



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 07:45 AM UTC

PDB ID : 7X8X / pdb_00007x8x
Title : structural insights into Mycobacterium tuberculosis ClpP1P2 inhibition by Cediranib: implications for developing antimicrobial agents targeting Clp protease
Authors : Bao, R.; Luo, Y.F.; Zhu, Y.B.; Yang, Y.; Zhou, Y.Z.
Deposited on : 2022-03-15
Resolution : 3.24 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

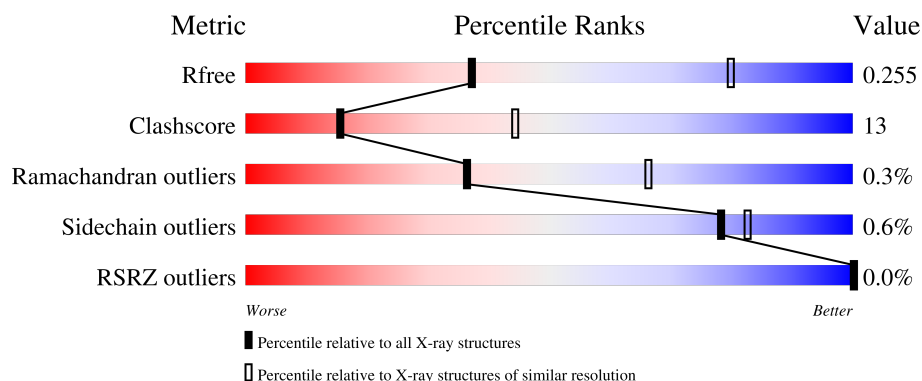
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

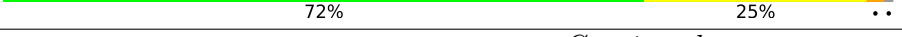
The reported resolution of this entry is 3.24 Å.

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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	197	 72% 26% ..
1	C	197	 71% 28% ..
1	E	197	 67% 31% .
1	F	197	 72% 25% ..

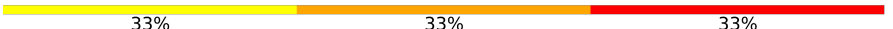
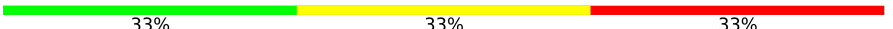
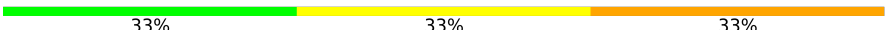
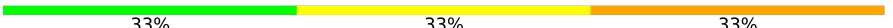
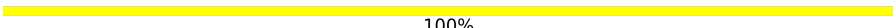
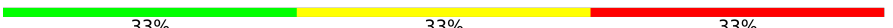
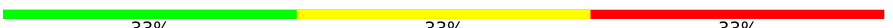
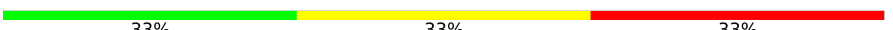
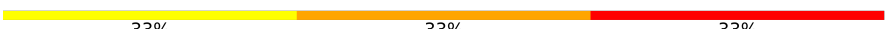
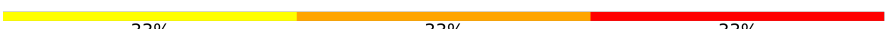
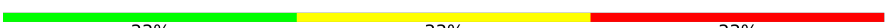
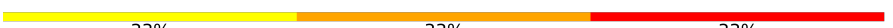
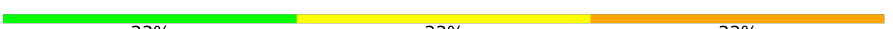
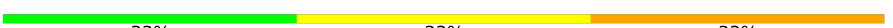
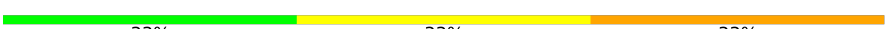
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Mol	Chain	Length	Quality of chain
1	H	197	74% 25% ..
1	J	197	76% 22% ..
1	L	197	69% 28% ..
1	O	197	71% 27% ..
1	Q	197	76% 23% ..
1	S	197	73% 27% .
1	T	197	76% 23% ..
1	V	197	68% 31% .
1	X	197	75% 23% .
1	a	197	73% 25% .
2	B	177	73% 27% .
2	D	177	72% 26% ..
2	G	177	72% 26% ..
2	I	177	70% 28% ..
2	K	177	68% 30% ..
2	M	177	71% 29% .
2	N	177	72% 27% ..
2	P	177	77% 23%
2	R	177	77% 21% ..
2	U	177	69% 30% .
2	W	177	80% 19% .
2	Y	177	71% 28% ..
2	Z	177	76% 23% ..
2	b	177	73% 27% .
3	0	3	67% 33%

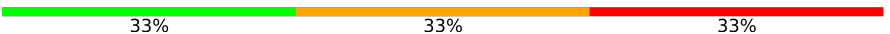
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Mol	Chain	Length	Quality of chain
3	1	3	 33% 67%
3	2	3	 33% 67%
3	3	3	 33% 33% 33%
3	4	3	 33% 33% 33%
3	c	3	 33% 33% 33%
3	e	3	 33% 33% 33%
3	f	3	 33% 67%
3	g	3	 100%
3	h	3	 33% 33% 33%
3	i	3	 33% 67%
3	j	3	 33% 67%
3	k	3	 33% 33% 33%
3	l	3	 33% 33% 33%
3	m	3	 33% 33% 33%
3	n	3	 33% 33% 33%
3	o	3	 67% 33%
3	p	3	 33% 67%
3	q	3	 33% 33% 33%
3	r	3	 33% 33% 33%
3	s	3	 33% 67%
3	t	3	 33% 33% 33%
3	u	3	 33% 33% 33%
3	v	3	 33% 67%
3	w	3	 33% 33% 33%
3	x	3	 33% 67%

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Mol	Chain	Length	Quality of chain
3	y	3	 67% 33%
3	z	3	 33% 33% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AI4	B	201	-	X	-	-
4	AI4	F	301	-	X	-	-
4	AI4	G	201	-	X	-	-
4	AI4	I	201	-	X	-	-
4	AI4	K	201	-	X	-	-
4	AI4	M	201	-	X	-	-
4	AI4	N	301	-	X	-	-
4	AI4	R	201	-	X	-	-
4	AI4	U	201	-	X	-	-
4	AI4	V	301	-	X	-	-
4	AI4	W	201	-	X	-	-
4	AI4	Y	201	-	X	-	-
4	AI4	Z	201	-	X	-	-
4	AI4	b	201	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 81239 atoms, of which 40443 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 ATP-dependent Clp protease proteolytic subunit 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	194	Total	C	H	N	O	S	0	0	0
			2986	936	1495	255	292	8			
1	O	194	Total	C	H	N	O	S	0	0	0
			2986	936	1495	255	292	8			
1	C	196	Total	C	H	N	O	S	0	0	0
			2993	940	1496	256	293	8			
1	Q	196	Total	C	H	N	O	S	0	0	0
			2993	940	1496	256	293	8			
1	F	196	Total	C	H	N	O	S	0	0	0
			2993	940	1496	256	293	8			
1	S	196	Total	C	H	N	O	S	0	0	0
			2993	940	1496	256	293	8			
1	H	196	Total	C	H	N	O	S	0	0	0
			3008	943	1507	257	293	8			
1	T	196	Total	C	H	N	O	S	0	0	0
			3008	943	1507	257	293	8			
1	J	195	Total	C	H	N	O	S	0	0	0
			3011	946	1509	256	292	8			
1	V	195	Total	C	H	N	O	S	0	0	0
			3010	946	1508	256	292	8			
1	L	193	Total	C	H	N	O	S	0	0	0
			2941	925	1467	252	289	8			
1	X	193	Total	C	H	N	O	S	0	0	0
			2941	925	1467	252	289	8			
1	E	193	Total	C	H	N	O	S	0	0	0
			2941	925	1467	252	289	8			
1	a	193	Total	C	H	N	O	S	0	0	0
			2941	925	1467	252	289	8			

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	177	Total	C	H	N	O	S	0	0	0
			2695	855	1344	228	259	9			
2	P	177	Total	C	H	N	O	S	0	0	0
			2695	855	1344	228	259	9			
2	D	175	Total	C	H	N	O	S	0	0	0
			2652	843	1320	223	257	9			
2	R	175	Total	C	H	N	O	S	0	0	0
			2652	843	1320	223	257	9			
2	I	175	Total	C	H	N	O	S	0	0	0
			2644	841	1316	223	255	9			
2	U	175	Total	C	H	N	O	S	0	0	0
			2644	841	1316	223	255	9			
2	K	175	Total	C	H	N	O	S	0	0	0
			2627	838	1305	220	255	9			
2	W	175	Total	C	H	N	O	S	0	0	0
			2627	838	1305	220	255	9			
2	M	176	Total	C	H	N	O	S	0	0	0
			2629	841	1305	218	256	9			
2	Y	176	Total	C	H	N	O	S	0	0	0
			2629	841	1305	218	256	9			
2	N	176	Total	C	H	N	O	S	0	0	0
			2629	841	1305	218	256	9			
2	Z	176	Total	C	H	N	O	S	0	0	0
			2629	841	1305	218	256	9			
2	G	176	Total	C	H	N	O	S	0	0	0
			2646	844	1316	221	256	9			
2	b	176	Total	C	H	N	O	S	0	0	0
			2646	844	1316	221	256	9			

- Molecule 3 is a protein called 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	c	3	Total	C	H	N	O		0	0	0
			52	19	27	2	4				
3	e	3	Total	C	H	N	O		0	0	0
			52	19	27	2	4				
3	f	3	Total	C	H	N	O		0	0	0
			52	19	27	2	4				
3	g	3	Total	C	H	N	O		0	0	0
			52	19	27	2	4				
3	h	3	Total	C	H	N	O		0	0	0
			52	19	27	2	4				

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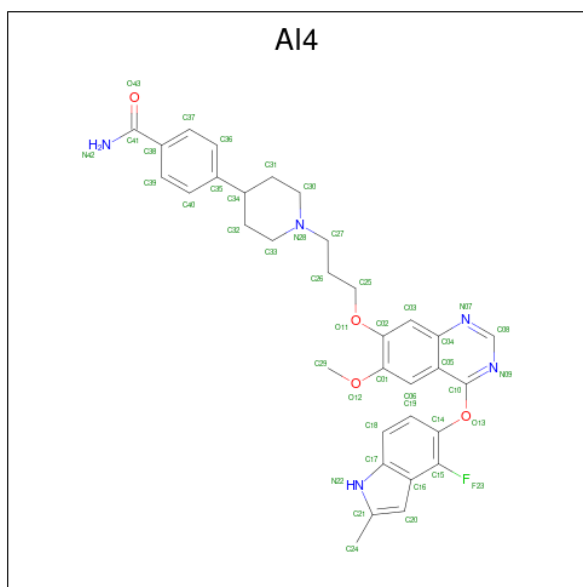
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	i	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	j	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	k	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	l	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	m	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	n	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	o	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	p	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	q	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	r	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	s	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	t	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	u	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	v	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	w	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	x	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	y	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	z	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	0	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	1	3	Total 52	C 19	H 27	N 2	O 4	0	0	0
3	2	3	Total 52	C 19	H 27	N 2	O 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	3	Total	C	H	N	O	0	0	0
			52	19	27	2	4			
3	4	3	Total	C	H	N	O	0	0	0
			52	19	27	2	4			

- Molecule 4 is 4-[1-[3-[4-[(4-fluoranyl-2-methyl-1H-indol-5-yl)oxy]-6-methoxy-quinazolin-7-yl]oxypropyl]piperidin-4-yl]benzamide (CCD ID: AI4) (formula: C₃₃H₃₄FN₅O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total 71	C 33	F 1	H 28	N 5	O 4	0	0
4	R	1	Total 71	C 33	F 1	H 28	N 5	O 4	0	0
4	F	1	Total 71	C 33	F 1	H 28	N 5	O 4	0	0
4	I	1	Total 71	C 33	F 1	H 28	N 5	O 4	0	0
4	U	1	Total 71	C 33	F 1	H 28	N 5	O 4	0	0
4	V	1	Total 71	C 33	F 1	H 28	N 5	O 4	0	0
4	K	1	Total 71	C 33	F 1	H 28	N 5	O 4	0	0
4	W	1	Total 71	C 33	F 1	H 28	N 5	O 4	0	0

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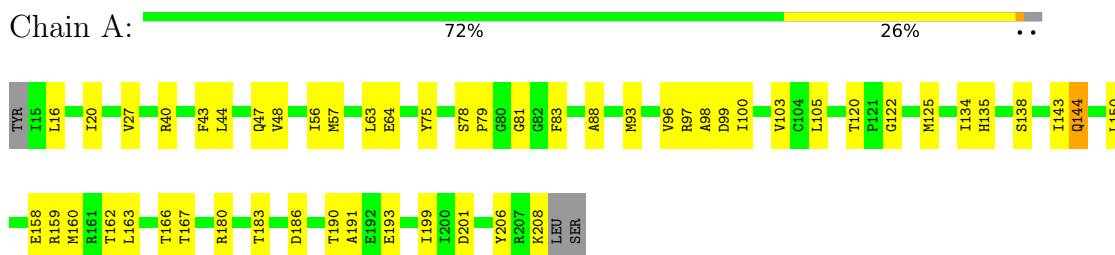
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	M	1	Total	C	F	H	N	O	0	0
			71	33	1	28	5	4		
4	Y	1	Total	C	F	H	N	O	0	0
			71	33	1	28	5	4		
4	N	1	Total	C	F	H	N	O	0	0
			71	33	1	28	5	4		
4	Z	1	Total	C	F	H	N	O	0	0
			71	33	1	28	5	4		
4	G	1	Total	C	F	H	N	O	0	0
			71	33	1	28	5	4		
4	b	1	Total	C	F	H	N	O	0	0
			71	33	1	28	5	4		

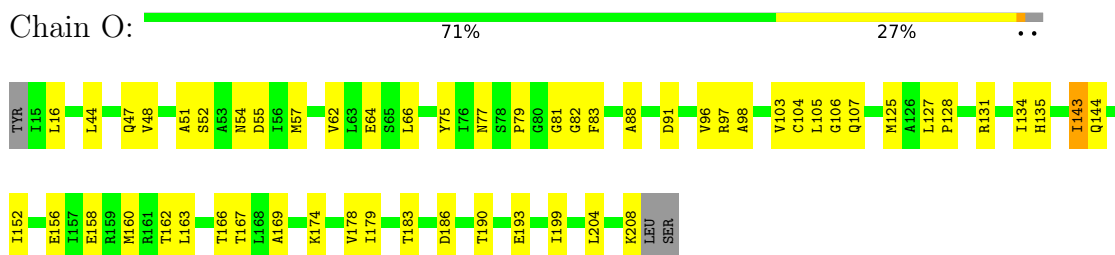
3 Residue-property plots

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

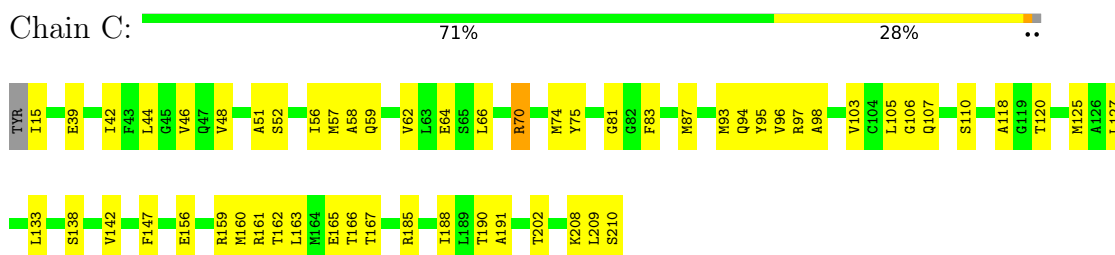
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



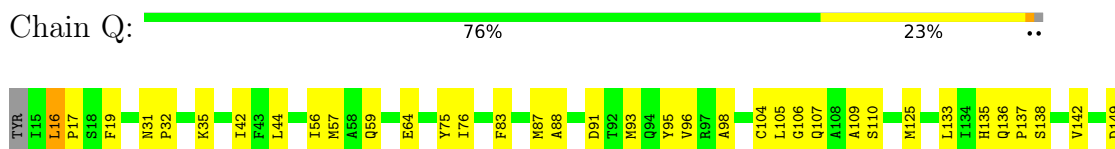
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2





- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain F: 72% 25% ..



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain S: 73% 27% .



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain H: 74% 25% ..



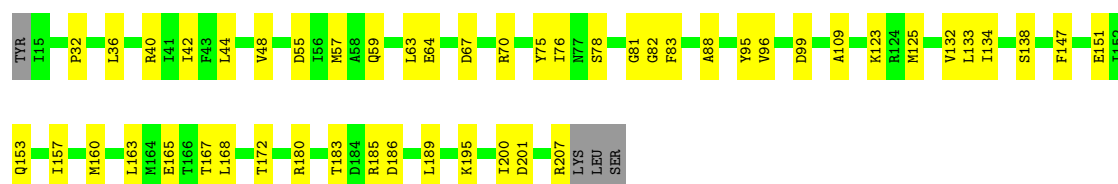
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain T: 76% 23% ..



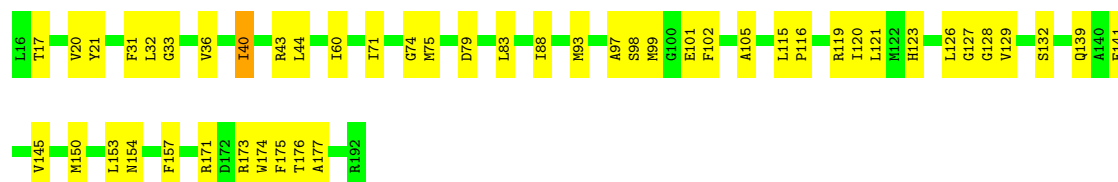
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain J: 76% 22% ..



- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain B: 73% 27% .



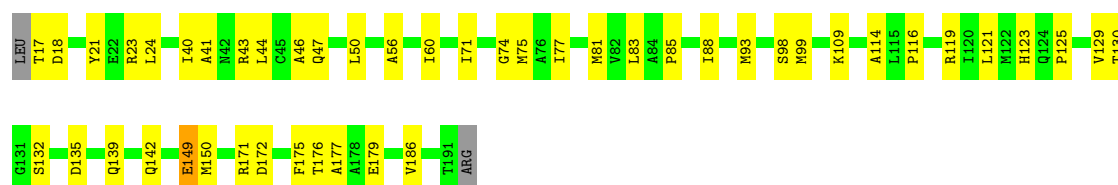
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain P: 77% 23%



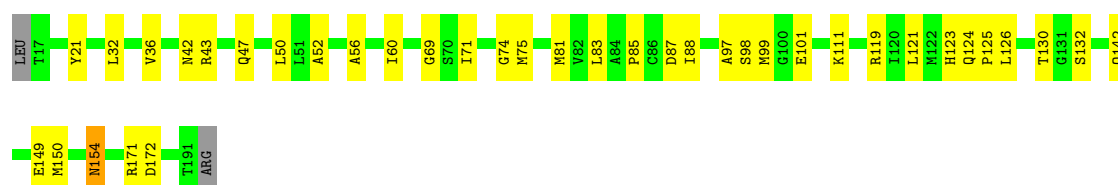
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain D: 72% 26% ..



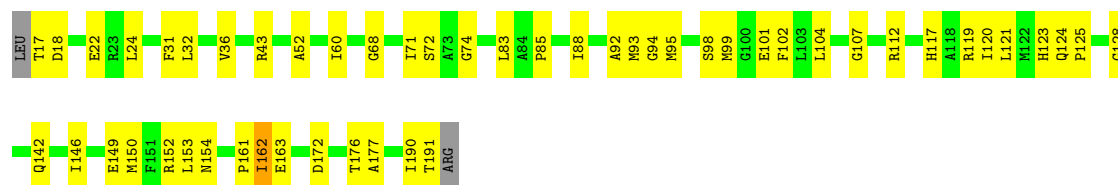
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain R: 77% 21% ..



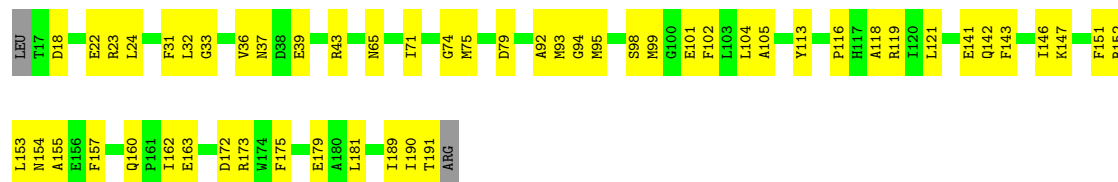
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain I: 70% 28% ..



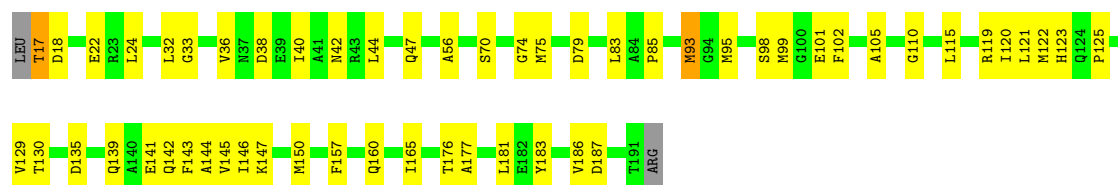
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain U: 69% 30% .



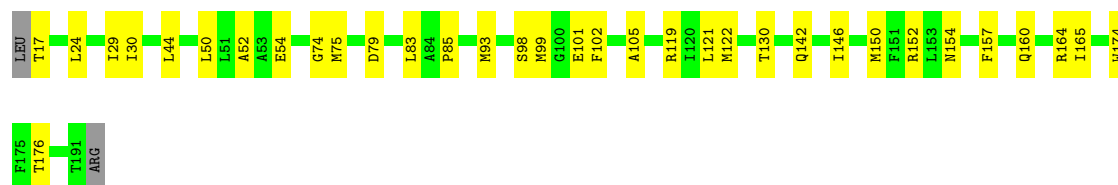
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain K: 68% 30% ..



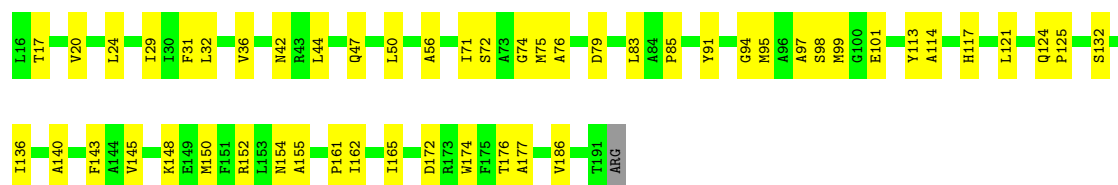
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain W: 80% 19% .



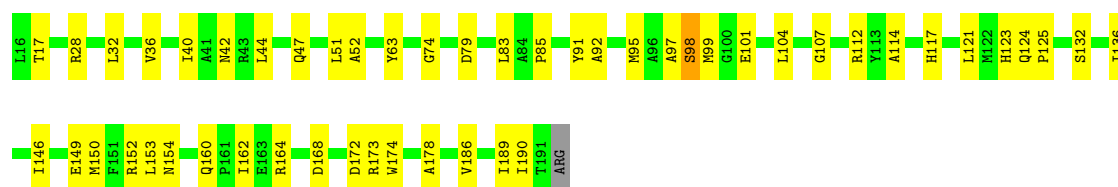
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain M: 71% 29% .



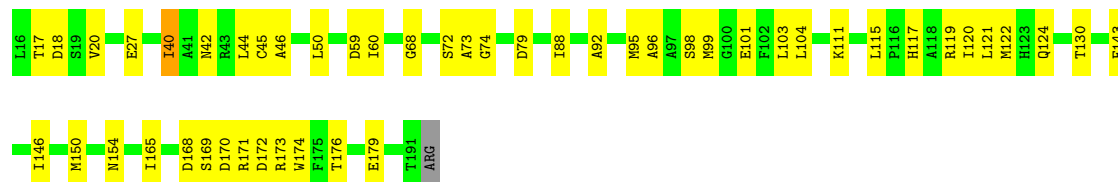
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain Y: 71% 28% ..



- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain N: 72% 27% ..



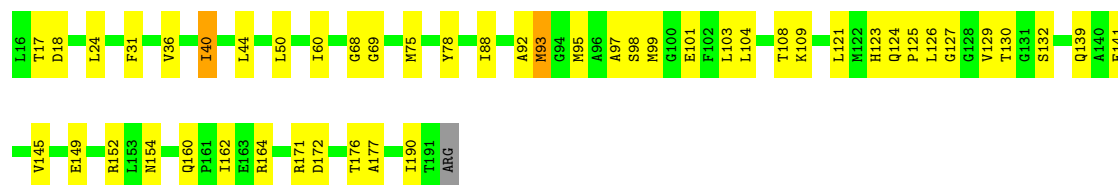
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain Z: 76% 23% ..



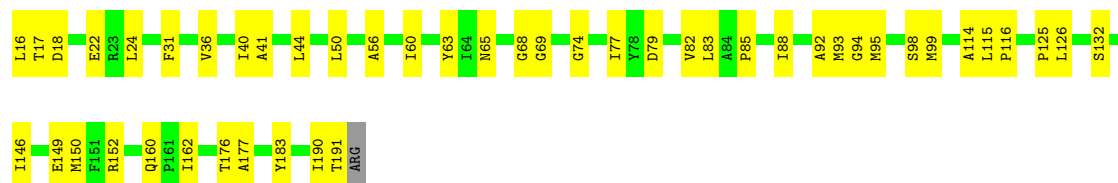
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain G: 72% 26% ..

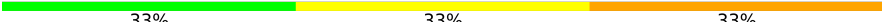


- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain b: 73% 27% .

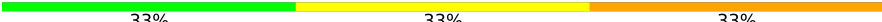


- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain c:  33% 33% 33%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain e:  33% 33% 33%

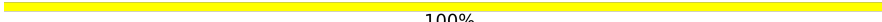


- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain f:  33% 67%

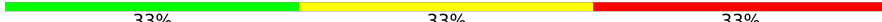


- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain g:  100%

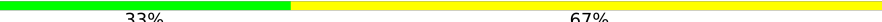


- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain h:  33% 33% 33%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain i:  33% 67%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain j:  33% 67%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain k:  33% 33% 33%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain l:  33% 33% 33%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain m:  33% 33% 33%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain n:  33% 33% 33%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain o:  67% 33%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain p:  33% 67%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain q:  33% 33% 33%



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide



- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

Chain x:  33% 67%

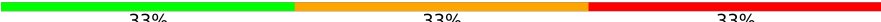
BEZ1
L2
L3

- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain y:  67% 33%

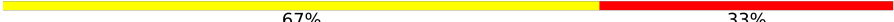
BEZ1
L2
L3

- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain z:  33% 33% 33%

BEZ1
L2
L3

- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain 0:  67% 33%

BEZ1
L2
L3

- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain 1:  33% 67%

BEZ1
L2
L3

- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain 2:  33% 67%

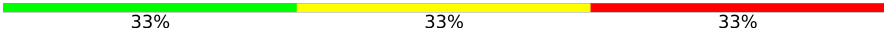
BEZ1
L2
L3

- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain 3:  33% 33% 33%

BEZ1
L2
L3

- Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide

Chain 4: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.51Å 182.50Å 188.70Å 90.00° 95.02° 90.00°	Depositor
Resolution (Å)	33.31 – 3.24 33.31 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.31-3.24) 99.7 (33.31-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.179 , 0.254 0.182 , 0.255	Depositor DCC
R_{free} test set	5566 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	98.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	81239	wwPDB-VP
Average B, all atoms (Å ²)	105.0	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 38.33 % 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 3.7473e-04. 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: BEZ, AI4

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	1.05	3/1512 (0.2%)	1.18	1/2045 (0.0%)
1	C	1.09	2/1518 (0.1%)	1.31	7/2055 (0.3%)
1	E	0.95	1/1495 (0.1%)	1.12	1/2025 (0.0%)
1	F	1.11	4/1518 (0.3%)	1.30	3/2055 (0.1%)
1	H	1.07	1/1522 (0.1%)	1.27	7/2059 (0.3%)
1	J	0.90	0/1524	1.10	3/2062 (0.1%)
1	L	0.89	0/1495	1.10	1/2025 (0.0%)
1	O	0.88	0/1512	1.08	2/2045 (0.1%)
1	Q	0.85	1/1518 (0.1%)	1.09	2/2055 (0.1%)
1	S	0.86	1/1518 (0.1%)	1.06	0/2055
1	T	0.93	0/1522	1.13	1/2059 (0.0%)
1	V	0.89	2/1524 (0.1%)	1.13	2/2062 (0.1%)
1	X	0.89	0/1495	1.10	0/2025
1	a	0.91	2/1495 (0.1%)	1.11	0/2025
2	B	0.95	2/1373 (0.1%)	1.14	0/1856
2	D	1.03	1/1354 (0.1%)	1.21	2/1831 (0.1%)
2	G	0.93	1/1352 (0.1%)	1.18	1/1830 (0.1%)
2	I	1.06	0/1350	1.25	2/1826 (0.1%)
2	K	0.96	3/1344 (0.2%)	1.13	3/1819 (0.2%)
2	M	1.03	3/1346 (0.2%)	1.20	3/1823 (0.2%)
2	N	0.91	1/1346 (0.1%)	1.19	1/1823 (0.1%)
2	P	0.95	1/1373 (0.1%)	1.19	0/1856
2	R	0.95	0/1354	1.12	1/1831 (0.1%)
2	U	0.96	0/1350	1.20	1/1826 (0.1%)
2	W	0.92	1/1344 (0.1%)	1.11	0/1819
2	Y	0.93	0/1346	1.13	1/1823 (0.1%)
2	Z	0.83	0/1346	1.12	1/1823 (0.1%)
2	b	0.86	0/1352	1.11	1/1830 (0.1%)
3	0	3.04	1/16 (6.2%)	1.77	0/19
3	1	2.20	1/16 (6.2%)	2.29	0/19
3	2	3.20	1/16 (6.2%)	1.66	0/19
3	3	2.17	1/16 (6.2%)	1.90	1/19 (5.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	4	3.17	1/16 (6.2%)	2.58	1/19 (5.3%)
3	c	2.40	1/16 (6.2%)	2.40	0/19
3	e	2.59	1/16 (6.2%)	1.68	0/19
3	f	2.78	1/16 (6.2%)	2.34	1/19 (5.3%)
3	g	3.41	1/16 (6.2%)	2.62	2/19 (10.5%)
3	h	2.11	1/16 (6.2%)	2.36	1/19 (5.3%)
3	i	2.92	1/16 (6.2%)	2.27	0/19
3	j	3.03	1/16 (6.2%)	2.27	1/19 (5.3%)
3	k	3.26	1/16 (6.2%)	2.54	1/19 (5.3%)
3	l	2.96	1/16 (6.2%)	2.68	1/19 (5.3%)
3	m	2.56	1/16 (6.2%)	2.73	2/19 (10.5%)
3	n	2.20	1/16 (6.2%)	3.10	3/19 (15.8%)
3	o	3.43	1/16 (6.2%)	3.49	2/19 (10.5%)
3	p	2.80	1/16 (6.2%)	2.78	0/19
3	q	3.84	1/16 (6.2%)	3.28	1/19 (5.3%)
3	r	2.16	1/16 (6.2%)	2.90	2/19 (10.5%)
3	s	3.34	1/16 (6.2%)	3.22	3/19 (15.8%)
3	t	3.07	1/16 (6.2%)	2.24	1/19 (5.3%)
3	u	3.57	1/16 (6.2%)	2.99	2/19 (10.5%)
3	v	2.62	1/16 (6.2%)	2.21	0/19
3	w	2.90	1/16 (6.2%)	2.31	0/19
3	x	2.90	1/16 (6.2%)	2.11	0/19
3	y	2.79	1/16 (6.2%)	3.32	1/19 (5.3%)
3	z	2.64	1/16 (6.2%)	3.04	2/19 (10.5%)
All	All	0.99	58/40546 (0.1%)	1.18	75/54800 (0.1%)

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
2	N	0	1
2	Z	0	1
All	All	0	2

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	q	2	LEU	C-N	13.53	1.52	1.33
3	u	2	LEU	C-N	12.72	1.51	1.33
3	g	2	LEU	C-N	12.31	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	s	2	LEU	C-N	12.22	1.50	1.33
3	2	2	LEU	C-N	11.72	1.49	1.33

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	y	2	LEU	O-C-N	-11.27	104.96	123.00
3	o	2	LEU	O-C-N	-10.39	106.38	123.00
3	k	2	LEU	O-C-N	-8.86	108.82	123.00
3	q	2	LEU	O-C-N	-8.82	108.88	123.00
3	u	2	LEU	O-C-N	-8.47	109.45	123.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	18	ASP	Peptide
2	Z	18	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1491	1495	1495	49	0
1	C	1497	1496	1496	46	0
1	E	1474	1467	1467	49	0
1	F	1497	1496	1496	45	0
1	H	1501	1507	1507	43	0
1	J	1502	1509	1509	39	1
1	L	1474	1467	1467	48	0
1	O	1491	1495	1495	47	0
1	Q	1497	1496	1496	38	1
1	S	1497	1496	1496	42	0
1	T	1501	1507	1507	41	0
1	V	1502	1508	1508	58	0
1	X	1474	1467	1467	41	0
1	a	1474	1467	1467	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1351	1344	1344	38	0
2	D	1332	1320	1320	53	0
2	G	1330	1316	1316	49	0
2	I	1328	1316	1316	60	0
2	K	1322	1305	1305	42	0
2	M	1324	1305	1305	45	0
2	N	1324	1305	1305	41	0
2	P	1351	1344	1344	35	0
2	R	1332	1320	1320	31	0
2	U	1328	1316	1316	42	0
2	W	1322	1305	1305	32	0
2	Y	1324	1305	1305	40	0
2	Z	1324	1305	1305	37	0
2	b	1330	1316	1316	40	0
3	0	25	27	27	6	0
3	1	25	27	27	6	0
3	2	25	27	27	4	0
3	3	25	27	27	5	0
3	4	25	27	27	2	0
3	c	25	27	27	5	0
3	e	25	27	27	2	0
3	f	25	27	27	1	0
3	g	25	27	27	4	0
3	h	25	27	27	3	0
3	i	25	27	27	1	0
3	j	25	27	27	8	0
3	k	25	27	27	3	0
3	l	25	27	27	4	0
3	m	25	27	27	8	0
3	n	25	27	27	5	0
3	o	25	27	27	2	0
3	p	25	27	27	4	0
3	q	25	27	27	3	0
3	r	25	27	27	4	0
3	s	25	27	27	7	0
3	t	25	27	27	3	0
3	u	25	27	27	2	0
3	v	25	27	27	4	0
3	w	25	27	27	7	0
3	x	25	27	27	7	0
3	y	25	27	27	4	0
3	z	25	27	27	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	28	0	3	0
4	F	43	28	0	2	0
4	G	43	28	0	0	0
4	I	43	28	0	4	0
4	K	43	28	0	1	0
4	M	43	28	0	2	0
4	N	43	28	0	1	0
4	R	43	28	0	1	0
4	U	43	28	0	3	0
4	V	43	28	0	1	0
4	W	43	28	0	2	0
4	Y	43	28	0	1	0
4	Z	43	28	0	1	0
4	b	43	28	0	1	0
All	All	40796	40443	40051	1086	1

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 13.

The worst 5 of 1086 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)
2:B:40:ILE:CD1	2:B:40:ILE:CG1	1.77	1.60
2:G:40:ILE:CD1	2:G:40:ILE:CG1	1.75	1.58
1:O:64:GLU:OE1	1:O:96:VAL:HG13	1.57	1.05
2:Z:74:GLY:HA3	2:Z:99:MET:HE2	1.34	1.04
1:O:134:ILE:HG22	1:O:183:THR:HG22	1.48	0.95

All (1) 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:Q:170:ARG:O	1:J:175:ASP:OD2[1_554]	2.12	0.08

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	192/197 (98%)	183 (95%)	8 (4%)	1 (0%)	24	56
1	C	194/197 (98%)	186 (96%)	7 (4%)	1 (0%)	24	56
1	E	191/197 (97%)	180 (94%)	11 (6%)	0	100	100
1	F	194/197 (98%)	185 (95%)	7 (4%)	2 (1%)	12	42
1	H	194/197 (98%)	184 (95%)	10 (5%)	0	100	100
1	J	193/197 (98%)	182 (94%)	11 (6%)	0	100	100
1	L	191/197 (97%)	183 (96%)	8 (4%)	0	100	100
1	O	192/197 (98%)	181 (94%)	10 (5%)	1 (0%)	24	56
1	Q	194/197 (98%)	186 (96%)	7 (4%)	1 (0%)	24	56
1	S	194/197 (98%)	183 (94%)	10 (5%)	1 (0%)	24	56
1	T	194/197 (98%)	188 (97%)	6 (3%)	0	100	100
1	V	193/197 (98%)	182 (94%)	10 (5%)	1 (0%)	24	56
1	X	191/197 (97%)	181 (95%)	9 (5%)	1 (0%)	24	56
1	a	191/197 (97%)	182 (95%)	9 (5%)	0	100	100
2	B	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	D	173/177 (98%)	168 (97%)	5 (3%)	0	100	100
2	G	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	I	173/177 (98%)	170 (98%)	2 (1%)	1 (1%)	21	53
2	K	173/177 (98%)	166 (96%)	7 (4%)	0	100	100
2	M	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	21	53
2	N	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	P	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	21	53
2	R	173/177 (98%)	168 (97%)	5 (3%)	0	100	100
2	U	173/177 (98%)	169 (98%)	3 (2%)	1 (1%)	21	53
2	W	173/177 (98%)	167 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	Z	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	b	174/177 (98%)	168 (97%)	5 (3%)	1 (1%)	21	53
3	0	1/3 (33%)	1 (100%)	0	0	100	100
3	1	1/3 (33%)	1 (100%)	0	0	100	100
3	2	1/3 (33%)	1 (100%)	0	0	100	100
3	3	1/3 (33%)	1 (100%)	0	0	100	100
3	4	1/3 (33%)	1 (100%)	0	0	100	100
3	c	1/3 (33%)	1 (100%)	0	0	100	100
3	e	1/3 (33%)	1 (100%)	0	0	100	100
3	f	1/3 (33%)	1 (100%)	0	0	100	100
3	g	1/3 (33%)	1 (100%)	0	0	100	100
3	h	1/3 (33%)	1 (100%)	0	0	100	100
3	i	1/3 (33%)	0	1 (100%)	0	100	100
3	j	1/3 (33%)	1 (100%)	0	0	100	100
3	k	1/3 (33%)	1 (100%)	0	0	100	100
3	l	1/3 (33%)	1 (100%)	0	0	100	100
3	m	1/3 (33%)	0	0	1 (100%)	0	0
3	n	1/3 (33%)	1 (100%)	0	0	100	100
3	o	1/3 (33%)	1 (100%)	0	0	100	100
3	p	1/3 (33%)	1 (100%)	0	0	100	100
3	q	1/3 (33%)	0	1 (100%)	0	100	100
3	r	1/3 (33%)	1 (100%)	0	0	100	100
3	s	1/3 (33%)	0	1 (100%)	0	100	100
3	t	1/3 (33%)	1 (100%)	0	0	100	100
3	u	1/3 (33%)	1 (100%)	0	0	100	100
3	v	1/3 (33%)	1 (100%)	0	0	100	100
3	w	1/3 (33%)	1 (100%)	0	0	100	100
3	x	1/3 (33%)	1 (100%)	0	0	100	100
3	y	1/3 (33%)	1 (100%)	0	0	100	100
3	z	1/3 (33%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5158/5320 (97%)	4946 (96%)	197 (4%)	15 (0%)	36	66

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	94	GLY
2	U	94	GLY
1	V	106	GLY
2	b	94	GLY
3	m	2	LEU

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	160/164 (98%)	160 (100%)	0	100	100
1	C	160/164 (98%)	160 (100%)	0	100	100
1	E	157/164 (96%)	157 (100%)	0	100	100
1	F	160/164 (98%)	160 (100%)	0	100	100
1	H	161/164 (98%)	161 (100%)	0	100	100
1	J	161/164 (98%)	161 (100%)	0	100	100
1	L	157/164 (96%)	157 (100%)	0	100	100
1	O	160/164 (98%)	160 (100%)	0	100	100
1	Q	160/164 (98%)	160 (100%)	0	100	100
1	S	160/164 (98%)	160 (100%)	0	100	100
1	T	161/164 (98%)	161 (100%)	0	100	100
1	V	161/164 (98%)	161 (100%)	0	100	100
1	X	157/164 (96%)	157 (100%)	0	100	100
1	a	157/164 (96%)	157 (100%)	0	100	100
2	B	138/138 (100%)	138 (100%)	0	100	100
2	D	136/138 (99%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	135/138 (98%)	135 (100%)	0	100	100
2	I	135/138 (98%)	135 (100%)	0	100	100
2	K	134/138 (97%)	134 (100%)	0	100	100
2	M	134/138 (97%)	134 (100%)	0	100	100
2	N	134/138 (97%)	134 (100%)	0	100	100
2	P	138/138 (100%)	138 (100%)	0	100	100
2	R	136/138 (99%)	136 (100%)	0	100	100
2	U	135/138 (98%)	135 (100%)	0	100	100
2	W	134/138 (97%)	134 (100%)	0	100	100
2	Y	134/138 (97%)	134 (100%)	0	100	100
2	Z	134/138 (97%)	134 (100%)	0	100	100
2	b	135/138 (98%)	135 (100%)	0	100	100
3	0	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	1	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	2	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	3	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	4	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	c	2/2 (100%)	2 (100%)	0	100	100
3	e	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	f	2/2 (100%)	2 (100%)	0	100	100
3	g	2/2 (100%)	2 (100%)	0	100	100
3	h	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	i	2/2 (100%)	2 (100%)	0	100	100
3	j	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	k	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	l	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	m	2/2 (100%)	0	2 (100%)	0	0
3	n	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	o	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	p	2/2 (100%)	0	2 (100%)	0	0
3	q	2/2 (100%)	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	r	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	s	2/2 (100%)	2 (100%)	0	100	100
3	t	2/2 (100%)	2 (100%)	0	100	100
3	u	2/2 (100%)	2 (100%)	0	100	100
3	v	2/2 (100%)	0	2 (100%)	0	0
3	w	2/2 (100%)	2 (100%)	0	100	100
3	x	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	y	2/2 (100%)	0	2 (100%)	0	0
3	z	2/2 (100%)	0	2 (100%)	0	0
All	All	4180/4284 (98%)	4155 (99%)	25 (1%)	78	83

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	v	3	LEU
3	y	3	LEU
3	4	2	LEU
3	y	2	LEU
3	z	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	42	ASN
1	L	94	GLN
2	I	65	ASN
2	K	42	ASN
1	X	94	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 ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AI4	R	201	-	48,48,48	5.72	26 (54%)	63,68,68	4.81	35 (55%)
4	AI4	K	201	-	48,48,48	5.74	26 (54%)	63,68,68	4.99	35 (55%)
4	AI4	N	301	-	48,48,48	5.84	24 (50%)	63,68,68	8.51	40 (63%)
4	AI4	I	201	-	48,48,48	5.76	31 (64%)	63,68,68	5.17	34 (53%)
4	AI4	Z	201	-	48,48,48	5.87	28 (58%)	63,68,68	5.09	34 (53%)
4	AI4	V	301	-	48,48,48	5.83	29 (60%)	63,68,68	4.93	34 (53%)
4	AI4	b	201	-	48,48,48	5.76	28 (58%)	63,68,68	5.14	35 (55%)
4	AI4	F	301	-	48,48,48	5.83	29 (60%)	63,68,68	4.94	33 (52%)
4	AI4	U	201	-	48,48,48	5.68	28 (58%)	63,68,68	5.27	35 (55%)
4	AI4	G	201	-	48,48,48	5.79	30 (62%)	63,68,68	5.14	38 (60%)
4	AI4	Y	201	-	48,48,48	5.86	28 (58%)	63,68,68	5.21	34 (53%)
4	AI4	B	201	-	48,48,48	5.71	28 (58%)	63,68,68	5.59	41 (65%)
4	AI4	W	201	-	48,48,48	5.80	27 (56%)	63,68,68	4.47	34 (53%)
4	AI4	M	201	-	48,48,48	5.79	31 (64%)	63,68,68	4.83	36 (57%)

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	AI4	R	201	-	-	11/21/31/31	0/6/6/6
4	AI4	K	201	-	-	10/21/31/31	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AI4	N	301	-	-	10/21/31/31	0/6/6/6
4	AI4	I	201	-	-	10/21/31/31	0/6/6/6
4	AI4	Z	201	-	-	11/21/31/31	0/6/6/6
4	AI4	V	301	-	-	10/21/31/31	0/6/6/6
4	AI4	b	201	-	-	11/21/31/31	0/6/6/6
4	AI4	F	301	-	-	9/21/31/31	0/6/6/6
4	AI4	U	201	-	-	13/21/31/31	0/6/6/6
4	AI4	G	201	-	-	11/21/31/31	0/6/6/6
4	AI4	Y	201	-	-	11/21/31/31	0/6/6/6
4	AI4	B	201	-	-	10/21/31/31	0/6/6/6
4	AI4	W	201	-	-	9/21/31/31	0/6/6/6
4	AI4	M	201	-	-	13/21/31/31	0/6/6/6

The worst 5 of 393 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	201	AI4	C37-C38	18.13	1.66	1.39
4	Y	201	AI4	C37-C38	17.90	1.66	1.39
4	U	201	AI4	C37-C38	17.84	1.66	1.39
4	V	301	AI4	C37-C38	17.74	1.66	1.39
4	N	301	AI4	C37-C38	17.55	1.66	1.39

The worst 5 of 498 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	301	AI4	O43-C41-N42	-41.27	62.98	122.62
4	N	301	AI4	O43-C41-C38	-35.95	75.63	119.60
4	Y	201	AI4	C38-C41-N42	17.64	139.48	117.74
4	F	301	AI4	C39-C38-C37	-17.55	96.25	118.57
4	B	201	AI4	C39-C38-C37	-17.23	96.65	118.57

There are no chirality outliers.

5 of 149 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	201	AI4	C15-C14-O13-C10
4	K	201	AI4	C15-C14-O13-C10
4	M	201	AI4	C15-C14-O13-C10
4	b	201	AI4	C15-C14-O13-C10

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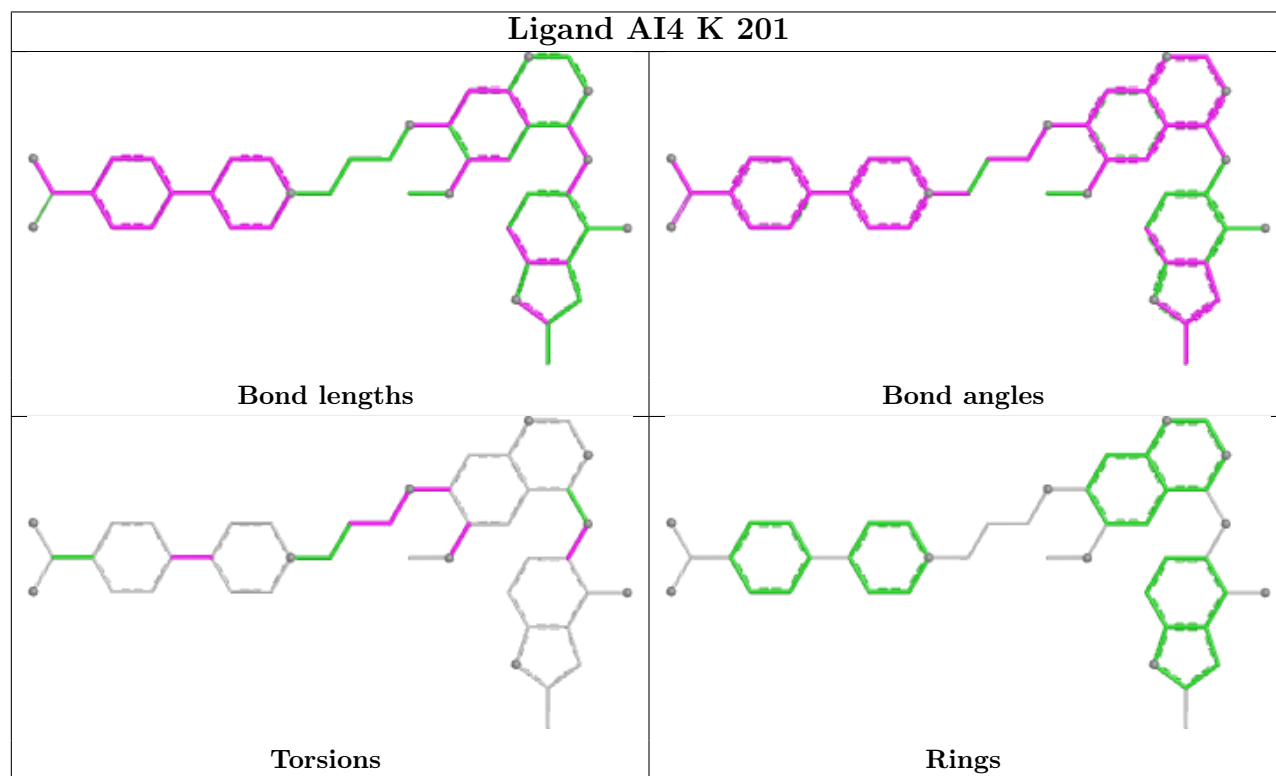
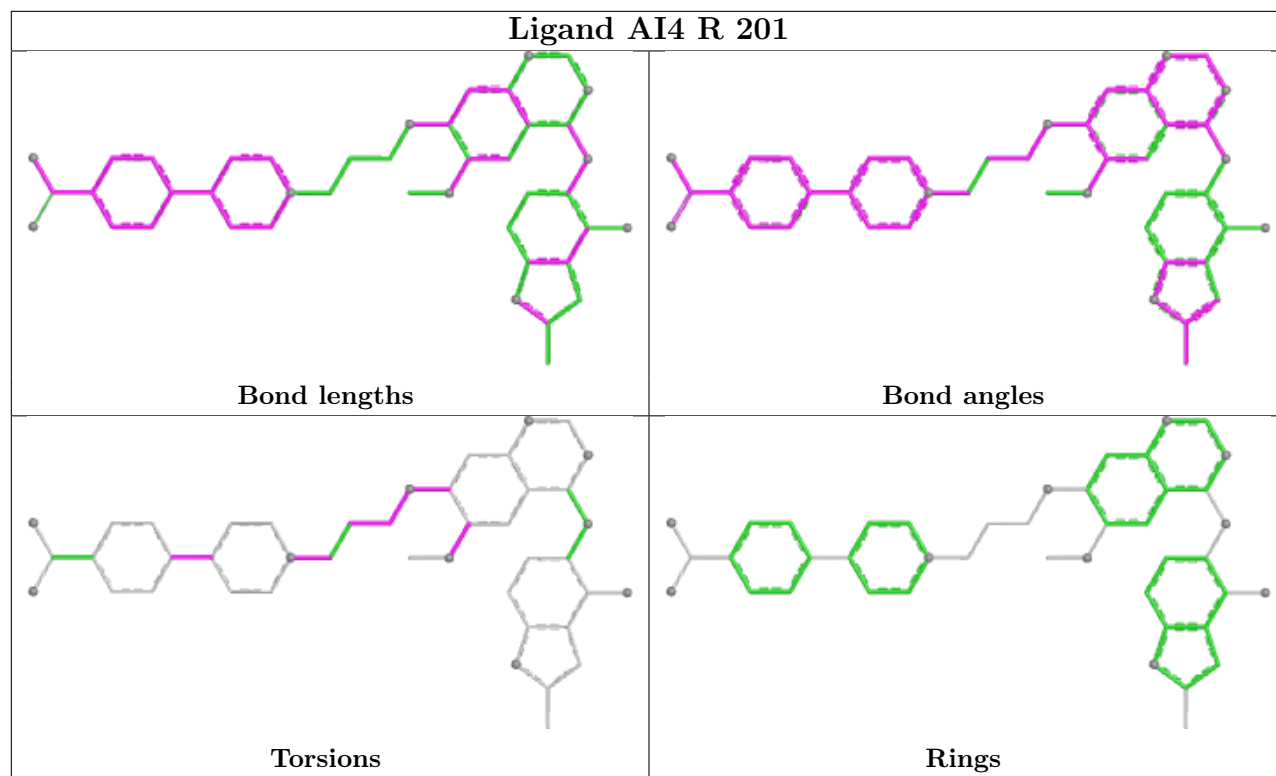
Mol	Chain	Res	Type	Atoms
4	W	201	AI4	C26-C27-N28-C30

There are no ring outliers.

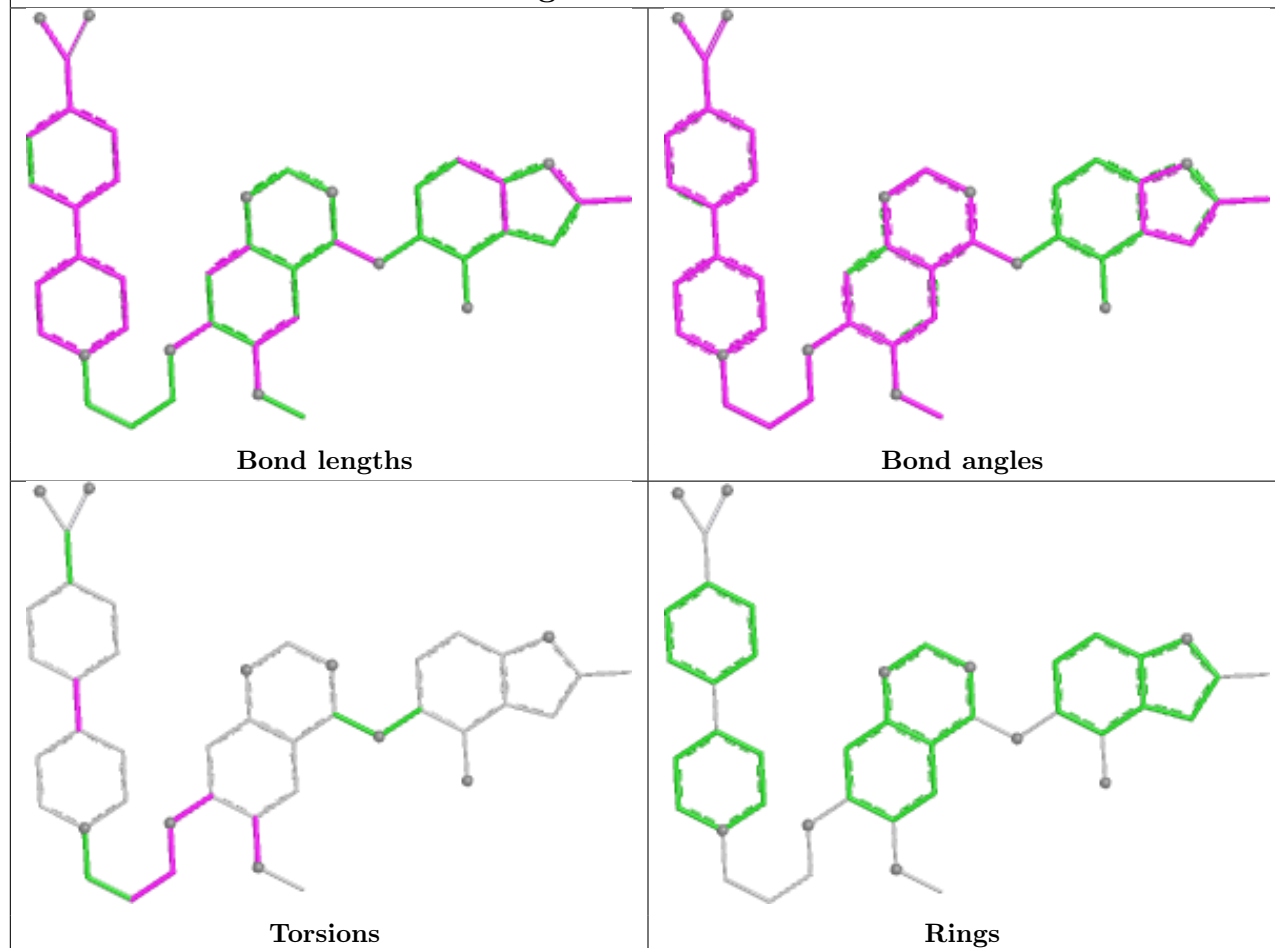
13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	201	AI4	1	0
4	K	201	AI4	1	0
4	N	301	AI4	1	0
4	I	201	AI4	4	0
4	Z	201	AI4	1	0
4	V	301	AI4	1	0
4	b	201	AI4	1	0
4	F	301	AI4	2	0
4	U	201	AI4	3	0
4	Y	201	AI4	1	0
4	B	201	AI4	3	0
4	W	201	AI4	2	0
4	M	201	AI4	2	0

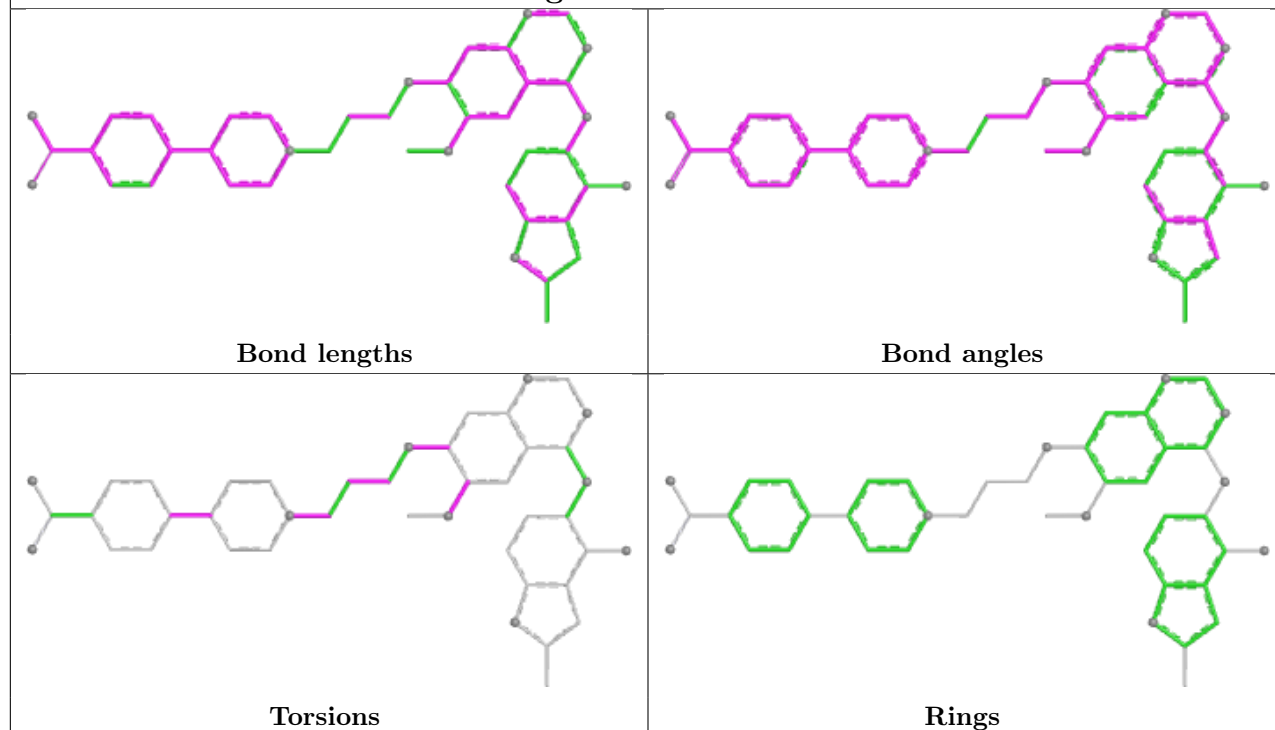
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

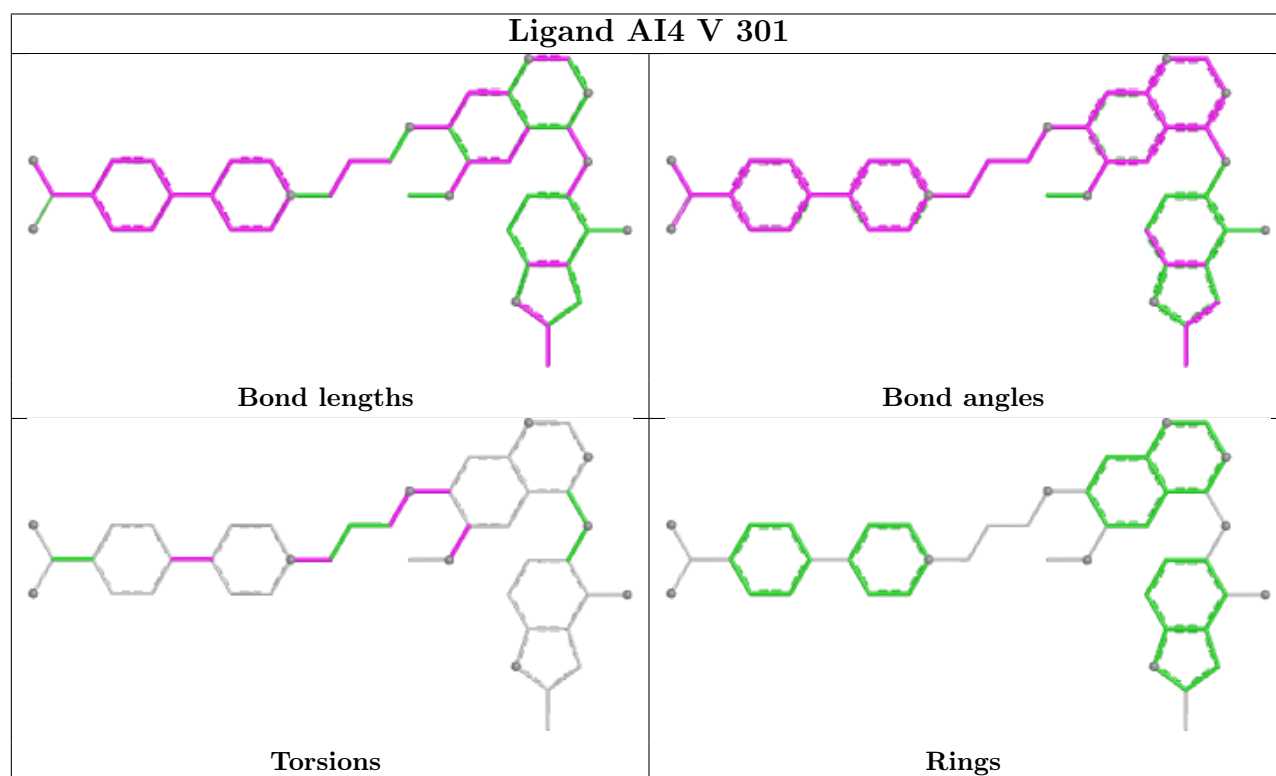
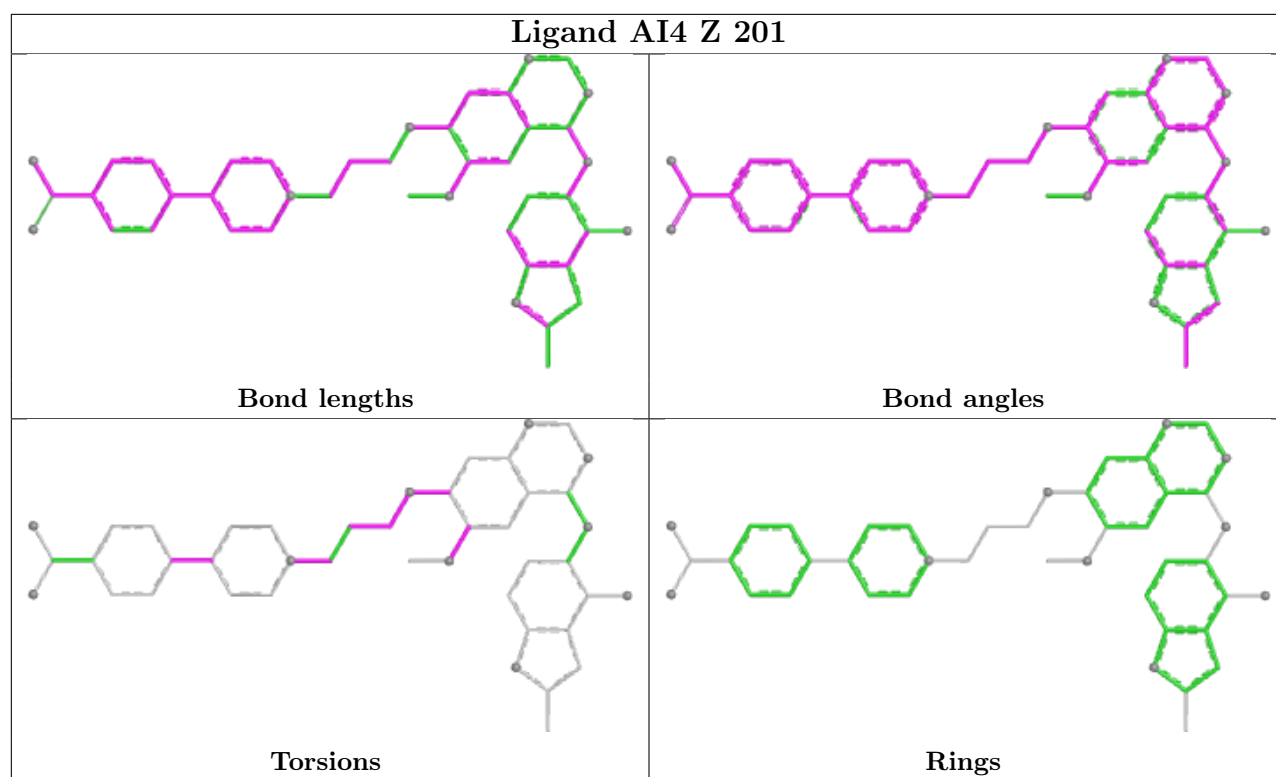


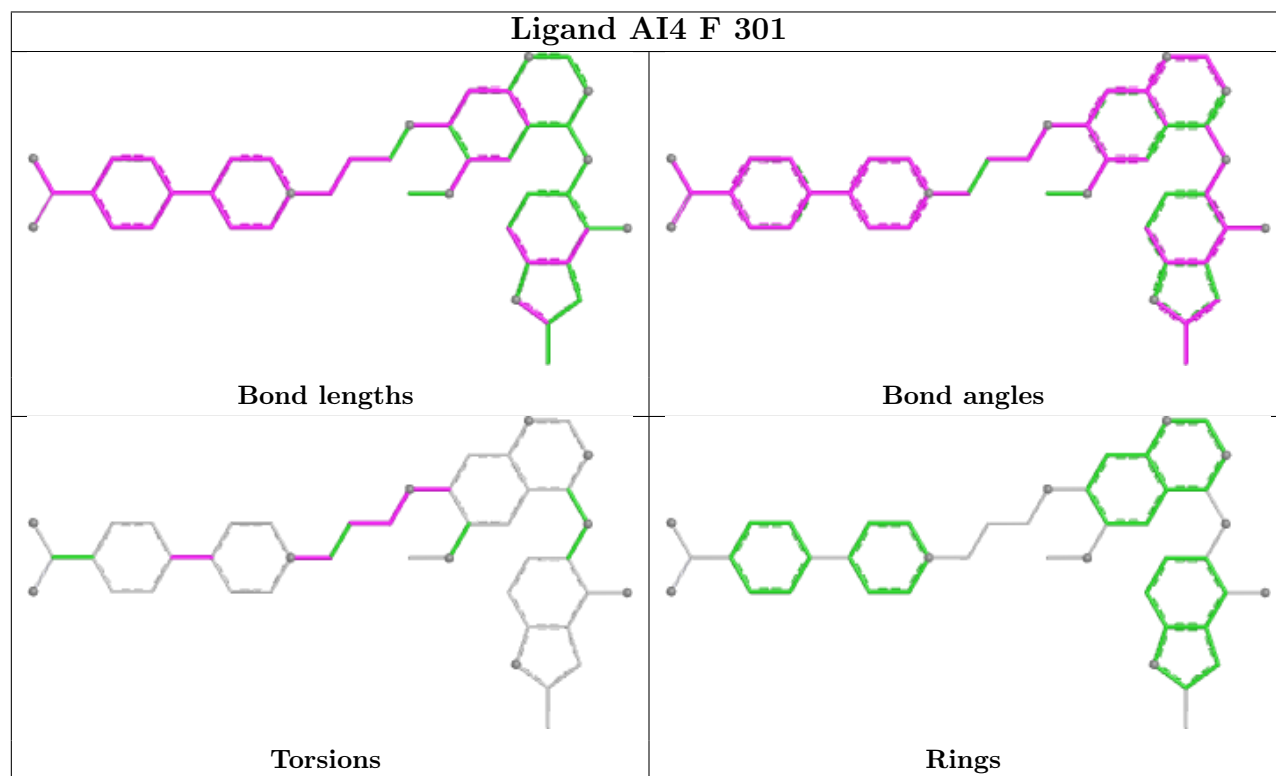
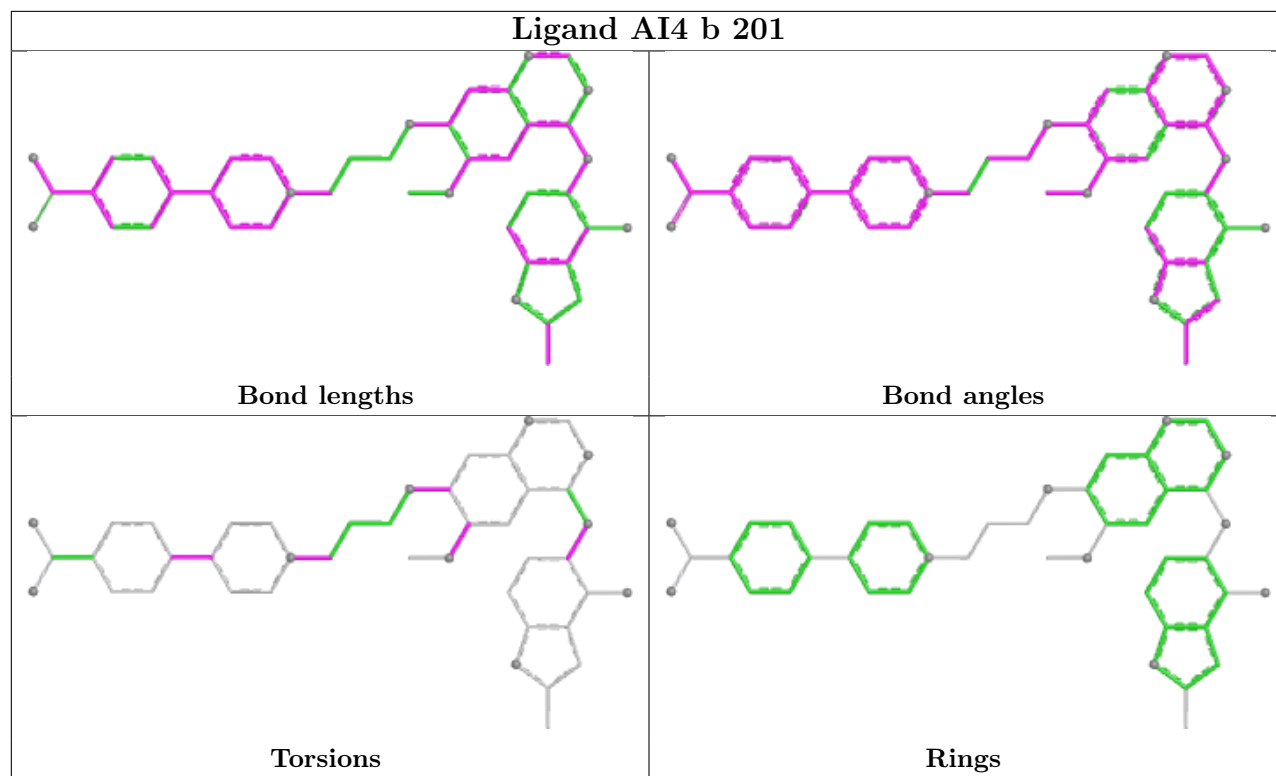
Ligand AI4 N 301

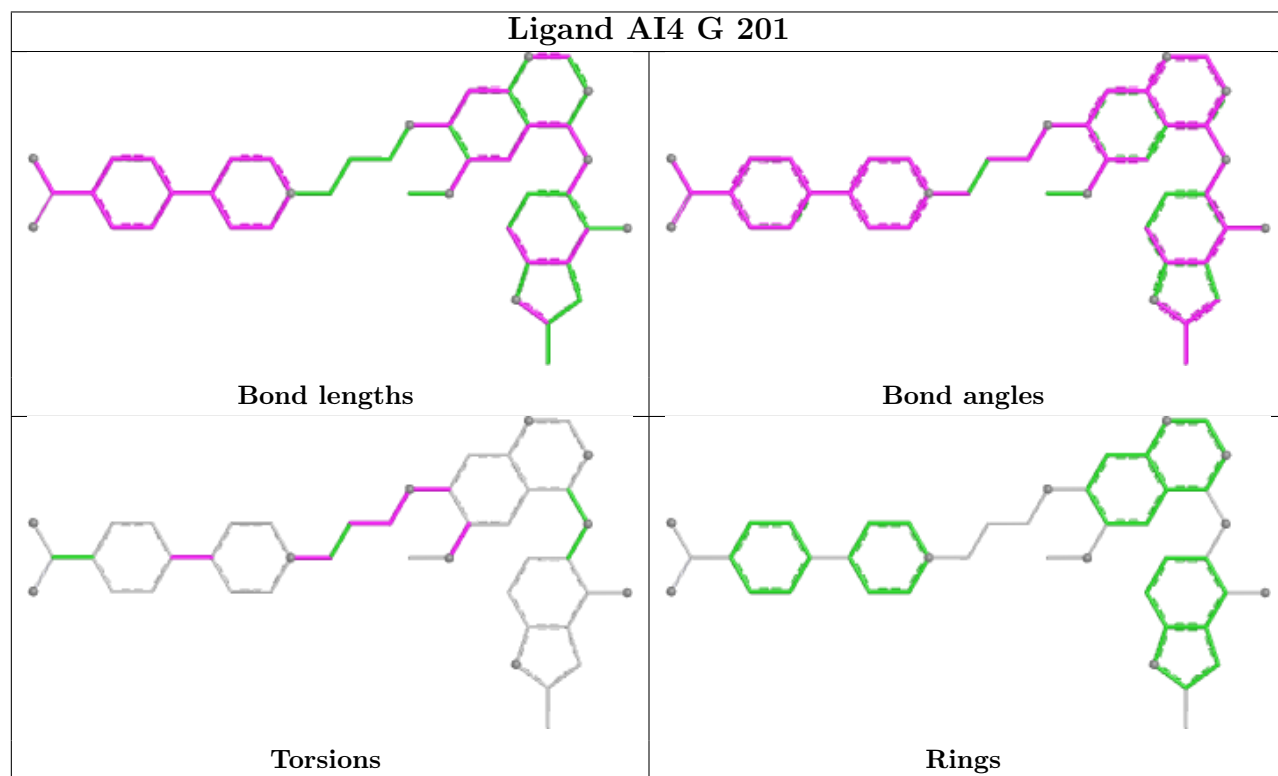
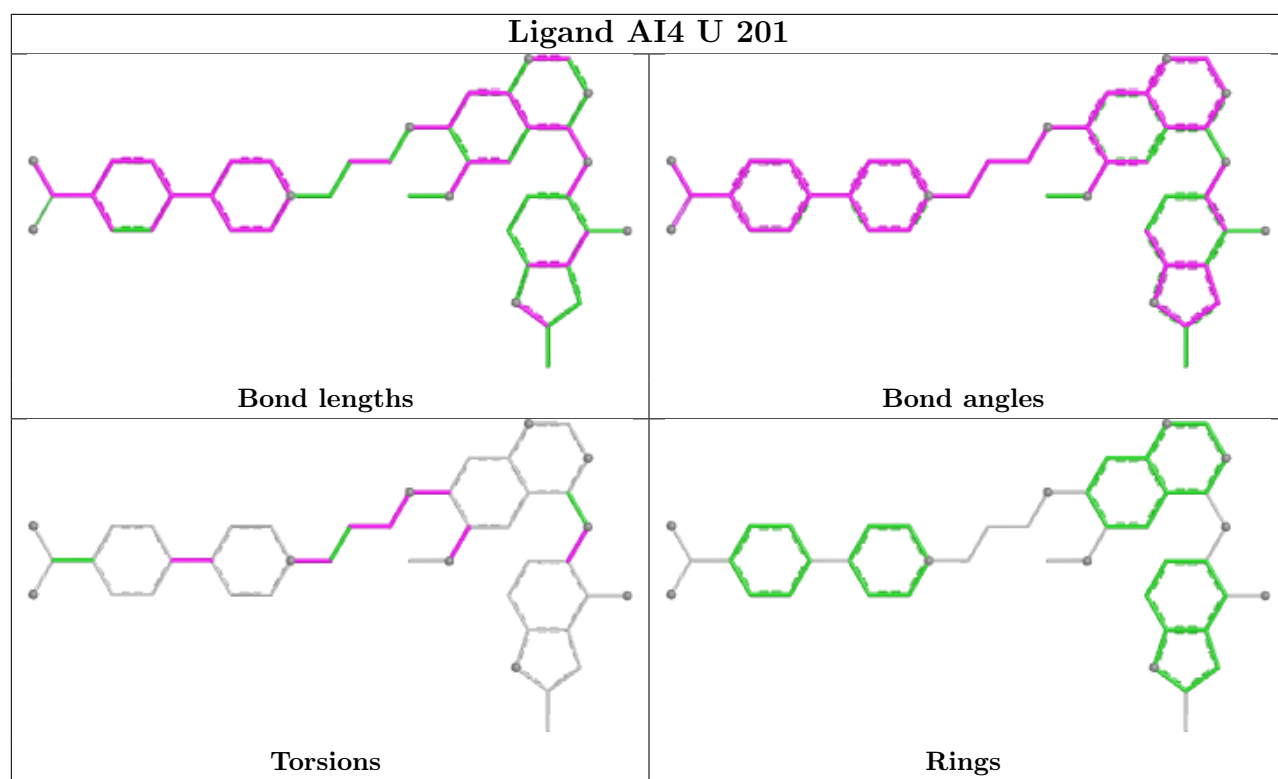


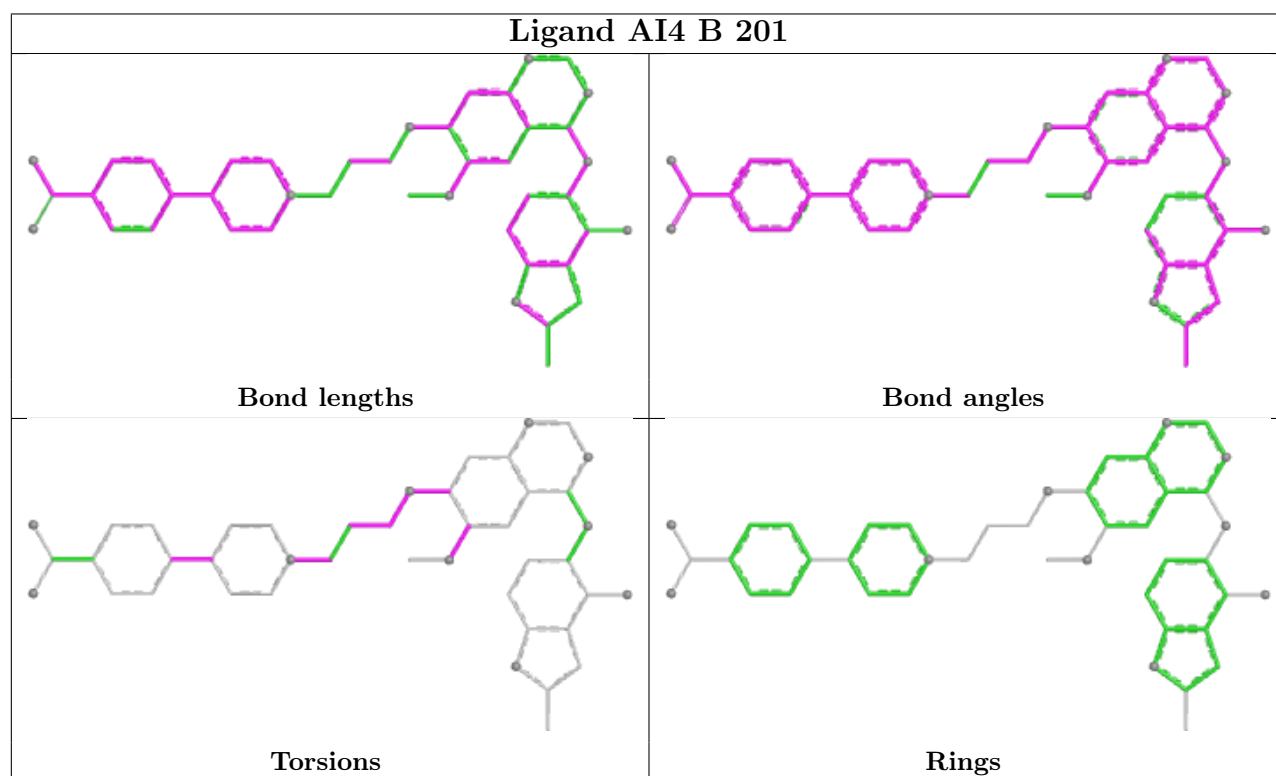
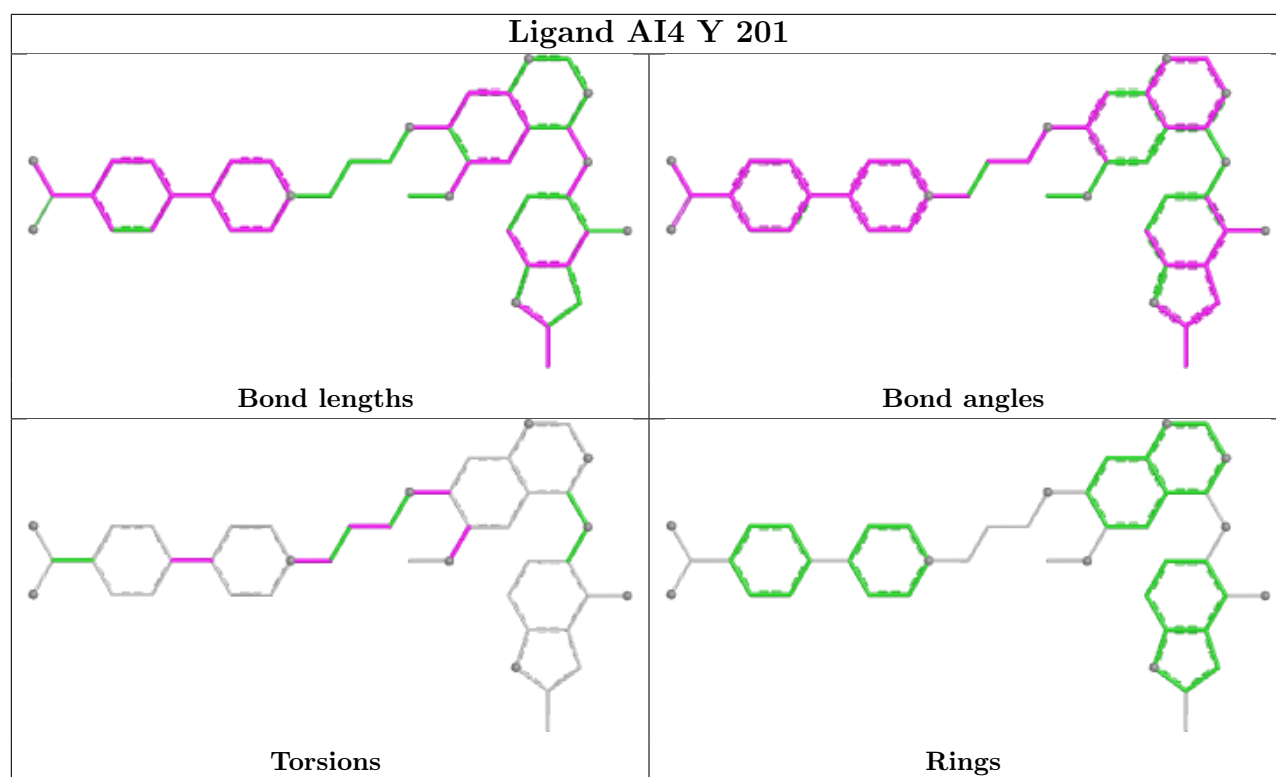
Ligand AI4 I 201

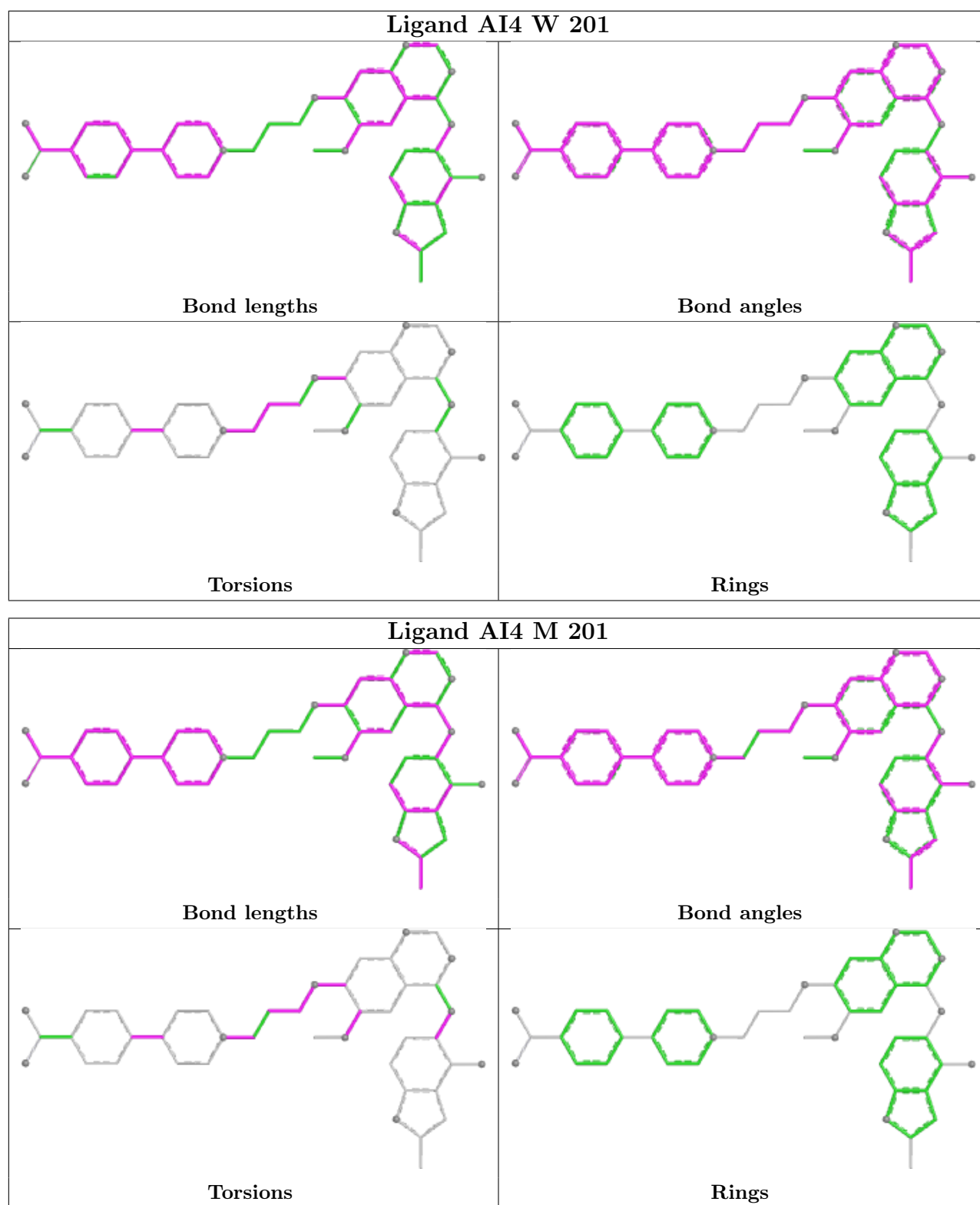












5.7 Other polymers ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9
1	A	194/197 (98%)	-0.83	0	100	100	71, 96, 130, 153	0
1	C	196/197 (99%)	-0.72	0	100	100	65, 91, 125, 170	0
1	E	193/197 (97%)	-0.77	0	100	100	74, 99, 130, 151	0
1	F	196/197 (99%)	-0.74	0	100	100	72, 91, 122, 190	0
1	H	196/197 (99%)	-0.78	0	100	100	70, 90, 138, 190	0
1	J	195/197 (98%)	-0.74	0	100	100	82, 106, 138, 167	0
1	L	193/197 (97%)	-0.70	0	100	100	81, 107, 131, 159	0
1	O	194/197 (98%)	-0.74	0	100	100	85, 106, 149, 167	0
1	Q	196/197 (99%)	-0.69	0	100	100	84, 112, 147, 171	0
1	S	196/197 (99%)	-0.71	0	100	100	83, 116, 154, 191	0
1	T	196/197 (99%)	-0.71	1 (0%)	87	76	85, 106, 141, 209	0
1	V	195/197 (98%)	-0.67	0	100	100	85, 111, 148, 181	0
1	X	193/197 (97%)	-0.61	0	100	100	85, 112, 143, 159	0
1	a	193/197 (97%)	-0.63	0	100	100	82, 107, 137, 154	0
2	B	177/177 (100%)	-0.79	0	100	100	71, 95, 137, 166	0
2	D	175/177 (98%)	-0.85	0	100	100	70, 92, 126, 148	0
2	G	176/177 (99%)	-0.75	0	100	100	68, 96, 130, 160	0
2	I	175/177 (98%)	-0.78	0	100	100	73, 90, 120, 153	0
2	K	175/177 (98%)	-0.69	0	100	100	79, 103, 130, 156	0
2	M	176/177 (99%)	-0.85	0	100	100	68, 90, 120, 153	0
2	N	176/177 (99%)	-0.73	0	100	100	70, 98, 135, 172	0
2	P	177/177 (100%)	-0.74	0	100	100	74, 98, 127, 158	0
2	R	175/177 (98%)	-0.77	0	100	100	78, 99, 132, 160	0
2	U	175/177 (98%)	-0.75	0	100	100	78, 96, 125, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	175/177 (98%)	-0.71	0 100 100	81, 101, 136, 153	0
2	Y	176/177 (99%)	-0.78	0 100 100	75, 97, 127, 157	0
2	Z	176/177 (99%)	-0.73	0 100 100	79, 106, 137, 171	0
2	b	176/177 (99%)	-0.78	0 100 100	80, 101, 128, 157	0
3	0	2/3 (66%)	-0.13	0 100 100	133, 133, 133, 146	0
3	1	2/3 (66%)	-0.31	0 100 100	112, 112, 112, 132	0
3	2	2/3 (66%)	-0.50	0 100 100	135, 135, 135, 141	0
3	3	2/3 (66%)	-0.12	0 100 100	115, 115, 115, 123	0
3	4	2/3 (66%)	-0.36	0 100 100	136, 136, 136, 149	0
3	c	2/3 (66%)	-0.30	0 100 100	116, 116, 116, 120	0
3	e	2/3 (66%)	-0.35	0 100 100	130, 130, 130, 136	0
3	f	2/3 (66%)	-0.60	0 100 100	106, 106, 106, 111	0
3	g	2/3 (66%)	-0.41	0 100 100	132, 132, 132, 151	0
3	h	2/3 (66%)	-0.33	0 100 100	105, 105, 105, 113	0
3	i	2/3 (66%)	-0.27	0 100 100	125, 125, 125, 128	0
3	j	2/3 (66%)	-0.64	0 100 100	100, 100, 100, 109	0
3	k	2/3 (66%)	-0.69	0 100 100	123, 123, 123, 146	0
3	l	2/3 (66%)	0.08	0 100 100	106, 106, 106, 121	0
3	m	2/3 (66%)	-0.14	0 100 100	131, 131, 131, 131	0
3	n	2/3 (66%)	-0.08	0 100 100	113, 113, 113, 118	0
3	o	2/3 (66%)	0.09	0 100 100	131, 131, 131, 138	0
3	p	2/3 (66%)	0.48	0 100 100	109, 109, 109, 117	0
3	q	2/3 (66%)	0.08	0 100 100	141, 141, 141, 144	0
3	r	2/3 (66%)	-0.04	0 100 100	109, 109, 109, 114	0
3	s	2/3 (66%)	-0.25	0 100 100	134, 134, 134, 138	0
3	t	2/3 (66%)	-0.05	0 100 100	113, 113, 113, 117	0
3	u	2/3 (66%)	-0.36	0 100 100	128, 128, 128, 146	0
3	v	2/3 (66%)	-0.23	0 100 100	110, 110, 110, 116	0
3	w	2/3 (66%)	-0.36	0 100 100	135, 135, 135, 138	0
3	x	2/3 (66%)	-0.16	0 100 100	112, 112, 112, 124	0
3	y	2/3 (66%)	-0.08	0 100 100	140, 140, 140, 156	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	z	2/3 (66%)	-0.38	0 100 100	109, 109, 109, 113	0
All	All	5242/5320 (98%)	-0.73	1 (0%) 100 100	65, 101, 137, 209	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	65	SER	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

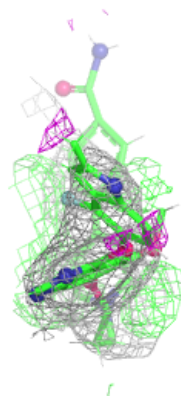
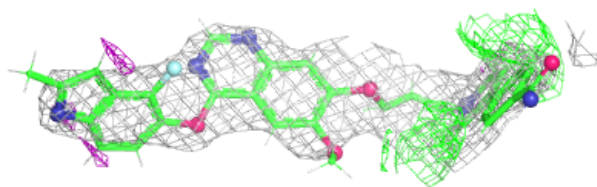
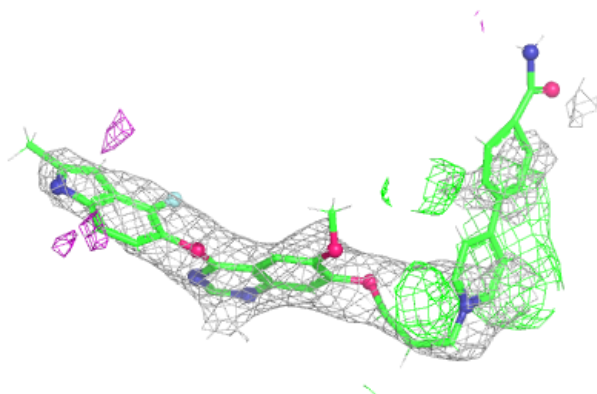
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AI4	U	201	43/43	0.79	0.17	103,148,191,204	0
4	AI4	W	201	43/43	0.81	0.16	111,157,195,219	0
4	AI4	F	301	43/43	0.82	0.15	96,133,190,200	0
4	AI4	I	201	43/43	0.84	0.13	104,137,196,215	0
4	AI4	Y	201	43/43	0.84	0.13	102,136,195,209	0
4	AI4	G	201	43/43	0.85	0.14	100,137,201,215	0
4	AI4	K	201	43/43	0.86	0.12	114,146,188,204	0
4	AI4	b	201	43/43	0.86	0.14	107,140,184,201	0
4	AI4	Z	201	43/43	0.87	0.13	99,149,213,226	0
4	AI4	B	201	43/43	0.88	0.12	105,138,204,223	0
4	AI4	V	301	43/43	0.89	0.12	101,135,192,215	0
4	AI4	M	201	43/43	0.90	0.12	99,135,199,215	0
4	AI4	R	201	43/43	0.90	0.12	94,136,203,221	0
4	AI4	N	301	43/43	0.90	0.12	90,134,190,200	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.

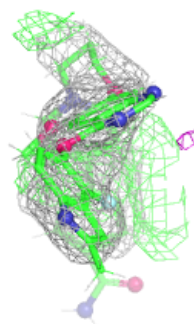
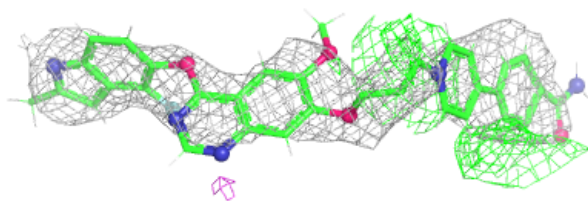
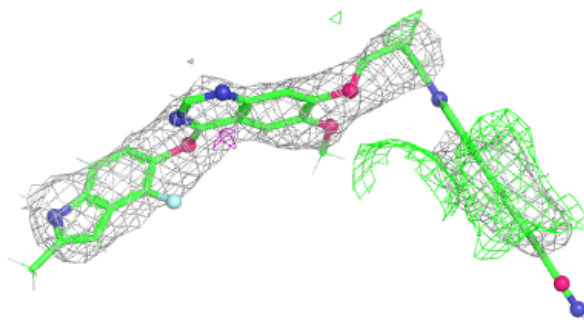
Electron density around AI4 U 201:

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

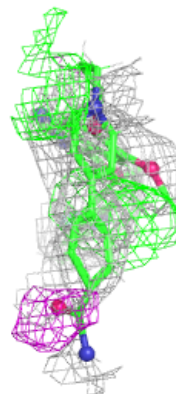
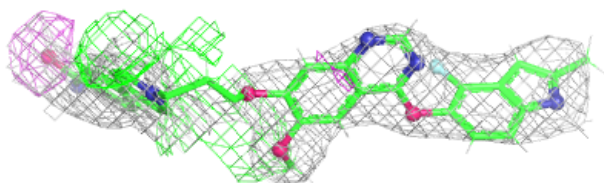
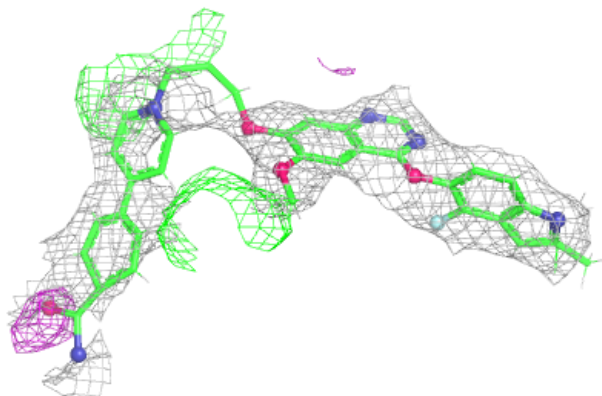


Electron density around AI4 W 201:

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

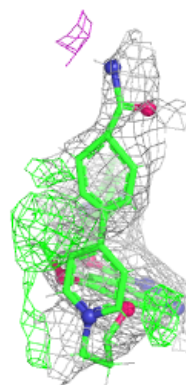
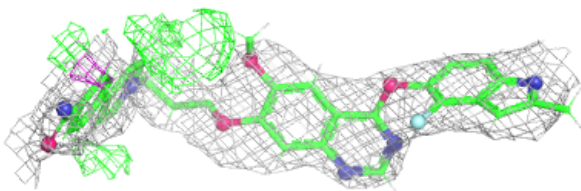
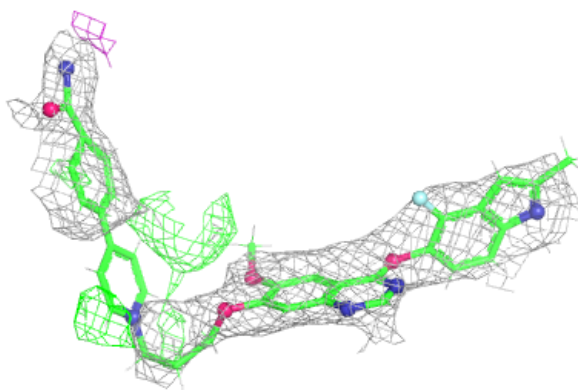
**Electron density around AI4 F 301:**

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

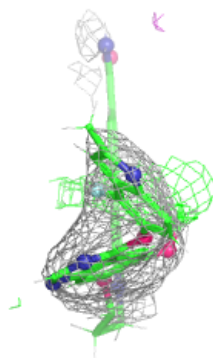
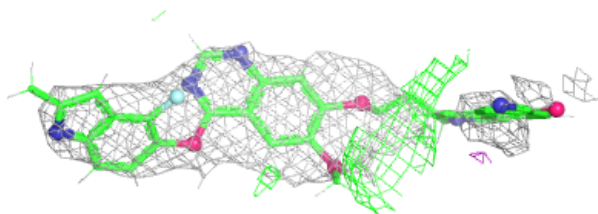
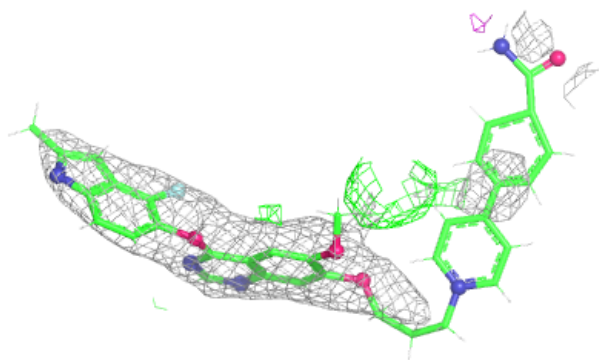


Electron density around AI4 I 201:

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

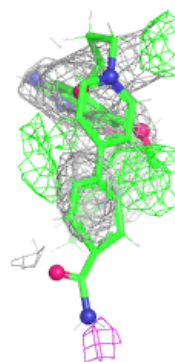
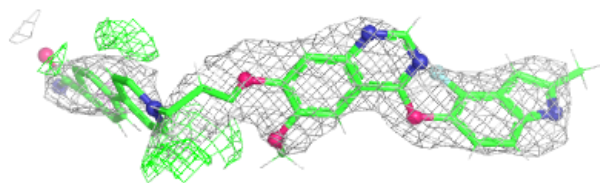
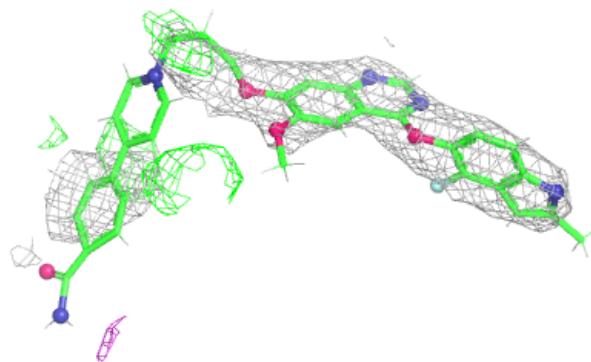
**Electron density around AI4 Y 201:**

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

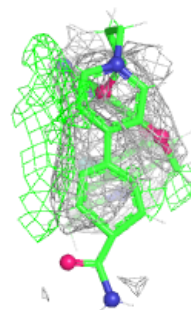
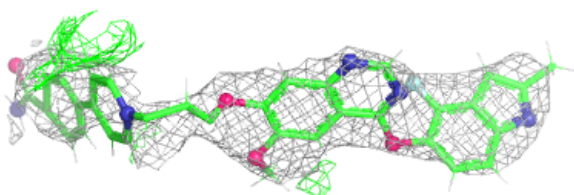
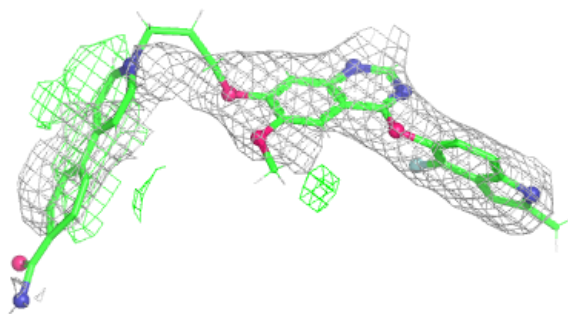


Electron density around AI4 G 201:

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

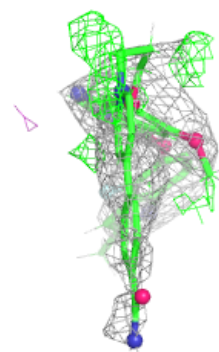
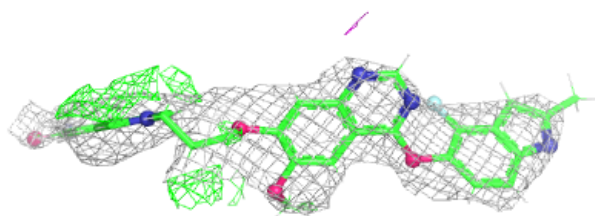
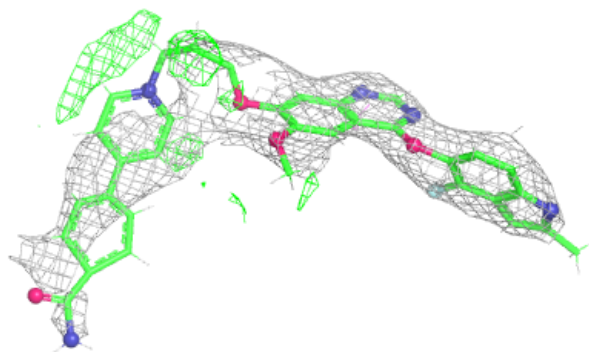
**Electron density around AI4 K 201:**

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

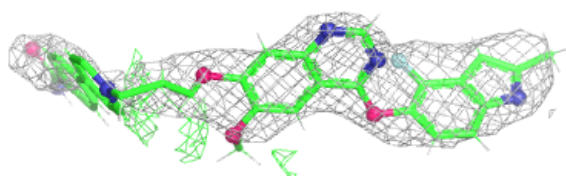
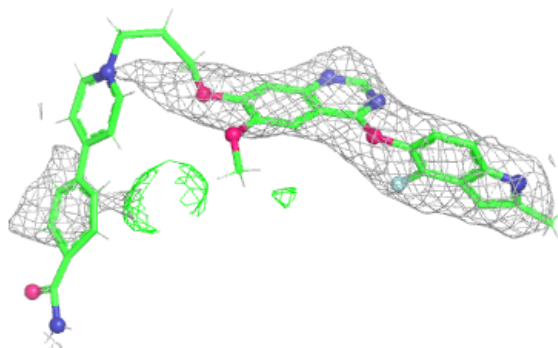


Electron density around AI4 b 201:

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

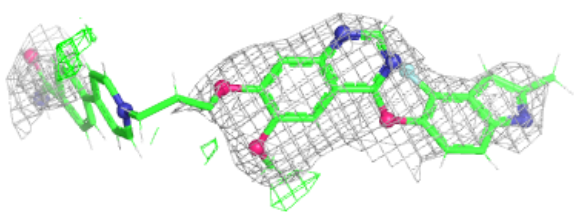
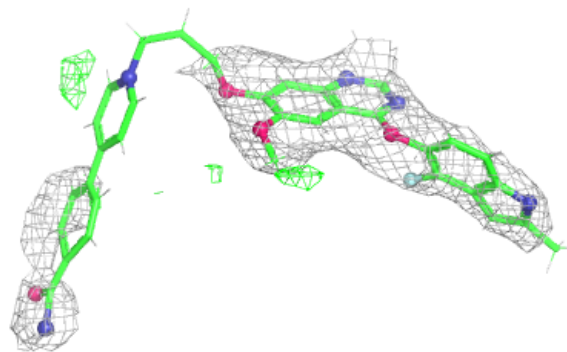
**Electron density around AI4 Z 201:**

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

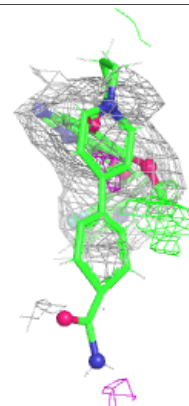
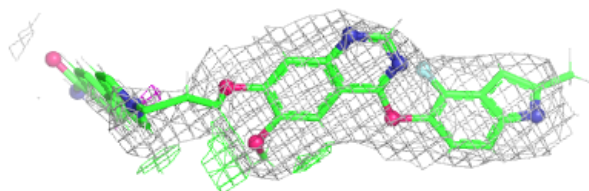
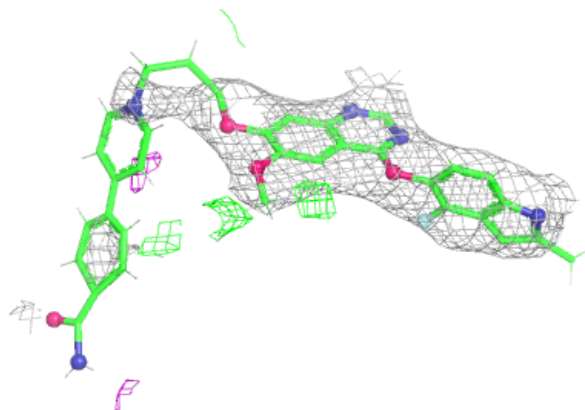


Electron density around AI4 B 201:

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and green (positive)

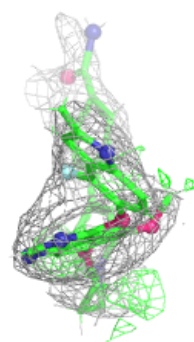
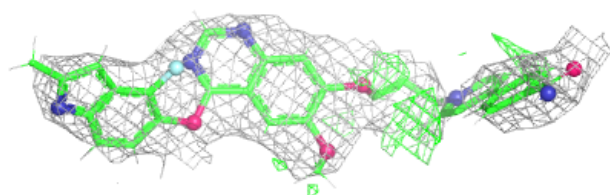
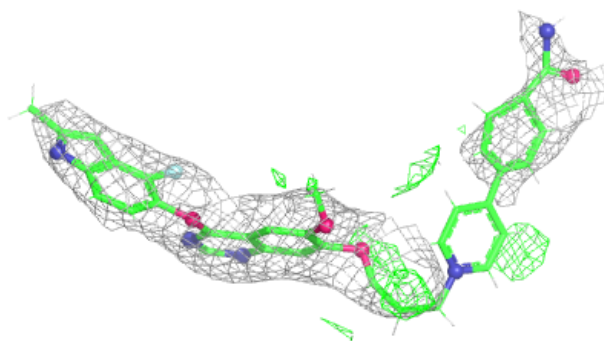
**Electron density around AI4 V 301:**

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

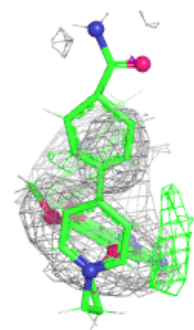
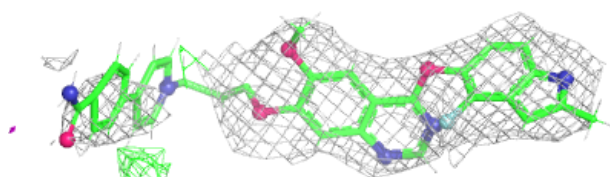
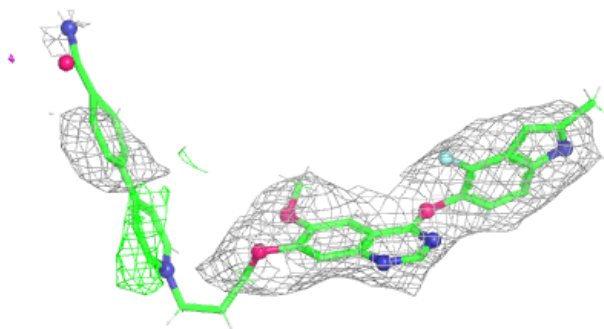


Electron density around AI4 M 201:

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

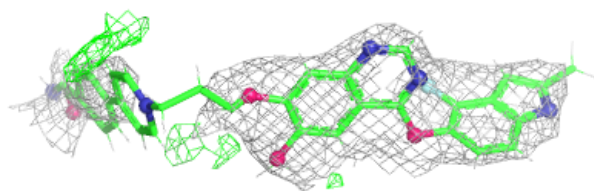
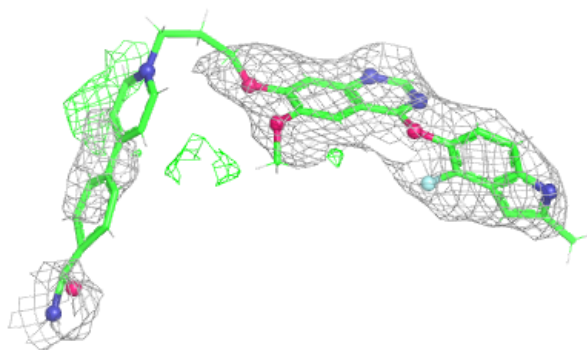
**Electron density around AI4 R 201:**

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



Electron density around AI4 N 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 ⓘ

There are no such residues in this entry.