:330:LYS:HG3	1:H:335:LEU:CD2	2.43	0.48
1:J:55:PHE:O	1:J:56:ALA:HB2	2.13	0.48
1:K:241:HIS:C	1:K:242:ARG:HG3	2.34	0.48
1:K:257:LYS:NZ	1:K:317:PRO:HB3	2.28	0.48
1:K:325:GLY:HA2	1:K:329:LEU:HA	1.96	0.48
1:L:374:ASP:OD2	1:L:376:LYS:HB2	2.13	0.48
1:L:53:ILE:HG21	1:L:200:TRP:CZ2	2.49	0.48
1:B:191:HIS:HB3	1:B:327:LEU:HD11	1.95	0.48
3:B:1280:SIA:H113	1:C:262:LYS:HZ3	1.78	0.48
1:D:34:LEU:HB3	1:D:79:ASN:CB	2.42	0.48
1:D:90:ASP:HB3	1:D:93:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:SER:O	1:E:383:TRP:HB3	2.13	0.48
1:F:452:ARG:NE	1:F:462:LYS:HA	2.29	0.48
1:F:88:THR:CG2	1:F:295:LEU:HD22	2.44	0.48
1:H:220:GLU:HA	1:H:246:GLU:O	2.12	0.48
1:J:134:PRO:CG	1:J:163:VAL:HG12	2.34	0.48
1:A:68:PRO:HG3	1:A:193:ASP:OD1	2.14	0.47
1:B:103:ASN:HD22	1:B:476:PHE:HB3	1.79	0.47
1:C:140:HIS:HD2	1:C:141:GLY:O	1.97	0.47
1:D:317:PRO:HG2	1:D:318:LEU:H	1.79	0.47
1:G:191:HIS:NE2	1:G:321:THR:OG1	2.41	0.47
1:H:215:VAL:N	1:H:241:HIS:HD2	2.11	0.47
1:I:55:PHE:CE1	1:I:197:ALA:HB2	2.49	0.47
1:I:428:VAL:N	1:I:429:PRO:CD	2.77	0.47
1:L:202:GLN:HG2	6:L:6395:HOH:O	2.14	0.47
1:A:461:PRO:HG2	1:A:464:VAL:HG23	1.96	0.47
1:B:211:ASN:HD22	1:B:214:SER:CB	2.26	0.47
1:C:452:ARG:NE	1:C:462:LYS:HA	2.29	0.47
1:E:184:HIS:O	1:E:185:SER:HB2	2.14	0.47
1:G:316:GLN:NE2	1:G:316:GLN:HA	2.29	0.47
1:H:215:VAL:H	1:H:241:HIS:CD2	2.32	0.47
1:H:262:LYS:N	1:H:263:PRO:CD	2.78	0.47
1:H:532:ASN:N	1:H:532:ASN:ND2	2.60	0.47
1:I:28:THR:HG23	1:I:31:GLY:O	2.14	0.47
1:I:357:TRP:O	1:I:360:PRO:HD2	2.14	0.47
1:J:312:PRO:HG2	1:J:383:TRP:CE2	2.50	0.47
1:K:59:PRO:HD3	1:K:117:LEU:HD12	1.96	0.47
1:L:498:LYS:CD	6:L:6137:HOH:O	2.59	0.47
1:D:172:LEU:HB2	6:D:6033:HOH:O	2.14	0.47
1:D:319:LEU:HG	1:D:319:LEU:O	2.13	0.47
1:D:381:LEU:HA	1:D:384:LYS:HD2	1.95	0.47
1:F:540:LYS:O	1:F:544:VAL:HG23	2.13	0.47
1:H:171:ARG:HB3	1:H:176:GLY:CA	2.44	0.47
1:H:194:GLN:HE22	1:H:226:SER:CB	2.26	0.47
1:K:211:ASN:C	1:K:211:ASN:OD1	2.53	0.47
1:B:453:PRO:HG2	1:B:456:SER:OG	2.14	0.47
1:C:228:SER:CB	1:C:250:ALA:H	2.27	0.47
1:D:283:VAL:HG12	1:D:287:ARG:NH1	2.28	0.47
1:E:33:VAL:CG1	1:E:34:LEU:N	2.78	0.47
1:E:385:SER:C	1:E:387:PRO:HD2	2.34	0.47
1:F:420:LEU:HD22	1:F:547:TRP:HZ2	1.79	0.47
1:G:431:VAL:HG22	1:G:446:MET:CE	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:LEU:HD13	1:H:35:GLY:N	2.28	0.47
1:I:217:ILE:O	1:I:243:ALA:HA	2.15	0.47
1:I:414:LYS:O	1:I:417:PHE:HB3	2.14	0.47
1:J:117:LEU:HD21	1:J:193:ASP:OD2	2.14	0.47
1:K:383:TRP:C	1:K:385:SER:H	2.17	0.47
1:B:132:ARG:HG3	1:B:211:ASN:HB2	1.97	0.47
1:E:149:ALA:HB2	1:E:168:ILE:O	2.15	0.47
1:G:264:LEU:CD1	1:G:316:GLN:HG2	2.44	0.47
1:G:333:GLU:CD	1:G:333:GLU:H	2.18	0.47
1:J:88:THR:HA	1:J:112:LEU:HD22	1.97	0.47
1:J:403:TYR:CG	1:J:420:LEU:HD23	2.49	0.47
1:K:97:LEU:HG	1:K:101:PHE:CD2	2.50	0.47
1:K:78:LYS:HE2	1:L:182:ASP:HB3	1.97	0.47
1:A:225:GLU:O	1:A:229:VAL:HG23	2.14	0.47
1:B:185:SER:HA	6:B:6123:HOH:O	2.14	0.47
1:D:23:PRO:HA	1:D:24:PRO:HD3	1.77	0.47
1:D:297:THR:O	1:D:301:MET:HG2	2.13	0.47
1:D:79:ASN:O	3:D:2180:SIA:O7	2.28	0.47
1:E:28:THR:HG23	1:E:31:GLY:O	2.14	0.47
1:E:487:GLU:HA	1:E:490:ILE:HD12	1.96	0.47
1:G:450:GLN:HG2	1:G:450:GLN:O	2.13	0.47
1:I:34:LEU:HA	1:I:34:LEU:HD22	1.61	0.47
3:L:1282:SIA:H113	3:L:1282:SIA:H31	1.95	0.47
1:L:316:GLN:HE21	1:L:316:GLN:HA	1.79	0.47
1:A:95:GLN:O	1:A:99:GLU:HG3	2.15	0.47
1:D:156:ALA:O	1:D:157:LEU:C	2.52	0.47
1:I:242:ARG:CG	1:I:242:ARG:NH1	2.72	0.47
1:I:264:LEU:O	1:I:268:ILE:HG13	2.13	0.47
1:J:103:ASN:O	1:J:482:LYS:HG3	2.14	0.47
1:K:312:PRO:HG2	1:K:383:TRP:CE2	2.50	0.47
1:D:409:ASP:O	1:D:413:LYS:HG3	2.15	0.47
1:D:426:PHE:N	1:D:426:PHE:CD1	2.82	0.47
1:E:136:MET:HA	1:E:216:THR:O	2.15	0.47
1:E:113:SER:HB2	1:F:277:THR:HG21	1.95	0.47
1:F:499:PHE:CE2	1:F:514:LEU:HD13	2.50	0.47
1:I:220:GLU:HA	1:I:246:GLU:O	2.15	0.47
1:I:34:LEU:HD13	1:I:35:GLY:N	2.30	0.47
3:K:1182:SIA:C7	3:K:1182:SIA:O2	2.62	0.47
1:K:26:VAL:CG1	1:K:207:SER:HB3	2.44	0.47
1:K:447:TYR:HB3	1:K:517:TRP:CZ2	2.50	0.47
1:L:286:LEU:HA	1:L:286:LEU:HD23	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:TYR:CD1	1:C:420:LEU:HD23	2.49	0.47
1:E:242:ARG:HH11	1:E:242:ARG:CG	2.28	0.47
3:D:2180:SIA:H111	1:E:278:THR:HG22	1.96	0.47
1:G:306:LEU:HD22	1:G:366:TYR:CE1	2.49	0.47
1:G:438:ARG:HH12	1:G:524:GLU:HG2	1.80	0.47
1:H:487:GLU:HG3	1:H:491:ARG:HD2	1.97	0.47
1:I:199:ARG:HG2	1:I:199:ARG:HH11	1.80	0.47
1:I:478:ALA:N	1:I:479:PRO:CD	2.78	0.47
1:J:461:PRO:HB2	6:J:6348:HOH:O	2.14	0.47
1:K:237:LYS:HE3	1:K:342:HIS:HB2	1.97	0.47
1:L:428:VAL:N	1:L:429:PRO:CD	2.77	0.47
1:A:138:TRP:HH2	1:A:220:GLU:HB2	1.80	0.47
1:A:382:LEU:HB2	1:A:417:PHE:HE1	1.80	0.47
1:C:138:TRP:CZ3	1:C:219:GLY:HA2	2.50	0.47
1:C:540:LYS:O	1:C:544:VAL:HG23	2.15	0.47
1:G:121:ILE:HG12	1:G:166:VAL:HG13	1.97	0.47
1:H:330:LYS:HG3	1:H:335:LEU:HD21	1.97	0.47
1:H:413:LYS:O	1:H:416:LEU:HB2	2.14	0.47
1:L:312:PRO:HD2	1:L:383:TRP:CZ2	2.50	0.47
1:A:198:LEU:HB3	1:A:239:LEU:HB3	1.97	0.47
1:B:86:MET:HE3	1:B:110:LEU:HB2	1.96	0.47
1:D:487:GLU:OE2	1:D:491:ARG:HG2	2.15	0.47
1:D:395:LEU:HD22	1:D:550:LEU:CD1	2.44	0.47
1:E:290:THR:HG23	1:E:293:GLU:OE2	2.15	0.47
1:F:225:GLU:HG2	1:F:225:GLU:O	2.14	0.47
1:F:268:ILE:HG12	1:F:301:MET:HE2	1.95	0.47
1:G:461:PRO:HG2	1:G:464:VAL:CG2	2.45	0.47
1:G:86:MET:HG3	1:G:112:LEU:HD23	1.95	0.47
1:H:278:THR:O	1:H:282:MET:HG3	2.15	0.47
1:I:142:GLY:HA3	1:I:146:VAL:O	2.15	0.47
1:I:325:GLY:O	1:I:329:LEU:HD23	2.15	0.47
1:I:526:TYR:CE2	1:I:536:ALA:HB3	2.50	0.47
1:J:258:LYS:HA	6:J:6129:HOH:O	2.14	0.47
1:L:242:ARG:NH1	1:L:242:ARG:HG2	2.24	0.47
1:L:478:ALA:N	1:L:479:PRO:CD	2.78	0.47
1:A:386:TYR:N	1:A:387:PRO:CD	2.78	0.46
1:A:540:LYS:O	1:A:544:VAL:HG23	2.15	0.46
1:A:78:LYS:HE3	1:B:183:GLU:OE2	2.16	0.46
1:E:59:PRO:HD3	1:E:117:LEU:HD12	1.97	0.46
1:F:350:ILE:O	1:F:448:GLU:HA	2.15	0.46
1:F:396:ILE:HB	1:F:397:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:431:VAL:HG21	1:F:540:LYS:HB2	1.96	0.46
1:F:477:GLY:HA2	1:F:493:SER:OG	2.15	0.46
1:G:332:PRO:O	1:G:336:GLN:HG2	2.15	0.46
1:H:491:ARG:HG3	1:H:491:ARG:HH11	1.80	0.46
1:J:45:GLN:NE2	1:J:46:PRO:HD2	2.30	0.46
1:K:142:GLY:O	1:K:144:LEU:N	2.48	0.46
1:K:257:LYS:HE2	1:K:257:LYS:CA	2.40	0.46
1:K:290:THR:OG1	1:K:293:GLU:HG3	2.14	0.46
1:L:143:GLY:N	6:L:6474:HOH:O	2.43	0.46
1:L:141:GLY:HA2	1:L:223:GLY:H	1.80	0.46
1:L:480:PHE:CD1	1:L:480:PHE:N	2.82	0.46
1:L:64:ARG:HH11	1:L:294:LEU:CD1	2.28	0.46
1:A:241:HIS:N	1:A:241:HIS:CD2	2.83	0.46
1:C:97:LEU:HD22	1:C:146:VAL:HG23	1.97	0.46
1:D:395:LEU:HD22	1:D:550:LEU:HD12	1.98	0.46
1:F:222:ALA:HA	1:F:255:LEU:HD11	1.98	0.46
1:G:218:PHE:CB	1:G:244:ILE:HB	2.44	0.46
1:G:428:VAL:HG13	1:G:544:VAL:HG22	1.97	0.46
1:H:340:ASN:N	1:H:340:ASN:HD22	2.12	0.46
1:I:121:ILE:HD11	1:I:200:TRP:CZ3	2.50	0.46
1:K:278:THR:HG23	1:K:281:VAL:CG2	2.46	0.46
1:K:318:LEU:O	1:K:319:LEU:C	2.50	0.46
1:L:105:LYS:HG3	1:L:106:GLU:N	2.31	0.46
1:L:525:GLY:HA2	1:L:537:GLN:HA	1.97	0.46
3:A:1181:SIA:C7	6:A:6003:HOH:O	2.63	0.46
1:B:264:LEU:HD23	1:B:264:LEU:O	2.15	0.46
1:C:193:ASP:O	1:C:194:GLN:C	2.54	0.46
1:C:396:ILE:HB	1:C:397:PRO:HD3	1.97	0.46
1:C:381:LEU:HB3	1:C:417:PHE:CZ	2.51	0.46
1:E:218:PHE:HA	1:E:244:ILE:O	2.15	0.46
1:E:218:PHE:HB2	1:E:244:ILE:HB	1.97	0.46
1:E:242:ARG:HD3	1:E:503:PHE:O	2.16	0.46
1:F:179:SER:HB2	1:F:187:GLY:HA3	1.96	0.46
1:G:190:GLY:O	1:G:193:ASP:HB2	2.15	0.46
1:G:236:ALA:HB1	1:G:240:PHE:HE1	1.80	0.46
1:G:242:ARG:HG2	1:G:242:ARG:NH1	2.24	0.46
1:G:72:GLU:HB3	6:G:6098:HOH:O	2.15	0.46
1:H:84:PRO:HA	1:H:85:PRO:HD3	1.79	0.46
1:J:104:ARG:HD2	1:J:108:ILE:HG12	1.97	0.46
1:J:453:PRO:HG2	1:J:456:SER:OG	2.15	0.46
1:K:180:THR:HB	1:K:279:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:550:LEU:C	1:K:552:ALA:N	2.69	0.46
1:L:256:VAL:O	1:L:256:VAL:HG12	2.15	0.46
1:L:428:VAL:CG1	1:L:544:VAL:HG13	2.46	0.46
1:E:132:ARG:HH11	1:E:132:ARG:HG2	1.80	0.46
1:E:191:HIS:CD2	1:E:321:THR:HG23	2.50	0.46
1:E:438:ARG:HD2	1:E:521:ASN:HA	1.97	0.46
1:G:132:ARG:CB	1:G:211:ASN:HB2	2.45	0.46
1:I:257:LYS:CG	1:I:316:GLN:HE22	2.22	0.46
1:J:179:SER:HA	1:J:185:SER:O	2.15	0.46
1:J:393:LYS:C	1:J:395:LEU:H	2.19	0.46
1:K:178:PHE:CZ	1:K:286:LEU:HD12	2.50	0.46
1:K:201:VAL:HG13	1:K:205:ILE:HB	1.97	0.46
1:K:251:LEU:O	1:K:253:SER:N	2.49	0.46
1:K:333:GLU:CD	1:K:333:GLU:H	2.19	0.46
1:L:403:TYR:CE2	1:L:420:LEU:HA	2.50	0.46
1:A:447:TYR:C	1:A:447:TYR:CD2	2.87	0.46
1:C:135:VAL:CG2	1:C:205:ILE:HG12	2.45	0.46
1:D:57:LYS:HD3	1:D:63:LEU:HD11	1.96	0.46
1:F:316:GLN:HA	1:F:316:GLN:NE2	2.30	0.46
1:F:318:LEU:O	1:F:318:LEU:HD12	2.15	0.46
1:I:251:LEU:HD12	1:I:251:LEU:N	2.29	0.46
1:I:292:GLU:HG3	1:I:293:GLU:N	2.31	0.46
1:L:400:THR:HG22	1:L:404:LEU:CD1	2.45	0.46
1:A:499:PHE:HE2	1:A:514:LEU:HB3	1.81	0.46
1:B:385:SER:C	1:B:387:PRO:HD2	2.34	0.46
1:C:25:VAL:HG22	1:C:34:LEU:HD23	1.97	0.46
1:C:386:TYR:N	1:C:387:PRO:CD	2.78	0.46
1:D:254:VAL:HG13	1:D:255:LEU:HD12	1.96	0.46
1:D:480:PHE:N	1:D:480:PHE:CD1	2.83	0.46
1:D:65:PHE:O	1:D:66:THR:CG2	2.63	0.46
1:F:135:VAL:CG2	1:F:205:ILE:HG12	2.41	0.46
1:F:487:GLU:HG3	1:F:491:ARG:NH2	2.31	0.46
1:H:452:ARG:HH11	1:H:452:ARG:HG2	1.79	0.46
1:I:526:TYR:CD2	1:I:539:LEU:HB2	2.51	0.46
1:J:316:GLN:NE2	1:J:317:PRO:HD2	2.30	0.46
1:K:499:PHE:CE2	1:K:514:LEU:HD22	2.51	0.46
1:K:96:LEU:O	1:K:100:LEU:HD12	2.15	0.46
1:A:264:LEU:HD22	1:A:268:ILE:CD1	2.46	0.46
1:A:367:PRO:HB2	1:A:381:LEU:HD11	1.96	0.46
1:A:467:ASP:HB3	1:A:470:ASP:OD2	2.16	0.46
1:C:101:PHE:CE1	1:C:358:LEU:HD21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:ASP:HB3	1:D:314:GLU:CG	2.45	0.46
1:D:372:GLN:HB2	1:D:410:THR:O	2.14	0.46
1:E:355:PHE:CE2	1:E:421:ILE:HG21	2.51	0.46
1:E:87:CYS:HB3	6:E:6367:HOH:O	2.15	0.46
1:F:242:ARG:HD3	1:F:503:PHE:O	2.16	0.46
1:F:526:TYR:CE2	1:F:539:LEU:HB2	2.50	0.46
1:G:453:PRO:HG2	1:G:456:SER:OG	2.15	0.46
1:H:24:PRO:O	1:H:34:LEU:HD22	2.15	0.46
1:I:137:VAL:HA	1:I:166:VAL:O	2.16	0.46
1:I:24:PRO:C	1:I:24:PRO:HB2	2.35	0.46
1:I:287:ARG:HD2	4:I:3285:SO4:O3	2.16	0.46
1:I:358:LEU:O	1:I:363:LEU:HG	2.16	0.46
1:I:524:GLU:OE2	1:I:538:LYS:HG2	2.16	0.46
1:K:242:ARG:NH1	1:K:242:ARG:CG	2.79	0.46
1:L:186:ARG:HB3	1:L:324:ASP:HB2	1.96	0.46
1:L:380:SER:O	1:L:383:TRP:HB3	2.15	0.46
1:A:368:LEU:HD11	1:A:418:LEU:HD21	1.98	0.46
1:A:524:GLU:OE2	1:A:538:LYS:HG2	2.15	0.46
1:C:89:GLN:OE1	1:C:146:VAL:HA	2.16	0.46
1:C:330:LYS:HB3	1:C:330:LYS:HE2	1.74	0.46
1:C:55:PHE:CE1	1:C:197:ALA:HB2	2.51	0.46
1:E:51:LEU:HD13	1:E:83:TYR:CE1	2.51	0.46
1:F:31:GLY:HA3	1:F:74:TRP:NE1	2.31	0.46
1:F:414:LYS:C	1:F:414:LYS:HD2	2.36	0.46
1:F:40:LEU:O	1:F:41:GLU:C	2.55	0.46
1:F:478:ALA:N	1:F:479:PRO:CD	2.79	0.46
1:I:343:THR:HB	1:I:442:ALA:CB	2.46	0.46
1:I:539:LEU:C	1:I:541:ASP:H	2.17	0.46
1:J:381:LEU:HD22	1:J:417:PHE:CZ	2.51	0.46
1:K:308:LEU:HD21	1:K:367:PRO:HG2	1.98	0.46
1:K:351:ASN:ND2	1:K:351:ASN:N	2.63	0.46
1:B:104:ARG:HD2	1:B:108:ILE:HG12	1.98	0.46
1:B:84:PRO:HA	1:B:85:PRO:HD3	1.80	0.46
1:C:101:PHE:CZ	1:C:358:LEU:HD21	2.51	0.46
1:D:156:ALA:O	1:D:159:ALA:N	2.49	0.46
1:D:320:GLY:O	1:D:322:VAL:HG13	2.15	0.46
1:F:439:ASP:O	1:F:441:GLY:N	2.49	0.46
1:G:218:PHE:HA	1:G:244:ILE:O	2.16	0.46
1:H:38:VAL:HG21	1:H:49:ILE:HD12	1.97	0.46
1:J:88:THR:HB	1:J:175:TRP:CZ3	2.50	0.46
1:J:330:LYS:HG3	1:J:335:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HD12	1:A:119:LEU:C	2.37	0.46
1:B:160:HIS:NE2	1:B:480:PHE:CD2	2.83	0.46
1:B:352:LYS:HD3	1:B:450:GLN:HG3	1.98	0.46
1:D:449:PHE:HZ	1:D:474:SER:HG	1.64	0.46
1:E:348:VAL:O	1:E:446:MET:HG2	2.16	0.46
1:E:359:ILE:HA	1:E:363:LEU:HD12	1.97	0.46
1:E:51:LEU:HD13	1:E:83:TYR:CD1	2.51	0.46
1:F:404:LEU:O	1:F:406:GLY:N	2.49	0.46
1:G:372:GLN:NE2	1:G:410:THR:OG1	2.49	0.46
1:I:135:VAL:HG21	1:I:205:ILE:HG12	1.98	0.46
1:J:140:HIS:CE1	1:J:170:TYR:CE1	3.03	0.46
1:J:421:ILE:O	1:J:425:MET:HG3	2.16	0.46
1:L:64:ARG:NH1	1:L:289:LYS:O	2.48	0.46
1:A:226:SER:CA	1:A:229:VAL:HG23	2.44	0.45
1:B:24:PRO:O	1:B:34:LEU:HD22	2.16	0.45
1:B:403:TYR:HB3	1:B:404:LEU:HD23	1.97	0.45
1:D:101:PHE:O	1:D:102:THR:C	2.53	0.45
1:D:64:ARG:HG2	1:D:65:PHE:CE1	2.52	0.45
1:E:379:MET:HE1	1:E:397:PRO:HG3	1.98	0.45
1:E:426:PHE:C	1:E:429:PRO:HD2	2.37	0.45
1:E:435:ARG:O	1:E:438:ARG:HB3	2.15	0.45
1:F:420:LEU:CD2	1:F:547:TRP:HZ2	2.29	0.45
1:G:23:PRO:HB2	1:G:34:LEU:HD21	1.97	0.45
1:H:105:LYS:HG3	1:H:106:GLU:H	1.81	0.45
1:I:227:VAL:O	1:I:228:SER:C	2.55	0.45
1:J:59:PRO:HD3	1:J:117:LEU:CD1	2.46	0.45
1:L:318:LEU:HD12	1:L:318:LEU:O	2.16	0.45
1:A:184:HIS:O	1:A:283:VAL:HG21	2.16	0.45
1:C:107:ASN:ND2	1:C:108:ILE:H	2.14	0.45
1:G:86:MET:CE	1:G:110:LEU:HD12	2.46	0.45
1:H:30:HIS:HD2	6:H:6446:HOH:O	1.97	0.45
1:H:492:LEU:O	1:H:496:VAL:HG23	2.17	0.45
1:J:138:TRP:HH2	1:J:220:GLU:HB2	1.80	0.45
1:J:386:TYR:N	1:J:387:PRO:CD	2.79	0.45
1:K:171:ARG:HB3	1:K:176:GLY:HA3	1.99	0.45
1:L:112:LEU:O	1:L:113:SER:HB2	2.15	0.45
1:L:126:ASP:HB3	1:L:129:LYS:HG2	1.96	0.45
1:L:522:GLN:HB2	6:L:6288:HOH:O	2.16	0.45
1:B:420:LEU:HD21	1:B:547:TRP:CZ2	2.51	0.45
1:E:453:PRO:HG2	1:E:456:SER:OG	2.15	0.45
1:F:253:SER:O	1:F:254:VAL:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:ALA:O	1:G:201:VAL:HG23	2.16	0.45
1:H:161:GLU:CB	1:H:501:ALA:HB2	2.46	0.45
1:H:357:TRP:CZ2	1:H:361:MET:HG3	2.51	0.45
1:H:383:TRP:O	1:H:385:SER:N	2.50	0.45
1:I:404:LEU:HD22	1:I:413:LYS:O	2.15	0.45
1:J:349:GLY:HA3	1:J:447:TYR:CZ	2.51	0.45
1:K:161:GLU:HG3	1:K:501:ALA:HB2	1.98	0.45
1:L:257:LYS:HE2	1:L:316:GLN:CD	2.37	0.45
1:A:324:ASP:OD2	1:A:325:GLY:N	2.49	0.45
1:B:547:TRP:O	1:B:551:PHE:HB2	2.17	0.45
1:E:133:LEU:HD12	1:E:209:GLY:O	2.16	0.45
1:I:25:VAL:HG22	1:I:34:LEU:HD23	1.95	0.45
1:L:435:ARG:O	1:L:438:ARG:HB3	2.16	0.45
1:L:90:ASP:HB3	1:L:93:ALA:HB3	1.99	0.45
1:B:24:PRO:CA	1:B:25:VAL:N	2.66	0.45
1:G:262:LYS:HB3	1:G:263:PRO:HD3	1.99	0.45
1:G:335:LEU:O	1:G:338:GLU:HG2	2.17	0.45
1:H:143:GLY:O	1:H:144:LEU:HB2	2.16	0.45
1:H:318:LEU:HD12	1:H:318:LEU:O	2.16	0.45
1:J:121:ILE:HD11	1:J:200:TRP:HZ3	1.81	0.45
1:J:253:SER:O	1:J:254:VAL:C	2.54	0.45
1:K:34:LEU:HB3	1:K:79:ASN:HA	1.98	0.45
1:C:45:GLN:HB2	1:L:488:GLU:HG3	1.99	0.45
1:L:84:PRO:HA	1:L:85:PRO:HD3	1.78	0.45
1:A:152:TYR:CD1	1:A:152:TYR:N	2.85	0.45
1:A:529:ILE:N	1:A:529:ILE:CD1	2.80	0.45
1:A:547:TRP:CZ3	1:A:550:LEU:HD23	2.52	0.45
1:B:386:TYR:N	1:B:387:PRO:CD	2.80	0.45
1:C:237:LYS:O	1:C:238:ASN:HB2	2.16	0.45
1:C:51:LEU:HD13	1:C:83:TYR:CD1	2.52	0.45
1:D:31:GLY:HA3	1:D:74:TRP:NE1	2.30	0.45
1:G:105:LYS:CE	1:G:106:GLU:HG2	2.38	0.45
1:H:499:PHE:CE1	1:H:514:LEU:HD22	2.51	0.45
1:J:223:GLY:O	1:J:227:VAL:HG23	2.16	0.45
1:K:85:PRO:HD3	3:K:1182:SIA:H92	1.96	0.45
1:L:63:LEU:C	1:L:66:THR:HG23	2.36	0.45
1:A:343:THR:HB	1:A:442:ALA:HB2	1.99	0.45
1:A:88:THR:HB	1:A:175:TRP:CH2	2.51	0.45
1:C:142:GLY:HA3	1:C:146:VAL:O	2.17	0.45
1:C:264:LEU:CG	1:C:316:GLN:HG2	2.47	0.45
1:D:264:LEU:CD2	1:D:268:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:GLU:N	1:D:471:GLU:OE1	2.45	0.45
1:E:84:PRO:HA	1:E:85:PRO:HD3	1.85	0.45
1:F:86:MET:CE	1:F:110:LEU:HB2	2.46	0.45
1:I:431:VAL:O	1:I:434:ALA:HB3	2.16	0.45
1:J:339:ARG:O	1:J:341:PHE:N	2.50	0.45
1:K:199:ARG:NH1	1:K:199:ARG:HB3	2.24	0.45
1:K:386:TYR:N	1:K:387:PRO:HD2	2.32	0.45
1:B:218:PHE:HD1	1:B:218:PHE:N	2.15	0.45
1:B:320:GLY:O	1:B:322:VAL:HG13	2.17	0.45
1:C:24:PRO:HG3	1:C:37:PHE:CZ	2.51	0.45
1:C:421:ILE:HG22	1:C:425:MET:CE	2.46	0.45
1:I:56:ALA:CB	1:I:117:LEU:HD13	2.47	0.45
1:J:48:ALA:HB3	1:J:123:THR:HG23	1.99	0.45
1:J:60:LEU:N	1:J:60:LEU:HD23	2.32	0.45
1:A:221:SER:O	1:A:224:GLY:N	2.50	0.45
1:B:218:PHE:HA	1:B:244:ILE:O	2.16	0.45
1:C:86:MET:HG2	1:C:110:LEU:HB3	1.99	0.45
1:C:471:GLU:OE1	1:C:472:LEU:HG	2.17	0.45
1:D:119:LEU:HD12	1:D:119:LEU:O	2.17	0.45
1:D:132:ARG:HB3	1:D:211:ASN:HB2	1.98	0.45
1:G:236:ALA:O	1:G:239:LEU:HB2	2.17	0.45
1:G:231:VAL:HA	1:G:240:PHE:HZ	1.81	0.45
1:H:218:PHE:HB2	1:H:244:ILE:HB	1.98	0.45
1:I:105:LYS:HG3	1:I:106:GLU:N	2.21	0.45
1:J:204:ASN:O	1:J:206:ALA:N	2.49	0.45
1:J:64:ARG:HH11	1:J:287:ARG:HA	1.82	0.45
1:K:383:TRP:CE3	1:K:393:LYS:HB2	2.52	0.45
1:L:191:HIS:O	1:L:195:VAL:HG23	2.17	0.45
1:L:539:LEU:C	1:L:541:ASP:H	2.20	0.45
1:B:218:PHE:HB3	1:B:244:ILE:HD12	1.98	0.45
1:C:107:ASN:HB3	6:C:6463:HOH:O	2.16	0.45
1:C:124:PRO:HD3	1:C:158:ALA:HB1	1.99	0.45
1:C:24:PRO:HG3	1:C:37:PHE:CE1	2.52	0.45
1:D:97:LEU:HD11	1:D:101:PHE:CZ	2.52	0.45
1:G:217:ILE:HD12	1:G:227:VAL:HG13	1.99	0.45
1:G:317:PRO:O	1:G:318:LEU:CB	2.64	0.45
1:G:393:LYS:O	1:G:395:LEU:N	2.47	0.45
1:G:446:MET:CE	1:G:539:LEU:HD23	2.46	0.45
1:H:151:THR:HG22	1:H:152:TYR:CE1	2.52	0.45
1:I:65:PHE:O	1:I:189:TRP:CZ2	2.70	0.45
1:J:161:GLU:OE2	1:J:498:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:271:THR:HG22	1:J:297:THR:HG23	1.99	0.45
3:J:1082:SIA:C11	1:K:278:THR:HA	2.38	0.45
1:K:478:ALA:N	1:K:479:PRO:CD	2.80	0.45
1:K:61:GLY:HA3	1:K:62:PRO:HD2	1.84	0.45
1:L:396:ILE:O	1:L:399:ALA:HB3	2.16	0.45
1:L:254:VAL:HG11	5:L:4380:BEZ:H4	1.99	0.45
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.32	0.44
1:C:372:GLN:NE2	1:C:410:THR:OG1	2.50	0.44
1:C:526:TYR:CE1	1:C:528:GLN:HG2	2.52	0.44
1:H:34:LEU:HD13	1:H:34:LEU:C	2.38	0.44
1:H:526:TYR:CE1	1:H:539:LEU:HD13	2.52	0.44
1:J:377:THR:O	1:J:380:SER:HB3	2.17	0.44
1:J:221:SER:OG	1:J:222:ALA:N	2.48	0.44
1:J:528:GLN:HE21	1:J:536:ALA:HB2	1.81	0.44
1:K:211:ASN:C	1:K:213:GLY:H	2.21	0.44
1:L:38:VAL:CG2	1:L:49:ILE:HD12	2.46	0.44
1:A:312:PRO:HG2	1:A:383:TRP:NE1	2.32	0.44
1:B:34:LEU:HB3	1:B:79:ASN:HA	1.99	0.44
1:B:354:GLU:HB2	1:B:422:ALA:HB1	1.98	0.44
1:C:271:THR:CG2	1:C:297:THR:HG23	2.41	0.44
1:D:225:GLU:O	1:D:229:VAL:HG23	2.18	0.44
1:D:400:THR:HG23	1:D:404:LEU:HD12	1.98	0.44
1:D:68:PRO:HA	6:D:6276:HOH:O	2.18	0.44
1:E:461:PRO:HG2	1:E:464:VAL:HG23	1.99	0.44
1:F:245:SER:HB3	1:F:248:GLY:O	2.17	0.44
1:F:495:MET:CE	1:F:533:THR:HG21	2.43	0.44
1:G:393:LYS:O	1:G:396:ILE:HG12	2.18	0.44
1:G:471:GLU:HG2	1:G:472:LEU:N	2.31	0.44
1:H:184:HIS:HD2	1:H:279:SER:HB2	1.82	0.44
1:J:382:LEU:HD23	1:J:396:ILE:HG23	1.99	0.44
1:J:447:TYR:C	1:J:447:TYR:CD2	2.91	0.44
1:K:173:GLY:O	1:K:177:PHE:N	2.47	0.44
1:K:372:GLN:HB2	1:K:410:THR:O	2.17	0.44
1:L:131:ASN:O	1:L:132:ARG:HD2	2.17	0.44
1:L:544:VAL:HG12	1:L:548:THR:OG1	2.17	0.44
1:A:201:VAL:O	1:A:205:ILE:HG22	2.16	0.44
1:B:237:LYS:HG2	1:B:238:ASN:ND2	2.32	0.44
1:C:498:LYS:O	1:C:502:ASN:HB2	2.17	0.44
1:D:339:ARG:HD2	1:D:339:ARG:N	2.31	0.44
1:G:369:SER:O	1:G:371:GLY:N	2.50	0.44
1:I:260:ASP:O	1:I:263:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:76:PHE:N	1:I:76:PHE:CD1	2.86	0.44
1:J:102:THR:CG2	1:J:107:ASN:HD22	2.29	0.44
1:J:510:ASN:ND2	1:J:517:TRP:O	2.50	0.44
1:K:278:THR:HG23	1:K:281:VAL:HG21	1.99	0.44
1:K:309:GLN:N	1:K:309:GLN:OE1	2.50	0.44
1:A:191:HIS:CD2	1:A:321:THR:HG23	2.52	0.44
1:B:171:ARG:HG3	1:B:193:ASP:OD2	2.18	0.44
1:B:540:LYS:O	1:B:543:GLU:HB2	2.18	0.44
1:C:194:GLN:HE22	1:C:226:SER:CB	2.30	0.44
1:D:199:ARG:NH1	1:D:202:GLN:HE22	2.14	0.44
1:D:373:LEU:HG	1:D:378:ALA:HB2	1.98	0.44
1:F:198:LEU:HD21	1:F:217:ILE:CG2	2.48	0.44
1:G:133:LEU:HD22	1:G:162:ASN:O	2.17	0.44
1:G:388:LEU:HD22	1:G:425:MET:SD	2.58	0.44
1:H:355:PHE:CZ	1:H:360:PRO:HG3	2.53	0.44
1:H:399:ALA:HB2	1:H:550:LEU:CD2	2.45	0.44
1:H:437:HIS:HD2	1:H:444:THR:OG1	2.01	0.44
1:I:55:PHE:CD2	1:I:119:LEU:HD23	2.52	0.44
1:K:218:PHE:CB	1:K:244:ILE:HB	2.48	0.44
1:L:339:ARG:HG3	1:L:339:ARG:HH11	1.82	0.44
1:A:138:TRP:CH2	1:A:220:GLU:HB2	2.53	0.44
1:A:529:ILE:H	1:A:529:ILE:CD1	2.30	0.44
1:A:84:PRO:HA	1:A:85:PRO:HD3	1.72	0.44
1:C:193:ASP:O	1:C:195:VAL:N	2.50	0.44
1:D:26:VAL:HG12	1:D:27:ASP:N	2.33	0.44
1:H:103:ASN:ND2	1:H:481:LEU:HD12	2.33	0.44
1:I:104:ARG:O	1:I:482:LYS:HE2	2.17	0.44
1:I:241:HIS:O	1:I:242:ARG:HG2	2.18	0.44
1:I:416:LEU:O	1:I:419:ASP:HB2	2.17	0.44
1:J:538:LYS:HB3	1:J:541:ASP:HB2	1.99	0.44
1:K:245:SER:HB3	1:K:248:GLY:O	2.18	0.44
1:L:102:THR:HG23	1:L:103:ASN:N	2.32	0.44
1:L:339:ARG:HG2	1:L:440:ALA:HA	2.00	0.44
1:L:414:LYS:O	1:L:417:PHE:HB3	2.18	0.44
1:A:245:SER:HB3	1:A:248:GLY:O	2.18	0.44
1:A:550:LEU:C	1:A:552:ALA:H	2.21	0.44
1:C:517:TRP:CE3	1:C:527:LEU:HD23	2.53	0.44
1:F:376:LYS:HE3	1:F:376:LYS:HB2	1.80	0.44
1:G:152:TYR:HE2	1:G:472:LEU:HD13	1.81	0.44
1:H:255:LEU:HD23	1:H:318:LEU:HD11	1.99	0.44
1:K:217:ILE:HG13	1:K:227:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:461:PRO:HG2	1:L:464:VAL:HG23	2.00	0.44
1:A:461:PRO:C	1:A:463:THR:H	2.21	0.44
3:B:1280:SIA:C10	3:B:1280:SIA:HO4	2.31	0.44
1:B:242:ARG:HG2	1:B:242:ARG:HH11	1.83	0.44
1:B:374:ASP:OD2	1:B:376:LYS:HB2	2.18	0.44
1:C:230:LEU:O	1:C:236:ALA:HB3	2.17	0.44
1:D:144:LEU:HB3	1:D:177:PHE:CE2	2.52	0.44
1:D:198:LEU:HB3	1:D:239:LEU:HB3	2.00	0.44
1:D:242:ARG:HD3	1:D:503:PHE:O	2.18	0.44
3:E:582:SIA:C7	3:E:582:SIA:O2	2.66	0.44
1:F:338:GLU:OE2	1:F:341:PHE:HB2	2.17	0.44
1:F:45:GLN:NE2	1:F:46:PRO:HD2	2.32	0.44
1:G:220:GLU:HB2	1:G:472:LEU:HD21	1.99	0.44
1:H:104:ARG:HB3	1:H:104:ARG:HH11	1.83	0.44
1:H:161:GLU:HG3	1:H:501:ALA:HB2	2.00	0.44
1:H:87:CYS:O	1:H:88:THR:C	2.56	0.44
1:I:211:ASN:ND2	1:I:214:SER:HB2	2.33	0.44
1:J:224:GLY:O	1:J:227:VAL:HB	2.18	0.44
1:K:519:GLU:O	1:K:521:ASN:N	2.50	0.44
1:L:24:PRO:HD2	1:L:35:GLY:O	2.17	0.44
1:L:262:LYS:HE3	1:L:282:MET:HE1	2.00	0.44
1:L:447:TYR:C	1:L:447:TYR:CD2	2.91	0.44
1:A:414:LYS:NZ	5:A:1385:BEZ:H2	2.32	0.44
1:A:353:GLN:NE2	1:A:465:ILE:H	2.16	0.44
1:A:527:LEU:HD23	1:A:529:ILE:HD11	1.99	0.44
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.82	0.44
1:B:373:LEU:O	1:B:413:LYS:HD2	2.18	0.44
1:C:197:ALA:O	1:C:201:VAL:HG23	2.18	0.44
1:C:23:PRO:HB2	1:C:34:LEU:HD21	1.99	0.44
1:D:197:ALA:O	1:D:201:VAL:HG23	2.17	0.44
1:E:278:THR:OG1	1:E:281:VAL:HG23	2.18	0.44
1:F:51:LEU:HD13	1:F:83:TYR:CE1	2.53	0.44
1:G:467:ASP:HB3	1:G:470:ASP:OD2	2.18	0.44
1:G:52:GLY:HA2	1:G:118:TYR:HB3	1.98	0.44
1:H:140:HIS:CD2	1:H:140:HIS:C	2.91	0.44
1:H:26:VAL:CG1	1:H:207:SER:HB3	2.48	0.44
1:H:218:PHE:HB3	1:H:244:ILE:HB	1.99	0.44
1:H:420:LEU:C	1:H:420:LEU:HD13	2.37	0.44
1:J:136:MET:HB3	1:J:218:PHE:CE1	2.53	0.44
1:J:462:LYS:N	6:J:6348:HOH:O	2.50	0.44
1:L:257:LYS:HE2	1:L:316:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LYS:HE3	1:A:342:HIS:CB	2.47	0.44
1:B:187:GLY:O	1:B:188:ASN:HB2	2.18	0.44
1:C:316:GLN:CA	1:C:316:GLN:NE2	2.76	0.44
1:C:353:GLN:O	1:C:467:ASP:HA	2.17	0.44
1:D:188:ASN:OD1	1:D:322:VAL:HG22	2.17	0.44
1:E:428:VAL:N	1:E:429:PRO:CD	2.80	0.44
1:G:135:VAL:CG2	1:G:205:ILE:HG12	2.47	0.44
1:L:233:SER:HA	1:L:234:PRO:HD3	1.90	0.44
1:A:424:VAL:O	1:A:424:VAL:CG1	2.65	0.43
1:B:140:HIS:HE1	6:B:6392:HOH:O	2.01	0.43
1:B:221:SER:OG	6:B:6470:HOH:O	2.12	0.43
1:E:366:TYR:HE2	1:E:417:PHE:HE2	1.66	0.43
1:G:251:LEU:HD12	1:G:433:VAL:HG22	1.99	0.43
1:H:498:LYS:HB3	1:H:514:LEU:HD11	1.99	0.43
1:I:38:VAL:HG21	1:I:49:ILE:HD12	1.99	0.43
1:J:477:GLY:HA2	1:J:493:SER:OG	2.17	0.43
1:L:106:GLU:HG3	1:L:106:GLU:O	2.16	0.43
1:L:236:ALA:HB1	1:L:240:PHE:CE1	2.53	0.43
1:A:414:LYS:O	1:A:418:LEU:HG	2.18	0.43
1:B:104:ARG:O	1:B:482:LYS:HE3	2.18	0.43
1:C:27:ASP:CG	1:C:32:LYS:HG2	2.39	0.43
1:F:124:PRO:HG3	1:F:158:ALA:O	2.17	0.43
1:G:306:LEU:HD22	1:G:366:TYR:CD1	2.52	0.43
1:G:491:ARG:HH11	1:G:491:ARG:HG3	1.83	0.43
1:G:538:LYS:HB3	1:G:541:ASP:HB2	2.00	0.43
1:H:343:THR:HA	6:H:6072:HOH:O	2.17	0.43
1:H:359:ILE:CB	1:H:360:PRO:HD3	2.43	0.43
1:I:126:ASP:OD2	1:I:129:LYS:HE2	2.18	0.43
1:I:170:TYR:CD1	1:I:170:TYR:N	2.86	0.43
1:K:188:ASN:N	6:K:6038:HOH:O	2.37	0.43
1:A:414:LYS:HZ1	5:A:1385:BEZ:H2	1.83	0.43
1:A:222:ALA:HA	1:A:255:LEU:CD1	2.48	0.43
1:B:211:ASN:HD22	1:B:214:SER:HB3	1.83	0.43
1:B:220:GLU:HA	1:B:246:GLU:O	2.18	0.43
1:B:24:PRO:C	1:B:24:PRO:HB2	2.37	0.43
1:B:366:TYR:HA	1:B:367:PRO:HD3	1.74	0.43
1:B:435:ARG:O	1:B:438:ARG:HB3	2.18	0.43
1:C:420:LEU:CD2	1:C:547:TRP:HZ2	2.31	0.43
1:D:204:ASN:O	1:D:205:ILE:C	2.57	0.43
1:D:33:VAL:HA	1:D:78:LYS:O	2.18	0.43
1:G:152:TYR:CD1	1:G:152:TYR:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:GLY:HA2	1:G:189:TRP:HB2	2.00	0.43
1:G:361:MET:SD	1:G:363:LEU:HD23	2.58	0.43
1:H:120:ASN:HB2	1:H:167:THR:OG1	2.18	0.43
1:H:296:GLU:O	1:H:300:LYS:HG3	2.18	0.43
1:H:382:LEU:HB2	1:H:417:PHE:CE1	2.51	0.43
1:H:450:GLN:HG2	1:H:529:ILE:O	2.19	0.43
1:I:140:HIS:NE2	1:I:147:GLY:HA3	2.33	0.43
1:I:526:TYR:CE1	1:I:528:GLN:HG2	2.53	0.43
1:J:164:VAL:CG1	1:J:205:ILE:HD11	2.47	0.43
1:J:24:PRO:HG3	1:J:37:PHE:CE1	2.53	0.43
1:K:144:LEU:HD13	1:K:177:PHE:CE1	2.53	0.43
1:A:237:LYS:CG	6:A:6099:HOH:O	2.66	0.43
1:A:290:THR:OG1	1:A:293:GLU:HG3	2.19	0.43
1:B:327:LEU:O	1:B:327:LEU:HD23	2.17	0.43
1:C:97:LEU:CD2	1:C:146:VAL:HG23	2.48	0.43
1:C:300:LYS:NZ	6:C:6102:HOH:O	2.42	0.43
1:F:29:VAL:HG23	1:F:204:ASN:OD1	2.19	0.43
1:H:266:GLU:O	1:H:270:ILE:HG13	2.19	0.43
1:H:316:GLN:NE2	1:H:316:GLN:HA	2.33	0.43
1:H:403:TYR:O	1:H:416:LEU:HD13	2.18	0.43
1:H:59:PRO:HD3	1:H:117:LEU:CD1	2.47	0.43
1:I:355:PHE:HD1	1:I:418:LEU:HD22	1.83	0.43
1:I:445:TYR:CE1	1:I:519:GLU:HA	2.53	0.43
1:J:161:GLU:CD	1:J:498:LYS:HG2	2.37	0.43
1:K:84:PRO:HA	3:K:1182:SIA:H91	1.99	0.43
1:K:420:LEU:HD13	1:K:421:ILE:N	2.33	0.43
1:L:129:LYS:HG2	1:L:129:LYS:H	1.53	0.43
1:B:304:LEU:O	1:B:364:MET:HG2	2.18	0.43
1:D:152:TYR:N	1:D:152:TYR:CD1	2.86	0.43
1:D:249:VAL:HB	1:D:433:VAL:HG21	2.01	0.43
1:E:343:THR:HB	1:E:442:ALA:CB	2.49	0.43
1:G:138:TRP:CH2	1:G:220:GLU:HB2	2.53	0.43
1:G:369:SER:C	1:G:371:GLY:N	2.72	0.43
1:H:253:SER:O	1:H:254:VAL:C	2.56	0.43
1:H:333:GLU:CD	1:H:333:GLU:H	2.21	0.43
1:I:249:VAL:HB	1:I:433:VAL:HG21	2.00	0.43
1:I:52:GLY:HA3	3:I:982:SIA:O9	2.19	0.43
1:J:143:GLY:O	1:J:144:LEU:HB2	2.17	0.43
1:J:104:ARG:CZ	1:J:153:ASP:HB2	2.48	0.43
1:J:157:LEU:HD13	1:J:475:VAL:O	2.18	0.43
1:J:366:TYR:CE2	1:J:381:LEU:HD21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:428:VAL:HG22	1:J:544:VAL:HA	2.01	0.43
1:J:447:TYR:HB3	1:J:517:TRP:CZ2	2.53	0.43
1:J:488:GLU:HA	1:J:491:ARG:NH1	2.34	0.43
1:K:319:LEU:HB2	6:K:6148:HOH:O	2.18	0.43
1:A:195:VAL:HG22	1:A:230:LEU:HD22	2.00	0.43
1:A:257:LYS:NZ	1:A:257:LYS:HA	2.34	0.43
1:C:478:ALA:N	1:C:479:PRO:CD	2.81	0.43
1:D:170:TYR:N	6:D:6060:HOH:O	2.51	0.43
1:E:139:ILE:HD12	1:E:227:VAL:HG22	1.99	0.43
1:E:260:ASP:O	1:E:263:PRO:HD2	2.18	0.43
1:E:409:ASP:O	1:E:413:LYS:HG3	2.19	0.43
1:F:218:PHE:HA	1:F:244:ILE:O	2.19	0.43
1:G:332:PRO:HD2	1:G:333:GLU:OE2	2.18	0.43
1:I:368:LEU:CD1	1:I:418:LEU:HD21	2.48	0.43
1:I:526:TYR:HE2	6:I:6336:HOH:O	2.00	0.43
1:I:52:GLY:HA2	1:I:118:TYR:HB3	2.00	0.43
1:I:547:TRP:O	1:I:551:PHE:HB2	2.18	0.43
1:J:190:GLY:O	1:J:193:ASP:HB2	2.19	0.43
1:K:143:GLY:N	1:K:222:ALA:HB2	2.34	0.43
1:A:529:ILE:HA	1:A:533:THR:CG2	2.46	0.43
1:B:242:ARG:CG	1:B:242:ARG:HH11	2.31	0.43
1:B:492:LEU:O	1:B:495:MET:HB3	2.19	0.43
1:C:357:TRP:O	1:C:360:PRO:CD	2.59	0.43
1:D:194:GLN:O	1:D:195:VAL:C	2.56	0.43
1:D:237:LYS:O	1:D:238:ASN:HB2	2.18	0.43
1:E:221:SER:CB	6:E:6472:HOH:O	2.66	0.43
1:E:431:VAL:O	1:E:435:ARG:HG3	2.19	0.43
1:F:222:ALA:HA	1:F:255:LEU:CD1	2.48	0.43
1:F:476:PHE:O	1:F:477:GLY:C	2.56	0.43
1:G:317:PRO:O	1:G:318:LEU:HB3	2.18	0.43
1:G:369:SER:C	1:G:371:GLY:H	2.22	0.43
1:H:174:ILE:HA	1:H:319:LEU:HD11	2.00	0.43
1:H:498:LYS:NZ	6:H:6303:HOH:O	2.43	0.43
1:I:499:PHE:CD2	1:I:509:PRO:HB2	2.53	0.43
1:K:40:LEU:O	1:K:41:GLU:C	2.57	0.43
1:K:528:GLN:O	1:K:533:THR:HA	2.19	0.43
1:L:101:PHE:O	1:L:102:THR:O	2.37	0.43
1:L:407:THR:C	1:L:409:ASP:H	2.21	0.43
1:B:119:LEU:C	1:B:119:LEU:HD12	2.39	0.43
1:B:301:MET:HB3	1:B:303:PHE:CE2	2.54	0.43
1:D:306:LEU:HD22	1:D:366:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:MET:HE3	1:E:397:PRO:HG3	1.98	0.43
1:F:290:THR:HG23	1:F:293:GLU:OE2	2.19	0.43
1:F:50:PHE:CD1	1:F:50:PHE:N	2.85	0.43
1:F:31:GLY:HA3	1:F:74:TRP:CE2	2.54	0.43
1:H:517:TRP:CE3	1:H:527:LEU:HD22	2.54	0.43
1:J:215:VAL:H	1:J:241:HIS:HD2	1.67	0.43
1:J:184:HIS:CE1	1:J:280:ALA:HB2	2.54	0.43
1:J:351:ASN:ND2	1:J:449:PHE:HB3	2.34	0.43
1:K:297:THR:O	1:K:301:MET:HG2	2.18	0.43
1:L:266:GLU:O	1:L:270:ILE:HG13	2.19	0.43
1:L:431:VAL:HG21	1:L:540:LYS:HB2	2.00	0.43
1:L:88:THR:HB	1:L:175:TRP:CZ3	2.54	0.43
1:A:249:VAL:HB	1:A:433:VAL:HG21	2.01	0.43
1:A:279:SER:HB2	3:A:1181:SIA:C11	2.48	0.43
1:A:312:PRO:HG2	1:A:383:TRP:CD1	2.54	0.43
1:A:264:LEU:HD13	1:A:319:LEU:HD23	2.00	0.43
1:A:134:PRO:HG3	1:A:505:ARG:CG	2.47	0.43
1:A:499:PHE:CZ	1:A:514:LEU:HD22	2.52	0.43
1:B:125:ALA:HB2	1:B:133:LEU:HD12	2.01	0.43
3:A:1180:SIA:C11	1:B:278:THR:HG22	2.41	0.43
1:C:140:HIS:CE1	1:C:170:TYR:CE1	3.07	0.43
1:D:445:TYR:CD1	1:D:519:GLU:HA	2.54	0.43
1:F:366:TYR:HB3	1:F:368:LEU:HG	2.00	0.43
1:G:351:ASN:ND2	1:G:351:ASN:N	2.65	0.43
1:H:257:LYS:HB2	1:H:322:VAL:HG12	2.01	0.43
1:I:379:MET:O	1:I:383:TRP:HB2	2.18	0.43
1:I:385:SER:C	1:I:387:PRO:HD2	2.38	0.43
1:I:90:ASP:OD1	1:I:91:PRO:HD2	2.18	0.43
1:J:308:LEU:HD12	1:J:309:GLN:HG2	2.00	0.43
1:L:218:PHE:HA	1:L:244:ILE:O	2.19	0.43
1:L:361:MET:SD	1:L:363:LEU:HD23	2.59	0.43
1:A:136:MET:HB3	1:A:218:PHE:CE1	2.54	0.43
1:A:366:TYR:CD2	1:A:367:PRO:HD2	2.54	0.43
1:B:230:LEU:O	1:B:236:ALA:HB3	2.19	0.43
1:C:215:VAL:H	1:C:241:HIS:CD2	2.30	0.43
1:C:450:GLN:O	1:C:450:GLN:HG2	2.19	0.43
1:D:186:ARG:HG3	1:D:186:ARG:NH1	2.34	0.43
1:D:353:GLN:OE1	1:D:464:VAL:HG13	2.19	0.43
1:E:141:GLY:HA2	1:E:222:ALA:HB3	2.01	0.43
1:E:251:LEU:CD1	1:E:336:GLN:HE22	2.27	0.43
1:F:199:ARG:HH11	1:F:199:ARG:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:GLN:O	1:F:467:ASP:HA	2.18	0.43
1:G:89:GLN:HE22	1:G:147:GLY:N	2.16	0.43
1:H:221:SER:O	1:H:224:GLY:N	2.51	0.43
1:I:425:MET:O	1:I:429:PRO:HG2	2.19	0.43
1:I:431:VAL:HA	1:I:446:MET:CE	2.49	0.43
1:I:517:TRP:CE3	1:I:527:LEU:HD22	2.54	0.43
1:J:436:ASN:HD22	1:J:436:ASN:HA	1.64	0.43
1:L:508:ASN:OD1	1:L:510:ASN:HB2	2.19	0.43
1:A:149:ALA:CB	1:A:169:GLN:HG3	2.49	0.42
1:A:218:PHE:HB2	1:A:244:ILE:HB	2.00	0.42
1:A:308:LEU:HB2	6:A:6331:HOH:O	2.19	0.42
1:A:242:ARG:HD2	1:A:504:ALA:HA	2.01	0.42
1:B:467:ASP:CG	1:B:468:HIS:H	2.21	0.42
1:B:455:PHE:HZ	1:B:479:PRO:HA	1.84	0.42
1:B:51:LEU:HD13	1:B:83:TYR:CE1	2.54	0.42
1:C:133:LEU:HD22	1:C:162:ASN:O	2.19	0.42
1:E:423:ASP:OD2	1:E:543:GLU:HG2	2.19	0.42
1:F:277:THR:HG22	1:F:278:THR:HG23	2.01	0.42
1:G:486:SER:O	1:G:490:ILE:HG13	2.19	0.42
1:G:51:LEU:HD13	1:G:83:TYR:CD1	2.53	0.42
1:G:56:ALA:C	1:G:71:ALA:HB2	2.39	0.42
1:H:416:LEU:HD23	1:H:416:LEU:HA	1.84	0.42
3:I:982:SIA:N5	3:I:982:SIA:O8	2.51	0.42
1:K:354:GLU:O	1:K:468:HIS:HB2	2.19	0.42
1:L:367:PRO:CB	1:L:381:LEU:HD21	2.49	0.42
1:B:308:LEU:HB2	1:B:309:GLN:OE1	2.19	0.42
1:B:348:VAL:O	1:B:446:MET:HG2	2.20	0.42
1:D:217:ILE:HD12	1:D:230:LEU:HD12	2.00	0.42
1:E:284:HIS:O	1:E:287:ARG:HB2	2.20	0.42
1:E:386:TYR:N	1:E:387:PRO:CD	2.82	0.42
1:E:442:ALA:HA	1:E:443:PRO:HD3	1.92	0.42
1:F:332:PRO:HA	1:F:335:LEU:HB2	2.01	0.42
1:F:373:LEU:HD21	1:F:378:ALA:HB2	2.01	0.42
1:F:51:LEU:HD13	1:F:83:TYR:CD1	2.54	0.42
1:G:220:GLU:CG	1:G:472:LEU:HD21	2.45	0.42
1:H:87:CYS:HB3	6:H:6073:HOH:O	2.17	0.42
1:I:474:SER:HB3	1:I:493:SER:HA	1.99	0.42
1:I:26:VAL:HG23	1:I:50:PHE:CZ	2.54	0.42
1:I:88:THR:HG21	1:I:291:GLU:HG3	2.00	0.42
1:J:479:PRO:HB3	1:J:490:ILE:HG12	2.01	0.42
1:J:499:PHE:HD2	1:J:499:PHE:HA	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:386:TYR:C	1:K:388:LEU:H	2.23	0.42
1:L:184:HIS:O	1:L:283:VAL:HG21	2.18	0.42
1:L:372:GLN:NE2	1:L:411:VAL:HG22	2.34	0.42
1:L:26:VAL:HG23	1:L:50:PHE:CZ	2.54	0.42
1:A:40:LEU:O	1:A:41:GLU:C	2.58	0.42
1:B:197:ALA:O	1:B:200:TRP:N	2.52	0.42
1:C:190:GLY:O	1:C:194:GLN:HG3	2.20	0.42
1:D:351:ASN:ND2	1:D:351:ASN:N	2.61	0.42
1:D:58:PRO:O	1:D:60:LEU:N	2.48	0.42
1:F:176:GLY:HA2	1:F:189:TRP:HB2	2.02	0.42
1:F:268:ILE:HG12	1:F:301:MET:HE1	2.01	0.42
1:G:517:TRP:HA	1:G:518:PRO:HD2	1.93	0.42
1:H:383:TRP:C	1:H:385:SER:N	2.71	0.42
1:H:487:GLU:OE2	1:H:491:ARG:NH1	2.50	0.42
1:J:28:THR:HB	1:J:204:ASN:OD1	2.18	0.42
1:J:382:LEU:HD11	1:J:391:ILE:CD1	2.46	0.42
1:J:59:PRO:C	1:J:60:LEU:HD23	2.40	0.42
1:K:372:GLN:HB3	1:K:372:GLN:HE21	1.63	0.42
1:L:329:LEU:HD13	1:L:335:LEU:HD21	2.00	0.42
1:L:485:ALA:HB1	1:L:489:GLU:OE2	2.19	0.42
1:A:103:ASN:HD22	1:A:476:PHE:HB3	1.80	0.42
1:B:495:MET:HE1	1:B:533:THR:HG21	1.97	0.42
1:C:132:ARG:NH1	1:C:132:ARG:HG2	2.32	0.42
1:C:193:ASP:O	1:C:196:ALA:N	2.52	0.42
1:C:251:LEU:HD11	1:C:336:GLN:HE22	1.83	0.42
1:E:276:THR:O	1:E:277:THR:C	2.57	0.42
1:F:228:SER:CB	1:F:250:ALA:H	2.33	0.42
1:G:226:SER:O	1:G:230:LEU:HG	2.19	0.42
1:H:45:GLN:HA	1:H:46:PRO:HD2	1.92	0.42
1:I:133:LEU:O	1:I:211:ASN:N	2.48	0.42
1:I:517:TRP:CG	1:I:527:LEU:HD13	2.53	0.42
1:J:49:ILE:HG12	1:J:122:TYR:CD2	2.55	0.42
1:K:134:PRO:HG2	1:K:163:VAL:HG12	2.01	0.42
1:A:170:TYR:N	1:A:170:TYR:CD1	2.87	0.42
1:A:206:ALA:HA	1:A:210:GLY:O	2.19	0.42
1:B:86:MET:HE2	1:B:110:LEU:HB2	2.00	0.42
1:B:241:HIS:O	1:B:344:VAL:HB	2.20	0.42
1:B:357:TRP:CE2	1:B:361:MET:HG3	2.55	0.42
1:B:420:LEU:HD21	1:B:547:TRP:HZ2	1.82	0.42
1:B:499:PHE:CE2	1:B:514:LEU:HB3	2.54	0.42
1:E:254:VAL:HG23	1:E:387:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:445:TYR:HA	6:E:6035:HOH:O	2.20	0.42
1:F:264:LEU:O	1:F:268:ILE:HG13	2.19	0.42
1:F:510:ASN:ND2	1:F:517:TRP:O	2.48	0.42
1:F:86:MET:HE3	1:F:110:LEU:HB2	2.01	0.42
1:G:222:ALA:HB2	6:G:6473:HOH:O	2.18	0.42
1:H:499:PHE:HD2	1:H:509:PRO:HB2	1.84	0.42
1:I:84:PRO:HA	1:I:85:PRO:HD3	1.81	0.42
1:J:36:LYS:HE3	1:J:38:VAL:CG2	2.49	0.42
1:A:220:GLU:HA	1:A:246:GLU:O	2.19	0.42
1:C:136:MET:HB3	1:C:218:PHE:CE1	2.55	0.42
1:C:276:THR:HG22	1:C:282:MET:SD	2.60	0.42
1:C:221:SER:HB2	1:C:468:HIS:NE2	2.35	0.42
1:D:294:LEU:HD23	1:D:294:LEU:HA	1.87	0.42
1:E:52:GLY:N	1:E:120:ASN:OD1	2.49	0.42
1:E:176:GLY:HA2	1:E:189:TRP:HB2	2.01	0.42
1:E:520:TYR:CE2	1:E:524:GLU:HG2	2.54	0.42
1:F:404:LEU:HD22	1:F:413:LYS:O	2.19	0.42
1:F:492:LEU:O	1:F:496:VAL:HG23	2.19	0.42
1:I:330:LYS:HE2	1:I:330:LYS:HB3	1.96	0.42
3:K:1182:SIA:H6	6:L:6046:HOH:O	2.19	0.42
1:K:191:HIS:HB2	1:K:327:LEU:HD22	2.01	0.42
1:K:44:ALA:N	6:K:6380:HOH:O	2.52	0.42
1:L:102:THR:OG1	1:L:103:ASN:N	2.52	0.42
1:L:211:ASN:C	1:L:213:GLY:H	2.23	0.42
1:A:383:TRP:C	1:A:385:SER:H	2.21	0.42
1:B:226:SER:O	1:B:230:LEU:HG	2.20	0.42
1:E:221:SER:OG	6:E:6469:HOH:O	1.90	0.42
1:G:428:VAL:HG21	1:G:547:TRP:CD1	2.55	0.42
1:H:97:LEU:HD11	1:H:101:PHE:CE2	2.54	0.42
1:H:413:LYS:O	1:H:414:LYS:C	2.58	0.42
1:L:428:VAL:HB	1:L:429:PRO:HD3	2.01	0.42
1:L:76:PHE:N	1:L:76:PHE:CD1	2.86	0.42
1:A:400:THR:O	1:A:404:LEU:HB2	2.19	0.42
1:C:428:VAL:HG13	1:C:544:VAL:HG22	2.00	0.42
1:C:51:LEU:HD13	1:C:83:TYR:CE1	2.55	0.42
1:D:332:PRO:O	1:D:336:GLN:HG3	2.19	0.42
1:D:435:ARG:HB3	1:D:438:ARG:HH22	1.80	0.42
1:D:84:PRO:HA	1:D:85:PRO:HD3	1.77	0.42
1:D:262:LYS:CE	2:F:2379:NAG:H82	2.49	0.42
2:G:3179:NAG:H81	6:G:6010:HOH:O	2.19	0.42
1:G:249:VAL:CG2	1:G:433:VAL:HG21	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:184:HIS:O	1:I:185:SER:HB2	2.19	0.42
1:I:190:GLY:O	1:I:193:ASP:HB2	2.20	0.42
1:J:400:THR:CG2	1:J:404:LEU:HD12	2.43	0.42
1:J:517:TRP:CE3	1:J:527:LEU:HD23	2.54	0.42
1:K:220:GLU:HA	1:K:246:GLU:HB2	2.01	0.42
1:K:314:GLU:O	1:K:316:GLN:N	2.53	0.42
1:K:63:LEU:HD23	1:K:63:LEU:HA	1.74	0.42
1:L:144:LEU:HG	1:L:222:ALA:HB1	2.02	0.42
1:L:33:VAL:HG12	1:L:34:LEU:N	2.35	0.42
1:L:366:TYR:HA	1:L:367:PRO:HD3	1.89	0.42
1:A:131:ASN:O	1:A:209:GLY:HA2	2.19	0.42
1:A:83:TYR:HD1	1:A:150:SER:HB3	1.85	0.42
1:A:526:TYR:CD2	1:A:539:LEU:HB2	2.55	0.42
1:B:297:THR:O	1:B:301:MET:HG2	2.19	0.42
1:B:400:THR:HG23	1:B:404:LEU:CD1	2.49	0.42
1:B:355:PHE:HD1	1:B:418:LEU:HD22	1.85	0.42
1:C:126:ASP:H	1:C:131:ASN:ND2	2.18	0.42
1:D:186:ARG:HG3	1:D:186:ARG:HH11	1.84	0.42
1:E:227:VAL:O	1:E:228:SER:C	2.56	0.42
1:F:386:TYR:N	1:F:387:PRO:CD	2.82	0.42
1:F:464:VAL:HG12	1:F:467:ASP:HB2	2.01	0.42
1:G:268:ILE:HG12	1:G:301:MET:HE1	2.02	0.42
1:I:218:PHE:CD1	1:I:218:PHE:N	2.88	0.42
1:J:121:ILE:HD11	1:J:200:TRP:CZ3	2.55	0.42
1:J:452:ARG:NE	1:J:462:LYS:HA	2.35	0.42
1:K:132:ARG:HB3	1:K:211:ASN:HB2	2.01	0.42
1:K:317:PRO:C	1:K:318:LEU:HD13	2.40	0.42
1:K:325:GLY:HA2	1:K:329:LEU:HD23	2.01	0.42
1:A:109:PRO:O	1:A:110:LEU:HD23	2.20	0.42
1:A:237:LYS:HG2	6:A:6099:HOH:O	2.19	0.42
1:A:311:ASP:HA	1:A:312:PRO:HD3	1.94	0.42
1:C:194:GLN:NE2	1:C:226:SER:HB3	2.35	0.42
1:C:319:LEU:HD23	1:C:319:LEU:N	2.21	0.42
1:D:379:MET:HG2	1:D:400:THR:HG21	2.02	0.42
1:E:383:TRP:C	1:E:385:SER:H	2.23	0.42
1:E:403:TYR:CG	1:E:420:LEU:HD23	2.54	0.42
1:E:54:PRO:HD3	6:E:6015:HOH:O	2.20	0.42
1:E:61:GLY:HA3	1:E:62:PRO:HD2	1.83	0.42
1:F:268:ILE:HD11	1:F:319:LEU:HD23	2.01	0.42
1:F:428:VAL:HG13	1:F:544:VAL:HG13	2.02	0.42
1:I:292:GLU:HA	6:I:6339:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:252:THR:O	1:J:253:SER:C	2.57	0.42
1:J:268:ILE:HD11	1:J:319:LEU:HD22	2.02	0.42
1:J:357:TRP:O	1:J:358:LEU:C	2.58	0.42
1:A:132:ARG:HB3	1:A:211:ASN:HB2	2.02	0.41
1:A:180:THR:HB	1:A:279:SER:OG	2.20	0.41
1:A:279:SER:O	1:A:283:VAL:HG23	2.20	0.41
1:B:33:VAL:HG12	1:B:34:LEU:N	2.35	0.41
1:C:132:ARG:O	1:C:211:ASN:HB2	2.20	0.41
1:C:149:ALA:HB1	1:C:167:THR:HB	2.02	0.41
1:C:269:ALA:O	1:C:274:CYS:HB2	2.20	0.41
1:C:349:GLY:HA3	1:C:447:TYR:CE1	2.55	0.41
1:C:477:GLY:HA2	1:C:493:SER:OG	2.19	0.41
1:C:478:ALA:C	1:C:480:PHE:H	2.23	0.41
1:D:226:SER:O	1:D:229:VAL:N	2.52	0.41
1:E:262:LYS:HG3	1:E:266:GLU:OE2	2.19	0.41
1:E:274:CYS:SG	1:E:289:LYS:HE3	2.60	0.41
1:H:191:HIS:CD2	1:H:321:THR:HG23	2.55	0.41
1:H:313:ARG:HG2	1:H:386:TYR:CE2	2.54	0.41
1:J:185:SER:HA	6:J:6164:HOH:O	2.19	0.41
1:K:319:LEU:N	1:K:319:LEU:HD23	2.35	0.41
1:K:372:GLN:HB2	1:K:410:THR:CB	2.44	0.41
1:K:425:MET:HB2	1:K:426:PHE:CD1	2.55	0.41
1:K:78:LYS:HE2	1:L:182:ASP:CB	2.50	0.41
1:L:220:GLU:C	1:L:224:GLY:H	2.23	0.41
1:B:381:LEU:O	1:B:382:LEU:C	2.58	0.41
1:B:469:GLY:O	1:B:470:ASP:C	2.58	0.41
1:C:140:HIS:HB2	1:C:152:TYR:CE1	2.54	0.41
1:C:193:ASP:C	1:C:195:VAL:N	2.72	0.41
1:C:216:THR:CG2	1:C:242:ARG:HB2	2.41	0.41
1:C:301:MET:O	1:C:302:LYS:HB2	2.20	0.41
1:C:25:VAL:HG22	1:C:34:LEU:CD2	2.50	0.41
1:E:540:LYS:HA	1:E:543:GLU:OE2	2.20	0.41
1:F:88:THR:HG22	1:F:295:LEU:HD13	2.02	0.41
1:G:218:PHE:N	1:G:218:PHE:CD1	2.88	0.41
1:G:385:SER:C	1:G:387:PRO:HD2	2.40	0.41
3:G:782:SIA:H4	1:H:262:LYS:HZ1	1.85	0.41
1:H:495:MET:HE3	1:H:533:THR:CG2	2.48	0.41
1:I:133:LEU:HB3	1:I:134:PRO:HD2	2.02	0.41
1:J:132:ARG:HB3	1:J:211:ASN:HB2	2.02	0.41
1:J:51:LEU:HD13	1:J:83:TYR:CD1	2.55	0.41
1:K:51:LEU:O	1:K:80:ALA:HB1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:386:TYR:N	1:L:387:PRO:CD	2.82	0.41
1:A:101:PHE:O	1:A:102:THR:C	2.59	0.41
1:A:406:GLY:O	1:A:407:THR:C	2.58	0.41
1:A:508:ASN:OD1	1:A:510:ASN:HB2	2.18	0.41
1:A:526:TYR:CE2	1:A:539:LEU:HB2	2.55	0.41
1:B:135:VAL:HG21	1:B:205:ILE:HG12	2.02	0.41
1:B:194:GLN:OE1	1:B:226:SER:HB3	2.20	0.41
1:B:435:ARG:NH1	1:B:544:VAL:HG11	2.35	0.41
1:C:234:PRO:HA	1:C:341:PHE:CZ	2.44	0.41
1:D:357:TRP:CH2	1:D:361:MET:HE2	2.55	0.41
1:E:140:HIS:CD2	1:E:141:GLY:O	2.74	0.41
1:E:143:GLY:N	1:E:222:ALA:HB2	2.35	0.41
1:E:343:THR:CB	1:E:442:ALA:HB2	2.51	0.41
1:F:140:HIS:HB2	1:F:152:TYR:HE1	1.85	0.41
1:G:182:ASP:O	1:G:184:HIS:N	2.53	0.41
1:G:427:GLY:O	1:G:428:VAL:C	2.57	0.41
1:H:204:ASN:O	1:H:206:ALA:N	2.54	0.41
1:H:304:LEU:HD12	1:H:364:MET:CE	2.48	0.41
1:I:241:HIS:C	1:I:242:ARG:CG	2.88	0.41
1:I:312:PRO:CG	1:I:384:LYS:HA	2.50	0.41
1:I:477:GLY:HA2	1:I:493:SER:OG	2.20	0.41
1:J:216:THR:HG23	1:J:242:ARG:HB2	2.01	0.41
1:J:502:ASN:HB3	1:J:509:PRO:O	2.21	0.41
1:J:447:TYR:HA	1:J:527:LEU:O	2.21	0.41
1:L:116:CYS:O	1:L:118:TYR:N	2.50	0.41
1:A:23:PRO:HA	1:A:24:PRO:HD3	1.78	0.41
1:A:272:ALA:O	1:A:289:LYS:HE3	2.20	0.41
1:B:393:LYS:HA	1:B:396:ILE:HG12	2.03	0.41
1:D:361:MET:HE3	1:D:363:LEU:CD2	2.50	0.41
1:D:403:TYR:CG	1:D:420:LEU:HD23	2.54	0.41
1:H:306:LEU:HD22	1:H:366:TYR:CE1	2.56	0.41
1:I:48:ALA:HB3	1:I:123:THR:HG23	2.01	0.41
1:I:221:SER:OG	5:I:3380:BEZ:H2	2.21	0.41
1:I:431:VAL:HA	1:I:446:MET:HE3	2.02	0.41
1:J:133:LEU:CD2	1:J:134:PRO:HD2	2.50	0.41
1:J:261:VAL:O	1:J:262:LYS:C	2.59	0.41
1:J:86:MET:CE	1:J:110:LEU:HD13	2.50	0.41
1:K:304:LEU:HD12	1:K:364:MET:HE2	2.02	0.41
1:K:366:TYR:HA	1:K:367:PRO:HD3	1.84	0.41
1:L:195:VAL:HG13	1:L:239:LEU:CD1	2.51	0.41
1:L:221:SER:O	1:L:224:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:SER:O	1:B:254:VAL:C	2.58	0.41
1:B:486:SER:O	1:B:490:ILE:HG13	2.21	0.41
1:C:102:THR:OG1	1:C:104:ARG:HG2	2.20	0.41
1:C:143:GLY:N	5:C:5013:BEZ:O2	2.53	0.41
1:D:143:GLY:O	1:D:144:LEU:HB2	2.21	0.41
1:D:149:ALA:HB2	1:D:169:GLN:HG3	2.03	0.41
1:D:549:ASN:O	1:D:550:LEU:C	2.58	0.41
1:D:87:CYS:O	1:D:88:THR:C	2.57	0.41
1:E:107:ASN:HD22	1:E:108:ILE:H	1.68	0.41
1:E:139:ILE:O	1:E:223:GLY:HA3	2.19	0.41
1:F:426:PHE:O	1:F:430:SER:HB2	2.20	0.41
1:G:251:LEU:CD2	1:G:333:GLU:HG3	2.50	0.41
1:G:447:TYR:CD2	1:G:447:TYR:C	2.94	0.41
1:H:104:ARG:HD2	1:H:108:ILE:HG12	2.01	0.41
1:I:386:TYR:N	1:I:387:PRO:CD	2.84	0.41
1:I:543:GLU:OE2	1:I:543:GLU:N	2.46	0.41
1:I:76:PHE:H	1:I:76:PHE:HD1	1.67	0.41
1:J:343:THR:HB	1:J:442:ALA:CB	2.49	0.41
1:J:355:PHE:CD1	1:J:360:PRO:HG3	2.55	0.41
1:J:479:PRO:HG2	1:J:493:SER:HB2	2.02	0.41
1:K:449:PHE:CE2	1:K:471:GLU:HA	2.56	0.41
1:K:506:ASN:ND2	6:K:6453:HOH:O	2.38	0.41
1:L:354:GLU:O	1:L:468:HIS:HB2	2.20	0.41
1:A:233:SER:HA	1:A:234:PRO:HD3	1.74	0.41
1:B:227:VAL:O	1:B:228:SER:C	2.59	0.41
1:B:346:TYR:HB3	1:B:437:HIS:CD2	2.56	0.41
1:B:503:PHE:HD1	1:B:509:PRO:HD3	1.85	0.41
1:C:125:ALA:HB1	1:C:131:ASN:HD22	1.85	0.41
1:E:179:SER:HB2	1:E:187:GLY:HA3	2.02	0.41
1:E:438:ARG:HD2	1:E:521:ASN:CA	2.50	0.41
1:F:359:ILE:HB	1:F:360:PRO:HD3	2.02	0.41
1:G:261:VAL:O	1:G:262:LYS:C	2.59	0.41
1:G:316:GLN:HE21	1:G:316:GLN:HA	1.85	0.41
1:G:383:TRP:HA	1:G:383:TRP:CE3	2.55	0.41
1:G:526:TYR:CE1	1:G:528:GLN:HG2	2.56	0.41
1:H:426:PHE:O	1:H:427:GLY:C	2.58	0.41
1:I:257:LYS:HA	1:I:257:LYS:HD3	1.88	0.41
1:J:119:LEU:HD12	1:J:119:LEU:C	2.40	0.41
1:J:206:ALA:HA	1:J:210:GLY:O	2.21	0.41
1:J:237:LYS:HE3	1:J:342:HIS:CB	2.49	0.41
1:J:216:THR:HA	1:J:242:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:311:ASP:HA	1:J:312:PRO:HD3	1.95	0.41
1:J:366:TYR:HA	1:J:367:PRO:HD3	1.73	0.41
1:J:420:LEU:HD22	1:J:547:TRP:HZ2	1.85	0.41
1:K:131:ASN:O	1:K:209:GLY:HA2	2.21	0.41
1:K:400:THR:HG23	1:K:404:LEU:HD13	2.02	0.41
1:K:543:GLU:O	1:K:544:VAL:C	2.58	0.41
1:L:482:LYS:HB3	1:L:483:GLU:H	1.60	0.41
1:L:446:MET:CE	1:L:539:LEU:HD23	2.51	0.41
1:A:275:LYS:NZ	6:A:6039:HOH:O	2.36	0.41
1:A:549:ASN:O	1:A:550:LEU:C	2.59	0.41
1:B:113:SER:OG	1:C:281:VAL:HG21	2.21	0.41
1:B:428:VAL:HB	1:B:429:PRO:HD3	2.02	0.41
1:C:324:ASP:OD2	1:C:324:ASP:N	2.52	0.41
1:D:372:GLN:HA	1:D:414:LYS:HB2	2.02	0.41
1:E:363:LEU:C	1:E:365:SER:N	2.73	0.41
1:E:52:GLY:HA3	3:E:582:SIA:O9	2.19	0.41
1:G:114:GLU:CG	1:G:291:GLU:HG3	2.49	0.41
1:G:431:VAL:CG2	1:G:446:MET:HE1	2.51	0.41
1:J:97:LEU:CD2	1:J:146:VAL:HG23	2.45	0.41
1:J:151:THR:HG22	1:J:152:TYR:N	2.36	0.41
1:J:71:ALA:HB1	6:J:6057:HOH:O	2.20	0.41
1:K:105:LYS:CG	1:K:106:GLU:H	2.28	0.41
1:K:221:SER:O	1:K:222:ALA:C	2.59	0.41
1:L:101:PHE:CD2	1:L:472:LEU:HD11	2.56	0.41
1:L:374:ASP:OD1	1:L:377:THR:HB	2.19	0.41
1:L:452:ARG:HB2	1:L:465:ILE:HG12	2.03	0.41
1:A:205:ILE:HA	1:A:205:ILE:HD12	1.79	0.41
1:B:304:LEU:HD22	1:B:304:LEU:HA	1.87	0.41
1:C:194:GLN:HE22	1:C:226:SER:HB3	1.86	0.41
1:D:40:LEU:HD13	1:D:155:LEU:HD21	2.02	0.41
1:D:328:LEU:HD23	1:D:328:LEU:HA	1.94	0.41
1:D:352:LYS:HD2	1:D:448:GLU:OE1	2.21	0.41
1:E:121:ILE:HD11	1:E:200:TRP:CZ3	2.56	0.41
1:E:169:GLN:HB3	1:E:169:GLN:HE21	1.59	0.41
1:E:469:GLY:O	1:E:472:LEU:HG	2.21	0.41
1:E:492:LEU:HD12	1:E:492:LEU:O	2.20	0.41
1:F:186:ARG:HB3	1:F:324:ASP:HB2	2.02	0.41
1:F:352:LYS:HD2	1:F:450:GLN:HG3	2.01	0.41
1:H:475:VAL:O	1:H:497:MET:HG2	2.20	0.41
1:I:137:VAL:O	1:I:218:PHE:CD1	2.74	0.41
1:I:538:LYS:HB3	1:I:541:ASP:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:198:LEU:O	1:J:201:VAL:HB	2.21	0.41
1:L:404:LEU:HD23	1:L:404:LEU:N	2.36	0.41
3:A:1181:SIA:H7	6:A:6003:HOH:O	2.21	0.41
1:D:402:LYS:HG2	1:D:546:PHE:CE1	2.56	0.41
1:E:262:LYS:HB3	1:E:263:PRO:HD3	2.03	0.41
1:F:339:ARG:HG3	1:F:440:ALA:HA	2.03	0.41
1:G:324:ASP:N	1:G:324:ASP:OD2	2.51	0.41
1:G:366:TYR:HA	1:G:367:PRO:HD3	1.85	0.41
1:H:381:LEU:HD22	1:H:417:PHE:CZ	2.55	0.41
1:I:112:LEU:O	1:I:113:SER:HB2	2.20	0.41
1:I:179:SER:O	1:I:265:ALA:HB2	2.21	0.41
1:I:431:VAL:HG11	1:I:544:VAL:HG21	2.02	0.41
1:I:452:ARG:HA	1:I:453:PRO:HD2	1.94	0.41
1:J:45:GLN:NE2	6:J:6143:HOH:O	2.48	0.41
1:K:368:LEU:CD1	1:K:418:LEU:HD21	2.50	0.41
1:K:382:LEU:HD13	1:K:420:LEU:HD11	2.02	0.41
1:L:184:HIS:O	1:L:185:SER:CB	2.69	0.41
1:A:135:VAL:HA	1:A:164:VAL:HG23	2.03	0.41
1:B:332:PRO:C	1:B:334:GLU:H	2.25	0.41
1:B:43:PHE:HZ	1:B:160:HIS:ND1	2.18	0.41
1:C:103:ASN:HB2	1:C:478:ALA:HB2	2.03	0.41
1:D:186:ARG:HD3	1:D:324:ASP:O	2.21	0.41
1:E:145:MET:HE1	1:E:303:PHE:CD1	2.55	0.41
1:E:72:GLU:HA	1:E:73:PRO:HD2	1.92	0.41
1:F:138:TRP:CH2	1:F:220:GLU:HB2	2.56	0.41
1:F:381:LEU:HD23	1:F:381:LEU:HA	1.94	0.41
3:G:782:SIA:O10	3:G:782:SIA:O8	2.39	0.41
1:I:211:ASN:C	1:I:213:GLY:H	2.24	0.41
1:I:477:GLY:C	1:I:479:PRO:CD	2.89	0.41
1:J:149:ALA:HB1	1:J:167:THR:HB	2.03	0.41
1:J:403:TYR:CE2	1:J:420:LEU:HA	2.55	0.41
1:J:414:LYS:HZ2	5:J:5042:BEZ:H6	1.86	0.41
1:K:311:ASP:HA	1:K:312:PRO:HD3	1.96	0.41
1:K:384:LYS:HE2	6:K:6420:HOH:O	2.19	0.41
2:K:4279:NAG:H81	1:L:260:ASP:CB	2.48	0.41
1:L:134:PRO:HG3	1:L:505:ARG:HG3	2.03	0.41
1:L:154:GLY:O	1:L:155:LEU:C	2.59	0.41
1:L:205:ILE:HA	1:L:205:ILE:HD12	1.84	0.41
1:L:236:ALA:O	1:L:239:LEU:HB2	2.21	0.41
1:L:539:LEU:C	1:L:541:ASP:N	2.73	0.41
1:A:104:ARG:NH1	1:A:153:ASP:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:THR:HG21	1:A:412:LYS:HD2	2.03	0.41
1:B:141:GLY:CA	1:B:223:GLY:H	2.28	0.41
1:B:51:LEU:HA	1:B:120:ASN:OD1	2.20	0.41
1:C:140:HIS:CD2	1:C:147:GLY:HA3	2.56	0.41
1:E:222:ALA:HB3	6:E:6472:HOH:O	2.18	0.41
1:E:477:GLY:HA2	1:E:493:SER:OG	2.20	0.41
1:F:24:PRO:HG3	1:F:37:PHE:CZ	2.56	0.41
1:F:351:ASN:HD22	1:F:351:ASN:N	2.14	0.41
1:F:498:LYS:HB3	1:F:514:LEU:HD11	2.02	0.41
1:F:498:LYS:HE2	1:F:514:LEU:HD11	2.03	0.41
1:G:379:MET:O	1:G:396:ILE:HG21	2.21	0.41
1:H:194:GLN:O	1:H:195:VAL:C	2.59	0.41
1:I:125:ALA:HB2	1:I:133:LEU:HD12	2.03	0.41
1:J:389:VAL:HG23	1:J:391:ILE:HG13	2.03	0.41
1:J:393:LYS:O	1:J:396:ILE:HG12	2.21	0.41
1:K:296:GLU:O	1:K:300:LYS:HG3	2.21	0.41
1:L:137:VAL:HB	1:L:217:ILE:HG22	2.04	0.41
1:L:269:ALA:O	1:L:274:CYS:HB2	2.20	0.41
1:L:386:TYR:C	1:L:388:LEU:H	2.24	0.41
1:L:434:ALA:HB2	1:L:446:MET:HE3	2.02	0.41
3:A:1181:SIA:H113	3:A:1181:SIA:H31	2.03	0.40
1:A:173:GLY:O	1:A:174:ILE:C	2.57	0.40
1:A:266:GLU:HG2	1:A:282:MET:HE1	2.03	0.40
1:A:34:LEU:HD13	1:A:35:GLY:N	2.35	0.40
1:A:420:LEU:HD13	1:A:421:ILE:N	2.36	0.40
1:B:266:GLU:HG2	1:B:282:MET:CE	2.45	0.40
1:B:38:VAL:HG21	1:B:49:ILE:HD12	2.03	0.40
1:C:400:THR:HG23	1:C:404:LEU:HD12	2.03	0.40
1:D:399:ALA:HB2	1:D:550:LEU:CD2	2.50	0.40
1:E:126:ASP:H	1:E:131:ASN:HD22	1.68	0.40
1:E:124:PRO:HD3	1:E:158:ALA:HB1	2.03	0.40
1:E:57:LYS:HA	1:E:58:PRO:HD3	1.91	0.40
1:G:144:LEU:HD22	1:G:177:PHE:CZ	2.56	0.40
1:G:529:ILE:HA	1:G:533:THR:HG23	2.02	0.40
1:H:221:SER:O	1:H:222:ALA:C	2.59	0.40
1:H:244:ILE:HD11	1:H:503:PHE:CD2	2.55	0.40
1:H:257:LYS:HZ2	1:H:257:LYS:HA	1.85	0.40
1:J:194:GLN:HE22	1:J:226:SER:HB3	1.86	0.40
1:J:442:ALA:HA	1:J:443:PRO:HD3	1.92	0.40
1:K:290:THR:HG23	1:K:293:GLU:HG3	2.03	0.40
1:L:143:GLY:O	1:L:144:LEU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:140:HIS:CD2	1:L:147:GLY:HA3	2.56	0.40
1:L:257:LYS:CE	1:L:316:GLN:HE22	2.34	0.40
1:L:482:LYS:O	1:L:483:GLU:HG3	2.21	0.40
1:A:45:GLN:HE22	1:A:124:PRO:HB2	1.86	0.40
1:A:97:LEU:HD11	1:A:101:PHE:HE2	1.83	0.40
1:B:136:MET:CE	1:B:504:ALA:HB2	2.51	0.40
1:B:528:GLN:O	1:B:533:THR:HA	2.21	0.40
1:B:79:ASN:ND2	2:B:1279:NAG:H82	2.37	0.40
1:C:452:ARG:HA	1:C:453:PRO:HD2	1.91	0.40
1:D:319:LEU:N	1:D:319:LEU:CD2	2.83	0.40
1:D:520:TYR:CZ	1:D:524:GLU:HG2	2.56	0.40
1:D:495:MET:CE	1:D:533:THR:HG21	2.51	0.40
1:E:107:ASN:ND2	1:E:108:ILE:H	2.20	0.40
1:E:377:THR:O	1:E:380:SER:HB3	2.21	0.40
1:F:417:PHE:O	1:F:420:LEU:HB3	2.21	0.40
1:G:23:PRO:HA	1:G:24:PRO:HD3	1.78	0.40
1:G:372:GLN:HB2	1:G:410:THR:HB	2.03	0.40
1:G:375:GLN:HB3	1:G:375:GLN:HE21	1.56	0.40
1:H:221:SER:OG	5:H:3386:BEZ:H2	2.20	0.40
1:I:495:MET:CE	1:I:533:THR:HG21	2.48	0.40
1:J:36:LYS:HE3	1:J:38:VAL:HG21	2.03	0.40
1:K:372:GLN:CB	1:K:410:THR:HB	2.50	0.40
1:L:218:PHE:N	1:L:218:PHE:CD1	2.89	0.40
1:A:26:VAL:HG11	1:A:207:SER:HB3	2.00	0.40
1:B:133:LEU:HB3	1:B:134:PRO:HD2	2.03	0.40
1:B:378:ALA:O	1:B:379:MET:C	2.60	0.40
1:C:119:LEU:HD12	1:C:119:LEU:C	2.42	0.40
1:C:89:GLN:OE1	1:C:146:VAL:CA	2.69	0.40
1:D:351:ASN:N	1:D:354:GLU:OE2	2.54	0.40
1:E:297:THR:C	1:E:299:LEU:N	2.75	0.40
1:E:357:TRP:O	1:E:360:PRO:HD2	2.21	0.40
1:E:431:VAL:HG12	1:E:435:ARG:HE	1.87	0.40
1:E:517:TRP:HA	1:E:518:PRO:HD2	1.96	0.40
1:F:240:PHE:CD1	1:F:240:PHE:N	2.90	0.40
1:F:279:SER:C	1:F:281:VAL:N	2.72	0.40
1:G:297:THR:O	1:G:301:MET:HG2	2.22	0.40
1:H:186:ARG:HD3	1:H:324:ASP:HB2	2.02	0.40
1:I:375:GLN:O	1:I:379:MET:HG2	2.21	0.40
1:J:138:TRP:CZ3	1:J:219:GLY:HA2	2.56	0.40
1:J:233:SER:HA	1:J:234:PRO:HD3	1.92	0.40
1:J:231:VAL:HG22	1:J:240:PHE:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:488:GLU:O	1:J:491:ARG:HB3	2.22	0.40
1:J:474:SER:HB3	1:J:496:VAL:HG21	2.02	0.40
1:K:205:ILE:HG13	1:K:210:GLY:HA3	2.03	0.40
1:K:456:SER:HB3	1:K:460:LYS:HD3	2.02	0.40
1:L:64:ARG:HH11	1:L:294:LEU:HD12	1.85	0.40
1:L:491:ARG:HH11	1:L:491:ARG:HG3	1.87	0.40
1:A:257:LYS:HB2	1:A:322:VAL:HG12	2.02	0.40
1:C:89:GLN:OE1	1:C:146:VAL:HB	2.21	0.40
1:D:134:PRO:HG2	1:D:163:VAL:HG12	2.02	0.40
1:D:34:LEU:HB3	1:D:79:ASN:CA	2.51	0.40
1:E:283:VAL:HG12	1:E:287:ARG:NH1	2.36	0.40
1:E:449:PHE:CE2	1:E:451:TYR:HB3	2.56	0.40
1:G:34:LEU:C	1:G:34:LEU:HD13	2.42	0.40
1:G:383:TRP:O	1:G:386:TYR:HB2	2.21	0.40
1:H:225:GLU:O	1:H:229:VAL:HG23	2.21	0.40
1:H:236:ALA:HA	1:H:239:LEU:HD12	2.01	0.40
1:H:480:PHE:N	1:H:480:PHE:CD1	2.89	0.40
1:I:117:LEU:HD21	1:I:193:ASP:OD2	2.22	0.40
1:I:61:GLY:HA3	1:I:62:PRO:HD2	1.83	0.40
1:I:89:GLN:NE2	1:I:147:GLY:O	2.54	0.40
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.85	0.40
1:K:97:LEU:HD11	1:K:101:PHE:CE2	2.57	0.40
1:L:23:PRO:HB3	1:L:35:GLY:O	2.21	0.40
1:L:297:THR:O	1:L:301:MET:HG2	2.21	0.40
1:L:493:SER:O	1:L:497:MET:HG3	2.21	0.40
3:A:1181:SIA:H8	6:A:6003:HOH:O	2.21	0.40
1:A:252:THR:HG22	1:A:254:VAL:CG1	2.50	0.40
1:C:23:PRO:HA	1:C:24:PRO:HD3	1.85	0.40
1:C:415:ASP:HA	1:C:418:LEU:HD12	2.03	0.40
1:D:86:MET:CE	1:D:110:LEU:HD12	2.49	0.40
1:E:119:LEU:C	1:E:119:LEU:HD12	2.42	0.40
1:F:242:ARG:NH1	1:F:242:ARG:HG2	2.34	0.40
1:F:27:ASP:HA	1:F:32:LYS:HA	2.03	0.40
1:F:375:GLN:HE21	1:F:375:GLN:HB3	1.61	0.40
1:G:338:GLU:O	1:G:338:GLU:HG3	2.21	0.40
1:H:180:THR:O	1:H:262:LYS:HD3	2.22	0.40
1:H:447:TYR:HB3	1:H:517:TRP:CZ2	2.56	0.40
1:J:312:PRO:HG2	1:J:383:TRP:CD1	2.57	0.40
1:J:330:LYS:NZ	1:J:330:LYS:HB3	2.36	0.40
1:J:79:ASN:O	1:J:81:THR:N	2.54	0.40
1:J:83:TYR:CD1	1:J:150:SER:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:143:GLY:O	1:K:144:LEU:CB	2.70	0.40
1:K:182:ASP:OD2	1:K:182:ASP:N	2.52	0.40
1:K:176:GLY:HA2	1:K:189:TRP:HB2	2.03	0.40
1:K:225:GLU:O	1:K:228:SER:HB3	2.22	0.40
1:K:23:PRO:HA	1:K:24:PRO:HD3	1.80	0.40
1:K:372:GLN:HB2	1:K:410:THR:C	2.42	0.40
1:K:428:VAL:HB	1:K:429:PRO:HD3	2.03	0.40
1:L:133:LEU:O	1:L:211:ASN:N	2.54	0.40
1:L:220:GLU:HA	1:L:246:GLU:O	2.22	0.40
1:L:278:THR:OG1	1:L:281:VAL:HG23	2.22	0.40
1:L:367:PRO:HB2	1:L:381:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/532 (100%)	451 (85%)	67 (13%)	12 (2%)	6	34
1	B	530/532 (100%)	448 (84%)	65 (12%)	17 (3%)	4	26
1	C	530/532 (100%)	467 (88%)	54 (10%)	9 (2%)	9	42
1	D	530/532 (100%)	454 (86%)	60 (11%)	16 (3%)	4	28
1	E	530/532 (100%)	438 (83%)	80 (15%)	12 (2%)	6	34
1	F	530/532 (100%)	464 (88%)	51 (10%)	15 (3%)	5	29
1	G	530/532 (100%)	445 (84%)	62 (12%)	23 (4%)	2	20
1	H	530/532 (100%)	449 (85%)	71 (13%)	10 (2%)	8	39
1	I	530/532 (100%)	451 (85%)	60 (11%)	19 (4%)	3	23
1	J	530/532 (100%)	444 (84%)	74 (14%)	12 (2%)	6	34
1	K	530/532 (100%)	451 (85%)	64 (12%)	15 (3%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	530/532 (100%)	434 (82%)	80 (15%)	16 (3%)	4	28
All	All	6360/6384 (100%)	5396 (85%)	788 (12%)	176 (3%)	5	29

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	SER
1	B	358	LEU
1	E	185	SER
1	E	358	LEU
1	E	456	SER
1	F	238	ASN
1	F	253	SER
1	F	531	ALA
1	G	105	LYS
1	I	76	PHE
1	I	185	SER
1	I	254	VAL
1	I	308	LEU
1	I	540	LYS
1	J	253	SER
1	J	340	ASN
1	L	76	PHE
1	L	102	THR
1	L	185	SER
1	L	308	LEU
1	A	102	THR
1	A	185	SER
1	A	427	GLY
1	B	308	LEU
1	B	340	ASN
1	B	427	GLY
1	B	456	SER
1	B	538	LYS
1	C	105	LYS
1	C	357	TRP
1	C	427	GLY
1	D	185	SER
1	D	205	ILE
1	D	317	PRO
1	D	427	GLY
1	D	467	ASP

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Mol	Chain	Res	Type
1	D	484	GLY
1	E	320	GLY
1	E	427	GLY
1	E	520	TYR
1	F	105	LYS
1	F	185	SER
1	F	358	LEU
1	F	427	GLY
1	G	127	LEU
1	G	140	HIS
1	G	205	ILE
1	G	253	SER
1	G	307	ASP
1	G	427	GLY
1	G	538	LYS
1	H	427	GLY
1	I	253	SER
1	I	302	LYS
1	J	127	LEU
1	J	254	VAL
1	J	427	GLY
1	K	252	THR
1	K	406	GLY
1	K	427	GLY
1	L	103	ASN
1	L	427	GLY
1	A	317	PRO
1	A	367	PRO
1	A	485	ALA
1	B	105	LYS
1	B	182	ASP
1	B	254	VAL
1	B	302	LYS
1	C	185	SER
1	C	545	ALA
1	D	319	LEU
1	D	358	LEU
1	D	538	LYS
1	E	538	LYS
1	F	254	VAL
1	F	315	SER
1	F	406	GLY

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Mol	Chain	Res	Type
1	F	520	TYR
1	G	76	PHE
1	G	79	ASN
1	G	183	GLU
1	G	306	LEU
1	G	312	PRO
1	G	394	GLU
1	H	102	THR
1	H	185	SER
1	H	252	THR
1	H	384	LYS
1	H	484	GLY
1	I	142	GLY
1	I	358	LEU
1	I	397	PRO
1	I	406	GLY
1	I	510	ASN
1	J	41	GLU
1	J	185	SER
1	J	315	SER
1	K	102	THR
1	K	143	GLY
1	K	340	ASN
1	K	482	LYS
1	K	551	PHE
1	L	75	SER
1	L	358	LEU
1	L	482	LYS
1	B	80	ALA
1	D	156	ALA
1	D	340	ASN
1	E	127	LEU
1	E	254	VAL
1	E	364	MET
1	E	400	THR
1	G	65	PHE
1	G	156	ALA
1	G	318	LEU
1	G	370	GLU
1	G	456	SER
1	H	156	ALA
1	I	467	ASP

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Mol	Chain	Res	Type
1	J	105	LYS
1	J	205	ILE
1	K	76	PHE
1	K	407	THR
1	L	79	ASN
1	L	369	SER
1	L	409	ASP
1	L	540	LYS
1	A	212	PRO
1	A	253	SER
1	A	540	LYS
1	B	397	PRO
1	B	470	ASP
1	B	520	TYR
1	C	148	ALA
1	C	253	SER
1	C	479	PRO
1	D	127	LEU
1	D	406	GLY
1	E	406	GLY
1	G	308	LEU
1	G	340	ASN
1	G	368	LEU
1	H	254	VAL
1	I	105	LYS
1	I	538	LYS
1	J	255	LEU
1	K	185	SER
1	L	260	ASP
1	C	205	ILE
1	D	76	PHE
1	F	41	GLU
1	F	440	ALA
1	J	142	GLY
1	K	315	SER
1	K	367	PRO
1	L	275	LYS
1	D	254	VAL
1	F	477	GLY
1	G	406	GLY
1	H	544	VAL
1	I	205	ILE

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Mol	Chain	Res	Type
1	K	254	VAL
1	L	254	VAL
1	B	317	PRO
1	H	143	GLY
1	I	62	PRO
1	K	142	GLY
1	D	515	PRO
1	I	427	GLY
1	A	143	GLY
1	B	227	VAL
1	A	90	ASP
1	A	142	GLY
1	F	405	GLY
1	I	124	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	448/448 (100%)	423 (94%)	25 (6%)	21	57
1	B	448/448 (100%)	419 (94%)	29 (6%)	17	51
1	C	448/448 (100%)	419 (94%)	29 (6%)	17	51
1	D	448/448 (100%)	418 (93%)	30 (7%)	16	50
1	E	448/448 (100%)	417 (93%)	31 (7%)	15	49
1	F	448/448 (100%)	430 (96%)	18 (4%)	31	66
1	G	448/448 (100%)	423 (94%)	25 (6%)	21	57
1	H	448/448 (100%)	423 (94%)	25 (6%)	21	57
1	I	448/448 (100%)	418 (93%)	30 (7%)	16	50
1	J	448/448 (100%)	424 (95%)	24 (5%)	22	58
1	K	448/448 (100%)	417 (93%)	31 (7%)	15	49
1	L	448/448 (100%)	413 (92%)	35 (8%)	12	43
All	All	5376/5376 (100%)	5044 (94%)	332 (6%)	18	53

All (332) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	78	LYS
1	A	104	ARG
1	A	106	GLU
1	A	124	PRO
1	A	151	THR
1	A	162	ASN
1	A	164	VAL
1	A	221	SER
1	A	241	HIS
1	A	264	LEU
1	A	279	SER
1	A	304	LEU
1	A	338	GLU
1	A	339	ARG
1	A	344	VAL
1	A	346	TYR
1	A	381	LEU
1	A	390	CYS
1	A	420	LEU
1	A	425	MET
1	A	436	ASN
1	A	500	TRP
1	A	522	GLN
1	A	553	LYS
1	B	24	PRO
1	B	69	GLN
1	B	88	THR
1	B	132	ARG
1	B	162	ASN
1	B	186	ARG
1	B	218	PHE
1	B	225	GLU
1	B	249	VAL
1	B	251	LEU
1	B	257	LYS
1	B	261	VAL
1	B	292	GLU
1	B	304	LEU
1	B	329	LEU
1	B	338	GLU
1	B	339	ARG

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Mol	Chain	Res	Type
1	B	366	TYR
1	B	379	MET
1	B	404	LEU
1	B	410	THR
1	B	493	SER
1	B	499	PHE
1	B	500	TRP
1	B	506	ASN
1	B	523	LYS
1	B	532	ASN
1	B	542	LYS
1	B	551	PHE
1	C	86	MET
1	C	88	THR
1	C	105	LYS
1	C	111	LYS
1	C	123	THR
1	C	132	ARG
1	C	150	SER
1	C	151	THR
1	C	162	ASN
1	C	182	ASP
1	C	199	ARG
1	C	218	PHE
1	C	225	GLU
1	C	247	SER
1	C	264	LEU
1	C	318	LEU
1	C	319	LEU
1	C	338	GLU
1	C	339	ARG
1	C	346	TYR
1	C	366	TYR
1	C	373	LEU
1	C	375	GLN
1	C	463	THR
1	C	471	GLU
1	C	499	PHE
1	C	500	TRP
1	C	506	ASN
1	C	523	LYS
1	D	79	ASN

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Mol	Chain	Res	Type
1	D	102	THR
1	D	104	ARG
1	D	112	LEU
1	D	119	LEU
1	D	132	ARG
1	D	150	SER
1	D	151	THR
1	D	202	GLN
1	D	221	SER
1	D	225	GLU
1	D	242	ARG
1	D	261	VAL
1	D	264	LEU
1	D	278	THR
1	D	304	LEU
1	D	339	ARG
1	D	366	TYR
1	D	372	GLN
1	D	425	MET
1	D	455	PHE
1	D	458	ASP
1	D	462	LYS
1	D	499	PHE
1	D	500	TRP
1	D	523	LYS
1	D	528	GLN
1	D	532	ASN
1	D	534	GLN
1	D	551	PHE
1	E	24	PRO
1	E	27	ASP
1	E	28	THR
1	E	37	PHE
1	E	66	THR
1	E	69	GLN
1	E	79	ASN
1	E	104	ARG
1	E	106	GLU
1	E	107	ASN
1	E	124	PRO
1	E	132	ARG
1	E	218	PHE

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Mol	Chain	Res	Type
1	E	225	GLU
1	E	245	SER
1	E	264	LEU
1	E	287	ARG
1	E	298	THR
1	E	304	LEU
1	E	316	GLN
1	E	318	LEU
1	E	338	GLU
1	E	366	TYR
1	E	375	GLN
1	E	404	LEU
1	E	408	ASP
1	E	410	THR
1	E	420	LEU
1	E	459	MET
1	E	471	GLU
1	E	500	TRP
1	F	66	THR
1	F	79	ASN
1	F	132	ARG
1	F	162	ASN
1	F	182	ASP
1	F	218	PHE
1	F	225	GLU
1	F	264	LEU
1	F	293	GLU
1	F	319	LEU
1	F	339	ARG
1	F	363	LEU
1	F	375	GLN
1	F	383	TRP
1	F	419	ASP
1	F	489	GLU
1	F	523	LYS
1	F	534	GLN
1	G	37	PHE
1	G	69	GLN
1	G	111	LYS
1	G	132	ARG
1	G	151	THR
1	G	162	ASN

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Mol	Chain	Res	Type
1	G	172	LEU
1	G	182	ASP
1	G	202	GLN
1	G	218	PHE
1	G	225	GLU
1	G	264	LEU
1	G	278	THR
1	G	279	SER
1	G	292	GLU
1	G	335	LEU
1	G	366	TYR
1	G	375	GLN
1	G	420	LEU
1	G	457	SER
1	G	458	ASP
1	G	499	PHE
1	G	500	TRP
1	G	523	LYS
1	G	534	GLN
1	H	24	PRO
1	H	39	SER
1	H	79	ASN
1	H	104	ARG
1	H	132	ARG
1	H	151	THR
1	H	199	ARG
1	H	225	GLU
1	H	242	ARG
1	H	257	LYS
1	H	276	THR
1	H	278	THR
1	H	292	GLU
1	H	319	LEU
1	H	339	ARG
1	H	361	MET
1	H	366	TYR
1	H	419	ASP
1	H	420	LEU
1	H	479	PRO
1	H	500	TRP
1	H	528	GLN
1	H	532	ASN

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Mol	Chain	Res	Type
1	H	541	ASP
1	H	551	PHE
1	I	24	PRO
1	I	27	ASP
1	I	28	THR
1	I	78	LYS
1	I	79	ASN
1	I	82	SER
1	I	104	ARG
1	I	124	PRO
1	I	132	ARG
1	I	162	ASN
1	I	182	ASP
1	I	202	GLN
1	I	218	PHE
1	I	220	GLU
1	I	225	GLU
1	I	264	LEU
1	I	292	GLU
1	I	304	LEU
1	I	309	GLN
1	I	313	ARG
1	I	333	GLU
1	I	338	GLU
1	I	366	TYR
1	I	372	GLN
1	I	374	ASP
1	I	423	ASP
1	I	471	GLU
1	I	500	TRP
1	I	506	ASN
1	I	551	PHE
1	J	88	THR
1	J	89	GLN
1	J	110	LEU
1	J	113	SER
1	J	132	ARG
1	J	151	THR
1	J	162	ASN
1	J	182	ASP
1	J	215	VAL
1	J	218	PHE

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Mol	Chain	Res	Type
1	J	225	GLU
1	J	226	SER
1	J	264	LEU
1	J	279	SER
1	J	319	LEU
1	J	330	LYS
1	J	339	ARG
1	J	342	HIS
1	J	346	TYR
1	J	366	TYR
1	J	375	GLN
1	J	457	SER
1	J	471	GLU
1	J	499	PHE
1	K	33	VAL
1	K	39	SER
1	K	78	LYS
1	K	88	THR
1	K	104	ARG
1	K	107	ASN
1	K	131	ASN
1	K	132	ARG
1	K	199	ARG
1	K	207	SER
1	K	214	SER
1	K	221	SER
1	K	225	GLU
1	K	242	ARG
1	K	278	THR
1	K	279	SER
1	K	292	GLU
1	K	304	LEU
1	K	307	ASP
1	K	316	GLN
1	K	318	LEU
1	K	339	ARG
1	K	361	MET
1	K	366	TYR
1	K	372	GLN
1	K	420	LEU
1	K	425	MET
1	K	447	TYR

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Mol	Chain	Res	Type
1	K	455	PHE
1	K	471	GLU
1	K	523	LYS
1	L	28	THR
1	L	66	THR
1	L	79	ASN
1	L	81	THR
1	L	88	THR
1	L	129	LYS
1	L	132	ARG
1	L	133	LEU
1	L	135	VAL
1	L	162	ASN
1	L	163	VAL
1	L	182	ASP
1	L	199	ARG
1	L	203	ASP
1	L	218	PHE
1	L	220	GLU
1	L	225	GLU
1	L	264	LEU
1	L	302	LYS
1	L	304	LEU
1	L	329	LEU
1	L	338	GLU
1	L	339	ARG
1	L	346	TYR
1	L	366	TYR
1	L	375	GLN
1	L	400	THR
1	L	404	LEU
1	L	411	VAL
1	L	471	GLU
1	L	491	ARG
1	L	497	MET
1	L	500	TRP
1	L	523	LYS
1	L	551	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (171) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	107	ASN
1	A	140	HIS
1	A	162	ASN
1	A	184	HIS
1	A	241	HIS
1	A	351	ASN
1	A	353	GLN
1	A	372	GLN
1	A	450	GLN
1	A	510	ASN
1	A	537	GLN
1	A	549	ASN
1	B	131	ASN
1	B	140	HIS
1	B	162	ASN
1	B	169	GLN
1	B	211	ASN
1	B	238	ASN
1	B	241	HIS
1	B	351	ASN
1	B	436	ASN
1	B	437	HIS
1	B	468	HIS
1	B	528	GLN
1	B	532	ASN
1	B	537	GLN
1	C	69	GLN
1	C	107	ASN
1	C	131	ASN
1	C	140	HIS
1	C	162	ASN
1	C	202	GLN
1	C	238	ASN
1	C	241	HIS
1	C	336	GLN
1	C	351	ASN
1	C	372	GLN
1	C	436	ASN
1	C	537	GLN
1	D	30	HIS
1	D	131	ASN
1	D	140	HIS

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Mol	Chain	Res	Type
1	D	162	ASN
1	D	202	GLN
1	D	241	HIS
1	D	351	ASN
1	D	372	GLN
1	D	436	ASN
1	D	437	HIS
1	D	528	GLN
1	D	537	GLN
1	E	107	ASN
1	E	131	ASN
1	E	140	HIS
1	E	162	ASN
1	E	169	GLN
1	E	184	HIS
1	E	211	ASN
1	E	241	HIS
1	E	316	GLN
1	E	336	GLN
1	E	351	ASN
1	E	372	GLN
1	E	375	GLN
1	E	436	ASN
1	E	528	GLN
1	E	532	ASN
1	E	534	GLN
1	E	537	GLN
1	F	45	GLN
1	F	131	ASN
1	F	160	HIS
1	F	211	ASN
1	F	241	HIS
1	F	316	GLN
1	F	351	ASN
1	F	353	GLN
1	F	372	GLN
1	F	375	GLN
1	F	450	GLN
1	F	528	GLN
1	F	534	GLN
1	F	537	GLN
1	G	45	GLN

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Mol	Chain	Res	Type
1	G	95	GLN
1	G	107	ASN
1	G	140	HIS
1	G	169	GLN
1	G	241	HIS
1	G	316	GLN
1	G	351	ASN
1	G	372	GLN
1	G	375	GLN
1	G	436	ASN
1	G	528	GLN
1	G	534	GLN
1	G	537	GLN
1	H	30	HIS
1	H	69	GLN
1	H	162	ASN
1	H	184	HIS
1	H	241	HIS
1	H	316	GLN
1	H	340	ASN
1	H	351	ASN
1	H	353	GLN
1	H	372	GLN
1	H	375	GLN
1	H	436	ASN
1	H	437	HIS
1	H	528	GLN
1	H	532	ASN
1	H	534	GLN
1	H	537	GLN
1	H	549	ASN
1	I	140	HIS
1	I	162	ASN
1	I	169	GLN
1	I	241	HIS
1	I	309	GLN
1	I	336	GLN
1	I	351	ASN
1	I	372	GLN
1	I	375	GLN
1	I	436	ASN
1	I	437	HIS

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Mol	Chain	Res	Type
1	I	450	GLN
1	I	537	GLN
1	J	45	GLN
1	J	107	ASN
1	J	131	ASN
1	J	140	HIS
1	J	241	HIS
1	J	336	GLN
1	J	351	ASN
1	J	353	GLN
1	J	372	GLN
1	J	436	ASN
1	J	450	GLN
1	J	528	GLN
1	J	534	GLN
1	J	537	GLN
1	J	549	ASN
1	K	30	HIS
1	K	69	GLN
1	K	107	ASN
1	K	140	HIS
1	K	162	ASN
1	K	241	HIS
1	K	267	GLN
1	K	316	GLN
1	K	336	GLN
1	K	351	ASN
1	K	372	GLN
1	K	436	ASN
1	K	450	GLN
1	K	537	GLN
1	L	131	ASN
1	L	162	ASN
1	L	169	GLN
1	L	241	HIS
1	L	316	GLN
1	L	336	GLN
1	L	351	ASN
1	L	372	GLN
1	L	375	GLN
1	L	436	ASN
1	L	437	HIS

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Mol	Chain	Res	Type
1	L	468	HIS
1	L	534	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

72 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
5	BEZ	L	4381	-	7,9,9	3.32	1 (14%)	8,11,11	0.87	0
3	SIA	K	1182	-	18,21,21	0.96	1 (5%)	21,31,31	0.96	0
2	NAG	H	3279	1	14,14,15	0.75	0	17,19,21	0.86	0
2	NAG	L	4379	1	14,14,15	0.57	0	17,19,21	0.82	1 (5%)
4	SO4	I	3285	-	4,4,4	0.33	0	6,6,6	0.13	0
5	BEZ	A	1385	-	7,9,9	5.45	3 (42%)	8,11,11	1.63	2 (25%)
2	NAG	D	2179	1	14,14,15	0.72	0	17,19,21	0.65	1 (5%)
4	SO4	I	3185	-	4,4,4	0.27	0	6,6,6	0.13	0
3	SIA	A	1181	-	18,21,21	1.15	3 (16%)	21,31,31	0.68	0
4	SO4	E	2284	-	4,4,4	0.31	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SIA	J	1082	-	18,21,21	1.06	2 (11%)	21,31,31	0.91	1 (4%)
3	SIA	F	682	-	18,21,21	1.22	3 (16%)	21,31,31	0.84	1 (4%)
4	SO4	K	4284	-	4,4,4	0.29	0	6,6,6	0.05	0
5	BEZ	C	5013	1	8,8,9	2.18	3 (37%)	9,9,11	0.78	1 (11%)
4	SO4	F	2285	-	4,4,4	0.32	0	6,6,6	0.13	0
4	SO4	G	3384	-	4,4,4	0.30	0	6,6,6	0.16	0
2	NAG	E	2279	1	14,14,15	0.54	0	17,19,21	1.05	1 (5%)
5	BEZ	H	3386	-	7,9,9	4.10	1 (14%)	8,11,11	0.87	0
5	BEZ	C	5014	-	7,9,9	5.52	1 (14%)	8,11,11	0.71	0
2	NAG	I	3379	1	14,14,15	0.64	0	17,19,21	0.89	1 (5%)
4	SO4	B	1385	-	4,4,4	0.27	0	6,6,6	0.13	0
4	SO4	H	3385	-	4,4,4	0.33	0	6,6,6	0.11	0
3	SIA	E	582	-	18,21,21	0.91	1 (5%)	21,31,31	0.92	0
4	SO4	E	2385	-	4,4,4	0.27	0	6,6,6	0.12	0
5	BEZ	H	3387	-	7,9,9	7.93	5 (71%)	8,11,11	1.73	3 (37%)
4	SO4	H	3284	-	4,4,4	0.34	0	6,6,6	0.10	0
4	SO4	J	4185	-	4,4,4	0.31	0	6,6,6	0.23	0
5	BEZ	I	3381	-	7,9,9	3.19	3 (42%)	8,11,11	0.34	0
5	BEZ	J	5041	1	8,8,9	2.21	3 (37%)	9,9,11	0.63	0
3	SIA	I	982	-	18,21,21	0.86	1 (5%)	21,31,31	0.79	1 (4%)
5	BEZ	G	3386	-	7,9,9	9.63	6 (85%)	8,11,11	3.49	4 (50%)
5	BEZ	G	3385	-	7,9,9	4.79	1 (14%)	8,11,11	1.05	0
2	NAG	B	1279	1	14,14,15	0.67	0	17,19,21	0.81	1 (5%)
4	SO4	D	2384	-	4,4,4	0.35	0	6,6,6	0.14	0
2	NAG	J	4179	1	14,14,15	0.79	0	17,19,21	1.33	4 (23%)
5	BEZ	E	2387	-	7,9,9	3.64	1 (14%)	8,11,11	0.97	0
4	SO4	J	4384	-	4,4,4	0.34	0	6,6,6	0.14	0
3	SIA	L	1282	-	18,21,21	0.79	0	21,31,31	0.94	0
4	SO4	L	4285	-	4,4,4	0.32	0	6,6,6	0.07	0
5	BEZ	L	4380	-	7,9,9	3.42	1 (14%)	8,11,11	0.68	0
5	BEZ	K	4386	-	7,9,9	4.00	1 (14%)	8,11,11	0.83	0
3	SIA	D	2180	-	18,21,21	0.92	1 (5%)	21,31,31	0.72	0
4	SO4	F	2185	-	4,4,4	0.31	0	6,6,6	0.15	0
2	NAG	F	2379	1	14,14,15	1.18	2 (14%)	17,19,21	1.56	3 (17%)
5	BEZ	K	4387	-	7,9,9	4.75	5 (71%)	8,11,11	1.00	0
2	NAG	A	1179	1	14,14,15	0.70	0	17,19,21	0.70	1 (5%)
4	SO4	C	1185	-	4,4,4	0.32	0	6,6,6	0.16	0
4	SO4	D	2184	-	4,4,4	0.28	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	1285	-	4,4,4	0.33	0	6,6,6	0.17	0
2	NAG	G	3179	1	14,14,15	0.84	0	17,19,21	0.92	1 (5%)
5	BEZ	F	5024	-	7,9,9	3.52	1 (14%)	8,11,11	0.52	0
5	BEZ	A	11	-	7,9,9	5.04	5 (71%)	8,11,11	1.36	1 (12%)
4	SO4	A	1384	-	4,4,4	0.31	0	6,6,6	0.16	0
5	BEZ	E	2386	-	7,9,9	3.74	1 (14%)	8,11,11	0.71	0
3	SIA	G	782	-	18,21,21	0.95	2 (11%)	21,31,31	0.79	0
5	BEZ	D	2385	-	7,9,9	14.36	7 (100%)	8,11,11	2.18	5 (62%)
5	BEZ	J	5042	-	7,9,9	6.40	3 (42%)	8,11,11	2.39	3 (37%)
2	NAG	K	4279	1	14,14,15	0.84	0	17,19,21	0.67	0
3	SIA	B	1280	-	18,21,21	0.80	0	21,31,31	1.08	2 (9%)
4	SO4	G	3184	-	4,4,4	0.27	0	6,6,6	0.13	0
5	BEZ	B	12	-	7,9,9	17.97	7 (100%)	8,11,11	1.34	1 (12%)
2	NAG	C	1379	1	14,14,15	0.69	0	17,19,21	0.86	1 (5%)
4	SO4	J	4184	-	4,4,4	0.28	0	6,6,6	0.14	0
3	SIA	H	882	-	18,21,21	1.11	2 (11%)	21,31,31	0.87	0
5	BEZ	B	1386	-	7,9,9	3.50	3 (42%)	8,11,11	0.40	0
5	BEZ	I	3380	-	7,9,9	3.79	1 (14%)	8,11,11	1.05	1 (12%)
3	SIA	A	1180	-	18,21,21	0.83	1 (5%)	21,31,31	0.80	0
4	SO4	B	1284	-	4,4,4	0.32	0	6,6,6	0.08	0
5	BEZ	D	2386	-	7,9,9	5.44	6 (85%)	8,11,11	0.91	0
4	SO4	K	4385	-	4,4,4	0.29	0	6,6,6	0.07	0
5	BEZ	F	5023	1	8,8,9	2.14	4 (50%)	9,9,11	0.66	0
4	SO4	A	1184	-	4,4,4	0.25	0	6,6,6	0.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BEZ	L	4381	-	-	0/0/4/4	0/1/1/1
3	SIA	K	1182	-	-	10/14/38/38	0/1/1/1
2	NAG	H	3279	1	-	6/6/23/26	0/1/1/1
2	NAG	D	2179	1	-	2/6/23/26	0/1/1/1
3	SIA	A	1181	-	-	8/14/38/38	0/1/1/1
3	SIA	J	1082	-	-	8/14/38/38	0/1/1/1
3	SIA	I	982	-	-	11/14/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BEZ	H	3386	-	-	0/0/4/4	0/1/1/1
5	BEZ	C	5014	-	-	0/0/4/4	0/1/1/1
2	NAG	I	3379	1	-	3/6/23/26	0/1/1/1
5	BEZ	A	11	-	-	0/0/4/4	0/1/1/1
5	BEZ	D	2385	-	-	0/0/4/4	0/1/1/1
5	BEZ	E	2387	-	-	0/0/4/4	0/1/1/1
5	BEZ	C	5013	1	-	0/2/2/4	0/1/1/1
5	BEZ	I	3381	-	-	0/0/4/4	0/1/1/1
5	BEZ	J	5041	1	-	0/2/2/4	0/1/1/1
5	BEZ	G	3386	-	-	0/0/4/4	0/1/1/1
5	BEZ	G	3385	-	-	0/0/4/4	0/1/1/1
2	NAG	B	1279	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	E	2279	1	-	2/6/23/26	0/1/1/1
2	NAG	J	4179	1	1/1/5/7	4/6/23/26	0/1/1/1
5	BEZ	F	5024	-	-	0/0/4/4	0/1/1/1
3	SIA	L	1282	-	-	9/14/38/38	0/1/1/1
5	BEZ	A	1385	-	-	0/0/4/4	0/1/1/1
5	BEZ	L	4380	-	-	0/0/4/4	0/1/1/1
5	BEZ	K	4386	-	-	0/0/4/4	0/1/1/1
3	SIA	D	2180	-	-	9/14/38/38	0/1/1/1
2	NAG	F	2379	1	1/1/5/7	2/6/23/26	0/1/1/1
5	BEZ	K	4387	-	-	0/0/4/4	0/1/1/1
3	SIA	F	682	-	-	5/14/38/38	0/1/1/1
2	NAG	A	1179	1	-	6/6/23/26	0/1/1/1
3	SIA	E	582	-	-	10/14/38/38	0/1/1/1
2	NAG	G	3179	1	1/1/5/7	4/6/23/26	0/1/1/1
5	BEZ	H	3387	-	-	0/0/4/4	0/1/1/1
3	SIA	G	782	-	-	6/14/38/38	0/1/1/1
5	BEZ	J	5042	-	-	0/0/4/4	0/1/1/1
2	NAG	K	4279	1	1/1/5/7	3/6/23/26	0/1/1/1
3	SIA	B	1280	-	-	8/14/38/38	0/1/1/1
5	BEZ	F	5023	1	-	0/2/2/4	0/1/1/1
5	BEZ	B	12	-	-	0/0/4/4	0/1/1/1
2	NAG	C	1379	1	-	3/6/23/26	0/1/1/1
3	SIA	H	882	-	-	7/14/38/38	0/1/1/1
5	BEZ	B	1386	-	-	0/0/4/4	0/1/1/1
5	BEZ	I	3380	-	-	0/0/4/4	0/1/1/1
3	SIA	A	1180	-	-	6/14/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BEZ	D	2386	-	-	0/0/4/4	0/1/1/1
5	BEZ	E	2386	-	-	0/0/4/4	0/1/1/1
2	NAG	L	4379	1	-	6/6/23/26	0/1/1/1

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3386	BEZ	C1-C	23.60	1.70	1.47
5	H	3387	BEZ	C1-C	19.87	1.66	1.47
5	B	12	BEZ	C6-C1	18.46	1.78	1.39
5	B	12	BEZ	C1-C	18.34	1.65	1.47
5	B	12	BEZ	C2-C1	18.29	1.78	1.39
5	B	12	BEZ	C3-C2	17.98	1.76	1.38
5	B	12	BEZ	C4-C3	17.92	1.85	1.38
5	B	12	BEZ	C5-C4	17.62	1.84	1.38
5	D	2385	BEZ	C1-C	17.48	1.64	1.47
5	B	12	BEZ	C5-C6	17.11	1.74	1.38
5	D	2385	BEZ	C4-C3	16.58	1.82	1.38
5	D	2385	BEZ	C5-C4	16.53	1.81	1.38
5	D	2385	BEZ	C3-C2	15.52	1.71	1.38
5	C	5014	BEZ	C1-C	14.31	1.61	1.47
5	D	2385	BEZ	C5-C6	13.59	1.67	1.38
5	J	5042	BEZ	C1-C	13.31	1.60	1.47
5	G	3385	BEZ	C1-C	12.50	1.59	1.47
5	D	2386	BEZ	C1-C	11.98	1.59	1.47
5	A	1385	BEZ	C1-C	11.28	1.58	1.47
5	A	11	BEZ	C1-C	10.75	1.57	1.47
5	H	3386	BEZ	C1-C	10.70	1.57	1.47
5	K	4386	BEZ	C1-C	10.32	1.57	1.47
5	K	4387	BEZ	C1-C	9.97	1.57	1.47
5	I	3380	BEZ	C1-C	9.83	1.56	1.47
5	E	2386	BEZ	C1-C	9.69	1.56	1.47
5	D	2385	BEZ	C2-C1	9.44	1.59	1.39
5	E	2387	BEZ	C1-C	9.37	1.56	1.47
5	D	2385	BEZ	C6-C1	8.65	1.57	1.39
5	L	4381	BEZ	C1-C	8.52	1.55	1.47
5	L	4380	BEZ	C1-C	8.51	1.55	1.47
5	F	5024	BEZ	C1-C	8.50	1.55	1.47
5	J	5042	BEZ	C2-C1	7.96	1.56	1.39
5	B	1386	BEZ	C1-C	7.82	1.55	1.47
5	I	3381	BEZ	C1-C	7.12	1.54	1.47
5	A	1385	BEZ	C2-C1	6.67	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	5042	BEZ	C6-C1	6.57	1.53	1.39
5	G	3386	BEZ	C2-C1	-5.85	1.26	1.39
5	A	1385	BEZ	C6-C1	5.83	1.51	1.39
5	G	3386	BEZ	C6-C1	-5.71	1.27	1.39
5	A	11	BEZ	C5-C4	4.62	1.50	1.38
5	K	4387	BEZ	C5-C4	4.53	1.50	1.38
5	K	4387	BEZ	C4-C3	4.49	1.49	1.38
5	D	2386	BEZ	C5-C4	4.39	1.49	1.38
5	A	11	BEZ	C4-C3	4.31	1.49	1.38
5	H	3387	BEZ	C4-C3	-4.26	1.26	1.38
5	D	2386	BEZ	C4-C3	4.23	1.49	1.38
5	C	5013	BEZ	O2-C	-4.03	1.24	1.41
5	J	5041	BEZ	O2-C	-3.87	1.25	1.41
5	F	5023	BEZ	O2-C	-3.60	1.26	1.41
5	H	3387	BEZ	C2-C1	-3.39	1.32	1.39
5	G	3386	BEZ	C5-C4	3.35	1.46	1.38
5	D	2386	BEZ	C5-C6	3.26	1.45	1.38
5	A	11	BEZ	C5-C6	3.10	1.45	1.38
2	F	2379	NAG	C1-C2	3.09	1.56	1.52
5	K	4387	BEZ	C5-C6	2.93	1.45	1.38
5	A	11	BEZ	C3-C2	2.86	1.45	1.38
5	B	1386	BEZ	C6-C1	2.86	1.45	1.39
3	K	1182	SIA	C4-C5	2.83	1.55	1.53
5	D	2386	BEZ	C3-C2	2.77	1.44	1.38
5	G	3386	BEZ	C4-C3	2.77	1.45	1.38
5	J	5041	BEZ	C6-C1	2.75	1.44	1.38
3	F	682	SIA	O6-C2	2.67	1.45	1.43
5	H	3387	BEZ	C6-C1	-2.67	1.33	1.39
5	J	5041	BEZ	C2-C1	2.65	1.44	1.38
5	C	5013	BEZ	C2-C1	2.60	1.44	1.38
5	B	1386	BEZ	C2-C1	2.52	1.44	1.39
5	H	3387	BEZ	C5-C4	-2.48	1.31	1.38
3	A	1181	SIA	C4-C5	2.47	1.55	1.53
3	E	582	SIA	C4-C5	2.44	1.55	1.53
5	I	3381	BEZ	C2-C1	2.41	1.44	1.39
5	F	5023	BEZ	C6-C1	2.40	1.44	1.38
3	F	682	SIA	C4-C5	2.38	1.55	1.53
3	I	982	SIA	C3-C2	2.37	1.54	1.51
5	G	3386	BEZ	C3-C2	-2.33	1.34	1.38
3	J	1082	SIA	O6-C2	2.30	1.45	1.43
5	C	5013	BEZ	C6-C1	2.29	1.43	1.38
3	F	682	SIA	C3-C2	2.26	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1082	SIA	C4-C5	2.23	1.55	1.53
5	F	5023	BEZ	C2-C1	2.23	1.43	1.38
3	H	882	SIA	C7-C6	2.21	1.55	1.53
3	A	1181	SIA	C3-C2	2.19	1.54	1.51
3	A	1180	SIA	C3-C2	2.15	1.54	1.51
5	K	4387	BEZ	C3-C2	2.13	1.43	1.38
3	H	882	SIA	C6-C5	2.13	1.56	1.53
3	A	1181	SIA	C6-C5	2.09	1.56	1.53
2	F	2379	NAG	C4-C5	2.09	1.57	1.53
3	D	2180	SIA	O6-C2	2.08	1.45	1.43
3	G	782	SIA	C4-C5	2.06	1.55	1.53
3	G	782	SIA	C3-C2	2.05	1.54	1.51
5	I	3381	BEZ	C6-C1	2.03	1.43	1.39
5	D	2386	BEZ	C6-C1	2.03	1.43	1.39
5	F	5023	BEZ	C3-C2	2.00	1.43	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3386	BEZ	C5-C4-C3	-5.62	109.49	119.93
5	G	3386	BEZ	C3-C2-C1	5.52	127.50	120.56
5	G	3386	BEZ	C5-C6-C1	5.44	127.39	120.56
5	J	5042	BEZ	C6-C1-C2	-4.71	108.20	117.59
2	F	2379	NAG	O5-C1-C2	-3.47	105.80	111.29
5	A	1385	BEZ	C6-C1-C2	-3.46	110.70	117.59
2	J	4179	NAG	O5-C1-C2	-3.40	105.92	111.29
5	J	5042	BEZ	C3-C2-C1	-3.34	116.37	120.56
2	E	2279	NAG	C2-N2-C7	-3.10	118.49	122.90
2	I	3379	NAG	C2-N2-C7	-3.09	118.50	122.90
2	F	2379	NAG	C1-C2-N2	3.02	115.64	110.49
5	J	5042	BEZ	C5-C6-C1	-3.00	116.78	120.56
5	A	11	BEZ	C5-C4-C3	-2.92	114.51	119.93
5	D	2385	BEZ	C4-C3-C2	-2.82	115.89	120.19
3	J	1082	SIA	C9-C8-C7	-2.77	106.40	112.41
3	B	1280	SIA	C9-C8-C7	-2.75	106.46	112.41
5	H	3387	BEZ	C4-C3-C2	2.73	124.35	120.19
2	B	1279	NAG	C2-N2-C7	-2.62	119.17	122.90
5	D	2385	BEZ	C5-C6-C1	2.59	123.82	120.56
2	F	2379	NAG	C3-C4-C5	2.53	114.76	110.24
5	H	3387	BEZ	C5-C6-C1	-2.41	117.53	120.56
5	A	1385	BEZ	C6-C1-C	2.40	123.59	120.37
3	F	682	SIA	O6-C6-C7	2.39	110.98	107.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	4379	NAG	C2-N2-C7	-2.38	119.52	122.90
5	D	2385	BEZ	C2-C1-C	-2.37	117.19	120.37
5	B	12	BEZ	C2-C1-C	-2.30	117.28	120.37
5	D	2385	BEZ	C4-C5-C6	-2.29	116.71	120.19
3	I	982	SIA	C9-C8-C7	-2.28	107.46	112.41
5	D	2385	BEZ	C6-C1-C2	2.25	122.08	117.59
2	A	1179	NAG	C2-N2-C7	-2.22	119.74	122.90
2	J	4179	NAG	C1-C2-N2	2.20	114.25	110.49
5	H	3387	BEZ	C5-C4-C3	-2.18	115.88	119.93
3	B	1280	SIA	O6-C6-C7	2.17	110.64	107.29
5	C	5013	BEZ	O2-C-C1	2.15	119.95	112.03
2	C	1379	NAG	C2-N2-C7	-2.14	119.86	122.90
2	J	4179	NAG	C4-C3-C2	-2.13	107.90	111.02
2	J	4179	NAG	C2-N2-C7	-2.11	119.90	122.90
5	G	3386	BEZ	C6-C1-C2	-2.10	113.41	117.59
5	I	3380	BEZ	C3-C2-C1	2.09	123.19	120.56
2	D	2179	NAG	C2-N2-C7	-2.06	119.96	122.90
2	G	3179	NAG	C3-C4-C5	2.01	113.83	110.24

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1279	NAG	C1
2	J	4179	NAG	C1
2	F	2379	NAG	C1
2	G	3179	NAG	C1
2	K	4279	NAG	C1

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1182	SIA	C5-C6-C7-C8
3	K	1182	SIA	C5-C6-C7-O7
3	K	1182	SIA	O6-C6-C7-C8
3	K	1182	SIA	O6-C6-C7-O7
3	K	1182	SIA	C11-C10-N5-C5
3	K	1182	SIA	O10-C10-N5-C5
2	H	3279	NAG	C8-C7-N2-C2
2	H	3279	NAG	O7-C7-N2-C2
3	A	1181	SIA	C4-C5-N5-C10
3	A	1181	SIA	C5-C6-C7-C8
3	A	1181	SIA	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
3	A	1181	SIA	O6-C6-C7-C8
3	A	1181	SIA	O6-C6-C7-O7
3	A	1181	SIA	C11-C10-N5-C5
3	A	1181	SIA	O10-C10-N5-C5
3	J	1082	SIA	C5-C6-C7-C8
3	J	1082	SIA	C5-C6-C7-O7
3	J	1082	SIA	O6-C6-C7-C8
3	J	1082	SIA	O6-C6-C7-O7
3	J	1082	SIA	C11-C10-N5-C5
3	J	1082	SIA	O10-C10-N5-C5
3	F	682	SIA	O6-C6-C7-O7
3	F	682	SIA	C11-C10-N5-C5
3	F	682	SIA	O10-C10-N5-C5
2	I	3379	NAG	C8-C7-N2-C2
2	I	3379	NAG	O7-C7-N2-C2
2	B	1279	NAG	C8-C7-N2-C2
2	B	1279	NAG	O7-C7-N2-C2
2	E	2279	NAG	C8-C7-N2-C2
2	E	2279	NAG	O7-C7-N2-C2
2	J	4179	NAG	C8-C7-N2-C2
2	J	4179	NAG	O7-C7-N2-C2
3	I	982	SIA	C5-C6-C7-C8
3	I	982	SIA	C5-C6-C7-O7
3	I	982	SIA	O6-C6-C7-C8
3	I	982	SIA	O6-C6-C7-O7
3	I	982	SIA	C11-C10-N5-C5
3	I	982	SIA	O10-C10-N5-C5
3	L	1282	SIA	C4-C5-N5-C10
3	L	1282	SIA	C5-C6-C7-C8
3	L	1282	SIA	C5-C6-C7-O7
3	L	1282	SIA	O6-C6-C7-C8
3	L	1282	SIA	O6-C6-C7-O7
3	L	1282	SIA	C11-C10-N5-C5
3	L	1282	SIA	O10-C10-N5-C5
3	D	2180	SIA	C5-C6-C7-C8
3	D	2180	SIA	C5-C6-C7-O7
3	D	2180	SIA	O6-C6-C7-C8
3	D	2180	SIA	O6-C6-C7-O7
3	D	2180	SIA	C11-C10-N5-C5
3	D	2180	SIA	O10-C10-N5-C5
2	F	2379	NAG	C8-C7-N2-C2
2	F	2379	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	A	1179	NAG	C8-C7-N2-C2
2	A	1179	NAG	O7-C7-N2-C2
3	E	582	SIA	C5-C6-C7-C8
3	E	582	SIA	C5-C6-C7-O7
3	E	582	SIA	O6-C6-C7-C8
3	E	582	SIA	O6-C6-C7-O7
3	E	582	SIA	C6-C7-C8-C9
3	E	582	SIA	C6-C7-C8-O8
3	E	582	SIA	O7-C7-C8-C9
3	E	582	SIA	O7-C7-C8-O8
3	E	582	SIA	C11-C10-N5-C5
3	E	582	SIA	O10-C10-N5-C5
2	G	3179	NAG	C8-C7-N2-C2
2	G	3179	NAG	O7-C7-N2-C2
3	G	782	SIA	C5-C6-C7-C8
3	G	782	SIA	C5-C6-C7-O7
3	G	782	SIA	O6-C6-C7-C8
3	G	782	SIA	O6-C6-C7-O7
3	G	782	SIA	C11-C10-N5-C5
3	G	782	SIA	O10-C10-N5-C5
2	K	4279	NAG	C8-C7-N2-C2
2	K	4279	NAG	O7-C7-N2-C2
3	B	1280	SIA	C4-C5-N5-C10
3	B	1280	SIA	C5-C6-C7-C8
3	B	1280	SIA	C5-C6-C7-O7
3	B	1280	SIA	O6-C6-C7-C8
3	B	1280	SIA	O6-C6-C7-O7
3	B	1280	SIA	C11-C10-N5-C5
3	B	1280	SIA	O10-C10-N5-C5
2	L	4379	NAG	C8-C7-N2-C2
2	L	4379	NAG	O7-C7-N2-C2
2	C	1379	NAG	C8-C7-N2-C2
2	C	1379	NAG	O7-C7-N2-C2
3	H	882	SIA	C4-C5-N5-C10
3	H	882	SIA	C5-C6-C7-C8
3	H	882	SIA	C5-C6-C7-O7
3	H	882	SIA	O6-C6-C7-C8
3	H	882	SIA	O6-C6-C7-O7
3	H	882	SIA	C11-C10-N5-C5
3	H	882	SIA	O10-C10-N5-C5
3	A	1180	SIA	C5-C6-C7-C8
3	A	1180	SIA	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
3	A	1180	SIA	O6-C6-C7-C8
3	A	1180	SIA	O6-C6-C7-O7
3	A	1180	SIA	C11-C10-N5-C5
3	A	1180	SIA	O10-C10-N5-C5
2	L	4379	NAG	C1-C2-N2-C7
2	A	1179	NAG	O5-C5-C6-O6
2	A	1179	NAG	C4-C5-C6-O6
2	G	3179	NAG	O5-C5-C6-O6
3	K	1182	SIA	O8-C8-C9-O9
2	J	4179	NAG	C4-C5-C6-O6
3	K	1182	SIA	C6-C5-N5-C10
3	K	1182	SIA	C7-C8-C9-O9
2	G	3179	NAG	C4-C5-C6-O6
2	B	1279	NAG	C1-C2-N2-C7
2	C	1379	NAG	O5-C5-C6-O6
2	D	2179	NAG	C8-C7-N2-C2
3	I	982	SIA	C7-C8-C9-O9
2	J	4179	NAG	O5-C5-C6-O6
2	H	3279	NAG	C1-C2-N2-C7
2	A	1179	NAG	C1-C2-N2-C7
3	J	1082	SIA	C7-C8-C9-O9
2	D	2179	NAG	O7-C7-N2-C2
3	K	1182	SIA	C4-C5-N5-C10
3	F	682	SIA	C4-C5-N5-C10
3	I	982	SIA	C4-C5-N5-C10
2	K	4279	NAG	O5-C5-C6-O6
3	I	982	SIA	O8-C8-C9-O9
3	L	1282	SIA	C7-C8-C9-O9
2	H	3279	NAG	C4-C5-C6-O6
3	A	1181	SIA	C7-C8-C9-O9
2	I	3379	NAG	C1-C2-N2-C7
2	H	3279	NAG	O5-C5-C6-O6
2	L	4379	NAG	C3-C2-N2-C7
3	D	2180	SIA	O7-C7-C8-O8
2	L	4379	NAG	C4-C5-C6-O6
3	I	982	SIA	C6-C5-N5-C10
3	D	2180	SIA	O7-C7-C8-C9
3	F	682	SIA	C6-C5-N5-C10
3	D	2180	SIA	C6-C7-C8-C9
3	L	1282	SIA	O8-C8-C9-O9
2	B	1279	NAG	C4-C5-C6-O6
2	H	3279	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	A	1179	NAG	C3-C2-N2-C7
3	B	1280	SIA	C7-C8-C9-O9
3	I	982	SIA	O7-C7-C8-C9
2	L	4379	NAG	O5-C5-C6-O6
3	J	1082	SIA	O8-C8-C9-O9

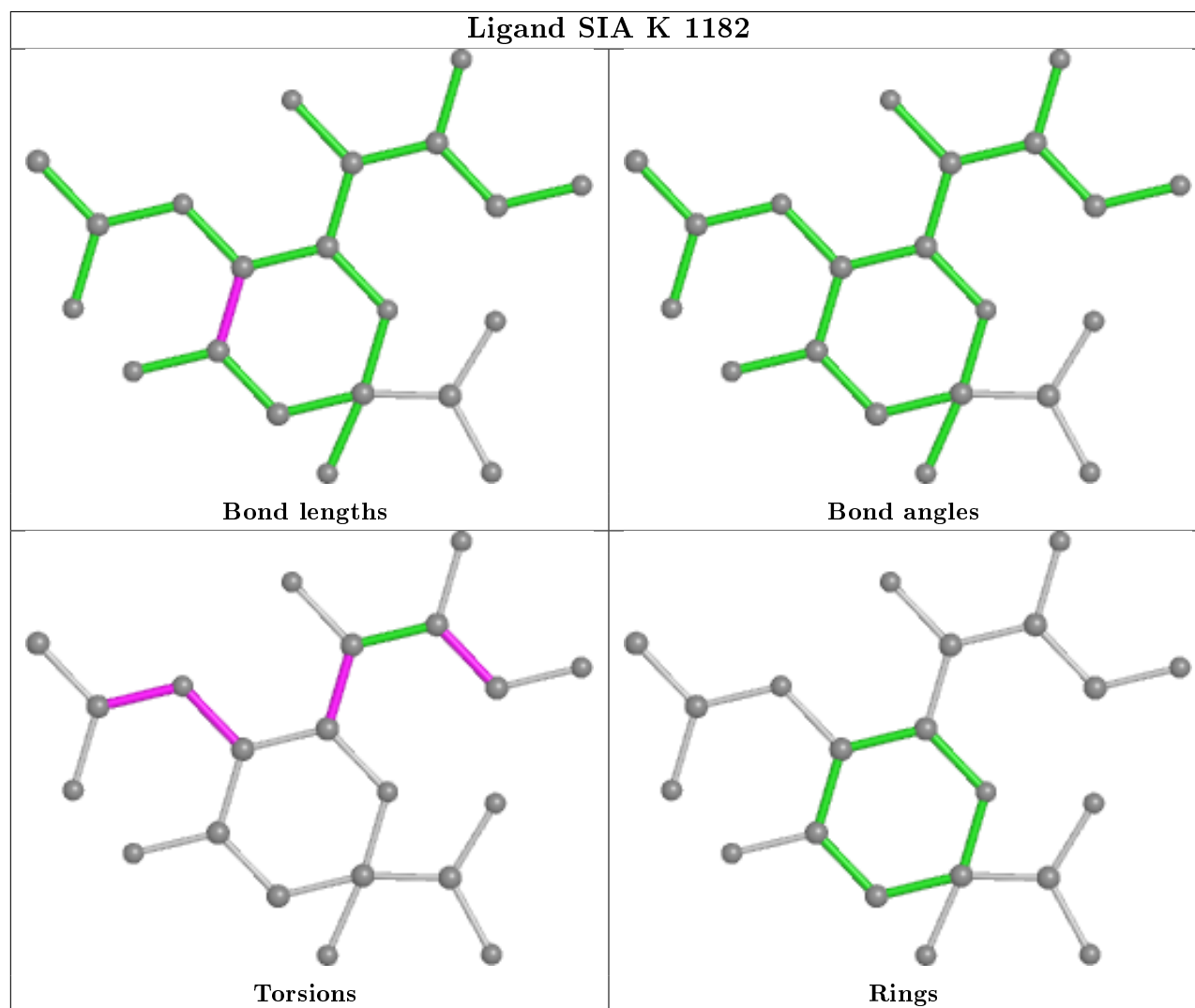
There are no ring outliers.

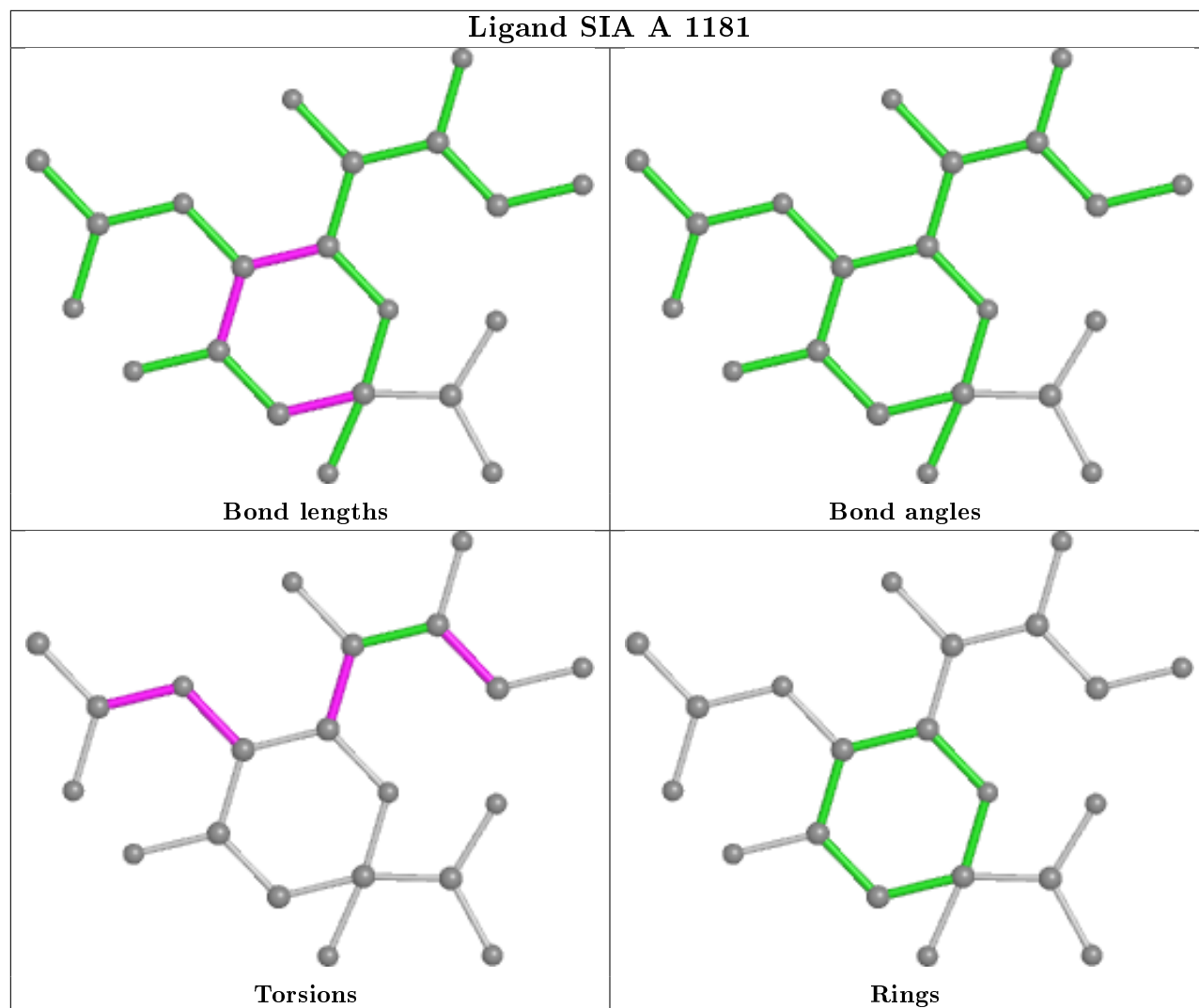
28 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1182	SIA	7	0
4	I	3285	SO4	1	0
5	A	1385	BEZ	2	0
3	A	1181	SIA	10	0
3	J	1082	SIA	5	0
3	F	682	SIA	1	0
5	C	5013	BEZ	3	0
5	H	3386	BEZ	1	0
5	C	5014	BEZ	1	0
3	E	582	SIA	2	0
3	I	982	SIA	5	0
5	G	3385	BEZ	1	0
2	B	1279	NAG	1	0
2	J	4179	NAG	1	0
3	L	1282	SIA	7	0
5	L	4380	BEZ	1	0
3	D	2180	SIA	8	0
2	F	2379	NAG	3	0
2	G	3179	NAG	1	0
3	G	782	SIA	6	0
5	D	2385	BEZ	3	0
5	J	5042	BEZ	1	0
2	K	4279	NAG	2	0
3	B	1280	SIA	5	0
5	B	12	BEZ	6	0
3	H	882	SIA	1	0
5	I	3380	BEZ	1	0
3	A	1180	SIA	3	0

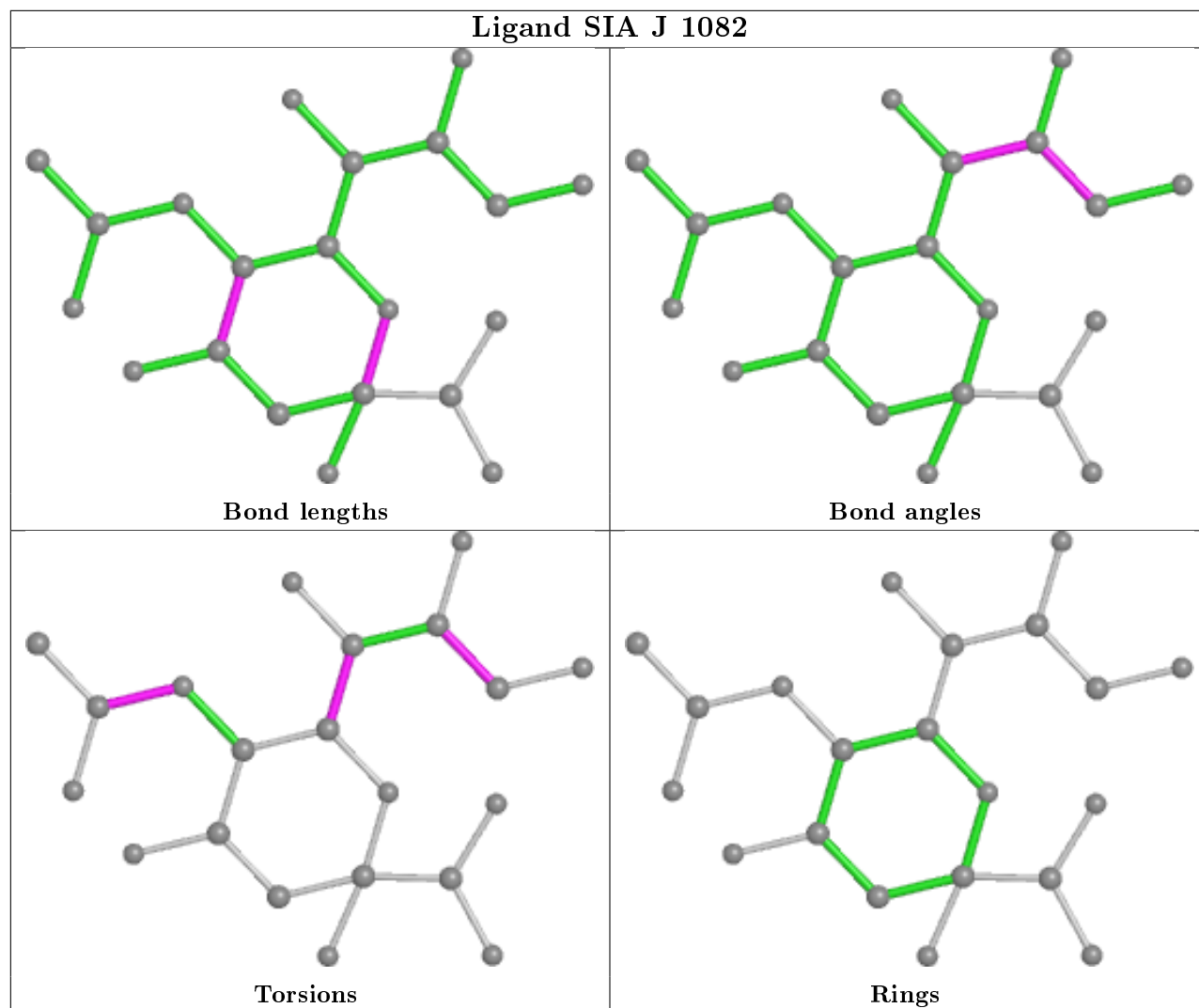
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

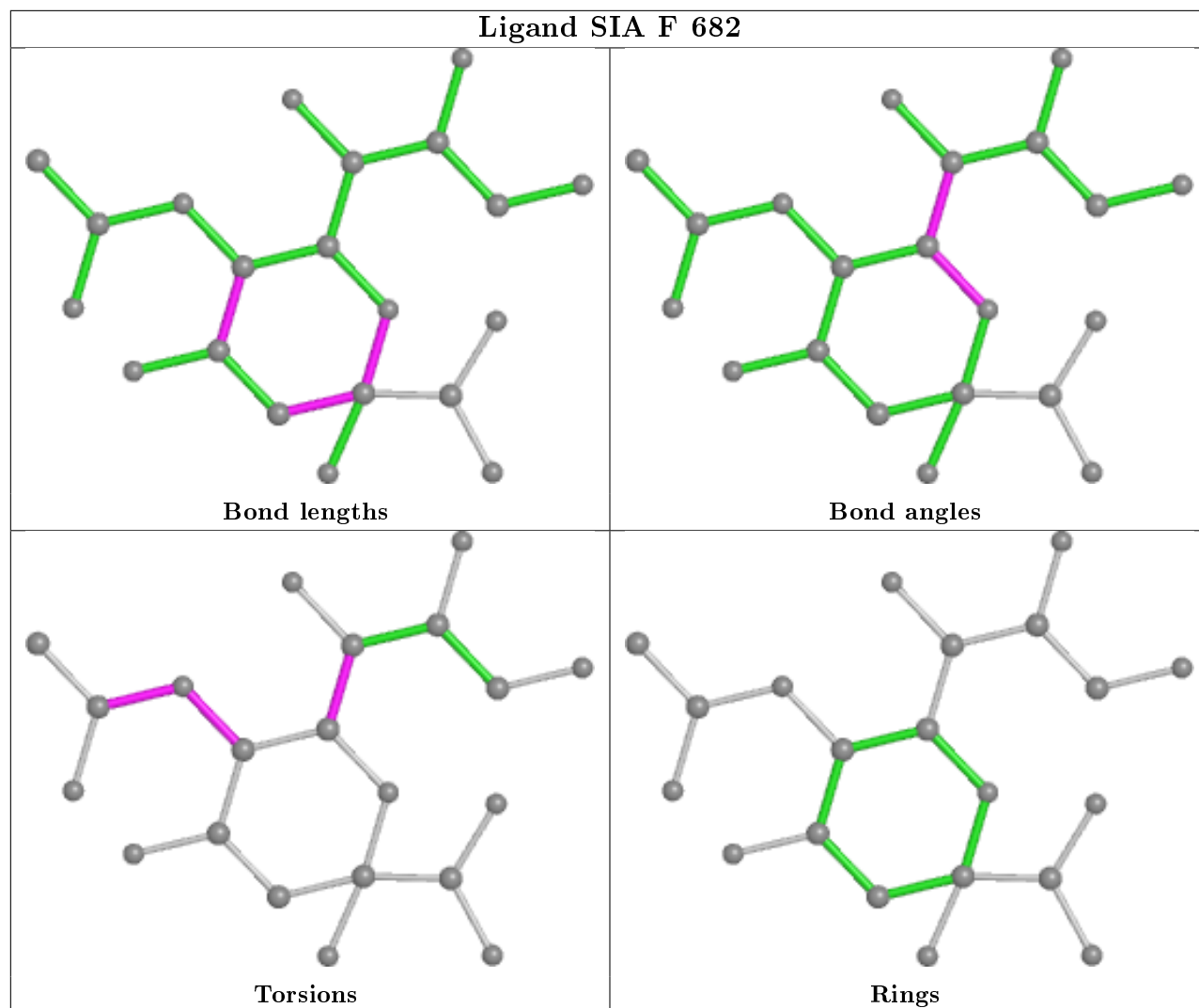




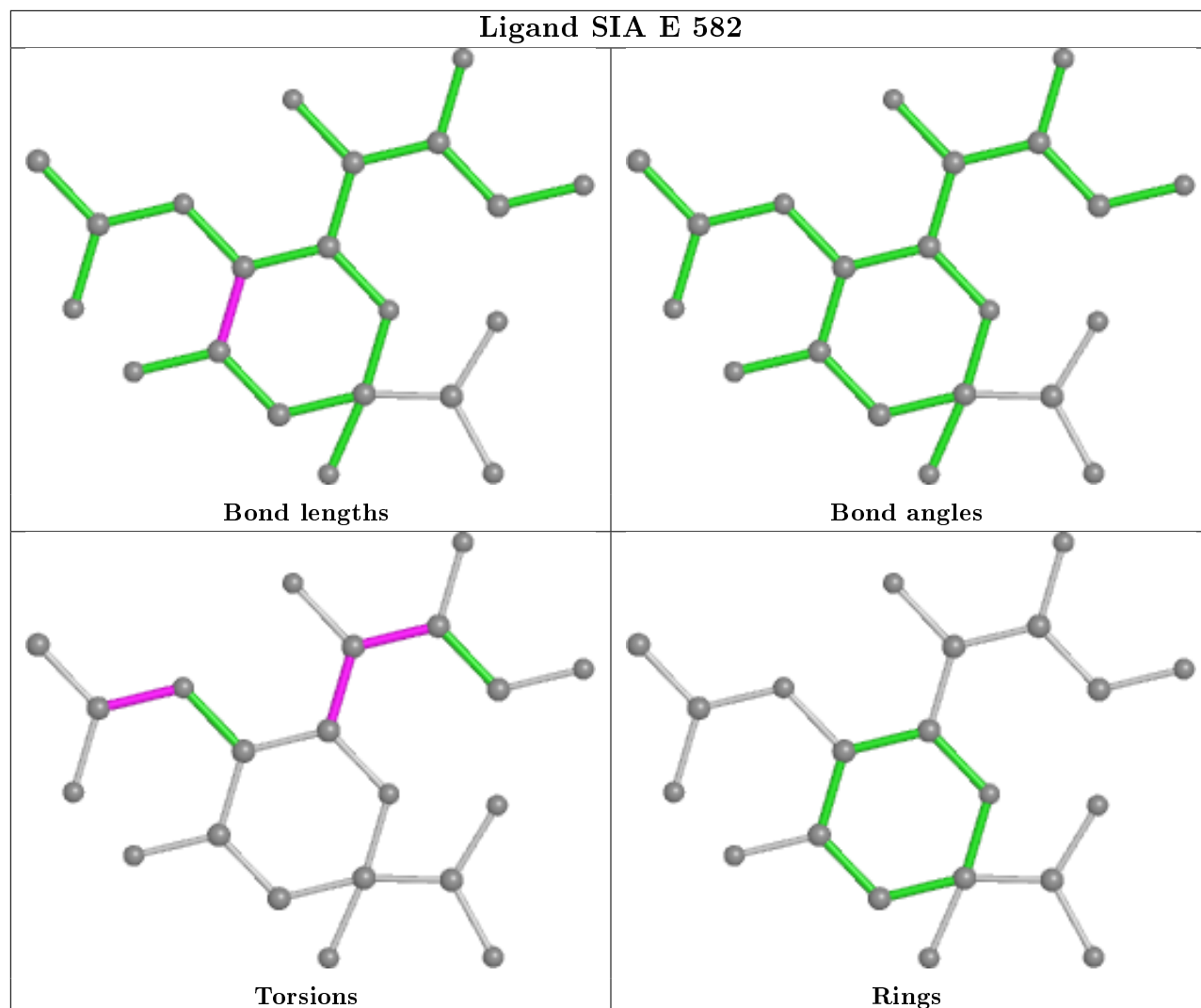
Ligand SIA J 1082



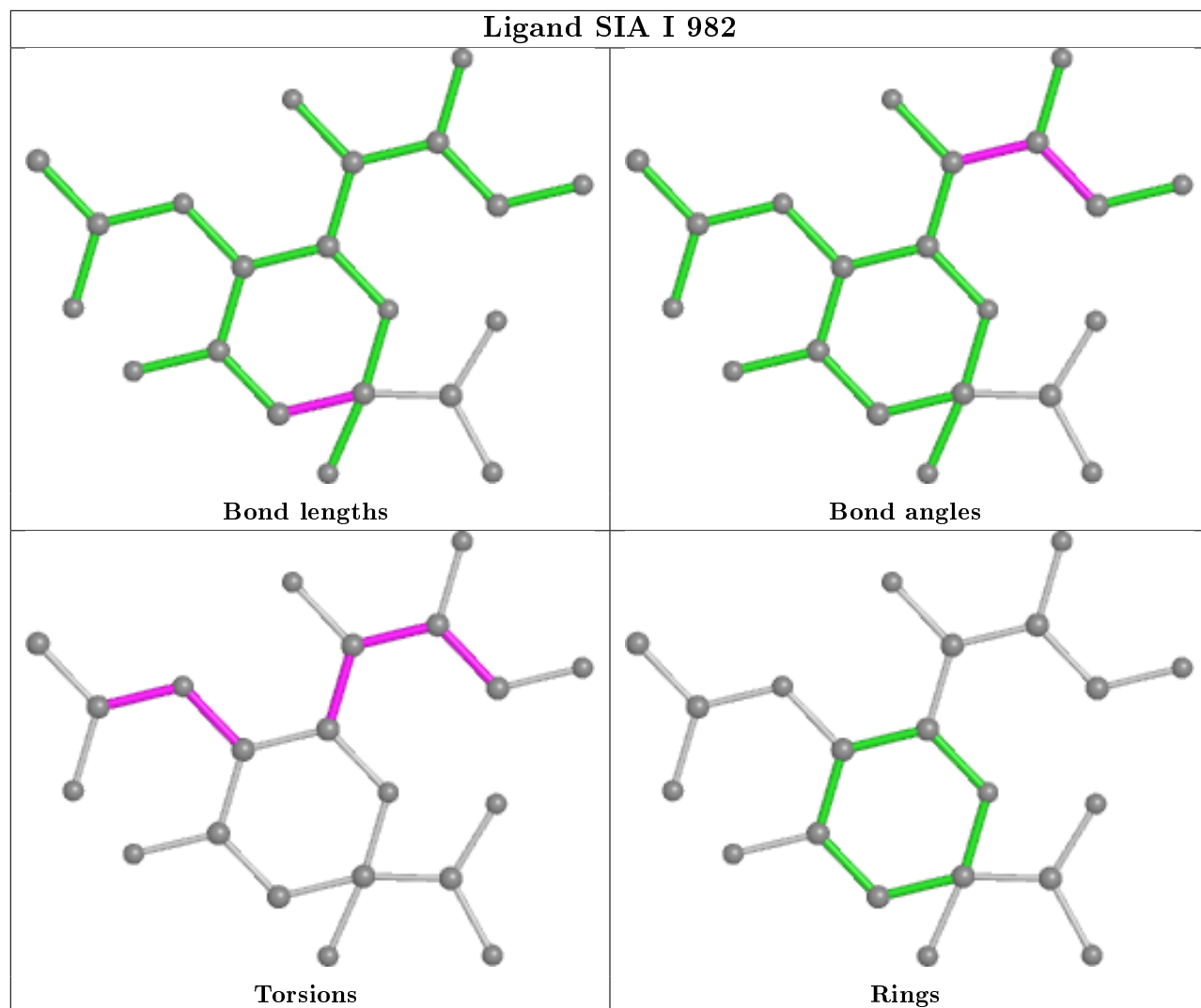
Ligand SIA F 682



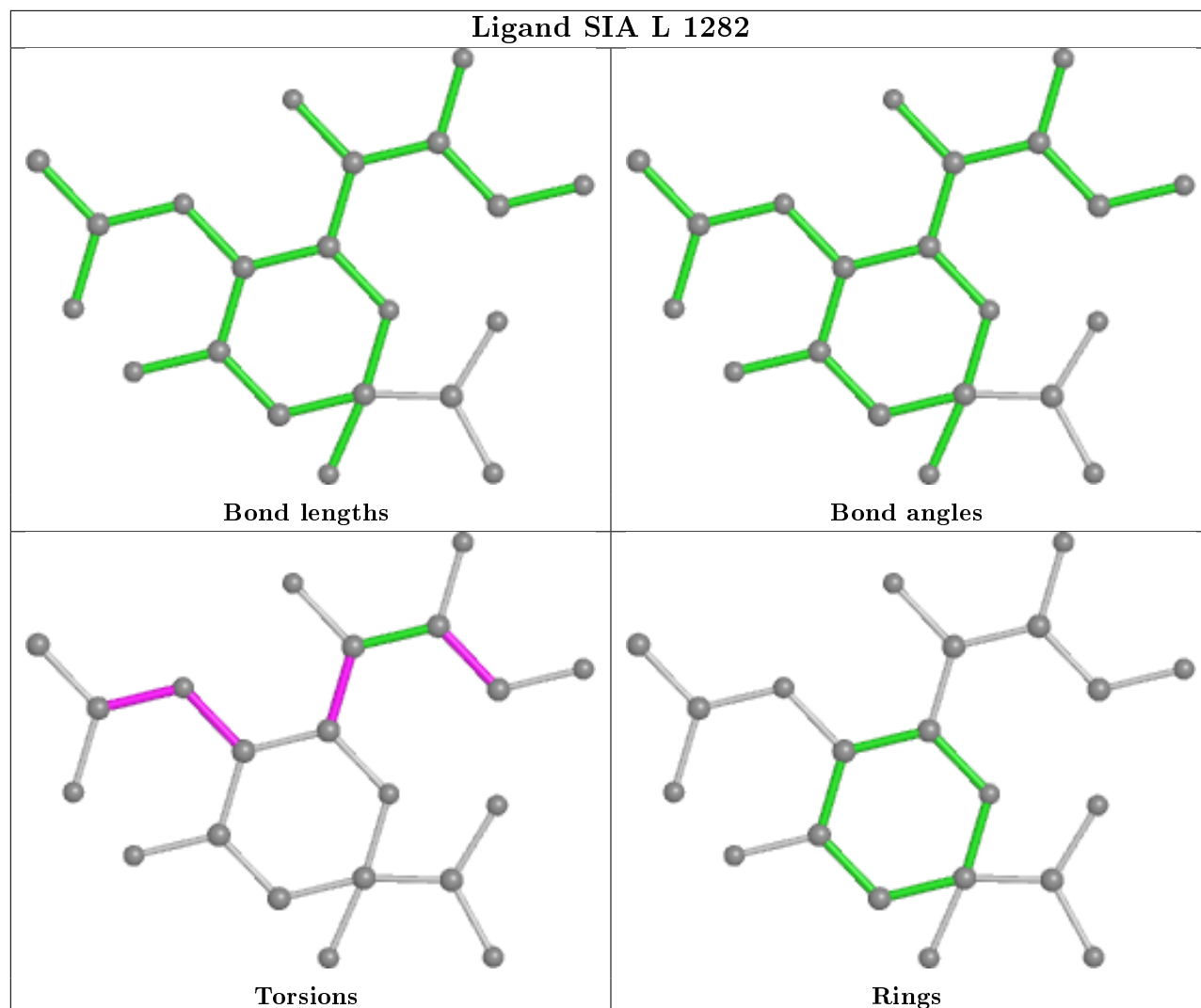
Ligand SIA E 582

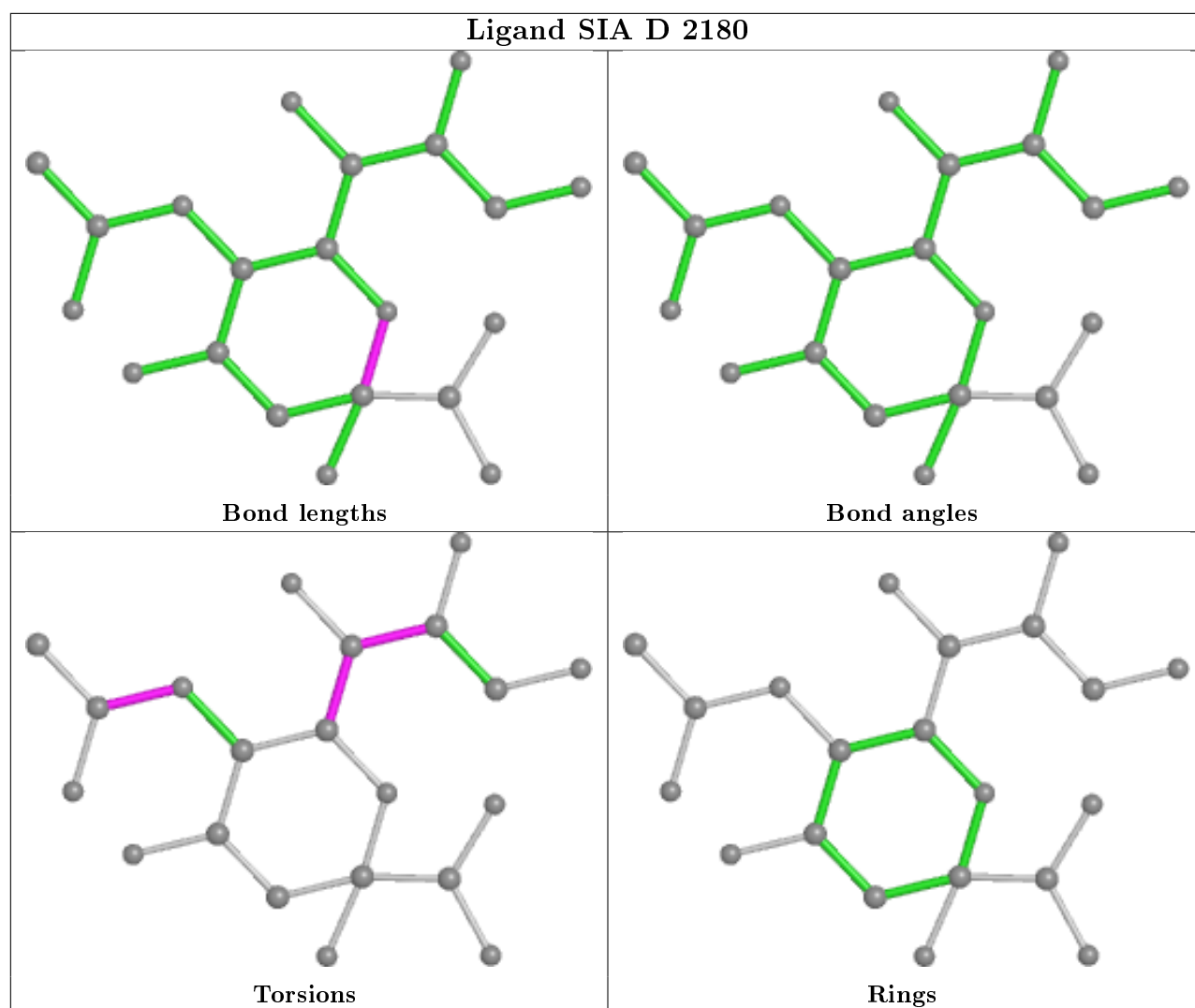


Ligand SIA I 982

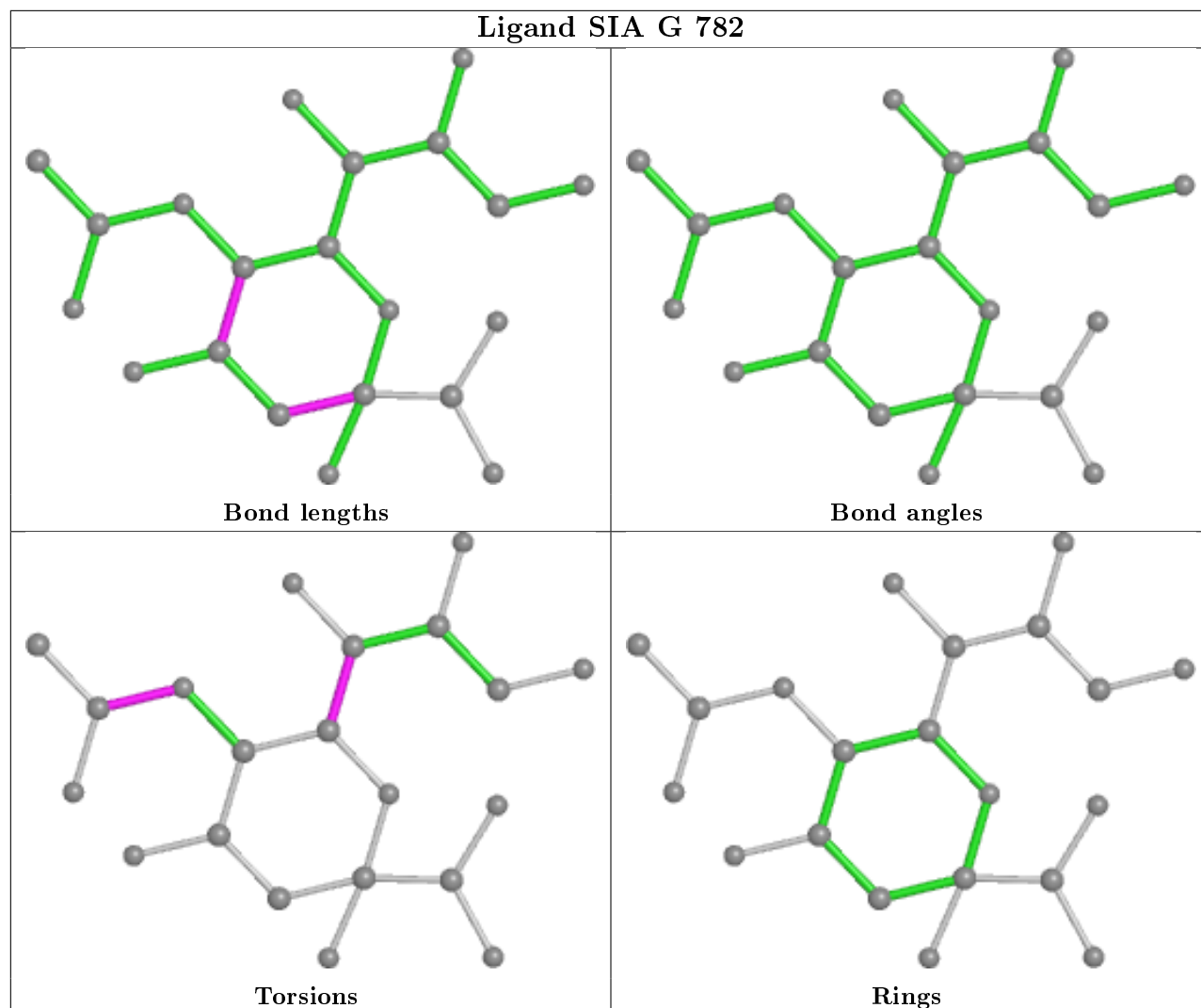


Ligand SIA L 1282

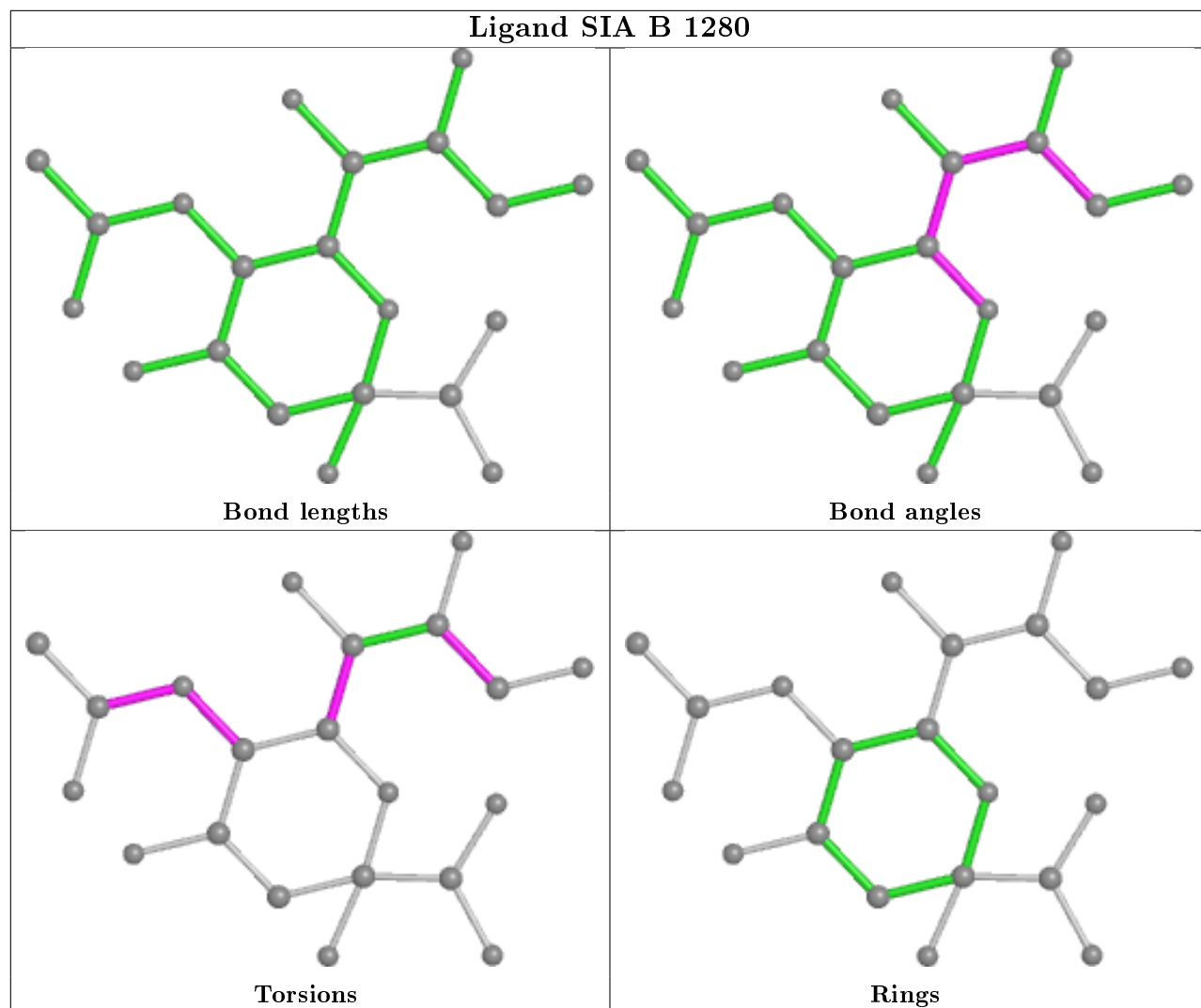




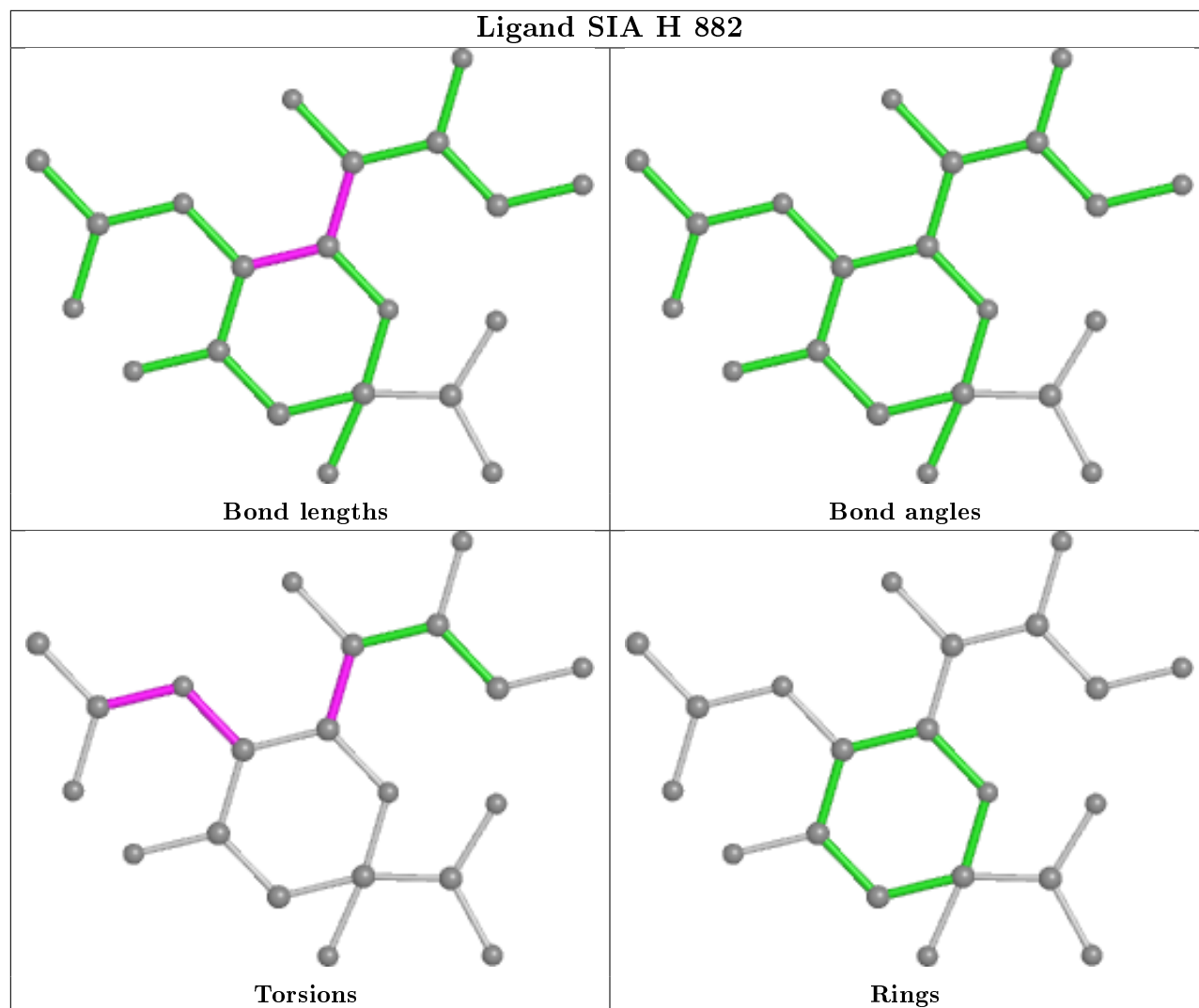
Ligand SIA G 782

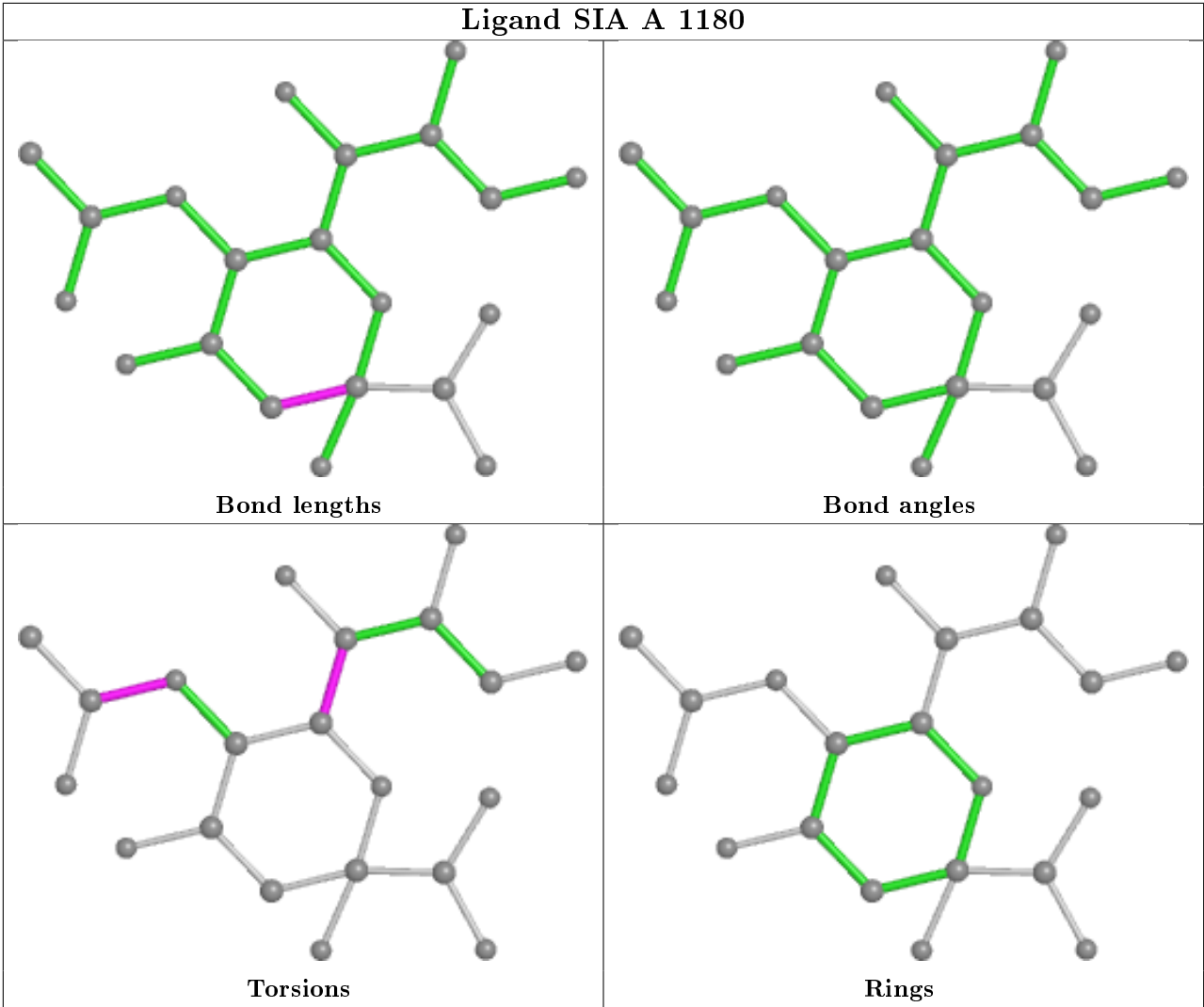


Ligand SIA B 1280



Ligand SIA H 882





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	550:LEU	C	551:PHE	N	1.00

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	532/532 (100%)	-0.06	1 (0%) 95 94	2, 25, 69, 83	0
1	B	532/532 (100%)	0.01	5 (0%) 84 75	4, 29, 74, 86	0
1	C	532/532 (100%)	-0.03	3 (0%) 89 83	2, 26, 64, 85	0
1	D	532/532 (100%)	-0.05	3 (0%) 89 83	2, 25, 70, 84	0
1	E	532/532 (100%)	0.01	5 (0%) 84 75	4, 30, 73, 86	0
1	F	532/532 (100%)	-0.05	5 (0%) 84 75	3, 26, 65, 81	0
1	G	532/532 (100%)	-0.08	0 100 100	3, 26, 67, 85	0
1	H	532/532 (100%)	-0.02	3 (0%) 89 83	3, 27, 71, 84	0
1	I	532/532 (100%)	0.05	8 (1%) 73 61	3, 31, 74, 85	0
1	J	532/532 (100%)	-0.04	2 (0%) 92 89	2, 26, 64, 83	0
1	K	532/532 (100%)	-0.01	3 (0%) 89 83	3, 27, 71, 85	0
1	L	532/532 (100%)	0.02	2 (0%) 92 89	2, 31, 73, 83	0
All	All	6384/6384 (100%)	-0.02	40 (0%) 89 83	2, 27, 70, 86	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	306	LEU	4.5
1	E	307	ASP	3.9
1	H	400	THR	3.7
1	A	315	SER	3.4
1	I	318	LEU	3.2
1	I	317	PRO	3.2
1	H	396	ILE	3.1
1	D	368	LEU	2.8
1	I	311	ASP	2.8
1	F	371	GLY	2.8
1	C	318	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	340	ASN	2.6
1	E	373	LEU	2.6
1	C	317	PRO	2.6
1	J	336	GLN	2.6
1	B	395	LEU	2.5
1	I	404	LEU	2.4
1	E	314	GLU	2.4
1	I	249	VAL	2.4
1	K	317	PRO	2.4
1	F	509	PRO	2.4
1	D	367	PRO	2.3
1	F	508	ASN	2.3
1	D	383	TRP	2.3
1	I	306	LEU	2.3
1	L	317	PRO	2.3
1	K	312	PRO	2.2
1	C	341	PHE	2.2
1	L	406	GLY	2.2
1	F	207	SER	2.2
1	J	373	LEU	2.2
1	B	307	ASP	2.1
1	B	318	LEU	2.1
1	E	236	ALA	2.1
1	H	307	ASP	2.1
1	B	388	LEU	2.1
1	F	342	HIS	2.0
1	B	387	PRO	2.0
1	I	339	ARG	2.0
1	I	372	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1179	14/15	0.76	0.53	70,76,78,78	0
2	NAG	H	3279	14/15	0.83	0.28	63,66,69,69	0
5	BEZ	H	3387	9/9	0.84	0.21	41,43,45,46	0
4	SO4	A	1384	5/5	0.84	0.38	76,76,77,77	0
5	BEZ	L	4380	9/9	0.85	0.55	59,59,60,60	0
4	SO4	C	1185	5/5	0.85	0.28	100,100,101,101	0
2	NAG	K	4279	14/15	0.85	0.23	63,67,71,71	0
5	BEZ	B	1386	9/9	0.85	0.23	54,55,56,56	0
4	SO4	K	4385	5/5	0.85	0.44	97,98,98,99	0
4	SO4	F	2185	5/5	0.86	0.28	106,106,106,106	0
4	SO4	H	3385	5/5	0.86	0.28	97,97,97,97	0
3	SIA	B	1280	21/21	0.86	0.28	45,61,66,67	0
2	NAG	D	2179	14/15	0.86	0.45	70,76,78,79	0
2	NAG	G	3179	14/15	0.86	0.24	67,72,75,75	0
4	SO4	D	2184	5/5	0.87	0.38	100,100,101,101	0
2	NAG	J	4179	14/15	0.87	0.36	69,75,78,78	0
4	SO4	J	4185	5/5	0.87	0.25	96,96,97,97	0
5	BEZ	K	4386	9/9	0.87	0.54	48,49,50,50	0
5	BEZ	B	12	9/9	0.88	0.41	52,53,54,55	0
3	SIA	J	1082	21/21	0.88	0.28	59,71,76,77	0
3	SIA	A	1180	21/21	0.88	0.25	64,71,74,75	0
5	BEZ	L	4381	9/9	0.88	0.20	54,55,55,55	0
3	SIA	E	582	21/21	0.89	0.24	42,60,70,70	0
5	BEZ	A	1385	9/9	0.89	0.19	49,50,52,52	0
3	SIA	I	982	21/21	0.89	0.29	51,60,64,65	0
2	NAG	C	1379	14/15	0.89	0.23	59,64,68,68	0
3	SIA	H	882	21/21	0.89	0.23	52,66,69,70	0
4	SO4	I	3185	5/5	0.89	0.27	95,95,96,96	0
5	BEZ	C	5014	9/9	0.89	0.20	36,40,40,41	0
5	BEZ	G	3385	9/9	0.89	0.32	58,59,60,60	0
3	SIA	A	1181	21/21	0.90	0.20	44,57,67,68	0
3	SIA	D	2180	21/21	0.90	0.27	57,69,72,73	0
5	BEZ	I	3381	9/9	0.90	0.19	52,52,53,54	0
2	NAG	F	2379	14/15	0.90	0.16	59,64,66,66	0
5	BEZ	K	4387	9/9	0.90	0.26	36,39,40,41	0
5	BEZ	G	3386	9/9	0.90	0.20	45,47,48,49	0
3	SIA	G	782	21/21	0.90	0.27	61,69,73,74	0

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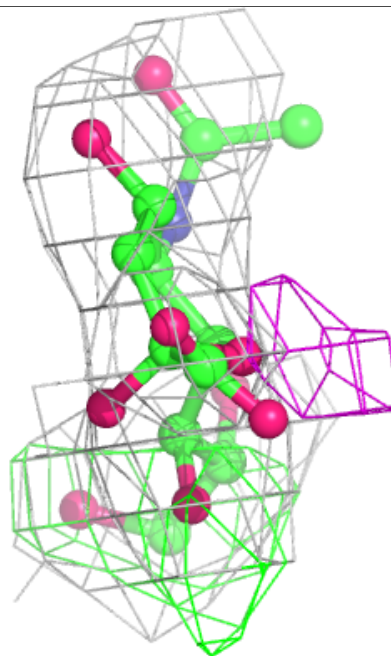
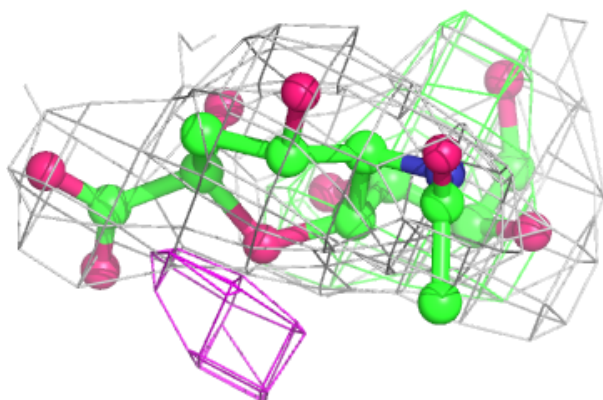
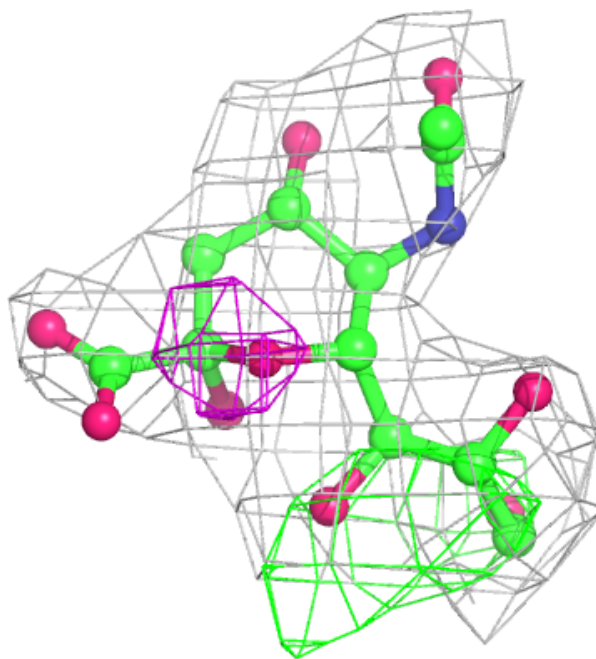
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	BEZ	D	2385	9/9	0.90	0.44	51,51,53,53	0
2	NAG	I	3379	14/15	0.91	0.32	57,61,62,63	0
5	BEZ	I	3380	9/9	0.91	0.33	53,53,54,55	0
5	BEZ	F	5024	9/9	0.91	0.23	42,44,46,46	0
2	NAG	L	4379	14/15	0.91	0.23	56,59,62,63	0
3	SIA	F	682	21/21	0.92	0.25	52,56,62,62	0
5	BEZ	E	2386	9/9	0.92	0.15	47,47,49,50	0
3	SIA	L	1282	21/21	0.92	0.24	50,55,63,65	0
5	BEZ	E	2387	9/9	0.92	0.22	42,43,43,44	0
4	SO4	D	2384	5/5	0.92	0.34	76,77,77,77	0
3	SIA	K	1182	21/21	0.93	0.23	60,63,67,69	0
2	NAG	B	1279	14/15	0.93	0.30	59,64,68,70	0
4	SO4	B	1385	5/5	0.93	0.16	96,97,97,98	0
5	BEZ	D	2386	9/9	0.93	0.16	44,45,46,46	0
4	SO4	F	2285	5/5	0.93	0.24	80,80,81,81	0
4	SO4	B	1284	5/5	0.94	0.23	80,80,81,81	0
4	SO4	J	4384	5/5	0.94	0.19	84,85,85,86	0
4	SO4	J	4184	5/5	0.94	0.22	94,94,95,95	0
4	SO4	E	2284	5/5	0.94	0.16	85,86,86,86	0
5	BEZ	H	3386	9/9	0.94	0.26	49,51,51,51	0
4	SO4	H	3284	5/5	0.94	0.33	84,84,85,85	0
2	NAG	E	2279	14/15	0.94	0.29	57,60,62,63	0
4	SO4	E	2385	5/5	0.94	0.17	94,94,94,95	0
5	BEZ	A	11	9/9	0.94	0.43	49,51,52,52	0
4	SO4	I	3285	5/5	0.95	0.23	79,79,79,80	0
4	SO4	K	4284	5/5	0.95	0.29	85,85,86,86	0
4	SO4	G	3384	5/5	0.95	0.33	81,81,81,81	0
5	BEZ	J	5042	9/9	0.95	0.16	44,45,46,46	0
5	BEZ	F	5023	8/9	0.96	0.24	46,49,50,51	0
4	SO4	L	4285	5/5	0.96	0.25	74,74,75,75	0
4	SO4	C	1285	5/5	0.96	0.19	76,76,77,77	0
5	BEZ	J	5041	8/9	0.96	0.35	41,45,45,46	0
4	SO4	G	3184	5/5	0.96	0.27	86,86,87,88	0
4	SO4	A	1184	5/5	0.96	0.28	94,94,94,95	0
5	BEZ	C	5013	8/9	0.97	0.20	40,44,46,46	0

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

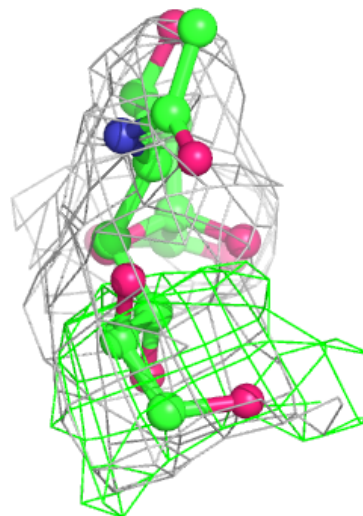
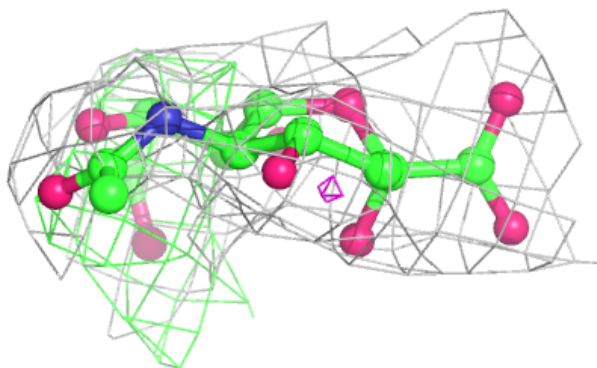
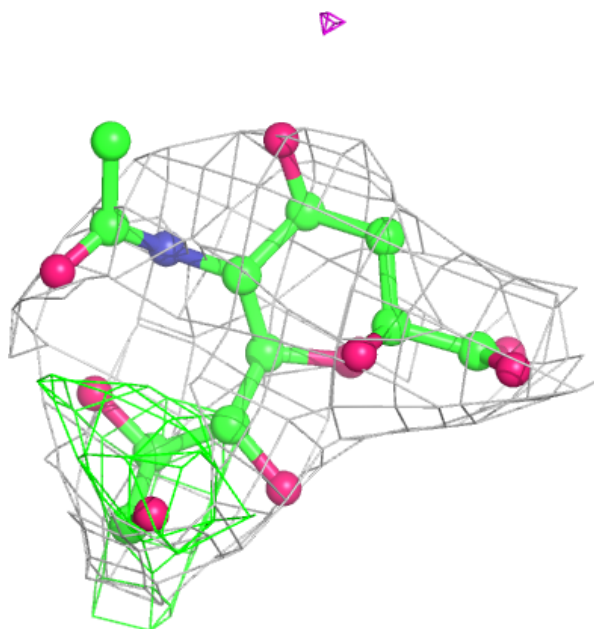
Electron density around SIA B 1280:

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



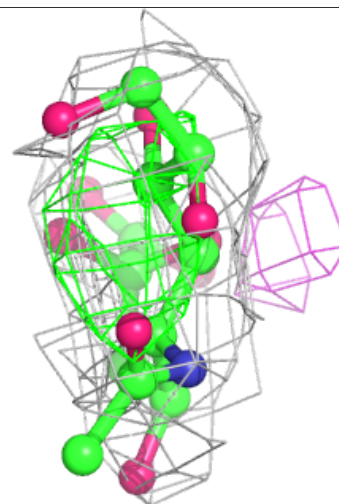
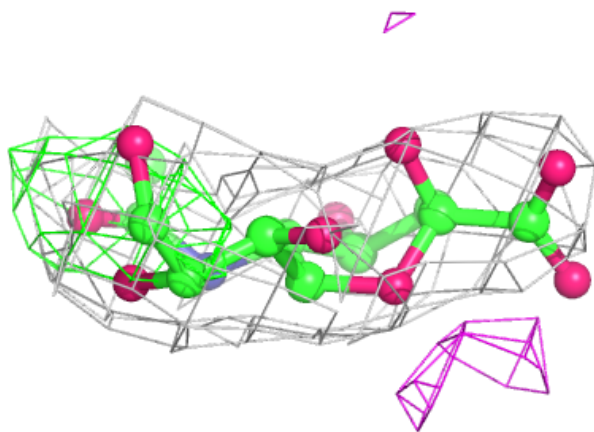
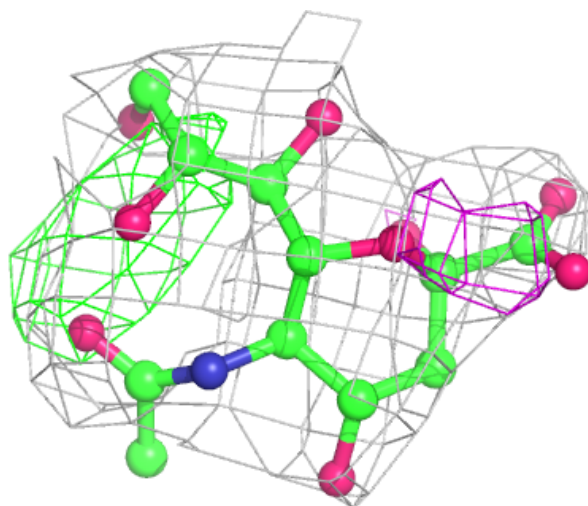
Electron density around SIA J 1082:

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



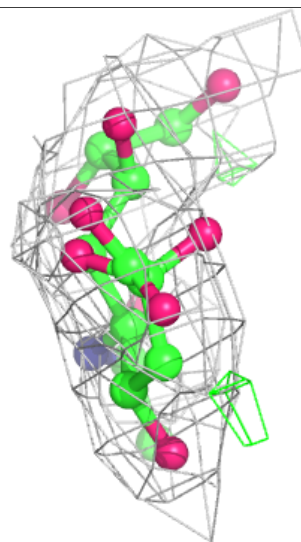
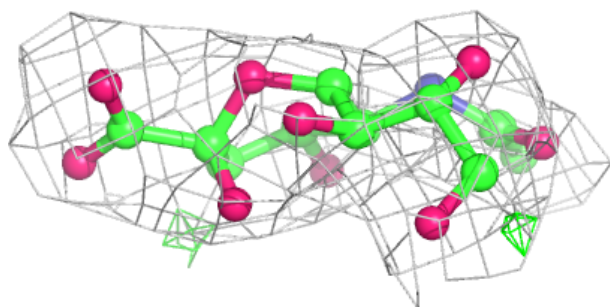
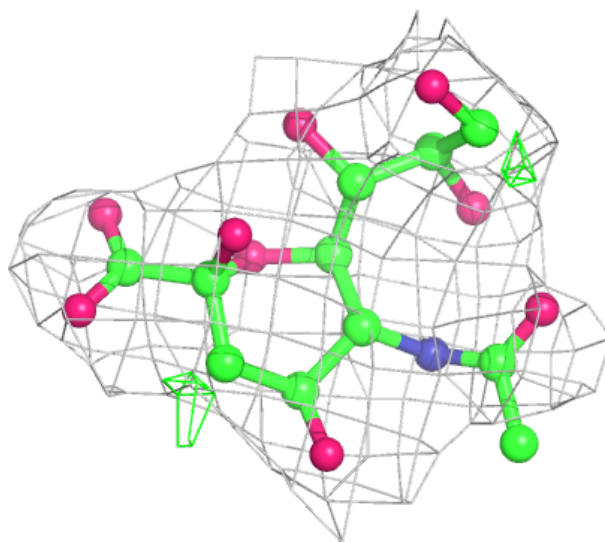
Electron density around SIA A 1180:

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



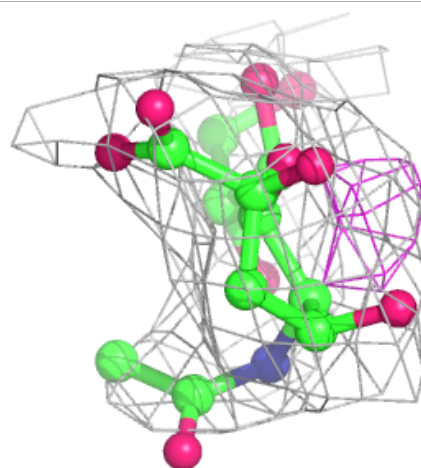
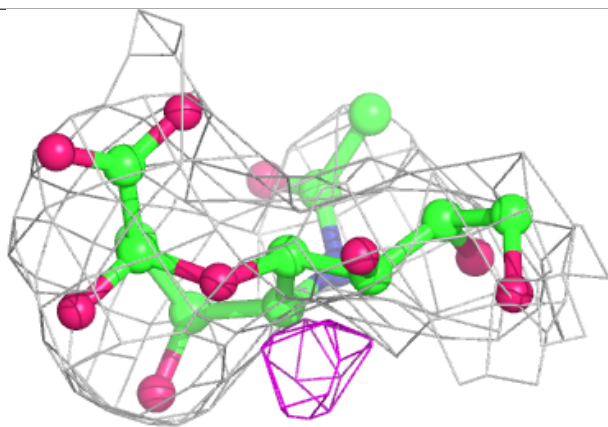
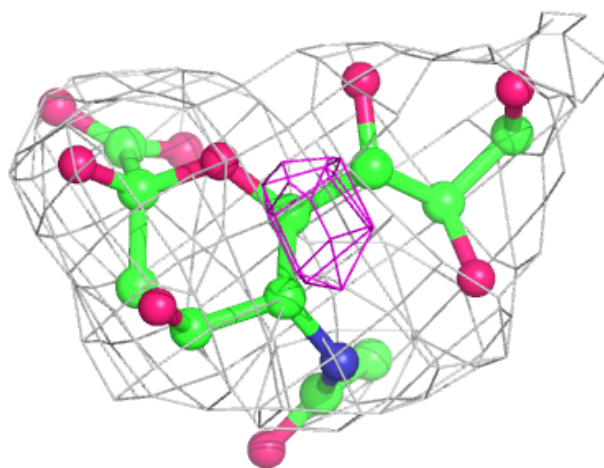
Electron density around SIA E 582:

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



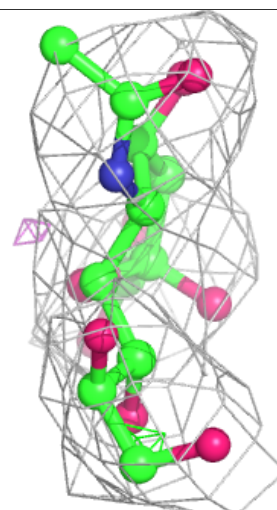
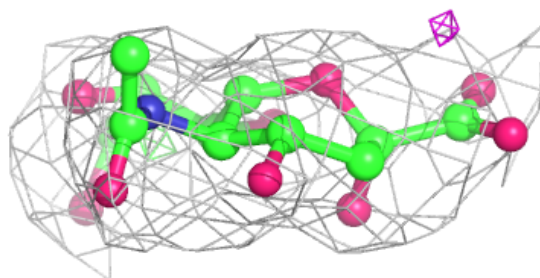
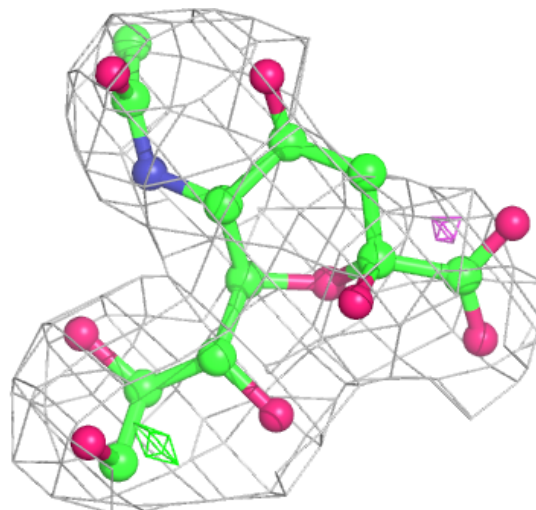
Electron density around SIA I 982:

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



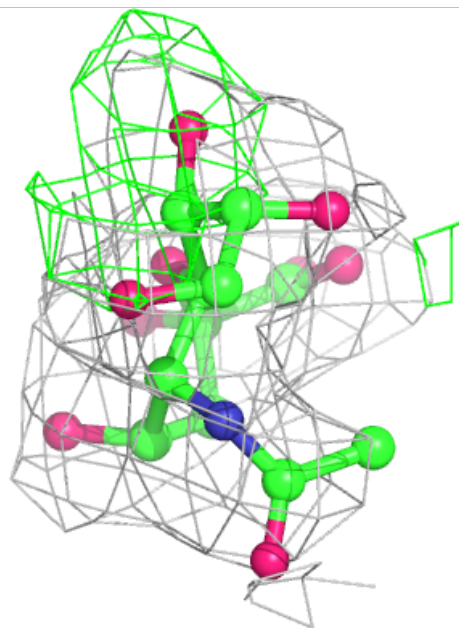
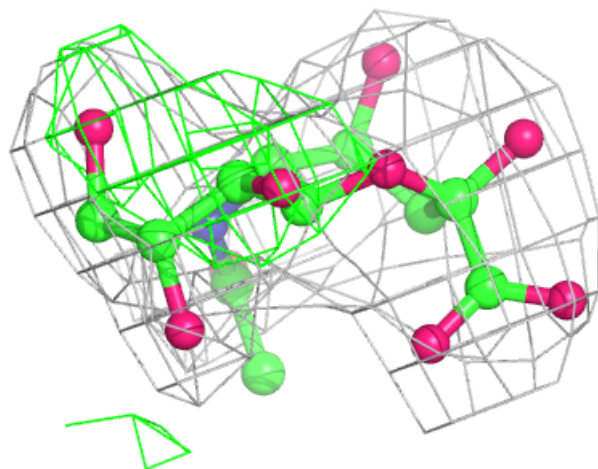
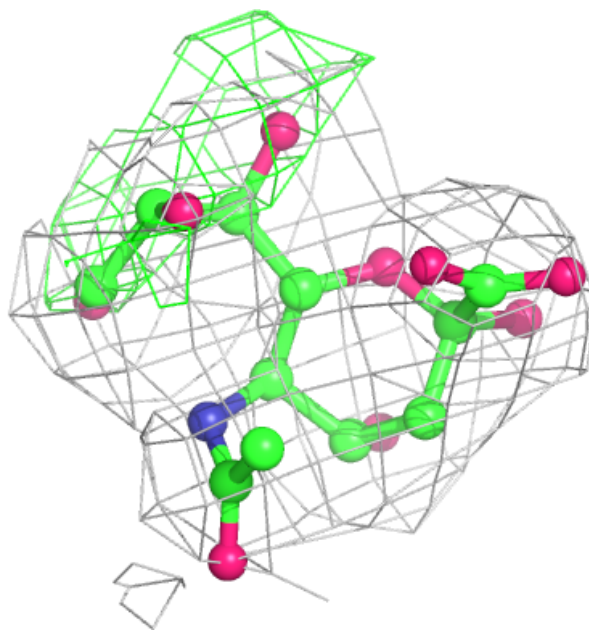
Electron density around SIA H 882:

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



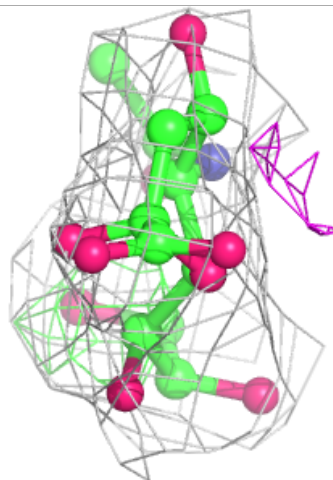
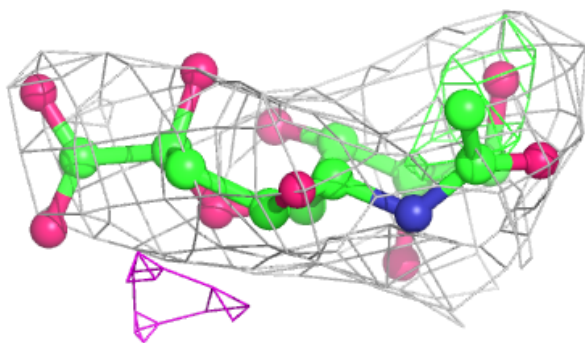
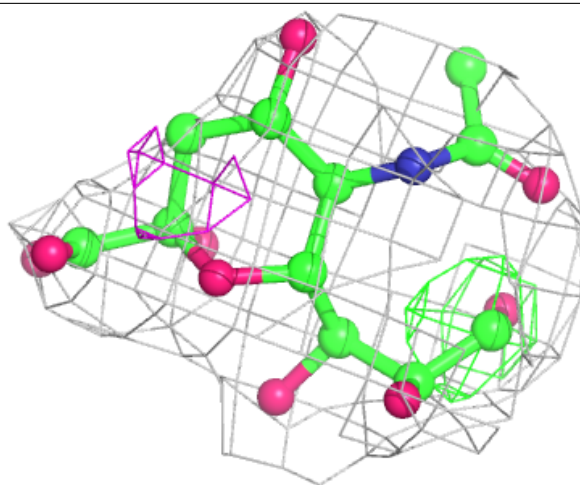
Electron density around SIA A 1181:

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



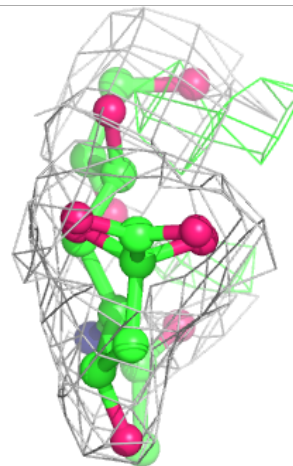
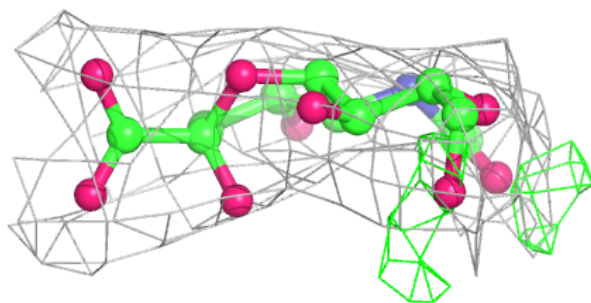
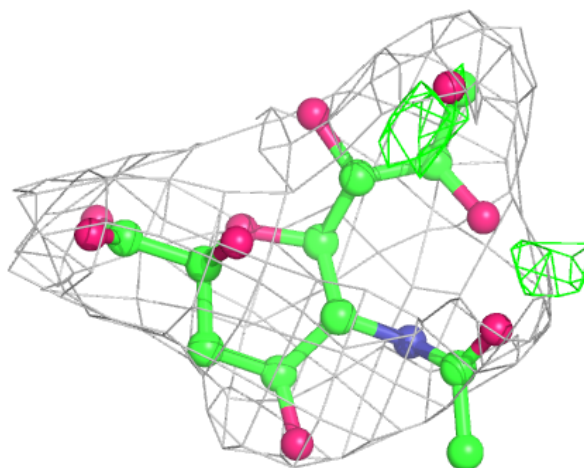
Electron density around SIA D 2180:

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



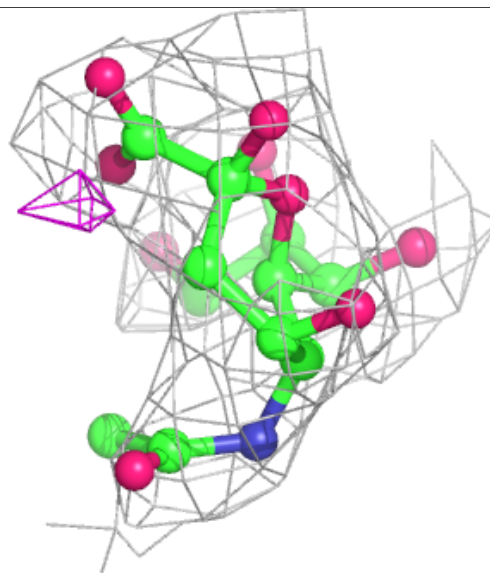
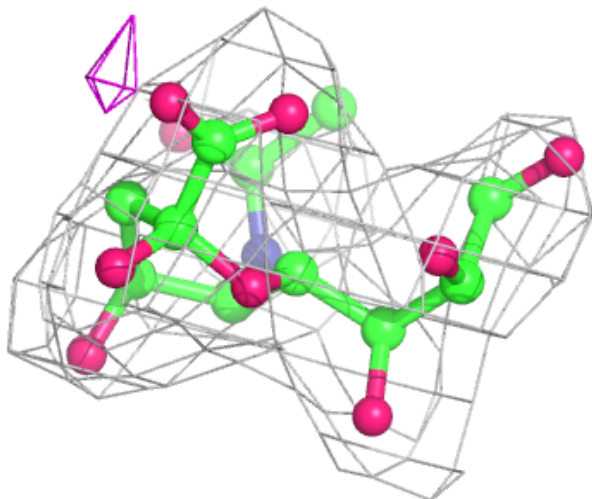
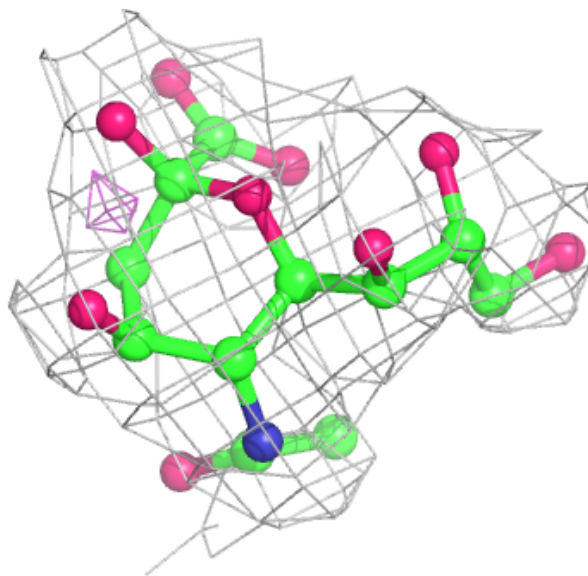
Electron density around SIA G 782:

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



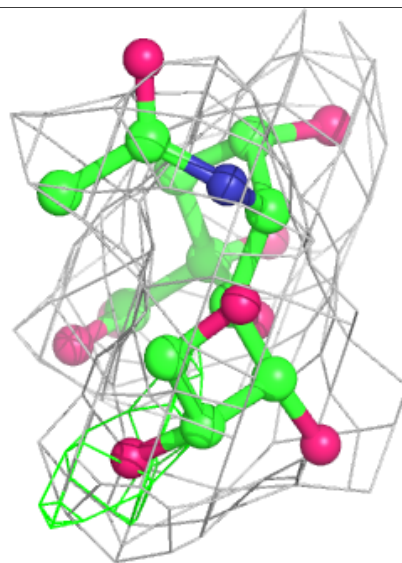
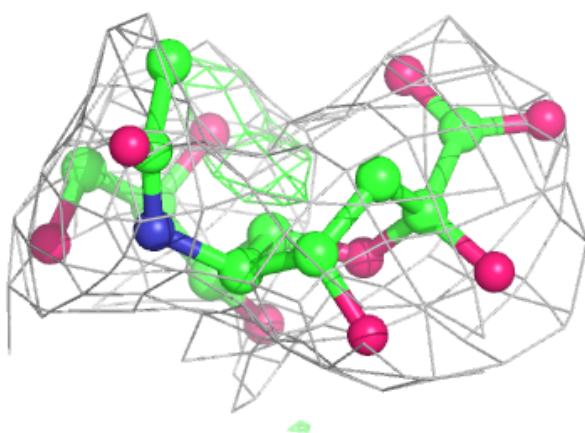
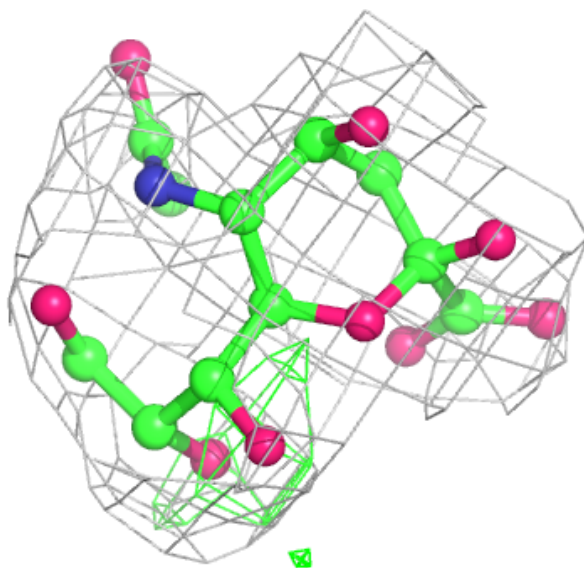
Electron density around SIA F 682:

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



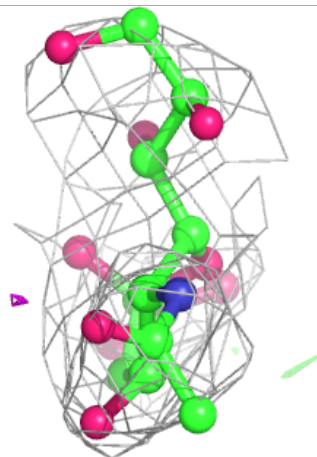
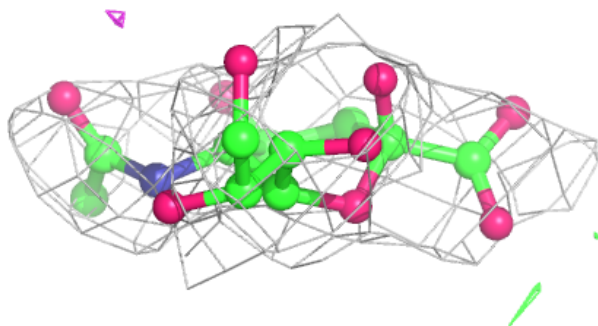
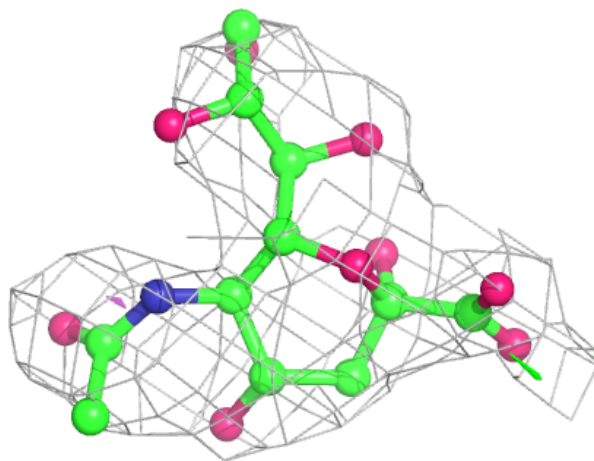
Electron density around SIA L 1282:

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



Electron density around SIA K 1182:

$2mF_o-DF_c$ (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.