



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2025 – 04:24 PM EDT

PDB ID : 9E2U / pdb_00009e2u
Title : Crystal structure of DDB1-CRBN-ALV1 complex bound to triple ZnF of Helios (IKZF2 ZF1-3)
Authors : Nowak, R.P.; Fischer, E.S.
Deposited on : 2024-10-23
Resolution : 4.11 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

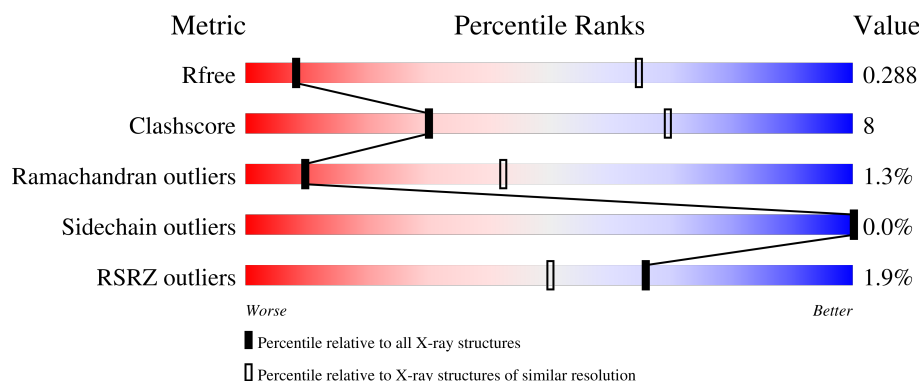
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

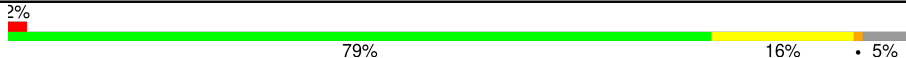
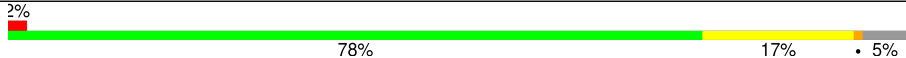



The reported resolution of this entry is 4.11 Å.

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}	164625	1151 (4.44-3.80)
Clashscore	180529	1218 (4.44-3.80)
Ramachandran outliers	177936	1145 (4.44-3.80)
Sidechain outliers	177891	1132 (4.44-3.80)
RSRZ outliers	164620	1149 (4.44-3.80)

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	864	
1	C	864	
1	E	864	
1	G	864	
1	I	864	

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Mol	Chain	Length	Quality of chain
1	K	864	
1	M	864	
1	O	864	
2	B	463	
2	D	463	
2	F	463	
2	H	463	
2	J	463	
2	L	463	
2	N	463	
2	P	463	
3	R	182	
3	S	182	
3	T	182	
3	U	182	
3	V	182	
3	W	182	
3	X	182	
3	Y	182	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 81784 atoms, of which 184 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 damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	0	0
			6445	4082	1089	1238	36			
1	C	820	Total	C	N	O	S	0	0	0
			6426	4070	1084	1236	36			
1	E	822	Total	C	N	O	S	0	0	0
			6445	4082	1089	1238	36			
1	G	821	Total	C	N	O	S	0	0	0
			6437	4078	1087	1236	36			
1	I	821	Total	C	N	O	S	0	0	0
			6434	4076	1085	1237	36			
1	K	822	Total	C	N	O	S	0	0	0
			6445	4082	1089	1238	36			
1	M	822	Total	C	N	O	S	0	0	0
			6445	4082	1089	1238	36			
1	O	822	Total	C	N	O	S	0	0	0
			6445	4082	1089	1238	36			

There are 272 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q16531
A	-26	GLY	-	expression tag	UNP Q16531
A	-25	SER	-	expression tag	UNP Q16531
A	-24	SER	-	expression tag	UNP Q16531
A	-23	HIS	-	expression tag	UNP Q16531
A	-22	HIS	-	expression tag	UNP Q16531
A	-21	HIS	-	expression tag	UNP Q16531
A	-20	HIS	-	expression tag	UNP Q16531
A	-19	HIS	-	expression tag	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	SER	-	expression tag	UNP Q16531
A	-16	ALA	-	expression tag	UNP Q16531
A	-15	ALA	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	ILE	-	expression tag	UNP Q16531
A	-12	VAL	-	expression tag	UNP Q16531
A	-11	MET	-	expression tag	UNP Q16531
A	-10	VAL	-	expression tag	UNP Q16531
A	-9	ASP	-	expression tag	UNP Q16531
A	-8	ALA	-	expression tag	UNP Q16531
A	-7	TYR	-	expression tag	UNP Q16531
A	-6	LYS	-	expression tag	UNP Q16531
A	-5	PRO	-	expression tag	UNP Q16531
A	-4	THR	-	expression tag	UNP Q16531
A	-3	LYS	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531
C	-27	MET	-	initiating methionine	UNP Q16531
C	-26	GLY	-	expression tag	UNP Q16531
C	-25	SER	-	expression tag	UNP Q16531
C	-24	SER	-	expression tag	UNP Q16531
C	-23	HIS	-	expression tag	UNP Q16531
C	-22	HIS	-	expression tag	UNP Q16531
C	-21	HIS	-	expression tag	UNP Q16531
C	-20	HIS	-	expression tag	UNP Q16531
C	-19	HIS	-	expression tag	UNP Q16531
C	-18	HIS	-	expression tag	UNP Q16531
C	-17	SER	-	expression tag	UNP Q16531
C	-16	ALA	-	expression tag	UNP Q16531
C	-15	ALA	-	expression tag	UNP Q16531
C	-14	HIS	-	expression tag	UNP Q16531
C	-13	ILE	-	expression tag	UNP Q16531
C	-12	VAL	-	expression tag	UNP Q16531
C	-11	MET	-	expression tag	UNP Q16531
C	-10	VAL	-	expression tag	UNP Q16531
C	-9	ASP	-	expression tag	UNP Q16531
C	-8	ALA	-	expression tag	UNP Q16531
C	-7	TYR	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LYS	-	expression tag	UNP Q16531
C	-5	PRO	-	expression tag	UNP Q16531
C	-4	THR	-	expression tag	UNP Q16531
C	-3	LYS	-	expression tag	UNP Q16531
C	-2	GLY	-	expression tag	UNP Q16531
C	-1	GLY	-	expression tag	UNP Q16531
C	0	ARG	-	expression tag	UNP Q16531
C	700	GLY	-	linker	UNP Q16531
C	701	ASN	-	linker	UNP Q16531
C	702	GLY	-	linker	UNP Q16531
C	703	ASN	-	linker	UNP Q16531
C	704	SER	-	linker	UNP Q16531
C	705	GLY	-	linker	UNP Q16531
E	-27	MET	-	initiating methionine	UNP Q16531
E	-26	GLY	-	expression tag	UNP Q16531
E	-25	SER	-	expression tag	UNP Q16531
E	-24	SER	-	expression tag	UNP Q16531
E	-23	HIS	-	expression tag	UNP Q16531
E	-22	HIS	-	expression tag	UNP Q16531
E	-21	HIS	-	expression tag	UNP Q16531
E	-20	HIS	-	expression tag	UNP Q16531
E	-19	HIS	-	expression tag	UNP Q16531
E	-18	HIS	-	expression tag	UNP Q16531
E	-17	SER	-	expression tag	UNP Q16531
E	-16	ALA	-	expression tag	UNP Q16531
E	-15	ALA	-	expression tag	UNP Q16531
E	-14	HIS	-	expression tag	UNP Q16531
E	-13	ILE	-	expression tag	UNP Q16531
E	-12	VAL	-	expression tag	UNP Q16531
E	-11	MET	-	expression tag	UNP Q16531
E	-10	VAL	-	expression tag	UNP Q16531
E	-9	ASP	-	expression tag	UNP Q16531
E	-8	ALA	-	expression tag	UNP Q16531
E	-7	TYR	-	expression tag	UNP Q16531
E	-6	LYS	-	expression tag	UNP Q16531
E	-5	PRO	-	expression tag	UNP Q16531
E	-4	THR	-	expression tag	UNP Q16531
E	-3	LYS	-	expression tag	UNP Q16531
E	-2	GLY	-	expression tag	UNP Q16531
E	-1	GLY	-	expression tag	UNP Q16531
E	0	ARG	-	expression tag	UNP Q16531
E	700	GLY	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
E	701	ASN	-	linker	UNP Q16531
E	702	GLY	-	linker	UNP Q16531
E	703	ASN	-	linker	UNP Q16531
E	704	SER	-	linker	UNP Q16531
E	705	GLY	-	linker	UNP Q16531
G	-27	MET	-	initiating methionine	UNP Q16531
G	-26	GLY	-	expression tag	UNP Q16531
G	-25	SER	-	expression tag	UNP Q16531
G	-24	SER	-	expression tag	UNP Q16531
G	-23	HIS	-	expression tag	UNP Q16531
G	-22	HIS	-	expression tag	UNP Q16531
G	-21	HIS	-	expression tag	UNP Q16531
G	-20	HIS	-	expression tag	UNP Q16531
G	-19	HIS	-	expression tag	UNP Q16531
G	-18	HIS	-	expression tag	UNP Q16531
G	-17	SER	-	expression tag	UNP Q16531
G	-16	ALA	-	expression tag	UNP Q16531
G	-15	ALA	-	expression tag	UNP Q16531
G	-14	HIS	-	expression tag	UNP Q16531
G	-13	ILE	-	expression tag	UNP Q16531
G	-12	VAL	-	expression tag	UNP Q16531
G	-11	MET	-	expression tag	UNP Q16531
G	-10	VAL	-	expression tag	UNP Q16531
G	-9	ASP	-	expression tag	UNP Q16531
G	-8	ALA	-	expression tag	UNP Q16531
G	-7	TYR	-	expression tag	UNP Q16531
G	-6	LYS	-	expression tag	UNP Q16531
G	-5	PRO	-	expression tag	UNP Q16531
G	-4	THR	-	expression tag	UNP Q16531
G	-3	LYS	-	expression tag	UNP Q16531
G	-2	GLY	-	expression tag	UNP Q16531
G	-1	GLY	-	expression tag	UNP Q16531
G	0	ARG	-	expression tag	UNP Q16531
G	700	GLY	-	linker	UNP Q16531
G	701	ASN	-	linker	UNP Q16531
G	702	GLY	-	linker	UNP Q16531
G	703	ASN	-	linker	UNP Q16531
G	704	SER	-	linker	UNP Q16531
G	705	GLY	-	linker	UNP Q16531
I	-27	MET	-	initiating methionine	UNP Q16531
I	-26	GLY	-	expression tag	UNP Q16531
I	-25	SER	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-24	SER	-	expression tag	UNP Q16531
I	-23	HIS	-	expression tag	UNP Q16531
I	-22	HIS	-	expression tag	UNP Q16531
I	-21	HIS	-	expression tag	UNP Q16531
I	-20	HIS	-	expression tag	UNP Q16531
I	-19	HIS	-	expression tag	UNP Q16531
I	-18	HIS	-	expression tag	UNP Q16531
I	-17	SER	-	expression tag	UNP Q16531
I	-16	ALA	-	expression tag	UNP Q16531
I	-15	ALA	-	expression tag	UNP Q16531
I	-14	HIS	-	expression tag	UNP Q16531
I	-13	ILE	-	expression tag	UNP Q16531
I	-12	VAL	-	expression tag	UNP Q16531
I	-11	MET	-	expression tag	UNP Q16531
I	-10	VAL	-	expression tag	UNP Q16531
I	-9	ASP	-	expression tag	UNP Q16531
I	-8	ALA	-	expression tag	UNP Q16531
I	-7	TYR	-	expression tag	UNP Q16531
I	-6	LYS	-	expression tag	UNP Q16531
I	-5	PRO	-	expression tag	UNP Q16531
I	-4	THR	-	expression tag	UNP Q16531
I	-3	LYS	-	expression tag	UNP Q16531
I	-2	GLY	-	expression tag	UNP Q16531
I	-1	GLY	-	expression tag	UNP Q16531
I	0	ARG	-	expression tag	UNP Q16531
I	700	GLY	-	linker	UNP Q16531
I	701	ASN	-	linker	UNP Q16531
I	702	GLY	-	linker	UNP Q16531
I	703	ASN	-	linker	UNP Q16531
I	704	SER	-	linker	UNP Q16531
I	705	GLY	-	linker	UNP Q16531
K	-27	MET	-	initiating methionine	UNP Q16531
K	-26	GLY	-	expression tag	UNP Q16531
K	-25	SER	-	expression tag	UNP Q16531
K	-24	SER	-	expression tag	UNP Q16531
K	-23	HIS	-	expression tag	UNP Q16531
K	-22	HIS	-	expression tag	UNP Q16531
K	-21	HIS	-	expression tag	UNP Q16531
K	-20	HIS	-	expression tag	UNP Q16531
K	-19	HIS	-	expression tag	UNP Q16531
K	-18	HIS	-	expression tag	UNP Q16531
K	-17	SER	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-16	ALA	-	expression tag	UNP Q16531
K	-15	ALA	-	expression tag	UNP Q16531
K	-14	HIS	-	expression tag	UNP Q16531
K	-13	ILE	-	expression tag	UNP Q16531
K	-12	VAL	-	expression tag	UNP Q16531
K	-11	MET	-	expression tag	UNP Q16531
K	-10	VAL	-	expression tag	UNP Q16531
K	-9	ASP	-	expression tag	UNP Q16531
K	-8	ALA	-	expression tag	UNP Q16531
K	-7	TYR	-	expression tag	UNP Q16531
K	-6	LYS	-	expression tag	UNP Q16531
K	-5	PRO	-	expression tag	UNP Q16531
K	-4	THR	-	expression tag	UNP Q16531
K	-3	LYS	-	expression tag	UNP Q16531
K	-2	GLY	-	expression tag	UNP Q16531
K	-1	GLY	-	expression tag	UNP Q16531
K	0	ARG	-	expression tag	UNP Q16531
K	700	GLY	-	linker	UNP Q16531
K	701	ASN	-	linker	UNP Q16531
K	702	GLY	-	linker	UNP Q16531
K	703	ASN	-	linker	UNP Q16531
K	704	SER	-	linker	UNP Q16531
K	705	GLY	-	linker	UNP Q16531
M	-27	MET	-	initiating methionine	UNP Q16531
M	-26	GLY	-	expression tag	UNP Q16531
M	-25	SER	-	expression tag	UNP Q16531
M	-24	SER	-	expression tag	UNP Q16531
M	-23	HIS	-	expression tag	UNP Q16531
M	-22	HIS	-	expression tag	UNP Q16531
M	-21	HIS	-	expression tag	UNP Q16531
M	-20	HIS	-	expression tag	UNP Q16531
M	-19	HIS	-	expression tag	UNP Q16531
M	-18	HIS	-	expression tag	UNP Q16531
M	-17	SER	-	expression tag	UNP Q16531
M	-16	ALA	-	expression tag	UNP Q16531
M	-15	ALA	-	expression tag	UNP Q16531
M	-14	HIS	-	expression tag	UNP Q16531
M	-13	ILE	-	expression tag	UNP Q16531
M	-12	VAL	-	expression tag	UNP Q16531
M	-11	MET	-	expression tag	UNP Q16531
M	-10	VAL	-	expression tag	UNP Q16531
M	-9	ASP	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-8	ALA	-	expression tag	UNP Q16531
M	-7	TYR	-	expression tag	UNP Q16531
M	-6	LYS	-	expression tag	UNP Q16531
M	-5	PRO	-	expression tag	UNP Q16531
M	-4	THR	-	expression tag	UNP Q16531
M	-3	LYS	-	expression tag	UNP Q16531
M	-2	GLY	-	expression tag	UNP Q16531
M	-1	GLY	-	expression tag	UNP Q16531
M	0	ARG	-	expression tag	UNP Q16531
M	700	GLY	-	linker	UNP Q16531
M	701	ASN	-	linker	UNP Q16531
M	702	GLY	-	linker	UNP Q16531
M	703	ASN	-	linker	UNP Q16531
M	704	SER	-	linker	UNP Q16531
M	705	GLY	-	linker	UNP Q16531
O	-27	MET	-	initiating methionine	UNP Q16531
O	-26	GLY	-	expression tag	UNP Q16531
O	-25	SER	-	expression tag	UNP Q16531
O	-24	SER	-	expression tag	UNP Q16531
O	-23	HIS	-	expression tag	UNP Q16531
O	-22	HIS	-	expression tag	UNP Q16531
O	-21	HIS	-	expression tag	UNP Q16531
O	-20	HIS	-	expression tag	UNP Q16531
O	-19	HIS	-	expression tag	UNP Q16531
O	-18	HIS	-	expression tag	UNP Q16531
O	-17	SER	-	expression tag	UNP Q16531
O	-16	ALA	-	expression tag	UNP Q16531
O	-15	ALA	-	expression tag	UNP Q16531
O	-14	HIS	-	expression tag	UNP Q16531
O	-13	ILE	-	expression tag	UNP Q16531
O	-12	VAL	-	expression tag	UNP Q16531
O	-11	MET	-	expression tag	UNP Q16531
O	-10	VAL	-	expression tag	UNP Q16531
O	-9	ASP	-	expression tag	UNP Q16531
O	-8	ALA	-	expression tag	UNP Q16531
O	-7	TYR	-	expression tag	UNP Q16531
O	-6	LYS	-	expression tag	UNP Q16531
O	-5	PRO	-	expression tag	UNP Q16531
O	-4	THR	-	expression tag	UNP Q16531
O	-3	LYS	-	expression tag	UNP Q16531
O	-2	GLY	-	expression tag	UNP Q16531
O	-1	GLY	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
O	0	ARG	-	expression tag	UNP Q16531
O	700	GLY	-	linker	UNP Q16531
O	701	ASN	-	linker	UNP Q16531
O	702	GLY	-	linker	UNP Q16531
O	703	ASN	-	linker	UNP Q16531
O	704	SER	-	linker	UNP Q16531
O	705	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	396	Total	C	N	O	S	0	0	0
			3157	2011	538	583	25			
2	D	396	Total	C	N	O	S	0	0	0
			3157	2011	538	583	25			
2	F	396	Total	C	N	O	S	0	0	0
			3157	2011	538	583	25			
2	H	396	Total	C	N	O	S	0	0	0
			3157	2011	538	583	25			
2	J	396	Total	C	N	O	S	0	0	0
			3157	2011	538	583	25			
2	L	396	Total	C	N	O	S	0	0	0
			3157	2011	538	583	25			
2	N	396	Total	C	N	O	S	0	0	0
			3157	2011	538	583	25			
2	P	396	Total	C	N	O	S	0	0	0
			3157	2011	538	583	25			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP Q96SW2
B	-19	GLY	-	expression tag	UNP Q96SW2
B	-18	SER	-	expression tag	UNP Q96SW2
B	-17	SER	-	expression tag	UNP Q96SW2
B	-16	HIS	-	expression tag	UNP Q96SW2
B	-15	HIS	-	expression tag	UNP Q96SW2
B	-14	HIS	-	expression tag	UNP Q96SW2
B	-13	HIS	-	expression tag	UNP Q96SW2
B	-12	HIS	-	expression tag	UNP Q96SW2
B	-11	HIS	-	expression tag	UNP Q96SW2
B	-10	SER	-	expression tag	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	ALA	-	expression tag	UNP Q96SW2
B	-8	VAL	-	expression tag	UNP Q96SW2
B	-7	ASP	-	expression tag	UNP Q96SW2
B	-6	GLU	-	expression tag	UNP Q96SW2
B	-5	ASN	-	expression tag	UNP Q96SW2
B	-4	LEU	-	expression tag	UNP Q96SW2
B	-3	TYR	-	expression tag	UNP Q96SW2
B	-2	PHE	-	expression tag	UNP Q96SW2
B	-1	GLN	-	expression tag	UNP Q96SW2
B	0	GLY	-	expression tag	UNP Q96SW2
B	1	GLY	-	expression tag	UNP Q96SW2
D	-20	MET	-	initiating methionine	UNP Q96SW2
D	-19	GLY	-	expression tag	UNP Q96SW2
D	-18	SER	-	expression tag	UNP Q96SW2
D	-17	SER	-	expression tag	UNP Q96SW2
D	-16	HIS	-	expression tag	UNP Q96SW2
D	-15	HIS	-	expression tag	UNP Q96SW2
D	-14	HIS	-	expression tag	UNP Q96SW2
D	-13	HIS	-	expression tag	UNP Q96SW2
D	-12	HIS	-	expression tag	UNP Q96SW2
D	-11	HIS	-	expression tag	UNP Q96SW2
D	-10	SER	-	expression tag	UNP Q96SW2
D	-9	ALA	-	expression tag	UNP Q96SW2
D	-8	VAL	-	expression tag	UNP Q96SW2
D	-7	ASP	-	expression tag	UNP Q96SW2
D	-6	GLU	-	expression tag	UNP Q96SW2
D	-5	ASN	-	expression tag	UNP Q96SW2
D	-4	LEU	-	expression tag	UNP Q96SW2
D	-3	TYR	-	expression tag	UNP Q96SW2
D	-2	PHE	-	expression tag	UNP Q96SW2
D	-1	GLN	-	expression tag	UNP Q96SW2
D	0	GLY	-	expression tag	UNP Q96SW2
D	1	GLY	-	expression tag	UNP Q96SW2
F	-20	MET	-	initiating methionine	UNP Q96SW2
F	-19	GLY	-	expression tag	UNP Q96SW2
F	-18	SER	-	expression tag	UNP Q96SW2
F	-17	SER	-	expression tag	UNP Q96SW2
F	-16	HIS	-	expression tag	UNP Q96SW2
F	-15	HIS	-	expression tag	UNP Q96SW2
F	-14	HIS	-	expression tag	UNP Q96SW2
F	-13	HIS	-	expression tag	UNP Q96SW2
F	-12	HIS	-	expression tag	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	HIS	-	expression tag	UNP Q96SW2
F	-10	SER	-	expression tag	UNP Q96SW2
F	-9	ALA	-	expression tag	UNP Q96SW2
F	-8	VAL	-	expression tag	UNP Q96SW2
F	-7	ASP	-	expression tag	UNP Q96SW2
F	-6	GLU	-	expression tag	UNP Q96SW2
F	-5	ASN	-	expression tag	UNP Q96SW2
F	-4	LEU	-	expression tag	UNP Q96SW2
F	-3	TYR	-	expression tag	UNP Q96SW2
F	-2	PHE	-	expression tag	UNP Q96SW2
F	-1	GLN	-	expression tag	UNP Q96SW2
F	0	GLY	-	expression tag	UNP Q96SW2
F	1	GLY	-	expression tag	UNP Q96SW2
H	-20	MET	-	initiating methionine	UNP Q96SW2
H	-19	GLY	-	expression tag	UNP Q96SW2
H	-18	SER	-	expression tag	UNP Q96SW2
H	-17	SER	-	expression tag	UNP Q96SW2
H	-16	HIS	-	expression tag	UNP Q96SW2
H	-15	HIS	-	expression tag	UNP Q96SW2
H	-14	HIS	-	expression tag	UNP Q96SW2
H	-13	HIS	-	expression tag	UNP Q96SW2
H	-12	HIS	-	expression tag	UNP Q96SW2
H	-11	HIS	-	expression tag	UNP Q96SW2
H	-10	SER	-	expression tag	UNP Q96SW2
H	-9	ALA	-	expression tag	UNP Q96SW2
H	-8	VAL	-	expression tag	UNP Q96SW2
H	-7	ASP	-	expression tag	UNP Q96SW2
H	-6	GLU	-	expression tag	UNP Q96SW2
H	-5	ASN	-	expression tag	UNP Q96SW2
H	-4	LEU	-	expression tag	UNP Q96SW2
H	-3	TYR	-	expression tag	UNP Q96SW2
H	-2	PHE	-	expression tag	UNP Q96SW2
H	-1	GLN	-	expression tag	UNP Q96SW2
H	0	GLY	-	expression tag	UNP Q96SW2
H	1	GLY	-	expression tag	UNP Q96SW2
J	-20	MET	-	initiating methionine	UNP Q96SW2
J	-19	GLY	-	expression tag	UNP Q96SW2
J	-18	SER	-	expression tag	UNP Q96SW2
J	-17	SER	-	expression tag	UNP Q96SW2
J	-16	HIS	-	expression tag	UNP Q96SW2
J	-15	HIS	-	expression tag	UNP Q96SW2
J	-14	HIS	-	expression tag	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-13	HIS	-	expression tag	UNP Q96SW2
J	-12	HIS	-	expression tag	UNP Q96SW2
J	-11	HIS	-	expression tag	UNP Q96SW2
J	-10	SER	-	expression tag	UNP Q96SW2
J	-9	ALA	-	expression tag	UNP Q96SW2
J	-8	VAL	-	expression tag	UNP Q96SW2
J	-7	ASP	-	expression tag	UNP Q96SW2
J	-6	GLU	-	expression tag	UNP Q96SW2
J	-5	ASN	-	expression tag	UNP Q96SW2
J	-4	LEU	-	expression tag	UNP Q96SW2
J	-3	TYR	-	expression tag	UNP Q96SW2
J	-2	PHE	-	expression tag	UNP Q96SW2
J	-1	GLN	-	expression tag	UNP Q96SW2
J	0	GLY	-	expression tag	UNP Q96SW2
J	1	GLY	-	expression tag	UNP Q96SW2
L	-20	MET	-	initiating methionine	UNP Q96SW2
L	-19	GLY	-	expression tag	UNP Q96SW2
L	-18	SER	-	expression tag	UNP Q96SW2
L	-17	SER	-	expression tag	UNP Q96SW2
L	-16	HIS	-	expression tag	UNP Q96SW2
L	-15	HIS	-	expression tag	UNP Q96SW2
L	-14	HIS	-	expression tag	UNP Q96SW2
L	-13	HIS	-	expression tag	UNP Q96SW2
L	-12	HIS	-	expression tag	UNP Q96SW2
L	-11	HIS	-	expression tag	UNP Q96SW2
L	-10	SER	-	expression tag	UNP Q96SW2
L	-9	ALA	-	expression tag	UNP Q96SW2
L	-8	VAL	-	expression tag	UNP Q96SW2
L	-7	ASP	-	expression tag	UNP Q96SW2
L	-6	GLU	-	expression tag	UNP Q96SW2
L	-5	ASN	-	expression tag	UNP Q96SW2
L	-4	LEU	-	expression tag	UNP Q96SW2
L	-3	TYR	-	expression tag	UNP Q96SW2
L	-2	PHE	-	expression tag	UNP Q96SW2
L	-1	GLN	-	expression tag	UNP Q96SW2
L	0	GLY	-	expression tag	UNP Q96SW2
L	1	GLY	-	expression tag	UNP Q96SW2
N	-20	MET	-	initiating methionine	UNP Q96SW2
N	-19	GLY	-	expression tag	UNP Q96SW2
N	-18	SER	-	expression tag	UNP Q96SW2
N	-17	SER	-	expression tag	UNP Q96SW2
N	-16	HIS	-	expression tag	UNP Q96SW2

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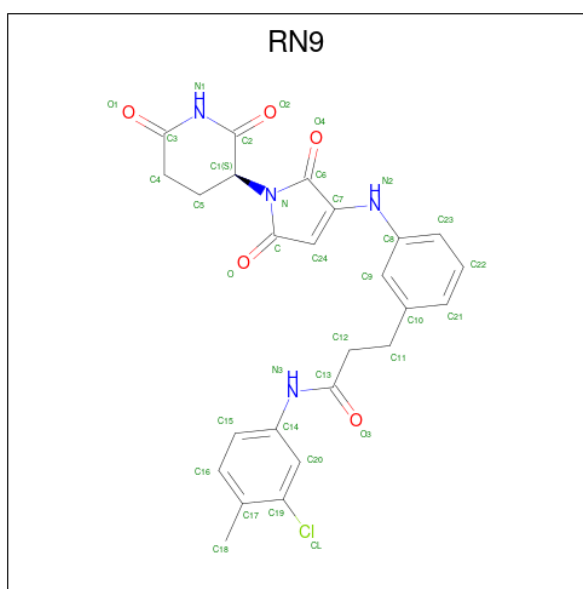
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Chain	Residue	Modelled	Actual	Comment	Reference
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N	-14	HIS	-	expression tag	UNP Q96SW2
N	-13	HIS	-	expression tag	UNP Q96SW2
N	-12	HIS	-	expression tag	UNP Q96SW2
N	-11	HIS	-	expression tag	UNP Q96SW2
N	-10	SER	-	expression tag	UNP Q96SW2
N	-9	ALA	-	expression tag	UNP Q96SW2
N	-8	VAL	-	expression tag	UNP Q96SW2
N	-7	ASP	-	expression tag	UNP Q96SW2
N	-6	GLU	-	expression tag	UNP Q96SW2
N	-5	ASN	-	expression tag	UNP Q96SW2
N	-4	LEU	-	expression tag	UNP Q96SW2
N	-3	TYR	-	expression tag	UNP Q96SW2
N	-2	PHE	-	expression tag	UNP Q96SW2
N	-1	GLN	-	expression tag	UNP Q96SW2
N	0	GLY	-	expression tag	UNP Q96SW2
N	1	GLY	-	expression tag	UNP Q96SW2
P	-20	MET	-	initiating methionine	UNP Q96SW2
P	-19	GLY	-	expression tag	UNP Q96SW2
P	-18	SER	-	expression tag	UNP Q96SW2
P	-17	SER	-	expression tag	UNP Q96SW2
P	-16	HIS	-	expression tag	UNP Q96SW2
P	-15	HIS	-	expression tag	UNP Q96SW2
P	-14	HIS	-	expression tag	UNP Q96SW2
P	-13	HIS	-	expression tag	UNP Q96SW2
P	-12	HIS	-	expression tag	UNP Q96SW2
P	-11	HIS	-	expression tag	UNP Q96SW2
P	-10	SER	-	expression tag	UNP Q96SW2
P	-9	ALA	-	expression tag	UNP Q96SW2
P	-8	VAL	-	expression tag	UNP Q96SW2
P	-7	ASP	-	expression tag	UNP Q96SW2
P	-6	GLU	-	expression tag	UNP Q96SW2
P	-5	ASN	-	expression tag	UNP Q96SW2
P	-4	LEU	-	expression tag	UNP Q96SW2
P	-3	TYR	-	expression tag	UNP Q96SW2
P	-2	PHE	-	expression tag	UNP Q96SW2
P	-1	GLN	-	expression tag	UNP Q96SW2
P	0	GLY	-	expression tag	UNP Q96SW2
P	1	GLY	-	expression tag	UNP Q96SW2

- Molecule 3 is a protein called Zinc finger protein Helios.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	83	Total	C	N	O	S	0	0	0
			647	399	131	107	10			
3	S	82	Total	C	N	O	S	0	0	0
			641	396	130	105	10			
3	T	82	Total	C	N	O	S	0	0	0
			641	396	130	105	10			
3	U	58	Total	C	N	O	S	0	0	0
			444	273	89	75	7			
3	V	56	Total	C	N	O	S	0	0	0
			426	262	86	71	7			
3	W	56	Total	C	N	O	S	0	0	0
			426	262	86	71	7			
3	X	83	Total	C	N	O	S	0	0	0
			647	399	131	107	10			
3	Y	82	Total	C	N	O	S	0	0	0
			641	396	130	105	10			

- Molecule 4 is 3-[3-[[1-[(3 {S})-2,6-bis(oxidanylidene)piperidin-3-yl]-2,5-bis(oxidanylidene)pyrrol-3-yl]amino]phenyl]-{N}-(3-chloranyl-4-methyl-phenyl)propanamide (CCD ID: RN9) (formula: C₂₅H₂₃ClN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total 58	C 25	Cl 1	H 23	N 4	O 5	0	0
4	D	1	Total 58	C 25	Cl 1	H 23	N 4	O 5	0	0
4	F	1	Total 58	C 25	Cl 1	H 23	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	H	1	Total	C	Cl	H	N	O	0	0
			58	25	1	23	4	5		
4	J	1	Total	C	Cl	H	N	O	0	0
			58	25	1	23	4	5		
4	L	1	Total	C	Cl	H	N	O	0	0
			58	25	1	23	4	5		
4	N	1	Total	C	Cl	H	N	O	0	0
			58	25	1	23	4	5		
4	P	1	Total	C	Cl	H	N	O	0	0
			58	25	1	23	4	5		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		
5	F	1	Total	Zn	0	0
			1	1		
5	H	1	Total	Zn	0	0
			1	1		
5	J	1	Total	Zn	0	0
			1	1		
5	L	1	Total	Zn	0	0
			1	1		
5	N	1	Total	Zn	0	0
			1	1		
5	P	1	Total	Zn	0	0
			1	1		
5	R	3	Total	Zn	0	0
			3	3		
5	S	3	Total	Zn	0	0
			3	3		
5	T	3	Total	Zn	0	0
			3	3		
5	U	2	Total	Zn	0	0
			2	2		
5	V	2	Total	Zn	0	0
			2	2		
5	W	2	Total	Zn	0	0
			2	2		

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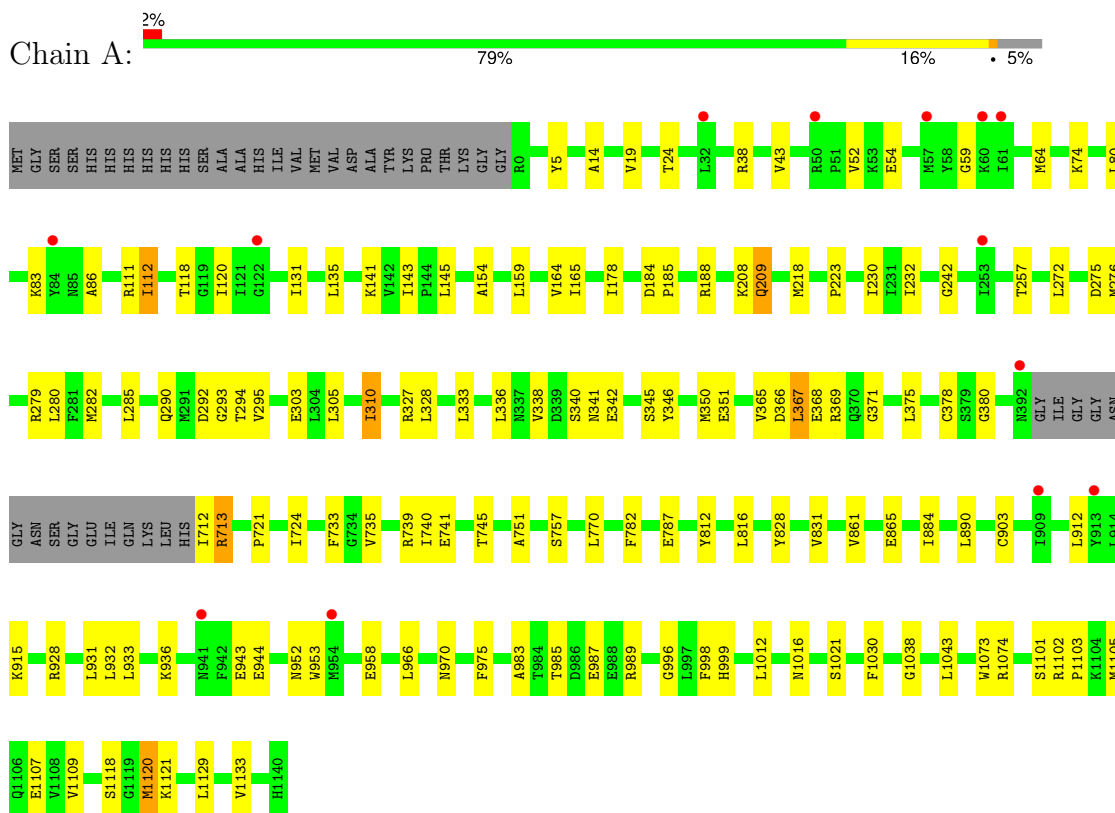
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	3	Total 3	Zn 3	0	0
5	Y	3	Total 3	Zn 3	0	0

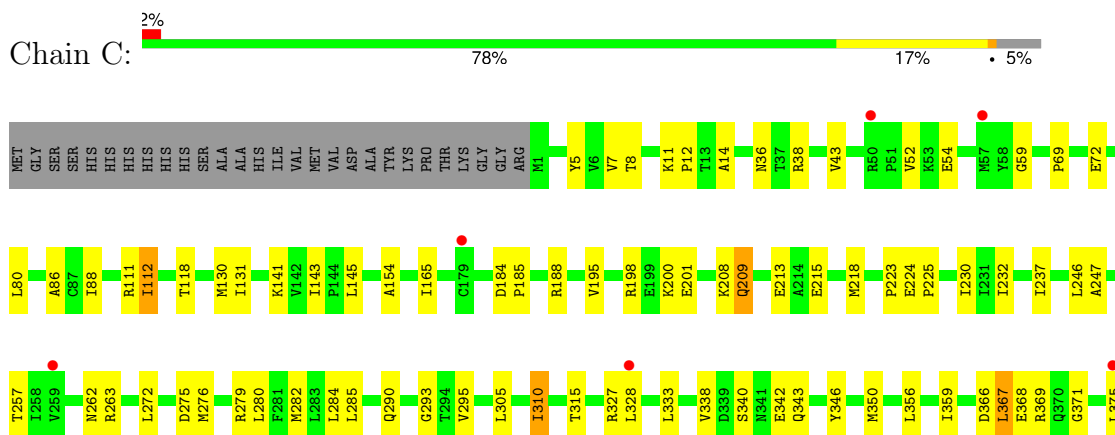
3 Residue-property plots [i](#)

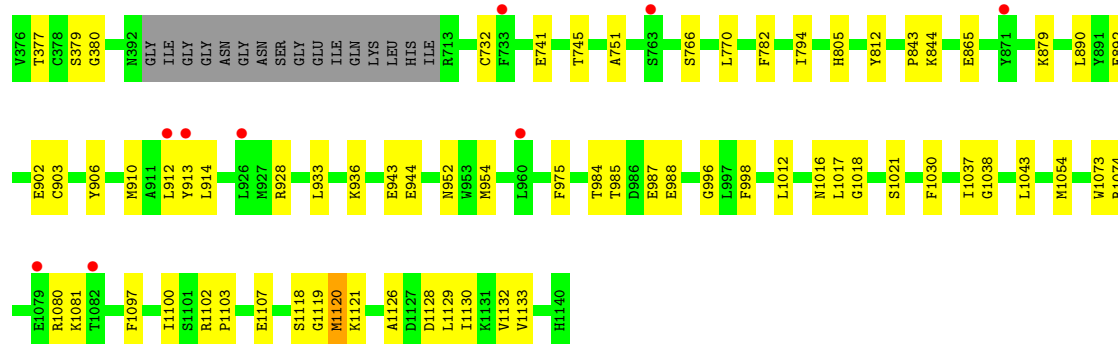
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 damage-binding protein 1

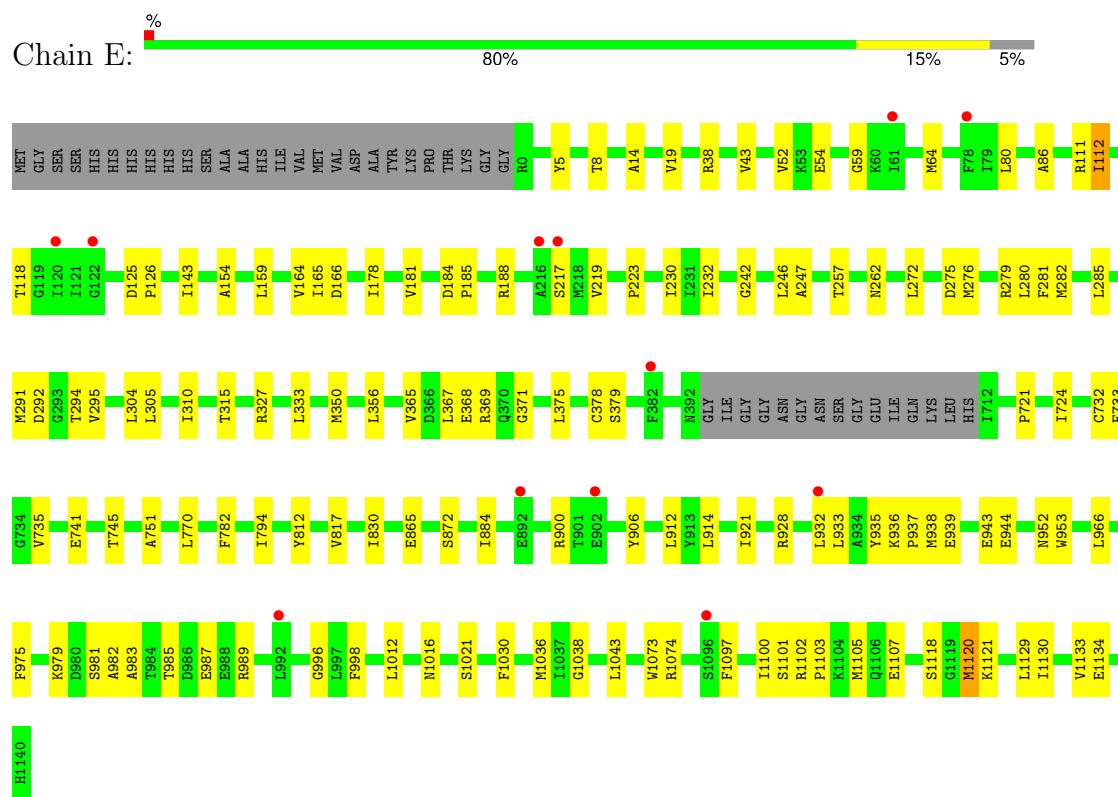


• Molecule 1: DNA damage-binding protein 1

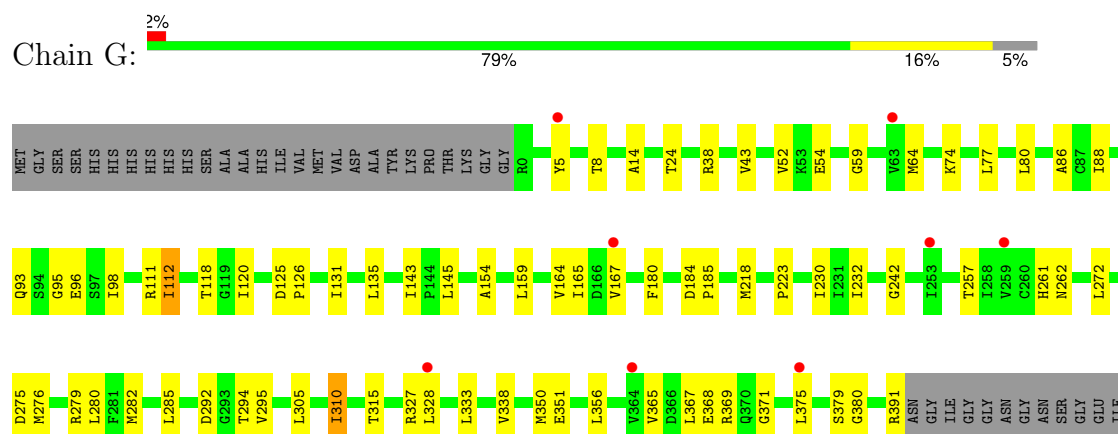


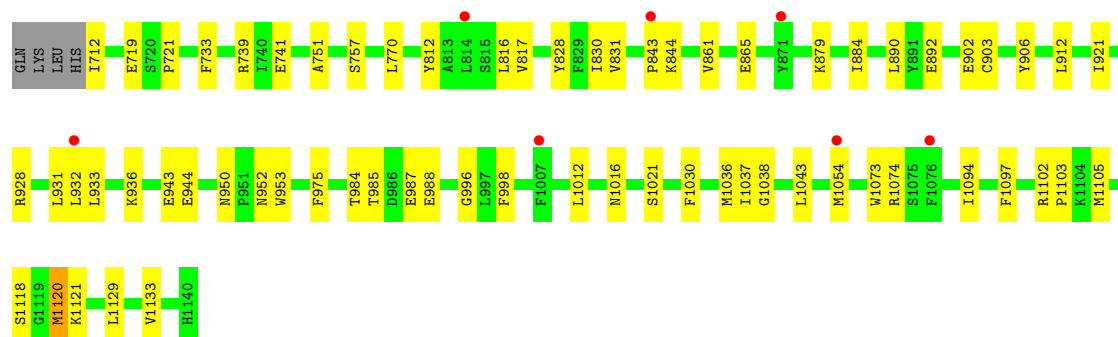


• Molecule 1: DNA damage-binding protein 1

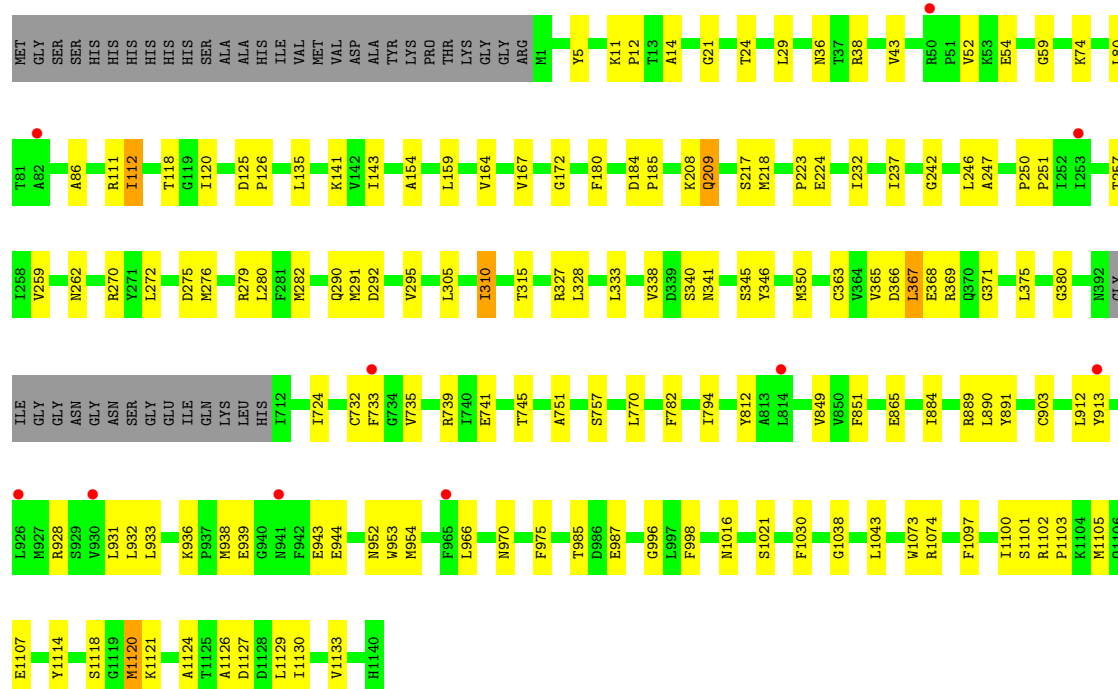
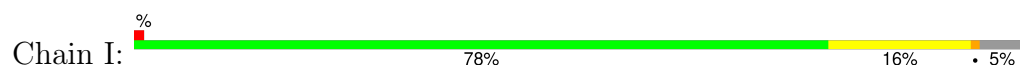


• Molecule 1: DNA damage-binding protein 1

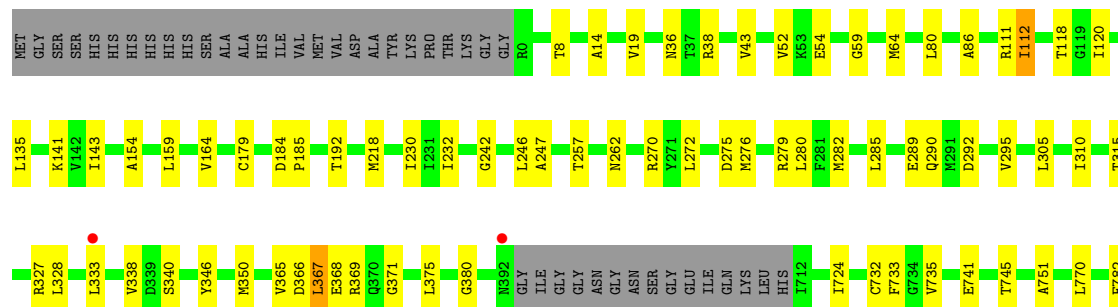
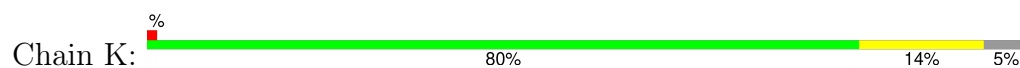


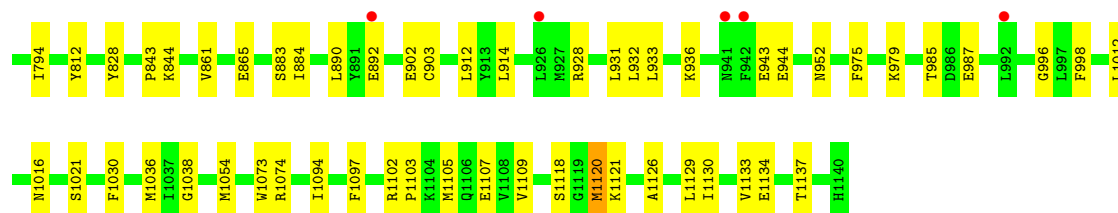


• Molecule 1: DNA damage-binding protein 1

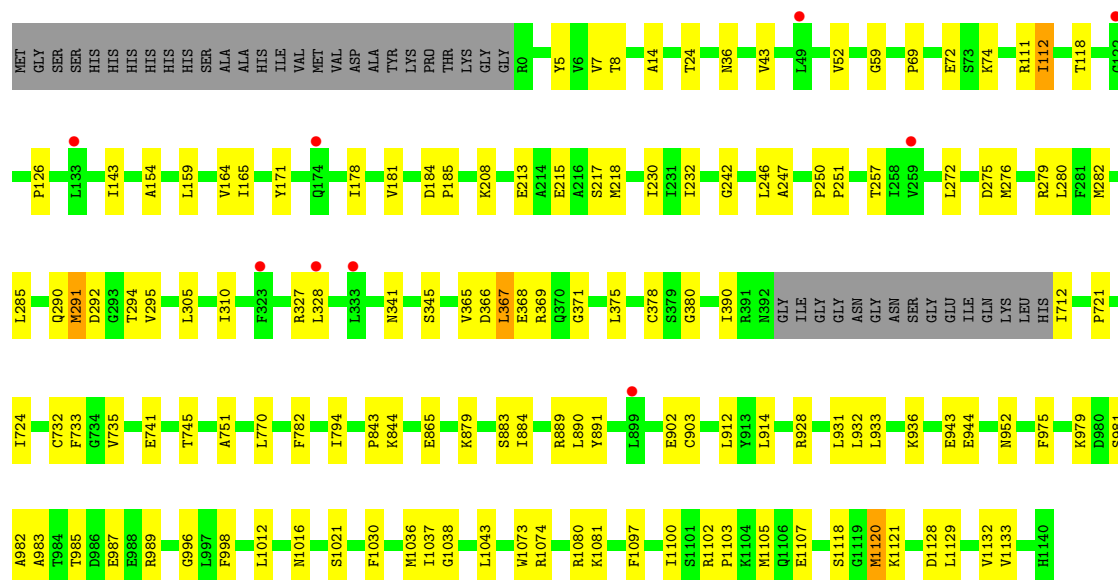
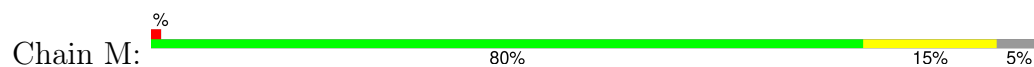


• Molecule 1: DNA damage-binding protein 1

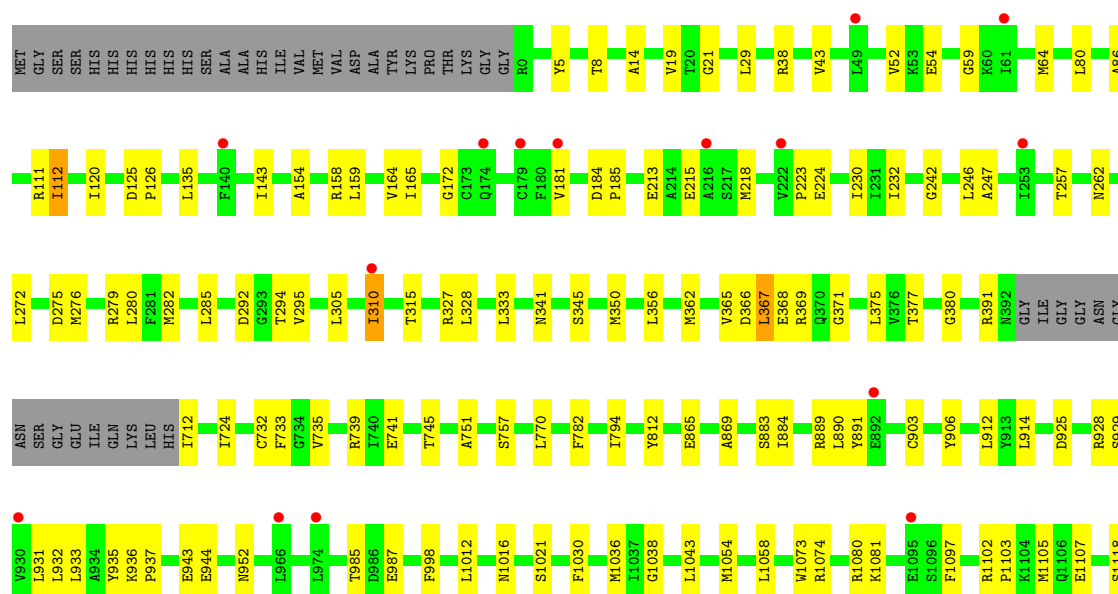
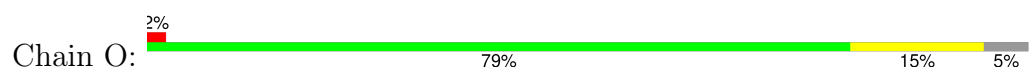


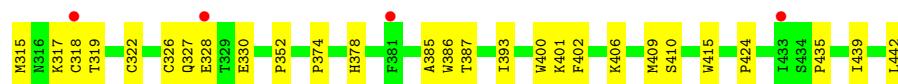


• Molecule 1: DNA damage-binding protein 1

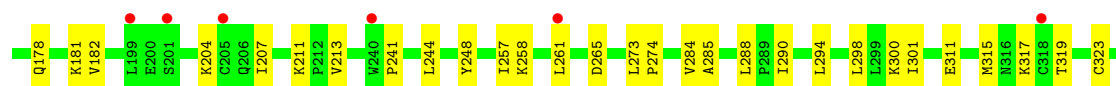
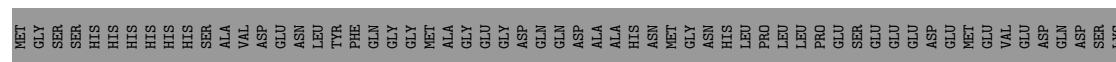


• Molecule 1: DNA damage-binding protein 1

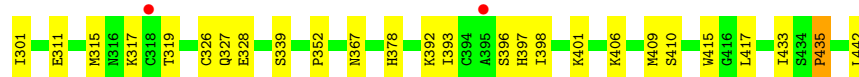
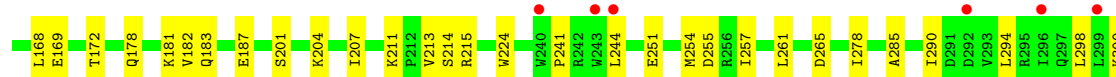
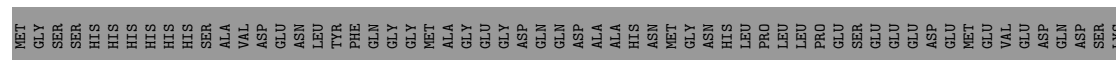




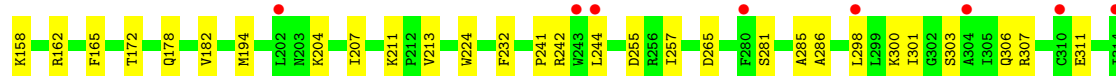
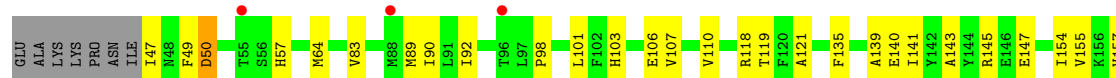
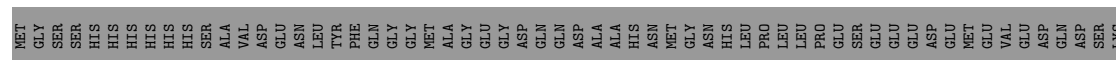
• Molecule 2: Protein cereblon



• Molecule 2: Protein cereblon

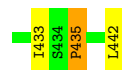
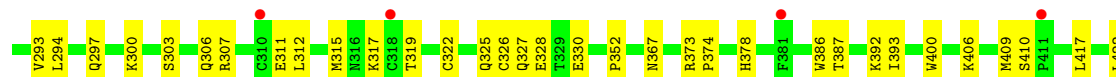
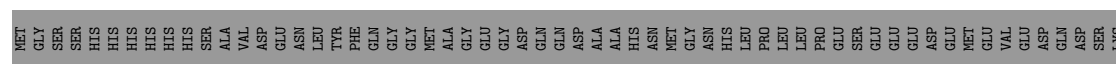


• Molecule 2: Protein cereblon

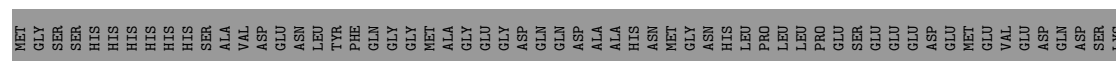




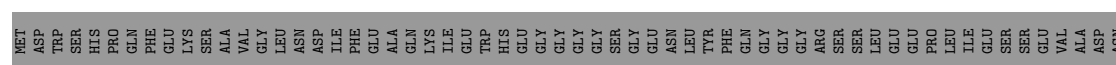
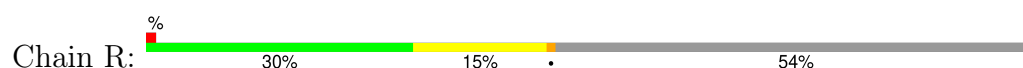
• Molecule 2: Protein cereblon

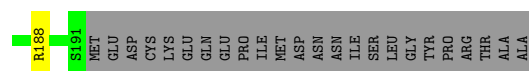


• Molecule 2: Protein cereblon

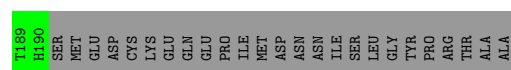
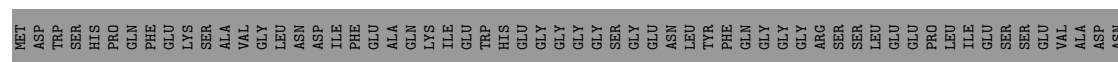
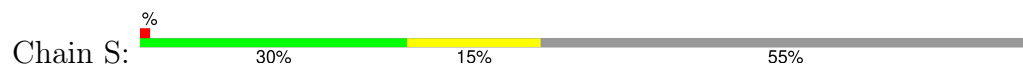


• Molecule 3: Zinc finger protein Helios

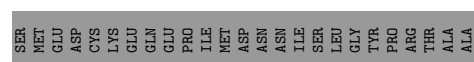
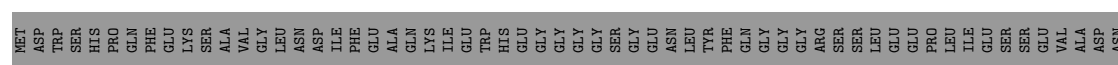
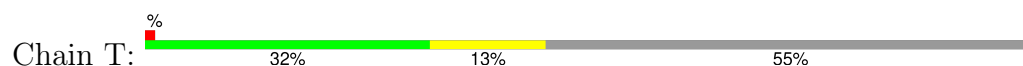




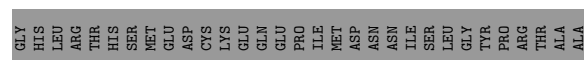
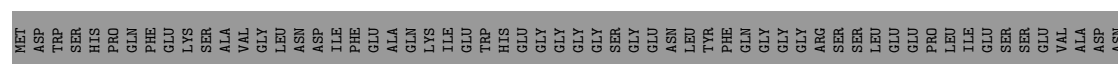
• Molecule 3: Zinc finger protein Helios



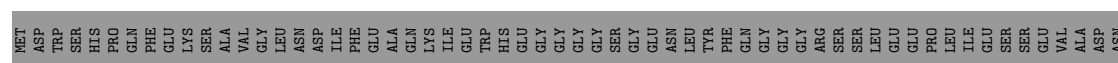
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• Molecule 3: Zinc finger protein Helios



• Molecule 3: Zinc finger protein Helios



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• Molecule 3: Zinc finger protein Helios



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• Molecule 3: Zinc finger protein Helios

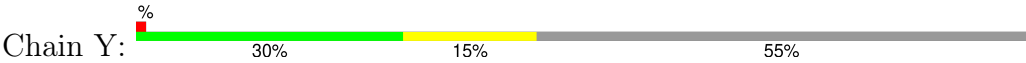


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• Molecule 3: Zinc finger protein Helios



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.59Å 279.06Å 286.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.33 – 4.11 69.33 – 4.11	Depositor EDS
% Data completeness (in resolution range)	99.7 (69.33-4.11) 99.7 (69.33-4.11)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.235 , 0.289 0.236 , 0.288	Depositor DCC
R_{free} test set	6419 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	188.0	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 208.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	81784	wwPDB-VP
Average B, all atoms (Å ²)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8731e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: RN9, ZN

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	0.11	0/6561	0.29	0/8874
1	C	0.12	0/6542	0.31	0/8849
1	E	0.10	0/6561	0.28	0/8874
1	G	0.11	0/6553	0.29	0/8863
1	I	0.11	0/6550	0.29	0/8860
1	K	0.11	0/6561	0.29	0/8874
1	M	0.10	0/6561	0.28	0/8874
1	O	0.11	0/6561	0.28	0/8874
2	B	0.12	0/3232	0.28	0/4390
2	D	0.13	0/3232	0.28	0/4390
2	F	0.11	0/3232	0.27	0/4390
2	H	0.14	0/3232	0.30	0/4390
2	J	0.13	0/3232	0.29	0/4390
2	L	0.12	0/3232	0.28	0/4390
2	N	0.12	0/3232	0.28	0/4390
2	P	0.13	0/3232	0.30	0/4390
3	R	0.13	0/662	0.29	0/885
3	S	0.15	0/656	0.31	0/877
3	T	0.13	0/656	0.30	0/877
3	U	0.20	0/452	0.34	0/602
3	V	0.11	0/434	0.25	0/579
3	W	0.12	0/434	0.23	0/579
3	X	0.17	0/662	0.38	0/885
3	Y	0.19	0/656	0.35	0/877
All	All	0.12	0/82918	0.29	0/112223

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6445	0	6398	98	0
1	C	6426	0	6374	109	0
1	E	6445	0	6398	87	0
1	G	6437	0	6392	100	0
1	I	6434	0	6385	93	0
1	K	6445	0	6398	92	0
1	M	6445	0	6398	87	0
1	O	6445	0	6398	83	0
2	B	3157	0	3114	88	0
2	D	3157	0	3114	62	0
2	F	3157	0	3114	74	0
2	H	3157	0	3114	61	0
2	J	3157	0	3114	68	0
2	L	3157	0	3114	65	0
2	N	3157	0	3114	74	0
2	P	3157	0	3114	75	0
3	R	647	0	642	28	0
3	S	641	0	637	35	0
3	T	641	0	637	22	0
3	U	444	0	446	13	0
3	V	426	0	427	10	0
3	W	426	0	427	10	0
3	X	647	0	642	22	0
3	Y	641	0	638	23	0
4	B	35	23	0	2	0
4	D	35	23	0	0	0
4	F	35	23	0	1	0
4	H	35	23	0	0	0
4	J	35	23	0	0	0
4	L	35	23	0	4	0
4	N	35	23	0	3	0
4	P	35	23	0	3	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	1	0	0	0	0
5	N	1	0	0	0	0
5	P	1	0	0	0	0
5	R	3	0	0	0	0
5	S	3	0	0	0	0
5	T	3	0	0	0	0
5	U	2	0	0	0	0
5	V	2	0	0	0	0
5	W	2	0	0	0	0
5	X	3	0	0	0	0
5	Y	3	0	0	0	0
All	All	81600	184	80549	1343	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1343 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:C:111:ARG:O	1:C:112:ILE:HG12	1.57	1.00
3:S:161:LEU:HD21	3:S:167:PRO:HB3	1.44	0.98
1:A:1120:MET:HA	1:A:1121:LYS:HB2	1.54	0.90
1:O:1120:MET:HA	1:O:1121:LYS:HB2	1.54	0.90
1:M:1120:MET:HA	1:M:1121:LYS:HB2	1.54	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	818/864 (95%)	756 (92%)	49 (6%)	13 (2%)	8 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	816/864 (94%)	755 (92%)	49 (6%)	12 (2%)	8	40
1	E	818/864 (95%)	751 (92%)	55 (7%)	12 (2%)	8	40
1	G	817/864 (95%)	755 (92%)	50 (6%)	12 (2%)	8	40
1	I	817/864 (95%)	755 (92%)	49 (6%)	13 (2%)	8	39
1	K	818/864 (95%)	748 (91%)	59 (7%)	11 (1%)	10	42
1	M	818/864 (95%)	758 (93%)	48 (6%)	12 (2%)	8	40
1	O	818/864 (95%)	754 (92%)	53 (6%)	11 (1%)	10	42
2	B	394/463 (85%)	376 (95%)	15 (4%)	3 (1%)	16	53
2	D	394/463 (85%)	376 (95%)	15 (4%)	3 (1%)	16	53
2	F	394/463 (85%)	377 (96%)	14 (4%)	3 (1%)	16	53
2	H	394/463 (85%)	377 (96%)	14 (4%)	3 (1%)	16	53
2	J	394/463 (85%)	376 (95%)	15 (4%)	3 (1%)	16	53
2	L	394/463 (85%)	371 (94%)	21 (5%)	2 (0%)	25	62
2	N	394/463 (85%)	375 (95%)	16 (4%)	3 (1%)	16	53
2	P	394/463 (85%)	375 (95%)	16 (4%)	3 (1%)	16	53
3	R	81/182 (44%)	76 (94%)	2 (2%)	3 (4%)	2	23
3	S	80/182 (44%)	76 (95%)	4 (5%)	0	100	100
3	T	80/182 (44%)	75 (94%)	5 (6%)	0	100	100
3	U	56/182 (31%)	52 (93%)	2 (4%)	2 (4%)	3	23
3	V	54/182 (30%)	51 (94%)	1 (2%)	2 (4%)	2	23
3	W	54/182 (30%)	48 (89%)	6 (11%)	0	100	100
3	X	81/182 (44%)	76 (94%)	1 (1%)	4 (5%)	2	19
3	Y	80/182 (44%)	73 (91%)	5 (6%)	2 (2%)	4	30
All	All	10258/12072 (85%)	9562 (93%)	564 (6%)	132 (1%)	10	42

5 of 132 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ILE
1	A	295	VAL
1	A	713	ARG
2	B	50	ASP
1	C	295	VAL

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	711/749 (95%)	711 (100%)	0	100	100
1	C	709/749 (95%)	709 (100%)	0	100	100
1	E	711/749 (95%)	711 (100%)	0	100	100
1	G	710/749 (95%)	710 (100%)	0	100	100
1	I	710/749 (95%)	710 (100%)	0	100	100
1	K	711/749 (95%)	711 (100%)	0	100	100
1	M	711/749 (95%)	711 (100%)	0	100	100
1	O	711/749 (95%)	711 (100%)	0	100	100
2	B	350/416 (84%)	350 (100%)	0	100	100
2	D	350/416 (84%)	350 (100%)	0	100	100
2	F	350/416 (84%)	350 (100%)	0	100	100
2	H	350/416 (84%)	349 (100%)	1 (0%)	91	92
2	J	350/416 (84%)	350 (100%)	0	100	100
2	L	350/416 (84%)	350 (100%)	0	100	100
2	N	350/416 (84%)	350 (100%)	0	100	100
2	P	350/416 (84%)	350 (100%)	0	100	100
3	R	72/153 (47%)	72 (100%)	0	100	100
3	S	71/153 (46%)	71 (100%)	0	100	100
3	T	71/153 (46%)	71 (100%)	0	100	100
3	U	50/153 (33%)	50 (100%)	0	100	100
3	V	48/153 (31%)	48 (100%)	0	100	100
3	W	48/153 (31%)	48 (100%)	0	100	100
3	X	72/153 (47%)	72 (100%)	0	100	100
3	Y	71/153 (46%)	71 (100%)	0	100	100
All	All	8987/10544 (85%)	8986 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	323	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	163	HIS
1	O	234	GLN
3	T	143	ASN
1	G	337	ASN
2	F	378	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 29 are monoatomic - leaving 8 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	$\# Z > 2$
4	RN9	F	501	-	38,38,38	0.35	0	53,54,54	0.76	1 (1%)
4	RN9	P	501	-	38,38,38	0.23	0	53,54,54	0.68	2 (3%)
4	RN9	D	501	-	38,38,38	0.28	0	53,54,54	0.67	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	RN9	L	501	-	38,38,38	0.23	0	53,54,54	0.67	2 (3%)
4	RN9	N	501	-	38,38,38	0.25	0	53,54,54	0.62	1 (1%)
4	RN9	B	501	-	38,38,38	0.21	0	53,54,54	0.67	2 (3%)
4	RN9	J	501	-	38,38,38	0.26	0	53,54,54	0.70	3 (5%)
4	RN9	H	501	-	38,38,38	0.46	0	53,54,54	0.76	1 (1%)

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
4	RN9	F	501	-	-	6/17/46/46	0/4/4/4
4	RN9	P	501	-	-	6/17/46/46	0/4/4/4
4	RN9	D	501	-	-	6/17/46/46	0/4/4/4
4	RN9	L	501	-	-	6/17/46/46	0/4/4/4
4	RN9	N	501	-	-	5/17/46/46	0/4/4/4
4	RN9	B	501	-	-	6/17/46/46	0/4/4/4
4	RN9	J	501	-	-	6/17/46/46	0/4/4/4
4	RN9	H	501	-	-	6/17/46/46	0/4/4/4

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	RN9	C23-C8-N2	-2.83	110.90	120.41
4	P	501	RN9	C23-C8-N2	-2.80	111.02	120.41
4	J	501	RN9	C23-C8-N2	-2.79	111.04	120.41
4	B	501	RN9	C23-C8-N2	-2.72	111.26	120.41
4	L	501	RN9	C23-C8-N2	-2.70	111.35	120.41

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	RN9	C24-C7-N2-C8
4	B	501	RN9	C6-C7-N2-C8
4	D	501	RN9	C24-C7-N2-C8

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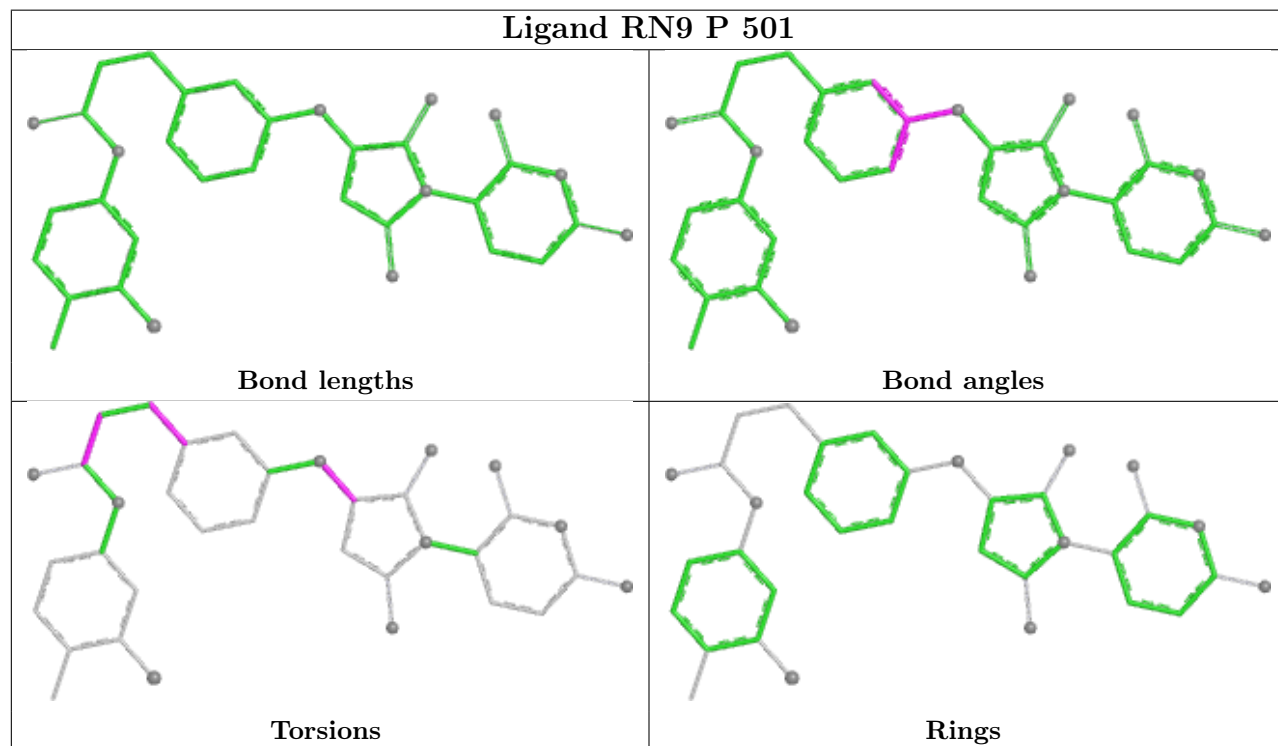
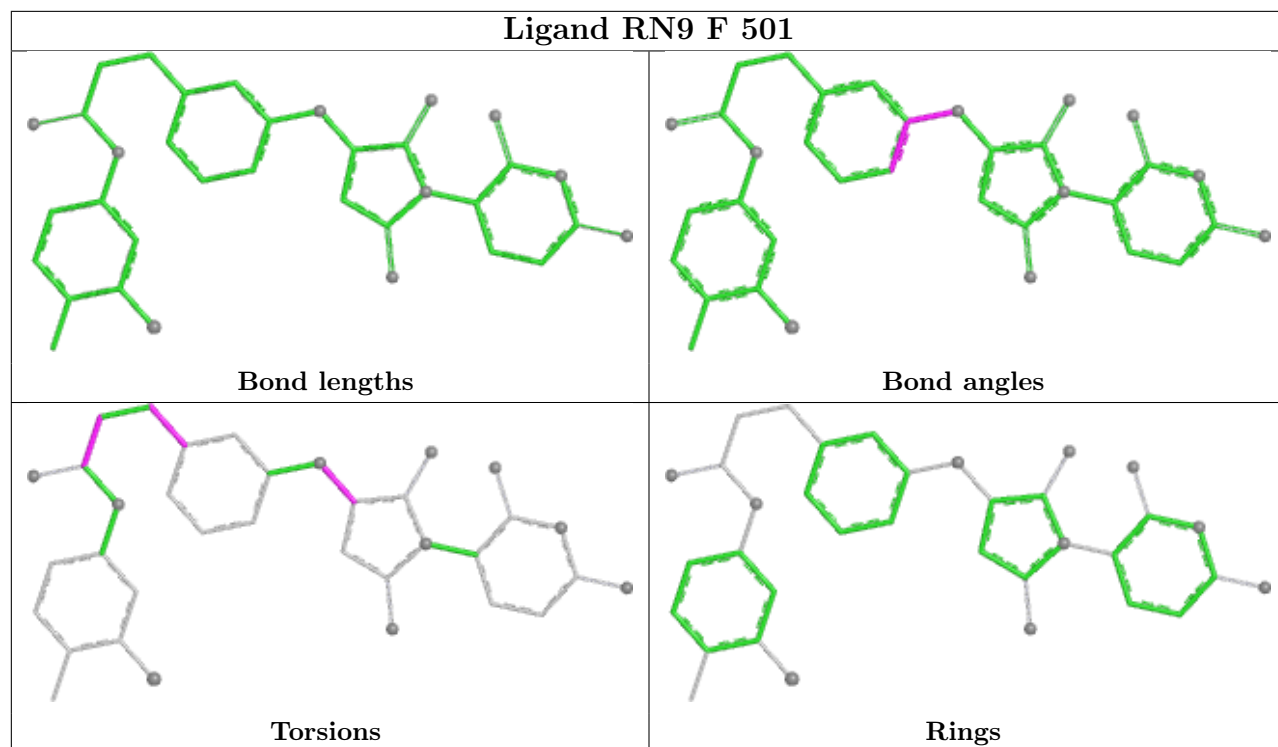
Mol	Chain	Res	Type	Atoms
4	D	501	RN9	C6-C7-N2-C8
4	F	501	RN9	C24-C7-N2-C8

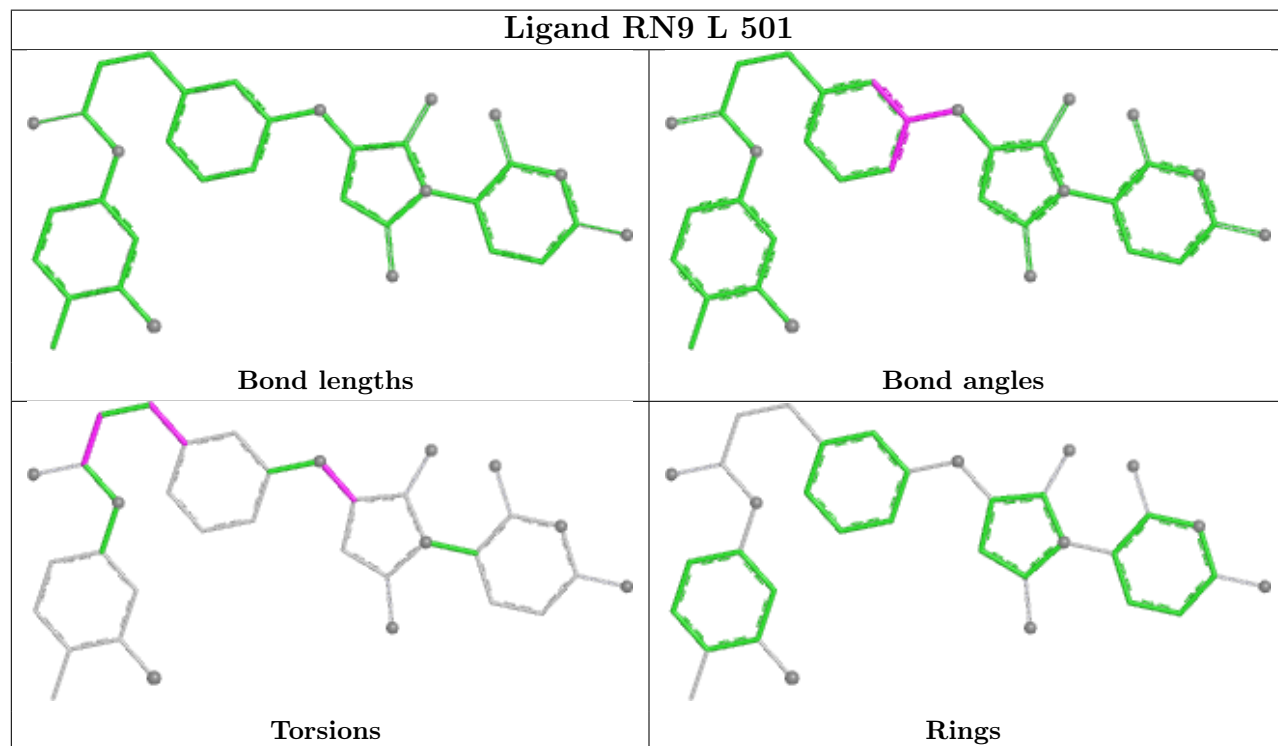
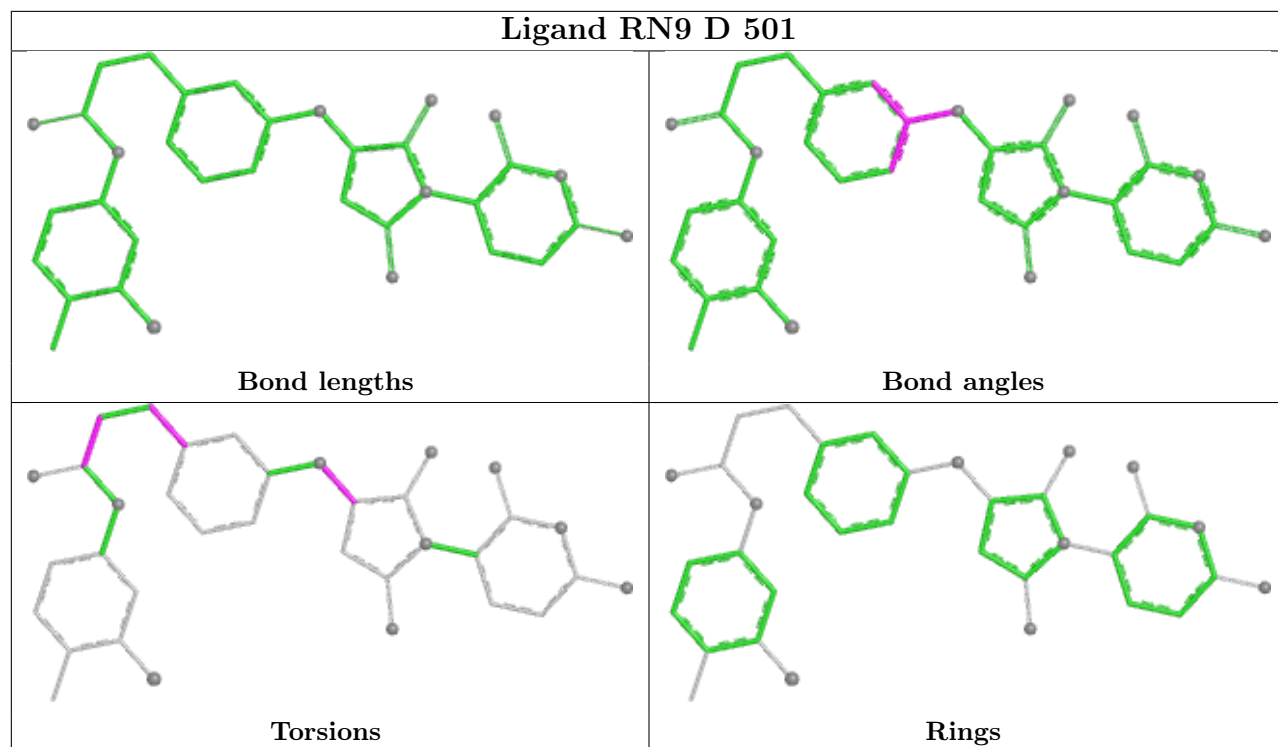
There are no ring outliers.

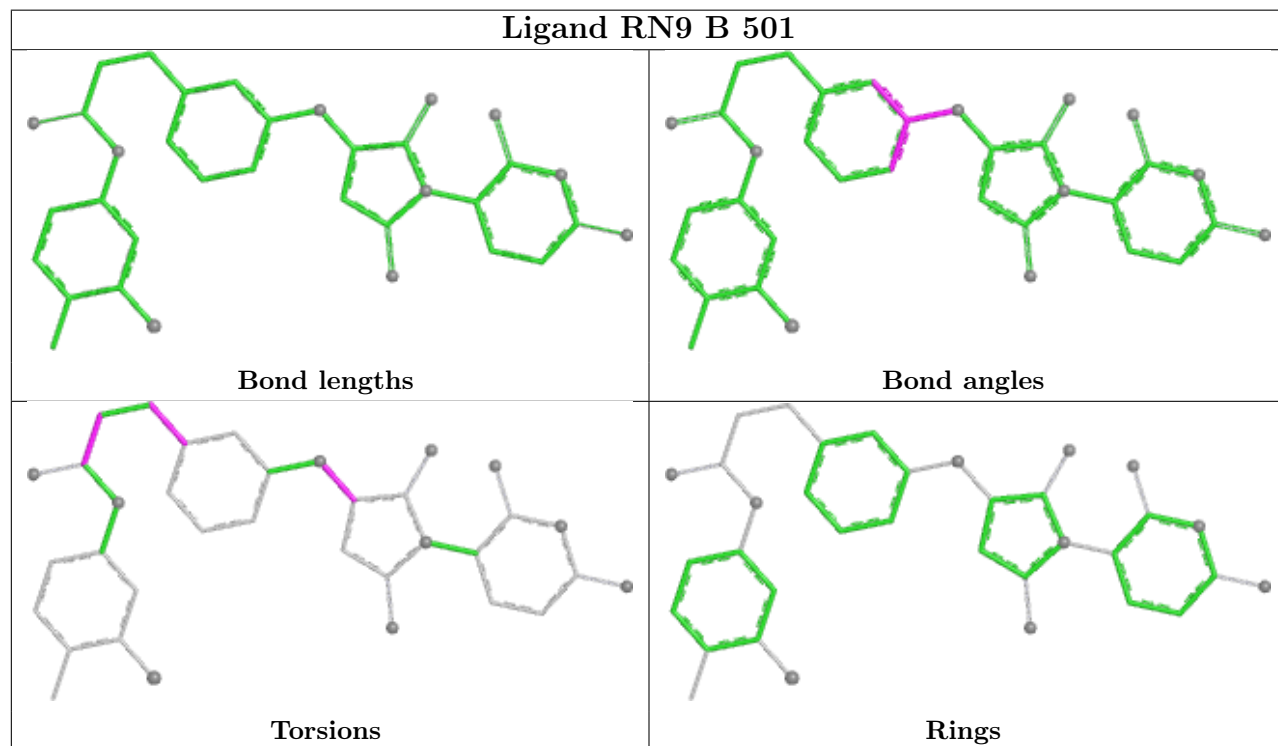
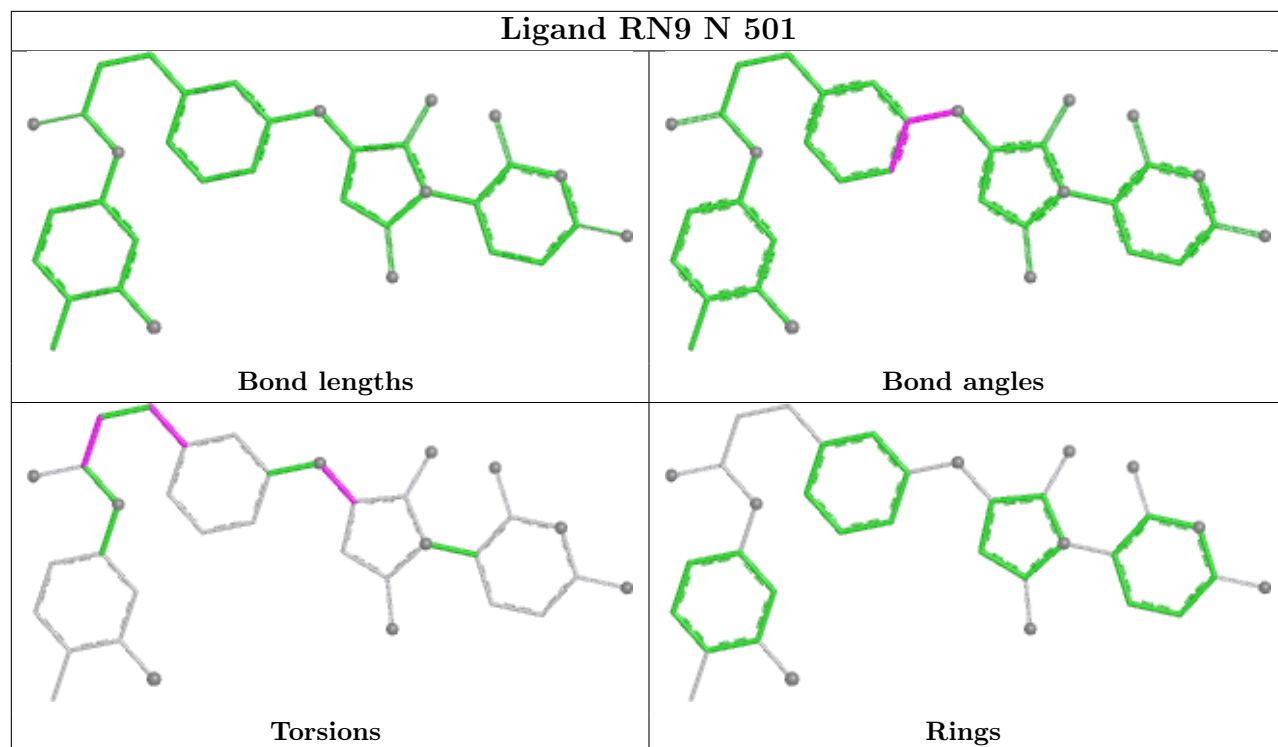
5 monomers are involved in 13 short contacts:

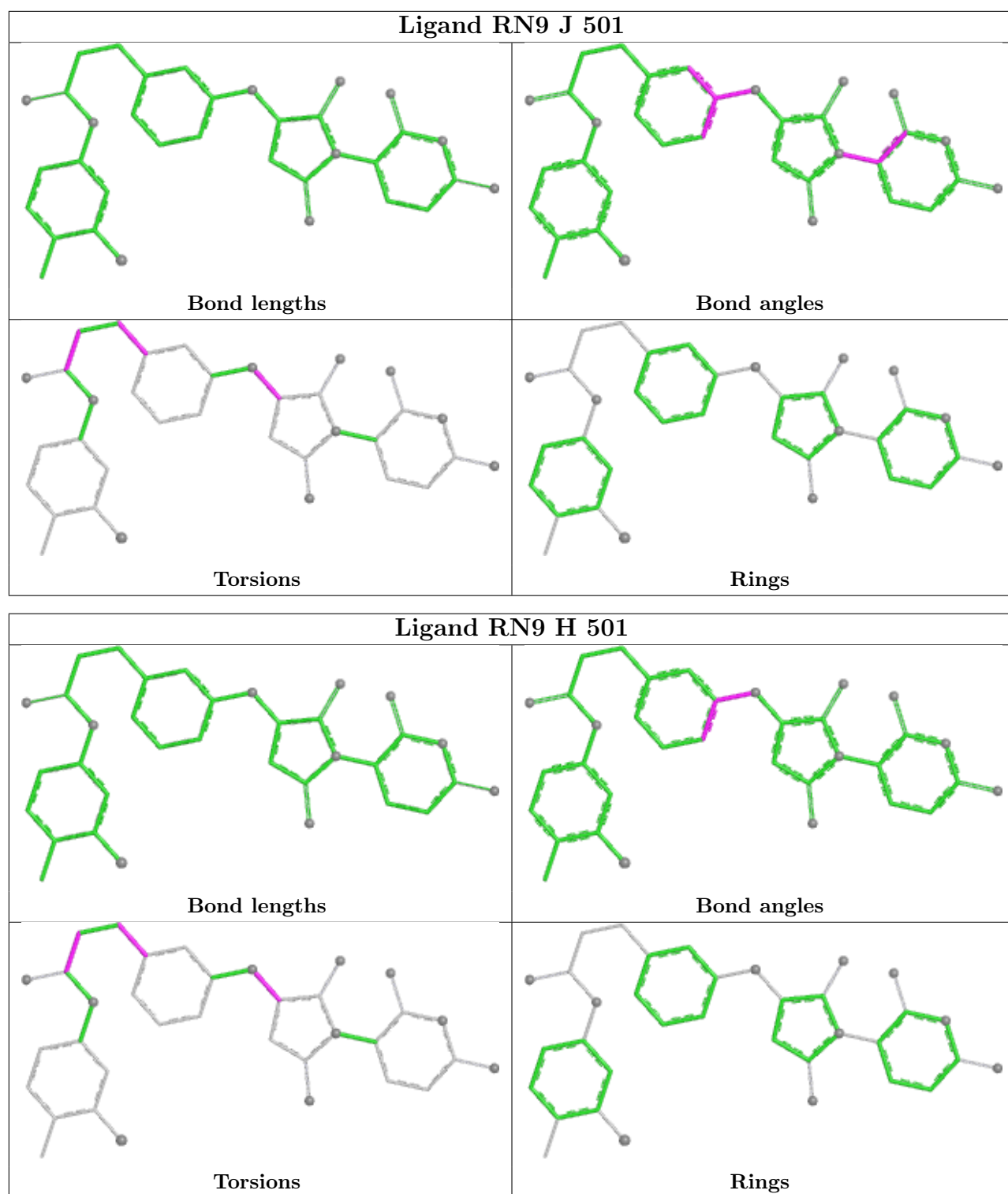
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	501	RN9	1	0
4	P	501	RN9	3	0
4	L	501	RN9	4	0
4	N	501	RN9	3	0
4	B	501	RN9	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	822/864 (95%)	-0.01	13 (1%) 70 55	143, 212, 280, 355	0
1	C	820/864 (94%)	0.01	15 (1%) 67 51	127, 188, 269, 362	0
1	E	822/864 (95%)	0.01	12 (1%) 71 56	174, 278, 332, 362	0
1	G	821/864 (95%)	-0.03	15 (1%) 67 51	147, 208, 288, 366	0
1	I	821/864 (95%)	-0.10	10 (1%) 76 61	141, 206, 277, 351	0
1	K	822/864 (95%)	-0.11	7 (0%) 81 67	144, 215, 281, 370	0
1	M	822/864 (95%)	-0.14	9 (1%) 77 64	149, 225, 290, 362	0
1	O	822/864 (95%)	0.03	15 (1%) 67 51	147, 222, 291, 361	0
2	B	396/463 (85%)	0.14	12 (3%) 52 39	129, 184, 268, 342	0
2	D	396/463 (85%)	0.02	7 (1%) 67 51	129, 174, 271, 331	0
2	F	396/463 (85%)	0.15	15 (3%) 44 34	151, 209, 287, 373	0
2	H	396/463 (85%)	0.11	9 (2%) 61 46	147, 184, 270, 345	0
2	J	396/463 (85%)	0.24	11 (2%) 55 41	140, 179, 274, 339	0
2	L	396/463 (85%)	0.29	17 (4%) 40 32	142, 197, 270, 354	0
2	N	396/463 (85%)	0.09	8 (2%) 64 49	130, 192, 277, 340	0
2	P	396/463 (85%)	0.06	7 (1%) 67 51	137, 178, 276, 334	0
3	R	83/182 (45%)	0.05	2 (2%) 59 45	154, 213, 250, 272	0
3	S	82/182 (45%)	0.19	2 (2%) 59 45	167, 237, 285, 300	0
3	T	82/182 (45%)	0.23	2 (2%) 59 45	149, 235, 289, 307	0
3	U	58/182 (31%)	0.07	0 100 100	179, 228, 280, 309	0
3	V	56/182 (30%)	0.11	1 (1%) 67 51	169, 218, 260, 296	0
3	W	56/182 (30%)	-0.08	0 100 100	149, 202, 260, 291	0
3	X	83/182 (45%)	0.16	1 (1%) 76 61	144, 219, 271, 292	0
3	Y	82/182 (45%)	0.10	1 (1%) 76 61	156, 234, 275, 308	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	10322/12072 (85%)	0.02	191 (1%)	66	50	127, 208, 298, 373	0

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	912	LEU	5.7
1	O	174	GLN	4.8
1	A	913	TYR	4.6
2	D	197	VAL	4.2
1	E	217	SER	4.1

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
4	RN9	H	501	35/35	0.77	0.12	165,194,262,304	0
4	RN9	F	501	35/35	0.83	0.10	171,205,272,273	0
4	RN9	L	501	35/35	0.84	0.15	173,228,297,303	0
4	RN9	B	501	35/35	0.85	0.15	147,182,250,260	0
4	RN9	J	501	35/35	0.86	0.14	153,186,235,242	0
5	ZN	S	301	1/1	0.87	0.10	272,272,272,272	0
5	ZN	T	302	1/1	0.88	0.12	257,257,257,257	0
4	RN9	N	501	35/35	0.89	0.11	151,207,268,274	0
4	RN9	D	501	35/35	0.90	0.13	132,172,232,255	0
4	RN9	P	501	35/35	0.90	0.10	137,190,246,248	0
5	ZN	X	303	1/1	0.91	0.15	295,295,295,295	0
5	ZN	R	301	1/1	0.95	0.05	225,225,225,225	0
5	ZN	S	302	1/1	0.95	0.05	202,202,202,202	0

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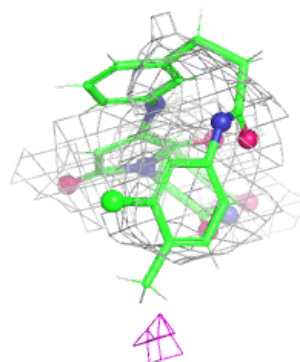
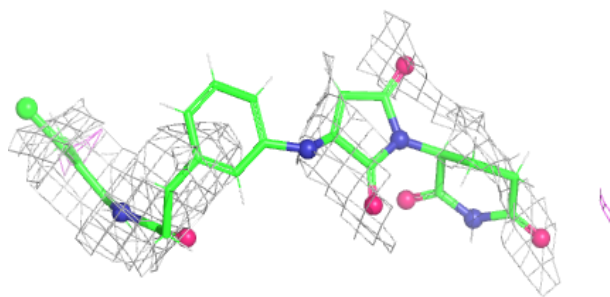
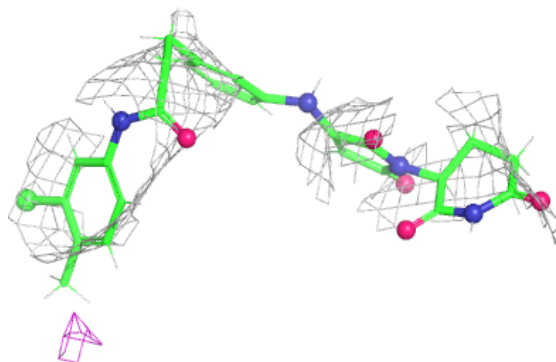
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ZN	U	301	1/1	0.96	0.05	276,276,276,276	0
5	ZN	V	301	1/1	0.97	0.06	214,214,214,214	0
5	ZN	T	301	1/1	0.97	0.05	205,205,205,205	0
5	ZN	W	301	1/1	0.98	0.06	212,212,212,212	0
5	ZN	X	301	1/1	0.98	0.04	183,183,183,183	0
5	ZN	R	302	1/1	0.98	0.06	227,227,227,227	0
5	ZN	Y	302	1/1	0.98	0.03	238,238,238,238	0
5	ZN	R	303	1/1	0.99	0.07	152,152,152,152	0
5	ZN	U	302	1/1	0.99	0.05	163,163,163,163	0
5	ZN	J	502	1/1	0.99	0.11	153,153,153,153	0
5	ZN	V	302	1/1	0.99	0.08	169,169,169,169	0
5	ZN	L	502	1/1	0.99	0.12	184,184,184,184	0
5	ZN	S	303	1/1	0.99	0.04	176,176,176,176	0
5	ZN	X	302	1/1	0.99	0.04	151,151,151,151	0
5	ZN	B	502	1/1	0.99	0.09	160,160,160,160	0
5	ZN	Y	301	1/1	0.99	0.03	206,206,206,206	0
5	ZN	H	502	1/1	0.99	0.12	170,170,170,170	0
5	ZN	Y	303	1/1	0.99	0.13	156,156,156,156	0
5	ZN	F	502	1/1	1.00	0.09	203,203,203,203	0
5	ZN	D	502	1/1	1.00	0.09	166,166,166,166	0
5	ZN	N	502	1/1	1.00	0.10	159,159,159,159	0
5	ZN	P	502	1/1	1.00	0.09	148,148,148,148	0
5	ZN	T	303	1/1	1.00	0.04	128,128,128,128	0
5	ZN	W	302	1/1	1.00	0.06	142,142,142,142	0

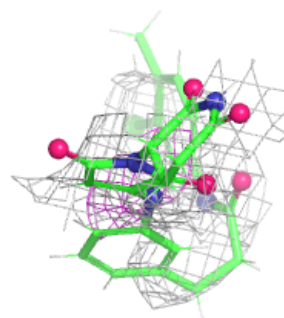
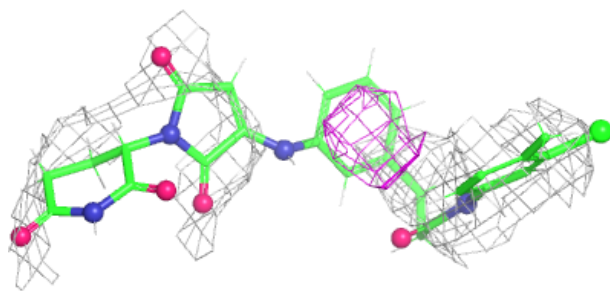
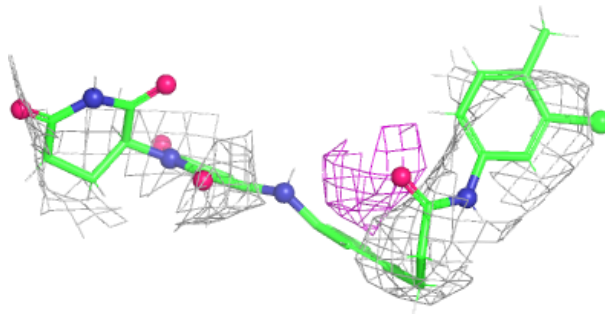
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RN9 H 501:

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

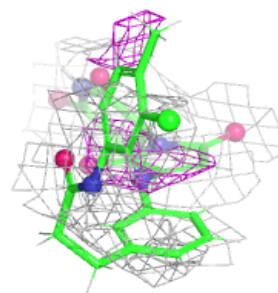
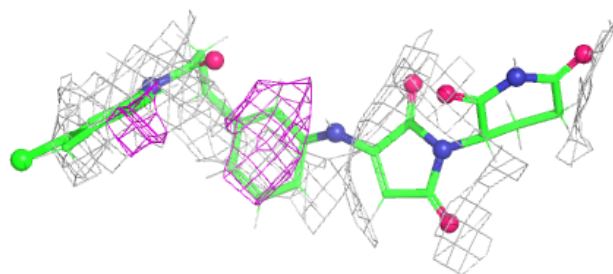
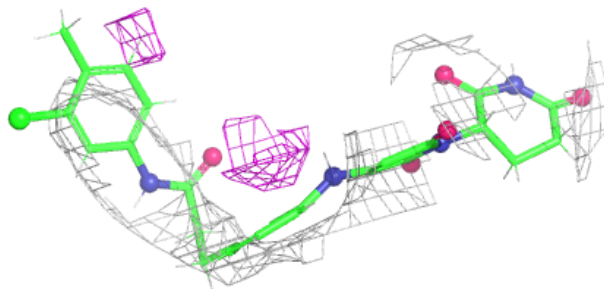
**Electron density around RN9 F 501:**

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

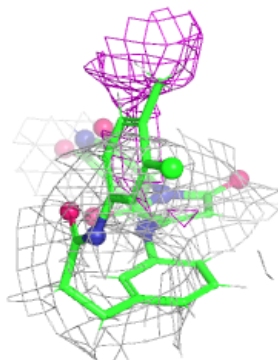
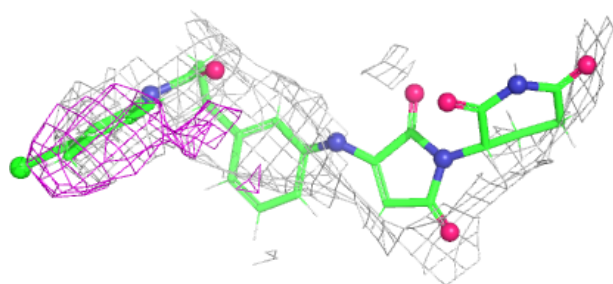
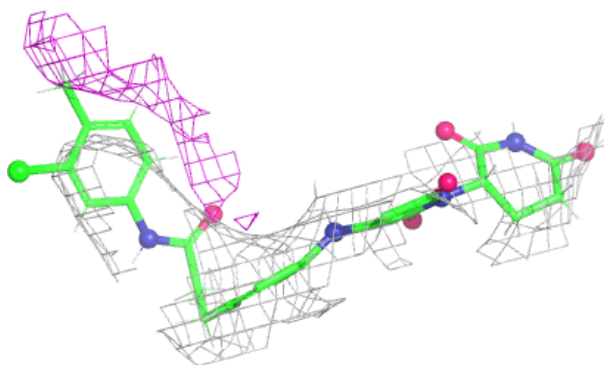


Electron density around RN9 L 501:

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

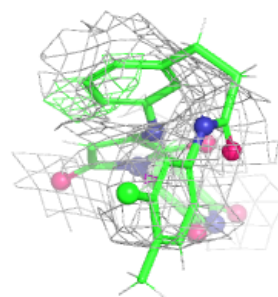
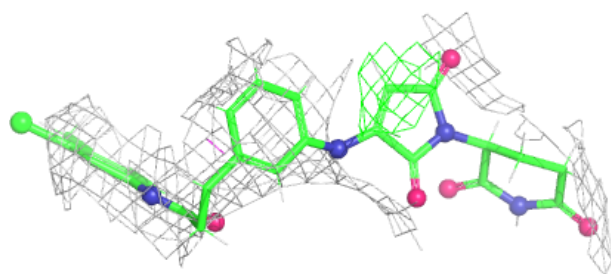
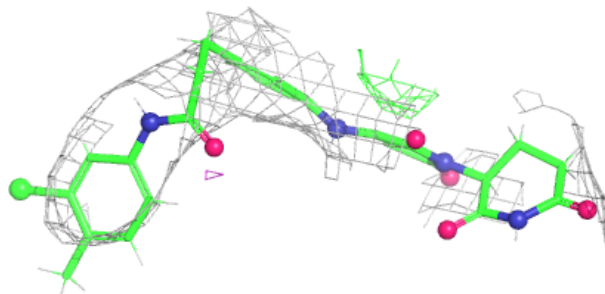
**Electron density around RN9 B 501:**

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

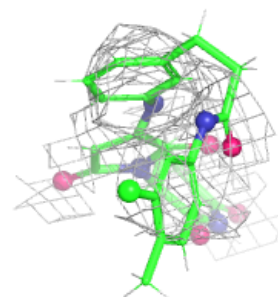
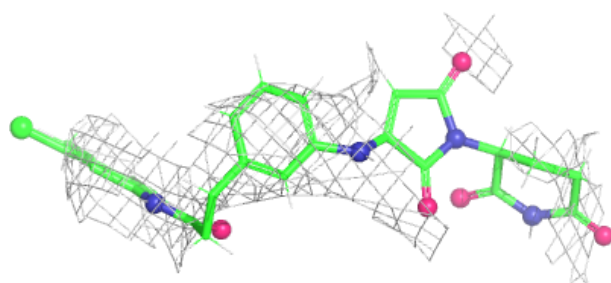
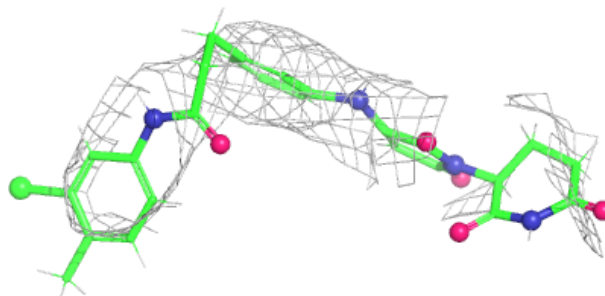


Electron density around RN9 J 501:

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

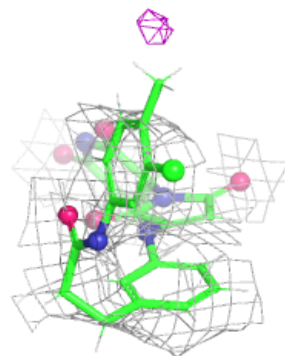
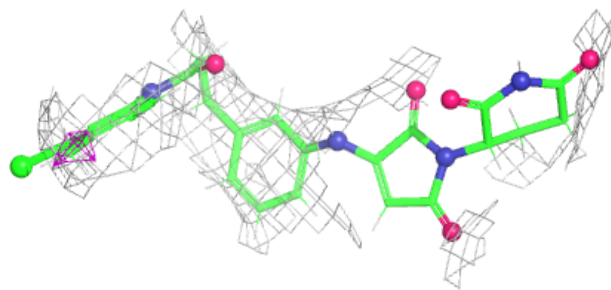
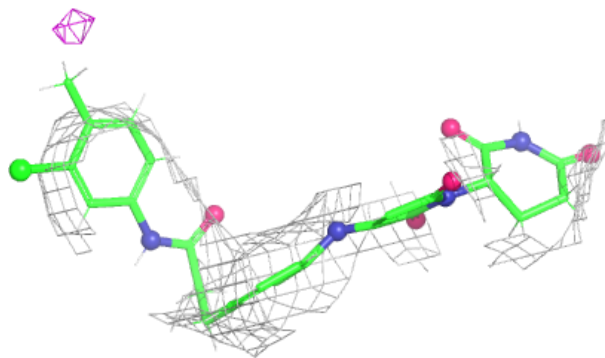
**Electron density around RN9 N 501:**

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

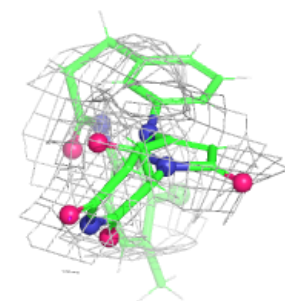
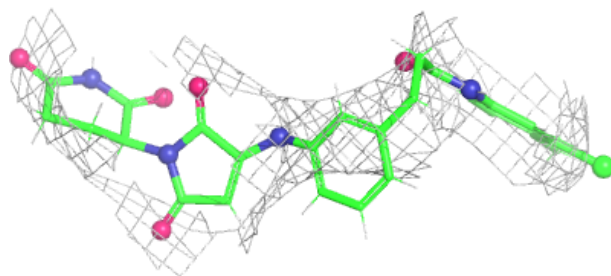
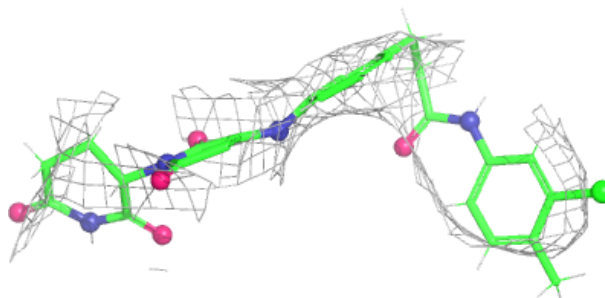


Electron density around RN9 D 501:

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

**Electron density around RN9 P 501:**

$2mF_o-DF_c$ (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.