



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 05:13 PM BST

PDB ID : 4I9D  
Title : X-ray structure of NikA in complex with Fe-N,N'-Bis(2-pyridylmethyl)-N-carboxymethyl-N'-methyl  
Authors : Cherrier, M.V.; Amara, P.; Iannello, M.; Cavazza, C.  
Deposited on : 2012-12-05  
Resolution : 1.70 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

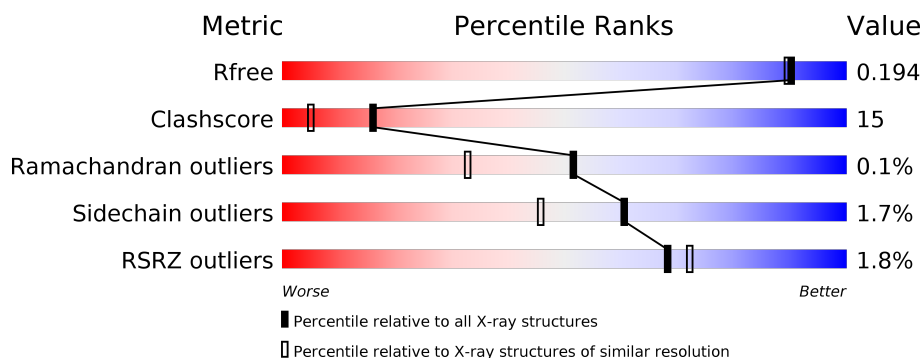
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	502	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 79%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>79%</span> <span>18%</span> <span>..</span> </div> </div>
1	B	502	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 19%, green 80%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>3%</span> <span>80%</span> <span>19%</span> <span>..</span> </div> </div>

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
2	ACT	A	607	-	-	X	-
2	ACT	A	611	-	-	X	-
2	ACT	A	617	-	-	X	-
2	ACT	A	621	-	-	X	-
2	ACT	A	625	-	-	X	-
2	ACT	A	627	-	-	X	-
2	ACT	A	628	-	-	X	-
2	ACT	B	609	-	-	X	-
2	ACT	B	615	-	-	X	-
3	GOL	A	608	-	-	X	-
3	GOL	A	619	-	-	X	-
3	GOL	A	626	-	-	X	-
3	GOL	A	633	-	-	X	-
3	GOL	B	604	-	-	X	-
3	GOL	B	610	-	-	X	-
3	GOL	B	611	-	-	X	-
3	GOL	B	616	-	-	X	-
5	L4D	A	631[B]	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9819 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 Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	33	0
			4143	2663	691	776	13			
1	B	497	Total	C	N	O	S	11	33	0
			4143	2667	691	771	14			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

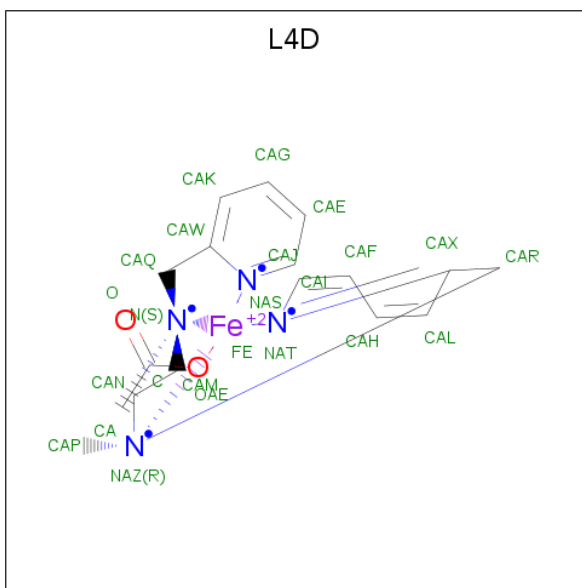
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

- Molecule 5 is {(S)-N-(2-{methyl[(pyridin-2-yl-kappaN)methyl]amino-kappaN}ethyl)-N-[(pyridin-2-yl-kappaN)methyl]glycinato-kappa 2 N,O}iron(2+) (three-letter code: L4D)

(formula: C<sub>17</sub>H<sub>21</sub>FeN<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 47	C 34	Fe 1	N 8	O 4	0	1
5	B	1	Total 47	C 34	Fe 1	N 8	O 4	0	1

- Molecule 6 is water.

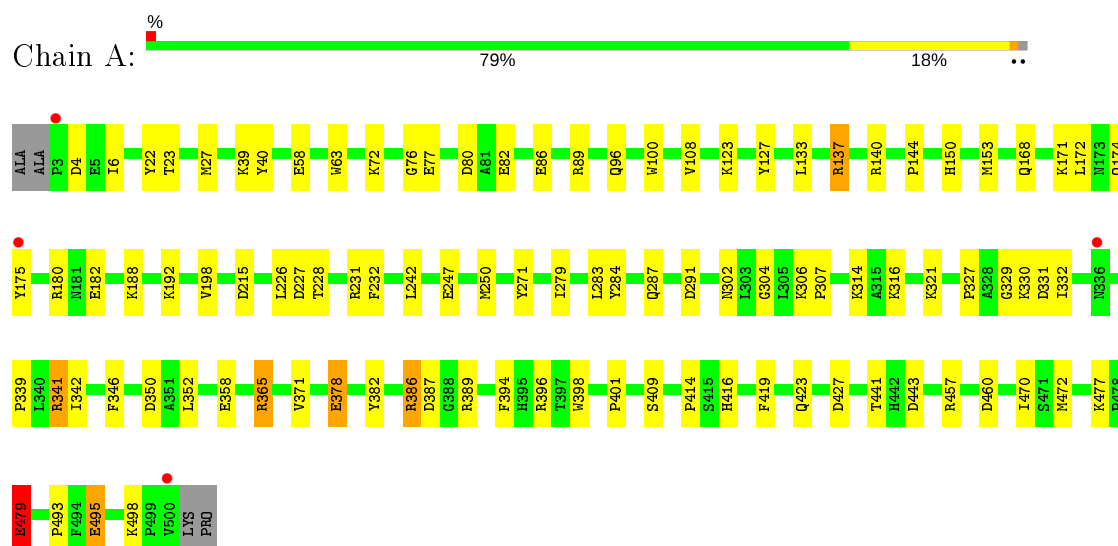
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	665	Total O 665 665	0	0
6	B	532	Total O 532 532	0	0



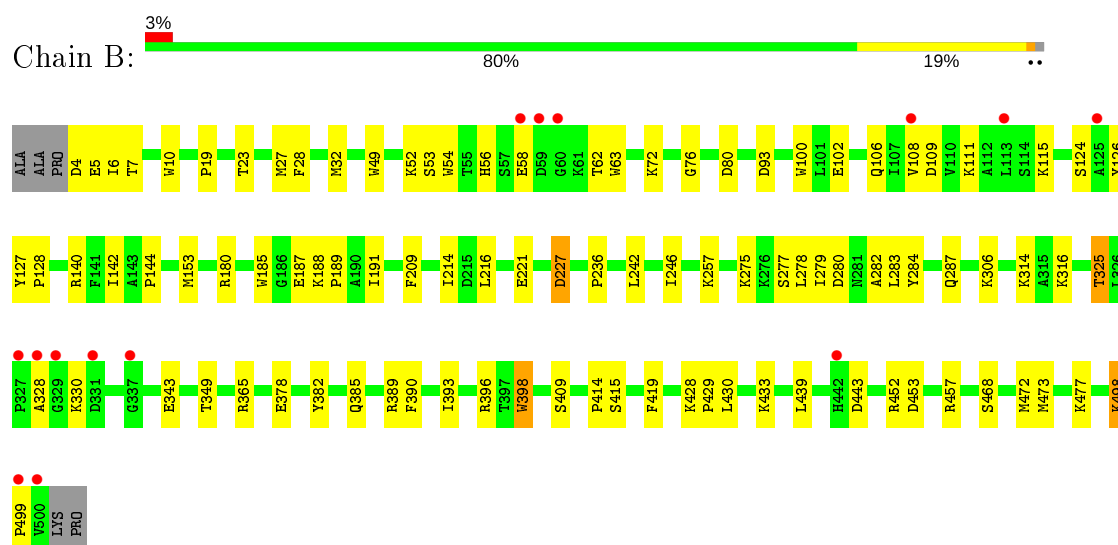
### 3 Residue-property plots [i](#)

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

- Molecule 1: Nickel-binding periplasmic protein



- Molecule 1: Nickel-binding periplasmic protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.67Å 94.73Å 124.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.94 – 1.70 47.37 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.94-1.70) 99.7 (47.37-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.81 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, $R_{free}$	0.152 , 0.195 0.151 , 0.194	Depositor DCC
$R_{free}$ test set	5653 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, SO4, L4D

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.20	11/4337 (0.3%)	1.18	19/5899 (0.3%)
1	B	1.13	8/4334 (0.2%)	1.07	11/5897 (0.2%)
All	All	1.17	19/8671 (0.2%)	1.13	30/11796 (0.3%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	330	LYS	CD-CE	-12.39	1.20	1.51
1	A	479[A]	GLU	CD-OE1	-8.64	1.16	1.25
1	A	479[B]	GLU	CD-OE1	-8.64	1.16	1.25
1	B	187	GLU	CB-CG	-8.07	1.36	1.52
1	B	49	TRP	CD2-CE2	7.00	1.49	1.41

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD1	13.47	130.43	118.30
1	B	452	ARG	NE-CZ-NH1	-8.87	115.87	120.30
1	A	389	ARG	NE-CZ-NH1	-8.67	115.97	120.30
1	B	58	GLU	CB-CA-C	7.61	125.63	110.40
1	A	227	ASP	CB-CG-OD2	-7.55	111.50	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4143	0	4166	115	1
1	B	4143	0	4169	95	0
2	A	72	0	54	24	0
2	B	28	0	21	8	0
3	A	84	0	112	37	0
3	B	48	0	64	26	0
4	A	10	0	0	0	0
5	A	47	0	36	12	0
5	B	47	0	36	5	0
6	A	665	0	0	58	3
6	B	532	0	0	25	2
All	All	9819	0	8658	251	3

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 15.

The worst 5 of 251 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:B:257[A]:LYS:HE2	3:B:616:GOL:O2	1.19	1.29
1:A:387:ASP:HB2	6:A:1353:HOH:O	1.36	1.19
5:A:631[B]:L4D:CAF	6:A:1365:HOH:O	1.92	1.18
5:A:631[B]:L4D:CAJ	6:A:1365:HOH:O	1.88	1.18
1:B:4:ASP:N	3:B:610:GOL:HO1	1.48	1.12

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358[A]:GLU:OE2	6:A:1218:HOH:O[3_554]	1.97	0.23
6:A:1019:HOH:O	6:B:1080:HOH:O[3_444]	2.11	0.09
6:A:1162:HOH:O	6:B:1092:HOH:O[2_454]	2.13	0.07

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/502 (106%)	518 (98%)	12 (2%)	0	100	100
1	B	531/502 (106%)	513 (97%)	17 (3%)	1 (0%)	47	30
All	All	1061/1004 (106%)	1031 (97%)	29 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	328	ALA

### 5.3.2 Protein sidechains [i](#)

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	457/425 (108%)	447 (98%)	10 (2%)	52	34
1	B	457/425 (108%)	450 (98%)	7 (2%)	65	51
All	All	914/850 (108%)	897 (98%)	17 (2%)	60	41

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	GLU
1	A	479[A]	GLU
1	B	124	SER
1	A	341[B]	ARG
1	B	325[A]	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

53 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ACT	A	602	-	1,3,3	1.86	0	0,3,3	0.00	-
2	ACT	A	624	-	1,3,3	2.22	1 (100%)	0,3,3	0.00	-
2	ACT	A	627	-	1,3,3	2.18	1 (100%)	0,3,3	0.00	-
3	GOL	B	614	-	5,5,5	0.15	0	5,5,5	0.51	0
3	GOL	A	632	-	5,5,5	0.36	0	5,5,5	1.42	1 (20%)
2	ACT	B	607	-	1,3,3	2.27	1 (100%)	0,3,3	0.00	-
2	ACT	A	607	-	1,3,3	2.54	1 (100%)	0,3,3	0.00	-
3	GOL	A	603	-	5,5,5	0.30	0	5,5,5	0.80	0
5	L4D	B	613[A]	-	28,29,29	5.08	18 (64%)	20,51,51	2.64	8 (40%)
2	ACT	A	617	-	1,3,3	0.75	0	0,3,3	0.00	-
2	ACT	B	608	-	1,3,3	2.20	1 (100%)	0,3,3	0.00	-
4	SO4	A	604	-	4,4,4	0.60	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ACT	A	613	-	1,3,3	1.59	0	0,3,3	0.00	-
2	ACT	B	605	-	1,3,3	1.89	0	0,3,3	0.00	-
3	GOL	A	606	-	5,5,5	0.47	0	5,5,5	0.88	0
3	GOL	A	622	-	5,5,5	0.60	0	5,5,5	1.36	1 (20%)
2	ACT	A	615	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
3	GOL	A	608	-	5,5,5	0.23	0	5,5,5	0.26	0
3	GOL	B	611	-	5,5,5	0.51	0	5,5,5	0.75	0
2	ACT	A	611	-	1,3,3	0.59	0	0,3,3	0.00	-
5	L4D	A	631[B]	-	28,29,29	5.75	17 (60%)	20,51,51	2.52	9 (45%)
2	ACT	B	609	-	1,3,3	1.29	0	0,3,3	0.00	-
2	ACT	A	625	-	1,3,3	1.35	0	0,3,3	0.00	-
3	GOL	B	606	-	5,5,5	0.71	0	5,5,5	1.13	0
3	GOL	A	626	-	5,5,5	0.49	0	5,5,5	0.46	0
3	GOL	A	633	-	5,5,5	0.75	0	5,5,5	1.04	0
3	GOL	B	602	-	5,5,5	0.54	0	5,5,5	1.55	1 (20%)
2	ACT	A	630	-	1,3,3	1.49	0	0,3,3	0.00	-
3	GOL	B	610	-	5,5,5	0.23	0	5,5,5	0.71	0
2	ACT	A	621	-	1,3,3	0.63	0	0,3,3	0.00	-
2	ACT	A	620	-	1,3,3	1.97	0	0,3,3	0.00	-
2	ACT	B	603	-	1,3,3	1.63	0	0,3,3	0.00	-
3	GOL	B	604	-	5,5,5	0.69	0	5,5,5	1.01	0
2	ACT	A	618	-	1,3,3	1.79	0	0,3,3	0.00	-
2	ACT	A	616	-	1,3,3	0.00	0	0,3,3	0.00	-
3	GOL	B	616	-	5,5,5	0.54	0	5,5,5	0.74	0
2	ACT	A	629	-	1,3,3	3.24	1 (100%)	0,3,3	0.00	-
2	ACT	B	615	-	1,3,3	3.25	1 (100%)	0,3,3	0.00	-
5	L4D	A	631[A]	-	28,29,29	4.66	16 (57%)	20,51,51	2.68	7 (35%)
3	GOL	A	610[A]	-	5,5,5	1.22	0	5,5,5	0.73	0
3	GOL	B	601	-	5,5,5	1.20	1 (20%)	5,5,5	0.69	0
3	GOL	A	619	-	5,5,5	0.98	0	5,5,5	1.45	1 (20%)
3	GOL	A	634	-	5,5,5	0.53	0	5,5,5	1.04	0
3	GOL	A	612	-	5,5,5	0.49	0	5,5,5	0.44	0
5	L4D	B	613[B]	-	28,29,29	5.60	17 (60%)	20,51,51	2.89	11 (55%)
2	ACT	A	601	-	1,3,3	1.91	0	0,3,3	0.00	-
3	GOL	A	609	-	5,5,5	0.48	0	5,5,5	0.54	0
4	SO4	A	605	-	4,4,4	0.51	0	6,6,6	0.73	0
2	ACT	A	628	-	1,3,3	2.73	1 (100%)	0,3,3	0.00	-
2	ACT	B	612	-	1,3,3	2.95	1 (100%)	0,3,3	0.00	-
3	GOL	A	614	-	5,5,5	0.72	0	5,5,5	1.10	0
2	ACT	A	623	-	1,3,3	2.58	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	610[B]	-	5,5,5	0.33	0	5,5,5	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	614	-	-	4/4/4/4	-
3	GOL	A	632	-	-	3/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
5	L4D	B	613[A]	-	-	-	0/6/6/6
5	L4D	B	613[B]	-	-	-	0/6/6/6
3	GOL	A	608	-	-	2/4/4/4	-
3	GOL	A	606	-	-	2/4/4/4	-
3	GOL	B	604	-	-	4/4/4/4	-
3	GOL	B	611	-	-	1/4/4/4	-
5	L4D	A	631[B]	-	-	-	0/6/6/6
3	GOL	A	622	-	-	2/4/4/4	-
3	GOL	B	606	-	-	2/4/4/4	-
3	GOL	A	626	-	-	2/4/4/4	-
3	GOL	A	633	-	-	4/4/4/4	-
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	B	610	-	-	0/4/4/4	-
5	L4D	A	631[A]	-	-	-	0/6/6/6
3	GOL	B	616	-	-	4/4/4/4	-
3	GOL	A	610[B]	-	-	4/4/4/4	-
3	GOL	A	610[A]	-	-	0/4/4/4	-
3	GOL	B	601	-	-	0/4/4/4	-
3	GOL	A	619	-	-	4/4/4/4	-
3	GOL	A	634	-	-	2/4/4/4	-
3	GOL	A	612	-	-	2/4/4/4	-
3	GOL	A	609	-	-	1/4/4/4	-
3	GOL	A	614	-	-	2/4/4/4	-

The worst 5 of 80 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	631[B]	L4D	CAW-NAS	-16.39	1.33	1.49
5	B	613[A]	L4D	CAX-NAT	-15.07	1.34	1.49
5	A	631[B]	L4D	CAX-NAT	-14.62	1.35	1.49
5	B	613[A]	L4D	CAW-NAS	-14.23	1.35	1.49
5	B	613[B]	L4D	CAW-NAS	-14.22	1.35	1.49

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	631[A]	L4D	CAJ-CAF-CAH	6.54	122.52	111.44
5	B	613[B]	L4D	CAI-CAE-CAG	6.06	121.70	111.44
5	A	631[A]	L4D	CAI-CAE-CAG	5.54	120.83	111.44
5	A	631[B]	L4D	CAF-CAH-CAL	5.07	121.76	111.42
5	B	613[A]	L4D	CAH-CAL-CAX	4.88	121.21	110.83

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	614	GOL	C1-C2-C3-O3
3	A	632	GOL	O1-C1-C2-C3
3	A	603	GOL	O1-C1-C2-C3
3	A	606	GOL	O1-C1-C2-C3
3	A	622	GOL	C1-C2-C3-O3

There are no ring outliers.

37 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	624	ACT	1	0
2	A	627	ACT	3	0
3	B	614	GOL	2	0
3	A	632	GOL	3	0
2	A	607	ACT	3	0
3	A	603	GOL	1	0
5	B	613[A]	L4D	3	0
2	A	617	ACT	3	0
2	A	613	ACT	1	0
3	A	622	GOL	3	0
3	A	608	GOL	4	0
3	B	611	GOL	4	0
2	A	611	ACT	2	0

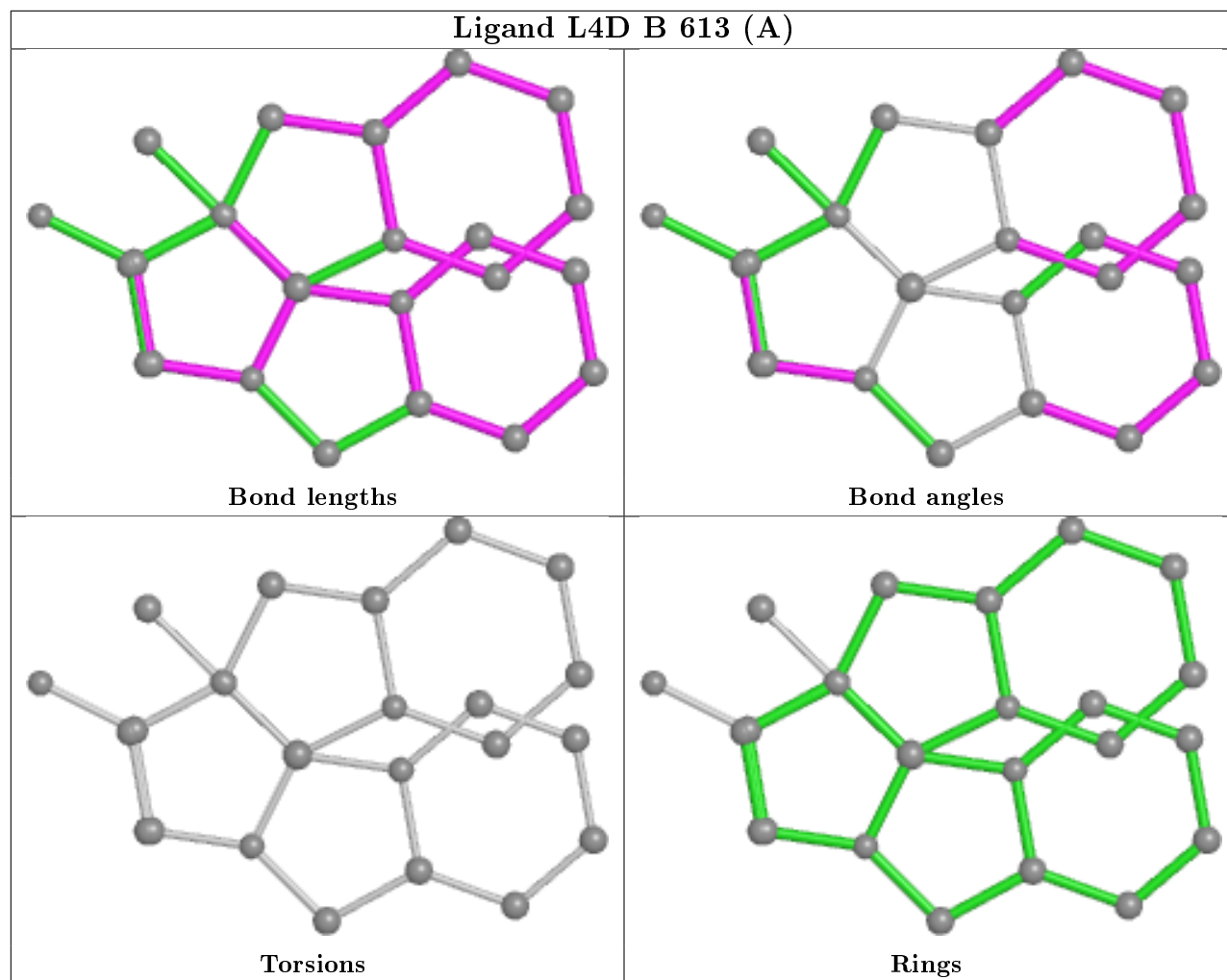
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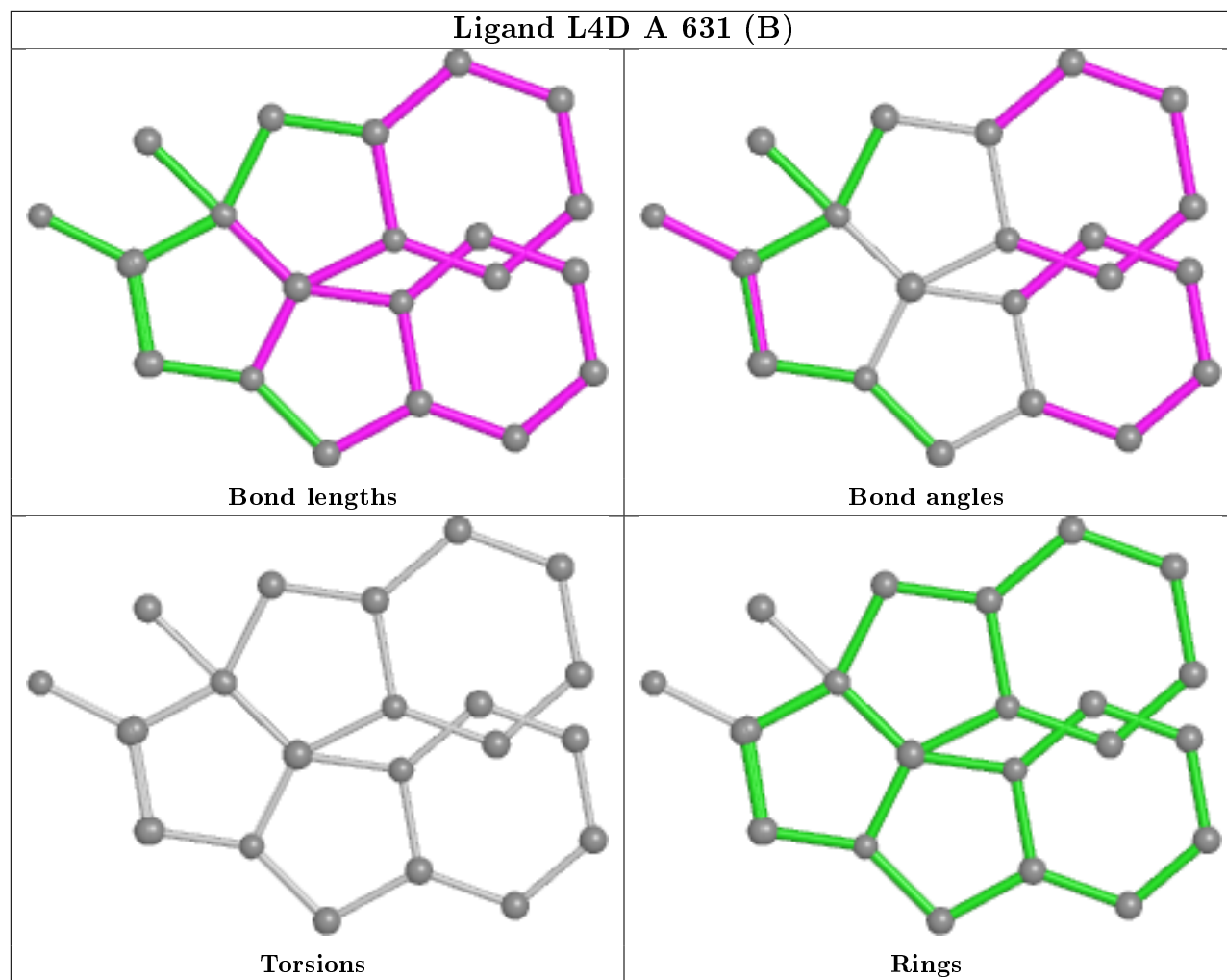
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	631[B]	L4D	9	0
2	B	609	ACT	2	0
2	A	625	ACT	3	0
3	A	626	GOL	5	0
3	A	633	GOL	4	0
3	B	602	GOL	2	0
2	A	630	ACT	1	0
3	B	610	GOL	4	0
2	A	621	ACT	2	0
2	B	603	ACT	1	0
3	B	604	GOL	4	0
3	B	616	GOL	10	0
2	B	615	ACT	4	0
5	A	631[A]	L4D	3	0
3	A	610[A]	GOL	2	0
3	A	619	GOL	5	0
3	A	634	GOL	2	0
3	A	612	GOL	2	0
5	B	613[B]	L4D	2	0
3	A	609	GOL	2	0
2	A	628	ACT	5	0
2	B	612	ACT	1	0
3	A	614	GOL	3	0
3	A	610[B]	GOL	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.

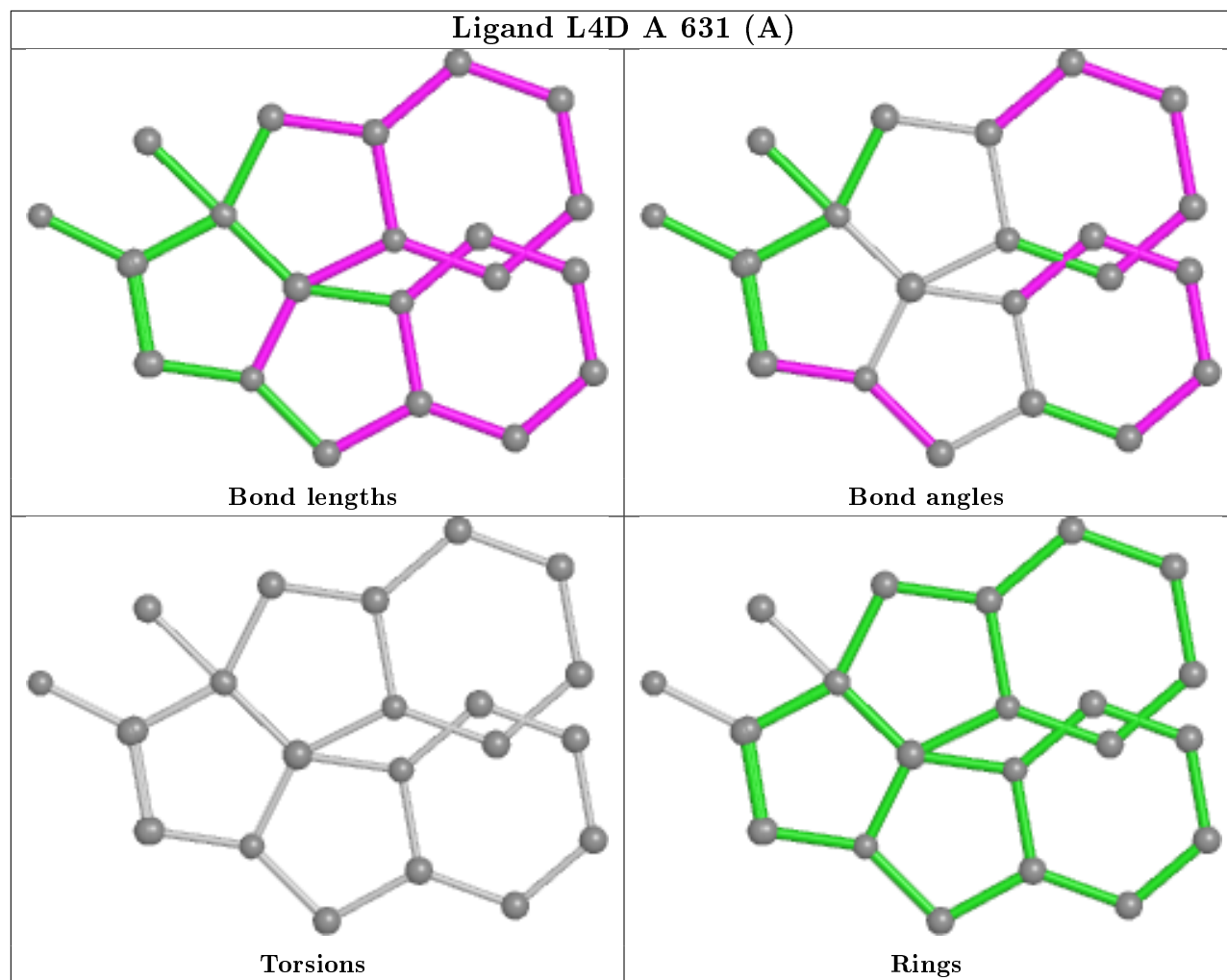
## Ligand L4D B 613 (A)

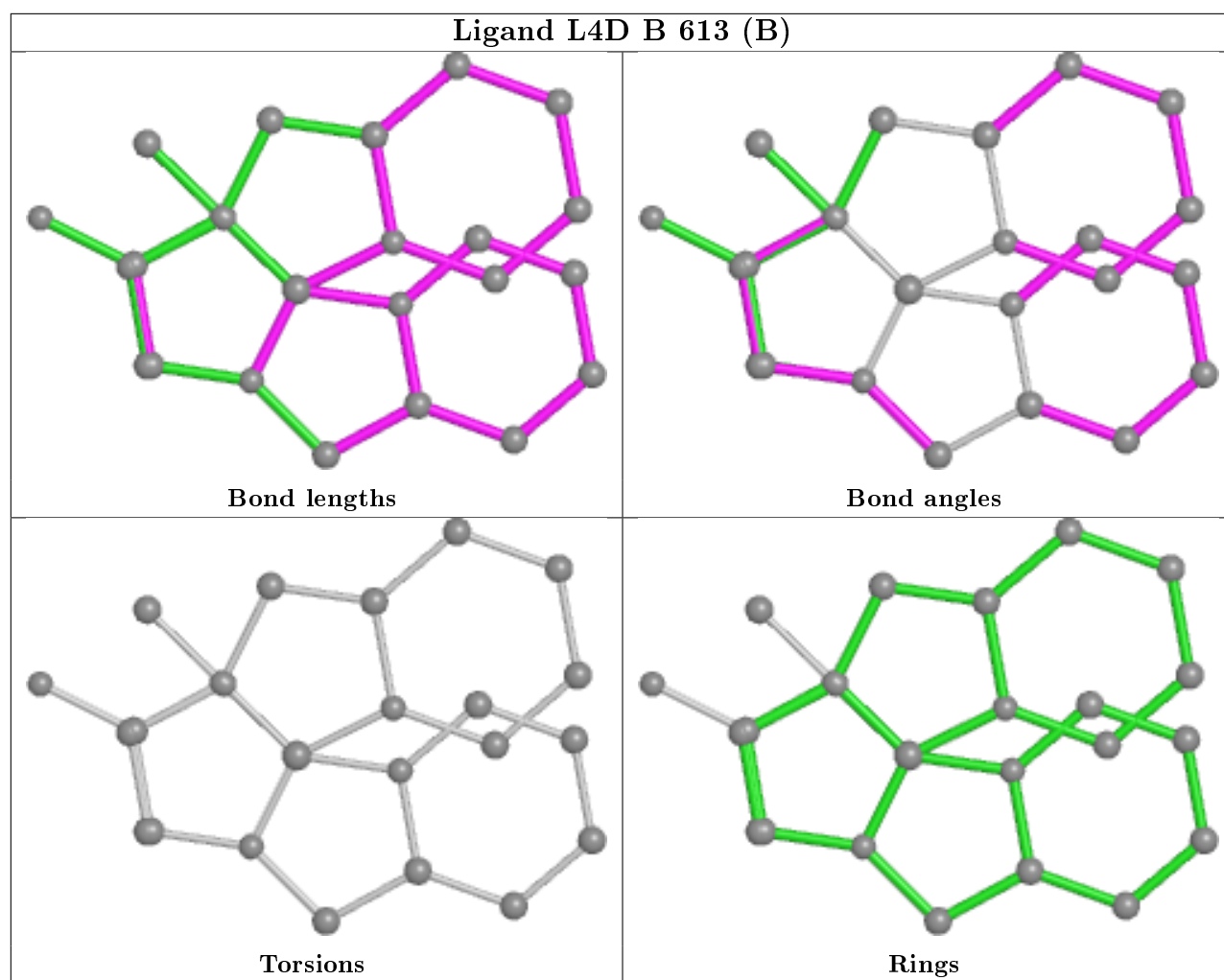


## Ligand L4D A 631 (B)



## Ligand L4D A 631 (A)





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	498/502 (99%)	-0.46	4 (0%) 86 88	10, 17, 34, 56	0
1	B	497/502 (99%)	-0.24	14 (2%) 53 57	10, 23, 46, 58	9 (1%)
All	All	995/1004 (99%)	-0.35	18 (1%) 68 72	10, 19, 41, 58	9 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	500	VAL	6.4
1	B	328	ALA	5.9
1	A	500	VAL	5.5
1	B	125	ALA	5.1
1	B	337	GLY	4.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	609	6/6	0.41	0.27	66,74,75,76	0
2	ACT	B	605	4/4	0.65	0.20	70,70,72,74	0
2	ACT	A	628	4/4	0.72	0.22	45,46,47,47	4
2	ACT	A	616	4/4	0.76	0.24	31,32,37,43	4
3	GOL	A	626	6/6	0.80	0.22	43,48,51,51	0
3	GOL	A	633	6/6	0.81	0.17	41,50,51,55	0
2	ACT	A	617	4/4	0.82	0.20	48,52,57,65	0
2	ACT	A	623	4/4	0.82	0.34	37,51,53,57	0
3	GOL	B	616	6/6	0.83	0.34	51,55,56,61	0
2	ACT	A	621	4/4	0.83	0.28	44,45,48,49	0
2	ACT	A	601	4/4	0.84	0.16	29,35,42,51	0
3	GOL	B	614	6/6	0.85	0.14	54,59,61,62	0
3	GOL	A	612	6/6	0.85	0.18	45,57,61,65	0
2	ACT	A	629	4/4	0.86	0.26	42,51,52,54	0
2	ACT	B	612	4/4	0.86	0.13	48,56,57,58	0
3	GOL	B	611	6/6	0.86	0.18	51,53,55,57	0
2	ACT	A	625	4/4	0.87	0.11	44,49,51,52	0
2	ACT	A	611	4/4	0.88	0.13	45,52,53,53	0
3	GOL	A	608	6/6	0.89	0.18	51,53,56,57	0
3	GOL	B	610	6/6	0.89	0.23	59,59,62,65	0
3	GOL	A	622	6/6	0.89	0.16	21,27,29,38	6
2	ACT	A	620	4/4	0.89	0.13	57,60,61,61	0
2	ACT	A	618	4/4	0.89	0.18	62,63,64,64	0
2	ACT	A	624	4/4	0.90	0.15	36,41,49,51	0
3	GOL	A	632	6/6	0.90	0.19	36,48,52,53	0
3	GOL	B	604	6/6	0.90	0.12	23,34,39,40	0
3	GOL	B	601	6/6	0.90	0.10	25,30,34,37	0
3	GOL	A	619	6/6	0.90	0.16	22,29,34,38	0
2	ACT	B	609	4/4	0.90	0.13	52,53,55,60	0
3	GOL	A	634	6/6	0.91	0.12	36,38,48,53	0
3	GOL	B	602	6/6	0.91	0.14	21,30,33,35	6
2	ACT	B	615	4/4	0.92	0.22	37,40,42,44	0
2	ACT	A	613	4/4	0.92	0.15	57,62,65,66	0
2	ACT	B	607	4/4	0.92	0.09	38,41,44,45	0
2	ACT	B	603	4/4	0.92	0.17	54,57,58,62	0
2	ACT	B	608	4/4	0.92	0.12	40,41,43,46	0
3	GOL	A	614	6/6	0.93	0.17	27,40,44,44	0
3	GOL	A	606	6/6	0.93	0.10	26,31,38,38	0
3	GOL	B	606	6/6	0.94	0.11	17,30,45,47	0
2	ACT	A	627	4/4	0.94	0.21	27,45,45,54	0
2	ACT	A	602	4/4	0.94	0.11	34,40,41,51	0
3	GOL	A	610[A]	6/6	0.94	0.16	12,23,25,25	6
2	ACT	A	630	4/4	0.94	0.09	53,54,54,55	0

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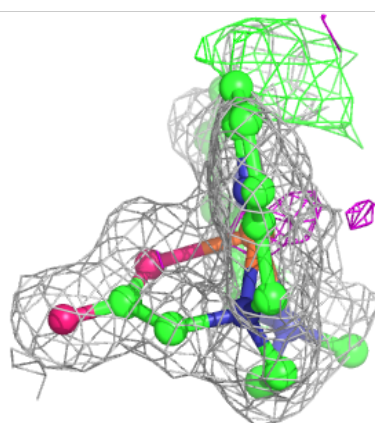
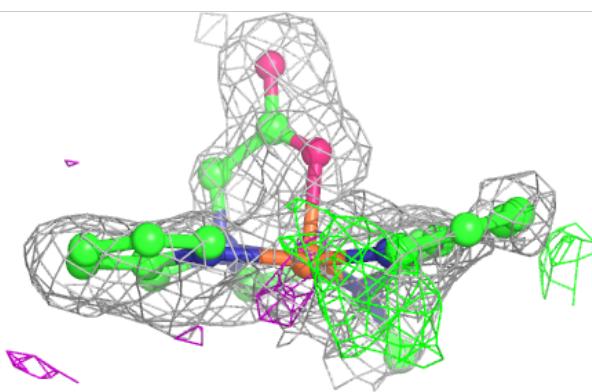
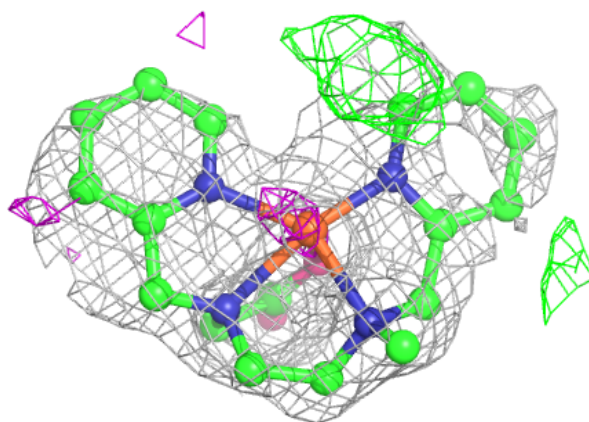
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	610[B]	6/6	0.94	0.16	14,17,22,26	6
4	SO4	A	605	5/5	0.95	0.10	49,57,59,63	0
3	GOL	A	603	6/6	0.95	0.09	22,36,43,43	0
4	SO4	A	604	5/5	0.96	0.17	43,48,51,51	0
2	ACT	A	615	4/4	0.96	0.09	29,33,40,41	0
2	ACT	A	607	4/4	0.96	0.08	26,37,38,50	0
5	L4D	A	631[A]	24/24	0.97	0.11	13,21,28,32	23
5	L4D	B	613[A]	24/24	0.97	0.11	13,26,31,31	23
5	L4D	A	631[B]	24/24	0.97	0.11	7,19,26,27	23
5	L4D	B	613[B]	24/24	0.97	0.11	15,25,27,30	23

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.

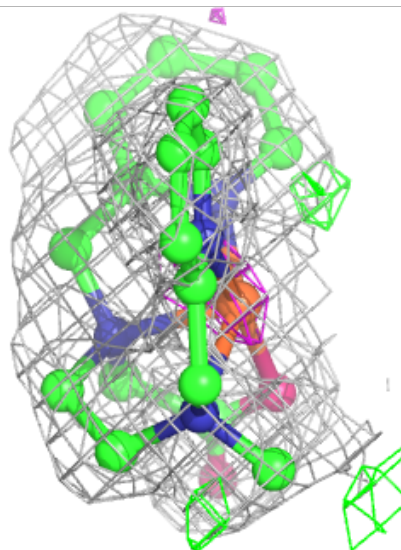
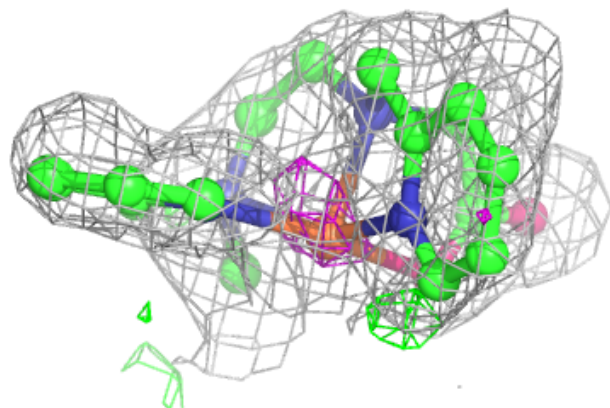
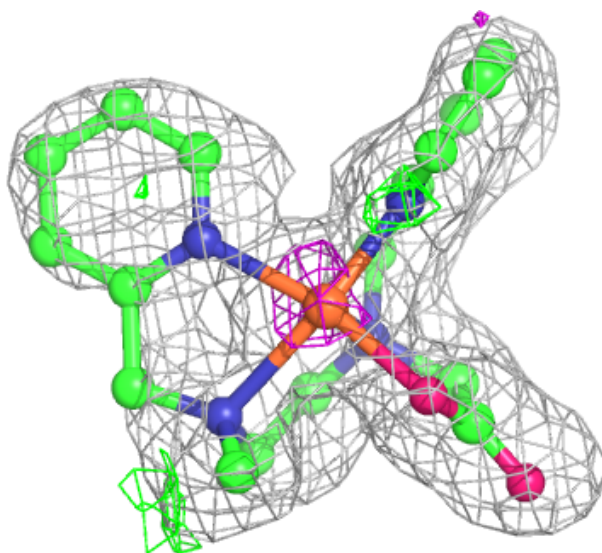
**Electron density around L4D A 631 (A):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



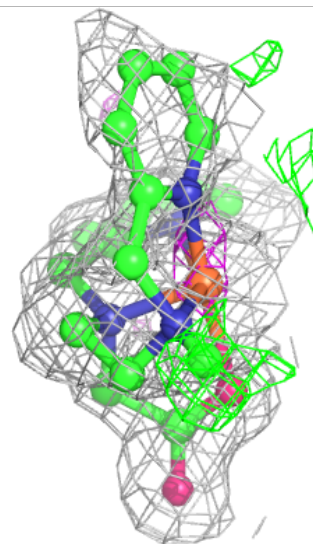
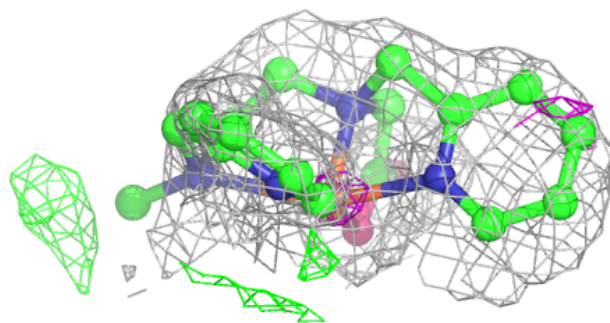
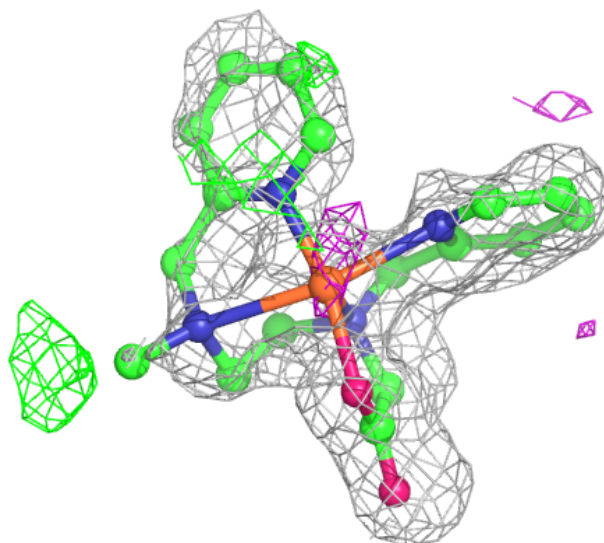
**Electron density around L4D B 613 (A):**

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



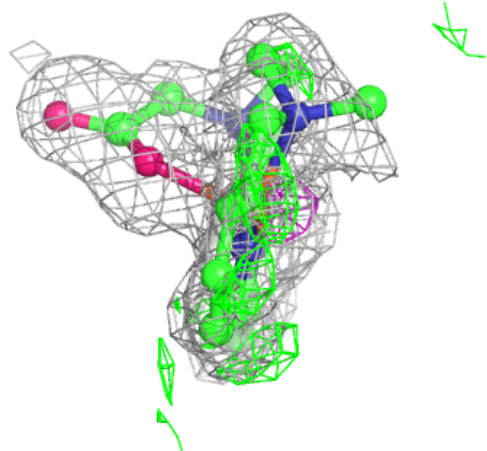
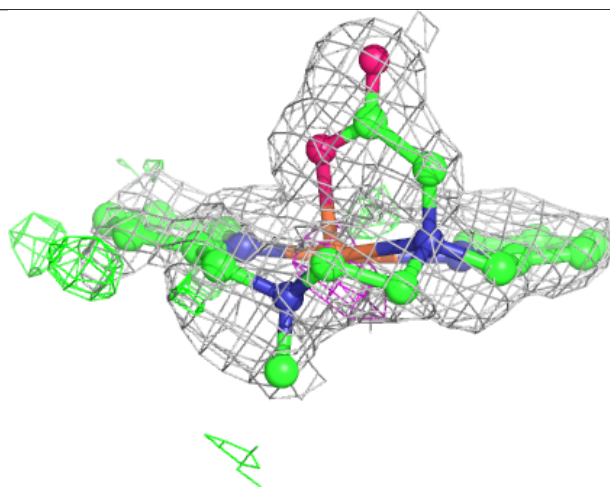
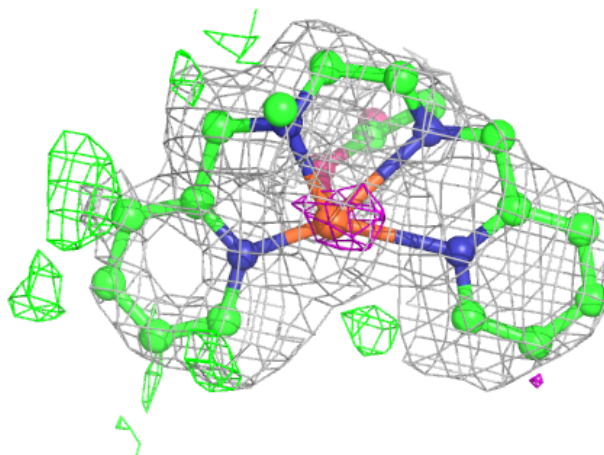
**Electron density around L4D A 631 (B):**

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



**Electron density around L4D B 613 (B):**

$2mF_o-DF_c$  (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.