



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2026 – 03:36 pm BST

PDB ID : 3IZI / pdb_000031zi
Title : Crystal structure of RAD52 N-terminal domain in complex with fragment Z271005800
Authors : Bocquet, N.; Powell, A.J.; Barker, I.A.
Deposited on : 2026-06-30
Resolution : 2.10 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 Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

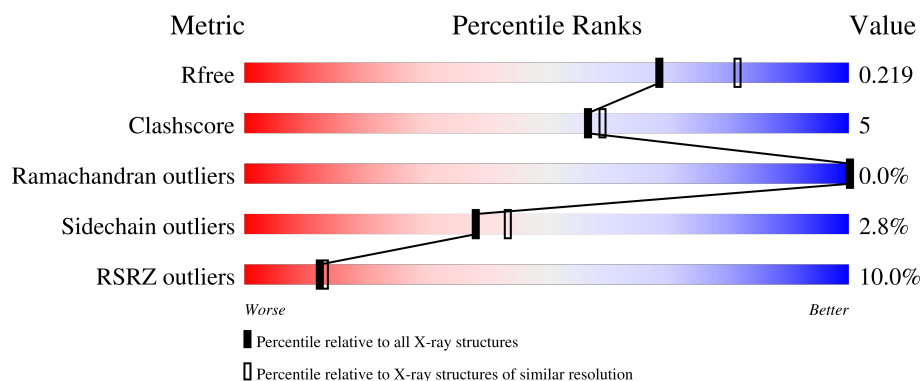
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	215	5% 77% 9% • 13%
1	B	215	6% 80% 6% • 13%
1	C	215	6% 76% 10% • 13%
1	D	215	6% 80% 7% • 12%
1	E	215	4% 80% 7% • 12%

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Mol	Chain	Length	Quality of chain
1	F	215	
1	G	215	
1	H	215	
1	I	215	
1	J	215	
1	K	215	
1	L	215	
1	M	215	
1	N	215	
1	O	215	
1	P	215	
1	Q	215	
1	R	215	
1	S	215	
1	T	215	
1	U	215	
1	V	215	

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
3	EDO	C	304	-	-	X	-
3	EDO	G	305	-	-	X	-
3	EDO	K	302	-	-	X	-
3	EDO	N	306	-	-	X	-
3	EDO	S	305	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35092 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 DNA repair protein RAD52 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	2	0
			1479	922	270	279	8			
1	B	188	Total	C	N	O	S	0	3	0
			1504	938	274	284	8			
1	C	188	Total	C	N	O	S	0	2	0
			1492	929	271	283	9			
1	D	189	Total	C	N	O	S	0	1	0
			1486	925	270	282	9			
1	E	189	Total	C	N	O	S	0	2	0
			1498	933	272	284	9			
1	F	187	Total	C	N	O	S	0	2	0
			1487	926	272	281	8			
1	G	187	Total	C	N	O	S	0	0	0
			1465	913	266	278	8			
1	H	189	Total	C	N	O	S	0	0	0
			1481	924	268	280	9			
1	I	186	Total	C	N	O	S	0	2	0
			1476	919	270	279	8			
1	J	187	Total	C	N	O	S	0	1	0
			1473	917	268	280	8			
1	K	187	Total	C	N	O	S	0	1	0
			1476	920	268	280	8			
1	L	188	Total	C	N	O	S	0	2	0
			1489	926	273	282	8			
1	M	189	Total	C	N	O	S	0	0	0
			1478	921	268	280	9			
1	N	187	Total	C	N	O	S	0	1	0
			1473	919	267	279	8			
1	O	187	Total	C	N	O	S	0	3	0
			1496	933	271	284	8			
1	P	187	Total	C	N	O	S	0	1	0
			1476	920	268	280	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	188	Total	C	N	O	S	0	3	0
			1504	938	274	284	8			
1	R	187	Total	C	N	O	S	0	1	0
			1476	920	268	280	8			
1	S	188	Total	C	N	O	S	0	1	0
			1481	923	269	281	8			
1	T	187	Total	C	N	O	S	0	2	0
			1487	926	272	281	8			
1	U	188	Total	C	N	O	S	0	0	0
			1473	919	267	279	8			
1	V	187	Total	C	N	O	S	0	2	0
			1487	926	272	281	8			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P43351
A	-1	SER	-	expression tag	UNP P43351
A	0	HIS	-	expression tag	UNP P43351
A	102	ALA	LYS	engineered mutation	UNP P43351
A	133	ALA	LYS	engineered mutation	UNP P43351
B	-2	GLY	-	expression tag	UNP P43351
B	-1	SER	-	expression tag	UNP P43351
B	0	HIS	-	expression tag	UNP P43351
B	102	ALA	LYS	engineered mutation	UNP P43351
B	133	ALA	LYS	engineered mutation	UNP P43351
C	-2	GLY	-	expression tag	UNP P43351
C	-1	SER	-	expression tag	UNP P43351
C	0	HIS	-	expression tag	UNP P43351
C	102	ALA	LYS	engineered mutation	UNP P43351
C	133	ALA	LYS	engineered mutation	UNP P43351
D	-2	GLY	-	expression tag	UNP P43351
D	-1	SER	-	expression tag	UNP P43351
D	0	HIS	-	expression tag	UNP P43351
D	102	ALA	LYS	engineered mutation	UNP P43351
D	133	ALA	LYS	engineered mutation	UNP P43351
E	-2	GLY	-	expression tag	UNP P43351
E	-1	SER	-	expression tag	UNP P43351
E	0	HIS	-	expression tag	UNP P43351
E	102	ALA	LYS	engineered mutation	UNP P43351
E	133	ALA	LYS	engineered mutation	UNP P43351
F	-2	GLY	-	expression tag	UNP P43351
F	-1	SER	-	expression tag	UNP P43351

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP P43351
F	102	ALA	LYS	engineered mutation	UNP P43351
F	133	ALA	LYS	engineered mutation	UNP P43351
G	-2	GLY	-	expression tag	UNP P43351
G	-1	SER	-	expression tag	UNP P43351
G	0	HIS	-	expression tag	UNP P43351
G	102	ALA	LYS	engineered mutation	UNP P43351
G	133	ALA	LYS	engineered mutation	UNP P43351
H	-2	GLY	-	expression tag	UNP P43351
H	-1	SER	-	expression tag	UNP P43351
H	0	HIS	-	expression tag	UNP P43351
H	102	ALA	LYS	engineered mutation	UNP P43351
H	133	ALA	LYS	engineered mutation	UNP P43351
I	-2	GLY	-	expression tag	UNP P43351
I	-1	SER	-	expression tag	UNP P43351
I	0	HIS	-	expression tag	UNP P43351
I	102	ALA	LYS	engineered mutation	UNP P43351
I	133	ALA	LYS	engineered mutation	UNP P43351
J	-2	GLY	-	expression tag	UNP P43351
J	-1	SER	-	expression tag	UNP P43351
J	0	HIS	-	expression tag	UNP P43351
J	102	ALA	LYS	engineered mutation	UNP P43351
J	133	ALA	LYS	engineered mutation	UNP P43351
K	-2	GLY	-	expression tag	UNP P43351
K	-1	SER	-	expression tag	UNP P43351
K	0	HIS	-	expression tag	UNP P43351
K	102	ALA	LYS	engineered mutation	UNP P43351
K	133	ALA	LYS	engineered mutation	UNP P43351
L	-2	GLY	-	expression tag	UNP P43351
L	-1	SER	-	expression tag	UNP P43351
L	0	HIS	-	expression tag	UNP P43351
L	102	ALA	LYS	engineered mutation	UNP P43351
L	133	ALA	LYS	engineered mutation	UNP P43351
M	-2	GLY	-	expression tag	UNP P43351
M	-1	SER	-	expression tag	UNP P43351
M	0	HIS	-	expression tag	UNP P43351
M	102	ALA	LYS	engineered mutation	UNP P43351
M	133	ALA	LYS	engineered mutation	UNP P43351
N	-2	GLY	-	expression tag	UNP P43351
N	-1	SER	-	expression tag	UNP P43351
N	0	HIS	-	expression tag	UNP P43351
N	102	ALA	LYS	engineered mutation	UNP P43351

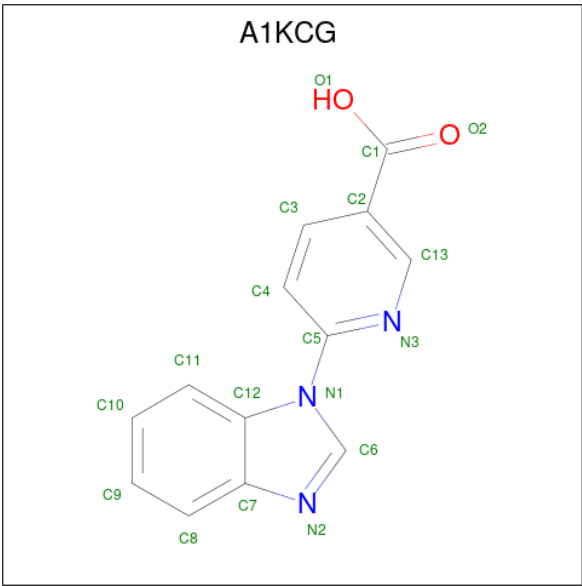
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Chain	Residue	Modelled	Actual	Comment	Reference
N	133	ALA	LYS	engineered mutation	UNP P43351
O	-2	GLY	-	expression tag	UNP P43351
O	-1	SER	-	expression tag	UNP P43351
O	0	HIS	-	expression tag	UNP P43351
O	102	ALA	LYS	engineered mutation	UNP P43351
O	133	ALA	LYS	engineered mutation	UNP P43351
P	-2	GLY	-	expression tag	UNP P43351
P	-1	SER	-	expression tag	UNP P43351
P	0	HIS	-	expression tag	UNP P43351
P	102	ALA	LYS	engineered mutation	UNP P43351
P	133	ALA	LYS	engineered mutation	UNP P43351
Q	-2	GLY	-	expression tag	UNP P43351
Q	-1	SER	-	expression tag	UNP P43351
Q	0	HIS	-	expression tag	UNP P43351
Q	102	ALA	LYS	engineered mutation	UNP P43351
Q	133	ALA	LYS	engineered mutation	UNP P43351
R	-2	GLY	-	expression tag	UNP P43351
R	-1	SER	-	expression tag	UNP P43351
R	0	HIS	-	expression tag	UNP P43351
R	102	ALA	LYS	engineered mutation	UNP P43351
R	133	ALA	LYS	engineered mutation	UNP P43351
S	-2	GLY	-	expression tag	UNP P43351
S	-1	SER	-	expression tag	UNP P43351
S	0	HIS	-	expression tag	UNP P43351
S	102	ALA	LYS	engineered mutation	UNP P43351
S	133	ALA	LYS	engineered mutation	UNP P43351
T	-2	GLY	-	expression tag	UNP P43351
T	-1	SER	-	expression tag	UNP P43351
T	0	HIS	-	expression tag	UNP P43351
T	102	ALA	LYS	engineered mutation	UNP P43351
T	133	ALA	LYS	engineered mutation	UNP P43351
U	-2	GLY	-	expression tag	UNP P43351
U	-1	SER	-	expression tag	UNP P43351
U	0	HIS	-	expression tag	UNP P43351
U	102	ALA	LYS	engineered mutation	UNP P43351
U	133	ALA	LYS	engineered mutation	UNP P43351
V	-2	GLY	-	expression tag	UNP P43351
V	-1	SER	-	expression tag	UNP P43351
V	0	HIS	-	expression tag	UNP P43351
V	102	ALA	LYS	engineered mutation	UNP P43351
V	133	ALA	LYS	engineered mutation	UNP P43351

- Molecule 2 is 6-(benzimidazol-1-yl)pyridine-3-carboxylic acid (CCD ID: A1KCG) (formula:

C₁₃H₉N₃O₂) (labeled as "Ligand of Interest" by depositor).



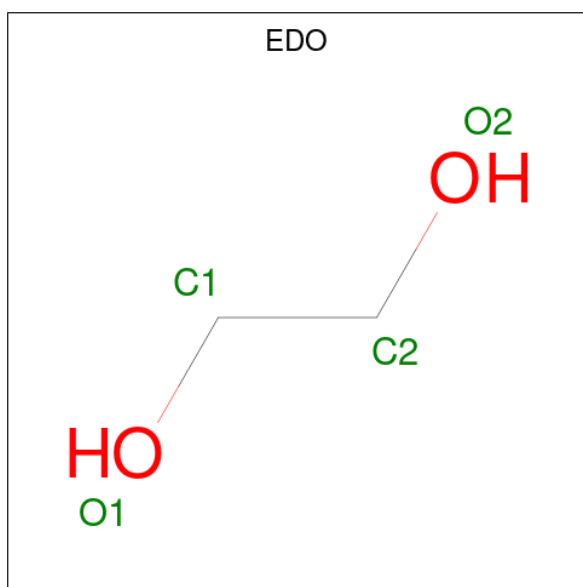
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	13	3	2		
2	B	1	Total	C	N	O	0	0
			18	13	3	2		
2	B	1	Total	C	N	O	0	0
			18	13	3	2		
2	C	1	Total	C	N	O	0	0
			18	13	3	2		
2	C	1	Total	C	N	O	0	0
			18	13	3	2		
2	D	1	Total	C	N	O	0	0
			18	13	3	2		
2	D	1	Total	C	N	O	0	0
			18	13	3	2		
2	E	1	Total	C	N	O	0	0
			18	13	3	2		
2	F	1	Total	C	N	O	0	0
			18	13	3	2		
2	F	1	Total	C	N	O	0	0
			18	13	3	2		
2	G	1	Total	C	N	O	0	0
			18	13	3	2		
2	G	1	Total	C	N	O	0	0
			18	13	3	2		
2	H	1	Total	C	N	O	0	0
			18	13	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	K	1	Total	C	N	O	0	0
			18	13	3	2		
2	L	1	Total	C	N	O	0	0
			18	13	3	2		
2	L	1	Total	C	N	O	0	0
			18	13	3	2		
2	M	1	Total	C	N	O	0	0
			18	13	3	2		
2	N	1	Total	C	N	O	0	0
			18	13	3	2		
2	O	1	Total	C	N	O	0	0
			18	13	3	2		
2	P	1	Total	C	N	O	0	0
			18	13	3	2		
2	Q	1	Total	C	N	O	0	0
			18	13	3	2		
2	Q	1	Total	C	N	O	0	0
			18	13	3	2		
2	R	1	Total	C	N	O	0	0
			18	13	3	2		
2	R	1	Total	C	N	O	0	0
			18	13	3	2		
2	S	1	Total	C	N	O	0	0
			18	13	3	2		
2	S	1	Total	C	N	O	0	0
			18	13	3	2		
2	T	1	Total	C	N	O	0	0
			18	13	3	2		
2	U	1	Total	C	N	O	0	0
			18	13	3	2		
2	V	1	Total	C	N	O	0	0
			18	13	3	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	N	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	N	1	Total 4	C 2	O 2	0	0
3	N	1	Total 4	C 2	O 2	0	0
3	N	1	Total 4	C 2	O 2	0	0
3	N	1	Total 4	C 2	O 2	0	0
3	O	1	Total 4	C 2	O 2	0	0
3	O	1	Total 4	C 2	O 2	0	0
3	O	1	Total 4	C 2	O 2	0	0
3	P	1	Total 4	C 2	O 2	0	0
3	P	1	Total 4	C 2	O 2	0	0
3	P	1	Total 4	C 2	O 2	0	0
3	P	1	Total 4	C 2	O 2	0	0
3	P	1	Total 4	C 2	O 2	0	0
3	P	1	Total 4	C 2	O 2	0	0
3	Q	1	Total 4	C 2	O 2	0	0
3	Q	1	Total 4	C 2	O 2	0	0
3	Q	1	Total 4	C 2	O 2	0	0
3	Q	1	Total 4	C 2	O 2	0	0
3	R	1	Total 4	C 2	O 2	0	0
3	R	1	Total 4	C 2	O 2	0	0
3	R	1	Total 4	C 2	O 2	0	0
3	R	1	Total 4	C 2	O 2	0	0
3	R	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	R	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	T	1	Total C O 4 2 2	0	0
3	T	1	Total C O 4 2 2	0	0
3	T	1	Total C O 4 2 2	0	0
3	T	1	Total C O 4 2 2	0	0
3	U	1	Total C O 4 2 2	0	0
3	U	1	Total C O 4 2 2	0	0
3	V	1	Total C O 4 2 2	0	0
3	V	1	Total C O 4 2 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0
4	O	1	Total Mg 1 1	0	0
4	Q	1	Total Mg 1 1	0	0
4	R	1	Total Mg 1 1	0	0
4	V	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	2	Total	Cl	0	0
			2	2		
5	C	2	Total	Cl	0	0
			2	2		
5	D	1	Total	Cl	0	0
			1	1		
5	E	2	Total	Cl	0	0
			2	2		
5	F	1	Total	Cl	0	0
			1	1		
5	G	1	Total	Cl	0	0
			1	1		
5	H	1	Total	Cl	0	0
			1	1		
5	L	2	Total	Cl	0	0
			2	2		
5	M	1	Total	Cl	0	0
			1	1		
5	N	1	Total	Cl	0	0
			1	1		
5	O	3	Total	Cl	0	0
			3	3		
5	P	2	Total	Cl	0	0
			2	2		
5	Q	1	Total	Cl	0	0
			1	1		
5	R	1	Total	Cl	0	0
			1	1		
5	S	1	Total	Cl	0	0
			1	1		
5	T	1	Total	Cl	0	0
			1	1		
5	U	1	Total	Cl	0	0
			1	1		
5	V	1	Total	Cl	0	0
			1	1		

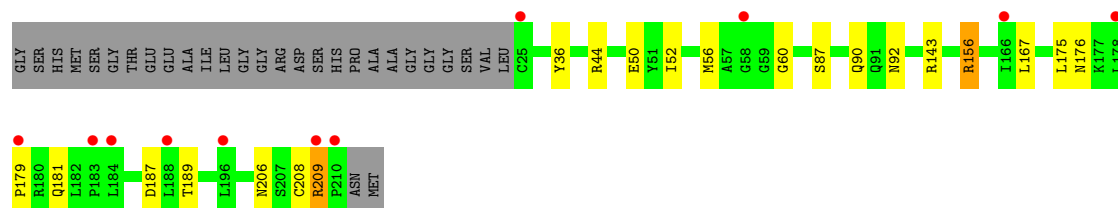
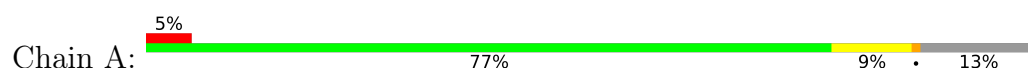
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	82	Total O 82 82	0	0
6	B	91	Total O 91 91	0	0
6	C	102	Total O 102 102	0	0
6	D	86	Total O 86 86	0	0
6	E	80	Total O 80 80	0	0
6	F	77	Total O 77 77	0	0
6	G	50	Total O 50 50	0	0
6	H	49	Total O 49 49	0	0
6	I	22	Total O 22 22	0	0
6	J	34	Total O 34 34	0	0
6	K	31	Total O 31 31	0	0
6	L	78	Total O 78 78	0	0
6	M	77	Total O 77 77	0	0
6	N	81	Total O 81 81	0	0
6	O	84	Total O 84 84	0	0
6	P	98	Total O 98 98	0	0
6	Q	94	Total O 94 94	0	0
6	R	92	Total O 92 92	0	0
6	S	75	Total O 75 75	0	0
6	T	80	Total O 80 80	0	0
6	U	88	Total O 88 88	0	0
6	V	76	Total O 76 76	0	0

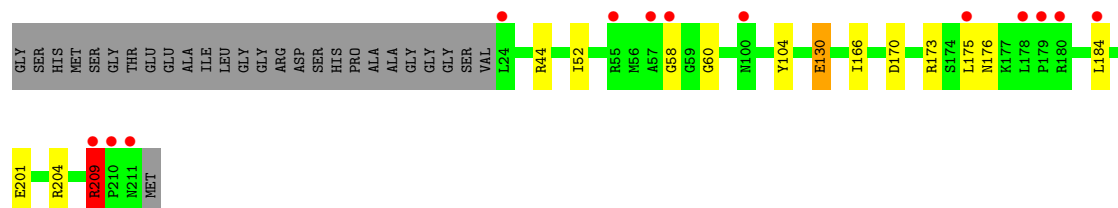
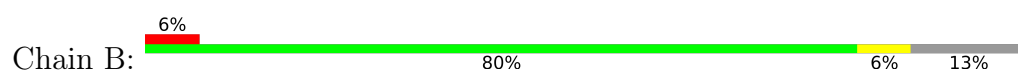
3 Residue-property plots [i](#)

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

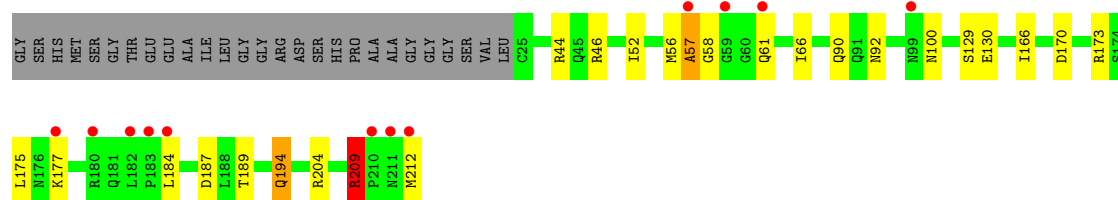
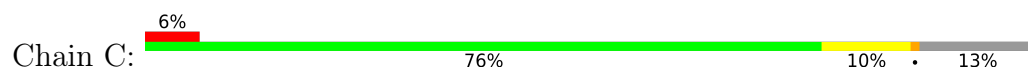
- Molecule 1: DNA repair protein RAD52 homolog



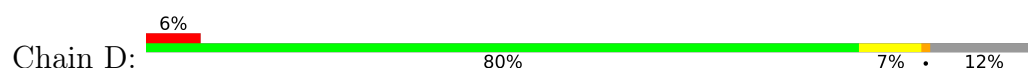
- Molecule 1: DNA repair protein RAD52 homolog

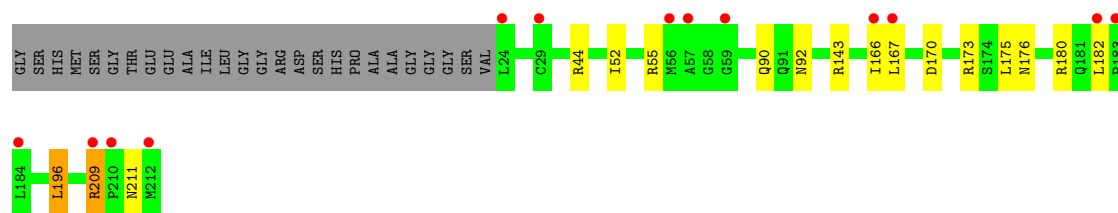


- Molecule 1: DNA repair protein RAD52 homolog

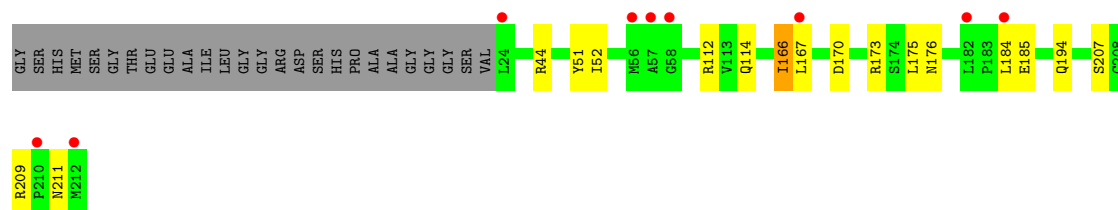
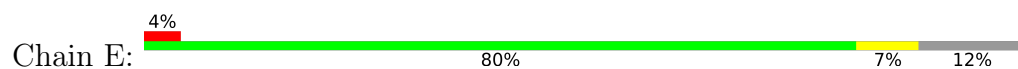


- Molecule 1: DNA repair protein RAD52 homolog

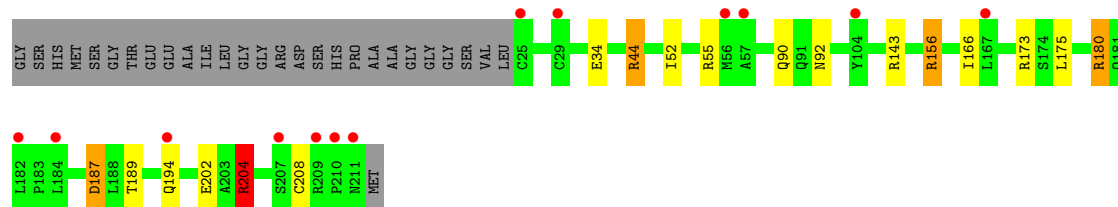
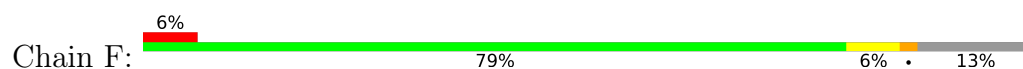




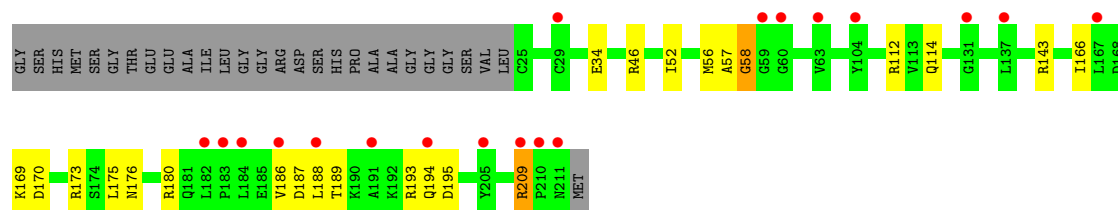
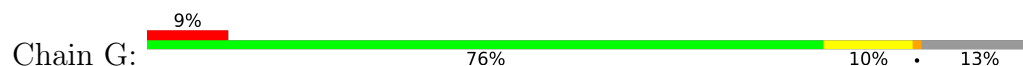
- Molecule 1: DNA repair protein RAD52 homolog



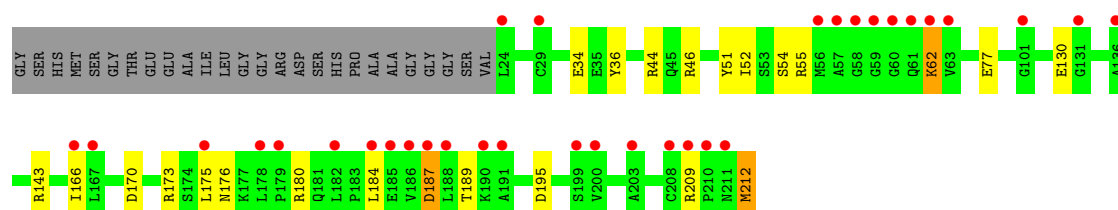
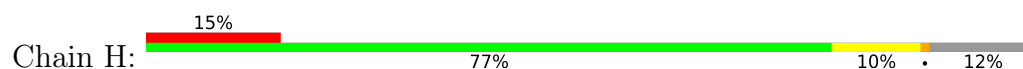
- Molecule 1: DNA repair protein RAD52 homolog



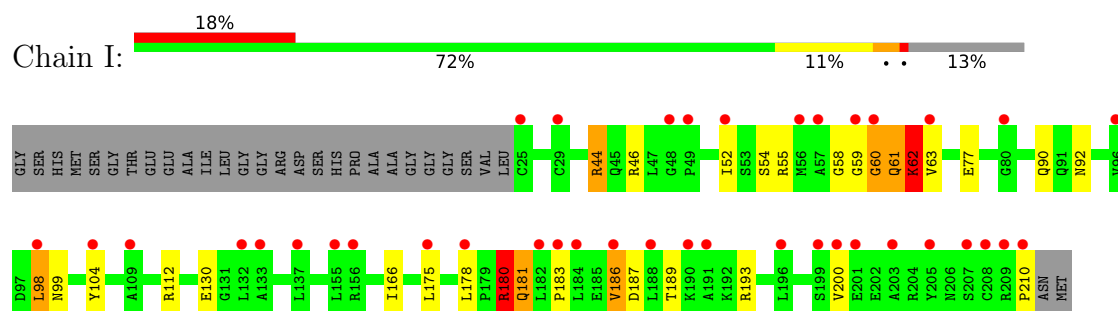
- Molecule 1: DNA repair protein RAD52 homolog



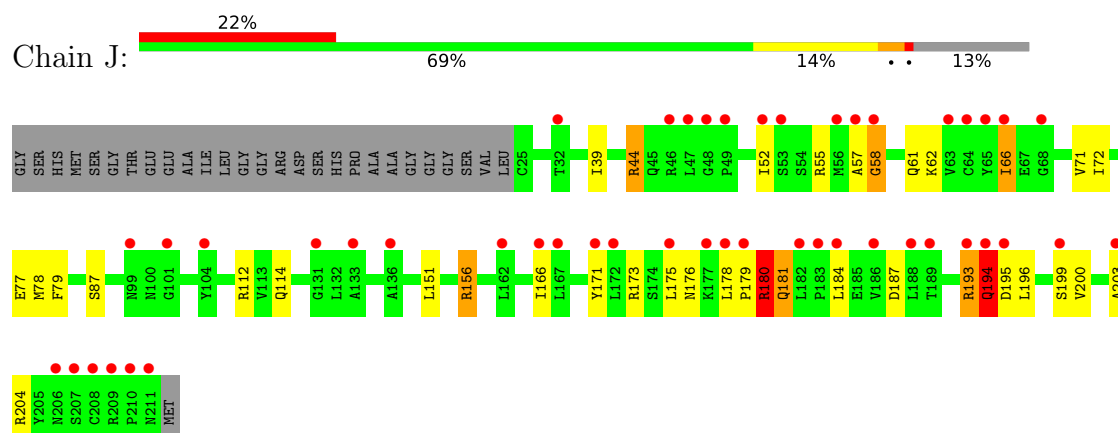
- Molecule 1: DNA repair protein RAD52 homolog



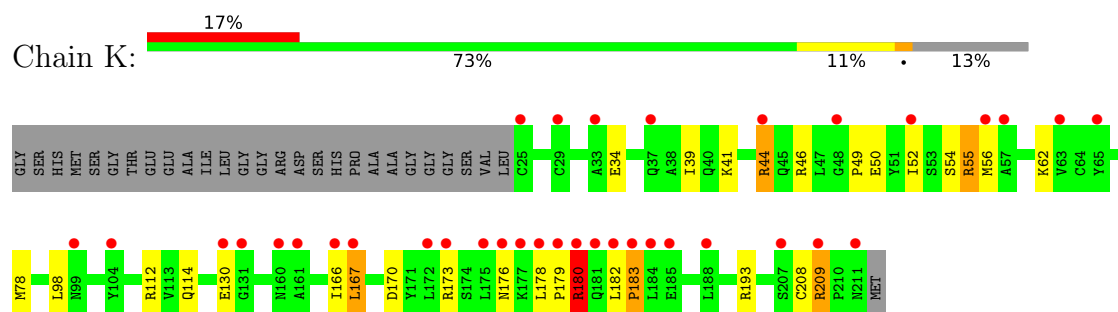
• Molecule 1: DNA repair protein RAD52 homolog



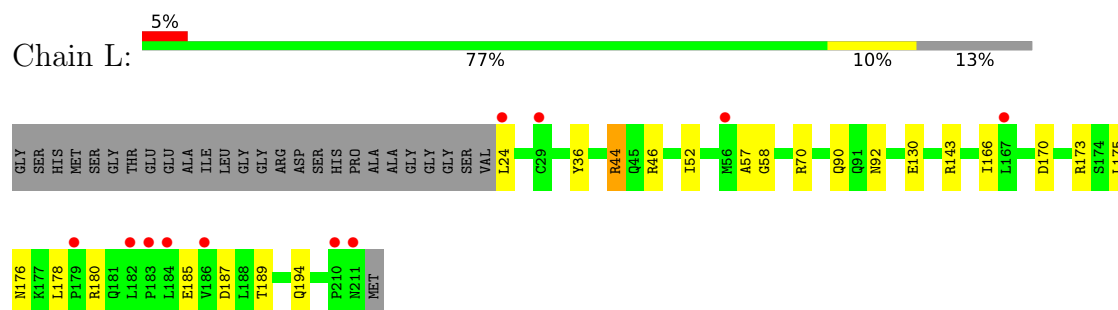
• Molecule 1: DNA repair protein RAD52 homolog



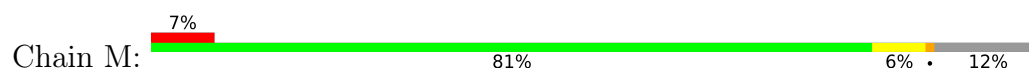
• Molecule 1: DNA repair protein RAD52 homolog

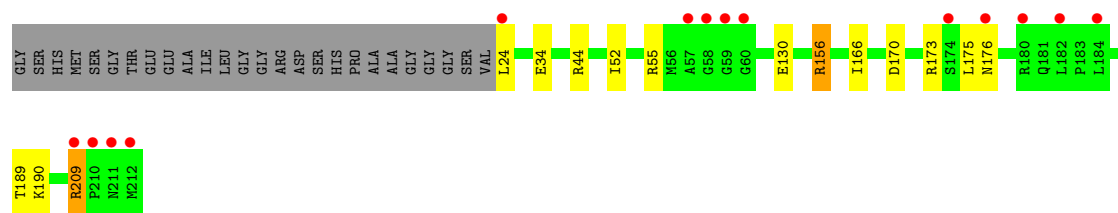


• Molecule 1: DNA repair protein RAD52 homolog

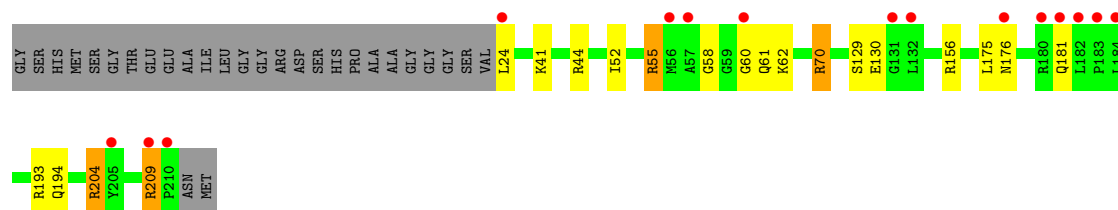
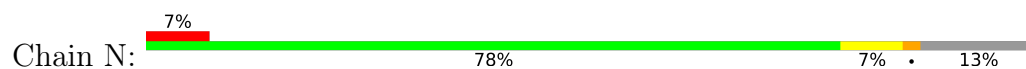


• Molecule 1: DNA repair protein RAD52 homolog

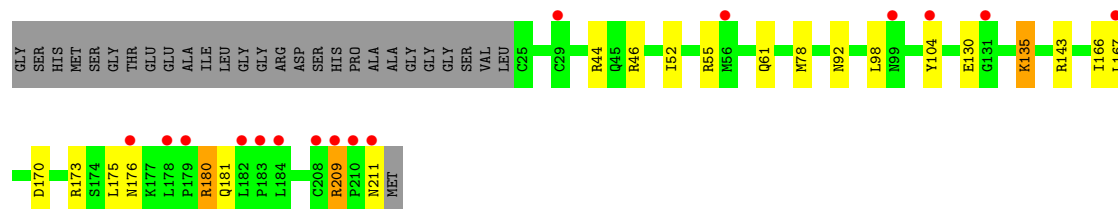
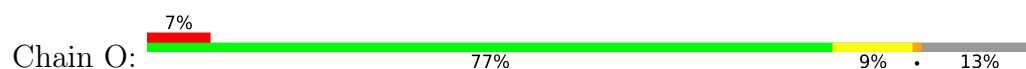




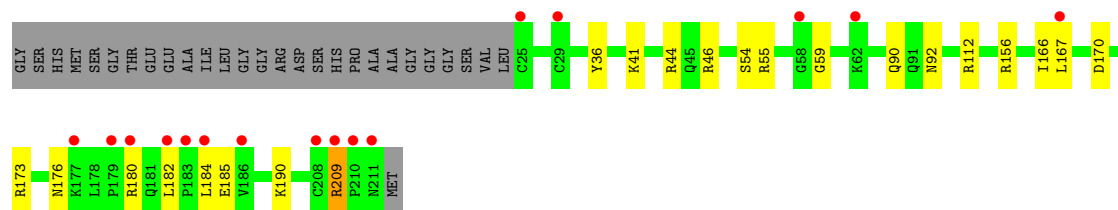
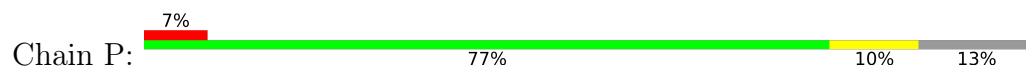
- Molecule 1: DNA repair protein RAD52 homolog



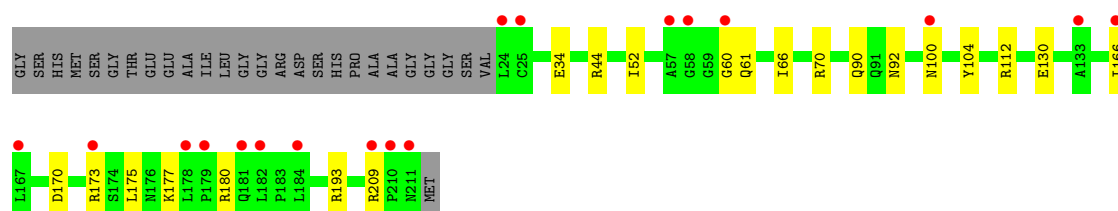
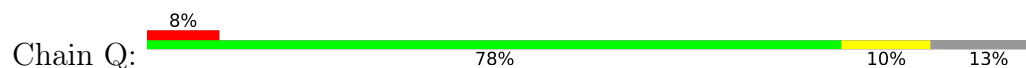
- Molecule 1: DNA repair protein RAD52 homolog



- Molecule 1: DNA repair protein RAD52 homolog

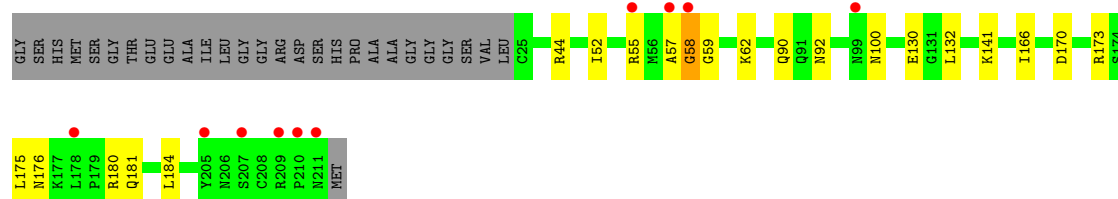


- Molecule 1: DNA repair protein RAD52 homolog



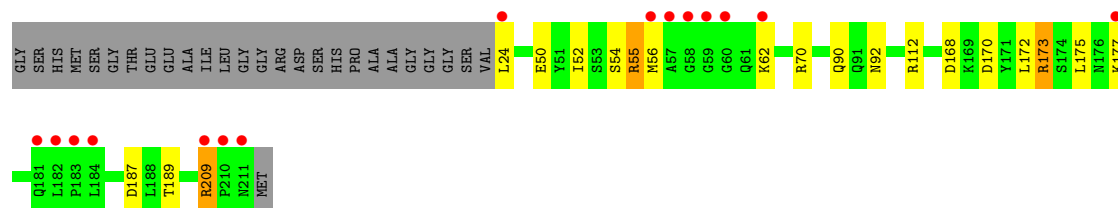
- Molecule 1: DNA repair protein RAD52 homolog

Chain R: 



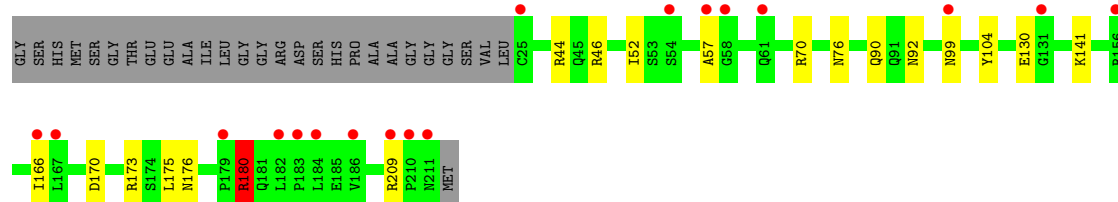
- Molecule 1: DNA repair protein RAD52 homolog

Chain S: 



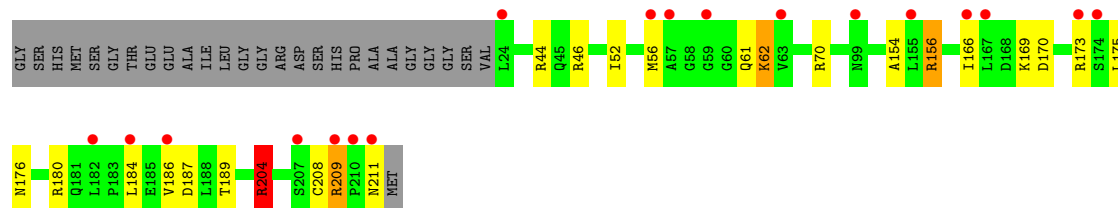
- Molecule 1: DNA repair protein RAD52 homolog

Chain T: 



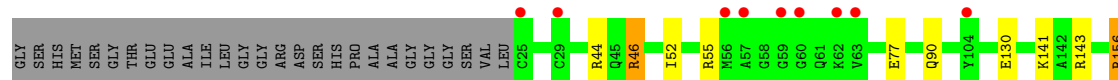
- Molecule 1: DNA repair protein RAD52 homolog

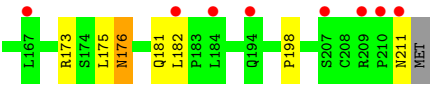
Chain U: 



- Molecule 1: DNA repair protein RAD52 homolog

Chain V: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	144.87Å 147.19Å 251.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.88 – 2.10 79.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (79.88-2.10) 100.0 (79.88-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.182 , 0.210 0.193 , 0.219	Depositor DCC
R_{free} test set	21080 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	35092	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: EDO, CL, MG, A1KCG

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	0.71	1/1504 (0.1%)	1.08	6/2024 (0.3%)
1	B	0.72	0/1530	1.07	4/2060 (0.2%)
1	C	0.70	0/1517	1.16	7/2042 (0.3%)
1	D	0.72	0/1511	1.05	2/2034 (0.1%)
1	E	0.72	0/1523	1.06	3/2050 (0.1%)
1	F	0.76	1/1512 (0.1%)	1.08	4/2035 (0.2%)
1	G	0.70	0/1490	1.02	2/2006 (0.1%)
1	H	0.66	0/1506	1.06	4/2027 (0.2%)
1	I	0.68	1/1501 (0.1%)	1.12	10/2020 (0.5%)
1	J	0.71	0/1498	1.64	11/2017 (0.5%)
1	K	0.75	1/1501 (0.1%)	1.13	6/2021 (0.3%)
1	L	0.71	1/1514 (0.1%)	1.05	4/2038 (0.2%)
1	M	0.69	0/1503	1.03	1/2023 (0.0%)
1	N	0.69	0/1498	1.10	8/2017 (0.4%)
1	O	0.70	0/1522	1.06	4/2050 (0.2%)
1	P	0.79	3/1501 (0.2%)	1.12	8/2021 (0.4%)
1	Q	0.84	3/1530 (0.2%)	1.03	2/2060 (0.1%)
1	R	0.72	0/1501	1.08	4/2021 (0.2%)
1	S	0.73	1/1506 (0.1%)	1.14	9/2028 (0.4%)
1	T	0.66	0/1512	1.07	6/2035 (0.3%)
1	U	0.69	0/1498	1.17	10/2017 (0.5%)
1	V	0.68	0/1512	1.08	5/2035 (0.2%)
All	All	0.72	12/33190 (0.0%)	1.12	120/44681 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
1	D	0	4
1	E	0	1
1	F	0	6
1	G	0	4
1	H	0	4
1	I	0	4
1	J	0	6
1	K	0	6
1	L	0	4
1	M	0	4
1	N	0	4
1	O	0	4
1	P	0	3
1	Q	0	3
1	R	0	2
1	S	0	3
1	T	0	4
1	U	0	6
1	V	0	5
All	All	0	85

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	60	GLY	C-N	14.56	1.54	1.33
1	Q	61	GLN	C-N	9.97	1.47	1.33
1	P	209	ARG	C-N	-8.64	1.22	1.33
1	S	173	ARG	C-N	-7.89	1.23	1.33
1	A	208	CYS	C-N	7.33	1.45	1.33
1	F	208	CYS	C-N	6.67	1.54	1.33
1	K	209	ARG	C-N	-6.05	1.25	1.33
1	P	112	ARG	NE-CZ	5.33	1.39	1.33
1	P	156	ARG	NE-CZ	5.22	1.38	1.33
1	I	44	ARG	NE-CZ	-5.20	1.27	1.33
1	L	44	ARG	NE-CZ	-5.16	1.27	1.33
1	Q	112	ARG	NE-CZ	5.07	1.38	1.33

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	194	GLN	CB-CA-C	-25.78	74.48	112.11
1	J	194	GLN	N-CA-C	25.07	145.12	111.28
1	J	194	GLN	CA-C-N	24.83	156.63	120.38
1	J	194	GLN	C-N-CA	24.83	156.63	120.38
1	J	195	ASP	N-CA-C	-23.01	82.30	111.75
1	C	57	ALA	N-CA-C	-13.71	93.55	110.41
1	A	209	ARG	O-C-N	-13.25	106.56	121.66
1	C	57	ALA	CB-CA-C	12.90	138.31	110.19
1	S	56	MET	O-C-N	11.87	138.28	123.21
1	U	209	ARG	O-C-N	-11.84	109.05	121.60
1	R	59	GLY	N-CA-C	11.38	131.12	115.30
1	K	209	ARG	O-C-N	-10.79	108.82	121.12
1	T	57	ALA	N-CA-C	-10.42	97.60	110.41
1	T	57	ALA	CB-CA-C	10.31	132.66	110.19
1	U	204	ARG	CD-NE-CZ	9.81	138.14	124.40
1	S	172	LEU	O-C-N	9.09	131.75	122.12
1	P	209	ARG	O-C-N	-7.78	111.05	121.64
1	V	46	ARG	CA-CB-CG	7.58	129.27	114.10
1	N	156	ARG	CA-CB-CG	7.58	129.26	114.10
1	D	44	ARG	CG-CD-NE	-7.57	95.36	112.00
1	N	70	ARG	NE-CZ-NH2	7.44	125.90	119.20
1	V	181	GLN	CB-CA-C	7.42	122.62	110.22
1	N	70	ARG	NE-CZ-NH1	-7.41	114.09	121.50
1	O	44	ARG	CG-CD-NE	-7.40	95.72	112.00
1	S	56	MET	CA-C-N	-7.32	109.87	121.87
1	S	56	MET	C-N-CA	-7.32	109.87	121.87
1	I	62	LYS	N-CA-C	-7.26	95.33	110.80
1	Q	44	ARG	CG-CD-NE	-7.20	96.17	112.00
1	V	44	ARG	CG-CD-NE	-7.02	96.56	112.00
1	C	58	GLY	N-CA-C	-6.96	96.69	113.18
1	I	60	GLY	N-CA-C	-6.86	96.93	113.18
1	U	44	ARG	CG-CD-NE	-6.85	96.93	112.00
1	T	44	ARG	CG-CD-NE	-6.81	97.01	112.00
1	P	185	GLU	CB-CG-CD	-6.77	101.09	112.60
1	U	208	CYS	CA-C-N	-6.76	110.20	121.03
1	U	208	CYS	C-N-CA	-6.76	110.20	121.03
1	P	44	ARG	CG-CD-NE	-6.76	97.12	112.00
1	R	181	GLN	CB-CA-C	6.72	121.08	110.19
1	H	44	ARG	CG-CD-NE	-6.69	97.28	112.00
1	P	59	GLY	N-CA-C	-6.67	105.90	115.64
1	G	58	GLY	N-CA-C	-6.58	97.59	113.18
1	E	44	ARG	CG-CD-NE	-6.55	97.60	112.00
1	N	44	ARG	CG-CD-NE	-6.49	97.71	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	204	ARG	NH1-CZ-NH2	6.47	127.71	119.30
1	K	176	ASN	CB-CA-C	6.47	123.01	110.46
1	B	44	ARG	CG-CD-NE	-6.46	97.80	112.00
1	I	180	ARG	N-CA-C	-6.45	100.70	110.70
1	S	177	LYS	CB-CG-CD	6.43	126.09	111.30
1	C	44	ARG	CG-CD-NE	-6.40	97.92	112.00
1	I	98	LEU	CB-CG-CD1	6.39	129.87	110.70
1	I	210	PRO	N-CA-CB	-6.32	96.05	103.00
1	F	204	ARG	CD-NE-CZ	6.27	133.17	124.40
1	O	44	ARG	CB-CA-C	-6.26	97.23	110.31
1	O	135	LYS	CG-CD-CE	6.24	125.66	111.30
1	L	44	ARG	CB-CA-C	-6.24	97.27	110.31
1	N	58	GLY	N-CA-C	-6.23	98.41	113.18
1	S	54	SER	O-C-N	6.23	130.87	123.33
1	T	44	ARG	CB-CA-C	-6.22	97.30	110.31
1	D	44	ARG	CB-CA-C	-6.21	97.32	110.31
1	P	209	ARG	CA-C-N	6.20	126.66	120.52
1	P	209	ARG	C-N-CA	6.20	126.66	120.52
1	E	44	ARG	CB-CA-C	-6.17	97.42	110.31
1	V	44	ARG	CB-CA-C	-6.15	97.47	110.31
1	N	204	ARG	CD-NE-CZ	6.14	133.00	124.40
1	T	130	GLU	CB-CG-CD	6.11	122.98	112.60
1	J	44	ARG	CB-CA-C	-6.08	97.60	110.31
1	J	58	GLY	N-CA-C	-6.05	98.83	113.18
1	Q	44	ARG	CB-CA-C	-6.05	97.66	110.31
1	U	208	CYS	O-C-N	6.04	129.73	122.85
1	A	44	ARG	CG-CD-NE	-6.00	98.80	112.00
1	I	44	ARG	CB-CA-C	-5.98	97.80	110.31
1	P	44	ARG	CB-CA-C	-5.97	97.83	110.31
1	F	204	ARG	NE-CZ-NH1	-5.95	115.55	121.50
1	I	44	ARG	CB-CG-CD	5.93	124.94	111.30
1	U	44	ARG	CB-CA-C	-5.93	97.92	110.31
1	H	44	ARG	CB-CA-C	-5.91	97.95	110.31
1	N	204	ARG	NH1-CZ-NH2	5.90	126.97	119.30
1	K	44	ARG	CB-CA-C	-5.90	97.98	110.31
1	V	181	GLN	N-CA-CB	-5.86	100.33	110.17
1	B	44	ARG	CB-CA-C	-5.82	98.14	110.31
1	A	44	ARG	CB-CA-C	-5.80	98.20	110.31
1	C	44	ARG	CB-CA-C	-5.76	98.26	110.31
1	H	130	GLU	CB-CG-CD	5.74	122.35	112.60
1	J	180	ARG	N-CA-C	-5.70	100.70	109.76
1	C	177	LYS	CB-CG-CD	5.69	124.38	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	63	VAL	N-CA-C	-5.68	99.70	107.99
1	N	44	ARG	CB-CA-C	-5.66	98.48	110.31
1	U	204	ARG	NE-CZ-NH2	-5.65	114.12	119.20
1	U	154	ALA	O-C-N	-5.62	115.97	122.03
1	C	194	GLN	CB-CA-C	5.58	121.24	109.79
1	J	62	LYS	N-CA-C	-5.53	99.78	108.63
1	L	178	LEU	O-C-N	-5.50	115.37	121.53
1	J	66	ILE	CA-CB-CG1	5.47	119.70	110.40
1	B	130	GLU	CA-CB-CG	5.45	124.99	114.10
1	I	130	GLU	CB-CG-CD	5.44	121.85	112.60
1	A	206	ASN	CB-CG-ND2	5.43	124.55	116.40
1	S	172	LEU	CA-C-N	-5.34	112.20	120.31
1	S	172	LEU	C-N-CA	-5.34	112.20	120.31
1	T	180	ARG	CA-CB-CG	5.34	124.77	114.10
1	L	130	GLU	CB-CG-CD	5.32	121.65	112.60
1	B	201	GLU	CB-CG-CD	5.32	121.64	112.60
1	K	130	GLU	CB-CG-CD	5.30	121.61	112.60
1	K	183	PRO	N-CA-C	-5.25	101.66	112.47
1	R	130	GLU	CB-CG-CD	5.22	121.48	112.60
1	J	187	ASP	CA-CB-CG	5.21	117.81	112.60
1	O	143	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	S	168	ASP	CA-CB-CG	5.20	117.80	112.60
1	M	130	GLU	CB-CG-CD	5.19	121.42	112.60
1	R	58	GLY	N-CA-C	-5.16	100.94	113.18
1	U	156	ARG	CB-CA-C	-5.16	100.44	110.46
1	G	195	ASP	CA-CB-CG	5.16	117.76	112.60
1	E	207	SER	CA-CB-OG	5.14	121.39	111.10
1	K	50	GLU	CB-CG-CD	5.11	121.29	112.60
1	I	62	LYS	CB-CA-C	5.10	120.56	110.42
1	A	208	CYS	CA-C-N	-5.08	112.73	120.86
1	A	208	CYS	C-N-CA	-5.08	112.73	120.86
1	H	187	ASP	CA-CB-CG	5.08	117.67	112.60
1	P	180	ARG	CB-CA-C	5.01	118.22	109.65
1	L	44	ARG	CB-CG-CD	5.01	122.82	111.30
1	F	187	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (85) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ARG	Sidechain
1	A	156[A]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	209	ARG	Sidechain,Mainchain
1	B	204	ARG	Sidechain
1	B	209	ARG	Sidechain
1	C	209	ARG	Sidechain
1	C	46	ARG	Sidechain
1	D	143	ARG	Sidechain
1	D	180	ARG	Sidechain
1	D	209	ARG	Sidechain
1	D	55	ARG	Sidechain
1	E	209	ARG	Sidechain
1	F	143	ARG	Sidechain
1	F	156[A]	ARG	Sidechain
1	F	180	ARG	Sidechain
1	F	204	ARG	Sidechain
1	F	44	ARG	Sidechain
1	F	55	ARG	Sidechain
1	G	143	ARG	Sidechain
1	G	180	ARG	Sidechain
1	G	209	ARG	Sidechain
1	G	46	ARG	Sidechain
1	H	143	ARG	Sidechain
1	H	180	ARG	Sidechain
1	H	46	ARG	Sidechain
1	H	55	ARG	Sidechain
1	I	180	ARG	Sidechain
1	I	193	ARG	Sidechain
1	I	46	ARG	Sidechain
1	I	55	ARG	Sidechain
1	J	156	ARG	Sidechain
1	J	173	ARG	Sidechain
1	J	180	ARG	Sidechain
1	J	193	ARG	Sidechain
1	J	194	GLN	Peptide
1	J	55	ARG	Sidechain
1	K	180	ARG	Sidechain
1	K	208	CYS	Mainchain
1	K	209	ARG	Sidechain,Mainchain
1	K	46	ARG	Sidechain
1	K	55	ARG	Sidechain
1	L	143	ARG	Sidechain
1	L	180	ARG	Sidechain
1	L	46	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	L	70	ARG	Sidechain
1	M	156	ARG	Sidechain
1	M	209	ARG	Sidechain
1	M	44	ARG	Sidechain
1	M	55	ARG	Sidechain
1	N	193	ARG	Sidechain
1	N	209	ARG	Sidechain
1	N	55	ARG	Sidechain
1	N	70	ARG	Sidechain
1	O	180	ARG	Sidechain
1	O	209	ARG	Sidechain
1	O	46	ARG	Sidechain
1	O	55	ARG	Sidechain
1	P	209	ARG	Sidechain
1	P	46	ARG	Sidechain
1	P	55	ARG	Sidechain
1	Q	180	ARG	Sidechain
1	Q	193	ARG	Sidechain
1	Q	209	ARG	Sidechain
1	R	44	ARG	Sidechain
1	R	55	ARG	Sidechain
1	S	209	ARG	Sidechain
1	S	55	ARG	Sidechain
1	S	70	ARG	Sidechain
1	T	180	ARG	Sidechain
1	T	209	ARG	Sidechain
1	T	46	ARG	Sidechain
1	T	70	ARG	Sidechain
1	U	156	ARG	Sidechain
1	U	180	ARG	Sidechain
1	U	204	ARG	Sidechain
1	U	209	ARG	Mainchain
1	U	46	ARG	Sidechain
1	U	70	ARG	Sidechain
1	V	143	ARG	Sidechain
1	V	156[A]	ARG	Sidechain
1	V	173	ARG	Sidechain
1	V	46	ARG	Sidechain
1	V	55	ARG	Sidechain

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	1479	0	1454	14	0
1	B	1504	0	1470	7	0
1	C	1492	0	1462	23	0
1	D	1486	0	1450	10	0
1	E	1498	0	1466	9	0
1	F	1487	0	1460	20	0
1	G	1465	0	1434	20	2
1	H	1481	0	1454	17	0
1	I	1476	0	1445	30	0
1	J	1473	0	1438	36	0
1	K	1476	0	1448	28	0
1	L	1489	0	1453	16	0
1	M	1478	0	1445	6	0
1	N	1473	0	1444	12	0
1	O	1496	0	1461	12	0
1	P	1476	0	1448	11	0
1	Q	1504	0	1470	19	0
1	R	1476	0	1448	12	0
1	S	1481	0	1450	14	0
1	T	1487	0	1460	10	0
1	U	1473	0	1445	11	0
1	V	1487	0	1460	11	2
2	A	18	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
2	D	36	0	0	0	0
2	E	18	0	0	0	0
2	F	36	0	0	0	0
2	G	36	0	0	0	0
2	H	18	0	0	0	0
2	K	18	0	0	0	0
2	L	36	0	0	0	0
2	M	18	0	0	1	0
2	N	18	0	0	0	0
2	O	18	0	0	0	0
2	P	18	0	0	0	0
2	Q	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	36	0	0	0	0
2	S	36	0	0	0	0
2	T	18	0	0	0	0
2	U	18	0	0	0	0
2	V	18	0	0	0	0
3	A	20	0	30	0	0
3	B	16	0	24	1	0
3	C	12	0	18	4	0
3	D	8	0	12	0	0
3	E	12	0	18	1	0
3	F	4	0	6	0	0
3	G	12	0	18	8	0
3	H	4	0	6	0	0
3	I	8	0	12	3	0
3	J	8	0	12	0	0
3	K	4	0	6	7	0
3	L	16	0	24	3	0
3	M	12	0	18	0	0
3	N	20	0	30	5	0
3	O	12	0	18	0	0
3	P	20	0	30	2	0
3	Q	16	0	24	1	0
3	R	24	0	36	2	0
3	S	12	0	18	7	0
3	T	16	0	24	1	0
3	U	8	0	11	1	0
3	V	8	0	12	5	0
4	A	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	V	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	2	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	3	0	0	0	0
5	P	2	0	0	0	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
5	U	1	0	0	0	0
5	V	1	0	0	0	0
6	A	82	0	0	4	0
6	B	91	0	0	0	2
6	C	102	0	0	0	0
6	D	86	0	0	0	2
6	E	80	0	0	0	0
6	F	77	0	0	4	0
6	G	50	0	0	0	0
6	H	49	0	0	0	0
6	I	22	0	0	0	0
6	J	34	0	0	1	0
6	K	31	0	0	0	0
6	L	78	0	0	2	0
6	M	77	0	0	1	0
6	N	81	0	0	2	0
6	O	84	0	0	0	0
6	P	98	0	0	2	0
6	Q	94	0	0	1	0
6	R	92	0	0	1	0
6	S	75	0	0	1	0
6	T	80	0	0	0	0
6	U	88	0	0	1	0
6	V	76	0	0	3	0
All	All	35092	0	32372	305	4

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 5.

All (305) 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:Q:66:ILE:HG13	1:Q:166:ILE:HD11	1.31	1.06
1:C:66:ILE:CG1	1:C:166:ILE:HD11	1.90	1.02
1:Q:66:ILE:CG1	1:Q:166:ILE:HD11	1.90	1.01
1:C:66:ILE:HG13	1:C:166:ILE:HD11	1.38	1.01
1:I:61:GLN:O	1:I:62:LYS:O	1.79	1.01
1:T:90:GLN:HE21	1:T:92[B]:ASN:HD21	1.01	0.96
1:K:78:MET:HE3	1:K:78:MET:HA	1.48	0.95
1:C:66:ILE:CD1	1:C:166:ILE:HD11	1.95	0.95
1:T:90:GLN:NE2	1:T:92[B]:ASN:HD21	1.64	0.94
1:J:112:ARG:HH12	1:J:114:GLN:HE21	1.16	0.94
3:P:305:EDO:H11	6:P:455:HOH:O	1.66	0.93
1:G:112:ARG:HE	3:G:305:EDO:C1	1.82	0.93
1:F:173:ARG:NE	6:F:401:HOH:O	1.99	0.93
1:G:112:ARG:HH22	1:G:114:GLN:HE21	1.17	0.92
1:K:112:ARG:HH22	1:K:114:GLN:HE21	1.17	0.92
1:J:78:MET:HA	1:J:78:MET:HE3	1.49	0.92
1:I:61:GLN:O	1:I:62:LYS:C	2.12	0.92
1:Q:66:ILE:HG13	1:Q:166:ILE:CD1	2.01	0.90
1:I:200:VAL:HG21	1:J:78:MET:HE1	1.54	0.89
1:R:141:LYS:HE3	3:R:309:EDO:H12	1.54	0.87
1:E:112:ARG:HH22	1:E:114:GLN:HE21	1.19	0.86
1:J:200:VAL:HG21	1:K:78:MET:HE1	1.57	0.86
1:O:104[A]:TYR:CE1	1:O:130:GLU:OE2	2.30	0.85
1:J:194:GLN:O	1:J:196:LEU:N	2.10	0.85
1:E:211:ASN:HD21	1:G:34:GLU:H	1.23	0.84
1:S:112:ARG:HE	3:S:305:EDO:C1	1.90	0.84
1:T:90:GLN:HE21	1:T:92[B]:ASN:ND2	1.75	0.83
1:C:66:ILE:HG13	1:C:166:ILE:CD1	2.11	0.79
1:Q:104[A]:TYR:HD1	1:Q:130:GLU:HG2	1.48	0.76
1:V:130:GLU:H	3:V:302:EDO:H21	1.52	0.74
1:Q:66:ILE:CD1	1:Q:166:ILE:HD11	2.18	0.74
1:N:130:GLU:H	3:N:306:EDO:C1	2.01	0.73
1:I:112:ARG:HE	3:I:301:EDO:H12	1.52	0.73
1:G:112:ARG:NE	3:G:305:EDO:H12	2.04	0.72
1:L:36:TYR:OH	1:U:204:ARG:HD2	1.88	0.72
1:C:130:GLU:H	3:C:304:EDO:C2	2.01	0.72
1:O:104[A]:TYR:HD1	1:O:130:GLU:HG2	1.53	0.72
1:C:66:ILE:HD11	1:C:166:ILE:HD11	1.71	0.72
1:Q:104[A]:TYR:CD1	1:Q:130:GLU:HG2	2.24	0.72
1:I:112:ARG:HE	3:I:301:EDO:C1	2.03	0.72
1:O:104[A]:TYR:CD1	1:O:130:GLU:HG2	2.26	0.71
1:F:204:ARG:HD2	1:H:36:TYR:OH	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:GLY:C	1:I:60:GLY:H	1.99	0.70
1:A:50:GLU:OE2	1:K:193:ARG:NH1	2.25	0.70
1:D:211:ASN:HD21	1:F:34:GLU:H	1.37	0.70
3:L:303:EDO:H12	1:V:90:GLN:HA	1.74	0.70
1:J:194:GLN:C	1:J:196:LEU:N	2.39	0.69
1:V:211:ASN:ND2	6:V:402:HOH:O	2.26	0.69
1:L:36:TYR:CZ	1:U:204:ARG:HD3	2.27	0.69
1:O:52:ILE:HD12	1:O:166:ILE:HD11	1.74	0.69
1:G:112:ARG:HE	3:G:305:EDO:H12	1.58	0.69
1:S:112:ARG:HE	3:S:305:EDO:H12	1.56	0.69
1:R:90:GLN:HE21	1:R:92[B]:ASN:HD21	1.39	0.68
1:S:112:ARG:NE	3:S:305:EDO:H12	2.08	0.68
1:K:98:LEU:HD23	1:R:100:ASN:O	1.93	0.68
1:G:112:ARG:NE	3:G:305:EDO:C1	2.55	0.68
1:D:90:GLN:HE21	1:D:92[B]:ASN:HD21	1.42	0.67
1:K:52:ILE:HD12	1:K:166:ILE:HD11	1.74	0.67
1:J:194:GLN:O	1:J:196:LEU:HB3	1.94	0.67
1:O:211:ASN:HD22	1:Q:34:GLU:CD	2.03	0.67
1:J:194:GLN:C	1:J:196:LEU:H	1.96	0.67
1:M:52:ILE:HD12	1:M:166:ILE:HD11	1.76	0.67
1:C:129:SER:HA	3:C:304:EDO:H21	1.77	0.66
1:A:36:TYR:OH	1:J:204:ARG:HD2	1.96	0.66
1:L:90:GLN:HE21	1:L:92[A]:ASN:HD21	1.44	0.66
1:C:100:ASN:O	1:O:98:LEU:HD23	1.96	0.65
1:T:52:ILE:HD12	1:T:166:ILE:HD11	1.76	0.65
1:A:90:GLN:CD	1:A:92[B]:ASN:HD21	2.04	0.65
1:K:182:LEU:O	1:K:183:PRO:C	2.39	0.65
1:J:180:ARG:HH21	1:J:181:GLN:H	1.45	0.65
1:I:112:ARG:NE	3:I:301:EDO:H12	2.12	0.64
1:L:36:TYR:OH	1:U:204:ARG:CD	2.45	0.64
1:C:130:GLU:H	3:C:304:EDO:H21	1.63	0.64
1:K:112:ARG:HE	3:K:302:EDO:C1	2.11	0.64
1:I:52:ILE:HD12	1:I:166:ILE:HD11	1.80	0.64
1:N:129:SER:HA	3:N:306:EDO:H12	1.80	0.64
1:C:66:ILE:CD1	1:C:166:ILE:CD1	2.73	0.63
1:I:59:GLY:O	1:I:60:GLY:C	2.41	0.63
1:B:52:ILE:HD12	1:B:166:ILE:HD11	1.81	0.63
1:A:156[B]:ARG:NH1	6:A:401:HOH:O	2.32	0.62
1:S:24:LEU:N	6:S:401:HOH:O	2.32	0.62
1:J:57:ALA:O	1:J:58:GLY:C	2.41	0.62
1:K:78:MET:HE3	1:K:78:MET:CA	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:104[A]:TYR:HE1	1:O:130:GLU:OE2	1.79	0.62
1:S:90:GLN:HE21	1:S:92[A]:ASN:HD21	1.48	0.62
1:U:52:ILE:HD12	1:U:166:ILE:HD11	1.81	0.61
1:I:186:VAL:HG11	1:J:171:TYR:HA	1.81	0.61
1:I:58:GLY:C	1:I:60:GLY:N	2.58	0.61
1:L:36:TYR:CZ	1:U:204:ARG:CD	2.84	0.60
1:R:90:GLN:HE21	1:R:92[B]:ASN:ND2	1.99	0.60
1:I:90:GLN:HE21	1:I:92[B]:ASN:HD21	1.48	0.60
1:R:52:ILE:HD12	1:R:166:ILE:HD11	1.82	0.60
1:H:52:ILE:HD12	1:H:166:ILE:HD11	1.82	0.59
1:N:41:LYS:NZ	6:N:1501:HOH:O	2.26	0.59
1:N:204:ARG:HD2	1:P:36:TYR:OH	2.03	0.59
1:I:181:GLN:C	1:I:183:PRO:HD3	2.28	0.59
1:J:52:ILE:HD12	1:J:166:ILE:HD11	1.85	0.59
1:I:52:ILE:HG13	1:I:175:LEU:HD21	1.85	0.59
1:A:87:SER:CB	3:B:306:EDO:H21	2.32	0.59
1:V:130:GLU:H	3:V:302:EDO:C2	2.16	0.59
1:K:112:ARG:HH22	1:K:114:GLN:NE2	1.97	0.58
1:N:60:GLY:O	1:N:61:GLN:C	2.46	0.58
1:D:90:GLN:HE21	1:D:92[B]:ASN:ND2	2.01	0.58
1:G:112:ARG:HE	3:G:305:EDO:H11	1.66	0.58
1:I:61:GLN:C	1:I:62:LYS:O	2.40	0.58
1:J:203:ALA:HB1	1:K:34:GLU:HB3	1.84	0.58
1:F:90:GLN:HE21	1:F:92[B]:ASN:ND2	2.02	0.58
1:A:60:GLY:HA3	6:A:421:HOH:O	2.04	0.57
1:C:130:GLU:H	3:C:304:EDO:H22	1.68	0.57
1:D:211:ASN:ND2	1:F:34:GLU:H	2.03	0.57
1:R:141:LYS:CE	3:R:309:EDO:H12	2.31	0.57
1:B:104[B]:TYR:CE2	1:B:130:GLU:HG3	2.39	0.57
1:J:39:ILE:HG12	1:J:78:MET:HE2	1.87	0.57
1:L:90:GLN:HE21	1:L:92[A]:ASN:ND2	2.01	0.57
1:F:156[A]:ARG:NE	6:F:402:HOH:O	2.37	0.56
1:M:189:THR:HG23	1:M:190:LYS:HG3	1.88	0.56
1:M:24:LEU:N	6:M:402:HOH:O	2.38	0.56
1:Q:90:GLN:HE21	1:Q:92[A]:ASN:HD21	1.52	0.56
1:C:90:GLN:NE2	1:C:92[B]:ASN:HD21	2.04	0.55
1:L:57:ALA:O	1:L:58:GLY:C	2.48	0.55
1:N:130:GLU:H	3:N:306:EDO:H11	1.71	0.55
1:S:90:GLN:HE21	1:S:92[A]:ASN:ND2	2.04	0.55
1:A:90:GLN:NE2	1:A:92[B]:ASN:OD1	2.40	0.55
1:L:24:LEU:N	6:L:402:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLY:C	1:B:60:GLY:N	2.64	0.55
1:M:34:GLU:HG3	6:V:445:HOH:O	2.07	0.55
1:F:52:ILE:HG13	1:F:175:LEU:HD11	1.89	0.55
1:J:58:GLY:O	1:J:61:GLN:OE1	2.25	0.55
1:K:112:ARG:NE	3:K:302:EDO:H11	2.22	0.55
1:Q:66:ILE:HD11	1:Q:166:ILE:HD11	1.89	0.55
1:J:200:VAL:HG21	1:K:78:MET:CE	2.32	0.54
1:P:90:GLN:HE21	1:P:92[B]:ASN:HD21	1.54	0.54
1:I:90:GLN:HE21	1:I:92[B]:ASN:ND2	2.05	0.54
1:F:204:ARG:CD	1:H:36:TYR:CZ	2.90	0.54
1:J:112:ARG:HH12	1:J:114:GLN:NE2	1.97	0.54
1:E:51:TYR:CE1	3:E:304:EDO:H22	2.43	0.54
1:G:112:ARG:HH22	1:G:114:GLN:NE2	1.98	0.54
1:K:39:ILE:HG12	1:K:78:MET:HE2	1.89	0.54
1:J:78:MET:HE3	1:J:78:MET:CA	2.29	0.53
1:K:112:ARG:HD2	3:K:302:EDO:H11	1.89	0.53
1:R:90:GLN:NE2	1:R:92[B]:ASN:HD21	2.05	0.53
1:A:56:MET:HB3	6:A:403:HOH:O	2.08	0.53
3:L:303:EDO:H22	6:L:407:HOH:O	2.09	0.52
1:T:52:ILE:HG13	1:T:175:LEU:HD11	1.90	0.52
1:Q:66:ILE:CD1	1:Q:166:ILE:CD1	2.87	0.52
1:K:112:ARG:CD	3:K:302:EDO:H11	2.39	0.52
1:Q:90:GLN:HE21	1:Q:92[A]:ASN:ND2	2.08	0.52
1:J:77:GLU:OE1	1:K:44:ARG:HD3	2.10	0.52
1:R:57:ALA:O	1:R:58:GLY:C	2.51	0.52
1:H:77:GLU:OE2	1:I:44:ARG:HD3	2.10	0.52
1:I:90:GLN:NE2	1:I:92[B]:ASN:HD21	2.08	0.52
1:F:204:ARG:HD3	1:H:36:TYR:CZ	2.45	0.51
1:P:90:GLN:NE2	1:P:92[B]:ASN:HD21	2.09	0.51
1:K:56:MET:HA	1:K:62:LYS:HA	1.92	0.51
1:B:58:GLY:C	1:B:60:GLY:H	2.19	0.51
1:P:90:GLN:HE21	1:P:92[B]:ASN:ND2	2.08	0.51
1:V:156[B]:ARG:NH1	6:V:405:HOH:O	2.40	0.51
1:L:90:GLN:NE2	1:L:92[A]:ASN:HD21	2.09	0.51
1:L:52:ILE:HG13	1:L:175:LEU:HD21	1.93	0.51
1:C:90:GLN:HE21	1:C:92[B]:ASN:HD21	1.59	0.50
1:C:194:GLN:OE1	1:C:194:GLN:N	2.44	0.50
1:D:90:GLN:NE2	1:D:92[B]:ASN:HD21	2.07	0.50
1:V:198:PRO:O	3:V:304:EDO:H21	2.11	0.50
1:I:200:VAL:HG21	1:J:78:MET:CE	2.36	0.50
1:Q:90:GLN:NE2	1:Q:92[A]:ASN:HD21	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:180:ARG:NH2	1:J:181:GLN:H	2.08	0.50
1:D:211:ASN:ND2	1:F:34:GLU:HB2	2.26	0.50
1:S:112:ARG:NH2	3:S:305:EDO:H12	2.27	0.50
1:G:112:ARG:CZ	3:G:305:EDO:H12	2.42	0.50
1:S:112:ARG:CZ	3:S:305:EDO:H12	2.42	0.49
1:J:87:SER:HB2	3:K:302:EDO:H21	1.94	0.49
1:N:52:ILE:HG13	1:N:175:LEU:HD21	1.95	0.49
1:D:196:LEU:HD11	1:F:44:ARG:HD3	1.95	0.49
1:K:112:ARG:NE	3:K:302:EDO:C1	2.75	0.49
1:H:195:ASP:HB3	1:I:77:GLU:HG3	1.94	0.49
1:U:56:MET:SD	1:U:62:LYS:HG3	2.53	0.48
3:P:304:EDO:H11	1:Q:92[A]:ASN:CG	2.38	0.48
1:E:211:ASN:HD21	1:G:34:GLU:N	2.01	0.48
1:J:193:ARG:HH21	1:K:49:PRO:HD2	1.78	0.48
1:K:112:ARG:HD2	3:K:302:EDO:C1	2.43	0.48
1:E:211:ASN:ND2	1:G:34:GLU:H	2.02	0.48
1:J:66:ILE:HG12	1:J:71:VAL:HG23	1.96	0.48
3:L:303:EDO:C1	1:V:90:GLN:HA	2.43	0.48
1:S:170:ASP:HA	1:S:173:ARG:NH2	2.29	0.48
1:S:112:ARG:HH21	3:S:305:EDO:H12	1.78	0.48
1:S:90:GLN:NE2	1:S:92[A]:ASN:HD21	2.09	0.48
1:B:52:ILE:HG13	1:B:175:LEU:HD21	1.96	0.47
1:K:167:LEU:H	1:K:167:LEU:HD22	1.79	0.47
1:H:212:MET:HE2	1:H:212:MET:HB2	1.73	0.47
1:J:52:ILE:HG13	1:J:175:LEU:HD21	1.95	0.47
1:L:36:TYR:CE1	1:U:204:ARG:HD3	2.48	0.47
1:V:52:ILE:HG13	1:V:175:LEU:HD21	1.96	0.47
1:C:90:GLN:HE21	1:C:92[B]:ASN:ND2	2.13	0.47
1:M:52:ILE:HG13	1:M:175:LEU:HD21	1.96	0.47
1:N:204:ARG:CD	1:P:36:TYR:OH	2.61	0.47
1:F:204:ARG:CD	1:H:36:TYR:OH	2.61	0.47
1:I:77:GLU:OE2	1:J:44:ARG:HD3	2.15	0.47
1:K:78:MET:HA	1:K:78:MET:CE	2.34	0.47
1:P:170:ASP:OD1	1:P:173:ARG:NH2	2.48	0.47
1:A:60:GLY:HA2	6:A:403:HOH:O	2.14	0.47
1:C:66:ILE:HD11	1:C:166:ILE:CD1	2.43	0.47
1:O:52:ILE:HG13	1:O:175:LEU:HD21	1.96	0.47
1:F:90:GLN:NE2	1:F:92[B]:ASN:HD21	2.13	0.46
3:N:302:EDO:H11	1:O:92[B]:ASN:ND2	2.31	0.46
1:R:52:ILE:HG13	1:R:175:LEU:HD21	1.97	0.46
1:E:194[A]:GLN:N	1:E:194[A]:GLN:CD	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:ASN:HB3	1:I:104:TYR:HE2	1.81	0.46
1:A:156[B]:ARG:HH21	1:A:167:LEU:HD11	1.80	0.46
1:D:170:ASP:OD1	1:D:173:ARG:NH2	2.48	0.46
1:F:204:ARG:HD3	1:H:36:TYR:CE1	2.51	0.46
1:G:112:ARG:HH11	3:G:305:EDO:C1	2.29	0.46
1:S:52:ILE:HG13	1:S:175:LEU:HD21	1.98	0.46
1:T:99:ASN:HB2	1:T:104:TYR:HE2	1.81	0.45
1:H:77:GLU:CD	1:I:44:ARG:HH11	2.24	0.45
1:O:211:ASN:ND2	1:Q:34:GLU:OE2	2.49	0.45
1:T:76:ASN:HB3	3:U:303:EDO:H12	1.98	0.45
1:H:52:ILE:HG13	1:H:175:LEU:HD21	1.99	0.45
1:A:52:ILE:HG13	1:A:175:LEU:HD21	1.98	0.45
1:J:194:GLN:O	1:J:196:LEU:CB	2.63	0.45
1:V:198:PRO:HA	3:V:304:EDO:H21	1.98	0.45
1:F:173:ARG:CZ	6:F:401:HOH:O	2.55	0.45
1:T:141:LYS:HE3	3:T:305:EDO:H11	1.98	0.45
1:G:170:ASP:OD1	1:G:173:ARG:NH2	2.49	0.45
1:G:194:GLN:C	1:H:51:TYR:OH	2.60	0.45
1:J:178:LEU:O	1:J:179:PRO:C	2.58	0.44
1:P:90:GLN:HE21	1:P:92[B]:ASN:CG	2.25	0.44
1:F:90:GLN:HE21	1:F:92[B]:ASN:HD21	1.62	0.44
1:J:180:ARG:HD2	1:J:180:ARG:HA	1.39	0.44
1:O:170:ASP:OD1	1:O:173:ARG:NH2	2.48	0.44
1:I:175:LEU:HD12	1:I:175:LEU:HA	1.91	0.44
1:Q:170:ASP:OD1	1:Q:173:ARG:NH2	2.49	0.44
1:U:52:ILE:HG13	1:U:175:LEU:HD21	2.00	0.44
1:F:204:ARG:HD2	1:H:36:TYR:CZ	2.51	0.44
1:L:90:GLN:HE21	1:L:92[A]:ASN:CG	2.25	0.44
1:P:190:LYS:HE3	6:P:423:HOH:O	2.17	0.44
1:J:194:GLN:O	1:J:196:LEU:CA	2.65	0.44
1:Q:100:ASN:HB3	6:Q:480:HOH:O	2.17	0.44
1:V:141:LYS:HE3	3:V:302:EDO:H12	2.00	0.44
1:C:52:ILE:HG13	1:C:175:LEU:HD21	1.99	0.43
1:C:56:MET:C	1:C:57:ALA:O	2.51	0.43
1:G:52:ILE:HG13	1:G:175:LEU:HD21	1.99	0.43
1:H:187:ASP:OD1	1:H:189:THR:HG23	2.18	0.43
1:I:90:GLN:HE21	1:I:92[B]:ASN:CG	2.26	0.43
1:N:130:GLU:H	3:N:306:EDO:H12	1.77	0.43
1:E:52:ILE:HG13	1:E:175:LEU:HD21	1.99	0.43
1:F:52:ILE:HD12	1:F:166:ILE:CD1	2.48	0.43
1:S:90:GLN:HE21	1:S:92[A]:ASN:CG	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:GLN:HE21	1:D:92[B]:ASN:CG	2.26	0.43
1:B:209:ARG:H	1:B:209:ARG:HG3	1.46	0.43
1:F:187:ASP:OD1	1:F:189:THR:HG23	2.17	0.43
1:G:112:ARG:NH1	3:G:305:EDO:H12	2.34	0.43
1:Q:90:GLN:HE21	1:Q:92[A]:ASN:CG	2.26	0.43
1:K:179:PRO:O	1:K:180:ARG:C	2.62	0.43
1:F:173:ARG:NH1	6:F:401:HOH:O	2.51	0.43
1:H:170:ASP:OD1	1:H:173:ARG:NH2	2.50	0.43
1:J:79:PHE:O	6:J:401:HOH:O	2.21	0.43
1:L:170:ASP:OD1	1:L:173:ARG:NH2	2.50	0.43
1:L:187:ASP:OD1	1:L:189:THR:HG23	2.19	0.42
1:Q:52:ILE:HG13	1:Q:175:LEU:HD21	2.01	0.42
1:R:170:ASP:OD1	1:R:173:ARG:NH2	2.49	0.42
1:B:170:ASP:OD1	1:B:173:ARG:NH2	2.50	0.42
1:D:52:ILE:HG13	1:D:175:LEU:HD21	2.01	0.42
1:P:41:LYS:HB3	1:P:41:LYS:HE3	1.64	0.42
1:T:170:ASP:OD1	1:T:173:ARG:NH2	2.48	0.42
1:G:57:ALA:O	1:G:58:GLY:C	2.63	0.42
1:H:77:GLU:OE1	1:I:44:ARG:NH1	2.52	0.42
1:K:62:LYS:HB3	1:K:62:LYS:HE3	1.69	0.42
1:P:184:LEU:HD12	1:P:184:LEU:HA	1.84	0.42
1:N:204:ARG:HD3	1:P:36:TYR:CZ	2.54	0.42
1:A:187:ASP:OD1	1:A:189:THR:HG23	2.19	0.42
1:G:52:ILE:HD12	1:G:166:ILE:CD1	2.50	0.42
1:K:98:LEU:CD2	1:R:100:ASN:O	2.67	0.42
1:C:170:ASP:OD1	1:C:173:ARG:NH2	2.49	0.42
1:C:209:ARG:H	1:C:209:ARG:HG3	1.63	0.42
1:E:52:ILE:HD12	1:E:166:ILE:HD12	2.02	0.42
1:I:187:ASP:OD1	1:I:189:THR:HG23	2.20	0.42
1:R:132:LEU:HB2	6:R:414:HOH:O	2.19	0.42
1:U:170:ASP:OD1	1:U:173:ARG:NH2	2.49	0.42
1:U:187:ASP:OD1	1:U:189:THR:HG23	2.20	0.42
1:C:90:GLN:HE21	1:C:92[B]:ASN:CG	2.27	0.41
1:C:187:ASP:OD1	1:C:189:THR:HG23	2.20	0.41
1:J:180:ARG:HH21	1:J:181:GLN:N	2.14	0.41
1:A:90:GLN:NE2	1:A:92[B]:ASN:HD21	2.19	0.41
1:U:211:ASN:ND2	6:U:407:HOH:O	2.54	0.41
1:E:170:ASP:OD1	1:E:173:ARG:NH2	2.50	0.41
1:I:77:GLU:CD	1:J:44:ARG:HH11	2.28	0.41
1:L:44:ARG:HH11	1:V:77:GLU:CD	2.28	0.41
1:J:72:ILE:HD11	1:J:151:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:167:LEU:HD22	1:K:167:LEU:N	2.35	0.41
1:M:170:ASP:OD1	1:M:173:ARG:NH2	2.50	0.41
1:H:54:SER:HB2	1:H:62:LYS:HG3	2.02	0.41
1:K:170:ASP:OD1	1:K:173:ARG:NH2	2.49	0.41
1:Q:70:ARG:HH11	3:Q:307:EDO:C1	2.34	0.41
1:S:187:ASP:OD1	1:S:189:THR:HG23	2.20	0.41
1:C:204:ARG:HH21	1:C:204:ARG:HD3	1.75	0.41
1:G:187:ASP:OD1	1:G:189:THR:HG23	2.20	0.41
2:M:301:A1KCG:C11	2:M:301:A1KCG:N3	2.83	0.41
3:S:304:EDO:H11	1:T:92[B]:ASN:ND2	2.36	0.41
1:A:179:PRO:HB2	1:A:181:GLN:HE21	1.86	0.41
1:L:52:ILE:HD12	1:L:166:ILE:CD1	2.51	0.41
1:I:77:GLU:OE1	1:J:44:ARG:NH1	2.53	0.40
1:N:204:ARG:NH2	1:O:78:MET:O	2.45	0.40
1:N:24:LEU:N	6:N:1507:HOH:O	2.54	0.40
1:I:54:SER:HB2	1:I:62:LYS:HG2	2.04	0.40
1:G:188:LEU:O	1:G:193:ARG:NH2	2.54	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:GLN:NE2	1:V:176:ASN:OD1[3_555]	1.69	0.51
6:B:485:HOH:O	6:D:476:HOH:O[4_445]	1.71	0.49
6:B:486:HOH:O	6:D:482:HOH:O[4_445]	1.91	0.29
1:G:194:GLN:CD	1:V:176:ASN:OD1[3_555]	1.95	0.25

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	186/215 (86%)	186 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	189/215 (88%)	188 (100%)	1 (0%)	0	100	100
1	C	188/215 (87%)	187 (100%)	1 (0%)	0	100	100
1	D	188/215 (87%)	186 (99%)	2 (1%)	0	100	100
1	E	189/215 (88%)	189 (100%)	0	0	100	100
1	F	187/215 (87%)	187 (100%)	0	0	100	100
1	G	185/215 (86%)	185 (100%)	0	0	100	100
1	H	187/215 (87%)	184 (98%)	3 (2%)	0	100	100
1	I	186/215 (86%)	181 (97%)	4 (2%)	1 (0%)	24	22
1	J	186/215 (86%)	181 (97%)	5 (3%)	0	100	100
1	K	186/215 (86%)	181 (97%)	5 (3%)	0	100	100
1	L	188/215 (87%)	186 (99%)	2 (1%)	0	100	100
1	M	187/215 (87%)	187 (100%)	0	0	100	100
1	N	186/215 (86%)	185 (100%)	1 (0%)	0	100	100
1	O	188/215 (87%)	188 (100%)	0	0	100	100
1	P	186/215 (86%)	186 (100%)	0	0	100	100
1	Q	189/215 (88%)	187 (99%)	2 (1%)	0	100	100
1	R	186/215 (86%)	186 (100%)	0	0	100	100
1	S	187/215 (87%)	184 (98%)	3 (2%)	0	100	100
1	T	187/215 (87%)	186 (100%)	1 (0%)	0	100	100
1	U	186/215 (86%)	186 (100%)	0	0	100	100
1	V	187/215 (87%)	187 (100%)	0	0	100	100
All	All	4114/4730 (87%)	4083 (99%)	30 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	62	LYS

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	155/172 (90%)	154 (99%)	1 (1%)	78	86
1	B	157/172 (91%)	154 (98%)	3 (2%)	50	58
1	C	157/172 (91%)	153 (98%)	4 (2%)	42	48
1	D	155/172 (90%)	149 (96%)	6 (4%)	28	31
1	E	157/172 (91%)	152 (97%)	5 (3%)	34	38
1	F	156/172 (91%)	153 (98%)	3 (2%)	50	58
1	G	153/172 (89%)	148 (97%)	5 (3%)	33	37
1	H	155/172 (90%)	149 (96%)	6 (4%)	28	31
1	I	154/172 (90%)	147 (96%)	7 (4%)	24	25
1	J	154/172 (90%)	148 (96%)	6 (4%)	28	31
1	K	155/172 (90%)	149 (96%)	6 (4%)	28	31
1	L	155/172 (90%)	152 (98%)	3 (2%)	50	58
1	M	154/172 (90%)	151 (98%)	3 (2%)	50	58
1	N	154/172 (90%)	148 (96%)	6 (4%)	28	31
1	O	157/172 (91%)	150 (96%)	7 (4%)	24	25
1	P	155/172 (90%)	150 (97%)	5 (3%)	34	38
1	Q	157/172 (91%)	156 (99%)	1 (1%)	78	86
1	R	155/172 (90%)	151 (97%)	4 (3%)	40	46
1	S	155/172 (90%)	151 (97%)	4 (3%)	40	46
1	T	156/172 (91%)	154 (99%)	2 (1%)	61	69
1	U	154/172 (90%)	148 (96%)	6 (4%)	28	31
1	V	156/172 (91%)	154 (99%)	2 (1%)	61	69
All	All	3416/3784 (90%)	3321 (97%)	95 (3%)	38	43

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	B	176	ASN
1	B	184	LEU
1	B	209	ARG
1	C	61	GLN
1	C	184	LEU

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Mol	Chain	Res	Type
1	C	209	ARG
1	C	212	MET
1	D	166	ILE
1	D	167	LEU
1	D	176	ASN
1	D	182	LEU
1	D	196	LEU
1	D	209	ARG
1	E	166	ILE
1	E	167	LEU
1	E	176	ASN
1	E	184	LEU
1	E	185	GLU
1	F	180	ARG
1	F	194	GLN
1	F	202	GLU
1	G	56	MET
1	G	169	LYS
1	G	176	ASN
1	G	186	VAL
1	G	209	ARG
1	H	34	GLU
1	H	62	LYS
1	H	176	ASN
1	H	184	LEU
1	H	209	ARG
1	H	212	MET
1	I	61	GLN
1	I	62	LYS
1	I	98	LEU
1	I	178	LEU
1	I	180	ARG
1	I	181	GLN
1	I	186	VAL
1	J	156	ARG
1	J	176	ASN
1	J	180	ARG
1	J	181	GLN
1	J	184	LEU
1	J	199	SER
1	K	41	LYS
1	K	54	SER

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Mol	Chain	Res	Type
1	K	55	ARG
1	K	167	LEU
1	K	178	LEU
1	K	180	ARG
1	L	176	ASN
1	L	185	GLU
1	L	194	GLN
1	M	156	ARG
1	M	176	ASN
1	M	209	ARG
1	N	55	ARG
1	N	62	LYS
1	N	176	ASN
1	N	181	GLN
1	N	194	GLN
1	N	209	ARG
1	O	61	GLN
1	O	135	LYS
1	O	167	LEU
1	O	176	ASN
1	O	180	ARG
1	O	181	GLN
1	O	209	ARG
1	P	54	SER
1	P	166	ILE
1	P	167	LEU
1	P	176	ASN
1	P	182	LEU
1	Q	177	LYS
1	R	62	LYS
1	R	176	ASN
1	R	180	ARG
1	R	184	LEU
1	S	50	GLU
1	S	55	ARG
1	S	62	LYS
1	S	209	ARG
1	T	176	ASN
1	T	180	ARG
1	U	61	GLN
1	U	62	LYS
1	U	169	LYS

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Mol	Chain	Res	Type
1	U	176	ASN
1	U	184	LEU
1	U	186	VAL
1	V	176	ASN
1	V	182	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	90	GLN
1	B	28	GLN
1	B	37	GLN
1	B	211	ASN
1	C	30	GLN
1	C	37	GLN
1	C	61	GLN
1	C	90	GLN
1	D	69	HIS
1	D	90	GLN
1	D	211	ASN
1	E	90	GLN
1	E	114	GLN
1	E	206	ASN
1	E	211	ASN
1	F	37	GLN
1	F	45	GLN
1	F	90	GLN
1	F	181	GLN
1	G	45	GLN
1	G	69	HIS
1	G	114	GLN
1	G	181	GLN
1	H	69	HIS
1	H	181	GLN
1	I	30	GLN
1	I	45	GLN
1	I	61	GLN
1	I	69	HIS
1	I	90	GLN
1	I	100	ASN
1	I	181	GLN

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Mol	Chain	Res	Type
1	J	61	GLN
1	J	114	GLN
1	J	181	GLN
1	J	194	GLN
1	K	114	GLN
1	L	45	GLN
1	L	90	GLN
1	L	211	ASN
1	M	45	GLN
1	M	61	GLN
1	M	90	GLN
1	M	92	ASN
1	N	30	GLN
1	N	45	GLN
1	N	90	GLN
1	O	211	ASN
1	P	37	GLN
1	P	61	GLN
1	P	69	HIS
1	P	90	GLN
1	Q	90	GLN
1	Q	100	ASN
1	Q	176	ASN
1	Q	181	GLN
1	Q	211	ASN
1	R	30	GLN
1	R	61	GLN
1	R	90	GLN
1	R	181	GLN
1	R	211	ASN
1	S	45	GLN
1	S	69	HIS
1	S	90	GLN
1	T	45	GLN
1	T	61	GLN
1	T	90	GLN
1	U	28	GLN
1	U	90	GLN
1	U	181	GLN
1	V	69	HIS
1	V	181	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 131 ligands modelled in this entry, 34 are monoatomic - leaving 97 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	$\# Z > 2$
2	A1KCG	L	304	-	20,20,20	0.64	0	28,28,28	0.86	1 (3%)
2	A1KCG	F	301	-	20,20,20	0.72	0	28,28,28	0.61	0
2	A1KCG	B	302	-	20,20,20	0.93	1 (5%)	28,28,28	0.74	1 (3%)
3	EDO	A	305	-	3,3,3	0.29	0	2,2,2	0.69	0
3	EDO	O	305	-	3,3,3	0.34	0	2,2,2	0.35	0
3	EDO	N	302	-	3,3,3	0.25	0	2,2,2	0.29	0
3	EDO	B	306	-	3,3,3	0.29	0	2,2,2	0.60	0
3	EDO	N	306	-	3,3,3	0.45	0	2,2,2	0.49	0
2	A1KCG	R	301	-	20,20,20	0.73	0	28,28,28	0.91	1 (3%)
2	A1KCG	V	301	-	20,20,20	0.59	0	28,28,28	0.64	0
3	EDO	P	303	-	3,3,3	0.33	0	2,2,2	0.25	0
2	A1KCG	C	302	-	20,20,20	0.84	1 (5%)	28,28,28	0.70	0
3	EDO	G	303	-	3,3,3	0.34	0	2,2,2	0.69	0
3	EDO	J	301	-	3,3,3	0.25	0	2,2,2	0.23	0
2	A1KCG	T	301	-	20,20,20	0.67	0	28,28,28	0.62	0
3	EDO	H	302	-	3,3,3	0.50	0	2,2,2	0.61	0
3	EDO	I	302	-	3,3,3	0.22	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1KCG	S	302	-	20,20,20	0.61	0	28,28,28	0.77	1 (3%)
2	A1KCG	S	301	-	20,20,20	0.71	0	28,28,28	0.80	1 (3%)
3	EDO	E	303	-	3,3,3	0.49	0	2,2,2	0.24	0
3	EDO	M	303	-	3,3,3	0.79	0	2,2,2	0.83	0
2	A1KCG	K	301	-	20,20,20	0.69	1 (5%)	28,28,28	0.65	0
3	EDO	R	304	-	3,3,3	0.21	0	2,2,2	0.08	0
3	EDO	I	301	-	3,3,3	0.70	0	2,2,2	0.46	0
3	EDO	N	301	-	3,3,3	0.24	0	2,2,2	0.16	0
2	A1KCG	H	301	-	20,20,20	0.52	0	28,28,28	0.78	2 (7%)
3	EDO	O	302	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	L	307	-	3,3,3	0.48	0	2,2,2	0.28	0
3	EDO	M	305	-	3,3,3	0.70	0	2,2,2	0.43	0
2	A1KCG	L	301	-	20,20,20	0.64	0	28,28,28	0.93	1 (3%)
3	EDO	R	306	-	3,3,3	0.33	0	2,2,2	0.04	0
3	EDO	Q	303	-	3,3,3	0.23	0	2,2,2	0.36	0
2	A1KCG	F	302	-	20,20,20	0.63	0	28,28,28	0.73	0
3	EDO	P	306	-	3,3,3	0.20	0	2,2,2	0.09	0
3	EDO	S	305	-	3,3,3	0.62	0	2,2,2	0.78	0
2	A1KCG	N	303	-	20,20,20	0.68	0	28,28,28	0.77	0
3	EDO	L	306	-	3,3,3	0.27	0	2,2,2	0.48	0
3	EDO	S	303	-	3,3,3	0.39	0	2,2,2	0.25	0
2	A1KCG	Q	301	-	20,20,20	0.67	0	28,28,28	0.73	0
3	EDO	C	305	-	3,3,3	0.31	0	2,2,2	0.24	0
3	EDO	G	302	-	3,3,3	0.38	0	2,2,2	0.46	0
3	EDO	R	308	-	3,3,3	0.35	0	2,2,2	0.56	0
3	EDO	J	302	-	3,3,3	0.30	0	2,2,2	0.30	0
3	EDO	A	307	-	3,3,3	0.29	0	2,2,2	0.38	0
2	A1KCG	D	303	-	20,20,20	0.71	0	28,28,28	0.82	1 (3%)
3	EDO	L	302	-	3,3,3	0.50	0	2,2,2	0.49	0
2	A1KCG	M	301	-	20,20,20	0.58	0	28,28,28	0.94	2 (7%)
3	EDO	E	301	-	3,3,3	0.41	0	2,2,2	0.32	0
3	EDO	M	302	-	3,3,3	0.21	0	2,2,2	0.25	0
2	A1KCG	A	301	-	20,20,20	0.74	0	28,28,28	1.09	3 (10%)
3	EDO	Q	304	-	3,3,3	0.54	0	2,2,2	0.36	0
3	EDO	T	305	-	3,3,3	0.24	0	2,2,2	0.18	0
2	A1KCG	D	301	-	20,20,20	0.66	1 (5%)	28,28,28	0.68	0
3	EDO	U	303	-	3,3,3	0.87	0	2,2,2	0.35	0
3	EDO	P	305	-	3,3,3	0.21	0	2,2,2	0.18	0
3	EDO	G	305	-	3,3,3	0.69	0	2,2,2	0.58	0
3	EDO	A	304	-	3,3,3	0.89	0	2,2,2	0.57	0
3	EDO	Q	306	-	3,3,3	0.25	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	S	304	-	3,3,3	0.45	0	2,2,2	0.39	0
3	EDO	A	302	-	3,3,3	0.13	0	2,2,2	0.44	0
3	EDO	D	304	-	3,3,3	0.47	0	2,2,2	0.67	0
3	EDO	V	304	-	3,3,3	0.21	0	2,2,2	0.41	0
3	EDO	N	304	-	3,3,3	0.19	0	2,2,2	0.28	0
3	EDO	T	304	-	3,3,3	0.18	0	2,2,2	0.25	0
2	A1KCG	U	302	-	20,20,20	0.70	0	28,28,28	0.74	0
3	EDO	L	303	-	3,3,3	0.57	0	2,2,2	1.18	0
2	A1KCG	B	301	-	20,20,20	0.68	0	28,28,28	0.68	0
3	EDO	E	304	-	3,3,3	0.39	0	2,2,2	0.57	0
2	A1KCG	E	302	-	20,20,20	0.71	0	28,28,28	1.07	2 (7%)
2	A1KCG	P	302	-	20,20,20	0.82	0	28,28,28	0.99	1 (3%)
2	A1KCG	G	301	-	20,20,20	0.73	0	28,28,28	0.69	0
3	EDO	P	304	-	3,3,3	0.60	0	2,2,2	0.21	0
3	EDO	C	303	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	B	303	-	3,3,3	0.15	0	2,2,2	0.11	0
2	A1KCG	G	304	-	20,20,20	0.67	1 (5%)	28,28,28	0.72	0
3	EDO	O	303	-	3,3,3	0.43	0	2,2,2	0.21	0
3	EDO	C	304	-	3,3,3	0.60	0	2,2,2	1.17	0
3	EDO	F	303	-	3,3,3	0.29	0	2,2,2	0.39	0
3	EDO	A	303	-	3,3,3	1.02	0	2,2,2	0.93	0
3	EDO	R	307	-	3,3,3	0.59	0	2,2,2	0.37	0
2	A1KCG	R	302	-	20,20,20	0.93	1 (5%)	28,28,28	0.69	0
3	EDO	V	302	-	3,3,3	0.23	0	2,2,2	0.58	0
2	A1KCG	Q	302	-	20,20,20	0.74	0	28,28,28	0.79	0
3	EDO	T	302	-	3,3,3	0.31	0	2,2,2	0.21	0
2	A1KCG	O	301	-	20,20,20	0.61	0	28,28,28	0.68	0
3	EDO	B	304	-	3,3,3	0.44	0	2,2,2	0.70	0
3	EDO	U	301	-	3,3,3	0.29	0	2,2,2	0.17	0
2	A1KCG	C	301	-	20,20,20	0.66	0	28,28,28	0.89	2 (7%)
3	EDO	R	309	-	3,3,3	0.29	0	2,2,2	0.74	0
3	EDO	D	302	-	3,3,3	0.53	0	2,2,2	0.34	0
3	EDO	K	302	-	3,3,3	0.75	0	2,2,2	0.90	0
3	EDO	R	303	-	3,3,3	0.64	0	2,2,2	0.37	0
3	EDO	T	303	-	3,3,3	0.54	0	2,2,2	0.44	0
3	EDO	B	305	-	3,3,3	0.27	0	2,2,2	0.31	0
3	EDO	N	305	-	3,3,3	0.54	0	2,2,2	0.51	0
3	EDO	Q	307	-	3,3,3	0.34	0	2,2,2	0.35	0
3	EDO	P	301	-	3,3,3	0.51	0	2,2,2	0.44	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
2	A1KCG	L	304	-	-	4/8/8/8	0/3/3/3
2	A1KCG	F	301	-	-	2/8/8/8	0/3/3/3
2	A1KCG	B	302	-	-	0/8/8/8	0/3/3/3
3	EDO	A	305	-	-	1/1/1/1	-
3	EDO	O	305	-	-	1/1/1/1	-
3	EDO	N	302	-	-	1/1/1/1	-
3	EDO	B	306	-	-	1/1/1/1	-
3	EDO	N	306	-	-	0/1/1/1	-
2	A1KCG	R	301	-	-	0/8/8/8	0/3/3/3
2	A1KCG	V	301	-	-	2/8/8/8	0/3/3/3
3	EDO	P	303	-	-	1/1/1/1	-
2	A1KCG	C	302	-	-	0/8/8/8	0/3/3/3
3	EDO	G	303	-	-	1/1/1/1	-
3	EDO	J	301	-	-	1/1/1/1	-
2	A1KCG	T	301	-	-	0/8/8/8	0/3/3/3
3	EDO	H	302	-	-	1/1/1/1	-
3	EDO	I	302	-	-	0/1/1/1	-
2	A1KCG	S	302	-	-	2/8/8/8	0/3/3/3
2	A1KCG	S	301	-	-	0/8/8/8	0/3/3/3
3	EDO	E	303	-	-	1/1/1/1	-
3	EDO	M	303	-	-	1/1/1/1	-
2	A1KCG	K	301	-	-	4/8/8/8	0/3/3/3
3	EDO	R	304	-	-	1/1/1/1	-
3	EDO	I	301	-	-	0/1/1/1	-
3	EDO	N	301	-	-	1/1/1/1	-
2	A1KCG	H	301	-	-	2/8/8/8	0/3/3/3
3	EDO	O	302	-	-	0/1/1/1	-
3	EDO	L	307	-	-	1/1/1/1	-
3	EDO	M	305	-	-	1/1/1/1	-
2	A1KCG	L	301	-	-	0/8/8/8	0/3/3/3
3	EDO	R	306	-	-	0/1/1/1	-
3	EDO	Q	303	-	-	1/1/1/1	-
2	A1KCG	F	302	-	-	0/8/8/8	0/3/3/3
3	EDO	P	306	-	-	0/1/1/1	-
3	EDO	S	305	-	-	1/1/1/1	-
2	A1KCG	N	303	-	-	0/8/8/8	0/3/3/3
3	EDO	L	306	-	-	1/1/1/1	-
3	EDO	S	303	-	-	1/1/1/1	-
2	A1KCG	Q	301	-	-	1/8/8/8	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	305	-	-	1/1/1/1	-
3	EDO	G	302	-	-	1/1/1/1	-
3	EDO	R	308	-	-	1/1/1/1	-
3	EDO	J	302	-	-	1/1/1/1	-
3	EDO	A	307	-	-	1/1/1/1	-
2	A1KCG	D	303	-	-	0/8/8/8	0/3/3/3
3	EDO	L	302	-	-	1/1/1/1	-
2	A1KCG	M	301	-	-	0/8/8/8	0/3/3/3
3	EDO	E	301	-	-	1/1/1/1	-
3	EDO	M	302	-	-	1/1/1/1	-
2	A1KCG	A	301	-	-	0/8/8/8	0/3/3/3
3	EDO	Q	304	-	-	1/1/1/1	-
3	EDO	T	305	-	-	1/1/1/1	-
2	A1KCG	D	301	-	-	2/8/8/8	0/3/3/3
3	EDO	U	303	-	-	1/1/1/1	-
3	EDO	P	305	-	-	1/1/1/1	-
3	EDO	G	305	-	-	1/1/1/1	-
3	EDO	A	304	-	-	1/1/1/1	-
3	EDO	Q	306	-	-	1/1/1/1	-
3	EDO	S	304	-	-	1/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	D	304	-	-	1/1/1/1	-
3	EDO	V	304	-	-	1/1/1/1	-
3	EDO	N	304	-	-	1/1/1/1	-
3	EDO	T	304	-	-	1/1/1/1	-
2	A1KCG	U	302	-	-	0/8/8/8	0/3/3/3
3	EDO	L	303	-	-	1/1/1/1	-
2	A1KCG	B	301	-	-	0/8/8/8	0/3/3/3
3	EDO	E	304	-	-	1/1/1/1	-
2	A1KCG	E	302	-	-	0/8/8/8	0/3/3/3
2	A1KCG	P	302	-	-	0/8/8/8	0/3/3/3
2	A1KCG	G	301	-	-	0/8/8/8	0/3/3/3
3	EDO	P	304	-	-	1/1/1/1	-
3	EDO	C	303	-	-	1/1/1/1	-
3	EDO	B	303	-	-	1/1/1/1	-
2	A1KCG	G	304	-	-	0/8/8/8	0/3/3/3
3	EDO	O	303	-	-	1/1/1/1	-
3	EDO	C	304	-	-	1/1/1/1	-
3	EDO	F	303	-	-	1/1/1/1	-
3	EDO	A	303	-	-	1/1/1/1	-
3	EDO	R	307	-	-	1/1/1/1	-
2	A1KCG	R	302	-	-	0/8/8/8	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	V	302	-	-	1/1/1/1	-
2	A1KCG	Q	302	-	-	0/8/8/8	0/3/3/3
3	EDO	T	302	-	-	1/1/1/1	-
2	A1KCG	O	301	-	-	0/8/8/8	0/3/3/3
3	EDO	B	304	-	-	1/1/1/1	-
3	EDO	U	301	-	-	1/1/1/1	-
2	A1KCG	C	301	-	-	0/8/8/8	0/3/3/3
3	EDO	R	309	-	-	1/1/1/1	-
3	EDO	D	302	-	-	1/1/1/1	-
3	EDO	K	302	-	-	0/1/1/1	-
3	EDO	R	303	-	-	1/1/1/1	-
3	EDO	T	303	-	-	1/1/1/1	-
3	EDO	B	305	-	-	0/1/1/1	-
3	EDO	N	305	-	-	1/1/1/1	-
3	EDO	Q	307	-	-	1/1/1/1	-
3	EDO	P	301	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	A1KCG	O2-C1	3.25	1.32	1.22
2	R	302	A1KCG	O2-C1	2.72	1.30	1.22
2	G	304	A1KCG	O2-C1	2.23	1.29	1.22
2	C	302	A1KCG	O2-C1	2.08	1.28	1.22
2	D	301	A1KCG	O1-C1	-2.07	1.24	1.30
2	K	301	A1KCG	O2-C1	2.04	1.28	1.22

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	302	A1KCG	O1-C1-C2	3.32	123.47	114.85
2	P	302	A1KCG	O1-C1-C2	2.83	122.20	114.85
2	R	301	A1KCG	O1-C1-C2	2.73	121.93	114.85
2	L	301	A1KCG	N3-C5-N1	2.72	117.50	115.09
2	A	301	A1KCG	O2-C1-C2	-2.66	114.35	121.45
2	M	301	A1KCG	C12-N1-C5	-2.65	125.28	128.91
2	M	301	A1KCG	C5-N1-C6	2.47	127.98	124.20
2	A	301	A1KCG	O1-C1-C2	2.42	121.13	114.85
2	A	301	A1KCG	N3-C5-N1	2.39	117.21	115.09
2	C	301	A1KCG	O1-C1-C2	2.34	120.91	114.85
2	C	301	A1KCG	O2-C1-C2	-2.26	115.44	121.45
2	H	301	A1KCG	O2-C1-C2	-2.21	115.56	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	A1KCG	O1-C1-C2	2.21	120.58	114.85
2	S	301	A1KCG	O1-C1-C2	2.21	120.57	114.85
2	D	303	A1KCG	N3-C5-N1	2.19	117.03	115.09
2	S	302	A1KCG	O1-C1-C2	2.16	120.46	114.85
2	L	304	A1KCG	C5-N1-C6	2.06	127.35	124.20
2	E	302	A1KCG	N3-C5-N1	2.05	116.90	115.09
2	B	302	A1KCG	C5-N1-C6	2.03	127.31	124.20

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	A1KCG	C4-C5-N1-C6
2	F	301	A1KCG	C4-C5-N1-C6
2	H	301	A1KCG	C4-C5-N1-C6
2	L	304	A1KCG	N3-C5-N1-C12
2	Q	301	A1KCG	C4-C5-N1-C6
2	S	302	A1KCG	C4-C5-N1-C6
2	V	301	A1KCG	C4-C5-N1-C6
2	K	301	A1KCG	O1-C1-C2-C13
2	K	301	A1KCG	O2-C1-C2-C13
2	K	301	A1KCG	O1-C1-C2-C3
3	N	301	EDO	O1-C1-C2-O2
3	N	304	EDO	O1-C1-C2-O2
3	O	303	EDO	O1-C1-C2-O2
3	P	305	EDO	O1-C1-C2-O2
3	R	307	EDO	O1-C1-C2-O2
2	K	301	A1KCG	O2-C1-C2-C3
3	A	302	EDO	O1-C1-C2-O2
3	B	306	EDO	O1-C1-C2-O2
3	C	303	EDO	O1-C1-C2-O2
3	C	305	EDO	O1-C1-C2-O2
3	E	301	EDO	O1-C1-C2-O2
3	E	304	EDO	O1-C1-C2-O2
3	G	302	EDO	O1-C1-C2-O2
3	H	302	EDO	O1-C1-C2-O2
3	J	301	EDO	O1-C1-C2-O2
3	M	302	EDO	O1-C1-C2-O2
3	M	303	EDO	O1-C1-C2-O2
3	N	305	EDO	O1-C1-C2-O2
3	P	303	EDO	O1-C1-C2-O2
3	P	304	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	Q	303	EDO	O1-C1-C2-O2
3	R	304	EDO	O1-C1-C2-O2
3	S	304	EDO	O1-C1-C2-O2
3	U	301	EDO	O1-C1-C2-O2
3	V	302	EDO	O1-C1-C2-O2
3	V	304	EDO	O1-C1-C2-O2
3	A	303	EDO	O1-C1-C2-O2
3	C	304	EDO	O1-C1-C2-O2
3	D	302	EDO	O1-C1-C2-O2
2	D	301	A1KCG	C4-C5-N1-C12
2	F	301	A1KCG	C4-C5-N1-C12
2	H	301	A1KCG	C4-C5-N1-C12
2	S	302	A1KCG	C4-C5-N1-C12
2	V	301	A1KCG	C4-C5-N1-C12
2	L	304	A1KCG	C4-C5-N1-C6
3	B	303	EDO	O1-C1-C2-O2
3	P	301	EDO	O1-C1-C2-O2
3	R	309	EDO	O1-C1-C2-O2
3	S	303	EDO	O1-C1-C2-O2
3	T	302	EDO	O1-C1-C2-O2
3	T	305	EDO	O1-C1-C2-O2
3	A	304	EDO	O1-C1-C2-O2
3	A	305	EDO	O1-C1-C2-O2
3	B	304	EDO	O1-C1-C2-O2
3	D	304	EDO	O1-C1-C2-O2
3	E	303	EDO	O1-C1-C2-O2
3	G	303	EDO	O1-C1-C2-O2
3	L	302	EDO	O1-C1-C2-O2
3	L	307	EDO	O1-C1-C2-O2
3	M	305	EDO	O1-C1-C2-O2
3	R	308	EDO	O1-C1-C2-O2
3	T	304	EDO	O1-C1-C2-O2
3	U	303	EDO	O1-C1-C2-O2
3	G	305	EDO	O1-C1-C2-O2
3	L	303	EDO	O1-C1-C2-O2
3	T	303	EDO	O1-C1-C2-O2
2	L	304	A1KCG	N3-C5-N1-C6
3	L	306	EDO	O1-C1-C2-O2
3	Q	307	EDO	O1-C1-C2-O2
3	F	303	EDO	O1-C1-C2-O2
3	J	302	EDO	O1-C1-C2-O2
3	N	302	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	R	303	EDO	O1-C1-C2-O2
3	S	305	EDO	O1-C1-C2-O2
2	L	304	A1KCG	C4-C5-N1-C12
3	A	307	EDO	O1-C1-C2-O2
3	O	305	EDO	O1-C1-C2-O2
3	Q	304	EDO	O1-C1-C2-O2
3	Q	306	EDO	O1-C1-C2-O2

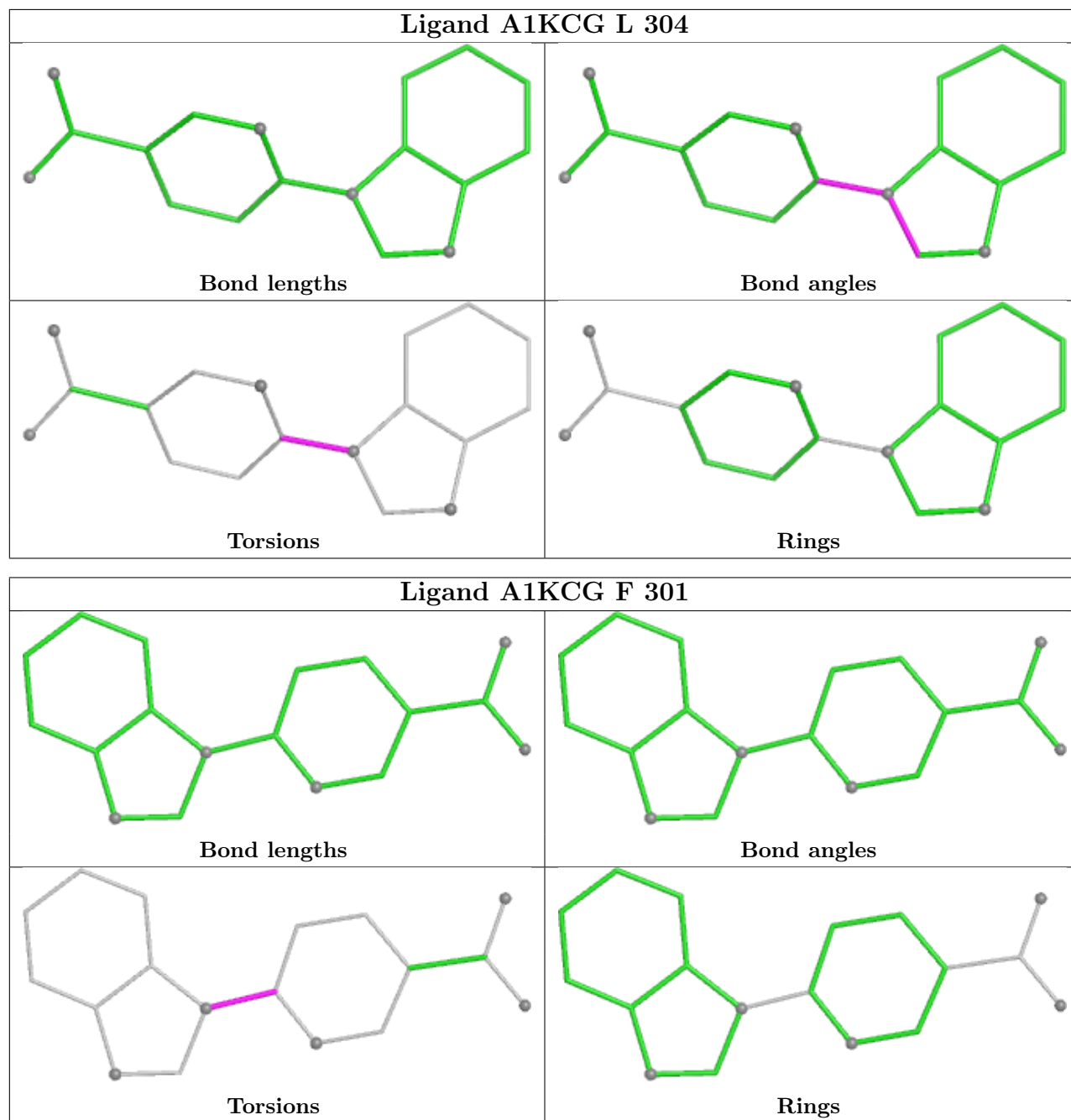
There are no ring outliers.

20 monomers are involved in 52 short contacts:

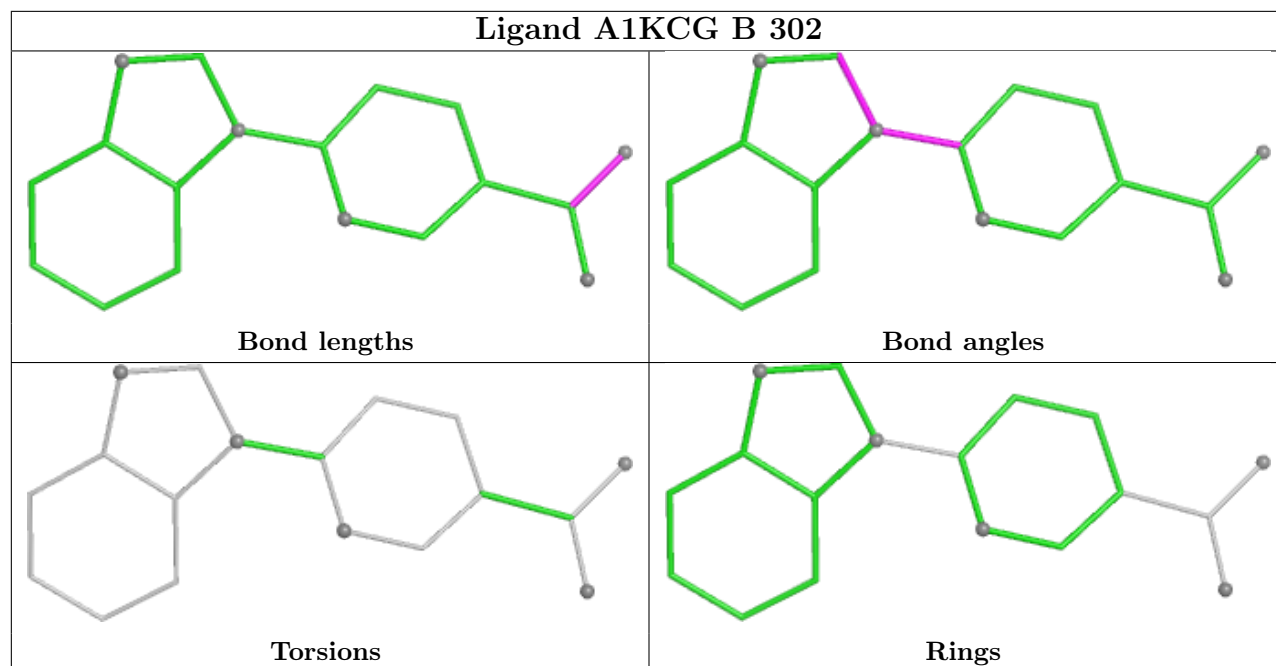
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	302	EDO	1	0
3	B	306	EDO	1	0
3	N	306	EDO	4	0
3	I	301	EDO	3	0
3	S	305	EDO	6	0
2	M	301	A1KCG	1	0
3	T	305	EDO	1	0
3	U	303	EDO	1	0
3	P	305	EDO	1	0
3	G	305	EDO	8	0
3	S	304	EDO	1	0
3	V	304	EDO	2	0
3	L	303	EDO	3	0
3	E	304	EDO	1	0
3	P	304	EDO	1	0
3	C	304	EDO	4	0
3	V	302	EDO	3	0
3	R	309	EDO	2	0
3	K	302	EDO	7	0
3	Q	307	EDO	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

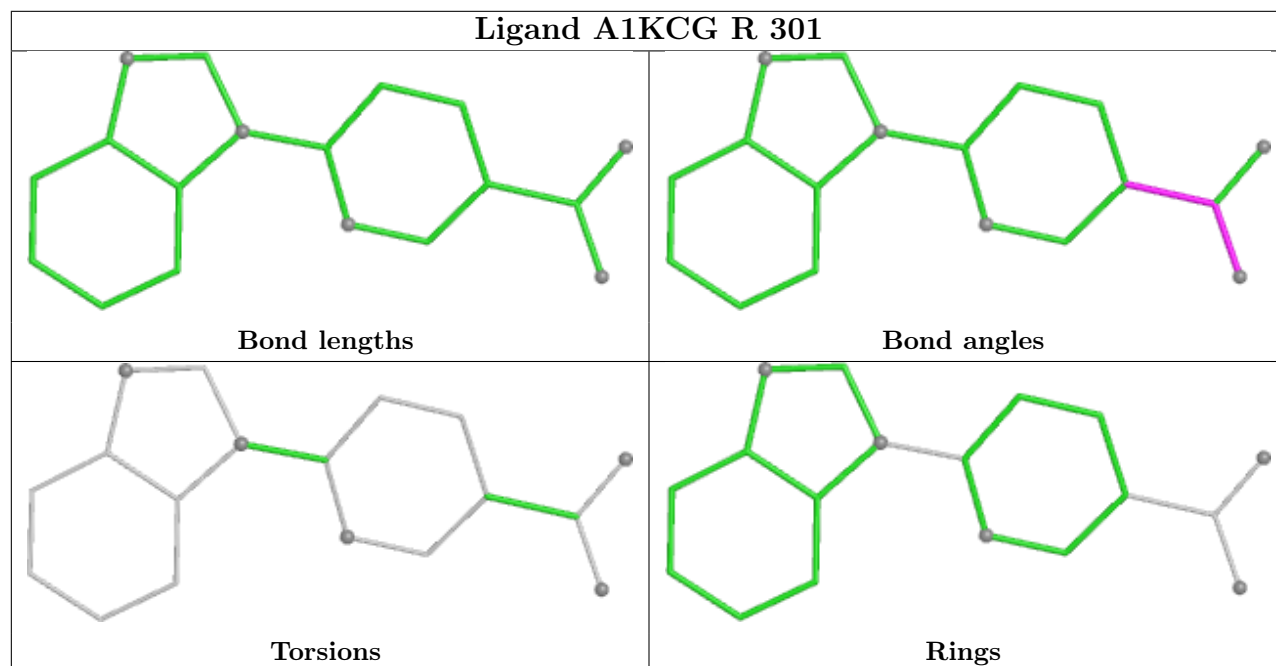
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



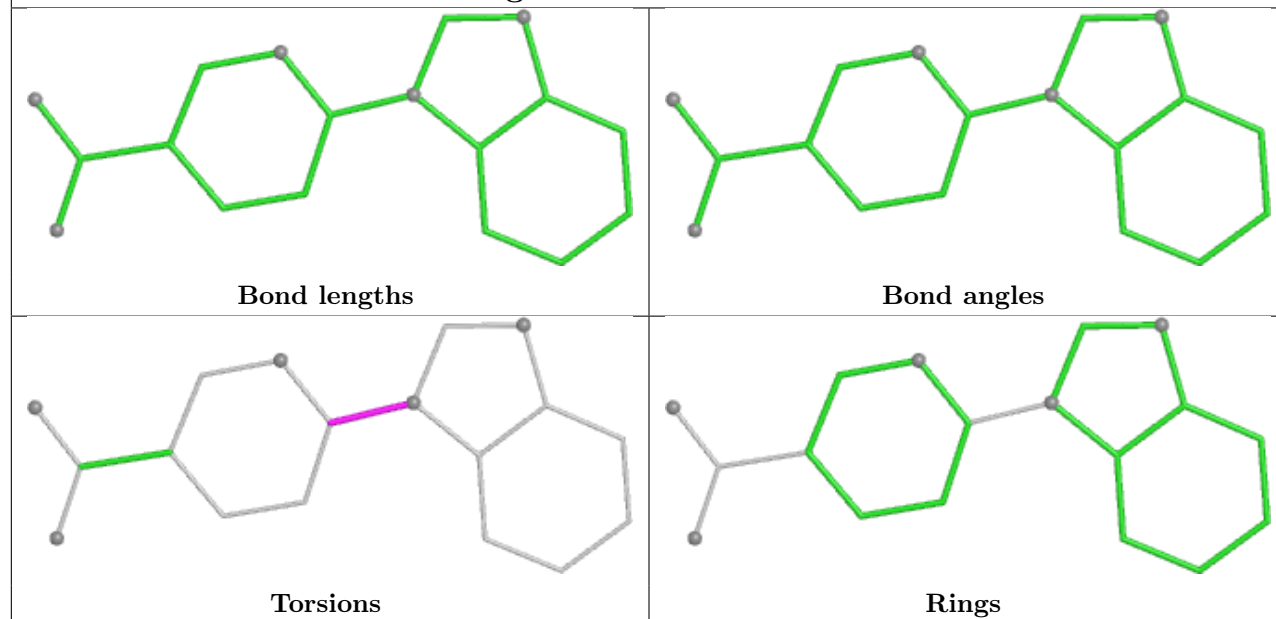
Ligand A1KCG B 302



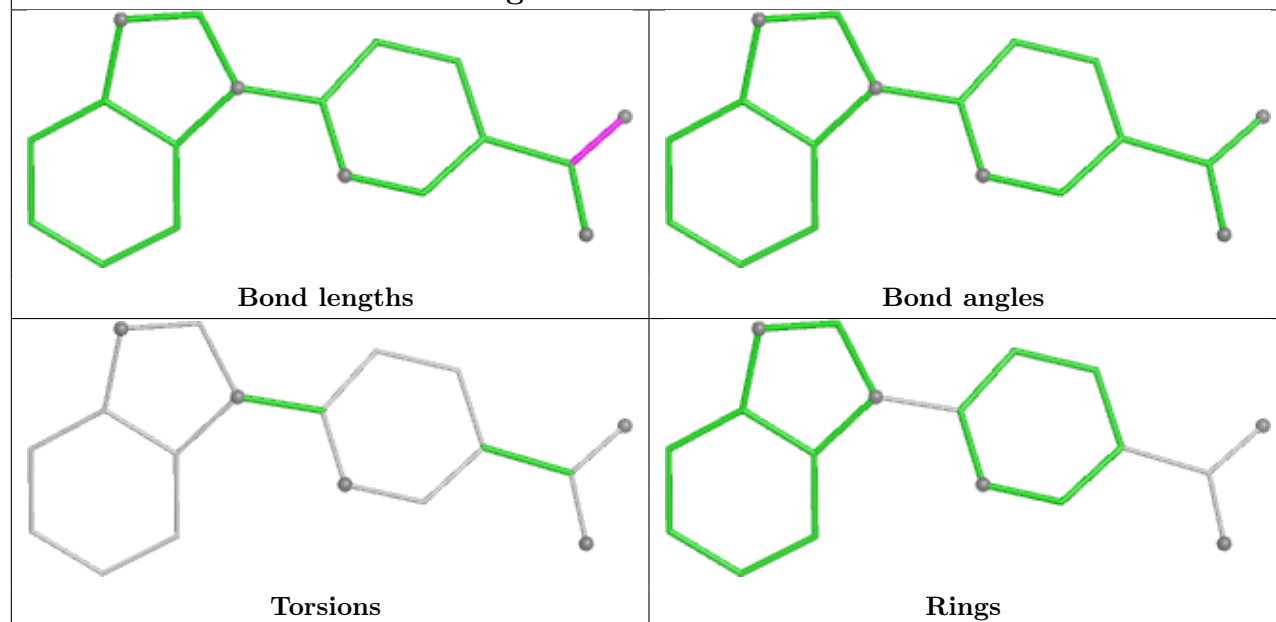
Ligand A1KCG R 301



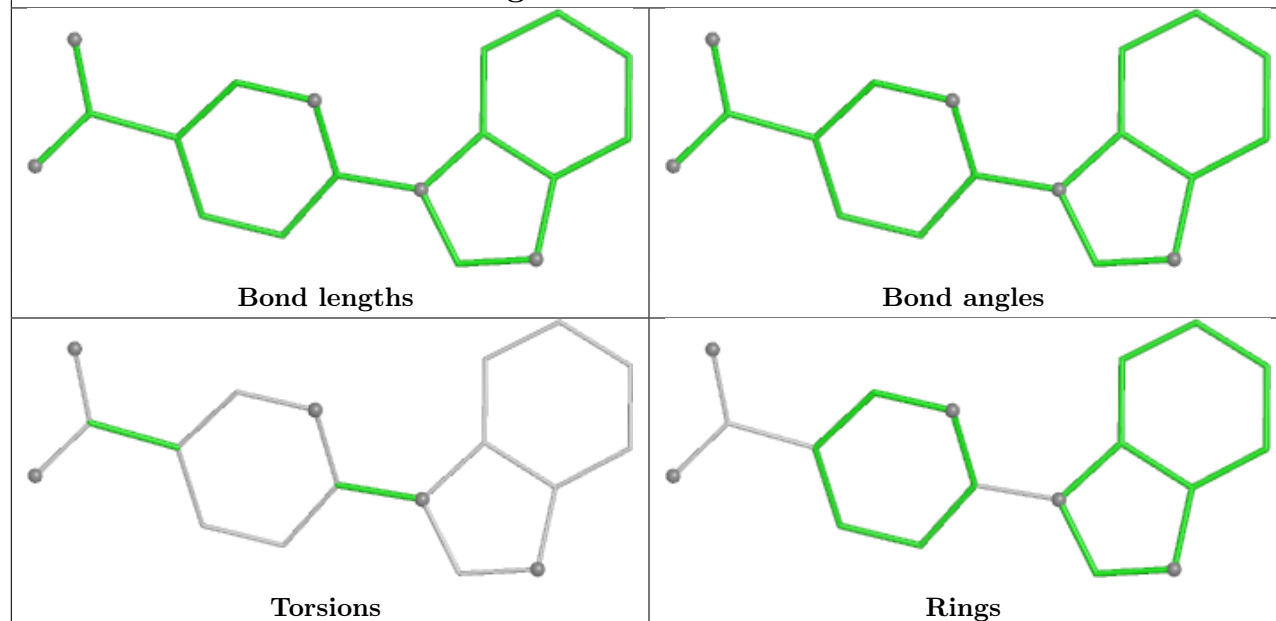
Ligand A1KCG V 301



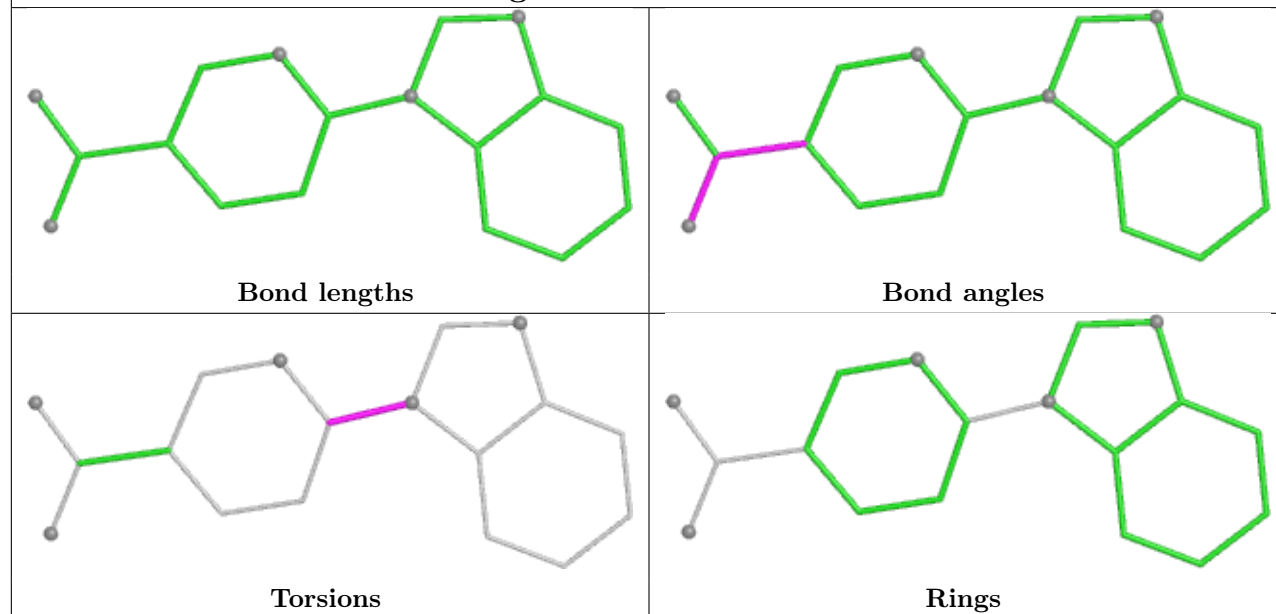
Ligand A1KCG C 302

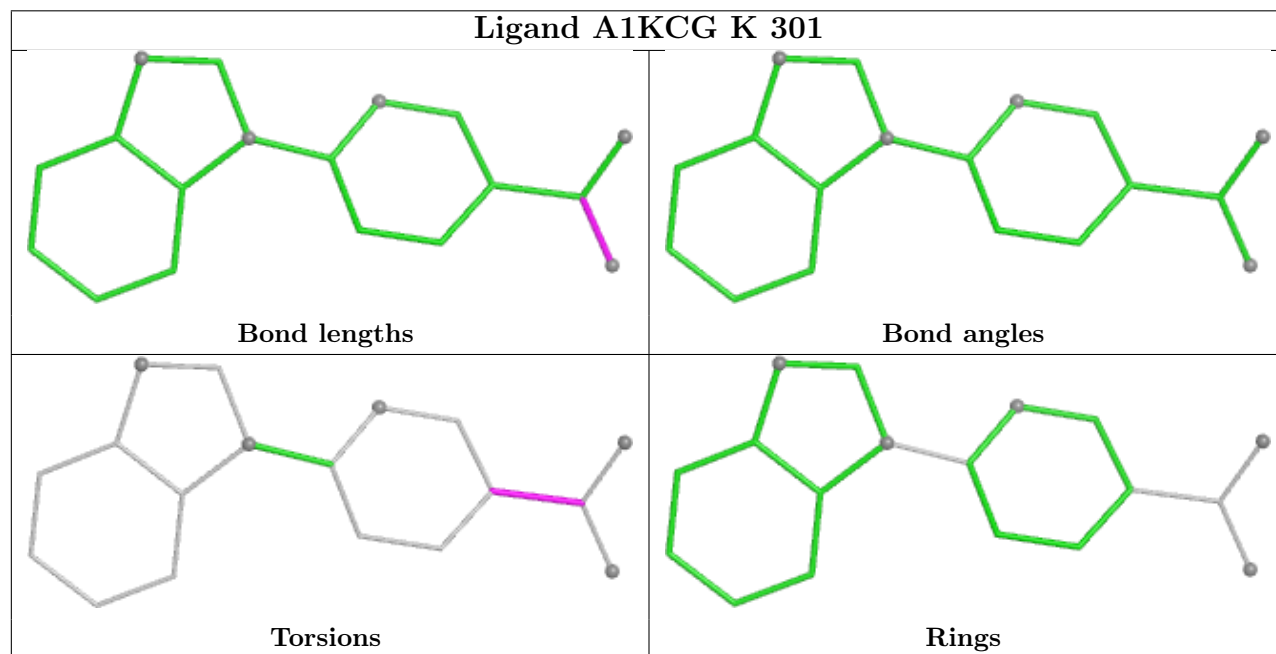
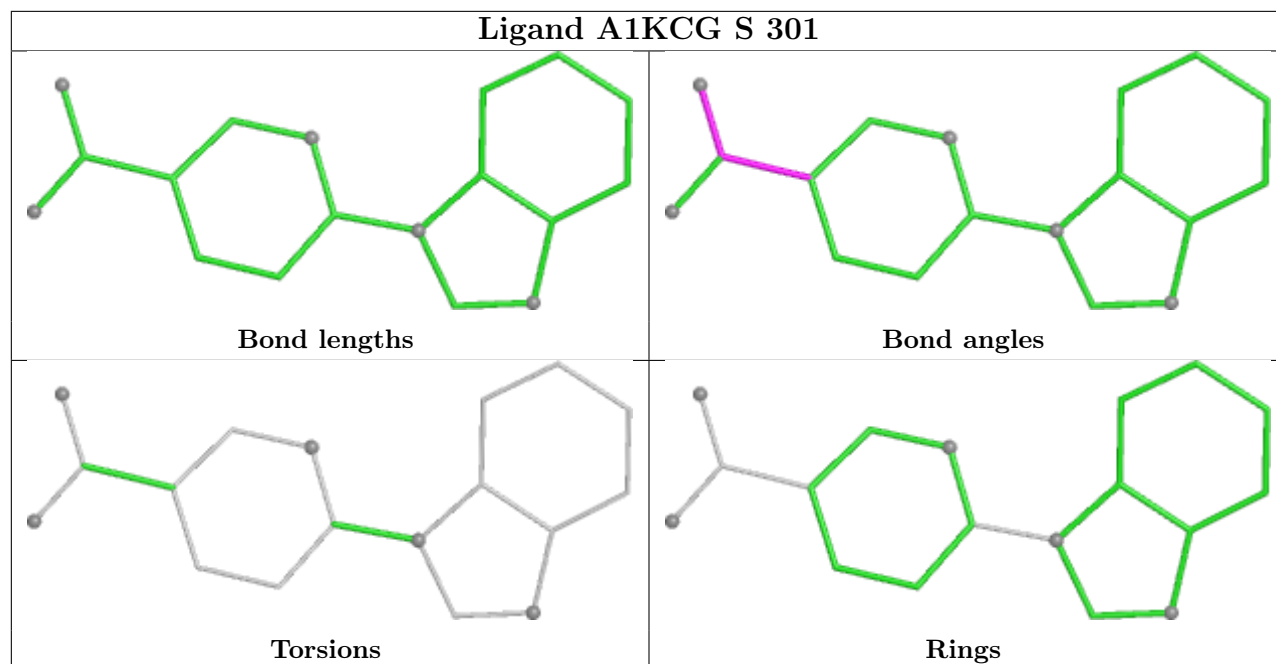


Ligand A1KCG T 301

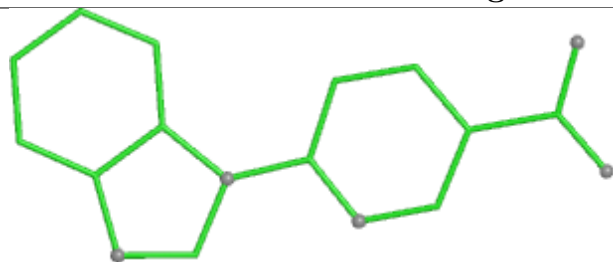


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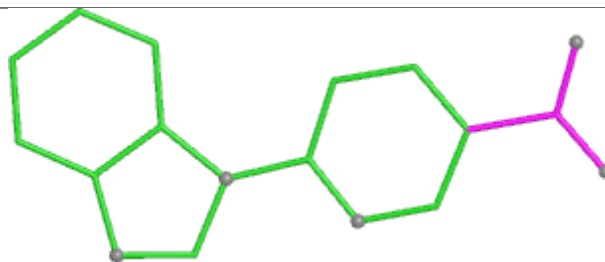




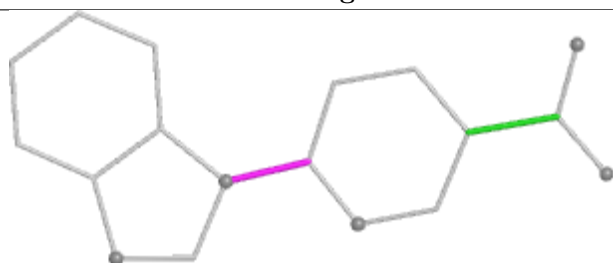
Ligand A1KCG H 301



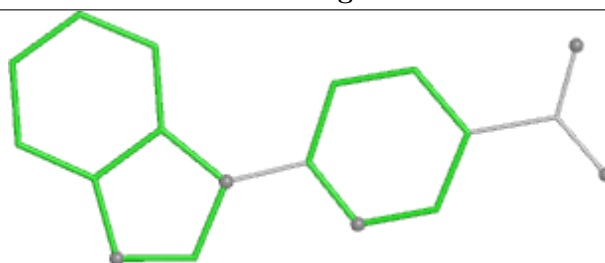
Bond lengths



Bond angles

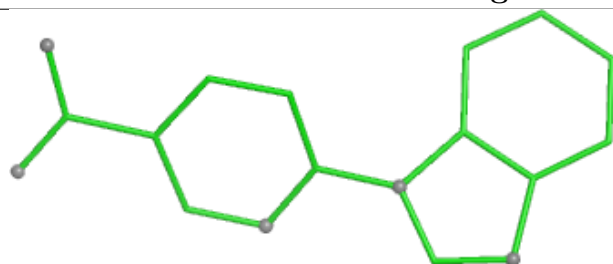


Torsions

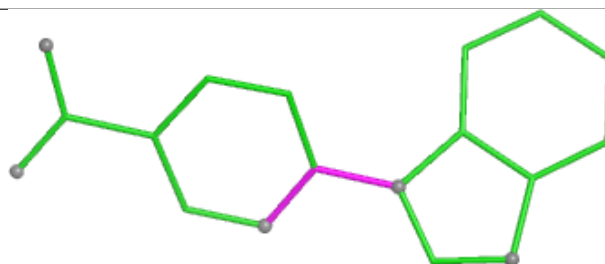


Rings

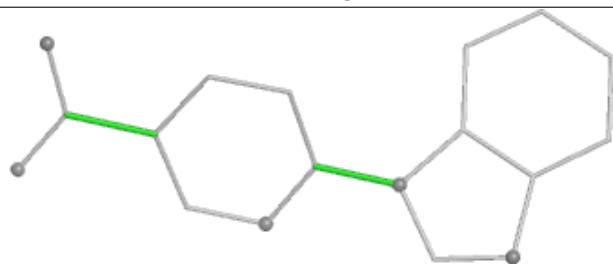
Ligand A1KCG L 301



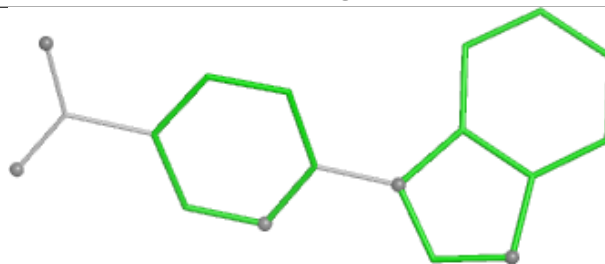
Bond lengths



Bond angles

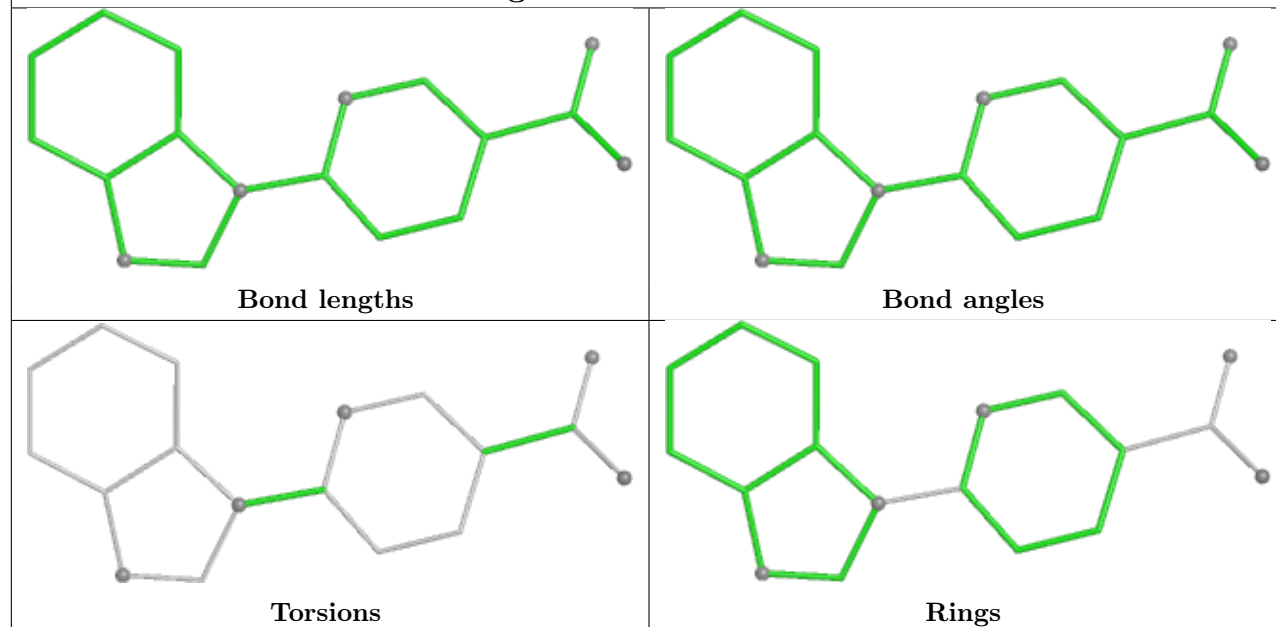


Torsions

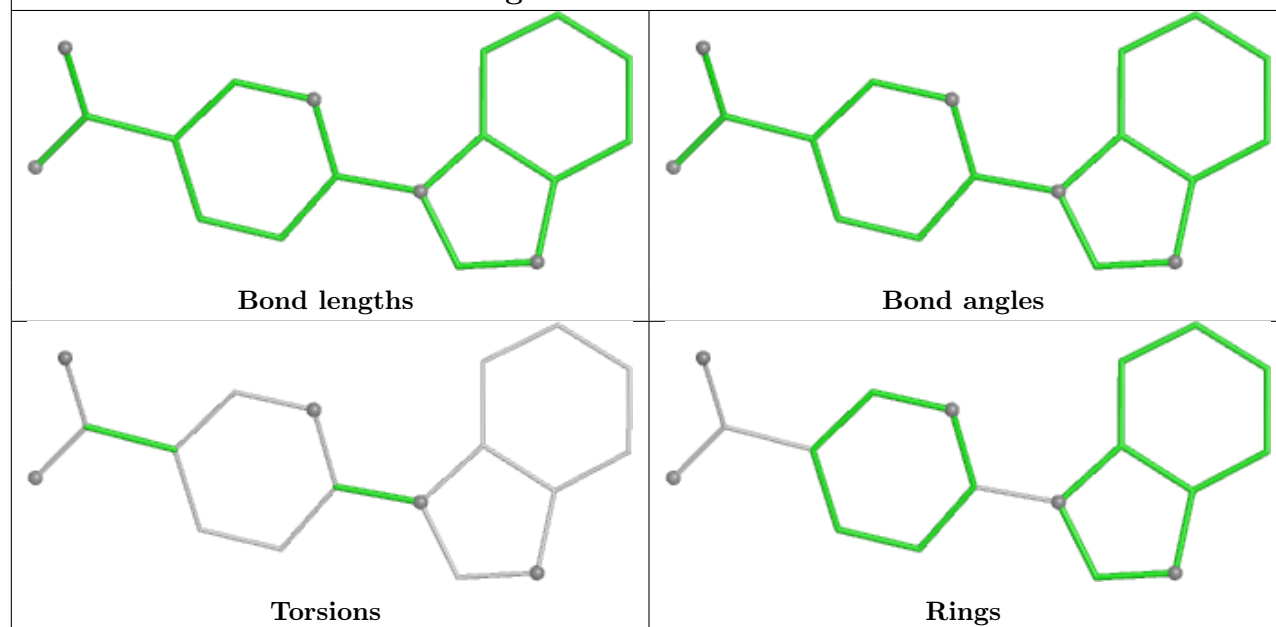


Rings

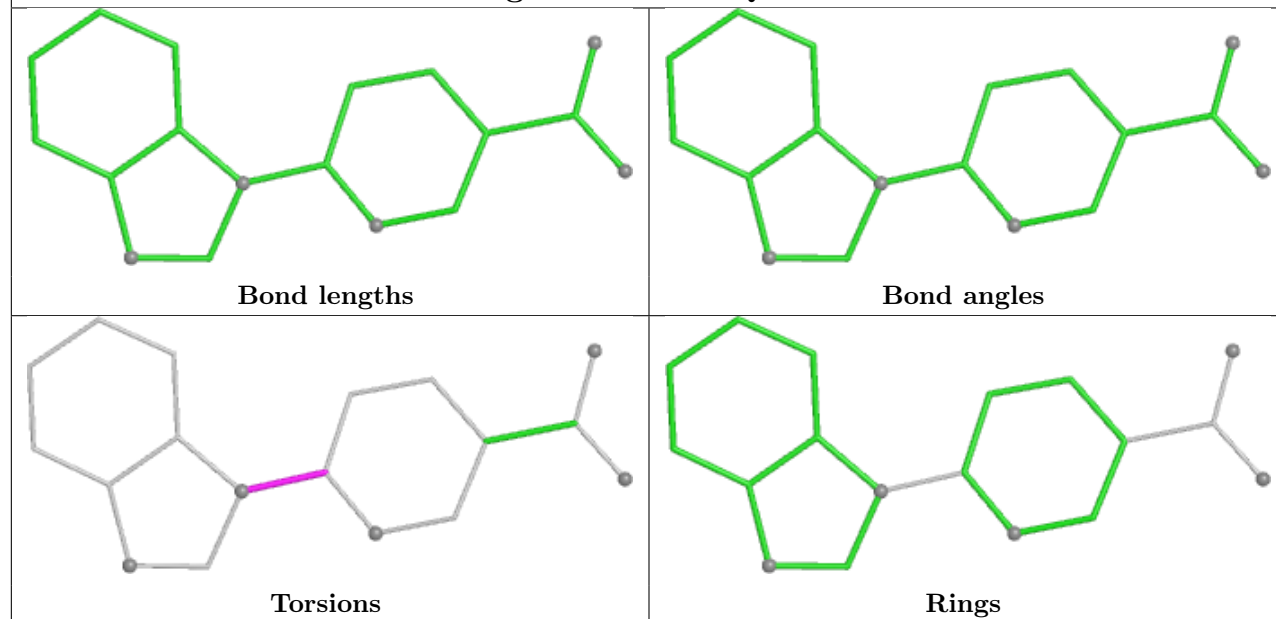
Ligand A1KCG F 302



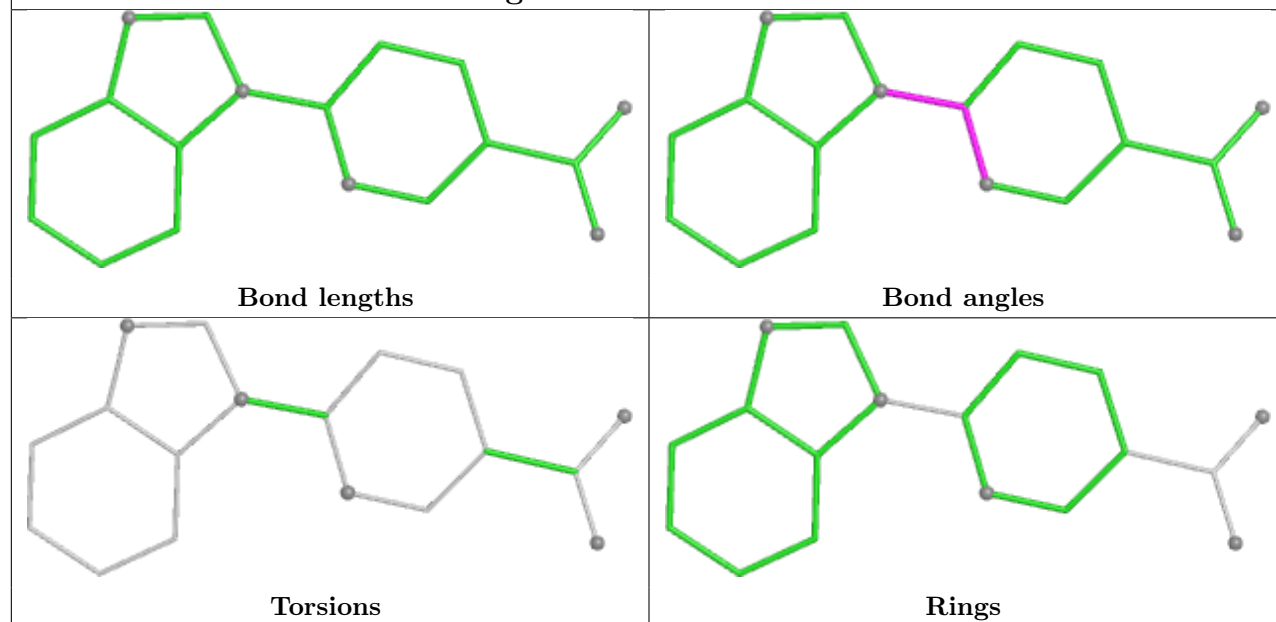
Ligand A1KCG N 303



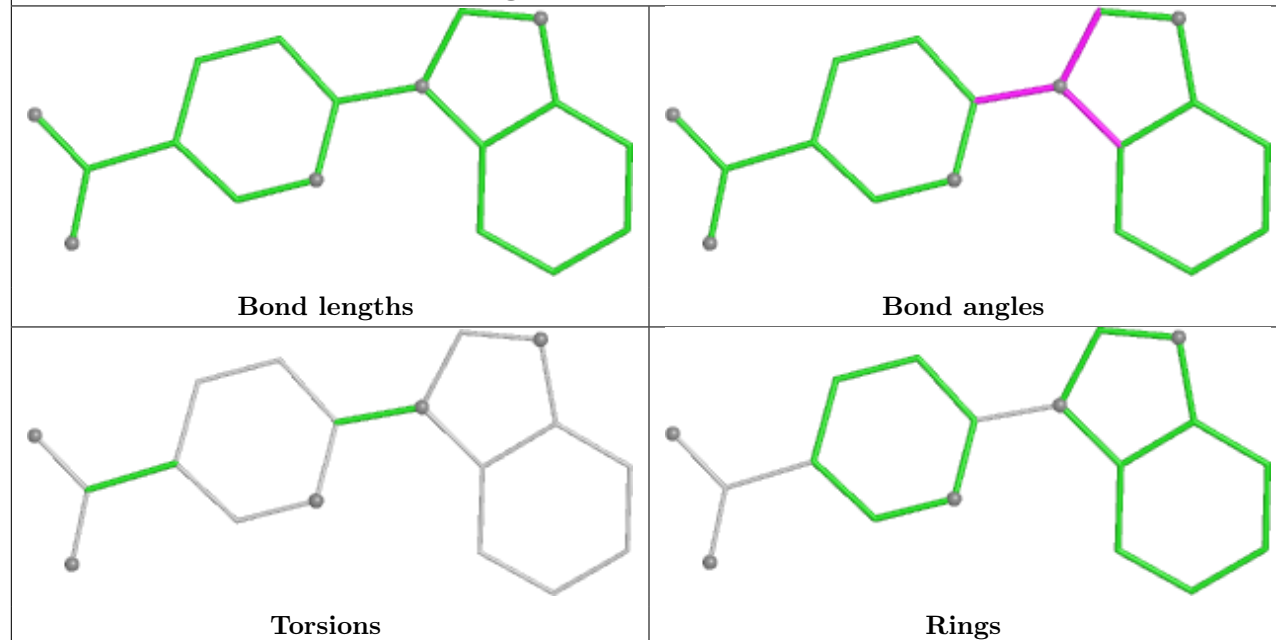
Ligand A1KCG Q 301



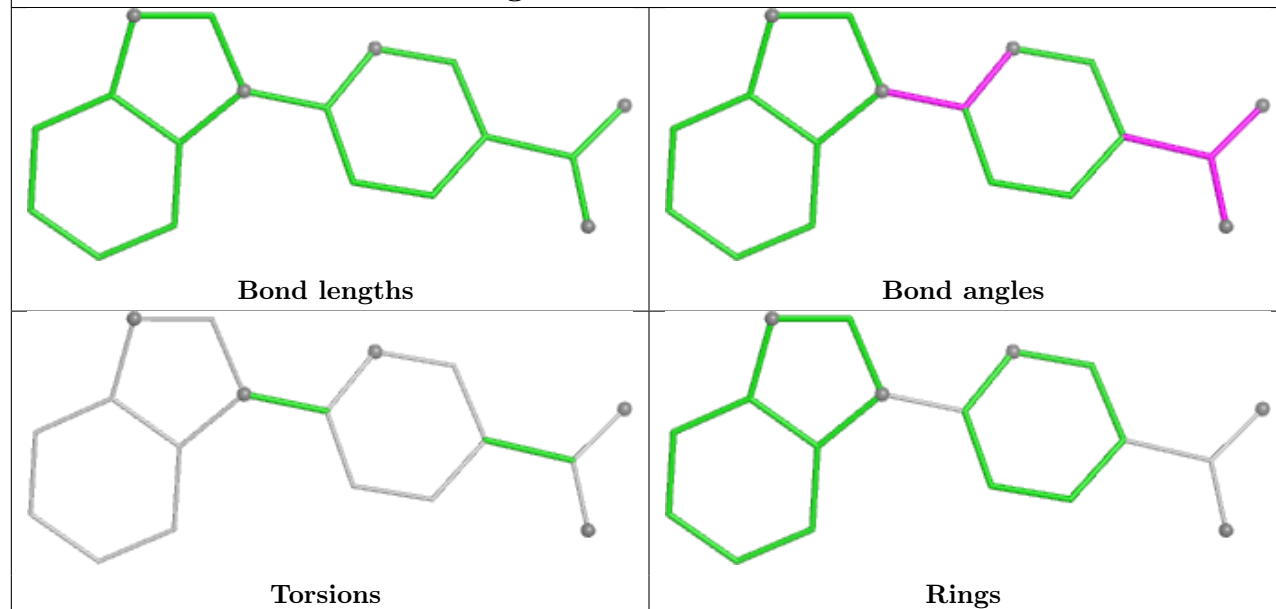
Ligand A1KCG D 303



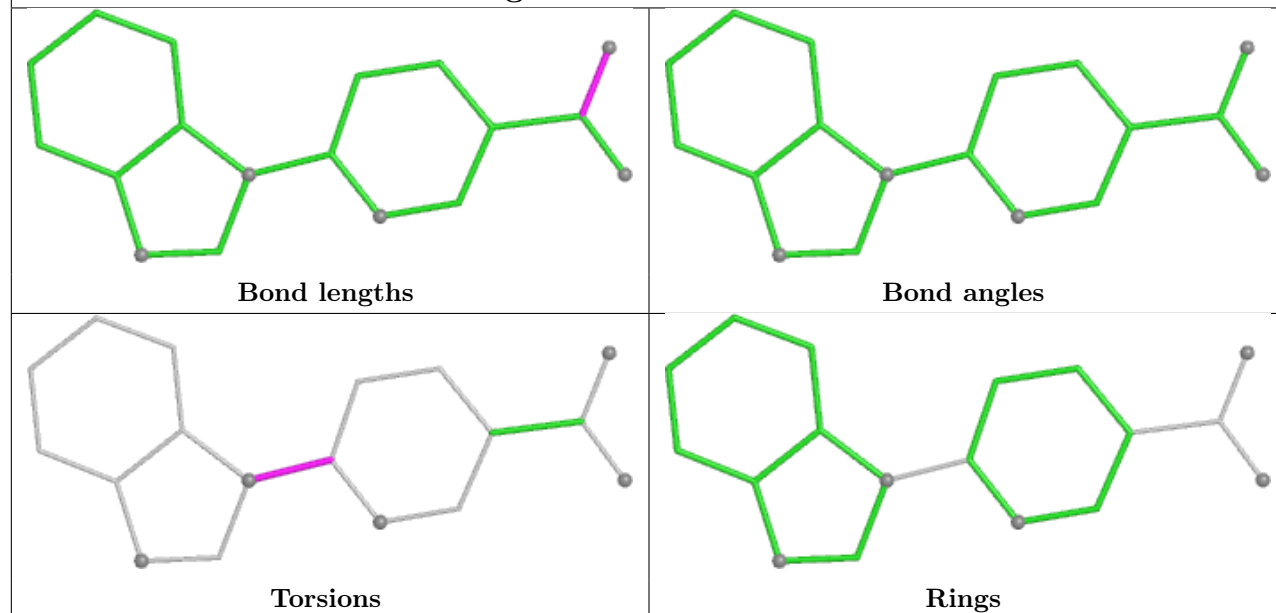
Ligand A1KCG M 301



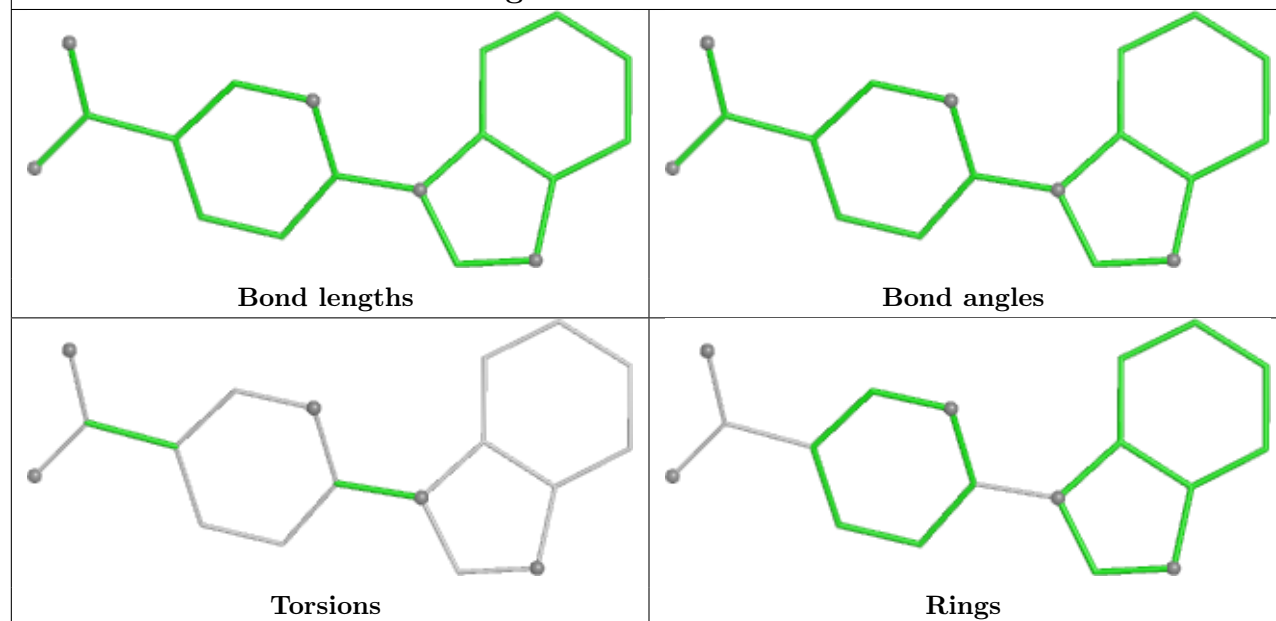
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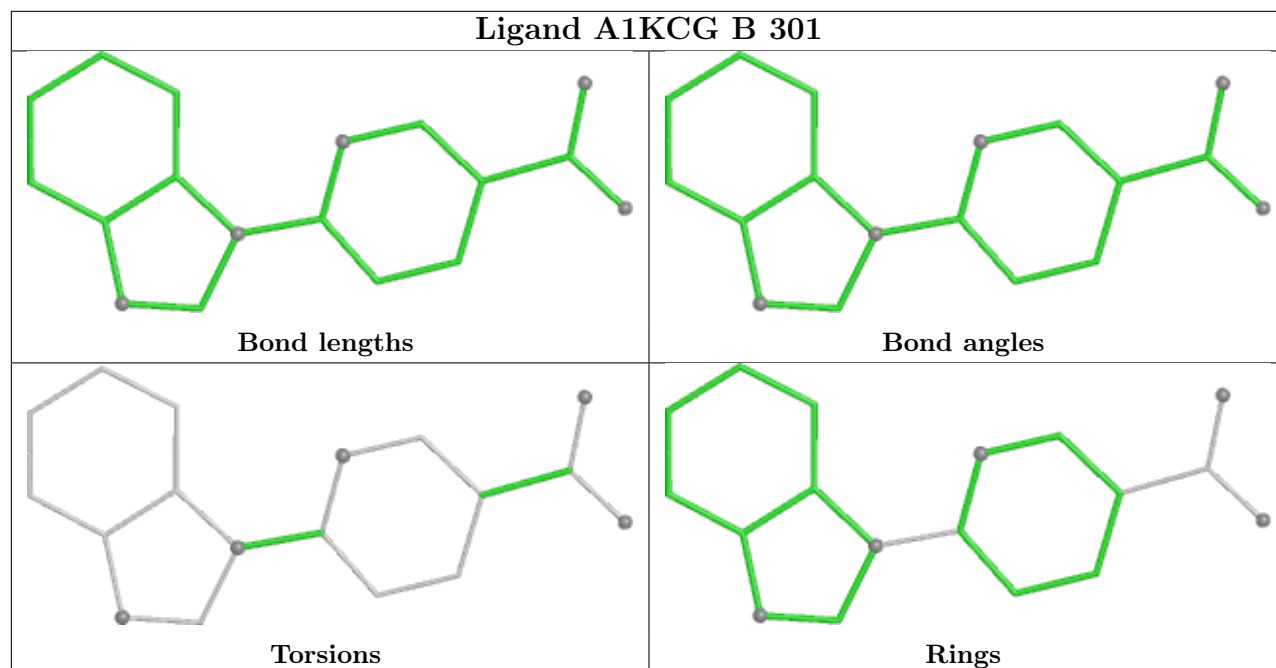
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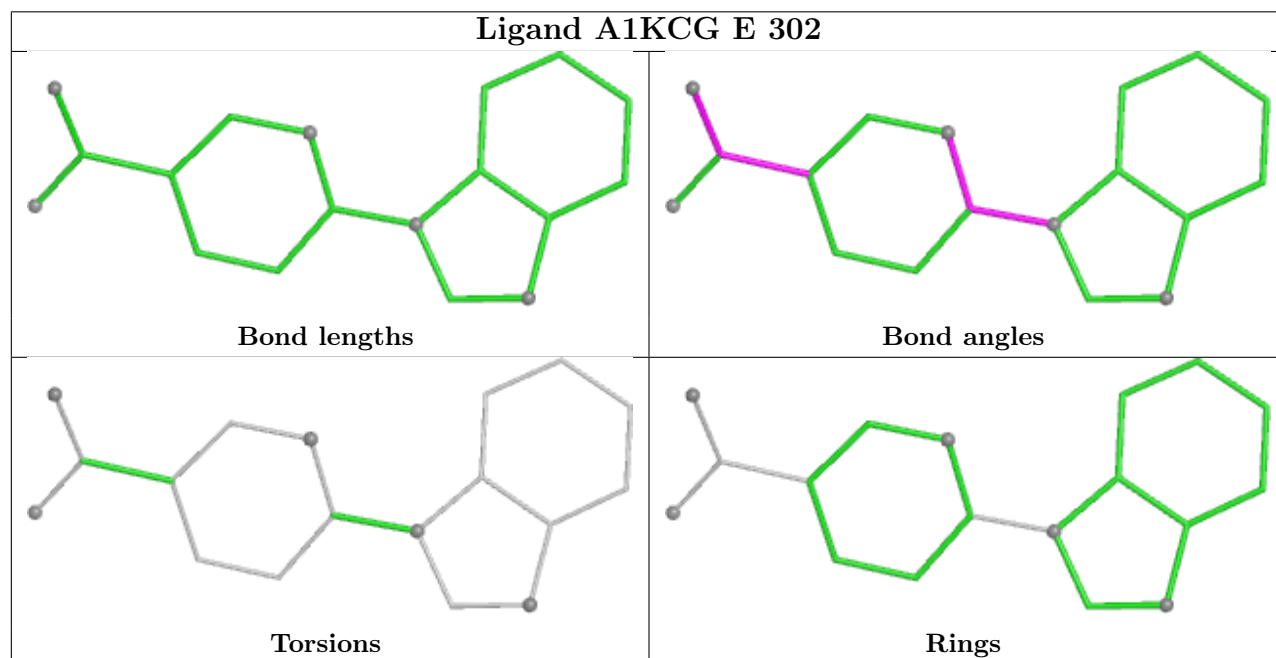
Ligand A1KCG U 302



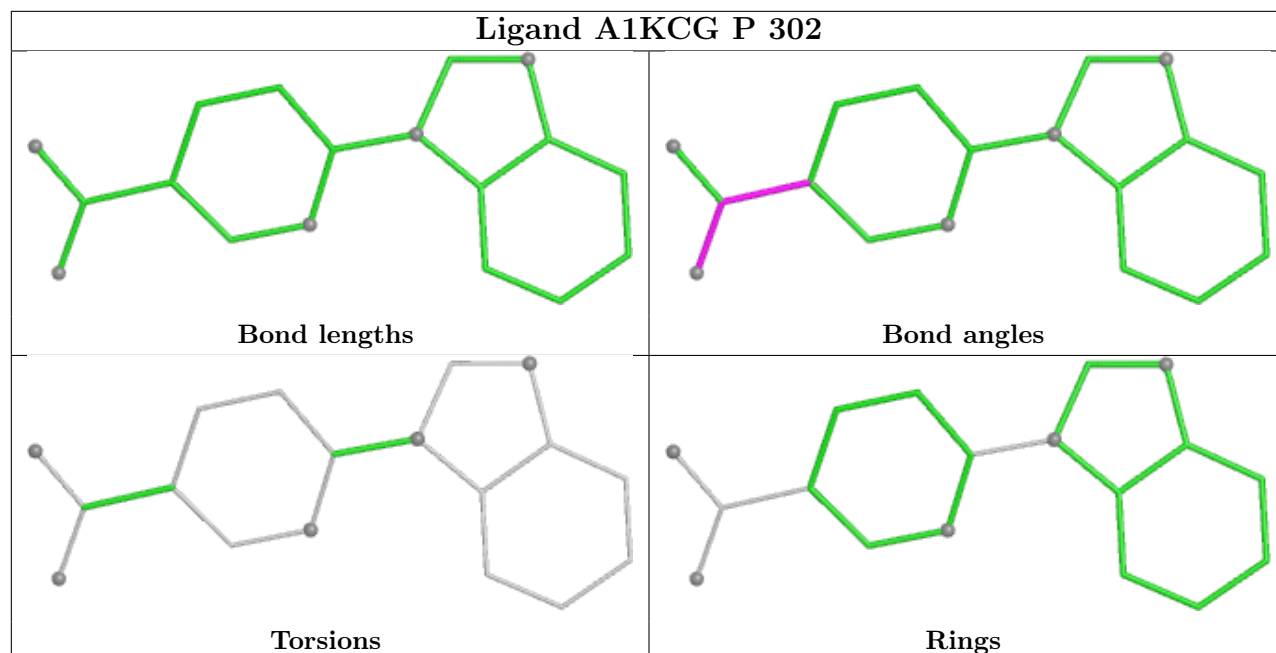
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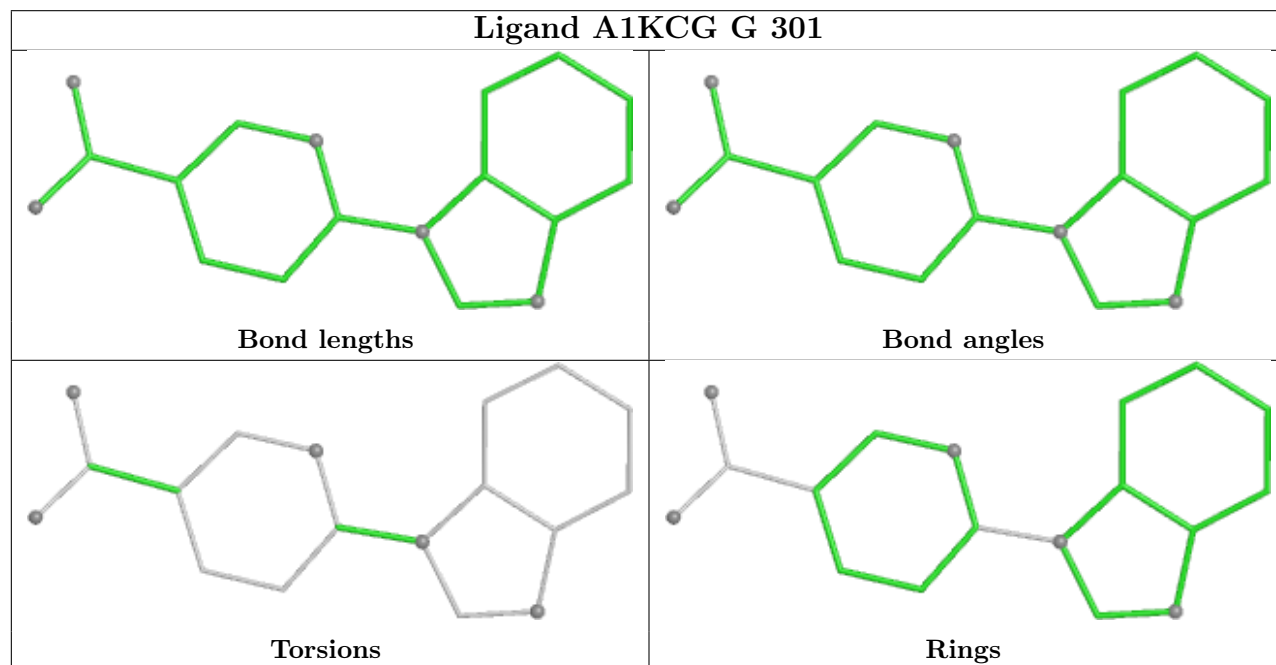
Ligand A1KCG E 302



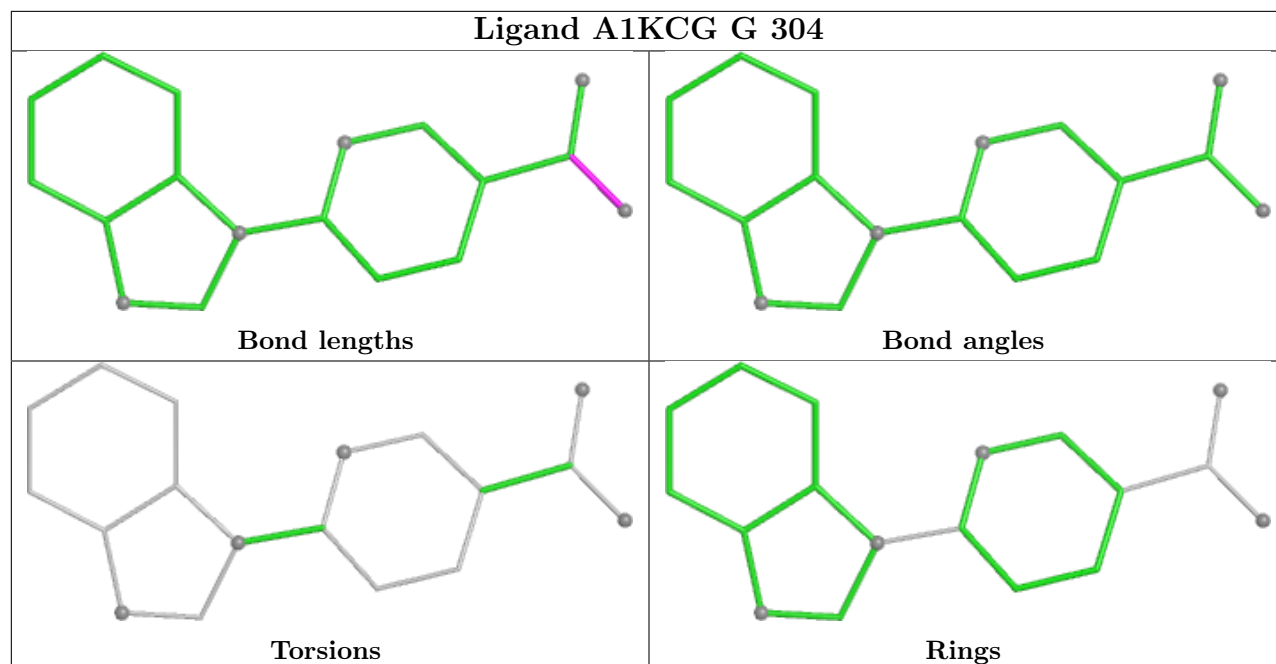
Ligand A1KCG P 302



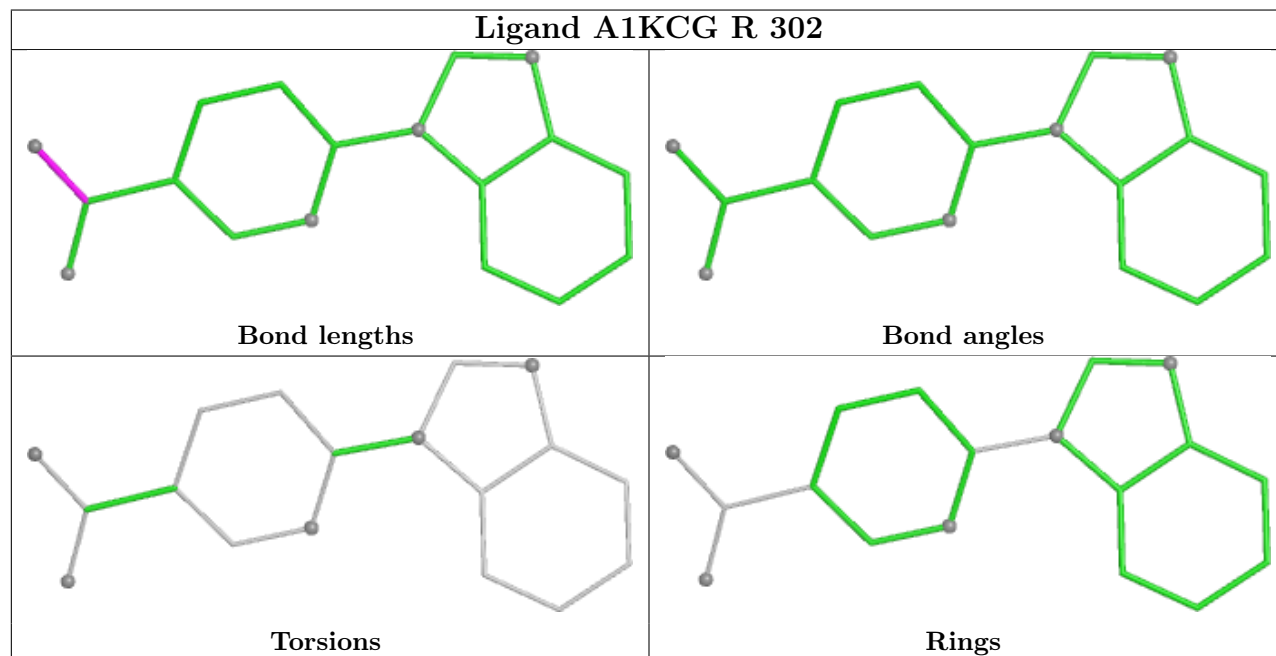
Ligand A1KCG G 301



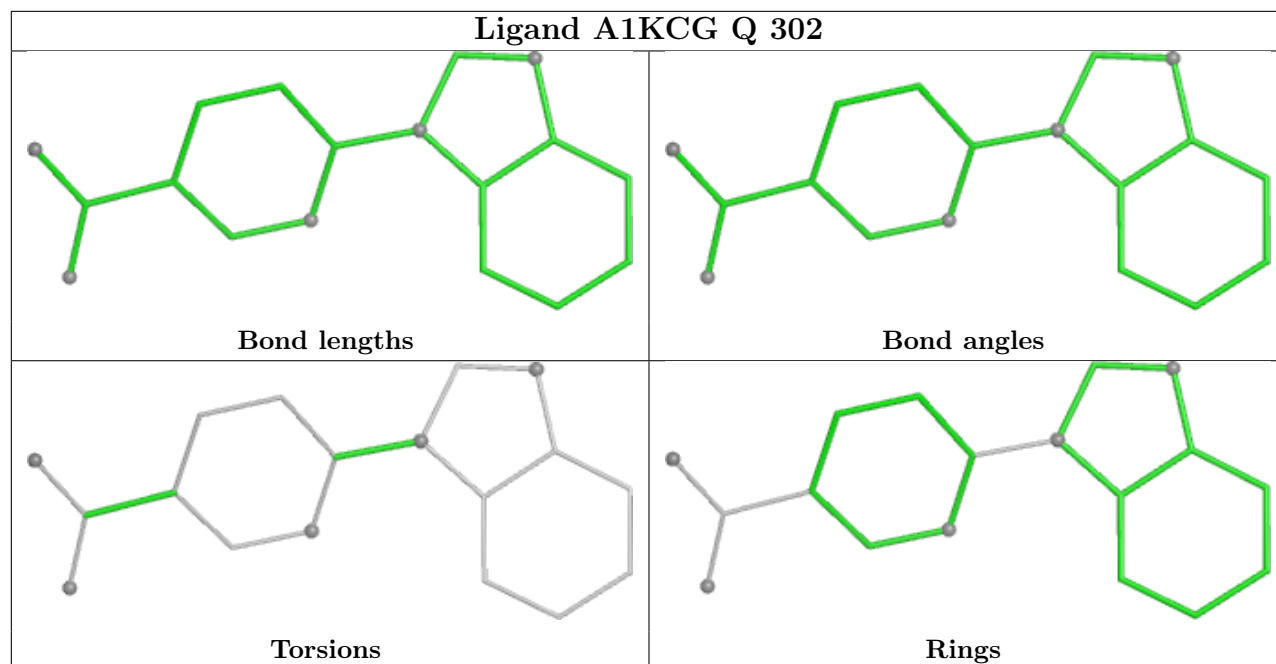
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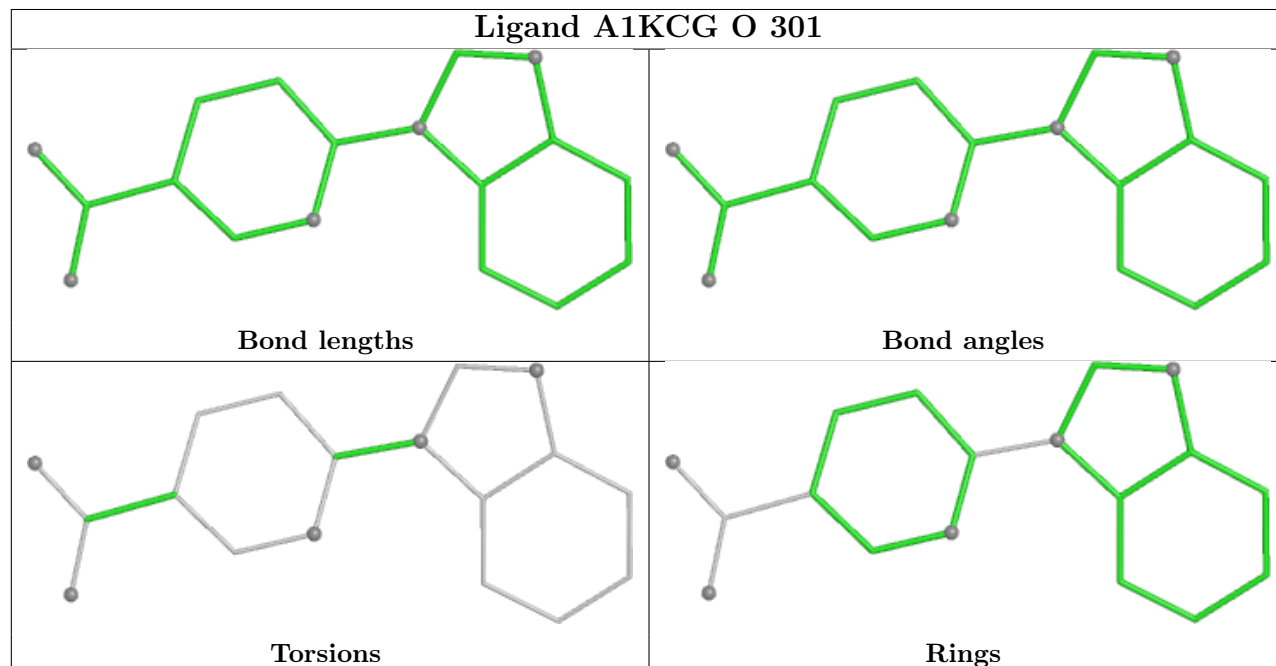
Ligand A1KCG R 302

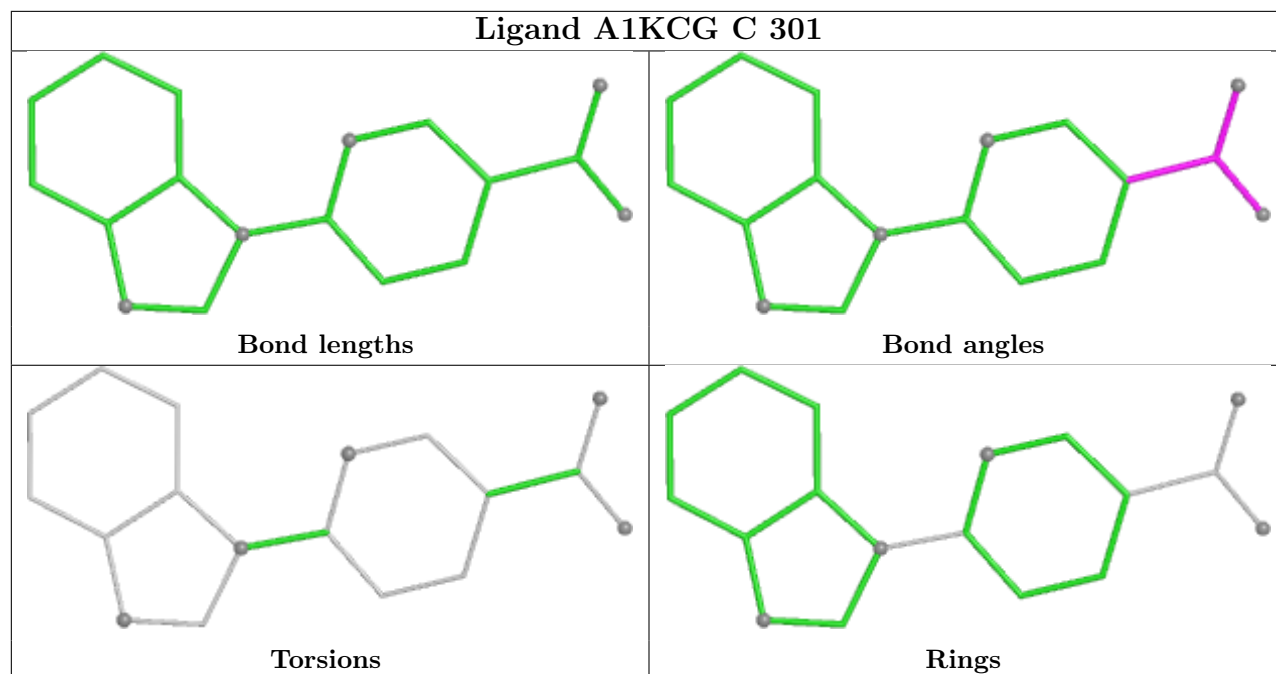


Ligand A1KCG Q 302



Ligand A1KCG O 301





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	186/215 (86%)	0.33	11 (5%)	28 30	16, 44, 108, 135	2 (1%)
1	B	188/215 (87%)	0.17	13 (6%)	23 24	15, 39, 87, 127	3 (1%)
1	C	188/215 (87%)	0.13	12 (6%)	25 27	15, 37, 99, 132	2 (1%)
1	D	189/215 (87%)	0.21	13 (6%)	23 24	16, 37, 105, 138	1 (0%)
1	E	189/215 (87%)	0.14	9 (4%)	35 38	17, 36, 85, 129	2 (1%)
1	F	187/215 (86%)	0.22	13 (6%)	22 24	17, 40, 87, 122	2 (1%)
1	G	187/215 (86%)	0.49	19 (10%)	12 12	26, 48, 110, 135	0
1	H	189/215 (87%)	0.92	33 (17%)	4 4	31, 55, 105, 132	0
1	I	186/215 (86%)	1.26	39 (20%)	2 2	25, 63, 136, 168	2 (1%)
1	J	187/215 (86%)	1.42	47 (25%)	1 2	28, 61, 137, 167	1 (0%)
1	K	187/215 (86%)	1.09	36 (19%)	3 3	21, 56, 132, 156	1 (0%)
1	L	188/215 (87%)	0.25	11 (5%)	28 30	17, 39, 103, 134	2 (1%)
1	M	189/215 (87%)	0.39	14 (7%)	20 22	24, 40, 82, 116	0
1	N	187/215 (86%)	0.39	15 (8%)	18 19	27, 42, 100, 134	1 (0%)
1	O	187/215 (86%)	0.36	16 (8%)	16 17	17, 40, 104, 137	3 (1%)
1	P	187/215 (86%)	0.26	16 (8%)	16 17	15, 37, 87, 141	1 (0%)
1	Q	188/215 (87%)	0.29	18 (9%)	13 14	16, 37, 97, 129	3 (1%)
1	R	187/215 (86%)	0.20	10 (5%)	32 34	17, 39, 83, 137	1 (0%)
1	S	188/215 (87%)	0.30	15 (7%)	18 19	18, 42, 102, 138	1 (0%)
1	T	187/215 (86%)	0.42	18 (9%)	13 14	18, 43, 109, 139	2 (1%)
1	U	188/215 (87%)	0.35	18 (9%)	13 14	26, 41, 94, 135	0
1	V	187/215 (86%)	0.32	17 (9%)	15 15	18, 40, 93, 133	2 (1%)
All	All	4126/4730 (87%)	0.45	413 (10%)	12 13	15, 44, 105, 168	32 (0%)

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	25	CYS	6.2
1	T	184	LEU	5.5
1	N	184	LEU	5.5
1	Q	184	LEU	5.4
1	H	60	GLY	5.3
1	M	184	LEU	5.2
1	Q	25	CYS	5.1
1	K	179	PRO	5.0
1	C	211	ASN	5.0
1	A	184	LEU	5.0
1	K	29	CYS	4.9
1	H	59	GLY	4.9
1	U	24	LEU	4.7
1	D	24	LEU	4.7
1	P	182	LEU	4.7
1	J	184	LEU	4.7
1	L	184	LEU	4.6
1	U	210	PRO	4.6
1	K	57	ALA	4.6
1	B	24	LEU	4.6
1	D	167	LEU	4.6
1	I	210	PRO	4.5
1	S	210	PRO	4.5
1	T	209	ARG	4.5
1	K	182	LEU	4.4
1	Q	24	LEU	4.4
1	G	210	PRO	4.3
1	H	210	PRO	4.3
1	H	56	MET	4.3
1	K	25	CYS	4.2
1	C	184	LEU	4.2
1	H	184	LEU	4.2
1	N	24	LEU	4.2
1	F	25	CYS	4.1
1	M	210	PRO	4.1
1	K	167	LEU	4.1
1	P	184	LEU	4.1
1	T	210	PRO	4.1
1	H	24	LEU	4.1
1	E	184	LEU	4.0
1	F	182	LEU	4.0
1	V	211	ASN	4.0
1	L	24	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	J	52	ILE	3.9
1	R	210	PRO	3.9
1	M	24	LEU	3.9
1	S	24	LEU	3.9
1	M	57	ALA	3.9
1	U	184	LEU	3.9
1	L	210	PRO	3.9
1	K	104	TYR	3.8
1	M	211	ASN	3.8
1	E	24	LEU	3.8
1	P	210	PRO	3.8
1	M	60	GLY	3.8
1	O	209	ARG	3.8
1	K	37	GLN	3.8
1	O	167	LEU	3.8
1	H	57	ALA	3.7
1	I	208	CYS	3.7
1	E	167	LEU	3.7
1	J	179	PRO	3.7
1	D	212	MET	3.7
1	N	182	LEU	3.6
1	D	183	PRO	3.6
1	T	57	ALA	3.6
1	S	184	LEU	3.6
1	H	188	LEU	3.6
1	N	210	PRO	3.6
1	V	184	LEU	3.6
1	K	209	ARG	3.6
1	J	210	PRO	3.6
1	G	167	LEU	3.6
1	H	211	ASN	3.5
1	T	211	ASN	3.5
1	J	194	GLN	3.5
1	I	48	GLY	3.5
1	I	182	LEU	3.5
1	O	184	LEU	3.5
1	K	180	ARG	3.5
1	I	59	GLY	3.4
1	D	182	LEU	3.4
1	I	175	LEU	3.4
1	H	190	LYS	3.4
1	C	210	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	O	210	PRO	3.4
1	J	172	LEU	3.4
1	K	175	LEU	3.4
1	I	104	TYR	3.4
1	B	55[A]	ARG	3.4
1	D	184	LEU	3.4
1	S	59	GLY	3.3
1	U	166	ILE	3.3
1	I	183	PRO	3.3
1	V	60	GLY	3.3
1	V	104	TYR	3.3
1	B	210	PRO	3.3
1	J	171	TYR	3.3
1	J	199	SER	3.2
1	U	209	ARG	3.2
1	H	58	GLY	3.2
1	B	179	PRO	3.2
1	E	57	ALA	3.2
1	R	211	ASN	3.2
1	B	175	LEU	3.2
1	K	184	LEU	3.2
1	L	167	LEU	3.2
1	K	48	GLY	3.2
1	A	210	PRO	3.2
1	K	183	PRO	3.2
1	Q	210	PRO	3.2
1	G	211	ASN	3.2
1	F	57	ALA	3.2
1	K	188	LEU	3.2
1	T	167	LEU	3.2
1	V	209	ARG	3.2
1	O	29	CYS	3.2
1	J	167	LEU	3.1
1	H	62	LYS	3.1
1	V	29	CYS	3.1
1	I	57	ALA	3.1
1	J	188	LEU	3.1
1	O	104[A]	TYR	3.1
1	K	56	MET	3.1
1	P	183	PRO	3.1
1	H	200	VAL	3.1
1	I	205	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	211	ASN	3.1
1	C	99[A]	ASN	3.1
1	O	179	PRO	3.1
1	U	211	ASN	3.1
1	O	182	LEU	3.1
1	V	210	PRO	3.0
1	D	29	CYS	3.0
1	H	208	CYS	3.0
1	K	177	LYS	3.0
1	T	182	LEU	3.0
1	M	209	ARG	3.0
1	P	211	ASN	3.0
1	H	186	VAL	3.0
1	J	186	VAL	3.0
1	J	166	ILE	3.0
1	Q	57	ALA	2.9
1	J	211	ASN	2.9
1	S	211	ASN	2.9
1	M	58	GLY	2.9
1	Q	58	GLY	2.9
1	S	60	GLY	2.9
1	T	25	CYS	2.9
1	J	193	ARG	2.9
1	K	176	ASN	2.9
1	I	133	ALA	2.9
1	V	59	GLY	2.9
1	P	29	CYS	2.9
1	I	52	ILE	2.9
1	P	209	ARG	2.9
1	J	183	PRO	2.9
1	J	207	SER	2.9
1	J	57	ALA	2.9
1	J	58	GLY	2.9
1	H	182	LEU	2.8
1	H	209	ARG	2.8
1	K	44	ARG	2.8
1	N	205	TYR	2.8
1	F	209	ARG	2.8
1	J	209	ARG	2.8
1	S	58	GLY	2.8
1	I	178	LEU	2.8
1	P	167	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	V	167	LEU	2.8
1	P	208	CYS	2.8
1	E	210	PRO	2.8
1	K	52	ILE	2.8
1	Q	166	ILE	2.8
1	T	156[A]	ARG	2.8
1	E	182	LEU	2.8
1	H	199	SER	2.8
1	F	194	GLN	2.8
1	G	60	GLY	2.8
1	K	33	ALA	2.8
1	I	186	VAL	2.8
1	I	190	LYS	2.7
1	K	178	LEU	2.7
1	M	182	LEU	2.7
1	O	178	LEU	2.7
1	B	184	LEU	2.7
1	I	98	LEU	2.7
1	K	172	LEU	2.7
1	Q	167	LEU	2.7
1	R	205	TYR	2.7
1	D	210	PRO	2.7
1	F	210	PRO	2.7
1	K	211	ASN	2.7
1	O	211	ASN	2.7
1	J	56	MET	2.7
1	K	63	VAL	2.7
1	S	56	MET	2.7
1	J	208	CYS	2.7
1	L	29	CYS	2.7
1	G	131	GLY	2.7
1	N	209	ARG	2.7
1	S	209	ARG	2.7
1	V	57	ALA	2.7
1	L	179	PRO	2.7
1	G	104	TYR	2.7
1	J	68	GLY	2.7
1	P	58	GLY	2.7
1	D	57	ALA	2.6
1	G	182	LEU	2.6
1	I	196	LEU	2.6
1	J	47	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	Q	100	ASN	2.6
1	Q	182	LEU	2.6
1	L	183	PRO	2.6
1	J	66	ILE	2.6
1	M	212	MET	2.6
1	I	191	ALA	2.6
1	J	206	ASN	2.6
1	R	99	ASN	2.6
1	I	137	LEU	2.6
1	F	207	SER	2.6
1	G	205	TYR	2.6
1	I	25	CYS	2.6
1	H	131	GLY	2.6
1	A	188	LEU	2.6
1	H	187	ASP	2.6
1	I	156[A]	ARG	2.6
1	F	104	TYR	2.6
1	K	131	GLY	2.6
1	U	59	GLY	2.6
1	C	212	MET	2.6
1	K	99	ASN	2.6
1	P	180	ARG	2.6
1	R	55	ARG	2.6
1	C	182	LEU	2.6
1	J	175	LEU	2.6
1	J	182	LEU	2.6
1	D	166	ILE	2.5
1	T	166	ILE	2.5
1	A	209	ARG	2.5
1	G	191	ALA	2.5
1	U	57	ALA	2.5
1	N	181	GLN	2.5
1	G	186	VAL	2.5
1	H	63	VAL	2.5
1	I	63	VAL	2.5
1	B	180	ARG	2.5
1	L	211	ASN	2.5
1	J	189	THR	2.5
1	C	183	PRO	2.5
1	T	183	PRO	2.5
1	E	212	MET	2.5
1	A	25	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	29	CYS	2.5
1	J	104	TYR	2.5
1	N	57	ALA	2.5
1	I	132	LEU	2.5
1	B	100	ASN	2.5
1	F	211	ASN	2.5
1	Q	211	ASN	2.5
1	P	25	CYS	2.4
1	G	184	LEU	2.4
1	C	180	ARG	2.4
1	R	209	ARG	2.4
1	T	58	GLY	2.4
1	I	56	MET	2.4
1	H	29	CYS	2.4
1	S	62	LYS	2.4
1	H	167	LEU	2.4
1	M	59	GLY	2.4
1	N	131	GLY	2.4
1	I	49	PRO	2.4
1	K	65	TYR	2.3
1	H	191	ALA	2.3
1	H	175	LEU	2.3
1	H	178	LEU	2.3
1	R	178	LEU	2.3
1	G	209	ARG	2.3
1	J	53	SER	2.3
1	P	186	VAL	2.3
1	V	207	SER	2.3
1	G	29	CYS	2.3
1	B	57	ALA	2.3
1	I	203	ALA	2.3
1	S	57	ALA	2.3
1	M	176	ASN	2.3
1	N	176	ASN	2.3
1	U	99	ASN	2.3
1	V	182	LEU	2.3
1	I	209	ARG	2.3
1	O	56	MET	2.3
1	I	207	SER	2.3
1	H	185	GLU	2.3
1	I	96	VAL	2.3
1	J	49	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	99[A]	ASN	2.3
1	H	203	ALA	2.3
1	A	178	LEU	2.3
1	J	48	GLY	2.3
1	N	60	GLY	2.3
1	S	177	LYS	2.3
1	L	56	MET	2.3
1	J	32	THR	2.3
1	K	160	ASN	2.3
1	C	177	LYS	2.3
1	G	188	LEU	2.3
1	J	178	LEU	2.3
1	U	155	LEU	2.3
1	G	63	VAL	2.2
1	J	63	VAL	2.2
1	N	183	PRO	2.2
1	M	180	ARG	2.2
1	P	177	LYS	2.2
1	B	58	GLY	2.2
1	G	59	GLY	2.2
1	O	131	GLY	2.2
1	V	56	MET	2.2
1	F	184	LEU	2.2
1	L	182	LEU	2.2
1	M	174	SER	2.2
1	D	209	ARG	2.2
1	L	186	VAL	2.2
1	D	59	GLY	2.2
1	Q	133	ALA	2.2
1	F	29	CYS	2.2
1	A	196	LEU	2.2
1	I	188	LEU	2.2
1	U	167	LEU	2.2
1	U	182	LEU	2.2
1	K	181	GLN	2.2
1	J	65	TYR	2.2
1	D	56	MET	2.2
1	F	56	MET	2.2
1	K	166	ILE	2.2
1	T	179	PRO	2.2
1	T	186	VAL	2.2
1	V	63	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	130	GLU	2.2
1	K	185	GLU	2.2
1	I	109	ALA	2.2
1	J	203	ALA	2.2
1	I	155	LEU	2.2
1	J	162	LEU	2.2
1	N	132	LEU	2.2
1	S	182	LEU	2.2
1	Q	209	ARG	2.2
1	C	61	GLN	2.1
1	H	136	ALA	2.1
1	I	184	LEU	2.1
1	Q	173	ARG	2.1
1	J	64	CYS	2.1
1	I	199	SER	2.1
1	U	174	SER	2.1
1	J	177	LYS	2.1
1	P	62	LYS	2.1
1	O	176	ASN	2.1
1	H	166	ILE	2.1
1	C	59	GLY	2.1
1	H	101	GLY	2.1
1	J	101	GLY	2.1
1	Q	60	GLY	2.1
1	R	58	GLY	2.1
1	U	63	VAL	2.1
1	U	186	VAL	2.1
1	K	173	ARG	2.1
1	U	173	ARG	2.1
1	C	57	ALA	2.1
1	R	57	ALA	2.1
1	B	178	LEU	2.1
1	O	208	CYS	2.1
1	U	207	SER	2.1
1	A	183	PRO	2.1
1	H	61	GLN	2.1
1	H	179	PRO	2.1
1	Q	179	PRO	2.1
1	S	181	GLN	2.1
1	S	183	PRO	2.1
1	B	209	ARG	2.1
1	J	133	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	Q	178	LEU	2.1
1	R	207	SER	2.1
1	T	54	SER	2.1
1	I	201	GLU	2.1
1	N	56	MET	2.1
1	T	99	ASN	2.1
1	G	194	GLN	2.1
1	A	179	PRO	2.1
1	O	183	PRO	2.1
1	P	179	PRO	2.1
1	J	131	GLY	2.1
1	A	166	ILE	2.1
1	V	62	LYS	2.1
1	K	161	ALA	2.1
1	K	207	SER	2.1
1	E	56	MET	2.0
1	F	167	LEU	2.0
1	G	137	LEU	2.0
1	J	195	ASP	2.0
1	T	61	GLN	2.0
1	V	194	GLN	2.0
1	J	46	ARG	2.0
1	G	183	PRO	2.0
1	I	80	GLY	2.0
1	I	200	VAL	2.0
1	U	56	MET	2.0
1	J	136	ALA	2.0
1	J	99	ASN	2.0
1	Q	181	GLN	2.0
1	N	180	ARG	2.0
1	A	58	GLY	2.0
1	E	58	GLY	2.0
1	I	60	GLY	2.0
1	T	131	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1KCG	G	301	18/18	0.68	0.21	53,110,139,140	0
2	A1KCG	V	301	18/18	0.73	0.17	60,96,110,112	0
2	A1KCG	C	302	18/18	0.74	0.17	46,69,74,78	0
2	A1KCG	R	302	18/18	0.74	0.17	43,68,74,75	0
2	A1KCG	D	303	18/18	0.74	0.19	44,92,120,121	0
2	A1KCG	K	301	18/18	0.75	0.20	57,101,110,113	0
2	A1KCG	F	301	18/18	0.75	0.17	53,98,108,108	0
2	A1KCG	D	301	18/18	0.75	0.17	42,89,108,110	0
2	A1KCG	L	304	18/18	0.76	0.18	47,85,102,103	0
2	A1KCG	O	301	18/18	0.76	0.17	51,90,113,114	0
2	A1KCG	T	301	18/18	0.77	0.18	53,107,127,127	0
2	A1KCG	M	301	18/18	0.78	0.15	48,84,103,108	0
3	EDO	I	301	4/4	0.78	0.19	52,60,63,64	0
3	EDO	N	306	4/4	0.78	0.18	61,67,71,79	0
2	A1KCG	U	302	18/18	0.79	0.17	56,86,95,101	0
2	A1KCG	L	301	18/18	0.79	0.17	57,79,88,89	0
2	A1KCG	C	301	18/18	0.79	0.16	43,64,93,98	0
2	A1KCG	F	302	18/18	0.79	0.16	56,89,96,96	0
2	A1KCG	S	301	18/18	0.80	0.17	46,88,111,113	0
3	EDO	P	301	4/4	0.80	0.18	56,56,57,62	0
2	A1KCG	E	302	18/18	0.81	0.16	42,73,83,84	0
2	A1KCG	S	302	18/18	0.81	0.16	62,80,84,90	0
3	EDO	M	303	4/4	0.81	0.17	61,62,66,73	0
3	EDO	M	305	4/4	0.81	0.19	50,55,60,66	0
2	A1KCG	R	301	18/18	0.81	0.16	39,57,82,84	0
2	A1KCG	B	302	18/18	0.81	0.14	43,54,58,59	0
2	A1KCG	H	301	18/18	0.82	0.15	53,88,113,114	0
3	EDO	R	308	4/4	0.82	0.16	65,76,77,77	0
2	A1KCG	Q	301	18/18	0.83	0.14	46,69,86,90	0
3	EDO	S	305	4/4	0.83	0.17	47,56,60,64	0
3	EDO	C	304	4/4	0.84	0.16	56,57,57,57	0
2	A1KCG	N	303	18/18	0.84	0.15	53,80,90,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	J	302	4/4	0.84	0.17	55,63,65,65	0
5	CL	G	306	1/1	0.84	0.20	79,79,79,79	0
3	EDO	K	302	4/4	0.85	0.17	45,53,60,63	0
4	MG	A	306	1/1	0.85	0.20	70,70,70,70	0
4	MG	M	304	1/1	0.85	0.10	70,70,70,70	0
5	CL	E	306	1/1	0.85	0.18	67,67,67,67	0
3	EDO	O	303	4/4	0.85	0.17	45,51,54,54	0
3	EDO	Q	306	4/4	0.86	0.18	61,66,67,71	0
2	A1KCG	B	301	18/18	0.86	0.12	43,54,88,89	0
3	EDO	E	303	4/4	0.86	0.15	42,55,56,57	0
3	EDO	L	306	4/4	0.86	0.17	44,59,60,65	0
3	EDO	A	303	4/4	0.86	0.19	47,56,56,64	0
3	EDO	Q	303	4/4	0.86	0.18	36,46,48,54	0
3	EDO	Q	304	4/4	0.86	0.15	42,53,58,58	0
3	EDO	R	307	4/4	0.87	0.16	50,60,62,63	0
2	A1KCG	G	304	18/18	0.87	0.13	59,77,84,85	0
3	EDO	O	305	4/4	0.87	0.20	58,68,68,77	0
3	EDO	H	302	4/4	0.87	0.15	59,62,64,67	0
4	MG	L	305	1/1	0.87	0.11	71,71,71,71	0
3	EDO	N	305	4/4	0.87	0.16	44,59,60,62	0
2	A1KCG	P	302	18/18	0.87	0.12	46,55,60,61	0
3	EDO	O	302	4/4	0.87	0.14	40,49,50,56	0
3	EDO	Q	307	4/4	0.88	0.17	59,62,64,65	0
3	EDO	R	303	4/4	0.88	0.15	45,58,58,59	0
2	A1KCG	Q	302	18/18	0.88	0.11	38,51,57,61	0
3	EDO	A	304	4/4	0.88	0.14	44,48,50,57	0
5	CL	A	308	1/1	0.88	0.14	79,79,79,79	0
3	EDO	R	309	4/4	0.88	0.14	52,54,57,58	0
3	EDO	S	304	4/4	0.88	0.13	46,52,60,60	0
5	CL	N	307	1/1	0.88	0.19	88,88,88,88	0
3	EDO	G	305	4/4	0.89	0.14	49,55,57,59	0
3	EDO	B	304	4/4	0.89	0.14	42,55,56,57	0
4	MG	V	303	1/1	0.89	0.10	59,59,59,59	0
3	EDO	D	302	4/4	0.89	0.14	38,46,50,58	0
3	EDO	I	302	4/4	0.89	0.14	53,54,59,61	0
3	EDO	B	306	4/4	0.89	0.15	41,55,61,63	0
5	CL	M	306	1/1	0.89	0.11	76,76,76,76	0
3	EDO	R	306	4/4	0.89	0.16	56,61,64,67	0
5	CL	T	306	1/1	0.89	0.14	78,78,78,78	0
3	EDO	T	303	4/4	0.90	0.18	50,59,60,63	0
4	MG	Q	305	1/1	0.90	0.14	68,68,68,68	0
5	CL	H	303	1/1	0.90	0.15	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	R	305	1/1	0.90	0.10	66,66,66,66	0
3	EDO	P	306	4/4	0.90	0.12	47,52,57,65	0
5	CL	R	310	1/1	0.90	0.16	65,65,65,65	0
3	EDO	B	305	4/4	0.90	0.17	48,56,60,62	0
3	EDO	N	304	4/4	0.91	0.15	69,71,72,73	0
2	A1KCG	A	301	18/18	0.91	0.09	42,49,52,53	0
4	MG	O	304	1/1	0.91	0.08	62,62,62,62	0
3	EDO	A	302	4/4	0.91	0.13	36,41,45,52	0
3	EDO	L	302	4/4	0.91	0.13	41,51,51,65	0
3	EDO	L	303	4/4	0.91	0.15	41,49,56,59	0
3	EDO	D	304	4/4	0.91	0.12	46,52,55,61	0
5	CL	B	307	1/1	0.91	0.14	70,70,70,70	0
3	EDO	L	307	4/4	0.91	0.12	44,56,57,62	0
3	EDO	P	305	4/4	0.91	0.12	69,69,69,71	0
3	EDO	A	307	4/4	0.91	0.14	58,59,61,71	0
3	EDO	J	301	4/4	0.91	0.14	55,56,59,61	0
3	EDO	U	301	4/4	0.91	0.12	40,46,49,57	0
3	EDO	V	302	4/4	0.91	0.12	58,62,64,68	0
3	EDO	N	301	4/4	0.91	0.12	40,46,47,55	0
5	CL	L	308	1/1	0.92	0.17	74,74,74,74	0
3	EDO	C	303	4/4	0.92	0.14	44,53,56,66	0
3	EDO	M	302	4/4	0.92	0.11	44,49,55,58	0
3	EDO	F	303	4/4	0.92	0.12	53,53,55,66	0
5	CL	S	306	1/1	0.92	0.18	79,79,79,79	0
3	EDO	E	301	4/4	0.92	0.11	43,47,52,56	0
5	CL	V	305	1/1	0.92	0.15	80,80,80,80	0
3	EDO	C	305	4/4	0.93	0.13	62,62,63,64	0
3	EDO	G	303	4/4	0.93	0.16	54,68,73,73	0
3	EDO	P	304	4/4	0.93	0.11	37,47,50,51	0
3	EDO	N	302	4/4	0.93	0.10	47,53,56,62	0
3	EDO	V	304	4/4	0.93	0.18	52,53,59,65	0
5	CL	U	304	1/1	0.93	0.12	72,72,72,72	0
3	EDO	E	304	4/4	0.93	0.11	46,49,53,62	0
3	EDO	B	303	4/4	0.94	0.09	35,43,46,53	0
3	EDO	T	304	4/4	0.94	0.12	54,63,64,65	0
3	EDO	T	305	4/4	0.94	0.09	54,56,58,59	0
5	CL	A	309	1/1	0.94	0.17	74,74,74,74	0
5	CL	O	306	1/1	0.94	0.09	83,83,83,83	0
5	CL	O	308	1/1	0.94	0.11	74,74,74,74	0
5	CL	Q	308	1/1	0.94	0.17	72,72,72,72	0
3	EDO	P	303	4/4	0.94	0.10	36,43,48,49	0
5	CL	B	308	1/1	0.94	0.10	74,74,74,74	0

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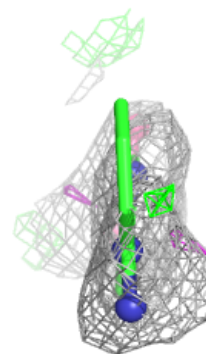
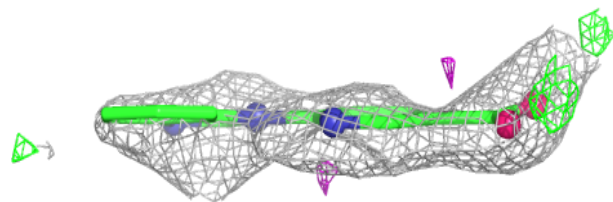
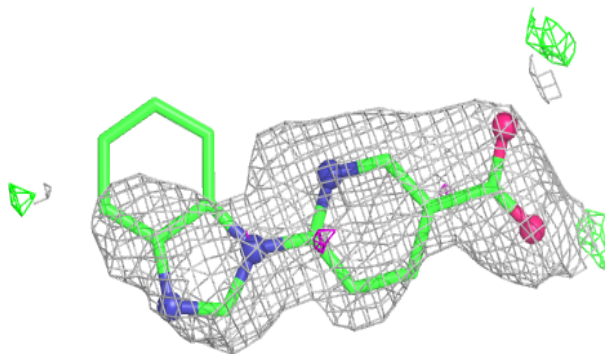
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	C	306	1/1	0.94	0.16	75,75,75,75	0
3	EDO	U	303	4/4	0.94	0.18	43,48,53,54	0
3	EDO	R	304	4/4	0.94	0.11	40,52,55,61	0
5	CL	L	309	1/1	0.95	0.09	79,79,79,79	0
5	CL	P	308	1/1	0.95	0.20	79,79,79,79	0
3	EDO	G	302	4/4	0.95	0.09	44,54,58,59	0
5	CL	O	307	1/1	0.95	0.13	77,77,77,77	0
3	EDO	T	302	4/4	0.96	0.11	47,51,54,63	0
3	EDO	A	305	4/4	0.96	0.10	43,43,51,53	0
3	EDO	S	303	4/4	0.96	0.10	42,51,52,60	0
5	CL	F	304	1/1	0.96	0.17	69,69,69,69	0
5	CL	C	307	1/1	0.97	0.09	77,77,77,77	0
5	CL	D	305	1/1	0.97	0.15	74,74,74,74	0
5	CL	E	305	1/1	0.97	0.15	75,75,75,75	0
5	CL	P	307	1/1	0.98	0.14	67,67,67,67	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.

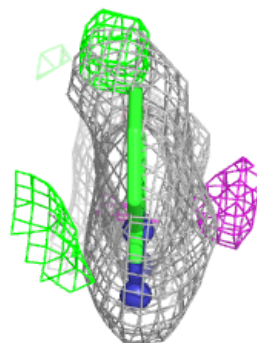
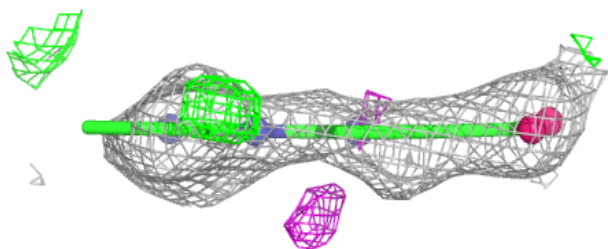
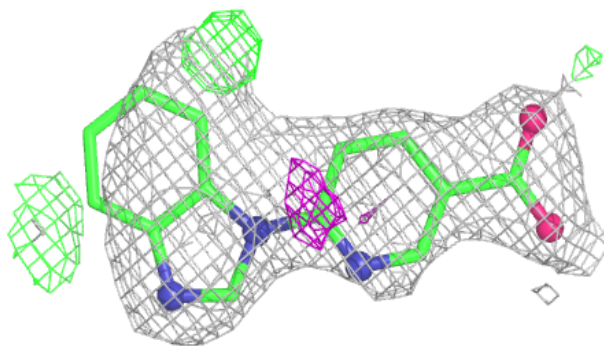
Electron density around A1KCG G 301:

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

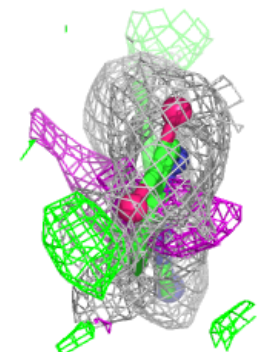
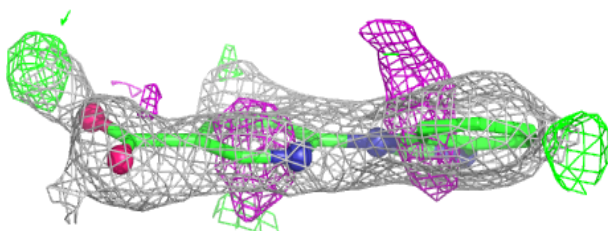
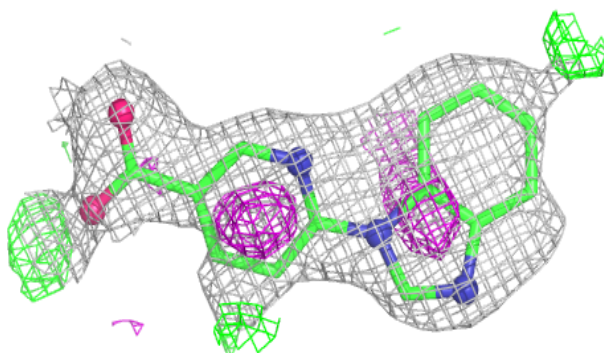


Electron density around A1KCG V 301:

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

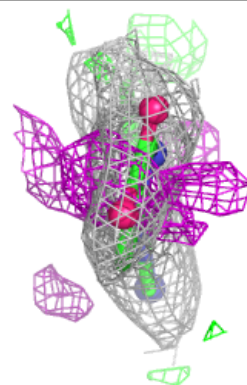
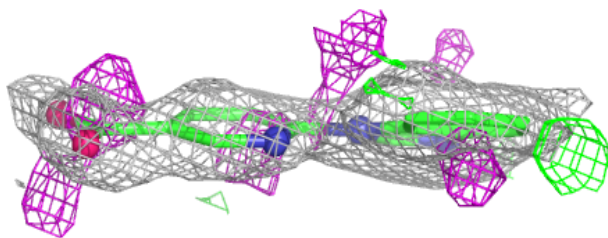
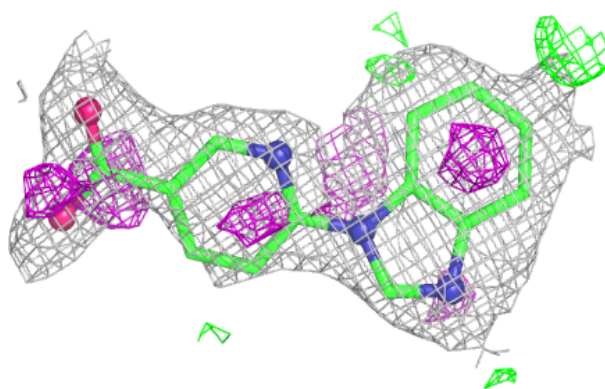
**Electron density around A1KCG C 302:**

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

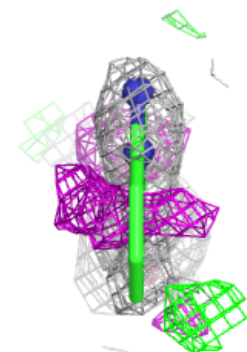
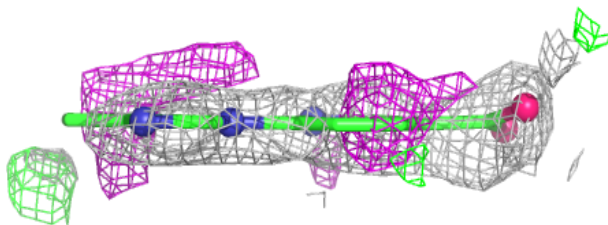
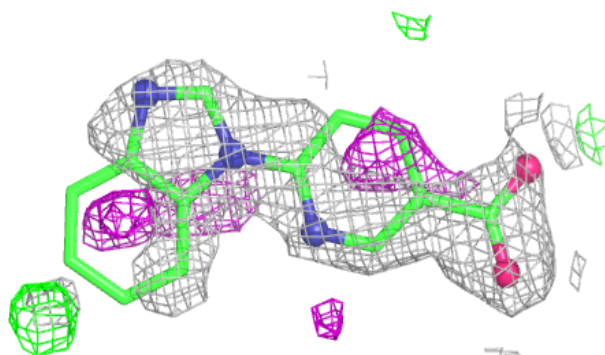


Electron density around A1KCG R 302:

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

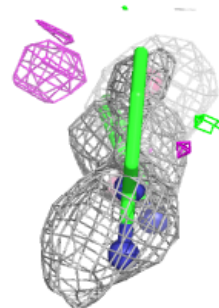
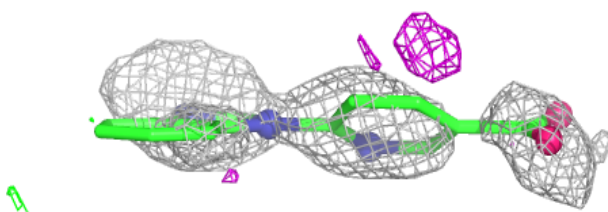
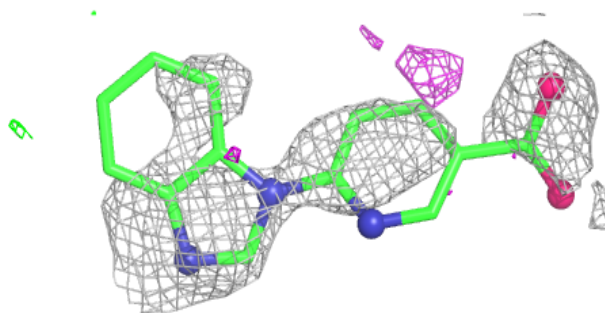
**Electron density around A1KCG D 303:**

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

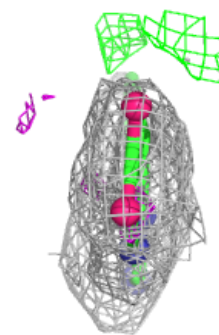
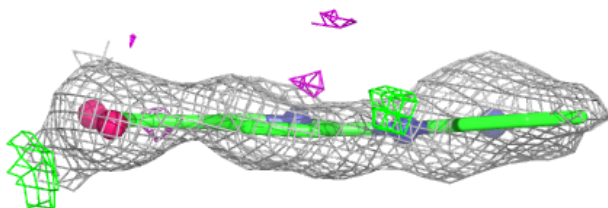
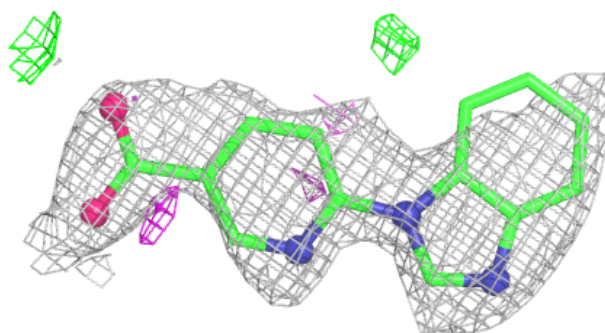


Electron density around A1KCG K 301:

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

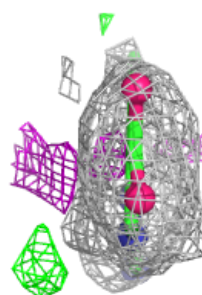
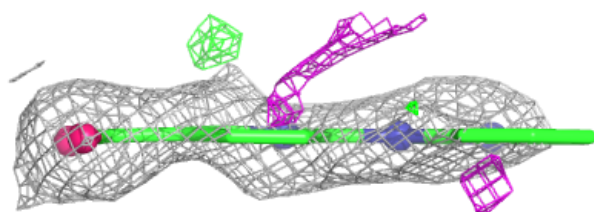
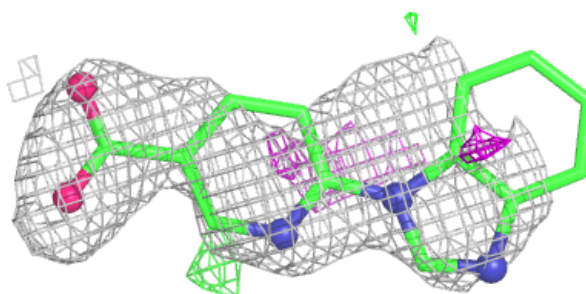
**Electron density around A1KCG F 301:**

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

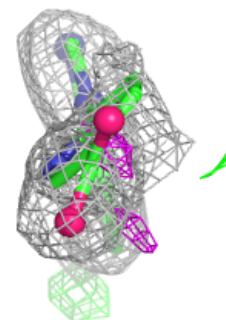
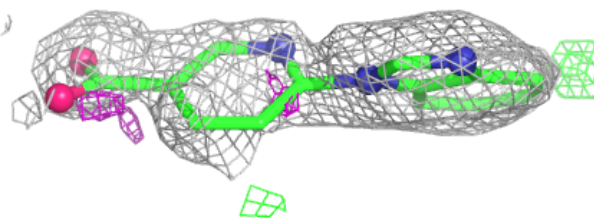
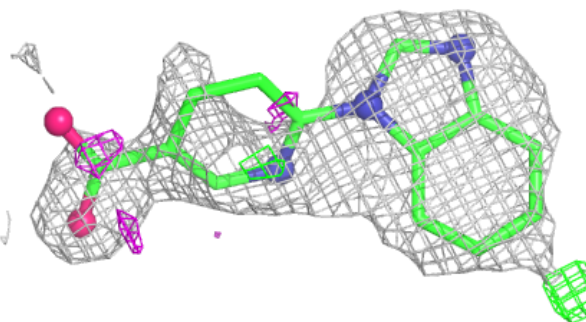


Electron density around A1KCG D 301:

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

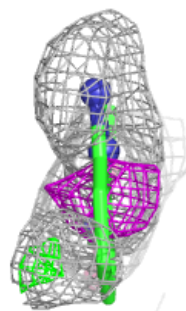
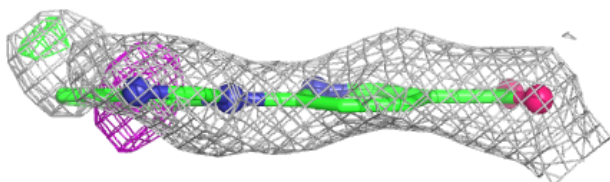
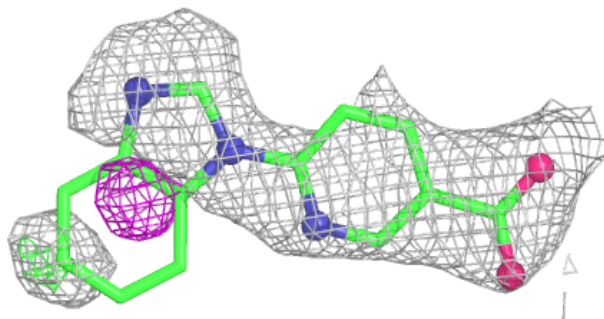
**Electron density around A1KCG L 304:**

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

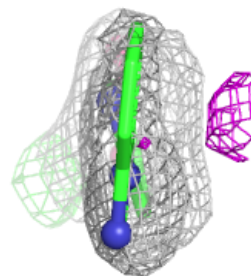
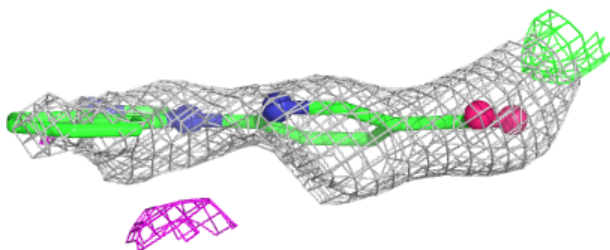
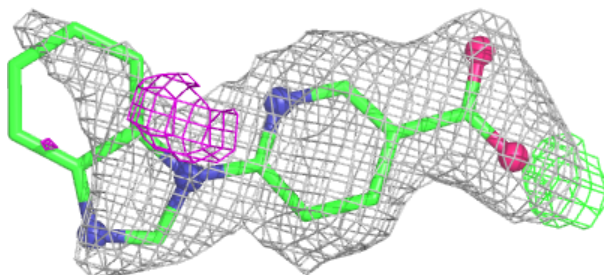


Electron density around A1KCG O 301:

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

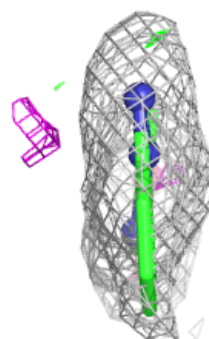
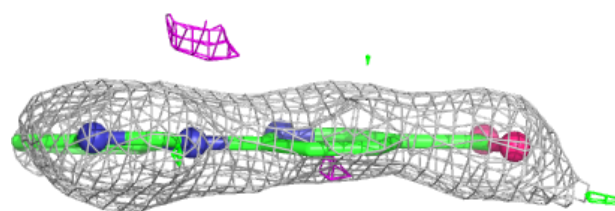
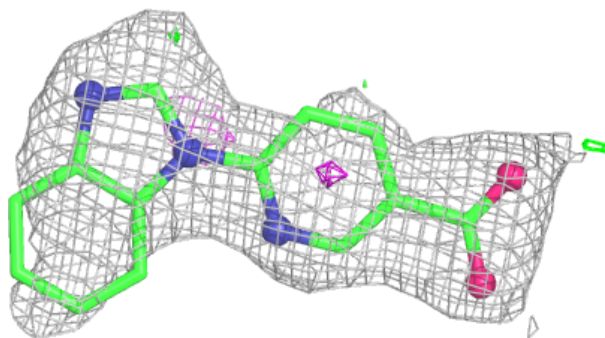
**Electron density around A1KCG T 301:**

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

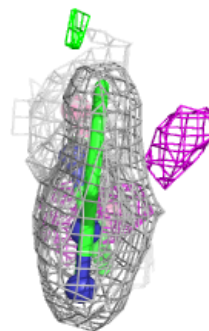
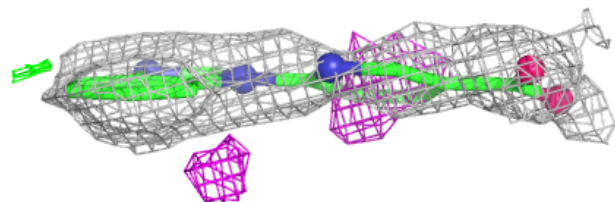
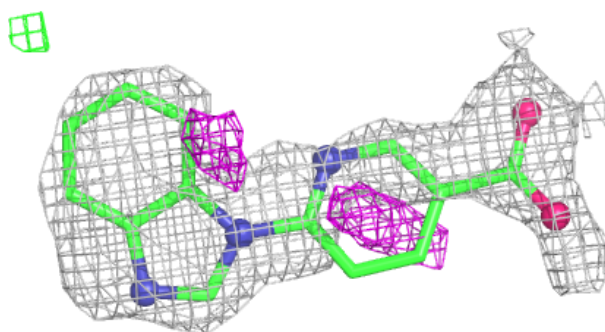


Electron density around A1KCG M 301:

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

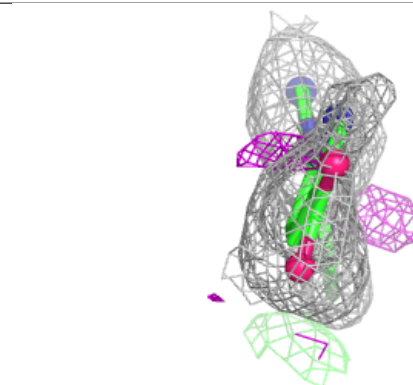
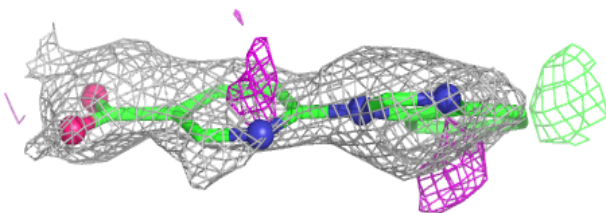
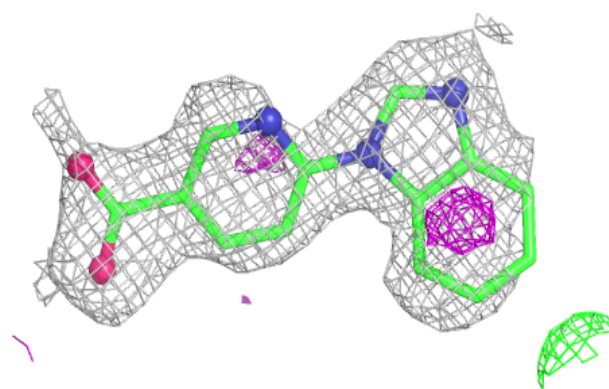
**Electron density around A1KCG U 302:**

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

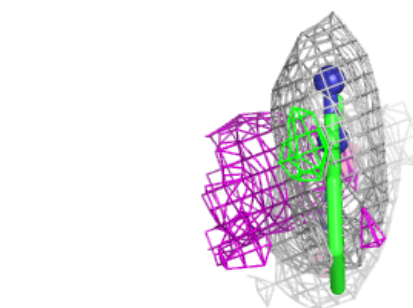
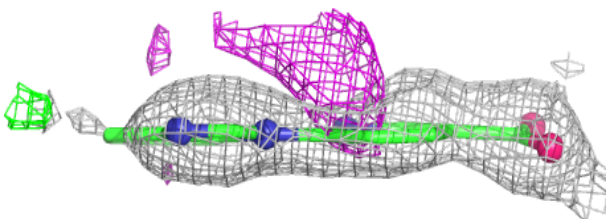
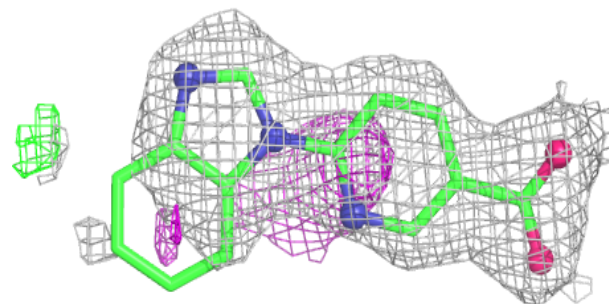


Electron density around A1KCG L 301:

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

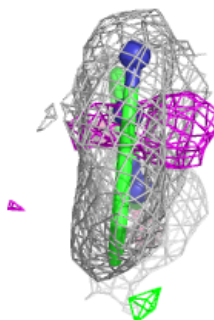
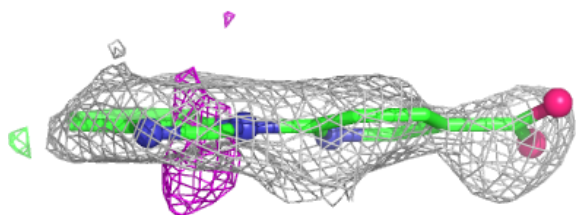
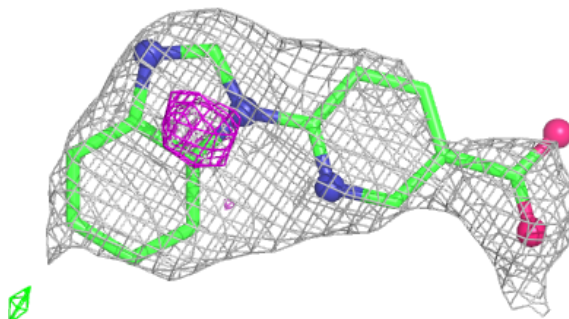
**Electron density around A1KCG C 301:**

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

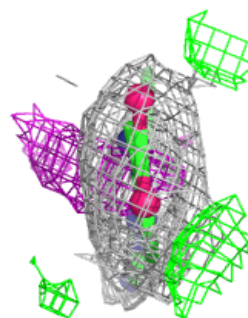
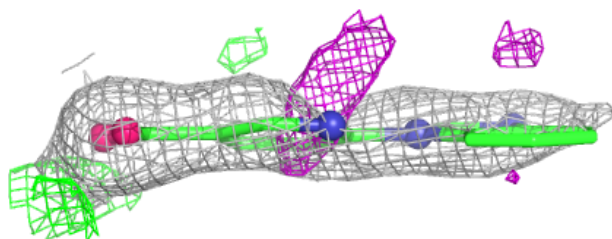
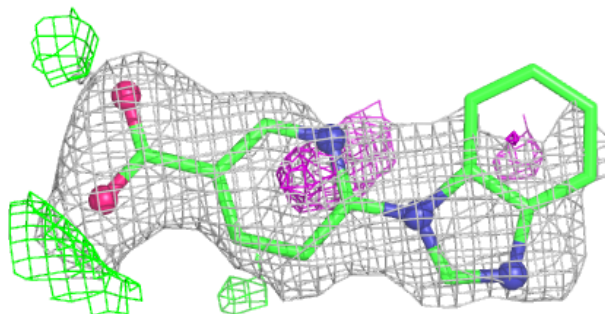


Electron density around A1KCG F 302:

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

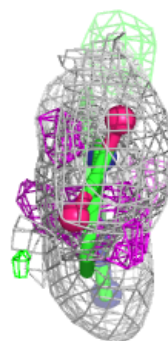
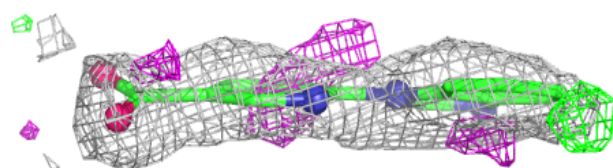
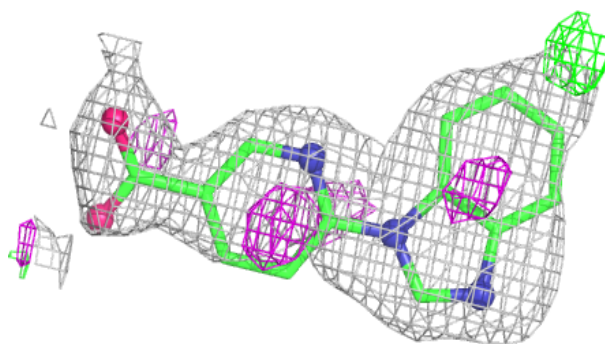
**Electron density around A1KCG S 301:**

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

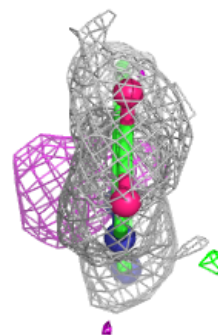
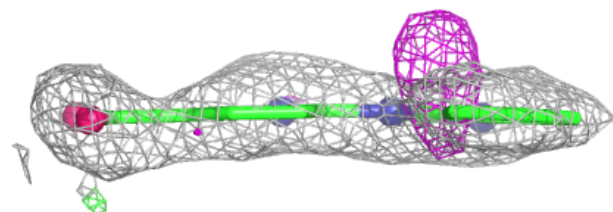
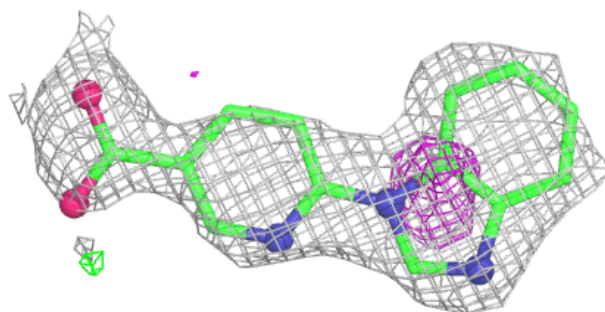


Electron density around A1KCG E 302:

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

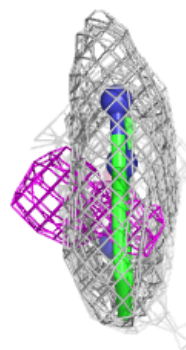
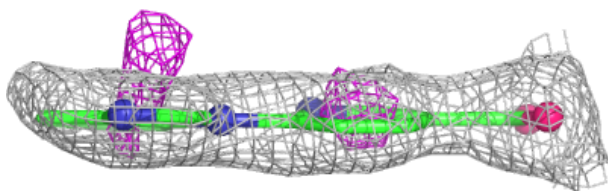
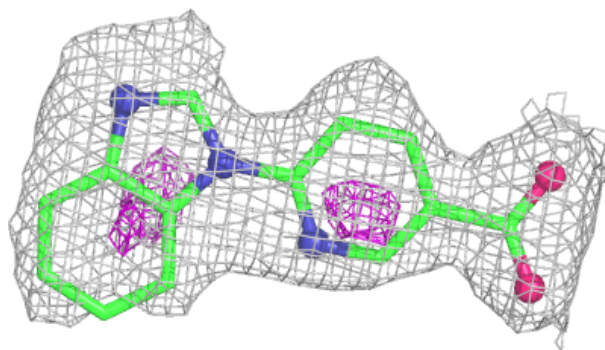
**Electron density around A1KCG S 302:**

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

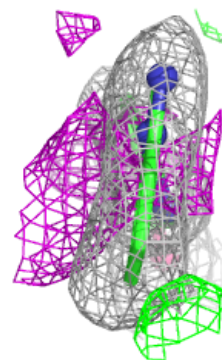
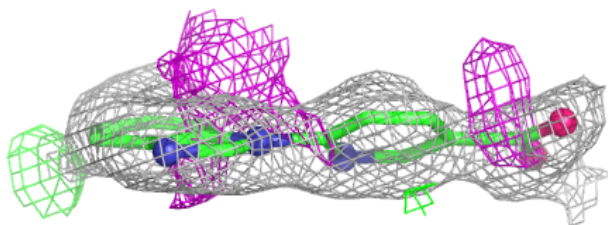
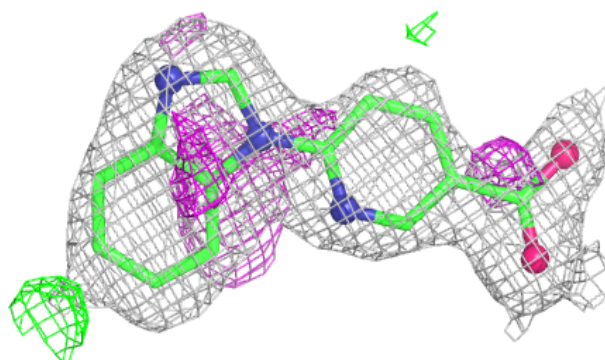


Electron density around A1KCG R 301:

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

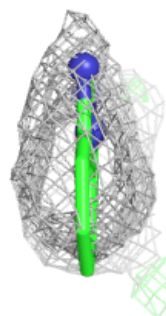
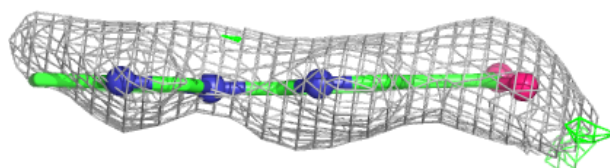
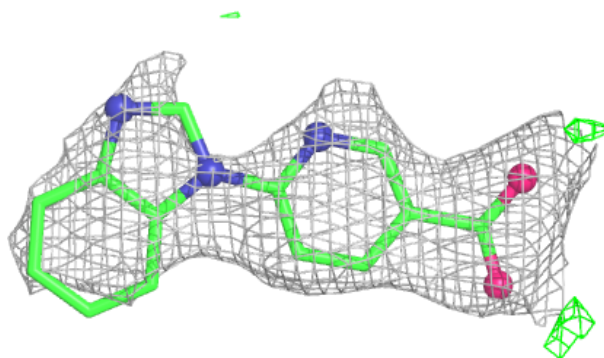
**Electron density around A1KCG B 302:**

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

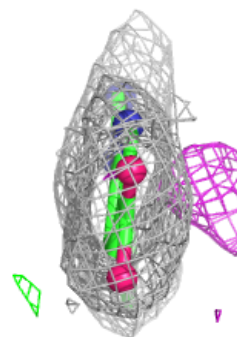
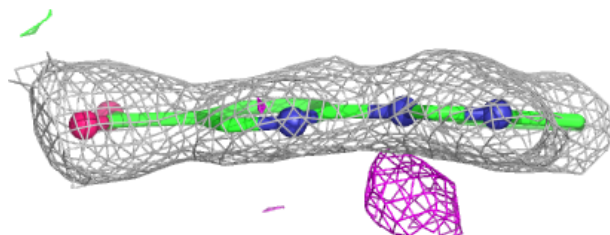
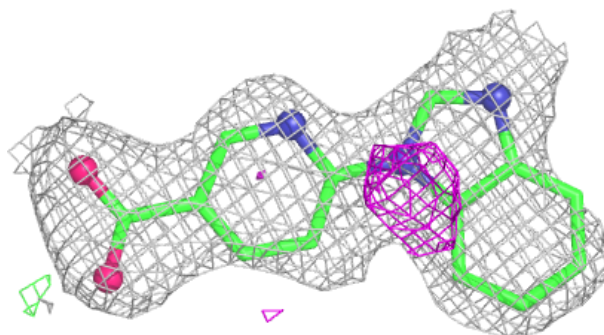


Electron density around A1KCG H 301:

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

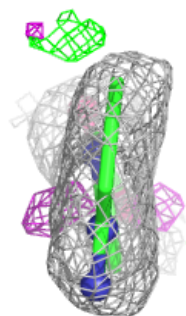
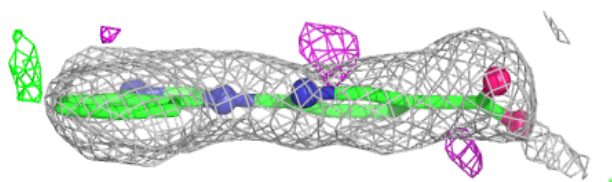
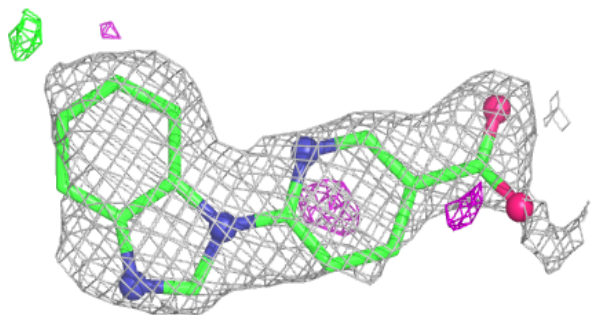
**Electron density around A1KCG Q 301:**

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

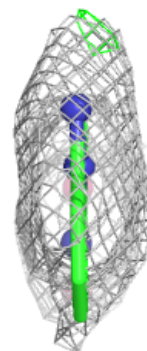
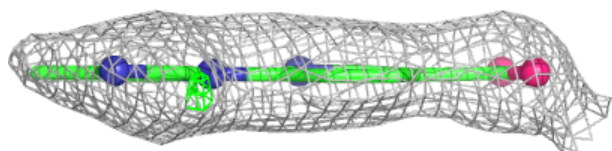


Electron density around A1KCG N 303:

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

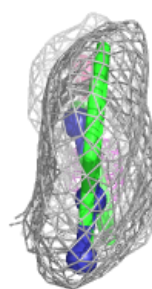
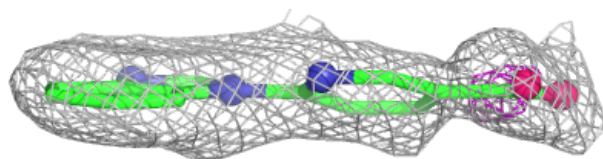
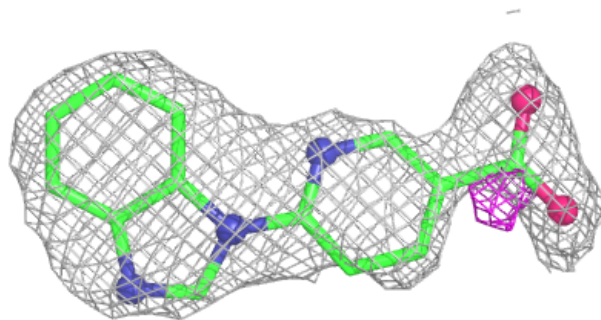
**Electron density around A1KCG B 301:**

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

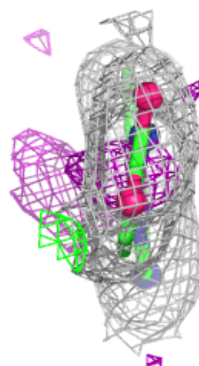
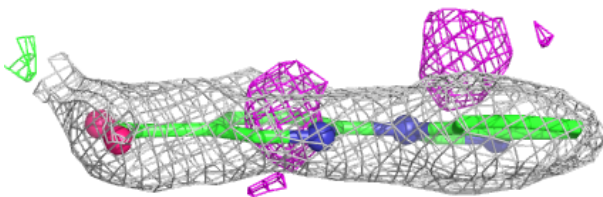
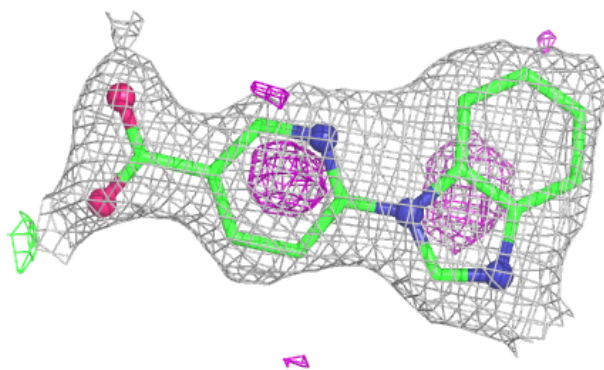


Electron density around A1KCG G 304:

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

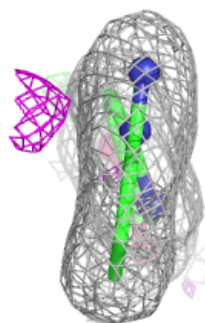
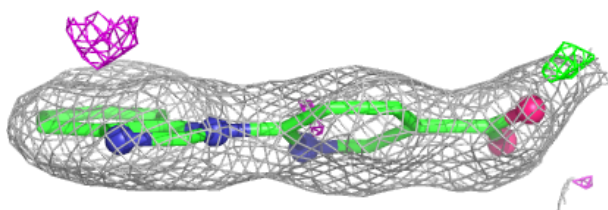
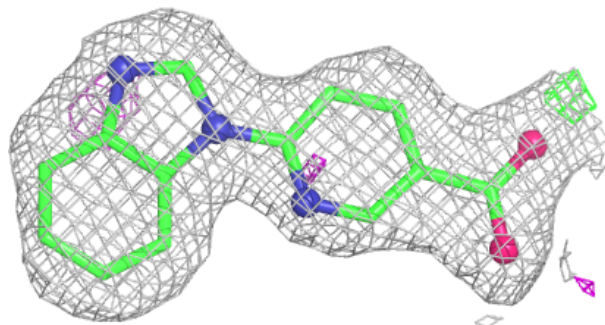
**Electron density around A1KCG P 302:**

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

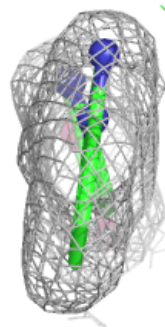
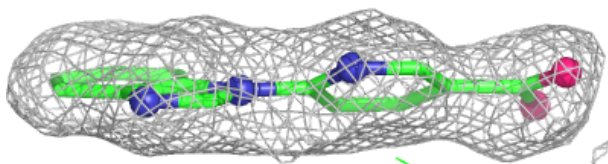
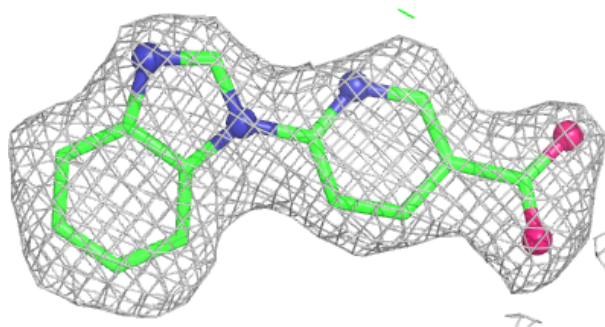


Electron density around A1KCG Q 302:

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

**Electron density around A1KCG A 301:**

$2mF_o-DF_c$ (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.