



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:33 PM UTC

PDB ID : 5YJ1 / pdb_00005yj1
Title : Mouse Cereblon thalidomide binding domain complexed with R-form thalidomide
Authors : Mori, T.; Hakoshima, T.
Deposited on : 2017-10-06
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

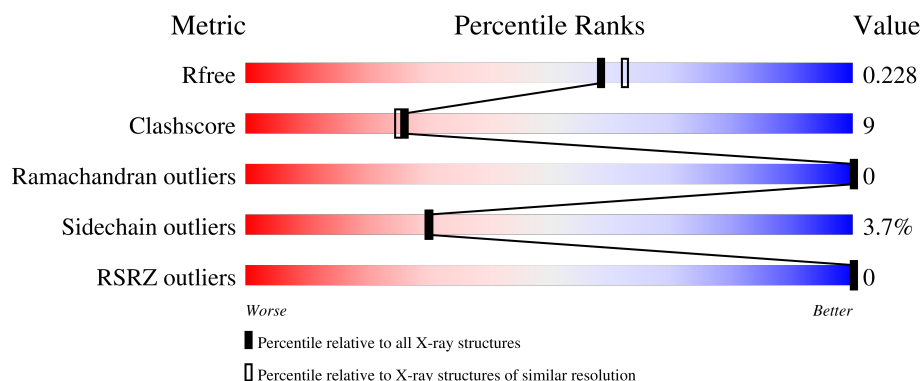
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	111	
1	D	111	
1	G	111	
1	J	111	
1	M	111	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	111	
1	S	111	
1	V	111	
1	Y	111	
1	b	111	
1	e	111	
1	h	111	
1	k	111	
1	n	111	
1	q	111	
1	t	111	

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	SO4	A	503	-	-	X	-
4	SO4	J	504	-	-	X	-
4	SO4	n	503	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13054 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

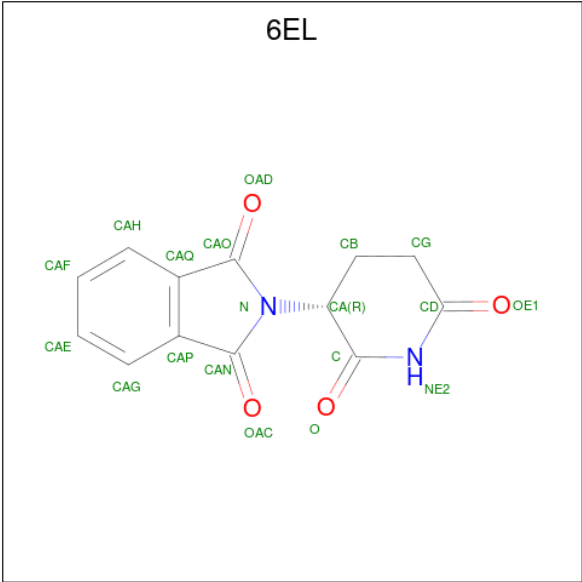
- Molecule 1 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	96	Total	C	N	O	S	0	0	0
			753	484	127	135	7			
1	D	96	Total	C	N	O	S	0	0	0
			753	484	127	135	7			
1	G	98	Total	C	N	O	S	0	0	0
			765	491	129	137	8			
1	J	91	Total	C	N	O	S	0	0	0
			721	463	122	130	6			
1	M	93	Total	C	N	O	S	0	0	0
			732	470	124	132	6			
1	P	93	Total	C	N	O	S	0	0	0
			732	470	124	132	6			
1	S	93	Total	C	N	O	S	0	0	0
			732	470	124	132	6			
1	V	93	Total	C	N	O	S	0	0	0
			732	470	124	132	6			
1	Y	93	Total	C	N	O	S	0	0	0
			732	470	124	132	6			
1	b	93	Total	C	N	O	S	0	0	0
			732	470	124	132	6			
1	e	93	Total	C	N	O	S	0	0	0
			732	470	124	132	6			
1	h	93	Total	C	N	O	S	0	0	0
			732	470	124	132	6			
1	k	94	Total	C	N	O	S	0	0	0
			740	476	125	133	6			
1	n	91	Total	C	N	O	S	0	0	0
			721	463	122	130	6			
1	q	93	Total	C	N	O	S	0	0	0
			732	470	124	132	6			
1	t	97	Total	C	N	O	S	0	0	0
			757	486	128	136	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLY	-	expression tag	UNP Q8C7D2
A	321	PRO	-	expression tag	UNP Q8C7D2
D	320	GLY	-	expression tag	UNP Q8C7D2
D	321	PRO	-	expression tag	UNP Q8C7D2
G	320	GLY	-	expression tag	UNP Q8C7D2
G	321	PRO	-	expression tag	UNP Q8C7D2
J	320	GLY	-	expression tag	UNP Q8C7D2
J	321	PRO	-	expression tag	UNP Q8C7D2
M	320	GLY	-	expression tag	UNP Q8C7D2
M	321	PRO	-	expression tag	UNP Q8C7D2
P	320	GLY	-	expression tag	UNP Q8C7D2
P	321	PRO	-	expression tag	UNP Q8C7D2
S	320	GLY	-	expression tag	UNP Q8C7D2
S	321	PRO	-	expression tag	UNP Q8C7D2
V	320	GLY	-	expression tag	UNP Q8C7D2
V	321	PRO	-	expression tag	UNP Q8C7D2
Y	320	GLY	-	expression tag	UNP Q8C7D2
Y	321	PRO	-	expression tag	UNP Q8C7D2
b	320	GLY	-	expression tag	UNP Q8C7D2
b	321	PRO	-	expression tag	UNP Q8C7D2
e	320	GLY	-	expression tag	UNP Q8C7D2
e	321	PRO	-	expression tag	UNP Q8C7D2
h	320	GLY	-	expression tag	UNP Q8C7D2
h	321	PRO	-	expression tag	UNP Q8C7D2
k	320	GLY	-	expression tag	UNP Q8C7D2
k	321	PRO	-	expression tag	UNP Q8C7D2
n	320	GLY	-	expression tag	UNP Q8C7D2
n	321	PRO	-	expression tag	UNP Q8C7D2
q	320	GLY	-	expression tag	UNP Q8C7D2
q	321	PRO	-	expression tag	UNP Q8C7D2
t	320	GLY	-	expression tag	UNP Q8C7D2
t	321	PRO	-	expression tag	UNP Q8C7D2

- Molecule 2 is 2-[(3 {R})-2,6-bis(oxidanylidene)piperidin-3-yl]isoindole-1,3-dione (CCD ID: 6EL) (formula: C₁₃H₁₀N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	13	2	4		
2	D	1	Total	C	N	O	0	0
			19	13	2	4		
2	G	1	Total	C	N	O	0	0
			19	13	2	4		
2	J	1	Total	C	N	O	0	0
			19	13	2	4		
2	M	1	Total	C	N	O	0	0
			19	13	2	4		
2	P	1	Total	C	N	O	0	0
			19	13	2	4		
2	S	1	Total	C	N	O	0	0
			19	13	2	4		
2	V	1	Total	C	N	O	0	0
			19	13	2	4		
2	Y	1	Total	C	N	O	0	0
			19	13	2	4		
2	b	1	Total	C	N	O	0	0
			19	13	2	4		
2	e	1	Total	C	N	O	0	0
			19	13	2	4		
2	h	1	Total	C	N	O	0	0
			19	13	2	4		
2	k	1	Total	C	N	O	0	0
			19	13	2	4		
2	n	1	Total	C	N	O	0	0
			19	13	2	4		

Continued on next page...

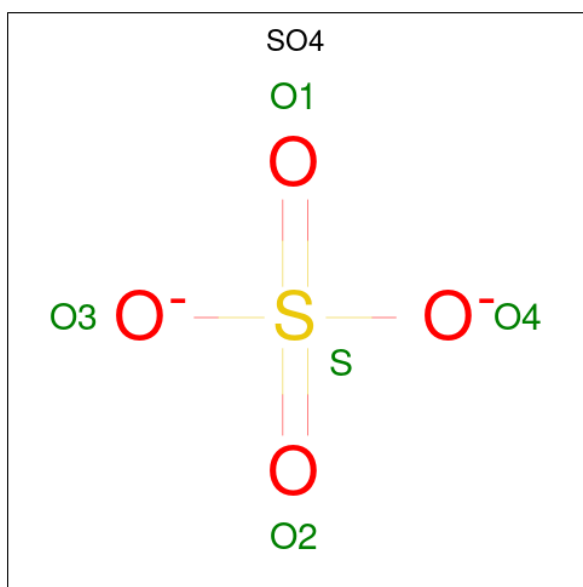
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	q	1	Total	C	N	O	0	0
			19	13	2	4		
2	t	1	Total	C	N	O	0	0
			19	13	2	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	M	1	Total	Zn	0	0
			1	1		
3	P	1	Total	Zn	0	0
			1	1		
3	S	1	Total	Zn	0	0
			1	1		
3	V	1	Total	Zn	0	0
			1	1		
3	Y	1	Total	Zn	0	0
			1	1		
3	b	1	Total	Zn	0	0
			1	1		
3	e	1	Total	Zn	0	0
			1	1		
3	h	1	Total	Zn	0	0
			1	1		
3	k	1	Total	Zn	0	0
			1	1		
3	n	1	Total	Zn	0	0
			1	1		
3	q	1	Total	Zn	0	0
			1	1		
3	t	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		
4	S	1	Total	O	S	0	0
			5	4	1		
4	S	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Y	1	Total O S 5 4 1	0	0
4	Y	1	Total O S 5 4 1	0	0
4	Y	1	Total O S 5 4 1	0	0
4	b	1	Total O S 5 4 1	0	0
4	b	1	Total O S 5 4 1	0	0
4	e	1	Total O S 5 4 1	0	0
4	e	1	Total O S 5 4 1	0	0
4	h	1	Total O S 5 4 1	0	0
4	k	1	Total O S 5 4 1	0	0
4	k	1	Total O S 5 4 1	0	0
4	n	1	Total O S 5 4 1	0	0
4	n	1	Total O S 5 4 1	0	0
4	n	1	Total O S 5 4 1	0	0
4	q	1	Total O S 5 4 1	0	0
4	t	1	Total O S 5 4 1	0	0
4	t	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	42	Total O 42 42	0	0
5	D	47	Total O 47 47	0	0
5	G	43	Total O 43 43	0	0

Continued on next page...

Continued from previous page...

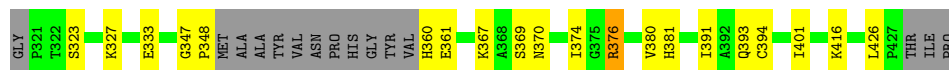
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	50	Total	O	0	0
			50	50		
5	M	54	Total	O	0	0
			54	54		
5	P	50	Total	O	0	0
			50	50		
5	S	54	Total	O	0	0
			54	54		
5	V	50	Total	O	0	0
			50	50		
5	Y	49	Total	O	0	0
			49	49		
5	b	51	Total	O	0	0
			51	51		
5	e	51	Total	O	0	0
			51	51		
5	h	50	Total	O	0	0
			50	50		
5	k	55	Total	O	0	0
			55	55		
5	n	56	Total	O	0	0
			56	56		
5	q	44	Total	O	0	0
			44	44		
5	t	40	Total	O	0	0
			40	40		

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.

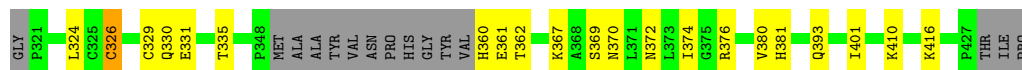
- Molecule 1: Protein cereblon

Chain A: 



- Molecule 1: Protein cereblon

Chain D: 



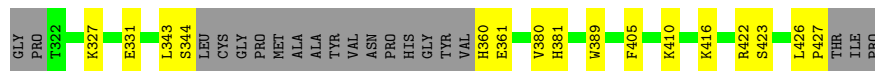
- Molecule 1: Protein cereblon

Chain G: 



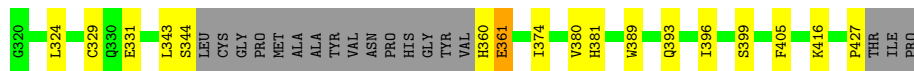
- Molecule 1: Protein cereblon

Chain J: 



- Molecule 1: Protein cereblon

Chain M: 

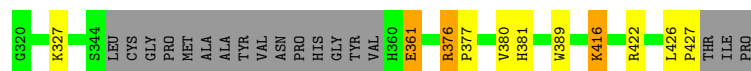


- Molecule 1: Protein cereblon

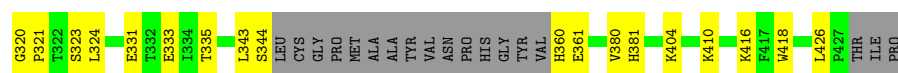
Chain P: 



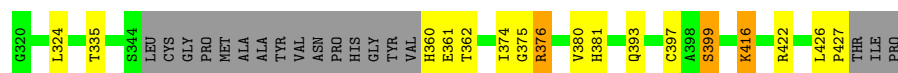
- Molecule 1: Protein cereblon



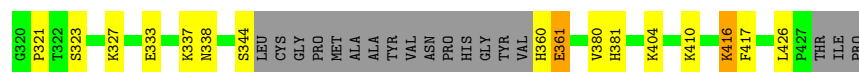
- Molecule 1: Protein cereblon



- Molecule 1: Protein cereblon



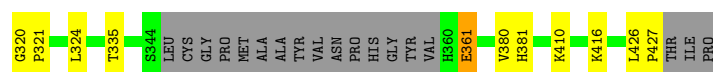
- Molecule 1: Protein cereblon



- Molecule 1: Protein cereblon

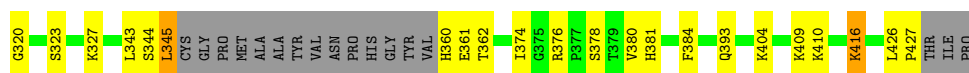


- Molecule 1: Protein cereblon

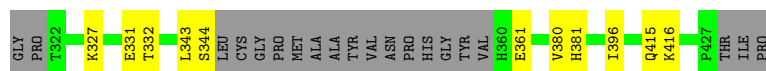


- Molecule 1: Protein cereblon

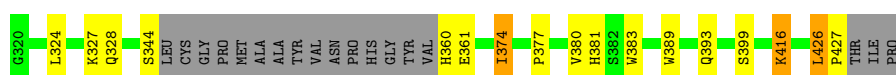




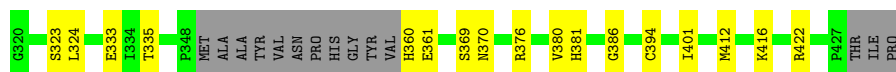
- Molecule 1: Protein cereblon



- Molecule 1: Protein cereblon



- Molecule 1: Protein cereblon



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	201.62Å 201.62Å 123.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.78 – 2.00 19.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.78-2.00) 99.8 (19.78-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.199 , 0.228 0.199 , 0.228	Depositor DCC
R_{free} test set	6364 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.020 for $-1/3^*h+1/3^*k+4/3^*l, -k, 2/3^*h+1/3^*k+1/3^*l$ 0.021 for $-2/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+4/3^*l, -1/3^*h+1/3^*k+1/3^*l$ 0.019 for $-h, 1/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+1/3^*l$ 0.477 for $-1/3^*h-2/3^*k+4/3^*l, -2/3^*h-1/3^*k-4/3^*l, 1/3^*h-1/3^*k-1/3^*l$ 0.477 for $-h, 2/3^*h+1/3^*k+4/3^*l, 1/3^*h+2/3^*k-1/3^*l$ 0.477 for $1/3^*h+2/3^*k-4/3^*l, -k, -2/3^*h-1/3^*k-1/3^*l$ 0.022 for $h, -h-k, -l$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13054	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 75.60 % 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 1.2262e-06. 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: 6EL, ZN, SO4

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	0.38	0/774	0.60	0/1050
1	D	0.41	0/774	0.60	0/1050
1	G	0.32	0/786	0.58	0/1066
1	J	0.41	0/740	0.57	0/1003
1	M	0.33	0/752	0.60	0/1020
1	P	0.33	0/752	0.58	0/1020
1	S	0.32	0/752	0.61	0/1020
1	V	0.33	0/752	0.58	0/1020
1	Y	0.32	0/752	0.59	0/1020
1	b	0.32	0/752	0.58	0/1020
1	e	0.34	0/752	0.62	0/1020
1	h	0.33	0/752	0.56	0/1020
1	k	0.33	0/760	0.62	0/1031
1	n	0.40	0/740	0.57	0/1003
1	q	0.33	0/752	0.62	0/1020
1	t	0.32	0/778	0.58	0/1056
All	All	0.35	0/12120	0.59	0/16439

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	753	0	749	25	0
1	D	753	0	749	20	0
1	G	765	0	760	18	0
1	J	721	0	715	13	0
1	M	732	0	725	11	0
1	P	732	0	725	13	0
1	S	732	0	725	13	0
1	V	732	0	725	12	0
1	Y	732	0	725	14	0
1	b	732	0	725	12	0
1	e	732	0	725	14	0
1	h	732	0	725	5	0
1	k	740	0	736	26	0
1	n	721	0	715	11	0
1	q	732	0	725	14	0
1	t	757	0	751	14	0
2	A	19	0	0	0	0
2	D	19	0	0	0	0
2	G	19	0	0	0	0
2	J	19	0	0	0	0
2	M	19	0	0	0	0
2	P	19	0	0	0	0
2	S	19	0	0	0	0
2	V	19	0	0	0	0
2	Y	19	0	0	0	0
2	b	19	0	0	0	0
2	e	19	0	0	0	0
2	h	19	0	0	0	0
2	k	19	0	0	0	0
2	n	19	0	0	0	0
2	q	19	0	0	1	0
2	t	19	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
3	M	1	0	0	0	0
3	P	1	0	0	0	0
3	S	1	0	0	0	0
3	V	1	0	0	0	0
3	Y	1	0	0	0	0
3	b	1	0	0	0	0
3	e	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	h	1	0	0	0	0
3	k	1	0	0	0	0
3	n	1	0	0	0	0
3	q	1	0	0	0	0
3	t	1	0	0	0	0
4	A	10	0	0	2	0
4	D	10	0	0	0	0
4	J	10	0	0	2	0
4	M	15	0	0	1	0
4	P	5	0	0	1	0
4	S	10	0	0	2	0
4	V	10	0	0	1	0
4	Y	15	0	0	1	0
4	b	10	0	0	0	0
4	e	10	0	0	1	0
4	h	5	0	0	0	0
4	k	10	0	0	1	0
4	n	15	0	0	3	0
4	q	5	0	0	0	0
4	t	10	0	0	0	0
5	A	42	0	0	0	0
5	D	47	0	0	0	0
5	G	43	0	0	0	0
5	J	50	0	0	2	0
5	M	54	0	0	0	0
5	P	50	0	0	0	0
5	S	54	0	0	0	0
5	V	50	0	0	1	0
5	Y	49	0	0	0	0
5	b	51	0	0	1	0
5	e	51	0	0	1	0
5	h	50	0	0	2	0
5	k	55	0	0	3	0
5	n	56	0	0	4	0
5	q	44	0	0	0	0
5	t	40	0	0	0	0
All	All	13054	0	11700	225	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 9.

All (225) 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:S:376:ARG:HG3	1:S:376:ARG:HH11	0.99	1.10
1:k:360:HIS:CG	1:k:361:GLU:H	1.74	1.06
1:G:376:ARG:HG2	1:G:376:ARG:HH11	0.88	1.03
1:G:376:ARG:HH11	1:G:376:ARG:CG	1.77	0.97
1:A:348:PRO:HD2	1:D:331:GLU:OE2	1.67	0.95
1:S:376:ARG:HG3	1:S:376:ARG:NH1	1.77	0.93
1:e:360:HIS:CG	1:e:361:GLU:H	1.86	0.92
1:G:376:ARG:HG2	1:G:376:ARG:NH1	1.69	0.91
1:Y:360:HIS:CG	1:Y:361:GLU:H	1.93	0.86
1:k:360:HIS:CD2	1:k:361:GLU:H	1.94	0.86
1:e:374:ILE:HD11	1:e:393:GLN:NE2	1.91	0.85
1:h:361:GLU:HG2	5:h:634:HOH:O	1.75	0.85
1:D:360:HIS:CE1	1:D:362:THR:HB	2.14	0.83
1:S:422:ARG:HH22	1:S:427:PRO:HG3	1.44	0.83
1:k:360:HIS:CG	1:k:361:GLU:N	2.44	0.83
1:G:374:ILE:HD11	1:G:391:ILE:HG21	1.61	0.81
1:J:426:LEU:HA	1:J:427:PRO:C	2.05	0.81
1:e:360:HIS:CG	1:e:361:GLU:N	2.50	0.80
1:M:360:HIS:CG	1:M:361:GLU:H	2.01	0.78
1:q:380:VAL:HG12	1:q:381:HIS:CD2	2.19	0.76
1:A:374:ILE:HD11	1:A:393:GLN:HG2	1.65	0.76
1:M:374:ILE:HD11	1:M:393:GLN:NE2	2.01	0.76
1:P:360:HIS:CD2	1:P:361:GLU:H	2.05	0.73
1:b:360:HIS:CG	1:b:361:GLU:H	2.07	0.73
1:Y:360:HIS:CG	1:Y:361:GLU:N	2.56	0.72
1:k:426:LEU:HA	1:k:427:PRO:C	2.15	0.71
1:S:376:ARG:HH11	1:S:376:ARG:CG	1.88	0.71
1:k:344:SER:O	1:k:345:LEU:CB	2.38	0.71
1:M:380:VAL:HG12	1:M:381:HIS:CD2	2.26	0.71
1:k:344:SER:O	1:k:345:LEU:HB2	1.88	0.70
1:t:360:HIS:CD2	1:t:361:GLU:H	2.09	0.70
1:k:344:SER:C	1:k:345:LEU:HD23	2.19	0.68
1:A:360:HIS:CD2	1:A:361:GLU:H	2.12	0.68
1:k:380:VAL:HG12	1:k:381:HIS:CD2	2.29	0.68
1:G:376:ARG:CG	1:G:376:ARG:NH1	2.46	0.67
1:A:374:ILE:HD11	1:A:393:GLN:CD	2.20	0.67
1:D:360:HIS:HE1	1:D:362:THR:HB	1.61	0.66
1:A:374:ILE:HD11	1:A:393:GLN:CG	2.25	0.65
1:k:374:ILE:HD11	1:k:393:GLN:NE2	2.10	0.65
1:k:416:LYS:HD2	5:k:606:HOH:O	1.97	0.65
1:q:327:LYS:HG3	1:q:426:LEU:HD13	1.79	0.64
1:D:326:CYS:HB2	1:D:401:ILE:HD11	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:361:GLU:O	1:b:361:GLU:HG3	1.97	0.64
1:q:327:LYS:HG3	1:q:426:LEU:CD1	2.28	0.63
1:Y:380:VAL:HG12	1:Y:381:HIS:CD2	2.33	0.63
1:A:347:GLY:N	1:D:331:GLU:HG2	2.14	0.63
1:b:360:HIS:CD2	1:b:361:GLU:H	2.17	0.63
1:h:426:LEU:HA	1:h:427:PRO:C	2.23	0.62
1:J:380:VAL:HG12	1:J:381:HIS:CD2	2.35	0.62
1:Y:374:ILE:HD11	1:Y:393:GLN:NE2	2.14	0.62
1:e:381:HIS:ND1	4:e:504:SO4:O2	2.32	0.62
1:b:380:VAL:HG12	1:b:381:HIS:CD2	2.36	0.61
1:G:374:ILE:CD1	1:G:391:ILE:HG21	2.30	0.61
1:G:374:ILE:HD11	1:G:391:ILE:CG2	2.31	0.61
1:t:323:SER:HB2	1:t:333:GLU:OE1	2.01	0.61
1:G:380:VAL:HG12	1:G:381:HIS:CD2	2.36	0.60
1:V:360:HIS:CD2	1:V:361:GLU:H	2.19	0.60
1:Y:376:ARG:CD	1:Y:376:ARG:N	2.63	0.60
1:q:360:HIS:HB2	1:q:361:GLU:OE2	2.01	0.60
1:M:360:HIS:CG	1:M:361:GLU:N	2.67	0.60
1:V:381:HIS:ND1	4:V:504:SO4:O2	2.35	0.60
1:k:409:LYS:HE2	5:k:614:HOH:O	2.01	0.60
1:D:380:VAL:HG12	1:D:381:HIS:CD2	2.37	0.60
1:t:394:CYS:HB2	1:t:401:ILE:HD11	1.83	0.60
1:t:386:GLY:C	1:t:412:MET:HE1	2.27	0.59
1:Y:376:ARG:N	1:Y:376:ARG:HD2	2.16	0.59
1:D:326:CYS:HB2	1:D:401:ILE:CD1	2.32	0.59
1:b:360:HIS:CG	1:b:361:GLU:N	2.66	0.58
1:A:360:HIS:CG	1:A:361:GLU:H	2.22	0.58
1:S:380:VAL:HG12	1:S:381:HIS:CD2	2.39	0.58
1:k:345:LEU:HB2	5:n:624:HOH:O	2.04	0.57
1:e:380:VAL:HG12	1:e:381:HIS:CD2	2.40	0.57
1:S:376:ARG:NH1	1:S:376:ARG:CG	2.55	0.57
1:P:360:HIS:CG	1:P:361:GLU:H	2.18	0.56
1:S:361:GLU:O	1:S:361:GLU:HG3	2.05	0.56
1:n:343:LEU:O	1:n:344:SER:HB2	2.04	0.56
1:n:361:GLU:HG3	5:n:647:HOH:O	2.05	0.55
1:P:324:LEU:HD23	1:P:427:PRO:HD2	1.88	0.55
1:V:343:LEU:O	1:V:344:SER:HB2	2.05	0.55
1:J:327:LYS:HE2	1:J:423:SER:O	2.06	0.55
1:A:374:ILE:HD13	1:A:391:ILE:HG22	1.88	0.55
1:t:394:CYS:HB2	1:t:401:ILE:CD1	2.37	0.55
1:t:360:HIS:CG	1:t:361:GLU:H	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:327:LYS:HD3	1:J:426:LEU:HD13	1.89	0.54
1:b:404:LYS:HE3	1:b:416:LYS:HD2	1.89	0.54
1:Y:360:HIS:CD2	1:Y:361:GLU:H	2.26	0.54
1:e:426:LEU:HA	1:e:427:PRO:C	2.31	0.54
1:A:348:PRO:CD	1:D:331:GLU:OE2	2.50	0.54
1:D:360:HIS:CD2	1:D:361:GLU:H	2.26	0.54
1:n:381:HIS:ND1	4:n:505:SO4:O1	2.36	0.54
1:J:331:GLU:HG3	5:J:604:HOH:O	2.08	0.53
1:J:343:LEU:O	1:J:344:SER:HB2	2.08	0.53
1:q:377:PRO:HA	1:q:389:TRP:O	2.09	0.53
1:b:416:LYS:HG2	1:b:417:PHE:N	2.22	0.53
1:k:345:LEU:HB3	1:n:331:GLU:O	2.09	0.53
1:G:374:ILE:CD1	1:G:391:ILE:CG2	2.87	0.52
1:k:343:LEU:HD23	1:k:384:PHE:CD1	2.44	0.52
1:A:327:LYS:HE2	1:A:426:LEU:HD13	1.92	0.52
1:e:397:CYS:SG	1:e:399:SER:HB3	2.50	0.52
1:k:345:LEU:O	1:n:331:GLU:HG3	2.10	0.52
1:D:369:SER:O	1:D:370:ASN:HB2	2.09	0.52
1:b:338:ASN:ND2	5:b:601:HOH:O	2.43	0.52
1:h:320:GLY:N	1:h:321:PRO:CD	2.72	0.52
1:D:329:CYS:O	1:D:330:GLN:HB2	2.10	0.51
1:A:347:GLY:HA3	1:D:331:GLU:CG	2.41	0.51
5:h:603:HOH:O	1:n:327:LYS:HE2	2.09	0.51
1:M:360:HIS:CD2	1:M:361:GLU:H	2.28	0.51
1:S:377:PRO:HA	1:S:389:TRP:O	2.11	0.51
1:k:344:SER:O	1:k:345:LEU:CG	2.59	0.51
1:P:380:VAL:HG12	1:P:381:HIS:CD2	2.46	0.51
1:e:374:ILE:HD11	1:e:393:GLN:HE21	1.72	0.51
1:k:360:HIS:CD2	1:k:361:GLU:N	2.72	0.51
1:M:343:LEU:O	1:M:344:SER:C	2.54	0.51
1:t:380:VAL:HG12	1:t:381:HIS:CD2	2.46	0.51
1:S:422:ARG:NH2	1:S:427:PRO:HG3	2.20	0.50
1:V:380:VAL:HG12	1:V:381:HIS:CD2	2.47	0.50
1:n:415:GLN:HB2	4:n:503:SO4:O2	2.11	0.50
1:e:416:LYS:NZ	5:e:603:HOH:O	2.43	0.50
1:S:381:HIS:ND1	4:S:504:SO4:O4	2.44	0.50
1:A:347:GLY:CA	1:D:331:GLU:HG2	2.42	0.50
1:V:320:GLY:N	1:V:321:PRO:HD3	2.26	0.50
1:A:347:GLY:HA3	1:D:331:GLU:HG2	1.94	0.50
4:M:503:SO4:O2	1:P:415:GLN:HB2	2.10	0.50
1:V:320:GLY:N	1:V:321:PRO:CD	2.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.77	0.50
1:D:361:GLU:O	1:D:361:GLU:HG3	2.11	0.49
1:Y:375:GLY:C	1:Y:376:ARG:HD2	2.37	0.49
1:t:323:SER:HB2	1:t:333:GLU:HG3	1.94	0.49
1:P:426:LEU:HA	1:P:427:PRO:C	2.38	0.49
1:D:324:LEU:HD12	1:D:335:THR:HG23	1.94	0.49
1:n:332:THR:OG1	1:n:396:ILE:HG13	2.13	0.49
1:n:380:VAL:HG12	1:n:381:HIS:CD2	2.48	0.48
1:P:343:LEU:O	1:P:344:SER:HB2	2.14	0.48
1:S:416:LYS:HE3	4:S:503:SO4:O1	2.13	0.48
1:A:380:VAL:HG12	1:A:381:HIS:CD2	2.49	0.48
1:G:374:ILE:CG1	1:G:391:ILE:HB	2.44	0.47
1:M:324:LEU:HD23	1:M:427:PRO:HD2	1.95	0.47
1:P:360:HIS:CG	1:P:361:GLU:N	2.82	0.47
1:b:323:SER:OG	1:b:333:GLU:OE1	2.26	0.47
1:k:416:LYS:CD	5:k:606:HOH:O	2.58	0.47
1:G:360:HIS:O	1:G:422:ARG:NE	2.48	0.47
1:t:324:LEU:HD12	1:t:335:THR:HG23	1.97	0.47
1:k:360:HIS:CD2	1:k:362:THR:H	2.33	0.47
1:q:361:GLU:H	1:q:361:GLU:CD	2.22	0.47
1:A:369:SER:O	1:A:370:ASN:HB2	2.14	0.47
1:M:329:CYS:O	1:M:331:GLU:N	2.48	0.46
1:t:386:GLY:O	1:t:412:MET:HE1	2.16	0.46
1:A:374:ILE:CD1	1:A:391:ILE:HG22	2.45	0.46
1:q:426:LEU:HA	1:q:427:PRO:C	2.40	0.46
1:S:327:LYS:HA	1:S:426:LEU:HG	1.98	0.46
1:D:374:ILE:HD11	1:D:393:GLN:CD	2.40	0.46
1:G:394:CYS:HB2	1:G:401:ILE:CD1	2.46	0.46
1:P:377:PRO:HA	1:P:389:TRP:O	2.16	0.46
1:Y:360:HIS:CD2	1:Y:362:THR:H	2.34	0.46
1:t:324:LEU:HD12	1:t:335:THR:CG2	2.45	0.46
1:A:376:ARG:HH11	1:A:376:ARG:CG	2.29	0.45
1:Y:397:CYS:SG	1:Y:399:SER:HB3	2.56	0.45
1:M:329:CYS:C	1:M:331:GLU:H	2.25	0.45
1:e:343:LEU:HD23	1:e:384:PHE:CD1	2.52	0.45
4:n:503:SO4:O1	1:q:416:LYS:HE3	2.16	0.45
1:q:328:GLN:NE2	1:q:399:SER:HB2	2.32	0.45
1:Y:361:GLU:O	1:Y:361:GLU:HG3	2.17	0.45
1:k:378:SER:OG	1:k:380:VAL:HG23	2.17	0.45
1:n:344:SER:HB3	5:n:650:HOH:O	2.16	0.45
1:k:320:GLY:O	1:k:323:SER:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:422:ARG:HH22	1:S:427:PRO:CG	2.21	0.45
4:A:503:SO4:O2	1:D:367:LYS:NZ	2.47	0.44
1:J:360:HIS:O	1:J:422:ARG:NE	2.49	0.44
1:J:381:HIS:HA	4:J:504:SO4:O4	2.17	0.44
1:M:389:TRP:HB3	1:M:405:PHE:CE1	2.53	0.44
1:A:323:SER:OG	1:A:333:GLU:HG3	2.18	0.44
1:G:327:LYS:HE2	1:G:426:LEU:HD13	1.99	0.44
1:D:360:HIS:CG	1:D:361:GLU:H	2.35	0.44
1:G:331:GLU:OE2	1:e:396:ILE:O	2.36	0.44
1:J:426:LEU:HD21	1:V:426:LEU:HD21	2.00	0.44
1:Y:426:LEU:HA	1:Y:427:PRO:C	2.43	0.44
1:h:380:VAL:HG12	1:h:381:HIS:CD2	2.52	0.44
1:Y:416:LYS:HE2	4:Y:504:SO4:O1	2.17	0.44
1:P:323:SER:OG	1:P:333:GLU:OE2	2.32	0.43
1:P:397:CYS:O	1:P:398:ALA:HB3	2.18	0.43
1:q:380:VAL:CG1	1:q:381:HIS:CD2	2.98	0.43
1:A:360:HIS:CG	1:A:361:GLU:N	2.86	0.43
1:Y:324:LEU:HD12	1:Y:335:THR:HG23	2.00	0.43
1:q:360:HIS:ND1	1:q:361:GLU:CD	2.76	0.43
1:A:367:LYS:NZ	4:A:503:SO4:O3	2.50	0.43
1:k:361:GLU:O	1:k:361:GLU:HG3	2.19	0.43
1:k:381:HIS:ND1	4:k:503:SO4:O3	2.49	0.43
1:h:324:LEU:HD12	1:h:335:THR:HG23	2.00	0.43
1:J:381:HIS:ND1	4:J:504:SO4:O4	2.37	0.43
1:b:410:LYS:HA	1:b:410:LYS:HD2	1.80	0.43
1:D:360:HIS:CG	1:D:361:GLU:N	2.87	0.43
1:V:331:GLU:HG3	5:V:609:HOH:O	2.19	0.42
1:t:360:HIS:O	1:t:422:ARG:NE	2.51	0.42
1:J:360:HIS:N	5:J:601:HOH:O	2.52	0.42
1:k:345:LEU:HD23	1:k:345:LEU:N	2.33	0.42
1:V:323:SER:HB2	1:V:333:GLU:OE1	2.20	0.42
1:t:360:HIS:CG	1:t:361:GLU:N	2.87	0.42
1:G:386:GLY:C	1:G:412:MET:HE1	2.44	0.42
1:A:361:GLU:O	1:A:361:GLU:HG3	2.19	0.42
1:A:394:CYS:HB2	1:A:401:ILE:CD1	2.50	0.42
1:P:389:TRP:HB3	1:P:405:PHE:CE1	2.55	0.42
1:k:416:LYS:HE2	1:k:416:LYS:HB3	1.20	0.42
1:e:329:CYS:C	1:e:331:GLU:H	2.28	0.41
1:q:324:LEU:HD23	1:q:427:PRO:HD2	2.02	0.41
1:A:394:CYS:HB2	1:A:401:ILE:HD11	2.02	0.41
1:t:369:SER:O	1:t:370:ASN:HB2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ILE:HD13	1:A:391:ILE:CG2	2.51	0.41
1:b:321:PRO:O	1:b:337:LYS:HE3	2.19	0.41
1:G:340:ILE:HA	1:G:365:VAL:HG12	2.03	0.41
1:q:374:ILE:HD13	1:q:393:GLN:OE1	2.20	0.41
1:V:324:LEU:HD12	1:V:335:THR:HG23	2.02	0.41
1:e:378:SER:OG	1:e:380:VAL:HG23	2.21	0.41
1:b:327:LYS:HA	1:b:426:LEU:HG	2.02	0.41
1:G:374:ILE:HG12	1:G:391:ILE:HB	2.02	0.41
1:J:327:LYS:CE	1:J:423:SER:O	2.68	0.41
1:k:404:LYS:HE2	1:k:416:LYS:HG3	2.02	0.41
1:P:416:LYS:HE3	4:P:503:SO4:O2	2.21	0.41
1:q:383:TRP:CE2	2:q:501:6EL:NE2	2.89	0.41
1:n:327:LYS:HD2	5:n:613:HOH:O	2.21	0.40
1:G:374:ILE:O	1:G:374:ILE:HG13	2.20	0.40
1:J:389:TRP:HB3	1:J:405:PHE:CE1	2.57	0.40
1:V:360:HIS:HD2	1:V:361:GLU:H	1.64	0.40
1:V:404:LYS:HE3	1:V:418:TRP:CZ2	2.56	0.40
1:e:343:LEU:HD22	1:e:417:PHE:CZ	2.56	0.40
1:M:396:ILE:HD13	1:M:396:ILE:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/111 (83%)	92 (100%)	0	0	100	100
1	D	92/111 (83%)	91 (99%)	1 (1%)	0	100	100
1	G	94/111 (85%)	94 (100%)	0	0	100	100
1	J	87/111 (78%)	85 (98%)	2 (2%)	0	100	100
1	M	89/111 (80%)	88 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	89/111 (80%)	87 (98%)	2 (2%)	0	100	100
1	S	89/111 (80%)	87 (98%)	2 (2%)	0	100	100
1	V	89/111 (80%)	86 (97%)	3 (3%)	0	100	100
1	Y	89/111 (80%)	87 (98%)	2 (2%)	0	100	100
1	b	89/111 (80%)	88 (99%)	1 (1%)	0	100	100
1	e	89/111 (80%)	88 (99%)	1 (1%)	0	100	100
1	h	89/111 (80%)	86 (97%)	3 (3%)	0	100	100
1	k	90/111 (81%)	89 (99%)	1 (1%)	0	100	100
1	n	87/111 (78%)	85 (98%)	2 (2%)	0	100	100
1	q	89/111 (80%)	88 (99%)	1 (1%)	0	100	100
1	t	93/111 (84%)	92 (99%)	1 (1%)	0	100	100
All	All	1436/1776 (81%)	1413 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	85/96 (88%)	83 (98%)	2 (2%)	43	47
1	D	85/96 (88%)	80 (94%)	5 (6%)	18	14
1	G	86/96 (90%)	82 (95%)	4 (5%)	23	22
1	J	81/96 (84%)	78 (96%)	3 (4%)	30	30
1	M	82/96 (85%)	79 (96%)	3 (4%)	30	30
1	P	82/96 (85%)	80 (98%)	2 (2%)	43	47
1	S	82/96 (85%)	79 (96%)	3 (4%)	30	30
1	V	82/96 (85%)	80 (98%)	2 (2%)	43	47
1	Y	82/96 (85%)	78 (95%)	4 (5%)	22	20
1	b	82/96 (85%)	79 (96%)	3 (4%)	30	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	82/96 (85%)	79 (96%)	3 (4%)	30	30
1	h	82/96 (85%)	79 (96%)	3 (4%)	30	30
1	k	83/96 (86%)	78 (94%)	5 (6%)	17	14
1	n	81/96 (84%)	80 (99%)	1 (1%)	63	70
1	q	82/96 (85%)	78 (95%)	4 (5%)	22	20
1	t	85/96 (88%)	83 (98%)	2 (2%)	43	47
All	All	1324/1536 (86%)	1275 (96%)	49 (4%)	30	30

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	ARG
1	A	416	LYS
1	D	326	CYS
1	D	372	ASN
1	D	376	ARG
1	D	410	LYS
1	D	416	LYS
1	G	345	LEU
1	G	372	ASN
1	G	376	ARG
1	G	416	LYS
1	J	361	GLU
1	J	410	LYS
1	J	416	LYS
1	M	361	GLU
1	M	399	SER
1	M	416	LYS
1	P	410	LYS
1	P	416	LYS
1	S	361	GLU
1	S	376	ARG
1	S	416	LYS
1	V	410	LYS
1	V	416	LYS
1	Y	376	ARG
1	Y	399	SER
1	Y	416	LYS
1	Y	422	ARG
1	b	344	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	361	GLU
1	b	416	LYS
1	e	376	ARG
1	e	399	SER
1	e	416	LYS
1	h	361	GLU
1	h	410	LYS
1	h	416	LYS
1	k	327	LYS
1	k	345	LEU
1	k	376	ARG
1	k	410	LYS
1	k	416	LYS
1	n	416	LYS
1	q	344	SER
1	q	374	ILE
1	q	416	LYS
1	q	426	LEU
1	t	376	ARG
1	t	416	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	338	ASN
1	A	360	HIS
1	A	381	HIS
1	D	338	ASN
1	D	360	HIS
1	D	372	ASN
1	D	381	HIS
1	G	338	ASN
1	G	393	GLN
1	M	372	ASN
1	M	393	GLN
1	P	360	HIS
1	P	381	HIS
1	P	393	GLN
1	S	338	ASN
1	V	338	ASN
1	V	360	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	372	ASN
1	V	393	GLN
1	Y	360	HIS
1	Y	372	ASN
1	Y	393	GLN
1	Y	400	HIS
1	b	338	ASN
1	b	360	HIS
1	b	372	ASN
1	b	381	HIS
1	e	372	ASN
1	e	393	GLN
1	h	338	ASN
1	h	372	ASN
1	h	381	HIS
1	h	393	GLN
1	k	360	HIS
1	k	372	ASN
1	k	393	GLN
1	k	400	HIS
1	n	360	HIS
1	n	372	ASN
1	q	328	GLN
1	q	372	ASN
1	q	381	HIS
1	t	330	GLN
1	t	360	HIS
1	t	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 62 ligands modelled in this entry, 16 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6EL	t	501	-	21,21,21	2.28	4 (19%)	31,31,31	2.21	11 (35%)
4	SO4	V	504	-	4,4,4	0.27	0	6,6,6	0.08	0
2	6EL	D	501	-	21,21,21	2.21	4 (19%)	31,31,31	2.29	13 (41%)
4	SO4	A	503	-	4,4,4	0.29	0	6,6,6	0.08	0
2	6EL	M	501	-	21,21,21	2.21	4 (19%)	31,31,31	2.63	14 (45%)
4	SO4	e	504	-	4,4,4	0.29	0	6,6,6	0.07	0
4	SO4	n	505	-	4,4,4	0.29	0	6,6,6	0.07	0
2	6EL	e	501	-	21,21,21	2.21	4 (19%)	31,31,31	2.66	12 (38%)
4	SO4	J	503	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	D	503	-	4,4,4	0.28	0	6,6,6	0.06	0
4	SO4	A	504	-	4,4,4	0.27	0	6,6,6	0.08	0
4	SO4	J	504	-	4,4,4	0.29	0	6,6,6	0.08	0
4	SO4	S	504	-	4,4,4	0.28	0	6,6,6	0.08	0
4	SO4	k	503	-	4,4,4	0.29	0	6,6,6	0.06	0
2	6EL	h	501	-	21,21,21	2.23	5 (23%)	31,31,31	2.55	14 (45%)
4	SO4	t	504	-	4,4,4	0.37	0	6,6,6	0.20	0
4	SO4	b	503	-	4,4,4	0.28	0	6,6,6	0.08	0
2	6EL	b	501	-	21,21,21	2.22	4 (19%)	31,31,31	2.48	13 (41%)
2	6EL	G	501	-	21,21,21	2.30	4 (19%)	31,31,31	2.24	12 (38%)
4	SO4	M	505	-	4,4,4	0.29	0	6,6,6	0.05	0
4	SO4	V	503	-	4,4,4	0.28	0	6,6,6	0.07	0
4	SO4	Y	505	-	4,4,4	0.28	0	6,6,6	0.07	0
4	SO4	P	503	-	4,4,4	0.28	0	6,6,6	0.08	0
2	6EL	P	501	-	21,21,21	2.18	5 (23%)	31,31,31	2.51	13 (41%)
4	SO4	M	504	-	4,4,4	0.28	0	6,6,6	0.08	0
4	SO4	t	503	-	4,4,4	0.28	0	6,6,6	0.08	0
4	SO4	q	503	-	4,4,4	0.29	0	6,6,6	0.08	0
2	6EL	n	501	-	21,21,21	2.32	4 (19%)	31,31,31	2.58	14 (45%)
2	6EL	J	501	-	21,21,21	2.25	4 (19%)	31,31,31	2.53	12 (38%)
4	SO4	S	503	-	4,4,4	0.28	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6EL	k	501	-	21,21,21	2.20	5 (23%)	31,31,31	2.63	14 (45%)
4	SO4	M	503	-	4,4,4	0.26	0	6,6,6	0.07	0
2	6EL	A	501	-	21,21,21	2.25	4 (19%)	31,31,31	2.23	13 (41%)
4	SO4	e	503	-	4,4,4	0.29	0	6,6,6	0.08	0
4	SO4	h	503	-	4,4,4	0.28	0	6,6,6	0.07	0
4	SO4	b	504	-	4,4,4	0.28	0	6,6,6	0.08	0
4	SO4	n	504	-	4,4,4	0.27	0	6,6,6	0.07	0
4	SO4	n	503	-	4,4,4	0.29	0	6,6,6	0.07	0
4	SO4	D	504	-	4,4,4	0.28	0	6,6,6	0.08	0
2	6EL	Y	501	-	21,21,21	2.23	5 (23%)	31,31,31	2.59	14 (45%)
4	SO4	k	504	-	4,4,4	0.28	0	6,6,6	0.08	0
2	6EL	V	501	-	21,21,21	2.27	4 (19%)	31,31,31	2.53	14 (45%)
4	SO4	Y	504	-	4,4,4	0.28	0	6,6,6	0.07	0
4	SO4	Y	503	-	4,4,4	0.28	0	6,6,6	0.06	0
2	6EL	S	501	-	21,21,21	2.24	5 (23%)	31,31,31	2.43	14 (45%)
2	6EL	q	501	-	21,21,21	2.23	4 (19%)	31,31,31	2.52	13 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6EL	A	501	-	-	2/4/33/33	0/3/3/3
2	6EL	P	501	-	-	2/4/33/33	0/3/3/3
2	6EL	t	501	-	-	2/4/33/33	0/3/3/3
2	6EL	h	501	-	-	1/4/33/33	0/3/3/3
2	6EL	D	501	-	-	2/4/33/33	0/3/3/3
2	6EL	b	501	-	-	2/4/33/33	0/3/3/3
2	6EL	n	501	-	-	1/4/33/33	0/3/3/3
2	6EL	J	501	-	-	1/4/33/33	0/3/3/3
2	6EL	Y	501	-	-	1/4/33/33	0/3/3/3
2	6EL	G	501	-	-	2/4/33/33	0/3/3/3
2	6EL	M	501	-	-	1/4/33/33	0/3/3/3
2	6EL	k	501	-	-	1/4/33/33	0/3/3/3
2	6EL	V	501	-	-	0/4/33/33	0/3/3/3
2	6EL	e	501	-	-	1/4/33/33	0/3/3/3
2	6EL	S	501	-	-	2/4/33/33	0/3/3/3
2	6EL	q	501	-	-	2/4/33/33	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	501	6EL	CAQ-CAO	-6.61	1.38	1.48
2	G	501	6EL	CAQ-CAO	-6.53	1.38	1.48
2	n	501	6EL	CAQ-CAO	-6.47	1.38	1.48
2	V	501	6EL	CAQ-CAO	-6.41	1.38	1.48
2	t	501	6EL	CAQ-CAO	-6.36	1.38	1.48
2	Y	501	6EL	CAQ-CAO	-6.25	1.38	1.48
2	A	501	6EL	CAQ-CAO	-6.24	1.38	1.48
2	h	501	6EL	CAQ-CAO	-6.24	1.38	1.48
2	S	501	6EL	CAQ-CAO	-6.23	1.38	1.48
2	e	501	6EL	CAQ-CAO	-6.21	1.38	1.48
2	q	501	6EL	CAQ-CAO	-6.20	1.38	1.48
2	M	501	6EL	CAP-CAN	-6.17	1.38	1.48
2	k	501	6EL	CAQ-CAO	-6.14	1.39	1.48
2	D	501	6EL	CAP-CAN	-6.12	1.39	1.48
2	b	501	6EL	CAQ-CAO	-6.10	1.39	1.48
2	G	501	6EL	CAP-CAN	-5.60	1.39	1.48
2	n	501	6EL	CAP-CAN	-5.58	1.39	1.48
2	t	501	6EL	CAP-CAN	-5.50	1.40	1.48
2	P	501	6EL	CAP-CAN	-5.48	1.40	1.48
2	P	501	6EL	CAQ-CAO	-5.46	1.40	1.48
2	h	501	6EL	CAP-CAN	-5.43	1.40	1.48
2	b	501	6EL	CAP-CAN	-5.43	1.40	1.48
2	A	501	6EL	CAP-CAN	-5.42	1.40	1.48
2	q	501	6EL	CAP-CAN	-5.39	1.40	1.48
2	V	501	6EL	CAP-CAN	-5.37	1.40	1.48
2	M	501	6EL	CAQ-CAO	-5.32	1.40	1.48
2	D	501	6EL	CAQ-CAO	-5.26	1.40	1.48
2	e	501	6EL	CAP-CAN	-5.22	1.40	1.48
2	k	501	6EL	CAP-CAN	-5.22	1.40	1.48
2	J	501	6EL	CAP-CAN	-5.20	1.40	1.48
2	Y	501	6EL	CAP-CAN	-5.18	1.40	1.48
2	S	501	6EL	CAP-CAN	-5.15	1.40	1.48
2	q	501	6EL	CAO-N	-4.00	1.32	1.40
2	S	501	6EL	CAO-N	-3.98	1.32	1.40
2	V	501	6EL	CAO-N	-3.96	1.32	1.40
2	n	501	6EL	CAO-N	-3.92	1.32	1.40
2	J	501	6EL	CAO-N	-3.82	1.32	1.40
2	b	501	6EL	CAO-N	-3.82	1.32	1.40
2	t	501	6EL	CAO-N	-3.81	1.32	1.40
2	Y	501	6EL	CAO-N	-3.80	1.32	1.40
2	G	501	6EL	CAO-N	-3.77	1.32	1.40
2	P	501	6EL	CAN-N	-3.77	1.32	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	501	6EL	CAO-N	-3.77	1.32	1.40
2	A	501	6EL	CAO-N	-3.75	1.32	1.40
2	h	501	6EL	CAO-N	-3.74	1.32	1.40
2	k	501	6EL	CAO-N	-3.69	1.32	1.40
2	D	501	6EL	CAN-N	-3.67	1.32	1.40
2	M	501	6EL	CAN-N	-3.65	1.32	1.40
2	P	501	6EL	CAO-N	-3.09	1.34	1.40
2	t	501	6EL	CAN-N	-3.05	1.34	1.40
2	A	501	6EL	CAN-N	-2.99	1.34	1.40
2	G	501	6EL	CAN-N	-2.98	1.34	1.40
2	D	501	6EL	CAO-N	-2.91	1.34	1.40
2	n	501	6EL	CAN-N	-2.87	1.34	1.40
2	S	501	6EL	CAN-N	-2.81	1.34	1.40
2	e	501	6EL	CAN-N	-2.79	1.34	1.40
2	b	501	6EL	CAN-N	-2.78	1.34	1.40
2	q	501	6EL	CAN-N	-2.74	1.34	1.40
2	Y	501	6EL	CAN-N	-2.73	1.34	1.40
2	h	501	6EL	CAN-N	-2.69	1.34	1.40
2	k	501	6EL	CAN-N	-2.66	1.34	1.40
2	V	501	6EL	CAN-N	-2.64	1.34	1.40
2	J	501	6EL	CAN-N	-2.59	1.35	1.40
2	M	501	6EL	CAO-N	-2.49	1.35	1.40
2	k	501	6EL	CG-CD	2.16	1.54	1.50
2	S	501	6EL	CG-CD	2.14	1.54	1.50
2	Y	501	6EL	CG-CD	2.11	1.54	1.50
2	h	501	6EL	CG-CD	2.03	1.54	1.50
2	P	501	6EL	CG-CD	2.00	1.54	1.50

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	501	6EL	C-CA-N	6.94	115.28	109.08
2	M	501	6EL	C-CA-N	6.73	115.09	109.08
2	Y	501	6EL	C-CA-N	6.58	114.95	109.08
2	k	501	6EL	C-CA-N	6.56	114.94	109.08
2	q	501	6EL	C-CA-N	6.15	114.57	109.08
2	n	501	6EL	C-CA-N	5.75	114.21	109.08
2	V	501	6EL	C-CA-N	5.67	114.14	109.08
2	h	501	6EL	C-CA-N	5.67	114.14	109.08
2	J	501	6EL	C-CA-N	5.60	114.07	109.08
2	J	501	6EL	CAQ-CAO-N	5.47	112.00	105.96
2	n	501	6EL	CG-CD-NE2	5.43	122.47	116.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	501	6EL	C-CA-N	5.22	113.74	109.08
2	e	501	6EL	CAQ-CAO-N	5.18	111.69	105.96
2	b	501	6EL	C-CA-N	5.13	113.65	109.08
2	h	501	6EL	CAQ-CAO-N	5.08	111.57	105.96
2	M	501	6EL	CAO-N-CAN	-4.99	105.88	111.55
2	V	501	6EL	CG-CD-NE2	4.97	121.98	116.69
2	b	501	6EL	CG-CD-NE2	4.97	121.97	116.69
2	e	501	6EL	CG-CD-NE2	4.93	121.94	116.69
2	S	501	6EL	CG-CD-NE2	4.90	121.91	116.69
2	t	501	6EL	CG-CD-NE2	4.90	121.90	116.69
2	k	501	6EL	CAO-N-CAN	-4.87	106.02	111.55
2	P	501	6EL	CG-CD-NE2	4.86	121.86	116.69
2	G	501	6EL	CAQ-CAO-N	4.85	111.32	105.96
2	t	501	6EL	CAQ-CAO-N	4.81	111.27	105.96
2	n	501	6EL	CAQ-CAO-N	4.78	111.24	105.96
2	D	501	6EL	CG-CD-NE2	4.77	121.77	116.69
2	S	501	6EL	C-CA-N	4.73	113.30	109.08
2	P	501	6EL	OAC-CAN-N	-4.72	118.35	124.99
2	V	501	6EL	CAQ-CAO-N	4.71	111.17	105.96
2	J	501	6EL	CG-CD-NE2	4.70	121.69	116.69
2	Y	501	6EL	CAO-N-CAN	-4.70	106.21	111.55
2	k	501	6EL	CG-CD-NE2	4.67	121.66	116.69
2	A	501	6EL	CG-CD-NE2	4.66	121.65	116.69
2	Y	501	6EL	CG-CD-NE2	4.66	121.64	116.69
2	D	501	6EL	CAO-N-CAN	-4.65	106.27	111.55
2	q	501	6EL	CAQ-CAO-N	4.63	111.08	105.96
2	G	501	6EL	CG-CD-NE2	4.61	121.59	116.69
2	M	501	6EL	CG-CD-NE2	4.57	121.55	116.69
2	h	501	6EL	CG-CD-NE2	4.53	121.51	116.69
2	J	501	6EL	CAO-N-CAN	-4.52	106.41	111.55
2	S	501	6EL	CAO-N-CAN	-4.45	106.49	111.55
2	q	501	6EL	CG-CD-NE2	4.44	121.41	116.69
2	q	501	6EL	CAO-N-CAN	-4.42	106.53	111.55
2	b	501	6EL	CD-NE2-C	-4.42	120.86	126.69
2	h	501	6EL	CAO-N-CAN	-4.41	106.54	111.55
2	Y	501	6EL	CAQ-CAO-N	4.36	110.78	105.96
2	e	501	6EL	CAO-N-CAN	-4.35	106.61	111.55
2	e	501	6EL	CD-NE2-C	-4.35	120.96	126.69
2	S	501	6EL	CAQ-CAO-N	4.34	110.75	105.96
2	M	501	6EL	CAP-CAN-N	4.34	110.75	105.96
2	b	501	6EL	CAO-N-CAN	-4.33	106.64	111.55
2	k	501	6EL	CD-NE2-C	-4.29	121.03	126.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	501	6EL	CD-NE2-C	-4.28	121.05	126.69
2	t	501	6EL	CD-NE2-C	-4.27	121.07	126.69
2	k	501	6EL	CAQ-CAO-N	4.19	110.59	105.96
2	P	501	6EL	CD-NE2-C	-4.17	121.19	126.69
2	A	501	6EL	CAO-N-CAN	-4.13	106.86	111.55
2	n	501	6EL	CAO-N-CAN	-4.13	106.86	111.55
2	A	501	6EL	CAQ-CAO-N	4.09	110.48	105.96
2	n	501	6EL	CD-NE2-C	-4.04	121.37	126.69
2	G	501	6EL	CAO-N-CAN	-3.99	107.02	111.55
2	Y	501	6EL	CD-NE2-C	-3.95	121.49	126.69
2	G	501	6EL	CD-NE2-C	-3.94	121.50	126.69
2	S	501	6EL	CD-NE2-C	-3.82	121.65	126.69
2	D	501	6EL	CD-NE2-C	-3.82	121.65	126.69
2	M	501	6EL	CD-NE2-C	-3.81	121.67	126.69
2	e	501	6EL	CAP-CAN-N	3.79	110.15	105.96
2	V	501	6EL	CAO-N-CAN	-3.79	107.25	111.55
2	t	501	6EL	CAO-N-CAN	-3.78	107.25	111.55
2	b	501	6EL	CAQ-CAO-N	3.78	110.14	105.96
2	V	501	6EL	CD-NE2-C	-3.77	121.72	126.69
2	q	501	6EL	CD-NE2-C	-3.75	121.74	126.69
2	b	501	6EL	OAD-CAO-N	-3.75	119.72	124.99
2	A	501	6EL	CD-NE2-C	-3.71	121.80	126.69
2	h	501	6EL	CAP-CAN-N	3.70	110.05	105.96
2	P	501	6EL	OAC-CAN-CAP	-3.65	121.59	128.66
2	n	501	6EL	CAP-CAN-N	3.61	109.95	105.96
2	J	501	6EL	CD-NE2-C	-3.61	121.93	126.69
2	P	501	6EL	CAO-N-CAN	-3.61	107.45	111.55
2	P	501	6EL	CAQ-CAO-N	3.54	109.87	105.96
2	D	501	6EL	CAP-CAN-N	3.54	109.87	105.96
2	M	501	6EL	OAD-CAO-CAQ	-3.53	121.82	128.66
2	D	501	6EL	CAQ-CAP-CAN	-3.51	105.18	108.26
2	G	501	6EL	CAP-CAN-N	3.49	109.81	105.96
2	t	501	6EL	CAP-CAN-N	3.47	109.79	105.96
2	J	501	6EL	CAP-CAN-N	3.47	109.79	105.96
2	V	501	6EL	CAP-CAQ-CAO	-3.44	105.25	108.26
2	q	501	6EL	CAP-CAN-N	3.38	109.70	105.96
2	k	501	6EL	OAD-CAO-N	-3.38	120.24	124.99
2	h	501	6EL	CAP-CAQ-CAO	-3.36	105.31	108.26
2	A	501	6EL	CAP-CAQ-CAO	-3.35	105.32	108.26
2	P	501	6EL	CAP-CAN-N	3.35	109.66	105.96
2	V	501	6EL	OAC-CAN-CAP	-3.33	122.21	128.66
2	S	501	6EL	CAP-CAQ-CAO	-3.31	105.36	108.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	6EL	CA-N-CAN	3.31	133.56	123.91
2	A	501	6EL	C-CA-N	3.29	112.01	109.08
2	k	501	6EL	CAP-CAQ-CAO	-3.28	105.39	108.26
2	Y	501	6EL	CAP-CAQ-CAO	-3.27	105.40	108.26
2	q	501	6EL	CA-N-CAN	3.25	133.38	123.91
2	V	501	6EL	CA-N-CAN	3.21	133.27	123.91
2	D	501	6EL	C-CA-N	3.19	111.92	109.08
2	h	501	6EL	CA-N-CAN	3.19	133.20	123.91
2	G	501	6EL	CAP-CAQ-CAO	-3.18	105.47	108.26
2	e	501	6EL	CAP-CAQ-CAO	-3.18	105.47	108.26
2	n	501	6EL	CAP-CAQ-CAO	-3.18	105.48	108.26
2	b	501	6EL	CAP-CAQ-CAO	-3.17	105.48	108.26
2	M	501	6EL	CA-N-CAO	3.15	133.10	123.91
2	P	501	6EL	CAQ-CAP-CAN	-3.15	105.50	108.26
2	A	501	6EL	CAP-CAN-N	3.15	109.44	105.96
2	P	501	6EL	CAP-CAQ-CAO	-3.14	105.51	108.26
2	G	501	6EL	C-CA-N	3.14	111.88	109.08
2	M	501	6EL	CAQ-CAP-CAN	-3.14	105.51	108.26
2	q	501	6EL	CAP-CAQ-CAO	-3.13	105.52	108.26
2	Y	501	6EL	OAD-CAO-N	-3.10	120.64	124.99
2	Y	501	6EL	CA-N-CAN	3.09	132.91	123.91
2	n	501	6EL	CA-N-CAN	3.08	132.90	123.91
2	t	501	6EL	CAP-CAQ-CAO	-3.07	105.57	108.26
2	k	501	6EL	OAC-CAN-CAP	-3.06	122.73	128.66
2	Y	501	6EL	OAC-CAN-CAP	-3.06	122.73	128.66
2	V	501	6EL	OAD-CAO-N	-3.05	120.70	124.99
2	e	501	6EL	CA-N-CAN	3.05	132.80	123.91
2	J	501	6EL	CAP-CAQ-CAO	-3.04	105.59	108.26
2	D	501	6EL	OAC-CAN-CAP	-3.04	122.77	128.66
2	M	501	6EL	OAC-CAN-N	-3.03	120.74	124.99
2	b	501	6EL	CA-N-CAN	3.02	132.73	123.91
2	k	501	6EL	CA-N-CAN	3.00	132.65	123.91
2	b	501	6EL	CAQ-CAP-CAN	-2.98	105.65	108.26
2	P	501	6EL	CA-N-CAO	2.97	132.56	123.91
2	V	501	6EL	CAQ-CAP-CAN	-2.96	105.67	108.26
2	D	501	6EL	OAC-CAN-N	-2.95	120.83	124.99
2	n	501	6EL	CAQ-CAP-CAN	-2.95	105.67	108.26
2	S	501	6EL	CA-N-CAN	2.95	132.50	123.91
2	S	501	6EL	CAQ-CAP-CAN	-2.94	105.68	108.26
2	b	501	6EL	CAP-CAN-N	2.94	109.21	105.96
2	q	501	6EL	CAQ-CAP-CAN	-2.92	105.70	108.26
2	M	501	6EL	CAQ-CAO-N	2.90	109.17	105.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	6EL	CAP-CAQ-CAO	-2.89	105.73	108.26
2	M	501	6EL	CAP-CAQ-CAO	-2.89	105.73	108.26
2	S	501	6EL	OAD-CAO-N	-2.88	120.94	124.99
2	e	501	6EL	CAQ-CAP-CAN	-2.87	105.75	108.26
2	k	501	6EL	CAQ-CAP-CAN	-2.86	105.76	108.26
2	Y	501	6EL	CAQ-CAP-CAN	-2.84	105.77	108.26
2	J	501	6EL	CAQ-CAP-CAN	-2.83	105.78	108.26
2	k	501	6EL	CAP-CAN-N	2.82	109.08	105.96
2	D	501	6EL	OAD-CAO-CAQ	-2.80	123.24	128.66
2	h	501	6EL	CAQ-CAP-CAN	-2.80	105.81	108.26
2	V	501	6EL	CAP-CAN-N	2.78	109.03	105.96
2	Y	501	6EL	CAP-CAN-N	2.75	109.00	105.96
2	J	501	6EL	OAC-CAN-CAP	-2.74	123.34	128.66
2	n	501	6EL	OAD-CAO-CAQ	-2.74	123.35	128.66
2	b	501	6EL	OAD-CAO-CAQ	-2.73	123.37	128.66
2	G	501	6EL	CA-N-CAN	2.73	131.86	123.91
2	D	501	6EL	CA-N-CAO	2.72	131.85	123.91
2	S	501	6EL	CAP-CAN-N	2.72	108.97	105.96
2	J	501	6EL	CB-CA-N	2.71	119.63	113.60
2	A	501	6EL	CAQ-CAP-CAN	-2.69	105.90	108.26
2	A	501	6EL	CAG-CAP-CAN	2.69	134.10	129.59
2	A	501	6EL	CA-N-CAN	2.68	131.72	123.91
2	k	501	6EL	OAD-CAO-CAQ	-2.65	123.53	128.66
2	t	501	6EL	CA-N-CAN	2.63	131.59	123.91
2	e	501	6EL	CAG-CAP-CAN	2.63	134.01	129.59
2	k	501	6EL	CAG-CAP-CAN	2.63	134.00	129.59
2	q	501	6EL	OAD-CAO-N	-2.62	121.30	124.99
2	P	501	6EL	CAH-CAQ-CAO	2.61	133.97	129.59
2	D	501	6EL	CAQ-CAO-N	2.61	108.84	105.96
2	q	501	6EL	CAG-CAP-CAN	2.60	133.95	129.59
2	J	501	6EL	CAG-CAP-CAN	2.60	133.95	129.59
2	t	501	6EL	CAQ-CAP-CAN	-2.59	105.99	108.26
2	n	501	6EL	CAG-CAP-CAN	2.58	133.92	129.59
2	S	501	6EL	OAC-CAN-CAP	-2.58	123.66	128.66
2	h	501	6EL	CAG-CAP-CAN	2.58	133.91	129.59
2	M	501	6EL	OAC-CAN-CAP	-2.58	123.67	128.66
2	A	501	6EL	OAD-CAO-CAQ	-2.56	123.70	128.66
2	G	501	6EL	CAQ-CAP-CAN	-2.56	106.02	108.26
2	h	501	6EL	OAD-CAO-CAQ	-2.55	123.71	128.66
2	Y	501	6EL	CAG-CAP-CAN	2.52	133.81	129.59
2	n	501	6EL	OAC-CAN-CAP	-2.52	123.78	128.66
2	S	501	6EL	OAD-CAO-CAQ	-2.51	123.79	128.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	501	6EL	OAC-CAN-CAP	-2.51	123.79	128.66
2	e	501	6EL	OAC-CAN-CAP	-2.48	123.86	128.66
2	t	501	6EL	CAG-CAP-CAN	2.47	133.74	129.59
2	n	501	6EL	CB-CA-N	2.47	119.11	113.60
2	q	501	6EL	OAC-CAN-CAP	-2.45	123.91	128.66
2	h	501	6EL	OAD-CAO-N	-2.41	121.60	124.99
2	S	501	6EL	CAG-CAP-CAN	2.40	133.61	129.59
2	b	501	6EL	CAG-CAP-CAN	2.39	133.60	129.59
2	b	501	6EL	OAC-CAN-CAP	-2.39	124.03	128.66
2	t	501	6EL	C-CA-N	2.38	111.20	109.08
2	V	501	6EL	CB-CA-N	2.38	118.90	113.60
2	V	501	6EL	OAD-CAO-CAQ	-2.38	124.06	128.66
2	Y	501	6EL	OAD-CAO-CAQ	-2.35	124.11	128.66
2	G	501	6EL	CAG-CAP-CAN	2.33	133.50	129.59
2	M	501	6EL	CAH-CAQ-CAO	2.33	133.50	129.59
2	h	501	6EL	CB-CA-N	2.33	118.79	113.60
2	S	501	6EL	CB-CA-N	2.32	118.78	113.60
2	D	501	6EL	CAH-CAQ-CAO	2.30	133.44	129.59
2	M	501	6EL	CB-CA-N	2.28	118.68	113.60
2	V	501	6EL	CAG-CAP-CAN	2.23	133.32	129.59
2	A	501	6EL	OAC-CAN-CAP	-2.21	124.38	128.66
2	n	501	6EL	OAD-CAO-N	-2.19	121.90	124.99
2	e	501	6EL	OAD-CAO-N	-2.15	121.96	124.99
2	k	501	6EL	CB-CA-N	2.15	118.39	113.60
2	G	501	6EL	OAC-CAN-CAP	-2.15	124.50	128.66
2	q	501	6EL	OAD-CAO-CAQ	-2.14	124.52	128.66
2	t	501	6EL	OAC-CAN-CAP	-2.08	124.63	128.66
2	Y	501	6EL	CB-CA-N	2.06	118.19	113.60
2	A	501	6EL	OAD-CAO-N	-2.05	122.10	124.99
2	G	501	6EL	CG-CB-CA	-2.04	106.09	109.77
2	P	501	6EL	OAD-CAO-CAQ	-2.03	124.73	128.66

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	501	6EL	CB-CA-N-CAO
2	P	501	6EL	CB-CA-N-CAO
2	Y	501	6EL	CB-CA-N-CAN
2	k	501	6EL	CB-CA-N-CAN
2	t	501	6EL	CB-CA-N-CAN
2	A	501	6EL	CB-CA-N-CAO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	501	6EL	CB-CA-N-CAN
2	G	501	6EL	CB-CA-N-CAO
2	S	501	6EL	CB-CA-N-CAO
2	b	501	6EL	CB-CA-N-CAO
2	P	501	6EL	CB-CA-N-CAN
2	q	501	6EL	CB-CA-N-CAO
2	t	501	6EL	CB-CA-N-CAO
2	A	501	6EL	CB-CA-N-CAN
2	D	501	6EL	CB-CA-N-CAO
2	G	501	6EL	CB-CA-N-CAN
2	S	501	6EL	CB-CA-N-CAN
2	b	501	6EL	CB-CA-N-CAN
2	e	501	6EL	CB-CA-N-CAN
2	h	501	6EL	CB-CA-N-CAN
2	n	501	6EL	CB-CA-N-CAN
2	q	501	6EL	CB-CA-N-CAN
2	J	501	6EL	CB-CA-N-CAN

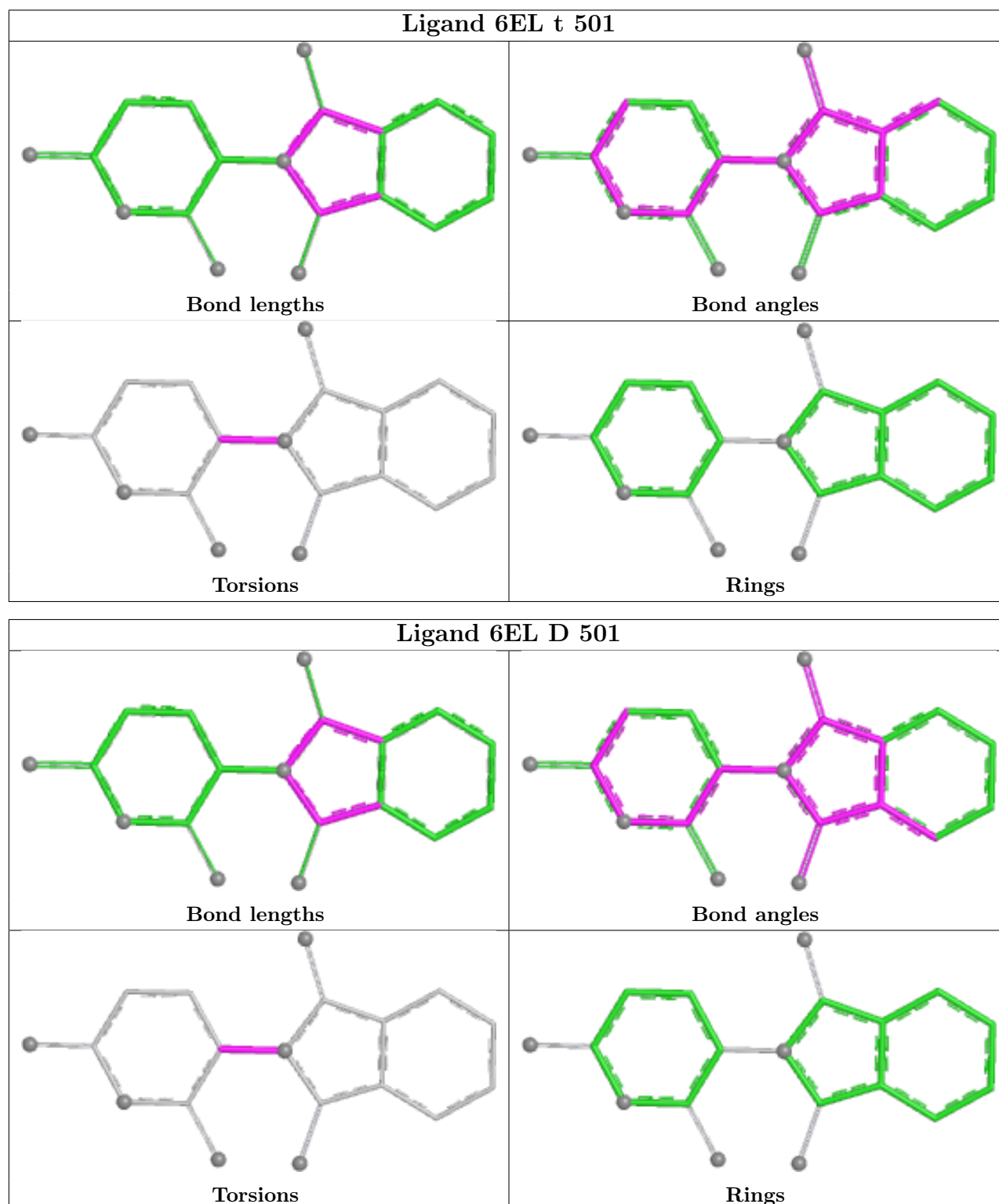
There are no ring outliers.

13 monomers are involved in 16 short contacts:

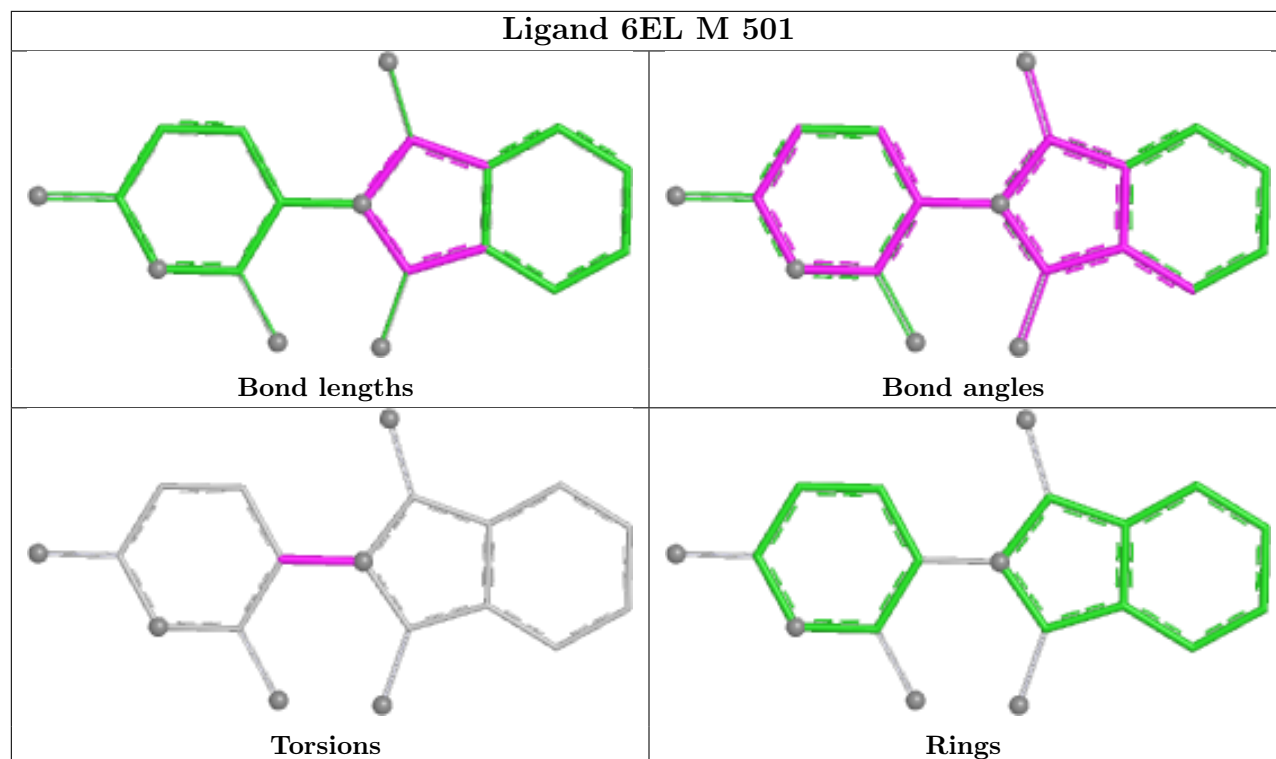
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	V	504	SO4	1	0
4	A	503	SO4	2	0
4	e	504	SO4	1	0
4	n	505	SO4	1	0
4	J	504	SO4	2	0
4	S	504	SO4	1	0
4	k	503	SO4	1	0
4	P	503	SO4	1	0
4	S	503	SO4	1	0
4	M	503	SO4	1	0
4	n	503	SO4	2	0
4	Y	504	SO4	1	0
2	q	501	6EL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

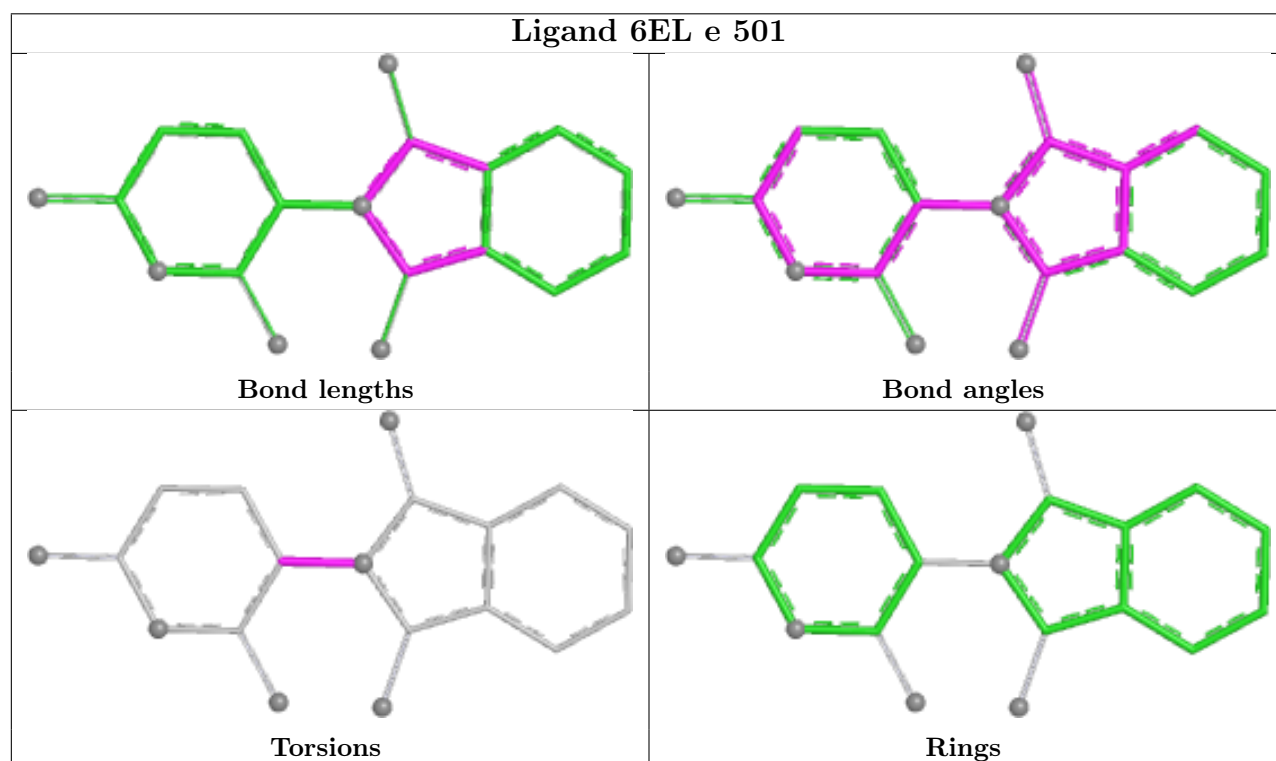
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



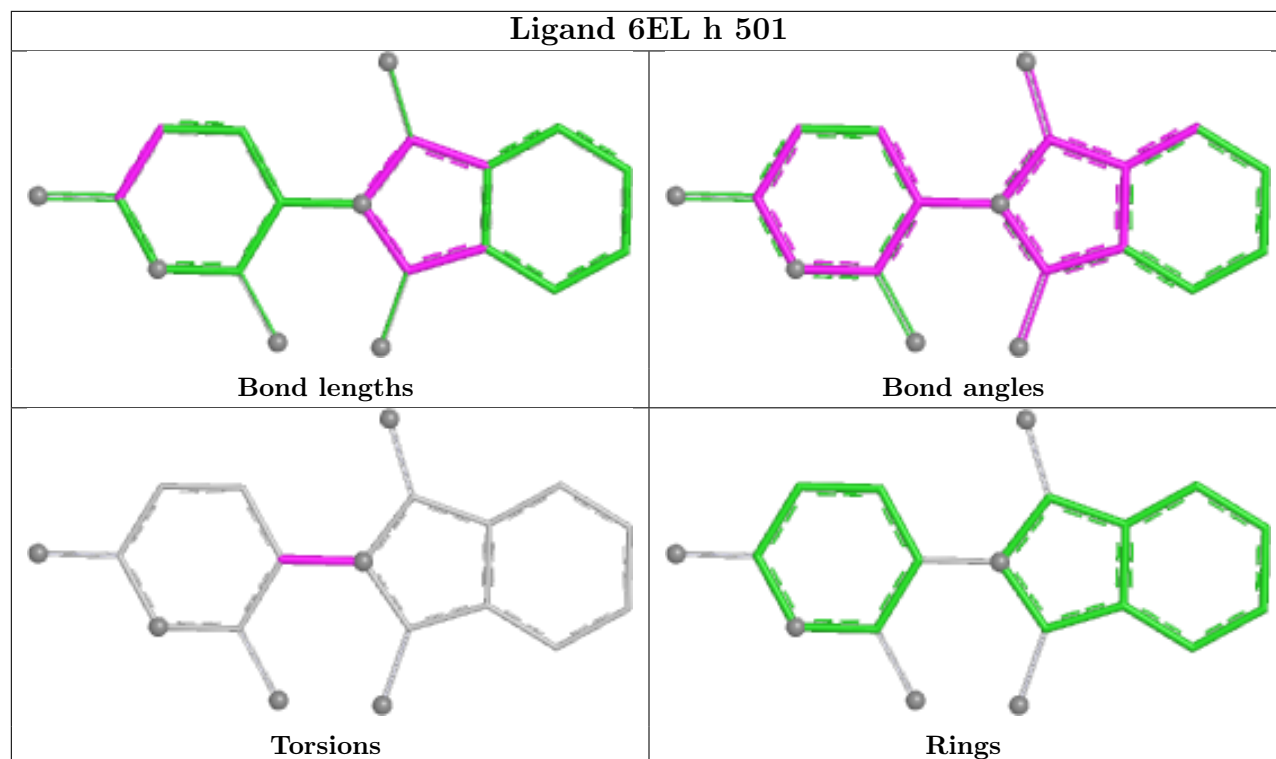
Ligand 6EL M 501



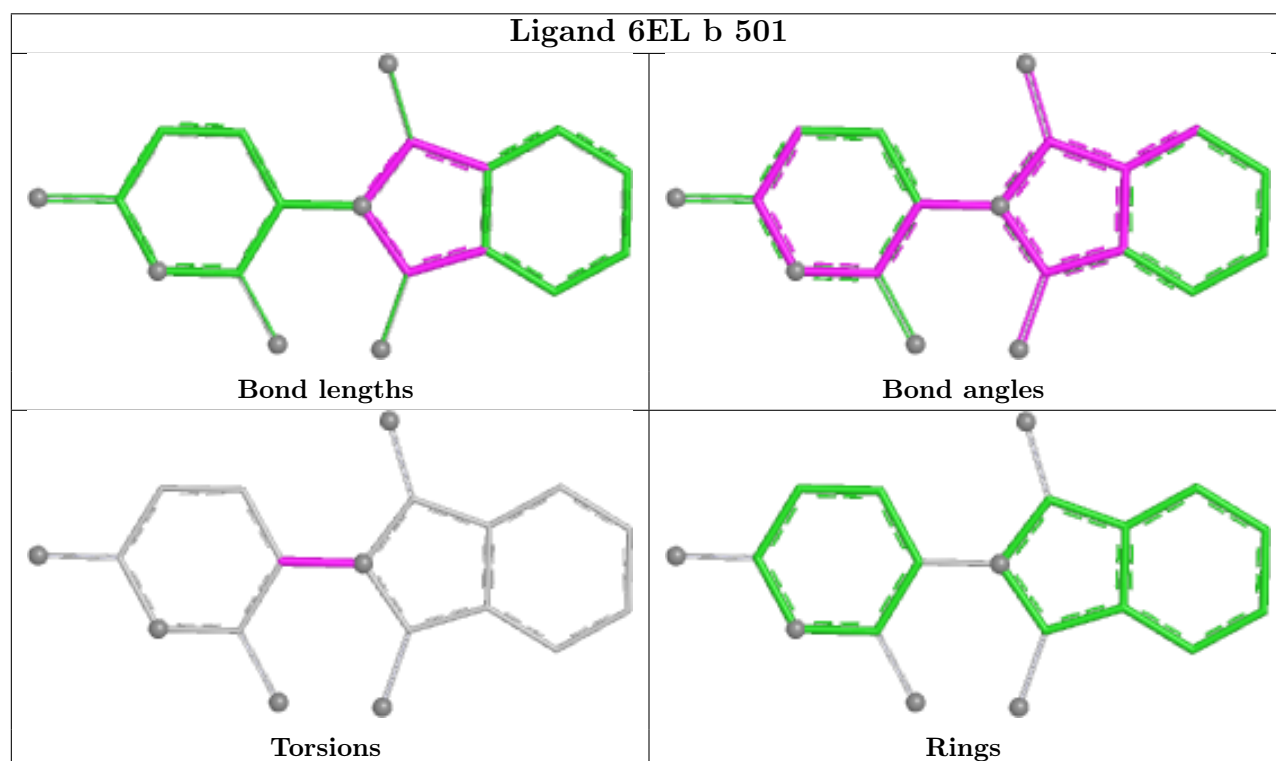
Ligand 6EL e 501



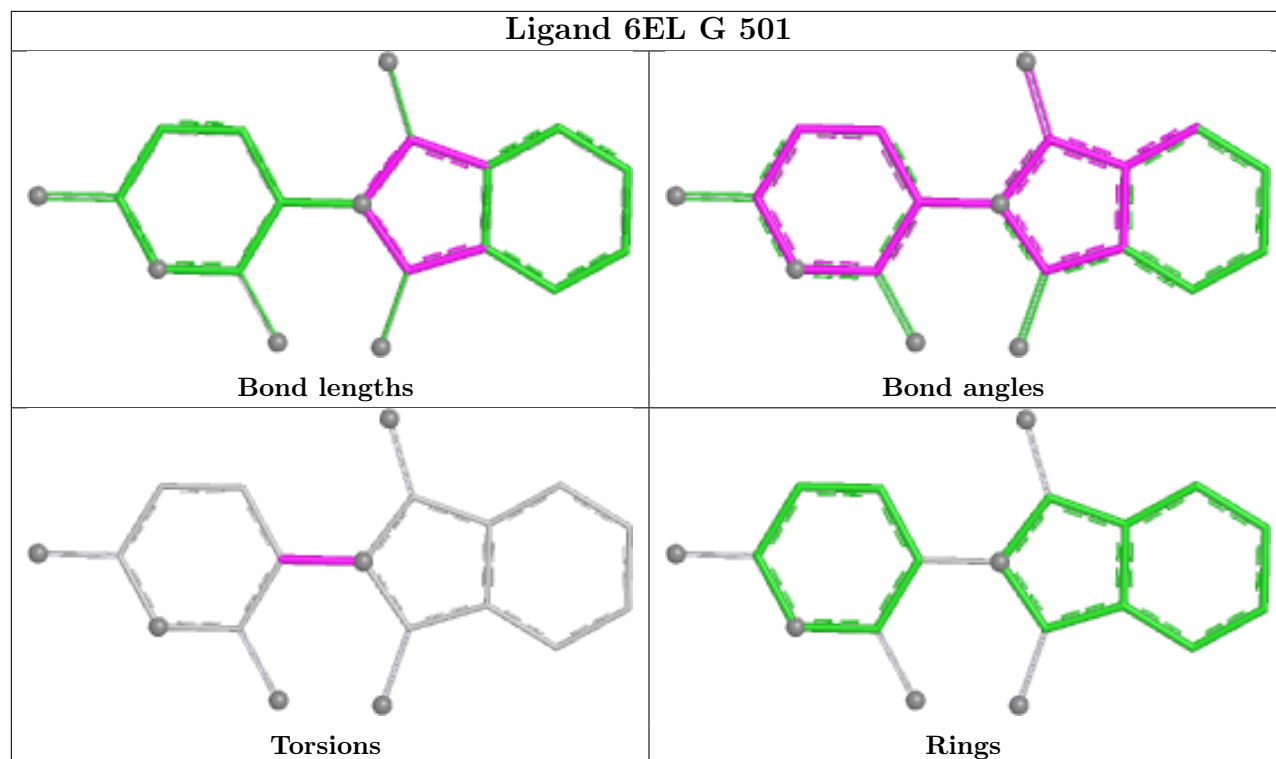
Ligand 6EL h 501



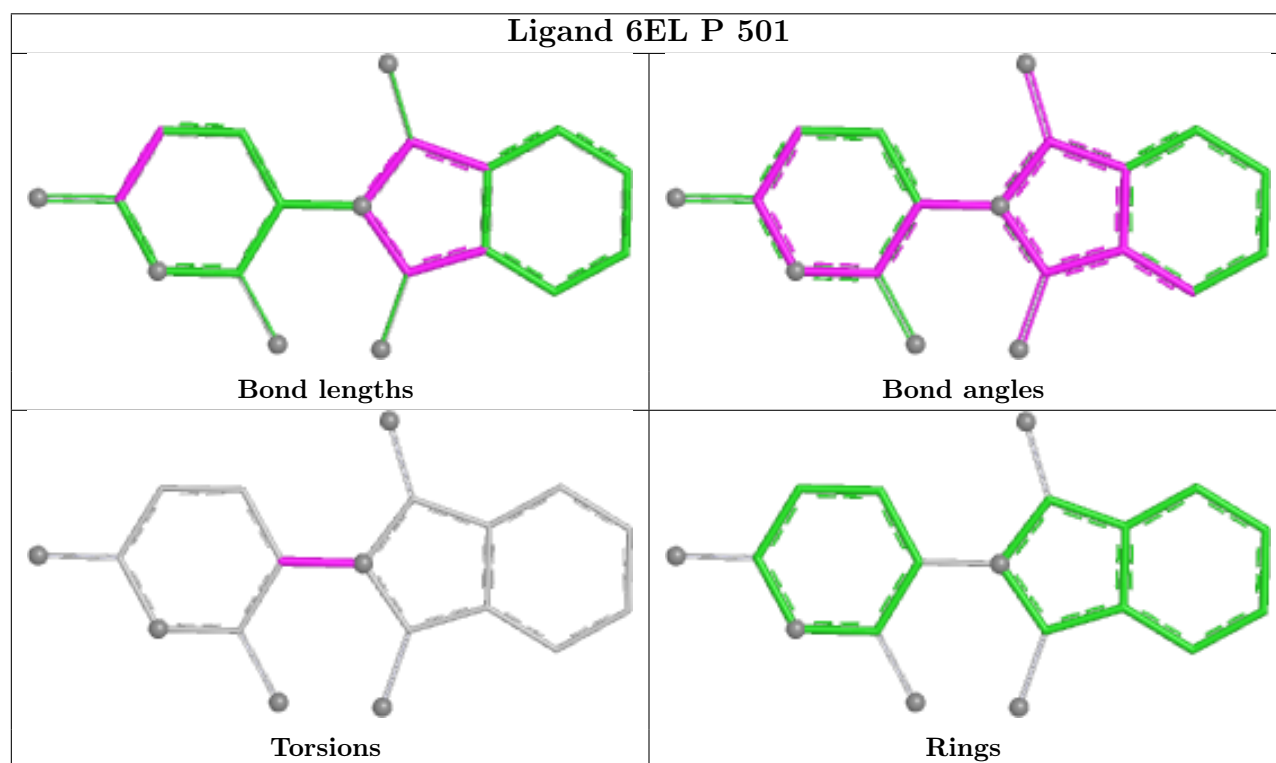
Ligand 6EL b 501



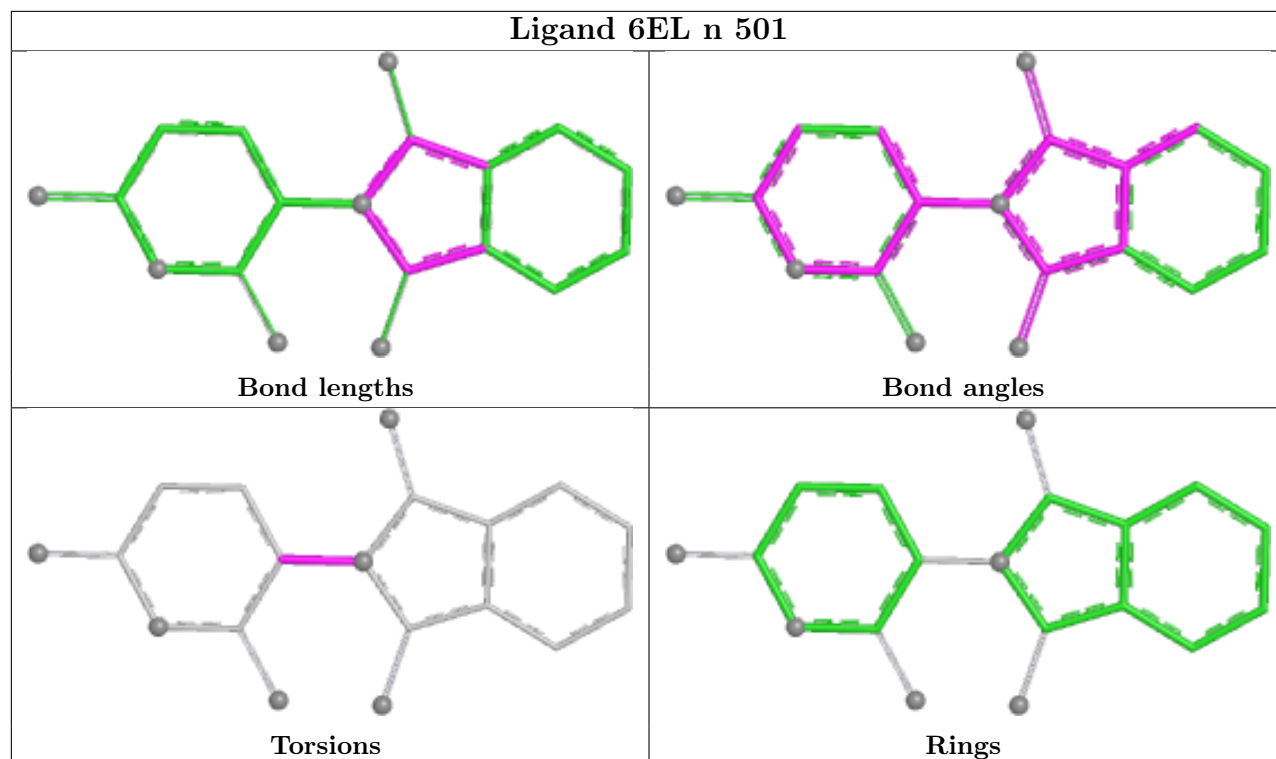
Ligand 6EL G 501



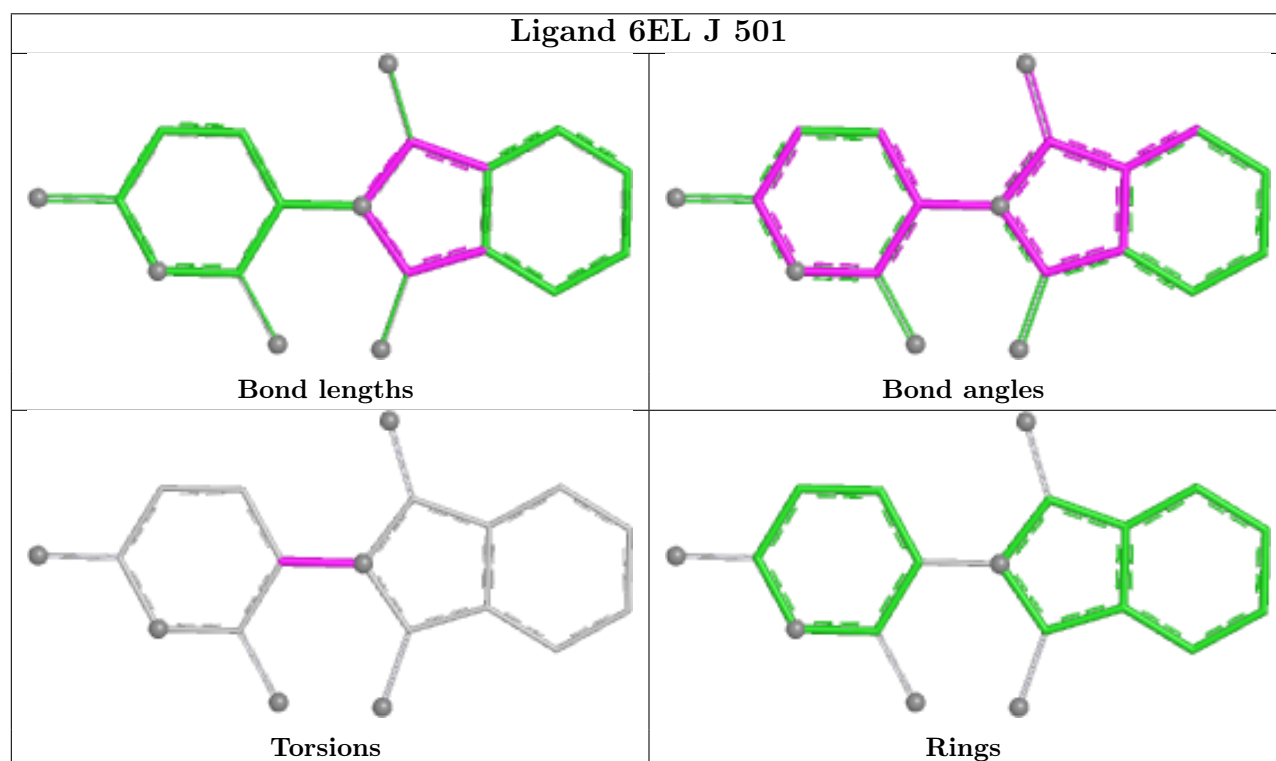
Ligand 6EL P 501



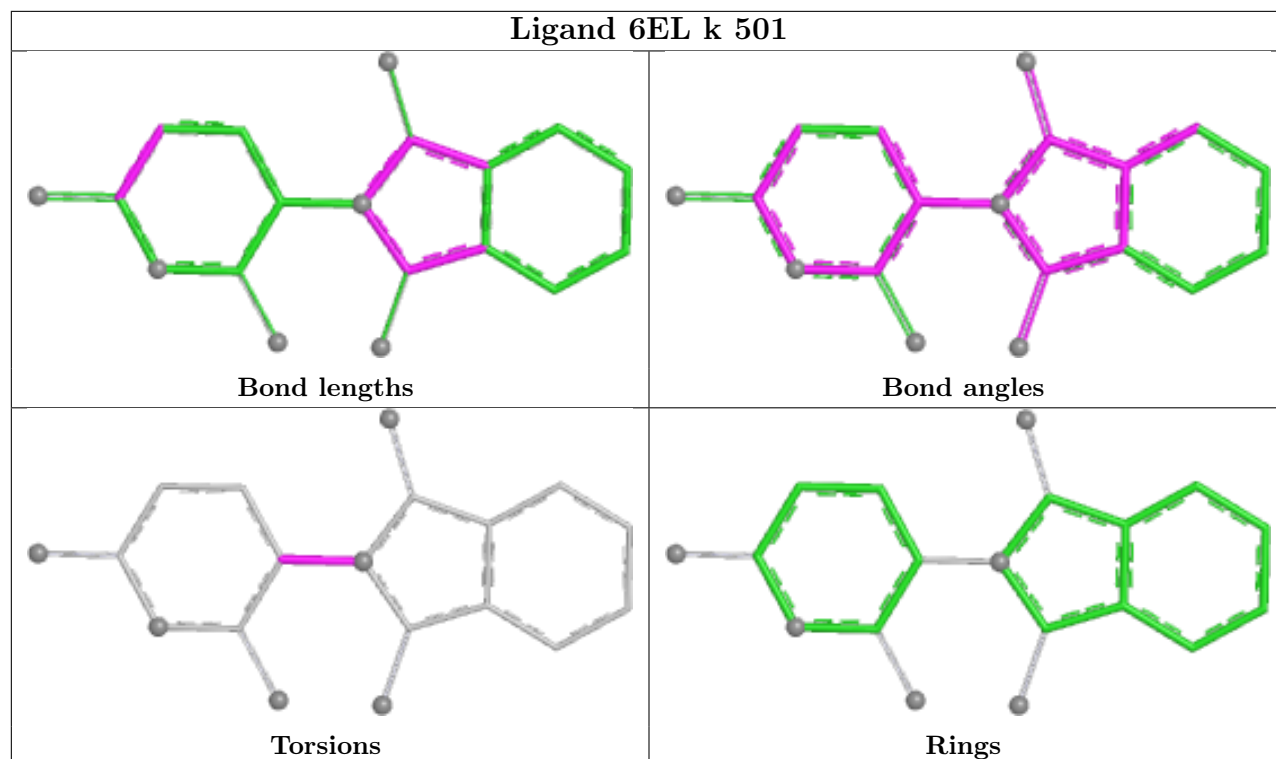
Ligand 6EL n 501



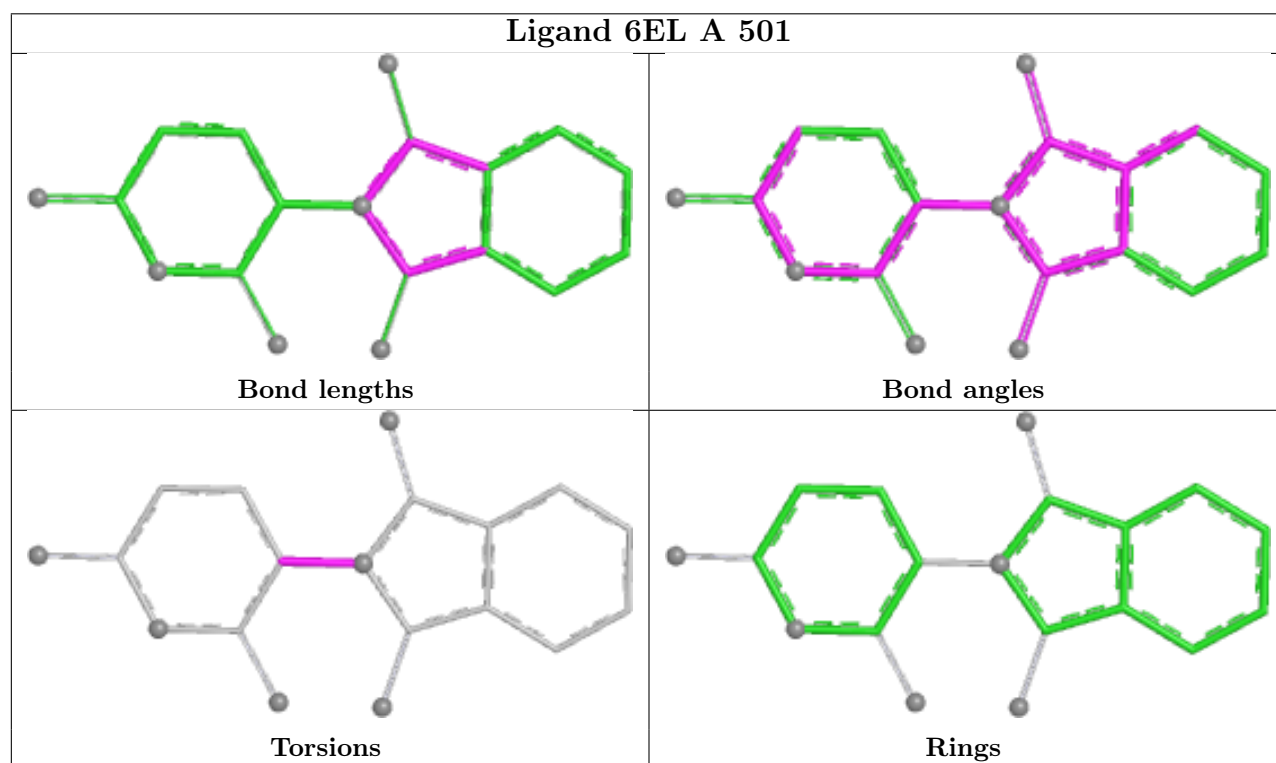
Ligand 6EL J 501



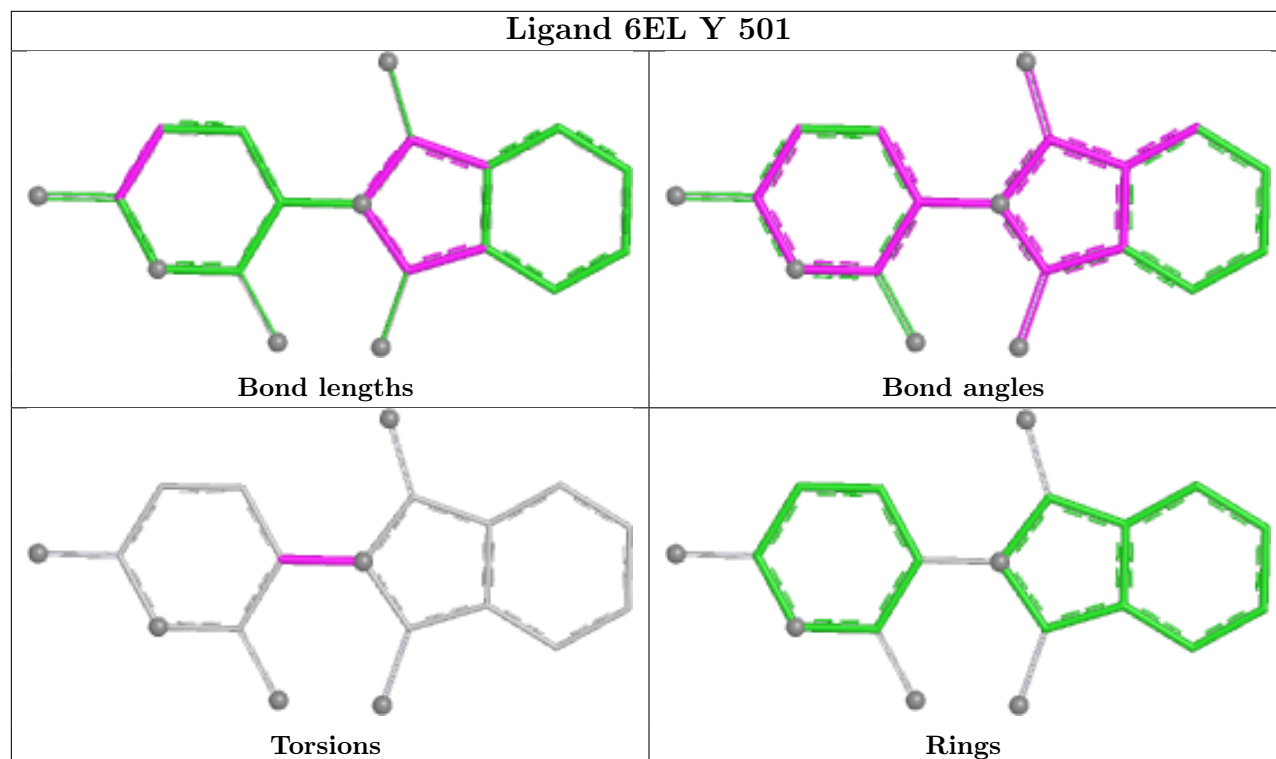
Ligand 6EL k 501



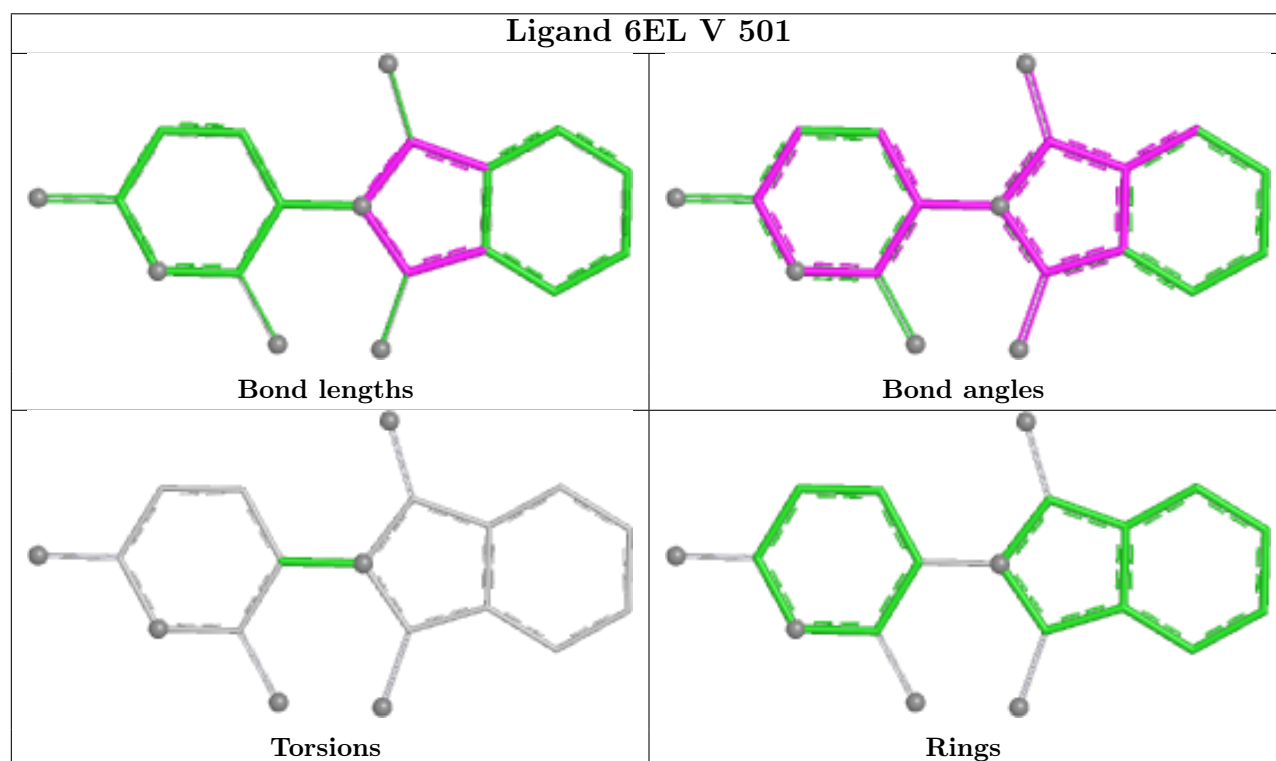
Ligand 6EL A 501

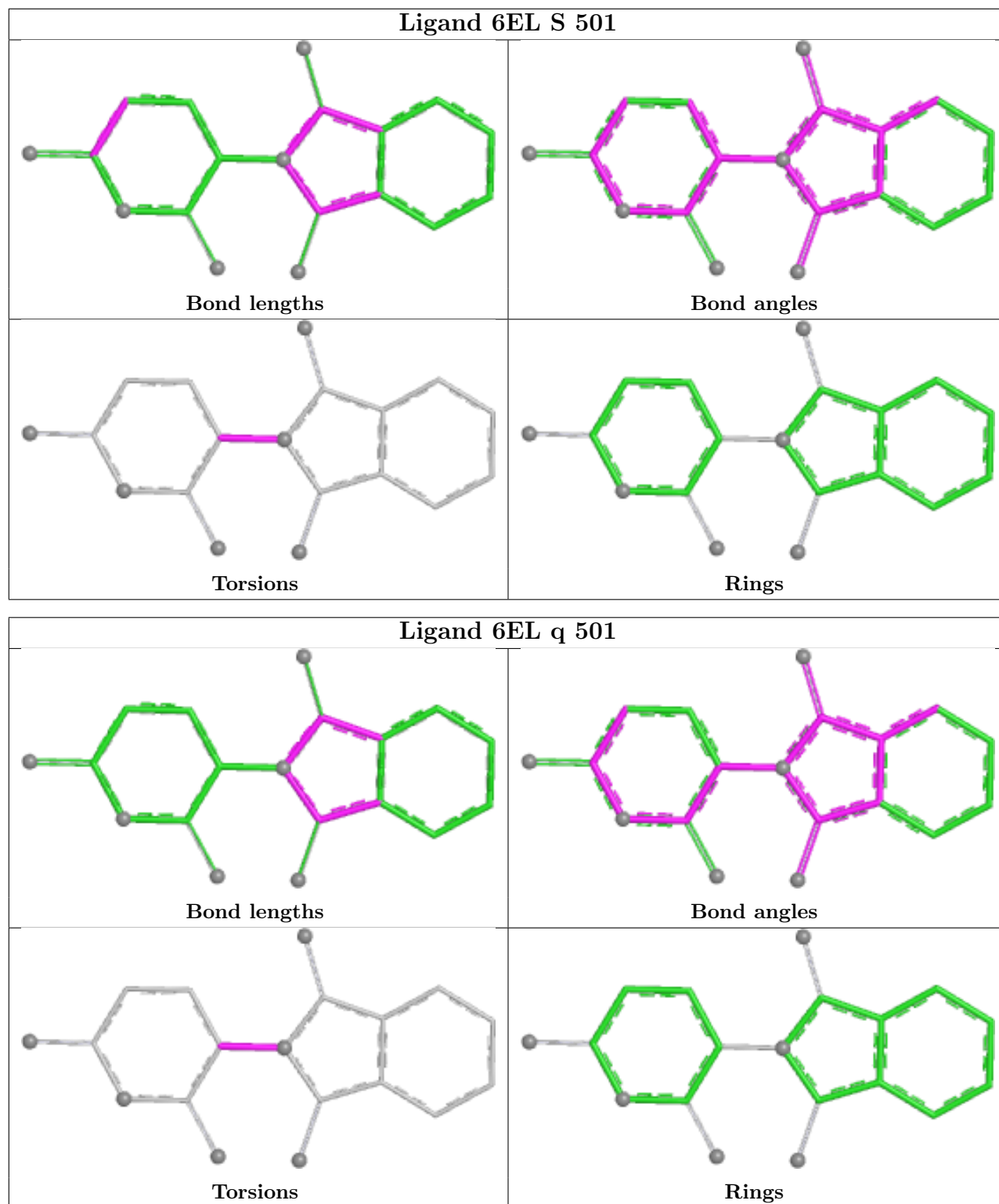


Ligand 6EL Y 501



Ligand 6EL V 501





5.7 Other polymers [i](#)

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	96/111 (86%)	-1.07	0 100 100	22, 34, 60, 71	0
1	D	96/111 (86%)	-1.12	0 100 100	21, 34, 61, 76	0
1	G	98/111 (88%)	-1.09	0 100 100	21, 34, 65, 80	0
1	J	91/111 (81%)	-1.35	0 100 100	18, 27, 42, 65	0
1	M	93/111 (83%)	-1.20	0 100 100	17, 30, 48, 62	0
1	P	93/111 (83%)	-1.31	0 100 100	17, 27, 47, 63	0
1	S	93/111 (83%)	-1.33	0 100 100	17, 28, 49, 61	0
1	V	93/111 (83%)	-1.31	0 100 100	17, 27, 45, 64	0
1	Y	93/111 (83%)	-1.18	0 100 100	18, 30, 49, 59	0
1	b	93/111 (83%)	-1.34	0 100 100	17, 28, 48, 65	0
1	e	93/111 (83%)	-1.18	0 100 100	18, 30, 50, 67	0
1	h	93/111 (83%)	-1.31	0 100 100	18, 27, 45, 66	0
1	k	94/111 (84%)	-1.18	0 100 100	18, 30, 53, 62	0
1	n	91/111 (81%)	-1.34	0 100 100	18, 26, 44, 64	0
1	q	93/111 (83%)	-1.37	0 100 100	17, 28, 48, 62	0
1	t	97/111 (87%)	-1.04	0 100 100	21, 34, 63, 75	0
All	All	1500/1776 (84%)	-1.23	0 100 100	17, 30, 54, 80	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	6EL	e	501	19/19	0.97	0.05	24,35,42,42	0
2	6EL	t	501	19/19	0.97	0.05	34,40,42,43	0
2	6EL	Y	501	19/19	0.98	0.04	26,34,44,45	0
2	6EL	b	501	19/19	0.98	0.04	28,36,41,41	0
2	6EL	D	501	19/19	0.98	0.04	34,39,42,44	0
2	6EL	h	501	19/19	0.98	0.04	30,36,39,39	0
2	6EL	k	501	19/19	0.98	0.04	24,34,42,43	0
2	6EL	M	501	19/19	0.98	0.04	26,34,43,44	0
4	SO4	J	504	5/5	0.98	0.04	65,68,70,71	0
4	SO4	M	505	5/5	0.98	0.04	65,72,75,79	0
4	SO4	S	504	5/5	0.98	0.04	64,67,68,72	0
4	SO4	e	504	5/5	0.98	0.04	65,69,74,76	0
2	6EL	S	501	19/19	0.99	0.03	25,37,41,41	0
2	6EL	n	501	19/19	0.99	0.03	26,34,38,39	0
2	6EL	q	501	19/19	0.99	0.03	26,34,37,38	0
2	6EL	V	501	19/19	0.99	0.03	25,35,40,40	0
3	ZN	A	502	1/1	0.99	0.06	46,46,46,46	0
3	ZN	D	502	1/1	0.99	0.04	45,45,45,45	0
3	ZN	G	502	1/1	0.99	0.08	46,46,46,46	0
3	ZN	M	502	1/1	0.99	0.07	39,39,39,39	0
3	ZN	e	502	1/1	0.99	0.05	38,38,38,38	0
3	ZN	k	502	1/1	0.99	0.04	38,38,38,38	0
3	ZN	q	502	1/1	0.99	0.08	37,37,37,37	0
3	ZN	t	502	1/1	0.99	0.06	47,47,47,47	0
4	SO4	D	503	5/5	0.99	0.03	37,38,43,44	0
2	6EL	G	501	19/19	0.99	0.04	33,38,42,43	0
2	6EL	J	501	19/19	0.99	0.03	27,34,37,39	0
4	SO4	S	503	5/5	0.99	0.03	32,32,42,42	0
2	6EL	A	501	19/19	0.99	0.04	32,41,46,46	0
4	SO4	V	504	5/5	0.99	0.03	64,66,71,73	0
4	SO4	Y	505	5/5	0.99	0.04	65,68,74,77	0
4	SO4	b	504	5/5	0.99	0.04	33,35,39,41	0

Continued on next page...

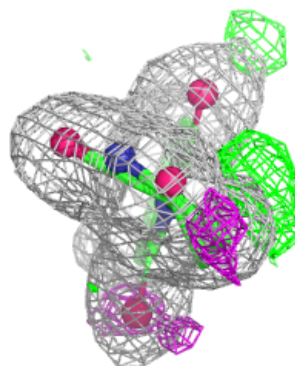
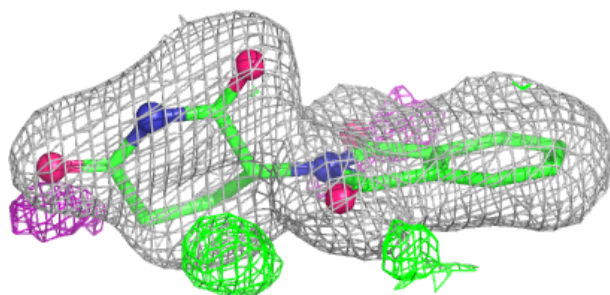
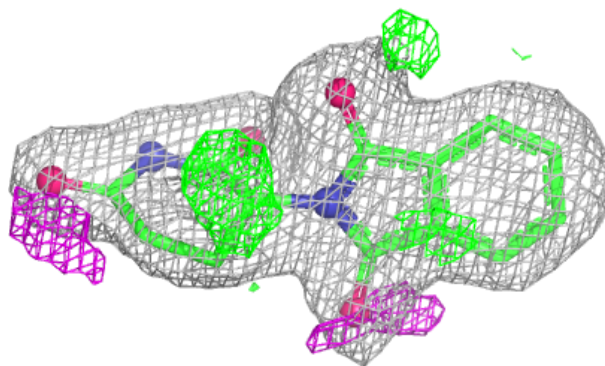
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	e	503	5/5	0.99	0.03	33,33,34,38	0
2	6EL	P	501	19/19	0.99	0.03	26,35,42,42	0
4	SO4	k	503	5/5	0.99	0.04	64,70,72,75	0
4	SO4	n	503	5/5	0.99	0.03	32,33,45,46	0
4	SO4	n	505	5/5	0.99	0.04	63,66,67,68	0
4	SO4	t	503	5/5	0.99	0.04	37,38,43,44	0
4	SO4	t	504	5/5	0.99	0.04	37,39,39,43	5
4	SO4	M	504	5/5	1.00	0.02	29,29,33,38	0
3	ZN	J	502	1/1	1.00	0.03	33,33,33,33	0
4	SO4	P	503	5/5	1.00	0.03	31,33,42,43	0
3	ZN	h	502	1/1	1.00	0.05	33,33,33,33	0
3	ZN	P	502	1/1	1.00	0.05	36,36,36,36	0
4	SO4	V	503	5/5	1.00	0.02	28,33,36,40	0
3	ZN	n	502	1/1	1.00	0.04	33,33,33,33	0
4	SO4	Y	503	5/5	1.00	0.02	31,32,36,40	0
4	SO4	Y	504	5/5	1.00	0.03	27,30,32,37	0
3	ZN	S	502	1/1	1.00	0.04	35,35,35,35	0
4	SO4	b	503	5/5	1.00	0.03	27,29,34,38	0
3	ZN	V	502	1/1	1.00	0.06	34,34,34,34	0
4	SO4	A	503	5/5	1.00	0.03	37,37,41,42	0
4	SO4	A	504	5/5	1.00	0.03	37,38,47,51	0
4	SO4	h	503	5/5	1.00	0.02	29,34,35,44	0
3	ZN	Y	502	1/1	1.00	0.06	38,38,38,38	0
4	SO4	k	504	5/5	1.00	0.03	30,31,34,36	0
4	SO4	D	504	5/5	1.00	0.02	37,37,45,45	0
4	SO4	n	504	5/5	1.00	0.03	28,34,38,41	0
4	SO4	J	503	5/5	1.00	0.03	28,30,36,41	0
4	SO4	q	503	5/5	1.00	0.03	26,32,32,37	0
3	ZN	b	502	1/1	1.00	0.06	37,37,37,37	0
4	SO4	M	503	5/5	1.00	0.03	28,30,35,40	0

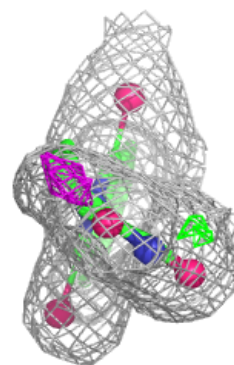
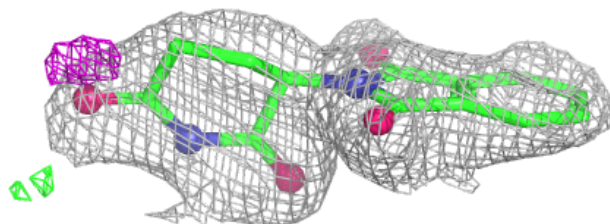
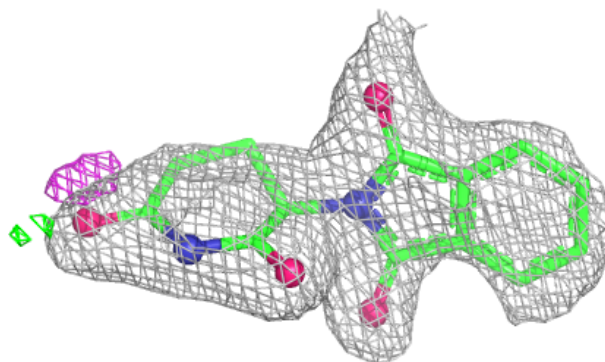
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6EL e 501:

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

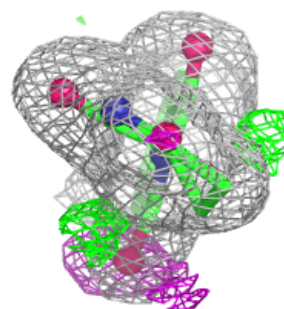
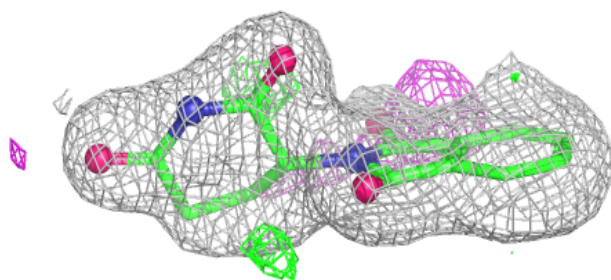
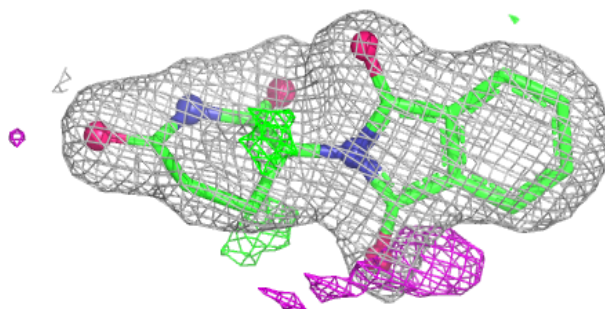
**Electron density around 6EL t 501:**

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

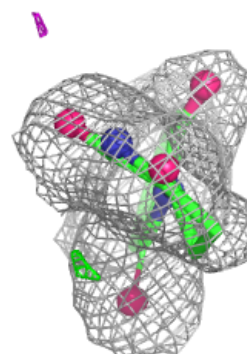
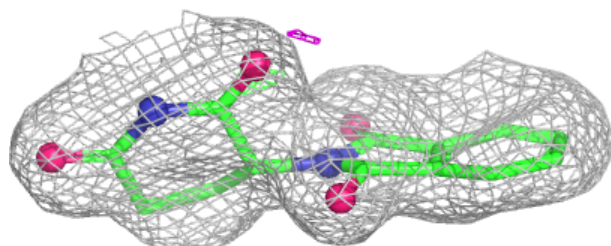
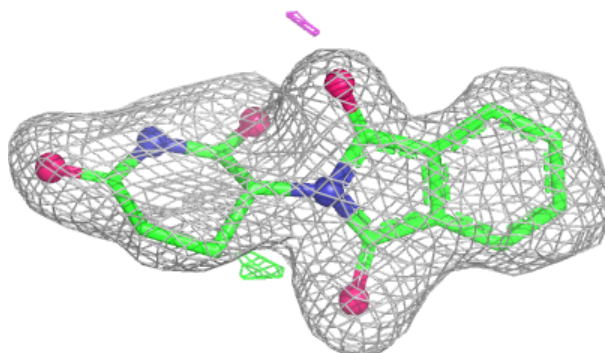


Electron density around 6EL Y 501:

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

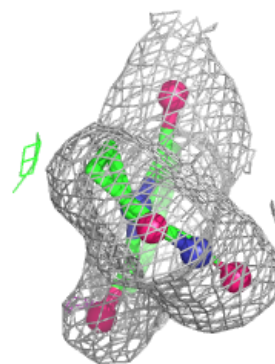
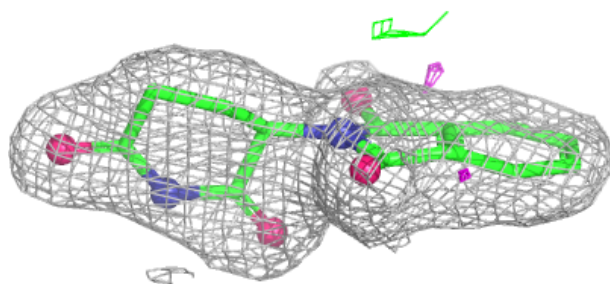
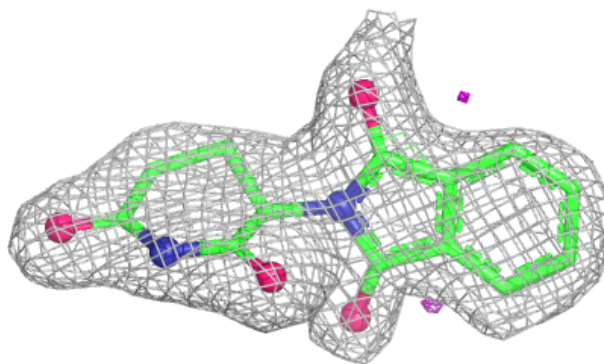
**Electron density around 6EL b 501:**

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

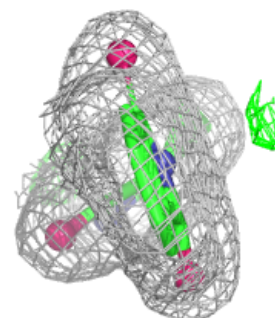
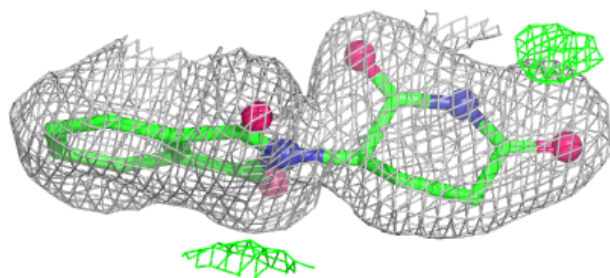
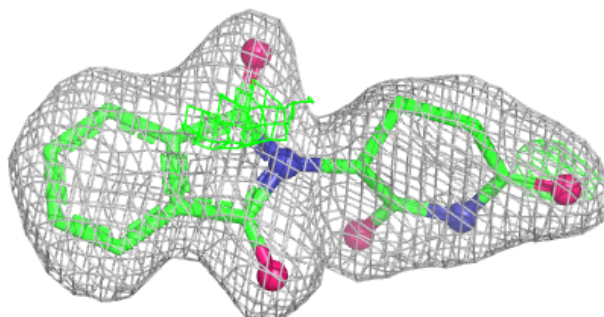


Electron density around 6EL D 501:

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

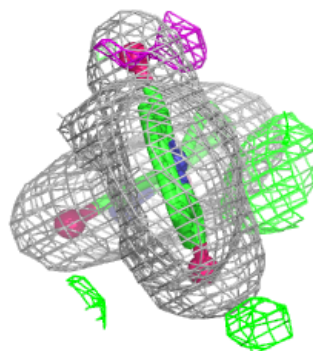
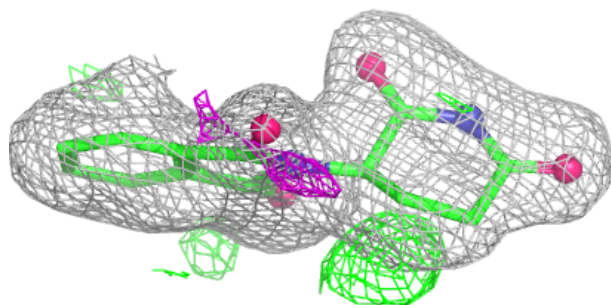
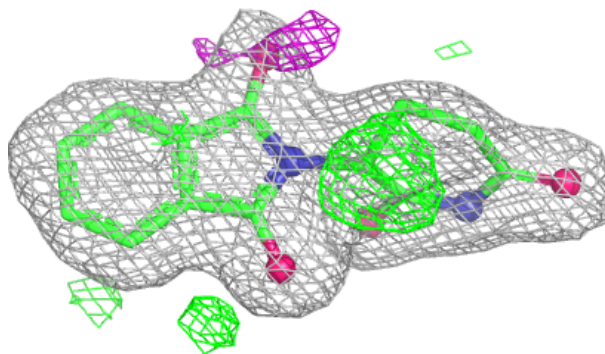
**Electron density around 6EL h 501:**

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

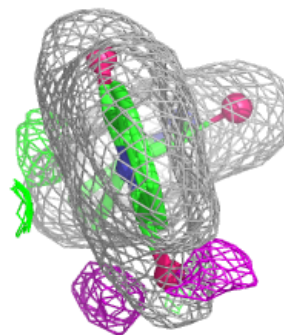
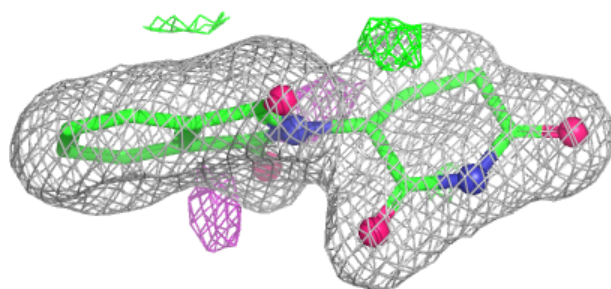
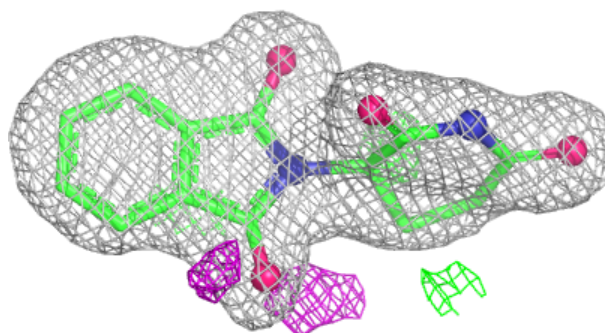


Electron density around 6EL k 501:

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

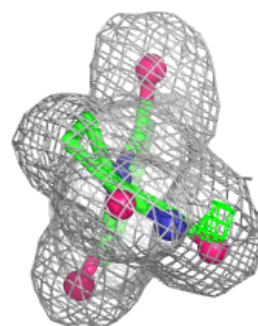
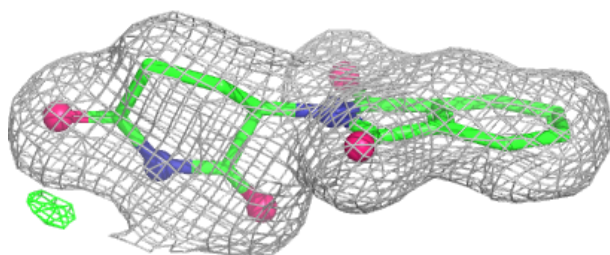
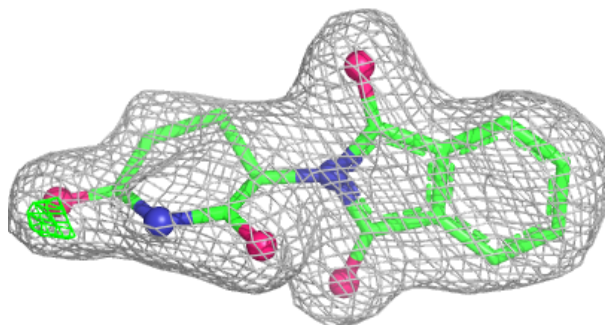
**Electron density around 6EL M 501:**

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

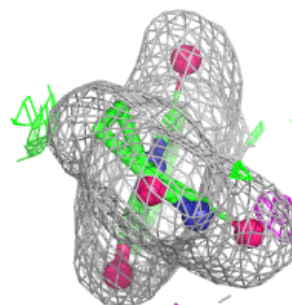
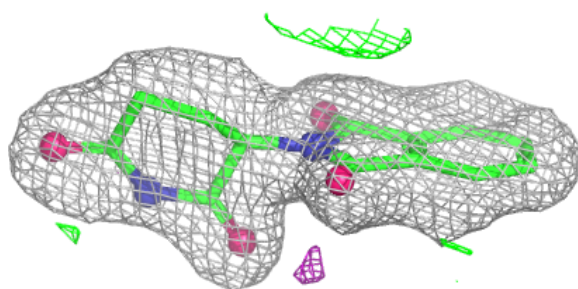
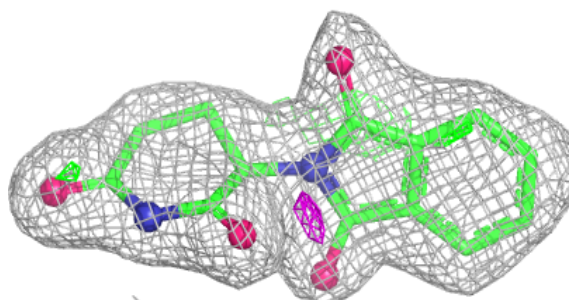


Electron density around 6EL S 501:

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

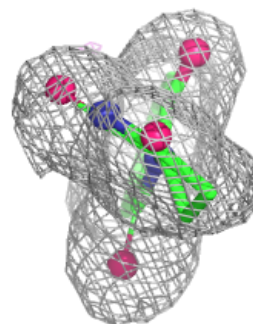
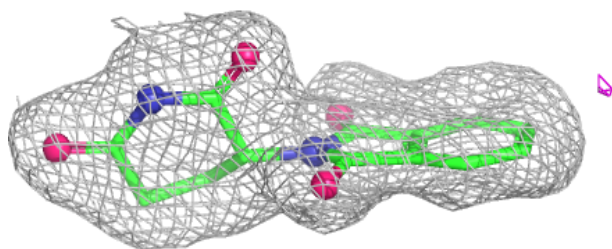
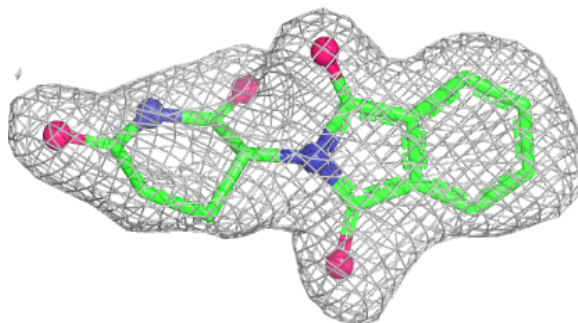
**Electron density around 6EL n 501:**

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

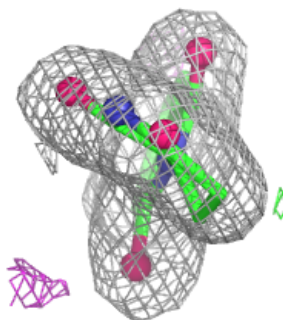
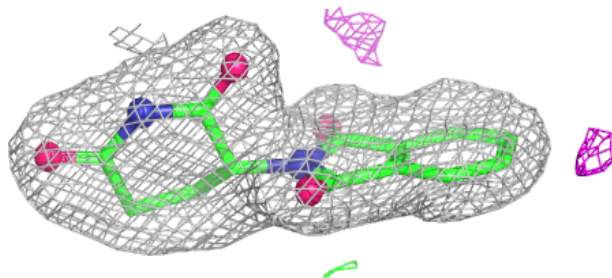
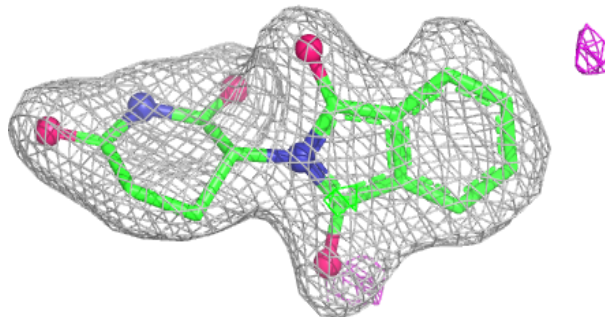


Electron density around 6EL q 501:

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

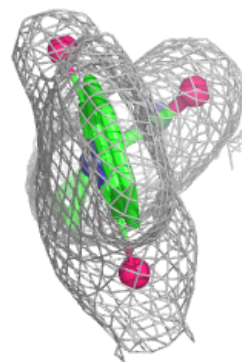
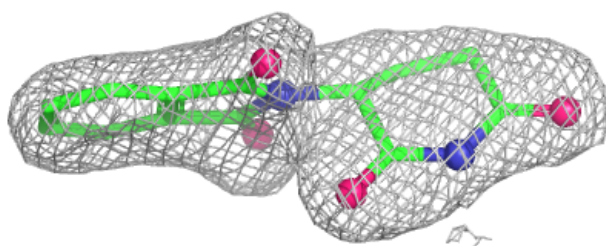
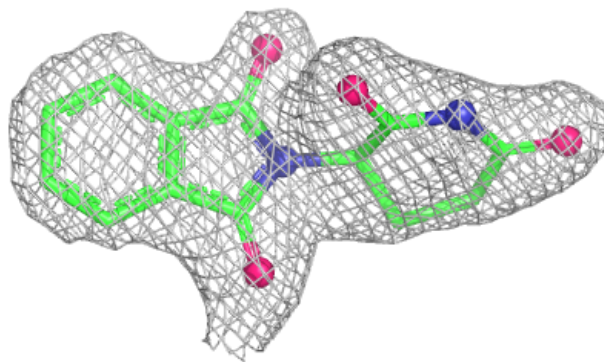
**Electron density around 6EL V 501:**

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

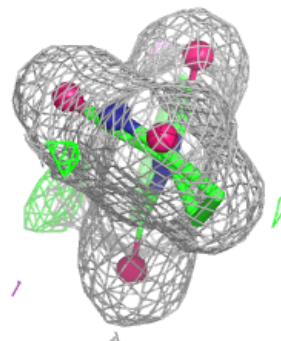
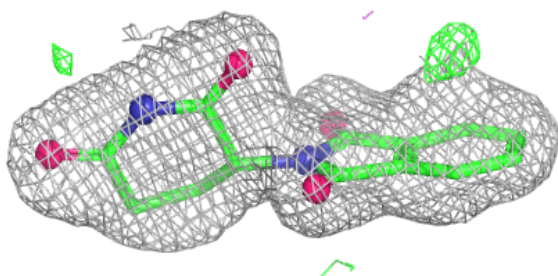
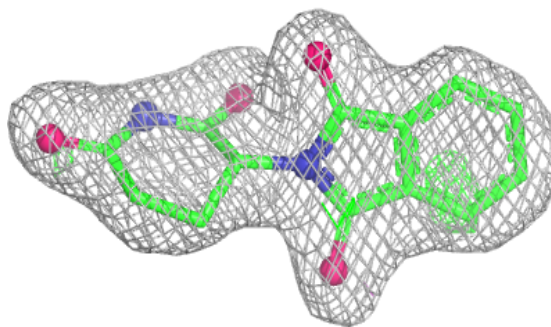


Electron density around 6EL G 501:

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

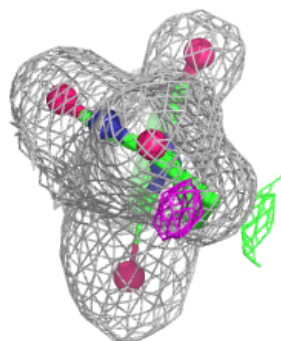
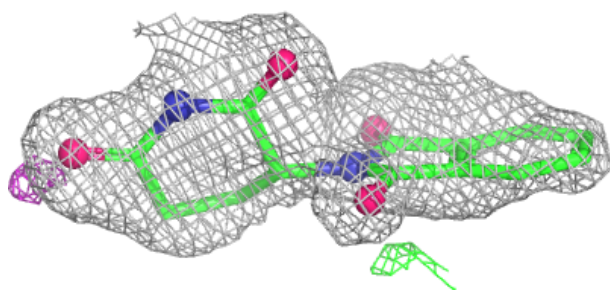
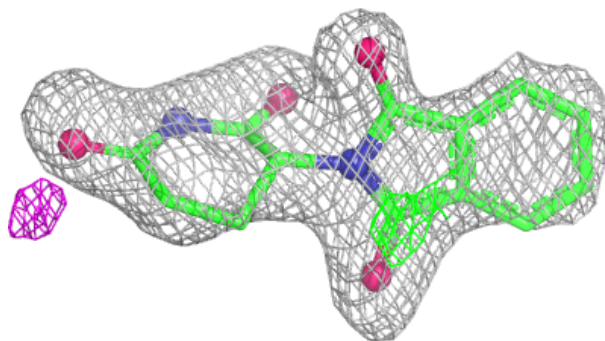
**Electron density around 6EL J 501:**

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

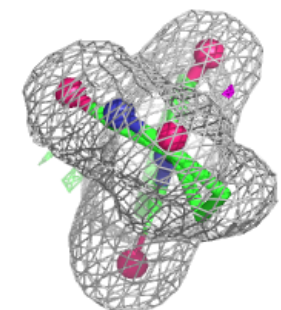
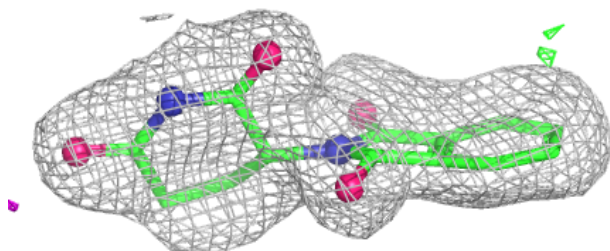
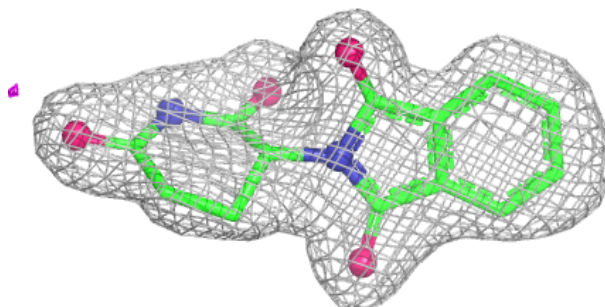


Electron density around 6EL A 501:

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

**Electron density around 6EL 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.