Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2023 – 08:17 am BST

PDB ID	:	8P5R
Title	:	Crystal structure of full-length, homohexameric 2-oxoglutarate dehydrogenase KGD from Mycobacterium smegmatis in complex with GarA
Authors	:	Wagner, T.; Mechaly, A.M.; Alzari, P.M.; Bellinzoni, M.
Deposited on	:	2023-05-24
Resolution	:	4.56 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

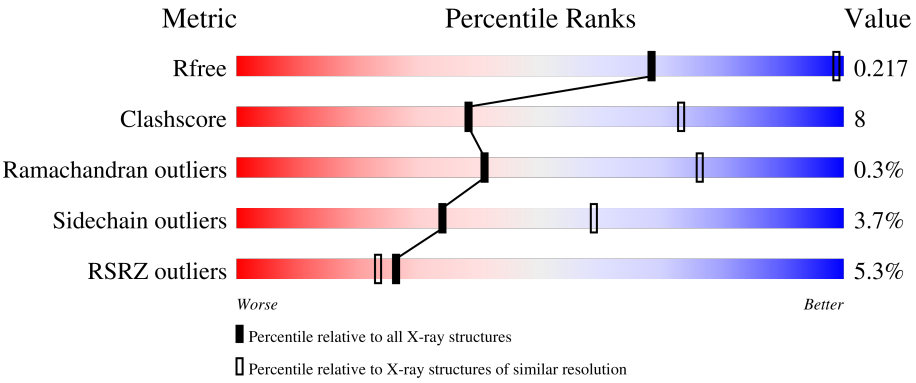
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 4.56 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	1060 (5.30-3.80)
Clashscore	141614	1128 (5.30-3.80)
Ramachandran outliers	138981	1072 (5.30-3.80)
Sidechain outliers	138945	1053 (5.30-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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	1250	4% 73% 15% • 12%
1	B	1250	3% 72% 16% • 11%
1	C	1250	4% 73% 15% 11%
1	D	1250	4% 73% 15% • 11%
1	E	1250	3% 73% 15% • 11%

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Mol	Chain	Length	Quality of chain
1	F	1250	4% 74% 14% 12%
1	N	1250	98%
1	O	1250	98%
1	P	1250	98%
1	Q	1250	98%
2	G	158	11% 49% 13% 38%
2	H	158	47% 11% 39%
2	I	158	8% 49% 13% 39%
2	J	158	10% 49% 11% 39%
2	K	158	3% 53% 8% 39%
2	L	158	9% 51% 10% 39%

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
4	CA	A	1302	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 57005 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 Multifunctional 2-oxoglutarate metabolism enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1106	Total	C	N	O	S	0	0	0
			8579	5394	1535	1619	31			
1	B	1108	Total	C	N	O	S	0	0	0
			8591	5404	1534	1622	31			
1	C	1109	Total	C	N	O	S	0	0	0
			8593	5407	1531	1624	31			
1	D	1107	Total	C	N	O	S	0	0	0
			8544	5379	1519	1615	31			
1	E	1109	Total	C	N	O	S	0	0	0
			8537	5373	1516	1617	31			
1	F	1105	Total	C	N	O	S	0	0	0
			8513	5357	1517	1608	31			
1	N	30	Total	C	N	O	S	0	0	0
			266	172	41	52	1			
1	O	30	Total	C	N	O	S	0	0	0
			266	172	41	52	1			
1	P	30	Total	C	N	O	S	0	0	0
			266	172	41	52	1			
1	Q	30	Total	C	N	O	S	0	0	0
			266	172	41	52	1			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP A0R2B1
A	-21	GLY	-	expression tag	UNP A0R2B1
A	-20	SER	-	expression tag	UNP A0R2B1
A	-19	SER	-	expression tag	UNP A0R2B1
A	-18	HIS	-	expression tag	UNP A0R2B1
A	-17	HIS	-	expression tag	UNP A0R2B1
A	-16	HIS	-	expression tag	UNP A0R2B1
A	-15	HIS	-	expression tag	UNP A0R2B1
A	-14	HIS	-	expression tag	UNP A0R2B1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP A0R2B1
A	-12	SER	-	expression tag	UNP A0R2B1
A	-11	SER	-	expression tag	UNP A0R2B1
A	-10	GLY	-	expression tag	UNP A0R2B1
A	-9	LEU	-	expression tag	UNP A0R2B1
A	-8	VAL	-	expression tag	UNP A0R2B1
A	-7	PRO	-	expression tag	UNP A0R2B1
A	-6	ARG	-	expression tag	UNP A0R2B1
A	-5	GLY	-	expression tag	UNP A0R2B1
A	-4	SER	-	expression tag	UNP A0R2B1
A	-3	HIS	-	expression tag	UNP A0R2B1
A	-2	MET	-	expression tag	UNP A0R2B1
A	-1	ALA	-	expression tag	UNP A0R2B1
A	0	SER	-	expression tag	UNP A0R2B1
A	1	VAL	-	expression tag	UNP A0R2B1
B	-22	MET	-	initiating methionine	UNP A0R2B1
B	-21	GLY	-	expression tag	UNP A0R2B1
B	-20	SER	-	expression tag	UNP A0R2B1
B	-19	SER	-	expression tag	UNP A0R2B1
B	-18	HIS	-	expression tag	UNP A0R2B1
B	-17	HIS	-	expression tag	UNP A0R2B1
B	-16	HIS	-	expression tag	UNP A0R2B1
B	-15	HIS	-	expression tag	UNP A0R2B1
B	-14	HIS	-	expression tag	UNP A0R2B1
B	-13	HIS	-	expression tag	UNP A0R2B1
B	-12	SER	-	expression tag	UNP A0R2B1
B	-11	SER	-	expression tag	UNP A0R2B1
B	-10	GLY	-	expression tag	UNP A0R2B1
B	-9	LEU	-	expression tag	UNP A0R2B1
B	-8	VAL	-	expression tag	UNP A0R2B1
B	-7	PRO	-	expression tag	UNP A0R2B1
B	-6	ARG	-	expression tag	UNP A0R2B1
B	-5	GLY	-	expression tag	UNP A0R2B1
B	-4	SER	-	expression tag	UNP A0R2B1
B	-3	HIS	-	expression tag	UNP A0R2B1
B	-2	MET	-	expression tag	UNP A0R2B1
B	-1	ALA	-	expression tag	UNP A0R2B1
B	0	SER	-	expression tag	UNP A0R2B1
B	1	VAL	-	expression tag	UNP A0R2B1
C	-22	MET	-	initiating methionine	UNP A0R2B1
C	-21	GLY	-	expression tag	UNP A0R2B1
C	-20	SER	-	expression tag	UNP A0R2B1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	SER	-	expression tag	UNP A0R2B1
C	-18	HIS	-	expression tag	UNP A0R2B1
C	-17	HIS	-	expression tag	UNP A0R2B1
C	-16	HIS	-	expression tag	UNP A0R2B1
C	-15	HIS	-	expression tag	UNP A0R2B1
C	-14	HIS	-	expression tag	UNP A0R2B1
C	-13	HIS	-	expression tag	UNP A0R2B1
C	-12	SER	-	expression tag	UNP A0R2B1
C	-11	SER	-	expression tag	UNP A0R2B1
C	-10	GLY	-	expression tag	UNP A0R2B1
C	-9	LEU	-	expression tag	UNP A0R2B1
C	-8	VAL	-	expression tag	UNP A0R2B1
C	-7	PRO	-	expression tag	UNP A0R2B1
C	-6	ARG	-	expression tag	UNP A0R2B1
C	-5	GLY	-	expression tag	UNP A0R2B1
C	-4	SER	-	expression tag	UNP A0R2B1
C	-3	HIS	-	expression tag	UNP A0R2B1
C	-2	MET	-	expression tag	UNP A0R2B1
C	-1	ALA	-	expression tag	UNP A0R2B1
C	0	SER	-	expression tag	UNP A0R2B1
C	1	VAL	-	expression tag	UNP A0R2B1
D	-22	MET	-	initiating methionine	UNP A0R2B1
D	-21	GLY	-	expression tag	UNP A0R2B1
D	-20	SER	-	expression tag	UNP A0R2B1
D	-19	SER	-	expression tag	UNP A0R2B1
D	-18	HIS	-	expression tag	UNP A0R2B1
D	-17	HIS	-	expression tag	UNP A0R2B1
D	-16	HIS	-	expression tag	UNP A0R2B1
D	-15	HIS	-	expression tag	UNP A0R2B1
D	-14	HIS	-	expression tag	UNP A0R2B1
D	-13	HIS	-	expression tag	UNP A0R2B1
D	-12	SER	-	expression tag	UNP A0R2B1
D	-11	SER	-	expression tag	UNP A0R2B1
D	-10	GLY	-	expression tag	UNP A0R2B1
D	-9	LEU	-	expression tag	UNP A0R2B1
D	-8	VAL	-	expression tag	UNP A0R2B1
D	-7	PRO	-	expression tag	UNP A0R2B1
D	-6	ARG	-	expression tag	UNP A0R2B1
D	-5	GLY	-	expression tag	UNP A0R2B1
D	-4	SER	-	expression tag	UNP A0R2B1
D	-3	HIS	-	expression tag	UNP A0R2B1
D	-2	MET	-	expression tag	UNP A0R2B1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ALA	-	expression tag	UNP A0R2B1
D	0	SER	-	expression tag	UNP A0R2B1
D	1	VAL	-	expression tag	UNP A0R2B1
E	-22	MET	-	initiating methionine	UNP A0R2B1
E	-21	GLY	-	expression tag	UNP A0R2B1
E	-20	SER	-	expression tag	UNP A0R2B1
E	-19	SER	-	expression tag	UNP A0R2B1
E	-18	HIS	-	expression tag	UNP A0R2B1
E	-17	HIS	-	expression tag	UNP A0R2B1
E	-16	HIS	-	expression tag	UNP A0R2B1
E	-15	HIS	-	expression tag	UNP A0R2B1
E	-14	HIS	-	expression tag	UNP A0R2B1
E	-13	HIS	-	expression tag	UNP A0R2B1
E	-12	SER	-	expression tag	UNP A0R2B1
E	-11	SER	-	expression tag	UNP A0R2B1
E	-10	GLY	-	expression tag	UNP A0R2B1
E	-9	LEU	-	expression tag	UNP A0R2B1
E	-8	VAL	-	expression tag	UNP A0R2B1
E	-7	PRO	-	expression tag	UNP A0R2B1
E	-6	ARG	-	expression tag	UNP A0R2B1
E	-5	GLY	-	expression tag	UNP A0R2B1
E	-4	SER	-	expression tag	UNP A0R2B1
E	-3	HIS	-	expression tag	UNP A0R2B1
E	-2	MET	-	expression tag	UNP A0R2B1
E	-1	ALA	-	expression tag	UNP A0R2B1
E	0	SER	-	expression tag	UNP A0R2B1
E	1	VAL	-	expression tag	UNP A0R2B1
F	-22	MET	-	initiating methionine	UNP A0R2B1
F	-21	GLY	-	expression tag	UNP A0R2B1
F	-20	SER	-	expression tag	UNP A0R2B1
F	-19	SER	-	expression tag	UNP A0R2B1
F	-18	HIS	-	expression tag	UNP A0R2B1
F	-17	HIS	-	expression tag	UNP A0R2B1
F	-16	HIS	-	expression tag	UNP A0R2B1
F	-15	HIS	-	expression tag	UNP A0R2B1
F	-14	HIS	-	expression tag	UNP A0R2B1
F	-13	HIS	-	expression tag	UNP A0R2B1
F	-12	SER	-	expression tag	UNP A0R2B1
F	-11	SER	-	expression tag	UNP A0R2B1
F	-10	GLY	-	expression tag	UNP A0R2B1
F	-9	LEU	-	expression tag	UNP A0R2B1
F	-8	VAL	-	expression tag	UNP A0R2B1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	PRO	-	expression tag	UNP A0R2B1
F	-6	ARG	-	expression tag	UNP A0R2B1
F	-5	GLY	-	expression tag	UNP A0R2B1
F	-4	SER	-	expression tag	UNP A0R2B1
F	-3	HIS	-	expression tag	UNP A0R2B1
F	-2	MET	-	expression tag	UNP A0R2B1
F	-1	ALA	-	expression tag	UNP A0R2B1
F	0	SER	-	expression tag	UNP A0R2B1
F	1	VAL	-	expression tag	UNP A0R2B1
N	-22	MET	-	initiating methionine	UNP A0R2B1
N	-21	GLY	-	expression tag	UNP A0R2B1
N	-20	SER	-	expression tag	UNP A0R2B1
N	-19	SER	-	expression tag	UNP A0R2B1
N	-18	HIS	-	expression tag	UNP A0R2B1
N	-17	HIS	-	expression tag	UNP A0R2B1
N	-16	HIS	-	expression tag	UNP A0R2B1
N	-15	HIS	-	expression tag	UNP A0R2B1
N	-14	HIS	-	expression tag	UNP A0R2B1
N	-13	HIS	-	expression tag	UNP A0R2B1
N	-12	SER	-	expression tag	UNP A0R2B1
N	-11	SER	-	expression tag	UNP A0R2B1
N	-10	GLY	-	expression tag	UNP A0R2B1
N	-9	LEU	-	expression tag	UNP A0R2B1
N	-8	VAL	-	expression tag	UNP A0R2B1
N	-7	PRO	-	expression tag	UNP A0R2B1
N	-6	ARG	-	expression tag	UNP A0R2B1
N	-5	GLY	-	expression tag	UNP A0R2B1
N	-4	SER	-	expression tag	UNP A0R2B1
N	-3	HIS	-	expression tag	UNP A0R2B1
N	-2	MET	-	expression tag	UNP A0R2B1
N	-1	ALA	-	expression tag	UNP A0R2B1
N	0	SER	-	expression tag	UNP A0R2B1
N	1	VAL	-	expression tag	UNP A0R2B1
O	-22	MET	-	initiating methionine	UNP A0R2B1
O	-21	GLY	-	expression tag	UNP A0R2B1
O	-20	SER	-	expression tag	UNP A0R2B1
O	-19	SER	-	expression tag	UNP A0R2B1
O	-18	HIS	-	expression tag	UNP A0R2B1
O	-17	HIS	-	expression tag	UNP A0R2B1
O	-16	HIS	-	expression tag	UNP A0R2B1
O	-15	HIS	-	expression tag	UNP A0R2B1
O	-14	HIS	-	expression tag	UNP A0R2B1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-13	HIS	-	expression tag	UNP A0R2B1
O	-12	SER	-	expression tag	UNP A0R2B1
O	-11	SER	-	expression tag	UNP A0R2B1
O	-10	GLY	-	expression tag	UNP A0R2B1
O	-9	LEU	-	expression tag	UNP A0R2B1
O	-8	VAL	-	expression tag	UNP A0R2B1
O	-7	PRO	-	expression tag	UNP A0R2B1
O	-6	ARG	-	expression tag	UNP A0R2B1
O	-5	GLY	-	expression tag	UNP A0R2B1
O	-4	SER	-	expression tag	UNP A0R2B1
O	-3	HIS	-	expression tag	UNP A0R2B1
O	-2	MET	-	expression tag	UNP A0R2B1
O	-1	ALA	-	expression tag	UNP A0R2B1
O	0	SER	-	expression tag	UNP A0R2B1
O	1	VAL	-	expression tag	UNP A0R2B1
P	-22	MET	-	initiating methionine	UNP A0R2B1
P	-21	GLY	-	expression tag	UNP A0R2B1
P	-20	SER	-	expression tag	UNP A0R2B1
P	-19	SER	-	expression tag	UNP A0R2B1
P	-18	HIS	-	expression tag	UNP A0R2B1
P	-17	HIS	-	expression tag	UNP A0R2B1
P	-16	HIS	-	expression tag	UNP A0R2B1
P	-15	HIS	-	expression tag	UNP A0R2B1
P	-14	HIS	-	expression tag	UNP A0R2B1
P	-13	HIS	-	expression tag	UNP A0R2B1
P	-12	SER	-	expression tag	UNP A0R2B1
P	-11	SER	-	expression tag	UNP A0R2B1
P	-10	GLY	-	expression tag	UNP A0R2B1
P	-9	LEU	-	expression tag	UNP A0R2B1
P	-8	VAL	-	expression tag	UNP A0R2B1
P	-7	PRO	-	expression tag	UNP A0R2B1
P	-6	ARG	-	expression tag	UNP A0R2B1
P	-5	GLY	-	expression tag	UNP A0R2B1
P	-4	SER	-	expression tag	UNP A0R2B1
P	-3	HIS	-	expression tag	UNP A0R2B1
P	-2	MET	-	expression tag	UNP A0R2B1
P	-1	ALA	-	expression tag	UNP A0R2B1
P	0	SER	-	expression tag	UNP A0R2B1
P	1	VAL	-	expression tag	UNP A0R2B1
Q	-22	MET	-	initiating methionine	UNP A0R2B1
Q	-21	GLY	-	expression tag	UNP A0R2B1
Q	-20	SER	-	expression tag	UNP A0R2B1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-19	SER	-	expression tag	UNP A0R2B1
Q	-18	HIS	-	expression tag	UNP A0R2B1
Q	-17	HIS	-	expression tag	UNP A0R2B1
Q	-16	HIS	-	expression tag	UNP A0R2B1
Q	-15	HIS	-	expression tag	UNP A0R2B1
Q	-14	HIS	-	expression tag	UNP A0R2B1
Q	-13	HIS	-	expression tag	UNP A0R2B1
Q	-12	SER	-	expression tag	UNP A0R2B1
Q	-11	SER	-	expression tag	UNP A0R2B1
Q	-10	GLY	-	expression tag	UNP A0R2B1
Q	-9	LEU	-	expression tag	UNP A0R2B1
Q	-8	VAL	-	expression tag	UNP A0R2B1
Q	-7	PRO	-	expression tag	UNP A0R2B1
Q	-6	ARG	-	expression tag	UNP A0R2B1
Q	-5	GLY	-	expression tag	UNP A0R2B1
Q	-4	SER	-	expression tag	UNP A0R2B1
Q	-3	HIS	-	expression tag	UNP A0R2B1
Q	-2	MET	-	expression tag	UNP A0R2B1
Q	-1	ALA	-	expression tag	UNP A0R2B1
Q	0	SER	-	expression tag	UNP A0R2B1
Q	1	VAL	-	expression tag	UNP A0R2B1

- Molecule 2 is a protein called Glycogen accumulation regulator GarA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	98	Total	C	N	O	0	0	0
			744	464	135	145			
2	H	96	Total	C	N	O	0	0	0
			710	438	131	141			
2	I	97	Total	C	N	O	0	0	0
			740	462	134	144			
2	J	97	Total	C	N	O	0	0	0
			740	462	134	144			
2	K	97	Total	C	N	O	0	0	0
			740	462	134	144			
2	L	97	Total	C	N	O	0	0	0
			740	462	134	144			

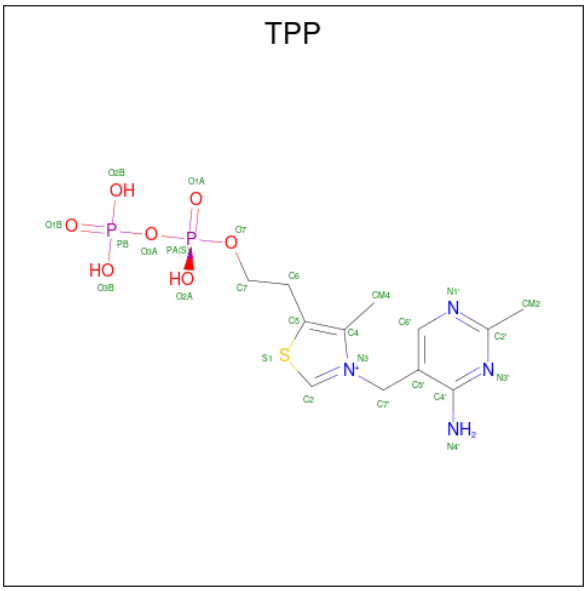
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



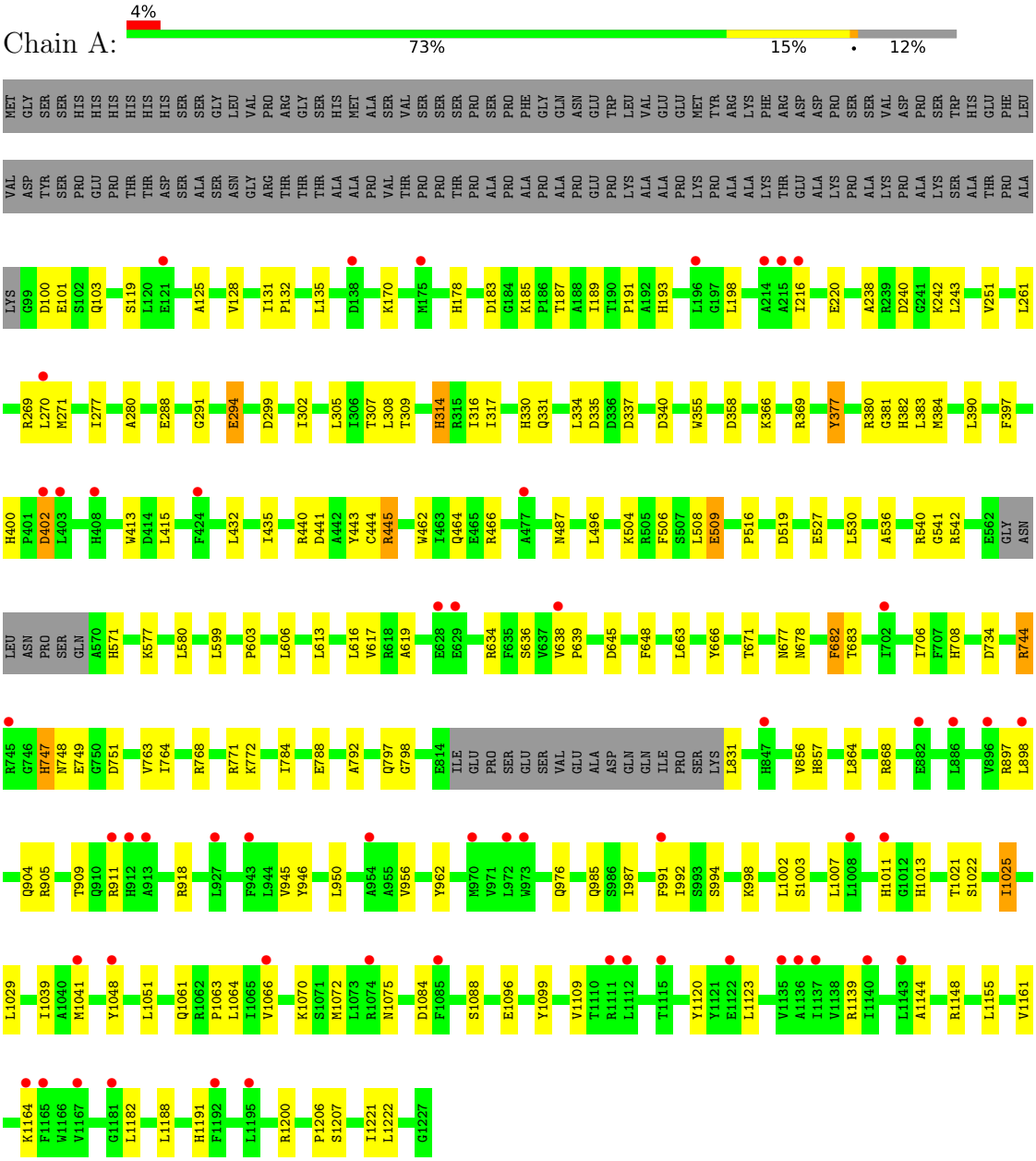
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
5	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
5	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
5	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
5	E	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
5	F	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

3 Residue-property plots (i)

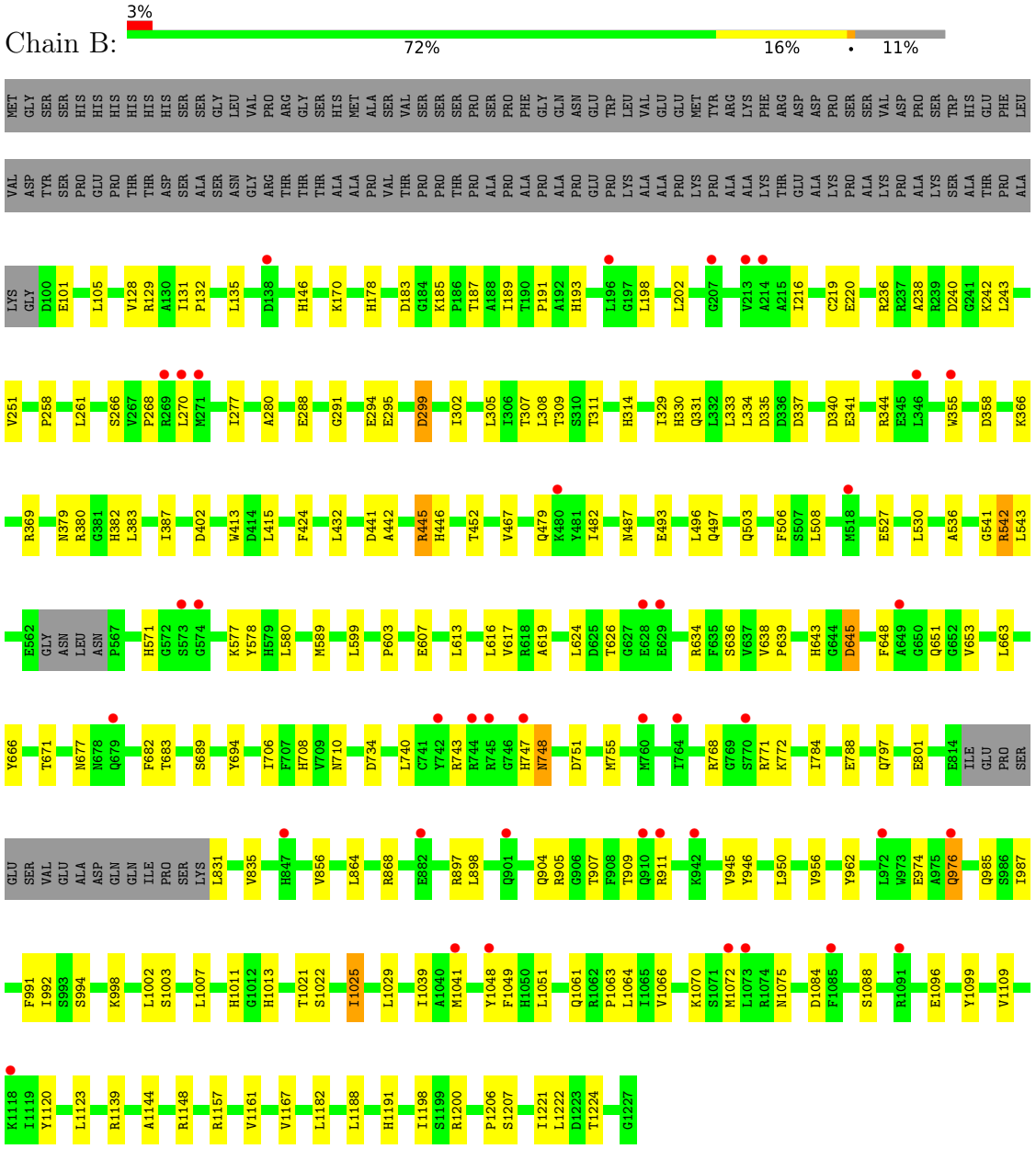
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Multifunctional 2-oxoglutarate metabolism enzyme

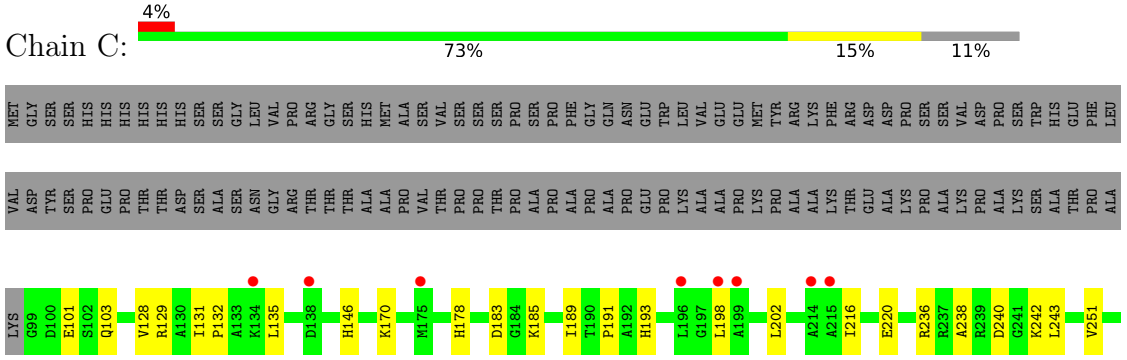
Chain A:

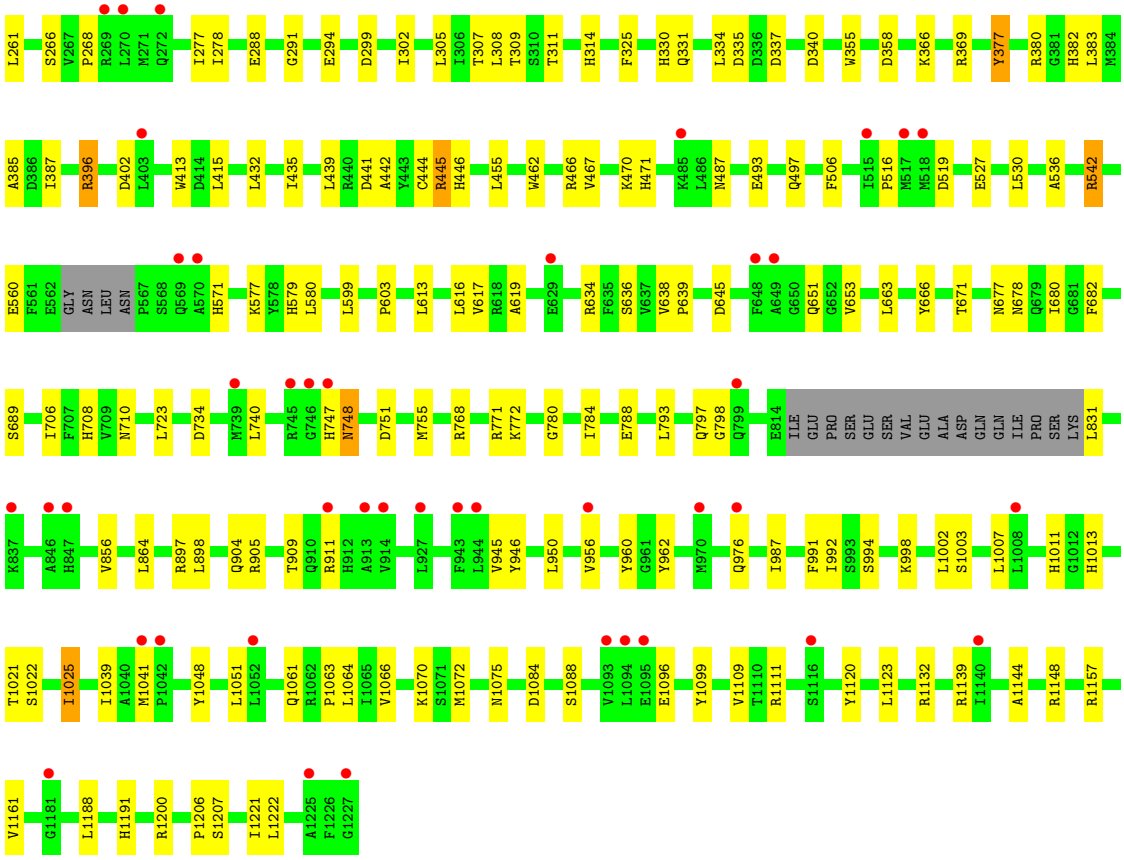


• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

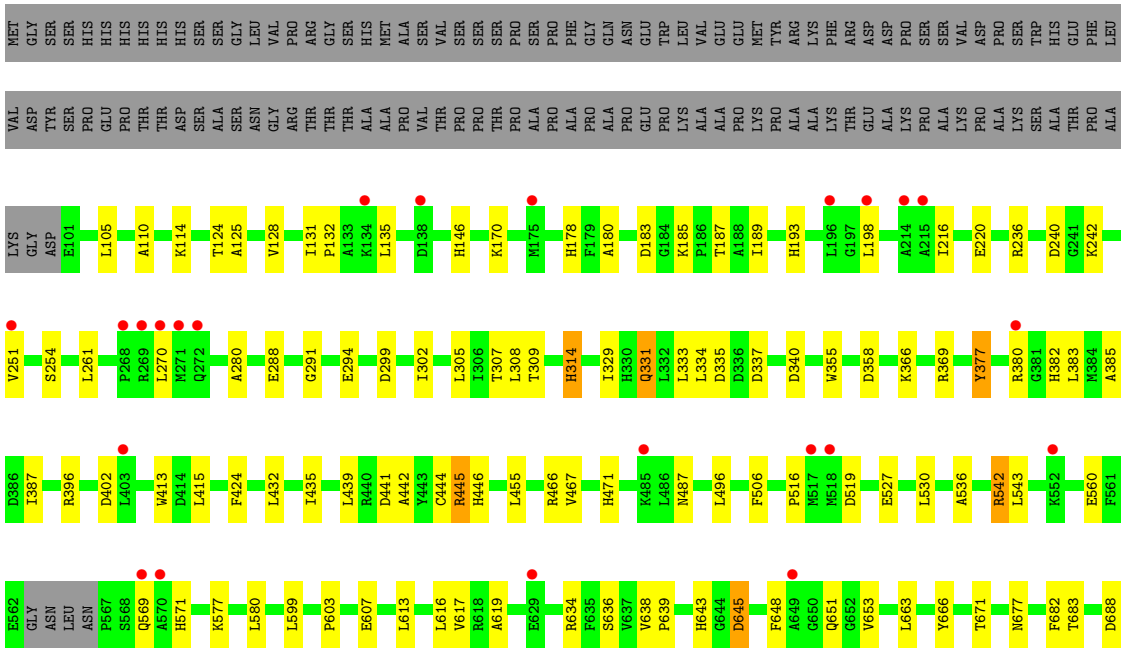


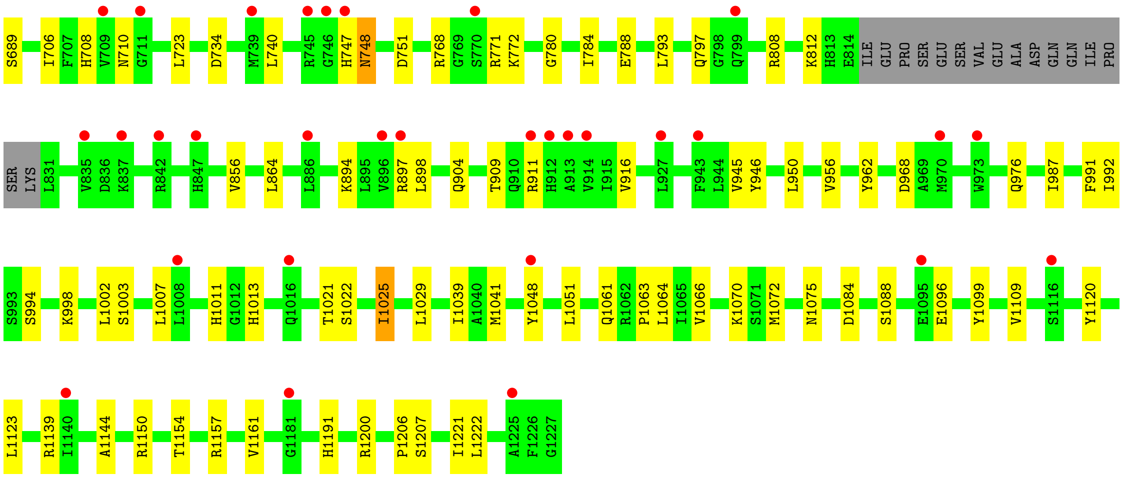
• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme





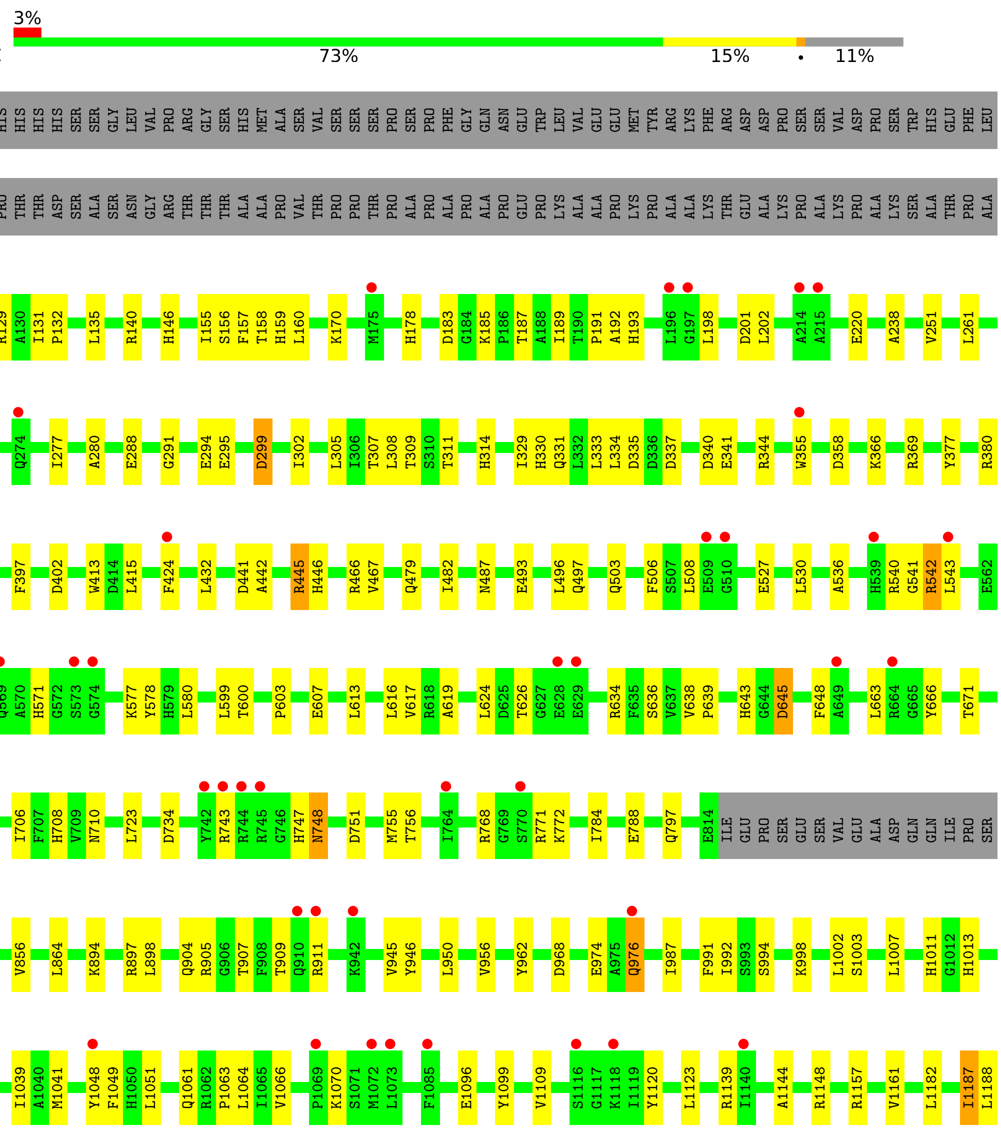
• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

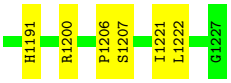




• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

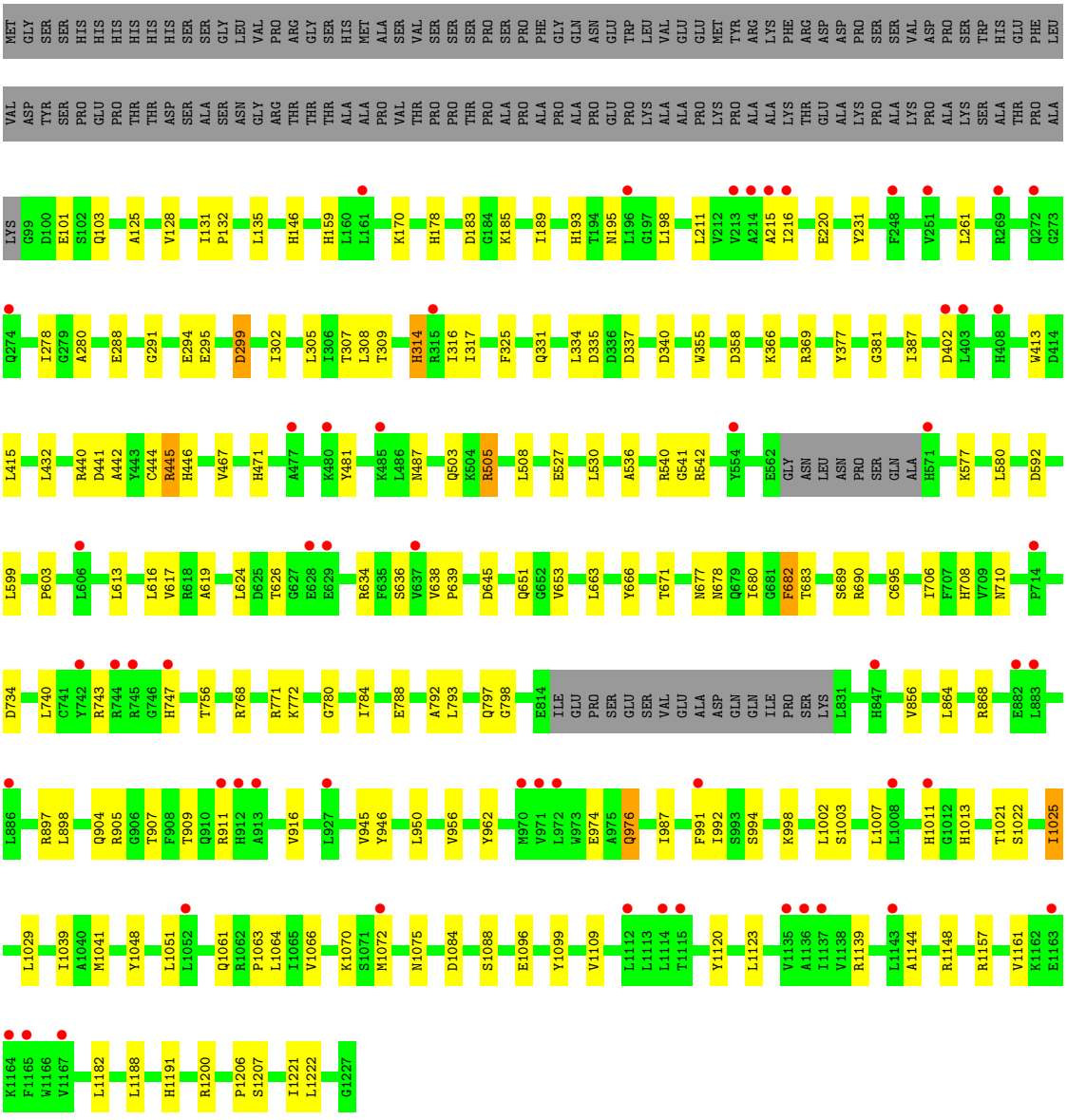
Chain E:





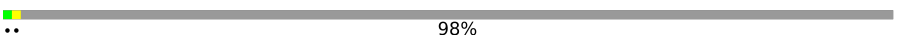
• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

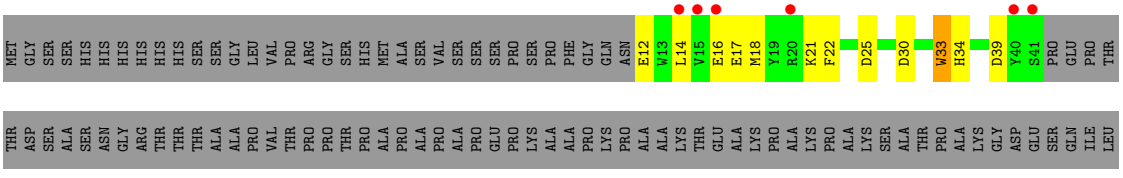
Chain F:

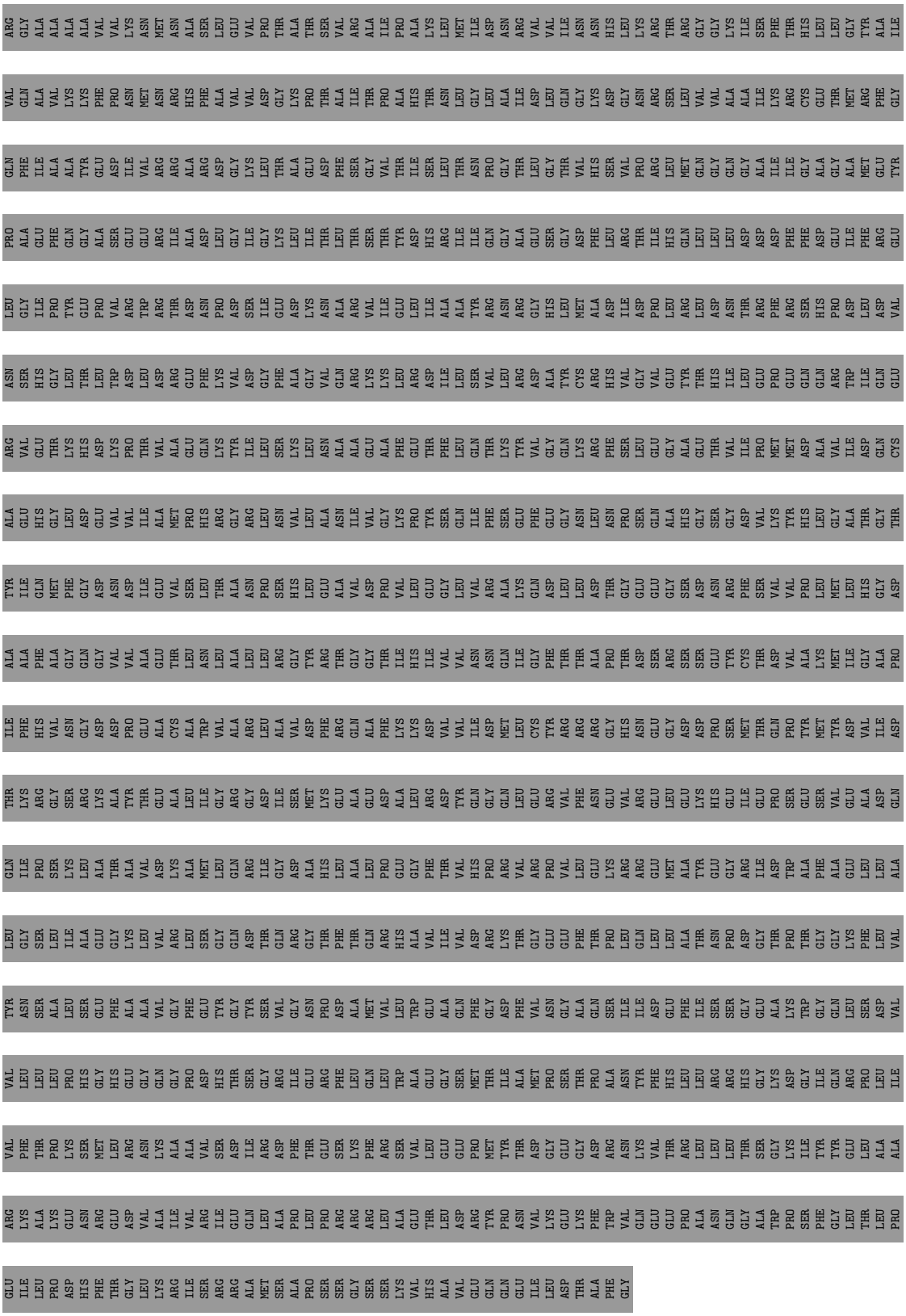


• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

Chain N:

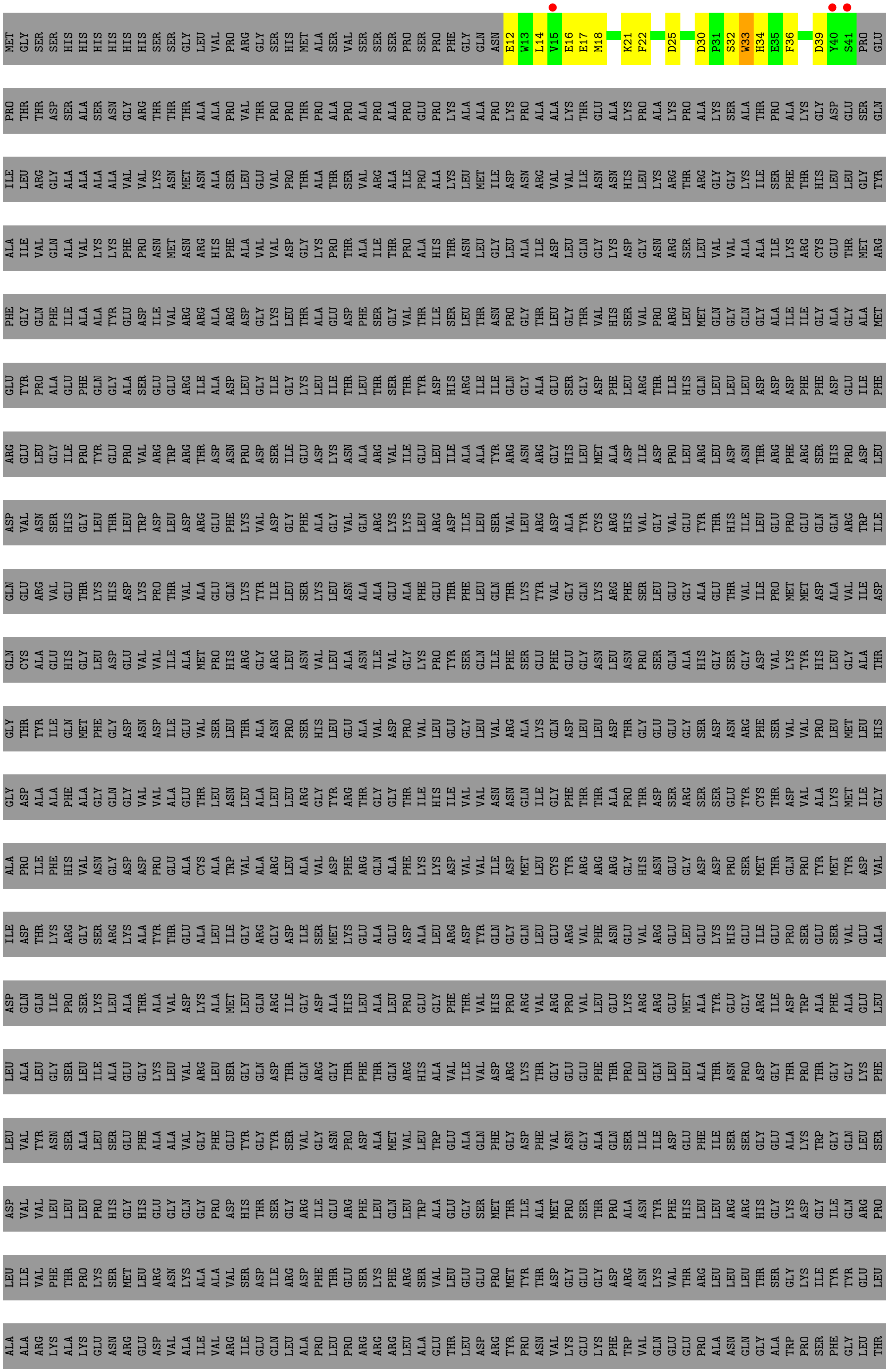




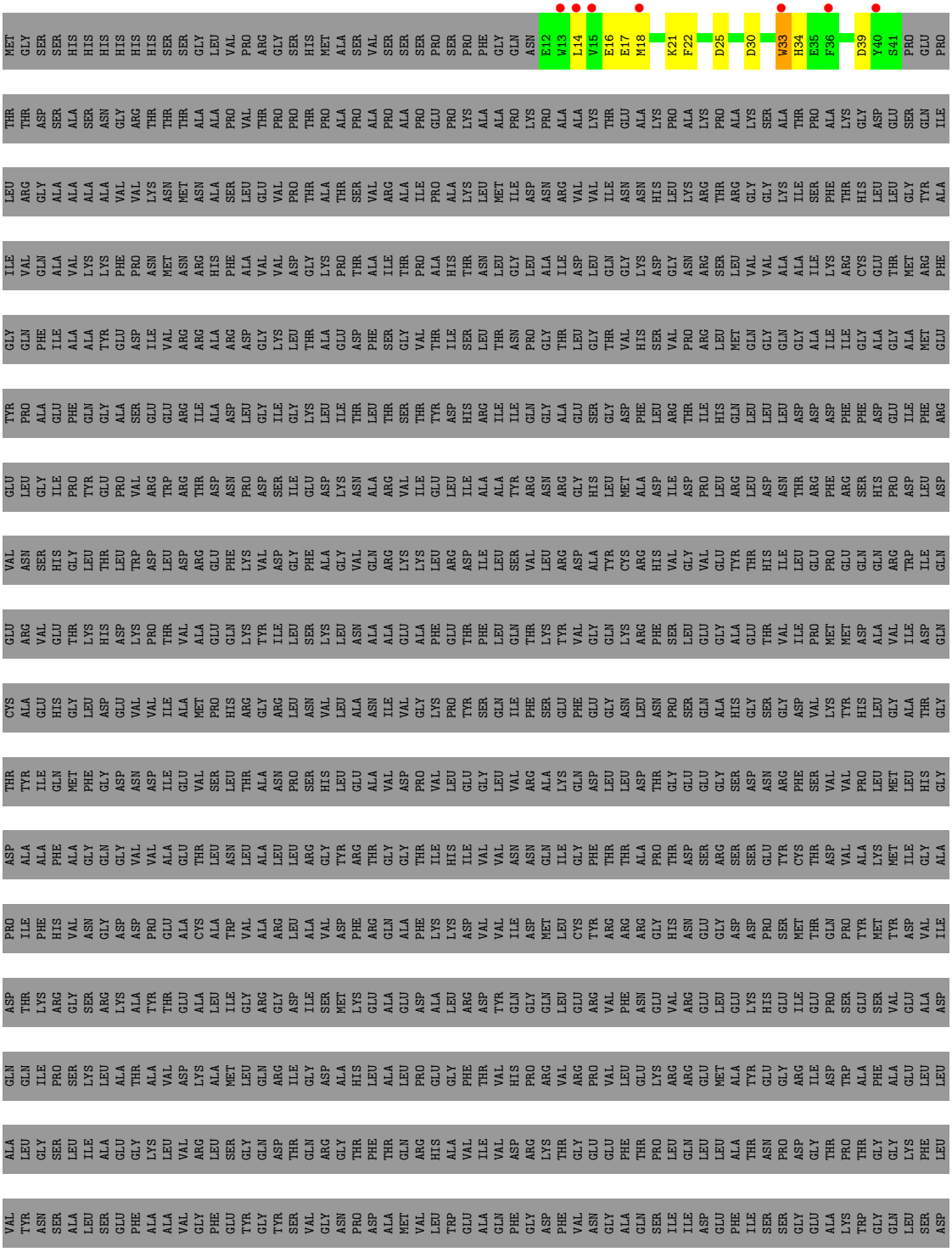


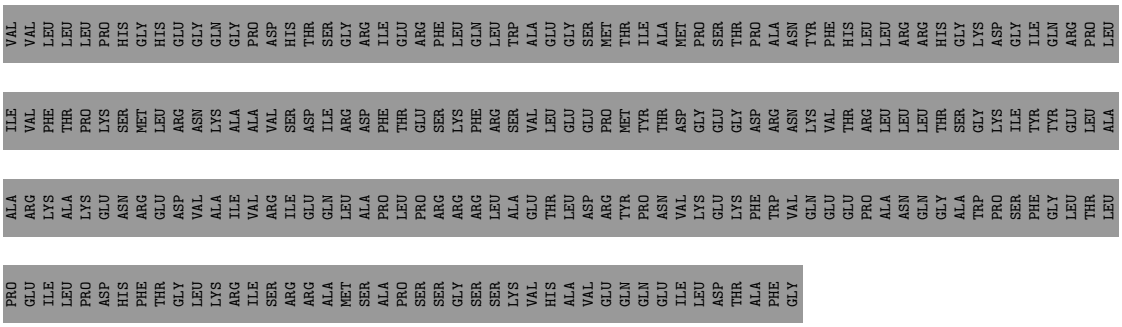
• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

Chain O: 98%


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER VAL SER SER SER PRO SER PRO PHE GLY GLN ASN E12 W13 L14 V15 E16 E17 M18 K21 F22 D25 D30 P31 S32 W33 H34 E35 F36 D39 Y40 S41 PRO GLU
PRO THR THR ASP SER ALA SER ASN GLY ARG THR THR THR ALA ALA PRO VAL THR PRO PRO THR PRO ALA PRO ALA PRO ALA PRO GLU PRO LYS ALA ALA PRO LYS PRO ALA ALA LYS THR GLU ALA LYS PRO ALA LYS PRO ALA LYS SER ALA THR PRO ALA LYS GLY ASP GLU SER GLN
ILE LEU ARG GLY ALA ALA ALA ALA VAL VAL LYS ASN MET ASN ALA SER LEU GLU VAL PRO THR ALA THR SER VAL ARG ALA ILE PRO ALA LYS LEU MET ILE ASP ASN ARG VAL VAL ILE ASN ASN HIS LEU LYS ARG THR ARG GLY GLY LYS ILE SER PHE THR HIS LEU LEU GLY TYR
ALA ILE VAL GLN ALA VAL LYS LYS PHE PRO ASN MET ASN ARG HIS PHE ALA VAL VAL ASP GLY LYS PRO THR ALA ILE THR PRO ALA HIS THR ASN LEU GLY LEU ALA ILE ASP LEU GLN GLY LYS ASP GLY ASN ARG SER LEU VAL VAL ALA ALA ILE LYS ARG CYS GLU THR MET ARG
PHE GLY GLN PHE ILE ALA ALA TYR GLU ASP ILE VAL ARG ARG ALA ARG ASP GLY LYS LEU THR ALA GLU ASP PHE SER GLY VAL THR ILE SER LEU THR ASN PRO GLY THR LEU GLY THR VAL HIS SER VAL PRO ARG LEU MET GLN GLY GLN GLY ALA ILE ILE GLY ALA GLY ALA MET
GLU TYR PRO ALA GLU PHE GLN GLY ALA SER GLU GLU ARG ILE ALA ASP LEU GLY ILE GLY LYS LEU ILE THR LEU THR SER THR TYR ASP HIS ARG ILE ILE GLN GLY ALA GLU SER GLY ASP PHE LEU ARG THR ILE HIS GLN LEU LEU LEU ASP ASP ASP PHE PHE ASP GLU ILE PHE
ARG GLU LEU GLY ILE PRO TYR GLU PRO VAL ARG TRP ARG THR ASP ASN PRO ASP SER ILE GLU ASP LYS ASN ALA ARG VAL ILE GLU LEU ILE ALA ALA TYR ARG ASN ARG GLY HIS LEU MET ALA ASP ILE ASP PRO LEU ARG LEU ASP ASN THR ARG PHE ARG SER HIS PRO ASP LEU
ASP VAL ASN SER HIS GLY LEU THR LEU TRP ASP LEU ASP ARG GLU PHE LYS VAL ASP GLY PHE ALA GLY VAL GLN ARG LYS LYS LEU ARG ASP ILE LEU SER VAL LEU ARG ASP ALA TYR CYS ARG HIS VAL GLY VAL GLU TYR THR HIS ILE LEU GLU PRO GLU GLN GLN ARG TRP ILE
GLN GLU ARG VAL GLU THR LYS HIS ASP LYS PRO THR VAL ALA GLU GLN LYS TYR ILE LEU SER LYS LEU ASN ALA ALA GLU ALA PHE GLU THR PHE LEU GLN THR LYS TYR VAL GLY GLN LYS ARG PHE SER LEU GLU GLY ALA GLU THR VAL ILE PRO MET MET ASP ALA VAL ILE ASP
GLN CYS ALA GLU HIS GLY LEU ASP GLU VAL VAL ILE ALA MET PRO HIS ARG GLY ARG LEU ASN VAL LEU ALA ASN ILE VAL GLY LYS PRO TYR SER GLN ILE PHE SER GLU PHE GLU GLY ASN LEU ASN PRO SER GLN ALA HIS GLY SER GLY ASP VAL LYS TYR HIS LEU GLY ALA THR
GLY THR TYR ILE GLN MET PHE GLY ASP ASN ASP ILE GLU VAL SER LEU THR ALA ASN PRO SER HIS LEU GLU ALA VAL ASP PRO VAL LEU GLU GLY LEU VAL ARG ALA LYS GLN ASP LEU LEU ASP THR GLY GLU GLU GLY SER ASP ASN ARG PHE SER VAL VAL PRO LEU MET LEU HIS
GLY ASP ALA ALA PHE ALA GLY GLN GLY VAL VAL ALA GLU THR LEU ASN LEU ALA LEU ARG GLY TYR ARG THR GLY GLY THR ILE HIS ILE VAL VAL ASN ASN GLN ILE GLY PHE THR THR ALA PRO THR ASP SER ARG SER SER GLU TYR CYS THR ASP VAL ALA LYS MET ILE GLY
ALA PRO ILE PHE HIS VAL ASN GLY ASP ASP PRO GLU ALA CYS ALA TRP VAL ALA ARG LEU ALA VAL ASP PHE ARG GLN ALA PHE LYS LYS ASP VAL VAL ILE ASP MET LEU CYS TYR ARG ARG ARG GLY HIS ASN GLU GLY ASP PRO SER MET THR GLN PRO TYR MET TYR ASP VAL
ILE ASP THR LYS ARG GLY SER ARG LYS ALA TYR THR GLU ALA LEU ILE GLY ARG GLY ASP ILE SER MET LYS GLU ALA GLU ASP ALA LEU ARG ASP TYR GLN GLY GLN LEU GLU ARG VAL PHE ASN GLU VAL ARG GLU LEU GLU LYS HIS GLU ILE GLU PRO SER GLU SER VAL GLU ALA
ASP GLN GLN ILE PRO SER LYS LEU ALA THR ALA VAL ASP LYS ALA MET LEU GLN ARG ILE GLY ASP ALA HIS LEU ALA LEU PRO GLU GLY PHE THR VAL HIS PRO ARG VAL ARG PRO VAL LEU GLU LYS ARG ARG GLU MET ALA TYR GLU GLY ARG ILE ASP TRP ALA PHE ALA GLU LEU
LEU ALA LEU GLY SER LEU ILE ALA GLU GLY LYS LEU VAL ARG LEU SER GLY GLN ASP THR GLN ARG GLY THR PHE THR GLN ARG HIS ALA VAL ILE VAL ASP ARG LYS THR GLY GLU GLU PHE THR PRO LEU GLN LEU LEU ALA THR ASN PRO ASP GLY THR PRO THR GLY GLY LYS PHE
LEU VAL TYR ASN SER ALA LEU SER GLU PHE ALA ALA VAL GLY PHE GLU TYR GLY TYR SER VAL GLY ASN PRO ASP ALA MET VAL LEU TRP GLU ALA GLN PHE GLY ASP PHE VAL ASN GLY ALA GLN SER ILE ILE ASP GLU PHE ILE SER SER GLY GLU ALA LYS TRP GLY GLN LEU SER
ASP VAL VAL LEU LEU LEU PRO HIS GLY HIS GLU GLY GLN GLY PRO ASP HIS THR SER GLY ARG ILE GLU ARG PHE LEU GLN LEU TRP ALA GLU GLY SER MET THR ILE ALA MET PRO SER THR PRO ALA ASN TYR PHE HIS LEU LEU ARG ARG HIS GLY LYS ASP GLY ILE GLN ARG PRO
LEU ILE VAL PHE THR PRO LYS SER MET LEU ARG ASN LYS ALA ALA VAL SER ASP ILE ARG ASP PHE THR GLU SER LYS PHE ARG SER VAL LEU GLU GLU PRO MET TYR THR ASP GLY GLU GLY ASP ARG ASN LYS VAL THR ARG LEU LEU LEU THR SER GLY LYS ILE TYR TYR GLU LEU
ALA ALA ARG LYS ALA LYS GLU ASN ARG GLU ASP VAL ALA ILE VAL ARG ILE GLU GLN LEU ALA PRO LEU PRO ARG ARG ARG LEU ALA GLU THR LEU ASP ARG TYR PRO ASN VAL LYS GLU LYS PHE TRP VAL GLN GLU GLU PRO ALA ASN GLN GLY ALA TRP PRO SER PHE GLY LEU THR

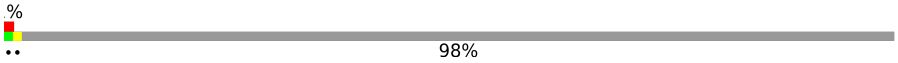
• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

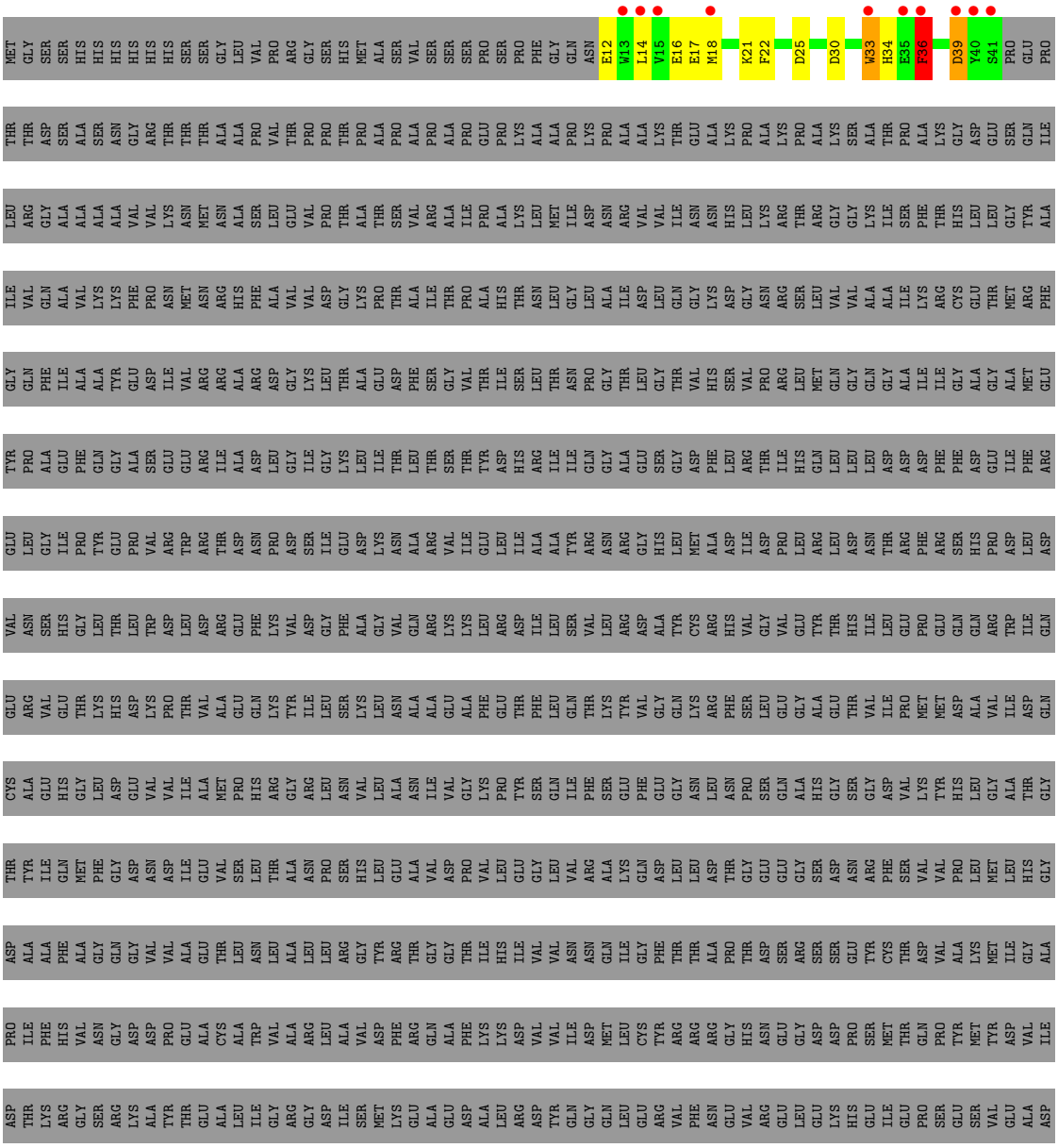


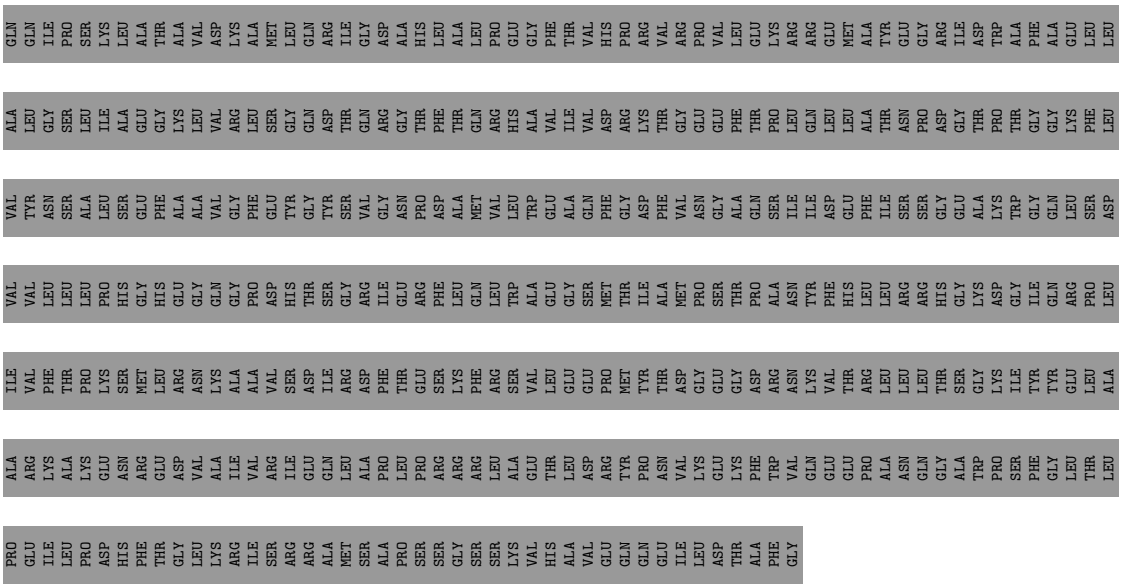


• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

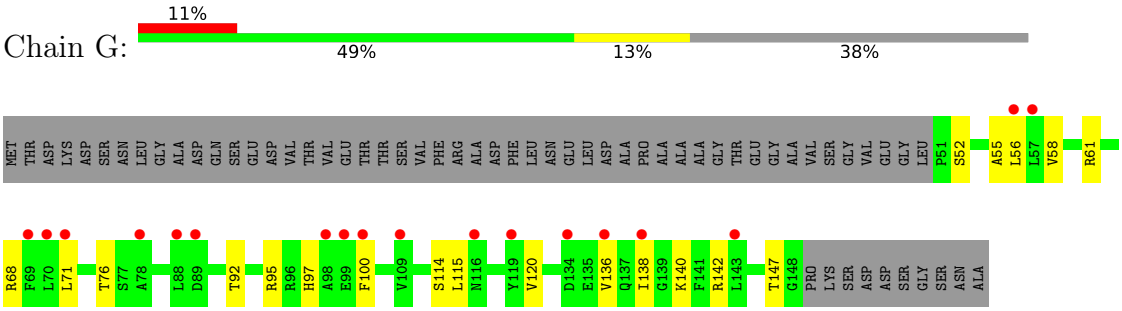
Chain Q:



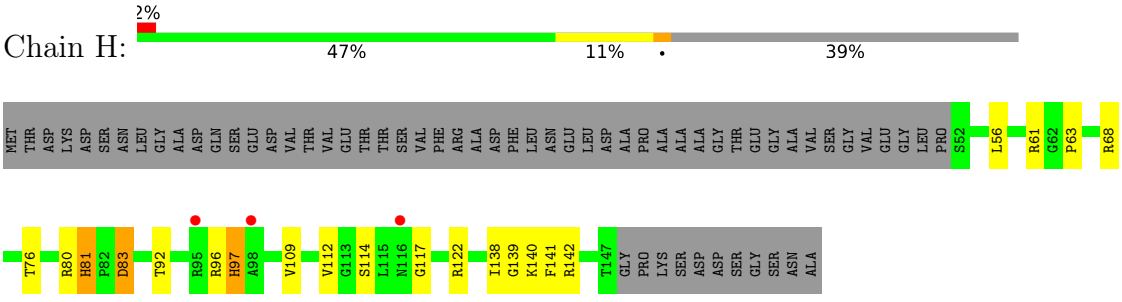




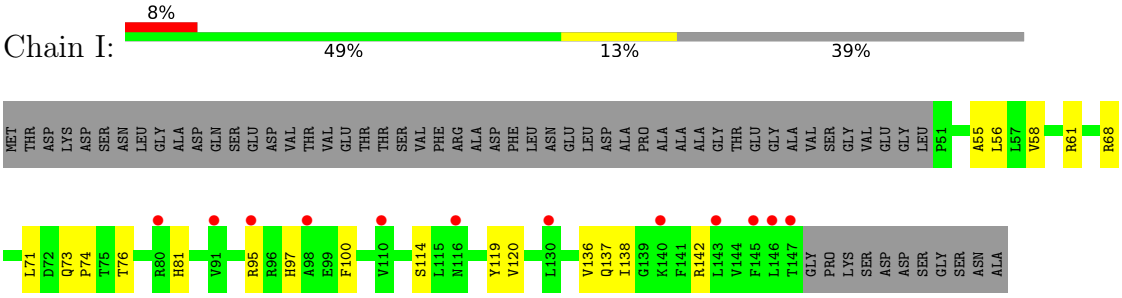
• Molecule 2: Glycogen accumulation regulator GarA



• Molecule 2: Glycogen accumulation regulator GarA

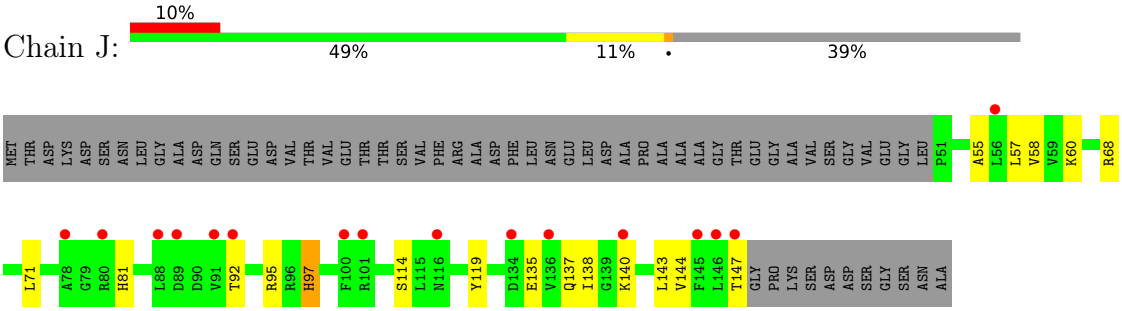


• Molecule 2: Glycogen accumulation regulator GarA



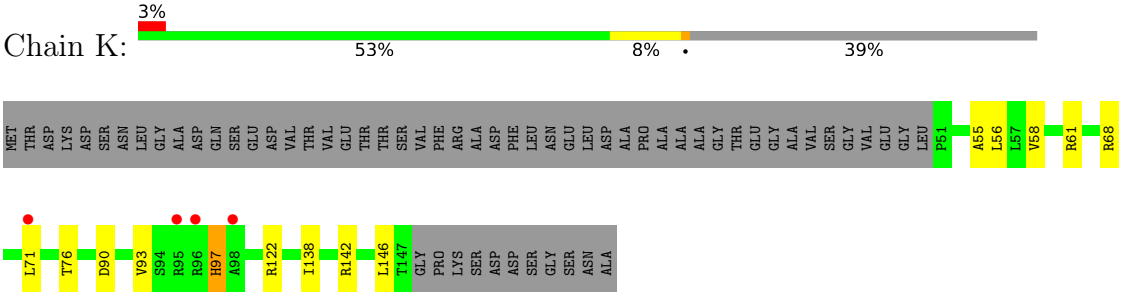
• Molecule 2: Glycogen accumulation regulator GarA

Chain J:



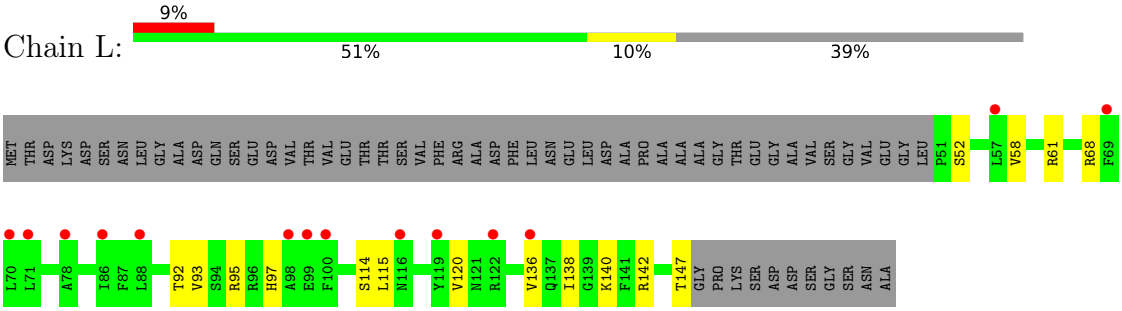
• Molecule 2: Glycogen accumulation regulator GarA

Chain K:



• Molecule 2: Glycogen accumulation regulator GarA

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	325.75Å 325.75Å 396.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.99 – 4.56 45.99 – 4.56	Depositor EDS
% Data completeness (in resolution range)	89.6 (45.99-4.56) 89.6 (45.99-4.56)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 4.64Å)	Xtriage
Refinement program	BUSTER 2.10.4 (8-JUN-2022)	Depositor
R, R_{free}	0.198 , 0.229 0.193 , 0.217	Depositor DCC
R_{free} test set	6055 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	197.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 338.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.390 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	57005	wwPDB-VP
Average B, all atoms (Å^2)	236.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: CA, TPP, MG

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	0.28	0/8751	0.45	0/11855
1	B	0.29	0/8764	0.45	0/11874
1	C	0.28	0/8767	0.45	0/11877
1	D	0.28	0/8717	0.45	0/11816
1	E	0.29	0/8710	0.45	0/11812
1	F	0.28	0/8685	0.45	0/11776
1	N	0.37	0/276	0.49	0/375
1	O	0.37	0/276	0.49	0/375
1	P	0.38	0/276	0.49	0/375
1	Q	0.40	0/276	0.49	0/375
2	G	0.25	0/757	0.43	0/1025
2	H	0.31	0/722	0.52	0/980
2	I	0.23	0/753	0.42	0/1020
2	J	0.23	0/753	0.42	0/1020
2	K	0.28	0/753	0.44	0/1020
2	L	0.26	0/753	0.43	0/1020
All	All	0.29	0/57989	0.45	0/78595

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8579	0	8402	136	0
1	B	8591	0	8414	135	0
1	C	8593	0	8408	129	0
1	D	8544	0	8341	128	0
1	E	8537	0	8299	130	0
1	F	8513	0	8287	126	0
1	N	266	0	233	13	0
1	O	266	0	233	15	0
1	P	266	0	233	11	0
1	Q	266	0	233	15	0
2	G	744	0	730	13	0
2	H	710	0	656	12	0
2	I	740	0	727	14	0
2	J	740	0	727	17	0
2	K	740	0	727	9	0
2	L	740	0	727	13	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	26	0	16	2	0
5	B	26	0	16	1	0
5	C	26	0	16	1	0
5	D	26	0	16	1	0
5	E	26	0	16	0	0
5	F	26	0	16	2	0
All	All	57005	0	55473	857	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 8.

All (857) 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:B:634:ARG:HE	1:B:636:SER:HB3	1.05	1.08
1:E:542:ARG:HE	1:E:599:LEU:HD21	1.15	1.05
1:E:634:ARG:HE	1:E:636:SER:HB3	1.16	1.05
1:F:645:ASP:HB3	1:F:677:ASN:HA	1.41	1.01
1:F:634:ARG:HE	1:F:636:SER:HB3	1.26	1.01
1:D:542:ARG:HE	1:D:599:LEU:HD21	1.25	1.00
1:C:542:ARG:HE	1:C:599:LEU:HD21	1.27	0.99
1:A:645:ASP:HB3	1:A:677:ASN:HA	1.44	0.98
1:F:780:GLY:HA2	1:Q:12:GLU:HB2	1.42	0.98
2:K:97:HIS:CD2	2:K:138:ILE:HG23	2.00	0.96
2:L:97:HIS:CD2	2:L:138:ILE:HG23	2.01	0.96
1:C:240:ASP:HB2	1:C:242:LYS:NZ	1.81	0.96
1:B:240:ASP:HB2	1:B:242:LYS:NZ	1.81	0.95
1:A:240:ASP:HB2	1:A:242:LYS:NZ	1.82	0.95
2:H:97:HIS:CD2	2:H:138:ILE:HG23	2.02	0.94
1:D:240:ASP:HB2	1:D:242:LYS:NZ	1.82	0.94
2:G:97:HIS:CD2	2:G:138:ILE:HG23	2.01	0.94
2:J:97:HIS:CD2	2:J:138:ILE:HG23	2.02	0.94
1:C:645:ASP:HB3	1:C:677:ASN:HA	1.50	0.94
1:A:377:TYR:HE2	1:A:444:CYS:HG	1.07	0.92
2:I:97:HIS:CD2	2:I:138:ILE:HG23	2.06	0.91
1:C:131:ILE:HG23	1:C:330:HIS:CD2	2.06	0.91
1:B:542:ARG:HE	1:B:599:LEU:HD21	1.35	0.91
1:A:504:LYS:CB	1:A:749:GLU:HA	2.01	0.90
1:N:14:LEU:HG	1:N:18:MET:HB3	1.52	0.90
2:J:60:LYS:NZ	2:J:135:GLU:HG3	1.86	0.90
1:P:14:LEU:HG	1:P:18:MET:HB3	1.52	0.89
1:O:14:LEU:HG	1:O:18:MET:HB3	1.52	0.89
2:J:60:LYS:HZ1	2:J:135:GLU:HG3	1.36	0.88
1:Q:14:LEU:HG	1:Q:18:MET:HB3	1.52	0.88
1:D:780:GLY:HA2	1:N:12:GLU:HB2	1.56	0.87
1:F:366:LYS:HA	1:F:369:ARG:HD2	1.58	0.86
1:B:634:ARG:NE	1:B:636:SER:HB3	1.91	0.86
2:J:60:LYS:HD2	2:J:144:VAL:HB	1.56	0.85
1:A:441:ASP:HA	1:A:445:ARG:HG3	1.57	0.85
1:E:441:ASP:HA	1:E:445:ARG:HG2	1.60	0.84
1:C:442:ALA:HB1	1:C:467:VAL:HG12	1.59	0.83
1:A:634:ARG:HE	1:A:636:SER:HB3	1.42	0.83
1:B:366:LYS:HA	1:B:369:ARG:HD2	1.58	0.83
1:A:366:LYS:HA	1:A:369:ARG:HD2	1.58	0.83
1:D:366:LYS:HA	1:D:369:ARG:HD2	1.58	0.83
1:E:366:LYS:HA	1:E:369:ARG:HD2	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:LYS:HA	1:C:369:ARG:HD2	1.58	0.82
1:C:240:ASP:HB2	1:C:242:LYS:HZ3	1.47	0.81
1:C:131:ILE:HG23	1:C:330:HIS:HD2	1.42	0.80
1:B:240:ASP:HB2	1:B:242:LYS:HZ2	1.42	0.80
1:E:645:ASP:HB2	1:E:677:ASN:HA	1.63	0.80
1:A:240:ASP:HB2	1:A:242:LYS:HZ2	1.44	0.79
1:A:748:ASN:HB2	1:A:751:ASP:HB2	1.63	0.79
2:G:97:HIS:CG	2:G:138:ILE:HG23	2.17	0.79
2:L:97:HIS:CG	2:L:138:ILE:HG23	2.18	0.79
1:C:634:ARG:HE	1:C:636:SER:HB3	1.47	0.79
1:D:240:ASP:HB2	1:D:242:LYS:HZ3	1.46	0.78
1:E:441:ASP:HA	1:E:445:ARG:CG	2.14	0.77
1:A:540:ARG:NH2	1:A:747:HIS:NE2	2.33	0.77
2:K:56:LEU:HD11	2:K:68:ARG:HB3	1.65	0.76
1:B:187:THR:HB	1:F:103:GLN:HB3	1.68	0.76
1:F:542:ARG:HE	1:F:599:LEU:HD21	1.50	0.76
1:F:768:ARG:HG3	1:F:772:LYS:HZ2	1.53	0.74
1:D:1011:HIS:CE1	1:D:1025:ILE:HD11	2.23	0.73
1:E:1011:HIS:CE1	1:E:1025:ILE:HD11	2.23	0.73
1:E:496:LEU:HD21	1:E:543:LEU:HD12	1.70	0.73
2:J:97:HIS:HA	2:J:114:SER:HB3	1.69	0.73
1:C:1011:HIS:CE1	1:C:1025:ILE:HD11	2.24	0.73
1:D:634:ARG:HE	1:D:636:SER:HB3	1.53	0.73
2:J:97:HIS:CG	2:J:138:ILE:HG23	2.23	0.73
1:B:1011:HIS:CE1	1:B:1025:ILE:HD11	2.23	0.72
1:C:780:GLY:HA2	1:O:12:GLU:HB2	1.71	0.72
1:D:645:ASP:HB3	1:D:677:ASN:HA	1.70	0.72
1:F:1011:HIS:CE1	1:F:1025:ILE:HD11	2.24	0.72
1:B:1021:THR:HA	1:B:1070:LYS:NZ	2.05	0.72
1:E:1021:THR:HA	1:E:1070:LYS:NZ	2.05	0.72
1:C:240:ASP:HB2	1:C:242:LYS:HZ2	1.53	0.72
1:E:129:ARG:NH1	1:E:330:HIS:ND1	2.38	0.72
1:E:542:ARG:NE	1:E:599:LEU:HD21	1.98	0.72
1:A:1011:HIS:CE1	1:A:1025:ILE:HD11	2.24	0.72
1:D:240:ASP:HB2	1:D:242:LYS:HZ2	1.55	0.71
1:D:808:ARG:HG2	1:D:812:LYS:NZ	2.05	0.71
1:D:131:ILE:HD12	1:D:308:LEU:HD12	1.72	0.71
1:A:103:GLN:HB3	1:E:187:THR:HB	1.72	0.71
1:D:1021:THR:HA	1:D:1070:LYS:NZ	2.06	0.71
1:C:441:ASP:HA	1:C:445:ARG:CG	2.21	0.71
1:C:1021:THR:HA	1:C:1070:LYS:NZ	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:THR:HA	1:A:1070:LYS:NZ	2.05	0.70
1:C:542:ARG:NE	1:C:599:LEU:HD21	2.04	0.70
1:F:1021:THR:HA	1:F:1070:LYS:NZ	2.05	0.70
1:B:441:ASP:HA	1:B:445:ARG:CG	2.23	0.69
1:F:131:ILE:HD12	1:F:308:LEU:HD12	1.74	0.69
1:C:441:ASP:HA	1:C:445:ARG:HG2	1.75	0.69
1:E:493:GLU:O	1:E:497:GLN:HG2	1.92	0.69
1:E:442:ALA:HB1	1:E:467:VAL:HG12	1.73	0.69
1:D:441:ASP:HA	1:D:445:ARG:CG	2.23	0.69
1:C:131:ILE:HD12	1:C:308:LEU:HD12	1.75	0.69
1:A:634:ARG:NE	1:A:636:SER:HB3	2.07	0.68
1:B:240:ASP:HB2	1:B:242:LYS:HZ3	1.56	0.68
1:C:170:LYS:HE2	1:C:220:GLU:HA	1.75	0.68
1:D:442:ALA:HB1	1:D:467:VAL:HG12	1.74	0.68
1:A:240:ASP:HB2	1:A:242:LYS:HZ3	1.56	0.68
1:Q:14:LEU:HG	1:Q:18:MET:CB	2.24	0.68
1:D:170:LYS:HE2	1:D:220:GLU:HA	1.75	0.68
2:K:97:HIS:CG	2:K:138:ILE:HG23	2.29	0.68
1:B:131:ILE:HD12	1:B:308:LEU:HD12	1.76	0.68
1:P:14:LEU:HG	1:P:18:MET:CB	2.24	0.67
1:B:170:LYS:HE2	1:B:220:GLU:HA	1.77	0.67
1:B:178:HIS:CD2	1:B:189:ILE:HD12	2.29	0.67
1:C:302:ILE:HG23	1:E:288:GLU:HB2	1.76	0.67
1:D:178:HIS:CD2	1:D:189:ILE:HD12	2.30	0.67
1:F:415:LEU:HA	1:F:432:LEU:HB3	1.77	0.67
1:F:441:ASP:HA	1:F:445:ARG:CG	2.25	0.67
1:A:131:ILE:HD12	1:A:308:LEU:HD12	1.76	0.67
1:E:683:THR:HG21	1:F:905:ARG:HD3	1.77	0.67
1:A:191:PRO:HA	1:C:101:GLU:HG2	1.76	0.67
1:C:415:LEU:HA	1:C:432:LEU:HB3	1.77	0.67
1:A:170:LYS:HE2	1:A:220:GLU:HA	1.77	0.67
1:D:415:LEU:HA	1:D:432:LEU:HB3	1.77	0.67
1:F:542:ARG:NE	1:F:599:LEU:HD21	2.10	0.67
1:A:302:ILE:HG23	1:C:288:GLU:HB2	1.75	0.66
1:A:415:LEU:HA	1:A:432:LEU:HB3	1.77	0.66
1:B:496:LEU:HD21	1:B:543:LEU:HD12	1.77	0.66
1:C:178:HIS:CD2	1:C:189:ILE:HD12	2.30	0.66
2:L:120:VAL:HG22	2:L:136:VAL:HG22	1.77	0.66
1:E:178:HIS:CD2	1:E:189:ILE:HD12	2.30	0.66
1:N:14:LEU:HG	1:N:18:MET:CB	2.24	0.66
1:D:542:ARG:NE	1:D:599:LEU:HD21	2.05	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:743:ARG:NH1	1:E:747:HIS:ND1	2.43	0.66
1:E:170:LYS:HE2	1:E:220:GLU:HA	1.77	0.66
1:B:508:LEU:HD13	1:B:541:GLY:HA3	1.78	0.66
1:E:131:ILE:HD12	1:E:308:LEU:HD12	1.77	0.66
1:E:540:ARG:HH21	1:E:747:HIS:CE1	2.13	0.66
1:E:415:LEU:HA	1:E:432:LEU:HB3	1.77	0.66
1:A:119:SER:HB3	1:A:271:MET:HA	1.78	0.65
1:A:178:HIS:CD2	1:A:189:ILE:HD12	2.31	0.65
1:F:634:ARG:NE	1:F:636:SER:HB3	2.06	0.65
1:O:14:LEU:HG	1:O:18:MET:CB	2.24	0.65
1:A:856:VAL:HG11	1:A:864:LEU:HD11	1.79	0.65
1:B:415:LEU:HA	1:B:432:LEU:HB3	1.77	0.65
1:B:503:GLN:NE2	1:B:578:TYR:OH	2.29	0.65
2:L:58:VAL:HG22	2:L:68:ARG:HG2	1.79	0.65
1:F:178:HIS:CD2	1:F:189:ILE:HD12	2.31	0.65
2:J:81:HIS:HD2	2:J:95:ARG:HD2	1.61	0.65
1:A:1021:THR:HA	1:A:1070:LYS:HZ3	1.61	0.64
1:E:508:LEU:HD13	1:E:541:GLY:HA3	1.78	0.64
1:F:663:LEU:HB2	1:F:666:TYR:HB2	1.79	0.64
1:B:288:GLU:HB2	1:D:302:ILE:HG23	1.80	0.64
1:B:1051:LEU:HD11	1:B:1064:LEU:HD11	1.78	0.64
1:E:1051:LEU:HD11	1:E:1064:LEU:HD11	1.78	0.64
1:Q:18:MET:HA	1:Q:21:LYS:HD2	1.79	0.64
1:D:441:ASP:HA	1:D:445:ARG:HG2	1.80	0.64
1:P:18:MET:HA	1:P:21:LYS:HD2	1.80	0.64
1:F:768:ARG:HG2	1:F:772:LYS:HG3	1.80	0.64
1:F:1051:LEU:HD11	1:F:1064:LEU:HD11	1.79	0.64
2:H:56:LEU:HD11	2:H:68:ARG:HB3	1.78	0.64
1:D:1051:LEU:HD11	1:D:1064:LEU:HD11	1.79	0.64
1:F:170:LYS:HE2	1:F:220:GLU:HA	1.80	0.63
1:E:1187:ILE:HG22	1:E:1188:LEU:HG	1.80	0.63
1:B:441:ASP:HA	1:B:445:ARG:HG2	1.78	0.63
1:C:1051:LEU:HD11	1:C:1064:LEU:HD11	1.79	0.63
1:E:178:HIS:NE2	1:E:189:ILE:HD12	2.14	0.63
1:B:178:HIS:NE2	1:B:189:ILE:HD12	2.13	0.63
1:D:288:GLU:HB2	1:F:302:ILE:HG23	1.79	0.63
1:F:178:HIS:NE2	1:F:189:ILE:HD12	2.14	0.63
1:F:442:ALA:HB1	1:F:467:VAL:HG12	1.81	0.63
1:F:772:LYS:HE3	1:Q:39:ASP:HB2	1.80	0.63
1:A:288:GLU:HB2	1:E:302:ILE:HG23	1.81	0.62
1:B:1013:HIS:HA	1:B:1021:THR:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:HIS:NE2	1:D:189:ILE:HD12	2.14	0.62
1:F:1013:HIS:HA	1:F:1021:THR:HG23	1.81	0.62
1:A:663:LEU:HB2	1:A:666:TYR:HB2	1.81	0.62
1:A:1013:HIS:HA	1:A:1021:THR:HG23	1.81	0.62
1:A:1051:LEU:HD11	1:A:1064:LEU:HD11	1.80	0.62
1:C:1021:THR:HA	1:C:1070:LYS:HZ3	1.64	0.62
1:N:18:MET:HA	1:N:21:LYS:HD2	1.81	0.62
1:O:18:MET:HA	1:O:21:LYS:HD2	1.80	0.62
1:C:178:HIS:NE2	1:C:189:ILE:HD12	2.14	0.62
1:E:1013:HIS:HA	1:E:1021:THR:HG23	1.82	0.62
1:A:178:HIS:NE2	1:A:189:ILE:HD12	2.15	0.62
1:C:1013:HIS:HA	1:C:1021:THR:HG23	1.82	0.62
1:N:14:LEU:CG	1:N:18:MET:HB3	2.28	0.62
1:A:377:TYR:HE2	1:A:444:CYS:SG	2.19	0.62
1:F:441:ASP:HA	1:F:445:ARG:HG2	1.80	0.62
1:D:1013:HIS:HA	1:D:1021:THR:HG23	1.82	0.61
1:F:505:ARG:HB3	1:F:747:HIS:HA	1.82	0.61
1:B:1003:SER:HB3	1:B:1063:PRO:HG3	1.82	0.61
2:I:58:VAL:HG22	2:I:68:ARG:HG2	1.82	0.61
1:B:1021:THR:HA	1:B:1070:LYS:HZ3	1.64	0.61
1:D:1003:SER:HB3	1:D:1063:PRO:HG3	1.83	0.61
1:E:1021:THR:HA	1:E:1070:LYS:HZ3	1.64	0.61
1:F:1003:SER:HB3	1:F:1063:PRO:HG3	1.82	0.61
1:A:1003:SER:HB3	1:A:1063:PRO:HG3	1.82	0.61
1:C:536:ALA:HB2	1:C:613:LEU:HD13	1.83	0.61
1:C:542:ARG:HE	1:C:599:LEU:CD2	2.08	0.61
1:C:1003:SER:HB3	1:C:1063:PRO:HG3	1.82	0.61
2:I:120:VAL:HG22	2:I:136:VAL:HG22	1.81	0.61
1:D:808:ARG:HG2	1:D:812:LYS:HZ1	1.65	0.61
1:B:277:ILE:HG23	1:B:311:THR:HG23	1.83	0.61
1:C:442:ALA:HB1	1:C:467:VAL:CG1	2.30	0.61
1:E:1003:SER:HB3	1:E:1063:PRO:HG3	1.82	0.61
2:H:97:HIS:CG	2:H:138:ILE:HG23	2.35	0.61
2:I:73:GLN:HG3	2:I:74:PRO:HD2	1.82	0.61
1:A:540:ARG:HH21	1:A:747:HIS:CE1	2.19	0.61
1:A:508:LEU:HD13	1:A:541:GLY:HA3	1.83	0.60
1:B:801:GLU:OE1	2:H:81:HIS:NE2	2.35	0.60
1:D:536:ALA:HB2	1:D:613:LEU:HD13	1.84	0.60
1:B:442:ALA:HB1	1:B:467:VAL:HG12	1.83	0.60
1:B:129:ARG:NH1	1:B:330:HIS:ND1	2.50	0.60
1:F:536:ALA:HB2	1:F:613:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:14:LEU:CG	1:O:18:MET:HB3	2.29	0.60
2:L:61:ARG:HB2	2:L:142:ARG:HB2	1.84	0.60
1:B:291:GLY:HA3	1:D:413:TRP:CZ2	2.36	0.60
1:B:645:ASP:CB	1:B:677:ASN:HA	2.32	0.60
2:G:120:VAL:HG22	2:G:136:VAL:HG22	1.83	0.60
1:A:125:ALA:CB	1:A:314:HIS:HD2	2.15	0.59
1:B:198:LEU:HD11	1:B:216:ILE:HD11	1.83	0.59
1:B:536:ALA:HB2	1:B:613:LEU:HD13	1.83	0.59
2:G:97:HIS:HA	2:G:114:SER:HB3	1.84	0.59
1:A:536:ALA:HB2	1:A:613:LEU:HD13	1.83	0.59
1:F:540:ARG:NH2	1:F:747:HIS:NE2	2.51	0.59
1:A:509:GLU:HB3	1:A:744:ARG:HB3	1.84	0.59
1:B:904:GLN:HG2	1:B:945:VAL:HG22	1.85	0.59
1:C:191:PRO:HA	1:E:101:GLU:HG3	1.85	0.59
1:F:508:LEU:HD13	1:F:541:GLY:HA3	1.85	0.59
2:I:97:HIS:CG	2:I:138:ILE:HG23	2.37	0.59
1:D:1021:THR:HA	1:D:1070:LYS:HZ3	1.67	0.59
1:B:302:ILE:HG23	1:F:288:GLU:HB2	1.84	0.59
1:E:277:ILE:HG23	1:E:311:THR:HG23	1.85	0.59
1:E:536:ALA:HB2	1:E:613:LEU:HD13	1.83	0.59
1:C:651:GLN:HE21	1:C:653:VAL:HG12	1.68	0.58
1:E:634:ARG:NE	1:E:636:SER:HB3	2.01	0.58
1:A:291:GLY:HA3	1:E:413:TRP:CZ2	2.39	0.58
1:F:904:GLN:HG2	1:F:945:VAL:HG22	1.85	0.58
1:A:198:LEU:HD11	1:A:216:ILE:HD11	1.85	0.58
1:C:413:TRP:CZ2	1:E:291:GLY:HA3	2.38	0.58
2:G:92:THR:HG21	2:G:140:LYS:HG3	1.84	0.58
1:Q:14:LEU:CG	1:Q:18:MET:HB3	2.29	0.58
1:C:904:GLN:HG2	1:C:945:VAL:HG22	1.86	0.58
2:J:55:ALA:HB3	2:J:71:LEU:HB2	1.86	0.58
1:F:1120:TYR:CE1	1:F:1139:ARG:NH1	2.72	0.58
2:I:55:ALA:HB3	2:I:71:LEU:HB2	1.85	0.58
2:I:97:HIS:HA	2:I:114:SER:HB3	1.84	0.58
1:B:413:TRP:CZ2	1:F:291:GLY:HA3	2.38	0.57
1:E:904:GLN:HG2	1:E:945:VAL:HG22	1.85	0.57
1:A:904:GLN:HG2	1:A:945:VAL:HG22	1.85	0.57
1:C:382:HIS:CE1	1:C:383:LEU:HG	2.39	0.57
1:D:645:ASP:CB	1:D:677:ASN:HA	2.34	0.57
1:A:441:ASP:HA	1:A:445:ARG:CG	2.31	0.57
1:A:768:ARG:CD	1:A:772:LYS:HZ2	2.17	0.57
1:B:645:ASP:HB3	1:B:677:ASN:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASP:HB2	1:E:192:ALA:HB2	1.86	0.57
1:B:105:LEU:HD21	1:D:185:LYS:HD3	1.87	0.57
1:B:1013:HIS:ND1	1:B:1021:THR:HG21	2.20	0.57
1:C:798:GLY:HA2	2:I:95:ARG:HD3	1.87	0.57
1:D:193:HIS:ND1	1:D:220:GLU:OE2	2.28	0.57
1:D:380:ARG:HB2	1:D:383:LEU:HD12	1.87	0.57
1:D:1120:TYR:CE1	1:D:1139:ARG:NH1	2.72	0.57
1:E:768:ARG:CD	1:E:772:LYS:HZ2	2.18	0.57
1:F:1013:HIS:ND1	1:F:1021:THR:HG21	2.20	0.57
1:A:1013:HIS:ND1	1:A:1021:THR:HG21	2.20	0.57
1:A:1120:TYR:CE1	1:A:1139:ARG:NH1	2.73	0.57
1:D:904:GLN:HG2	1:D:945:VAL:HG22	1.86	0.57
1:E:1120:TYR:CE1	1:E:1139:ARG:NH1	2.73	0.57
1:B:1198:ILE:HG22	1:B:1221:ILE:HG23	1.85	0.57
1:A:413:TRP:CZ2	1:C:291:GLY:HA3	2.39	0.57
1:A:542:ARG:HE	1:A:599:LEU:HD21	1.68	0.57
1:B:607:GLU:OE1	1:B:643:HIS:ND1	2.36	0.57
1:C:768:ARG:CD	1:C:772:LYS:HZ2	2.18	0.57
1:D:377:TYR:HB3	1:D:439:LEU:HD22	1.86	0.57
1:B:1120:TYR:CE1	1:B:1139:ARG:NH1	2.73	0.57
1:A:193:HIS:ND1	1:A:220:GLU:OE2	2.29	0.56
1:E:1013:HIS:ND1	1:E:1021:THR:HG21	2.20	0.56
1:B:146:HIS:ND1	1:B:445:ARG:NH1	2.53	0.56
1:B:193:HIS:ND1	1:B:220:GLU:OE2	2.29	0.56
1:C:1120:TYR:CE1	1:C:1139:ARG:NH1	2.73	0.56
1:D:291:GLY:HA3	1:F:413:TRP:CZ2	2.40	0.56
1:D:542:ARG:HE	1:D:599:LEU:CD2	2.09	0.56
1:B:135:LEU:HD22	1:B:355:TRP:HB2	1.87	0.56
1:D:768:ARG:CD	1:D:772:LYS:HZ2	2.18	0.56
1:E:135:LEU:HD22	1:E:355:TRP:HB2	1.87	0.56
1:E:202:LEU:HD21	1:E:238:ALA:HB1	1.87	0.56
2:G:58:VAL:HG22	2:G:68:ARG:HG2	1.88	0.56
1:B:743:ARG:NH1	1:B:747:HIS:ND1	2.53	0.56
1:F:135:LEU:HD22	1:F:355:TRP:HB2	1.87	0.56
1:A:606:LEU:HG	5:A:1303:TPP:N3'	2.20	0.56
1:C:146:HIS:ND1	1:C:445:ARG:NH1	2.51	0.56
1:N:18:MET:HE3	1:N:33:TRP:CD1	2.40	0.56
1:A:571:HIS:NE2	5:A:1303:TPP:H2	2.20	0.56
1:C:135:LEU:HD22	1:C:355:TRP:HB2	1.87	0.56
1:C:1013:HIS:ND1	1:C:1021:THR:HG21	2.20	0.56
1:B:441:ASP:HA	1:B:445:ARG:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1021:THR:HA	1:F:1070:LYS:HZ3	1.71	0.55
1:B:1013:HIS:CE1	1:B:1021:THR:HG21	2.42	0.55
1:D:198:LEU:HD11	1:D:216:ILE:HD11	1.88	0.55
1:D:1013:HIS:ND1	1:D:1021:THR:HG21	2.20	0.55
1:C:1013:HIS:CE1	1:C:1021:THR:HG21	2.42	0.55
1:E:1013:HIS:CE1	1:E:1021:THR:HG21	2.41	0.55
1:B:768:ARG:CD	1:B:772:LYS:HZ2	2.20	0.55
1:P:14:LEU:CG	1:P:18:MET:HB3	2.29	0.55
1:D:441:ASP:HA	1:D:445:ARG:HG3	1.87	0.55
1:A:135:LEU:HD22	1:A:355:TRP:HB2	1.88	0.55
1:E:663:LEU:HB2	1:E:666:TYR:HB2	1.87	0.55
1:F:768:ARG:CG	1:F:772:LYS:HZ2	2.18	0.55
2:J:57:LEU:HD13	2:J:143:LEU:HD13	1.87	0.55
2:K:61:ARG:HB2	2:K:142:ARG:HB2	1.89	0.55
1:D:135:LEU:HD22	1:D:355:TRP:HB2	1.88	0.55
1:F:1013:HIS:CE1	1:F:1021:THR:HG21	2.41	0.55
1:D:1013:HIS:CE1	1:D:1021:THR:HG21	2.42	0.55
1:A:1013:HIS:CE1	1:A:1021:THR:HG21	2.41	0.54
1:E:607:GLU:OE1	1:E:643:HIS:ND1	2.38	0.54
1:E:577:LYS:HD3	1:E:580:LEU:HD12	1.89	0.54
1:C:441:ASP:HA	1:C:445:ARG:HG3	1.88	0.54
1:C:383:LEU:HD21	1:D:455:LEU:HD21	1.88	0.54
1:P:14:LEU:HD12	1:P:17:GLU:HB3	1.89	0.54
1:E:193:HIS:ND1	1:E:220:GLU:OE2	2.29	0.54
1:E:624:LEU:HB2	1:E:626:THR:HG22	1.89	0.54
1:E:768:ARG:CG	1:E:772:LYS:HZ2	2.20	0.54
1:N:14:LEU:HD12	1:N:17:GLU:HB3	1.89	0.54
1:A:1022:SER:HB3	1:A:1206:PRO:HB3	1.90	0.54
1:B:1198:ILE:HD12	1:B:1224:THR:HG22	1.90	0.54
1:F:377:TYR:O	1:F:381:GLY:HA3	2.06	0.54
1:F:1022:SER:HB3	1:F:1206:PRO:HB3	1.90	0.54
1:A:384:MET:HG2	1:A:397:PHE:HA	1.90	0.54
1:D:124:THR:HG21	1:D:270:LEU:HB3	1.89	0.54
1:F:798:GLY:HA2	2:L:95:ARG:HD3	1.90	0.54
2:I:61:ARG:HB2	2:I:142:ARG:HB2	1.88	0.54
1:A:645:ASP:OD1	1:A:678:ASN:OD1	2.26	0.54
1:B:577:LYS:HD3	1:B:580:LEU:HD12	1.90	0.54
1:D:466:ARG:HD3	1:D:723:LEU:HD11	1.90	0.54
1:B:768:ARG:HG3	1:B:772:LYS:HZ1	1.73	0.54
1:F:195:ASN:HB3	1:F:215:ALA:HB1	1.89	0.54
1:D:146:HIS:ND1	1:D:445:ARG:NH1	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:HIS:CE1	1:D:383:LEU:HG	2.43	0.53
1:F:387:ILE:HB	1:F:740:LEU:HD13	1.90	0.53
1:C:198:LEU:HD11	1:C:216:ILE:HD11	1.90	0.53
1:C:571:HIS:NE2	5:C:1303:TPP:H2	2.24	0.53
1:E:183:ASP:HB2	1:E:185:LYS:HE2	1.90	0.53
1:O:14:LEU:HD12	1:O:17:GLU:HB3	1.89	0.53
1:B:183:ASP:HB2	1:B:185:LYS:HE2	1.90	0.53
1:C:462:TRP:CZ2	1:C:466:ARG:NH1	2.76	0.53
1:F:183:ASP:HB2	1:F:185:LYS:HE2	1.90	0.53
1:F:441:ASP:HA	1:F:445:ARG:HG3	1.89	0.53
1:A:798:GLY:HA2	2:G:95:ARG:HD3	1.90	0.53
1:C:748:ASN:HB2	1:C:751:ASP:HB2	1.91	0.53
1:E:140:ARG:HH21	1:E:156:SER:HA	1.74	0.53
1:E:441:ASP:HA	1:E:445:ARG:HG3	1.90	0.53
1:B:898:LEU:HD21	1:B:911:ARG:HD3	1.91	0.53
1:A:683:THR:HG21	1:B:905:ARG:HD3	1.90	0.53
2:J:57:LEU:HB3	2:J:143:LEU:HD22	1.90	0.53
1:A:183:ASP:HB2	1:A:185:LYS:HE2	1.90	0.53
1:D:183:ASP:HB2	1:D:185:LYS:HE2	1.90	0.53
1:D:748:ASN:HB2	1:D:751:ASP:HB2	1.91	0.53
1:E:1182:LEU:HB2	1:F:1182:LEU:HD22	1.90	0.53
1:F:146:HIS:ND1	1:F:445:ARG:NH1	2.54	0.53
1:F:193:HIS:ND1	1:F:220:GLU:OE2	2.32	0.53
1:A:768:ARG:CG	1:A:772:LYS:HZ2	2.21	0.53
1:B:706:ILE:HG21	1:B:708:HIS:CE1	2.44	0.53
2:G:55:ALA:HB3	2:G:71:LEU:HB2	1.90	0.53
1:B:748:ASN:HB2	1:B:751:ASP:HB2	1.91	0.52
1:D:442:ALA:HB1	1:D:467:VAL:CG1	2.40	0.52
1:A:131:ILE:HG12	1:A:330:HIS:ND1	2.25	0.52
1:D:1022:SER:HB3	1:D:1206:PRO:HB3	1.90	0.52
1:E:898:LEU:HD21	1:E:911:ARG:HD3	1.91	0.52
1:Q:14:LEU:HD12	1:Q:17:GLU:HB3	1.90	0.52
1:A:1182:LEU:HB2	1:B:1182:LEU:HD22	1.92	0.52
1:E:1022:SER:HB3	1:E:1206:PRO:HB3	1.90	0.52
1:A:1182:LEU:HD22	1:B:1182:LEU:HB2	1.91	0.52
1:C:183:ASP:HB2	1:C:185:LYS:HE2	1.90	0.52
1:D:377:TYR:HE2	1:D:444:CYS:SG	2.32	0.52
1:A:128:VAL:HG13	1:A:309:THR:HG22	1.91	0.52
1:D:768:ARG:HG3	1:D:772:LYS:HZ1	1.75	0.52
1:E:132:PRO:HG2	1:E:334:LEU:HD11	1.92	0.52
1:C:1022:SER:HB3	1:C:1206:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLY:HA3	1:A:443:TYR:HB3	1.91	0.52
1:F:680:ILE:O	5:F:1303:TPP:O2B	2.27	0.52
1:A:125:ALA:HB3	1:A:314:HIS:HD2	1.73	0.52
1:D:132:PRO:HG2	1:D:334:LEU:HD11	1.91	0.52
1:D:496:LEU:HD21	1:D:543:LEU:HD12	1.91	0.52
1:D:577:LYS:HD3	1:D:580:LEU:HD12	1.90	0.52
1:B:132:PRO:HG2	1:B:334:LEU:HD11	1.92	0.52
1:B:663:LEU:HB2	1:B:666:TYR:HB2	1.90	0.51
1:C:768:ARG:HG3	1:C:772:LYS:NZ	2.25	0.51
1:F:898:LEU:HD21	1:F:911:ARG:HD3	1.92	0.51
1:E:743:ARG:NH1	1:E:747:HIS:CE1	2.78	0.51
1:F:198:LEU:HD11	1:F:216:ILE:HD11	1.93	0.51
1:P:18:MET:HE3	1:P:33:TRP:CD1	2.45	0.51
1:A:132:PRO:HG2	1:A:334:LEU:HD11	1.92	0.51
1:F:683:THR:HB	1:F:756:THR:HG21	1.93	0.51
1:D:768:ARG:HG3	1:D:772:LYS:NZ	2.25	0.51
1:E:157:PHE:HA	1:E:160:LEU:HD12	1.92	0.51
1:C:577:LYS:HD3	1:C:580:LEU:HD12	1.91	0.51
1:A:768:ARG:HG3	1:A:772:LYS:NZ	2.26	0.51
1:A:898:LEU:HD21	1:A:911:ARG:HD3	1.92	0.51
1:A:577:LYS:HD3	1:A:580:LEU:HD12	1.92	0.51
1:C:193:HIS:ND1	1:C:220:GLU:OE2	2.29	0.51
1:C:768:ARG:HG3	1:C:772:LYS:HZ1	1.76	0.51
2:H:63:PRO:HD2	2:H:141:PHE:CE1	2.46	0.51
1:B:1022:SER:HB3	1:B:1206:PRO:HB3	1.91	0.51
1:E:897:ARG:NH1	1:E:946:TYR:HE2	2.09	0.51
1:B:240:ASP:CB	1:B:242:LYS:HZ2	2.20	0.51
1:C:994:SER:HB2	1:C:998:LYS:HG3	1.92	0.51
1:E:994:SER:HB2	1:E:998:LYS:HG3	1.92	0.51
1:E:706:ILE:HG21	1:E:708:HIS:CE1	2.46	0.51
1:F:278:ILE:HD11	1:F:325:PHE:HE2	1.75	0.51
1:A:542:ARG:NE	1:A:599:LEU:HD21	2.26	0.50
1:B:768:ARG:HG3	1:B:772:LYS:NZ	2.25	0.50
1:E:743:ARG:HH11	1:E:747:HIS:CE1	2.28	0.50
2:J:119:TYR:HB2	2:J:137:GLN:HB3	1.93	0.50
1:C:639:PRO:HB2	1:C:671:THR:HG23	1.93	0.50
1:C:645:ASP:OD1	1:C:678:ASN:OD1	2.30	0.50
1:D:180:ALA:O	1:D:187:THR:O	2.29	0.50
1:F:132:PRO:HG2	1:F:334:LEU:HD11	1.92	0.50
1:F:577:LYS:HD3	1:F:580:LEU:HD12	1.91	0.50
1:F:651:GLN:HE21	1:F:653:VAL:HG12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:PRO:HG2	1:C:334:LEU:HD11	1.92	0.50
1:B:897:ARG:NH1	1:B:946:TYR:HE2	2.09	0.50
1:B:994:SER:HB2	1:B:998:LYS:HG3	1.92	0.50
1:D:377:TYR:HE2	1:D:444:CYS:HG	1.59	0.50
1:D:994:SER:HB2	1:D:998:LYS:HG3	1.92	0.50
1:E:540:ARG:NH2	1:E:747:HIS:CE1	2.80	0.50
1:E:768:ARG:HG3	1:E:772:LYS:NZ	2.25	0.50
1:F:540:ARG:NH2	1:F:747:HIS:CE1	2.79	0.50
1:F:645:ASP:OD1	1:F:678:ASN:OD1	2.29	0.50
2:H:61:ARG:HD3	2:H:142:ARG:HD3	1.93	0.50
1:A:270:LEU:HD13	1:A:277:ILE:HG22	1.94	0.50
1:B:380:ARG:HB2	1:B:383:LEU:HD12	1.92	0.50
2:J:58:VAL:HG22	2:J:68:ARG:HG2	1.93	0.50
1:A:540:ARG:NH2	1:A:747:HIS:CE1	2.79	0.50
1:N:14:LEU:HG	1:N:18:MET:CG	2.42	0.50
1:A:119:SER:CB	1:A:271:MET:HA	2.41	0.50
2:G:61:ARG:HB2	2:G:142:ARG:HB2	1.94	0.50
1:A:639:PRO:HB2	1:A:671:THR:HG23	1.94	0.49
1:B:268:PRO:HD2	1:B:311:THR:CG2	2.42	0.49
1:C:387:ILE:HB	1:C:740:LEU:HD13	1.93	0.49
1:D:639:PRO:HB2	1:D:671:THR:HG23	1.93	0.49
1:D:651:GLN:HE21	1:D:653:VAL:HG12	1.76	0.49
1:F:897:ARG:NH1	1:F:946:TYR:HE2	2.09	0.49
1:O:14:LEU:O	1:O:18:MET:HG2	2.12	0.49
1:A:994:SER:HB2	1:A:998:LYS:HG3	1.93	0.49
1:D:706:ILE:CG2	1:D:708:HIS:CE1	2.95	0.49
1:F:542:ARG:HE	1:F:599:LEU:CD2	2.23	0.49
1:O:14:LEU:HG	1:O:18:MET:CG	2.42	0.49
1:O:18:MET:HE3	1:O:33:TRP:CD1	2.47	0.49
1:Q:14:LEU:HG	1:Q:18:MET:CG	2.42	0.49
1:A:331:GLN:O	1:A:335:ASP:HB2	2.12	0.49
1:D:897:ARG:NH1	1:D:946:TYR:HE2	2.10	0.49
1:E:639:PRO:HB2	1:E:671:THR:HG23	1.94	0.49
1:E:683:THR:HB	1:E:756:THR:HG21	1.94	0.49
1:F:994:SER:HB2	1:F:998:LYS:HG3	1.94	0.49
1:O:21:LYS:O	1:O:25:ASP:O	2.31	0.49
1:Q:18:MET:HE3	1:Q:33:TRP:CD1	2.47	0.49
1:B:191:PRO:HA	1:F:101:GLU:HG2	1.94	0.49
1:E:442:ALA:HB1	1:E:467:VAL:CG1	2.39	0.49
1:P:14:LEU:HG	1:P:18:MET:CG	2.43	0.49
1:A:897:ARG:NH1	1:A:946:TYR:HE2	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:TYR:HE2	1:C:444:CYS:SG	2.35	0.49
1:E:1002:LEU:HB3	1:E:1061:GLN:HB2	1.95	0.49
1:F:768:ARG:HG3	1:F:772:LYS:NZ	2.25	0.49
2:K:58:VAL:HG22	2:K:68:ARG:HG2	1.95	0.49
1:C:897:ARG:NH1	1:C:946:TYR:HE2	2.10	0.49
1:E:748:ASN:HB2	1:E:751:ASP:HB2	1.94	0.49
1:N:21:LYS:O	1:N:25:ASP:O	2.30	0.49
1:A:125:ALA:HB3	1:A:314:HIS:CD2	2.47	0.49
1:C:898:LEU:HD21	1:C:911:ARG:HD3	1.94	0.49
1:F:793:LEU:CD2	1:Q:33:TRP:CD1	2.95	0.49
1:N:14:LEU:O	1:N:18:MET:HG2	2.12	0.49
1:C:1120:TYR:CZ	1:C:1139:ARG:NH1	2.81	0.49
1:D:603:PRO:HD3	1:D:991:PHE:CZ	2.48	0.49
1:C:663:LEU:HB2	1:C:666:TYR:HB2	1.94	0.49
1:D:706:ILE:HG21	1:D:708:HIS:CE1	2.48	0.49
1:D:898:LEU:HD21	1:D:911:ARG:HD3	1.94	0.49
1:C:768:ARG:CG	1:C:772:LYS:HZ2	2.25	0.48
1:F:481:TYR:HE1	2:L:92:THR:HG22	1.78	0.48
1:A:540:ARG:NH2	1:A:747:HIS:CD2	2.81	0.48
1:A:1120:TYR:CZ	1:A:1139:ARG:NH1	2.82	0.48
1:D:1120:TYR:CZ	1:D:1139:ARG:NH1	2.81	0.48
1:F:639:PRO:HB2	1:F:671:THR:HG23	1.94	0.48
1:P:21:LYS:O	1:P:25:ASP:O	2.31	0.48
1:B:1167:VAL:HG22	1:B:1198:ILE:HB	1.95	0.48
1:D:125:ALA:HB2	1:D:314:HIS:HD2	1.77	0.48
1:F:1120:TYR:CZ	1:F:1139:ARG:NH1	2.82	0.48
1:Q:21:LYS:O	1:Q:25:ASP:O	2.31	0.48
1:F:331:GLN:O	1:F:335:ASP:HB2	2.13	0.48
1:Q:14:LEU:O	1:Q:18:MET:HG2	2.13	0.48
1:A:125:ALA:CB	1:A:314:HIS:CD2	2.96	0.48
1:A:1002:LEU:HB3	1:A:1061:GLN:HB2	1.96	0.48
1:B:1002:LEU:HB3	1:B:1061:GLN:HB2	1.96	0.48
1:B:1120:TYR:CZ	1:B:1139:ARG:NH1	2.82	0.48
1:C:603:PRO:HD3	1:C:991:PHE:CZ	2.48	0.48
1:C:706:ILE:CG2	1:C:708:HIS:CE1	2.97	0.48
1:D:1120:TYR:CG	1:D:1139:ARG:HD3	2.49	0.48
1:E:1120:TYR:CZ	1:E:1139:ARG:NH1	2.82	0.48
2:J:81:HIS:CD2	2:J:95:ARG:HH11	2.32	0.48
1:B:493:GLU:O	1:B:497:GLN:HG2	2.14	0.48
1:B:706:ILE:CG2	1:B:708:HIS:CE1	2.97	0.48
1:D:617:VAL:HG11	1:D:639:PRO:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1120:TYR:CG	1:E:1139:ARG:HD3	2.49	0.48
1:E:1182:LEU:HD22	1:F:1182:LEU:HB2	1.95	0.48
1:B:639:PRO:HB2	1:B:671:THR:HG23	1.95	0.48
1:B:1039:ILE:HD12	1:B:1144:ALA:HB3	1.96	0.48
1:C:905:ARG:HD3	1:D:683:THR:HG21	1.94	0.48
1:E:331:GLN:O	1:E:335:ASP:HB2	2.14	0.48
1:P:14:LEU:O	1:P:18:MET:HG2	2.13	0.48
1:C:617:VAL:HG11	1:C:639:PRO:HG3	1.96	0.48
1:E:706:ILE:CG2	1:E:708:HIS:CE1	2.97	0.48
1:F:1002:LEU:HB3	1:F:1061:GLN:HB2	1.95	0.48
1:F:1120:TYR:CG	1:F:1139:ARG:HD3	2.49	0.48
1:A:1120:TYR:CG	1:A:1139:ARG:HD3	2.49	0.47
1:C:277:ILE:HG23	1:C:311:THR:HG23	1.95	0.47
1:C:1039:ILE:HD12	1:C:1144:ALA:HB3	1.96	0.47
1:D:793:LEU:CD2	1:N:33:TRP:CD1	2.97	0.47
2:H:61:ARG:NH2	2:H:142:ARG:NH1	2.62	0.47
1:N:18:MET:CE	1:N:33:TRP:CD1	2.97	0.47
1:E:645:ASP:CB	1:E:677:ASN:HA	2.40	0.47
1:C:128:VAL:HG13	1:C:309:THR:HG22	1.96	0.47
1:C:1120:TYR:CG	1:C:1139:ARG:HD3	2.49	0.47
1:A:617:VAL:HG11	1:A:639:PRO:HG3	1.96	0.47
1:C:129:ARG:NH1	1:C:330:HIS:ND1	2.62	0.47
1:C:706:ILE:HG21	1:C:708:HIS:CE1	2.50	0.47
1:D:432:LEU:HA	1:D:435:ILE:HD12	1.96	0.47
1:D:1002:LEU:HB3	1:D:1061:GLN:HB2	1.95	0.47
1:E:146:HIS:ND1	1:E:445:ARG:NH1	2.61	0.47
2:L:97:HIS:HA	2:L:114:SER:HB3	1.94	0.47
1:A:603:PRO:HD3	1:A:991:PHE:CZ	2.49	0.47
1:B:651:GLN:HE21	1:B:653:VAL:HG12	1.79	0.47
1:E:1039:ILE:HD12	1:E:1144:ALA:HB3	1.96	0.47
1:B:331:GLN:O	1:B:335:ASP:HB2	2.14	0.47
1:D:331:GLN:O	1:D:335:ASP:HB2	2.14	0.47
1:B:624:LEU:HB2	1:B:626:THR:HG22	1.97	0.47
1:B:1120:TYR:CG	1:B:1139:ARG:HD3	2.50	0.47
1:C:793:LEU:HG	1:O:32:SER:HB2	1.97	0.47
1:D:663:LEU:HB2	1:D:666:TYR:HB2	1.97	0.47
1:F:682:PHE:H	1:F:743:ARG:HH12	1.63	0.47
2:H:92:THR:HG21	2:H:140:LYS:HG3	1.97	0.47
1:O:18:MET:CE	1:O:33:TRP:CD1	2.98	0.47
1:P:18:MET:CE	1:P:33:TRP:CD1	2.98	0.47
1:Q:18:MET:CE	1:Q:33:TRP:CD1	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:ASP:O	1:A:1088:SER:HB3	2.15	0.47
1:C:1002:LEU:HB3	1:C:1061:GLN:HB2	1.95	0.47
1:D:1039:ILE:HD12	1:D:1144:ALA:HB3	1.97	0.47
1:F:603:PRO:HD3	1:F:991:PHE:CZ	2.49	0.47
1:B:128:VAL:HG13	1:B:309:THR:HG22	1.97	0.47
1:E:128:VAL:HG13	1:E:309:THR:HG22	1.97	0.47
1:E:382:HIS:CE1	1:E:383:LEU:HG	2.50	0.47
1:E:384:MET:HG2	1:E:397:PHE:HA	1.97	0.47
1:D:128:VAL:HG13	1:D:309:THR:HG22	1.97	0.46
2:H:83:ASP:OD2	2:H:96:ARG:NH2	2.43	0.46
2:K:56:LEU:HD21	2:K:68:ARG:HD2	1.96	0.46
1:A:487:ASN:OD1	1:A:771:ARG:HD2	2.16	0.46
1:A:619:ALA:HB2	1:A:962:TYR:HA	1.98	0.46
1:D:768:ARG:CG	1:D:772:LYS:HZ2	2.27	0.46
1:F:617:VAL:HG11	1:F:639:PRO:HG3	1.97	0.46
1:F:856:VAL:HG11	1:F:864:LEU:HD11	1.98	0.46
1:F:1013:HIS:ND1	1:F:1021:THR:CG2	2.78	0.46
1:B:603:PRO:HD3	1:B:991:PHE:CZ	2.49	0.46
1:B:1013:HIS:ND1	1:B:1021:THR:CG2	2.79	0.46
1:C:331:GLN:O	1:C:335:ASP:HB2	2.16	0.46
1:D:768:ARG:CG	1:D:772:LYS:NZ	2.79	0.46
1:A:768:ARG:CG	1:A:772:LYS:NZ	2.79	0.46
1:C:466:ARG:HG3	1:C:723:LEU:HD11	1.96	0.46
1:C:856:VAL:HG11	1:C:864:LEU:HD11	1.97	0.46
1:E:856:VAL:HG11	1:E:864:LEU:HD11	1.98	0.46
1:F:706:ILE:CG2	1:F:708:HIS:CE1	2.99	0.46
1:A:1013:HIS:ND1	1:A:1021:THR:CG2	2.78	0.46
1:C:768:ARG:CG	1:C:772:LYS:NZ	2.79	0.46
1:D:387:ILE:HB	1:D:740:LEU:HD13	1.98	0.46
1:D:856:VAL:HG11	1:D:864:LEU:HD11	1.98	0.46
1:E:603:PRO:HD3	1:E:991:PHE:CZ	2.49	0.46
1:F:1039:ILE:HD12	1:F:1144:ALA:HB3	1.97	0.46
1:A:1039:ILE:HD12	1:A:1144:ALA:HB3	1.97	0.46
1:C:1013:HIS:ND1	1:C:1021:THR:CG2	2.79	0.46
1:C:487:ASN:OD1	1:C:771:ARG:HD2	2.16	0.46
1:C:793:LEU:CD2	1:O:33:TRP:CD1	2.99	0.46
1:E:155:ILE:HD13	1:E:159:HIS:ND1	2.31	0.46
1:A:187:THR:HB	1:C:103:GLN:HB3	1.98	0.46
1:A:857:HIS:CD2	1:A:918:ARG:HD3	2.50	0.46
1:B:856:VAL:HG11	1:B:864:LEU:HD11	1.98	0.46
1:D:487:ASN:OD1	1:D:771:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1013:HIS:ND1	1:E:1021:THR:CG2	2.79	0.46
1:A:240:ASP:CB	1:A:242:LYS:HZ2	2.21	0.46
1:B:619:ALA:HB2	1:B:962:TYR:HA	1.98	0.46
1:B:768:ARG:CG	1:B:772:LYS:NZ	2.78	0.46
1:E:487:ASN:OD1	1:E:771:ARG:HD2	2.16	0.46
1:A:101:GLU:HG2	1:E:191:PRO:HA	1.97	0.46
1:C:135:LEU:HD23	1:C:334:LEU:HA	1.98	0.46
1:F:768:ARG:CG	1:F:772:LYS:NZ	2.78	0.45
1:A:744:ARG:HD3	1:A:764:ILE:HG22	1.99	0.45
1:B:617:VAL:HG11	1:B:639:PRO:HG3	1.98	0.45
2:H:83:ASP:HB2	2:H:96:ARG:HH12	1.81	0.45
1:A:768:ARG:HG3	1:A:772:LYS:HZ1	1.81	0.45
1:D:385:ALA:H	1:D:396:ARG:HH12	1.65	0.45
1:D:1013:HIS:ND1	1:D:1021:THR:CG2	2.79	0.45
1:E:768:ARG:CG	1:E:772:LYS:NZ	2.79	0.45
2:J:92:THR:HG21	2:J:140:LYS:HG3	1.98	0.45
1:A:706:ILE:CG2	1:A:708:HIS:CE1	2.99	0.45
1:C:645:ASP:OD1	1:C:680:ILE:O	2.34	0.45
1:B:487:ASN:OD1	1:B:771:ARG:HD2	2.17	0.45
1:C:455:LEU:HD21	1:D:383:LEU:HD21	1.98	0.45
1:C:1084:ASP:O	1:C:1088:SER:HB3	2.17	0.45
1:E:617:VAL:HG11	1:E:639:PRO:HG3	1.98	0.45
1:E:619:ALA:HB2	1:E:962:TYR:HA	1.97	0.45
1:F:487:ASN:OD1	1:F:771:ARG:HD2	2.15	0.45
1:E:268:PRO:HD2	1:E:311:THR:CG2	2.47	0.45
1:A:462:TRP:O	1:A:466:ARG:HG2	2.17	0.45
1:C:619:ALA:HB2	1:C:962:TYR:HA	1.98	0.45
1:D:125:ALA:HB2	1:D:314:HIS:CD2	2.51	0.45
1:B:768:ARG:CG	1:B:772:LYS:HZ2	2.30	0.45
1:C:579:HIS:CE1	1:C:603:PRO:HA	2.52	0.45
1:D:1011:HIS:CE1	1:D:1025:ILE:CD1	2.98	0.45
1:E:1148:ARG:HG2	1:E:1188:LEU:HD21	1.99	0.45
1:F:128:VAL:HG13	1:F:309:THR:HG22	1.99	0.45
1:F:619:ALA:HB2	1:F:962:TYR:HA	1.98	0.45
1:B:542:ARG:NE	1:B:599:LEU:HD21	2.17	0.44
1:B:1148:ARG:HG2	1:B:1188:LEU:HD21	1.99	0.44
1:D:619:ALA:HB2	1:D:962:TYR:HA	1.98	0.44
1:C:337:ASP:HA	1:C:340:ASP:HB2	1.99	0.44
1:D:337:ASP:HA	1:D:340:ASP:HB2	2.00	0.44
1:D:671:THR:H	1:D:734:ASP:HA	1.83	0.44
1:D:1084:ASP:O	1:D:1088:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:HIS:H	1:A:382:HIS:CD2	2.35	0.44
1:A:1148:ARG:HG2	1:A:1188:LEU:HD21	1.99	0.44
1:C:1148:ARG:HG2	1:C:1188:LEU:HD21	1.98	0.44
1:D:1002:LEU:HB3	1:D:1061:GLN:CB	2.48	0.44
1:E:503:GLN:NE2	1:E:578:TYR:OH	2.48	0.44
1:D:135:LEU:HD23	1:D:334:LEU:HA	1.98	0.44
1:E:1002:LEU:HB3	1:E:1061:GLN:CB	2.47	0.44
1:N:18:MET:SD	1:N:33:TRP:CD2	3.11	0.44
1:A:400:HIS:HD2	1:A:402:ASP:OD1	2.01	0.44
1:C:377:TYR:HB3	1:C:439:LEU:HD22	1.98	0.44
1:C:1002:LEU:HB3	1:C:1061:GLN:CB	2.48	0.44
1:E:905:ARG:HD3	1:F:683:THR:HG21	1.98	0.44
1:F:1148:ARG:HG2	1:F:1188:LEU:HD21	1.97	0.44
1:P:18:MET:SD	1:P:33:TRP:CD2	3.11	0.44
1:B:268:PRO:HD2	1:B:311:THR:HG21	1.99	0.44
1:F:387:ILE:HA	1:F:710:ASN:HB2	2.00	0.44
2:K:122:ARG:HH12	2:K:142:ARG:HH21	1.66	0.44
1:O:18:MET:SD	1:O:33:TRP:CD2	3.11	0.44
1:C:432:LEU:HA	1:C:435:ILE:HD12	1.99	0.44
1:E:337:ASP:HA	1:E:340:ASP:HB2	2.00	0.44
1:F:337:ASP:HA	1:F:340:ASP:HB2	2.00	0.44
1:F:1011:HIS:CE1	1:F:1025:ILE:CD1	2.99	0.44
2:I:119:TYR:HB2	2:I:137:GLN:HB3	1.99	0.44
1:Q:18:MET:SD	1:Q:33:TRP:CD2	3.11	0.44
1:A:125:ALA:HB2	1:A:314:HIS:HD2	1.82	0.44
1:A:135:LEU:HD23	1:A:334:LEU:HA	1.99	0.44
1:B:135:LEU:HD23	1:B:334:LEU:HA	1.99	0.44
1:B:1002:LEU:HB3	1:B:1061:GLN:CB	2.48	0.44
1:D:894:LYS:HZ2	1:D:968:ASP:C	2.22	0.44
1:E:135:LEU:HD23	1:E:334:LEU:HA	1.99	0.44
1:C:240:ASP:CB	1:C:242:LYS:HZ2	2.28	0.44
1:F:592:ASP:HA	2:L:61:ARG:HH12	1.83	0.43
1:B:337:ASP:HA	1:B:340:ASP:HB2	2.00	0.43
1:F:135:LEU:HD23	1:F:334:LEU:HA	2.00	0.43
1:A:706:ILE:HG21	1:A:708:HIS:CE1	2.53	0.43
1:D:385:ALA:O	1:D:396:ARG:NH1	2.51	0.43
1:F:792:ALA:HA	2:L:115:LEU:HD22	2.00	0.43
2:I:56:LEU:HD11	2:I:68:ARG:HB3	2.01	0.43
1:B:382:HIS:ND1	1:B:694:TYR:OH	2.36	0.43
1:D:387:ILE:HA	1:D:710:ASN:HB2	2.01	0.43
1:D:1123:LEU:HD23	1:D:1222:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:LEU:HD13	1:E:277:ILE:HG22	2.01	0.43
1:F:280:ALA:HA	1:F:308:LEU:HD23	2.00	0.43
1:F:1002:LEU:HB3	1:F:1061:GLN:CB	2.48	0.43
2:I:76:THR:HB	2:I:100:PHE:HB2	2.00	0.43
2:K:90:ASP:HB3	2:K:93:VAL:HG23	2.00	0.43
1:A:1002:LEU:HB3	1:A:1061:GLN:CB	2.49	0.43
1:B:835:VAL:HG22	1:B:1049:PHE:HZ	1.82	0.43
1:E:155:ILE:HA	1:E:159:HIS:ND1	2.33	0.43
1:E:380:ARG:HB2	1:E:383:LEU:HD12	2.00	0.43
1:F:1013:HIS:CE1	1:F:1021:THR:CG2	3.02	0.43
1:E:768:ARG:HG3	1:E:772:LYS:HZ1	1.82	0.43
1:B:645:ASP:HB2	1:B:677:ASN:HA	2.01	0.43
1:D:446:HIS:HD2	1:D:710:ASN:HD22	1.66	0.43
1:D:1013:HIS:CE1	1:D:1021:THR:CG2	3.02	0.43
1:E:1011:HIS:CE1	1:E:1025:ILE:CD1	2.99	0.43
1:F:798:GLY:HA3	2:L:95:ARG:HB2	2.01	0.43
1:A:294:GLU:H	1:A:294:GLU:HG3	1.68	0.43
1:C:1109:VAL:HG12	1:C:1161:VAL:HG22	2.01	0.43
1:F:1084:ASP:O	1:F:1088:SER:HB3	2.18	0.43
1:A:384:MET:CG	1:A:397:PHE:HA	2.49	0.43
1:A:1013:HIS:CE1	1:A:1021:THR:CG2	3.02	0.43
1:B:329:ILE:O	1:B:333:LEU:HG	2.19	0.43
1:B:1123:LEU:HD23	1:B:1222:LEU:HD23	2.00	0.43
1:C:1123:LEU:HD23	1:C:1222:LEU:HD23	2.01	0.43
1:E:466:ARG:HG3	1:E:723:LEU:HD11	2.01	0.43
2:J:97:HIS:NE2	2:J:138:ILE:HG23	2.31	0.43
1:A:337:ASP:HA	1:A:340:ASP:HB2	2.00	0.43
1:B:280:ALA:HA	1:B:308:LEU:HD23	2.01	0.43
1:B:446:HIS:HD2	1:B:710:ASN:HD22	1.65	0.43
1:C:1013:HIS:CE1	1:C:1021:THR:CG2	3.02	0.43
1:D:240:ASP:CB	1:D:242:LYS:HZ2	2.30	0.43
1:E:755:MET:O	1:F:916:VAL:HB	2.19	0.43
1:A:280:ALA:HA	1:A:308:LEU:HD23	2.01	0.42
1:B:1200:ARG:HG3	1:B:1221:ILE:HD11	2.01	0.42
1:F:1109:VAL:HG12	1:F:1161:VAL:HG22	2.01	0.42
1:A:432:LEU:HA	1:A:435:ILE:HD12	2.00	0.42
1:A:905:ARG:HD3	1:B:683:THR:HG21	2.01	0.42
1:A:1123:LEU:HD23	1:A:1222:LEU:HD23	2.01	0.42
1:A:1200:ARG:HG3	1:A:1221:ILE:HD11	2.01	0.42
1:D:280:ALA:HA	1:D:308:LEU:HD23	2.00	0.42
1:E:835:VAL:HG22	1:E:1049:PHE:HZ	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1200:ARG:HG3	1:E:1221:ILE:HD11	2.01	0.42
2:G:56:LEU:HG	2:G:68:ARG:HB3	2.00	0.42
1:A:1096:GLU:HB2	1:A:1099:TYR:CD2	2.54	0.42
1:E:479:GLN:HA	1:E:482:ILE:HD12	2.00	0.42
1:A:857:HIS:CD2	1:B:755:MET:HA	2.53	0.42
1:A:1109:VAL:HG12	1:A:1161:VAL:HG22	2.02	0.42
1:B:1084:ASP:O	1:B:1088:SER:HB3	2.20	0.42
1:E:1013:HIS:CE1	1:E:1021:THR:CG2	3.02	0.42
1:A:380:ARG:HB2	1:A:383:LEU:HD12	2.00	0.42
1:B:1096:GLU:HB2	1:B:1099:TYR:CD2	2.54	0.42
1:D:1048:TYR:CE1	1:D:1066:VAL:HG11	2.54	0.42
1:D:1096:GLU:HB2	1:D:1099:TYR:CD2	2.55	0.42
1:D:1109:VAL:HG12	1:D:1161:VAL:HG22	2.02	0.42
1:F:682:PHE:HB2	5:F:1303:TPP:H62	2.00	0.42
1:C:671:THR:H	1:C:734:ASP:HA	1.84	0.42
1:D:607:GLU:OE1	1:D:643:HIS:ND1	2.51	0.42
1:F:1200:ARG:HG3	1:F:1221:ILE:HD11	2.02	0.42
2:J:97:HIS:CG	2:J:138:ILE:CG2	2.99	0.42
1:B:379:ASN:HA	1:B:452:THR:HG21	2.02	0.42
1:C:798:GLY:HA3	2:I:95:ARG:HB2	2.02	0.42
1:C:1096:GLU:HB2	1:C:1099:TYR:CD2	2.54	0.42
1:C:1200:ARG:HG3	1:C:1221:ILE:HD11	2.02	0.42
1:E:1109:VAL:HG12	1:E:1161:VAL:HG22	2.02	0.42
1:E:1123:LEU:HD23	1:E:1222:LEU:HD23	2.01	0.42
1:F:706:ILE:HG21	1:F:708:HIS:CE1	2.55	0.42
1:F:956:VAL:HG12	1:F:987:ILE:HG21	2.02	0.42
1:A:390:LEU:HB3	1:A:763:VAL:HG11	2.01	0.42
1:B:530:LEU:HD13	1:B:638:VAL:HG21	2.01	0.42
1:C:530:LEU:HD13	1:C:638:VAL:HG21	2.02	0.42
1:C:1011:HIS:CE1	1:C:1025:ILE:CD1	2.98	0.42
1:D:329:ILE:O	1:D:333:LEU:HG	2.20	0.42
1:D:530:LEU:HD13	1:D:638:VAL:HG21	2.02	0.42
1:F:1123:LEU:HD23	1:F:1222:LEU:HD23	2.01	0.42
1:A:985:GLN:HG2	1:B:985:GLN:HG2	2.02	0.42
1:A:1072:MET:HA	1:A:1075:ASN:HB2	2.02	0.42
1:B:784:ILE:HB	1:B:788:GLU:HB2	2.02	0.42
1:B:898:LEU:O	1:B:945:VAL:HA	2.20	0.42
1:B:992:ILE:HD13	1:B:1007:LEU:HD11	2.02	0.42
1:C:236:ARG:HD2	1:C:236:ARG:HA	1.93	0.42
1:C:266:SER:O	1:C:268:PRO:HD3	2.20	0.42
1:C:960:TYR:HE1	1:C:1003:SER:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:706:ILE:HG22	1:D:708:HIS:CE1	2.55	0.42
1:F:671:THR:H	1:F:734:ASP:HA	1.85	0.42
1:F:1096:GLU:HB2	1:F:1099:TYR:CD2	2.55	0.42
1:B:236:ARG:HA	1:B:236:ARG:HD2	1.93	0.41
1:B:238:ALA:HA	1:B:243:LEU:HG	2.02	0.41
1:C:202:LEU:HD21	1:C:238:ALA:HB1	2.02	0.41
1:C:992:ILE:HD13	1:C:1007:LEU:HD11	2.02	0.41
1:D:992:ILE:HD13	1:D:1007:LEU:HD11	2.02	0.41
1:E:266:SER:O	1:E:268:PRO:HD3	2.20	0.41
1:E:784:ILE:HB	1:E:788:GLU:HB2	2.02	0.41
1:F:1048:TYR:CE1	1:F:1066:VAL:HG11	2.55	0.41
2:L:93:VAL:HA	2:L:97:HIS:CE1	2.55	0.41
1:C:784:ILE:HB	1:C:788:GLU:HB2	2.02	0.41
1:D:125:ALA:CB	1:D:314:HIS:CD2	3.03	0.41
1:D:1072:MET:HA	1:D:1075:ASN:HB2	2.02	0.41
1:E:992:ILE:HD13	1:E:1007:LEU:HD11	2.02	0.41
1:E:1048:TYR:CE1	1:E:1066:VAL:HG11	2.54	0.41
1:E:1096:GLU:HB2	1:E:1099:TYR:CD2	2.55	0.41
1:A:238:ALA:HB2	1:A:243:LEU:HD11	2.02	0.41
1:A:956:VAL:HG12	1:A:987:ILE:HG21	2.02	0.41
1:B:956:VAL:HG12	1:B:987:ILE:HG21	2.02	0.41
1:B:1109:VAL:HG12	1:B:1161:VAL:HG22	2.02	0.41
1:D:236:ARG:O	1:D:240:ASP:OD1	2.38	0.41
1:E:898:LEU:O	1:E:945:VAL:HA	2.20	0.41
1:A:671:THR:H	1:A:734:ASP:HA	1.84	0.41
1:A:1048:TYR:CE1	1:A:1066:VAL:HG11	2.54	0.41
1:A:1155:LEU:HD22	1:A:1164:LYS:HE2	2.02	0.41
1:B:1013:HIS:CE1	1:B:1021:THR:CG2	3.02	0.41
1:C:516:PRO:HA	1:C:519:ASP:HB3	2.03	0.41
1:E:446:HIS:HD2	1:E:710:ASN:HD22	1.67	0.41
1:E:894:LYS:HZ2	1:E:968:ASP:C	2.24	0.41
1:F:772:LYS:HB3	1:Q:36:PHE:HE1	1.85	0.41
1:C:755:MET:O	1:D:916:VAL:HB	2.21	0.41
1:D:784:ILE:HB	1:D:788:GLU:HB2	2.02	0.41
1:E:671:THR:H	1:E:734:ASP:HA	1.86	0.41
1:B:266:SER:O	1:B:268:PRO:HD3	2.20	0.41
1:E:295:GLU:O	1:E:299:ASP:HB3	2.21	0.41
1:A:682:PHE:HA	1:A:747:HIS:ND1	2.36	0.41
1:A:992:ILE:HD13	1:A:1007:LEU:HD11	2.03	0.41
1:B:671:THR:H	1:B:734:ASP:HA	1.86	0.41
1:C:1048:TYR:CE1	1:C:1066:VAL:HG11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ALA:HA	1:E:308:LEU:HD23	2.02	0.41
1:E:956:VAL:HG12	1:E:987:ILE:HG21	2.02	0.41
1:E:1029:LEU:HD23	1:E:1039:ILE:HD13	2.03	0.41
1:F:440:ARG:HA	1:F:444:CYS:HB2	2.02	0.41
2:I:81:HIS:HD2	2:I:95:ARG:HD2	1.85	0.41
2:K:55:ALA:HB3	2:K:71:LEU:HB2	2.02	0.41
1:B:387:ILE:HB	1:B:740:LEU:HD13	2.01	0.41
1:B:589:MET:SD	2:H:139:GLY:O	2.79	0.41
1:B:1011:HIS:CE1	1:B:1025:ILE:CD1	2.98	0.41
1:B:1048:TYR:CE1	1:B:1066:VAL:HG11	2.55	0.41
1:C:772:LYS:HG3	1:O:36:PHE:CZ	2.55	0.41
1:D:110:ALA:O	1:D:114:LYS:HG2	2.20	0.41
1:E:387:ILE:HA	1:E:710:ASN:HB2	2.02	0.41
1:F:530:LEU:HD13	1:F:638:VAL:HG21	2.03	0.41
1:F:784:ILE:HB	1:F:788:GLU:HB2	2.02	0.41
1:F:898:LEU:O	1:F:945:VAL:HA	2.20	0.41
1:F:1072:MET:HA	1:F:1075:ASN:HB2	2.03	0.41
2:L:92:THR:HG21	2:L:140:LYS:HG3	2.01	0.41
1:A:530:LEU:HD13	1:A:638:VAL:HG21	2.02	0.41
1:B:341:GLU:HG2	1:B:344:ARG:HH12	1.85	0.41
1:B:907:THR:HG21	1:B:976:GLN:O	2.21	0.41
1:C:383:LEU:HD11	1:D:455:LEU:HG	2.03	0.41
1:C:898:LEU:O	1:C:945:VAL:HA	2.21	0.41
1:D:571:HIS:NE2	5:D:1303:TPP:H2	2.36	0.41
1:D:898:LEU:O	1:D:945:VAL:HA	2.20	0.41
1:E:530:LEU:HD13	1:E:638:VAL:HG21	2.01	0.41
1:F:125:ALA:CB	1:F:314:HIS:HD2	2.33	0.41
1:F:446:HIS:HD2	1:F:710:ASN:HD22	1.68	0.41
1:F:624:LEU:HB2	1:F:626:THR:HG22	2.02	0.41
1:F:690:ARG:HD2	1:F:695:CYS:HA	2.02	0.41
1:F:1021:THR:HA	1:F:1070:LYS:HZ1	1.82	0.41
2:J:81:HIS:HB2	2:J:95:ARG:HG3	2.03	0.41
1:A:798:GLY:HA3	2:G:95:ARG:HB2	2.03	0.41
1:B:1029:LEU:HD23	1:B:1039:ILE:HD13	2.02	0.41
1:C:956:VAL:HG12	1:C:987:ILE:HG21	2.03	0.41
1:D:1150:ARG:O	1:D:1154:THR:OG1	2.31	0.41
1:D:1200:ARG:HG3	1:D:1221:ILE:HD11	2.01	0.41
1:E:542:ARG:NH2	1:E:600:THR:O	2.54	0.41
1:E:907:THR:HG21	1:E:976:GLN:O	2.21	0.41
1:A:898:LEU:O	1:A:945:VAL:HA	2.20	0.40
1:A:1029:LEU:HD23	1:A:1039:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HD21	1:B:238:ALA:HB1	2.03	0.40
1:B:270:LEU:HD13	1:B:277:ILE:HG22	2.03	0.40
1:B:295:GLU:O	1:B:299:ASP:HB3	2.20	0.40
1:C:446:HIS:HD2	1:C:710:ASN:HD22	1.68	0.40
1:D:516:PRO:HA	1:D:519:ASP:HB3	2.03	0.40
1:E:329:ILE:O	1:E:333:LEU:HG	2.21	0.40
1:E:571:HIS:ND1	1:E:682:PHE:HE2	2.19	0.40
1:A:316:ILE:HG13	1:A:317:ILE:N	2.36	0.40
1:B:216:ILE:O	1:B:219:CYS:SG	2.79	0.40
1:B:479:GLN:HA	1:B:482:ILE:HD12	2.02	0.40
1:C:385:ALA:O	1:C:396:ARG:NH1	2.54	0.40
1:C:493:GLU:O	1:C:497:GLN:HG2	2.21	0.40
1:F:907:THR:HG21	1:F:976:GLN:O	2.21	0.40
1:F:992:ILE:HD13	1:F:1007:LEU:HD11	2.03	0.40
1:C:1072:MET:HA	1:C:1075:ASN:HB2	2.03	0.40
1:C:1111:ARG:NH1	1:C:1132:ARG:HH22	2.20	0.40
1:F:295:GLU:O	1:F:299:ASP:HB3	2.21	0.40
2:H:97:HIS:HA	2:H:114:SER:HB3	2.04	0.40
1:A:784:ILE:HB	1:A:788:GLU:HB2	2.02	0.40
1:A:792:ALA:HA	2:G:115:LEU:HD22	2.03	0.40
1:B:258:PRO:HG3	1:B:266:SER:OG	2.22	0.40
1:C:238:ALA:HA	1:C:243:LEU:HG	2.02	0.40
1:C:380:ARG:HB2	1:C:383:LEU:HD12	2.03	0.40
1:D:956:VAL:HG12	1:D:987:ILE:HG21	2.03	0.40
1:F:159:HIS:NE2	1:F:231:TYR:CE1	2.90	0.40
1:F:1029:LEU:HD23	1:F:1039:ILE:HD13	2.03	0.40
2:G:76:THR:HB	2:G:100:PHE:HB2	2.03	0.40
1:A:516:PRO:HA	1:A:519:ASP:HB3	2.03	0.40
1:B:571:HIS:NE2	5:B:1303:TPP:H2	2.37	0.40
1:B:1072:MET:HA	1:B:1075:ASN:HB2	2.02	0.40
1:C:278:ILE:HD11	1:C:325:PHE:HE2	1.85	0.40
1:D:569:GLN:NE2	1:D:748:ASN:HD22	2.20	0.40
1:D:1029:LEU:HD23	1:D:1039:ILE:HD13	2.04	0.40
1:E:341:GLU:HG2	1:E:344:ARG:HH12	1.86	0.40
1:F:316:ILE:HG13	1:F:317:ILE:H	1.87	0.40
1:F:638:VAL:HA	1:F:639:PRO:HD3	1.97	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	1100/1250 (88%)	1029 (94%)	68 (6%)	3 (0%)	41	76
1	B	1102/1250 (88%)	1022 (93%)	76 (7%)	4 (0%)	34	72
1	C	1103/1250 (88%)	1028 (93%)	72 (6%)	3 (0%)	41	76
1	D	1101/1250 (88%)	1026 (93%)	71 (6%)	4 (0%)	34	72
1	E	1103/1250 (88%)	1022 (93%)	77 (7%)	4 (0%)	34	72
1	F	1099/1250 (88%)	1018 (93%)	77 (7%)	4 (0%)	34	72
1	N	28/1250 (2%)	24 (86%)	4 (14%)	0	100	100
1	O	28/1250 (2%)	24 (86%)	4 (14%)	0	100	100
1	P	28/1250 (2%)	24 (86%)	4 (14%)	0	100	100
1	Q	28/1250 (2%)	25 (89%)	2 (7%)	1 (4%)	3	28
2	G	96/158 (61%)	87 (91%)	8 (8%)	1 (1%)	15	54
2	H	94/158 (60%)	79 (84%)	14 (15%)	1 (1%)	14	52
2	I	95/158 (60%)	87 (92%)	8 (8%)	0	100	100
2	J	95/158 (60%)	87 (92%)	8 (8%)	0	100	100
2	K	95/158 (60%)	87 (92%)	8 (8%)	0	100	100
2	L	95/158 (60%)	90 (95%)	5 (5%)	0	100	100
All	All	7290/13448 (54%)	6759 (93%)	506 (7%)	25 (0%)	41	76

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	ASP
1	B	358	ASP
1	C	358	ASP
1	C	445	ARG
1	D	358	ASP
1	E	358	ASP

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Mol	Chain	Res	Type
1	F	358	ASP
1	A	445	ARG
1	B	445	ARG
1	D	445	ARG
1	E	445	ARG
1	F	445	ARG
2	H	117	GLY
1	D	424	PHE
2	G	52	SER
1	A	682	PHE
1	B	424	PHE
1	B	682	PHE
1	C	682	PHE
1	D	682	PHE
1	E	682	PHE
1	F	682	PHE
1	E	424	PHE
1	F	503	GLN
1	Q	36	PHE

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	892/1037 (86%)	862 (97%)	30 (3%)	37 60
1	B	894/1037 (86%)	865 (97%)	29 (3%)	39 62
1	C	893/1037 (86%)	863 (97%)	30 (3%)	37 60
1	D	885/1037 (85%)	852 (96%)	33 (4%)	34 59
1	E	880/1037 (85%)	848 (96%)	32 (4%)	35 59
1	F	878/1037 (85%)	854 (97%)	24 (3%)	44 66
1	N	30/1037 (3%)	24 (80%)	6 (20%)	1 8
1	O	30/1037 (3%)	24 (80%)	6 (20%)	1 8
1	P	30/1037 (3%)	24 (80%)	6 (20%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Q	30/1037 (3%)	23 (77%)	7 (23%)	1 5
2	G	81/127 (64%)	80 (99%)	1 (1%)	71 84
2	H	72/127 (57%)	64 (89%)	8 (11%)	6 25
2	I	81/127 (64%)	81 (100%)	0	100 100
2	J	81/127 (64%)	79 (98%)	2 (2%)	47 68
2	K	81/127 (64%)	78 (96%)	3 (4%)	34 59
2	L	81/127 (64%)	79 (98%)	2 (2%)	47 68
All	All	5919/11132 (53%)	5700 (96%)	219 (4%)	34 59

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	VAL
1	A	261	LEU
1	A	269	ARG
1	A	294	GLU
1	A	299	ASP
1	A	305	LEU
1	A	307	THR
1	A	314	HIS
1	A	377	TYR
1	A	402	ASP
1	A	440	ARG
1	A	464	GLN
1	A	496	LEU
1	A	506	PHE
1	A	509	GLU
1	A	527	GLU
1	A	616	LEU
1	A	648	PHE
1	A	744	ARG
1	A	747	HIS
1	A	797	GLN
1	A	831	LEU
1	A	868	ARG
1	A	909	THR
1	A	950	LEU
1	A	976	GLN
1	A	1025	ILE
1	A	1041	MET

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Mol	Chain	Res	Type
1	A	1191	HIS
1	A	1207	SER
1	B	101	GLU
1	B	251	VAL
1	B	261	LEU
1	B	294	GLU
1	B	299	ASP
1	B	305	LEU
1	B	307	THR
1	B	314	HIS
1	B	402	ASP
1	B	506	PHE
1	B	527	GLU
1	B	542	ARG
1	B	616	LEU
1	B	645	ASP
1	B	648	PHE
1	B	689	SER
1	B	748	ASN
1	B	797	GLN
1	B	831	LEU
1	B	868	ARG
1	B	909	THR
1	B	950	LEU
1	B	974	GLU
1	B	976	GLN
1	B	1025	ILE
1	B	1041	MET
1	B	1157	ARG
1	B	1191	HIS
1	B	1207	SER
1	C	251	VAL
1	C	261	LEU
1	C	294	GLU
1	C	299	ASP
1	C	305	LEU
1	C	307	THR
1	C	314	HIS
1	C	377	TYR
1	C	396	ARG
1	C	402	ASP
1	C	470	LYS

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Mol	Chain	Res	Type
1	C	471	HIS
1	C	506	PHE
1	C	527	GLU
1	C	542	ARG
1	C	560	GLU
1	C	616	LEU
1	C	689	SER
1	C	747	HIS
1	C	748	ASN
1	C	797	GLN
1	C	831	LEU
1	C	909	THR
1	C	950	LEU
1	C	976	GLN
1	C	1025	ILE
1	C	1041	MET
1	C	1157	ARG
1	C	1191	HIS
1	C	1207	SER
1	D	105	LEU
1	D	251	VAL
1	D	254	SER
1	D	261	LEU
1	D	294	GLU
1	D	299	ASP
1	D	305	LEU
1	D	307	THR
1	D	314	HIS
1	D	331	GLN
1	D	377	TYR
1	D	402	ASP
1	D	471	HIS
1	D	506	PHE
1	D	527	GLU
1	D	542	ARG
1	D	560	GLU
1	D	616	LEU
1	D	645	ASP
1	D	648	PHE
1	D	688	ASP
1	D	689	SER
1	D	747	HIS

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Mol	Chain	Res	Type
1	D	748	ASN
1	D	797	GLN
1	D	909	THR
1	D	950	LEU
1	D	976	GLN
1	D	1025	ILE
1	D	1041	MET
1	D	1157	ARG
1	D	1191	HIS
1	D	1207	SER
1	E	158	THR
1	E	198	LEU
1	E	201	ASP
1	E	251	VAL
1	E	261	LEU
1	E	294	GLU
1	E	299	ASP
1	E	305	LEU
1	E	307	THR
1	E	314	HIS
1	E	377	TYR
1	E	402	ASP
1	E	506	PHE
1	E	527	GLU
1	E	542	ARG
1	E	616	LEU
1	E	645	ASP
1	E	648	PHE
1	E	682	PHE
1	E	689	SER
1	E	748	ASN
1	E	797	GLN
1	E	909	THR
1	E	950	LEU
1	E	974	GLU
1	E	976	GLN
1	E	1025	ILE
1	E	1041	MET
1	E	1157	ARG
1	E	1187	ILE
1	E	1191	HIS
1	E	1207	SER

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Mol	Chain	Res	Type
1	F	211	LEU
1	F	261	LEU
1	F	294	GLU
1	F	299	ASP
1	F	305	LEU
1	F	307	THR
1	F	314	HIS
1	F	402	ASP
1	F	471	HIS
1	F	505	ARG
1	F	527	GLU
1	F	616	LEU
1	F	689	SER
1	F	797	GLN
1	F	868	ARG
1	F	909	THR
1	F	950	LEU
1	F	974	GLU
1	F	976	GLN
1	F	1025	ILE
1	F	1041	MET
1	F	1157	ARG
1	F	1191	HIS
1	F	1207	SER
2	G	147	THR
2	H	76	THR
2	H	80	ARG
2	H	81	HIS
2	H	83	ASP
2	H	97	HIS
2	H	109	VAL
2	H	112	VAL
2	H	122	ARG
2	J	97	HIS
2	J	147	THR
2	K	76	THR
2	K	97	HIS
2	K	146	LEU
2	L	52	SER
2	L	147	THR
1	N	16	GLU
1	N	22	PHE

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Mol	Chain	Res	Type
1	N	30	ASP
1	N	33	TRP
1	N	34	HIS
1	N	39	ASP
1	O	16	GLU
1	O	22	PHE
1	O	30	ASP
1	O	33	TRP
1	O	34	HIS
1	O	39	ASP
1	P	16	GLU
1	P	22	PHE
1	P	30	ASP
1	P	33	TRP
1	P	34	HIS
1	P	39	ASP
1	Q	16	GLU
1	Q	22	PHE
1	Q	30	ASP
1	Q	33	TRP
1	Q	34	HIS
1	Q	36	PHE
1	Q	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	HIS
1	A	400	HIS
1	A	446	HIS
1	A	976	GLN
1	A	982	ASN
1	A	1016	GLN
1	A	1020	HIS
1	A	1061	GLN
1	A	1107	ASN
1	B	446	HIS
1	B	503	GLN
1	B	569	GLN
1	B	651	GLN
1	B	797	GLN
1	B	976	GLN

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Mol	Chain	Res	Type
1	B	982	ASN
1	B	1107	ASN
1	C	314	HIS
1	C	446	HIS
1	C	497	GLN
1	C	569	GLN
1	C	651	GLN
1	C	747	HIS
1	C	976	GLN
1	C	982	ASN
1	C	1061	GLN
1	C	1107	ASN
1	D	446	HIS
1	D	503	GLN
1	D	569	GLN
1	D	651	GLN
1	D	976	GLN
1	D	982	ASN
1	D	1016	GLN
1	D	1020	HIS
1	D	1107	ASN
1	E	400	HIS
1	E	408	HIS
1	E	446	HIS
1	E	497	GLN
1	E	503	GLN
1	E	797	GLN
1	E	976	GLN
1	E	982	ASN
1	E	1061	GLN
1	E	1107	ASN
1	F	446	HIS
1	F	651	GLN
1	F	976	GLN
1	F	982	ASN
1	F	1020	HIS
1	F	1061	GLN
1	F	1107	ASN
2	G	81	HIS
2	H	116	ASN
2	I	81	HIS
2	J	81	HIS

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Mol	Chain	Res	Type
2	K	116	ASN
2	L	81	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	TPP	A	1303	3	22,27,27	0.63	0	29,40,40	0.69	1 (3%)
5	TPP	E	1303	3	22,27,27	0.66	0	29,40,40	0.65	1 (3%)
5	TPP	C	1303	3	22,27,27	0.70	0	29,40,40	0.80	2 (6%)
5	TPP	B	1303	3	22,27,27	0.68	0	29,40,40	0.80	1 (3%)
5	TPP	F	1303	3	22,27,27	0.71	0	29,40,40	0.77	1 (3%)
5	TPP	D	1303	3	22,27,27	0.66	0	29,40,40	0.77	1 (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
5	TPP	A	1303	3	-	8/16/17/17	0/2/2/2
5	TPP	E	1303	3	-	8/16/17/17	0/2/2/2
5	TPP	C	1303	3	-	3/16/17/17	0/2/2/2
5	TPP	B	1303	3	-	8/16/17/17	0/2/2/2
5	TPP	F	1303	3	-	11/16/17/17	0/2/2/2
5	TPP	D	1303	3	-	8/16/17/17	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1303	TPP	C5-C4-N3	2.24	112.04	107.57
5	B	1303	TPP	C5-C4-N3	2.22	112.01	107.57
5	E	1303	TPP	C5-C4-N3	2.21	111.99	107.57
5	C	1303	TPP	C5-C4-N3	2.15	111.87	107.57
5	F	1303	TPP	C5-C4-N3	2.14	111.86	107.57
5	A	1303	TPP	C5-C4-N3	2.11	111.79	107.57
5	C	1303	TPP	O3B-PB-O3A	2.02	111.42	104.64

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1303	TPP	C4'-C5'-C7'-N3
5	A	1303	TPP	C4-C5-C6-C7
5	A	1303	TPP	C5-C6-C7-O7
5	A	1303	TPP	C7-O7-PA-O1A
5	A	1303	TPP	C7-O7-PA-O2A
5	A	1303	TPP	C7-O7-PA-O3A
5	A	1303	TPP	PA-O3A-PB-O3B
5	B	1303	TPP	C4'-C5'-C7'-N3
5	B	1303	TPP	C4-C5-C6-C7
5	B	1303	TPP	C5-C6-C7-O7
5	B	1303	TPP	C7-O7-PA-O2A
5	B	1303	TPP	C7-O7-PA-O3A
5	C	1303	TPP	C4'-C5'-C7'-N3
5	D	1303	TPP	C4-C5-C6-C7
5	D	1303	TPP	C5-C6-C7-O7
5	D	1303	TPP	C7-O7-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	D	1303	TPP	PA-O3A-PB-O3B
5	E	1303	TPP	C4'-C5'-C7'-N3
5	E	1303	TPP	C4-C5-C6-C7
5	E	1303	TPP	C5-C6-C7-O7
5	E	1303	TPP	C7-O7-PA-O1A
5	E	1303	TPP	C7-O7-PA-O2A
5	E	1303	TPP	C7-O7-PA-O3A
5	E	1303	TPP	PA-O3A-PB-O3B
5	F	1303	TPP	C4'-C5'-C7'-N3
5	F	1303	TPP	C4-C5-C6-C7
5	F	1303	TPP	C5-C6-C7-O7
5	F	1303	TPP	C7-O7-PA-O2A
5	F	1303	TPP	C7-O7-PA-O3A
5	F	1303	TPP	PA-O3A-PB-O2B
5	E	1303	TPP	PA-O3A-PB-O1B
5	C	1303	TPP	PA-O3A-PB-O2B
5	D	1303	TPP	PA-O3A-PB-O2B
5	B	1303	TPP	PB-O3A-PA-O1A
5	B	1303	TPP	C7-O7-PA-O1A
5	D	1303	TPP	C7-O7-PA-O1A
5	D	1303	TPP	C7-O7-PA-O2A
5	F	1303	TPP	C7-O7-PA-O1A
5	C	1303	TPP	C4-C5-C6-C7
5	F	1303	TPP	PB-O3A-PA-O1A
5	D	1303	TPP	C4'-C5'-C7'-N3
5	F	1303	TPP	PA-O3A-PB-O1B
5	A	1303	TPP	PA-O3A-PB-O2B
5	F	1303	TPP	PA-O3A-PB-O3B
5	B	1303	TPP	PB-O3A-PA-O2A
5	F	1303	TPP	C6'-C5'-C7'-N3

There are no ring outliers.

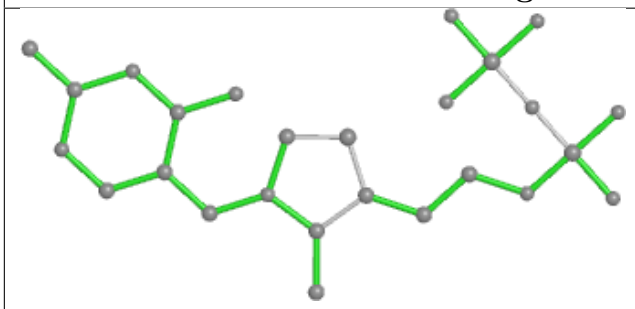
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1303	TPP	2	0
5	C	1303	TPP	1	0
5	B	1303	TPP	1	0
5	F	1303	TPP	2	0
5	D	1303	TPP	1	0

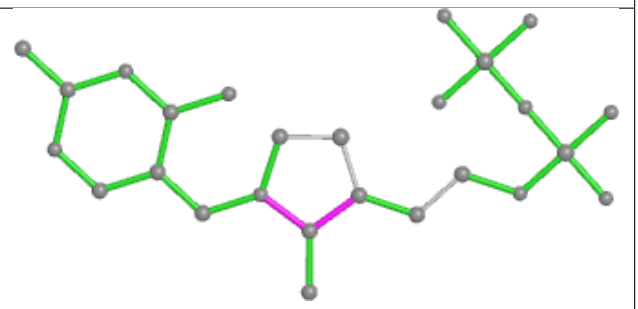
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

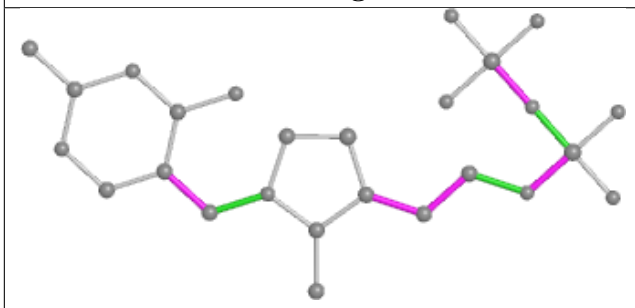
Ligand TPP A 1303



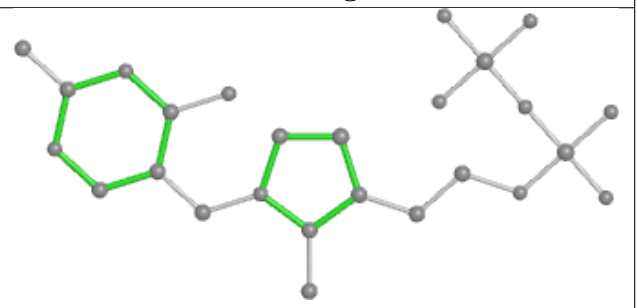
Bond lengths



Bond angles

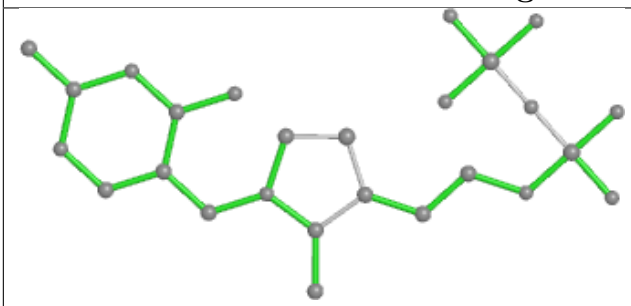


Torsions

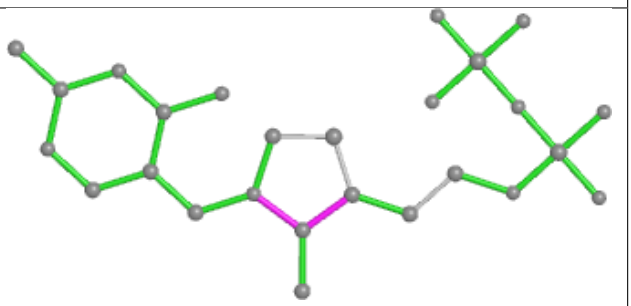


Rings

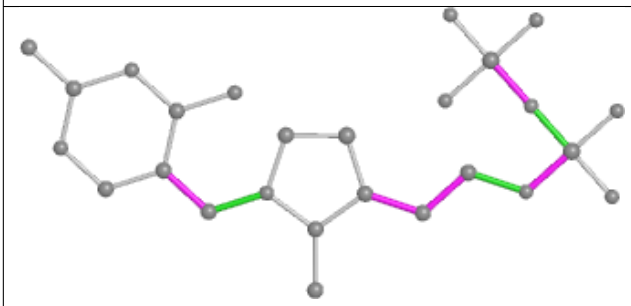
Ligand TPP E 1303



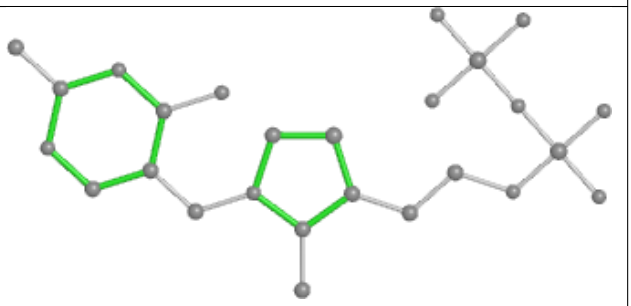
Bond lengths



Bond angles

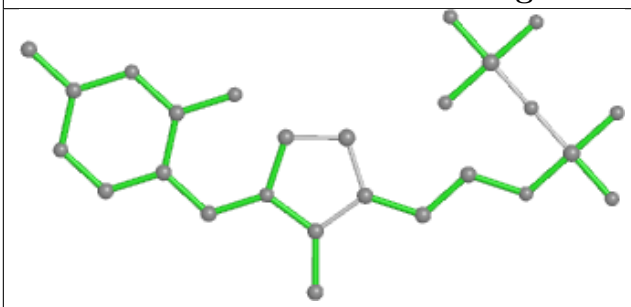


Torsions

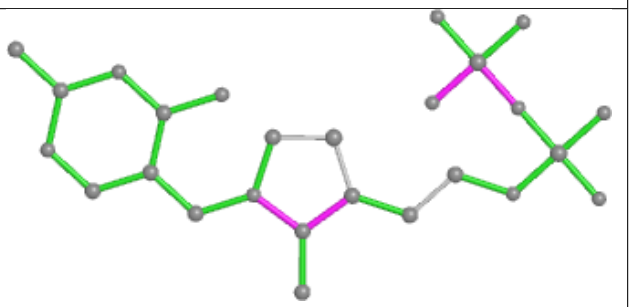


Rings

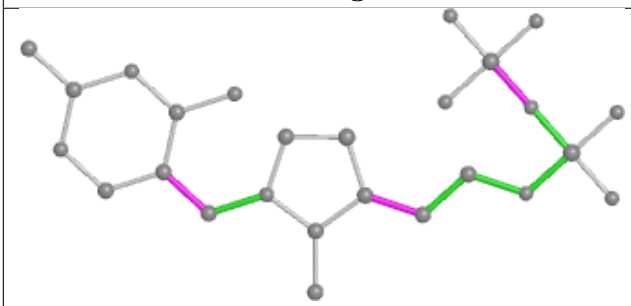
Ligand TPP C 1303



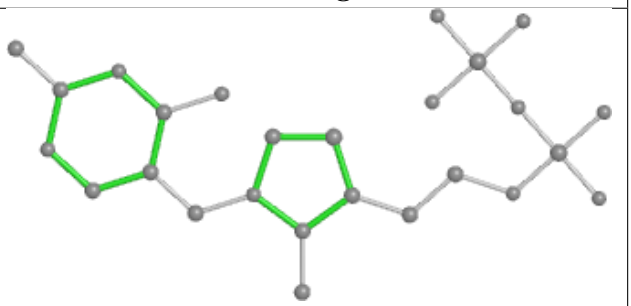
Bond lengths



Bond angles

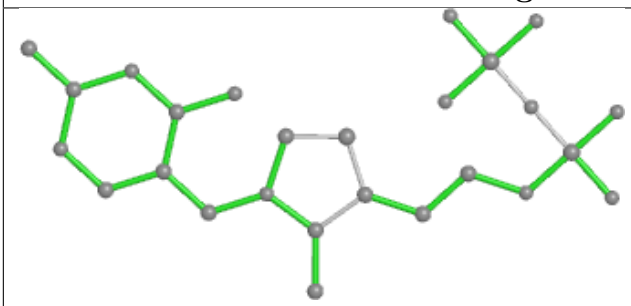


Torsions

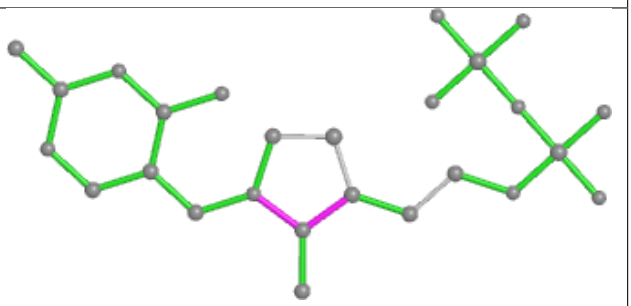


Rings

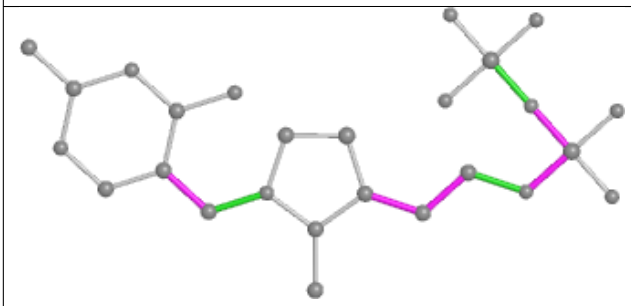
Ligand TPP B 1303



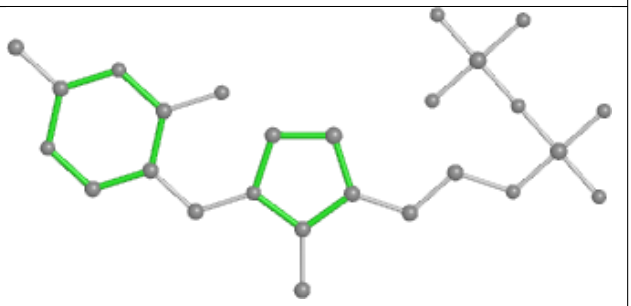
Bond lengths



Bond angles

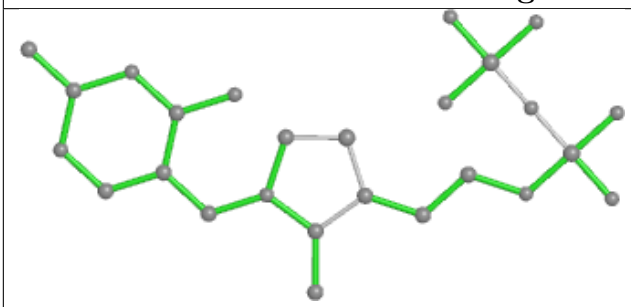


Torsions

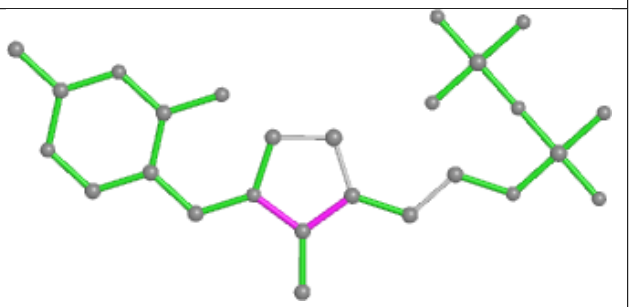


Rings

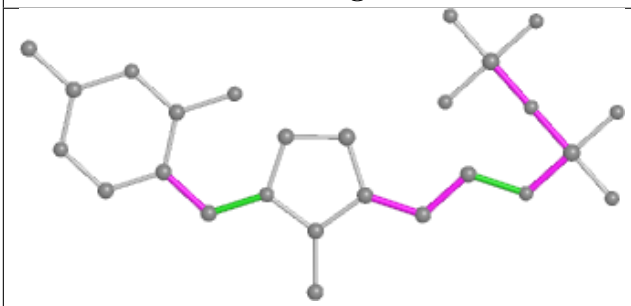
Ligand TPP F 1303



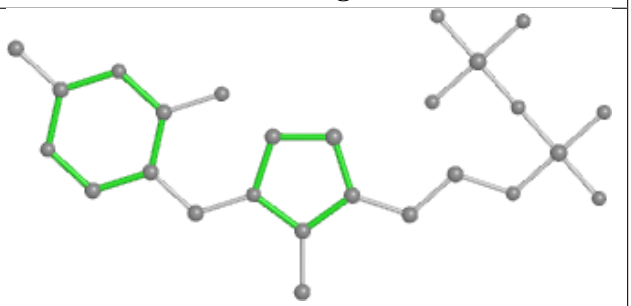
Bond lengths



Bond angles

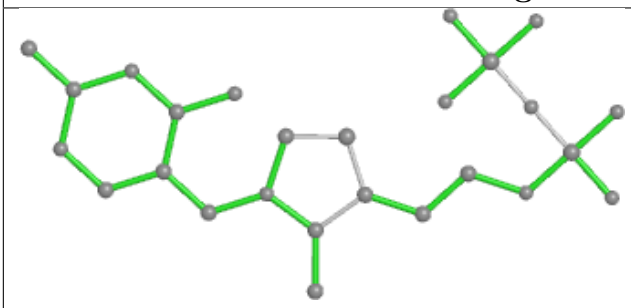


Torsions

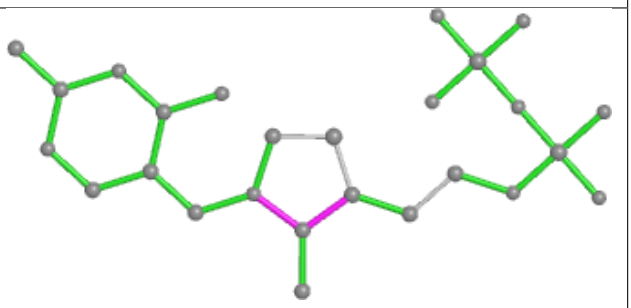


Rings

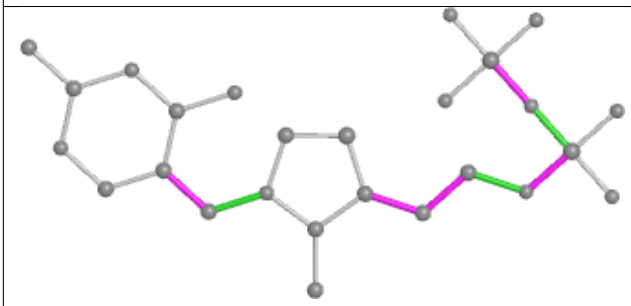
Ligand TPP D 1303



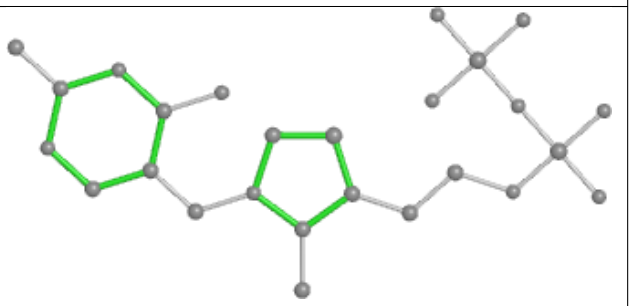
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1106/1250 (88%)	0.42	55 (4%) 28 25	155, 233, 300, 300	0
1	B	1108/1250 (88%)	0.40	40 (3%) 42 35	138, 225, 289, 300	0
1	C	1109/1250 (88%)	0.44	50 (4%) 33 28	148, 231, 298, 300	0
1	D	1107/1250 (88%)	0.44	54 (4%) 29 25	150, 232, 296, 300	0
1	E	1109/1250 (88%)	0.40	41 (3%) 41 33	145, 225, 290, 300	0
1	F	1105/1250 (88%)	0.41	56 (5%) 28 24	162, 233, 299, 300	0
1	N	30/1250 (2%)	1.02	6 (20%) 1 1	268, 300, 300, 300	0
1	O	30/1250 (2%)	0.91	3 (10%) 7 7	280, 300, 300, 300	0
1	P	30/1250 (2%)	0.77	7 (23%) 0 1	274, 300, 300, 300	0
1	Q	30/1250 (2%)	1.37	10 (33%) 0 1	259, 300, 300, 300	0
2	G	98/158 (62%)	0.83	18 (18%) 1 2	211, 283, 300, 300	0
2	H	96/158 (60%)	0.17	3 (3%) 49 39	179, 238, 300, 300	0
2	I	97/158 (61%)	0.58	12 (12%) 4 5	207, 279, 300, 300	0
2	J	97/158 (61%)	0.59	16 (16%) 1 2	218, 281, 300, 300	0
2	K	97/158 (61%)	0.29	4 (4%) 37 30	183, 236, 295, 300	0
2	L	97/158 (61%)	0.79	14 (14%) 2 3	230, 284, 300, 300	0
All	All	7346/13448 (54%)	0.44	389 (5%) 26 23	138, 233, 300, 300	0

All (389) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	629	GLU	11.4
1	B	629	GLU	9.1
1	A	629	GLU	6.9
1	F	629	GLU	6.6
1	C	747	HIS	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	629	GLU	5.3
1	D	269	ARG	5.3
1	D	629	GLU	5.0
1	A	911	ARG	4.9
1	A	215	ALA	4.8
1	Q	40	TYR	4.8
1	D	270	LEU	4.7
1	F	628	GLU	4.6
1	D	847	HIS	4.6
2	K	96	ARG	4.5
1	F	215	ALA	4.5
1	F	745	ARG	4.5
1	B	270	LEU	4.4
1	C	270	LEU	4.4
2	G	116	ASN	4.4
1	D	747	HIS	4.3
2	G	71	LEU	4.3
1	B	745	ARG	4.3
1	E	1072	MET	4.2
1	Q	15	VAL	4.2
1	Q	14	LEU	4.2
1	D	1116	SER	4.1
1	A	214	ALA	4.1
1	B	271	MET	4.0
1	D	911	ARG	3.9
1	N	15	VAL	3.9
2	I	147	THR	3.9
1	E	745	ARG	3.9
1	D	138	ASP	3.9
1	E	271	MET	3.8
1	E	270	LEU	3.8
1	F	214	ALA	3.8
1	C	746	GLY	3.8
1	O	15	VAL	3.8
2	G	88	LEU	3.7
1	F	911	ARG	3.7
1	E	355	TRP	3.6
2	G	57	LEU	3.6
1	Q	13	TRP	3.6
1	C	847	HIS	3.6
2	L	88	LEU	3.5
1	A	1164	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	I	140	LYS	3.5
1	D	799	GLN	3.5
1	P	14	LEU	3.4
1	P	33	TRP	3.4
1	B	976	GLN	3.4
1	E	269	ARG	3.4
1	D	175	MET	3.4
1	B	269	ARG	3.4
1	Q	36	PHE	3.4
2	G	136	VAL	3.4
2	L	100	PHE	3.3
1	C	1116	SER	3.3
1	D	745	ARG	3.3
2	L	99	GLU	3.3
1	F	927	LEU	3.3
1	C	927	LEU	3.3
1	F	972	LEU	3.3
1	E	1118	LYS	3.3
1	O	40	TYR	3.3
1	D	746	GLY	3.3
1	E	573	SER	3.3
1	D	913	ALA	3.3
2	K	95	ARG	3.3
1	C	269	ARG	3.3
1	A	745	ARG	3.3
1	A	1115	THR	3.3
1	E	539	HIS	3.3
1	E	744	ARG	3.3
1	A	1167	VAL	3.3
2	L	116	ASN	3.3
1	C	799	GLN	3.3
2	I	116	ASN	3.2
2	J	147	THR	3.2
2	L	57	LEU	3.2
1	A	270	LEU	3.2
1	F	1008	LEU	3.2
1	D	912	HIS	3.2
1	A	970	MET	3.2
1	D	1140	ILE	3.2
2	G	70	LEU	3.2
1	B	764	ILE	3.2
1	E	743	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	214	ALA	3.1
1	F	970	MET	3.1
1	A	1136	ALA	3.1
1	C	837	LYS	3.1
1	C	1140	ILE	3.1
1	D	271	MET	3.0
1	A	175	MET	3.0
1	D	198	LEU	3.0
1	B	742	TYR	3.0
1	D	517	MET	3.0
1	B	770	SER	3.0
1	Q	35	GLU	3.0
1	D	403	LEU	3.0
1	A	1135	VAL	3.0
1	E	911	ARG	3.0
2	J	140	LYS	3.0
1	B	628	GLU	3.0
2	J	116	ASN	3.0
1	E	509	GLU	2.9
1	B	744	ARG	2.9
1	B	1118	LYS	2.9
1	E	847	HIS	2.9
1	B	214	ALA	2.9
1	C	943	PHE	2.9
2	G	98	ALA	2.9
1	C	517	MET	2.9
1	C	569	GLN	2.9
1	C	1095	GLU	2.9
1	E	1116	SER	2.9
1	D	770	SER	2.9
1	E	628	GLU	2.9
1	B	1072	MET	2.8
2	J	100	PHE	2.8
1	F	847	HIS	2.8
2	L	86	ILE	2.8
2	G	119	TYR	2.8
1	E	910	GLN	2.8
1	P	15	VAL	2.8
1	F	1164	LYS	2.8
1	D	215	ALA	2.8
2	G	78	ALA	2.8
1	D	569	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	882	GLU	2.8
2	I	146	LEU	2.8
1	D	214	ALA	2.8
1	E	742	TYR	2.8
2	L	78	ALA	2.7
1	A	1137	ILE	2.7
2	I	145	PHE	2.7
1	A	628	GLU	2.7
1	F	912	HIS	2.7
1	Q	18	MET	2.7
1	Q	41	SER	2.7
1	E	574	GLY	2.7
2	G	100	PHE	2.7
1	E	214	ALA	2.7
1	F	1135	VAL	2.7
1	A	912	HIS	2.7
1	F	913	ALA	2.7
1	A	1048	TYR	2.7
1	C	913	ALA	2.7
1	A	896	VAL	2.7
1	D	709	VAL	2.7
1	B	911	ARG	2.7
1	A	1143	LEU	2.7
2	L	71	LEU	2.7
1	A	886	LEU	2.6
1	E	197	GLY	2.6
1	Q	33	TRP	2.6
1	C	570	ALA	2.6
1	P	13	TRP	2.6
1	F	403	LEU	2.6
2	K	71	LEU	2.6
1	D	1016	GLN	2.6
1	B	942	LYS	2.6
1	D	973	TRP	2.6
2	J	92	THR	2.6
1	N	16	GLU	2.6
1	D	649	ALA	2.6
1	C	911	ARG	2.6
1	N	14	LEU	2.6
1	C	745	ARG	2.5
2	H	95	ARG	2.5
1	A	402	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	927	LEU	2.5
1	N	40	TYR	2.5
2	J	134	ASP	2.5
1	C	846	ALA	2.5
1	F	883	LEU	2.5
1	A	196	LEU	2.5
1	A	973	TRP	2.5
2	L	69	PHE	2.5
2	J	136	VAL	2.5
1	C	196	LEU	2.5
2	L	119	TYR	2.5
1	E	510	GLY	2.5
1	Q	39	ASP	2.5
1	D	272	GLN	2.5
1	C	914	VAL	2.5
1	A	121	GLU	2.5
1	F	886	LEU	2.5
1	B	1085	PHE	2.5
2	I	91	VAL	2.5
1	B	355	TRP	2.5
1	D	196	LEU	2.5
1	F	742	TYR	2.4
1	B	1091	ARG	2.4
1	F	971	VAL	2.4
1	E	569	GLN	2.4
2	L	70	LEU	2.4
1	B	207	GLY	2.4
1	B	196	LEU	2.4
1	F	216	ILE	2.4
2	I	110	VAL	2.4
1	D	570	ALA	2.4
1	C	1008	LEU	2.4
1	B	882	GLU	2.4
1	F	315	ARG	2.4
1	B	679	GLN	2.4
1	F	251	VAL	2.4
1	F	269	ARG	2.4
1	P	36	PHE	2.4
1	C	272	GLN	2.4
2	I	98	ALA	2.4
1	A	424	PHE	2.4
1	A	882	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	175	MET	2.4
1	F	1163	GLU	2.4
1	A	913	ALA	2.4
1	C	199	ALA	2.4
1	A	1112	LEU	2.4
1	B	847	HIS	2.4
1	A	1165	PHE	2.4
2	J	80	ARG	2.4
1	A	847	HIS	2.4
1	F	1115	THR	2.4
1	B	1073	LEU	2.4
1	C	134	LYS	2.4
1	B	747	HIS	2.4
2	I	143	LEU	2.4
1	E	196	LEU	2.4
1	E	976	GLN	2.4
1	B	573	SER	2.4
2	G	143	LEU	2.4
1	A	1111	ARG	2.4
1	A	972	LEU	2.3
2	G	138	ILE	2.3
1	D	251	VAL	2.3
1	C	1227	GLY	2.3
1	E	942	LYS	2.3
1	F	991	PHE	2.3
1	F	1167	VAL	2.3
1	C	739	MET	2.3
1	E	424	PHE	2.3
1	E	770	SER	2.3
2	G	69	PHE	2.3
2	G	109	VAL	2.3
1	A	1192	PHE	2.3
1	C	1094	LEU	2.3
1	D	1008	LEU	2.3
1	F	747	HIS	2.3
2	J	145	PHE	2.3
1	D	1181	GLY	2.3
1	F	744	ARG	2.3
1	N	20	ARG	2.3
2	L	136	VAL	2.3
1	C	485	LYS	2.3
1	C	198	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1093	VAL	2.3
1	D	485	LYS	2.3
1	D	552	LYS	2.3
1	D	943	PHE	2.3
2	J	146	LEU	2.3
1	D	134	LYS	2.3
2	J	89	ASP	2.3
1	F	1072	MET	2.3
2	L	98	ALA	2.3
1	C	1052	LEU	2.3
1	F	1137	ILE	2.3
1	E	215	ALA	2.3
1	A	1074	ARG	2.3
1	F	213	VAL	2.3
1	A	216	ILE	2.2
1	E	649	ALA	2.2
2	G	99	GLU	2.2
1	A	1140	ILE	2.2
1	E	664	ARG	2.2
2	I	95	ARG	2.2
1	A	1011	HIS	2.2
1	C	215	ALA	2.2
1	F	1112	LEU	2.2
1	A	638	VAL	2.2
1	A	1008	LEU	2.2
1	F	1011	HIS	2.2
1	A	1066	VAL	2.2
1	F	606	LEU	2.2
1	B	518	MET	2.2
1	C	138	ASP	2.2
1	D	1225	ALA	2.2
1	E	175	MET	2.2
1	E	1085	PHE	2.2
1	A	954	ALA	2.2
1	C	1041	MET	2.2
1	D	1095	GLU	2.2
2	I	80	ARG	2.2
1	A	1085	PHE	2.2
1	E	1048	TYR	2.2
1	F	1052	LEU	2.2
1	D	711	GLY	2.2
1	O	41	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	480	LYS	2.2
2	G	56	LEU	2.2
1	B	649	ALA	2.2
1	D	837	LYS	2.2
1	D	914	VAL	2.2
1	B	910	GLN	2.2
1	D	835	VAL	2.2
1	F	1165	PHE	2.2
2	J	101	ARG	2.2
1	A	1181	GLY	2.2
1	B	760	MET	2.1
1	C	403	LEU	2.1
1	C	970	MET	2.1
1	E	543	LEU	2.1
1	F	1143	LEU	2.1
2	H	98	ALA	2.1
1	D	268	PRO	2.1
1	B	574	GLY	2.1
1	C	649	ALA	2.1
1	P	40	TYR	2.1
1	F	274	GLN	2.1
1	B	346	LEU	2.1
1	B	1048	TYR	2.1
1	P	18	MET	2.1
1	A	138	ASP	2.1
1	B	1041	MET	2.1
1	C	976	GLN	2.1
1	F	248	PHE	2.1
1	F	408	HIS	2.1
1	B	213	VAL	2.1
1	E	1069	PRO	2.1
1	F	571	HIS	2.1
1	F	477	ALA	2.1
1	D	518	MET	2.1
1	A	898	LEU	2.1
1	C	518	MET	2.1
1	E	274	GLN	2.1
1	F	272	GLN	2.1
2	H	116	ASN	2.1
1	C	1181	GLY	2.1
1	F	161	LEU	2.1
1	F	554	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1042	PRO	2.1
1	A	702	ILE	2.1
1	D	380	ARG	2.1
1	F	196	LEU	2.1
1	B	480	LYS	2.1
1	N	41	SER	2.1
1	C	956	VAL	2.1
2	J	91	VAL	2.1
1	A	403	LEU	2.1
1	D	886	LEU	2.1
1	C	515	ILE	2.1
2	L	122	ARG	2.1
1	B	138	ASP	2.1
1	F	637	VAL	2.1
1	D	927	LEU	2.1
1	A	408	HIS	2.1
1	A	1041	MET	2.1
1	E	764	ILE	2.1
1	A	477	ALA	2.1
1	E	1073	LEU	2.1
1	F	1114	LEU	2.1
2	J	78	ALA	2.1
2	K	98	ALA	2.1
1	D	842	ARG	2.0
1	C	1225	ALA	2.0
2	J	56	LEU	2.0
1	A	943	PHE	2.0
1	B	901	GLN	2.0
1	D	970	MET	2.0
1	D	897	ARG	2.0
2	G	134	ASP	2.0
2	I	130	LEU	2.0
1	D	739	MET	2.0
1	D	1048	TYR	2.0
1	F	714	PRO	2.0
1	C	648	PHE	2.0
1	E	1140	ILE	2.0
2	G	89	ASP	2.0
1	A	1195	LEU	2.0
1	F	485	LYS	2.0
1	F	1136	ALA	2.0
1	D	896	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1122	GLU	2.0
1	C	944	LEU	2.0
1	A	991	PHE	2.0
1	B	972	LEU	2.0
1	F	402	ASP	2.0
2	J	88	LEU	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
4	CA	A	1302	1/1	0.56	0.64	300,300,300,300	0
4	CA	B	1304	1/1	0.75	0.12	170,170,170,170	0
4	CA	F	1302	1/1	0.76	0.39	300,300,300,300	0
4	CA	B	1302	1/1	0.84	0.55	220,220,220,220	0
4	CA	E	1302	1/1	0.93	0.54	239,239,239,239	0
5	TPP	A	1303	26/26	0.93	0.48	226,226,226,226	0
4	CA	D	1302	1/1	0.94	0.21	298,298,298,298	0
5	TPP	B	1303	26/26	0.94	0.42	216,216,216,216	0
5	TPP	D	1303	26/26	0.94	0.42	223,223,223,223	0
5	TPP	F	1303	26/26	0.94	0.48	230,230,230,230	0
5	TPP	E	1303	26/26	0.95	0.42	223,223,223,223	0
4	CA	A	1304	1/1	0.95	0.12	176,176,176,176	0
5	TPP	C	1303	26/26	0.96	0.41	225,225,225,225	0
4	CA	C	1302	1/1	0.96	0.21	289,289,289,289	0
3	MG	B	1301	1/1	0.96	0.31	216,216,216,216	0
3	MG	E	1301	1/1	0.96	0.30	190,190,190,190	0
3	MG	D	1301	1/1	0.98	0.31	149,149,149,149	0

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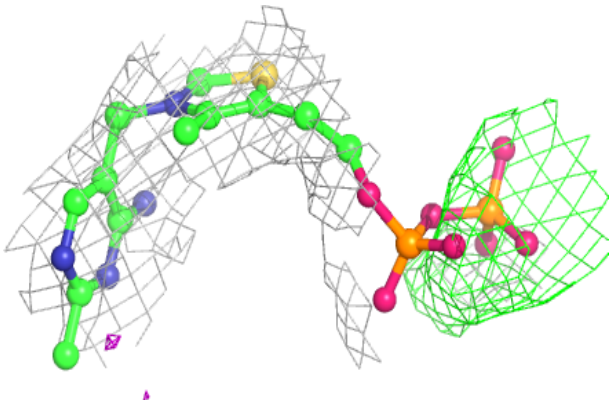
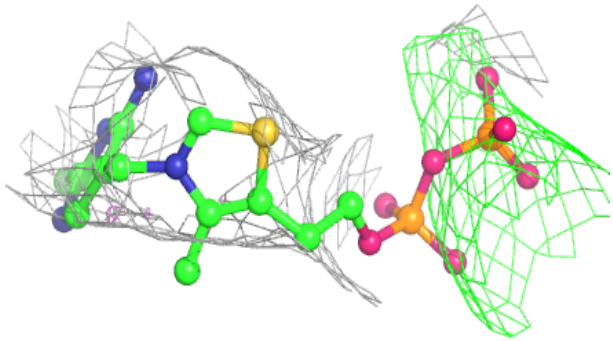
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	F	1301	1/1	0.99	0.30	119,119,119,119	0
3	MG	A	1301	1/1	0.99	0.24	106,106,106,106	0
3	MG	C	1301	1/1	0.99	0.32	160,160,160,160	0

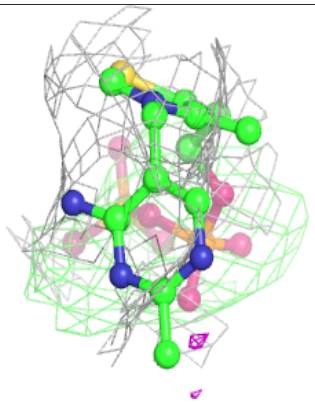
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 1303:

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

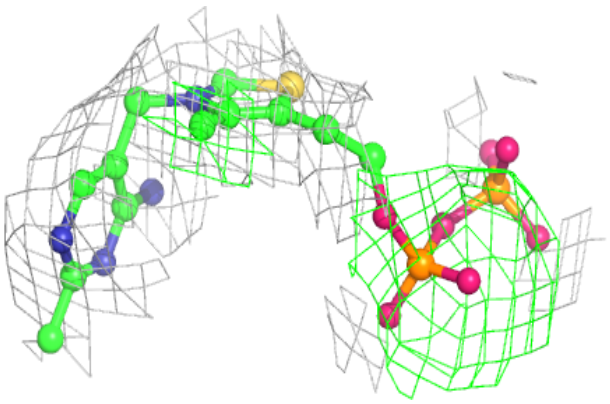


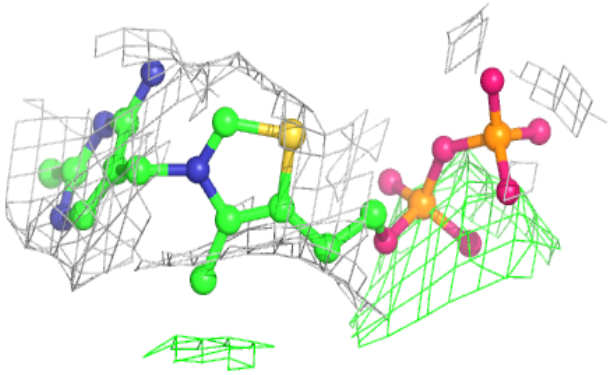


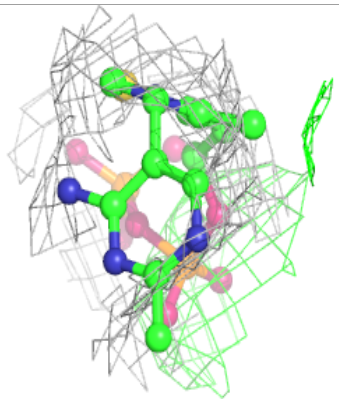


Electron density around TPP B 1303:

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

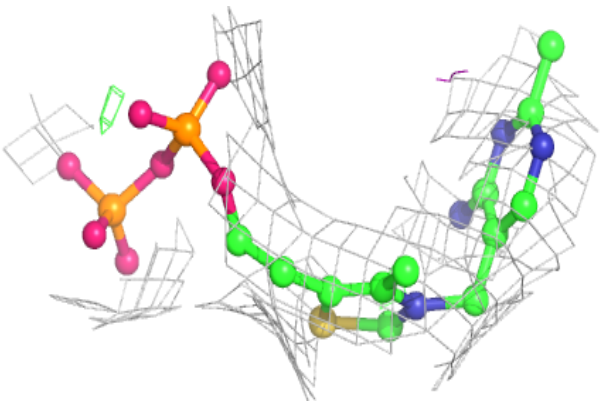


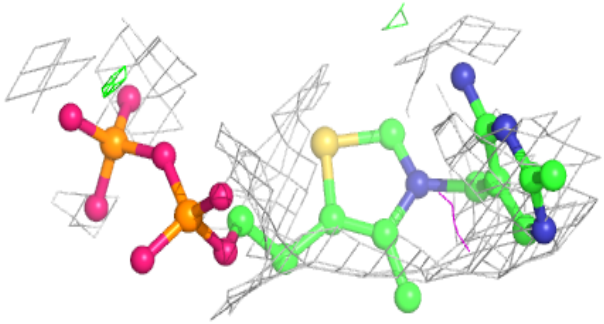


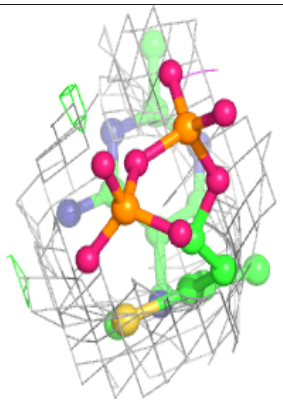


Electron density around TPP D 1303:

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

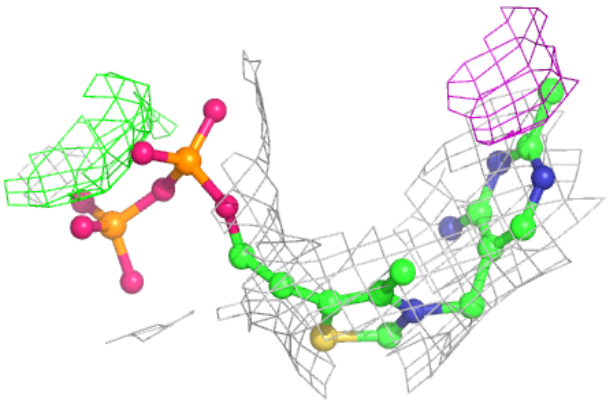


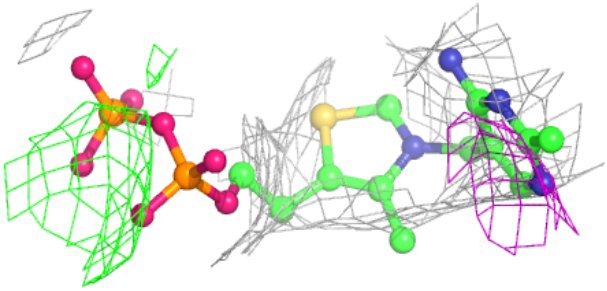


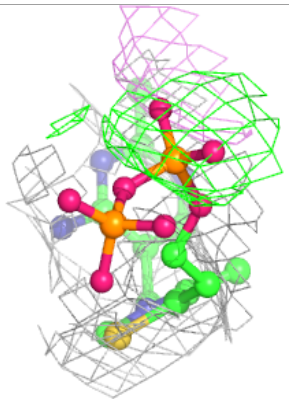


Electron density around TPP F 1303:

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

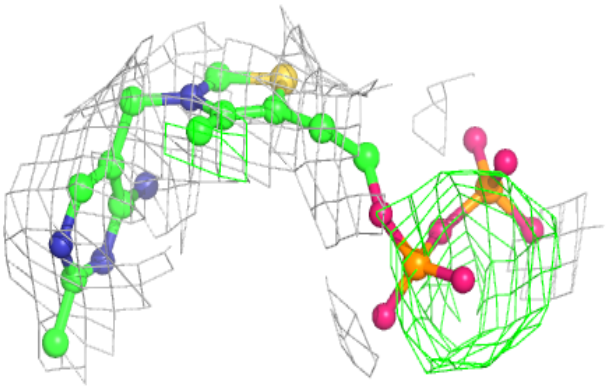


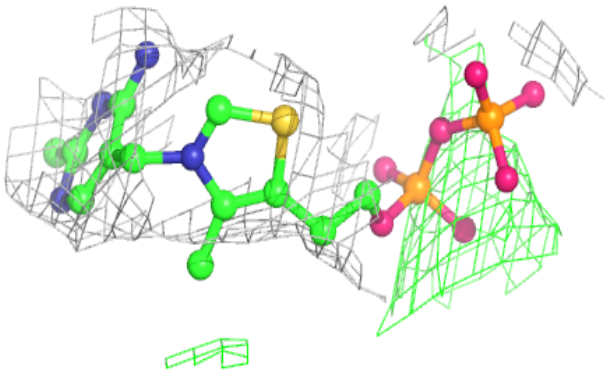


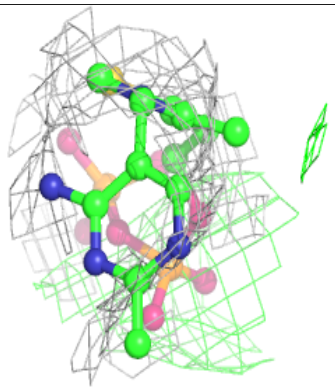


Electron density around TPP E 1303:

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

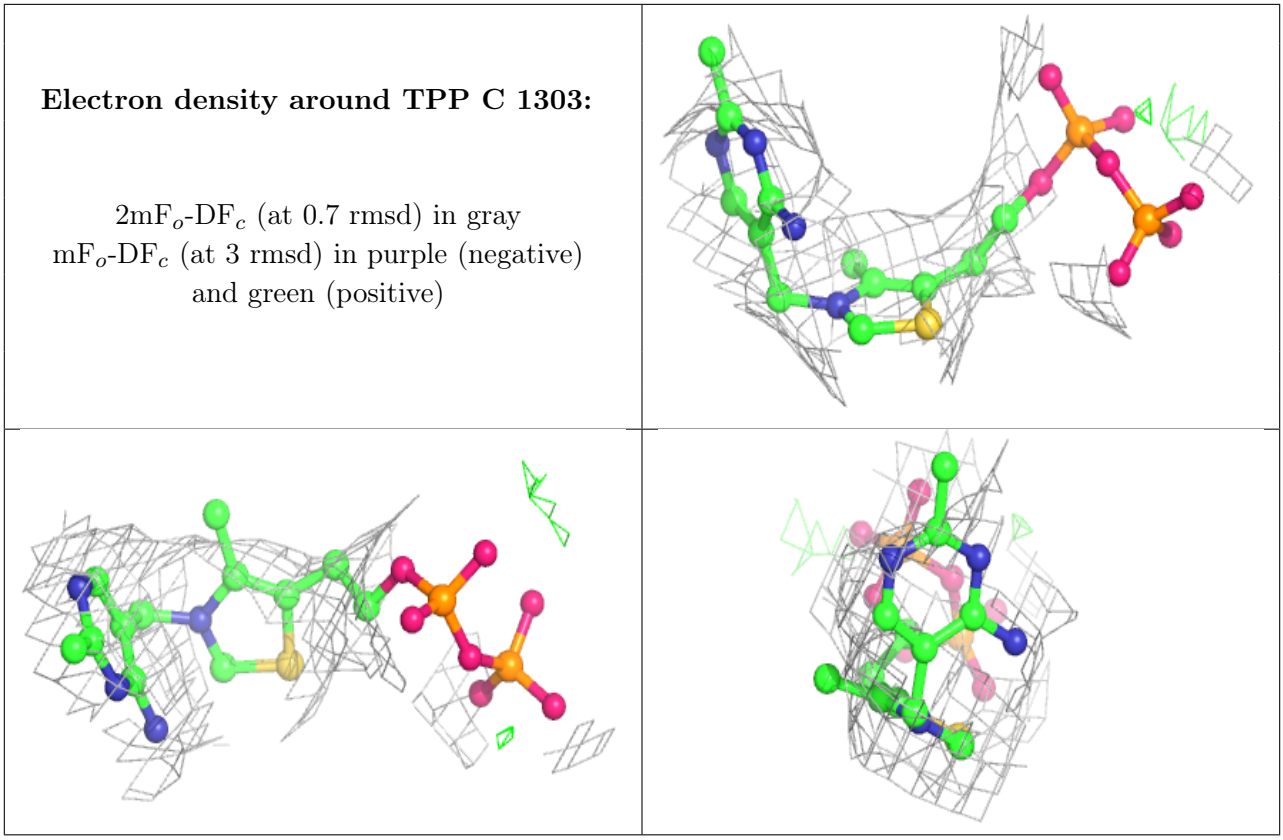






Electron density around TPP C 1303:

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



6.5 Other polymers (i)

There are no such residues in this entry.