



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:39 PM UTC

PDB ID : 7W1D / pdb_00007w1d
Title : Crystal structure of Klebsiella pneumoniae K1 capsule-specific polysaccharide lyase in a C2 crystal form
Authors : Tu, I.F.; Ko, T.P.; Huang, K.F.; Wu, S.H.
Deposited on : 2021-11-19
Resolution : 2.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

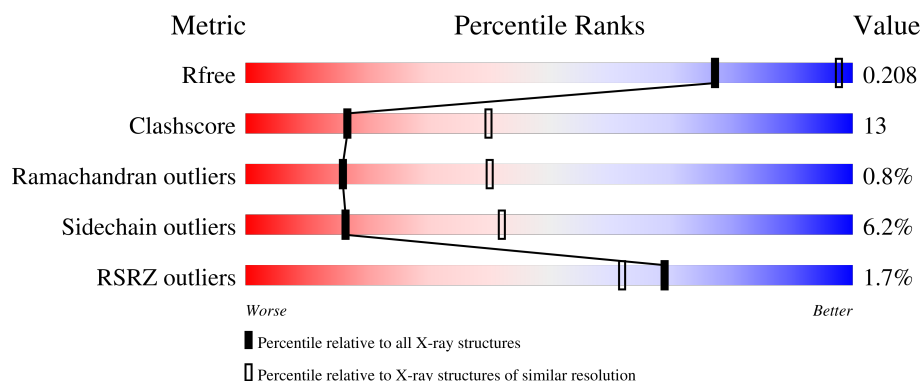
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	671	2% 68% 24% . .
1	B	671	2% 68% 26% . .
1	C	671	69% 25% . .
1	D	671	2% 67% 26% . .
1	E	671	2% 69% 24% . .

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Mol	Chain	Length	Quality of chain
1	F	671	2% 75% 20%
1	G	671	68% 26%
1	H	671	71% 23%
1	I	671	% 64% 30%
1	J	671	3% 62% 30%
1	K	671	3% 62% 31%
1	L	671	4% 59% 32%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 59973 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 K1 LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			4858	3055	840	944	19			
1	B	644	Total	C	N	O	S	0	0	0
			4870	3063	842	946	19			
1	C	644	Total	C	N	O	S	0	0	0
			4870	3063	842	946	19			
1	D	643	Total	C	N	O	S	0	0	0
			4865	3060	841	945	19			
1	E	643	Total	C	N	O	S	0	0	0
			4865	3060	841	945	19			
1	F	644	Total	C	N	O	S	0	0	0
			4870	3063	842	946	19			
1	G	642	Total	C	N	O	S	0	0	0
			4858	3055	840	944	19			
1	H	646	Total	C	N	O	S	0	0	0
			4885	3074	844	948	19			
1	I	644	Total	C	N	O	S	0	0	0
			4870	3063	842	946	19			
1	J	642	Total	C	N	O	S	0	0	0
			4858	3055	840	944	19			
1	K	642	Total	C	N	O	S	0	0	0
			4858	3055	840	944	19			
1	L	642	Total	C	N	O	S	0	0	0
			4858	3055	840	944	19			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
A	-18	GLY	-	expression tag	UNP A0A068Q5Q5
A	-17	SER	-	expression tag	UNP A0A068Q5Q5
A	-16	SER	-	expression tag	UNP A0A068Q5Q5
A	-15	HIS	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP A0A068Q5Q5
A	-13	HIS	-	expression tag	UNP A0A068Q5Q5
A	-12	HIS	-	expression tag	UNP A0A068Q5Q5
A	-11	HIS	-	expression tag	UNP A0A068Q5Q5
A	-10	HIS	-	expression tag	UNP A0A068Q5Q5
A	-9	SER	-	expression tag	UNP A0A068Q5Q5
A	-8	SER	-	expression tag	UNP A0A068Q5Q5
A	-7	GLY	-	expression tag	UNP A0A068Q5Q5
A	-6	LEU	-	expression tag	UNP A0A068Q5Q5
A	-5	VAL	-	expression tag	UNP A0A068Q5Q5
A	-4	PRO	-	expression tag	UNP A0A068Q5Q5
A	-3	ARG	-	expression tag	UNP A0A068Q5Q5
A	-2	GLY	-	expression tag	UNP A0A068Q5Q5
A	-1	SER	-	expression tag	UNP A0A068Q5Q5
A	0	HIS	-	expression tag	UNP A0A068Q5Q5
A	213	THR	ALA	conflict	UNP A0A068Q5Q5
A	256	ILE	SER	conflict	UNP A0A068Q5Q5
A	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
A	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
B	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
B	-18	GLY	-	expression tag	UNP A0A068Q5Q5
B	-17	SER	-	expression tag	UNP A0A068Q5Q5
B	-16	SER	-	expression tag	UNP A0A068Q5Q5
B	-15	HIS	-	expression tag	UNP A0A068Q5Q5
B	-14	HIS	-	expression tag	UNP A0A068Q5Q5
B	-13	HIS	-	expression tag	UNP A0A068Q5Q5
B	-12	HIS	-	expression tag	UNP A0A068Q5Q5
B	-11	HIS	-	expression tag	UNP A0A068Q5Q5
B	-10	HIS	-	expression tag	UNP A0A068Q5Q5
B	-9	SER	-	expression tag	UNP A0A068Q5Q5
B	-8	SER	-	expression tag	UNP A0A068Q5Q5
B	-7	GLY	-	expression tag	UNP A0A068Q5Q5
B	-6	LEU	-	expression tag	UNP A0A068Q5Q5
B	-5	VAL	-	expression tag	UNP A0A068Q5Q5
B	-4	PRO	-	expression tag	UNP A0A068Q5Q5
B	-3	ARG	-	expression tag	UNP A0A068Q5Q5
B	-2	GLY	-	expression tag	UNP A0A068Q5Q5
B	-1	SER	-	expression tag	UNP A0A068Q5Q5
B	0	HIS	-	expression tag	UNP A0A068Q5Q5
B	213	THR	ALA	conflict	UNP A0A068Q5Q5
B	256	ILE	SER	conflict	UNP A0A068Q5Q5
B	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
C	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
C	-18	GLY	-	expression tag	UNP A0A068Q5Q5
C	-17	SER	-	expression tag	UNP A0A068Q5Q5
C	-16	SER	-	expression tag	UNP A0A068Q5Q5
C	-15	HIS	-	expression tag	UNP A0A068Q5Q5
C	-14	HIS	-	expression tag	UNP A0A068Q5Q5
C	-13	HIS	-	expression tag	UNP A0A068Q5Q5
C	-12	HIS	-	expression tag	UNP A0A068Q5Q5
C	-11	HIS	-	expression tag	UNP A0A068Q5Q5
C	-10	HIS	-	expression tag	UNP A0A068Q5Q5
C	-9	SER	-	expression tag	UNP A0A068Q5Q5
C	-8	SER	-	expression tag	UNP A0A068Q5Q5
C	-7	GLY	-	expression tag	UNP A0A068Q5Q5
C	-6	LEU	-	expression tag	UNP A0A068Q5Q5
C	-5	VAL	-	expression tag	UNP A0A068Q5Q5
C	-4	PRO	-	expression tag	UNP A0A068Q5Q5
C	-3	ARG	-	expression tag	UNP A0A068Q5Q5
C	-2	GLY	-	expression tag	UNP A0A068Q5Q5
C	-1	SER	-	expression tag	UNP A0A068Q5Q5
C	0	HIS	-	expression tag	UNP A0A068Q5Q5
C	213	THR	ALA	conflict	UNP A0A068Q5Q5
C	256	ILE	SER	conflict	UNP A0A068Q5Q5
C	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
C	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
D	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
D	-18	GLY	-	expression tag	UNP A0A068Q5Q5
D	-17	SER	-	expression tag	UNP A0A068Q5Q5
D	-16	SER	-	expression tag	UNP A0A068Q5Q5
D	-15	HIS	-	expression tag	UNP A0A068Q5Q5
D	-14	HIS	-	expression tag	UNP A0A068Q5Q5
D	-13	HIS	-	expression tag	UNP A0A068Q5Q5
D	-12	HIS	-	expression tag	UNP A0A068Q5Q5
D	-11	HIS	-	expression tag	UNP A0A068Q5Q5
D	-10	HIS	-	expression tag	UNP A0A068Q5Q5
D	-9	SER	-	expression tag	UNP A0A068Q5Q5
D	-8	SER	-	expression tag	UNP A0A068Q5Q5
D	-7	GLY	-	expression tag	UNP A0A068Q5Q5
D	-6	LEU	-	expression tag	UNP A0A068Q5Q5
D	-5	VAL	-	expression tag	UNP A0A068Q5Q5
D	-4	PRO	-	expression tag	UNP A0A068Q5Q5
D	-3	ARG	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP A0A068Q5Q5
D	-1	SER	-	expression tag	UNP A0A068Q5Q5
D	0	HIS	-	expression tag	UNP A0A068Q5Q5
D	213	THR	ALA	conflict	UNP A0A068Q5Q5
D	256	ILE	SER	conflict	UNP A0A068Q5Q5
D	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
D	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
E	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
E	-18	GLY	-	expression tag	UNP A0A068Q5Q5
E	-17	SER	-	expression tag	UNP A0A068Q5Q5
E	-16	SER	-	expression tag	UNP A0A068Q5Q5
E	-15	HIS	-	expression tag	UNP A0A068Q5Q5
E	-14	HIS	-	expression tag	UNP A0A068Q5Q5
E	-13	HIS	-	expression tag	UNP A0A068Q5Q5
E	-12	HIS	-	expression tag	UNP A0A068Q5Q5
E	-11	HIS	-	expression tag	UNP A0A068Q5Q5
E	-10	HIS	-	expression tag	UNP A0A068Q5Q5
E	-9	SER	-	expression tag	UNP A0A068Q5Q5
E	-8	SER	-	expression tag	UNP A0A068Q5Q5
E	-7	GLY	-	expression tag	UNP A0A068Q5Q5
E	-6	LEU	-	expression tag	UNP A0A068Q5Q5
E	-5	VAL	-	expression tag	UNP A0A068Q5Q5
E	-4	PRO	-	expression tag	UNP A0A068Q5Q5
E	-3	ARG	-	expression tag	UNP A0A068Q5Q5
E	-2	GLY	-	expression tag	UNP A0A068Q5Q5
E	-1	SER	-	expression tag	UNP A0A068Q5Q5
E	0	HIS	-	expression tag	UNP A0A068Q5Q5
E	213	THR	ALA	conflict	UNP A0A068Q5Q5
E	256	ILE	SER	conflict	UNP A0A068Q5Q5
E	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
E	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
F	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
F	-18	GLY	-	expression tag	UNP A0A068Q5Q5
F	-17	SER	-	expression tag	UNP A0A068Q5Q5
F	-16	SER	-	expression tag	UNP A0A068Q5Q5
F	-15	HIS	-	expression tag	UNP A0A068Q5Q5
F	-14	HIS	-	expression tag	UNP A0A068Q5Q5
F	-13	HIS	-	expression tag	UNP A0A068Q5Q5
F	-12	HIS	-	expression tag	UNP A0A068Q5Q5
F	-11	HIS	-	expression tag	UNP A0A068Q5Q5
F	-10	HIS	-	expression tag	UNP A0A068Q5Q5
F	-9	SER	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-8	SER	-	expression tag	UNP A0A068Q5Q5
F	-7	GLY	-	expression tag	UNP A0A068Q5Q5
F	-6	LEU	-	expression tag	UNP A0A068Q5Q5
F	-5	VAL	-	expression tag	UNP A0A068Q5Q5
F	-4	PRO	-	expression tag	UNP A0A068Q5Q5
F	-3	ARG	-	expression tag	UNP A0A068Q5Q5
F	-2	GLY	-	expression tag	UNP A0A068Q5Q5
F	-1	SER	-	expression tag	UNP A0A068Q5Q5
F	0	HIS	-	expression tag	UNP A0A068Q5Q5
F	213	THR	ALA	conflict	UNP A0A068Q5Q5
F	256	ILE	SER	conflict	UNP A0A068Q5Q5
F	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
F	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
G	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
G	-18	GLY	-	expression tag	UNP A0A068Q5Q5
G	-17	SER	-	expression tag	UNP A0A068Q5Q5
G	-16	SER	-	expression tag	UNP A0A068Q5Q5
G	-15	HIS	-	expression tag	UNP A0A068Q5Q5
G	-14	HIS	-	expression tag	UNP A0A068Q5Q5
G	-13	HIS	-	expression tag	UNP A0A068Q5Q5
G	-12	HIS	-	expression tag	UNP A0A068Q5Q5
G	-11	HIS	-	expression tag	UNP A0A068Q5Q5
G	-10	HIS	-	expression tag	UNP A0A068Q5Q5
G	-9	SER	-	expression tag	UNP A0A068Q5Q5
G	-8	SER	-	expression tag	UNP A0A068Q5Q5
G	-7	GLY	-	expression tag	UNP A0A068Q5Q5
G	-6	LEU	-	expression tag	UNP A0A068Q5Q5
G	-5	VAL	-	expression tag	UNP A0A068Q5Q5
G	-4	PRO	-	expression tag	UNP A0A068Q5Q5
G	-3	ARG	-	expression tag	UNP A0A068Q5Q5
G	-2	GLY	-	expression tag	UNP A0A068Q5Q5
G	-1	SER	-	expression tag	UNP A0A068Q5Q5
G	0	HIS	-	expression tag	UNP A0A068Q5Q5
G	213	THR	ALA	conflict	UNP A0A068Q5Q5
G	256	ILE	SER	conflict	UNP A0A068Q5Q5
G	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
G	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
H	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
H	-18	GLY	-	expression tag	UNP A0A068Q5Q5
H	-17	SER	-	expression tag	UNP A0A068Q5Q5
H	-16	SER	-	expression tag	UNP A0A068Q5Q5
H	-15	HIS	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-14	HIS	-	expression tag	UNP A0A068Q5Q5
H	-13	HIS	-	expression tag	UNP A0A068Q5Q5
H	-12	HIS	-	expression tag	UNP A0A068Q5Q5
H	-11	HIS	-	expression tag	UNP A0A068Q5Q5
H	-10	HIS	-	expression tag	UNP A0A068Q5Q5
H	-9	SER	-	expression tag	UNP A0A068Q5Q5
H	-8	SER	-	expression tag	UNP A0A068Q5Q5
H	-7	GLY	-	expression tag	UNP A0A068Q5Q5
H	-6	LEU	-	expression tag	UNP A0A068Q5Q5
H	-5	VAL	-	expression tag	UNP A0A068Q5Q5
H	-4	PRO	-	expression tag	UNP A0A068Q5Q5
H	-3	ARG	-	expression tag	UNP A0A068Q5Q5
H	-2	GLY	-	expression tag	UNP A0A068Q5Q5
H	-1	SER	-	expression tag	UNP A0A068Q5Q5
H	0	HIS	-	expression tag	UNP A0A068Q5Q5
H	213	THR	ALA	conflict	UNP A0A068Q5Q5
H	256	ILE	SER	conflict	UNP A0A068Q5Q5
H	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
H	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
I	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
I	-18	GLY	-	expression tag	UNP A0A068Q5Q5
I	-17	SER	-	expression tag	UNP A0A068Q5Q5
I	-16	SER	-	expression tag	UNP A0A068Q5Q5
I	-15	HIS	-	expression tag	UNP A0A068Q5Q5
I	-14	HIS	-	expression tag	UNP A0A068Q5Q5
I	-13	HIS	-	expression tag	UNP A0A068Q5Q5
I	-12	HIS	-	expression tag	UNP A0A068Q5Q5
I	-11	HIS	-	expression tag	UNP A0A068Q5Q5
I	-10	HIS	-	expression tag	UNP A0A068Q5Q5
I	-9	SER	-	expression tag	UNP A0A068Q5Q5
I	-8	SER	-	expression tag	UNP A0A068Q5Q5
I	-7	GLY	-	expression tag	UNP A0A068Q5Q5
I	-6	LEU	-	expression tag	UNP A0A068Q5Q5
I	-5	VAL	-	expression tag	UNP A0A068Q5Q5
I	-4	PRO	-	expression tag	UNP A0A068Q5Q5
I	-3	ARG	-	expression tag	UNP A0A068Q5Q5
I	-2	GLY	-	expression tag	UNP A0A068Q5Q5
I	-1	SER	-	expression tag	UNP A0A068Q5Q5
I	0	HIS	-	expression tag	UNP A0A068Q5Q5
I	213	THR	ALA	conflict	UNP A0A068Q5Q5
I	256	ILE	SER	conflict	UNP A0A068Q5Q5
I	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5

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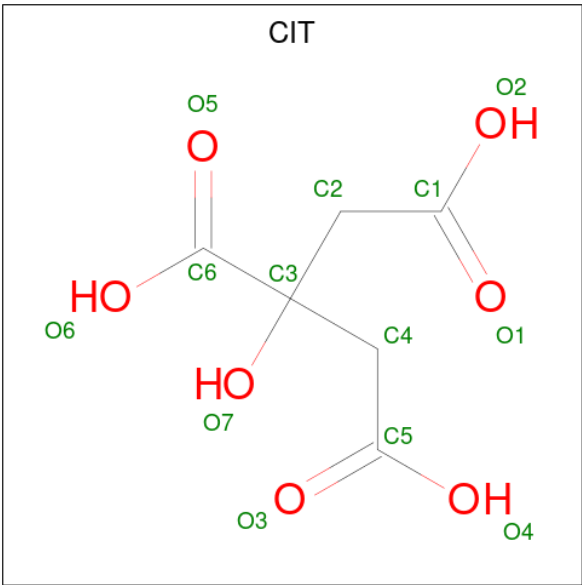
Chain	Residue	Modelled	Actual	Comment	Reference
I	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
J	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
J	-18	GLY	-	expression tag	UNP A0A068Q5Q5
J	-17	SER	-	expression tag	UNP A0A068Q5Q5
J	-16	SER	-	expression tag	UNP A0A068Q5Q5
J	-15	HIS	-	expression tag	UNP A0A068Q5Q5
J	-14	HIS	-	expression tag	UNP A0A068Q5Q5
J	-13	HIS	-	expression tag	UNP A0A068Q5Q5
J	-12	HIS	-	expression tag	UNP A0A068Q5Q5
J	-11	HIS	-	expression tag	UNP A0A068Q5Q5
J	-10	HIS	-	expression tag	UNP A0A068Q5Q5
J	-9	SER	-	expression tag	UNP A0A068Q5Q5
J	-8	SER	-	expression tag	UNP A0A068Q5Q5
J	-7	GLY	-	expression tag	UNP A0A068Q5Q5
J	-6	LEU	-	expression tag	UNP A0A068Q5Q5
J	-5	VAL	-	expression tag	UNP A0A068Q5Q5
J	-4	PRO	-	expression tag	UNP A0A068Q5Q5
J	-3	ARG	-	expression tag	UNP A0A068Q5Q5
J	-2	GLY	-	expression tag	UNP A0A068Q5Q5
J	-1	SER	-	expression tag	UNP A0A068Q5Q5
J	0	HIS	-	expression tag	UNP A0A068Q5Q5
J	213	THR	ALA	conflict	UNP A0A068Q5Q5
J	256	ILE	SER	conflict	UNP A0A068Q5Q5
J	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
J	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
K	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
K	-18	GLY	-	expression tag	UNP A0A068Q5Q5
K	-17	SER	-	expression tag	UNP A0A068Q5Q5
K	-16	SER	-	expression tag	UNP A0A068Q5Q5
K	-15	HIS	-	expression tag	UNP A0A068Q5Q5
K	-14	HIS	-	expression tag	UNP A0A068Q5Q5
K	-13	HIS	-	expression tag	UNP A0A068Q5Q5
K	-12	HIS	-	expression tag	UNP A0A068Q5Q5
K	-11	HIS	-	expression tag	UNP A0A068Q5Q5
K	-10	HIS	-	expression tag	UNP A0A068Q5Q5
K	-9	SER	-	expression tag	UNP A0A068Q5Q5
K	-8	SER	-	expression tag	UNP A0A068Q5Q5
K	-7	GLY	-	expression tag	UNP A0A068Q5Q5
K	-6	LEU	-	expression tag	UNP A0A068Q5Q5
K	-5	VAL	-	expression tag	UNP A0A068Q5Q5
K	-4	PRO	-	expression tag	UNP A0A068Q5Q5
K	-3	ARG	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	GLY	-	expression tag	UNP A0A068Q5Q5
K	-1	SER	-	expression tag	UNP A0A068Q5Q5
K	0	HIS	-	expression tag	UNP A0A068Q5Q5
K	213	THR	ALA	conflict	UNP A0A068Q5Q5
K	256	ILE	SER	conflict	UNP A0A068Q5Q5
K	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
K	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
L	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
L	-18	GLY	-	expression tag	UNP A0A068Q5Q5
L	-17	SER	-	expression tag	UNP A0A068Q5Q5
L	-16	SER	-	expression tag	UNP A0A068Q5Q5
L	-15	HIS	-	expression tag	UNP A0A068Q5Q5
L	-14	HIS	-	expression tag	UNP A0A068Q5Q5
L	-13	HIS	-	expression tag	UNP A0A068Q5Q5
L	-12	HIS	-	expression tag	UNP A0A068Q5Q5
L	-11	HIS	-	expression tag	UNP A0A068Q5Q5
L	-10	HIS	-	expression tag	UNP A0A068Q5Q5
L	-9	SER	-	expression tag	UNP A0A068Q5Q5
L	-8	SER	-	expression tag	UNP A0A068Q5Q5
L	-7	GLY	-	expression tag	UNP A0A068Q5Q5
L	-6	LEU	-	expression tag	UNP A0A068Q5Q5
L	-5	VAL	-	expression tag	UNP A0A068Q5Q5
L	-4	PRO	-	expression tag	UNP A0A068Q5Q5
L	-3	ARG	-	expression tag	UNP A0A068Q5Q5
L	-2	GLY	-	expression tag	UNP A0A068Q5Q5
L	-1	SER	-	expression tag	UNP A0A068Q5Q5
L	0	HIS	-	expression tag	UNP A0A068Q5Q5
L	213	THR	ALA	conflict	UNP A0A068Q5Q5
L	256	ILE	SER	conflict	UNP A0A068Q5Q5
L	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
L	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$) (labeled as "Ligand of Interest" by depositor).



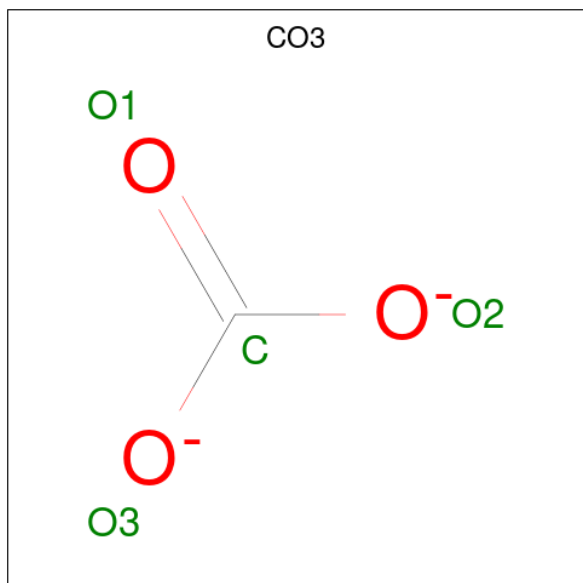
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		
2	I	1	Total	C	O	0	0
			13	6	7		
2	J	1	Total	C	O	0	0
			13	6	7		
2	K	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total	C	O	0	0
			13	6	7		
2	L	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	1	3		
3	H	1	Total	C	O	0	0
			4	1	3		
3	K	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	170	Total	O	0	0
			170	170		
4	B	151	Total	O	0	0
			151	151		
4	C	169	Total	O	0	0
			169	169		
4	D	117	Total	O	0	0
			117	117		

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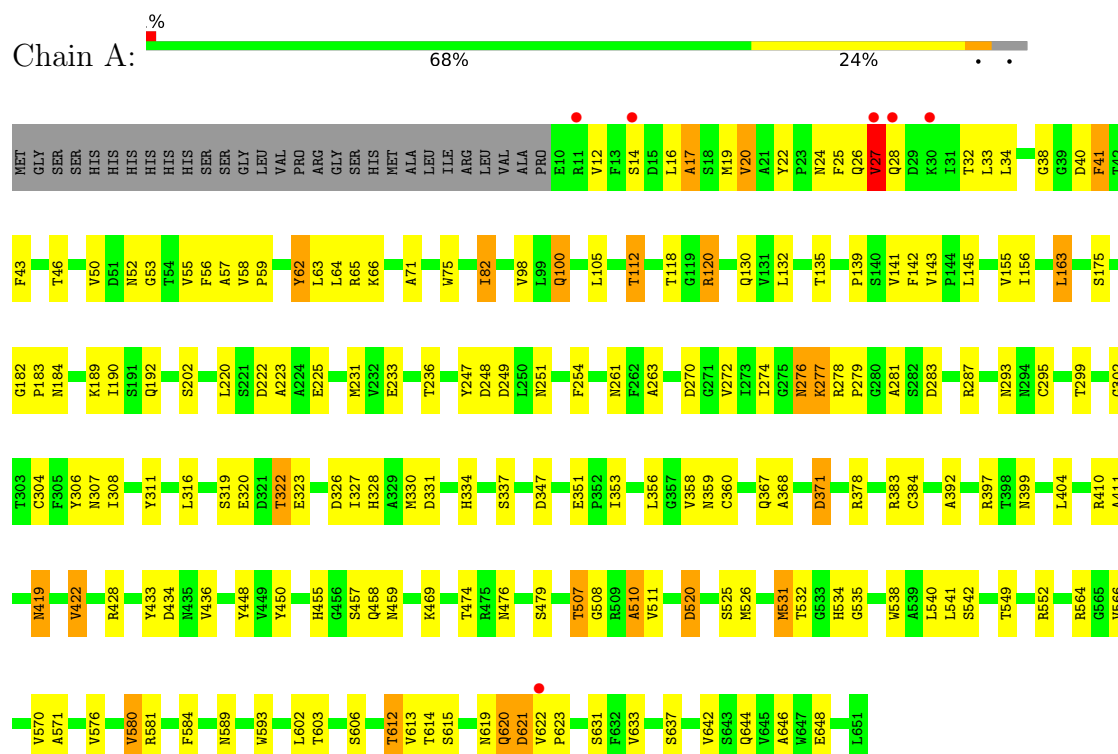
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	118	Total 118	O 118	0	0
4	F	164	Total 164	O 164	0	0
4	G	87	Total 87	O 87	0	0
4	H	106	Total 106	O 106	0	0
4	I	72	Total 72	O 72	0	0
4	J	72	Total 72	O 72	0	0
4	K	74	Total 74	O 74	0	0
4	L	68	Total 68	O 68	0	0

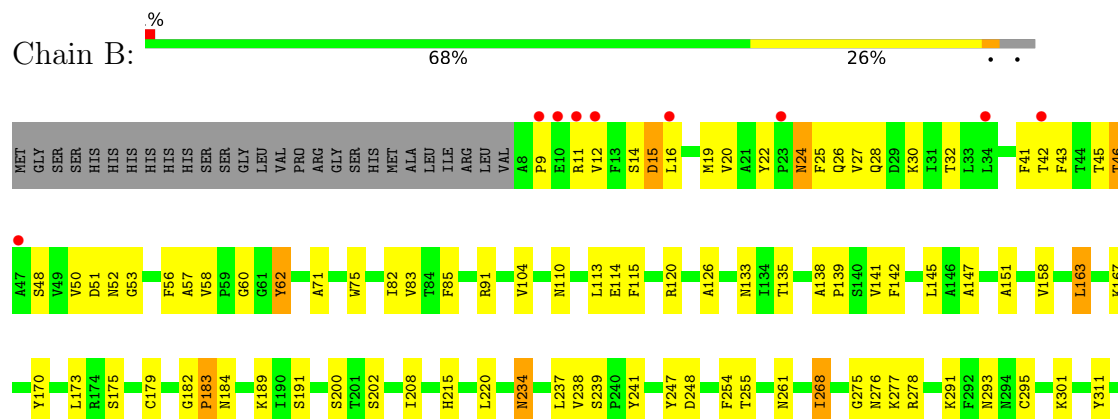
3 Residue-property plots

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

• Molecule 1: K1 LYASE



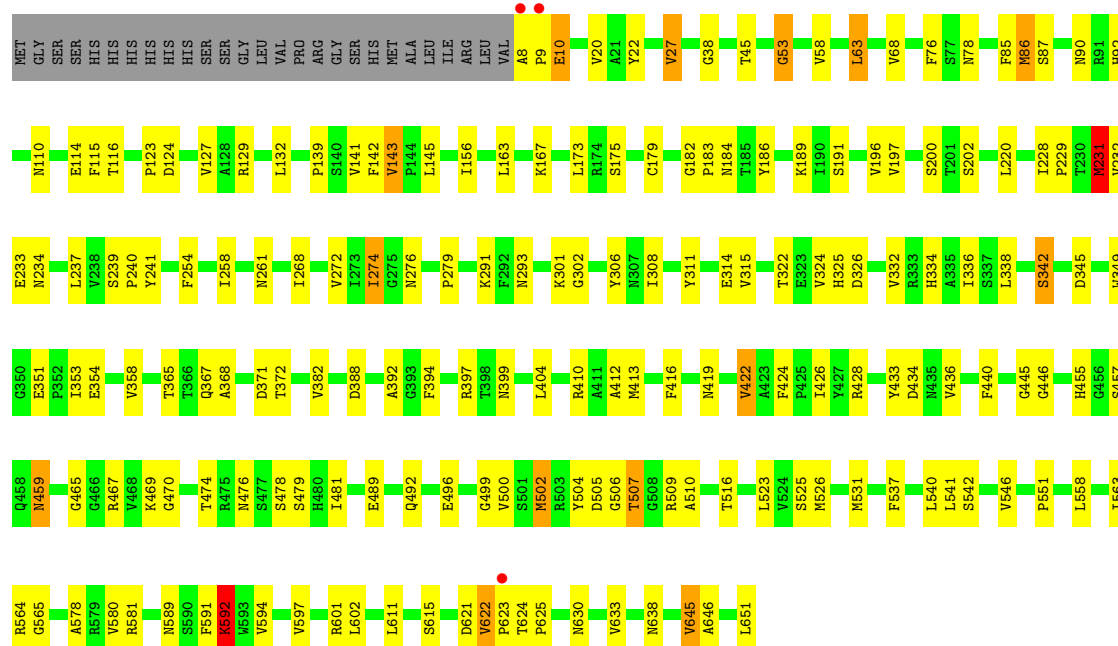
• Molecule 1: K1 LYASE





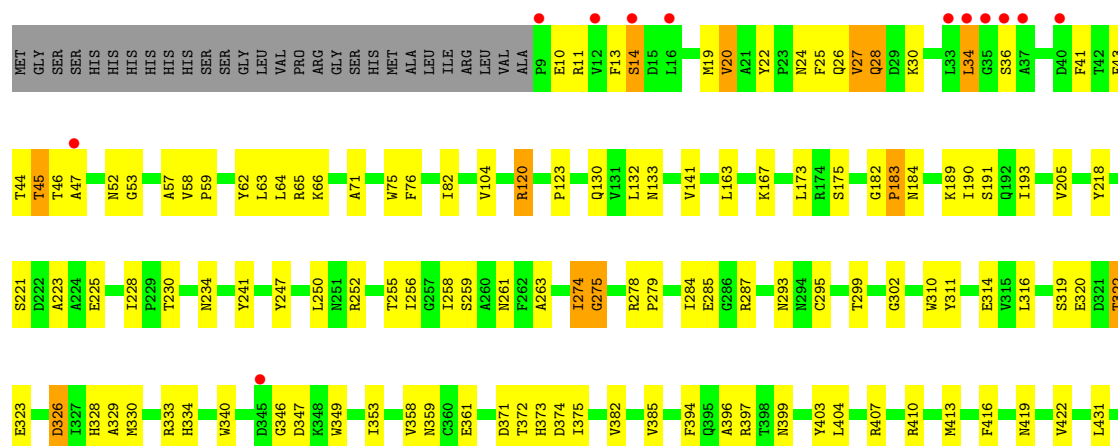
• Molecule 1: K1 LYASE

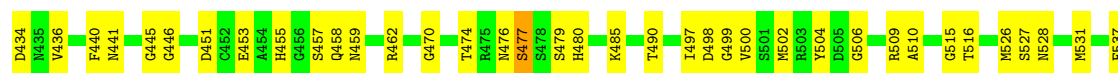
Chain C: 69% 25%



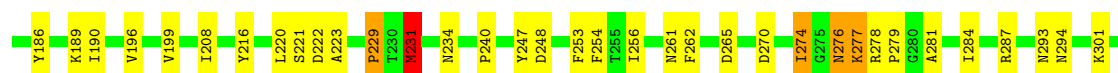
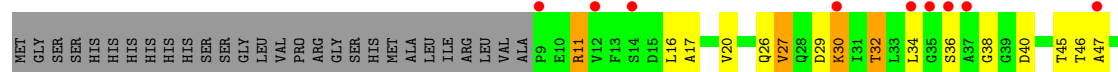
• Molecule 1: K1 LYASE

Chain D: 67% 26%

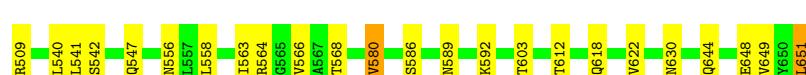
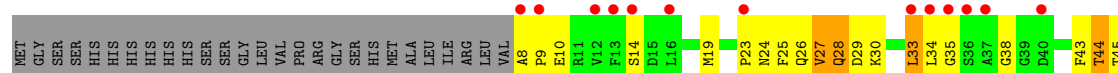
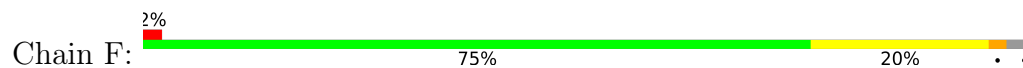




• Molecule 1: K1 LYASE

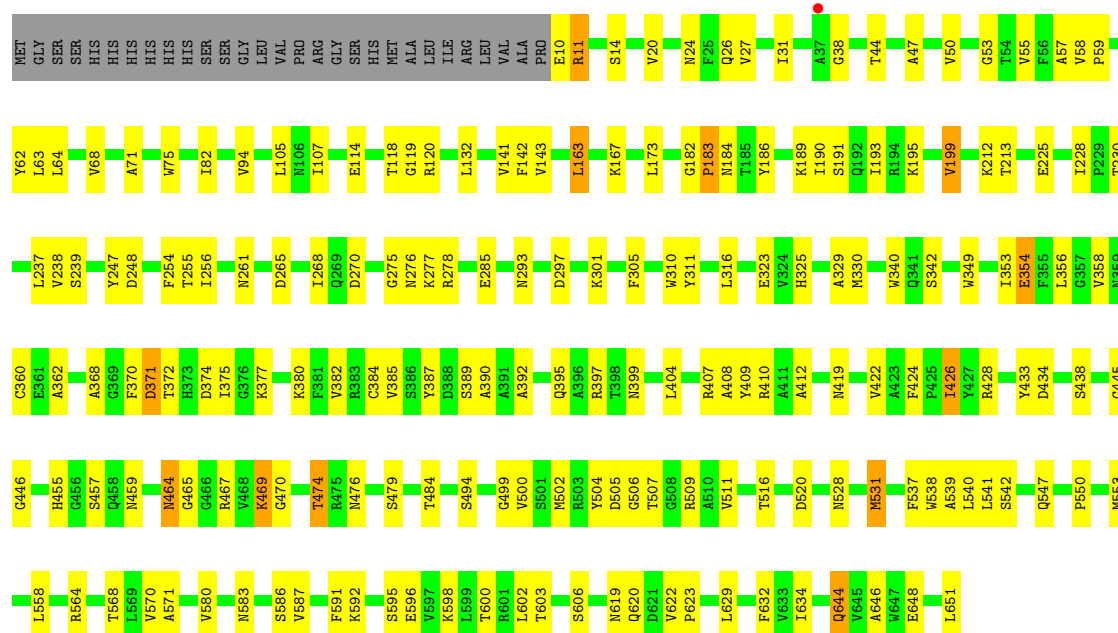


• Molecule 1: K1 LYASE



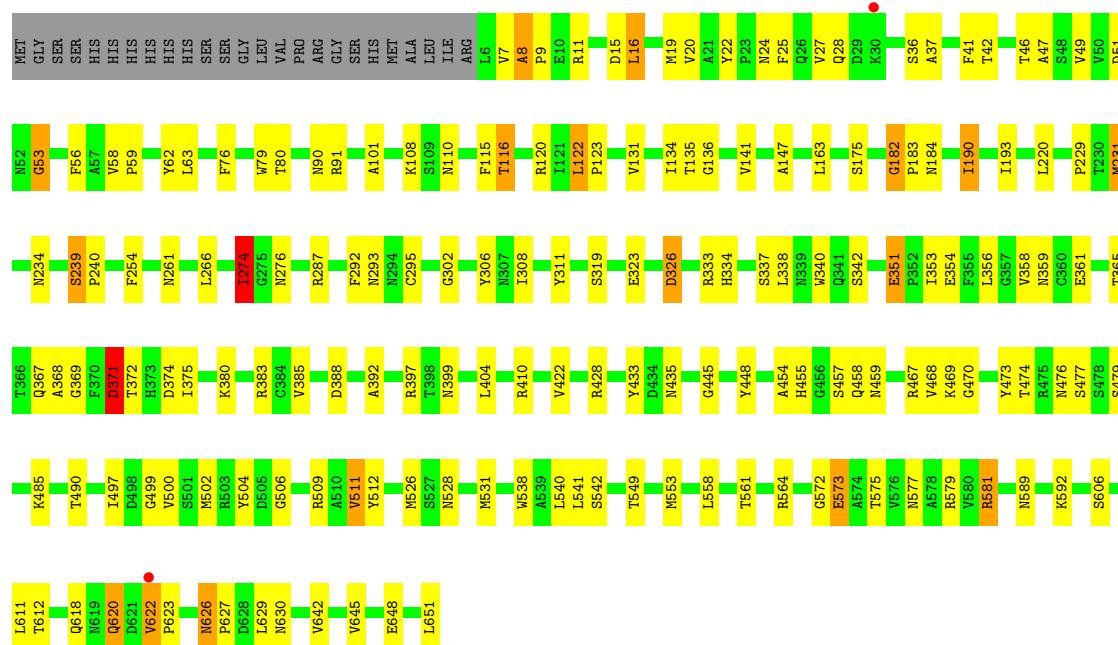
- Molecule 1: K1 LYASE

Chain G: 68% 26% . .



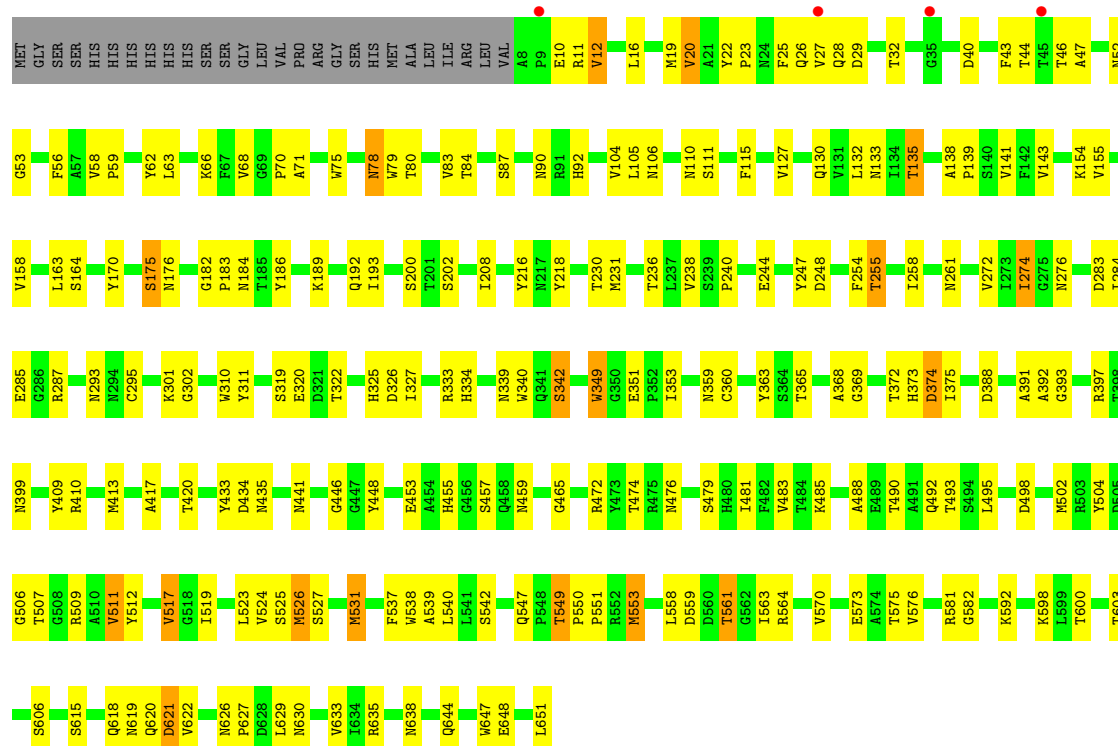
- Molecule 1: K1 LYASE

Chain H:  71% 23% 6%

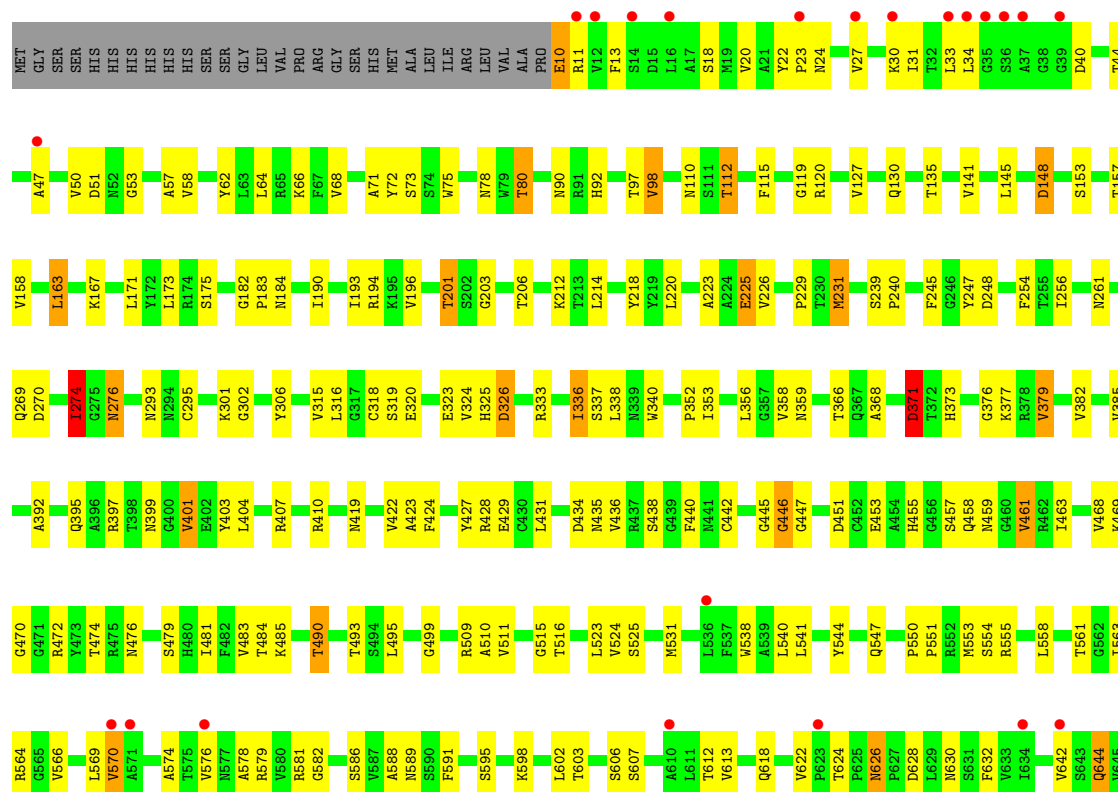


- Molecule 1: K1 LYASE

Chain I: %

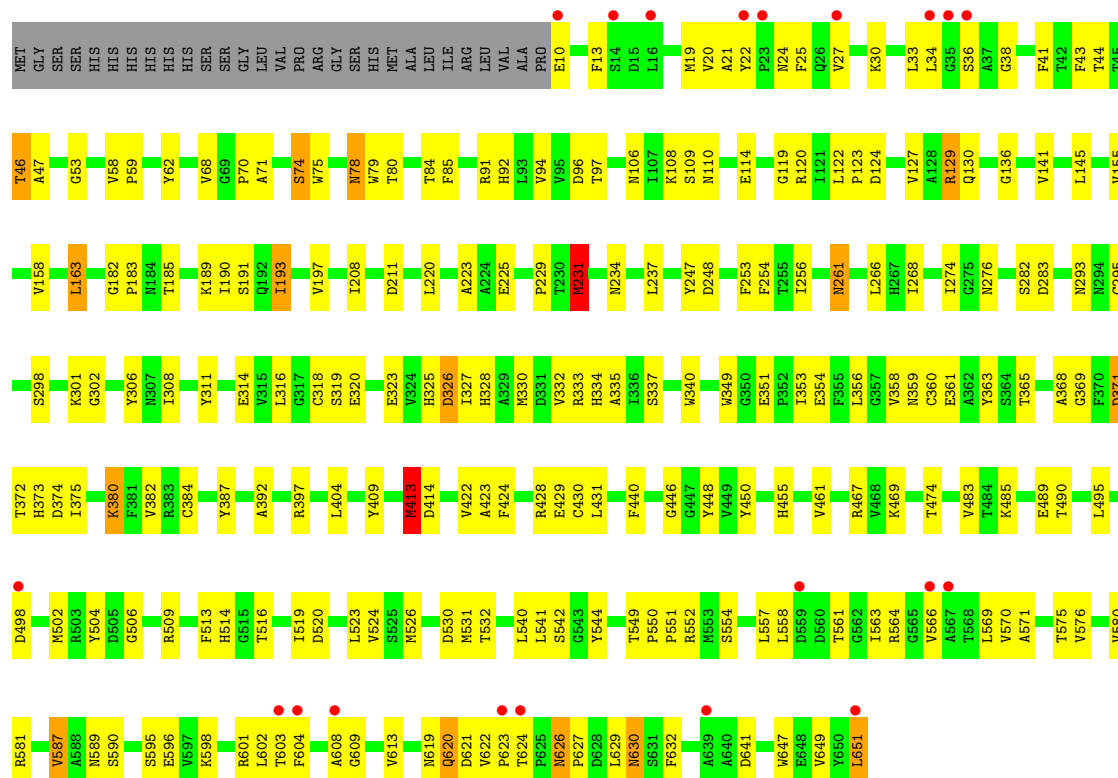


• Molecule 1: K1 LYASE

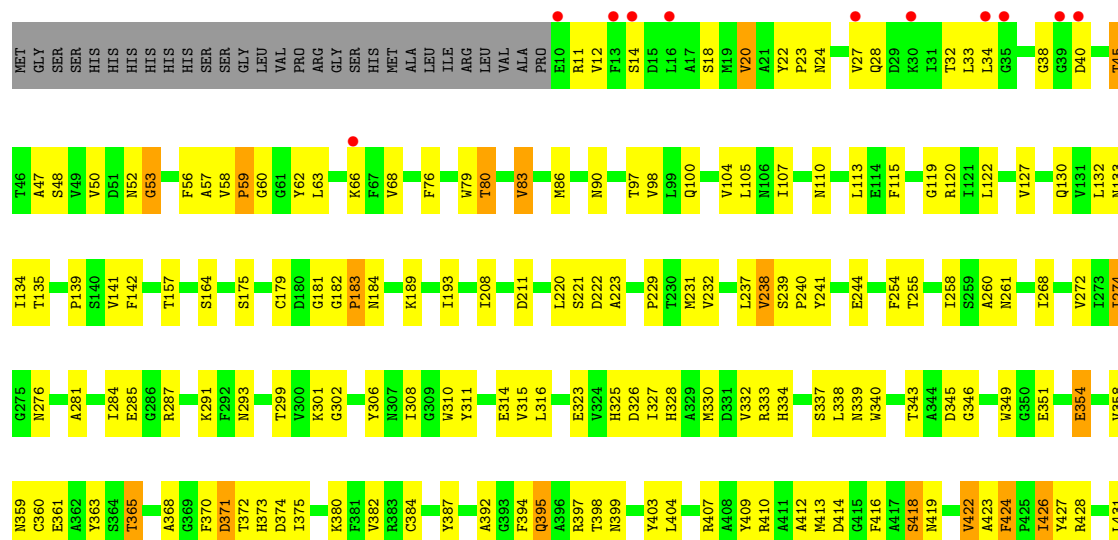


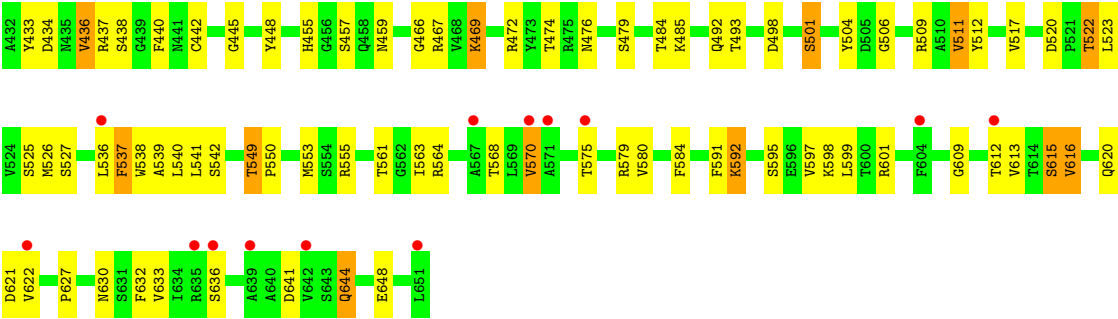


• Molecule 1: K1 LYASE



• Molecule 1: K1 LYASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	363.94Å 239.63Å 121.63Å 90.00° 100.13° 90.00°	Depositor
Resolution (Å)	29.95 – 2.78 29.95 – 2.78	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.95-2.78) 98.3 (29.95-2.78)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.76Å)	Xtriage
Refinement program	PHENIX Phenix1.17.1-3660	Depositor
R, R_{free}	0.182 , 0.219 0.178 , 0.208	Depositor DCC
R_{free} test set	12744 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	59973	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, CO3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.26	5/4962 (0.1%)	1.23	20/6755 (0.3%)
1	B	1.26	8/4975 (0.2%)	1.20	10/6774 (0.1%)
1	C	1.31	14/4975 (0.3%)	1.23	15/6774 (0.2%)
1	D	1.19	4/4970 (0.1%)	1.18	16/6766 (0.2%)
1	E	1.18	6/4970 (0.1%)	1.18	13/6766 (0.2%)
1	F	1.26	12/4975 (0.2%)	1.20	13/6774 (0.2%)
1	G	1.15	9/4962 (0.2%)	1.17	16/6755 (0.2%)
1	H	1.16	1/4990 (0.0%)	1.19	22/6795 (0.3%)
1	I	1.14	1/4975 (0.0%)	1.16	12/6774 (0.2%)
1	J	1.05	3/4962 (0.1%)	1.15	10/6755 (0.1%)
1	K	1.10	6/4962 (0.1%)	1.14	15/6755 (0.2%)
1	L	1.05	4/4962 (0.1%)	1.14	5/6755 (0.1%)
All	All	1.18	73/59640 (0.1%)	1.18	167/81198 (0.2%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	228	ILE	CA-C	-7.72	1.47	1.53
1	L	229	PRO	CA-C	-7.39	1.43	1.52
1	A	566	VAL	C-O	-6.84	1.17	1.24
1	E	498	ASP	CB-CG	6.76	1.69	1.52
1	C	86	MET	SD-CE	-6.47	1.63	1.79
1	C	141	VAL	C-O	-6.45	1.16	1.23
1	C	197	VAL	C-O	-6.44	1.16	1.24
1	C	228	ILE	N-CA	-6.40	1.41	1.46
1	G	190	ILE	C-O	-6.30	1.16	1.24
1	C	231	MET	SD-CE	-6.22	1.64	1.79
1	B	483	VAL	N-CA	-6.09	1.39	1.46
1	G	370	PHE	CA-C	-6.00	1.45	1.52
1	L	413	MET	CA-C	5.97	1.55	1.52
1	L	211	ASP	C-O	-5.96	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	172	TYR	C-O	-5.94	1.16	1.24
1	B	391	ALA	C-O	-5.90	1.18	1.23
1	D	413	MET	CA-C	5.90	1.55	1.52
1	F	185	THR	C-O	-5.84	1.17	1.24
1	C	492	GLN	C-O	-5.82	1.16	1.23
1	C	589	ASN	C-O	-5.82	1.17	1.23
1	F	387	TYR	C-O	-5.72	1.17	1.24
1	A	130	GLN	CA-C	-5.72	1.45	1.52
1	H	229	PRO	N-CA	-5.71	1.40	1.46
1	G	583	ASN	CA-C	-5.64	1.45	1.52
1	C	422	VAL	CA-CB	-5.59	1.47	1.54
1	E	113	LEU	CA-C	-5.58	1.46	1.52
1	F	502	MET	SD-CE	-5.56	1.65	1.79
1	F	391	ALA	C-O	-5.53	1.17	1.24
1	C	594	VAL	CA-CB	-5.52	1.49	1.55
1	C	502	MET	SD-CE	-5.50	1.65	1.79
1	G	193	ILE	CA-CB	-5.48	1.47	1.54
1	D	241	TYR	CA-C	-5.46	1.46	1.52
1	J	276	ASN	C-O	-5.46	1.16	1.24
1	B	215	HIS	C-O	-5.46	1.16	1.23
1	J	98	VAL	C-O	-5.38	1.18	1.24
1	G	362	ALA	C-O	-5.36	1.17	1.24
1	K	231	MET	SD-CE	-5.34	1.66	1.79
1	B	463	ILE	N-CA	-5.33	1.39	1.46
1	K	282	SER	CA-C	5.32	1.60	1.53
1	F	137	SER	CA-C	-5.29	1.45	1.52
1	I	448	TYR	N-CA	-5.28	1.40	1.46
1	A	510	ALA	N-CA	-5.27	1.40	1.46
1	A	192	GLN	C-O	-5.26	1.17	1.23
1	F	123	PRO	C-O	-5.26	1.17	1.23
1	F	115	PHE	C-O	-5.23	1.17	1.23
1	F	236	THR	C-O	5.23	1.29	1.24
1	F	328	HIS	N-CA	-5.22	1.40	1.46
1	K	127	VAL	C-O	-5.22	1.18	1.24
1	A	98	VAL	C-O	-5.21	1.18	1.24
1	B	485	LYS	CA-C	-5.21	1.46	1.52
1	E	525	SER	CA-C	-5.20	1.46	1.52
1	C	143	VAL	CA-C	-5.19	1.48	1.52
1	G	408	ALA	CA-C	5.18	1.58	1.52
1	E	231	MET	SD-CE	-5.17	1.66	1.79
1	F	232	VAL	CA-C	-5.17	1.46	1.52
1	G	467	ARG	CA-C	-5.16	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	106	ASN	CA-C	-5.16	1.46	1.52
1	F	55	VAL	C-O	-5.16	1.18	1.24
1	K	211	ASP	C-O	-5.15	1.18	1.24
1	L	316	LEU	CA-C	5.13	1.59	1.52
1	D	259	SER	CA-C	-5.11	1.46	1.52
1	B	644	GLN	C-O	-5.09	1.18	1.24
1	C	123	PRO	N-CA	-5.07	1.41	1.47
1	C	516	THR	C-O	-5.07	1.17	1.24
1	D	193	ILE	CA-CB	-5.06	1.48	1.54
1	G	419	ASN	CA-C	-5.05	1.46	1.53
1	G	469	LYS	CA-C	-5.05	1.46	1.52
1	F	190	ILE	C-O	-5.04	1.17	1.24
1	J	127	VAL	C-O	-5.04	1.19	1.24
1	B	484	THR	C-O	-5.04	1.19	1.24
1	E	229	PRO	C-O	-5.03	1.17	1.23
1	K	413	MET	CA-C	5.02	1.54	1.52
1	B	644	GLN	CA-CB	-5.00	1.46	1.53

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	ASP	CA-C-N	-8.15	111.41	119.64
1	A	520	ASP	C-N-CA	-8.15	111.41	119.64
1	J	371	ASP	N-CA-C	7.85	121.00	109.07
1	G	143	VAL	CA-C-N	-7.72	112.25	120.66
1	G	143	VAL	C-N-CA	-7.72	112.25	120.66
1	J	626	ASN	CA-C-N	7.58	127.25	119.82
1	J	626	ASN	C-N-CA	7.58	127.25	119.82
1	I	626	ASN	CA-C-N	7.38	127.09	119.56
1	I	626	ASN	C-N-CA	7.38	127.09	119.56
1	J	446	GLY	N-CA-C	7.20	122.00	112.65
1	E	127	VAL	CB-CA-C	-7.17	99.46	110.50
1	E	434	ASP	N-CA-C	7.00	121.20	112.24
1	K	351	GLU	CA-C-N	-6.96	112.82	119.85
1	K	351	GLU	C-N-CA	-6.96	112.82	119.85
1	A	531	MET	CG-SD-CE	-6.89	85.73	100.90
1	F	143	VAL	CA-C-N	-6.59	113.86	120.31
1	F	143	VAL	C-N-CA	-6.59	113.86	120.31
1	K	630	ASN	N-CA-C	-6.44	102.49	110.41
1	A	283	ASP	N-CA-C	6.43	119.24	110.55
1	I	393	GLY	N-CA-C	-6.43	104.71	112.49
1	E	374	ASP	N-CA-C	6.31	119.70	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	388	ASP	N-CA-C	6.28	120.05	111.39
1	D	477	SER	N-CA-C	6.26	118.90	111.33
1	H	326	ASP	CB-CA-C	-6.23	102.71	111.80
1	A	276	ASN	N-CA-C	-6.22	104.85	112.88
1	H	122	LEU	CA-C-N	6.21	126.18	119.78
1	H	122	LEU	C-N-CA	6.21	126.18	119.78
1	A	82	ILE	N-CA-C	-6.18	104.48	110.42
1	I	339	ASN	N-CA-C	6.18	119.55	110.59
1	I	274	ILE	N-CA-C	6.11	117.28	108.48
1	F	228	ILE	N-CA-C	6.08	113.57	107.55
1	C	592	LYS	N-CA-C	-6.06	98.85	108.73
1	H	371	ASP	N-CA-C	6.05	118.49	108.99
1	H	626	ASN	CA-C-N	5.98	125.66	119.56
1	H	626	ASN	C-N-CA	5.98	125.66	119.56
1	L	274	ILE	N-CA-C	5.97	116.47	107.75
1	K	274	ILE	CB-CA-C	-5.96	101.74	110.62
1	H	274	ILE	CB-CA-C	-5.95	101.75	110.62
1	C	116	THR	N-CA-C	-5.95	101.14	110.36
1	C	502	MET	CG-SD-CE	-5.94	87.83	100.90
1	D	190	ILE	N-CA-C	5.93	117.23	109.58
1	F	68	VAL	CB-CA-C	-5.91	102.73	111.19
1	E	483	VAL	CB-CA-C	-5.90	105.55	111.80
1	E	276	ASN	N-CA-C	-5.89	104.48	112.26
1	I	511	VAL	CB-CA-C	-5.89	101.84	110.62
1	J	276	ASN	N-CA-C	-5.88	104.77	112.41
1	F	358	VAL	N-CA-C	5.87	116.53	107.78
1	D	34	LEU	N-CA-C	5.86	118.94	109.40
1	I	483	VAL	CB-CA-C	-5.84	105.61	111.80
1	I	135	THR	N-CA-C	5.80	117.86	108.41
1	D	167	LYS	CD-CE-NZ	-5.80	93.35	111.90
1	D	446	GLY	N-CA-C	5.75	120.12	112.65
1	H	136	GLY	N-CA-C	-5.74	104.39	112.60
1	C	274	ILE	CB-CA-C	-5.74	102.07	110.62
1	G	374	ASP	N-CA-C	5.73	119.34	112.93
1	E	346	GLY	N-CA-C	5.72	117.76	110.96
1	K	136	GLY	N-CA-C	-5.71	104.43	112.60
1	B	46	THR	N-CA-C	-5.71	103.39	110.41
1	E	270	ASP	CB-CA-C	-5.71	110.01	116.63
1	J	274	ILE	CB-CA-C	-5.70	102.12	110.62
1	A	593	TRP	N-CA-C	5.67	117.41	108.96
1	D	346	GLY	N-CA-C	5.64	118.12	111.63
1	K	78	ASN	N-CA-C	5.63	117.40	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	424	PHE	CA-C-N	-5.60	114.48	120.03
1	G	424	PHE	C-N-CA	-5.60	114.48	120.03
1	D	326	ASP	CB-CA-C	-5.60	103.94	111.89
1	G	239	SER	CA-C-N	-5.59	114.17	119.76
1	G	239	SER	C-N-CA	-5.59	114.17	119.76
1	C	78	ASN	N-CA-C	5.59	116.76	108.60
1	E	65	ARG	N-CA-C	-5.59	101.37	110.20
1	C	228	ILE	CB-CA-C	-5.59	104.45	111.04
1	L	424	PHE	N-CA-C	5.59	122.16	109.81
1	A	358	VAL	N-CA-C	5.58	115.91	108.27
1	C	86	MET	CG-SD-CE	-5.56	88.67	100.90
1	G	305	PHE	N-CA-C	5.54	117.56	108.52
1	F	182	GLY	CA-C-N	5.52	125.87	119.47
1	F	182	GLY	C-N-CA	5.52	125.87	119.47
1	E	424	PHE	N-CA-C	5.51	121.98	109.81
1	D	82	ILE	CB-CA-C	-5.50	104.72	112.14
1	B	326	ASP	CB-CA-C	-5.48	103.80	111.80
1	H	190	ILE	N-CA-C	5.48	116.66	109.21
1	K	326	ASP	CB-CA-C	-5.48	104.11	111.89
1	A	411	ALA	N-CA-C	-5.47	101.62	110.32
1	L	592	LYS	N-CA-C	-5.47	99.81	108.73
1	B	83	VAL	CB-CA-C	-5.45	104.79	112.14
1	A	270	ASP	CB-CA-C	-5.43	108.73	116.34
1	I	349	TRP	N-CA-C	5.43	117.75	108.90
1	B	514	HIS	N-CA-C	5.43	118.00	108.56
1	H	351	GLU	CA-C-N	-5.42	114.37	119.85
1	H	351	GLU	C-N-CA	-5.42	114.37	119.85
1	H	49	VAL	CB-CA-C	-5.42	104.89	111.88
1	H	37	ALA	N-CA-C	-5.39	106.55	113.02
1	D	626	ASN	CA-C-N	5.38	125.72	119.47
1	D	626	ASN	C-N-CA	5.38	125.72	119.47
1	D	274	ILE	CB-CA-C	-5.38	102.08	110.69
1	J	274	ILE	N-CA-C	5.38	116.22	108.48
1	K	68	VAL	N-CA-C	-5.38	101.33	108.96
1	H	135	THR	N-CA-C	5.38	117.18	108.26
1	D	205	VAL	N-CA-C	5.37	115.59	107.75
1	H	116	THR	N-CA-C	-5.34	103.64	110.53
1	J	337	SER	N-CA-C	5.33	117.11	108.26
1	E	580	VAL	N-CA-C	-5.33	102.19	109.55
1	F	424	PHE	N-CA-C	5.33	121.59	109.81
1	G	424	PHE	N-CA-C	5.32	121.57	109.81
1	J	447	GLY	N-CA-C	5.32	119.07	110.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	274	ILE	N-CA-C	5.32	115.78	108.12
1	K	182	GLY	CA-C-N	5.32	125.14	119.28
1	K	182	GLY	C-N-CA	5.32	125.14	119.28
1	G	82	ILE	CB-CA-C	-5.31	104.98	112.14
1	I	374	ASP	N-CA-C	5.29	119.37	113.02
1	C	232	VAL	N-CA-C	-5.29	100.14	107.80
1	G	230	THR	CB-CA-C	-5.29	102.31	111.30
1	C	424	PHE	N-CA-C	5.28	121.47	109.81
1	L	157	THR	N-CA-C	5.28	118.00	109.40
1	L	238	VAL	CB-CA-C	-5.26	103.28	110.96
1	C	231	MET	N-CA-C	-5.24	102.30	110.42
1	B	151	ALA	N-CA-C	-5.23	102.64	110.23
1	H	358	VAL	N-CA-C	5.23	115.80	108.17
1	F	232	VAL	N-CA-C	-5.23	100.85	108.17
1	E	400	GLY	N-CA-C	5.22	121.10	113.48
1	I	10	GLU	N-CA-C	5.21	117.20	108.23
1	C	22	TYR	CA-C-N	-5.20	113.34	119.84
1	C	22	TYR	C-N-CA	-5.20	113.34	119.84
1	K	190	ILE	N-CA-C	5.20	116.28	109.21
1	G	277	LYS	N-CA-C	-5.20	101.01	108.60
1	H	134	ILE	N-CA-CB	-5.18	105.88	112.15
1	B	126	ALA	N-CA-C	5.17	117.82	111.82
1	I	12	VAL	N-CA-C	5.17	115.42	107.77
1	A	330	MET	CB-CG-SD	5.16	128.19	112.70
1	F	199	VAL	N-CA-C	5.16	116.15	108.46
1	B	399	ASN	N-CA-C	5.16	117.78	110.50
1	C	233	GLU	N-CA-C	5.15	117.96	109.72
1	K	335	ALA	N-CA-C	-5.15	105.36	111.69
1	B	531	MET	CG-SD-CE	-5.13	89.60	100.90
1	G	438	SER	N-CA-C	5.13	116.10	108.60
1	A	27	VAL	N-CA-C	5.12	119.99	109.34
1	D	228	ILE	CA-C-N	-5.12	114.96	120.03
1	D	228	ILE	C-N-CA	-5.12	114.96	120.03
1	A	41	PHE	N-CA-C	5.11	117.44	109.52
1	K	423	ALA	N-CA-C	5.10	117.80	109.59
1	A	419	ASN	N-CA-C	5.09	114.96	108.24
1	G	531	MET	CG-SD-CE	-5.09	89.69	100.90
1	K	626	ASN	CA-C-N	5.09	124.89	119.28
1	K	626	ASN	C-N-CA	5.09	124.89	119.28
1	B	138	ALA	CA-C-N	-5.09	114.71	119.85
1	B	138	ALA	C-N-CA	-5.09	114.71	119.85
1	E	274	ILE	CB-CA-C	-5.09	103.04	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	GLU	CA-C-N	-5.08	114.72	119.85
1	A	351	GLU	C-N-CA	-5.08	114.72	119.85
1	F	349	TRP	N-CA-C	5.07	117.71	109.24
1	J	438	SER	N-CA-C	5.06	116.53	108.79
1	H	182	GLY	CA-C-N	5.06	125.34	119.47
1	H	182	GLY	C-N-CA	5.06	125.34	119.47
1	H	302	GLY	N-CA-C	5.06	122.30	115.32
1	A	135	THR	N-CA-C	5.05	117.30	108.76
1	C	68	VAL	N-CA-C	-5.05	102.12	109.29
1	A	580	VAL	N-CA-C	-5.05	102.59	109.55
1	F	580	VAL	N-CA-C	-5.04	102.59	109.55
1	A	633	VAL	N-CA-C	5.03	115.09	107.75
1	A	378	ARG	CA-CB-CG	-5.03	104.05	114.10
1	C	38	GLY	N-CA-C	5.03	118.98	112.25
1	H	435	ASN	N-CA-C	-5.02	101.52	109.96
1	E	382	VAL	N-CA-C	5.01	115.25	107.28
1	G	11	ARG	N-CA-C	5.01	116.96	109.59
1	D	347	ASP	N-CA-C	5.01	117.70	110.28
1	G	270	ASP	CB-CA-C	-5.01	109.83	115.79
1	D	630	ASN	N-CA-C	-5.00	103.93	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4858	0	4712	124	0
1	B	4870	0	4724	123	0
1	C	4870	0	4724	104	0
1	D	4865	0	4720	129	0
1	E	4865	0	4720	129	0
1	F	4870	0	4724	77	0
1	G	4858	0	4712	112	0
1	H	4885	0	4744	108	0
1	I	4870	0	4724	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	4858	0	4712	144	0
1	K	4858	0	4712	152	0
1	L	4858	0	4712	180	0
2	A	26	0	8	2	0
2	B	26	0	10	7	0
2	C	13	0	5	2	0
2	D	13	0	5	4	0
2	E	13	0	5	3	0
2	F	26	0	10	2	0
2	G	13	0	5	2	0
2	H	13	0	5	1	0
2	I	13	0	5	3	0
2	J	13	0	5	3	0
2	K	26	0	8	1	0
2	L	13	0	5	2	0
3	C	4	0	0	0	0
3	H	4	0	0	0	0
3	K	4	0	0	0	0
4	A	170	0	0	3	0
4	B	151	0	0	4	0
4	C	169	0	0	3	0
4	D	117	0	0	4	0
4	E	118	0	0	6	0
4	F	164	0	0	1	0
4	G	87	0	0	0	0
4	H	106	0	0	1	0
4	I	72	0	0	1	0
4	J	72	0	0	2	0
4	K	74	0	0	1	0
4	L	68	0	0	2	0
All	All	59973	0	56716	1470	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 13.

All (1470) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:40:ASP:HB3	1:J:66:LYS:HE3	1.14	1.10
1:E:36:SER:HB2	4:E:829:HOH:O	1.55	1.07
1:I:526:MET:HE1	1:I:531:MET:HE1	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ARG:HH21	2:D:701:CIT:H41	1.23	1.03
1:D:120:ARG:HG2	1:D:120:ARG:HH11	1.27	0.98
1:C:467:ARG:NH2	1:C:469:LYS:HE2	1.80	0.97
1:D:603:THR:HG23	1:D:644:GLN:HB2	1.50	0.91
1:H:8:ALA:HB1	1:H:9:PRO:HA	1.53	0.91
1:I:627:PRO:HA	1:I:630:ASN:OD1	1.72	0.90
1:H:561:THR:O	1:H:579:ARG:HD2	1.72	0.89
1:L:301:LYS:HG2	1:L:325:HIS:HB2	1.54	0.89
1:B:622:VAL:HG12	1:B:623:PRO:HA	1.52	0.89
1:F:558:LEU:HD22	1:F:651:LEU:HD23	1.54	0.87
1:L:397:ARG:HH12	2:L:701:CIT:H42	1.39	0.87
1:H:182:GLY:HA2	1:H:399:ASN:ND2	1.89	0.86
1:F:8:ALA:HA	1:F:10:GLU:H	1.41	0.86
1:D:47:ALA:HA	1:D:62:TYR:HE2	1.41	0.85
1:I:549:THR:HG22	1:I:550:PRO:HD2	1.56	0.84
1:L:182:GLY:HA2	1:L:399:ASN:HD22	1.44	0.82
1:F:47:ALA:HA	1:F:62:TYR:HE2	1.42	0.82
1:H:274:ILE:HG23	1:H:306:TYR:HB2	1.58	0.82
1:C:481:ILE:HG12	1:C:502:MET:HE3	1.60	0.82
1:J:182:GLY:HA2	1:J:399:ASN:ND2	1.94	0.82
1:A:507:THR:OG1	1:A:508:GLY:N	2.09	0.81
1:A:112:THR:HG23	1:A:236:THR:HB	1.60	0.81
1:J:40:ASP:CB	1:J:66:LYS:HE3	2.06	0.81
1:L:308:ILE:HB	1:L:332:VAL:HG12	1.62	0.80
1:J:598:LYS:HE3	1:K:596:GLU:HG3	1.64	0.80
1:K:25:PHE:HB3	1:K:43:PHE:CD2	2.16	0.80
1:H:19:MET:HE3	1:H:63:LEU:HD13	1.64	0.80
1:D:34:LEU:HD21	1:E:30:LYS:HE3	1.64	0.79
1:F:58:VAL:HG11	1:F:63:LEU:HD22	1.64	0.78
1:H:8:ALA:CB	1:H:9:PRO:HA	2.14	0.78
1:H:8:ALA:HB1	1:H:9:PRO:CA	2.14	0.78
1:G:550:PRO:HA	1:G:591:PHE:CE1	2.19	0.78
1:I:19:MET:HE3	1:I:63:LEU:HD12	1.66	0.77
1:K:558:LEU:HD22	1:K:651:LEU:HD22	1.65	0.77
1:F:509:ARG:HD2	1:F:540:LEU:HB2	1.67	0.76
1:I:84:THR:O	1:I:87:SER:OG	2.04	0.76
1:J:47:ALA:HA	1:J:62:TYR:HE2	1.50	0.76
1:L:636:SER:OG	1:L:641:ASP:OD2	2.04	0.76
1:I:44:THR:OG1	1:I:46:THR:HG22	1.85	0.76
1:L:193:ILE:HG21	1:L:231:MET:HE2	1.68	0.76
1:D:558:LEU:HD22	1:D:651:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:ILE:HG12	1:B:502:MET:CE	2.17	0.75
1:L:244:GLU:OE2	4:L:801:HOH:O	2.04	0.75
1:B:9:PRO:HA	1:B:11:ARG:NH2	2.01	0.74
1:D:561:THR:HB	1:D:579:ARG:HE	1.52	0.74
1:I:397:ARG:HH12	2:I:701:CIT:H42	1.52	0.74
1:A:397:ARG:HH12	2:A:701:CIT:H41	1.52	0.74
1:B:45:THR:HG22	1:B:60:GLY:O	1.86	0.74
1:C:8:ALA:N	1:C:10:GLU:H	1.86	0.74
1:A:40:ASP:HB3	1:A:66:LYS:HD2	1.69	0.74
1:B:48:SER:HB2	1:B:62:TYR:CD1	2.22	0.74
1:F:8:ALA:HA	1:F:10:GLU:N	2.02	0.73
1:A:120:ARG:HH11	1:A:120:ARG:HG2	1.54	0.73
1:E:36:SER:CB	4:E:829:HOH:O	2.24	0.73
1:E:229:PRO:HB2	1:E:231:MET:HE1	1.70	0.73
1:K:467:ARG:NH2	1:K:469:LYS:HE2	2.04	0.73
1:D:14:SER:O	1:D:34:LEU:O	2.07	0.73
1:H:558:LEU:HD22	1:H:651:LEU:HD22	1.69	0.73
1:I:70:PRO:HB3	1:I:92:HIS:ND1	2.04	0.72
1:L:315:VAL:HB	1:L:338:LEU:HD23	1.69	0.72
1:G:47:ALA:HA	1:G:62:TYR:HE2	1.54	0.72
1:J:320:GLU:HG3	1:J:353:ILE:HB	1.70	0.72
1:B:481:ILE:HG12	1:B:502:MET:HE3	1.69	0.72
1:L:182:GLY:HA2	1:L:399:ASN:ND2	2.05	0.72
1:C:540:LEU:C	1:C:541:LEU:HD12	2.16	0.71
1:H:509:ARG:HD2	1:H:540:LEU:HB2	1.72	0.71
1:B:371:ASP:OD1	1:B:395:GLN:NE2	2.23	0.71
1:C:272:VAL:CG1	1:C:274:ILE:HD11	2.20	0.71
1:E:509:ARG:HD2	1:E:540:LEU:HB2	1.72	0.71
1:G:105:LEU:HD23	1:G:132:LEU:HD22	1.71	0.71
1:F:564:ARG:HD2	1:F:648:GLU:HG2	1.71	0.71
1:L:467:ARG:NH2	1:L:469:LYS:HE2	2.06	0.70
1:D:333:ARG:NH2	2:D:701:CIT:H41	2.03	0.70
1:E:419:ASN:HB3	4:E:876:HOH:O	1.90	0.70
1:D:563:ILE:HD12	1:E:552:ARG:NE	2.06	0.70
1:H:433:TYR:CE1	1:H:455:HIS:HD2	2.10	0.70
1:H:410:ARG:HD3	4:H:843:HOH:O	1.90	0.70
1:L:509:ARG:HD3	1:L:540:LEU:HB2	1.73	0.70
1:E:189:LYS:HB2	1:E:349:TRP:CD1	2.27	0.70
1:D:19:MET:HE1	1:D:41:PHE:CE1	2.27	0.69
1:J:40:ASP:HB3	1:J:66:LYS:CE	2.08	0.69
1:J:379:VAL:HB	1:J:401:VAL:HG22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:ALA:HA	1:K:62:TYR:HE2	1.57	0.69
1:D:34:LEU:CD2	1:E:30:LYS:HE3	2.23	0.69
1:G:105:LEU:HD23	1:G:132:LEU:CD2	2.22	0.69
1:I:182:GLY:HA2	1:I:399:ASN:ND2	2.07	0.69
1:B:622:VAL:CG1	1:B:623:PRO:HA	2.22	0.68
1:E:397:ARG:HH12	2:E:701:CIT:H42	1.58	0.68
1:C:308:ILE:HB	1:C:332:VAL:HG12	1.76	0.68
1:L:526:MET:HE2	1:L:553:MET:HE2	1.75	0.68
1:J:563:ILE:HD13	1:K:552:ARG:NE	2.07	0.68
1:F:603:THR:HG23	1:F:644:GLN:HB2	1.76	0.68
1:H:485:LYS:HD3	1:H:490:THR:O	1.93	0.68
1:E:404:LEU:CD2	1:E:428:ARG:HD2	2.24	0.68
1:F:558:LEU:HD22	1:F:651:LEU:CD2	2.24	0.68
1:B:340:TRP:HA	1:B:375:ILE:HD11	1.76	0.67
1:L:520:ASP:OD1	1:L:522:THR:OG1	2.12	0.67
1:L:132:LEU:HD12	1:L:258:ILE:HG12	1.76	0.67
1:L:340:TRP:HA	1:L:375:ILE:HD11	1.75	0.67
1:C:229:PRO:HB2	1:C:231:MET:HE1	1.76	0.67
1:D:261:ASN:HA	1:D:293:ASN:O	1.95	0.67
1:H:15:ASP:OD1	1:H:15:ASP:O	2.13	0.67
1:G:464:ASN:HD22	1:G:464:ASN:C	2.02	0.67
1:I:481:ILE:HD12	1:I:502:MET:SD	2.35	0.67
1:J:148:ASP:OD1	1:J:148:ASP:N	2.28	0.67
1:J:603:THR:HG23	1:J:644:GLN:HB2	1.75	0.67
1:E:47:ALA:HA	1:E:62:TYR:HE2	1.60	0.66
1:I:433:TYR:CE1	1:I:455:HIS:HD2	2.13	0.66
1:K:22:TYR:CE1	1:K:24:ASN:HB2	2.30	0.66
1:L:193:ILE:HD13	1:L:231:MET:HE1	1.76	0.66
1:D:541:LEU:HD12	1:D:541:LEU:N	2.11	0.66
1:H:15:ASP:OD1	1:H:15:ASP:C	2.38	0.66
1:B:241:TYR:HB3	4:B:881:HOH:O	1.96	0.66
1:C:301:LYS:HG2	1:C:325:HIS:HB2	1.77	0.66
1:H:19:MET:HE3	1:H:63:LEU:CD1	2.26	0.66
1:K:509:ARG:HD2	1:K:540:LEU:HB2	1.78	0.66
1:L:371:ASP:OD2	1:L:395:GLN:HG2	1.95	0.66
1:G:47:ALA:HA	1:G:62:TYR:CE2	2.30	0.66
1:D:526:MET:HE2	1:D:551:PRO:HG3	1.78	0.66
1:C:397:ARG:HH12	2:C:701:CIT:H41	1.60	0.65
1:H:542:SER:HA	1:H:589:ASN:ND2	2.12	0.65
1:I:301:LYS:HG2	1:I:325:HIS:HB2	1.78	0.65
1:K:340:TRP:HA	1:K:375:ILE:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:153:SER:HB2	1:J:214:LEU:HD12	1.76	0.65
1:E:32:THR:OG1	1:E:40:ASP:OD1	2.14	0.65
1:L:244:GLU:HA	1:L:274:ILE:HD12	1.79	0.65
1:A:251:ASN:OD1	1:A:278:ARG:NH2	2.29	0.65
1:F:155:VAL:HG13	1:F:208:ILE:O	1.97	0.65
1:A:540:LEU:C	1:A:541:LEU:HD12	2.22	0.65
1:H:182:GLY:HA2	1:H:399:ASN:HD22	1.59	0.65
1:H:581:ARG:HH11	1:H:581:ARG:HG2	1.62	0.65
1:K:601:ARG:NH2	1:K:609:GLY:O	2.29	0.65
1:K:627:PRO:HA	1:K:630:ASN:OD1	1.97	0.65
1:L:50:VAL:HG21	1:L:57:ALA:HB2	1.78	0.65
1:B:311:TYR:CE1	1:B:334:HIS:HD2	2.15	0.64
1:D:603:THR:CG2	1:D:644:GLN:HB2	2.25	0.64
1:H:333:ARG:HH21	2:H:702:CIT:H41	1.62	0.64
1:H:337:SER:HA	1:H:371:ASP:O	1.97	0.64
1:H:397:ARG:HA	1:H:422:VAL:HG21	1.79	0.64
1:L:33:LEU:HD12	1:L:34:LEU:H	1.62	0.64
1:J:326:ASP:HA	1:J:359:ASN:O	1.98	0.64
1:G:316:LEU:N	1:G:316:LEU:HD23	2.12	0.64
1:B:481:ILE:CG1	1:B:502:MET:HE3	2.28	0.64
1:K:301:LYS:HG2	1:K:325:HIS:HB2	1.78	0.64
1:F:14:SER:O	1:F:34:LEU:O	2.16	0.64
1:L:139:PRO:HG2	1:L:142:PHE:CZ	2.33	0.64
1:C:470:GLY:HA2	1:C:499:GLY:O	1.99	0.63
1:K:397:ARG:HA	1:K:422:VAL:HG21	1.79	0.63
1:A:311:TYR:CE1	1:A:334:HIS:HD2	2.16	0.63
1:G:316:LEU:HD23	1:G:316:LEU:H	1.63	0.63
1:I:564:ARG:HD2	1:I:648:GLU:HG2	1.80	0.63
1:I:615:SER:HB2	1:I:633:VAL:HG23	1.81	0.63
1:K:193:ILE:HD12	1:K:318:CYS:SG	2.38	0.63
1:D:622:VAL:HG12	1:D:623:PRO:HA	1.80	0.63
1:F:58:VAL:CG1	1:F:63:LEU:HD22	2.29	0.63
1:K:47:ALA:HA	1:K:62:TYR:CE2	2.32	0.63
1:A:277:LYS:HE3	1:A:281:ALA:O	1.98	0.63
1:L:306:TYR:CE1	1:L:330:MET:HE3	2.33	0.63
1:E:404:LEU:HD23	1:E:428:ARG:HD2	1.81	0.62
1:I:19:MET:HE3	1:I:63:LEU:CD1	2.29	0.62
1:H:22:TYR:HB3	1:H:25:PHE:CE2	2.35	0.62
1:L:370:PHE:HB2	1:L:394:PHE:CD1	2.34	0.62
1:A:272:VAL:HG22	1:A:304:CYS:HB2	1.80	0.62
1:K:542:SER:HA	1:K:589:ASN:ND2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:424:PHE:CD2	1:L:448:TYR:CE2	2.87	0.62
1:B:145:LEU:O	1:B:220:LEU:HD21	1.98	0.62
1:A:22:TYR:HB3	1:A:25:PHE:CE2	2.34	0.62
1:H:8:ALA:CB	1:H:9:PRO:CA	2.77	0.62
1:I:193:ILE:HG21	1:I:231:MET:CE	2.28	0.62
1:B:540:LEU:C	1:B:541:LEU:HD12	2.24	0.62
1:L:326:ASP:HA	1:L:359:ASN:O	1.99	0.62
1:E:315:VAL:HB	1:E:338:LEU:HD22	1.81	0.62
1:J:293:ASN:OD1	1:J:316:LEU:HG	2.00	0.62
1:A:50:VAL:HA	1:A:55:VAL:HG12	1.81	0.62
1:B:509:ARG:HD2	1:B:540:LEU:HB2	1.81	0.62
1:L:409:TYR:CE2	1:L:433:TYR:CD2	2.88	0.62
1:A:620:GLN:HA	1:A:620:GLN:HE21	1.65	0.62
1:B:498:ASP:OD2	1:B:527:SER:HB3	1.99	0.62
1:I:509:ARG:HD2	1:I:540:LEU:HB2	1.82	0.62
1:J:229:PRO:HB2	1:J:231:MET:HE1	1.82	0.62
1:L:370:PHE:CD2	1:L:394:PHE:CE1	2.88	0.62
1:E:100:GLN:HB2	4:E:806:HOH:O	1.99	0.61
1:B:254:PHE:O	1:B:276:ASN:HB2	2.00	0.61
1:D:189:LYS:O	1:D:349:TRP:HA	1.99	0.61
1:C:58:VAL:HG11	1:C:63:LEU:HD22	1.81	0.61
1:H:51:ASP:OD1	1:H:51:ASP:C	2.43	0.61
1:J:401:VAL:HG12	1:J:403:TYR:CE2	2.35	0.61
1:L:394:PHE:CD2	1:L:416:PHE:CE2	2.89	0.61
1:K:229:PRO:CG	1:K:231:MET:HE1	2.31	0.61
1:K:626:ASN:HD22	1:K:629:LEU:HG	1.64	0.61
1:K:145:LEU:O	1:K:220:LEU:HD21	2.01	0.61
1:J:167:LYS:HA	1:J:196:VAL:HG12	1.83	0.61
1:J:603:THR:CG2	1:J:644:GLN:HB2	2.30	0.61
1:A:564:ARG:HH11	1:A:648:GLU:CG	2.14	0.61
1:J:90:ASN:HA	1:J:110:ASN:O	2.01	0.61
1:L:181:GLY:O	1:L:399:ASN:HB2	2.00	0.61
1:H:564:ARG:CZ	1:I:550:PRO:HG2	2.30	0.60
1:L:579:ARG:HD3	1:L:627:PRO:HB2	1.82	0.60
1:E:284:ILE:CG2	1:E:287:ARG:HD2	2.31	0.60
1:G:397:ARG:HA	1:G:422:VAL:HG21	1.82	0.60
1:L:433:TYR:CE1	1:L:455:HIS:HD2	2.20	0.60
1:B:147:ALA:HA	1:B:220:LEU:HD11	1.82	0.60
1:B:558:LEU:HD22	1:B:651:LEU:HD22	1.83	0.60
1:G:602:LEU:HD11	1:G:646:ALA:HB2	1.83	0.60
1:L:83:VAL:HA	1:L:105:LEU:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:541:LEU:HD21	1:L:591:PHE:CE1	2.35	0.60
1:C:611:LEU:HD13	1:C:645:VAL:HG11	1.84	0.60
1:H:110:ASN:ND2	1:H:234:ASN:HB3	2.17	0.60
1:K:44:THR:HG1	1:K:46:THR:HG1	1.48	0.60
1:A:419:ASN:O	1:A:422:VAL:HG23	2.02	0.60
1:D:30:LYS:CG	1:F:34:LEU:HD11	2.31	0.60
1:E:526:MET:HE3	1:E:551:PRO:HG3	1.83	0.60
1:F:26:GLN:N	1:F:29:ASP:OD2	2.35	0.60
1:J:130:GLN:HG2	1:J:256:ILE:HB	1.84	0.60
1:D:47:ALA:HA	1:D:62:TYR:CE2	2.31	0.60
1:G:509:ARG:HD3	1:G:537:PHE:O	2.02	0.60
1:J:510:ALA:CB	1:J:531:MET:HE3	2.32	0.60
1:E:397:ARG:HH22	2:E:701:CIT:C4	2.15	0.60
1:G:410:ARG:HA	1:G:434:ASP:O	2.02	0.60
1:D:498:ASP:OD1	1:D:527:SER:HB2	2.02	0.60
1:I:25:PHE:HB3	1:I:43:PHE:CD1	2.36	0.60
1:I:582:GLY:O	1:I:618:GLN:NE2	2.35	0.60
1:J:440:PHE:HB2	1:J:461:VAL:HG13	1.83	0.60
1:K:360:CYS:HB2	1:K:384:CYS:SG	2.42	0.60
1:K:526:MET:HE1	1:K:531:MET:HE1	1.82	0.60
1:J:558:LEU:HD12	1:J:558:LEU:O	2.02	0.59
1:K:283:ASP:OD2	1:K:333:ARG:NH1	2.35	0.59
1:L:53:GLY:HA3	1:L:76:PHE:CD2	2.37	0.59
1:L:580:VAL:HG11	1:L:632:PHE:CD2	2.37	0.59
1:B:16:LEU:HD11	1:B:56:PHE:CE2	2.36	0.59
1:E:277:LYS:HE3	1:E:281:ALA:O	2.02	0.59
1:K:261:ASN:ND2	1:K:293:ASN:HB3	2.17	0.59
1:C:622:VAL:HG22	1:C:623:PRO:HA	1.83	0.59
1:D:25:PHE:HB3	1:D:43:PHE:CD1	2.38	0.59
1:I:498:ASP:OD2	1:I:527:SER:HB2	2.01	0.59
1:L:134:ILE:HG23	1:L:232:VAL:HG11	1.83	0.59
1:L:354:GLU:OE1	1:L:354:GLU:HA	2.02	0.59
1:D:485:LYS:HD3	1:D:490:THR:O	2.02	0.59
1:F:25:PHE:HB3	1:F:43:PHE:CD1	2.38	0.59
1:J:31:ILE:HD12	1:J:31:ILE:N	2.18	0.59
1:E:301:LYS:HG2	1:E:325:HIS:HB2	1.83	0.59
1:H:611:LEU:HD13	1:H:645:VAL:HG21	1.84	0.59
1:I:603:THR:HG23	1:I:644:GLN:HB2	1.84	0.59
1:K:74:SER:HB3	1:K:96:ASP:OD2	2.03	0.59
1:L:299:THR:HG22	1:L:323:GLU:HB2	1.85	0.59
1:D:455:HIS:HA	1:D:474:THR:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:457:SER:O	1:G:476:ASN:HA	2.03	0.58
1:D:540:LEU:C	1:D:541:LEU:HD12	2.28	0.58
1:E:549:THR:HG23	1:E:550:PRO:HD2	1.85	0.58
1:F:47:ALA:HA	1:F:62:TYR:CE2	2.31	0.58
1:G:213:THR:HG21	1:I:388:ASP:OD2	2.02	0.58
1:G:619:ASN:HD22	1:G:629:LEU:HB2	1.68	0.58
1:I:372:THR:O	1:I:397:ARG:HB2	2.03	0.58
1:J:245:PHE:HE1	1:K:197:VAL:HG12	1.69	0.58
1:I:526:MET:HE1	1:I:531:MET:CE	2.23	0.58
1:A:142:PHE:CD2	1:A:225:GLU:HG3	2.38	0.58
1:D:34:LEU:HD11	1:E:40:ASP:HB3	1.86	0.58
1:H:110:ASN:HD22	1:H:234:ASN:HB3	1.69	0.58
1:B:404:LEU:CD2	1:B:428:ARG:HD2	2.34	0.58
1:B:541:LEU:HD12	1:B:541:LEU:N	2.19	0.58
1:C:315:VAL:HB	1:C:338:LEU:HD23	1.85	0.58
1:D:326:ASP:HA	1:D:359:ASN:O	2.04	0.58
1:E:603:THR:HG23	1:E:644:GLN:HB2	1.86	0.58
1:J:550:PRO:HA	1:J:591:PHE:CE1	2.39	0.58
1:C:504:TYR:CZ	1:C:506:GLY:HA2	2.39	0.58
1:G:541:LEU:HD12	1:G:541:LEU:N	2.18	0.58
1:K:34:LEU:HA	1:L:66:LYS:HZ2	1.67	0.58
1:K:602:LEU:HD13	1:L:592:LYS:HG2	1.84	0.58
1:A:541:LEU:HD12	1:A:541:LEU:N	2.19	0.58
1:L:409:TYR:CE2	1:L:433:TYR:HD2	2.22	0.58
1:B:374:ASP:HA	1:B:397:ARG:O	2.04	0.58
1:D:30:LYS:HG3	1:F:34:LEU:HD11	1.86	0.58
1:F:459:ASN:HA	1:F:479:SER:O	2.03	0.58
1:G:558:LEU:HD22	1:G:651:LEU:HD22	1.85	0.58
1:A:261:ASN:HA	1:A:293:ASN:O	2.04	0.57
1:G:404:LEU:CD2	1:G:428:ARG:HD2	2.34	0.57
1:J:540:LEU:C	1:J:541:LEU:HD12	2.29	0.57
1:D:361:GLU:HG3	1:D:385:VAL:CG1	2.34	0.57
1:G:254:PHE:O	1:G:276:ASN:HB2	2.04	0.57
1:K:25:PHE:CB	1:K:43:PHE:CD2	2.88	0.57
1:L:237:LEU:HD12	1:L:268:ILE:HG12	1.85	0.57
1:L:360:CYS:HB2	1:L:384:CYS:SG	2.44	0.57
1:L:597:VAL:HG12	1:L:599:LEU:CD2	2.35	0.57
1:D:311:TYR:HD2	1:D:314:GLU:HG3	1.69	0.57
1:L:549:THR:HG22	1:L:550:PRO:HD2	1.86	0.57
1:F:23:PRO:HA	1:F:59:PRO:HB2	1.87	0.57
1:J:203:GLY:O	4:J:801:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:85:PHE:CE2	1:K:91:ARG:HD2	2.39	0.57
1:K:520:ASP:OD1	1:K:520:ASP:C	2.48	0.57
1:D:322:THR:HB	4:D:856:HOH:O	2.03	0.57
1:J:582:GLY:H	1:J:618:GLN:NE2	2.02	0.57
1:I:193:ILE:HG21	1:I:231:MET:HE2	1.86	0.57
1:L:40:ASP:O	1:L:66:LYS:HG2	2.05	0.57
1:E:561:THR:O	1:E:579:ARG:HD2	2.04	0.57
1:G:182:GLY:HA2	1:G:399:ASN:ND2	2.20	0.57
1:J:223:ALA:O	1:J:225:GLU:HG2	2.04	0.57
1:I:285:GLU:HA	1:I:310:TRP:CE3	2.39	0.56
1:L:122:LEU:HD21	1:L:244:GLU:HG2	1.88	0.56
1:L:284:ILE:HG21	1:L:287:ARG:HD2	1.86	0.56
1:L:351:GLU:HB2	1:L:375:ILE:HB	1.87	0.56
1:A:404:LEU:CD2	1:A:428:ARG:HD2	2.34	0.56
1:A:564:ARG:HE	1:B:550:PRO:HD2	1.70	0.56
1:E:177:LYS:HB3	1:E:190:ILE:HD13	1.87	0.56
1:J:98:VAL:HG13	1:J:120:ARG:HB2	1.87	0.56
1:J:410:ARG:HA	1:J:434:ASP:O	2.05	0.56
1:H:351:GLU:CB	1:H:375:ILE:HD12	2.36	0.56
1:L:327:ILE:HG12	1:L:360:CYS:SG	2.44	0.56
1:D:295:CYS:O	1:D:319:SER:HA	2.05	0.56
1:F:394:PHE:CD1	1:F:416:PHE:CE2	2.94	0.56
1:J:33:LEU:HD12	1:J:34:LEU:H	1.70	0.56
1:J:561:THR:HB	1:J:579:ARG:NH1	2.19	0.56
1:C:510:ALA:CB	1:C:531:MET:HE3	2.35	0.56
1:G:470:GLY:O	1:G:500:VAL:HG22	2.05	0.56
1:H:53:GLY:HA3	1:H:76:PHE:CE2	2.40	0.56
1:H:626:ASN:ND2	1:H:629:LEU:HG	2.21	0.56
1:C:241:TYR:HB3	4:C:818:HOH:O	2.06	0.56
1:A:603:THR:HG23	1:A:644:GLN:HB2	1.88	0.56
1:E:284:ILE:HB	1:E:287:ARG:HD2	1.88	0.56
1:H:541:LEU:N	1:H:541:LEU:HD12	2.20	0.56
1:G:191:SER:HB3	1:G:349:TRP:HB3	1.88	0.55
1:J:436:VAL:O	1:J:458:GLN:HG3	2.05	0.55
1:I:284:ILE:HG21	1:I:287:ARG:HD2	1.88	0.55
1:J:22:TYR:CE2	1:J:24:ASN:HB2	2.42	0.55
1:K:85:PHE:CZ	1:K:91:ARG:HD2	2.41	0.55
1:H:53:GLY:HA3	1:H:76:PHE:CD2	2.41	0.55
1:I:47:ALA:HA	1:I:62:TYR:HE2	1.72	0.55
1:B:320:GLU:HG3	1:B:353:ILE:HB	1.88	0.55
1:D:579:ARG:NH1	1:D:627:PRO:CG	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:464:ASN:HD22	1:G:465:GLY:N	2.05	0.55
1:H:7:VAL:HG12	1:H:8:ALA:N	2.20	0.55
1:J:20:VAL:HA	1:J:58:VAL:HG12	1.89	0.55
1:A:254:PHE:CZ	1:A:276:ASN:HB3	2.42	0.55
1:B:46:THR:O	1:B:62:TYR:HE1	1.89	0.55
1:K:469:LYS:HG2	1:K:498:ASP:HB3	1.88	0.55
1:L:416:PHE:CD1	1:L:440:PHE:CE1	2.94	0.55
1:B:301:LYS:HG2	1:B:325:HIS:HB2	1.87	0.55
1:C:139:PRO:HG2	1:C:142:PHE:CZ	2.42	0.55
1:D:328:HIS:HB3	1:D:330:MET:HE2	1.89	0.55
1:K:58:VAL:HB	1:K:59:PRO:CD	2.37	0.55
1:K:183:PRO:HD2	1:K:374:ASP:HB2	1.87	0.55
1:A:322:THR:HB	4:A:867:HOH:O	2.06	0.55
1:C:500:VAL:HG12	1:C:502:MET:HG3	1.89	0.55
1:L:541:LEU:HD12	1:L:541:LEU:N	2.22	0.55
1:D:579:ARG:NH1	1:D:627:PRO:HG2	2.22	0.55
1:F:8:ALA:CA	1:F:10:GLU:H	2.18	0.55
1:A:564:ARG:HH11	1:A:648:GLU:CD	2.15	0.55
1:C:426:ILE:N	1:C:426:ILE:HD12	2.23	0.55
1:I:52:ASN:HA	1:I:56:PHE:CE1	2.42	0.55
1:K:549:THR:HG22	1:K:550:PRO:HD2	1.87	0.55
1:C:410:ARG:HA	1:C:434:ASP:O	2.06	0.54
1:E:70:PRO:HB3	1:E:92:HIS:ND1	2.21	0.54
1:A:540:LEU:HD12	4:A:836:HOH:O	2.06	0.54
1:J:371:ASP:HB2	1:J:395:GLN:HB3	1.89	0.54
1:L:105:LEU:HD23	1:L:132:LEU:CD2	2.37	0.54
1:A:20:VAL:HA	1:A:58:VAL:HG12	1.89	0.54
1:D:120:ARG:HG2	1:D:120:ARG:NH1	2.02	0.54
1:G:596:GLU:HG3	1:I:598:LYS:HE3	1.90	0.54
1:K:254:PHE:CZ	1:K:276:ASN:HB3	2.42	0.54
1:K:483:VAL:HG12	1:K:519:ILE:HD12	1.89	0.54
1:K:570:VAL:O	1:K:571:ALA:HB3	2.08	0.54
1:J:315:VAL:HB	1:J:338:LEU:CD2	2.38	0.54
2:K:703:CIT:O3	2:K:703:CIT:O7	2.19	0.54
1:L:261:ASN:HA	1:L:293:ASN:O	2.07	0.54
1:L:374:ASP:HA	1:L:397:ARG:O	2.08	0.54
1:L:399:ASN:OD1	1:L:423:ALA:HB3	2.06	0.54
1:H:47:ALA:HA	1:H:62:TYR:CE2	2.43	0.54
1:K:34:LEU:HA	1:L:66:LYS:NZ	2.21	0.54
1:A:120:ARG:HG2	1:A:120:ARG:NH1	2.22	0.54
1:B:397:ARG:HA	1:B:422:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:619:ASN:HD22	1:K:629:LEU:HB2	1.73	0.54
1:L:79:TRP:O	1:L:83:VAL:HG22	2.08	0.54
1:D:284:ILE:CG2	1:D:287:ARG:HD2	2.37	0.54
1:L:538:TRP:CZ3	1:L:539:ALA:HB2	2.43	0.54
1:D:436:VAL:O	1:D:458:GLN:HG3	2.08	0.54
1:E:394:PHE:CD1	1:E:416:PHE:CE2	2.96	0.54
1:E:610:ALA:HA	1:F:612:THR:HB	1.90	0.54
1:G:228:ILE:HG22	1:G:228:ILE:O	2.06	0.54
1:I:20:VAL:HA	1:I:58:VAL:HG12	1.89	0.54
1:C:394:PHE:CD1	1:C:416:PHE:CE2	2.95	0.54
1:C:526:MET:CE	1:C:551:PRO:HG2	2.37	0.54
1:D:52:ASN:O	1:D:76:PHE:HA	2.08	0.54
1:F:179:CYS:HB3	1:F:351:GLU:CD	2.33	0.54
1:L:193:ILE:HG21	1:L:231:MET:CE	2.37	0.54
1:B:158:VAL:HG21	1:B:163:LEU:CD2	2.38	0.54
1:C:509:ARG:HD3	1:C:537:PHE:O	2.08	0.54
1:G:564:ARG:HD2	1:G:648:GLU:HG2	1.89	0.54
1:I:189:LYS:O	1:I:349:TRP:HA	2.08	0.54
1:K:327:ILE:HG12	1:K:360:CYS:SG	2.48	0.53
1:L:340:TRP:CD1	1:L:340:TRP:C	2.86	0.53
1:L:584:PHE:HZ	1:L:616:VAL:HG11	1.74	0.53
1:C:353:ILE:O	1:C:354:GLU:HB2	2.08	0.53
1:D:570:VAL:HG22	4:D:830:HOH:O	2.08	0.53
1:K:229:PRO:HB2	1:K:231:MET:HE1	1.90	0.53
1:K:604:PHE:CZ	1:L:616:VAL:HG12	2.44	0.53
1:B:459:ASN:HA	1:B:479:SER:O	2.08	0.53
1:C:145:LEU:O	1:C:220:LEU:HD21	2.09	0.53
1:C:459:ASN:HA	1:C:479:SER:O	2.08	0.53
1:E:425:PRO:C	1:E:426:ILE:HD13	2.33	0.53
1:I:551:PRO:HG2	1:I:553:MET:HE3	1.90	0.53
1:L:22:TYR:CE1	1:L:24:ASN:HB2	2.44	0.53
1:G:186:TYR:CE1	1:G:342:SER:HA	2.44	0.53
1:J:564:ARG:HD2	1:J:648:GLU:HG2	1.89	0.53
1:A:410:ARG:HA	1:A:434:ASP:O	2.08	0.53
1:E:339:ASN:HA	1:E:373:HIS:ND1	2.24	0.53
1:G:142:PHE:HB2	1:G:225:GLU:OE1	2.09	0.53
1:I:365:THR:HG21	1:I:369:GLY:HA2	1.91	0.53
1:J:71:ALA:HA	1:J:75:TRP:CZ3	2.44	0.53
1:J:254:PHE:CZ	1:J:276:ASN:HB3	2.43	0.53
1:L:97:THR:O	1:L:119:GLY:HA2	2.08	0.53
1:L:426:ILE:N	1:L:426:ILE:HD12	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ARG:CG	1:B:648:GLU:HG2	2.39	0.53
1:C:8:ALA:CA	1:C:10:GLU:H	2.22	0.53
1:D:515:GLY:O	1:D:516:THR:C	2.49	0.53
1:E:540:LEU:C	1:E:541:LEU:HD12	2.33	0.53
1:J:602:LEU:HD11	1:J:646:ALA:HB2	1.90	0.53
1:K:295:CYS:O	1:K:319:SER:HA	2.08	0.53
1:B:237:LEU:HD12	1:B:268:ILE:HD13	1.89	0.53
1:F:261:ASN:HA	1:F:293:ASN:O	2.08	0.53
1:J:484:THR:OG1	1:J:485:LYS:N	2.40	0.53
1:J:582:GLY:H	1:J:618:GLN:HE22	1.55	0.53
1:C:274:ILE:CD1	1:C:306:TYR:HD2	2.21	0.53
1:C:446:GLY:HA2	1:C:465:GLY:O	2.09	0.53
1:D:564:ARG:HD2	1:D:648:GLU:HG2	1.91	0.53
1:H:526:MET:SD	1:H:553:MET:HE3	2.49	0.53
1:I:261:ASN:HA	1:I:293:ASN:O	2.09	0.53
1:B:397:ARG:NH2	2:B:701:CIT:H42	2.24	0.53
1:J:245:PHE:CE1	1:K:197:VAL:HG12	2.44	0.53
1:L:45:THR:HG23	1:L:60:GLY:O	2.09	0.53
1:L:302:GLY:HA2	1:L:326:ASP:O	2.09	0.53
1:L:419:ASN:O	1:L:422:VAL:HG23	2.08	0.53
1:L:472:ARG:HG3	1:L:501:SER:HB3	1.90	0.53
1:C:229:PRO:HB2	1:C:231:MET:CE	2.39	0.52
1:D:20:VAL:HA	1:D:58:VAL:HG12	1.89	0.52
1:H:326:ASP:HA	1:H:359:ASN:O	2.09	0.52
1:I:302:GLY:HA2	1:I:326:ASP:O	2.09	0.52
1:L:363:TYR:CZ	1:L:387:TYR:CD2	2.97	0.52
1:L:403:TYR:CD2	1:L:427:TYR:CE1	2.96	0.52
1:A:540:LEU:HD12	1:A:541:LEU:N	2.24	0.52
1:A:278:ARG:NH1	1:A:278:ARG:HG2	2.25	0.52
1:B:22:TYR:CZ	1:B:24:ASN:HB2	2.44	0.52
1:F:540:LEU:HD12	1:F:541:LEU:N	2.24	0.52
1:H:193:ILE:HD13	1:H:231:MET:HE1	1.91	0.52
1:H:261:ASN:HA	1:H:293:ASN:O	2.10	0.52
1:H:374:ASP:HA	1:H:397:ARG:O	2.08	0.52
1:I:326:ASP:HA	1:I:359:ASN:O	2.09	0.52
1:G:547:GLN:HE22	1:G:592:LYS:HD3	1.74	0.52
1:B:435:ASN:O	1:B:457:SER:OG	2.24	0.52
1:F:254:PHE:CZ	1:F:276:ASN:HB3	2.44	0.52
1:G:382:VAL:HG22	1:G:404:LEU:HD12	1.92	0.52
1:H:459:ASN:HA	1:H:479:SER:O	2.10	0.52
1:I:155:VAL:HA	1:I:208:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:301:LYS:CG	1:I:325:HIS:HB2	2.39	0.52
1:J:78:ASN:OD1	1:J:80:THR:HB	2.10	0.52
1:K:130:GLN:HG2	1:K:256:ILE:HB	1.92	0.52
1:C:261:ASN:HA	1:C:293:ASN:O	2.10	0.52
1:E:340:TRP:HA	1:E:375:ILE:HD11	1.89	0.52
1:H:564:ARG:HD2	1:H:648:GLU:HG2	1.92	0.52
1:L:291:LYS:HE3	1:L:314:GLU:OE2	2.08	0.52
1:L:479:SER:HA	1:L:509:ARG:O	2.09	0.52
1:C:92:HIS:HB2	4:C:883:HOH:O	2.09	0.52
1:H:361:GLU:HG3	1:H:385:VAL:CG1	2.39	0.52
1:J:404:LEU:CD2	1:J:428:ARG:HD2	2.39	0.52
1:B:382:VAL:HG22	1:B:404:LEU:HD12	1.91	0.52
1:C:92:HIS:HE1	1:C:114:GLU:OE1	1.92	0.52
1:F:52:ASN:HA	1:F:56:PHE:CE2	2.45	0.52
1:I:154:LYS:HG3	4:I:846:HOH:O	2.10	0.52
1:K:10:GLU:HG3	1:K:30:LYS:O	2.09	0.52
1:B:20:VAL:HA	1:B:58:VAL:HG12	1.92	0.52
1:D:538:TRP:CE3	1:D:539:ALA:HB2	2.45	0.52
1:E:467:ARG:CZ	1:E:469:LYS:HD2	2.40	0.52
1:E:526:MET:HE3	1:E:551:PRO:CG	2.39	0.52
1:I:615:SER:HB2	1:I:633:VAL:CG2	2.39	0.52
1:L:570:VAL:HG12	1:L:570:VAL:O	2.08	0.52
1:C:324:VAL:HG11	1:C:336:ILE:HD11	1.92	0.52
1:J:231:MET:HA	1:J:231:MET:HE2	1.92	0.52
1:K:19:MET:HE2	1:K:33:LEU:HD22	1.91	0.52
1:A:510:ALA:CB	1:A:531:MET:HE3	2.40	0.51
1:B:295:CYS:O	1:B:319:SER:HA	2.09	0.51
1:E:426:ILE:HD13	1:E:426:ILE:N	2.25	0.51
1:H:504:TYR:CZ	1:H:506:GLY:HA2	2.45	0.51
1:I:182:GLY:HA2	1:I:399:ASN:HD22	1.74	0.51
1:K:231:MET:HE2	1:K:231:MET:CA	2.39	0.51
1:A:323:GLU:HG2	1:A:356:LEU:HB3	1.92	0.51
1:B:179:CYS:HB3	1:B:351:GLU:CD	2.35	0.51
1:D:404:LEU:HD21	1:F:405:ASN:HD21	1.75	0.51
1:E:340:TRP:CD1	1:E:340:TRP:C	2.87	0.51
1:G:426:ILE:HD12	1:G:426:ILE:N	2.26	0.51
1:L:139:PRO:HG2	1:L:142:PHE:CE1	2.45	0.51
2:D:701:CIT:C6	2:D:701:CIT:O4	2.57	0.51
1:I:186:TYR:CE1	1:I:342:SER:HA	2.45	0.51
1:C:564:ARG:HG3	1:C:565:GLY:N	2.25	0.51
1:D:526:MET:HE3	1:D:553:MET:SD	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:LEU:HD11	1:H:56:PHE:CE1	2.45	0.51
1:I:189:LYS:HB2	1:I:349:TRP:CD1	2.46	0.51
1:J:358:VAL:HA	1:J:382:VAL:O	2.10	0.51
1:J:399:ASN:OD1	1:J:423:ALA:HB3	2.10	0.51
1:J:403:TYR:CD2	1:J:427:TYR:CE1	2.97	0.51
1:C:397:ARG:NH1	2:C:701:CIT:H41	2.25	0.51
1:F:285:GLU:HA	1:F:310:TRP:CE3	2.45	0.51
1:F:470:GLY:HA2	1:F:499:GLY:O	2.10	0.51
1:G:20:VAL:HA	1:G:58:VAL:HG12	1.92	0.51
1:I:559:ASP:OD2	1:I:581:ARG:NE	2.36	0.51
1:J:541:LEU:HD12	1:J:541:LEU:N	2.25	0.51
1:K:44:THR:OG1	1:K:46:THR:OG1	2.19	0.51
1:L:537:PHE:HD1	1:L:537:PHE:N	2.08	0.51
1:C:457:SER:O	1:C:476:ASN:HA	2.11	0.51
1:G:540:LEU:C	1:G:541:LEU:HD12	2.36	0.51
1:L:512:TYR:CD1	1:L:540:LEU:HG	2.45	0.51
1:E:83:VAL:HA	1:E:105:LEU:HD12	1.93	0.51
1:J:13:PHE:HD2	1:J:18:SER:OG	1.94	0.51
1:J:115:PHE:HB2	1:J:239:SER:O	2.11	0.51
1:J:397:ARG:HA	1:J:422:VAL:HG21	1.90	0.51
1:J:558:LEU:HD22	1:J:651:LEU:HD22	1.93	0.51
1:K:13:PHE:CD2	1:K:19:MET:HA	2.46	0.51
1:K:20:VAL:HA	1:K:58:VAL:HG12	1.91	0.51
1:A:433:TYR:CE1	1:A:455:HIS:HD2	2.29	0.51
1:D:274:ILE:HG22	1:D:275:GLY:N	2.24	0.51
1:G:55:VAL:HG22	1:G:64:LEU:HD22	1.91	0.51
1:C:274:ILE:CD1	1:C:306:TYR:CD2	2.94	0.51
1:G:368:ALA:HA	1:G:392:ALA:O	2.11	0.51
1:H:404:LEU:HD23	1:H:428:ARG:HB2	1.93	0.51
1:J:377:LYS:HA	4:J:814:HOH:O	2.09	0.51
1:K:576:VAL:HG11	1:K:647:TRP:CE2	2.46	0.51
1:A:100:GLN:HE21	1:A:100:GLN:C	2.18	0.50
1:A:337:SER:HA	1:A:371:ASP:O	2.11	0.50
1:B:327:ILE:HG12	1:B:360:CYS:SG	2.51	0.50
1:G:340:TRP:CD1	1:G:340:TRP:C	2.88	0.50
1:G:459:ASN:HA	1:G:479:SER:O	2.11	0.50
1:K:429:GLU:HG2	1:L:428:ARG:NH1	2.26	0.50
1:A:63:LEU:C	1:A:64:LEU:HD23	2.36	0.50
1:A:564:ARG:HH21	1:B:550:PRO:HG2	1.76	0.50
1:F:397:ARG:HH12	2:F:702:CIT:H41	1.76	0.50
1:L:332:VAL:HG23	1:L:365:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:O	1:A:28:GLN:N	2.43	0.50
1:B:71:ALA:HA	1:B:75:TRP:CZ3	2.46	0.50
1:D:183:PRO:O	1:D:184:ASN:C	2.54	0.50
1:I:12:VAL:HG22	1:I:32:THR:HB	1.92	0.50
1:L:23:PRO:HA	1:L:59:PRO:HB2	1.93	0.50
1:L:339:ASN:HA	1:L:373:HIS:ND1	2.26	0.50
1:L:412:ALA:O	1:L:436:VAL:HB	2.10	0.50
1:E:231:MET:HA	1:E:231:MET:HE2	1.92	0.50
1:G:212:LYS:HD3	1:I:363:TYR:CE2	2.46	0.50
1:I:459:ASN:HA	1:I:479:SER:O	2.11	0.50
1:I:547:GLN:OE1	1:I:592:LYS:HE3	2.11	0.50
1:J:115:PHE:CD1	1:J:240:PRO:HA	2.46	0.50
1:B:237:LEU:HB2	1:B:268:ILE:HG23	1.93	0.50
1:B:481:ILE:CG1	1:B:502:MET:CE	2.87	0.50
1:I:311:TYR:CE1	1:I:334:HIS:HD2	2.30	0.50
1:I:368:ALA:HA	1:I:392:ALA:O	2.11	0.50
1:L:418:SER:OG	1:L:442:CYS:HA	2.12	0.50
1:C:416:PHE:CD1	1:C:440:PHE:CE2	3.00	0.50
1:F:142:PHE:CD2	1:F:225:GLU:HG3	2.47	0.50
1:G:455:HIS:HA	1:G:474:THR:O	2.11	0.50
1:L:537:PHE:N	1:L:537:PHE:CD1	2.78	0.50
1:E:231:MET:HE2	1:E:231:MET:CA	2.42	0.50
1:A:139:PRO:HG2	1:A:142:PHE:CZ	2.46	0.50
1:C:302:GLY:HA2	1:C:326:ASP:O	2.11	0.50
1:C:541:LEU:HD12	1:C:541:LEU:N	2.26	0.50
1:E:83:VAL:HA	1:E:105:LEU:CD1	2.42	0.50
1:H:22:TYR:CE2	1:H:24:ASN:HB2	2.47	0.50
1:H:380:LYS:HD2	1:H:404:LEU:HD12	1.94	0.50
1:I:193:ILE:HG21	1:I:231:MET:HE1	1.94	0.50
1:I:549:THR:CG2	1:I:550:PRO:HD2	2.36	0.50
1:L:459:ASN:HA	1:L:479:SER:O	2.11	0.50
1:A:459:ASN:HA	1:A:479:SER:O	2.12	0.50
1:G:71:ALA:HA	1:G:75:TRP:CZ3	2.47	0.50
1:G:500:VAL:HG12	1:G:502:MET:HG3	1.92	0.50
1:J:613:VAL:HG13	1:J:632:PHE:CD2	2.47	0.50
1:L:373:HIS:NE2	2:L:701:CIT:H41	2.27	0.50
1:F:426:ILE:HD12	1:F:426:ILE:N	2.27	0.49
1:J:194:ARG:NE	1:J:212:LYS:HB2	2.26	0.49
1:K:189:LYS:HB2	1:K:349:TRP:CD1	2.47	0.49
1:B:114:GLU:HG3	1:B:238:VAL:HB	1.93	0.49
1:B:261:ASN:HA	1:B:293:ASN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:ARG:HA	1:F:434:ASP:O	2.12	0.49
1:H:404:LEU:HD21	1:H:428:ARG:HD2	1.94	0.49
1:I:70:PRO:HB3	1:I:92:HIS:CE1	2.47	0.49
1:K:489:GLU:OE1	1:K:489:GLU:N	2.42	0.49
1:C:404:LEU:CD2	1:C:428:ARG:HD2	2.42	0.49
1:D:497:ILE:HG21	1:D:502:MET:HE1	1.94	0.49
1:D:564:ARG:NH1	1:E:551:PRO:O	2.46	0.49
1:F:44:THR:CG2	1:F:45:THR:N	2.75	0.49
1:F:71:ALA:HA	1:F:75:TRP:CZ3	2.47	0.49
1:F:372:THR:O	1:F:397:ARG:HB2	2.11	0.49
1:I:391:ALA:HA	1:I:413:MET:HE3	1.94	0.49
1:K:564:ARG:CZ	1:L:550:PRO:HG2	2.42	0.49
1:E:308:ILE:HB	1:E:332:VAL:HG12	1.94	0.49
1:G:504:TYR:CZ	1:G:506:GLY:HA2	2.48	0.49
1:I:435:ASN:O	1:I:457:SER:OG	2.17	0.49
1:J:550:PRO:HG3	1:J:591:PHE:CD1	2.47	0.49
1:J:598:LYS:HE3	1:K:596:GLU:CG	2.39	0.49
1:B:397:ARG:HH22	2:B:701:CIT:H42	1.77	0.49
1:D:284:ILE:HG21	1:D:287:ARG:HD2	1.93	0.49
1:E:512:TYR:HA	1:E:540:LEU:O	2.11	0.49
1:G:385:VAL:HA	1:G:407:ARG:O	2.13	0.49
1:E:278:ARG:O	1:E:279:PRO:C	2.56	0.49
1:F:316:LEU:HD23	1:F:316:LEU:N	2.27	0.49
1:H:579:ARG:HG2	1:H:627:PRO:HB2	1.95	0.49
1:K:448:TYR:HB3	1:K:450:TYR:CZ	2.48	0.49
1:B:580:VAL:HG23	1:B:595:SER:HB2	1.94	0.49
1:G:142:PHE:CB	1:G:225:GLU:OE1	2.61	0.49
1:H:311:TYR:CE1	1:H:334:HIS:HD2	2.31	0.49
1:J:315:VAL:HB	1:J:338:LEU:HD22	1.95	0.49
1:L:311:TYR:CE1	1:L:334:HIS:HD2	2.30	0.49
1:B:16:LEU:HD11	1:B:56:PHE:CD2	2.47	0.49
1:D:509:ARG:HD3	1:D:537:PHE:O	2.13	0.49
1:F:276:ASN:C	1:F:276:ASN:OD1	2.55	0.49
1:G:531:MET:HE2	1:G:538:TRP:HB2	1.94	0.49
1:J:261:ASN:HA	1:J:293:ASN:O	2.13	0.49
1:K:71:ALA:HA	1:K:75:TRP:CZ3	2.48	0.49
1:K:326:ASP:HA	1:K:359:ASN:O	2.13	0.49
1:B:104:VAL:HG11	1:B:133:ASN:OD1	2.13	0.49
1:E:512:TYR:CD2	1:E:540:LEU:HD23	2.48	0.49
1:F:563:ILE:C	1:F:563:ILE:HD12	2.38	0.49
1:I:638:ASN:C	1:I:638:ASN:OD1	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:LEU:HD12	1:C:258:ILE:HG12	1.95	0.49
1:G:163:LEU:HD23	1:G:163:LEU:O	2.13	0.49
1:G:537:PHE:CD1	1:G:537:PHE:N	2.81	0.49
1:I:186:TYR:CD1	1:I:342:SER:HA	2.48	0.49
1:J:463:ILE:O	1:J:483:VAL:HA	2.13	0.49
1:K:13:PHE:CE2	1:K:19:MET:HA	2.48	0.49
1:C:368:ALA:HA	1:C:392:ALA:O	2.12	0.48
1:C:541:LEU:HD21	1:C:591:PHE:CE1	2.48	0.48
1:D:564:ARG:NH2	4:D:805:HOH:O	2.46	0.48
1:E:130:GLN:HG2	1:E:256:ILE:HB	1.95	0.48
1:F:500:VAL:HG12	1:F:502:MET:CG	2.43	0.48
1:G:247:TYR:CG	1:G:248:ASP:N	2.81	0.48
1:I:104:VAL:CG2	1:I:130:GLN:HB2	2.42	0.48
1:I:285:GLU:HA	1:I:310:TRP:CZ3	2.47	0.48
1:I:488:ALA:CA	1:I:517:VAL:HG12	2.42	0.48
1:J:247:TYR:CD2	1:J:248:ASP:N	2.81	0.48
1:J:554:SER:OG	1:L:555:ARG:HD2	2.13	0.48
1:K:302:GLY:HA2	1:K:326:ASP:O	2.13	0.48
1:A:105:LEU:HD23	1:A:132:LEU:HD22	1.95	0.48
1:A:510:ALA:HB1	1:A:531:MET:HE3	1.94	0.48
1:G:120:ARG:NH1	1:G:120:ARG:HG2	2.28	0.48
1:H:295:CYS:O	1:H:319:SER:HA	2.14	0.48
1:I:16:LEU:O	1:I:20:VAL:HG23	2.13	0.48
1:I:71:ALA:HA	1:I:75:TRP:CZ3	2.48	0.48
1:J:269:GLN:HE21	1:J:270:ASP:CG	2.20	0.48
1:K:13:PHE:O	1:K:34:LEU:HG	2.12	0.48
1:C:455:HIS:HA	1:C:474:THR:O	2.13	0.48
1:K:46:THR:HG1	1:K:46:THR:H	1.41	0.48
1:K:311:TYR:CE1	1:K:334:HIS:CD2	3.01	0.48
1:A:455:HIS:HA	1:A:474:THR:O	2.13	0.48
1:D:480:HIS:CD2	1:D:502:MET:HB2	2.49	0.48
1:I:526:MET:HB2	1:I:553:MET:HE2	1.95	0.48
1:L:343:THR:HA	1:L:346:GLY:O	2.14	0.48
1:G:50:VAL:HG21	1:G:57:ALA:HB2	1.94	0.48
1:H:190:ILE:HG13	1:H:190:ILE:O	2.13	0.48
1:L:484:THR:OG1	1:L:485:LYS:N	2.46	0.48
1:D:459:ASN:HA	1:D:479:SER:O	2.13	0.48
1:I:52:ASN:HA	1:I:56:PHE:CD1	2.48	0.48
1:J:479:SER:OG	1:J:481:ILE:O	2.32	0.48
1:K:404:LEU:CD2	1:K:428:ARG:HD2	2.44	0.48
1:K:601:ARG:NH1	1:L:613:VAL:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LYS:HE2	1:C:499:GLY:O	2.14	0.48
1:B:397:ARG:NH1	2:B:701:CIT:H42	2.29	0.48
1:C:115:PHE:HB2	1:C:239:SER:O	2.13	0.48
1:D:34:LEU:CG	1:E:30:LYS:HE3	2.44	0.48
1:L:597:VAL:HG12	1:L:599:LEU:HD23	1.96	0.48
1:B:19:MET:HE1	1:B:41:PHE:CE1	2.48	0.48
1:C:291:LYS:HD2	1:C:314:GLU:OE1	2.13	0.48
1:E:337:SER:HA	1:E:371:ASP:O	2.13	0.48
1:E:540:LEU:O	1:E:541:LEU:HD12	2.13	0.48
1:I:561:THR:O	1:I:563:ILE:HG23	2.13	0.48
1:A:55:VAL:HG22	1:A:64:LEU:HD22	1.95	0.48
1:A:602:LEU:HD11	1:A:646:ALA:HB2	1.95	0.48
1:D:22:TYR:CE1	1:D:24:ASN:HB2	2.49	0.48
1:E:186:TYR:CD1	1:E:342:SER:HA	2.48	0.48
1:H:512:TYR:CD1	1:H:512:TYR:C	2.91	0.48
1:K:13:PHE:N	1:K:13:PHE:CD1	2.82	0.48
1:B:291:LYS:HE2	1:B:316:LEU:HD21	1.96	0.48
1:B:564:ARG:NH1	1:C:551:PRO:O	2.47	0.48
1:E:50:VAL:HG21	1:E:57:ALA:HB2	1.95	0.48
1:F:90:ASN:HA	1:F:110:ASN:O	2.14	0.48
1:H:455:HIS:HA	1:H:474:THR:O	2.13	0.48
1:H:618:GLN:HG2	1:H:630:ASN:ND2	2.29	0.48
1:I:488:ALA:HB2	1:I:517:VAL:HG12	1.96	0.48
1:J:333:ARG:HA	1:J:366:THR:OG1	2.14	0.48
1:J:442:CYS:SG	1:J:463:ILE:HD12	2.54	0.48
1:J:524:VAL:O	1:J:551:PRO:HB2	2.13	0.48
1:J:547:GLN:HA	1:J:588:ALA:O	2.14	0.48
1:J:613:VAL:HG13	1:J:632:PHE:HD2	1.79	0.48
1:K:380:LYS:HE2	4:K:827:HOH:O	2.13	0.48
1:D:63:LEU:C	1:D:64:LEU:HD23	2.39	0.47
1:E:254:PHE:O	1:E:276:ASN:HB2	2.14	0.47
1:E:315:VAL:HB	1:E:338:LEU:CD2	2.44	0.47
1:G:371:ASP:OD2	1:G:395:GLN:HG2	2.14	0.47
1:K:619:ASN:OD1	1:K:619:ASN:C	2.56	0.47
1:B:404:LEU:HD21	1:B:428:ARG:HD2	1.95	0.47
1:B:499:GLY:HA2	1:B:528:ASN:O	2.14	0.47
1:E:278:ARG:HB2	1:E:281:ALA:HB2	1.96	0.47
1:E:428:ARG:HG2	1:E:428:ARG:HH11	1.79	0.47
1:G:538:TRP:CZ3	1:G:553:MET:HE1	2.49	0.47
1:H:276:ASN:OD1	1:H:308:ILE:HA	2.14	0.47
1:K:185:THR:HG23	1:K:374:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:TRP:HE3	1:D:374:ASP:OD1	1.97	0.47
1:G:24:ASN:O	1:G:26:GLN:HG3	2.13	0.47
1:G:119:GLY:O	1:G:120:ARG:NH1	2.48	0.47
1:H:448:TYR:CD1	1:H:467:ARG:HG3	2.49	0.47
1:I:90:ASN:HA	1:I:110:ASN:O	2.14	0.47
1:J:72:TYR:O	1:J:73:SER:C	2.57	0.47
1:J:325:HIS:CD2	1:J:358:VAL:CG1	2.97	0.47
1:L:564:ARG:CG	1:L:648:GLU:HG2	2.44	0.47
1:A:436:VAL:O	1:A:458:GLN:HG3	2.14	0.47
1:B:182:GLY:HA2	1:B:399:ASN:ND2	2.29	0.47
1:C:90:ASN:HA	1:C:110:ASN:O	2.14	0.47
1:C:412:ALA:O	1:C:436:VAL:HB	2.15	0.47
1:D:285:GLU:HA	1:D:310:TRP:CE3	2.50	0.47
1:I:558:LEU:HD22	1:I:651:LEU:HD22	1.97	0.47
1:J:50:VAL:HG21	1:J:57:ALA:HB2	1.97	0.47
1:K:74:SER:HB3	1:K:96:ASP:CG	2.39	0.47
1:E:229:PRO:CB	1:E:231:MET:HE1	2.42	0.47
1:I:409:TYR:CD1	1:I:433:TYR:HB2	2.49	0.47
1:J:485:LYS:HD3	1:J:490:THR:O	2.15	0.47
1:E:284:ILE:CB	1:E:287:ARG:HD2	2.44	0.47
1:L:220:LEU:HD23	1:L:220:LEU:HA	1.67	0.47
1:L:457:SER:O	1:L:476:ASN:HA	2.14	0.47
1:A:278:ARG:HG2	1:A:278:ARG:HH11	1.80	0.47
1:A:368:ALA:HA	1:A:392:ALA:O	2.15	0.47
1:D:182:GLY:HA2	1:D:399:ASN:ND2	2.29	0.47
1:E:512:TYR:CG	1:E:540:LEU:HD23	2.49	0.47
1:F:547:GLN:NE2	1:F:586:SER:HA	2.30	0.47
1:I:183:PRO:O	1:I:184:ASN:C	2.57	0.47
1:I:236:THR:HG22	1:I:238:VAL:HG23	1.95	0.47
1:I:619:ASN:OD1	1:I:619:ASN:C	2.57	0.47
1:K:108:LYS:HD3	1:K:108:LYS:HA	1.58	0.47
1:K:311:TYR:CE1	1:K:334:HIS:HD2	2.32	0.47
1:K:320:GLU:HG3	1:K:353:ILE:HB	1.96	0.47
1:K:328:HIS:CD2	1:K:361:GLU:HB3	2.49	0.47
1:L:368:ALA:HA	1:L:392:ALA:O	2.14	0.47
1:L:370:PHE:HB2	1:L:394:PHE:HD1	1.79	0.47
1:L:598:LYS:C	1:L:599:LEU:HD23	2.39	0.47
1:A:56:PHE:O	1:A:62:TYR:HB3	2.15	0.47
1:A:189:LYS:HE3	1:A:347:ASP:CG	2.40	0.47
1:A:542:SER:HA	1:A:589:ASN:ND2	2.29	0.47
1:C:85:PHE:CD2	1:C:86:MET:CE	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLY:HA2	1:C:399:ASN:ND2	2.30	0.47
1:D:541:LEU:N	1:D:541:LEU:CD1	2.77	0.47
1:E:311:TYR:CE1	1:E:334:HIS:CD2	3.03	0.47
1:G:329:ALA:C	1:G:330:MET:HG3	2.39	0.47
1:H:365:THR:HG21	1:H:369:GLY:HA2	1.97	0.47
1:I:254:PHE:CZ	1:I:276:ASN:HB3	2.50	0.47
1:I:340:TRP:HA	1:I:375:ILE:HD11	1.97	0.47
1:J:569:LEU:HD23	1:J:574:ALA:HB2	1.96	0.47
1:B:446:GLY:HA2	1:B:465:GLY:O	2.14	0.47
1:B:500:VAL:HG12	1:B:502:MET:HG3	1.96	0.47
1:B:622:VAL:HG12	1:B:623:PRO:CA	2.36	0.47
1:I:23:PRO:HA	1:I:59:PRO:HG2	1.97	0.47
1:J:92:HIS:CD2	1:J:112:THR:HG22	2.50	0.47
1:J:397:ARG:HH22	2:J:701:CIT:H41	1.79	0.47
1:K:365:THR:HG21	1:K:369:GLY:HA2	1.97	0.47
1:K:558:LEU:HD22	1:K:651:LEU:CD2	2.39	0.47
1:L:52:ASN:HA	1:L:56:PHE:CE1	2.49	0.47
1:L:410:ARG:HA	1:L:434:ASP:O	2.15	0.47
1:L:433:TYR:CE1	1:L:455:HIS:CD2	3.01	0.47
1:A:564:ARG:NH1	1:A:648:GLU:CD	2.73	0.47
1:C:20:VAL:HA	1:C:58:VAL:HG12	1.97	0.47
1:E:182:GLY:HA2	1:E:399:ASN:ND2	2.29	0.47
1:E:216:TYR:OH	1:E:351:GLU:HG2	2.15	0.47
1:G:360:CYS:HB2	1:G:384:CYS:SG	2.55	0.47
1:I:115:PHE:CE1	1:I:240:PRO:HA	2.49	0.47
1:K:58:VAL:HB	1:K:59:PRO:HD2	1.97	0.47
1:A:287:ARG:NH1	2:A:702:CIT:O3	2.39	0.46
1:B:311:TYR:CE1	1:B:334:HIS:CD2	2.99	0.46
1:C:345:ASP:HA	1:F:135:THR:CG2	2.44	0.46
1:D:26:GLN:O	1:D:28:GLN:N	2.48	0.46
1:D:457:SER:O	1:D:476:ASN:HA	2.15	0.46
1:L:564:ARG:HG2	1:L:648:GLU:HG2	1.96	0.46
1:A:183:PRO:O	1:A:184:ASN:C	2.58	0.46
1:A:302:GLY:HA2	1:A:326:ASP:O	2.15	0.46
1:D:385:VAL:HG23	1:D:407:ARG:HB2	1.97	0.46
1:D:397:ARG:HA	1:D:422:VAL:HG21	1.98	0.46
1:E:504:TYR:CZ	1:E:506:GLY:HA2	2.50	0.46
1:F:433:TYR:CE1	1:F:455:HIS:HD2	2.33	0.46
1:G:31:ILE:HD13	1:G:63:LEU:CD2	2.46	0.46
1:I:40:ASP:HB3	1:I:66:LYS:HE2	1.97	0.46
1:I:495:LEU:HB3	1:I:524:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:619:ASN:OD1	1:K:620:GLN:N	2.48	0.46
1:A:25:PHE:HB3	1:A:43:PHE:CD1	2.51	0.46
1:B:120:ARG:HG2	1:B:120:ARG:HH11	1.80	0.46
1:B:527:SER:HB2	4:B:842:HOH:O	2.15	0.46
1:E:261:ASN:HD21	1:E:294:ASN:HD22	1.63	0.46
1:F:19:MET:HE3	1:F:63:LEU:HD23	1.96	0.46
1:F:326:ASP:HA	1:F:359:ASN:O	2.16	0.46
1:H:11:ARG:HD3	1:H:22:TYR:CZ	2.50	0.46
1:H:468:VAL:HG12	1:H:500:VAL:HG21	1.96	0.46
1:H:620:GLN:HA	1:H:620:GLN:OE1	2.16	0.46
1:I:255:THR:HA	1:I:287:ARG:HG2	1.97	0.46
1:J:254:PHE:CE1	1:J:276:ASN:HB3	2.51	0.46
1:K:94:VAL:HG22	1:K:114:GLU:HG2	1.97	0.46
1:K:110:ASN:HD22	1:K:234:ASN:HB3	1.80	0.46
1:K:191:SER:HB3	1:K:349:TRP:HB3	1.97	0.46
1:K:541:LEU:HD23	1:K:544:TYR:CE2	2.50	0.46
1:D:44:THR:OG1	1:D:45:THR:N	2.48	0.46
1:E:34:LEU:HD11	1:F:30:LYS:HG3	1.97	0.46
1:G:120:ARG:HG2	1:G:120:ARG:HH11	1.79	0.46
1:G:433:TYR:CE1	1:G:455:HIS:HD2	2.34	0.46
1:K:155:VAL:HA	1:K:208:ILE:O	2.15	0.46
1:L:135:THR:HG23	1:L:261:ASN:HB3	1.97	0.46
1:A:22:TYR:CE2	1:A:24:ASN:HB2	2.51	0.46
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.28	0.46
1:C:332:VAL:O	1:C:365:THR:HA	2.16	0.46
1:K:266:LEU:O	1:K:298:SER:HB3	2.15	0.46
1:L:568:THR:HG23	1:L:644:GLN:HE21	1.80	0.46
1:B:110:ASN:HD22	1:B:234:ASN:HB3	1.79	0.46
1:F:500:VAL:HG12	1:F:502:MET:HG2	1.97	0.46
1:J:435:ASN:O	1:J:457:SER:OG	2.31	0.46
1:K:526:MET:HE1	1:K:531:MET:CE	2.45	0.46
1:A:28:GLN:O	1:A:28:GLN:HG2	2.16	0.46
1:A:145:LEU:O	1:A:220:LEU:HD21	2.16	0.46
1:A:619:ASN:HD21	1:A:621:ASP:CG	2.24	0.46
1:B:25:PHE:HB3	1:B:43:PHE:CD2	2.50	0.46
1:B:110:ASN:ND2	1:B:234:ASN:HB3	2.31	0.46
2:B:702:CIT:O2	2:B:702:CIT:O7	2.31	0.46
1:E:361:GLU:HG3	1:E:385:VAL:CG1	2.45	0.46
1:H:457:SER:O	1:H:476:ASN:HA	2.15	0.46
1:H:497:ILE:HG21	1:H:502:MET:HE1	1.97	0.46
1:I:115:PHE:CD1	1:I:240:PRO:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:510:ALA:HB3	1:J:531:MET:HE3	1.97	0.46
1:K:523:LEU:HD23	1:K:523:LEU:HA	1.66	0.46
1:L:47:ALA:HA	1:L:62:TYR:HE2	1.80	0.46
1:L:80:THR:HA	1:L:83:VAL:HG23	1.96	0.46
1:L:100:GLN:HB2	4:L:808:HOH:O	2.14	0.46
1:A:520:ASP:OD1	1:A:520:ASP:C	2.57	0.46
1:G:390:ALA:O	1:G:412:ALA:HB3	2.16	0.46
1:G:538:TRP:CH2	1:G:553:MET:HE1	2.51	0.46
1:J:183:PRO:O	1:J:184:ASN:C	2.58	0.46
1:J:555:ARG:HD3	1:J:650:TYR:CD2	2.51	0.46
1:K:247:TYR:CG	1:K:248:ASP:N	2.84	0.46
1:A:327:ILE:HG12	1:A:360:CYS:SG	2.56	0.46
1:A:359:ASN:HA	1:A:383:ARG:O	2.16	0.46
1:C:467:ARG:NH2	1:C:469:LYS:CE	2.67	0.46
1:D:372:THR:O	1:D:397:ARG:HB2	2.15	0.46
1:D:410:ARG:HA	1:D:434:ASP:O	2.16	0.46
1:E:20:VAL:HA	1:E:58:VAL:HG12	1.98	0.46
1:H:448:TYR:HD1	1:H:467:ARG:HG3	1.81	0.46
1:I:283:ASP:OD2	1:I:333:ARG:NH1	2.45	0.46
1:I:619:ASN:ND2	1:I:629:LEU:HD12	2.31	0.46
1:E:170:TYR:O	1:E:171:LEU:HD23	2.16	0.46
1:E:558:LEU:HD22	1:E:651:LEU:HD22	1.98	0.46
1:I:104:VAL:CG1	1:I:105:LEU:N	2.77	0.46
1:I:327:ILE:O	1:I:327:ILE:HG13	2.16	0.46
1:K:70:PRO:HB3	1:K:92:HIS:ND1	2.31	0.46
1:K:368:ALA:HA	1:K:392:ALA:O	2.16	0.46
1:L:33:LEU:HD12	1:L:34:LEU:N	2.28	0.46
1:L:285:GLU:HA	1:L:310:TRP:CE3	2.50	0.46
1:L:433:TYR:HE1	1:L:455:HIS:CD2	2.34	0.46
1:L:609:GLY:N	1:L:641:ASP:OD2	2.49	0.46
1:A:71:ALA:HA	1:A:75:TRP:CZ3	2.51	0.45
1:A:316:LEU:HD23	1:A:316:LEU:N	2.32	0.45
1:B:85:PHE:CZ	1:B:91:ARG:HD2	2.51	0.45
1:B:183:PRO:O	1:B:184:ASN:C	2.58	0.45
1:C:254:PHE:O	1:C:276:ASN:HB2	2.16	0.45
1:D:263:ALA:O	1:D:295:CYS:HA	2.16	0.45
1:G:167:LYS:HE3	1:G:199:VAL:HG23	1.97	0.45
1:I:526:MET:HE2	1:I:553:MET:CE	2.46	0.45
1:A:24:ASN:O	1:A:25:PHE:C	2.58	0.45
1:B:22:TYR:CE1	1:B:24:ASN:HB2	2.50	0.45
1:F:58:VAL:HB	1:F:59:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:538:TRP:CH2	1:J:553:MET:SD	3.09	0.45
1:J:569:LEU:O	1:J:642:VAL:HA	2.16	0.45
1:K:392:ALA:HA	1:K:414:ASP:O	2.16	0.45
1:D:416:PHE:CD1	1:D:440:PHE:CE1	3.04	0.45
1:E:70:PRO:HB3	1:E:92:HIS:CE1	2.52	0.45
1:E:189:LYS:CB	1:E:349:TRP:CD1	2.99	0.45
1:E:365:THR:HG21	1:E:369:GLY:HA2	1.96	0.45
1:E:459:ASN:HA	1:E:479:SER:O	2.15	0.45
1:I:216:TYR:OH	1:I:351:GLU:HG2	2.16	0.45
1:K:223:ALA:O	1:K:225:GLU:HG2	2.16	0.45
1:A:311:TYR:CE1	1:A:334:HIS:CD2	3.02	0.45
1:E:526:MET:CE	1:E:551:PRO:HG3	2.45	0.45
1:E:538:TRP:CZ2	1:E:553:MET:HE1	2.51	0.45
1:G:387:TYR:CE1	1:G:409:TYR:CD2	3.04	0.45
1:G:516:THR:HG22	1:G:516:THR:O	2.15	0.45
1:I:326:ASP:OD1	1:I:359:ASN:HB3	2.16	0.45
1:J:51:ASP:C	1:J:51:ASP:OD1	2.59	0.45
1:K:110:ASN:ND2	1:K:234:ASN:HB3	2.31	0.45
1:K:337:SER:HA	1:K:371:ASP:O	2.17	0.45
1:L:83:VAL:HA	1:L:105:LEU:CD1	2.46	0.45
1:L:104:VAL:HG22	1:L:130:GLN:O	2.17	0.45
1:A:19:MET:HE1	1:A:33:LEU:HB2	1.98	0.45
1:B:189:LYS:HB2	1:B:349:TRP:CD1	2.51	0.45
1:E:261:ASN:HA	1:E:293:ASN:O	2.16	0.45
1:G:404:LEU:HD21	1:G:428:ARG:HD2	1.97	0.45
1:G:520:ASP:C	1:G:520:ASP:OD1	2.59	0.45
1:G:570:VAL:O	1:G:571:ALA:HB3	2.16	0.45
1:J:352:PRO:O	1:J:376:GLY:HA2	2.15	0.45
1:J:459:ASN:HA	1:J:479:SER:O	2.15	0.45
1:K:229:PRO:CB	1:K:231:MET:HE1	2.46	0.45
1:K:308:ILE:HB	1:K:332:VAL:HG12	1.98	0.45
1:K:557:LEU:HD11	1:L:525:SER:OG	2.17	0.45
1:L:115:PHE:CD1	1:L:240:PRO:HA	2.52	0.45
1:C:189:LYS:HB2	1:C:349:TRP:CD1	2.52	0.45
1:C:615:SER:HB2	1:C:633:VAL:HG23	1.99	0.45
1:I:78:ASN:O	1:I:79:TRP:C	2.60	0.45
1:K:253:PHE:CD1	1:K:253:PHE:N	2.84	0.45
1:K:306:TYR:CE1	1:K:330:MET:CE	3.00	0.45
1:A:190:ILE:O	1:A:190:ILE:HG13	2.15	0.45
1:A:552:ARG:NE	1:C:563:ILE:HD13	2.32	0.45
1:B:14:SER:O	1:B:15:ASP:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:PHE:CE2	1:B:91:ARG:HD2	2.52	0.45
1:B:158:VAL:HG21	1:B:163:LEU:HD22	1.98	0.45
1:B:564:ARG:HG2	1:B:648:GLU:HG2	1.99	0.45
1:D:71:ALA:HA	1:D:75:TRP:CZ3	2.51	0.45
1:D:223:ALA:O	1:D:225:GLU:HG2	2.16	0.45
1:E:47:ALA:HA	1:E:62:TYR:CE2	2.45	0.45
1:E:110:ASN:HD22	1:E:234:ASN:HD22	1.65	0.45
1:H:531:MET:HE2	1:H:538:TRP:HB2	1.97	0.45
1:I:537:PHE:CD1	1:I:537:PHE:N	2.84	0.45
1:J:323:GLU:HG2	1:J:356:LEU:HB3	1.99	0.45
1:D:293:ASN:HB2	1:D:316:LEU:HD21	1.99	0.45
1:E:564:ARG:HD2	1:E:648:GLU:HG2	1.99	0.45
1:H:372:THR:O	1:H:397:ARG:HB2	2.17	0.45
1:H:611:LEU:CD1	1:H:645:VAL:HG21	2.47	0.45
1:I:192:GLN:HG3	1:I:218:TYR:OH	2.17	0.45
1:I:373:HIS:NE2	2:I:701:CIT:H41	2.31	0.45
1:L:536:LEU:C	1:L:537:PHE:HD1	2.24	0.45
1:A:584:PHE:CD2	1:A:584:PHE:N	2.85	0.45
1:F:130:GLN:HG2	1:F:256:ILE:HB	1.99	0.45
1:I:247:TYR:CG	1:I:248:ASP:N	2.85	0.45
1:L:107:ILE:HB	1:L:134:ILE:HG13	1.98	0.45
1:B:510:ALA:CB	1:B:531:MET:HE3	2.47	0.45
1:C:85:PHE:CD2	1:C:86:MET:HE2	2.52	0.45
1:C:115:PHE:CD1	1:C:240:PRO:HA	2.52	0.45
1:D:255:THR:HA	1:D:287:ARG:HG2	1.98	0.45
1:E:541:LEU:N	1:E:541:LEU:CD1	2.79	0.45
1:I:433:TYR:CE1	1:I:455:HIS:CD2	3.00	0.45
1:J:247:TYR:CG	1:J:248:ASP:N	2.84	0.45
1:J:544:TYR:HB2	1:J:589:ASN:OD1	2.17	0.45
1:L:337:SER:HA	1:L:371:ASP:O	2.17	0.45
1:L:492:GLN:NE2	1:L:523:LEU:HB2	2.31	0.45
1:C:419:ASN:O	1:C:422:VAL:HG23	2.16	0.44
1:D:538:TRP:CZ3	1:D:539:ALA:HB2	2.52	0.44
1:E:463:ILE:O	1:E:483:VAL:HA	2.17	0.44
1:G:553:MET:O	1:I:598:LYS:NZ	2.49	0.44
1:H:20:VAL:HA	1:H:58:VAL:HG12	1.99	0.44
1:H:454:ALA:HB3	1:H:473:TYR:HD1	1.82	0.44
1:H:572:GLY:C	1:H:573:GLU:HG2	2.41	0.44
1:I:409:TYR:CE1	1:I:433:TYR:CD2	3.04	0.44
1:I:492:GLN:OE1	1:I:523:LEU:HD22	2.17	0.44
1:J:190:ILE:O	1:J:190:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:397:ARG:HH12	2:J:701:CIT:H42	1.81	0.44
1:K:22:TYR:HE1	1:K:24:ASN:HB2	1.81	0.44
1:K:229:PRO:HG2	1:K:231:MET:HE1	1.97	0.44
1:K:514:HIS:CD2	1:K:516:THR:HB	2.52	0.44
1:L:584:PHE:CD1	1:L:584:PHE:N	2.85	0.44
1:C:358:VAL:HA	1:C:382:VAL:O	2.16	0.44
1:E:11:ARG:HA	1:E:11:ARG:HH11	1.80	0.44
1:F:173:LEU:O	1:F:191:SER:HA	2.17	0.44
1:J:385:VAL:HA	1:J:407:ARG:O	2.18	0.44
1:J:457:SER:O	1:J:476:ASN:HA	2.16	0.44
1:K:155:VAL:HG13	1:K:208:ILE:O	2.16	0.44
1:K:158:VAL:HG21	1:K:163:LEU:HD23	2.00	0.44
1:K:550:PRO:HB2	1:K:551:PRO:HD2	2.00	0.44
1:A:52:ASN:HA	1:A:56:PHE:CE1	2.52	0.44
1:B:51:ASP:O	1:B:52:ASN:C	2.61	0.44
1:C:311:TYR:CE1	1:C:334:HIS:HD2	2.35	0.44
1:C:504:TYR:OH	1:C:506:GLY:HA2	2.17	0.44
1:D:25:PHE:CB	1:D:43:PHE:CD1	3.00	0.44
1:D:302:GLY:HA2	1:D:326:ASP:O	2.18	0.44
1:F:289:ALA:HB3	1:F:312:GLY:O	2.17	0.44
1:I:485:LYS:HD3	1:I:490:THR:O	2.17	0.44
1:I:526:MET:SD	1:I:553:MET:HE1	2.57	0.44
1:K:33:LEU:HD12	1:K:34:LEU:H	1.81	0.44
1:A:222:ASP:O	1:A:223:ALA:HB3	2.18	0.44
1:A:307:ASN:ND2	1:A:331:ASP:OD2	2.38	0.44
1:B:547:GLN:HG3	1:B:587:VAL:O	2.17	0.44
1:D:340:TRP:HA	1:D:375:ILE:HD11	2.00	0.44
1:E:163:LEU:C	1:E:163:LEU:HD12	2.43	0.44
1:F:316:LEU:HD23	1:F:316:LEU:H	1.81	0.44
1:F:556:ASN:HB2	1:F:651:LEU:HB3	2.00	0.44
1:I:175:SER:OG	1:I:176:ASN:N	2.47	0.44
1:I:526:MET:CE	1:I:553:MET:HE1	2.48	0.44
1:J:22:TYR:CZ	1:J:24:ASN:HB2	2.51	0.44
1:A:622:VAL:HA	1:A:623:PRO:C	2.43	0.44
1:D:470:GLY:HA2	1:D:499:GLY:O	2.16	0.44
1:E:247:TYR:CG	1:E:248:ASP:N	2.85	0.44
1:E:405:ASN:HA	1:E:429:GLU:O	2.17	0.44
1:G:255:THR:OG1	1:G:256:ILE:N	2.48	0.44
1:I:47:ALA:HA	1:I:62:TYR:CE2	2.53	0.44
1:I:526:MET:SD	1:I:553:MET:CE	3.06	0.44
1:I:538:TRP:CZ3	1:I:539:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:511:VAL:HG21	1:L:526:MET:SD	2.57	0.44
1:A:367:GLN:O	1:A:368:ALA:C	2.60	0.44
1:B:368:ALA:HA	1:B:392:ALA:O	2.18	0.44
1:B:470:GLY:HA2	1:B:499:GLY:O	2.18	0.44
1:C:481:ILE:CG1	1:C:502:MET:HE3	2.41	0.44
1:F:79:TRP:CD2	1:F:101:ALA:HA	2.52	0.44
1:G:499:GLY:HA2	1:G:528:ASN:O	2.18	0.44
1:G:538:TRP:CZ3	1:G:539:ALA:HB2	2.53	0.44
1:G:603:THR:CG2	1:G:644:GLN:HB2	2.48	0.44
2:G:701:CIT:O6	2:G:701:CIT:C5	2.64	0.44
1:H:90:ASN:HA	1:H:110:ASN:O	2.18	0.44
1:J:397:ARG:HH12	2:J:701:CIT:C4	2.31	0.44
1:K:530:ASP:OD1	1:K:532:THR:OG1	2.32	0.44
1:L:597:VAL:HG12	1:L:599:LEU:HD21	1.99	0.44
1:B:576:VAL:HG11	1:B:647:TRP:CE2	2.52	0.44
1:D:13:PHE:CD1	1:D:13:PHE:N	2.86	0.44
1:D:526:MET:HE1	1:D:538:TRP:CZ3	2.52	0.44
1:E:71:ALA:HA	1:E:75:TRP:CZ3	2.53	0.44
1:G:237:LEU:HD12	1:G:268:ILE:HG12	2.00	0.44
1:G:446:GLY:HA2	1:G:465:GLY:O	2.18	0.44
1:I:455:HIS:HA	1:I:474:THR:O	2.17	0.44
1:J:626:ASN:HD21	1:J:628:ASP:HB2	1.81	0.44
1:L:598:LYS:O	1:L:599:LEU:HD23	2.17	0.44
1:A:295:CYS:O	1:A:319:SER:HA	2.18	0.44
1:B:16:LEU:CD1	1:B:56:PHE:CE2	3.01	0.44
1:C:186:TYR:CZ	1:C:342:SER:HB2	2.53	0.44
1:D:218:TYR:N	1:D:218:TYR:CD1	2.86	0.44
1:E:34:LEU:HD11	1:F:30:LYS:CG	2.48	0.44
1:E:124:ASP:OD2	1:E:129:ARG:NH2	2.51	0.44
1:E:186:TYR:CE1	1:E:342:SER:HA	2.52	0.44
1:F:541:LEU:N	1:F:541:LEU:HD12	2.32	0.44
1:G:323:GLU:HG2	1:G:356:LEU:HB3	2.00	0.44
1:I:79:TRP:O	1:I:83:VAL:HG23	2.17	0.44
1:I:374:ASP:HA	1:I:397:ARG:O	2.18	0.44
1:K:613:VAL:HG13	1:K:632:PHE:HD2	1.82	0.44
1:L:570:VAL:O	1:L:570:VAL:CG1	2.66	0.44
1:A:614:THR:OG1	1:A:615:SER:N	2.50	0.44
2:B:702:CIT:O5	1:H:287:ARG:NH1	2.48	0.44
1:C:87:SER:HB3	4:C:942:HOH:O	2.17	0.44
1:C:526:MET:HE3	1:C:551:PRO:HG2	1.99	0.44
1:D:278:ARG:O	1:D:279:PRO:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:GLU:HA	1:D:353:ILE:O	2.17	0.44
1:D:608:ALA:O	1:E:635:ARG:NH1	2.49	0.44
1:E:45:THR:O	1:E:47:ALA:N	2.51	0.44
1:E:261:ASN:HD22	1:E:262:PHE:N	2.16	0.44
1:G:114:GLU:HG3	1:G:238:VAL:HB	2.00	0.44
1:G:261:ASN:HA	1:G:293:ASN:O	2.18	0.44
1:G:464:ASN:HB3	1:G:484:THR:O	2.17	0.44
1:G:580:VAL:HG23	1:G:595:SER:HB2	1.99	0.44
1:H:404:LEU:CD2	1:H:428:ARG:HD2	2.48	0.44
1:J:613:VAL:O	1:L:601:ARG:NH1	2.49	0.44
1:L:409:TYR:CD2	1:L:433:TYR:HB2	2.51	0.44
1:C:564:ARG:HG3	1:C:565:GLY:H	1.83	0.43
1:D:11:ARG:HH11	1:D:11:ARG:HG2	1.83	0.43
1:D:132:LEU:HD12	1:D:258:ILE:HG12	2.00	0.43
1:D:293:ASN:OD1	1:D:316:LEU:HG	2.18	0.43
1:D:504:TYR:CZ	1:D:506:GLY:HA2	2.53	0.43
1:E:254:PHE:CZ	1:E:276:ASN:HB3	2.53	0.43
1:G:509:ARG:HD2	1:G:540:LEU:HB2	1.99	0.43
1:H:115:PHE:CD1	1:H:240:PRO:HA	2.53	0.43
1:J:10:GLU:HA	1:J:30:LYS:HB3	1.99	0.43
1:J:324:VAL:HG21	1:J:336:ILE:HD13	2.00	0.43
1:L:12:VAL:HG22	1:L:32:THR:HB	1.99	0.43
1:L:285:GLU:HA	1:L:310:TRP:CZ3	2.53	0.43
1:B:277:LYS:HG3	1:B:278:ARG:N	2.32	0.43
1:C:433:TYR:CE1	1:C:455:HIS:HD2	2.36	0.43
1:D:173:LEU:O	1:D:191:SER:HA	2.18	0.43
1:E:120:ARG:HG2	1:E:120:ARG:HH11	1.82	0.43
1:E:301:LYS:HE2	1:E:325:HIS:CD2	2.53	0.43
1:G:632:PHE:HE1	1:G:634:ILE:HG13	1.83	0.43
1:H:351:GLU:HB2	1:H:375:ILE:HD12	2.00	0.43
1:I:138:ALA:HB1	1:I:139:PRO:CD	2.48	0.43
1:K:43:PHE:CD1	1:K:44:THR:N	2.86	0.43
1:K:120:ARG:HH11	1:K:120:ARG:HG2	1.83	0.43
1:A:531:MET:HE2	1:A:538:TRP:HB2	1.99	0.43
1:B:526:MET:HE1	1:B:531:MET:HE1	1.99	0.43
1:D:247:TYR:CZ	1:D:275:GLY:HA3	2.54	0.43
1:D:358:VAL:HA	1:D:382:VAL:O	2.18	0.43
1:E:196:VAL:HG13	1:E:208:ILE:HG23	2.01	0.43
1:E:371:ASP:OD2	1:E:395:GLN:HG2	2.19	0.43
1:G:505:ASP:OD1	1:G:507:THR:OG1	2.35	0.43
1:G:564:ARG:HG2	1:H:549:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:LEU:O	1:J:220:LEU:HD21	2.18	0.43
1:J:201:THR:HG23	1:J:206:THR:OG1	2.18	0.43
1:K:622:VAL:HA	1:K:623:PRO:C	2.42	0.43
1:G:538:TRP:CE3	1:G:539:ALA:HB2	2.54	0.43
1:H:470:GLY:HA2	1:H:499:GLY:O	2.18	0.43
1:J:13:PHE:CD1	1:J:13:PHE:N	2.85	0.43
1:L:284:ILE:HD13	1:L:287:ARG:HH11	1.83	0.43
1:A:276:ASN:OD1	1:A:308:ILE:HA	2.18	0.43
1:A:360:CYS:HB2	1:A:384:CYS:SG	2.59	0.43
1:B:397:ARG:HH12	2:B:701:CIT:H42	1.82	0.43
1:D:45:THR:O	1:D:47:ALA:N	2.51	0.43
1:D:299:THR:HG22	1:D:323:GLU:HB2	2.00	0.43
1:D:394:PHE:CD1	1:D:416:PHE:CE2	3.06	0.43
1:D:431:LEU:HD22	1:D:453:GLU:HB2	2.00	0.43
1:D:564:ARG:CZ	1:E:550:PRO:HG2	2.48	0.43
1:F:33:LEU:HD12	1:F:34:LEU:H	1.82	0.43
1:G:94:VAL:HA	1:G:114:GLU:O	2.18	0.43
1:H:120:ARG:HH11	1:H:120:ARG:HG2	1.83	0.43
1:H:340:TRP:CD1	1:H:340:TRP:C	2.96	0.43
1:J:274:ILE:HG23	1:J:306:TYR:HB2	2.01	0.43
1:K:604:PHE:HB3	1:L:615:SER:H	1.82	0.43
1:A:263:ALA:O	1:A:295:CYS:HA	2.19	0.43
1:B:50:VAL:HG21	1:B:57:ALA:HB2	1.99	0.43
1:B:247:TYR:CG	1:B:248:ASP:N	2.85	0.43
1:B:410:ARG:HA	1:B:434:ASP:O	2.19	0.43
1:B:626:ASN:HA	1:B:627:PRO:HD2	1.89	0.43
1:D:563:ILE:HD12	1:E:552:ARG:CZ	2.48	0.43
1:G:301:LYS:HG2	1:G:325:HIS:HB2	2.01	0.43
1:H:433:TYR:CE1	1:H:455:HIS:CD2	2.98	0.43
1:I:23:PRO:HA	1:I:59:PRO:CG	2.49	0.43
1:J:442:CYS:SG	1:J:463:ILE:CD1	3.06	0.43
1:L:455:HIS:HA	1:L:474:THR:O	2.19	0.43
1:A:40:ASP:CB	1:A:66:LYS:HD2	2.45	0.43
1:A:155:VAL:CG1	1:A:156:ILE:N	2.81	0.43
1:B:414:ASP:HA	1:B:438:SER:O	2.19	0.43
1:B:424:PHE:CD1	1:B:448:TYR:CE2	3.07	0.43
1:D:123:PRO:HD2	1:D:252:ARG:HD2	2.01	0.43
1:D:626:ASN:HA	1:D:627:PRO:HD2	1.76	0.43
1:J:22:TYR:HA	1:J:23:PRO:HD3	1.85	0.43
1:K:19:MET:HE1	1:K:41:PHE:CE1	2.54	0.43
1:K:608:ALA:HA	1:K:641:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:CYS:SG	1:L:351:GLU:HB3	2.59	0.43
1:B:602:LEU:HD13	1:C:592:LYS:HG2	2.00	0.43
1:D:66:LYS:HA	1:D:66:LYS:HD3	1.74	0.43
1:E:57:ALA:HA	1:E:62:TYR:HD1	1.84	0.43
1:E:609:GLY:N	1:E:641:ASP:OD2	2.50	0.43
1:I:410:ARG:HA	1:I:434:ASP:O	2.19	0.43
1:J:97:THR:O	1:J:119:GLY:HA2	2.19	0.43
1:J:231:MET:HB2	1:J:231:MET:HE3	1.87	0.43
1:J:429:GLU:HA	1:J:451:ASP:O	2.19	0.43
1:A:50:VAL:HA	1:A:55:VAL:CG1	2.48	0.43
1:B:340:TRP:CD1	1:B:340:TRP:C	2.97	0.43
1:C:459:ASN:OD1	1:C:478:SER:HB3	2.19	0.43
1:E:274:ILE:HG23	1:E:306:TYR:HB2	2.00	0.43
1:F:26:GLN:O	1:F:28:GLN:N	2.52	0.43
1:G:285:GLU:HA	1:G:310:TRP:CE3	2.54	0.43
1:H:47:ALA:HA	1:H:62:TYR:HE2	1.83	0.43
1:I:272:VAL:HG12	1:I:274:ILE:HG13	2.01	0.43
1:J:563:ILE:HD13	1:K:552:ARG:CZ	2.49	0.43
1:K:237:LEU:HD12	1:K:268:ILE:HG12	2.01	0.43
1:K:485:LYS:HD3	1:K:490:THR:O	2.19	0.43
1:L:237:LEU:HD12	1:L:268:ILE:CG1	2.47	0.43
1:L:466:GLY:C	1:L:467:ARG:HG3	2.43	0.43
1:A:163:LEU:HD23	1:A:163:LEU:O	2.18	0.43
1:D:130:GLN:HG2	1:D:256:ILE:HB	2.00	0.43
1:E:489:GLU:H	1:E:489:GLU:CD	2.27	0.43
1:K:358:VAL:HA	1:K:382:VAL:O	2.19	0.43
1:K:580:VAL:HG23	1:K:595:SER:HB2	2.01	0.43
1:A:534:HIS:O	1:A:535:GLY:C	2.62	0.42
1:B:170:TYR:N	1:B:170:TYR:CD1	2.87	0.42
1:B:333:ARG:HA	1:B:366:THR:OG1	2.20	0.42
1:B:541:LEU:N	1:B:541:LEU:CD1	2.81	0.42
1:C:372:THR:O	1:C:397:ARG:HB2	2.19	0.42
1:E:159:ALA:O	1:E:162:ALA:HB2	2.19	0.42
1:F:285:GLU:HA	1:F:310:TRP:CZ3	2.54	0.42
1:G:504:TYR:OH	1:G:506:GLY:HA2	2.19	0.42
1:I:22:TYR:O	1:I:59:PRO:HG2	2.18	0.42
1:J:254:PHE:O	1:J:276:ASN:HB2	2.19	0.42
1:K:97:THR:O	1:K:119:GLY:HA2	2.19	0.42
1:K:387:TYR:CE1	1:K:409:TYR:CD1	3.06	0.42
1:K:581:ARG:HG2	1:K:581:ARG:HH11	1.84	0.42
1:L:20:VAL:HA	1:L:58:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:512:TYR:HD1	1:L:540:LEU:O	2.02	0.42
1:A:50:VAL:HG21	1:A:57:ALA:HB2	2.01	0.42
1:A:163:LEU:HD23	1:A:163:LEU:C	2.44	0.42
1:A:327:ILE:C	1:A:328:HIS:HD2	2.27	0.42
1:B:173:LEU:O	1:B:191:SER:HA	2.19	0.42
1:C:173:LEU:O	1:C:191:SER:HA	2.19	0.42
1:C:624:THR:HA	1:C:625:PRO:HD3	1.90	0.42
1:D:64:LEU:HD23	1:D:64:LEU:N	2.34	0.42
1:D:499:GLY:HA2	1:D:528:ASN:O	2.19	0.42
1:E:284:ILE:HG21	1:E:287:ARG:HD2	2.01	0.42
1:E:333:ARG:HA	1:E:366:THR:OG1	2.19	0.42
1:G:316:LEU:N	1:G:316:LEU:CD2	2.81	0.42
1:G:598:LYS:NZ	1:H:553:MET:O	2.51	0.42
1:I:373:HIS:HE2	2:I:701:CIT:H41	1.84	0.42
1:K:21:ALA:O	1:K:22:TYR:C	2.62	0.42
1:K:323:GLU:HG2	1:K:356:LEU:HB3	2.02	0.42
1:L:469:LYS:HG3	1:L:498:ASP:HB3	2.01	0.42
1:B:113:LEU:HA	1:B:113:LEU:HD12	1.74	0.42
1:B:234:ASN:ND2	4:B:807:HOH:O	2.52	0.42
1:C:237:LEU:HD12	1:C:268:ILE:HG12	2.00	0.42
1:C:602:LEU:HD11	1:C:646:ALA:HB2	2.01	0.42
1:D:500:VAL:HB	1:D:502:MET:HE2	2.00	0.42
1:D:624:THR:HA	1:D:625:PRO:HD3	1.82	0.42
1:F:170:TYR:CZ	1:F:195:LYS:HE2	2.54	0.42
1:G:278:ARG:NH1	1:G:278:ARG:HB3	2.34	0.42
1:G:372:THR:O	1:G:397:ARG:HB2	2.19	0.42
1:H:458:GLN:HA	1:H:477:SER:OG	2.19	0.42
1:I:526:MET:HE2	1:I:553:MET:HE1	2.01	0.42
1:J:509:ARG:HD2	1:J:540:LEU:HB2	2.01	0.42
1:J:523:LEU:HD23	1:J:523:LEU:HA	1.94	0.42
1:K:363:TYR:CE1	1:K:387:TYR:CD2	3.07	0.42
1:K:513:PHE:N	1:K:513:PHE:CD1	2.86	0.42
1:L:183:PRO:O	1:L:184:ASN:C	2.60	0.42
1:L:492:GLN:HE22	1:L:523:LEU:HB2	1.84	0.42
1:A:12:VAL:HG22	1:A:32:THR:HB	2.01	0.42
1:A:511:VAL:HG21	1:A:526:MET:CE	2.49	0.42
1:A:549:THR:CG2	1:C:564:ARG:HG2	2.49	0.42
1:B:323:GLU:HG2	1:B:356:LEU:HB3	2.02	0.42
1:C:500:VAL:CG1	1:C:502:MET:HG3	2.48	0.42
1:D:329:ALA:C	1:D:330:MET:HG3	2.44	0.42
1:D:642:VAL:HG23	1:D:642:VAL:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:VAL:HB	1:E:59:PRO:HD2	2.01	0.42
2:F:701:CIT:O4	2:F:701:CIT:H22	2.19	0.42
1:G:547:GLN:NE2	1:G:586:SER:HA	2.34	0.42
1:H:115:PHE:HB2	1:H:239:SER:O	2.19	0.42
1:J:182:GLY:HA2	1:J:399:ASN:HD22	1.76	0.42
1:A:419:ASN:C	1:A:422:VAL:HG23	2.44	0.42
1:B:433:TYR:CE1	1:B:455:HIS:HD2	2.38	0.42
1:B:624:THR:HA	1:B:625:PRO:HD3	1.78	0.42
1:D:546:VAL:O	1:D:547:GLN:C	2.62	0.42
1:E:549:THR:CG2	1:E:550:PRO:HD2	2.48	0.42
1:F:135:THR:O	1:F:135:THR:HG22	2.18	0.42
1:G:353:ILE:O	1:G:354:GLU:HB2	2.19	0.42
1:I:170:TYR:CD1	1:I:231:MET:HG3	2.54	0.42
1:I:433:TYR:HE1	1:I:455:HIS:CD2	2.37	0.42
1:L:115:PHE:HB2	1:L:239:SER:O	2.20	0.42
1:B:12:VAL:HG22	1:B:32:THR:HB	2.02	0.42
1:B:510:ALA:HB1	1:B:531:MET:HE3	2.01	0.42
1:E:222:ASP:O	1:E:223:ALA:HB3	2.20	0.42
1:F:24:ASN:O	1:F:25:PHE:C	2.61	0.42
1:F:301:LYS:HG2	1:F:325:HIS:HB2	2.01	0.42
1:F:455:HIS:HA	1:F:474:THR:O	2.20	0.42
1:F:542:SER:HA	1:F:589:ASN:OD1	2.19	0.42
1:G:163:LEU:HD23	1:G:163:LEU:C	2.45	0.42
1:H:122:LEU:HA	1:H:123:PRO:HD3	1.84	0.42
1:I:340:TRP:CD1	1:I:340:TRP:C	2.96	0.42
1:I:509:ARG:NH2	1:I:537:PHE:HD2	2.17	0.42
1:K:372:THR:O	1:K:397:ARG:HB2	2.20	0.42
1:L:627:PRO:HA	1:L:630:ASN:OD1	2.20	0.42
1:A:41:PHE:CD1	1:A:65:ARG:HA	2.55	0.42
1:A:511:VAL:HG21	1:A:526:MET:HE1	2.02	0.42
1:A:564:ARG:HH11	1:A:648:GLU:HG2	1.83	0.42
1:B:120:ARG:HG2	1:B:120:ARG:NH1	2.34	0.42
1:B:163:LEU:HD23	1:B:163:LEU:O	2.20	0.42
1:C:345:ASP:HA	1:F:135:THR:HG21	2.01	0.42
1:C:388:ASP:HA	1:C:410:ARG:O	2.20	0.42
1:G:311:TYR:OH	2:G:701:CIT:H42	2.20	0.42
1:H:266:LEU:HD23	1:H:292:PHE:CE1	2.54	0.42
1:H:511:VAL:HG21	1:H:526:MET:HE1	2.02	0.42
1:I:132:LEU:HD12	1:I:258:ILE:HG12	2.00	0.42
1:J:470:GLY:HA2	1:J:499:GLY:O	2.20	0.42
1:K:220:LEU:HD23	1:K:220:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:424:PHE:CE1	1:K:446:GLY:HA3	2.55	0.42
1:K:504:TYR:CZ	1:K:506:GLY:HA2	2.54	0.42
1:K:564:ARG:HD3	1:L:550:PRO:O	2.20	0.42
1:L:255:THR:HA	1:L:287:ARG:HG2	2.02	0.42
1:A:16:LEU:O	1:A:17:ALA:C	2.63	0.42
1:B:397:ARG:CZ	2:B:701:CIT:H42	2.50	0.42
1:B:564:ARG:HG3	1:B:648:GLU:HG2	2.01	0.42
1:E:34:LEU:HD11	1:F:30:LYS:HB2	2.02	0.42
1:E:52:ASN:HA	1:E:56:PHE:CE1	2.54	0.42
1:G:189:LYS:HB2	1:G:349:TRP:CD1	2.55	0.42
1:G:433:TYR:CE1	1:G:455:HIS:CD2	3.08	0.42
1:H:454:ALA:HB3	1:H:473:TYR:CD1	2.55	0.42
1:I:104:VAL:HG21	1:I:130:GLN:HB2	2.02	0.42
1:I:457:SER:O	1:I:476:ASN:HA	2.20	0.42
1:J:424:PHE:CE1	1:J:446:GLY:HA3	2.55	0.42
1:J:515:GLY:O	1:J:516:THR:C	2.62	0.42
1:K:598:LYS:NZ	1:L:553:MET:O	2.53	0.42
1:L:58:VAL:HB	1:L:59:PRO:HD2	2.01	0.42
1:L:387:TYR:CE1	1:L:409:TYR:CD1	3.07	0.42
1:A:231:MET:HB3	1:A:231:MET:HE3	1.82	0.42
1:B:139:PRO:HG2	1:B:142:PHE:CZ	2.54	0.42
1:E:30:LYS:CD	1:E:30:LYS:C	2.93	0.42
1:E:520:ASP:OD1	1:E:520:ASP:C	2.63	0.42
1:J:302:GLY:HA2	1:J:326:ASP:O	2.20	0.42
1:K:122:LEU:HA	1:K:123:PRO:HD3	1.94	0.42
1:K:124:ASP:OD2	1:K:129:ARG:NH2	2.53	0.42
1:K:455:HIS:HA	1:K:474:THR:O	2.19	0.42
1:A:274:ILE:HG23	1:A:306:TYR:HB2	2.01	0.42
1:E:540:LEU:C	1:E:541:LEU:CD1	2.92	0.42
1:G:622:VAL:HA	1:G:623:PRO:C	2.45	0.42
1:H:622:VAL:HA	1:H:623:PRO:C	2.45	0.42
1:I:417:ALA:HA	1:I:441:ASN:O	2.20	0.42
1:I:519:ILE:HD13	1:I:519:ILE:HA	1.85	0.42
1:J:453:GLU:HG2	1:J:472:ARG:HB3	2.02	0.42
1:J:578:ALA:O	1:J:630:ASN:HB2	2.20	0.42
1:L:284:ILE:CG2	1:L:287:ARG:HD2	2.49	0.42
1:L:287:ARG:H	1:L:310:TRP:HB2	1.84	0.42
1:L:404:LEU:CD2	1:L:428:ARG:HD2	2.49	0.42
1:B:541:LEU:HD21	1:B:591:PHE:CE1	2.54	0.41
1:F:43:PHE:CG	1:F:44:THR:N	2.88	0.41
1:H:163:LEU:HD12	1:H:163:LEU:C	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:573:GLU:OE2	1:I:635:ARG:NE	2.53	0.41
1:K:78:ASN:O	1:K:79:TRP:C	2.63	0.41
1:L:90:ASN:HA	1:L:110:ASN:O	2.20	0.41
1:L:310:TRP:O	1:L:333:ARG:HB3	2.20	0.41
1:L:428:ARG:NH1	1:L:428:ARG:HG2	2.35	0.41
1:B:603:THR:C	1:B:605:PRO:HD3	2.45	0.41
1:C:638:ASN:OD1	1:C:638:ASN:C	2.61	0.41
1:E:16:LEU:O	1:E:17:ALA:C	2.63	0.41
1:E:129:ARG:HG2	4:E:848:HOH:O	2.20	0.41
1:G:58:VAL:HB	1:G:59:PRO:HD2	2.02	0.41
1:G:358:VAL:HA	1:G:382:VAL:O	2.21	0.41
1:G:389:SER:OG	1:G:392:ALA:O	2.34	0.41
1:I:78:ASN:OD1	1:I:80:THR:CB	2.68	0.41
1:K:549:THR:CG2	1:K:550:PRO:HD2	2.50	0.41
1:A:16:LEU:O	1:A:19:MET:N	2.51	0.41
1:A:247:TYR:CD2	1:A:247:TYR:C	2.98	0.41
1:C:531:MET:HE2	1:C:531:MET:HB3	1.88	0.41
1:D:373:HIS:NE2	2:D:701:CIT:O7	2.45	0.41
1:F:35:GLY:HA3	4:F:813:HOH:O	2.20	0.41
1:H:254:PHE:O	1:H:276:ASN:HB2	2.20	0.41
1:I:327:ILE:HG12	1:I:360:CYS:SG	2.60	0.41
1:I:446:GLY:HA2	1:I:465:GLY:O	2.20	0.41
1:K:293:ASN:HA	1:K:316:LEU:O	2.20	0.41
1:L:53:GLY:HA3	1:L:76:PHE:CE2	2.55	0.41
1:A:19:MET:HE1	1:A:33:LEU:HD22	2.02	0.41
1:A:105:LEU:HD23	1:A:132:LEU:CD2	2.50	0.41
1:A:249:ASP:OD2	1:B:167:LYS:HE3	2.20	0.41
1:B:504:TYR:CZ	1:B:506:GLY:HA2	2.56	0.41
1:D:531:MET:O	1:D:558:LEU:HD12	2.21	0.41
1:J:295:CYS:O	1:J:319:SER:HA	2.20	0.41
1:J:301:LYS:HG2	1:J:325:HIS:HB2	2.02	0.41
1:J:455:HIS:HA	1:J:474:THR:O	2.20	0.41
1:J:495:LEU:HB3	1:J:524:VAL:HG22	2.02	0.41
1:K:311:TYR:HD2	1:K:314:GLU:HG3	1.85	0.41
1:L:189:LYS:O	1:L:349:TRP:HA	2.20	0.41
1:L:340:TRP:C	1:L:340:TRP:HD1	2.28	0.41
1:L:504:TYR:CZ	1:L:506:GLY:HA2	2.55	0.41
1:L:509:ARG:HH11	1:L:540:LEU:HD13	1.85	0.41
1:A:182:GLY:HA2	1:A:399:ASN:ND2	2.36	0.41
1:B:457:SER:O	1:B:476:ASN:HA	2.20	0.41
1:C:433:TYR:CE1	1:C:455:HIS:CD2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:ILE:HB	1:F:332:VAL:HG12	2.00	0.41
1:G:31:ILE:HD13	1:G:63:LEU:HD22	2.03	0.41
1:G:142:PHE:N	1:G:142:PHE:CD1	2.88	0.41
1:G:189:LYS:O	1:G:349:TRP:HA	2.20	0.41
1:H:368:ALA:HA	1:H:392:ALA:O	2.21	0.41
1:I:504:TYR:CZ	1:I:506:GLY:HA2	2.56	0.41
1:K:495:LEU:HB3	1:K:524:VAL:HG22	2.02	0.41
1:L:80:THR:O	1:L:83:VAL:HG23	2.21	0.41
1:L:120:ARG:HD3	1:L:241:TYR:HB3	2.02	0.41
1:L:436:VAL:HG12	1:L:437:ARG:N	2.36	0.41
1:C:578:ALA:O	1:C:630:ASN:HB2	2.20	0.41
1:C:580:VAL:C	1:C:581:ARG:HG3	2.46	0.41
1:D:24:ASN:O	1:D:25:PHE:C	2.63	0.41
1:D:57:ALA:HA	1:D:62:TYR:HD1	1.85	0.41
1:D:526:MET:HE2	1:D:551:PRO:CG	2.46	0.41
1:D:558:LEU:HD22	1:D:651:LEU:CD2	2.46	0.41
1:E:529:ASN:N	1:E:556:ASN:OD1	2.45	0.41
1:F:24:ASN:O	1:F:26:GLN:HG3	2.20	0.41
1:G:464:ASN:C	1:G:464:ASN:ND2	2.70	0.41
1:G:550:PRO:HB3	1:G:591:PHE:CD1	2.55	0.41
1:H:323:GLU:HG2	1:H:356:LEU:HD23	2.03	0.41
1:I:576:VAL:HG11	1:I:647:TRP:CE2	2.56	0.41
1:I:620:GLN:O	1:I:621:ASP:C	2.64	0.41
1:J:340:TRP:CD1	1:J:340:TRP:C	2.98	0.41
1:L:98:VAL:HG13	1:L:120:ARG:HB2	2.03	0.41
1:L:189:LYS:HB3	1:L:349:TRP:CD1	2.56	0.41
1:L:345:ASP:OD1	1:L:345:ASP:N	2.53	0.41
1:L:358:VAL:HG23	1:L:382:VAL:HB	2.02	0.41
1:L:538:TRP:CE3	1:L:539:ALA:HB2	2.54	0.41
1:A:299:THR:HG22	1:A:323:GLU:HB2	2.03	0.41
1:A:581:ARG:NH1	4:A:803:HOH:O	2.54	0.41
1:A:612:THR:CG2	1:C:601:ARG:HH12	2.34	0.41
1:B:481:ILE:HG12	1:B:502:MET:HE2	2.01	0.41
1:C:179:CYS:HB3	1:C:351:GLU:CD	2.45	0.41
1:D:41:PHE:CD1	1:D:41:PHE:N	2.88	0.41
1:D:285:GLU:HA	1:D:310:TRP:CZ3	2.56	0.41
1:H:19:MET:HE1	1:H:41:PHE:CE1	2.55	0.41
1:H:183:PRO:O	1:H:184:ASN:C	2.63	0.41
1:H:311:TYR:CE1	1:H:334:HIS:CD2	3.09	0.41
1:I:26:GLN:N	1:I:29:ASP:OD1	2.52	0.41
1:J:220:LEU:HD23	1:J:220:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:601:ARG:HG2	1:K:603:THR:O	2.21	0.41
1:L:274:ILE:HG23	1:L:306:TYR:HB2	2.02	0.41
1:D:419:ASN:O	1:D:422:VAL:HB	2.20	0.41
1:H:46:THR:O	1:H:47:ALA:C	2.62	0.41
1:H:540:LEU:C	1:H:541:LEU:HD12	2.46	0.41
1:I:563:ILE:HD12	1:I:563:ILE:C	2.46	0.41
1:J:157:THR:HG22	1:J:206:THR:O	2.20	0.41
1:J:419:ASN:O	1:J:422:VAL:HG23	2.20	0.41
1:K:587:VAL:HG23	1:K:590:SER:OG	2.21	0.41
1:L:467:ARG:HH22	1:L:469:LYS:HE2	1.85	0.41
1:A:457:SER:O	1:A:476:ASN:HA	2.21	0.41
1:A:549:THR:HG22	1:C:564:ARG:HG2	2.03	0.41
1:B:46:THR:O	1:B:62:TYR:CE1	2.73	0.41
1:B:115:PHE:N	1:B:115:PHE:CD1	2.89	0.41
1:B:429:GLU:OE1	4:B:801:HOH:O	2.22	0.41
1:B:479:SER:HA	1:B:509:ARG:O	2.21	0.41
1:B:622:VAL:HA	1:B:623:PRO:C	2.46	0.41
1:C:92:HIS:CE1	1:C:114:GLU:OE1	2.73	0.41
1:C:231:MET:CA	1:C:231:MET:HE2	2.51	0.41
1:C:367:GLN:O	1:C:368:ALA:C	2.61	0.41
1:C:505:ASP:OD1	1:C:507:THR:OG1	2.39	0.41
1:D:25:PHE:HB3	1:D:43:PHE:CG	2.55	0.41
1:D:34:LEU:HD21	1:E:30:LYS:CE	2.44	0.41
1:D:311:TYR:CE1	1:D:334:HIS:CD2	3.09	0.41
1:D:510:ALA:HB1	1:D:531:MET:HE3	2.03	0.41
1:E:26:GLN:O	1:E:29:ASP:OD1	2.38	0.41
1:E:115:PHE:CD1	1:E:240:PRO:HA	2.56	0.41
1:E:231:MET:HB2	1:E:231:MET:HE3	1.76	0.41
1:E:457:SER:O	1:E:476:ASN:HA	2.20	0.41
1:G:340:TRP:C	1:G:340:TRP:HD1	2.27	0.41
1:H:351:GLU:HA	1:H:375:ILE:HD12	2.03	0.41
1:H:359:ASN:HA	1:H:383:ARG:O	2.21	0.41
1:I:295:CYS:O	1:I:319:SER:HA	2.21	0.41
1:I:453:GLU:HG2	1:I:472:ARG:HB3	2.03	0.41
1:J:173:LEU:HB3	1:J:218:TYR:CE2	2.55	0.41
1:J:407:ARG:HA	1:J:431:LEU:O	2.21	0.41
1:J:570:VAL:O	1:J:570:VAL:HG12	2.21	0.41
1:K:430:CYS:C	1:K:431:LEU:HD23	2.46	0.41
1:L:79:TRP:O	1:L:83:VAL:CG2	2.69	0.41
1:L:86:MET:HE2	1:L:113:LEU:HD13	2.01	0.41
1:L:134:ILE:O	1:L:260:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:254:PHE:O	1:L:276:ASN:HB2	2.20	0.41
1:A:58:VAL:HB	1:A:59:PRO:HD2	2.03	0.41
1:A:448:TYR:HB3	1:A:450:TYR:CZ	2.56	0.41
1:C:124:ASP:CB	1:C:129:ARG:HH12	2.34	0.41
1:C:274:ILE:HG23	1:C:306:TYR:HB2	2.02	0.41
1:E:148:ASP:OD1	1:E:220:LEU:N	2.47	0.41
1:E:345:ASP:HB2	4:E:893:HOH:O	2.21	0.41
1:E:624:THR:HG22	1:E:625:PRO:O	2.21	0.41
1:J:44:THR:HG21	1:J:64:LEU:HD11	2.03	0.41
1:L:407:ARG:HA	1:L:431:LEU:O	2.20	0.41
1:L:472:ARG:HG3	1:L:501:SER:CB	2.51	0.41
1:A:576:VAL:O	1:A:631:SER:HA	2.21	0.40
1:A:580:VAL:C	1:A:581:ARG:HG3	2.46	0.40
1:A:612:THR:HG23	1:A:613:VAL:N	2.36	0.40
1:E:253:PHE:CD1	1:E:253:PHE:N	2.89	0.40
1:F:446:GLY:HA2	1:F:465:GLY:O	2.21	0.40
1:H:79:TRP:CD2	1:H:101:ALA:HA	2.56	0.40
1:H:367:GLN:O	1:H:368:ALA:C	2.63	0.40
1:J:193:ILE:HG13	1:J:318:CYS:SG	2.61	0.40
1:J:581:ARG:H	1:J:595:SER:HG	1.66	0.40
1:A:247:TYR:CD2	1:A:248:ASP:N	2.89	0.40
1:A:404:LEU:HD21	1:A:428:ARG:HD2	2.02	0.40
1:B:26:GLN:O	1:B:28:GLN:N	2.54	0.40
1:B:558:LEU:HD22	1:B:651:LEU:CD2	2.51	0.40
1:C:558:LEU:HD22	1:C:651:LEU:HD22	2.04	0.40
1:E:159:ALA:O	1:E:162:ALA:CB	2.70	0.40
1:E:397:ARG:HH22	2:E:701:CIT:H41	1.85	0.40
1:H:108:LYS:HA	1:H:108:LYS:HD2	1.99	0.40
1:H:147:ALA:HA	1:H:220:LEU:HD11	2.02	0.40
1:J:158:VAL:HG21	1:J:163:LEU:CD2	2.51	0.40
1:J:368:ALA:HA	1:J:392:ALA:O	2.20	0.40
1:L:189:LYS:CB	1:L:349:TRP:CD1	3.04	0.40
1:A:320:GLU:HA	1:A:353:ILE:O	2.22	0.40
1:A:540:LEU:HD12	1:A:541:LEU:H	1.84	0.40
1:C:53:GLY:HA3	1:C:76:PHE:CD2	2.56	0.40
1:C:183:PRO:O	1:C:184:ASN:C	2.63	0.40
1:D:396:ALA:HB2	1:D:403:TYR:OH	2.21	0.40
1:F:58:VAL:HG11	1:F:63:LEU:CD2	2.44	0.40
1:G:632:PHE:HE1	1:G:634:ILE:CG1	2.34	0.40
1:H:58:VAL:O	1:H:59:PRO:C	2.63	0.40
1:I:193:ILE:CG2	1:I:231:MET:HE2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:LEU:HD13	1:J:226:VAL:HG21	2.04	0.40
1:K:413:MET:HE2	1:K:413:MET:HB2	1.86	0.40
1:K:440:PHE:HB2	1:K:461:VAL:HG22	2.03	0.40
1:A:112:THR:CG2	1:A:236:THR:HB	2.43	0.40
1:A:570:VAL:O	1:A:571:ALA:HB3	2.22	0.40
1:C:167:LYS:HA	1:C:196:VAL:HG12	2.03	0.40
1:D:36:SER:N	4:D:807:HOH:O	2.54	0.40
1:D:41:PHE:CE2	1:D:65:ARG:HB2	2.56	0.40
1:D:510:ALA:CB	1:D:531:MET:CE	3.00	0.40
1:F:603:THR:CG2	1:F:644:GLN:HB2	2.48	0.40
1:G:619:ASN:HD22	1:G:629:LEU:CB	2.33	0.40
1:I:512:TYR:CG	1:I:540:LEU:HD23	2.56	0.40
1:J:33:LEU:HD12	1:J:34:LEU:N	2.35	0.40
1:J:340:TRP:CE2	1:J:373:HIS:HD2	2.39	0.40
1:K:541:LEU:HD12	1:K:541:LEU:N	2.37	0.40
1:L:414:ASP:OD1	1:L:438:SER:OG	2.36	0.40
1:L:561:THR:O	1:L:579:ARG:HG3	2.21	0.40
1:B:277:LYS:HG3	1:B:278:ARG:O	2.22	0.40
1:B:358:VAL:HA	1:B:382:VAL:O	2.22	0.40
1:D:441:ASN:HA	1:D:462:ARG:HB2	2.03	0.40
1:D:602:LEU:HD11	1:D:646:ALA:HB2	2.04	0.40
1:F:618:GLN:HA	1:F:630:ASN:OD1	2.21	0.40
1:G:183:PRO:O	1:G:184:ASN:C	2.62	0.40
1:G:265:ASP:HA	1:G:297:ASP:O	2.22	0.40
1:H:353:ILE:O	1:H:354:GLU:HB2	2.21	0.40
1:H:499:GLY:HA2	1:H:528:ASN:O	2.22	0.40
1:I:320:GLU:HA	1:I:353:ILE:O	2.22	0.40
1:K:70:PRO:HB3	1:K:92:HIS:CE1	2.57	0.40
1:K:373:HIS:HA	1:K:397:ARG:HE	1.87	0.40
1:K:469:LYS:HA	1:K:498:ASP:O	2.21	0.40
1:L:222:ASP:O	1:L:223:ALA:HB3	2.21	0.40
1:L:328:HIS:CD2	1:L:361:GLU:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	640/671 (95%)	594 (93%)	41 (6%)	5 (1%)	16	40
1	B	642/671 (96%)	598 (93%)	38 (6%)	6 (1%)	14	37
1	C	642/671 (96%)	605 (94%)	32 (5%)	5 (1%)	16	40
1	D	641/671 (96%)	596 (93%)	38 (6%)	7 (1%)	11	32
1	E	641/671 (96%)	599 (93%)	36 (6%)	6 (1%)	14	37
1	F	642/671 (96%)	596 (93%)	40 (6%)	6 (1%)	14	37
1	G	640/671 (95%)	597 (93%)	38 (6%)	5 (1%)	16	40
1	H	644/671 (96%)	595 (92%)	45 (7%)	4 (1%)	21	47
1	I	642/671 (96%)	592 (92%)	48 (8%)	2 (0%)	36	63
1	J	640/671 (95%)	581 (91%)	57 (9%)	2 (0%)	36	63
1	K	640/671 (95%)	585 (91%)	51 (8%)	4 (1%)	21	47
1	L	640/671 (95%)	585 (91%)	47 (7%)	8 (1%)	9	28
All	All	7694/8052 (96%)	7123 (93%)	511 (7%)	60 (1%)	16	40

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	38	GLY
1	B	27	VAL
1	E	38	GLY
1	E	46	THR
1	F	27	VAL
1	H	8	ALA
1	L	621	ASP
1	A	53	GLY
1	C	27	VAL
1	C	53	GLY
1	C	621	ASP
1	D	46	THR
1	D	53	GLY
1	D	275	GLY
1	E	27	VAL
1	F	38	GLY
1	F	46	THR

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Mol	Chain	Res	Type
1	G	38	GLY
1	H	53	GLY
1	I	621	ASP
1	K	621	ASP
1	L	53	GLY
1	L	445	GLY
1	A	621	ASP
1	D	27	VAL
1	F	53	GLY
1	G	53	GLY
1	I	53	GLY
1	K	53	GLY
1	K	354	GLU
1	A	17	ALA
1	B	15	ASP
1	B	275	GLY
1	C	9	PRO
1	E	53	GLY
1	H	445	GLY
1	L	281	ALA
1	L	354	GLU
1	B	354	GLU
1	D	445	GLY
1	F	354	GLU
1	G	354	GLU
1	J	53	GLY
1	L	38	GLY
1	L	59	PRO
1	L	436	VAL
1	B	53	GLY
1	C	445	GLY
1	D	621	ASP
1	E	445	GLY
1	K	38	GLY
1	G	445	GLY
1	J	445	GLY
1	B	445	GLY
1	D	59	PRO
1	G	275	GLY
1	E	59	PRO
1	H	27	VAL
1	F	9	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	520/544 (96%)	490 (94%)	30 (6%)	18	45
1	B	521/544 (96%)	491 (94%)	30 (6%)	18	45
1	C	521/544 (96%)	491 (94%)	30 (6%)	18	45
1	D	521/544 (96%)	494 (95%)	27 (5%)	21	50
1	E	521/544 (96%)	496 (95%)	25 (5%)	23	53
1	F	521/544 (96%)	491 (94%)	30 (6%)	18	45
1	G	520/544 (96%)	489 (94%)	31 (6%)	17	43
1	H	523/544 (96%)	495 (95%)	28 (5%)	20	48
1	I	521/544 (96%)	480 (92%)	41 (8%)	11	31
1	J	520/544 (96%)	483 (93%)	37 (7%)	13	36
1	K	520/544 (96%)	492 (95%)	28 (5%)	20	48
1	L	520/544 (96%)	468 (90%)	52 (10%)	7	21
All	All	6249/6528 (96%)	5860 (94%)	389 (6%)	16	42

All (389) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	20	VAL
1	A	27	VAL
1	A	34	LEU
1	A	46	THR
1	A	62	TYR
1	A	82	ILE
1	A	100	GLN
1	A	112	THR
1	A	118	THR
1	A	120	ARG
1	A	141	VAL
1	A	143	VAL
1	A	163	LEU

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Mol	Chain	Res	Type
1	A	175	SER
1	A	202	SER
1	A	233	GLU
1	A	277	LYS
1	A	279	PRO
1	A	322	THR
1	A	371	ASP
1	A	422	VAL
1	A	507	THR
1	A	525	SER
1	A	532	THR
1	A	606	SER
1	A	612	THR
1	A	620	GLN
1	A	637	SER
1	A	642	VAL
1	B	24	ASN
1	B	30	LYS
1	B	42	THR
1	B	62	TYR
1	B	82	ILE
1	B	135	THR
1	B	141	VAL
1	B	163	LEU
1	B	175	SER
1	B	183	PRO
1	B	200	SER
1	B	202	SER
1	B	208	ILE
1	B	234	ASN
1	B	239	SER
1	B	255	THR
1	B	268	ILE
1	B	380	LYS
1	B	429	GLU
1	B	469	LYS
1	B	525	SER
1	B	541	LEU
1	B	545	THR
1	B	563	ILE
1	B	564	ARG
1	B	600	THR

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Mol	Chain	Res	Type
1	B	606	SER
1	B	620	GLN
1	B	622	VAL
1	B	624	THR
1	C	10	GLU
1	C	27	VAL
1	C	45	THR
1	C	63	LEU
1	C	127	VAL
1	C	143	VAL
1	C	156	ILE
1	C	163	LEU
1	C	175	SER
1	C	200	SER
1	C	202	SER
1	C	231	MET
1	C	234	ASN
1	C	279	PRO
1	C	322	THR
1	C	342	SER
1	C	371	ASP
1	C	413	MET
1	C	459	ASN
1	C	489	GLU
1	C	496	GLU
1	C	507	THR
1	C	523	LEU
1	C	525	SER
1	C	542	SER
1	C	546	VAL
1	C	592	LYS
1	C	597	VAL
1	C	622	VAL
1	C	645	VAL
1	D	10	GLU
1	D	14	SER
1	D	20	VAL
1	D	27	VAL
1	D	28	GLN
1	D	45	THR
1	D	104	VAL
1	D	120	ARG

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Mol	Chain	Res	Type
1	D	133	ASN
1	D	141	VAL
1	D	163	LEU
1	D	175	SER
1	D	183	PRO
1	D	221	SER
1	D	230	THR
1	D	234	ASN
1	D	250	LEU
1	D	322	THR
1	D	371	ASP
1	D	451	ASP
1	D	477	SER
1	D	541	LEU
1	D	553	MET
1	D	575	THR
1	D	620	GLN
1	D	622	VAL
1	D	642	VAL
1	E	11	ARG
1	E	27	VAL
1	E	30	LYS
1	E	32	THR
1	E	78	ASN
1	E	127	VAL
1	E	163	LEU
1	E	175	SER
1	E	199	VAL
1	E	221	SER
1	E	231	MET
1	E	265	ASP
1	E	277	LYS
1	E	321	ASP
1	E	327	ILE
1	E	395	GLN
1	E	413	MET
1	E	426	ILE
1	E	489	GLU
1	E	492	GLN
1	E	525	SER
1	E	561	THR
1	E	563	ILE

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Mol	Chain	Res	Type
1	E	620	GLN
1	E	622	VAL
1	F	27	VAL
1	F	28	GLN
1	F	33	LEU
1	F	44	THR
1	F	63	LEU
1	F	64	LEU
1	F	68	VAL
1	F	117	ASP
1	F	163	LEU
1	F	175	SER
1	F	183	PRO
1	F	200	SER
1	F	202	SER
1	F	230	THR
1	F	239	SER
1	F	256	ILE
1	F	371	ASP
1	F	380	LYS
1	F	395	GLN
1	F	413	MET
1	F	426	ILE
1	F	477	SER
1	F	493	THR
1	F	566	VAL
1	F	568	THR
1	F	580	VAL
1	F	592	LYS
1	F	622	VAL
1	F	649	VAL
1	F	651	LEU
1	G	10	GLU
1	G	11	ARG
1	G	14	SER
1	G	27	VAL
1	G	44	THR
1	G	68	VAL
1	G	107	ILE
1	G	118	THR
1	G	141	VAL
1	G	163	LEU

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Mol	Chain	Res	Type
1	G	173	LEU
1	G	183	PRO
1	G	195	LYS
1	G	199	VAL
1	G	371	ASP
1	G	375	ILE
1	G	377	LYS
1	G	380	LYS
1	G	426	ILE
1	G	464	ASN
1	G	469	LYS
1	G	474	THR
1	G	494	SER
1	G	511	VAL
1	G	542	SER
1	G	568	THR
1	G	587	VAL
1	G	600	THR
1	G	606	SER
1	G	620	GLN
1	G	644	GLN
1	H	16	LEU
1	H	28	GLN
1	H	36	SER
1	H	42	THR
1	H	80	THR
1	H	91	ARG
1	H	116	THR
1	H	131	VAL
1	H	141	VAL
1	H	175	SER
1	H	231	MET
1	H	239	SER
1	H	274	ILE
1	H	338	LEU
1	H	342	SER
1	H	371	ASP
1	H	469	LYS
1	H	511	VAL
1	H	573	GLU
1	H	575	THR
1	H	577	ASN

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Mol	Chain	Res	Type
1	H	581	ARG
1	H	592	LYS
1	H	606	SER
1	H	612	THR
1	H	620	GLN
1	H	622	VAL
1	H	642	VAL
1	I	11	ARG
1	I	20	VAL
1	I	27	VAL
1	I	28	GLN
1	I	68	VAL
1	I	78	ASN
1	I	106	ASN
1	I	111	SER
1	I	127	VAL
1	I	133	ASN
1	I	135	THR
1	I	141	VAL
1	I	143	VAL
1	I	158	VAL
1	I	163	LEU
1	I	164	SER
1	I	175	SER
1	I	200	SER
1	I	202	SER
1	I	230	THR
1	I	244	GLU
1	I	255	THR
1	I	322	THR
1	I	342	SER
1	I	420	THR
1	I	493	THR
1	I	507	THR
1	I	511	VAL
1	I	517	VAL
1	I	525	SER
1	I	526	MET
1	I	531	MET
1	I	542	SER
1	I	549	THR
1	I	553	MET

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Mol	Chain	Res	Type
1	I	561	THR
1	I	570	VAL
1	I	575	THR
1	I	600	THR
1	I	606	SER
1	I	622	VAL
1	J	10	GLU
1	J	11	ARG
1	J	27	VAL
1	J	68	VAL
1	J	80	THR
1	J	112	THR
1	J	135	THR
1	J	141	VAL
1	J	148	ASP
1	J	163	LEU
1	J	175	SER
1	J	201	THR
1	J	225	GLU
1	J	231	MET
1	J	274	ILE
1	J	326	ASP
1	J	336	ILE
1	J	371	ASP
1	J	379	VAL
1	J	401	VAL
1	J	461	VAL
1	J	468	VAL
1	J	469	LYS
1	J	490	THR
1	J	493	THR
1	J	511	VAL
1	J	525	SER
1	J	566	VAL
1	J	570	VAL
1	J	576	VAL
1	J	586	SER
1	J	606	SER
1	J	607	SER
1	J	612	THR
1	J	622	VAL
1	J	624	THR

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Mol	Chain	Res	Type
1	J	644	GLN
1	K	27	VAL
1	K	36	SER
1	K	46	THR
1	K	74	SER
1	K	80	THR
1	K	84	THR
1	K	109	SER
1	K	129	ARG
1	K	141	VAL
1	K	163	LEU
1	K	193	ILE
1	K	231	MET
1	K	261	ASN
1	K	371	ASP
1	K	380	LYS
1	K	413	MET
1	K	502	MET
1	K	554	SER
1	K	561	THR
1	K	563	ILE
1	K	566	VAL
1	K	569	LEU
1	K	575	THR
1	K	587	VAL
1	K	620	GLN
1	K	624	THR
1	K	649	VAL
1	K	651	LEU
1	L	11	ARG
1	L	14	SER
1	L	18	SER
1	L	20	VAL
1	L	27	VAL
1	L	28	GLN
1	L	45	THR
1	L	48	SER
1	L	63	LEU
1	L	68	VAL
1	L	80	THR
1	L	83	VAL
1	L	127	VAL

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Mol	Chain	Res	Type
1	L	133	ASN
1	L	141	VAL
1	L	164	SER
1	L	175	SER
1	L	183	PRO
1	L	208	ILE
1	L	221	SER
1	L	238	VAL
1	L	272	VAL
1	L	365	THR
1	L	371	ASP
1	L	372	THR
1	L	380	LYS
1	L	395	GLN
1	L	398	THR
1	L	418	SER
1	L	422	VAL
1	L	426	ILE
1	L	469	LYS
1	L	493	THR
1	L	501	SER
1	L	511	VAL
1	L	517	VAL
1	L	522	THR
1	L	527	SER
1	L	537	PHE
1	L	542	SER
1	L	549	THR
1	L	563	ILE
1	L	570	VAL
1	L	575	THR
1	L	595	SER
1	L	612	THR
1	L	615	SER
1	L	616	VAL
1	L	620	GLN
1	L	622	VAL
1	L	633	VAL
1	L	644	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	100	GLN
1	A	234	ASN
1	A	325	HIS
1	A	367	GLN
1	A	620	GLN
1	A	626	ASN
1	B	110	ASN
1	B	234	ASN
1	B	261	ASN
1	B	367	GLN
1	B	534	HIS
1	B	626	ASN
1	C	52	ASN
1	C	92	HIS
1	C	106	ASN
1	C	110	ASN
1	C	261	ASN
1	C	293	ASN
1	C	359	ASN
1	D	52	ASN
1	D	110	ASN
1	D	176	ASN
1	D	328	HIS
1	D	534	HIS
1	E	52	ASN
1	E	110	ASN
1	E	261	ASN
1	E	328	HIS
1	E	458	GLN
1	E	459	ASN
1	E	528	ASN
1	E	547	GLN
1	F	90	ASN
1	F	106	ASN
1	F	293	ASN
1	F	328	HIS
1	F	405	ASN
1	F	577	ASN
1	G	52	ASN
1	G	234	ASN
1	G	261	ASN
1	G	294	ASN

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Mol	Chain	Res	Type
1	G	328	HIS
1	G	455	HIS
1	G	458	GLN
1	G	464	ASN
1	G	644	GLN
1	H	106	ASN
1	H	110	ASN
1	H	130	GLN
1	H	133	ASN
1	H	234	ASN
1	H	261	ASN
1	H	455	HIS
1	H	459	ASN
1	H	534	HIS
1	H	577	ASN
1	H	626	ASN
1	H	644	GLN
1	I	269	GLN
1	I	328	HIS
1	I	626	ASN
1	J	106	ASN
1	J	130	GLN
1	J	133	ASN
1	J	215	HIS
1	J	234	ASN
1	J	269	GLN
1	J	325	HIS
1	J	395	GLN
1	J	441	ASN
1	J	459	ASN
1	J	618	GLN
1	J	626	ASN
1	K	26	GLN
1	K	28	GLN
1	K	110	ASN
1	K	176	ASN
1	K	234	ASN
1	K	261	ASN
1	K	328	HIS
1	K	367	GLN
1	K	405	ASN
1	K	458	GLN

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Mol	Chain	Res	Type
1	K	459	ASN
1	K	547	GLN
1	K	577	ASN
1	K	626	ASN
1	K	644	GLN
1	L	28	GLN
1	L	130	GLN
1	L	234	ASN
1	L	325	HIS
1	L	328	HIS
1	L	399	ASN
1	L	459	ASN
1	L	534	HIS
1	L	547	GLN
1	L	577	ASN
1	L	626	ASN
1	L	644	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	K	701	-	12,12,12	1.96	2 (16%)	17,17,17	1.99	2 (11%)
2	CIT	F	701	-	12,12,12	1.93	3 (25%)	17,17,17	2.27	7 (41%)
2	CIT	J	701	-	12,12,12	1.61	1 (8%)	17,17,17	1.50	4 (23%)
3	CO3	H	701	-	3,3,3	0.65	0	2,3,3	0.43	0
2	CIT	E	701	-	12,12,12	1.81	1 (8%)	17,17,17	1.67	4 (23%)
2	CIT	C	701	-	12,12,12	2.36	4 (33%)	17,17,17	1.66	5 (29%)
2	CIT	K	703	-	12,12,12	2.39	4 (33%)	17,17,17	1.22	1 (5%)
2	CIT	L	701	-	12,12,12	1.67	4 (33%)	17,17,17	1.04	1 (5%)
2	CIT	I	701	-	12,12,12	1.53	1 (8%)	17,17,17	1.18	2 (11%)
2	CIT	B	701	-	12,12,12	1.44	1 (8%)	17,17,17	1.60	4 (23%)
3	CO3	C	702	-	3,3,3	0.57	0	2,3,3	1.59	0
2	CIT	B	702	-	12,12,12	2.20	4 (33%)	17,17,17	1.61	2 (11%)
2	CIT	A	701	-	12,12,12	2.07	2 (16%)	17,17,17	1.55	4 (23%)
2	CIT	G	701	-	12,12,12	1.57	2 (16%)	17,17,17	1.12	1 (5%)
2	CIT	D	701	-	12,12,12	1.75	3 (25%)	17,17,17	1.76	3 (17%)
2	CIT	A	702	-	12,12,12	1.63	3 (25%)	17,17,17	1.41	3 (17%)
3	CO3	K	702	-	3,3,3	0.66	0	2,3,3	0.84	0
2	CIT	F	702	-	12,12,12	1.24	0	17,17,17	1.69	5 (29%)
2	CIT	H	702	-	12,12,12	1.87	3 (25%)	17,17,17	1.45	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	K	701	-	-	5/16/16/16	-
2	CIT	C	701	-	-	6/16/16/16	-
2	CIT	A	701	-	-	5/16/16/16	-
2	CIT	K	703	-	-	3/16/16/16	-
2	CIT	G	701	-	-	10/16/16/16	-
2	CIT	F	701	-	-	3/16/16/16	-
2	CIT	J	701	-	-	4/16/16/16	-
2	CIT	D	701	-	-	5/16/16/16	-
2	CIT	L	701	-	-	4/16/16/16	-
2	CIT	A	702	-	-	3/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	I	701	-	-	3/16/16/16	-
2	CIT	E	701	-	-	0/16/16/16	-
2	CIT	F	702	-	-	2/16/16/16	-
2	CIT	B	701	-	-	5/16/16/16	-
2	CIT	B	702	-	-	2/16/16/16	-
2	CIT	H	702	-	-	0/16/16/16	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CIT	C3-C6	6.07	1.59	1.53
2	B	702	CIT	C3-C6	5.60	1.59	1.53
2	C	701	CIT	C3-C6	5.59	1.59	1.53
2	K	701	CIT	C3-C6	4.90	1.58	1.53
2	E	701	CIT	C4-C3	-4.60	1.48	1.54
2	F	701	CIT	C3-C6	4.60	1.58	1.53
2	K	703	CIT	C3-C6	4.28	1.57	1.53
2	J	701	CIT	C3-C6	4.10	1.57	1.53
2	K	703	CIT	C2-C3	3.96	1.58	1.54
2	K	703	CIT	C2-C1	3.83	1.62	1.50
2	D	701	CIT	C3-C6	-3.44	1.49	1.53
2	C	701	CIT	C4-C3	3.32	1.58	1.54
2	H	702	CIT	C3-C6	-2.97	1.50	1.53
2	H	702	CIT	C2-C3	2.88	1.57	1.54
2	B	702	CIT	O2-C1	-2.66	1.22	1.30
2	G	701	CIT	C4-C3	2.61	1.57	1.54
2	A	702	CIT	C3-C6	2.55	1.56	1.53
2	C	701	CIT	C4-C5	2.54	1.58	1.50
2	B	701	CIT	C4-C3	2.54	1.57	1.54
2	H	702	CIT	C4-C3	2.50	1.57	1.54
2	F	701	CIT	O1-C1	2.49	1.30	1.22
2	K	701	CIT	O2-C1	-2.49	1.22	1.30
2	K	703	CIT	C4-C5	2.46	1.58	1.50
2	L	701	CIT	C4-C3	-2.46	1.50	1.54
2	B	702	CIT	C2-C3	-2.44	1.50	1.54
2	G	701	CIT	C2-C3	2.43	1.57	1.54
2	L	701	CIT	C4-C5	2.43	1.58	1.50
2	A	702	CIT	O2-C1	-2.32	1.23	1.30
2	D	701	CIT	C2-C1	2.29	1.57	1.50
2	D	701	CIT	C4-C5	2.28	1.57	1.50
2	F	701	CIT	O4-C5	-2.25	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	CIT	O4-C5	-2.22	1.23	1.30
2	I	701	CIT	C4-C3	-2.20	1.51	1.54
2	L	701	CIT	O3-C5	2.14	1.29	1.22
2	L	701	CIT	O2-C1	-2.13	1.23	1.30
2	A	701	CIT	O2-C1	-2.07	1.24	1.30
2	C	701	CIT	C2-C1	2.02	1.56	1.50
2	A	702	CIT	C4-C5	2.01	1.56	1.50

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	701	CIT	O7-C3-C6	7.20	119.18	108.96
2	F	701	CIT	O6-C6-C3	4.87	122.47	113.14
2	B	702	CIT	O6-C6-C3	4.27	121.33	113.14
2	A	702	CIT	O7-C3-C6	3.87	114.45	108.96
2	C	701	CIT	O7-C3-C6	3.85	114.42	108.96
2	D	701	CIT	O5-C6-C3	-3.83	114.68	122.09
2	E	701	CIT	O5-C6-C3	-3.72	114.89	122.09
2	F	701	CIT	C4-C3-C6	-3.67	101.91	110.03
2	F	701	CIT	C2-C3-C6	3.60	118.00	110.03
2	F	702	CIT	O5-C6-C3	-3.50	115.31	122.09
2	F	701	CIT	O5-C6-C3	-3.45	115.41	122.09
2	H	702	CIT	O5-C6-C3	-3.05	116.18	122.09
2	F	702	CIT	O6-C6-C3	3.00	118.89	113.14
2	D	701	CIT	O3-C5-C4	-2.97	114.53	122.95
2	B	701	CIT	O6-C6-C3	2.96	118.82	113.14
2	E	701	CIT	O7-C3-C4	-2.86	102.84	109.38
2	H	702	CIT	O3-C5-C4	-2.84	114.90	122.95
2	C	701	CIT	O6-C6-C3	2.81	118.54	113.14
2	A	701	CIT	O3-C5-C4	-2.79	115.05	122.95
2	D	701	CIT	O4-C5-C4	2.79	123.17	114.35
2	B	701	CIT	O5-C6-C3	-2.78	116.71	122.09
2	B	702	CIT	O5-C6-C3	-2.77	116.72	122.09
2	L	701	CIT	O5-C6-C3	-2.75	116.77	122.09
2	A	701	CIT	O6-C6-C3	2.64	118.21	113.14
2	J	701	CIT	O6-C6-C3	2.60	118.13	113.14
2	G	701	CIT	O3-C5-C4	-2.60	115.60	122.95
2	I	701	CIT	O7-C3-C4	-2.56	103.54	109.38
2	B	701	CIT	O1-C1-C2	-2.53	115.78	122.95
2	F	701	CIT	O7-C3-C6	-2.52	105.38	108.96
2	E	701	CIT	O1-C1-C2	-2.50	115.86	122.95
2	I	701	CIT	O5-C6-C3	-2.49	117.28	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	CIT	C3-C4-C5	2.47	120.68	113.92
2	J	701	CIT	O1-C1-C2	-2.40	116.16	122.95
2	A	701	CIT	C4-C3-C6	2.40	115.33	110.03
2	K	703	CIT	O7-C3-C6	2.35	112.30	108.96
2	C	701	CIT	O5-C6-C3	-2.35	117.55	122.09
2	C	701	CIT	O7-C3-C2	-2.33	104.05	109.38
2	F	702	CIT	O7-C3-C6	-2.29	105.71	108.96
2	A	702	CIT	O3-C5-C4	-2.28	116.50	122.95
2	F	702	CIT	O1-C1-C2	-2.28	116.50	122.95
2	J	701	CIT	O3-C5-C4	-2.24	116.60	122.95
2	F	702	CIT	C4-C3-C6	2.20	114.90	110.03
2	E	701	CIT	O6-C6-C3	2.18	117.33	113.14
2	B	701	CIT	O7-C3-C6	2.18	112.05	108.96
2	F	701	CIT	O7-C3-C4	2.17	114.33	109.38
2	K	701	CIT	C2-C3-C6	-2.17	105.23	110.03
2	A	702	CIT	O4-C5-C4	2.11	121.03	114.35
2	A	701	CIT	C4-C3-C2	-2.10	103.94	109.31
2	F	701	CIT	O2-C1-O1	2.04	128.59	123.33
2	J	701	CIT	O5-C6-C3	-2.00	118.22	122.09

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	CIT	O7-C3-C6-O5
2	A	701	CIT	O7-C3-C6-O6
2	A	701	CIT	C4-C3-C6-O5
2	A	701	CIT	C4-C3-C6-O6
2	B	701	CIT	O7-C3-C4-C5
2	B	701	CIT	C6-C3-C4-C5
2	C	701	CIT	O7-C3-C6-O5
2	C	701	CIT	O7-C3-C6-O6
2	C	701	CIT	C4-C3-C6-O5
2	C	701	CIT	C4-C3-C6-O6
2	G	701	CIT	C2-C3-C4-C5
2	G	701	CIT	O7-C3-C4-C5
2	G	701	CIT	C2-C3-C6-O5
2	G	701	CIT	C2-C3-C6-O6
2	G	701	CIT	O7-C3-C6-O5
2	G	701	CIT	O7-C3-C6-O6
2	J	701	CIT	C2-C3-C6-O5
2	J	701	CIT	C2-C3-C6-O6

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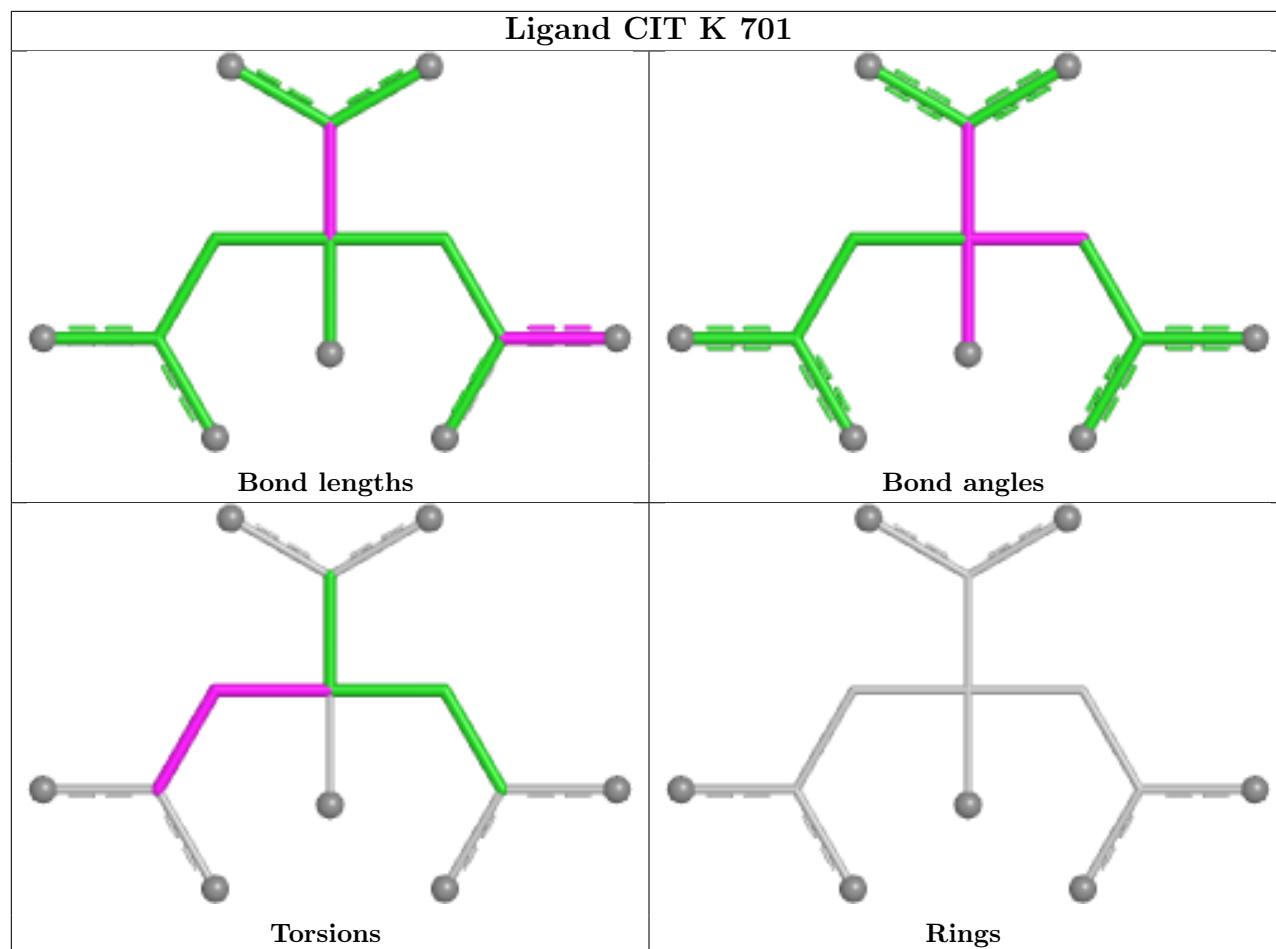
Mol	Chain	Res	Type	Atoms
2	J	701	CIT	O7-C3-C6-O5
2	J	701	CIT	O7-C3-C6-O6
2	K	701	CIT	C6-C3-C4-C5
2	L	701	CIT	C2-C3-C6-O5
2	L	701	CIT	C2-C3-C6-O6
2	L	701	CIT	O7-C3-C6-O5
2	L	701	CIT	O7-C3-C6-O6
2	B	701	CIT	C2-C3-C4-C5
2	G	701	CIT	C6-C3-C4-C5
2	A	702	CIT	O7-C3-C4-C5
2	A	702	CIT	C6-C3-C4-C5
2	K	701	CIT	C2-C3-C4-C5
2	K	701	CIT	O7-C3-C4-C5
2	G	701	CIT	C1-C2-C3-C6
2	I	701	CIT	C1-C2-C3-C6
2	K	703	CIT	O7-C3-C4-C5
2	K	703	CIT	C6-C3-C4-C5
2	A	702	CIT	C2-C3-C4-C5
2	D	701	CIT	C6-C3-C4-C5
2	G	701	CIT	C1-C2-C3-O7
2	I	701	CIT	C1-C2-C3-O7
2	I	701	CIT	C1-C2-C3-C4
2	K	703	CIT	C2-C3-C4-C5
2	D	701	CIT	O7-C3-C4-C5
2	D	701	CIT	C2-C3-C4-C5
2	G	701	CIT	C1-C2-C3-C4
2	B	702	CIT	O2-C1-C2-C3
2	D	701	CIT	C3-C4-C5-O4
2	F	701	CIT	C2-C3-C6-O5
2	F	702	CIT	C6-C3-C4-C5
2	B	702	CIT	O1-C1-C2-C3
2	D	701	CIT	C3-C4-C5-O3
2	A	701	CIT	C2-C3-C6-O6
2	C	701	CIT	C2-C3-C6-O6
2	F	701	CIT	C4-C3-C6-O5
2	B	701	CIT	C1-C2-C3-C6
2	F	702	CIT	O7-C3-C4-C5
2	F	701	CIT	O7-C3-C6-O5
2	B	701	CIT	C1-C2-C3-O7
2	C	701	CIT	O1-C1-C2-C3
2	K	701	CIT	C3-C4-C5-O3
2	K	701	CIT	C3-C4-C5-O4

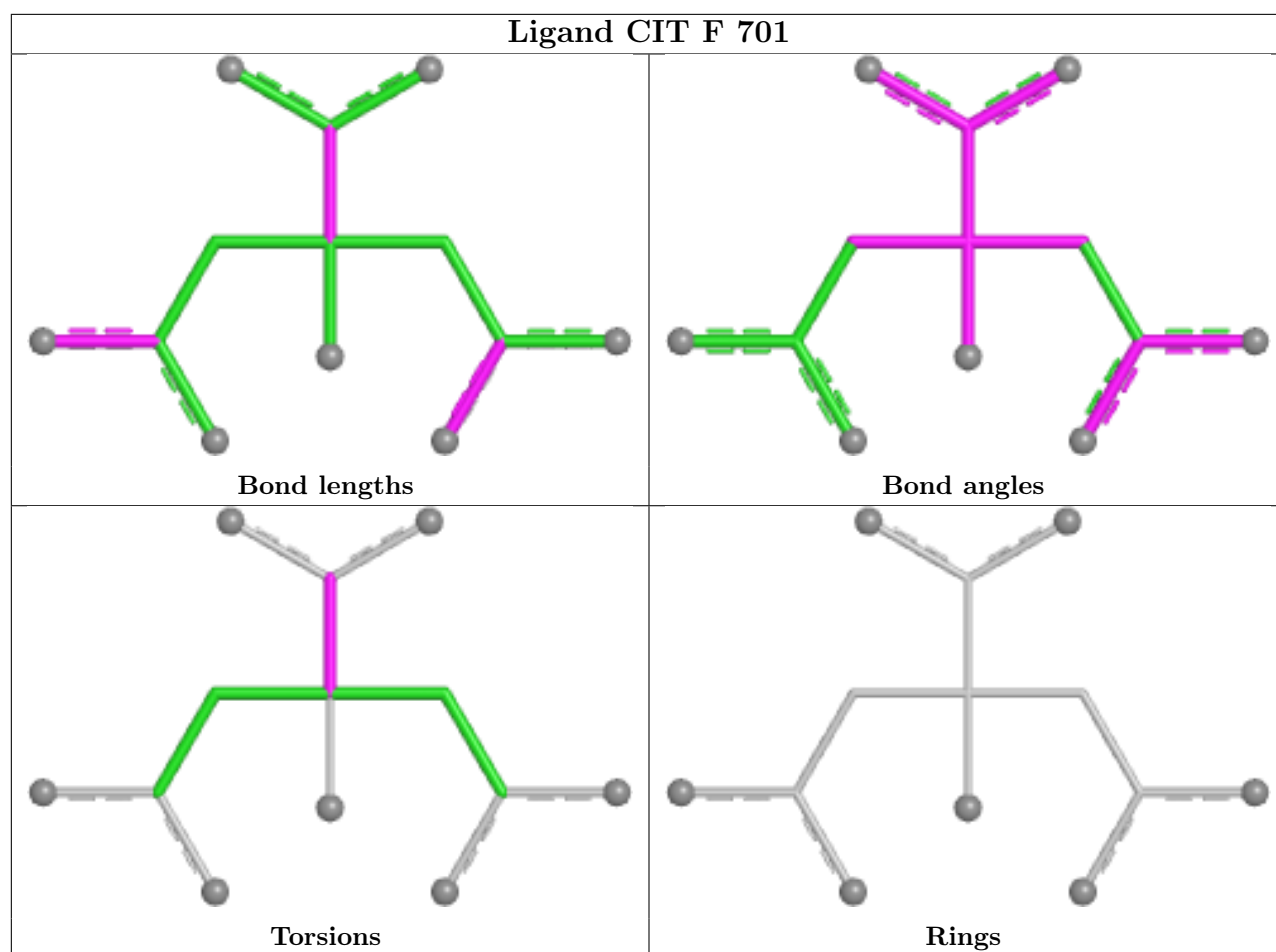
There are no ring outliers.

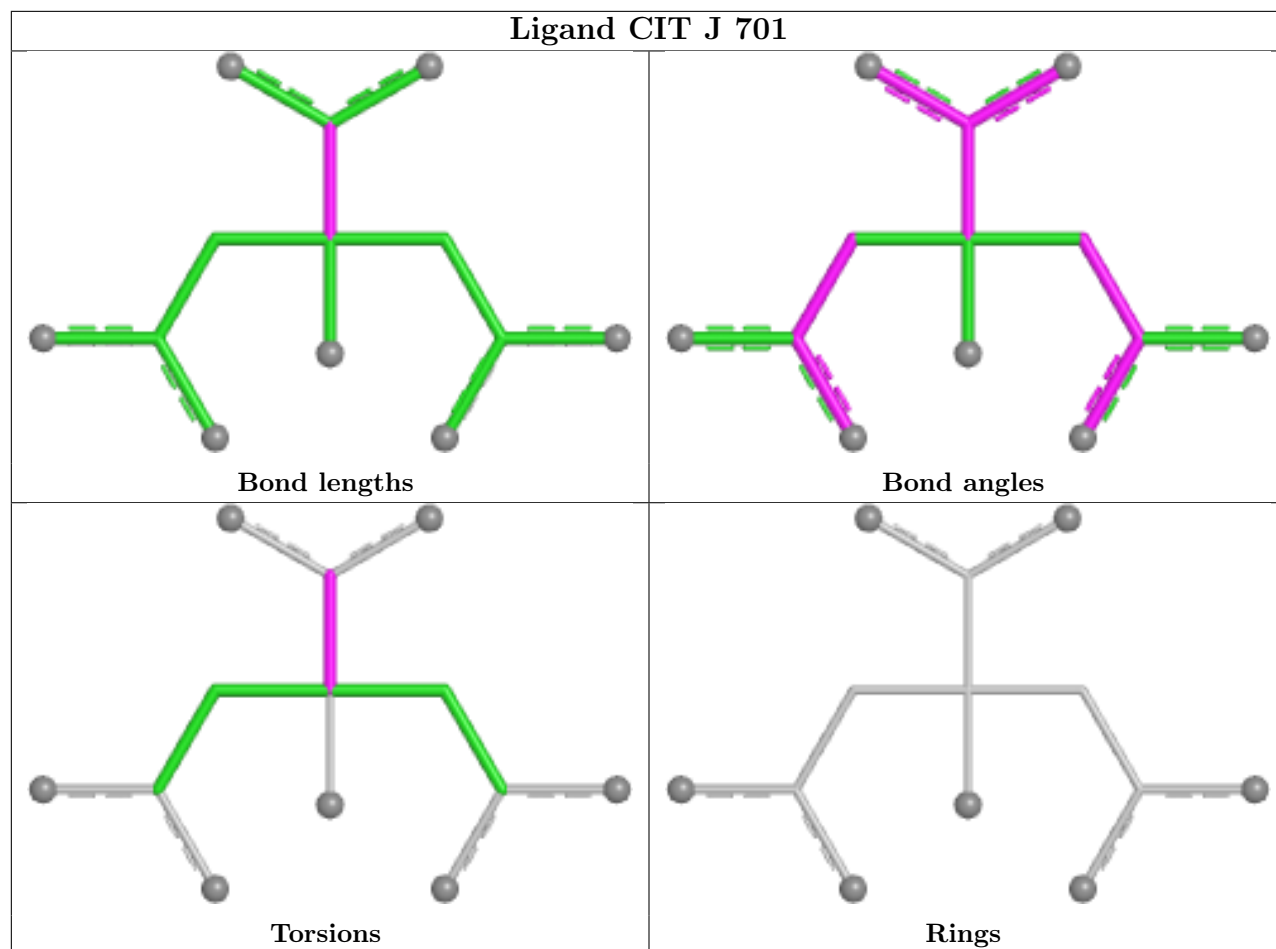
15 monomers are involved in 32 short contacts:

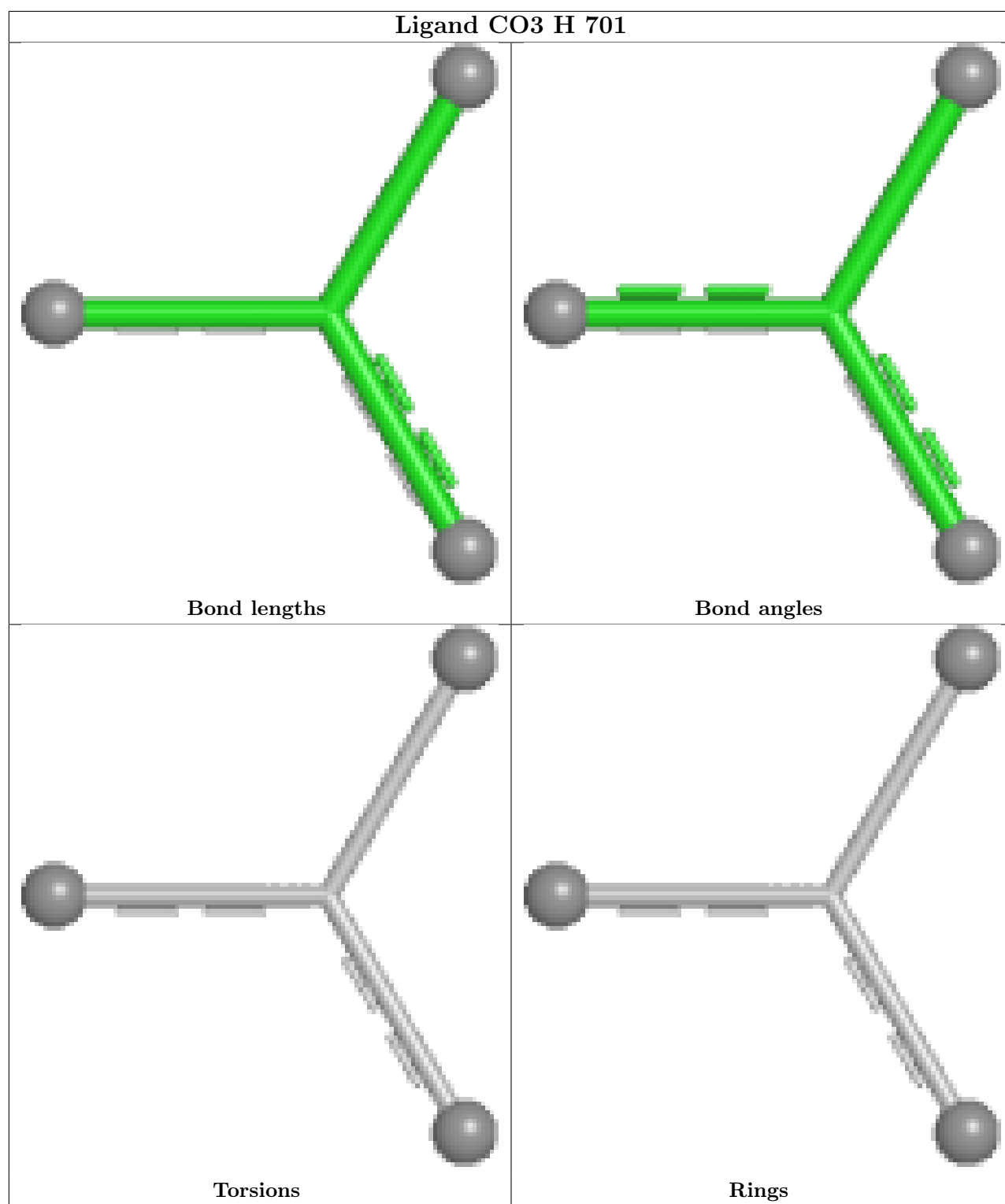
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	CIT	1	0
2	J	701	CIT	3	0
2	E	701	CIT	3	0
2	C	701	CIT	2	0
2	K	703	CIT	1	0
2	L	701	CIT	2	0
2	I	701	CIT	3	0
2	B	701	CIT	5	0
2	B	702	CIT	2	0
2	A	701	CIT	1	0
2	G	701	CIT	2	0
2	D	701	CIT	4	0
2	A	702	CIT	1	0
2	F	702	CIT	1	0
2	H	702	CIT	1	0

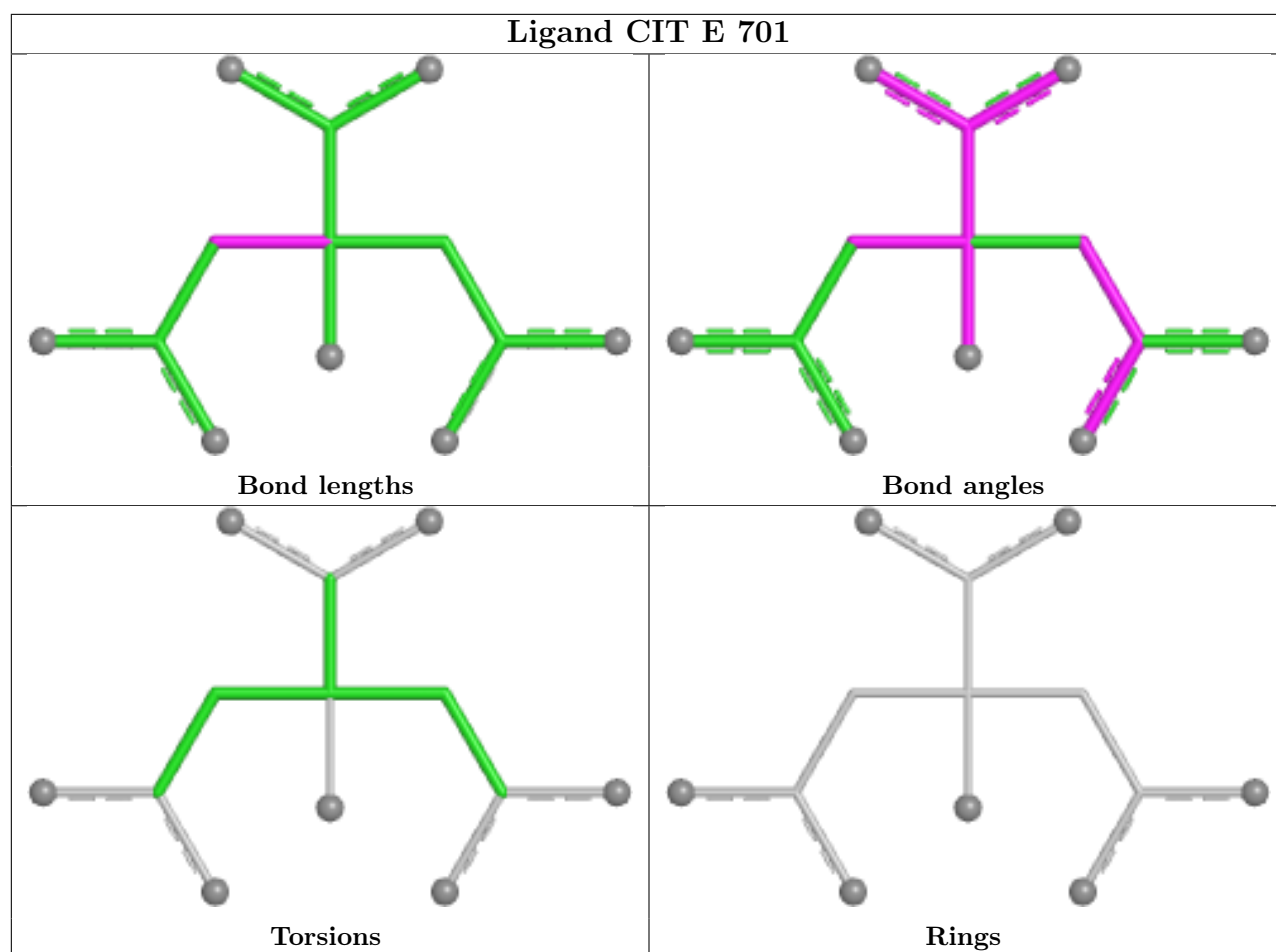
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

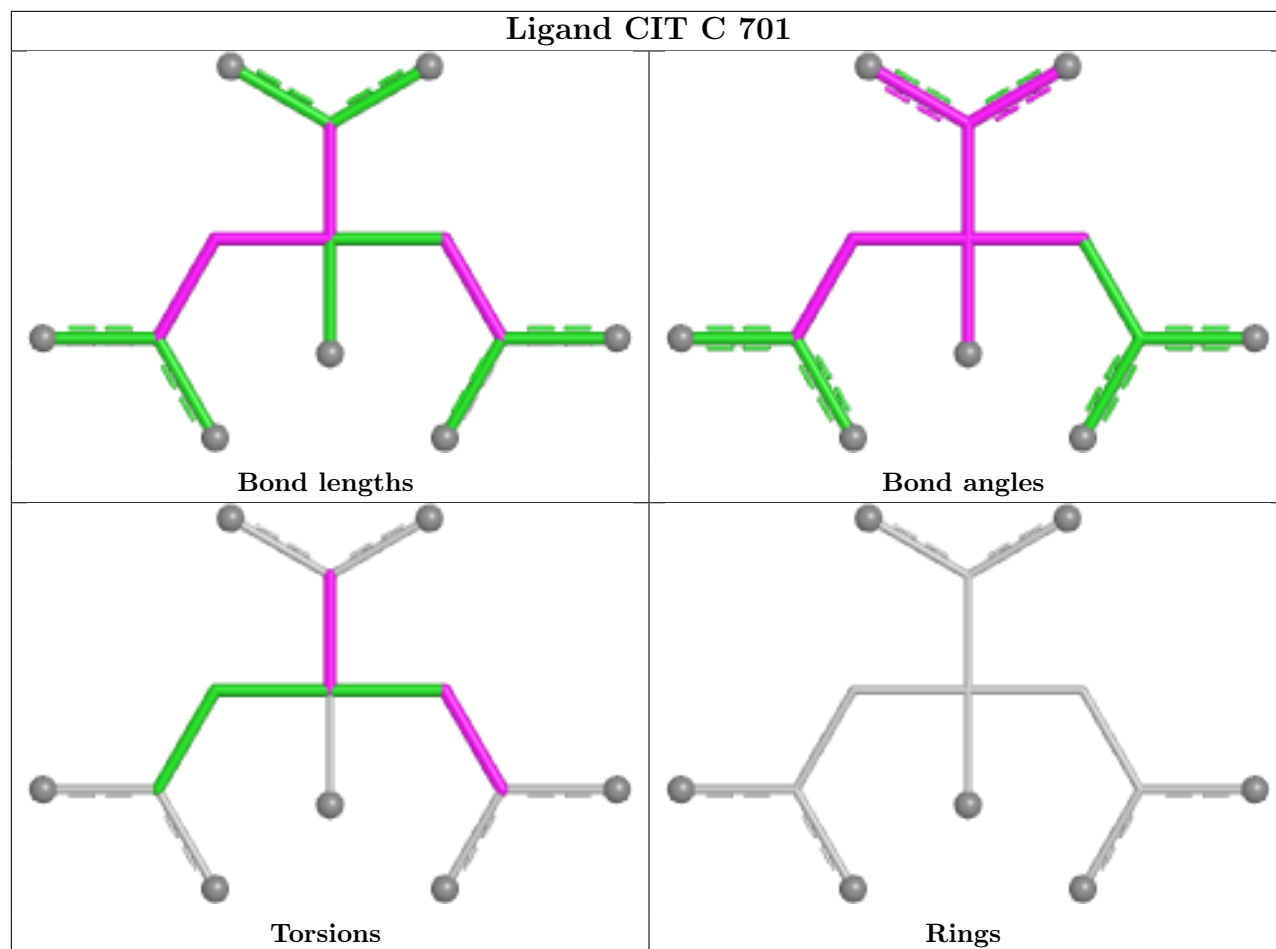


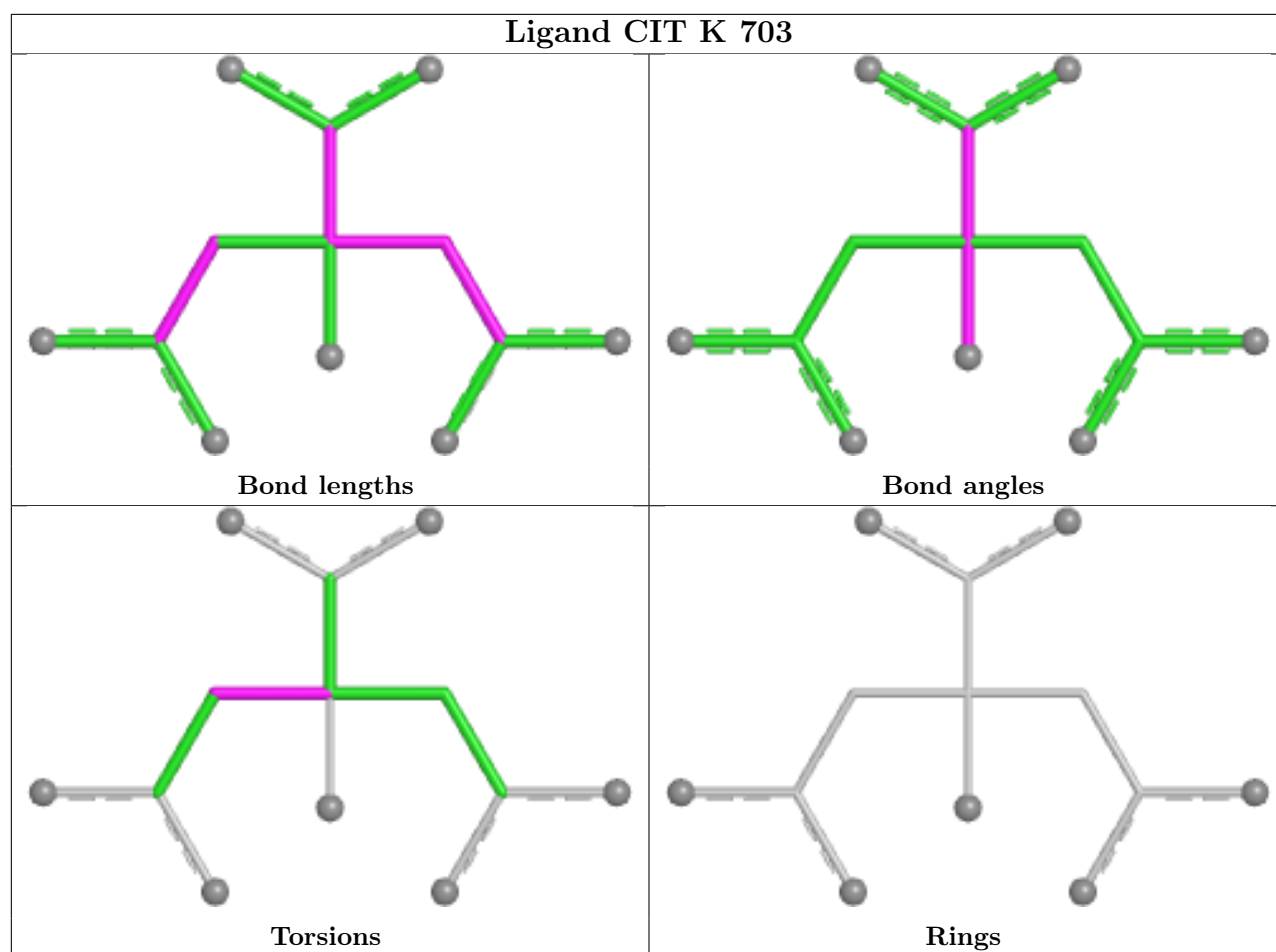


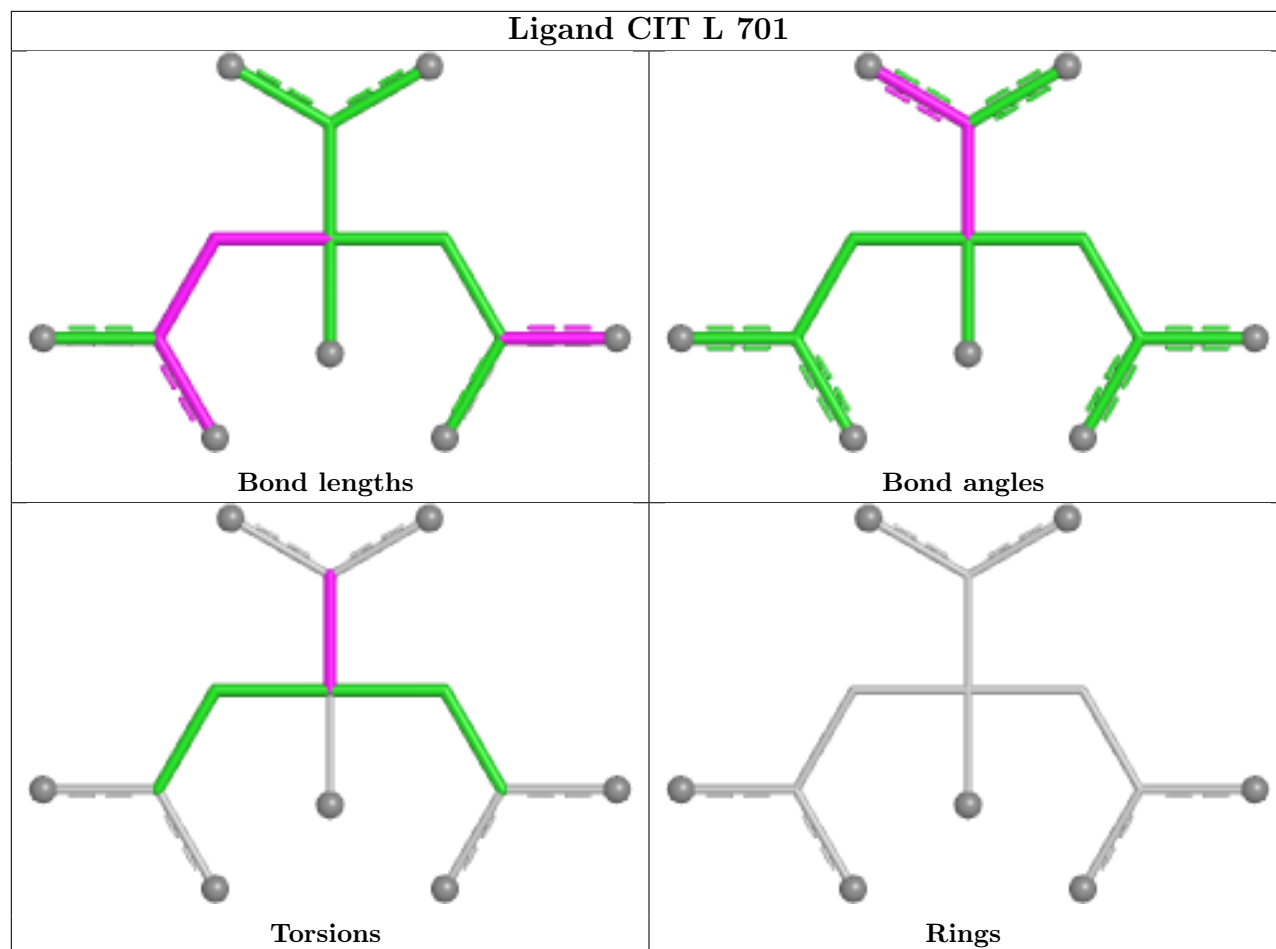


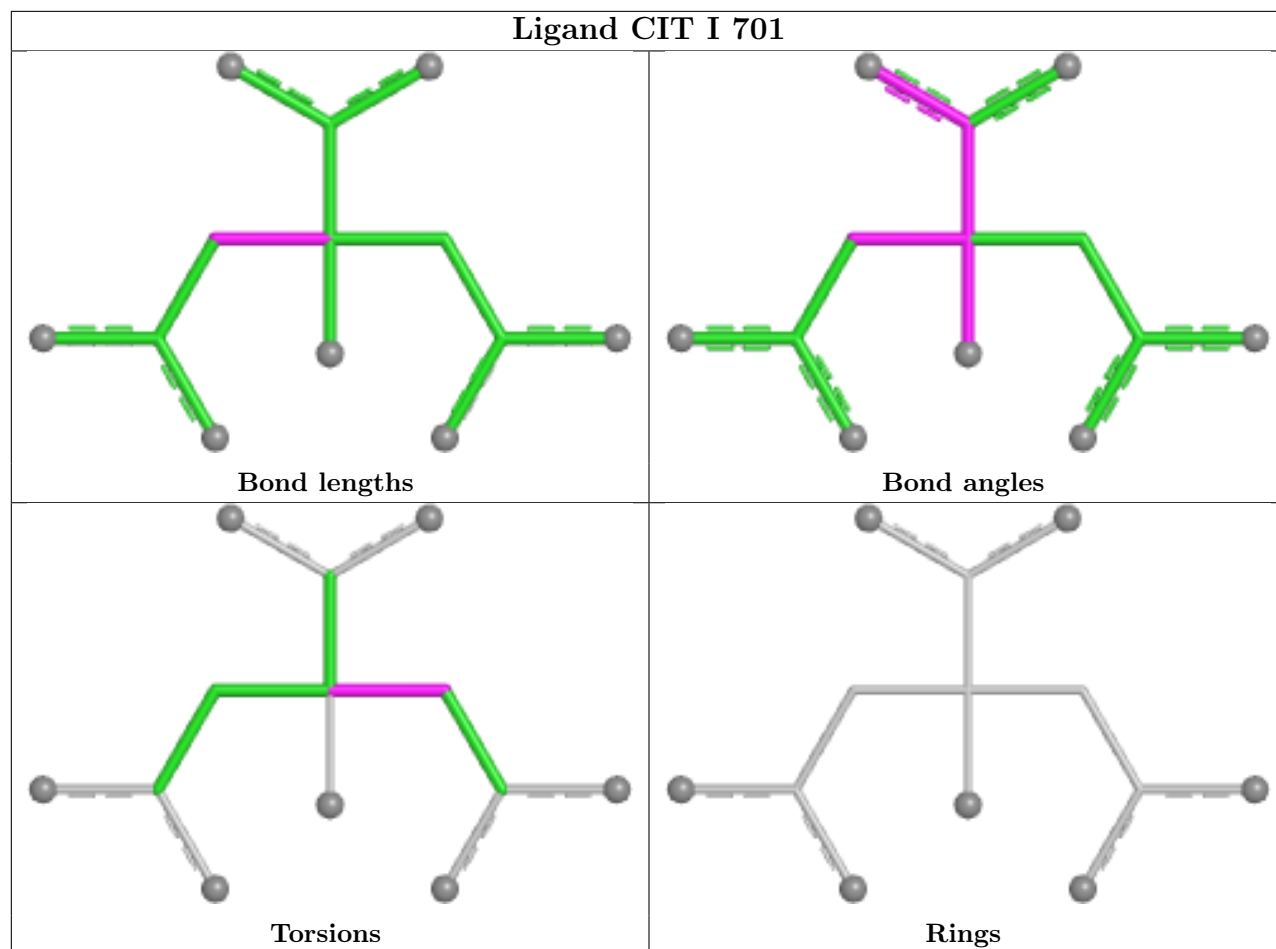


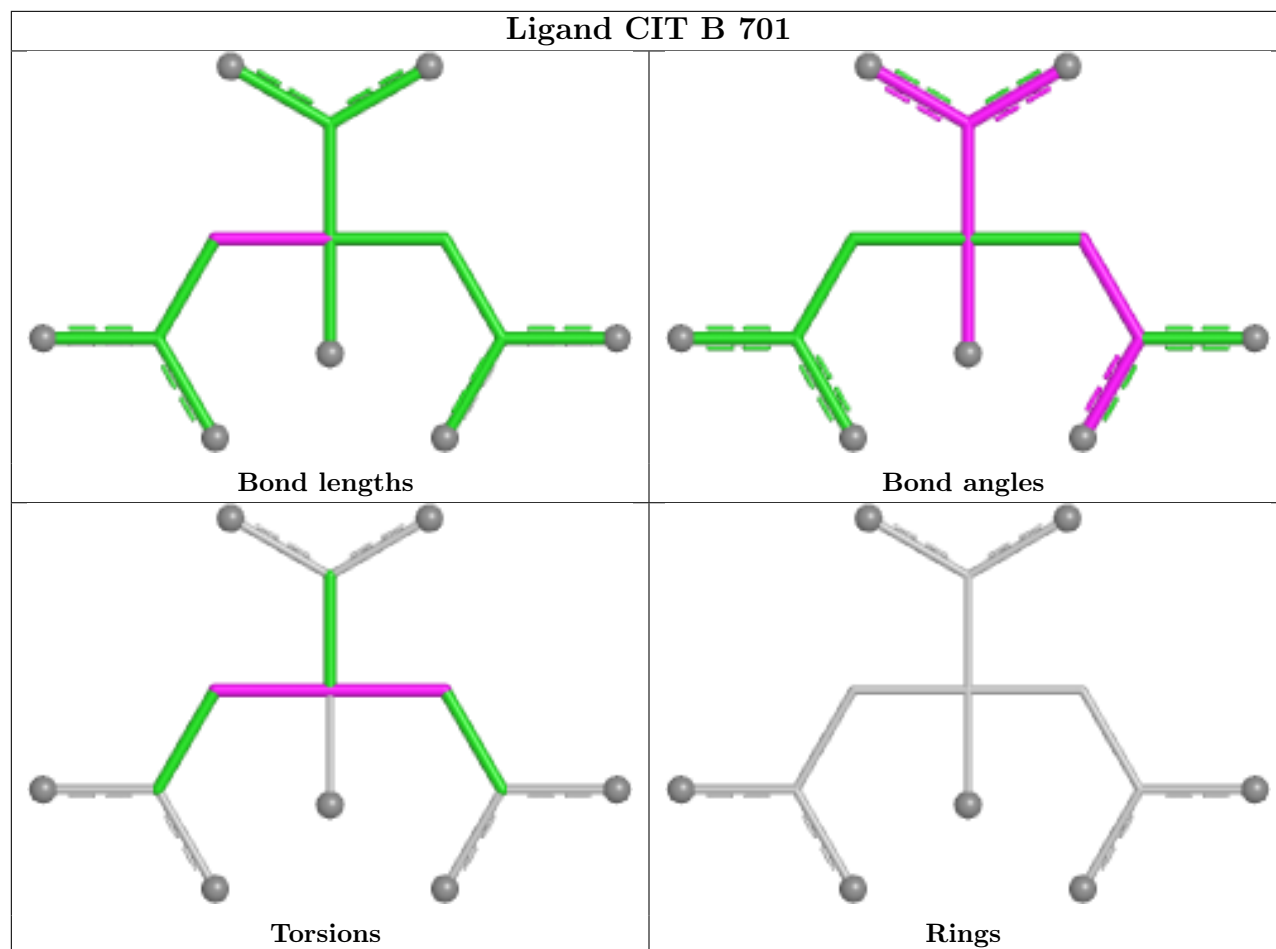


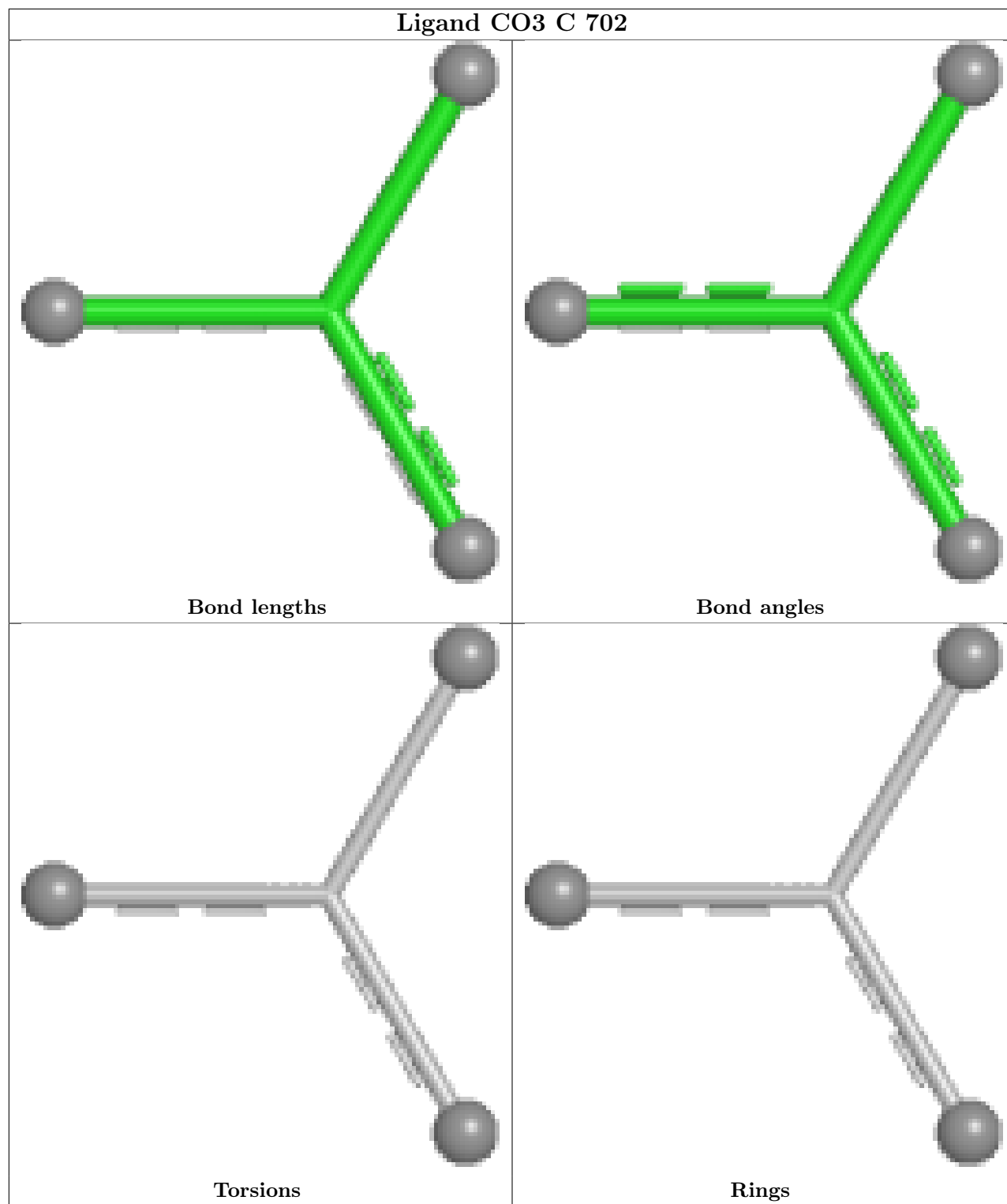


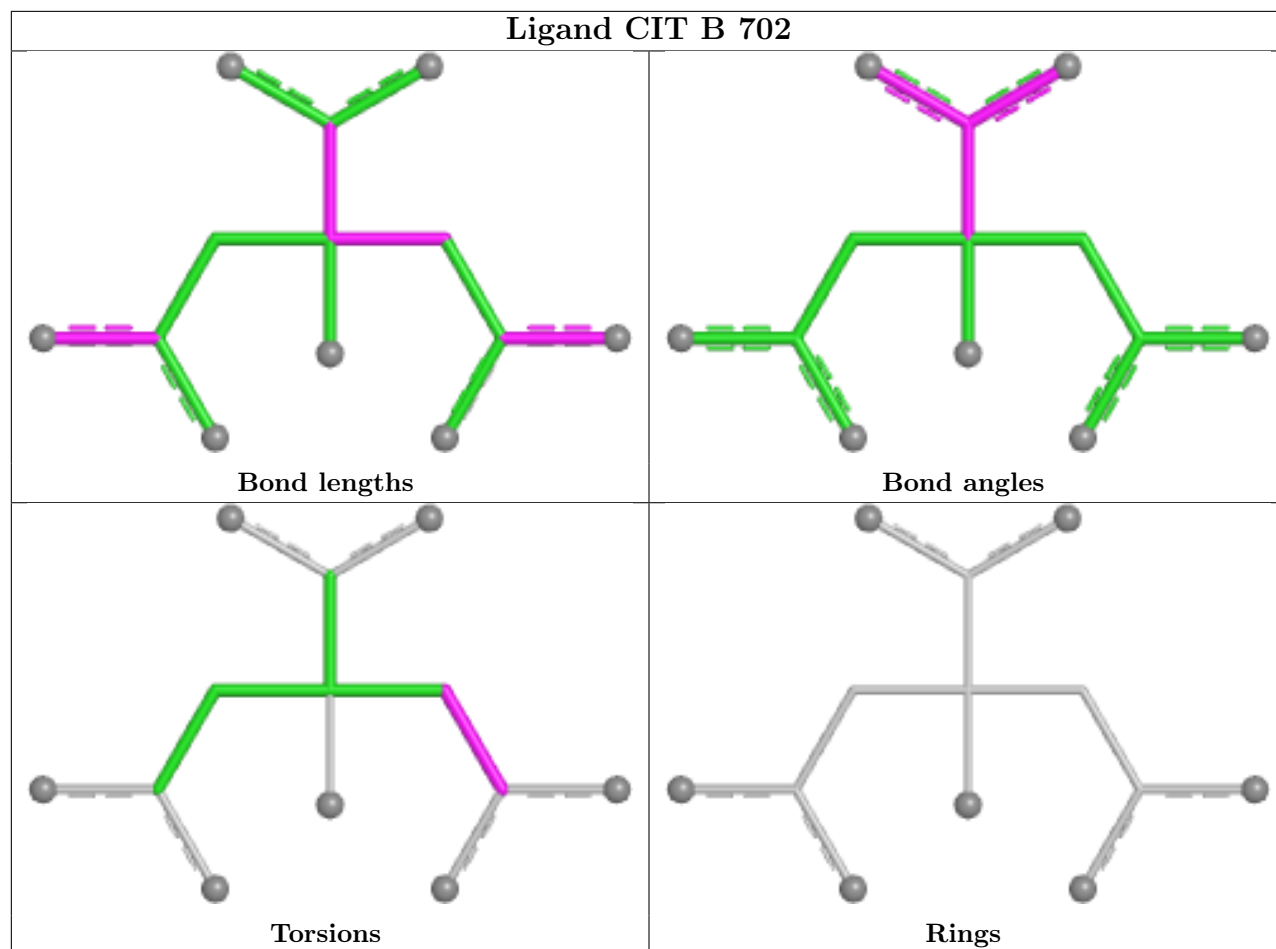


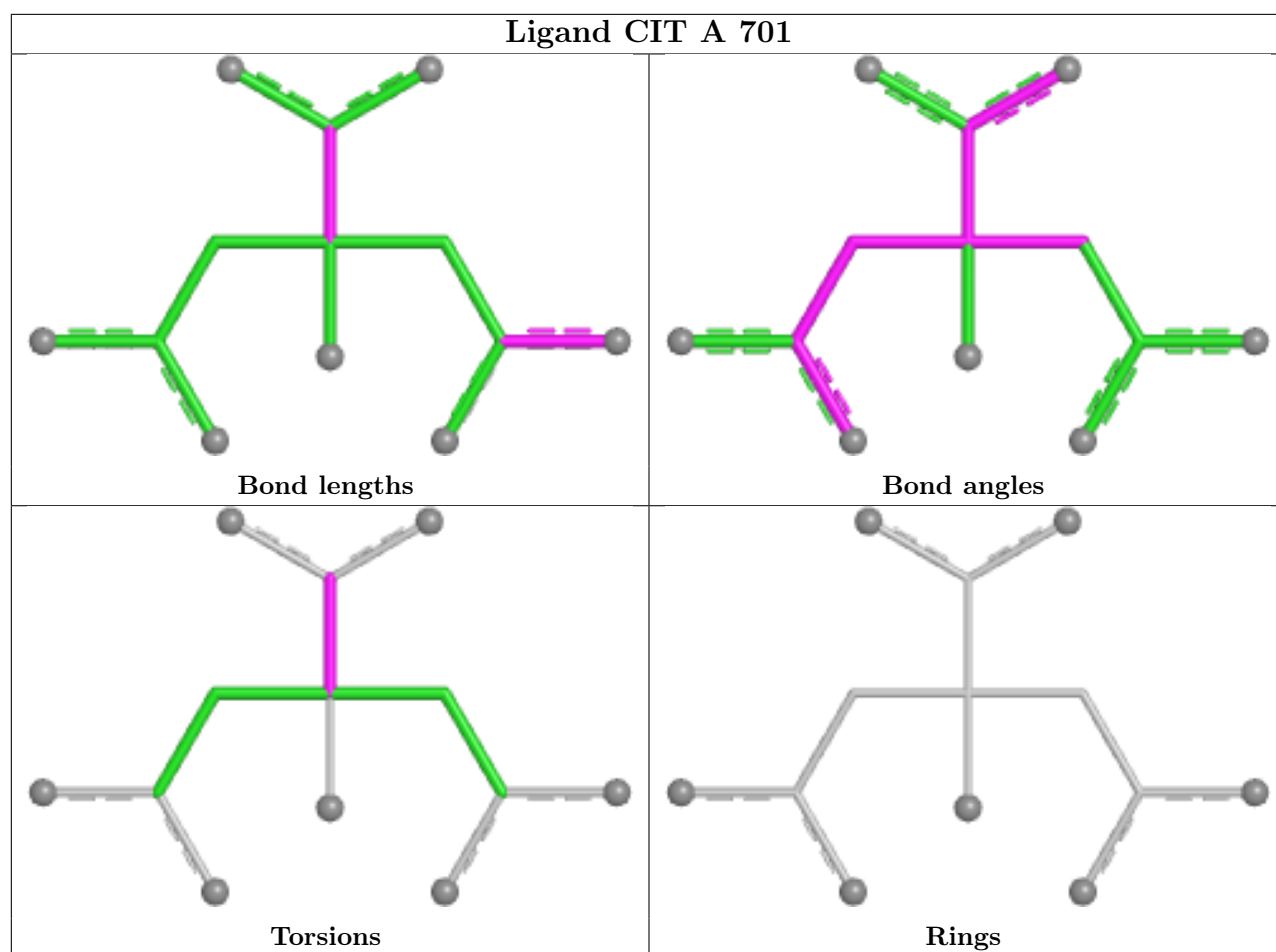


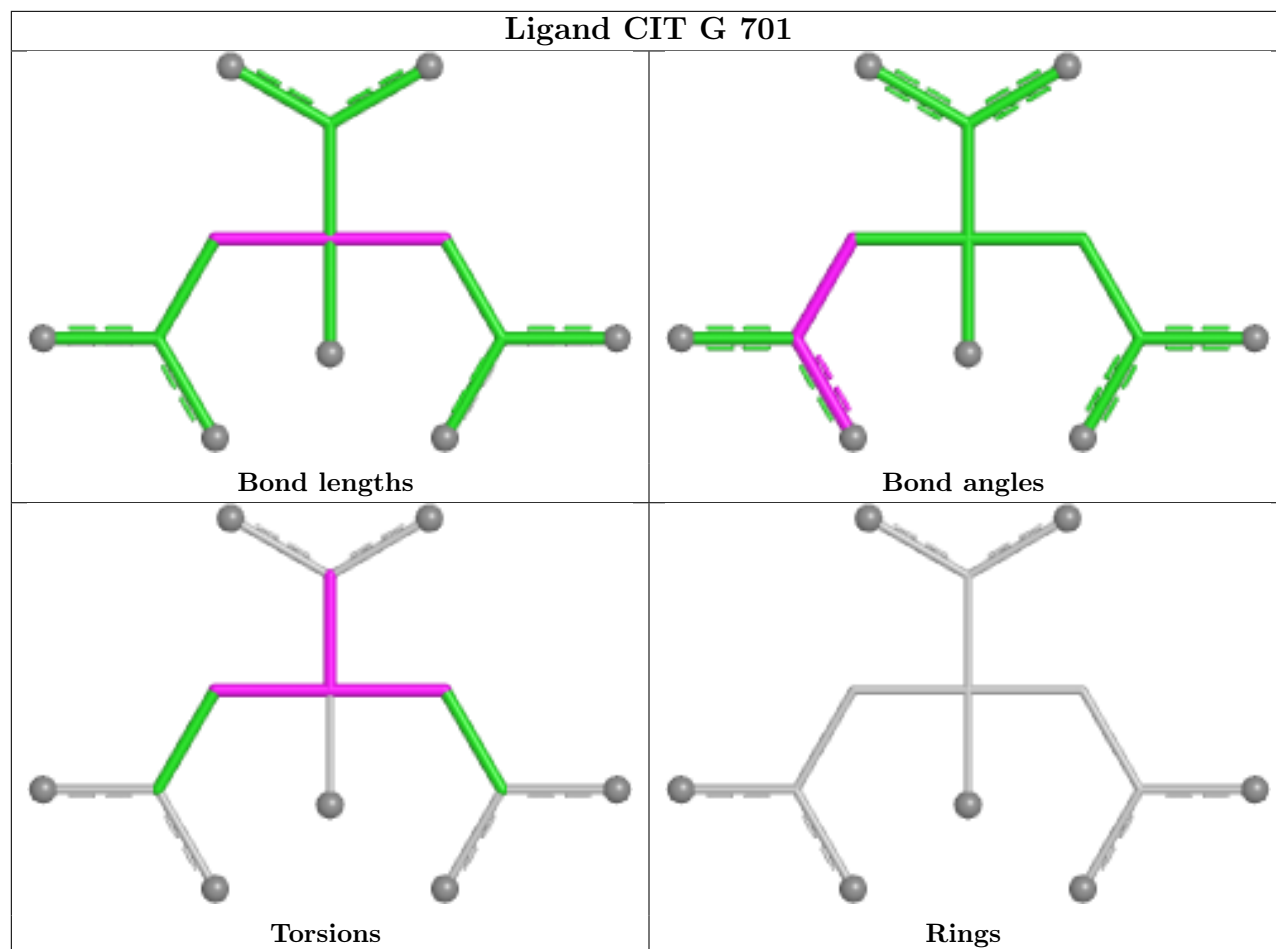


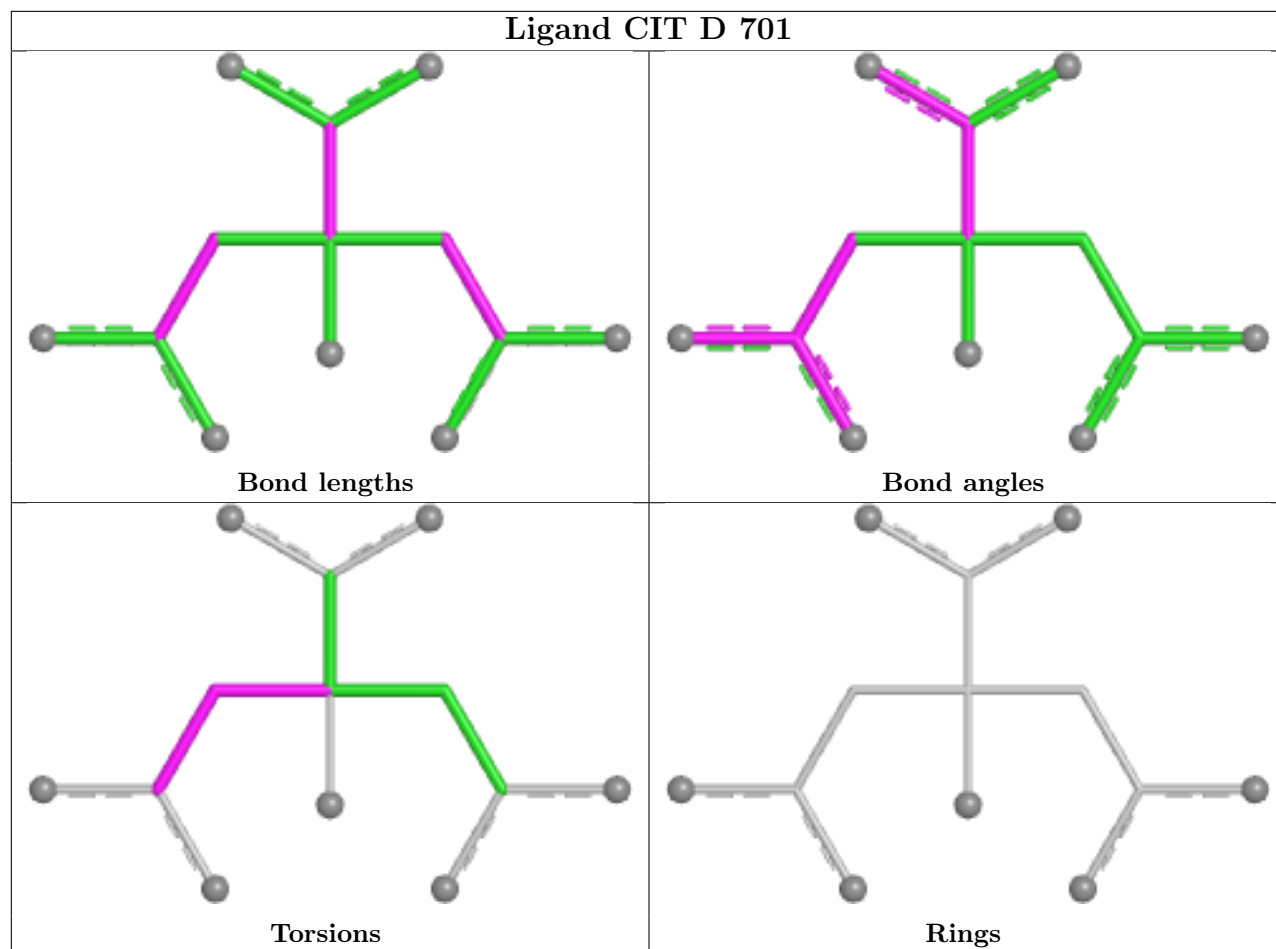


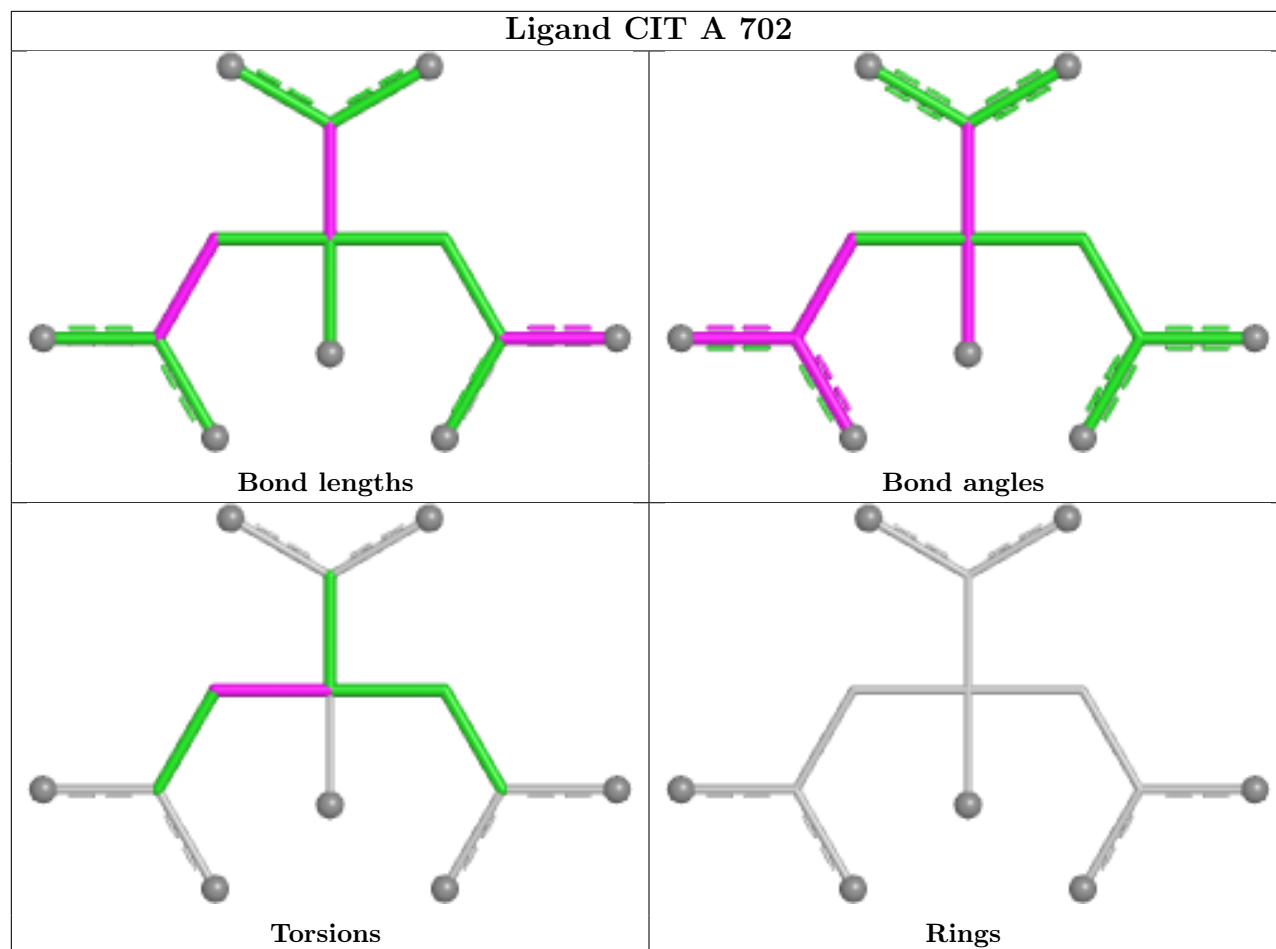


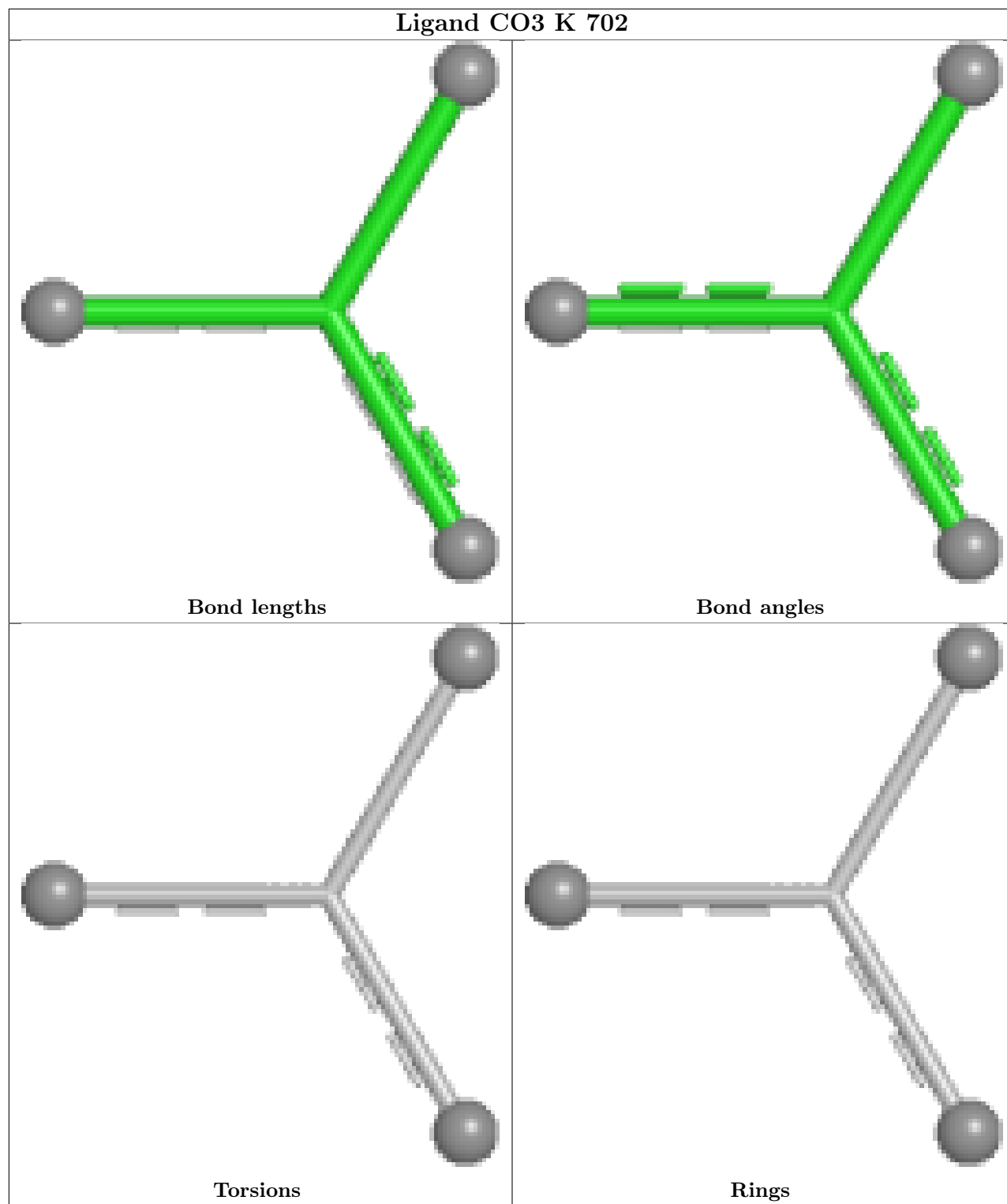


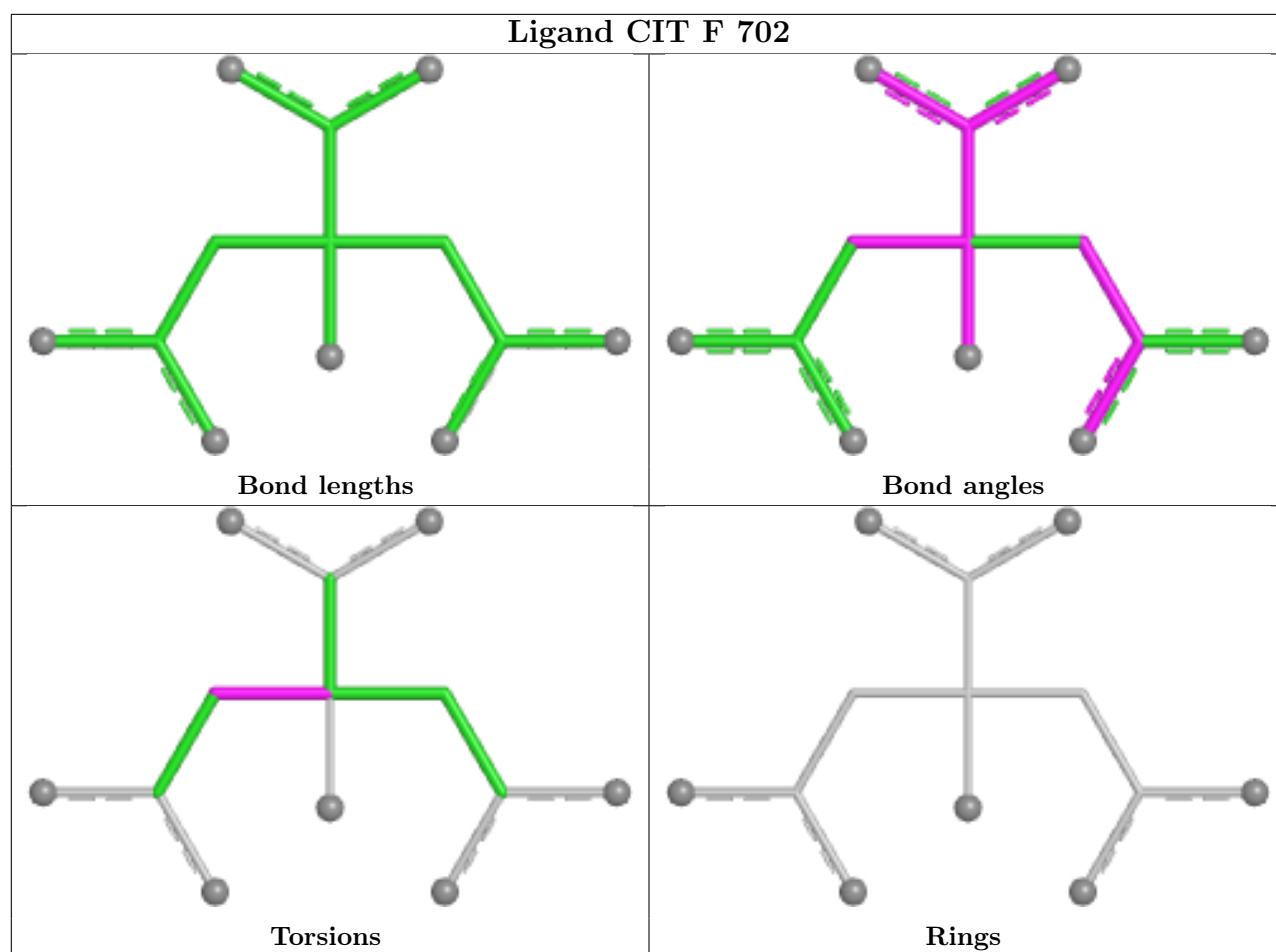


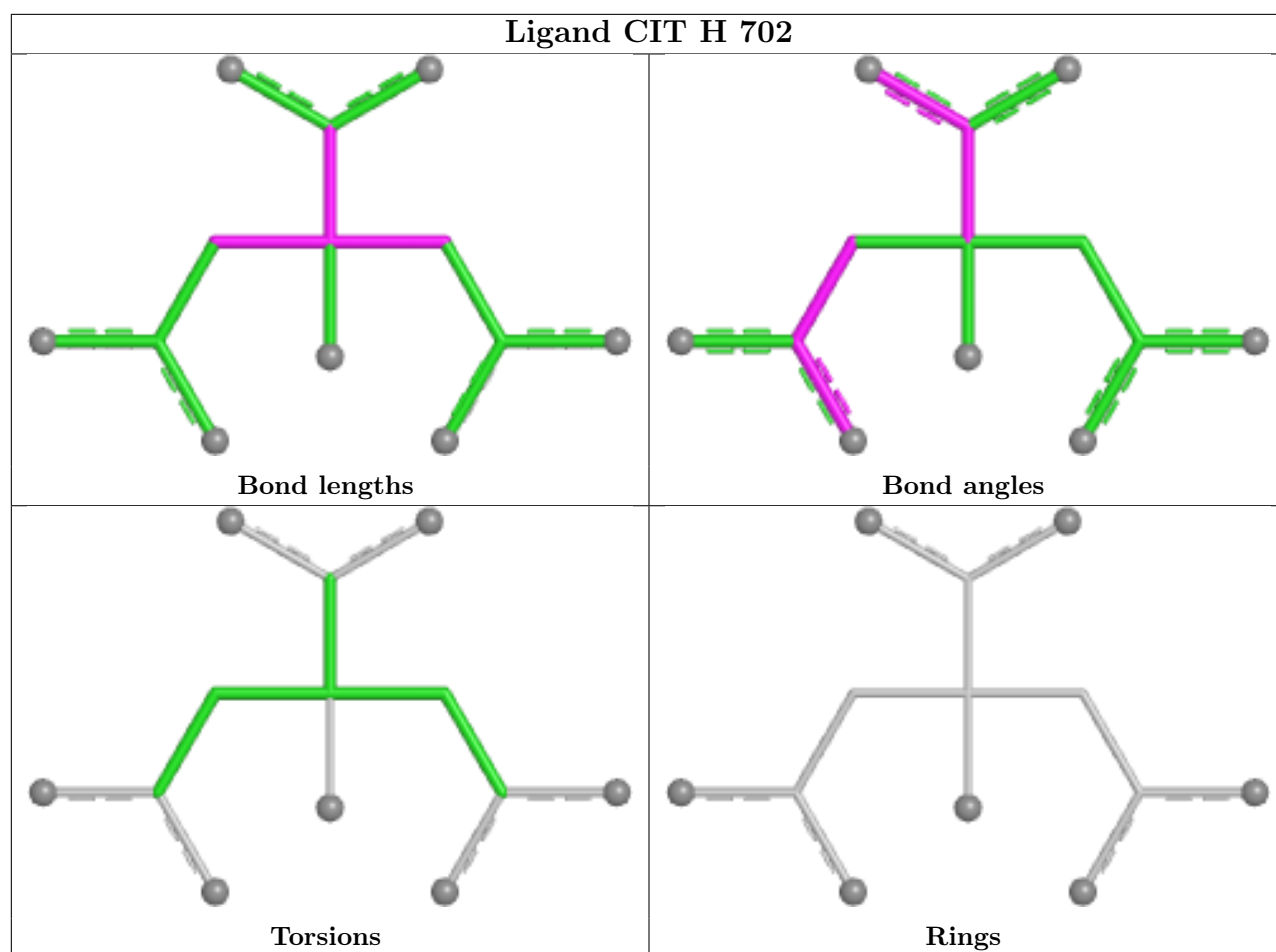












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	642/671 (95%)	-0.53	6 (0%) 81 76	9, 24, 70, 114	0
1	B	644/671 (95%)	-0.51	9 (1%) 73 67	9, 24, 74, 129	0
1	C	644/671 (95%)	-0.62	3 (0%) 87 83	8, 21, 48, 99	0
1	D	643/671 (95%)	-0.47	14 (2%) 62 55	12, 26, 65, 123	0
1	E	643/671 (95%)	-0.44	13 (2%) 65 58	12, 27, 69, 123	0
1	F	644/671 (95%)	-0.52	14 (2%) 62 55	8, 22, 62, 122	0
1	G	642/671 (95%)	-0.48	1 (0%) 91 89	9, 29, 53, 86	0
1	H	646/671 (96%)	-0.50	2 (0%) 90 88	10, 27, 57, 89	0
1	I	644/671 (95%)	-0.32	4 (0%) 85 81	12, 32, 64, 128	0
1	J	642/671 (95%)	0.06	23 (3%) 46 39	13, 39, 88, 112	0
1	K	642/671 (95%)	-0.09	20 (3%) 51 44	12, 34, 84, 109	0
1	L	642/671 (95%)	0.20	24 (3%) 45 38	19, 40, 88, 111	0
All	All	7718/8052 (95%)	-0.35	133 (1%) 69 62	8, 28, 75, 129	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	9	PRO	6.4
1	F	35	GLY	6.3
1	D	34	LEU	5.4
1	C	9	PRO	5.3
1	K	35	GLY	5.2
1	E	35	GLY	5.1
1	D	35	GLY	4.9
1	F	36	SER	4.9
1	F	34	LEU	4.8
1	D	36	SER	4.6
1	B	9	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	L	35	GLY	4.6
1	J	35	GLY	4.6
1	D	14	SER	4.4
1	J	34	LEU	4.3
1	F	9	PRO	4.1
1	F	14	SER	4.0
1	I	9	PRO	3.9
1	E	34	LEU	3.9
1	E	36	SER	3.8
1	L	34	LEU	3.8
1	E	623	PRO	3.7
1	F	12	VAL	3.6
1	K	36	SER	3.5
1	F	37	ALA	3.5
1	L	651	LEU	3.4
1	E	30	LYS	3.3
1	E	622	VAL	3.3
1	J	36	SER	3.3
1	K	566	VAL	3.3
1	E	47	ALA	3.2
1	E	14	SER	3.2
1	F	8	ALA	3.2
1	L	10	GLU	3.1
1	L	571	ALA	3.1
1	J	27	VAL	3.1
1	D	9	PRO	3.0
1	L	642	VAL	3.0
1	F	16	LEU	3.0
1	K	34	LEU	3.0
1	B	10	GLU	3.0
1	J	37	ALA	3.0
1	L	27	VAL	3.0
1	B	16	LEU	2.9
1	E	624	THR	2.9
1	L	570	VAL	2.9
1	K	623	PRO	2.9
1	A	27	VAL	2.9
1	D	16	LEU	2.9
1	A	30	LYS	2.8
1	E	37	ALA	2.8
1	J	570	VAL	2.8
1	J	16	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	16	LEU	2.8
1	J	571	ALA	2.8
1	G	37	ALA	2.7
1	D	33	LEU	2.7
1	J	536	LEU	2.7
1	A	11	ARG	2.7
1	F	46	THR	2.7
1	J	47	ALA	2.7
1	J	642	VAL	2.7
1	K	603	THR	2.6
1	B	34	LEU	2.6
1	J	623	PRO	2.6
1	L	567	ALA	2.6
1	K	16	LEU	2.6
1	B	47	ALA	2.6
1	L	40	ASP	2.5
1	L	30	LYS	2.5
1	A	28	GLN	2.5
1	B	42	THR	2.5
1	D	40	ASP	2.5
1	L	39	GLY	2.5
1	L	66	LYS	2.4
1	K	651	LEU	2.4
1	D	623	PRO	2.4
1	D	12	VAL	2.4
1	K	27	VAL	2.4
1	C	8	ALA	2.4
1	F	13	PHE	2.4
1	F	33	LEU	2.4
1	B	23	PRO	2.4
1	A	622	VAL	2.4
1	D	37	ALA	2.4
1	K	567	ALA	2.4
1	J	14	SER	2.3
1	J	33	LEU	2.3
1	D	345	ASP	2.3
1	C	623	PRO	2.3
1	L	622	VAL	2.3
1	L	639	ALA	2.3
1	L	575	THR	2.3
1	H	30	LYS	2.3
1	J	12	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	22	TYR	2.3
1	K	10	GLU	2.3
1	J	39	GLY	2.3
1	J	610	ALA	2.2
1	K	639	ALA	2.2
1	J	30	LYS	2.2
1	F	40	ASP	2.2
1	H	622	VAL	2.2
1	F	23	PRO	2.2
1	J	576	VAL	2.2
1	J	634	ILE	2.2
1	L	604	PHE	2.2
1	B	11	ARG	2.2
1	K	559	ASP	2.2
1	J	23	PRO	2.2
1	I	27	VAL	2.2
1	E	12	VAL	2.1
1	K	498	ASP	2.1
1	K	604	PHE	2.1
1	L	13	PHE	2.1
1	J	11	ARG	2.1
1	L	635	ARG	2.1
1	J	651	LEU	2.1
1	K	624	THR	2.1
1	L	612	THR	2.1
1	L	536	LEU	2.1
1	I	35	GLY	2.1
1	A	14	SER	2.1
1	K	14	SER	2.1
1	K	608	ALA	2.1
1	K	23	PRO	2.1
1	L	636	SER	2.0
1	E	620	GLN	2.0
1	D	622	VAL	2.0
1	D	47	ALA	2.0
1	L	14	SER	2.0
1	I	45	THR	2.0
1	B	12	VAL	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

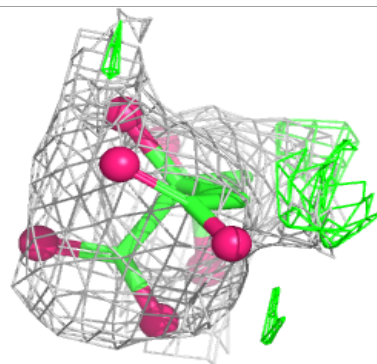
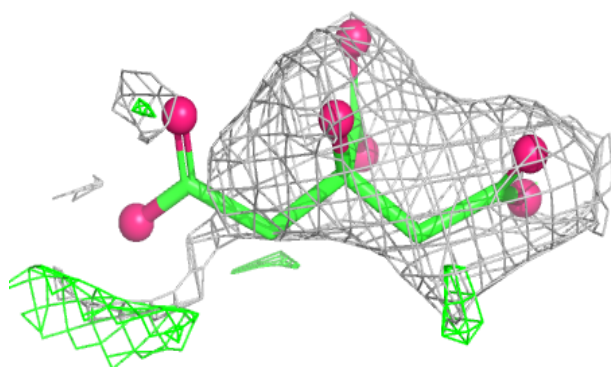
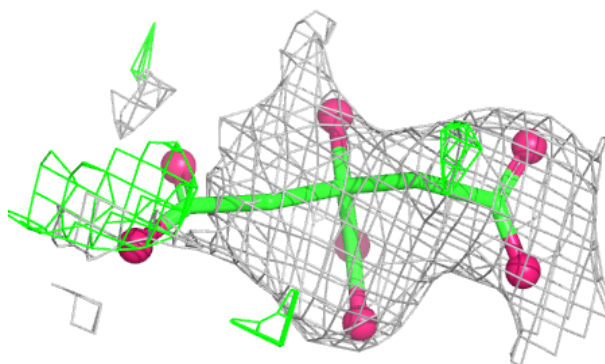
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	CIT	H	702	13/13	0.81	0.17	65,69,89,91	0
2	CIT	K	703	13/13	0.81	0.19	64,71,77,79	0
2	CIT	J	701	13/13	0.83	0.12	59,67,73,73	0
2	CIT	F	702	13/13	0.87	0.14	61,66,79,80	0
2	CIT	C	701	13/13	0.87	0.15	57,67,71,74	0
2	CIT	I	701	13/13	0.88	0.11	38,53,55,56	0
3	CO3	C	702	4/4	0.88	0.12	25,32,34,34	0
2	CIT	A	701	13/13	0.89	0.12	53,59,68,71	0
2	CIT	F	701	13/13	0.89	0.15	42,47,55,61	0
2	CIT	K	701	13/13	0.89	0.17	20,28,32,37	13
2	CIT	B	701	13/13	0.89	0.11	52,63,71,72	0
2	CIT	B	702	13/13	0.89	0.14	48,51,60,61	0
2	CIT	A	702	13/13	0.90	0.18	28,36,39,41	13
2	CIT	L	701	13/13	0.91	0.11	41,60,64,70	0
2	CIT	D	701	13/13	0.92	0.11	41,48,51,52	0
3	CO3	K	702	4/4	0.92	0.11	28,33,36,37	0
2	CIT	E	701	13/13	0.93	0.09	36,43,47,52	0
2	CIT	G	701	13/13	0.93	0.10	43,52,63,74	0
3	CO3	H	701	4/4	0.94	0.09	31,42,42,45	0

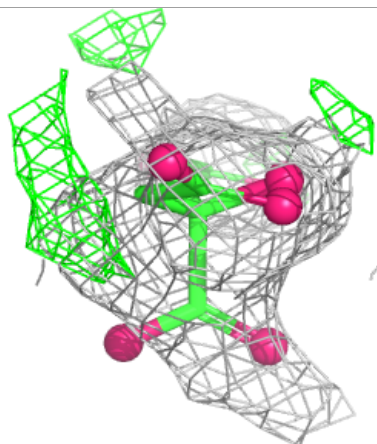
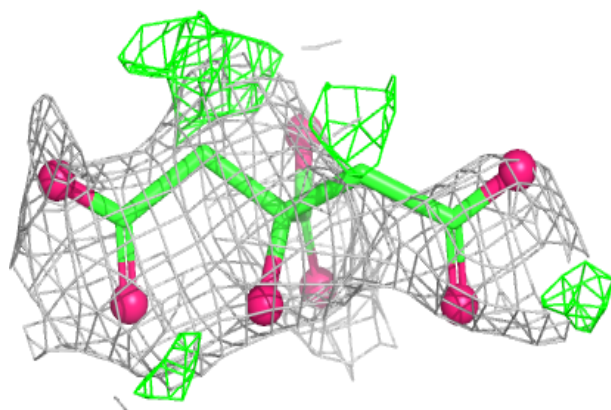
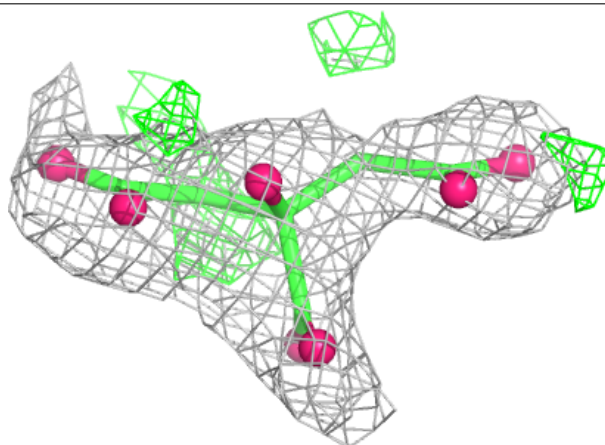
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CIT H 702:

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

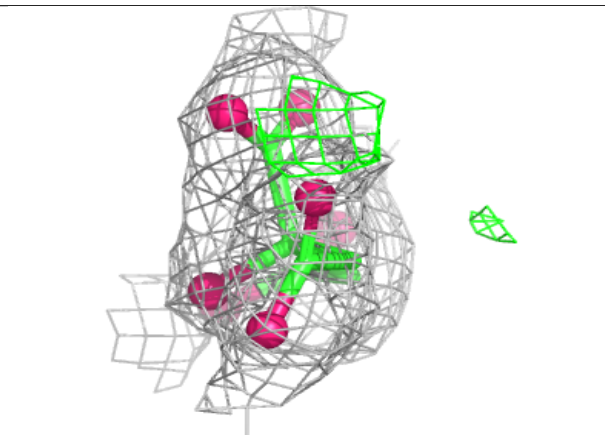
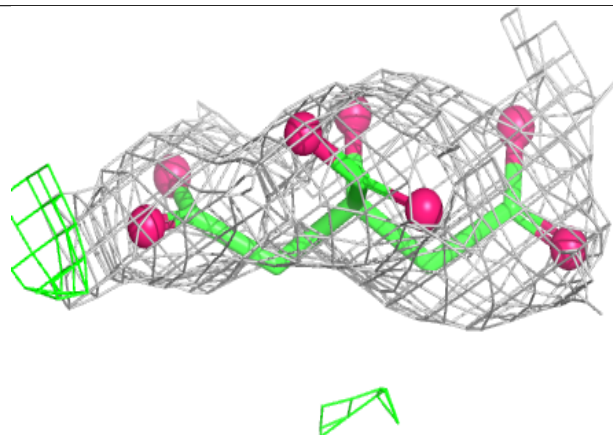
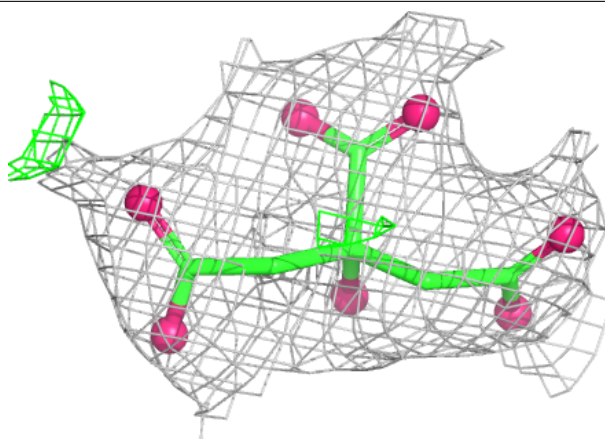
**Electron density around CIT K 703:**

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

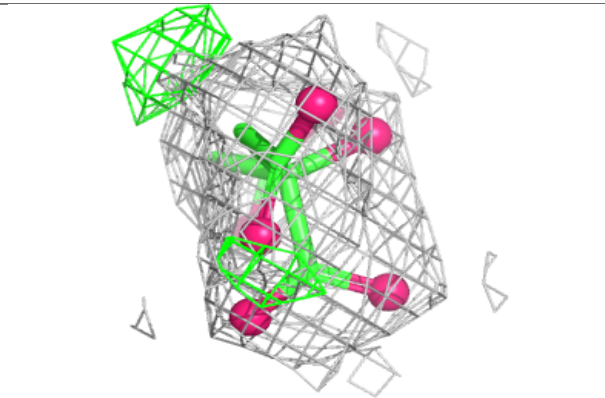
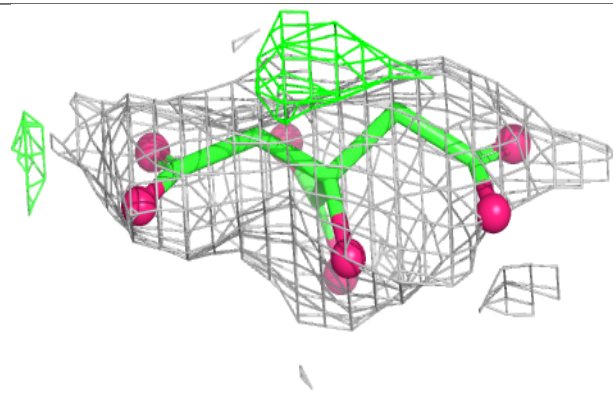
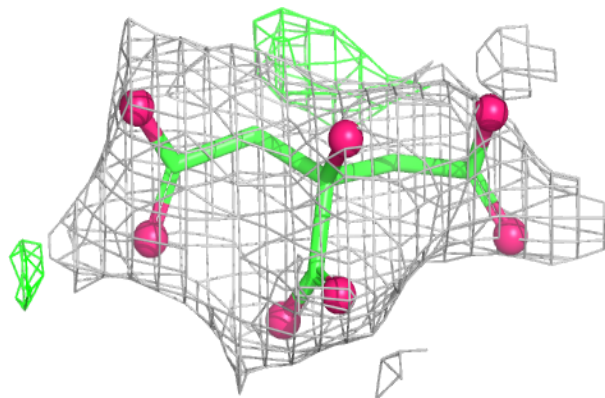


Electron density around CIT J 701:

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

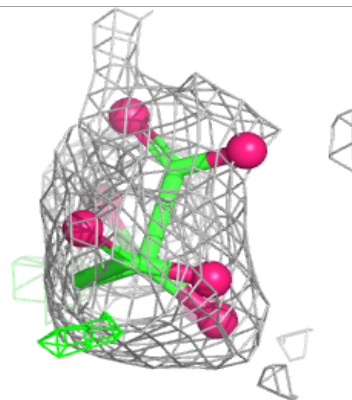
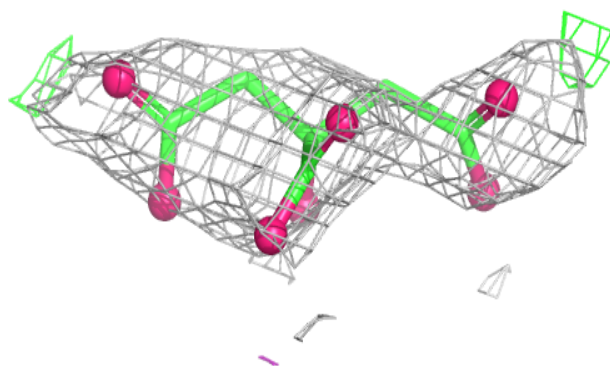
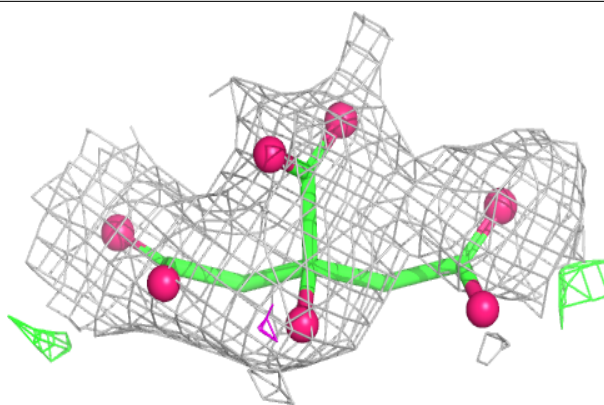
**Electron density around CIT F 702:**

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

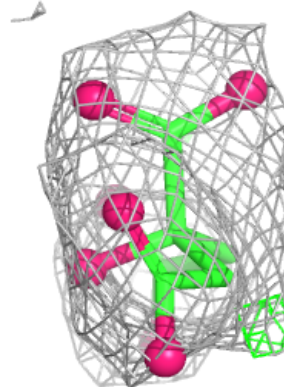
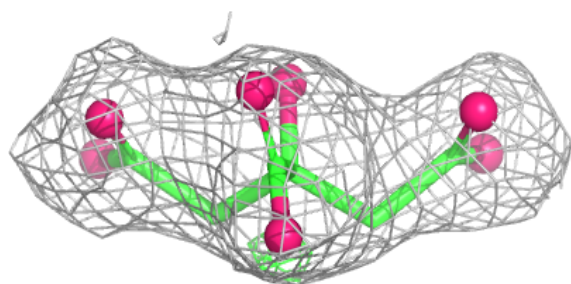
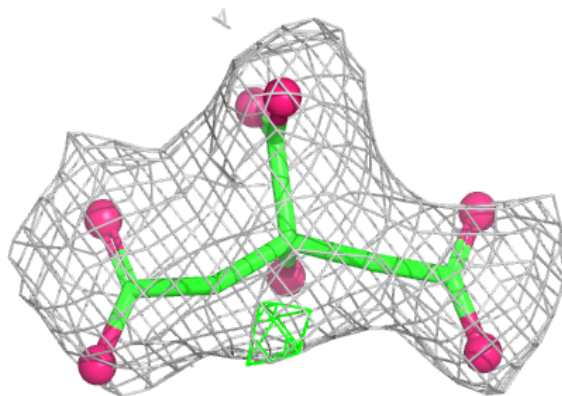


Electron density around CIT C 701:

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

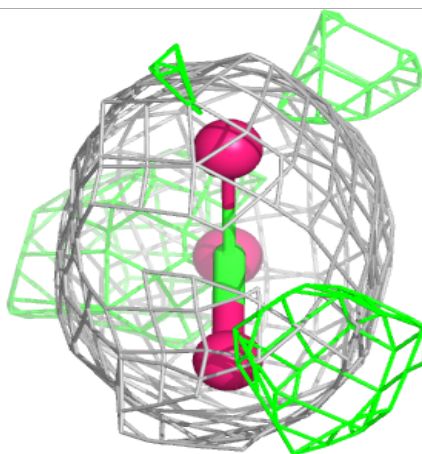
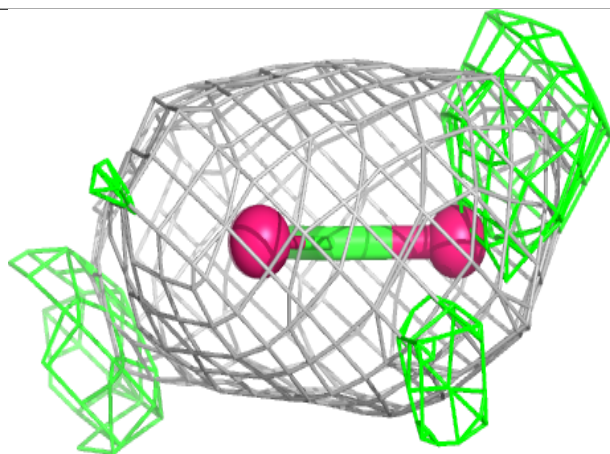
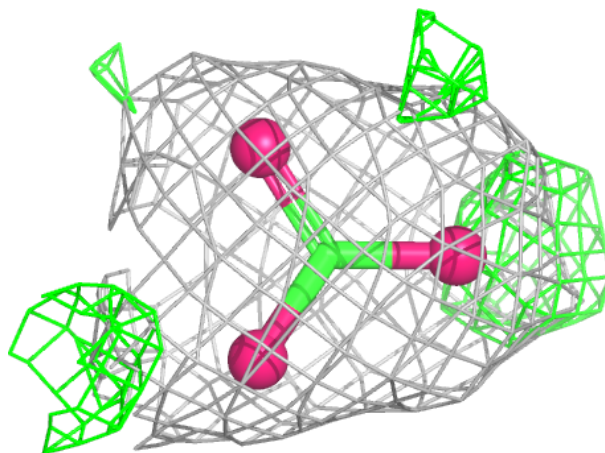
**Electron density around CIT I 701:**

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



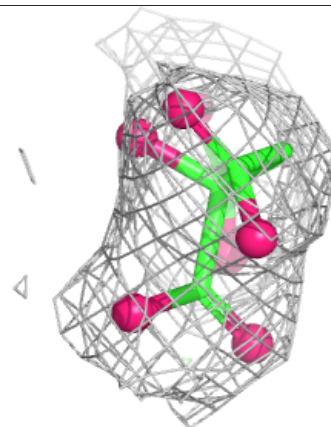
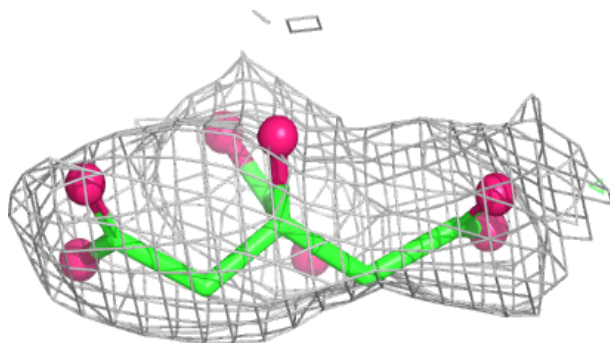
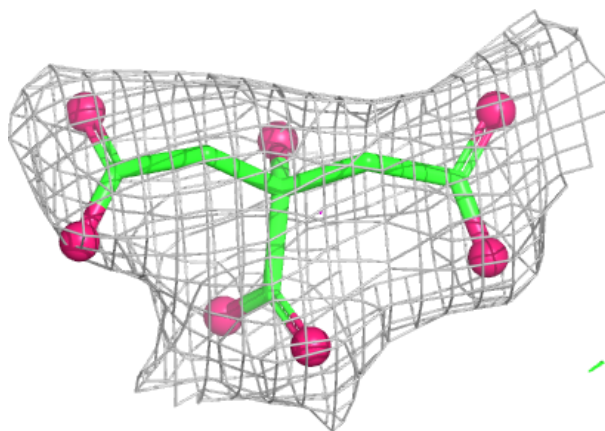
Electron density around CO3 C 702:

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

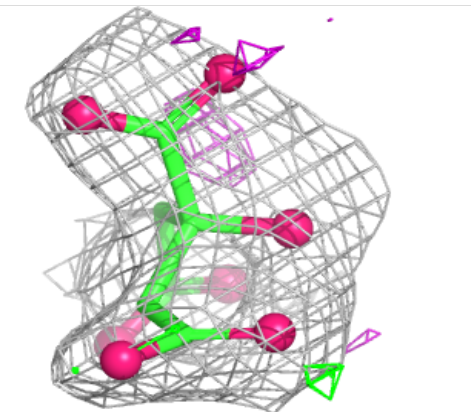
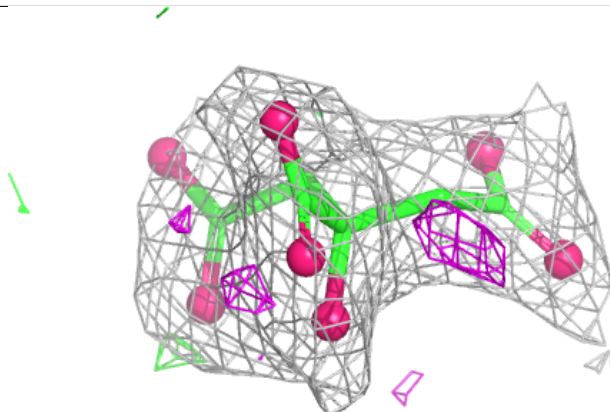
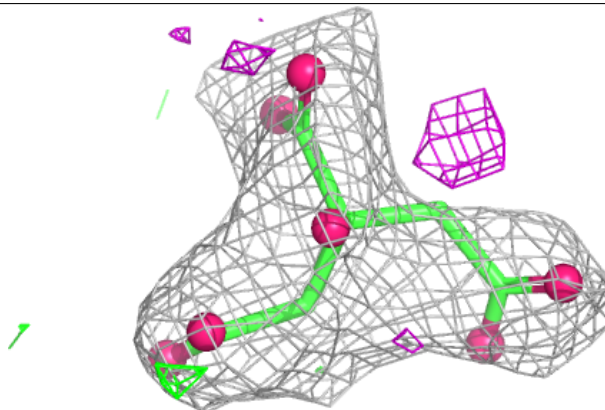


Electron density around CIT A 701:

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

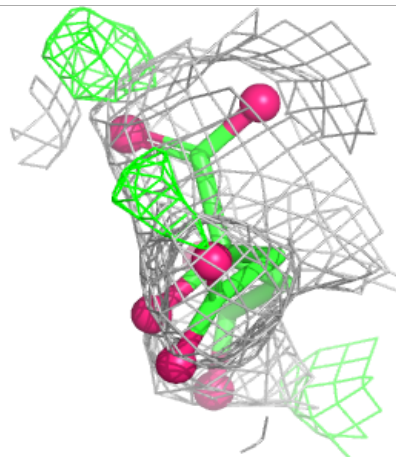
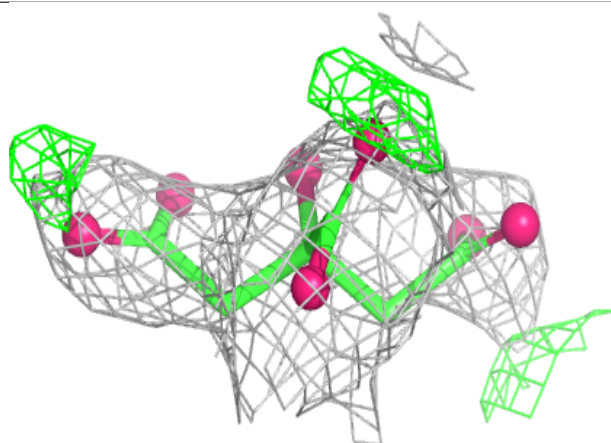
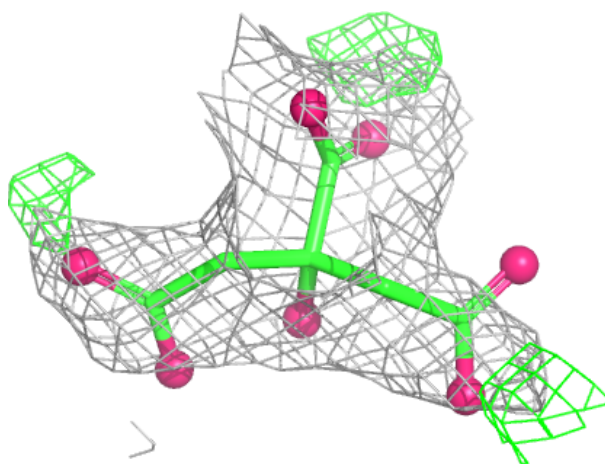
**Electron density around CIT F 701:**

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



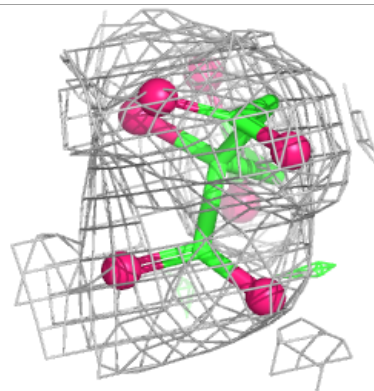
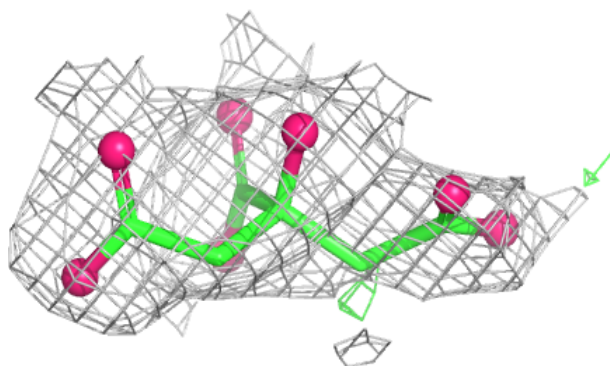
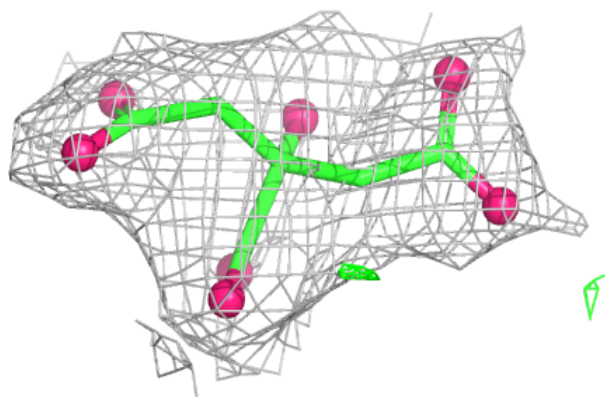
Electron density around CIT K 701:

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



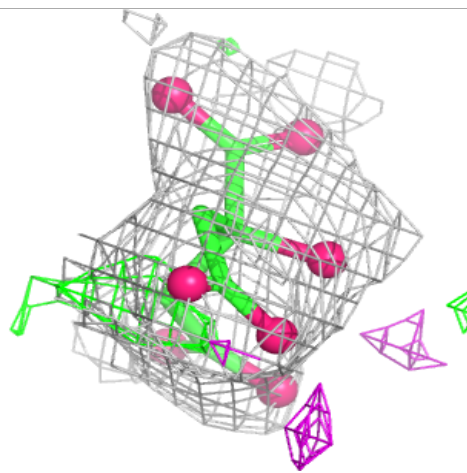
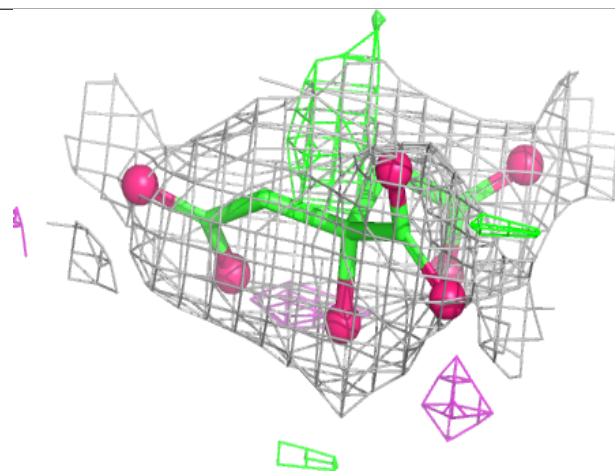
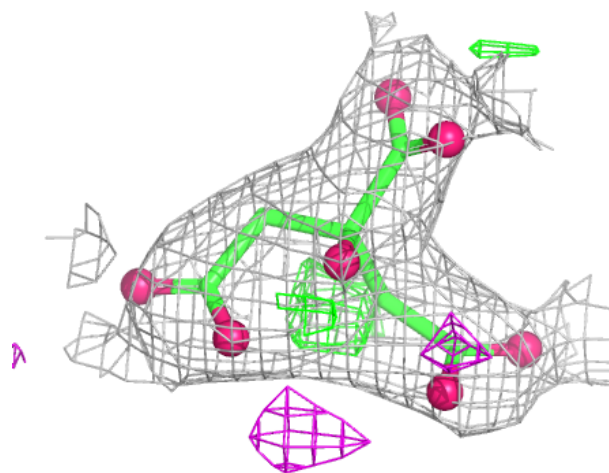
Electron density around CIT B 701:

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



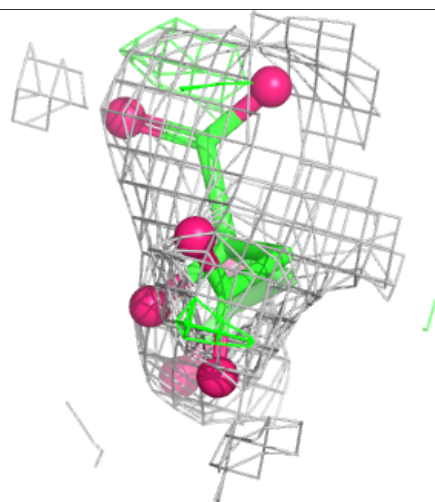
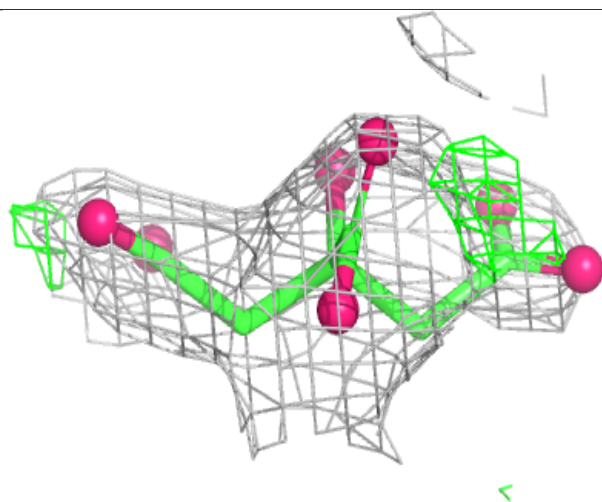
Electron density around CIT B 702:

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



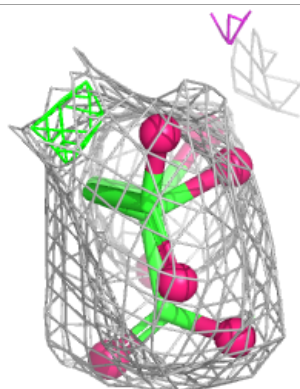
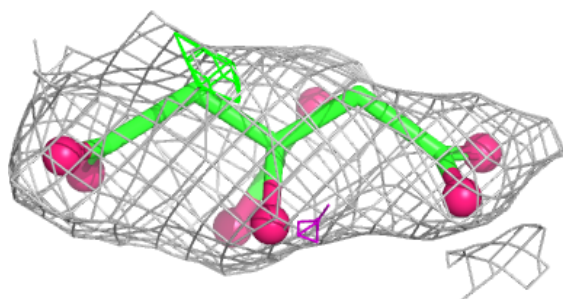
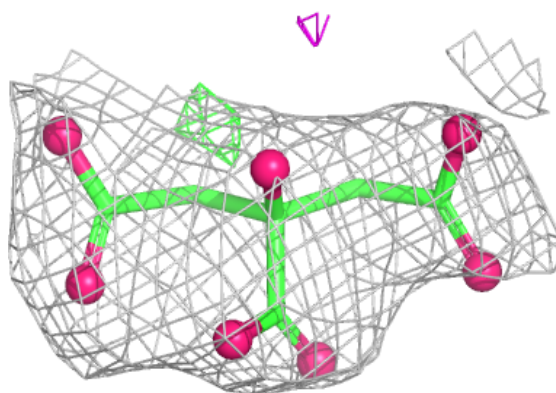
Electron density around CIT A 702:

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

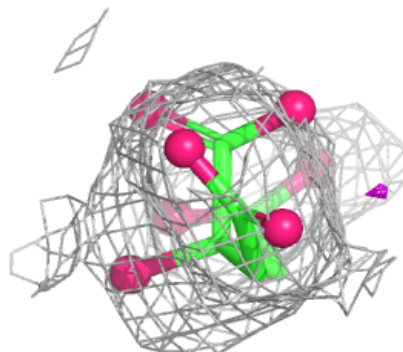
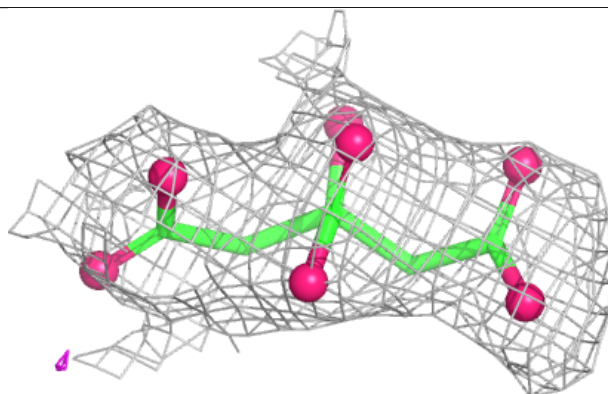
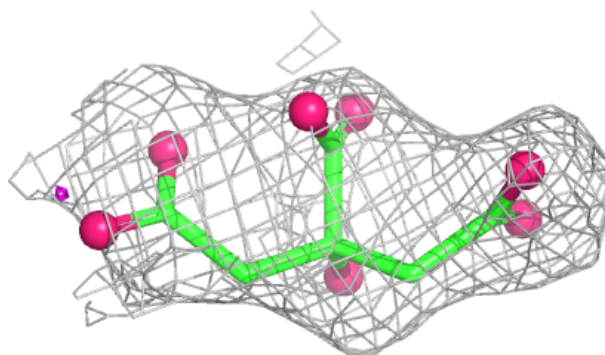


Electron density around CIT L 701:

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

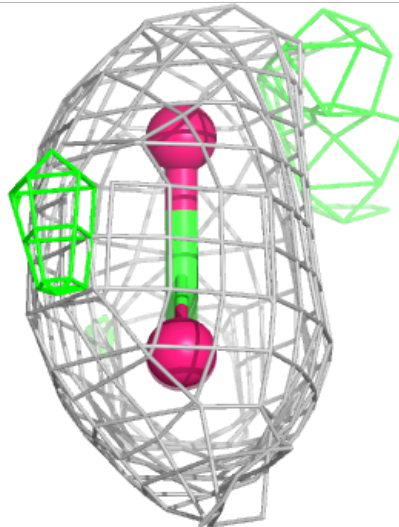
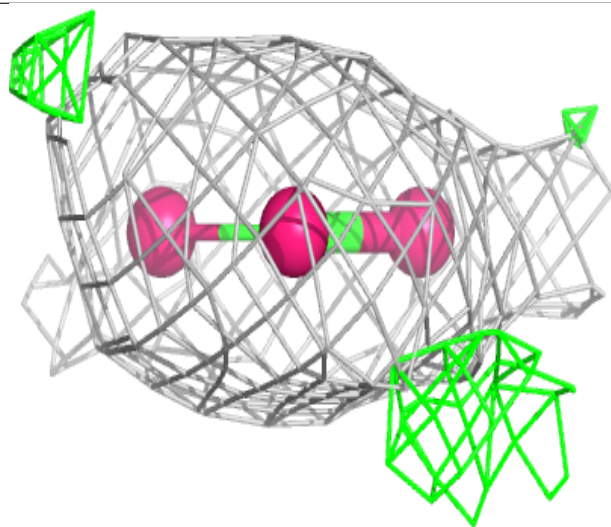
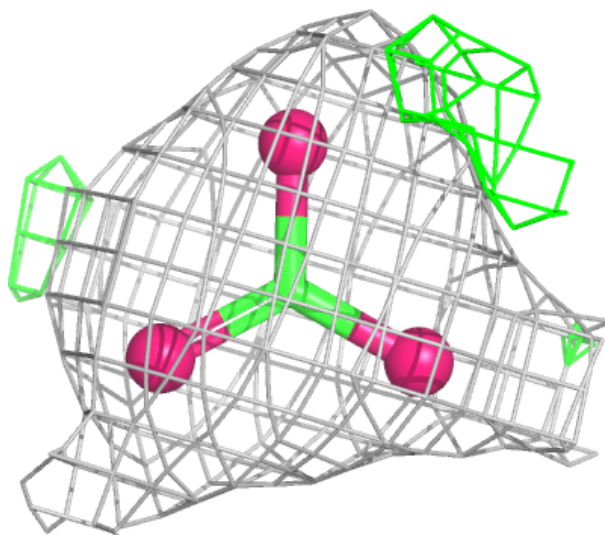
**Electron density around CIT D 701:**

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



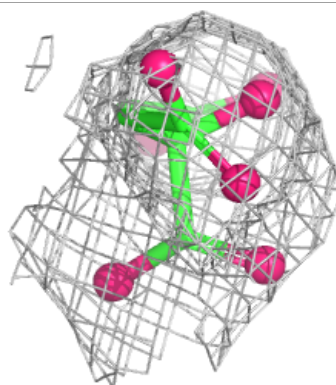
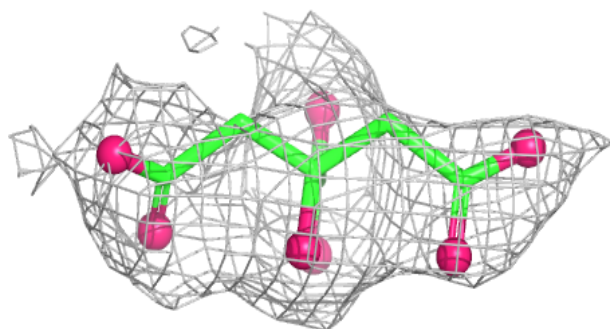
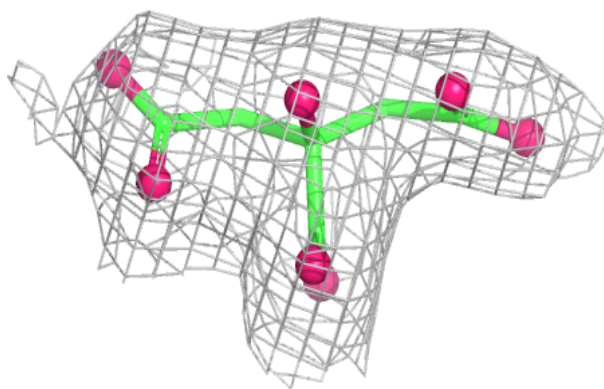
Electron density around CO3 K 702:

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

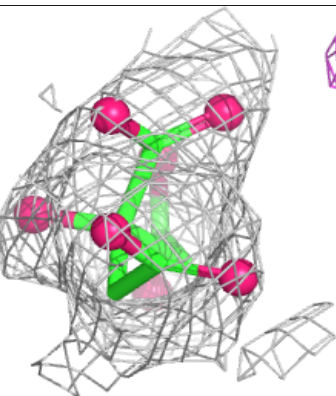
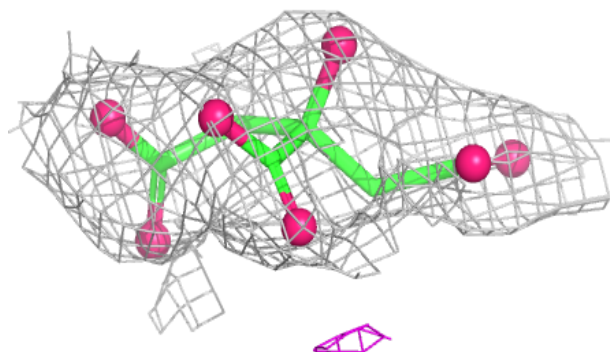
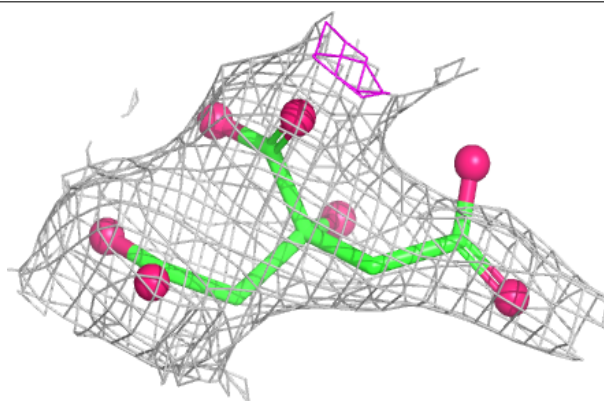


Electron density around CIT E 701:

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

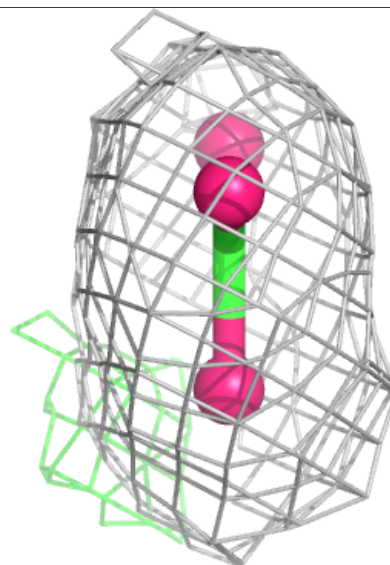
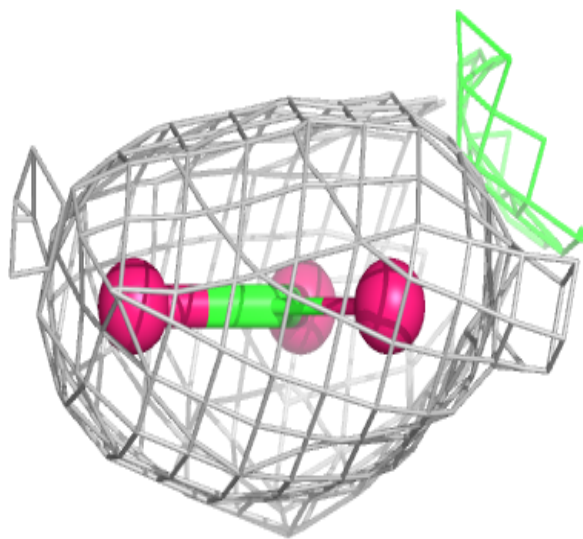
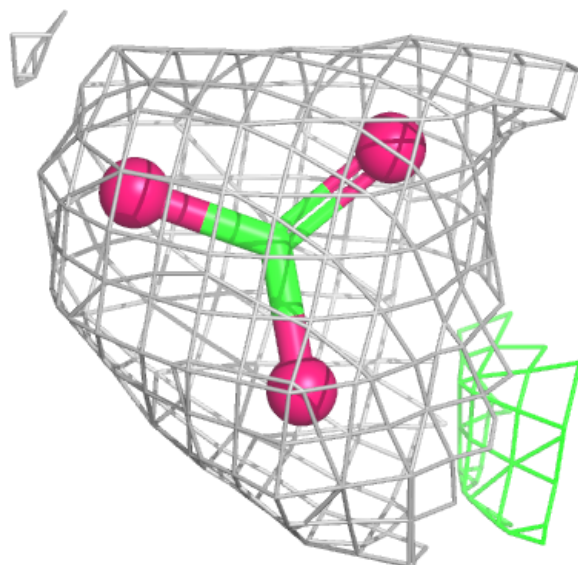
**Electron density around CIT G 701:**

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



Electron density around CO3 H 701:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.