



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:55 AM UTC

PDB ID : 8P5R / pdb_00008p5r
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

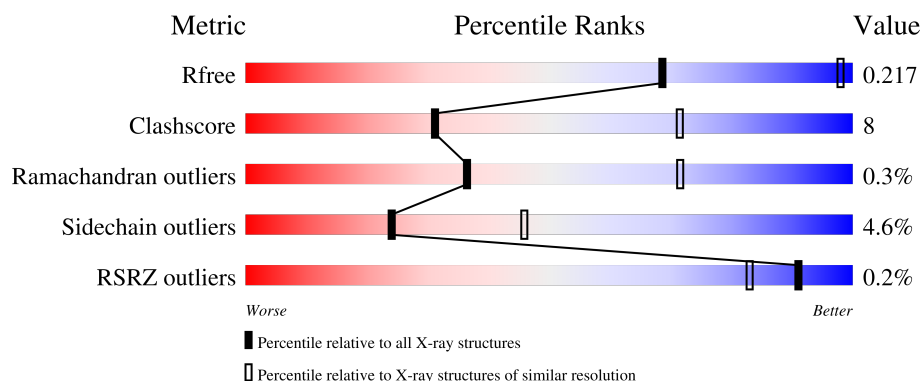
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



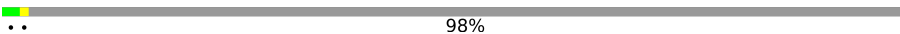
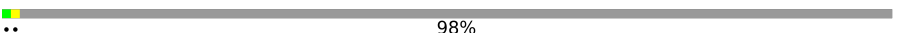
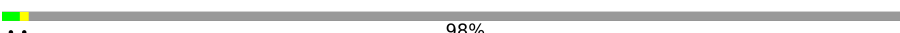
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1000 (5.20-3.92)
Clashscore	190562	1009 (5.14-3.94)
Ramachandran outliers	187476	1067 (5.22-3.90)
Sidechain outliers	187428	1049 (5.22-3.90)
RSRZ outliers	180081	1136 (5.22-3.90)

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

Mol	Chain	Length	Quality of chain
1	A	1250	
1	B	1250	
1	C	1250	
1	D	1250	
1	E	1250	

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Mol	Chain	Length	Quality of chain
1	F	1250	 72%15%12%
1	N	1250	 98%
1	O	1250	 98%
1	P	1250	 98%
1	Q	1250	 98%
2	G	158	 49%13%38%
2	H	158	 47%12%39%
2	I	158	 47%14%39%
2	J	158	 49%11%39%
2	K	158	 52%9%39%
2	L	158	 51%10%39%

2 Entry composition

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			

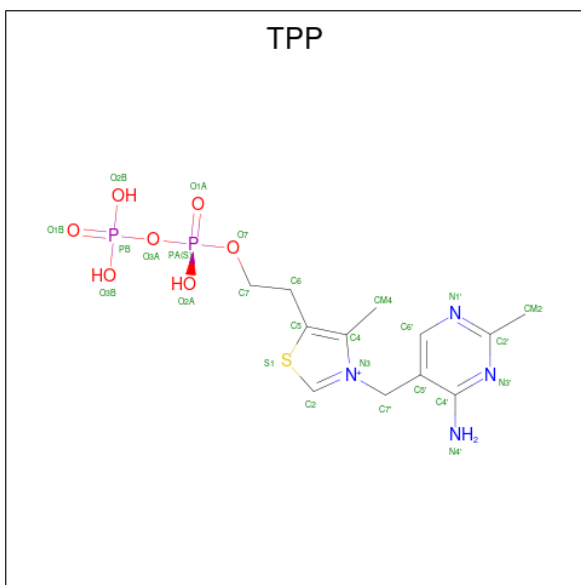
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: 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 (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S) (labeled as "Ligand of Interest" by depositor).



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

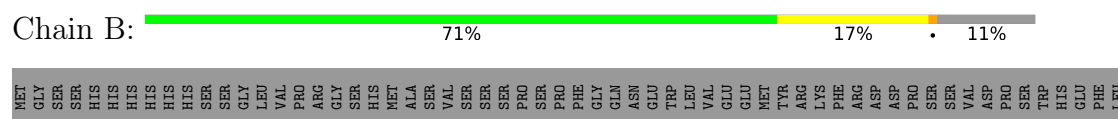
3 Residue-property plots

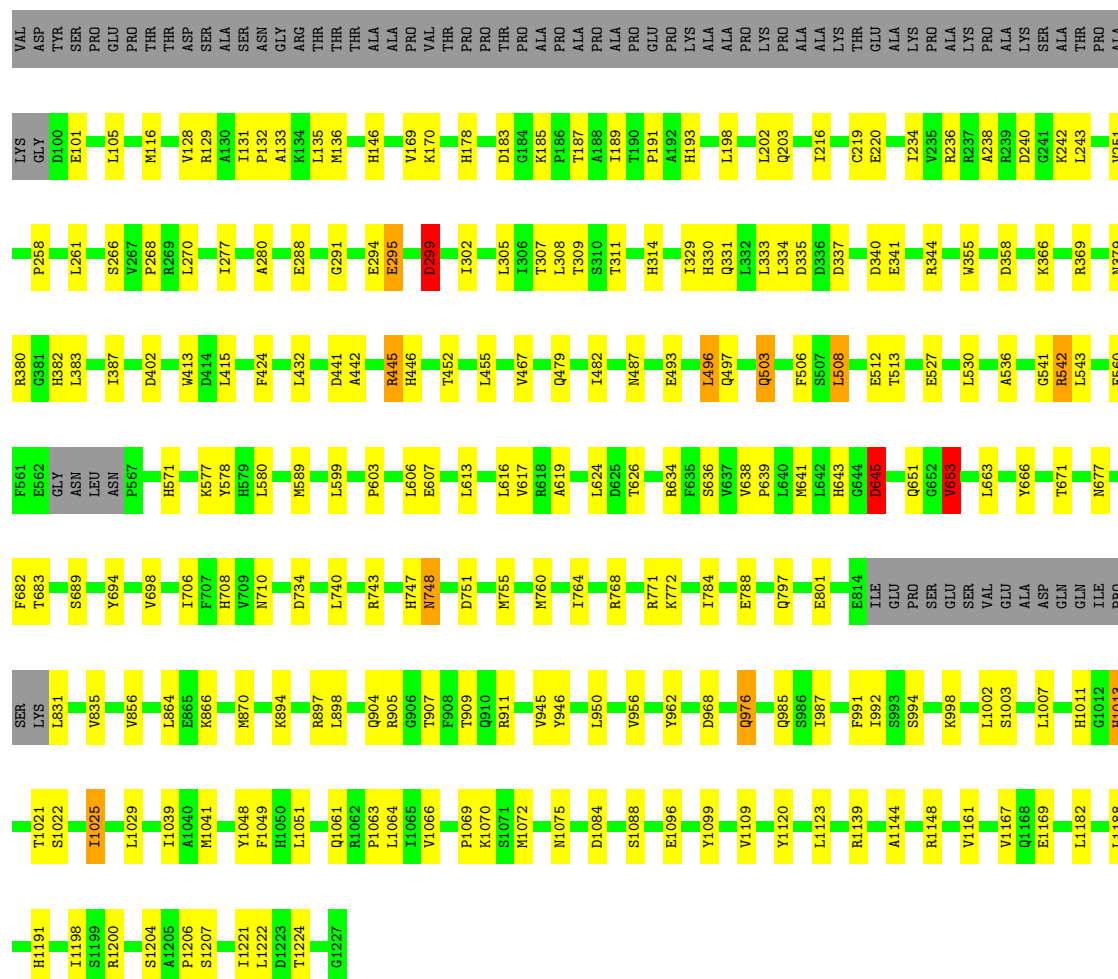
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

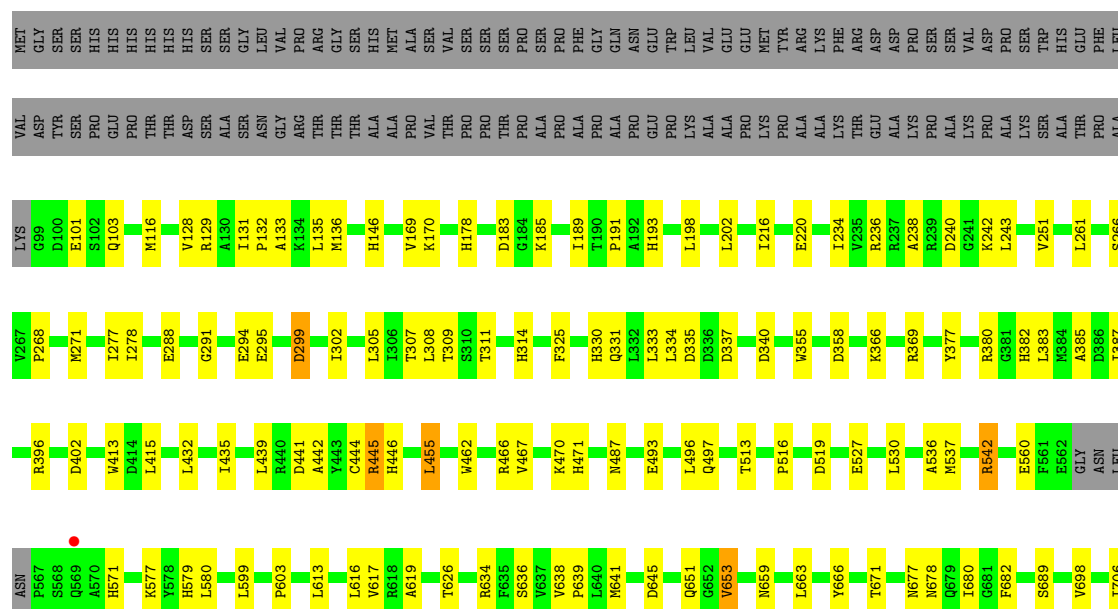


- Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

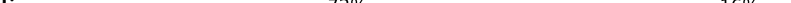


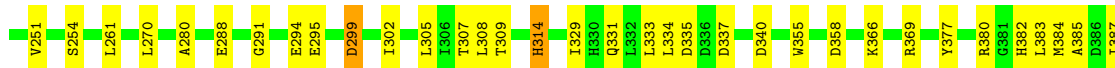


- Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme





- Chain D:  %



- Chain E:  71% 16% • 11%



[illegible]

- Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

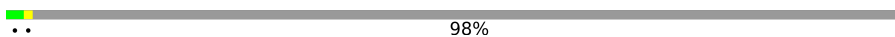
Chain 0: 

98%

[illegible]

[illegible]

- Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

Chain P: ..

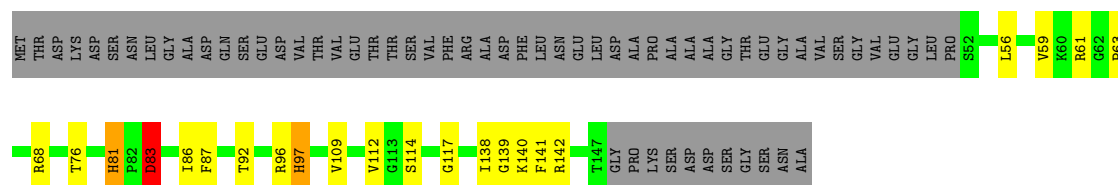
GLU	THR	HIS	ILE	GLU	ILE	GLU	ILE	ALA	ALA	SER	MET
THR	GLY	GLY	PRO	PHE	ALA	ALA	ALA	VAL	ALA	ALA	GLY
HIS	LEU	LEU	TYR	GLN	ALA	ALA	TYR	LYS	ALA	SER	ASN
ASP	THR	THR	GLU	GLY	GLU	ALA	GLU	PHE	VAL	GLY	HIS
LYS	TRP	TRP	VAL	SER	ASP	SER	ASP	ASN	VAL	ARG	HIS
PRO	ARG	ARG	ARG	GLU	ILE	GLU	ILE	ASN	LYS	THR	HIS
THR	TRP	TRP	TRP	GLU	VAL	GLU	VAL	MET	ASN	THR	HIS
VAL	ARG	ARG	ARG	ARG	ARG	ILE	ARG	ASN	MET	THR	HIS
ALA	ALA	ALA	THR	ILE	ALA	ARG	ARG	ASN	ASN	ALA	HIS
GLN	GLU	GLU	ASN	ASP	ALA	ASP	ARG	HIS	ALA	ALA	SER
GLY	PHE	PHE	PRO	LEU	ASP	LEU	ARG	ALA	LEU	PRO	SER
LYS	LYS	LYS	PRO	GLY	GLY	GLY	ASP	VAL	VAL	VAL	GLY
ILE	ASP	ASP	ASP	ILE	LYS	ILE	LYS	VAL	GLU	THR	LEU
SER	PHE	PHE	GLU	GLY	THR	LYS	THR	GLY	PRO	THR	ARG
LYS	ALA	ALA	ASP	LEU	ALA	ALA	ALA	LYS	ALA	PRO	GLY
LEU	GLY	GLY	LYS	ILE	GLU	ILE	GLU	THR	ALA	ALA	SER
ASN	VAL	VAL	ASN	THR	ASP	THR	ASP	PRO	SER	PRO	HIS
ALA	GLN	GLN	ALA	LEU	PHE	LEU	SER	ILE	VAL	ALA	MET
ALA	ALA	ALA	ARG	THR	SER	THR	ILE	THR	ARG	PRO	ALA
GLU	GLU	LYS	VAL	SER	VAL	SER	GLY	THR	ALA	ALA	ALA
ALA	LYS	LYS	ILE	THR	GLY	THR	VAL	PRO	ILE	PRO	VAL
PHE	LEU	LEU	GLU	TYR	THR	THR	THR	ALA	PRO	GLU	SER
GLU	ARG	ARG	ILE	ASP	ILE	ASP	ILE	HIS	ALA	PRO	SER
THR	THR	THR	ILE	HIS	SER	HIS	SER	THR	LYS	LYS	SER
PHE	LEU	ILE	ALA	ARG	LEU	ARG	LEU	ASN	LEU	ALA	PRO
GLN	SER	SER	TYR	ILE	THR	ILE	THR	LEU	MET	ALA	SER
THR	VAL	VAL	ARG	GLN	ASN	ILE	ASN	GLY	PRO	PRO	PRO
LYS	LEU	LEU	ASN	GLY	PRO	GLY	GLY	ALA	ASN	PRO	GLY
TYR	GLY	TYR	ARG	GLU	THR	ALA	THR	ILE	ARG	ALA	GLN
VAL	VAL	ASP	GLY	GLU	GLY	GLU	LEU	ASP	VAL	ALA	ASN
GLY	GLN	TYR	HIS	GLY	HIS	SER	THR	GLN	VAL	LYS	E12
LYS	CYS	CYS	MET	GLY	ALA	GLY	VAL	GLY	ASN	THR	M13
ARG	ARG	ARG	ALA	PHE	ALA	PHE	THR	GLY	ASN	GLU	L14
SER	LEU	LEU	ASP	LEU	ASP	LEU	SER	LYS	ASN	ALA	V15
LEU	GLY	VAL	ILE	ARG	VAL	GLY	VAL	GLY	HIS	LYS	E16
LEU	GLY	GLY	ASP	THR	ILE	THR	PRO	ASN	LEU	PRO	E17
GLU	GLU	VAL	PRO	ILE	PRO	ILE	ARG	LYS	LEU	ALA	M18
GLY	GLY	VAL	LEU	ILE	ARG	ARG	ARG	LYS	ARG	LYS	K21
ALA	ALA	TYR	LEU	GLN	LEU	HIS	SER	THR	THR	PRO	D25
GLU	THR	THR	LEU	LEU	GLN	LEU	GLN	VAL	GLY	LYS	V29
VAL	VAL	ILE	ASN	LEU	GLN	LEU	GLN	ALA	LYS	THR	D30
ILE	ILE	LEU	THR	ASP	GLY	ASP	GLY	ILE	ILE	ALA	W33
PRO	PRO	GLU	ARG	ASP	ALA	ASP	ALA	ILE	SER	PRO	V16
MET	MET	GLU	PHE	ASP	ILE	PHE	ILE	LYS	PHE	THR	W33
ASP	ASP	GLN	SER	PHE	ARG	PHE	GLY	ARG	LYS	LYS	D39
ALA	ALA	ASN	HIS	ASP	HIS	ASP	ALA	CYS	HIS	GLY	Y40
VAL	VAL	ARG	PRO	GLU	PRO	GLU	ALA	GLU	ASP	GLU	S41
ILE	ILE	TRP	ASP	ILE	ASP	ILE	ALA	MET	GLY	SER	PRO
GLN	GLN	GLN	ASP	PHE	GLN	PHE	GLN	THR	ILE	GLN	GLU
CYS	CYS	GLU	VAL	GLU	ASP	ARG	TYR	PHE	ALA	ILE	PRO
THR	THR	GLU	VAL	GLU	VAL	GLU	THR	ILE	ILE	LEU	THR
ASN	ASN	VAL	SER	GLY	ASN	GLY	ALA	GLN	ARG	THR	ASN

[illegible]

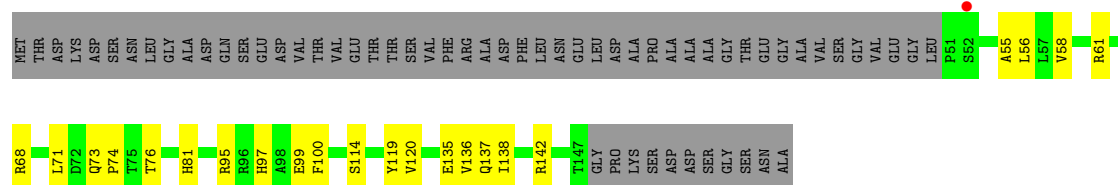
- Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

Chain Q:  98%

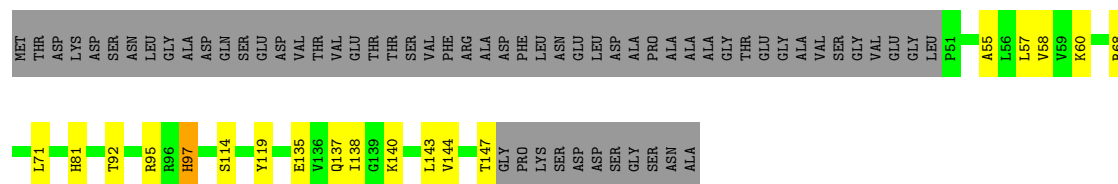
PRO	GLN	VAL	ARG	THR	MET
ALA	PHE	GLN	GLY	ASP	GLY
GLU	ILE	ALA	ALA	SER	SER
PHE	ALA	VAL	ALA	SER	ALA
GLN	ALA	LYS	ALA	SER	HIS
GLY	TYR	LYS	ALA	ASN	HIS
ALA	GLU	PHE	VAL	GLY	HIS
SER	ASP	PRO	VAL	ARG	HIS
GLU	ILE	ASN	LYS	THR	HIS
GLU	VAL	MET	ASN	THR	SER
ARG	ARG	ASN	MET	THR	SER
ILE	ARG	ARG	ASN	ALA	SER
ALA	ALA	HIS	ASN	ALA	GLY
ASP	ARG	PHE	SER	PRO	VAL
LEU	ASP	ALA	LEU	VAL	VAL
GLY	GLY	VAL	GLU	THR	VAL
ILE	LYS	VAL	VAL	PRO	ARG
GLY	LEU	ASP	PRO	PRO	GLY
LYS	THR	GLY	THR	THR	SER
LEU	ALA	LYS	ALA	PRO	HIS
ILE	GLU	PRO	THR	ALA	MET
THR	ASP	THR	SER	PRO	ALA
LEU	PHE	ALA	VAL	ALA	SER
THR	SER	ILE	ARG	PRO	VAL
SER	GLY	THR	ALA	ALA	SER
THR	VAL	PRO	ILE	PRO	SER
TYR	THR	ALA	PRO	GLU	SER
ASP	ILE	THR	ALA	PRO	SER
HIS	SER	HIS	LYS	LYS	SER
ARG	LEU	ASN	LEU	ALA	PRO
ILE	THR	LEU	MET	ALA	PHE
ILE	ASN	GLY	ILE	PRO	GLY
GLN	PRO	LEU	ASP	LYS	GLN
GLY	GLY	ALA	ASN	PRO	ASN
ALA	THR	ILE	ARG	ALA	E12
GLU	LEU	ASP	VAL	ALA	L13
SER	GLY	THR	VAL	LYS	L14
GLY	GLN	GLN	ILE	THR	V15
ASP	VAL	GLY	ASN	GLU	E16
PHE	HIS	LYS	ASN	ALA	E17
LEU	SER	ASP	HIS	LYS	M18
ARG	VAL	GLY	LEU	PRO	
THR	PRO	ASN	LYS	ALA	K21
ILE	ARG	ARG	ARG	LYS	
HIS	LEU	SER	THR	PRO	D25
GLN	MET	LEU	ARG	ALA	V29
LEU	GLN	VAL	GLY	LYS	D30
LEU	GLN	VAL	LYS	ALA	
ASP	GLY	ALA	ILE	THR	W33
ASP	ALA	ILE	SER	PRO	
ASP	ILE	LYS	PHE	ALA	F36
PHE	ILE	ARG	THR	LYS	
PHE	GLY	CYS	HIS	GLY	D39
ASP	ALA	GLU	LEU	ASP	Y40
GLU	GLY	THR	LEU	GLU	S41
ILE	ALA	MET	GLY	SER	PRO
PHE	MET	ARG	TYR	GLN	GLU
ARG	GLU	PHE	ILE	ILE	PRO
THR	TYR	GLY	ILE	THR	THR



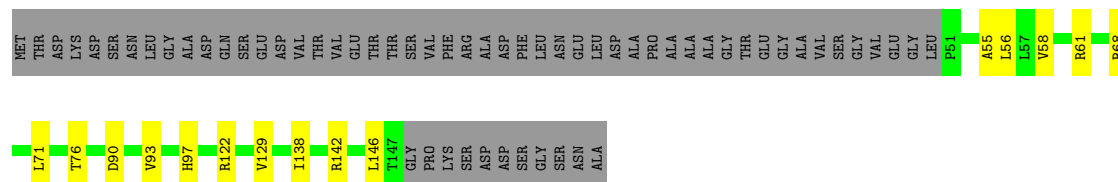
• Molecule 2: Glycogen accumulation regulator GarA



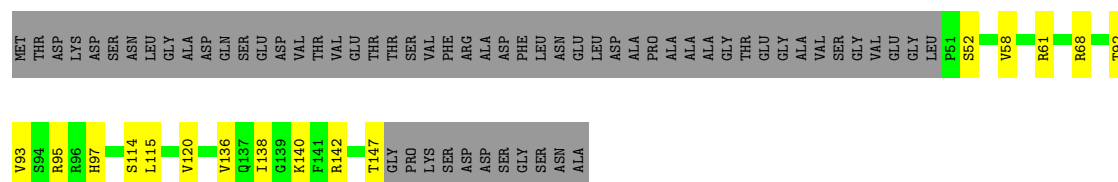
• Molecule 2: Glycogen accumulation regulator GarA



• Molecule 2: Glycogen accumulation regulator GarA



• Molecule 2: Glycogen accumulation regulator GarA



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 4.64Å)	Xtriage
Refinement program	BUSTER 2.10.4 (8-JUN-2022)	Depositor
R, R_{free}	0.198 , 0.229 0.190 , 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)	0.36 , 791.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.390 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CA, TPP

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	0.59	0/8751	0.97	3/11855 (0.0%)
1	B	0.60	0/8764	0.97	6/11874 (0.1%)
1	C	0.59	0/8767	0.96	1/11877 (0.0%)
1	D	0.59	0/8717	0.96	1/11816 (0.0%)
1	E	0.60	0/8710	0.97	6/11812 (0.1%)
1	F	0.59	0/8685	0.97	1/11776 (0.0%)
1	N	0.72	0/276	0.92	0/375
1	O	0.72	0/276	0.92	0/375
1	P	0.72	0/276	0.91	0/375
1	Q	0.75	0/276	0.96	1/375 (0.3%)
2	G	0.57	0/757	0.87	0/1025
2	H	0.65	0/722	1.03	2/980 (0.2%)
2	I	0.53	0/753	0.82	0/1020
2	J	0.53	0/753	0.85	0/1020
2	K	0.60	0/753	0.87	0/1020
2	L	0.58	0/753	0.89	0/1020
All	All	0.60	0/57989	0.96	21/78595 (0.0%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	39	ASP	CA-CB-CG	7.43	120.03	112.60
1	E	645	ASP	CA-CB-CG	7.29	119.89	112.60
2	H	87	PHE	CA-CB-CG	6.86	120.66	113.80
1	B	645	ASP	CA-CB-CG	6.63	119.23	112.60
1	B	653	VAL	CA-C-N	5.68	128.54	120.53
1	B	653	VAL	C-N-CA	5.68	128.54	120.53
2	H	83	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	381	GLY	CA-C-N	5.48	128.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	GLY	C-N-CA	5.48	128.18	120.28
1	A	299	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	299	ASP	CA-CB-CG	5.47	118.08	112.60
1	F	299	ASP	CA-CB-CG	5.37	117.97	112.60
1	D	299	ASP	CA-CB-CG	5.33	117.92	112.60
1	E	299	ASP	CA-CB-CG	5.28	117.88	112.60
1	E	512	GLU	CA-C-N	5.22	128.00	120.38
1	E	512	GLU	C-N-CA	5.22	128.00	120.38
1	E	653	VAL	CA-C-N	5.20	127.86	120.53
1	E	653	VAL	C-N-CA	5.20	127.86	120.53
1	B	512	GLU	CA-C-N	5.17	127.92	120.38
1	B	512	GLU	C-N-CA	5.17	127.92	120.38
1	C	299	ASP	CA-CB-CG	5.15	117.75	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8579	0	8402	144	0
1	B	8591	0	8414	143	0
1	C	8593	0	8408	141	0
1	D	8544	0	8341	137	0
1	E	8537	0	8299	140	0
1	F	8513	0	8287	136	0
1	N	266	0	233	15	0
1	O	266	0	233	17	0
1	P	266	0	233	13	0
1	Q	266	0	233	17	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	18	0
2	K	740	0	727	9	0
2	L	740	0	727	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	921	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 (921) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:240:ASP:HB2	1:A:242:LYS:HZ3	1.35	0.90
1:O:18:MET:HE1	1:O:33:TRP:CD1	2.07	0.89
1:P:14:LEU:HG	1:P:18:MET:HB3	1.52	0.89
1:P:18:MET:HE1	1:P:33:TRP:CD1	2.07	0.89
1:N:18:MET:HE1	1:N:33:TRP:CD1	2.07	0.89
1:O:14:LEU:HG	1:O:18:MET:HB3	1.52	0.89
1:Q:18:MET:HE1	1:Q:33:TRP:CD1	2.07	0.89
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
1:B:240:ASP:HB2	1:B:242:LYS:HZ3	1.36	0.85
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
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:E:645:ASP:HB2	1:E:677:ASN:HA	1.63	0.80
1:D:768:ARG:HG3	1:D:772:LYS:HZ1	1.46	0.79
1:A:748:ASN:HB2	1:A:751:ASP:HB2	1.63	0.79
1:C:768:ARG:HG3	1:C:772:LYS:HZ1	1.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:768:ARG:HG3	1:F:772:LYS:HZ2	1.54	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:170:LYS:HE2	1:C:220:GLU:HA	1.75	0.68
1:D:768:ARG:CG	1:D:772:LYS:HZ1	2.05	0.68
1:D:442:ALA:HB1	1:D:467:VAL:HG12	1.74	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:J:60:LYS:HZ1	2:J:135:GLU:HG3	1.56	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
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
2:J:60:LYS:HZ3	2:J:135:GLU:HG3	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:18:MET:HE1	1:N:33:TRP:NE1	2.11	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:Q:18:MET:HE1	1:Q:33:TRP:NE1	2.11	0.65
1:O:18:MET:HE1	1:O:33:TRP:NE1	2.12	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:P:18:MET:HE1	1:P:33:TRP:NE1	2.11	0.64
1:C:768:ARG:CG	1:C:772:LYS:HZ1	2.10	0.64
1:D:1051:LEU:HD11	1:D:1064:LEU:HD11	1.79	0.64
1:B:768:ARG:CG	1:B:772:LYS:HZ2	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:1003:SER:HB3	1:D:1063:PRO:HG3	1.83	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: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
1:F:866:LYS:HG3	1:F:870:MET:HE2	1.83	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:B:240:ASP:HB2	1:B:242:LYS:HZ2	1.64	0.61
1:C:866:LYS:HG3	1:C:870:MET:HE2	1.83	0.60
1:A:508:LEU:HD13	1:A:541:GLY:HA3	1.83	0.60
1:B:866:LYS:HG3	1:B:870:MET:HE2	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:A:866:LYS:HG3	1:A:870:MET:HE2	1.83	0.60
1:F:760:MET:HE2	1:F:764:ILE:HD11	1.83	0.60
1:B:129:ARG:NH1	1:B:330:HIS:ND1	2.50	0.60
1:D:866:LYS:HG3	1:D:870:MET:HE2	1.83	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:E:866:LYS:HG3	1:E:870:MET:HE2	1.83	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: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:E:760:MET:HE2	1:E:764:ILE:HD11	1.85	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:C:760:MET:HE2	1:C:764:ILE:HD11	1.85	0.57
1:D:760:MET:HE2	1:D:764:ILE:HD11	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASP:HB2	1:A:242:LYS:HZ2	1.67	0.57
1:A:441:ASP:HA	1:A:445:ARG:CG	2.31	0.57
1:B:645:ASP:HB3	1:B:677:ASN:HA	1.86	0.57
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:760:MET:HE2	1:B:764:ILE:HD11	1.86	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:1069:PRO:HG3	1:E:1072:MET:HE2	1.87	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:C:1069:PRO:HG3	1:C:1072:MET:HE2	1.87	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:D:377:TYR:HB3	1:D:439:LEU:HD22	1.86	0.57
1:F:1021:THR:HA	1:F:1070:LYS:HZ3	1.69	0.57
1:B:768:ARG:CD	1:B:772:LYS:HZ2	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:HIS:ND1	1:C:445:ARG:NH1	2.51	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:1069:PRO:HG3	1:B:1072:MET:HE2	1.87	0.56
1:B:441:ASP:HA	1:B:445:ARG:HG3	1.88	0.56
1:F:133:ALA:HA	1:F:136:MET:HE3	1.88	0.56
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:A:133:ALA:HA	1:A:136:MET:HE3	1.88	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:D:133:ALA:HA	1:D:136:MET:HE3	1.89	0.55
1:P:14:LEU:CG	1:P:18:MET:HB3	2.29	0.55
1:A:768:ARG:HG3	1:A:772:LYS:HZ1	1.70	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
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:A:1069:PRO:HG3	1:A:1072:MET:HE2	1.87	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:D:1069:PRO:HG3	1:D:1072:MET:HE2	1.87	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:133:ALA:HA	1:C:136:MET:HE3	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:B:133:ALA:HA	1:B:136:MET:HE3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1022:SER:HB3	1:F:1206:PRO:HB3	1.90	0.54
1:F:1069:PRO:HG3	1:F:1072:MET:HE2	1.88	0.54
1:A:384:MET:HG2	1:A:397:PHE:HA	1.90	0.54
1:A:768:ARG:CD	1:A:772:LYS:HZ2	2.20	0.54
1:D:124:THR:HG21	1:D:270:LEU:HB3	1.89	0.54
1:F:768:ARG:CG	1:F:772:LYS:HZ2	2.19	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:1021:THR:HA	1:B:1070:LYS:HZ3	1.71	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
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
1:E:133:ALA:HA	1:E:136:MET:HE3	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:C:1021:THR:HA	1:C:1070:LYS:HZ1	1.74	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:B:706:ILE:HG21	1:B:708:HIS:CE1	2.44	0.53
1:D:1021:THR:HA	1:D:1070:LYS:HZ1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:808:ARG:HG2	1:D:812:LYS:HZ1	1.71	0.52
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:A:136:MET:HE1	1:A:333:LEU:HB3	1.92	0.52
1:B:132:PRO:HG2	1:B:334:LEU:HD11	1.92	0.52
1:C:116:MET:HA	1:C:271:MET:HE1	1.92	0.52
1:F:136:MET:HE1	1:F:333:LEU:HB3	1.92	0.52
1:B:663:LEU:HB2	1:B:666:TYR:HB2	1.90	0.51
1:F:898:LEU:HD21	1:F:911:ARG:HD3	1.92	0.51
1:A:1021:THR:HA	1:A:1070:LYS:HZ3	1.73	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:A:132:PRO:HG2	1:A:334:LEU:HD11	1.92	0.51
1:A:760:MET:HE2	1:A:764:ILE:HD11	1.92	0.51
1:F:683:THR:HB	1:F:756:THR:HG21	1.93	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:D:136:MET:HE1	1:D:333:LEU:HB3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:136:MET:HE1	1:C:333:LEU:HB3	1.93	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:B:136:MET:HE1	1:B:333:LEU:HB3	1.92	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
1:C:132:PRO:HG2	1:C:334:LEU:HD11	1.92	0.50
1:E:613:LEU:HD23	1:E:641:MET:HE2	1.93	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: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:E:1021:THR:HA	1:E:1070:LYS:HZ1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:894:LYS:HZ2	1:A:968:ASP:C	2.20	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: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
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:D:613:LEU:HD23	1:D:641:MET:HE2	1.95	0.49
1:F:793:LEU:CD2	1:Q:33:TRP:CD1	2.95	0.49
1:F:894:LYS:HZ2	1:F:968:ASP:C	2.20	0.49
1:N:14:LEU:O	1:N:18:MET:HG2	2.12	0.49
1:B:613:LEU:HD23	1:B:641:MET:HE2	1.93	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:O:18:MET:HE1	1:O:33:TRP:CG	2.48	0.49
1:F:481:TYR:HE1	2:L:92:THR:HG22	1.78	0.48
1:D:894:LYS:HZ2	1:D:968:ASP:C	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:768:ARG:HG3	1:D:772:LYS:NZ	2.25	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:Q:18:MET:HE1	1:Q:33:TRP:CG	2.48	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:C:613:LEU:HD23	1:C:641:MET:HE2	1.96	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:P:18:MET:HE1	1:P:33:TRP:CG	2.48	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
1:E:136:MET:HE1	1:E:333:LEU:HB3	1.94	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:382:HIS:ND1	1:E:694:TYR:OH	2.37	0.47
1:E:1021:THR:HA	1:E:1070:LYS:HZ3	1.76	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:D:808:ARG:HG2	1:D:812:LYS:HZ2	1.77	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: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:F:617:VAL:HG11	1:F:639:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:613:LEU:HD23	1:F:641:MET:HE2	1.96	0.46
1:B:116:MET:HE3	1:D:314:HIS:ND1	2.31	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
1:E:894:LYS:HZ2	1:E:968:ASP:C	2.24	0.46
1:E:1013:HIS:ND1	1:E:1021:THR:CG2	2.79	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:C:1021:THR:HA	1:C:1070:LYS:HZ3	1.79	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:C:768:ARG:CG	1:C:772:LYS:NZ	2.79	0.46
1:P:18:MET:HE1	1:P:33:TRP:CE2	2.51	0.46
1:F:768:ARG:CG	1:F:772:LYS:NZ	2.78	0.45
1:N:18:MET:HE1	1:N:33:TRP:CE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1021:THR:HA	1:B:1070:LYS:HZ1	1.80	0.45
1:C:462:TRP:NE1	1:C:466:ARG:HH22	2.15	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:B:894:LYS:HZ2	1:B:968:ASP:C	2.25	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:O:18:MET:HE1	1:O:33:TRP:CE2	2.51	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:A:613:LEU:HD23	1:A:641:MET:HE2	1.98	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:Q:18:MET:HE1	1:Q:33:TRP:CE2	2.51	0.45
1:A:1021:THR:HA	1:A:1070:LYS:HZ1	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:18:MET:HE1	1:N:33:TRP:CG	2.48	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:D:768:ARG:CG	1:D:772:LYS:NZ	2.79	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: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:1021:THR:HA	1:D:1070:LYS:HZ3	1.80	0.43
1:D:1123:LEU:HD23	1:D:1222:LEU:HD23	2.01	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:768:ARG:CG	1:A:772:LYS:HZ2	2.33	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:537:MET:HE3	1:C:537:MET:HB2	1.96	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:659:ASN:O	1:D:691:SER:OG	2.34	0.42
1:C:960:TYR:HE1	1:C:1003:SER:HB2	1.85	0.42
1:D:706:ILE:HG22	1:D:708:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:772:LYS:HB3	1:Q:36:PHE:HE1	1.85	0.41
1:F:1072:MET:HE2	1:F:1072:MET:HB3	1.98	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:A:894:LYS:NZ	1:A:968:ASP:C	2.79	0.41
1:B:266:SER:O	1:B:268:PRO:HD3	2.20	0.41
1:C:768:ARG:HG3	1:C:772:LYS:NZ	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1048:TYR:CE1	1:C:1066:VAL:HG11	2.55	0.41
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:C:894:LYS:NZ	1:C:968:ASP:C	2.79	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:E:894:LYS:NZ	1:E:968:ASP:C	2.79	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:894:LYS:NZ	1:B:968:ASP:C	2.79	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:C:1072:MET:HE2	1:C:1072:MET:HB3	1.98	0.41
1:D:571:HIS:NE2	5:D:1303:TPP:H2	2.36	0.41
1:D:894:LYS:NZ	1:D:968:ASP:C	2.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1200:ARG:HG3	1:D:1221:ILE:HD11	2.01	0.41
1:E:537:MET:HE3	1:E:537:MET:HB2	1.96	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:F:894:LYS:NZ	1:F:968:ASP:C	2.78	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
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:768:ARG:CD	1:F:772:LYS:HZ3	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:537:MET:HE3	1:F:537:MET:HB2	1.97	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1100/1250 (88%)	1029 (94%)	68 (6%)	3 (0%)	36	71
1	B	1102/1250 (88%)	1022 (93%)	76 (7%)	4 (0%)	30	67
1	C	1103/1250 (88%)	1028 (93%)	72 (6%)	3 (0%)	36	71
1	D	1101/1250 (88%)	1026 (93%)	71 (6%)	4 (0%)	30	67
1	E	1103/1250 (88%)	1022 (93%)	77 (7%)	4 (0%)	30	67
1	F	1099/1250 (88%)	1018 (93%)	77 (7%)	4 (0%)	30	67
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%)	2	20
2	G	96/158 (61%)	87 (91%)	8 (8%)	1 (1%)	12	47
2	H	94/158 (60%)	79 (84%)	14 (15%)	1 (1%)	11	45
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7290/13448 (54%)	6759 (93%)	506 (7%)	25 (0%)	36	71

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
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 ⓘ

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%)	850 (95%)	42 (5%)	23	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	894/1037 (86%)	853 (95%)	41 (5%)	24	46
1	C	893/1037 (86%)	855 (96%)	38 (4%)	26	48
1	D	885/1037 (85%)	846 (96%)	39 (4%)	25	47
1	E	880/1037 (85%)	840 (96%)	40 (4%)	24	46
1	F	878/1037 (85%)	845 (96%)	33 (4%)	29	51
1	N	30/1037 (3%)	26 (87%)	4 (13%)	4	16
1	O	30/1037 (3%)	25 (83%)	5 (17%)	2	11
1	P	30/1037 (3%)	26 (87%)	4 (13%)	4	16
1	Q	30/1037 (3%)	25 (83%)	5 (17%)	2	11
2	G	81/127 (64%)	79 (98%)	2 (2%)	42	62
2	H	72/127 (57%)	64 (89%)	8 (11%)	6	20
2	I	81/127 (64%)	79 (98%)	2 (2%)	42	62
2	J	81/127 (64%)	79 (98%)	2 (2%)	42	62
2	K	81/127 (64%)	78 (96%)	3 (4%)	30	51
2	L	81/127 (64%)	79 (98%)	2 (2%)	42	62
All	All	5919/11132 (53%)	5649 (95%)	270 (5%)	24	46

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	GLU
1	A	169	VAL
1	A	234	ILE
1	A	251	VAL
1	A	253	ILE
1	A	261	LEU
1	A	269	ARG
1	A	294	GLU
1	A	295	GLU
1	A	299	ASP
1	A	305	LEU
1	A	307	THR
1	A	314	HIS
1	A	402	ASP
1	A	440	ARG
1	A	455	LEU
1	A	464	GLN

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Mol	Chain	Res	Type
1	A	496	LEU
1	A	503	GLN
1	A	506	PHE
1	A	509	GLU
1	A	513	THR
1	A	527	GLU
1	A	560	GLU
1	A	616	LEU
1	A	648	PHE
1	A	653	VAL
1	A	698	VAL
1	A	744	ARG
1	A	747	HIS
1	A	797	GLN
1	A	831	LEU
1	A	909	THR
1	A	950	LEU
1	A	976	GLN
1	A	1013	HIS
1	A	1025	ILE
1	A	1041	MET
1	A	1169	GLU
1	A	1191	HIS
1	A	1204	SER
1	A	1207	SER
1	B	101	GLU
1	B	169	VAL
1	B	203	GLN
1	B	234	ILE
1	B	251	VAL
1	B	261	LEU
1	B	294	GLU
1	B	295	GLU
1	B	299	ASP
1	B	305	LEU
1	B	307	THR
1	B	314	HIS
1	B	402	ASP
1	B	455	LEU
1	B	496	LEU
1	B	503	GLN
1	B	506	PHE

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Mol	Chain	Res	Type
1	B	508	LEU
1	B	513	THR
1	B	527	GLU
1	B	542	ARG
1	B	560	GLU
1	B	606	LEU
1	B	616	LEU
1	B	645	ASP
1	B	653	VAL
1	B	689	SER
1	B	698	VAL
1	B	748	ASN
1	B	797	GLN
1	B	831	LEU
1	B	909	THR
1	B	950	LEU
1	B	976	GLN
1	B	1013	HIS
1	B	1025	ILE
1	B	1041	MET
1	B	1169	GLU
1	B	1191	HIS
1	B	1204	SER
1	B	1207	SER
1	C	169	VAL
1	C	234	ILE
1	C	251	VAL
1	C	261	LEU
1	C	294	GLU
1	C	295	GLU
1	C	299	ASP
1	C	305	LEU
1	C	307	THR
1	C	314	HIS
1	C	402	ASP
1	C	455	LEU
1	C	470	LYS
1	C	471	HIS
1	C	496	LEU
1	C	513	THR
1	C	527	GLU
1	C	542	ARG

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Mol	Chain	Res	Type
1	C	560	GLU
1	C	616	LEU
1	C	626	THR
1	C	653	VAL
1	C	689	SER
1	C	698	VAL
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	1013	HIS
1	C	1025	ILE
1	C	1041	MET
1	C	1169	GLU
1	C	1191	HIS
1	C	1204	SER
1	C	1207	SER
1	D	105	LEU
1	D	169	VAL
1	D	234	ILE
1	D	251	VAL
1	D	254	SER
1	D	261	LEU
1	D	294	GLU
1	D	295	GLU
1	D	299	ASP
1	D	305	LEU
1	D	307	THR
1	D	314	HIS
1	D	384	MET
1	D	402	ASP
1	D	455	LEU
1	D	471	HIS
1	D	513	THR
1	D	527	GLU
1	D	542	ARG
1	D	560	GLU
1	D	616	LEU
1	D	626	THR

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Mol	Chain	Res	Type
1	D	648	PHE
1	D	653	VAL
1	D	689	SER
1	D	698	VAL
1	D	747	HIS
1	D	748	ASN
1	D	797	GLN
1	D	909	THR
1	D	950	LEU
1	D	976	GLN
1	D	1013	HIS
1	D	1025	ILE
1	D	1041	MET
1	D	1169	GLU
1	D	1191	HIS
1	D	1204	SER
1	D	1207	SER
1	E	158	THR
1	E	169	VAL
1	E	198	LEU
1	E	201	ASP
1	E	247	ASP
1	E	251	VAL
1	E	261	LEU
1	E	294	GLU
1	E	295	GLU
1	E	299	ASP
1	E	305	LEU
1	E	307	THR
1	E	314	HIS
1	E	402	ASP
1	E	455	LEU
1	E	496	LEU
1	E	503	GLN
1	E	506	PHE
1	E	513	THR
1	E	527	GLU
1	E	542	ARG
1	E	560	GLU
1	E	616	LEU
1	E	645	ASP
1	E	653	VAL

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Mol	Chain	Res	Type
1	E	689	SER
1	E	698	VAL
1	E	748	ASN
1	E	797	GLN
1	E	909	THR
1	E	950	LEU
1	E	976	GLN
1	E	1013	HIS
1	E	1025	ILE
1	E	1041	MET
1	E	1169	GLU
1	E	1187	ILE
1	E	1191	HIS
1	E	1204	SER
1	E	1207	SER
1	F	121	GLU
1	F	169	VAL
1	F	211	LEU
1	F	234	ILE
1	F	261	LEU
1	F	294	GLU
1	F	295	GLU
1	F	299	ASP
1	F	305	LEU
1	F	307	THR
1	F	314	HIS
1	F	402	ASP
1	F	455	LEU
1	F	471	HIS
1	F	505	ARG
1	F	513	THR
1	F	527	GLU
1	F	616	LEU
1	F	626	THR
1	F	653	VAL
1	F	689	SER
1	F	698	VAL
1	F	797	GLN
1	F	909	THR
1	F	950	LEU
1	F	976	GLN
1	F	1013	HIS

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Mol	Chain	Res	Type
1	F	1025	ILE
1	F	1041	MET
1	F	1169	GLU
1	F	1191	HIS
1	F	1204	SER
1	F	1207	SER
2	G	99	GLU
2	G	147	THR
2	H	59	VAL
2	H	76	THR
2	H	81	HIS
2	H	83	ASP
2	H	86	ILE
2	H	97	HIS
2	H	109	VAL
2	H	112	VAL
2	I	99	GLU
2	I	135	GLU
2	J	97	HIS
2	J	147	THR
2	K	76	THR
2	K	129	VAL
2	K	146	LEU
2	L	52	SER
2	L	147	THR
1	N	16	GLU
1	N	29	VAL
1	N	30	ASP
1	N	39	ASP
1	O	14	LEU
1	O	16	GLU
1	O	29	VAL
1	O	30	ASP
1	O	39	ASP
1	P	16	GLU
1	P	29	VAL
1	P	30	ASP
1	P	39	ASP
1	Q	16	GLU
1	Q	29	VAL
1	Q	30	ASP
1	Q	33	TRP

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Mol	Chain	Res	Type
1	Q	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	167	GLN
1	A	314	HIS
1	A	400	HIS
1	A	446	HIS
1	A	453	HIS
1	A	556	GLN
1	A	748	ASN
1	A	1061	GLN
1	B	167	GLN
1	B	497	GLN
1	B	503	GLN
1	B	544	ASN
1	B	548	ASN
1	B	556	GLN
1	B	651	GLN
1	B	710	ASN
1	B	748	ASN
1	B	799	GLN
1	B	1061	GLN
1	C	167	GLN
1	C	274	GLN
1	C	314	HIS
1	C	318	GLN
1	C	459	GLN
1	C	556	GLN
1	C	569	GLN
1	C	651	GLN
1	C	710	ASN
1	C	747	HIS
1	C	748	ASN
1	C	976	GLN
1	C	1061	GLN
1	D	167	GLN
1	D	379	ASN
1	D	459	GLN
1	D	556	GLN

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Mol	Chain	Res	Type
1	D	569	GLN
1	D	651	GLN
1	D	710	ASN
1	D	748	ASN
1	D	797	GLN
1	D	799	GLN
1	D	976	GLN
1	D	1061	GLN
1	E	167	GLN
1	E	400	HIS
1	E	497	GLN
1	E	503	GLN
1	E	556	GLN
1	E	710	ASN
1	E	1061	GLN
1	F	167	GLN
1	F	556	GLN
1	F	651	GLN
1	F	710	ASN
1	F	799	GLN
1	F	976	GLN
1	F	1061	GLN
2	G	81	HIS
2	G	132	ASN
2	I	81	HIS
2	J	81	HIS
2	K	132	ASN
2	L	81	HIS
2	L	132	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	26,27,27	0.46	0	38,40,40	0.48	0
5	TPP	E	1303	3	26,27,27	0.49	0	38,40,40	0.41	0
5	TPP	C	1303	3	26,27,27	0.57	0	38,40,40	0.58	1 (2%)
5	TPP	F	1303	3	26,27,27	0.56	0	38,40,40	0.50	0
5	TPP	B	1303	3	26,27,27	0.52	0	38,40,40	0.54	0
5	TPP	D	1303	3	26,27,27	0.51	0	38,40,40	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TPP	A	1303	3	-	7/17/17/17	0/2/2/2
5	TPP	E	1303	3	-	7/17/17/17	0/2/2/2
5	TPP	C	1303	3	-	3/17/17/17	0/2/2/2
5	TPP	F	1303	3	-	10/17/17/17	0/2/2/2
5	TPP	B	1303	3	-	7/17/17/17	0/2/2/2
5	TPP	D	1303	3	-	7/17/17/17	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1303	TPP	O3B-PB-O3A	2.02	111.42	104.64

There are no chirality outliers.

All (41) torsion outliers are listed below:

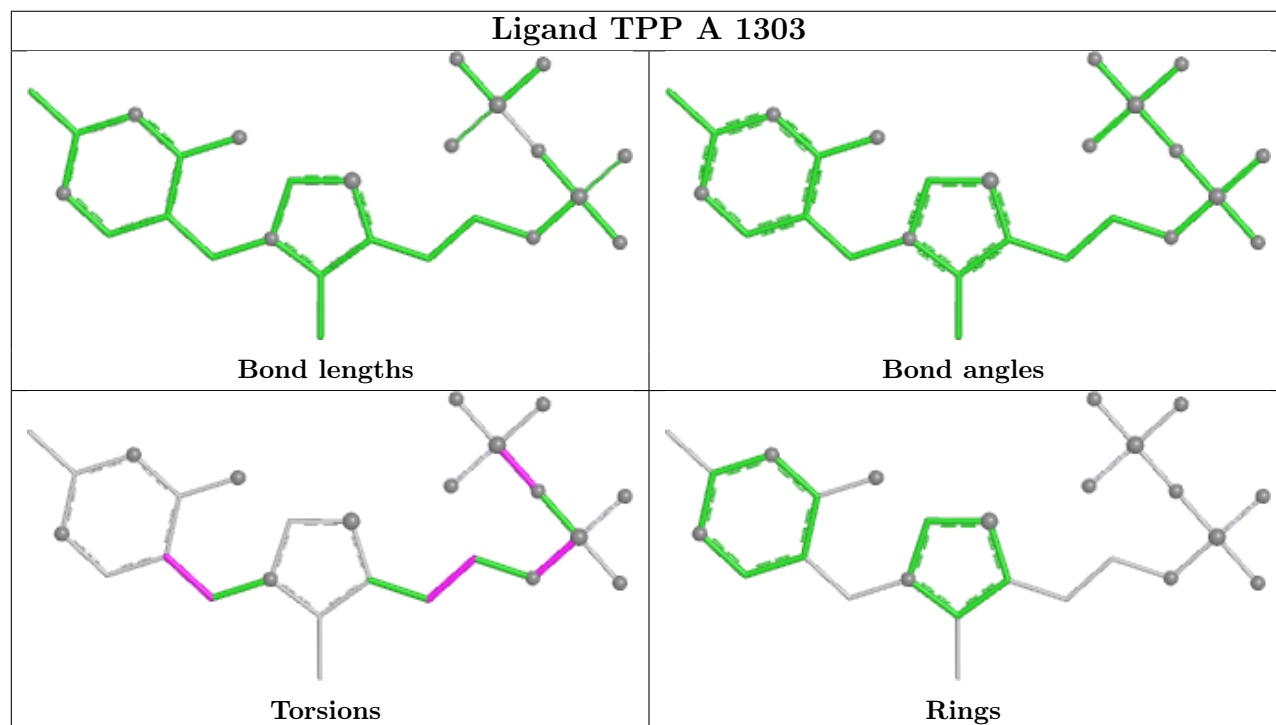
Mol	Chain	Res	Type	Atoms
5	A	1303	TPP	C5-C6-C7-O7
5	A	1303	TPP	C7-O7-PA-O1A
5	A	1303	TPP	C7-O7-PA-O2A
5	A	1303	TPP	PA-O3A-PB-O3B
5	B	1303	TPP	C5-C6-C7-O7
5	B	1303	TPP	C7-O7-PA-O2A
5	D	1303	TPP	C5-C6-C7-O7
5	D	1303	TPP	PA-O3A-PB-O3B
5	E	1303	TPP	C5-C6-C7-O7
5	E	1303	TPP	C7-O7-PA-O1A
5	E	1303	TPP	C7-O7-PA-O2A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

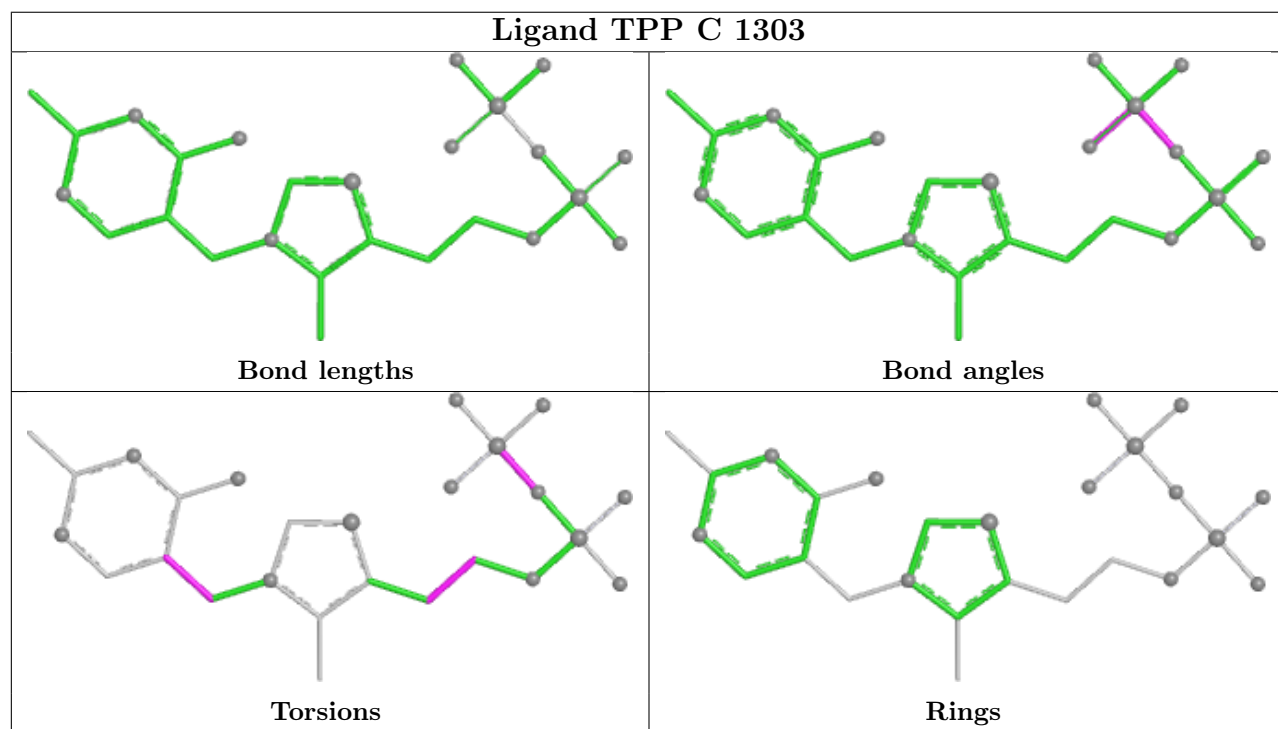
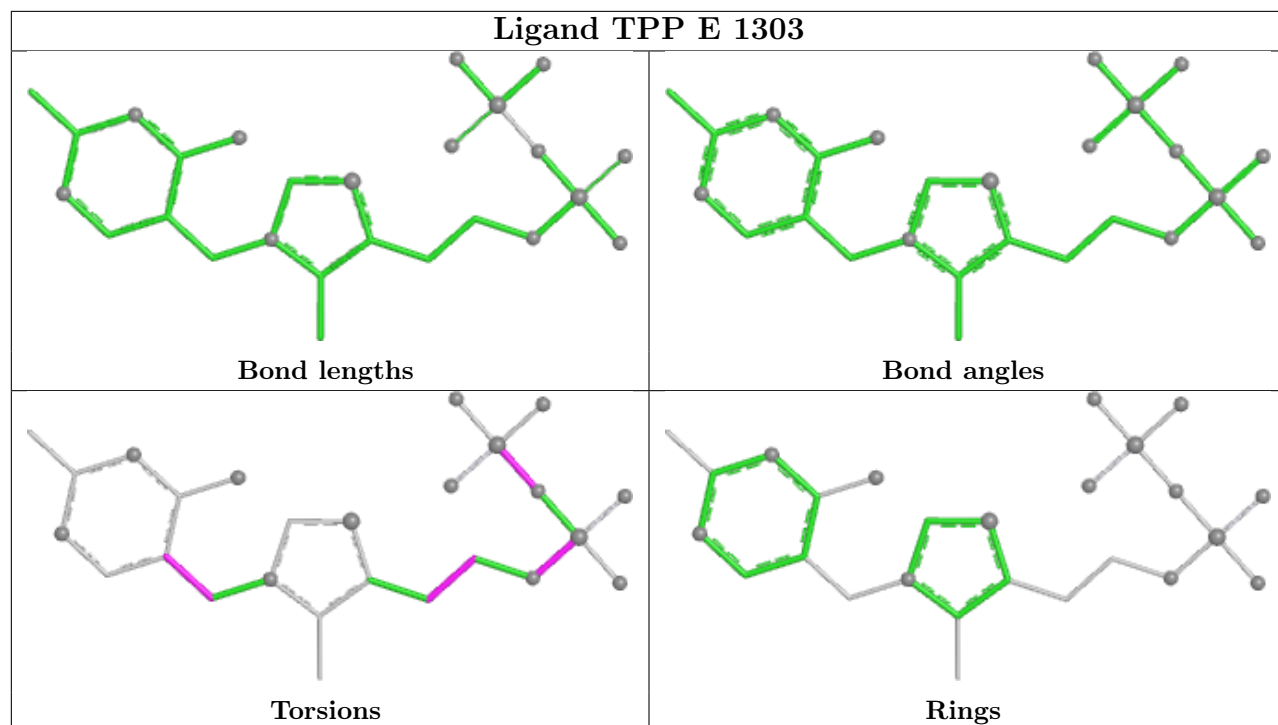
There are no ring outliers.

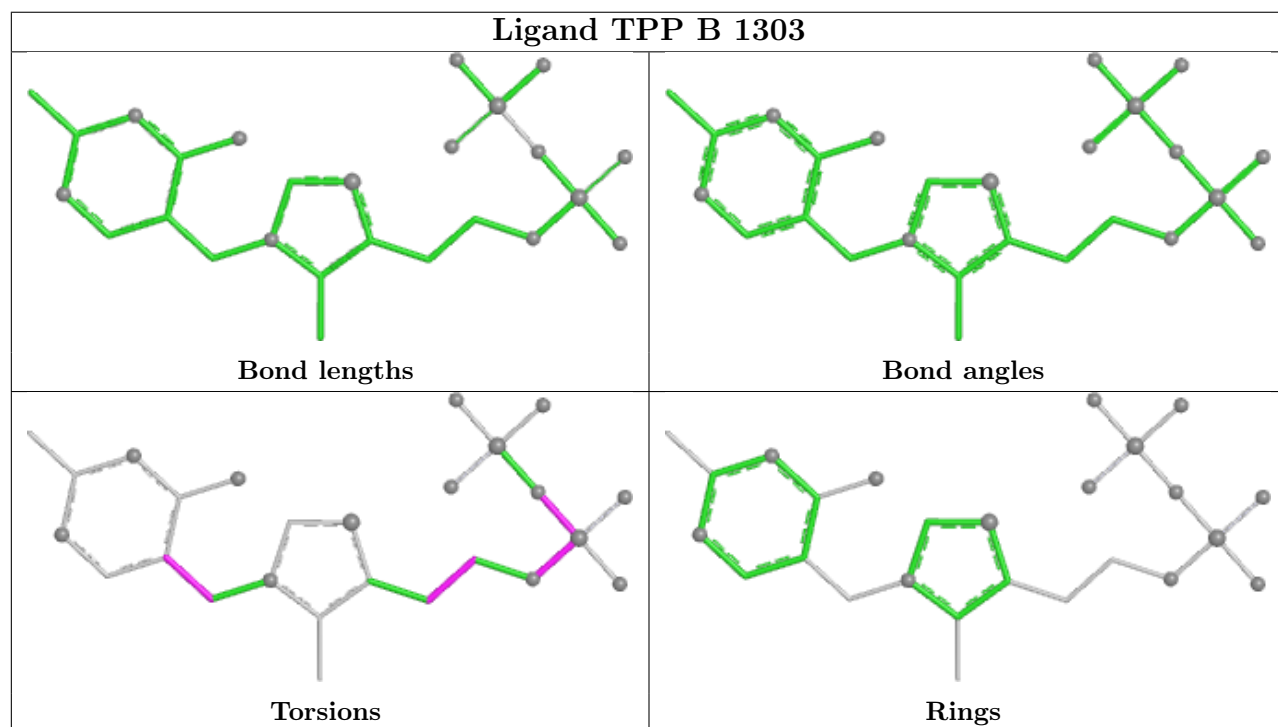
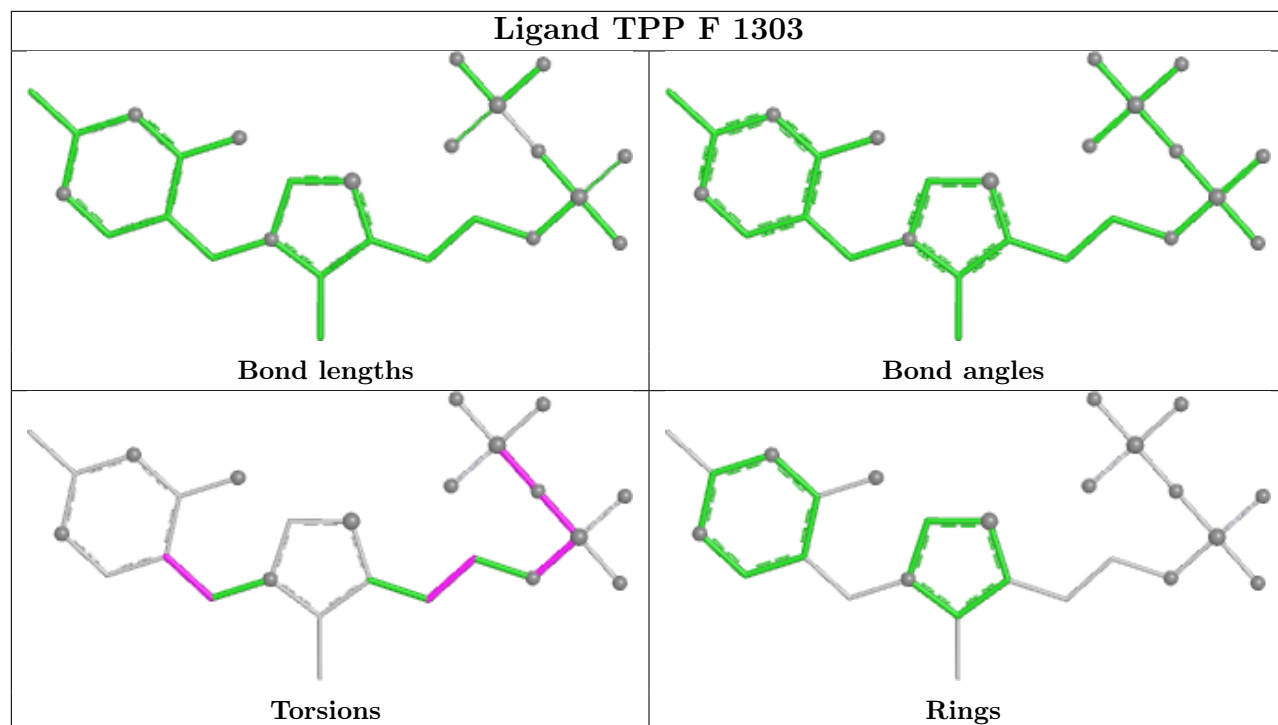
5 monomers are involved in 7 short contacts:

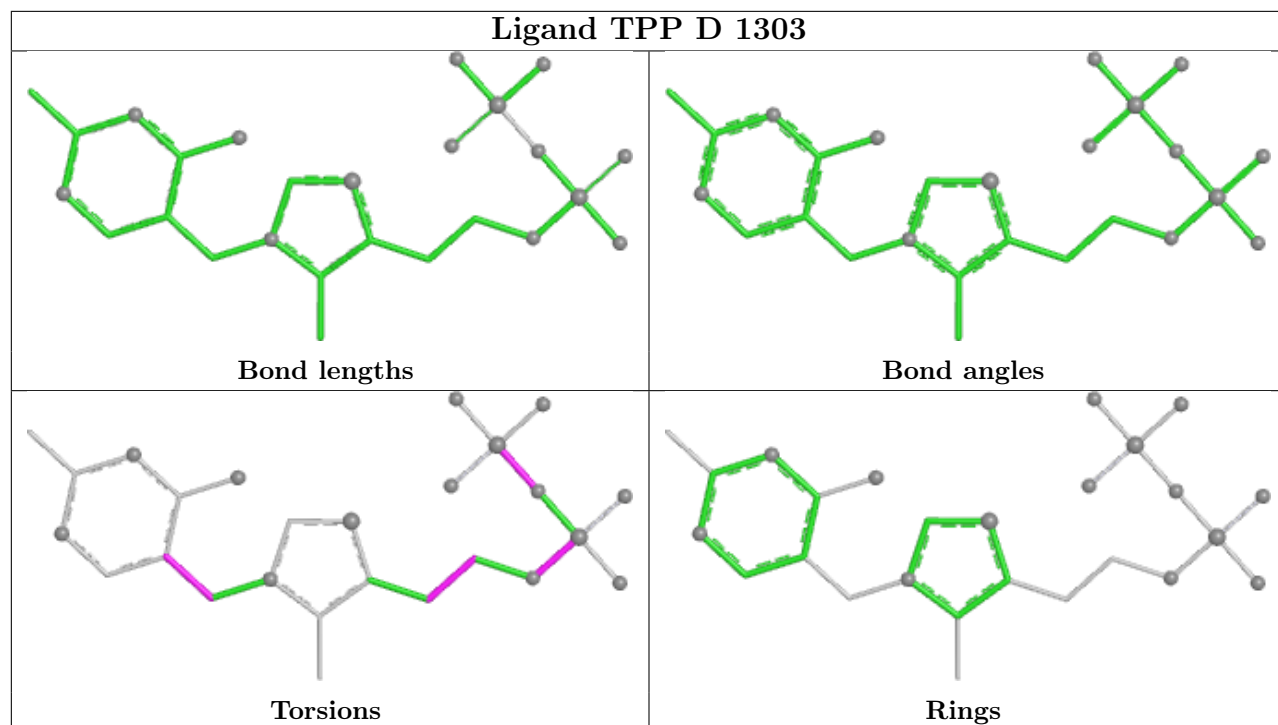
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1303	TPP	2	0
5	C	1303	TPP	1	0
5	F	1303	TPP	2	0
5	B	1303	TPP	1	0
5	D	1303	TPP	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1106/1250 (88%)	-0.69	0 100 100	155, 233, 300, 300	0
1	B	1108/1250 (88%)	-0.77	0 100 100	138, 225, 289, 300	0
1	C	1109/1250 (88%)	-0.64	1 (0%) 92 87	148, 231, 298, 300	0
1	D	1107/1250 (88%)	-0.64	7 (0%) 85 73	150, 232, 296, 300	0
1	E	1109/1250 (88%)	-0.78	3 (0%) 90 80	145, 225, 290, 300	0
1	F	1105/1250 (88%)	-0.67	2 (0%) 91 83	162, 233, 299, 300	0
1	N	30/1250 (2%)	0.18	1 (3%) 49 40	268, 300, 300, 300	0
1	O	30/1250 (2%)	0.05	0 100 100	280, 300, 300, 300	0
1	P	30/1250 (2%)	0.02	0 100 100	274, 300, 300, 300	0
1	Q	30/1250 (2%)	0.25	1 (3%) 49 40	259, 300, 300, 300	0
2	G	98/158 (62%)	-0.21	0 100 100	211, 283, 300, 300	0
2	H	96/158 (60%)	-0.61	0 100 100	179, 238, 300, 300	0
2	I	97/158 (61%)	-0.38	1 (1%) 79 64	207, 279, 300, 300	0
2	J	97/158 (61%)	-0.38	0 100 100	218, 281, 300, 300	0
2	K	97/158 (61%)	-0.63	0 100 100	183, 236, 295, 300	0
2	L	97/158 (61%)	-0.18	0 100 100	230, 284, 300, 300	0
All	All	7346/13448 (54%)	-0.66	16 (0%) 91 83	138, 233, 300, 300	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	746	GLY	3.5
1	Q	39	ASP	3.3
1	D	629	GLU	2.9
1	D	628	GLU	2.7
1	D	207	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	99	GLY	2.7
1	D	206	ASP	2.6
1	D	630	GLY	2.5
2	I	52	SER	2.5
1	E	206	ASP	2.5
1	D	209	ARG	2.4
1	E	207	GLY	2.3
1	F	1163	GLU	2.3
1	C	569	GLN	2.3
1	N	24	ASP	2.3
1	E	204	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	A	1302	1/1	0.97	0.06	300,300,300,300	0
4	CA	B	1302	1/1	0.98	0.07	220,220,220,220	0
4	CA	C	1302	1/1	0.98	0.11	289,289,289,289	0
4	CA	D	1302	1/1	0.98	0.12	298,298,298,298	0
3	MG	D	1301	1/1	0.99	0.06	149,149,149,149	0
4	CA	B	1304	1/1	0.99	0.07	170,170,170,170	0
3	MG	C	1301	1/1	0.99	0.06	160,160,160,160	0
4	CA	A	1304	1/1	0.99	0.08	176,176,176,176	0
4	CA	F	1302	1/1	0.99	0.07	300,300,300,300	0
5	TPP	A	1303	26/26	0.99	0.06	226,226,226,226	0
5	TPP	C	1303	26/26	0.99	0.06	225,225,225,225	0
5	TPP	F	1303	26/26	0.99	0.07	230,230,230,230	0

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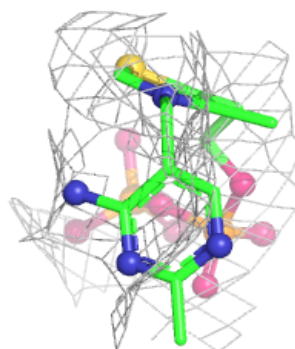
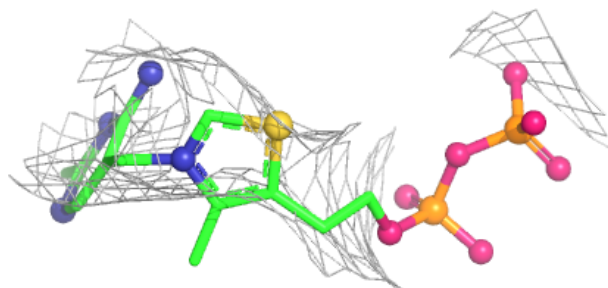
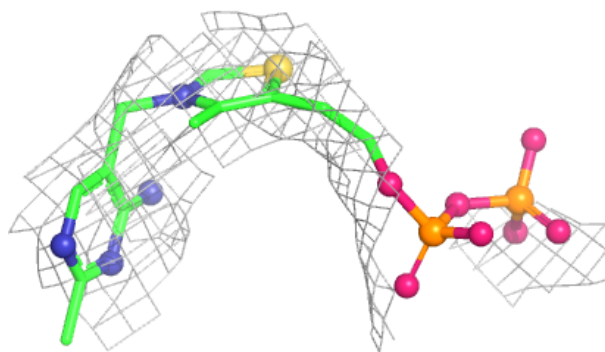
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	E	1302	1/1	1.00	0.04	239,239,239,239	0
3	MG	E	1301	1/1	1.00	0.03	190,190,190,190	0
3	MG	F	1301	1/1	1.00	0.05	119,119,119,119	0
5	TPP	B	1303	26/26	1.00	0.04	216,216,216,216	0
3	MG	A	1301	1/1	1.00	0.01	106,106,106,106	0
5	TPP	D	1303	26/26	1.00	0.04	223,223,223,223	0
5	TPP	E	1303	26/26	1.00	0.05	223,223,223,223	0
3	MG	B	1301	1/1	1.00	0.03	216,216,216,216	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.

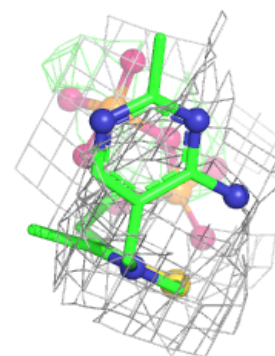
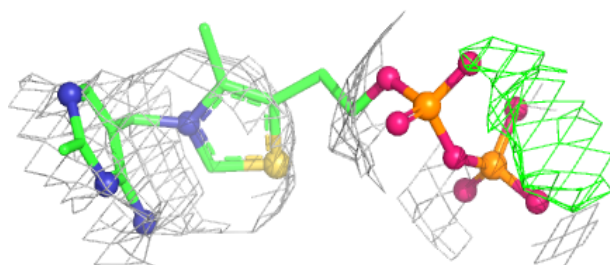
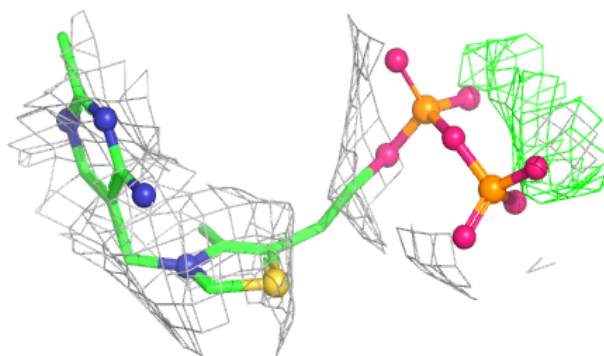
Electron density around TPP A 1303:

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

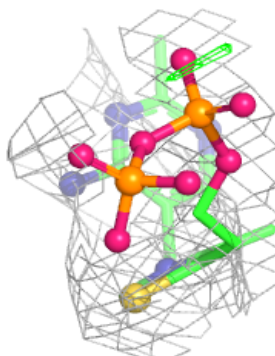
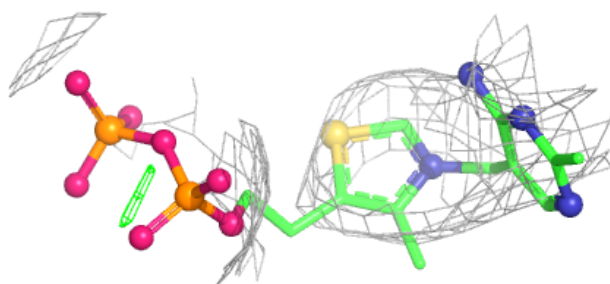
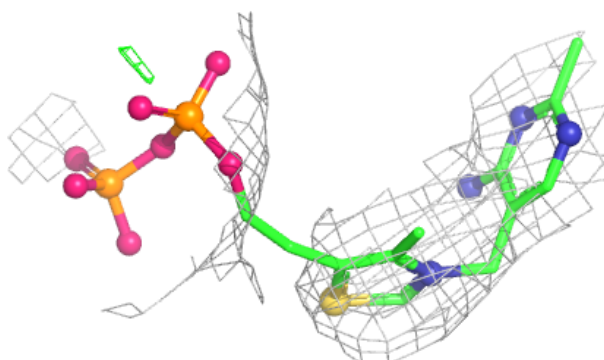


Electron density around TPP C 1303:

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

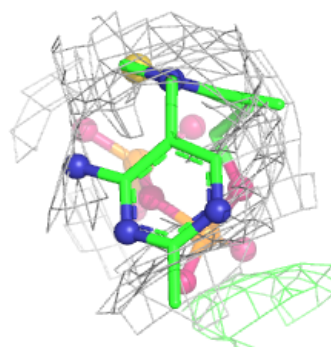
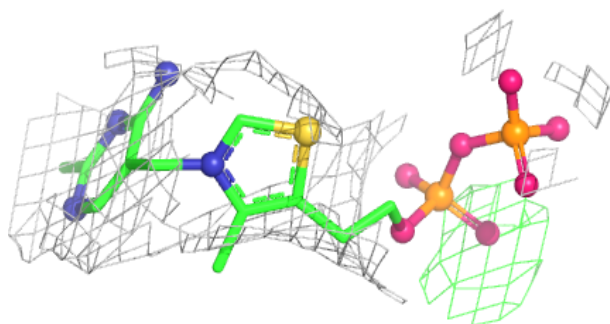
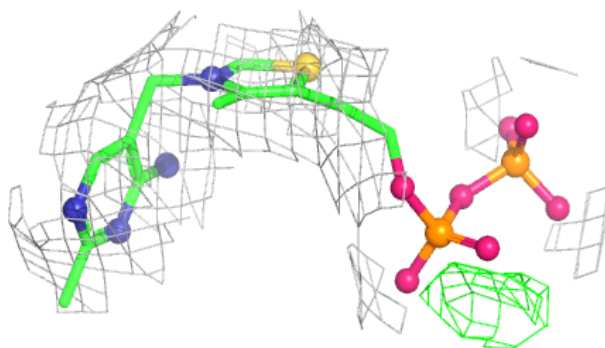
**Electron density around TPP F 1303:**

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

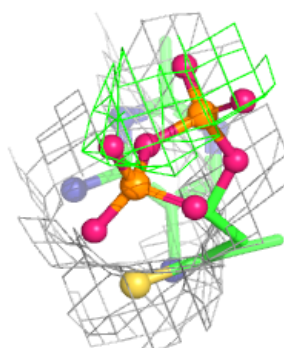
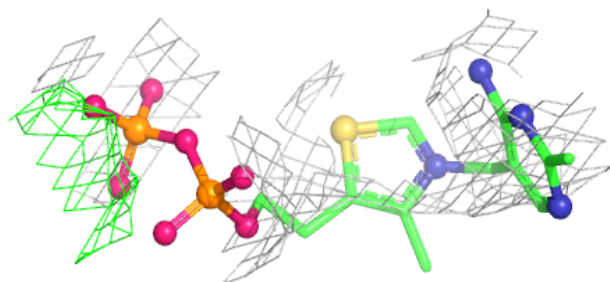
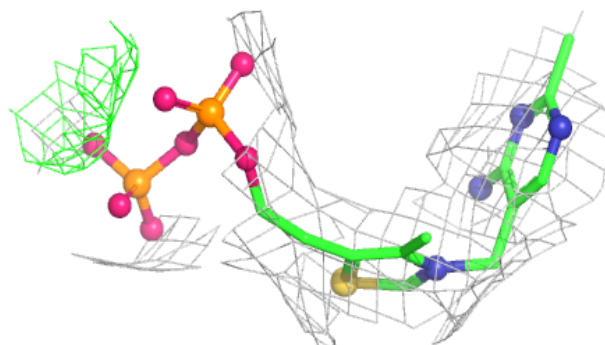


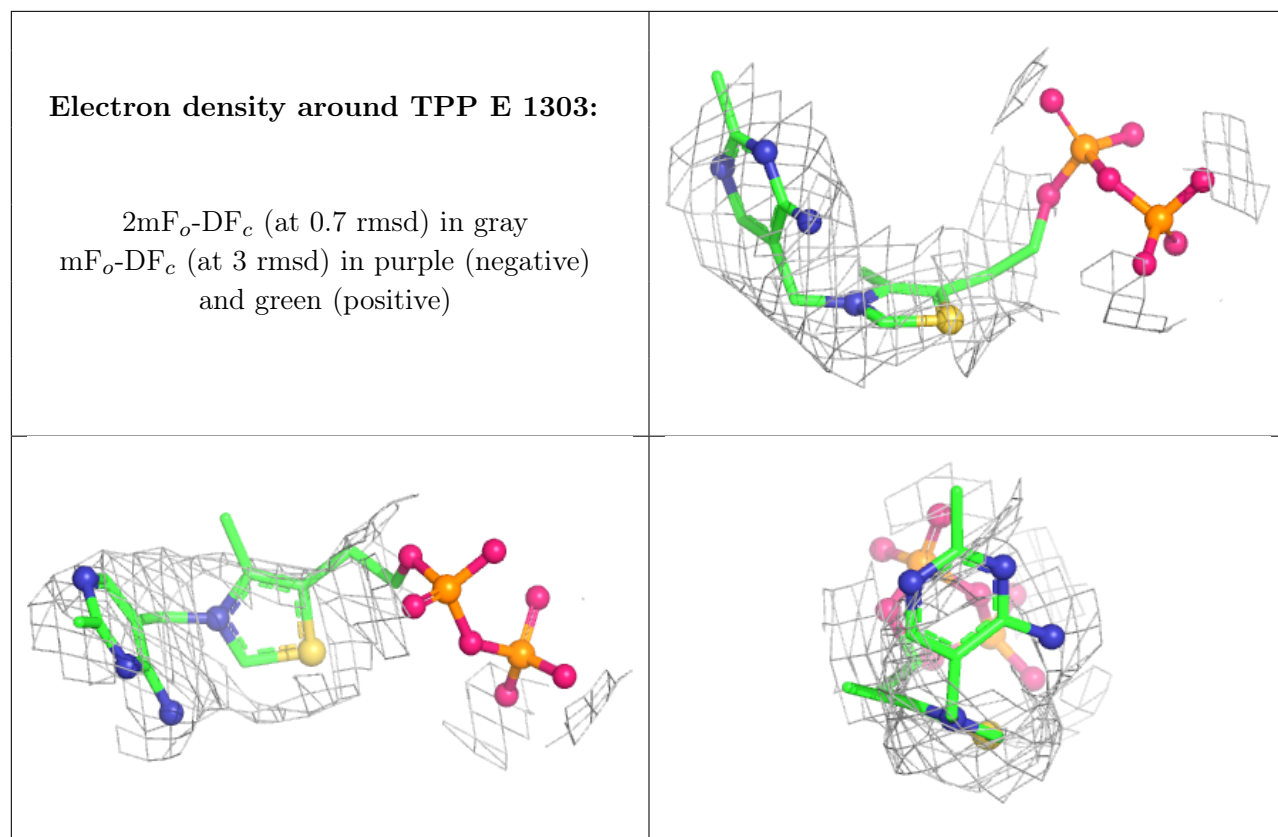
Electron density around TPP B 1303:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.