W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2023 – 01:54 am GMT

PDB ID	:	1OFI
Title	:	Asymmetric complex between HslV and I-domain deleted HslU (H. influenzae)
Authors	:	Kwon, A.R.; Kessler, B.M.; Overkleeft, H.S.; McKay, D.B.
Deposited on	:	2003-04-14
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

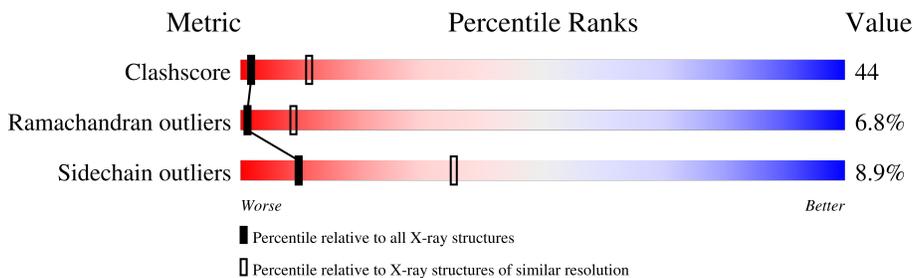|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	Percentile Ranks	Value
Clashscore		44
Ramachandran outliers		6.8%
Sidechain outliers		8.9%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	39% · 49% · 8% · ·
1	B	310	39% · 47% · 8% · 5%
1	C	310	37% · 49% · 10% · 5%
2	G	174	39% · 52% · 9% ·
2	H	174	36% · 54% · 10%
2	I	174	33% · 54% · 12% ·
2	L	174	37% · 54% · 9%
2	M	174	33% · 57% · 9% ·

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Mol	Chain	Length	Quality of chain
2	N	174	36% 55% 9%

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
5	PO4	B	452	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 15050 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.

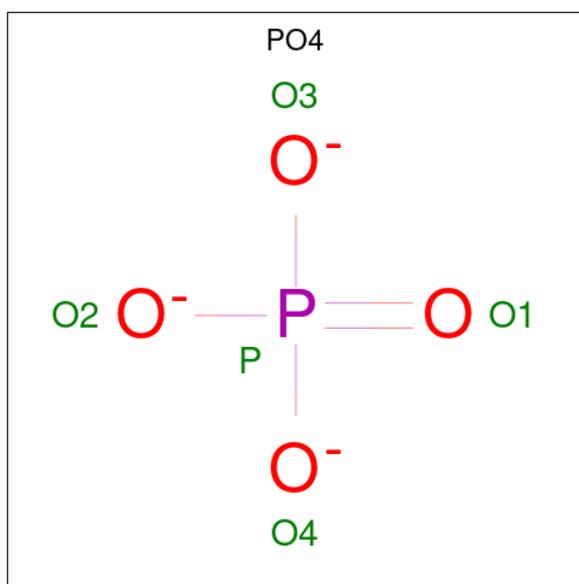- Molecule 1 is a protein called ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2312	1446	411	446	9			
1	B	295	Total	C	N	O	S	0	0	0
			2284	1430	407	438	9			
1	C	296	Total	C	N	O	S	0	0	0
			2288	1431	407	441	9			

- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	H	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	I	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	L	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	M	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	N	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	L	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		
4	N	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	P 1	0	0
5	B	1	Total 5	O 4	P 1	0	0
5	C	1	Total 5	O 4	P 1	0	0

- Molecule 6 is 4-IODO-3-NITROPHENYL ACETYL-LEUCINYL-LEUCINYL-LEUCINYL-VINYLSULFONE (three-letter code: LVS) (formula: $C_{28}H_{43}IN_4O_8S$).
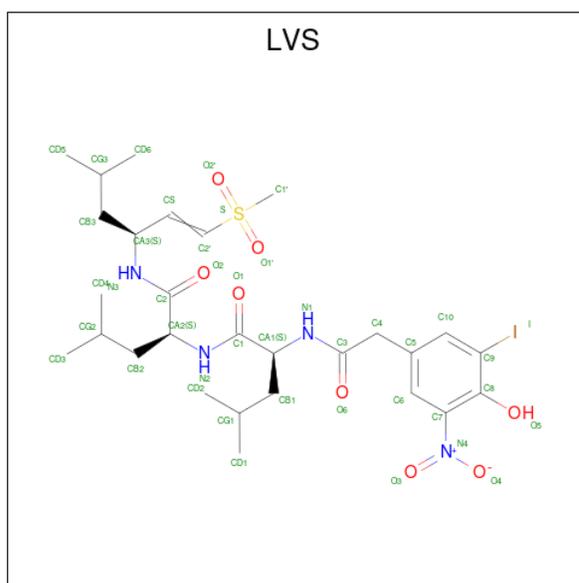
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	G	1	Total	C	N	O	S	0	0
			41	28	4	8	1		
6	H	1	Total	C	N	O	S	0	0
			41	28	4	8	1		
6	I	1	Total	C	N	O	S	0	0
			41	28	4	8	1		

• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total	O	0	0
			7	7		
7	B	7	Total	O	0	0
			7	7		
7	C	7	Total	O	0	0
			7	7		

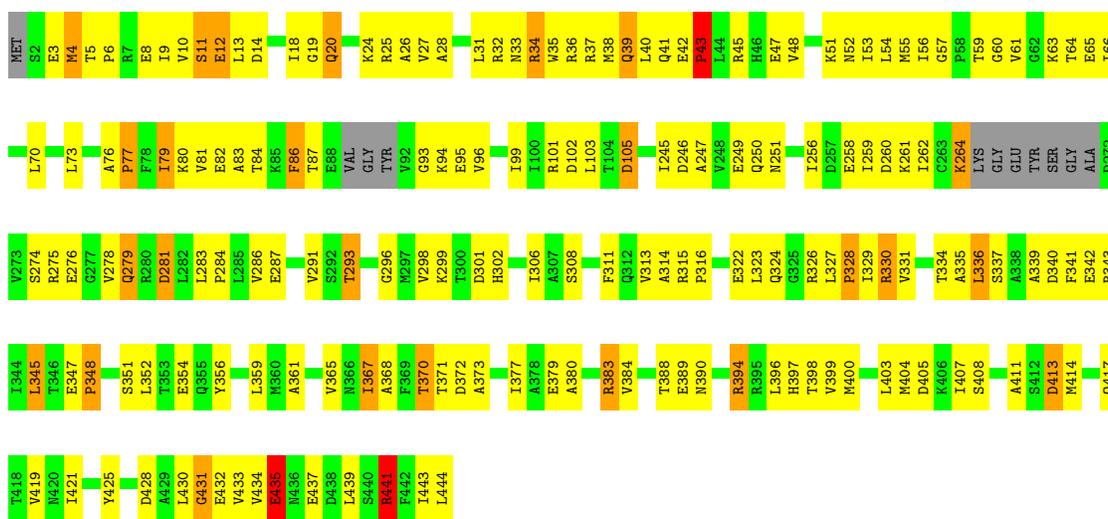# 3 Residue-property plots ⓘ

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. 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. 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.
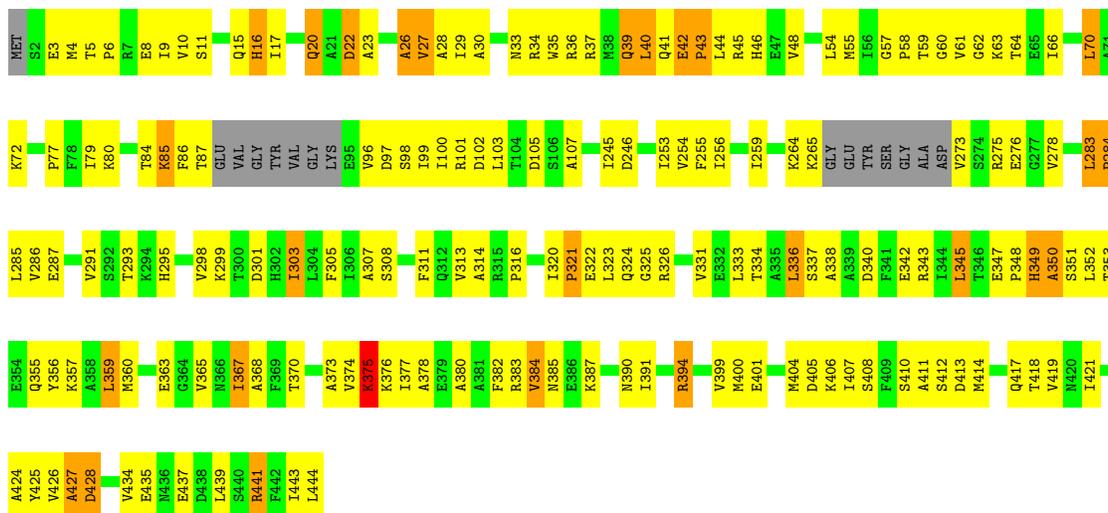
Note EDS was not executed.

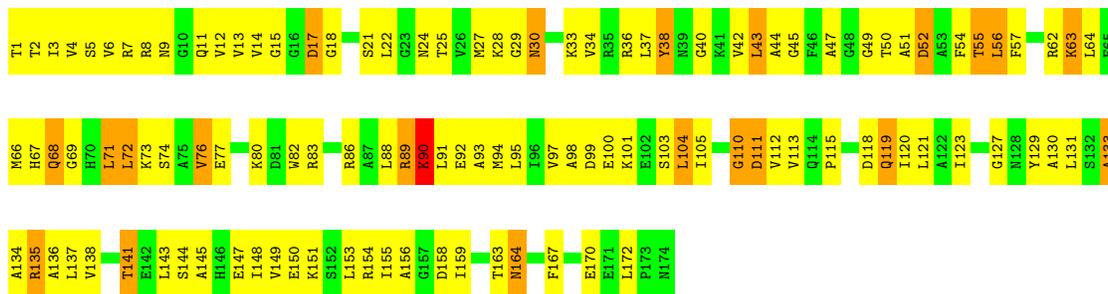• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain A:

• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain B:

• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU
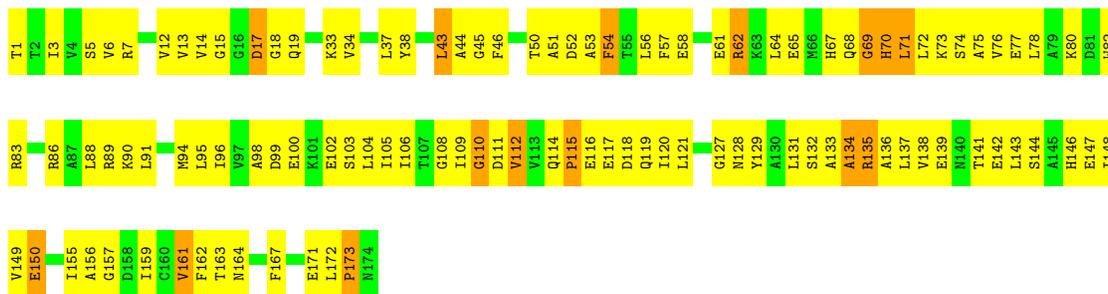
Chain C: 37%   49%   10%   5%
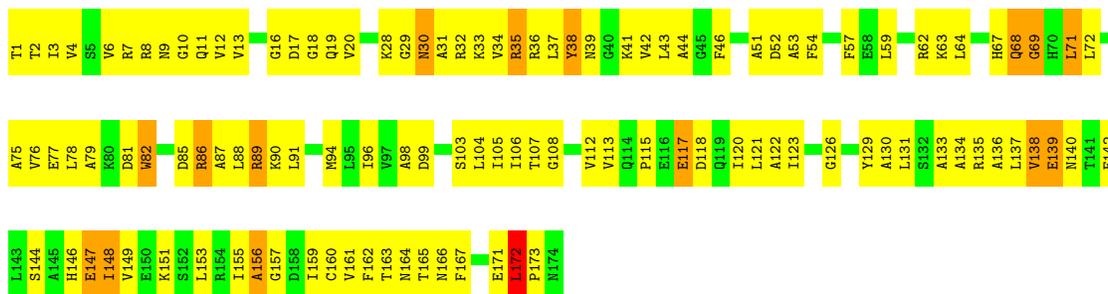

• Molecule 2: ATP-DEPENDENT PROTEASE HSLV
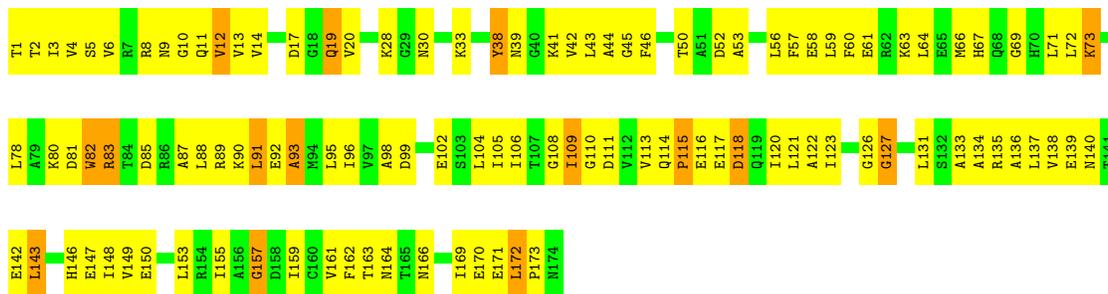
Chain G: 39%   52%   9%

• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain H: 36%   54%   10%

• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain I: 33%   54%   12%

T1 T2 I3 V4 S5 V6 R7 R8 N9 G10 Q11 V12 V13 V14 G15 G16 D17 G18 S21 L22 G23 N24 T25 V26 M27 K28 G29 N30 K33 V34 R35 R36 L37 Y38 N39 G40 K41 V42 L43 A44 G45 F46 A47 G48 Q49 T50 A51 D52 A53 F54 T55 L56 F57 R62 K63 L64 E65

M66 H67 Q68 G69 H70 L71 L72 K73 S74 A75 V76 E77 K80 D81 W82 R83 R86 A87 L88 R89 K90 L91 E92 A93 M94 L95 I96 V97 A98 D99 E100 K101 E102 S103 L104 I105 G110 D111 V112 V113 Q114 P115 D118 Q119 I120 L121 A122 I123 G127 N128 Y129 A130 L131 S132 A133

A134 R135 A136 L137 V138 T141 E142 L143 S144 A145 H146 E147 I148 V149 E150 K151 S152 L153 R154 A156 G157 D158 I159 T163 N164 F167 E170 E171 L172 P173 N174

● Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain L: ▰▰▰▰▰▰ 37% ▰▰▰▰▰▰▰▰▰▰▰ 54% ▰▰ 9%

T1 T2 I3 V4 S5 V6 R7 V12 V13 V14 G15 G16 D17 G18 Q19 K33 V34 L37 Y38 L43 A44 G45 F46 T50 A51 D52 A53 F54 T55 L56 F57 E58 E61 R62 K63 L64 E65 M66 H67 Q68 G69 H70 L71 L72 K73 S74 A75 V76 E77 L78 A79 K80 D81 W82

R83 R86 A87 L88 R89 K90 L91 M94 L95 I96 V97 A98 D99 E100 K101 E102 S103 L104 I105 I106 T107 G108 I109 G110 D111 V112 V113 Q114 P115 E116 E117 D118 Q119 I120 L121 G127 N128 Y129 A130 L131 S132 A133 A134 R135 L137 V138 E139 N140 T141 E142 L143 S144 A145 H146 E147 I148

V149 E150 I155 A156 G157 D158 I159 C160 V161 F162 T163 N164 F167 E171 L172 P173 N174

● Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain M: ▰▰▰▰▰ 33% ▰▰▰▰▰▰▰▰▰▰▰▰ 57% ▰▰ 9% ▪

T1 T2 I3 V4 S5 V6 R7 R8 N9 G10 Q11 V12 V13 G16 D17 G18 Q19 V20 K28 G29 N30 A31 R32 K33 V34 R35 R36 L37 Y38 N39 G40 K41 V42 L43 A44 G45 F46 A51 D52 A53 F54 F57 E58 L59 R62 K63 L64 H67 Q68 G69 H70 L71 L72

A75 V76 E77 L78 A79 K80 D81 W82 D85 R86 A87 L88 R89 K90 L91 M94 L95 I96 V97 A98 D99 S103 L104 I105 I106 T107 G108 V112 V113 Q114 P115 E116 E117 D118 Q119 I120 L121 A122 I123 G126 Y129 A130 L131 S132 A133 A134 R135 A136 L137 V138 E139 N140 T141 E142

L143 S144 A145 H146 E147 I148 V149 E150 K151 S152 L153 R154 I155 A156 G157 D158 I159 C160 V161 F162 T163 N164 T165 N166 F167 E171 L172 P173 N174

● Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain N: ▰▰▰▰▰▰ 36% ▰▰▰▰▰▰▰▰▰▰▰ 55% ▰▰ 9%

T1 T2 I3 V4 S5 V6 R7 R8 N9 G10 Q11 V12 V13 V14 D17 G18 Q19 V20 K28 G29 N30 K33 Y38 N39 G40 K41 V42 L43 A44 G45 F46 T50 A51 D52 A53 L56 F57 E58 L59 F60 E61 R62 K63 L64 E65 M66 H67 Q68 G69 H70 L71 L72 K73

L78 A79 K80 D81 W82 R83 T84 D85 R86 A87 L88 R89 K90 L91 E92 A93 M94 L95 I96 V97 A98 D99 E102 S103 L104 I105 I106 T107 G108 I109 G110 D111 V112 V113 Q114 P115 E116 E117 D118 Q119 I120 L121 A122 I123 G126 G127 L131 S132 A133 A134 R135 A136 L137 V138 E139 N140 T141

E142 L143 H146 E147 I148 V149 E150 L153 R154 I155 A156 G157 D158 I159 C160 V161 F162 T163 N164 T165 N166 I169 E170 E171 L172 P173 N174

4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α, β, γ	190.18Å 190.18Å 114.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20	Depositor
% Data completeness (in resolution range)	96.7 (50.00-3.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15050	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LVS, PO4, ADP, MG

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	0.44	0/2339	0.71	0/3156
1	B	0.44	0/2311	0.70	0/3118
1	C	0.41	0/2315	0.69	1/3125 (0.0%)
2	G	0.38	0/1333	0.63	0/1798
2	H	0.38	0/1333	0.61	0/1798
2	I	0.36	0/1333	0.62	0/1798
2	L	0.34	0/1333	0.60	0/1798
2	M	0.33	0/1333	0.58	0/1798
2	N	0.34	0/1333	0.60	0/1798
All	All	0.39	0/14963	0.65	1/20187 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	345	LEU	CA-CB-CG	6.12	129.39	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2312	0	2358	190	0
1	B	2284	0	2336	182	0
1	C	2288	0	2332	187	0
2	G	1319	0	1347	135	0
2	H	1319	0	1347	151	0
2	I	1319	0	1347	144	0
2	L	1319	0	1348	116	0
2	M	1319	0	1348	140	0
2	N	1319	0	1348	127	0
3	A	27	0	12	4	0
3	B	27	0	12	6	0
3	C	27	0	12	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	2	0
5	C	5	0	0	1	0
6	G	41	0	38	9	0
6	H	41	0	38	5	0
6	I	41	0	38	5	0
7	A	7	0	0	0	0
7	B	7	0	0	0	0
7	C	7	0	0	0	0
All	All	15050	0	15261	1331	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 44.

The worst 5 of 1331 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:GLU:HG3	1:C:4:MET:H	1.10	1.14
1:B:441:ARG:HH11	1:B:441:ARG:HB3	1.07	1.09
1:C:406:LYS:H	1:C:406:LYS:HD2	1.15	1.04
2:N:105:ILE:HG13	2:N:121:LEU:HD13	1.40	1.03
1:A:441:ARG:HH11	1:A:441:ARG:HB3	1.21	1.03

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	293/310 (94%)	229 (78%)	50 (17%)	14 (5%)	2	17
1	B	289/310 (93%)	217 (75%)	54 (19%)	18 (6%)	1	11
1	C	290/310 (94%)	219 (76%)	53 (18%)	18 (6%)	1	11
2	G	172/174 (99%)	128 (74%)	33 (19%)	11 (6%)	1	10
2	H	172/174 (99%)	131 (76%)	31 (18%)	10 (6%)	1	13
2	I	172/174 (99%)	128 (74%)	31 (18%)	13 (8%)	1	7
2	L	172/174 (99%)	122 (71%)	35 (20%)	15 (9%)	1	4
2	M	172/174 (99%)	109 (63%)	49 (28%)	14 (8%)	1	5
2	N	172/174 (99%)	121 (70%)	35 (20%)	16 (9%)	0	3
All	All	1904/1974 (96%)	1404 (74%)	371 (20%)	129 (7%)	1	9

5 of 129 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	VAL
1	A	435	GLU
1	B	42	GLU
1	B	85	LYS
1	C	47	GLU

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	249/256 (97%)	216 (87%)	33 (13%)	4	18
1	B	246/256 (96%)	224 (91%)	22 (9%)	9	35
1	C	246/256 (96%)	220 (89%)	26 (11%)	6	27
2	G	139/140 (99%)	130 (94%)	9 (6%)	17	51
2	H	139/140 (99%)	128 (92%)	11 (8%)	12	43
2	I	139/140 (99%)	122 (88%)	17 (12%)	5	22
2	L	139/140 (99%)	131 (94%)	8 (6%)	20	55
2	M	139/140 (99%)	129 (93%)	10 (7%)	14	47
2	N	139/140 (99%)	135 (97%)	4 (3%)	42	74
All	All	1575/1608 (98%)	1435 (91%)	140 (9%)	9	35

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	150	GLU
2	L	54	PHE
2	M	86	ARG
1	B	375	LYS
1	B	367	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	68	GLN
2	L	39	ASN
2	H	119	GLN
2	I	24	ASN
2	M	11	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	PO4	B	452	4	4,4,4	1.47	0	6,6,6	0.42	0
5	PO4	A	452	4	4,4,4	1.49	0	6,6,6	0.44	0
3	ADP	C	450	4	24,29,29	2.45	10 (41%)	29,45,45	2.09	6 (20%)
5	PO4	C	452	4	4,4,4	1.24	0	6,6,6	0.43	0
3	ADP	B	450	4	24,29,29	2.38	10 (41%)	29,45,45	1.96	4 (13%)
6	LVS	H	0	2	39,41,42	4.20	11 (28%)	49,57,59	1.54	6 (12%)
6	LVS	I	0	2	39,41,42	4.32	11 (28%)	49,57,59	1.56	5 (10%)
3	ADP	A	450	4	24,29,29	2.42	9 (37%)	29,45,45	1.93	4 (13%)
6	LVS	G	0	2	39,41,42	4.11	11 (28%)	49,57,59	1.61	8 (16%)

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
3	ADP	C	450	4	-	2/12/32/32	0/3/3/3
3	ADP	B	450	4	-	2/12/32/32	0/3/3/3
6	LVS	H	0	2	-	10/43/46/46	0/1/1/1
6	LVS	I	0	2	-	12/43/46/46	0/1/1/1
3	ADP	A	450	4	-	2/12/32/32	0/3/3/3
6	LVS	G	0	2	-	11/43/46/46	0/1/1/1

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	0	LVS	C2'-CS	16.69	1.58	1.31
6	I	0	LVS	C2'-CS	16.47	1.58	1.31
6	G	0	LVS	C2'-CS	15.46	1.56	1.31
6	I	0	LVS	O1'-S	10.58	1.58	1.44
6	I	0	LVS	O2'-S	10.18	1.58	1.44

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	450	ADP	PA-O3A-PB	-7.67	106.51	132.83
3	B	450	ADP	PA-O3A-PB	-7.02	108.73	132.83
3	A	450	ADP	PA-O3A-PB	-6.82	109.41	132.83
6	I	0	LVS	CD5-CG3-CB3	6.35	134.47	111.11
6	H	0	LVS	CD5-CG3-CB3	6.27	134.16	111.11

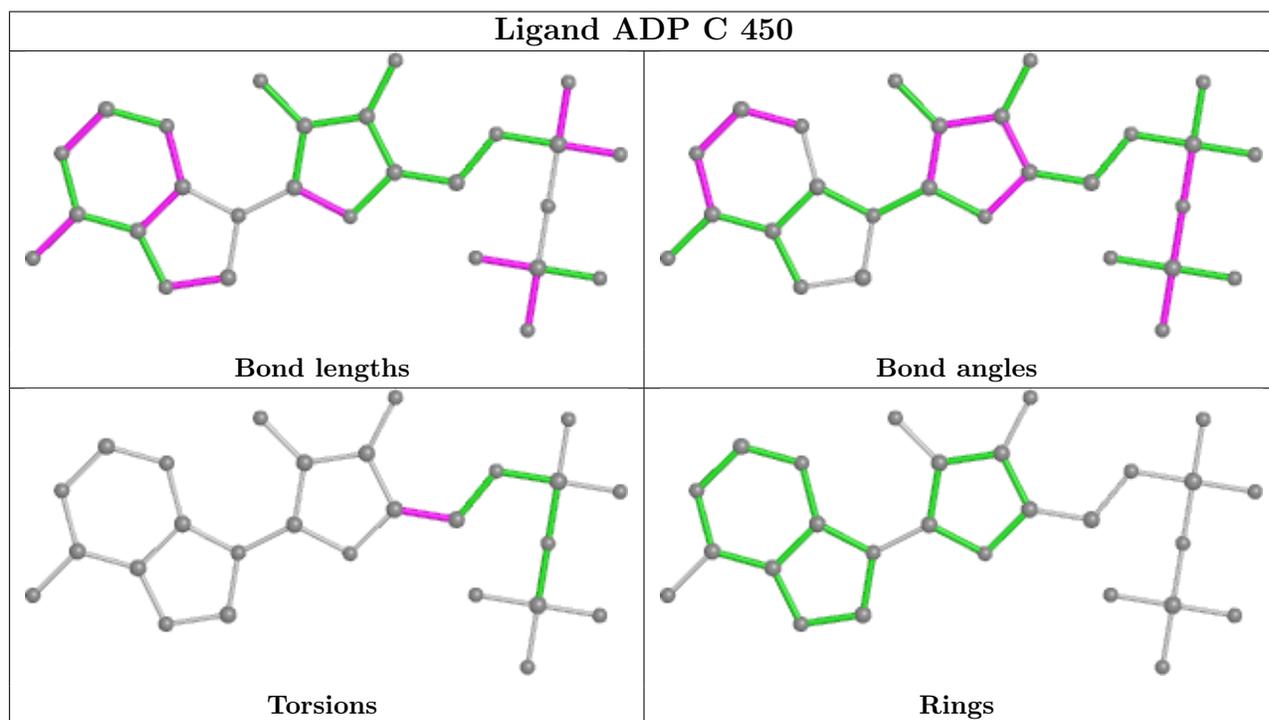There are no chirality outliers.

5 of 39 torsion outliers are listed below:

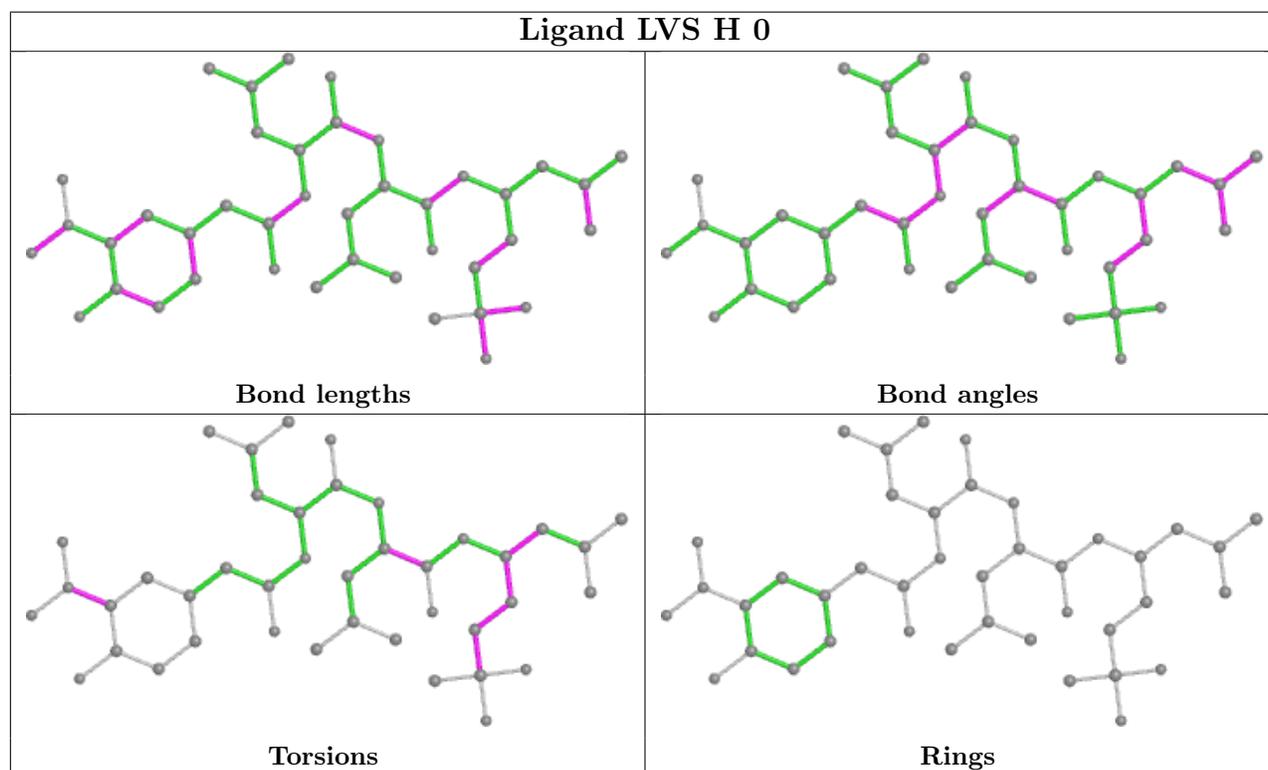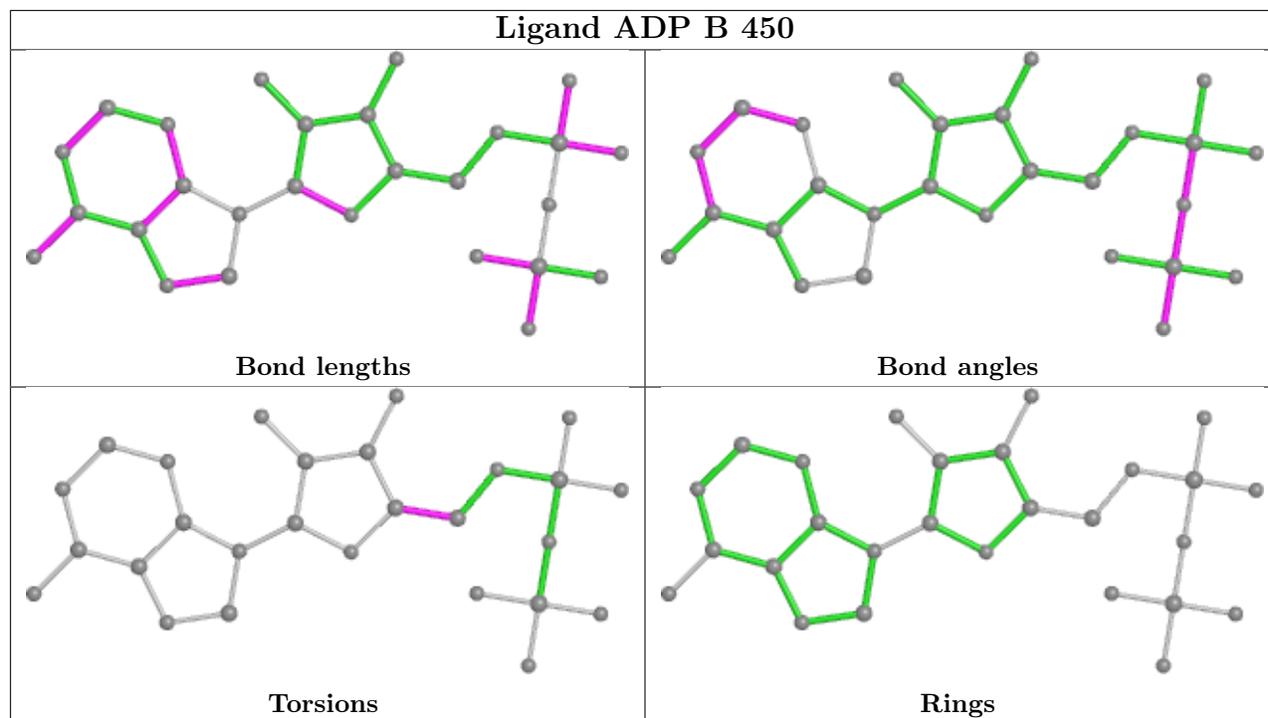| Mol	Chain	Res	Type	Atoms
6	G	0	LVS	N1-CA1-CB1-CG1
6	G	0	LVS	N3-CA3-CS-C2'
6	G	0	LVS	CB3-CA3-CS-C2'
6	G	0	LVS	S-C2'-CS-CA3
6	G	0	LVS	CS-C2'-S-O1'

There are no ring outliers.
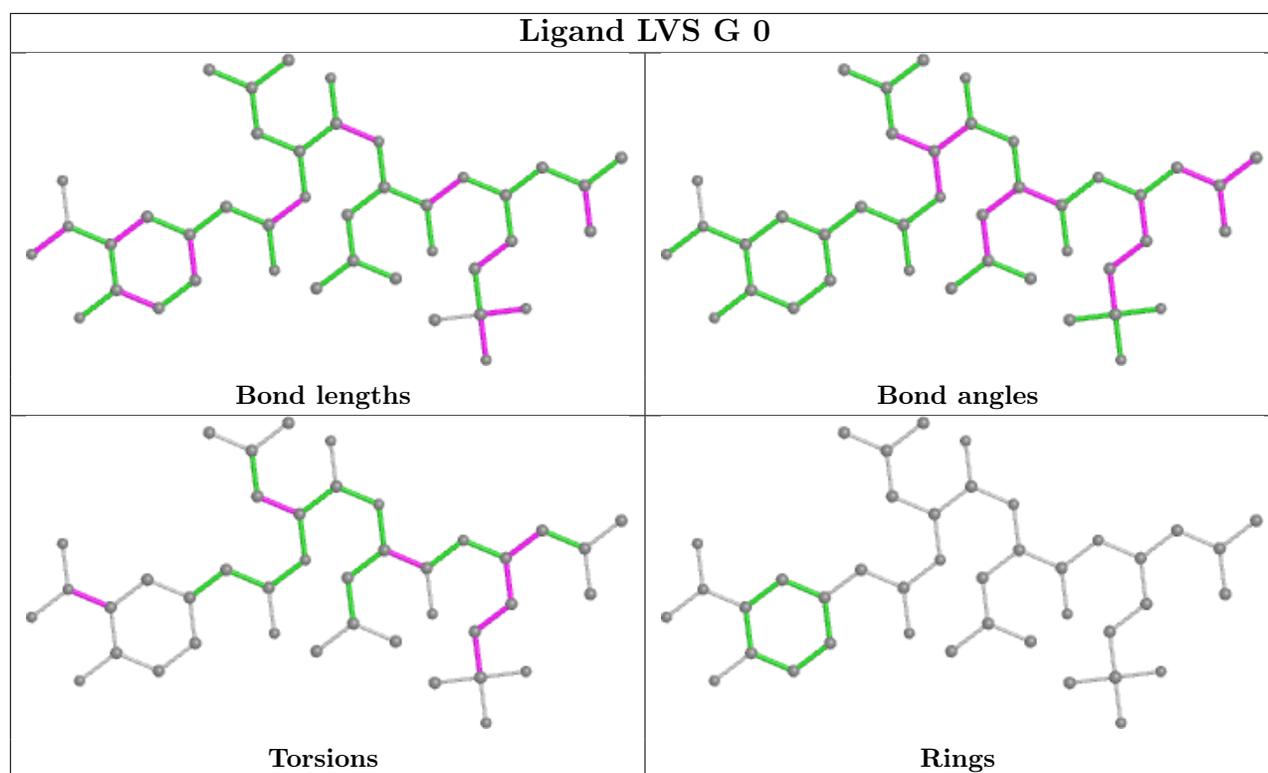
8 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	452	PO4	2	0
3	C	450	ADP	4	0
5	C	452	PO4	1	0
3	B	450	ADP	6	0
6	H	0	LVS	5	0
6	I	0	LVS	5	0
3	A	450	ADP	4	0
6	G	0	LVS	9	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 then 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 ADP C 450

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 450

Bond lengths

Bond angles

Torsions

Rings

Ligand LVS H 0

Bond lengths

Bond angles

Torsions

Rings

Ligand LVS I 0

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 450

Bond lengths

Bond angles

Torsions

Rings

Ligand LVS G 0

Bond lengths

Bond angles

Torsions

Rings
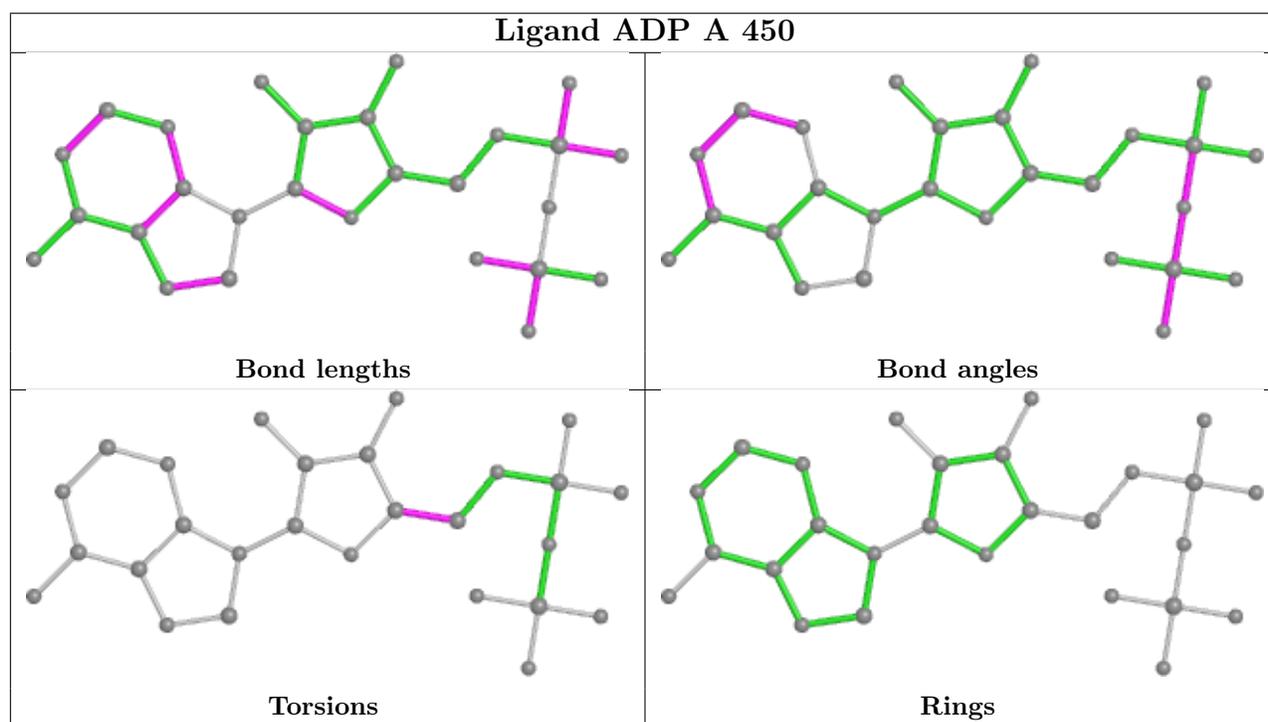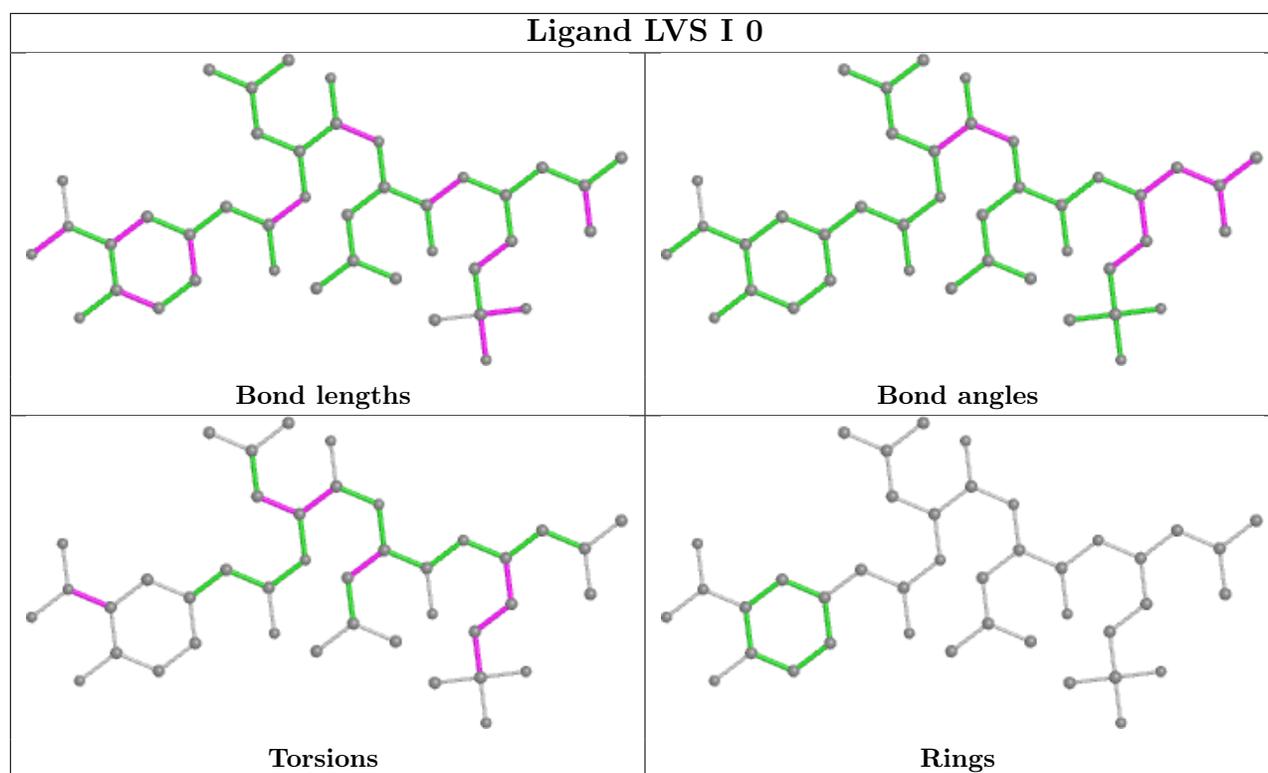
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3   Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4   Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5   Other polymers ⓘ

EDS was not executed - this section is therefore empty.