Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2022 – 06:32 PM JST

PDB ID	:	7W1D
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 following versions of software and data (see references ⓘ) were used in the production of this report:

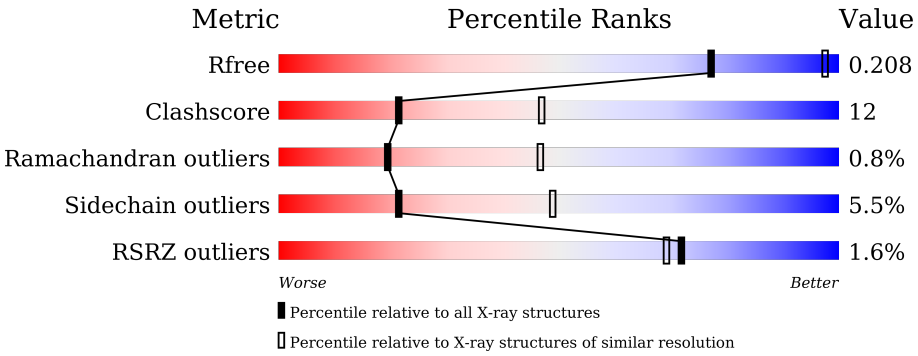
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (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 <=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	70% 23%
1	B	671	2% 71% 23%
1	C	671	72% 21%
1	D	671	% 71% 23%
1	E	671	% 71% 23%
1	F	671	% 78% 17%

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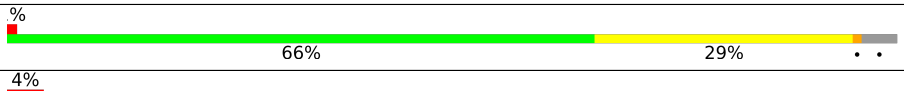
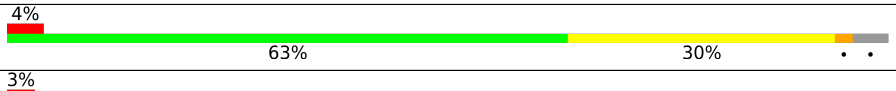
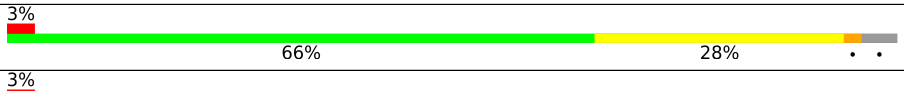
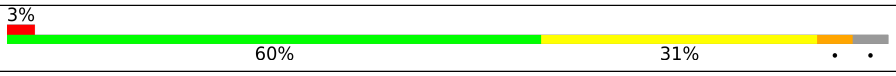
Mol	Chain	Length	Quality of chain
1	G	671	
1	H	671	
1	I	671	
1	J	671	
1	K	671	
1	L	671	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	A	702	-	-	X	-
2	CIT	K	701	-	-	X	-

2 Entry composition (i)

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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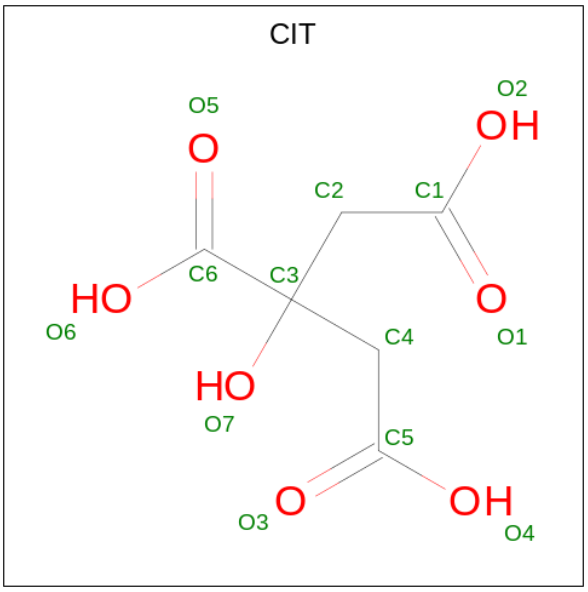
Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	GLY	-	expression tag	UNP A0A068Q5Q5
K	-1	SER	-	expression tag	UNP A0A068Q5Q5
K	0	HIS	-	expression tag	UNP A0A068Q5Q5
K	213	THR	ALA	conflict	UNP A0A068Q5Q5
K	256	ILE	SER	conflict	UNP A0A068Q5Q5
K	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
K	392	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 (three-letter code: 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 13 6 7	0	0
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0
2	I	1	Total C O 13 6 7	0	0
2	J	1	Total C O 13 6 7	0	0
2	K	1	Total C O 13 6 7	0	0

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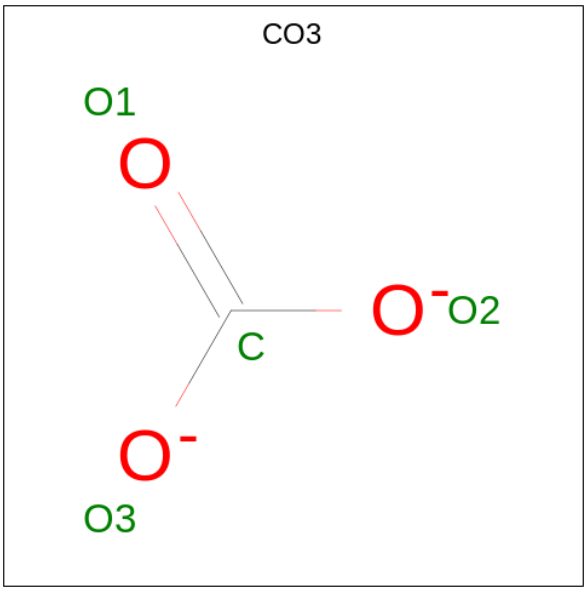
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	1	Total C O 13 6 7	0	0
2	L	1	Total C O 13 6 7	0	0

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

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

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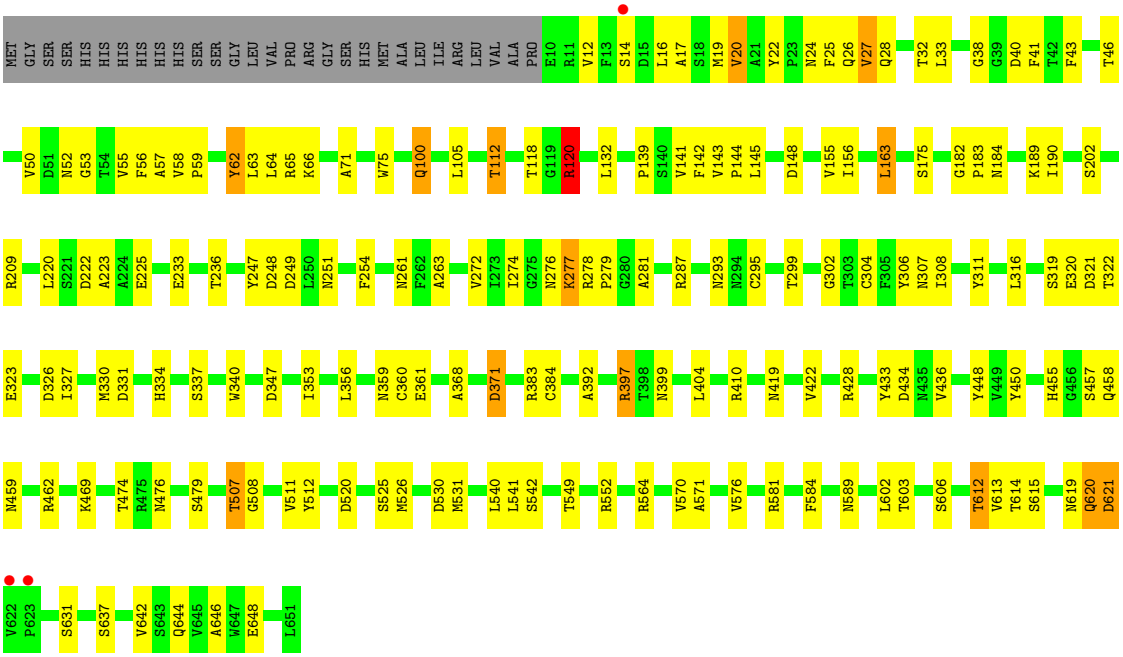
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	118	Total O 118 118	0	0
4	F	164	Total O 164 164	0	0
4	G	87	Total O 87 87	0	0
4	H	106	Total O 106 106	0	0
4	I	72	Total O 72 72	0	0
4	J	72	Total O 72 72	0	0
4	K	74	Total O 74 74	0	0
4	L	68	Total O 68 68	0	0

3 Residue-property plots (i)

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

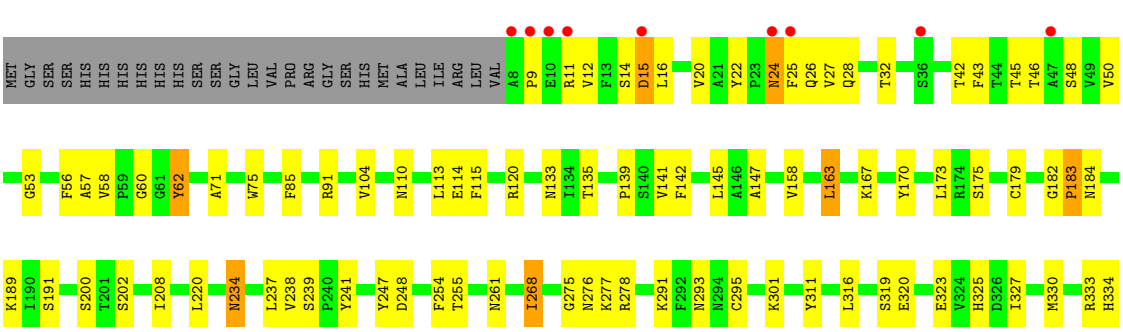
• Molecule 1: K1 LYASE

Chain A:



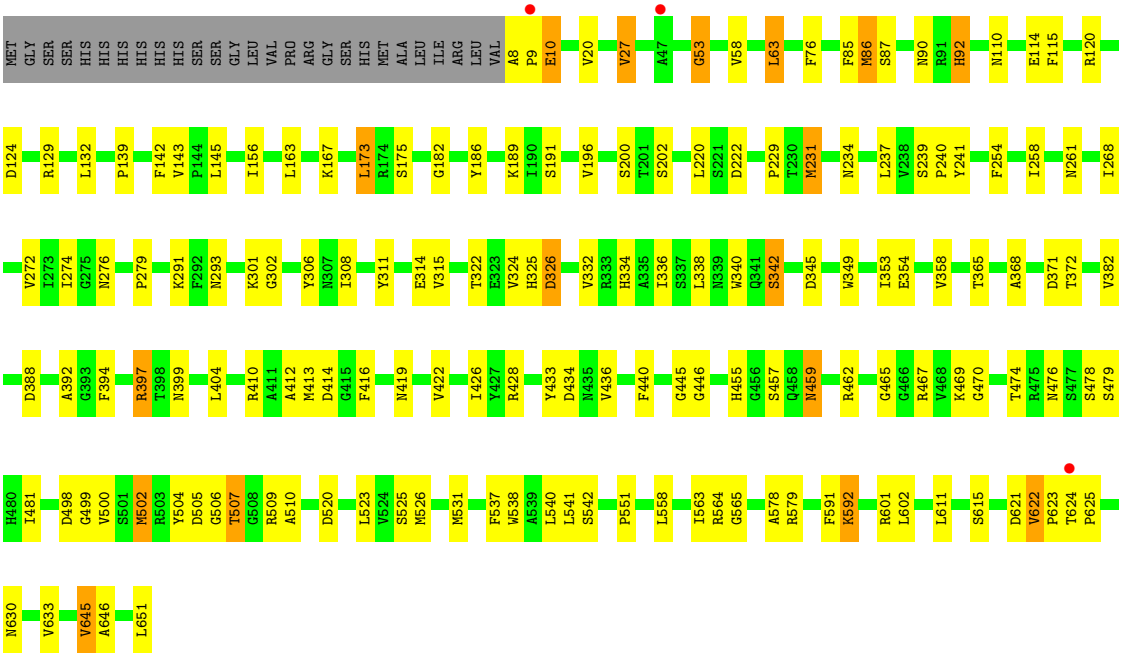
• Molecule 1: K1 LYASE

Chain B:



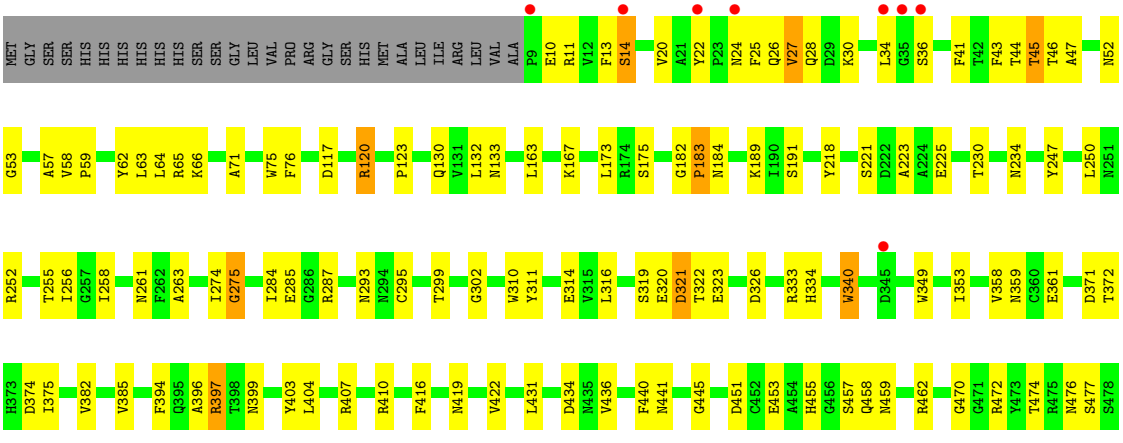
• Molecule 1: K1 LYASE

Chain C:



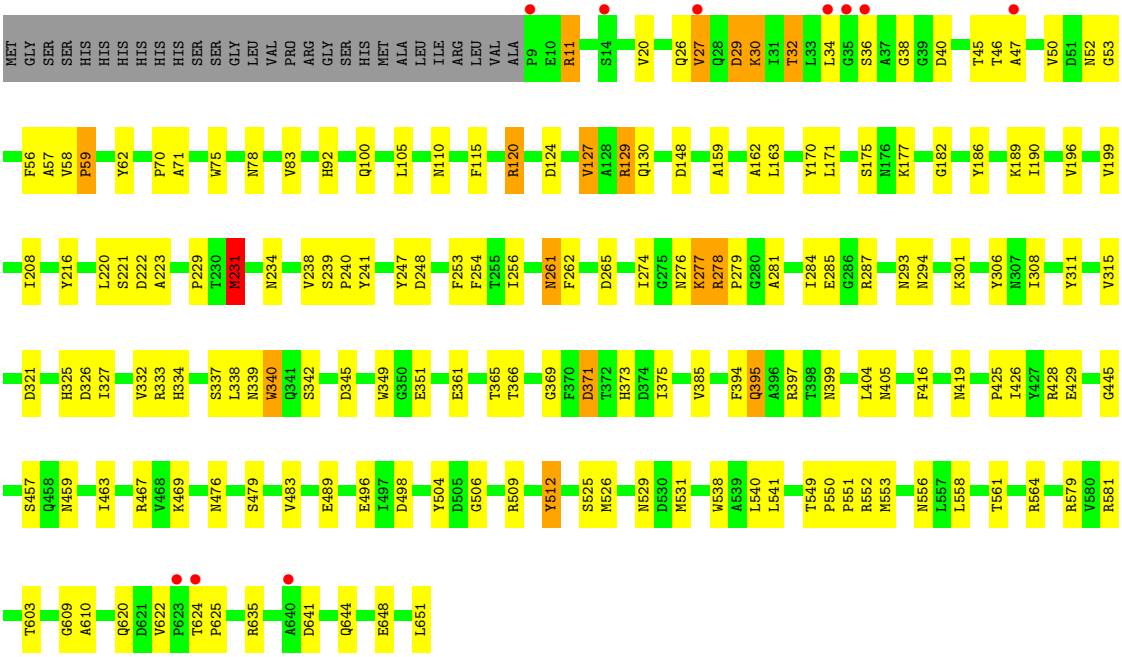
• Molecule 1: K1 LYASE

Chain D:



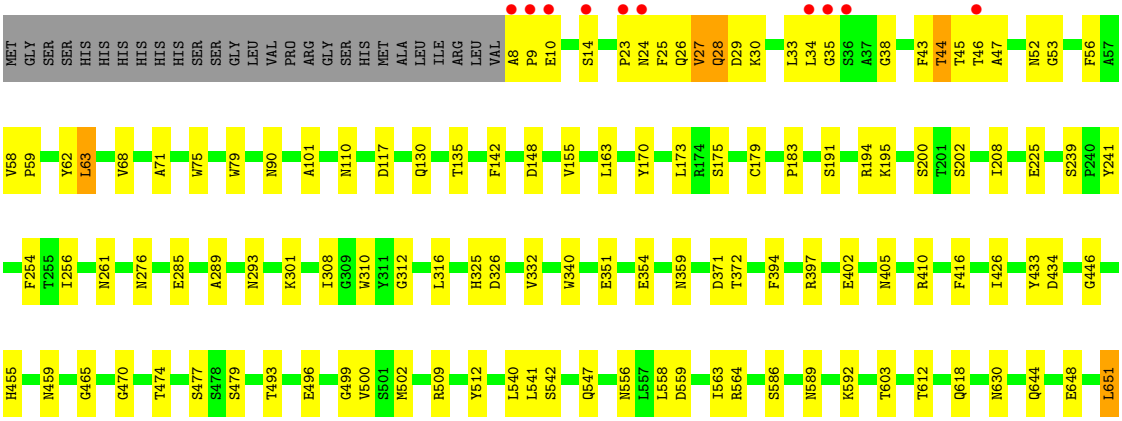
• Molecule 1: K1 LYASE

Chain E:



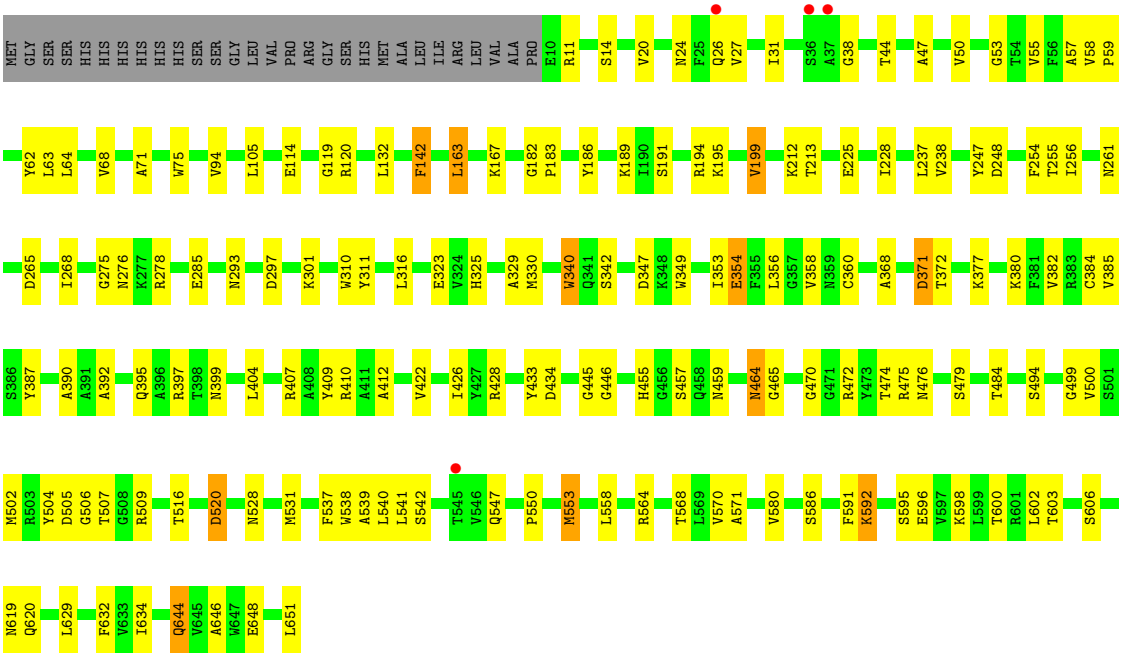
• Molecule 1: K1 LYASE

Chain F:



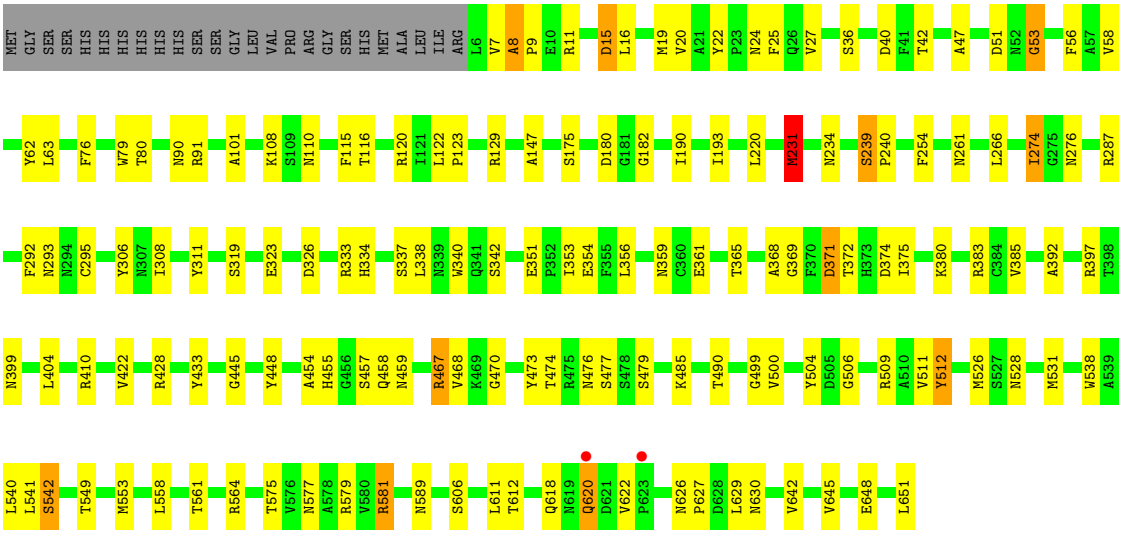
• Molecule 1: K1 LYASE

Chain G:



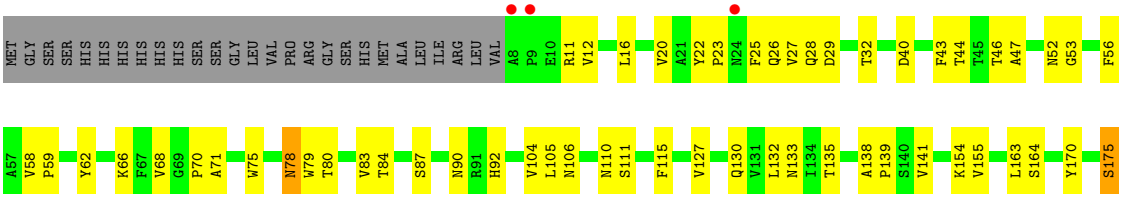
• Molecule 1: K1 LYASE

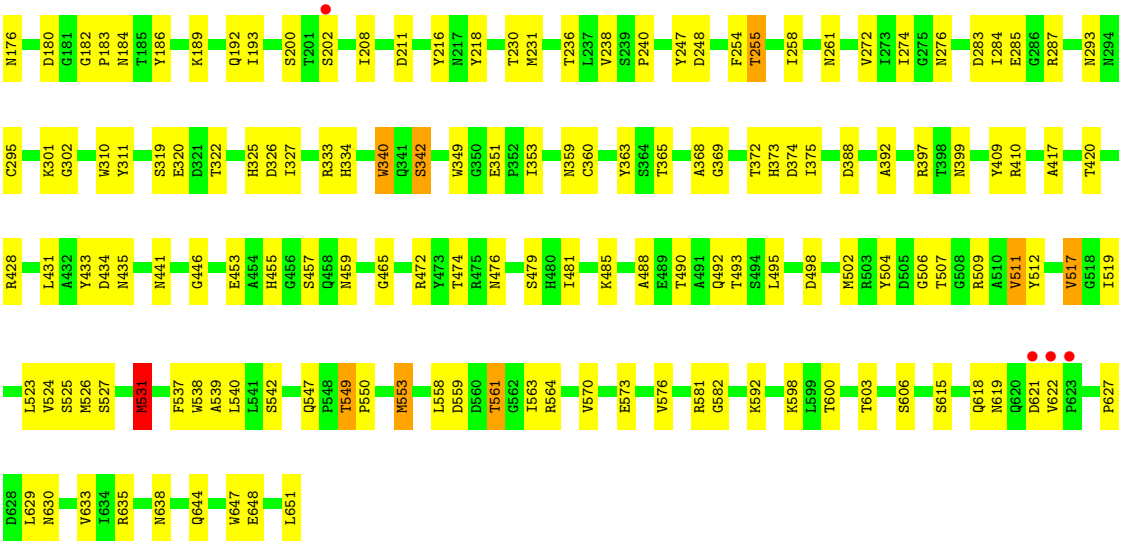
Chain H:



• Molecule 1: K1 LYASE

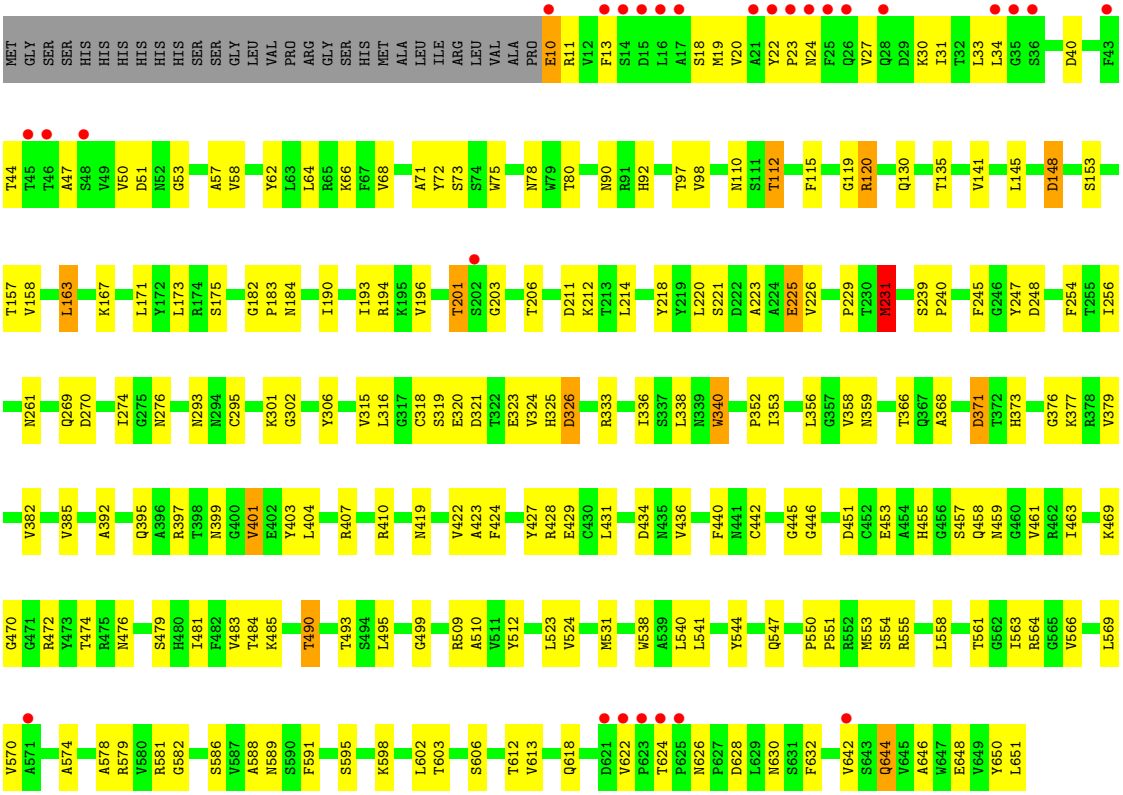
Chain I:





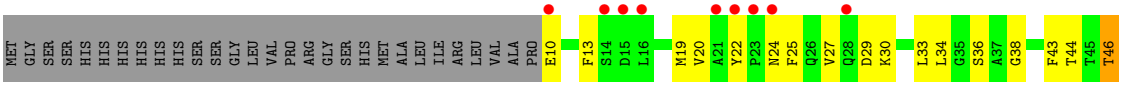
• Molecule 1: K1 LYASE

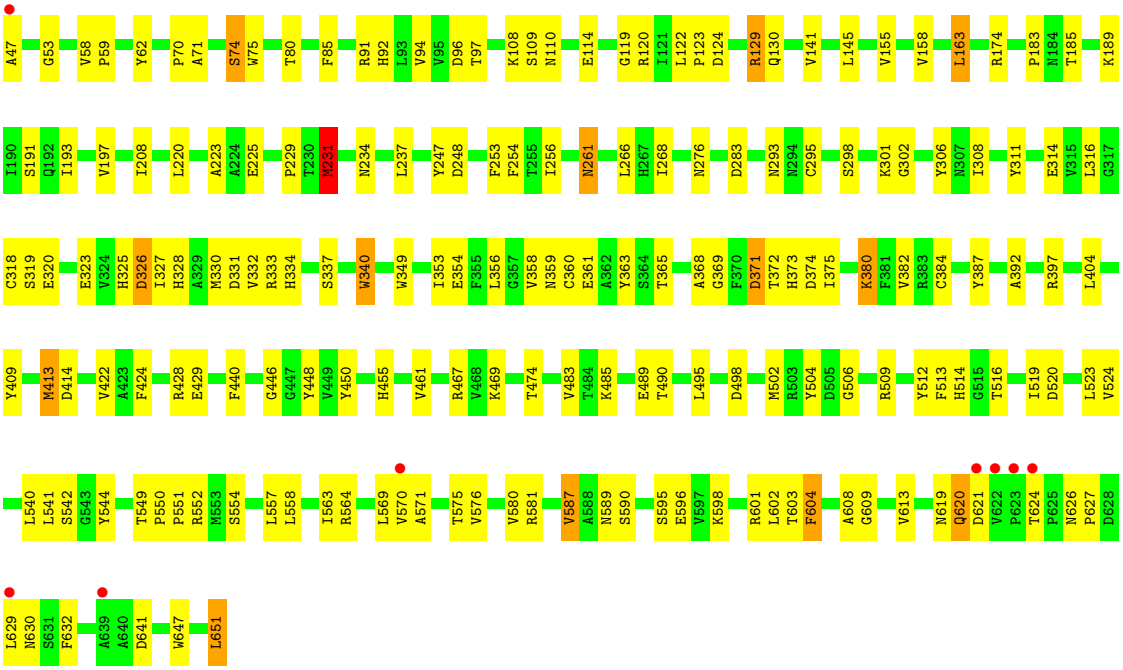
Chain J:



• Molecule 1: K1 LYASE

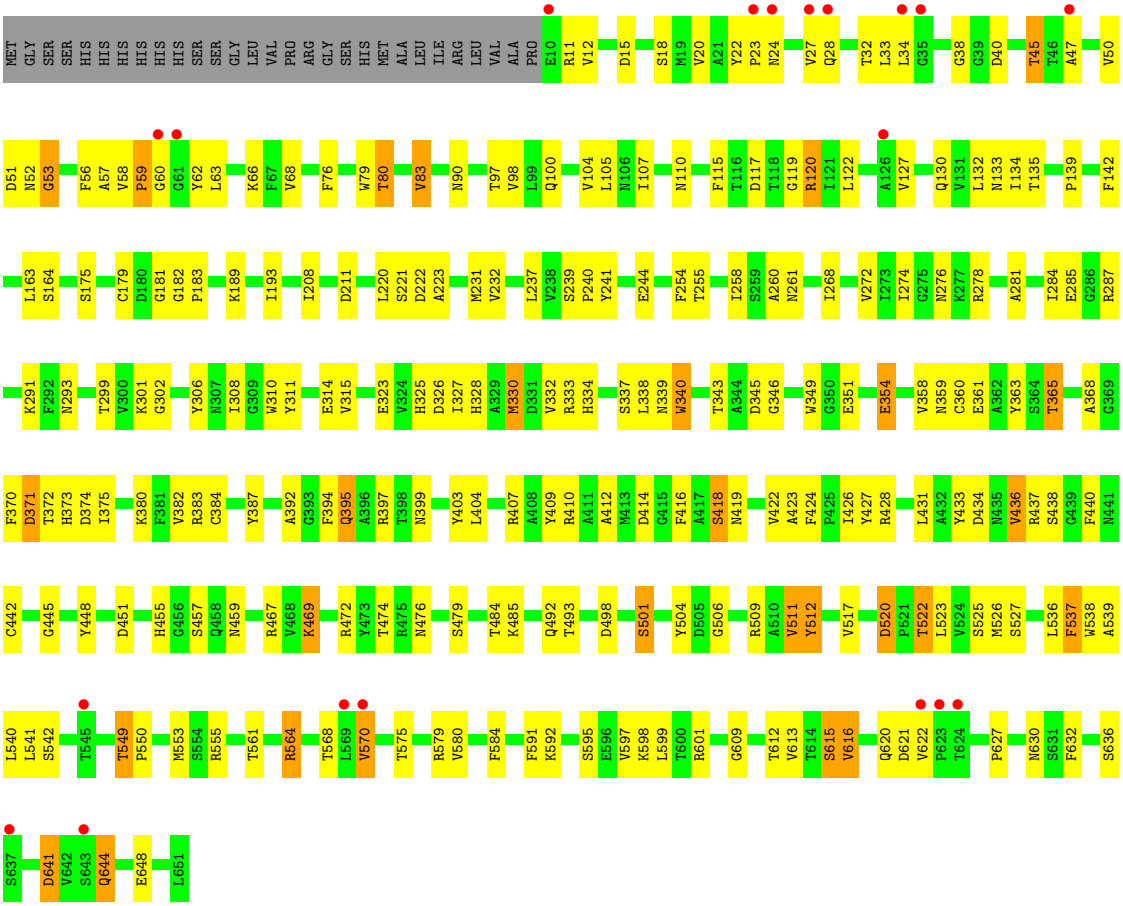
Chain K:





• Molecule 1: K1 LYASE

Chain L:



4 Data and refinement statistics (i)

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 29.86 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.95-2.78) 98.0 (29.86-2.77)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.02%)	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)	0.30 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.94	1/4962 (0.0%)	0.99	9/6755 (0.1%)
1	B	0.95	3/4975 (0.1%)	0.96	6/6774 (0.1%)
1	C	0.97	1/4975 (0.0%)	1.03	13/6774 (0.2%)
1	D	0.89	0/4970	0.95	7/6766 (0.1%)
1	E	0.90	4/4970 (0.1%)	0.96	7/6766 (0.1%)
1	F	0.95	3/4975 (0.1%)	0.97	3/6774 (0.0%)
1	G	0.87	0/4962	0.95	8/6755 (0.1%)
1	H	0.87	0/4990	0.97	3/6795 (0.0%)
1	I	0.84	0/4975	0.94	7/6774 (0.1%)
1	J	0.79	0/4962	0.93	3/6755 (0.0%)
1	K	0.83	0/4962	0.93	4/6755 (0.1%)
1	L	0.79	1/4962 (0.0%)	0.95	7/6755 (0.1%)
All	All	0.88	13/59640 (0.0%)	0.96	77/81198 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	498	ASP	CB-CG	8.19	1.69	1.51
1	B	361	GLU	CD-OE2	7.91	1.34	1.25
1	B	496	GLU	CG-CD	6.53	1.61	1.51
1	C	498	ASP	CB-CG	6.02	1.64	1.51
1	E	241	TYR	CG-CD2	5.77	1.46	1.39
1	F	241	TYR	CG-CD2	5.65	1.46	1.39
1	A	361	GLU	CD-OE2	5.53	1.31	1.25
1	E	496	GLU	CG-CD	5.50	1.60	1.51
1	F	496	GLU	CD-OE1	5.24	1.31	1.25
1	L	117	ASP	CB-CG	5.12	1.62	1.51
1	B	361	GLU	CD-OE1	5.09	1.31	1.25
1	E	285	GLU	CD-OE1	5.08	1.31	1.25
1	F	402	GLU	CG-CD	5.00	1.59	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	531	MET	CG-SD-CE	-9.04	85.73	100.20
1	D	167	LYS	CD-CE-NZ	-7.98	93.35	111.70
1	C	502	MET	CG-SD-CE	-7.73	87.83	100.20
1	D	397	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	G	472	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	G	472	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	462	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	C	86	MET	CG-SD-CE	-7.21	88.67	100.20
1	A	148	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	E	326	ASP	CB-CG-OD1	7.00	124.60	118.30
1	C	120	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	D	472	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	K	174	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	L	51	ASP	CB-CG-OD1	6.70	124.33	118.30
1	F	148	ASP	CB-CG-OD1	6.69	124.32	118.30
1	C	397	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	A	530	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	531	MET	CG-SD-CE	-6.62	89.60	100.20
1	G	531	MET	CG-SD-CE	-6.57	89.69	100.20
1	C	579	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	K	231	MET	CG-SD-CE	-6.44	89.90	100.20
1	B	553	MET	CG-SD-CE	-6.33	90.07	100.20
1	C	326	ASP	CB-CG-OD1	6.31	123.98	118.30
1	E	127	VAL	CB-CA-C	-6.29	99.46	111.40
1	J	120	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	E	531	MET	CG-SD-CE	-6.14	90.38	100.20
1	I	428	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	F	194	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	397	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	C	120	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	F	559	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	209	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	L	451	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	321	ASP	CB-CG-OD1	-5.85	113.03	118.30
1	B	428	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	I	428	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	173	LEU	CA-CB-CG	5.79	128.62	115.30
1	E	231	MET	CG-SD-CE	-5.75	91.00	100.20
1	A	397	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	J	211	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	410	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	L	383	ARG	NE-CZ-NH2	-5.68	117.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	278	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	321	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	K	331	ASP	CB-CG-OD1	5.59	123.33	118.30
1	G	347	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	I	531	MET	CG-SD-CE	-5.54	91.33	100.20
1	D	397	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	E	581	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	E	278	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	H	231	MET	CG-SD-CE	-5.44	91.50	100.20
1	C	462	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	C	520	ASP	CB-CG-OD1	5.36	123.13	118.30
1	G	194	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	120	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	222	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	H	467	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	330	MET	CB-CG-SD	5.26	128.19	112.40
1	B	581	ARG	CG-CD-NE	5.26	122.84	111.80
1	H	180	ASP	CB-CG-OD1	5.25	123.03	118.30
1	L	120	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	I	180	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	526	MET	CG-SD-CE	-5.18	91.91	100.20
1	G	520	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	L	520	ASP	CB-CG-OD1	5.14	122.92	118.30
1	L	211	ASP	CB-CG-OD1	5.13	122.92	118.30
1	L	120	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	K	326	ASP	CB-CG-OD1	5.10	122.89	118.30
1	G	475	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	I	211	ASP	CB-CG-OD1	5.05	122.85	118.30
1	G	553	MET	CG-SD-CE	-5.04	92.14	100.20
1	C	414	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	I	511	VAL	CB-CA-C	-5.03	101.84	111.40
1	D	472	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	J	231	MET	CG-SD-CE	-5.02	92.17	100.20
1	B	330	MET	CB-CG-SD	5.01	127.42	112.40
1	I	431	LEU	CB-CG-CD1	-5.01	102.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4858	0	4712	110	0
1	B	4870	0	4724	115	0
1	C	4870	0	4724	100	0
1	D	4865	0	4720	116	0
1	E	4865	0	4720	122	0
1	F	4870	0	4724	75	0
1	G	4858	0	4712	103	0
1	H	4885	0	4744	96	0
1	I	4870	0	4724	124	0
1	J	4858	0	4712	142	0
1	K	4858	0	4712	144	0
1	L	4858	0	4712	178	0
2	A	26	0	8	11	0
2	B	26	0	10	7	0
2	C	13	0	5	2	0
2	D	13	0	5	3	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	2	0
2	J	13	0	5	3	0
2	K	26	0	8	11	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	74	0	0	1	0
4	L	68	0	0	2	0
All	All	59973	0	56716	1385	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 12.

All (1385) 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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:550:PRO:HA	1:G:591:PHE:CE1	2.19	0.78
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:D:558:LEU:HD22	1:D:651:LEU:HD22	1.68	0.75
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:L:193:ILE:HG21	1:L:231:MET:HE2	1.69	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	1.71	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:L:182:GLY:HA2	1:L:399:ASN:ND2	2.05	0.72
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:B:481:ILE:HG12	1:B:502:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:L:193:ILE:HD13	1:L:231:MET:HE1	1.75	0.67
1:B:340:TRP:HA	1:B:375:ILE:HD11	1.76	0.67
1:C:229:PRO:HB2	1:C:231:MET:HE1	1.77	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: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:C:540:LEU:C	1:C:541:LEU:HD12	2.16	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:D:541:LEU:HD12	1:D:541:LEU:N	2.11	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: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:C:397:ARG:HH12	2:C:701:CIT:H41	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:K:701:CIT:O4	2:K:701:CIT:O7	2.16	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:K:229:PRO:CG	1:K:231:MET:HE1	2.28	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: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:B:481:ILE:CG1	1:B:502:MET:HE3	2.28	0.63
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:E:404:LEU:HD23	1:E:428:ARG:HD2	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:424:PHE:CD2	1:L:448:TYR:CE2	2.87	0.62
1:G:464:ASN:HD22	1:G:464:ASN:C	2.02	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:J:231:MET:HA	1:J:231:MET:HE2	1.82	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: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:15:ASP:OD1	1:H:15:ASP:C	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:VAL:HA	1:L:105:LEU:HD12	1.82	0.60
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: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:A:540:LEU:C	1:A:541:LEU:HD12	2.22	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: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: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:K:44:THR:HG1	1:K:46:THR:HG1	1.49	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:J:229:PRO:HB2	1:J:231:MET:HE1	1.85	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: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: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: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:B:540:LEU:C	1:B:541:LEU:HD12	2.24	0.57
1:G:404:LEU:CD2	1:G:428:ARG:HD2	2.34	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
1:K:85:PHE:CE2	1:K:91:ARG:HD2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:702:CIT:C5	2:K:701:CIT:H21	2.20	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:H:51:ASP:OD1	1:H:51:ASP:C	2.43	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
2:A:702:CIT:C5	2:K:701:CIT:C2	2.60	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: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:I:193:ILE:HG21	1:I:231:MET:HE2	1.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:J:484:THR:OG1	1:J:485:LYS:N	2.40	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: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
1:E:231:MET:CA	1:E:231:MET:HE2	2.38	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:540:LEU:C	1:D:541:LEU:HD12	2.28	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: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:E:231:MET:HE2	1:E:231:MET:HA	1.89	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:ASN:HA	1:F:293:ASN:O	2.08	0.53
1:J:540:LEU:C	1:J:541:LEU:HD12	2.29	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: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:H:193:ILE:HD13	1:H:231:MET:HE1	1.90	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:K:520:ASP:OD1	1:K:520:ASP:C	2.48	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: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:D:274:ILE:HG22	1:D:275:GLY:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:479:SER:HA	1:L:509:ARG:O	2.09	0.52
1:A:19:MET:HE2	1:A:33:LEU:HD13	1.90	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:231:MET:HE2	1:J:231:MET:CA	2.40	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: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: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:A:323:GLU:HG2	1:A:356:LEU:HB3	1.92	0.51
1:D:404:LEU:HD21	1:F:405:ASN:HD21	1.75	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: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:C:541:LEU:HD12	1:C:541:LEU:N	2.26	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:I:193:ILE:HG21	1:I:231:MET:HE1	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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:K:229:PRO:HG2	1:K:231:MET:HE1	1.92	0.50
1:L:332:VAL:HG23	1:L:365:THR:HG22	1.93	0.50
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:564:ARG:HH11	1:A:648:GLU:CD	2.15	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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:702:CIT:O4	2:K:701:CIT:C2	2.60	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:F:179:CYS:HB3	1:F:351:GLU:CD	2.33	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: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:L:340:TRP:CD1	1:L:340:TRP:C	2.86	0.49
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:E:425:PRO:C	1:E:426:ILE:HD13	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:ALA:HA	1:I:75:TRP:CZ3	2.48	0.48
1:K:13:PHE:O	1:K:34:LEU:HG	2.12	0.48
1:K:229:PRO:HB2	1:K:231:MET:HE1	1.95	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:C:510:ALA:CB	1:C:531:MET:HE3	2.43	0.48
1:D:480:HIS:CD2	1:D:502:MET:HB2	2.49	0.48
1:D:515:GLY:O	1:D:516:THR:C	2.49	0.48
1:L:343:THR:HA	1:L:346:GLY:O	2.14	0.48
1:E:540:LEU:C	1:E:541:LEU:HD12	2.33	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:702:CIT:C5	2:K:701:CIT:H22	2.25	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:I:526:MET:SD	1:I:553:MET:HE1	2.54	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: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
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: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: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:H:531:MET:HE2	1:H:538:TRP:HB2	1.96	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:C:481:ILE:HG12	1:C:502:MET:HE3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:547:GLN:NE2	1:F:586:SER:HA	2.30	0.47
1:H:511:VAL:HG21	1:H:526:MET:HE1	1.96	0.47
1:I:104:VAL:CG1	1:I:105:LEU:N	2.77	0.47
1:I:236:THR:HG22	1:I:238:VAL:HG23	1.95	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:A:56:PHE:O	1:A:62:TYR:HB3	2.15	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
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:H:365:THR:HG21	1:H:369:GLY:HA2	1.97	0.47
1:H:526:MET:SD	1:H:553:MET:HE3	2.55	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:E:340:TRP:CD1	1:E:340:TRP:C	2.87	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:B:179:CYS:HB3	1:B:351:GLU:CD	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:302:GLY:HA2	1:A:326:ASP:O	2.15	0.46
1:C:229:PRO:CB	1:C:231:MET:HE1	2.45	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
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: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:I:526:MET:HE1	1:I:531:MET:HE1	1.96	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:G:540:LEU:C	1:G:541:LEU:HD12	2.36	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:A:511:VAL:HG21	1:A:526:MET:HE1	1.98	0.46
2:A:702:CIT:O4	2:K:701:CIT:H21	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:340:TRP:CD1	1:G:340:TRP:C	2.88	0.46
1:H:457:SER:O	1:H:476:ASN:HA	2.15	0.46
1:I:115:PHE:CD1	1:I:240:PRO:HA	2.51	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:G:390:ALA:O	1:G:412:ALA:HB3	2.16	0.46
1:J:19:MET:HE2	1:J:33:LEU:HD22	1.97	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:63:LEU:C	1:A:64:LEU:HD23	2.36	0.46
1:A:100:GLN:HE21	1:A:100:GLN:C	2.18	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:D:183:PRO:O	1:D:184:ASN:C	2.54	0.46
1:E:170:TYR:O	1:E:171:LEU:HD23	2.16	0.46
1:E:229:PRO:CB	1:E:231:MET:HE1	2.44	0.46
1:E:558:LEU:HD22	1:E:651:LEU:HD22	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:526:MET:CE	1:E:551:PRO:HG3	2.45	0.45
1:G:167:LYS:HE3	1:G:199:VAL:HG23	1.97	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
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:231:MET:HE2	1:K:231:MET:CA	2.45	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
2:A:702:CIT:H21	2:K:701:CIT:C5	2.43	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:L:306:TYR:CE1	1:L:330:MET:HE3	2.52	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
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: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:C:531:MET:HE2	1:C:538:TRP:HB2	1.98	0.45
1:D:293:ASN:HB2	1:D:316:LEU:HD21	1.99	0.45
1:E:553:MET:HE1	1:E:651:LEU:HD11	1.98	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:E:278:ARG:O	1:E:279:PRO:C	2.56	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: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:F:276:ASN:C	1:F:276:ASN:OD1	2.55	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:F:563:ILE:C	1:F:563:ILE:HD12	2.38	0.44
1:I:175:SER:OG	1:I:176:ASN:N	2.47	0.44
1:J:22:TYR:CZ	1:J:24:ASN:HB2	2.51	0.44
1:J:531:MET:HE1	1:J:538:TRP:HB2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:638:ASN:C	1:I:638:ASN:OD1	2.54	0.44
1:L:511:VAL:HG21	1:L:526:MET:SD	2.57	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: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: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: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:J:269:GLN:HE21	1:J:270:ASP:CG	2.20	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:D:320:GLU:HA	1:D:353:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:A:702:CIT:H22	2:K:701:CIT:C5	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:510:ALA:CB	1:D:531:MET:HE2	2.49	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:C:85:PHE:CD2	1:C:86:MET:HE2	2.53	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:512:TYR:CD1	1:H:512:TYR:C	2.91	0.43
1:J:274:ILE:HG23	1:J:306:TYR:HB2	2.01	0.43
1:K:229:PRO:CB	1:K:231:MET:HE1	2.47	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:306:TYR:CZ	1:L:330:MET:HE1	2.54	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:C:502:MET:HE1	1:C:510:ALA:HB1	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:608:ALA:HA	1:K:641:ASP:OD2	2.18	0.43
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:63:LEU:C	1:D:64:LEU:HD23	2.39	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: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: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: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:J:72:TYR:O	1:J:73:SER:C	2.57	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
2:A:702:CIT:C2	2:K:701:CIT:C5	2.77	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:135:THR:O	1:F:135:THR:HG22	2.18	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: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: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:B:481:ILE:HG12	1:B:502:MET:HE2	1.99	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: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: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:74:SER:HB3	1:K:96:ASP:CG	2.39	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: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:A:564:ARG:NH1	1:A:648:GLU:CD	2.73	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:642:VAL:HG23	1:D:642:VAL:O	2.18	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:413:MET:HE2	1:K:413:MET:HB2	1.95	0.42
1:L:598:LYS:C	1:L:599:LEU:HD23	2.39	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:E:549:THR:CG2	1:E:550:PRO:HD2	2.48	0.42
1:G:329:ALA:C	1:G:330:MET:HG3	2.39	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:183:PRO:O	1:I:184:ASN:C	2.57	0.42
1:I:433:TYR:HE1	1:I:455:HIS:CD2	2.37	0.42
1:K:619:ASN:OD1	1:K:619:ASN:C	2.56	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:E:222:ASP:O	1:E:223:ALA:HB3	2.20	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:H:122:LEU:HA	1:H:123:PRO:HD3	1.84	0.42
1:I:509:ARG:NH2	1:I:537:PHE:HD2	2.17	0.42
1:I:619:ASN:OD1	1:I:619:ASN:C	2.57	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: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:C:481:ILE:HG12	1:C:502:MET:CE	2.50	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: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
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:189:LYS:HE3	1:A:347:ASP:CG	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:306:TYR:CE1	1:L:330:MET:CE	3.03	0.42
1:L:387:TYR:CE1	1:L:409:TYR:CD1	3.07	0.42
1:B:139:PRO:HG2	1:B:142:PHE:CZ	2.54	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:183:PRO:O	1:A:184:ASN:C	2.58	0.42
1:A:274:ILE:HG23	1:A:306:TYR:HB2	2.01	0.42
1:E:538:TRP:CZ2	1:E:553:MET:HE1	2.55	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:I:573:GLU:OE2	1:I:635:ARG:NE	2.53	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:C:526:MET:HE3	1:C:551:PRO:HG2	2.01	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:I:78:ASN:OD1	1:I:80:THR:CB	2.68	0.41
1:K:231:MET:HE3	1:K:231:MET:HB2	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:VAL:O	1:E:239:SER:HB2	2.20	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:J:510:ALA:CB	1:J:531:MET:HE2	2.50	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: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:H:19:MET:HE3	1:H:63:LEU:HD13	2.02	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: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
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:A:520:ASP:OD1	1:A:520:ASP:C	2.57	0.41
1:C:578:ALA:O	1:C:630:ASN:HB2	2.20	0.41
1:D:57:ALA:HA	1:D:62:TYR:HD1	1.85	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:550:PRO:HB3	1:G:591:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:183:PRO:O	1:J:184:ASN:C	2.58	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: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: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
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:A:619:ASN:HD21	1:A:621:ASP:CG	2.24	0.41
1:D:419:ASN:O	1:D:422:VAL:HB	2.20	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:34:LEU:HA	1:L:66:LYS:HZ2	1.84	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:183:PRO:O	1:B:184:ASN:C	2.58	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:C:92:HIS:CE1	1:C:114:GLU:OE1	2.73	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: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:457:SER:O	1:E:476:ASN:HA	2.20	0.41
1:H:351:GLU:HA	1:H:375:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:581:ARG:H	1:J:595:SER:HG	1.65	0.41
1:L:79:TRP:O	1:L:83:VAL:CG2	2.69	0.41
1:L:134:ILE:O	1:L:260:ALA:HA	2.20	0.41
1:L:254:PHE:O	1:L:276:ASN:HB2	2.20	0.41
1:A:24:ASN:O	1:A:25:PHE:C	2.58	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:J:479:SER:OG	1:J:481:ILE:O	2.32	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:L:636:SER:HG	1:L:641:ASP:CG	2.21	0.41
1:A:576:VAL:O	1:A:631:SER:HA	2.21	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:J:51:ASP:C	1:J:51:ASP:OD1	2.59	0.40
1:J:193:ILE:HG13	1:J:318:CYS:SG	2.61	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:G:520:ASP:OD1	1:G:520:ASP:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:78:ASN:O	1:I:79:TRP:C	2.60	0.40
1:J:171:LEU:HD13	1:J:226:VAL:HG21	2.04	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
2:A:702:CIT:O4	2:K:701:CIT:H22	2.20	0.40
1:B:24:ASN:N	1:B:24:ASN:OD1	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:536:LEU:C	1:L:537:PHE:HD1	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	640/671 (95%)	594 (93%)	41 (6%)	5 (1%)	19	47
1	B	642/671 (96%)	598 (93%)	38 (6%)	6 (1%)	17	44
1	C	642/671 (96%)	605 (94%)	32 (5%)	5 (1%)	19	47
1	D	641/671 (96%)	596 (93%)	38 (6%)	7 (1%)	14	38
1	E	641/671 (96%)	599 (93%)	36 (6%)	6 (1%)	17	44
1	F	642/671 (96%)	596 (93%)	40 (6%)	6 (1%)	17	44
1	G	640/671 (95%)	597 (93%)	38 (6%)	5 (1%)	19	47
1	H	644/671 (96%)	595 (92%)	45 (7%)	4 (1%)	25	54
1	I	642/671 (96%)	592 (92%)	48 (8%)	2 (0%)	41	70
1	J	640/671 (95%)	581 (91%)	57 (9%)	2 (0%)	41	70
1	K	640/671 (95%)	585 (91%)	51 (8%)	4 (1%)	25	54
1	L	640/671 (95%)	585 (91%)	47 (7%)	8 (1%)	12	33
All	All	7694/8052 (96%)	7123 (93%)	511 (7%)	60 (1%)	19	47

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	38	GLY
1	B	27	VAL

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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%)	492 (95%)	28 (5%)	22	50
1	B	521/544 (96%)	495 (95%)	26 (5%)	24	53
1	C	521/544 (96%)	495 (95%)	26 (5%)	24	53
1	D	521/544 (96%)	497 (95%)	24 (5%)	27	57
1	E	521/544 (96%)	494 (95%)	27 (5%)	23	52
1	F	521/544 (96%)	502 (96%)	19 (4%)	35	66
1	G	520/544 (96%)	497 (96%)	23 (4%)	28	58
1	H	523/544 (96%)	497 (95%)	26 (5%)	24	53
1	I	521/544 (96%)	485 (93%)	36 (7%)	15	38
1	J	520/544 (96%)	490 (94%)	30 (6%)	20	47
1	K	520/544 (96%)	493 (95%)	27 (5%)	23	52
1	L	520/544 (96%)	470 (90%)	50 (10%)	8	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6249/6528 (96%)	5907 (94%)	342 (6%)	21 49

All (342) 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	46	THR
1	A	62	TYR
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	144	PRO
1	A	163	LEU
1	A	175	SER
1	A	202	SER
1	A	233	GLU
1	A	277	LYS
1	A	279	PRO
1	A	340	TRP
1	A	371	ASP
1	A	507	THR
1	A	512	TYR
1	A	525	SER
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	42	THR
1	B	62	TYR
1	B	135	THR
1	B	141	VAL
1	B	163	LEU
1	B	175	SER
1	B	183	PRO
1	B	200	SER

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Mol	Chain	Res	Type
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	340	TRP
1	B	469	LYS
1	B	525	SER
1	B	545	THR
1	B	550	PRO
1	B	564	ARG
1	B	600	THR
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	63	LEU
1	C	92	HIS
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	340	TRP
1	C	342	SER
1	C	371	ASP
1	C	413	MET
1	C	459	ASN
1	C	507	THR
1	C	523	LEU
1	C	525	SER
1	C	542	SER
1	C	592	LYS
1	C	622	VAL

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Mol	Chain	Res	Type
1	C	645	VAL
1	D	10	GLU
1	D	14	SER
1	D	27	VAL
1	D	45	THR
1	D	117	ASP
1	D	120	ARG
1	D	133	ASN
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	321	ASP
1	D	340	TRP
1	D	371	ASP
1	D	451	ASP
1	D	477	SER
1	D	498	ASP
1	D	553	MET
1	D	620	GLN
1	D	622	VAL
1	D	642	VAL
1	E	11	ARG
1	E	27	VAL
1	E	29	ASP
1	E	30	LYS
1	E	32	THR
1	E	78	ASN
1	E	120	ARG
1	E	127	VAL
1	E	129	ARG
1	E	163	LEU
1	E	175	SER
1	E	199	VAL
1	E	221	SER
1	E	231	MET
1	E	261	ASN
1	E	265	ASP
1	E	277	LYS

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Mol	Chain	Res	Type
1	E	321	ASP
1	E	327	ILE
1	E	340	TRP
1	E	371	ASP
1	E	395	GLN
1	E	489	GLU
1	E	512	TYR
1	E	525	SER
1	E	620	GLN
1	E	622	VAL
1	F	27	VAL
1	F	28	GLN
1	F	44	THR
1	F	63	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	239	SER
1	F	340	TRP
1	F	371	ASP
1	F	477	SER
1	F	493	THR
1	F	512	TYR
1	F	592	LYS
1	F	651	LEU
1	G	11	ARG
1	G	14	SER
1	G	27	VAL
1	G	44	THR
1	G	68	VAL
1	G	142	PHE
1	G	163	LEU
1	G	183	PRO
1	G	195	LYS
1	G	199	VAL
1	G	340	TRP
1	G	371	ASP
1	G	377	LYS

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Mol	Chain	Res	Type
1	G	380	LYS
1	G	464	ASN
1	G	494	SER
1	G	542	SER
1	G	568	THR
1	G	592	LYS
1	G	600	THR
1	G	606	SER
1	G	620	GLN
1	G	644	GLN
1	H	15	ASP
1	H	36	SER
1	H	40	ASP
1	H	42	THR
1	H	80	THR
1	H	91	ARG
1	H	116	THR
1	H	129	ARG
1	H	175	SER
1	H	231	MET
1	H	239	SER
1	H	274	ILE
1	H	338	LEU
1	H	340	TRP
1	H	342	SER
1	H	371	ASP
1	H	512	TYR
1	H	542	SER
1	H	575	THR
1	H	577	ASN
1	H	581	ARG
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	27	VAL
1	I	28	GLN
1	I	68	VAL
1	I	78	ASN
1	I	106	ASN

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Mol	Chain	Res	Type
1	I	111	SER
1	I	127	VAL
1	I	133	ASN
1	I	135	THR
1	I	141	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	255	THR
1	I	322	THR
1	I	340	TRP
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	531	MET
1	I	542	SER
1	I	549	THR
1	I	553	MET
1	I	561	THR
1	I	570	VAL
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	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	221	SER

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Mol	Chain	Res	Type
1	J	225	GLU
1	J	231	MET
1	J	321	ASP
1	J	326	ASP
1	J	340	TRP
1	J	371	ASP
1	J	401	VAL
1	J	469	LYS
1	J	490	THR
1	J	493	THR
1	J	512	TYR
1	J	566	VAL
1	J	586	SER
1	J	606	SER
1	J	612	THR
1	J	622	VAL
1	J	624	THR
1	J	644	GLN
1	K	27	VAL
1	K	29	ASP
1	K	36	SER
1	K	46	THR
1	K	74	SER
1	K	80	THR
1	K	109	SER
1	K	129	ARG
1	K	141	VAL
1	K	163	LEU
1	K	231	MET
1	K	261	ASN
1	K	340	TRP
1	K	371	ASP
1	K	380	LYS
1	K	413	MET
1	K	502	MET
1	K	512	TYR
1	K	554	SER
1	K	563	ILE
1	K	569	LEU
1	K	575	THR
1	K	587	VAL
1	K	604	PHE

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Mol	Chain	Res	Type
1	K	620	GLN
1	K	624	THR
1	K	651	LEU
1	L	11	ARG
1	L	15	ASP
1	L	18	SER
1	L	27	VAL
1	L	28	GLN
1	L	45	THR
1	L	63	LEU
1	L	68	VAL
1	L	80	THR
1	L	83	VAL
1	L	127	VAL
1	L	133	ASN
1	L	163	LEU
1	L	164	SER
1	L	175	SER
1	L	183	PRO
1	L	208	ILE
1	L	221	SER
1	L	272	VAL
1	L	278	ARG
1	L	330	MET
1	L	340	TRP
1	L	365	THR
1	L	371	ASP
1	L	372	THR
1	L	380	LYS
1	L	395	GLN
1	L	418	SER
1	L	469	LYS
1	L	493	THR
1	L	501	SER
1	L	511	VAL
1	L	512	TYR
1	L	517	VAL
1	L	522	THR
1	L	527	SER
1	L	537	PHE
1	L	542	SER
1	L	549	THR

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Mol	Chain	Res	Type
1	L	564	ARG
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	641	ASP
1	L	644	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	325	HIS
1	A	367	GLN
1	A	395	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	458	GLN
1	B	534	HIS
1	C	92	HIS
1	C	328	HIS
1	D	367	GLN
1	D	534	HIS
1	E	110	ASN
1	E	261	ASN
1	E	269	GLN
1	E	458	GLN
1	F	28	GLN
1	F	328	HIS
1	F	367	GLN
1	F	405	ASN
1	G	234	ASN
1	G	328	HIS
1	G	464	ASN

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Mol	Chain	Res	Type
1	H	110	ASN
1	H	234	ASN
1	H	261	ASN
1	H	269	GLN
1	H	367	GLN
1	H	455	HIS
1	H	577	ASN
1	H	626	ASN
1	J	92	HIS
1	J	106	ASN
1	J	130	GLN
1	J	133	ASN
1	J	234	ASN
1	J	269	GLN
1	J	325	HIS
1	J	373	HIS
1	J	618	GLN
1	J	626	ASN
1	K	28	GLN
1	K	110	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
1	K	459	ASN
1	K	577	ASN
1	K	626	ASN
1	L	28	GLN
1	L	328	HIS
1	L	399	ASN
1	L	534	HIS
1	L	644	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	I	701	-	3,12,12	1.70	1 (33%)	3,17,17	0.67	0
2	CIT	A	701	-	3,12,12	1.02	0	3,17,17	2.34	2 (66%)
2	CIT	H	702	-	3,12,12	1.94	1 (33%)	3,17,17	0.87	0
2	CIT	F	701	-	3,12,12	0.88	0	3,17,17	1.65	1 (33%)
2	CIT	K	701	-	3,12,12	0.91	0	3,17,17	1.94	1 (33%)
2	CIT	J	701	-	3,12,12	0.30	0	3,17,17	2.02	1 (33%)
2	CIT	D	701	-	3,12,12	1.65	1 (33%)	3,17,17	2.45	1 (33%)
3	CO3	C	702	-	0,3,3	-	-	0,3,3	-	-
2	CIT	E	701	-	3,12,12	2.89	1 (33%)	3,17,17	1.51	1 (33%)
3	CO3	K	702	-	0,3,3	-	-	0,3,3	-	-
2	CIT	L	701	-	3,12,12	1.97	1 (33%)	3,17,17	1.59	1 (33%)
2	CIT	A	702	-	3,12,12	0.65	0	3,17,17	0.90	0
2	CIT	G	701	-	3,12,12	1.28	0	3,17,17	0.68	0
2	CIT	F	702	-	3,12,12	0.54	0	3,17,17	2.08	1 (33%)
2	CIT	B	702	-	3,12,12	1.72	1 (33%)	3,17,17	1.73	1 (33%)
2	CIT	B	701	-	3,12,12	1.00	0	3,17,17	1.86	1 (33%)
2	CIT	C	701	-	3,12,12	1.33	1 (33%)	3,17,17	2.36	2 (66%)
2	CIT	K	703	-	3,12,12	1.73	1 (33%)	3,17,17	2.04	2 (66%)
3	CO3	H	701	-	0,3,3	-	-	0,3,3	-	-

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	F	701	-	-	0/6/16/16	-
2	CIT	B	702	-	-	1/6/16/16	-
2	CIT	F	702	-	-	2/6/16/16	-
2	CIT	I	701	-	-	3/6/16/16	-
2	CIT	B	701	-	-	5/6/16/16	-
2	CIT	H	702	-	-	1/6/16/16	-
2	CIT	K	701	-	-	4/6/16/16	-
2	CIT	A	701	-	-	0/6/16/16	-
2	CIT	C	701	-	-	0/6/16/16	-
2	CIT	K	703	-	-	3/6/16/16	-
2	CIT	J	701	-	-	0/6/16/16	-
2	CIT	L	701	-	-	0/6/16/16	-
2	CIT	A	702	-	-	4/6/16/16	-
2	CIT	D	701	-	-	3/6/16/16	-
2	CIT	G	701	-	-	6/6/16/16	-
2	CIT	E	701	-	-	0/6/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	CIT	C4-C3	-4.70	1.48	1.54
2	L	701	CIT	C4-C3	-2.82	1.50	1.54
2	B	702	CIT	C2-C3	-2.81	1.50	1.54
2	K	703	CIT	C2-C3	2.80	1.58	1.54
2	I	701	CIT	C4-C3	-2.60	1.51	1.54
2	H	702	CIT	O7-C3	2.35	1.46	1.43
2	C	701	CIT	C4-C3	2.25	1.58	1.54
2	D	701	CIT	C4-C3	-2.19	1.51	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	CIT	C3-C2-C1	-3.80	108.90	114.98
2	C	701	CIT	C3-C4-C5	3.56	120.68	114.98
2	F	702	CIT	C3-C2-C1	-3.23	109.82	114.98
2	A	701	CIT	C3-C2-C1	-3.15	109.94	114.98
2	K	701	CIT	C3-C4-C5	-2.73	110.61	114.98
2	F	701	CIT	C3-C4-C5	2.72	119.33	114.98
2	B	702	CIT	C3-C2-C1	-2.68	110.70	114.98
2	K	703	CIT	C3-C2-C1	2.67	119.26	114.98
2	E	701	CIT	C3-C2-C1	-2.52	110.95	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	701	CIT	C3-C4-C5	2.51	119.00	114.98
2	L	701	CIT	C3-C2-C1	-2.45	111.07	114.98
2	B	701	CIT	C3-C4-C5	2.31	118.69	114.98
2	K	703	CIT	C3-C4-C5	-2.25	111.38	114.98
2	A	701	CIT	C4-C3-C2	-2.02	103.94	109.33
2	C	701	CIT	C3-C2-C1	-2.00	111.78	114.98

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	702	CIT	C6-C3-C4-C5
2	B	701	CIT	C2-C3-C4-C5
2	B	701	CIT	O7-C3-C4-C5
2	B	701	CIT	C6-C3-C4-C5
2	D	701	CIT	C6-C3-C4-C5
2	F	702	CIT	C6-C3-C4-C5
2	G	701	CIT	C1-C2-C3-C6
2	G	701	CIT	C2-C3-C4-C5
2	G	701	CIT	O7-C3-C4-C5
2	G	701	CIT	C6-C3-C4-C5
2	I	701	CIT	C1-C2-C3-C6
2	K	701	CIT	C6-C3-C4-C5
2	K	703	CIT	C6-C3-C4-C5
2	K	701	CIT	C2-C3-C4-C5
2	A	702	CIT	O7-C3-C4-C5
2	K	701	CIT	O7-C3-C4-C5
2	A	702	CIT	C2-C3-C4-C5
2	D	701	CIT	O7-C3-C4-C5
2	I	701	CIT	C1-C2-C3-C4
2	K	703	CIT	C2-C3-C4-C5
2	K	703	CIT	O7-C3-C4-C5
2	G	701	CIT	C1-C2-C3-O7
2	I	701	CIT	C1-C2-C3-O7
2	D	701	CIT	C2-C3-C4-C5
2	G	701	CIT	C1-C2-C3-C4
2	A	702	CIT	C1-C2-C3-C6
2	B	701	CIT	C1-C2-C3-C6
2	B	702	CIT	C6-C3-C4-C5
2	H	702	CIT	C6-C3-C4-C5
2	K	701	CIT	C1-C2-C3-C6
2	F	702	CIT	O7-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	B	701	CIT	C1-C2-C3-O7

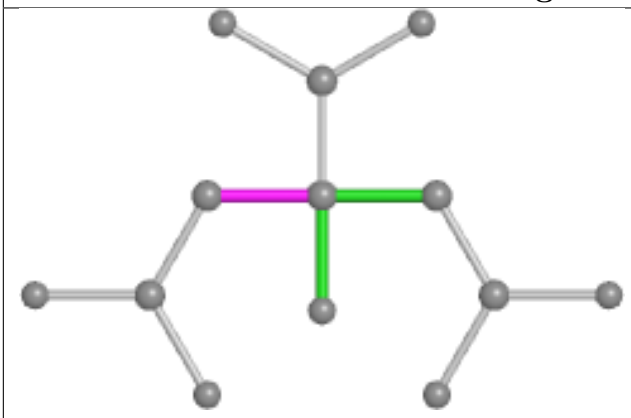
There are no ring outliers.

16 monomers are involved in 40 short contacts:

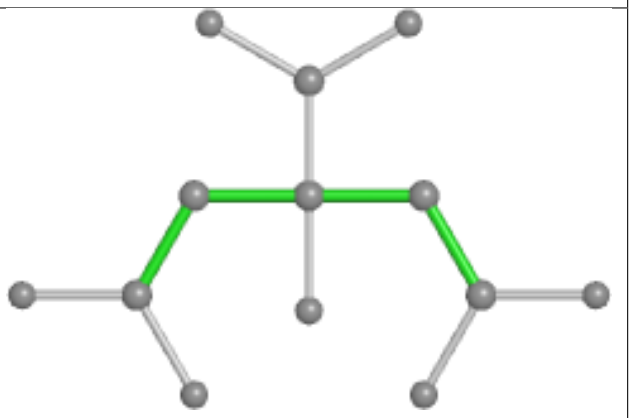
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	701	CIT	2	0
2	A	701	CIT	1	0
2	H	702	CIT	1	0
2	F	701	CIT	1	0
2	K	701	CIT	10	0
2	J	701	CIT	3	0
2	D	701	CIT	3	0
2	E	701	CIT	3	0
2	L	701	CIT	2	0
2	A	702	CIT	10	0
2	G	701	CIT	2	0
2	F	702	CIT	1	0
2	B	702	CIT	2	0
2	B	701	CIT	5	0
2	C	701	CIT	2	0
2	K	703	CIT	1	0

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

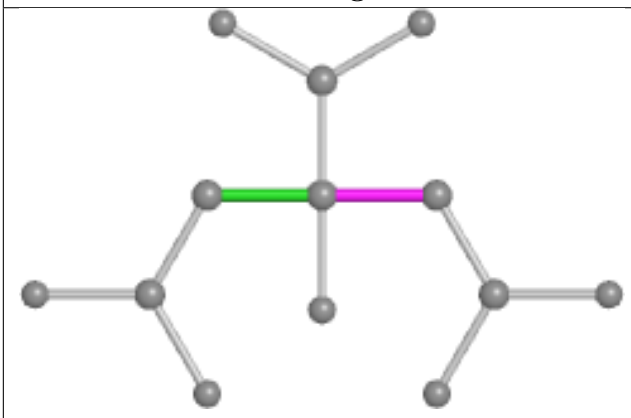
Ligand CIT I 701



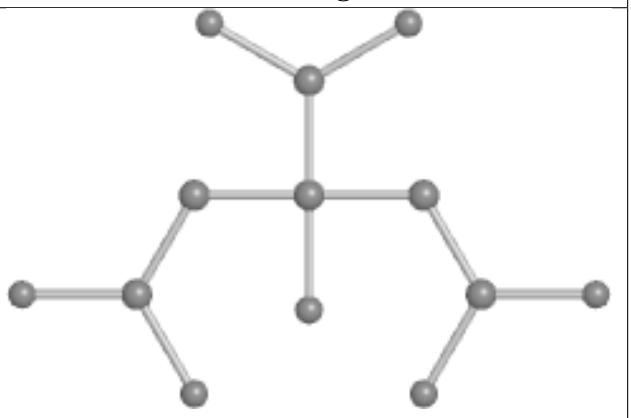
Bond lengths



Bond angles

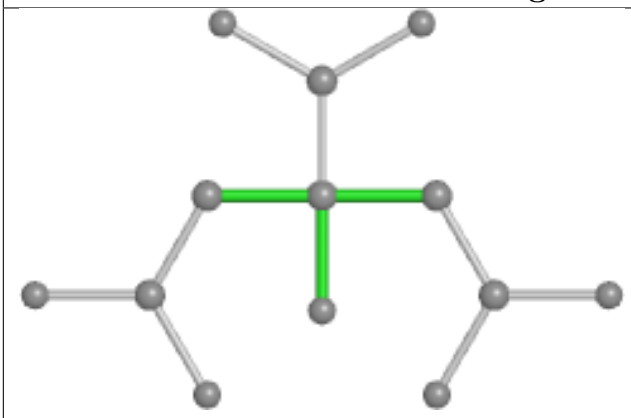


Torsions

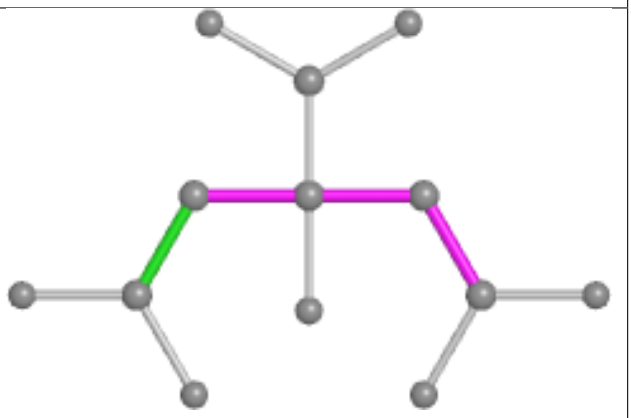


Rings

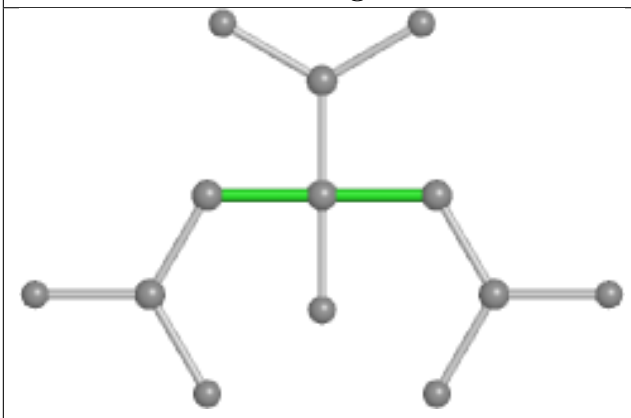
Ligand CIT A 701



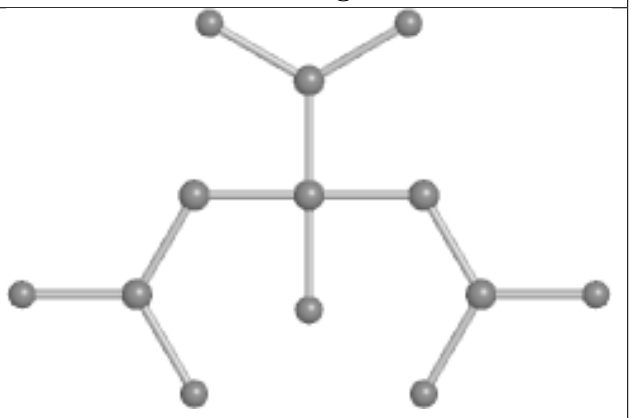
Bond lengths



Bond angles

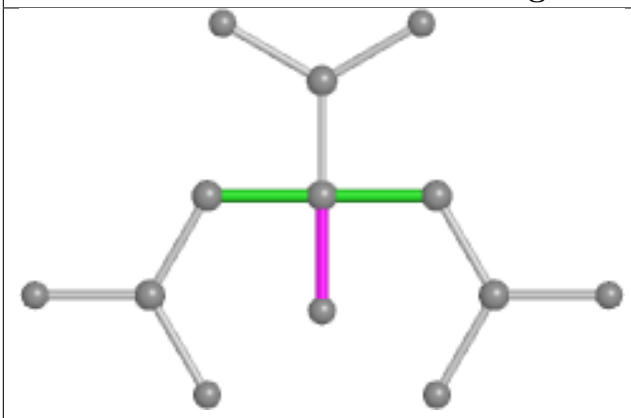


Torsions



Rings

Ligand CIT H 702



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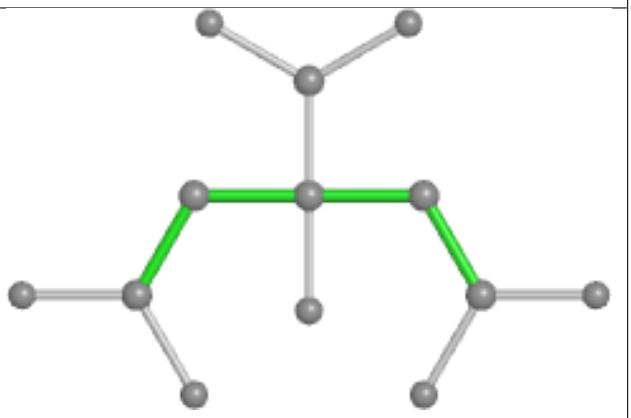

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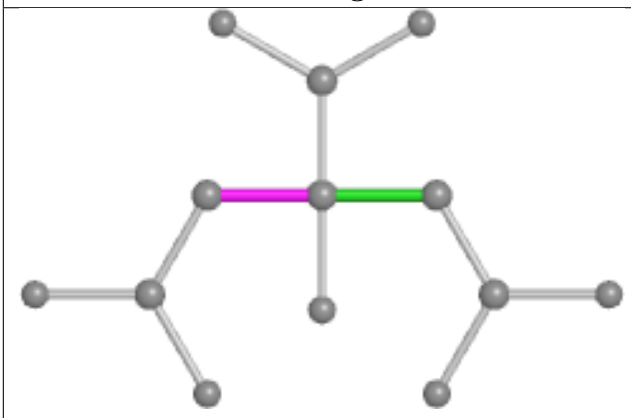

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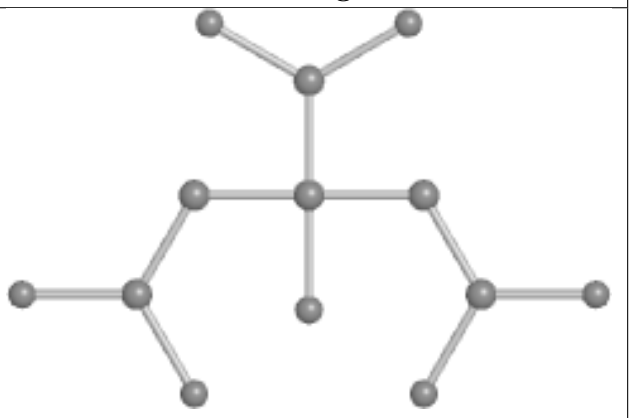
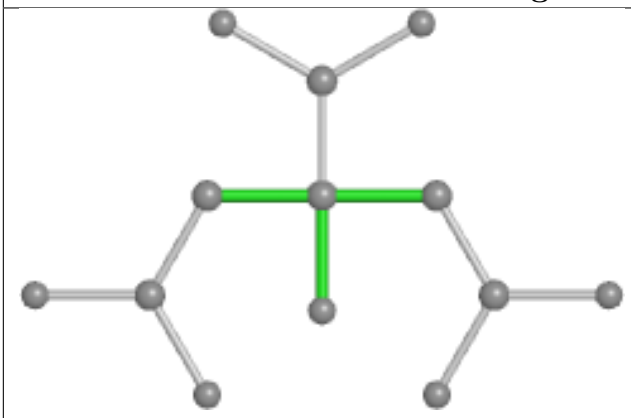


Rings

Ligand CIT F 701



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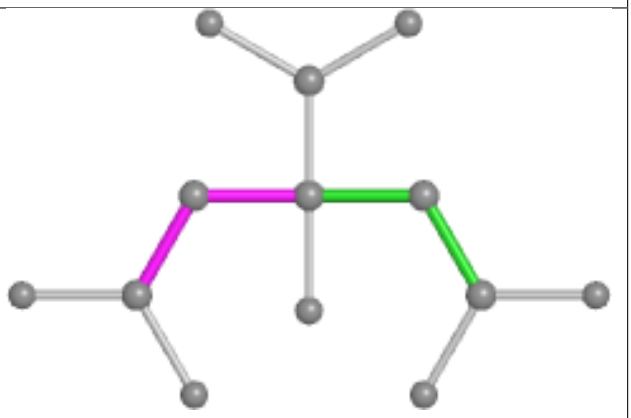

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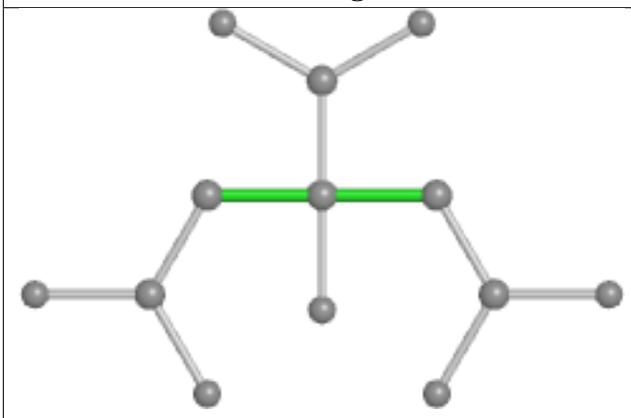

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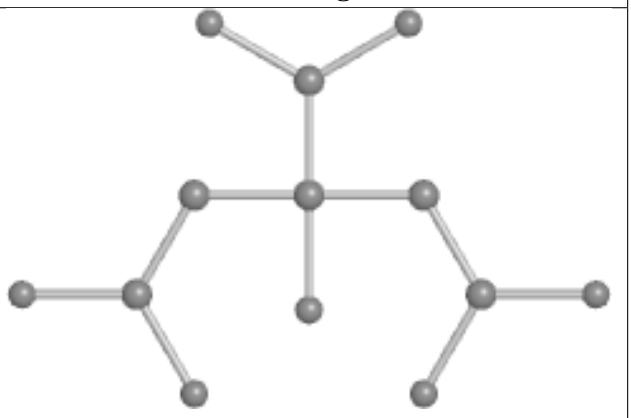
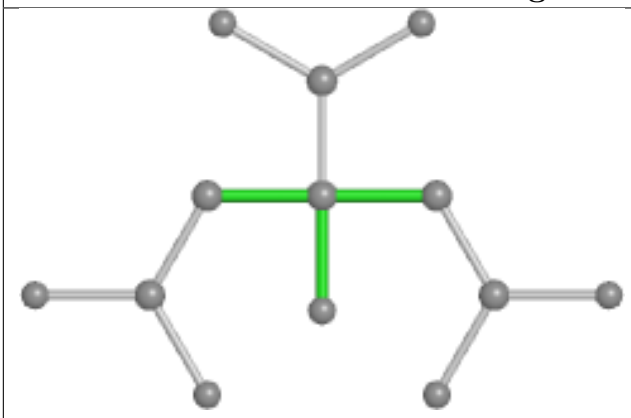


Rings

Ligand CIT K 701



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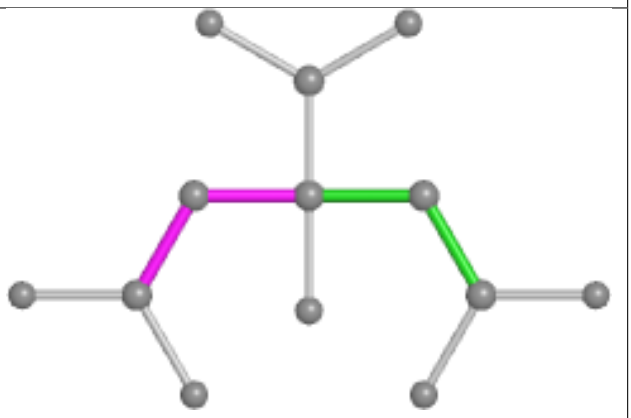

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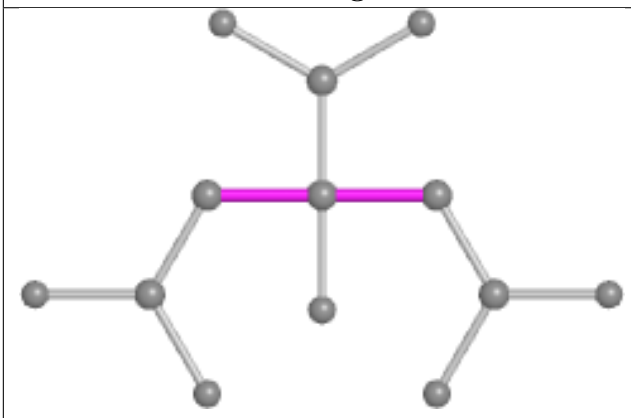

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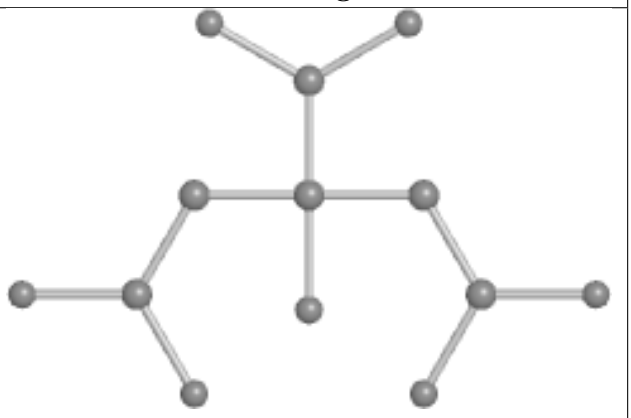
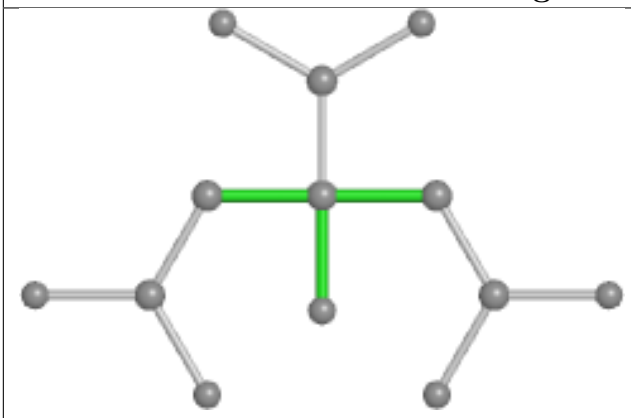


Rings

Ligand CIT J 701



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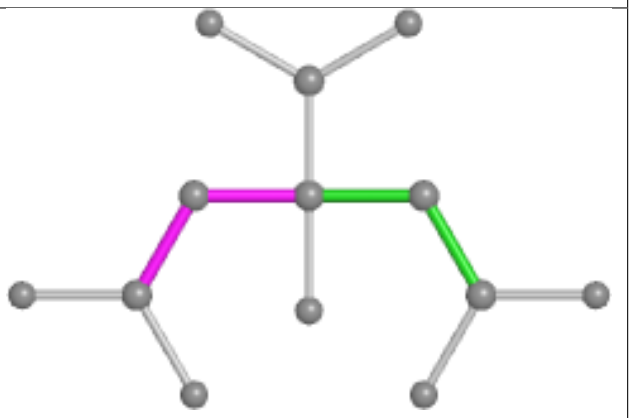

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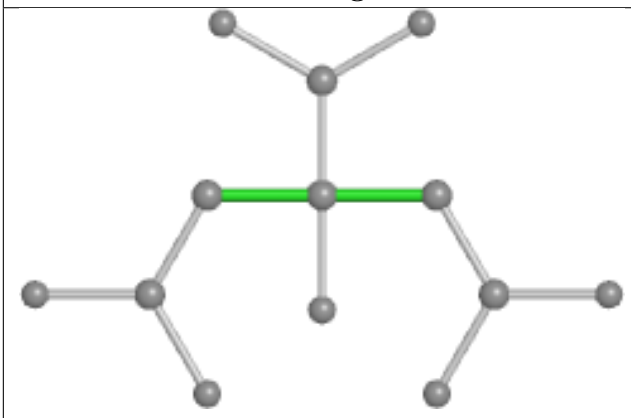

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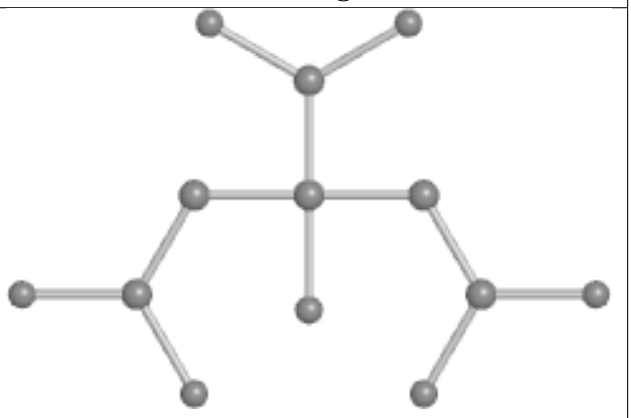
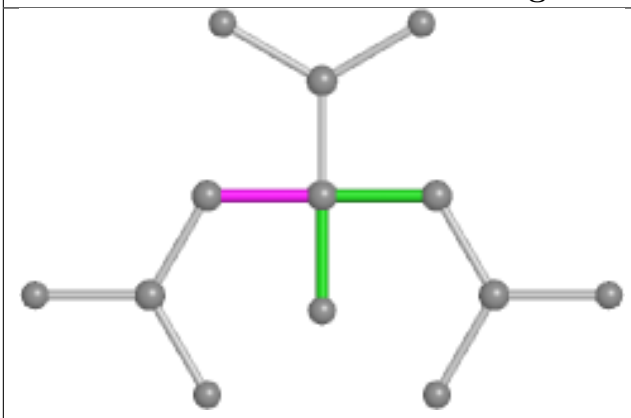


Rings

Ligand CIT D 701



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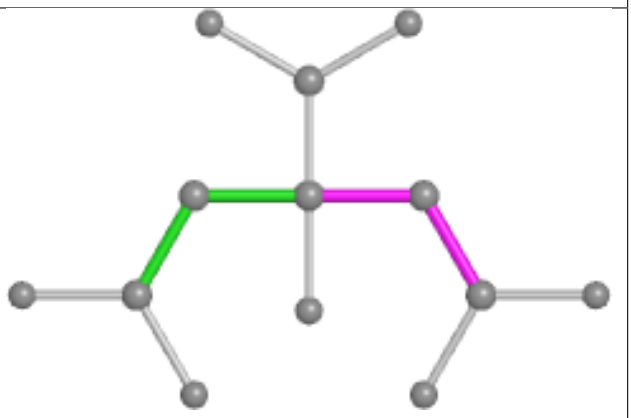

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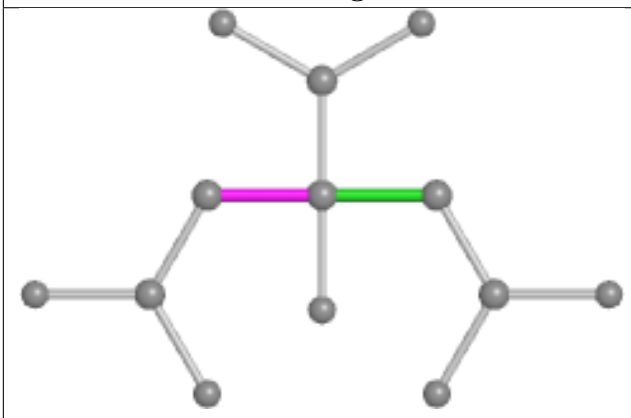

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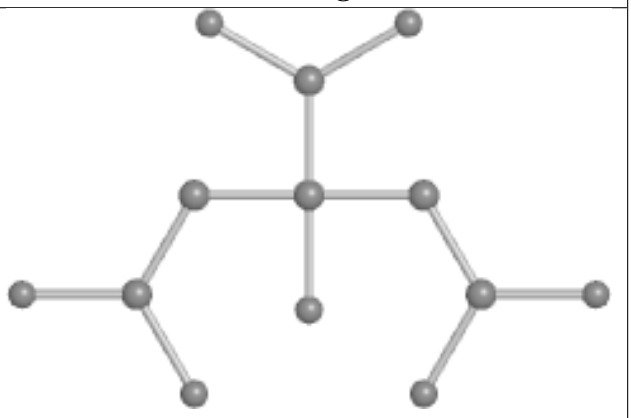
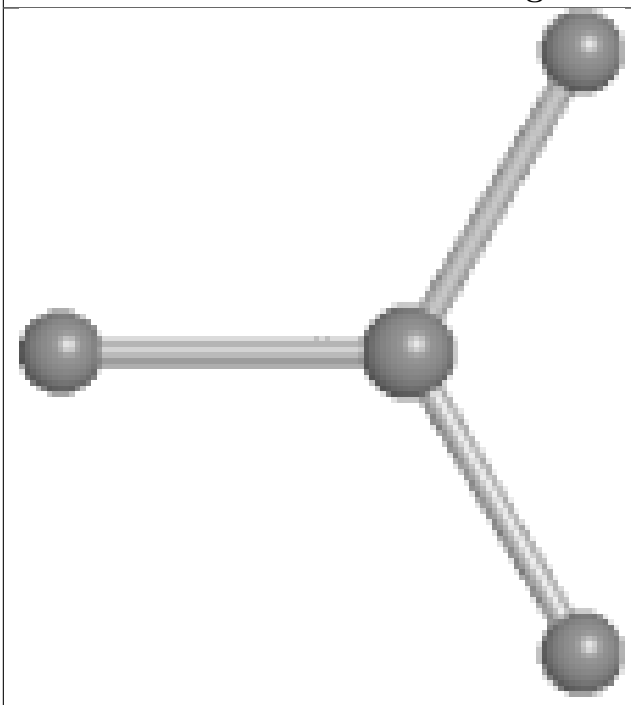


Rings

Ligand CO3 C 702



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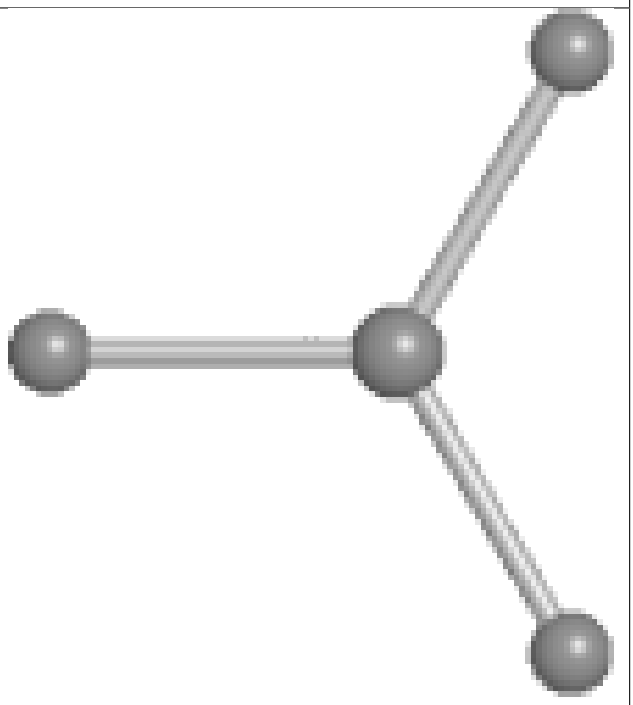

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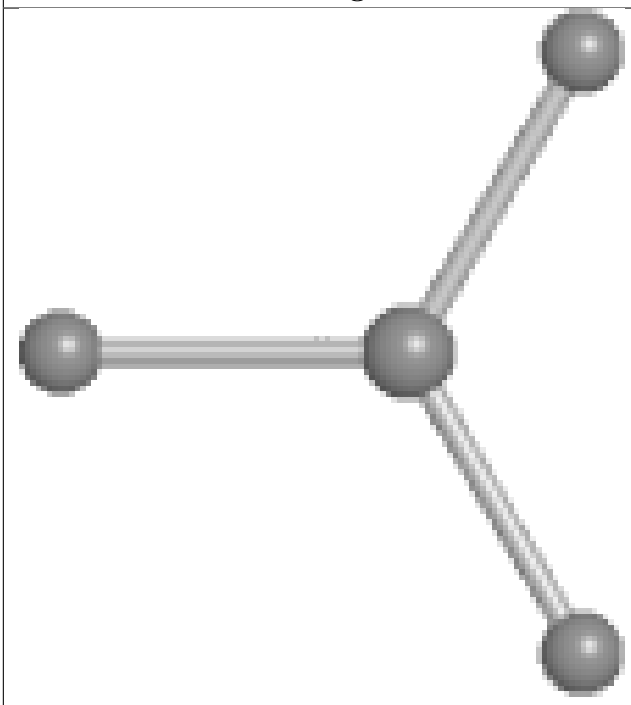

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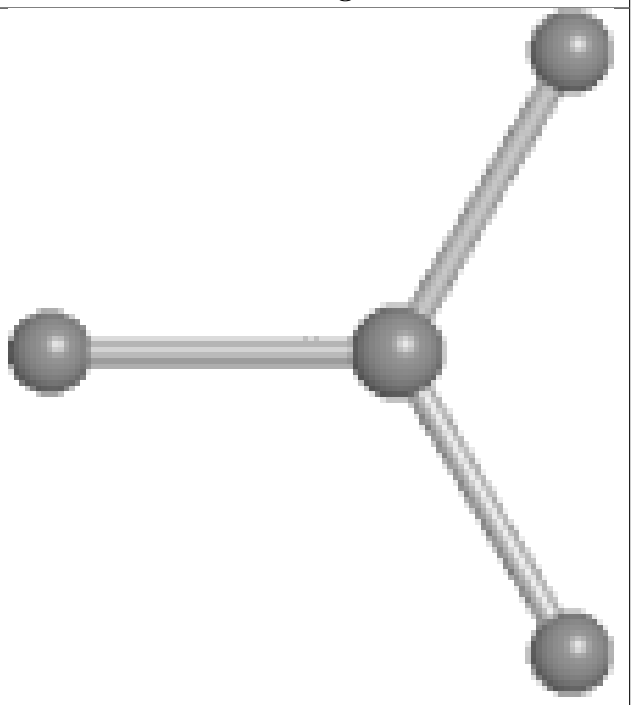
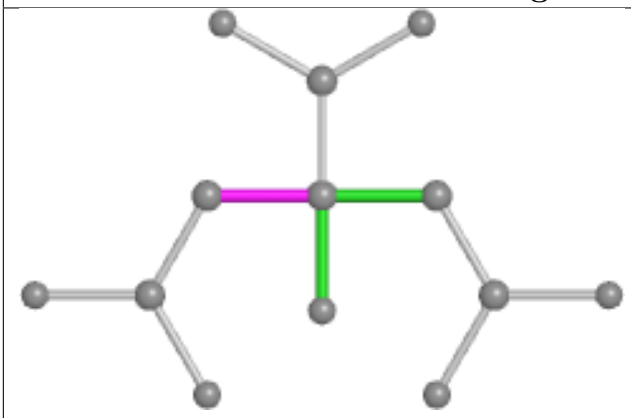


Rings

Ligand CIT E 701



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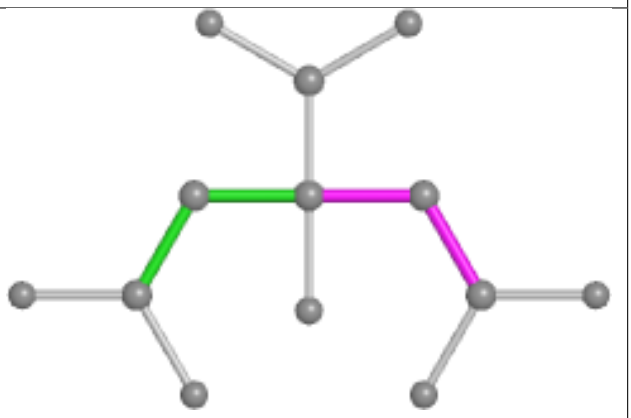

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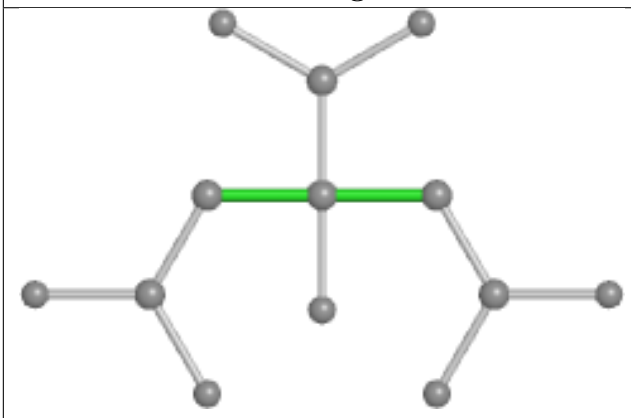

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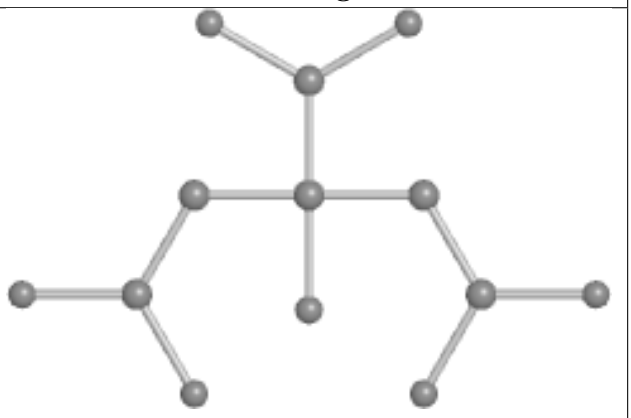
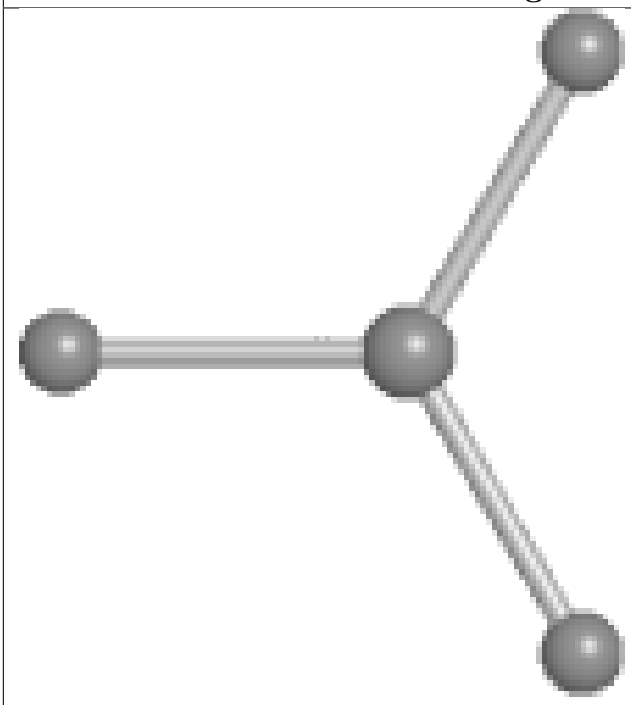


Rings

Ligand CO3 K 702



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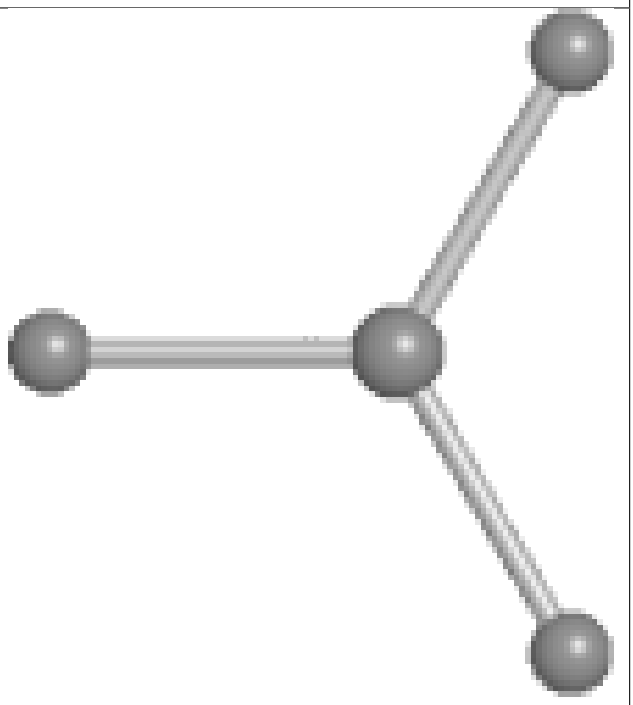

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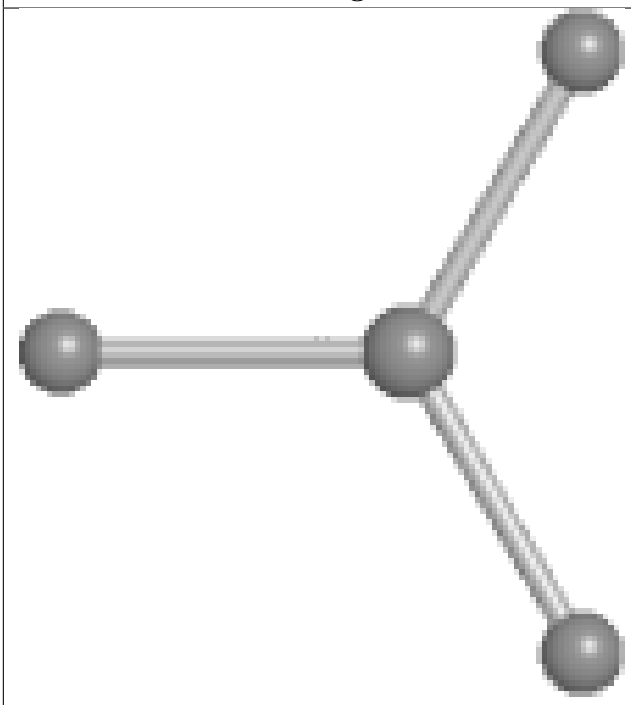

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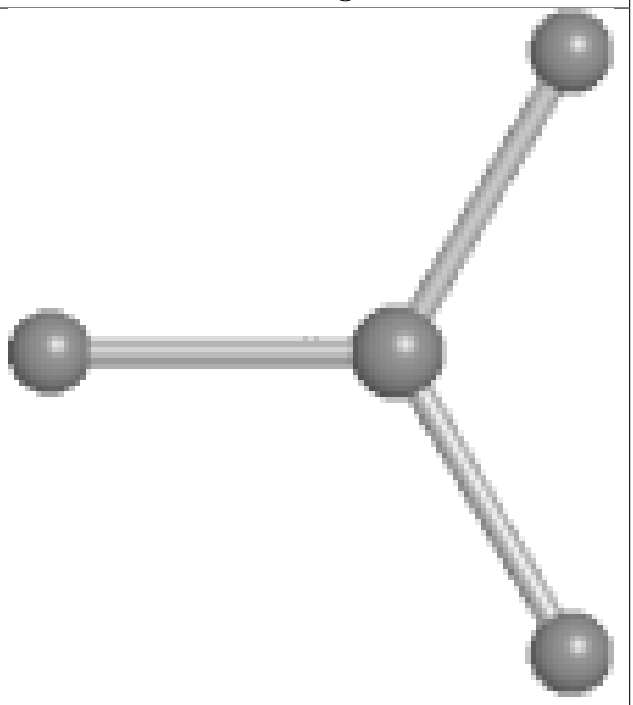

Rings

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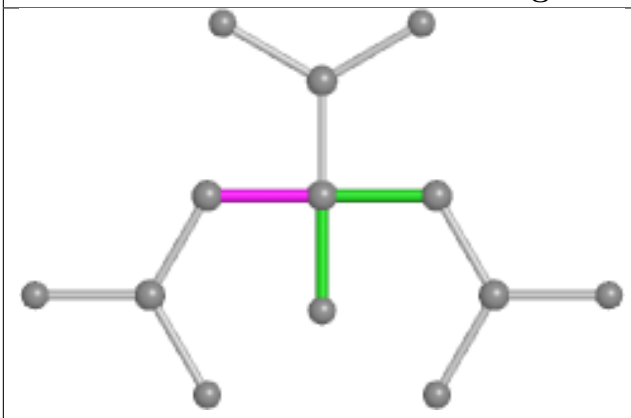

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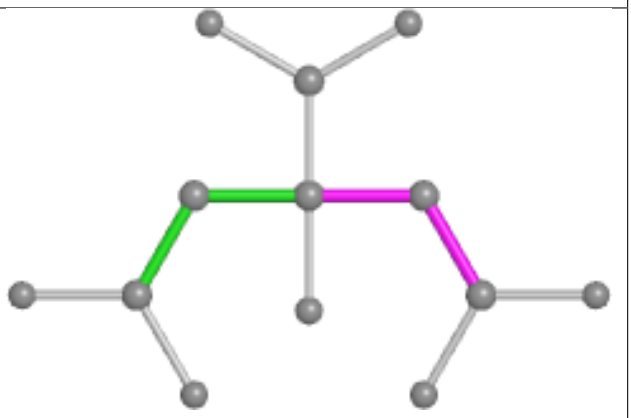

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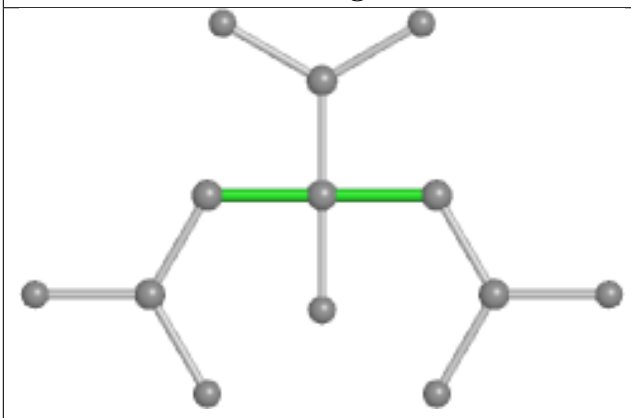

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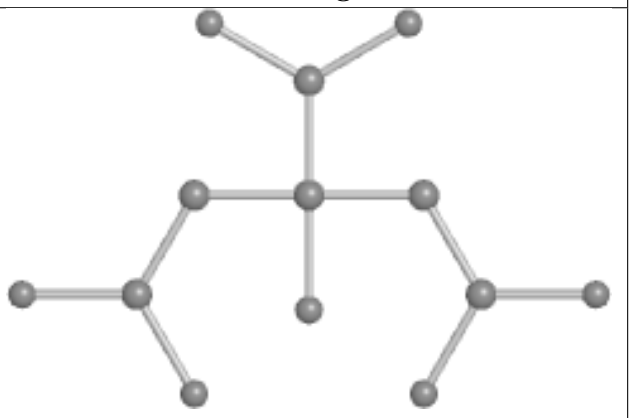
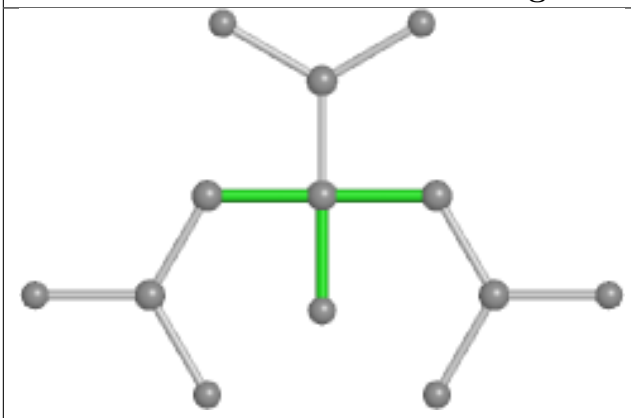


Rings

Ligand CIT A 702



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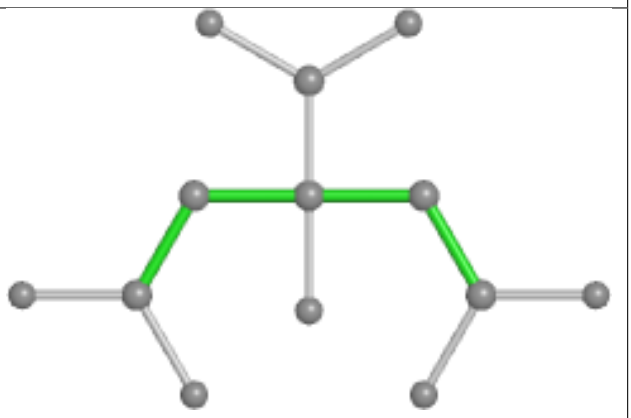

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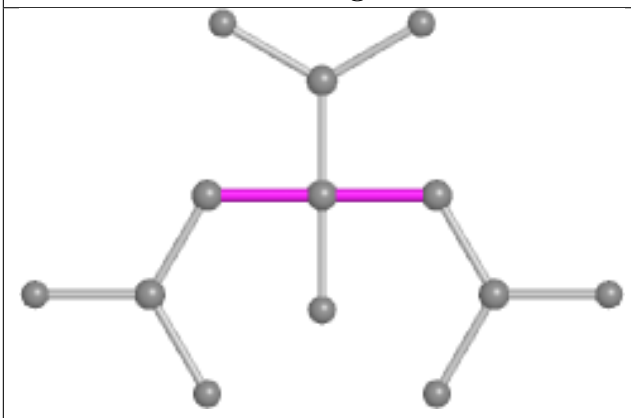

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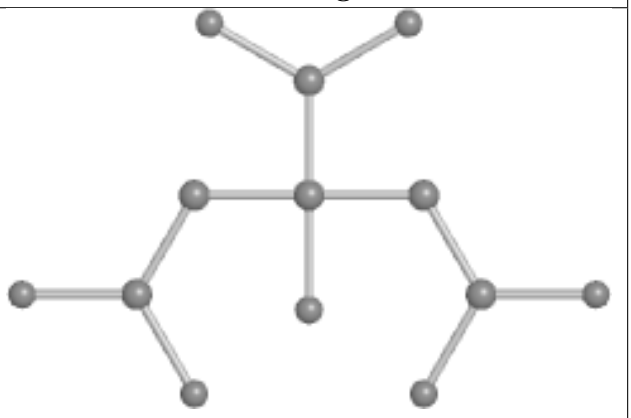
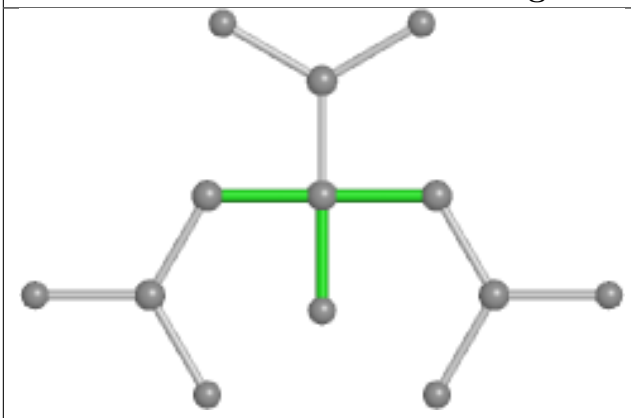


Rings

Ligand CIT G 701



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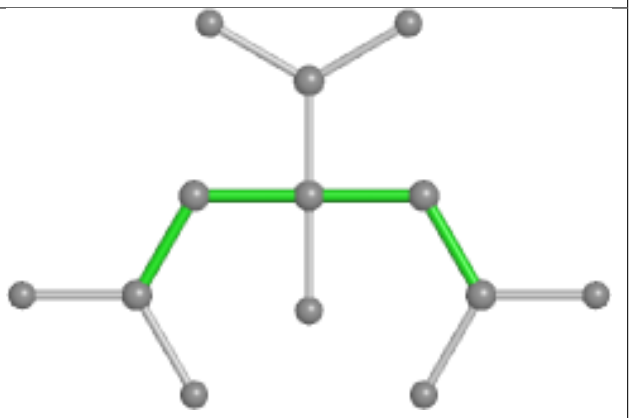

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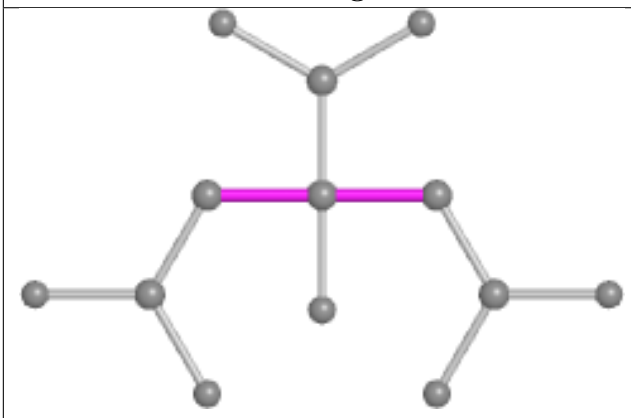

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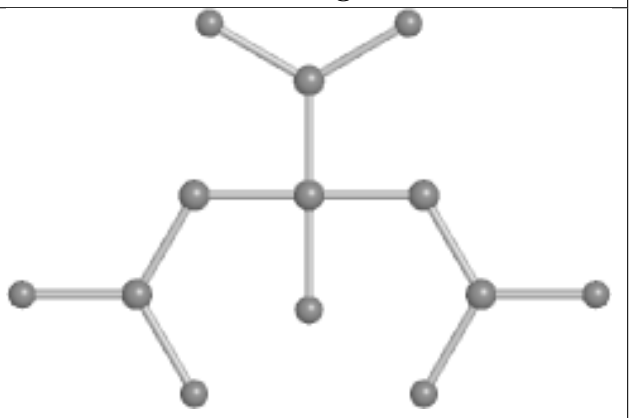
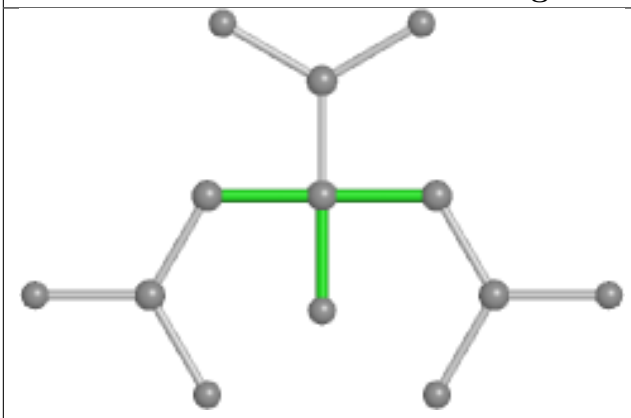


Rings

Ligand CIT F 702



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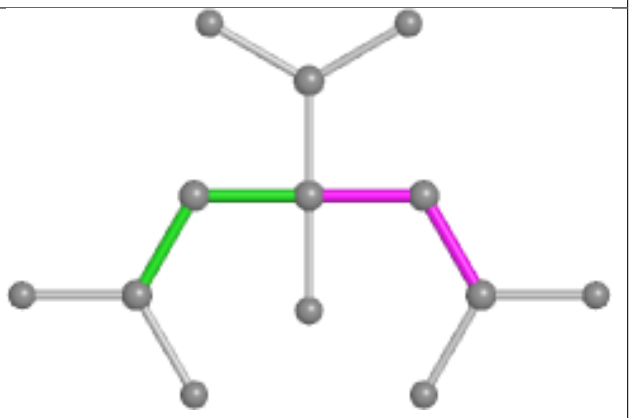

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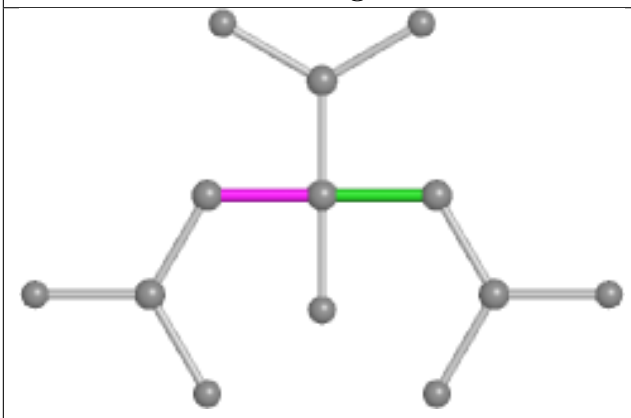

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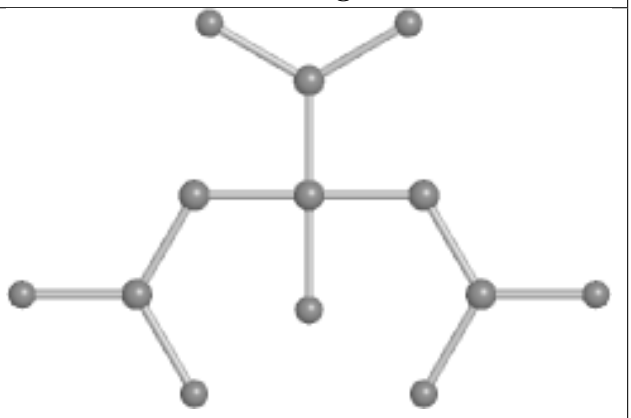
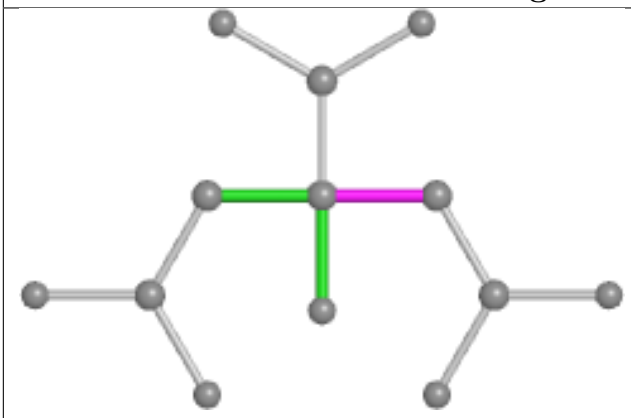


Rings

Ligand CIT B 702



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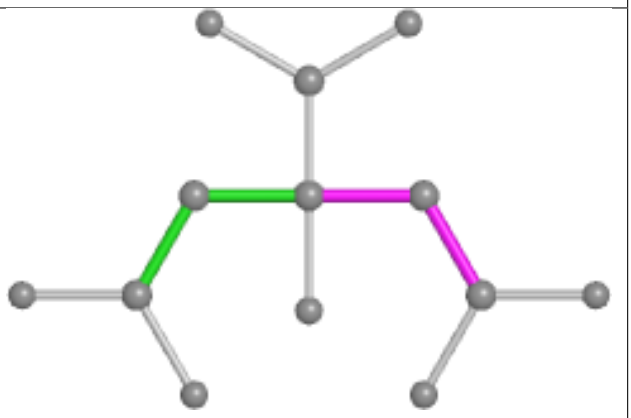

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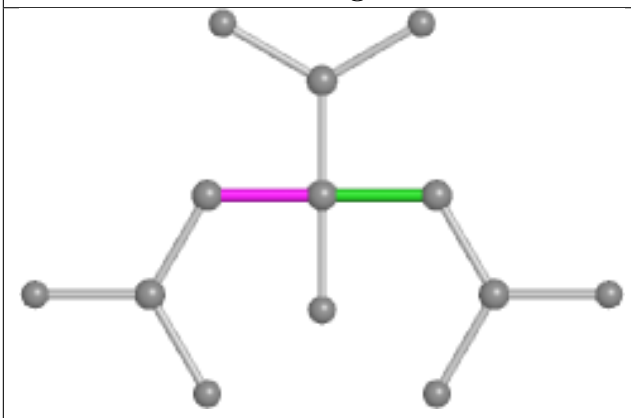

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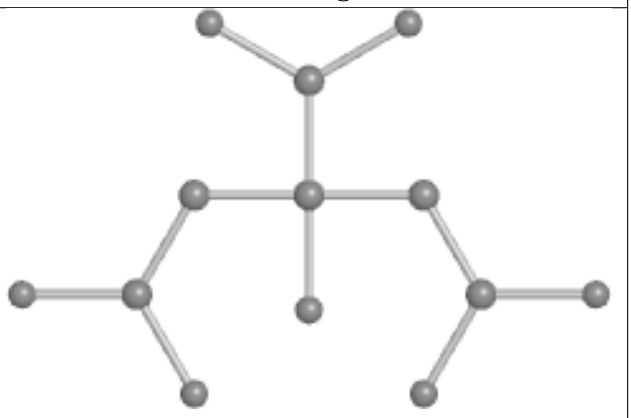
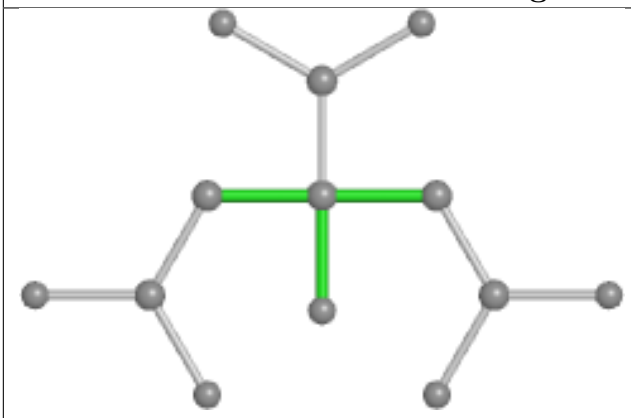


Rings

Ligand CIT B 701



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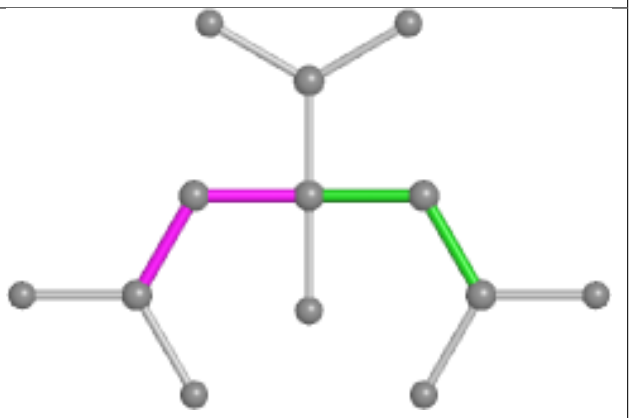

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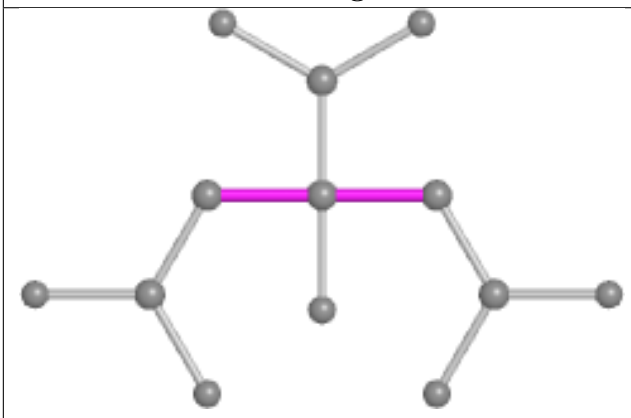

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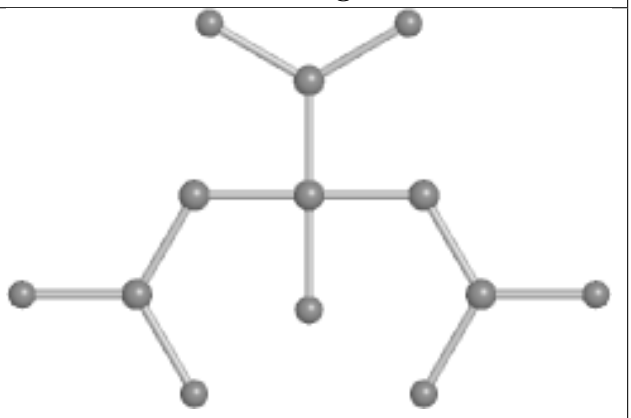
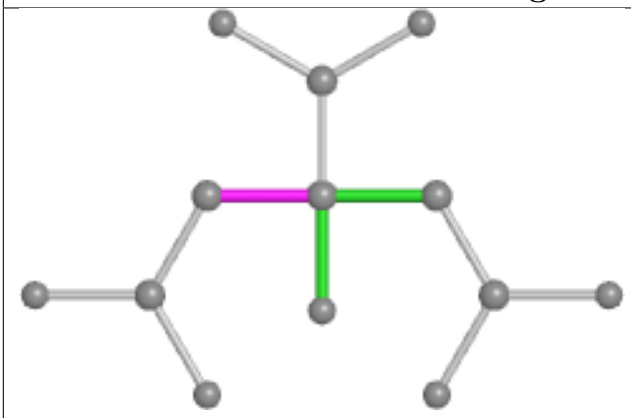
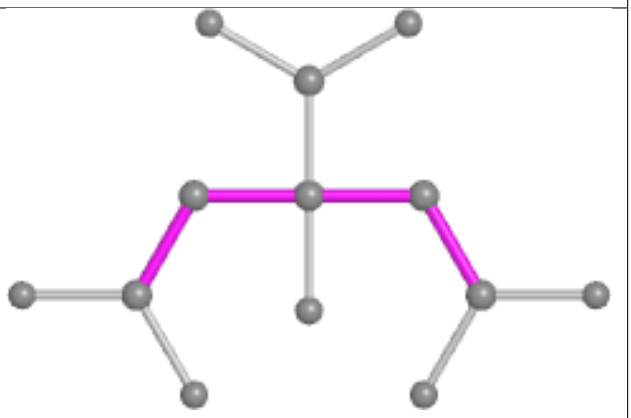


Rings

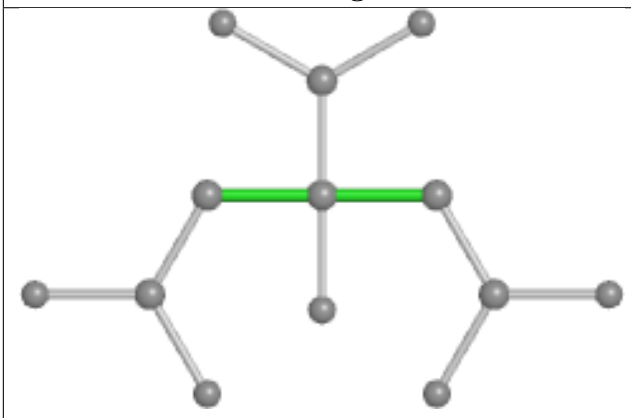
Ligand CIT C 701



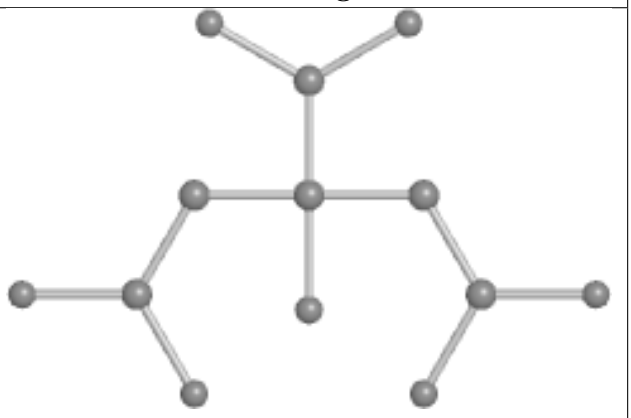
Bond lengths



Bond angles

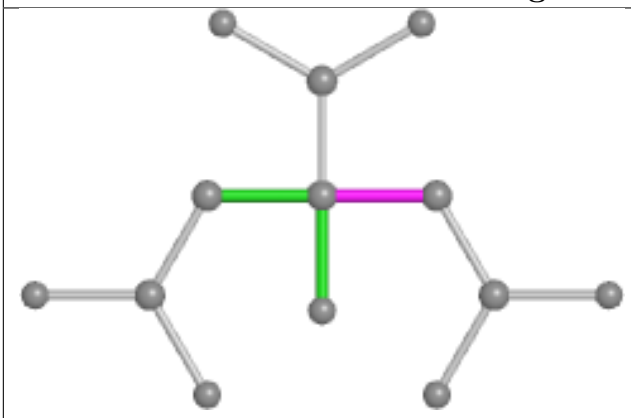


Torsions

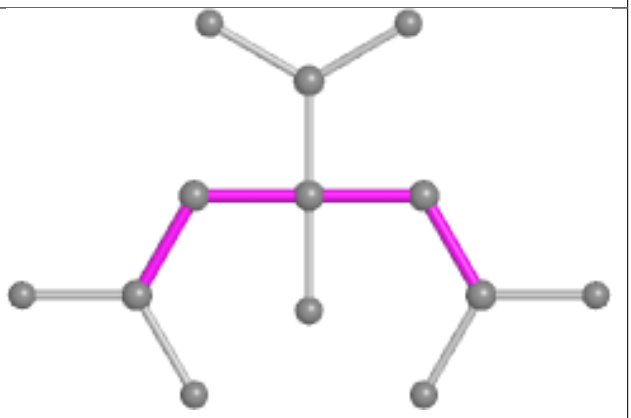


Rings

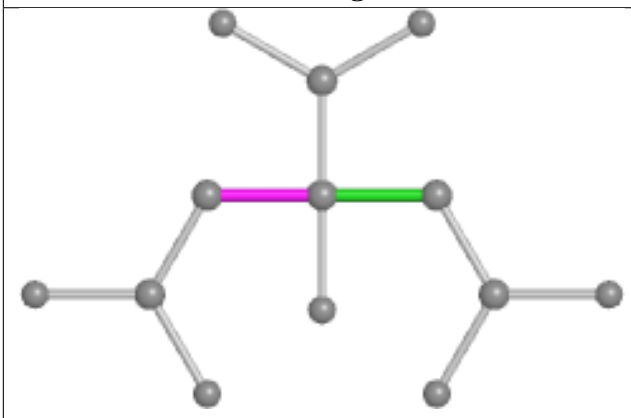
Ligand CIT K 703



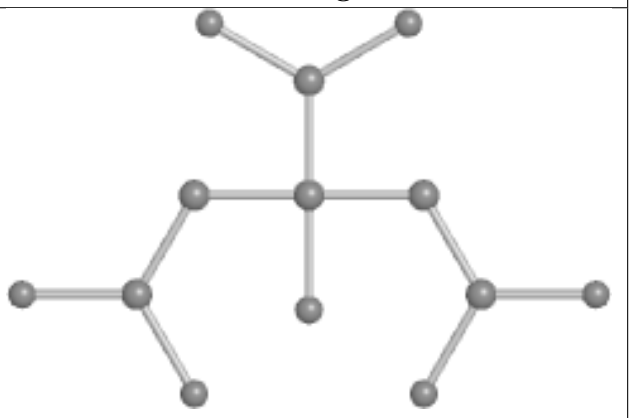
Bond lengths



Bond angles

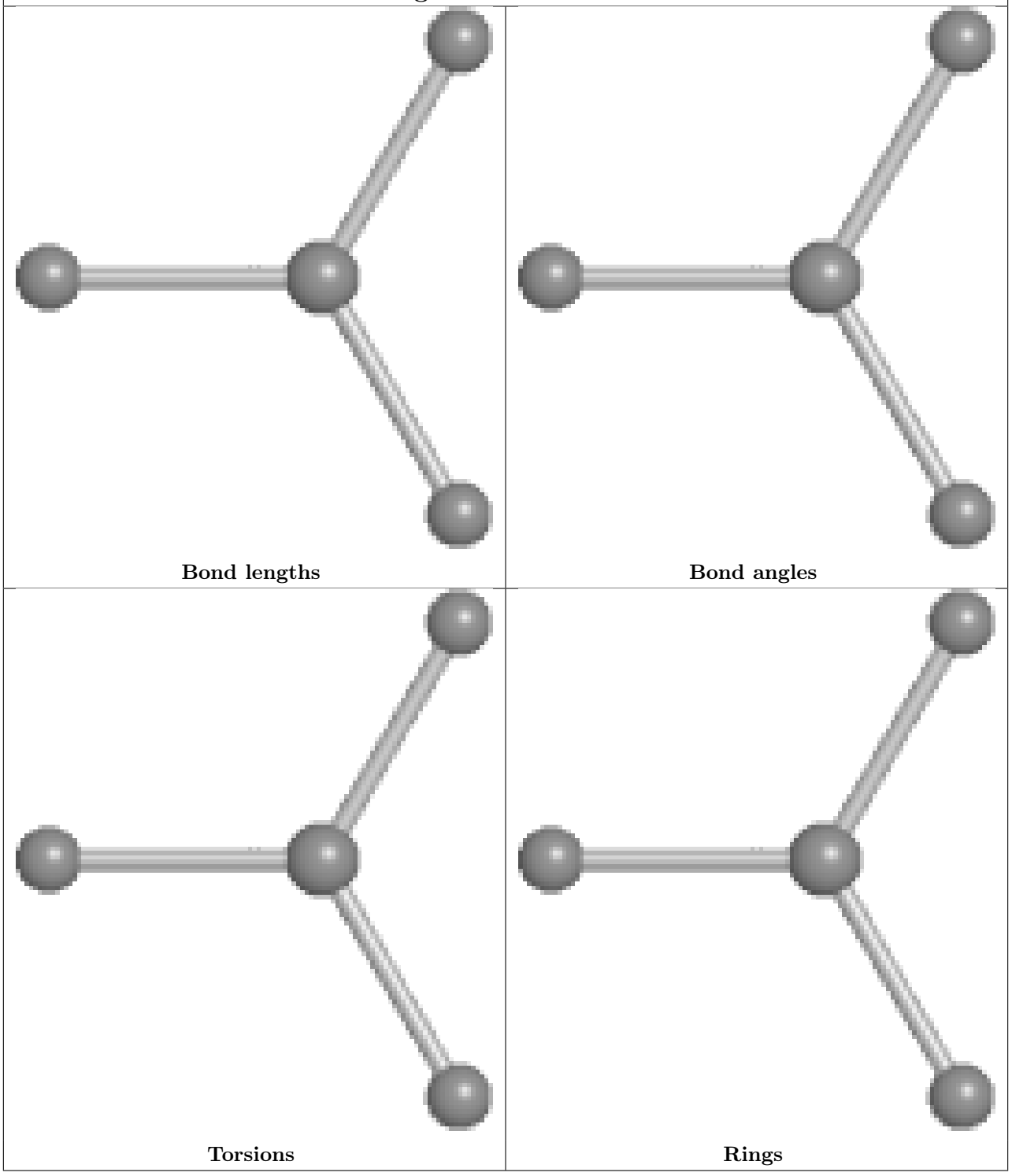


Torsions



Rings

Ligand CO3 H 701



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, 95^{th} 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%)	-0.69	3 (0%)	91	90	9, 24, 70, 114	0
1	B	644/671 (95%)	-0.58	11 (1%)	70	67	9, 24, 74, 129	0
1	C	644/671 (95%)	-0.72	3 (0%)	91	90	8, 21, 48, 99	0
1	D	643/671 (95%)	-0.55	9 (1%)	75	73	12, 26, 65, 123	0
1	E	643/671 (95%)	-0.54	10 (1%)	72	69	12, 27, 69, 123	0
1	F	644/671 (95%)	-0.59	10 (1%)	72	69	8, 22, 62, 122	0
1	G	642/671 (95%)	-0.60	4 (0%)	89	88	9, 29, 53, 86	0
1	H	646/671 (96%)	-0.68	2 (0%)	94	94	10, 27, 57, 89	0
1	I	644/671 (95%)	-0.47	7 (1%)	80	78	12, 32, 64, 128	0
1	J	642/671 (95%)	-0.20	28 (4%)	34	28	13, 39, 88, 112	0
1	K	642/671 (95%)	-0.31	17 (2%)	56	51	12, 34, 84, 109	0
1	L	642/671 (95%)	-0.18	19 (2%)	50	45	19, 40, 88, 111	0
All	All	7718/8052 (95%)	-0.51	123 (1%)	72	69	8, 28, 75, 129	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	35	GLY	7.7
1	B	9	PRO	5.5
1	F	34	LEU	5.5
1	E	36	SER	5.4
1	F	36	SER	5.1
1	B	8	ALA	5.1
1	B	10	GLU	5.1
1	E	9	PRO	4.7
1	J	35	GLY	4.5
1	D	35	GLY	4.5
1	K	623	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	L	23	PRO	4.5
1	J	622	VAL	4.3
1	K	24	ASN	4.1
1	D	14	SER	4.0
1	J	14	SER	4.0
1	E	35	GLY	4.0
1	F	14	SER	3.9
1	D	34	LEU	3.8
1	J	24	ASN	3.7
1	K	624	THR	3.7
1	K	16	LEU	3.7
1	J	17	ALA	3.7
1	L	623	PRO	3.6
1	D	345	ASP	3.6
1	L	35	GLY	3.6
1	K	47	ALA	3.5
1	D	24	ASN	3.5
1	K	629	LEU	3.5
1	E	623	PRO	3.5
1	F	8	ALA	3.4
1	J	15	ASP	3.4
1	L	24	ASN	3.4
1	F	46	THR	3.3
1	D	36	SER	3.3
1	J	36	SER	3.3
1	I	9	PRO	3.3
1	J	623	PRO	3.3
1	I	622	VAL	3.3
1	E	47	ALA	3.3
1	J	25	PHE	3.2
1	B	622	VAL	3.2
1	L	622	VAL	3.2
1	C	9	PRO	3.2
1	J	624	THR	3.1
1	J	22	TYR	3.1
1	D	622	VAL	3.1
1	L	27	VAL	3.1
1	A	622	VAL	3.0
1	L	28	GLN	3.0
1	J	16	LEU	3.0
1	B	47	ALA	3.0
1	K	14	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	21	ALA	3.0
1	K	22	TYR	3.0
1	J	48	SER	3.0
1	F	9	PRO	2.9
1	K	621	ASP	2.9
1	K	622	VAL	2.9
1	J	23	PRO	2.9
1	I	623	PRO	2.9
1	B	15	ASP	2.8
1	L	569	LEU	2.8
1	I	8	ALA	2.8
1	J	621	ASP	2.8
1	J	10	GLU	2.8
1	L	34	LEU	2.8
1	G	545	THR	2.7
1	E	27	VAL	2.7
1	L	637	SER	2.6
1	B	25	PHE	2.6
1	F	10	GLU	2.6
1	A	623	PRO	2.5
1	B	11	ARG	2.5
1	C	47	ALA	2.5
1	I	621	ASP	2.5
1	K	15	ASP	2.5
1	B	623	PRO	2.4
1	L	61	GLY	2.4
1	L	624	THR	2.4
1	L	10	GLU	2.4
1	F	23	PRO	2.4
1	L	545	THR	2.4
1	I	24	ASN	2.4
1	F	24	ASN	2.4
1	A	14	SER	2.3
1	J	34	LEU	2.3
1	E	34	LEU	2.3
1	L	60	GLY	2.3
1	L	643	SER	2.3
1	J	13	PHE	2.3
1	J	642	VAL	2.3
1	C	624	THR	2.3
1	G	37	ALA	2.3
1	E	624	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	10	GLU	2.2
1	E	640	ALA	2.2
1	L	47	ALA	2.2
1	K	23	PRO	2.2
1	D	22	TYR	2.2
1	G	26	GLN	2.2
1	B	36	SER	2.2
1	J	28	GLN	2.2
1	J	571	ALA	2.1
1	G	36	SER	2.1
1	I	202	SER	2.1
1	L	570	VAL	2.1
1	J	625	PRO	2.1
1	J	21	ALA	2.1
1	L	126	ALA	2.1
1	J	46	THR	2.1
1	K	28	GLN	2.1
1	K	570	VAL	2.1
1	B	24	ASN	2.1
1	K	639	ALA	2.1
1	E	14	SER	2.1
1	J	43	PHE	2.1
1	J	26	GLN	2.0
1	J	45	THR	2.0
1	H	620	GLN	2.0
1	D	9	PRO	2.0
1	J	202	SER	2.0
1	H	623	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

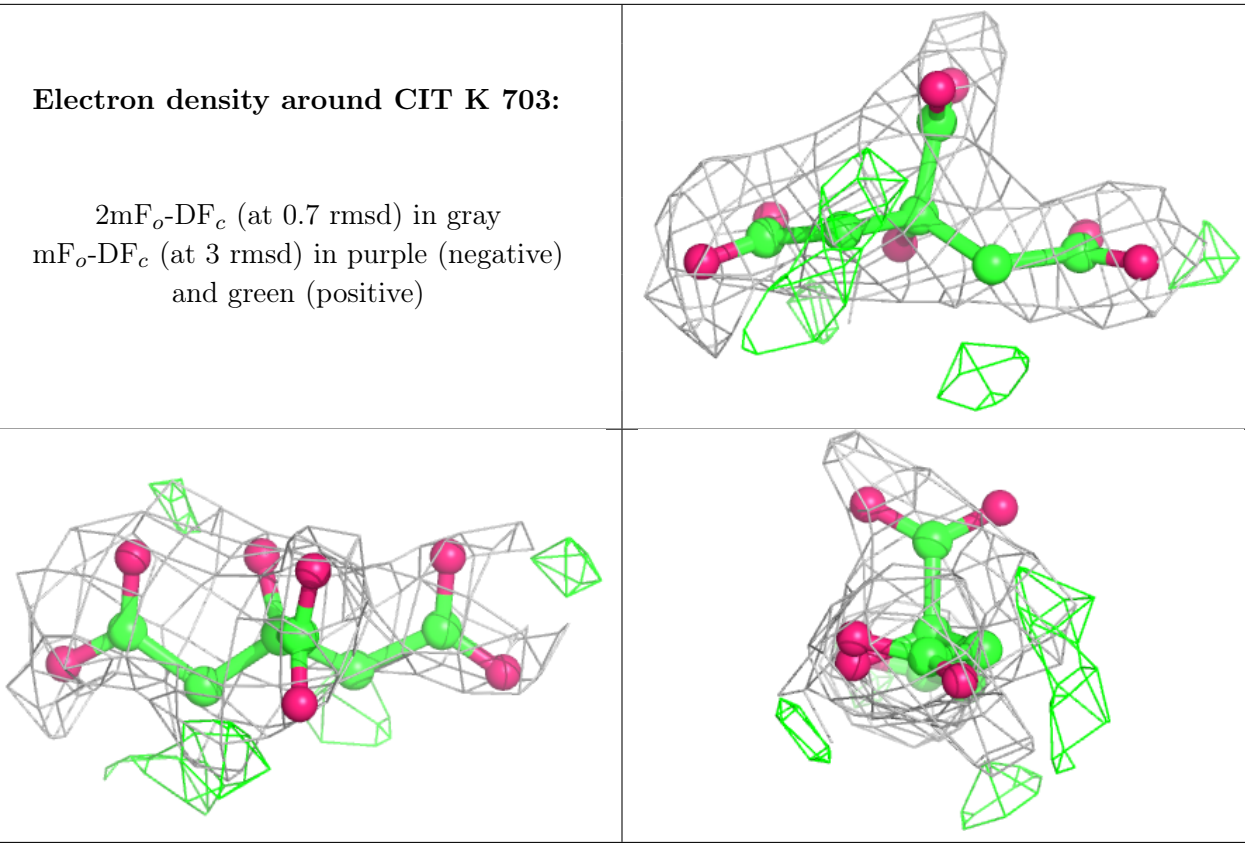
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	K	703	13/13	0.83	0.24	64,71,77,79	0
2	CIT	H	702	13/13	0.86	0.25	65,69,89,91	0
2	CIT	C	701	13/13	0.88	0.22	57,67,71,74	0
2	CIT	J	701	13/13	0.89	0.20	59,67,73,73	0
2	CIT	A	701	13/13	0.90	0.19	53,59,68,71	0
2	CIT	F	701	13/13	0.90	0.22	42,47,55,61	0
2	CIT	F	702	13/13	0.90	0.19	61,66,79,80	0
2	CIT	K	701	13/13	0.91	0.23	20,28,32,37	13
2	CIT	B	702	13/13	0.91	0.20	48,51,60,61	0
2	CIT	D	701	13/13	0.92	0.24	41,48,51,52	0
2	CIT	B	701	13/13	0.92	0.16	52,63,71,72	0
2	CIT	I	701	13/13	0.92	0.24	38,53,55,56	0
2	CIT	L	701	13/13	0.92	0.15	41,60,64,70	0
2	CIT	A	702	13/13	0.93	0.22	28,36,39,41	13
2	CIT	G	701	13/13	0.93	0.17	43,52,63,74	0
2	CIT	E	701	13/13	0.94	0.17	36,43,47,52	0
3	CO3	H	701	4/4	0.95	0.17	31,42,42,45	0
3	CO3	C	702	4/4	0.96	0.17	25,32,34,34	0
3	CO3	K	702	4/4	0.96	0.16	28,33,36,37	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.

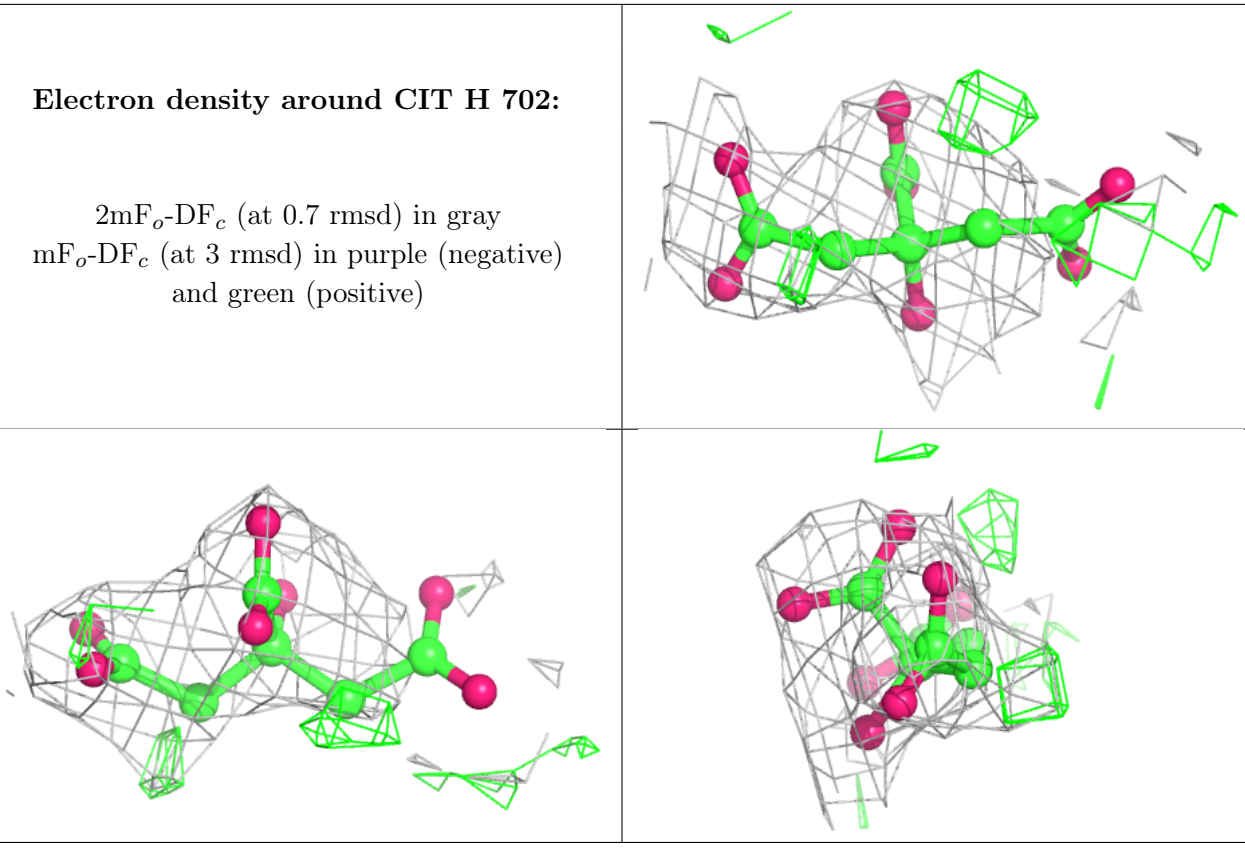
Electron density around CIT K 703:

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



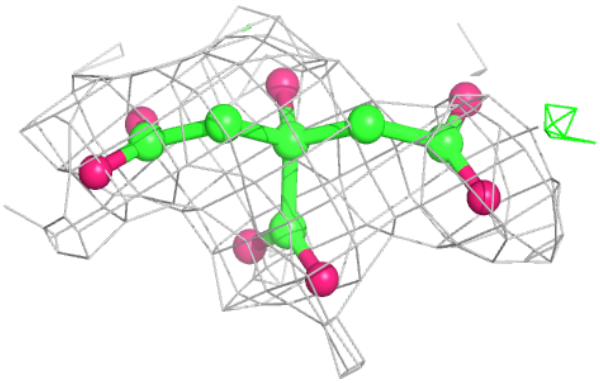
Electron density around CIT H 702:

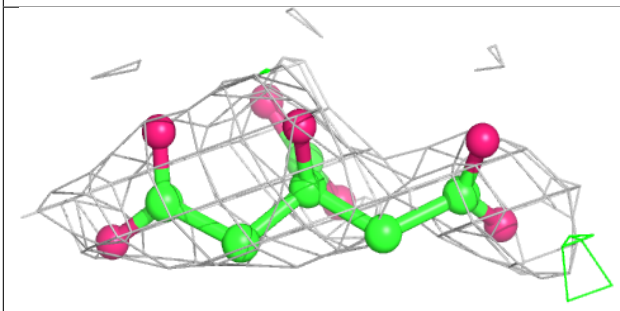
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

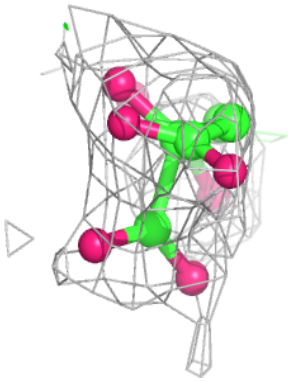


Electron density around CIT C 701:

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

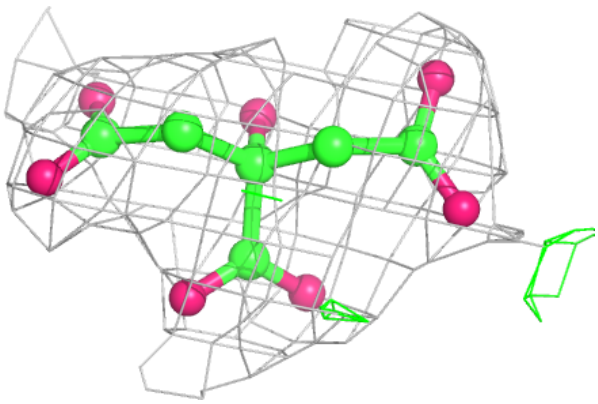


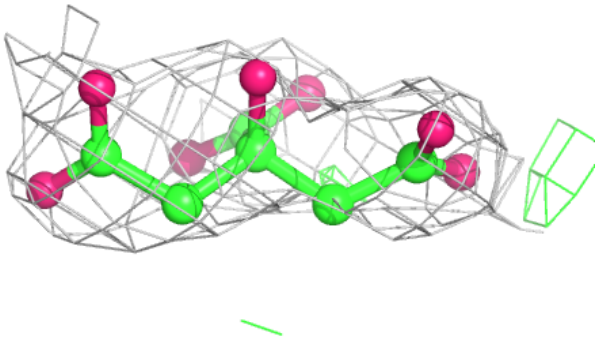


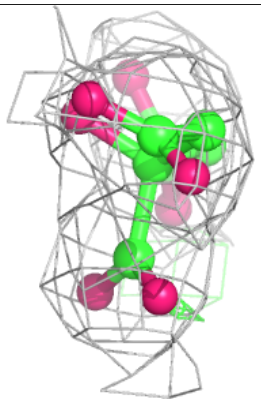


Electron density around CIT J 701:

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

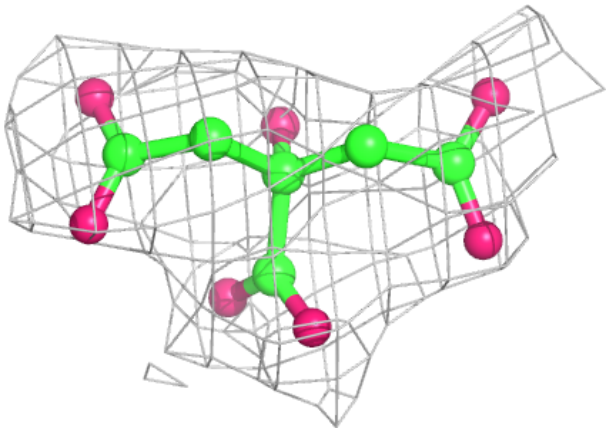


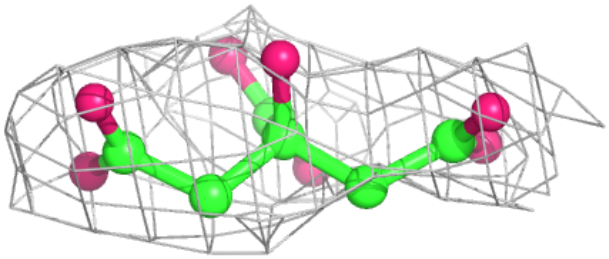


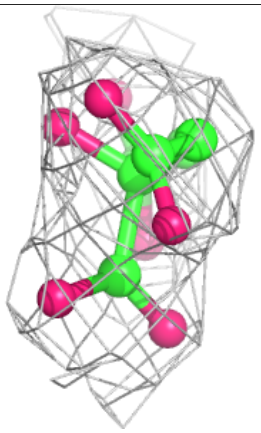


Electron density around CIT A 701:

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

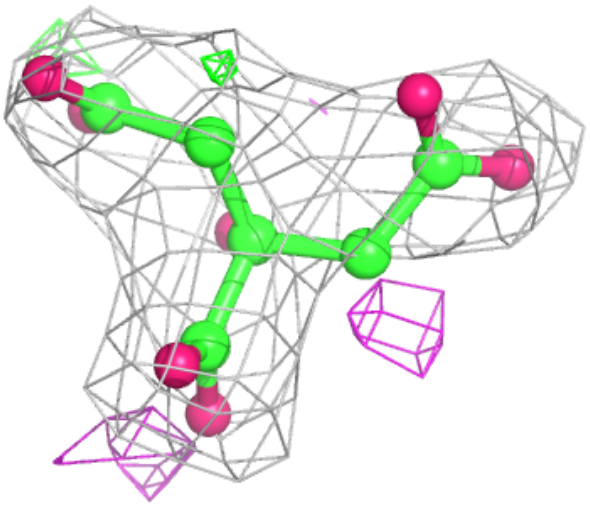


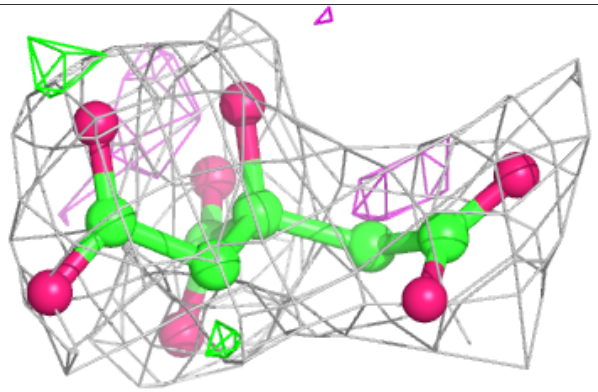


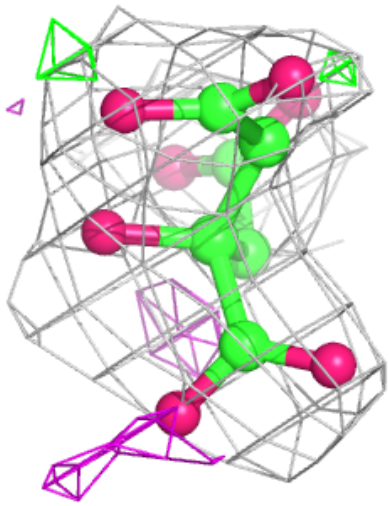


Electron density around CIT F 701:

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

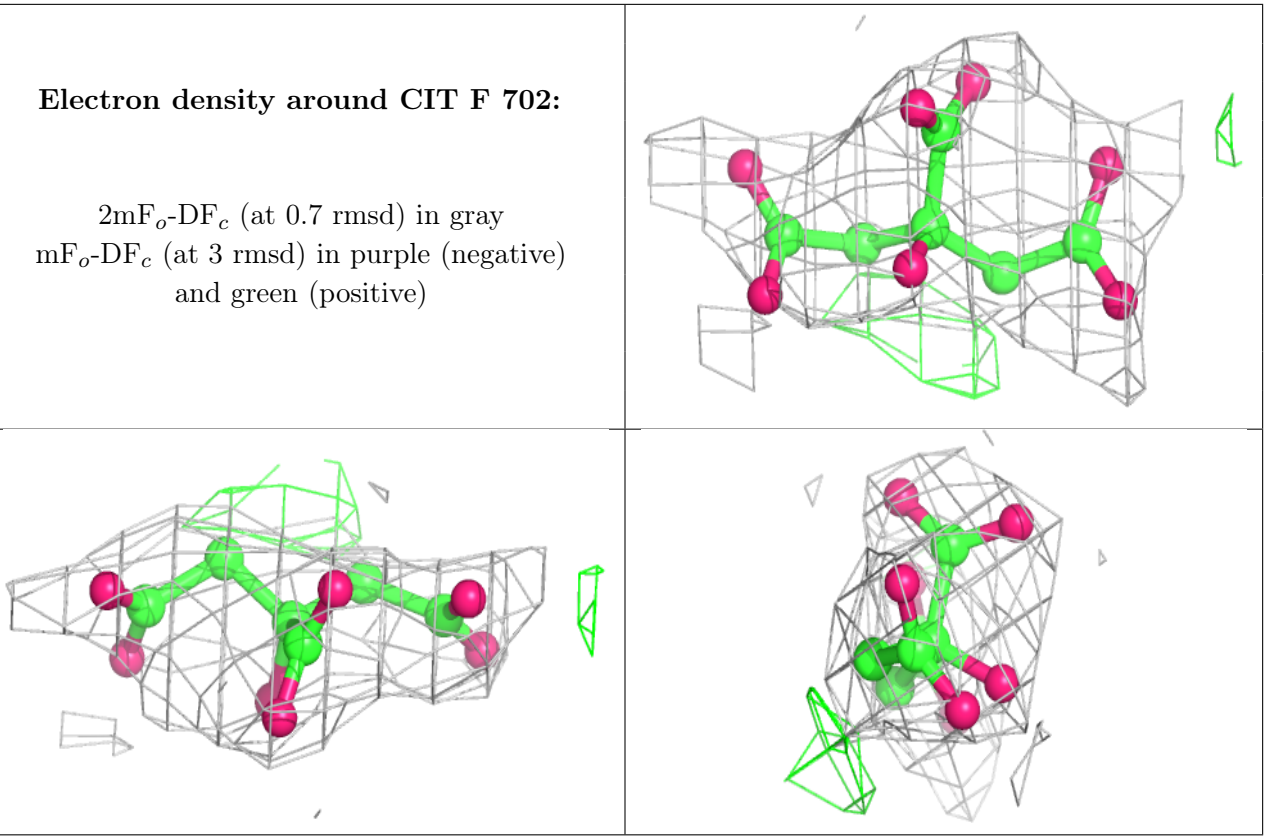






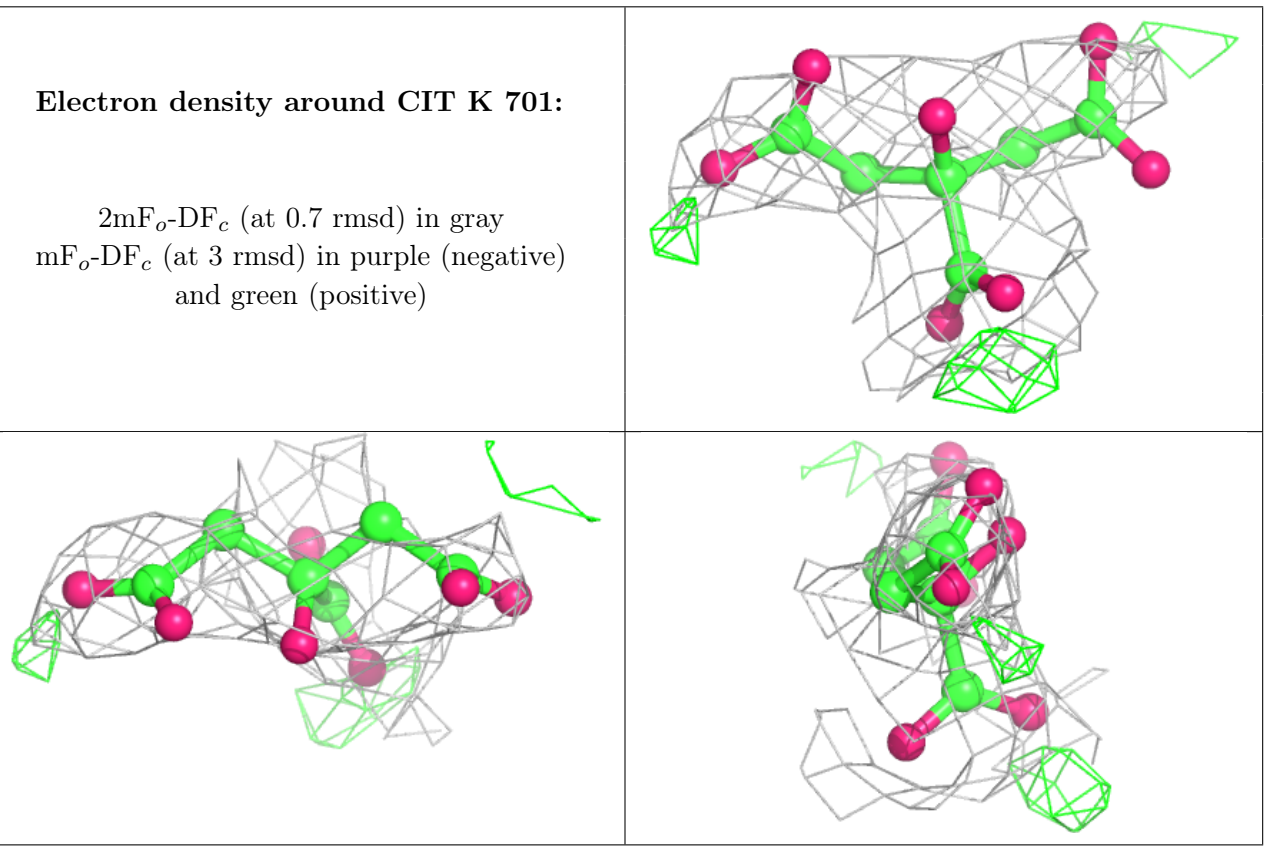
Electron density around CIT F 702:

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



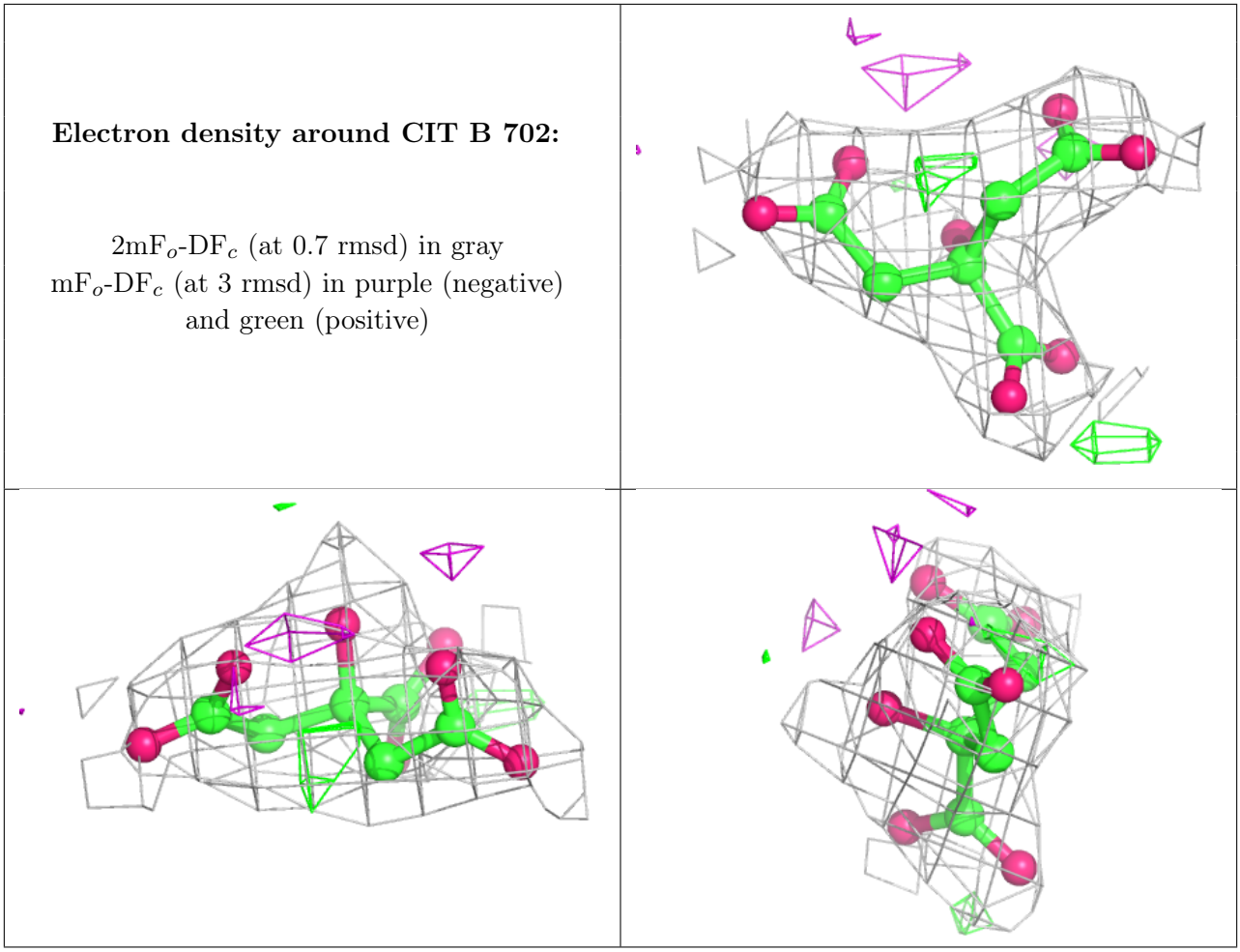
Electron density around CIT K 701:

$2mF_o$-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 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 D 701:

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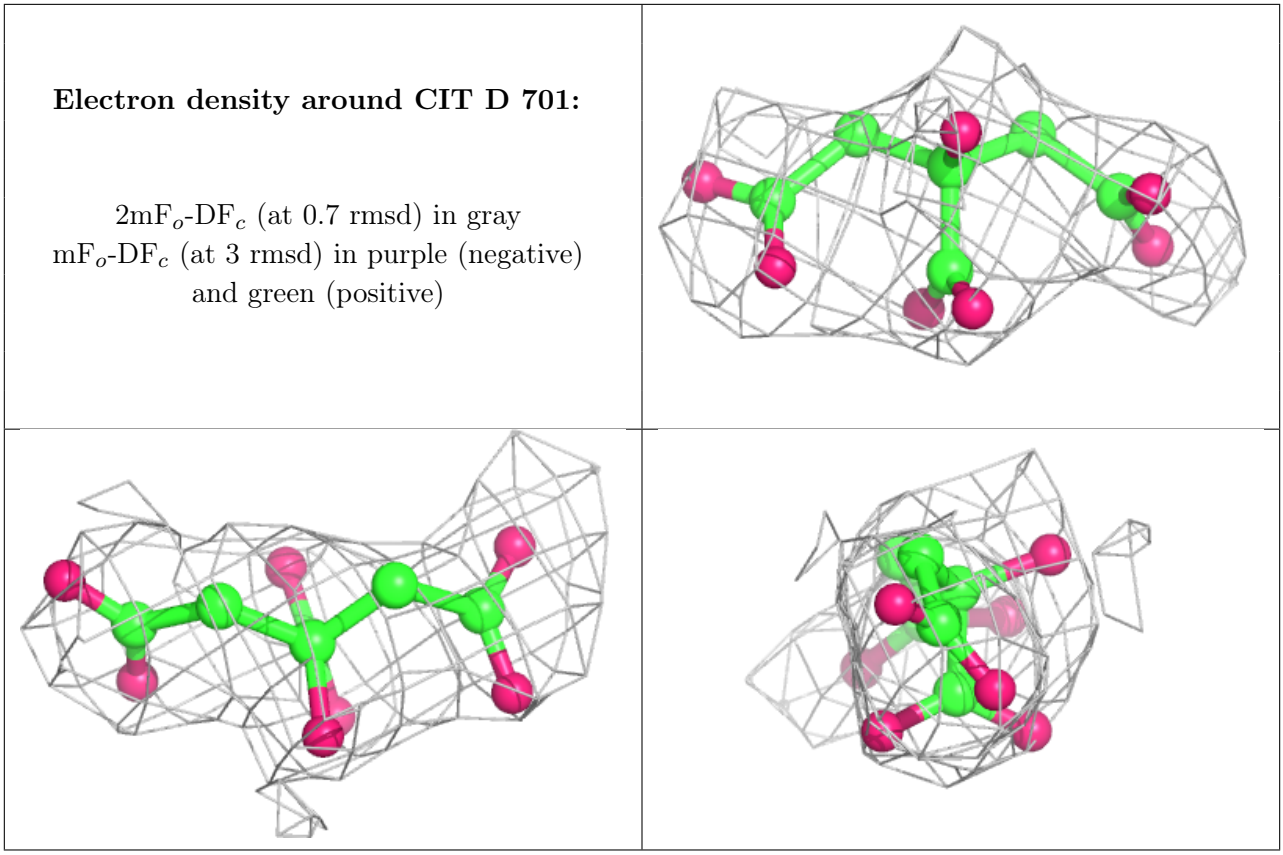
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CIT B 701:

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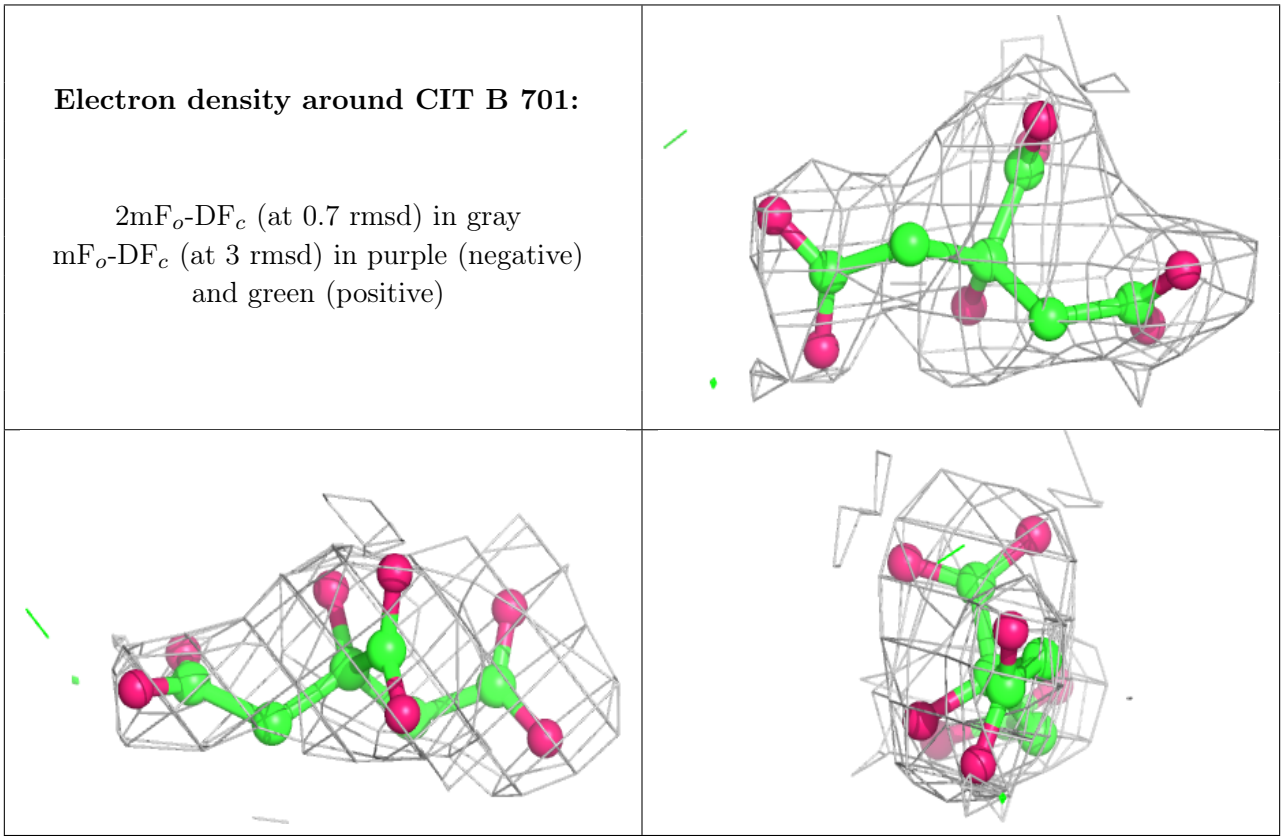
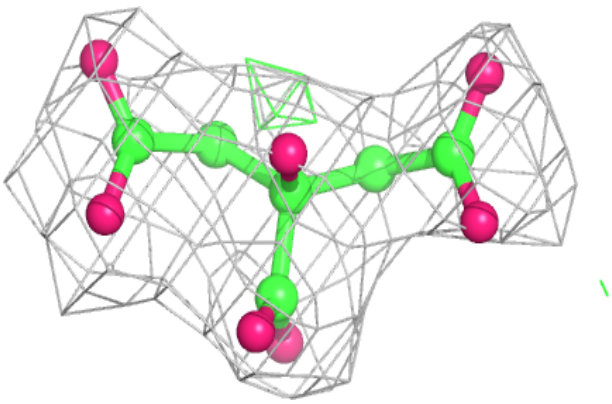
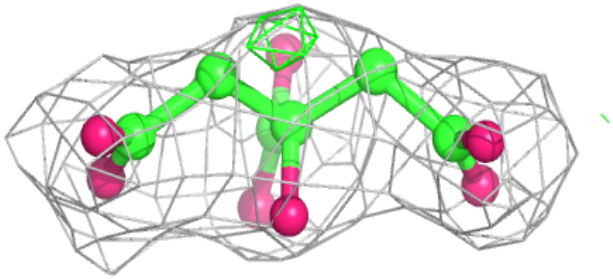
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

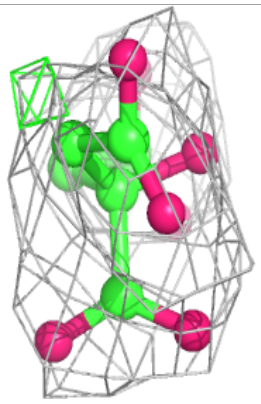


Electron density around CIT I 701:

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

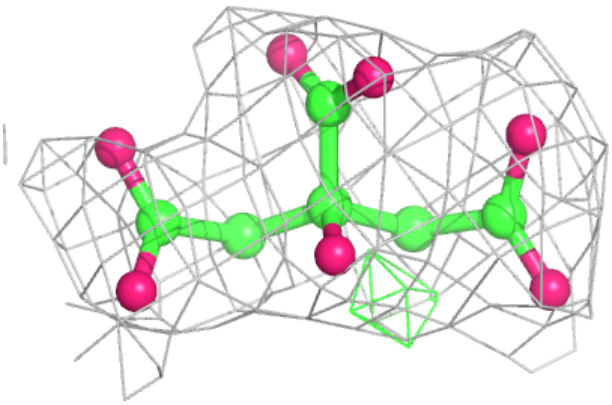


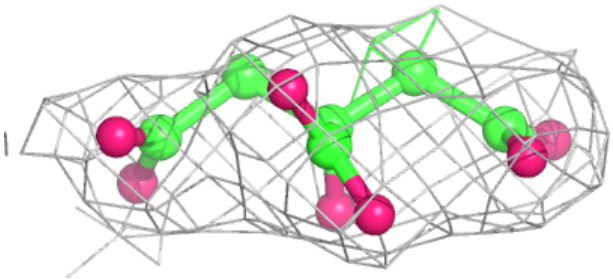


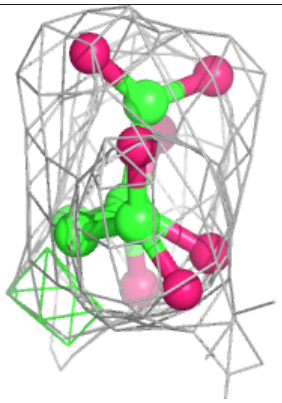


Electron density around CIT L 701:

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

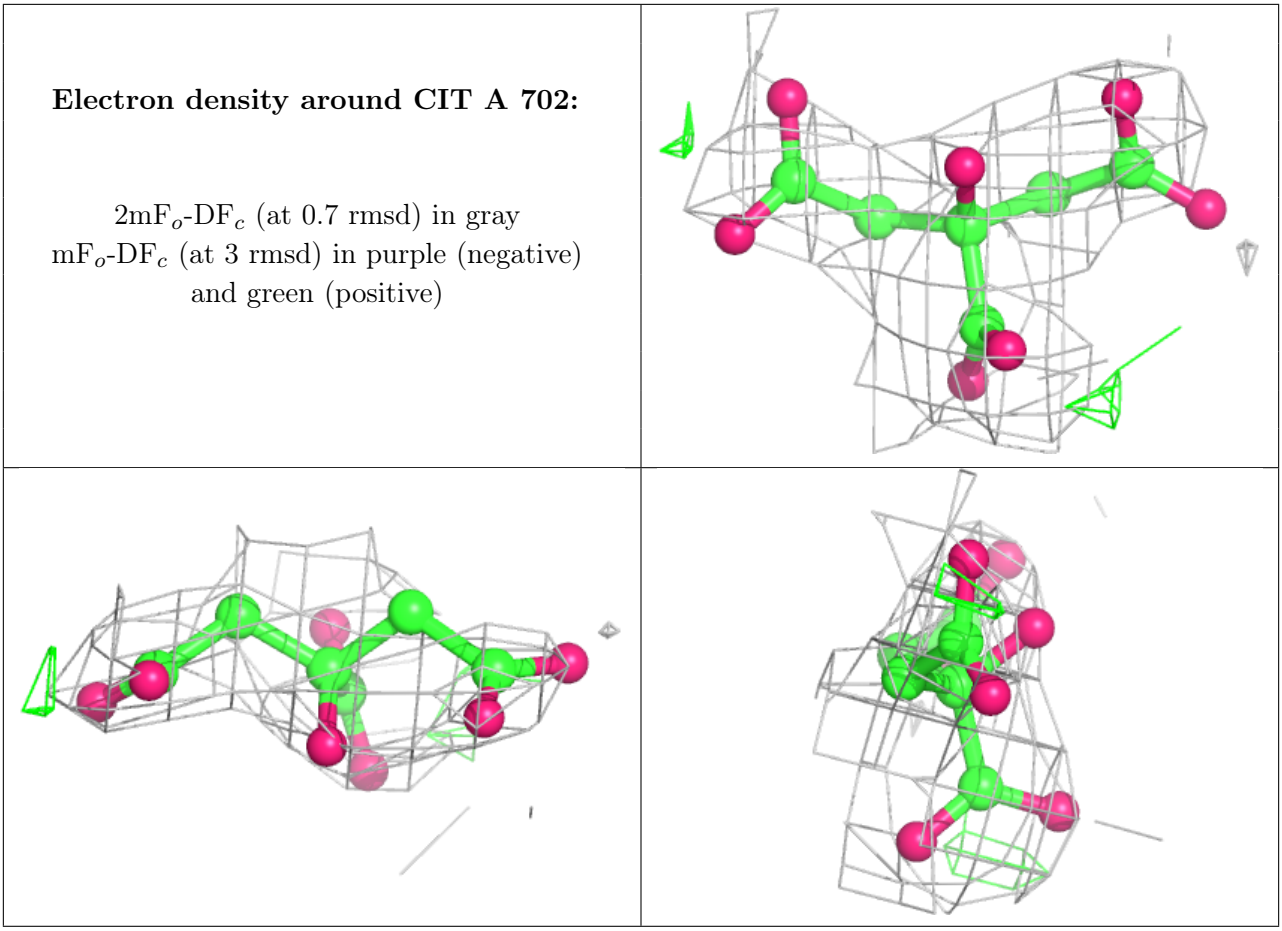






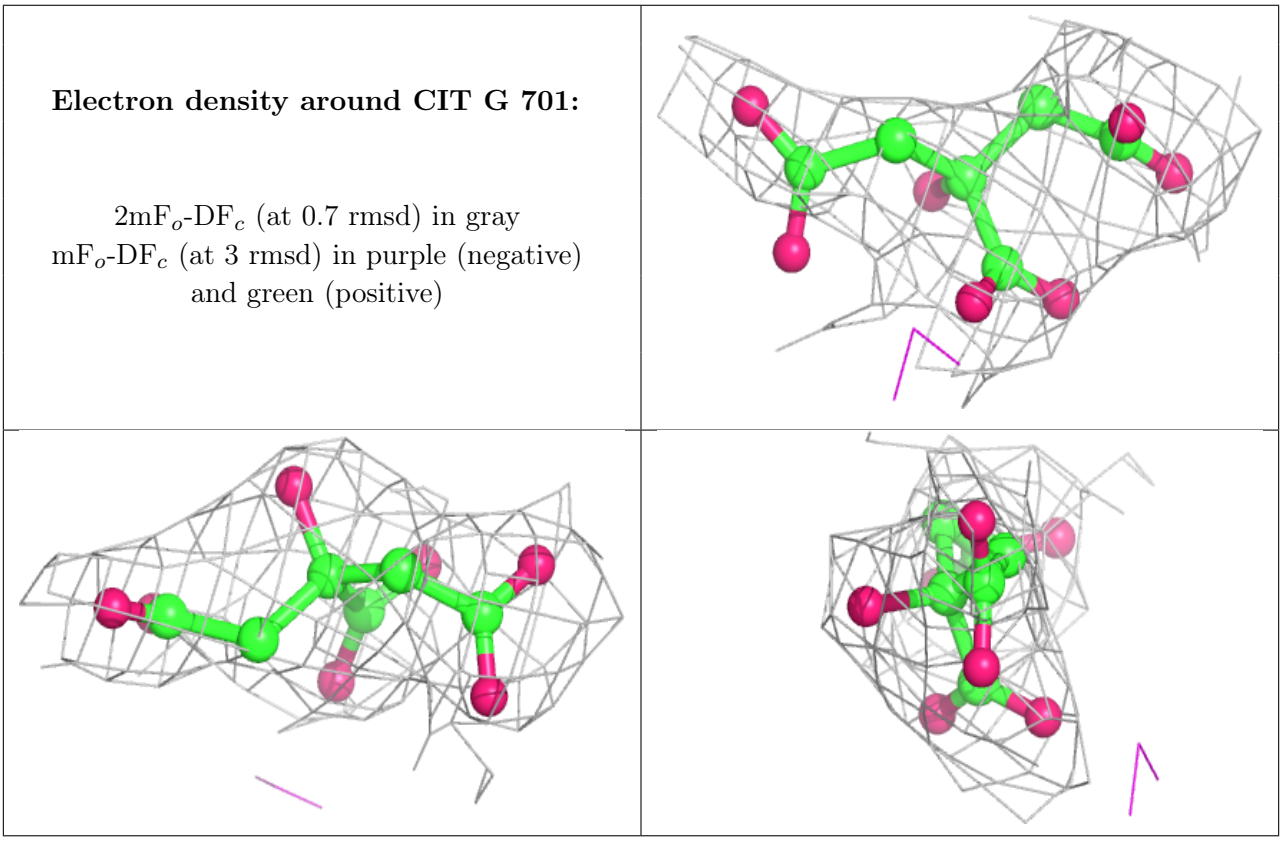
Electron density around CIT A 702:

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



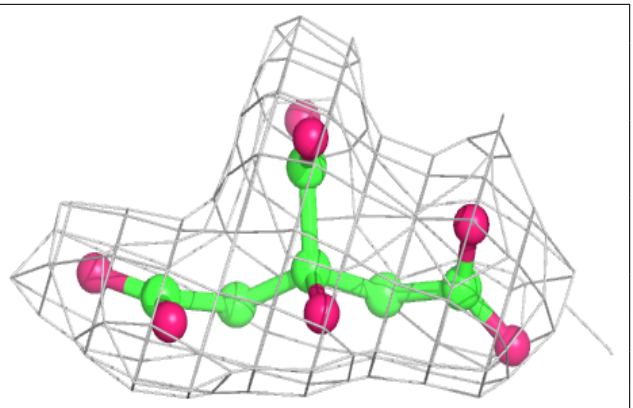
Electron density around CIT G 701:

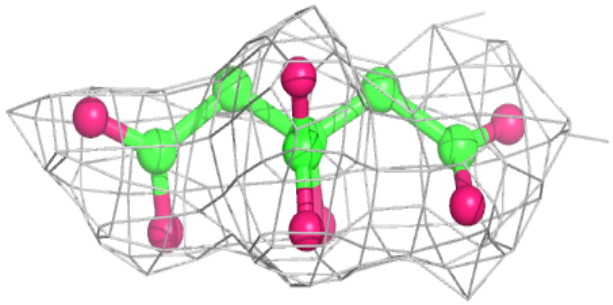
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

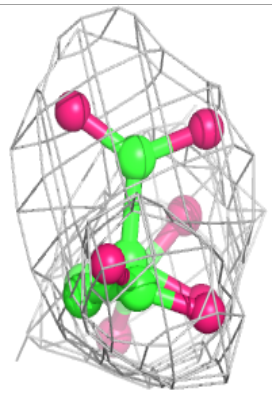


Electron density around CIT E 701:

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

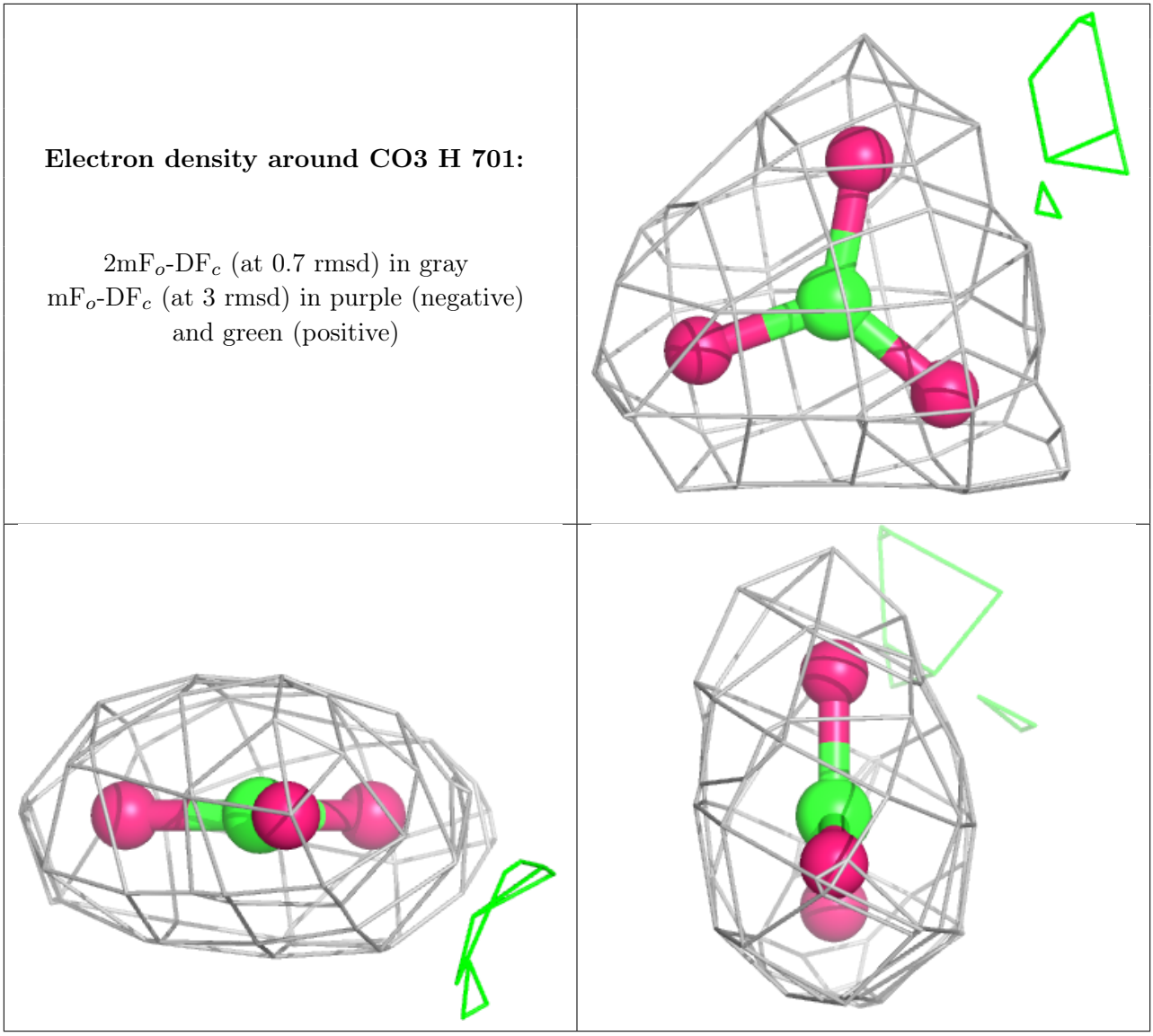






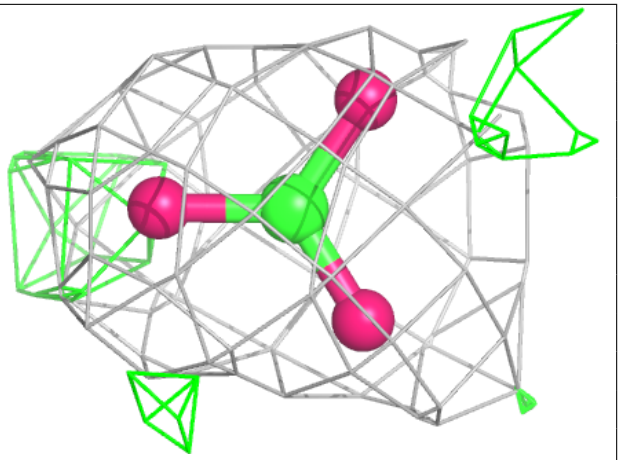
Electron density around CO3 H 701:

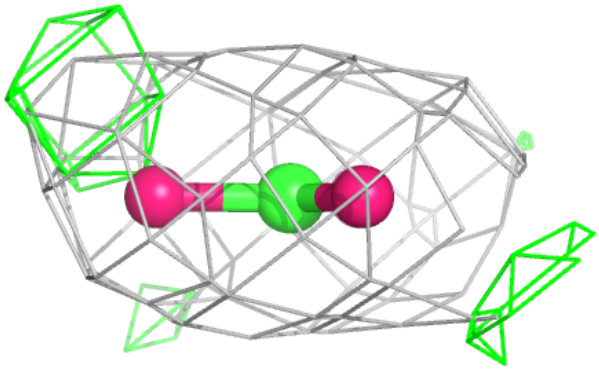
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

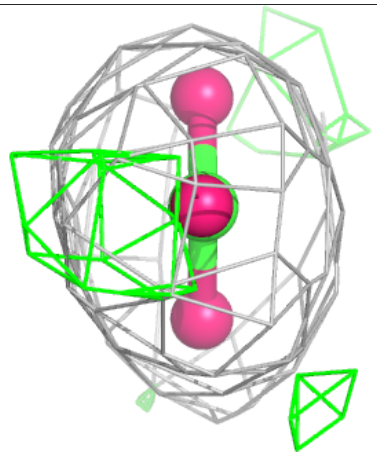


Electron density around CO3 C 702:

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

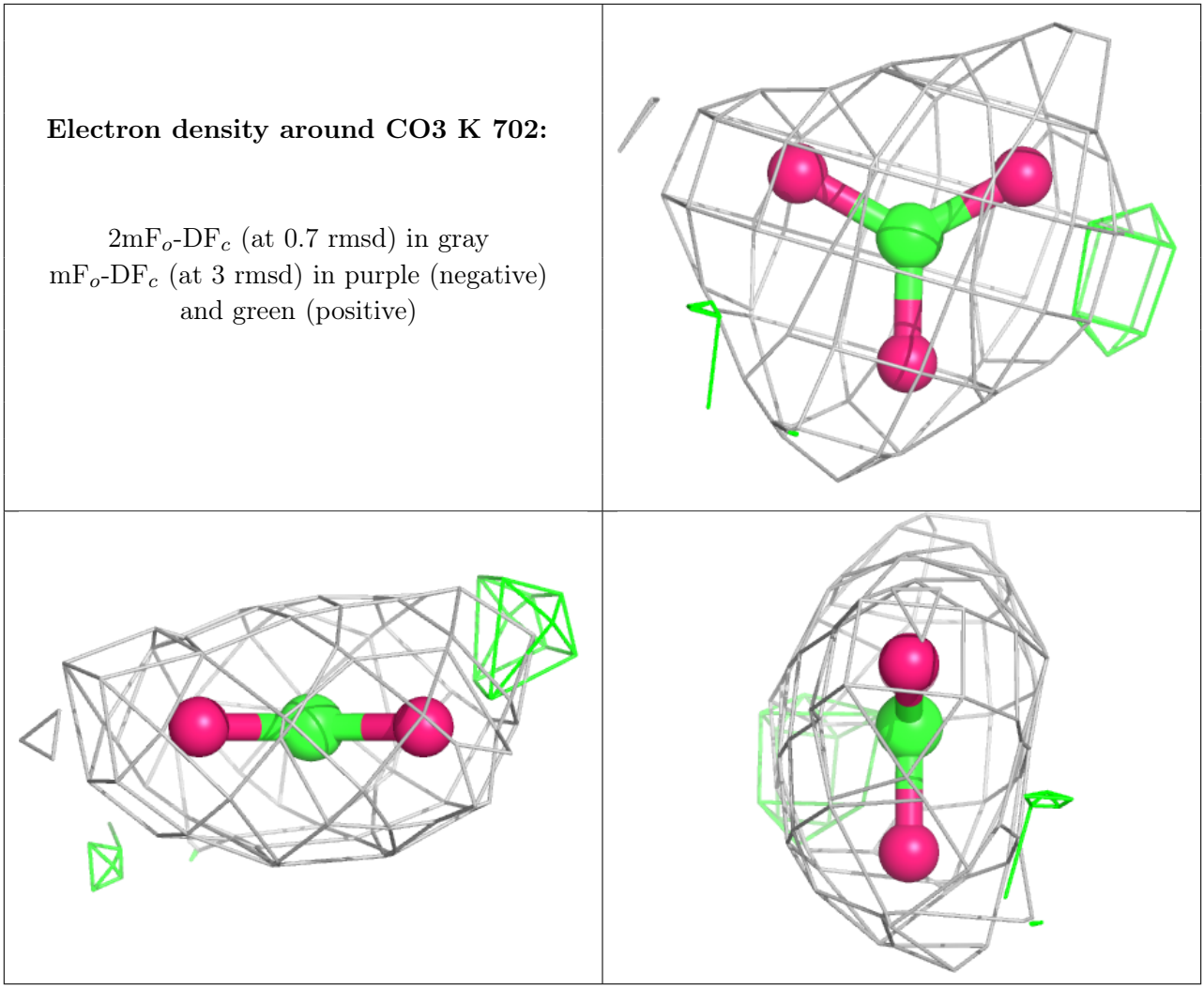






Electron density around CO3 K 702:

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



6.5 Other polymers

There are no such residues in this entry.