



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 12:36 am BST

PDB ID : 5NTD  
Title : Structure of Leucyl aminopeptidase from Trypanosoma brucei in complex with Bestatin  
Authors : Timm, J.; Wilson, K.  
Deposited on : 2017-04-27  
Resolution : 2.30 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 : 2.11  
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) : 2.11

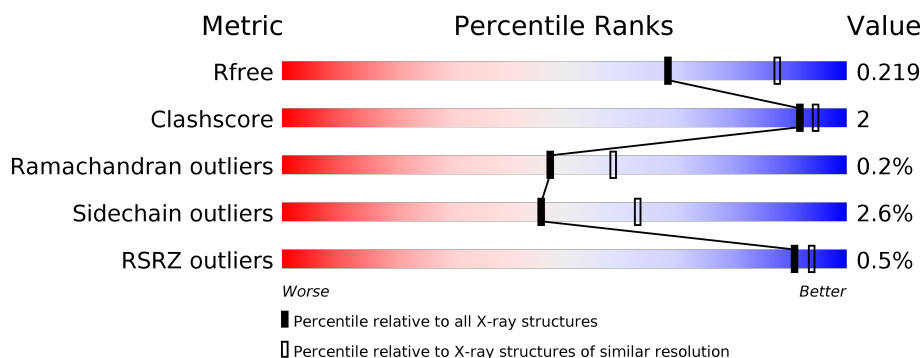
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	521	<div> <div style="width: 93%;"></div> <div style="width: 6%;"></div> <div style="width: 1%;"></div> </div> <div>93% 6% .</div>
1	B	521	<div> <div style="width: 94%;"></div> <div style="width: 5%;"></div> <div style="width: 1%;"></div> </div> <div>94% 5% .</div>
1	C	521	<div> <div style="width: 94%;"></div> <div style="width: 5%;"></div> <div style="width: 1%;"></div> </div> <div>94% 5% .</div>
1	D	521	<div> <div style="width: 94%;"></div> <div style="width: 5%;"></div> </div> <div>94% 5%</div>
1	E	521	<div> <div style="width: 94%;"></div> <div style="width: 5%;"></div> <div style="width: 1%;"></div> </div> <div>94% 5% .</div>
1	F	521	<div> <div style="width: 96%;"></div> <div style="width: 4%;"></div> </div> <div>96%</div>

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Mol	Chain	Length	Quality of chain
1	G	521	<div><div>%</div><div><div></div></div><div>94%6%</div></div>
1	H	521	<div><div></div><div>95%</div><div>.</div></div>
1	I	521	<div><div>2%</div><div><div></div></div><div>95%5%</div></div>
1	J	521	<div><div></div><div>95%</div><div>5%</div></div>
1	K	521	<div><div>%</div><div><div></div></div><div>94%5%</div></div>
1	L	521	<div><div></div><div>95%</div><div>.</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 48865 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 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	2	0
			3833	2427	647	737	22			
1	B	519	Total	C	N	O	S	0	2	0
			3805	2407	643	733	22			
1	D	519	Total	C	N	O	S	0	0	0
			3809	2412	645	730	22			
1	C	518	Total	C	N	O	S	0	1	0
			3807	2408	646	731	22			
1	E	519	Total	C	N	O	S	0	1	0
			3809	2411	646	730	22			
1	F	519	Total	C	N	O	S	0	0	0
			3808	2408	647	731	22			
1	G	520	Total	C	N	O	S	0	2	0
			3812	2411	642	737	22			
1	H	519	Total	C	N	O	S	0	0	0
			3790	2397	642	729	22			
1	I	519	Total	C	N	O	S	0	1	0
			3785	2397	646	720	22			
1	J	519	Total	C	N	O	S	0	0	0
			3811	2412	645	732	22			
1	K	519	Total	C	N	O	S	0	0	0
			3781	2395	642	722	22			
1	L	519	Total	C	N	O	S	0	0	0
			3781	2393	637	729	22			

There are 24 discrepancies between the modelled and reference sequences:

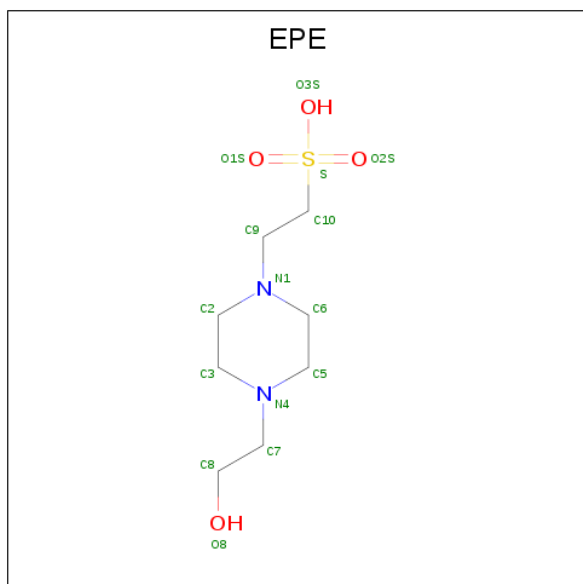
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	THR	conflict	UNP Q385B0
A	139	THR	ALA	conflict	UNP Q385B0
B	32	ALA	THR	conflict	UNP Q385B0
B	139	THR	ALA	conflict	UNP Q385B0
D	32	ALA	THR	conflict	UNP Q385B0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	139	THR	ALA	conflict	UNP Q385B0
C	32	ALA	THR	conflict	UNP Q385B0
C	139	THR	ALA	conflict	UNP Q385B0
E	32	ALA	THR	conflict	UNP Q385B0
E	139	THR	ALA	conflict	UNP Q385B0
F	32	ALA	THR	conflict	UNP Q385B0
F	139	THR	ALA	conflict	UNP Q385B0
G	32	ALA	THR	conflict	UNP Q385B0
G	139	THR	ALA	conflict	UNP Q385B0
H	32	ALA	THR	conflict	UNP Q385B0
H	139	THR	ALA	conflict	UNP Q385B0
I	32	ALA	THR	conflict	UNP Q385B0
I	139	THR	ALA	conflict	UNP Q385B0
J	32	ALA	THR	conflict	UNP Q385B0
J	139	THR	ALA	conflict	UNP Q385B0
K	32	ALA	THR	conflict	UNP Q385B0
K	139	THR	ALA	conflict	UNP Q385B0
L	32	ALA	THR	conflict	UNP Q385B0
L	139	THR	ALA	conflict	UNP Q385B0

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		

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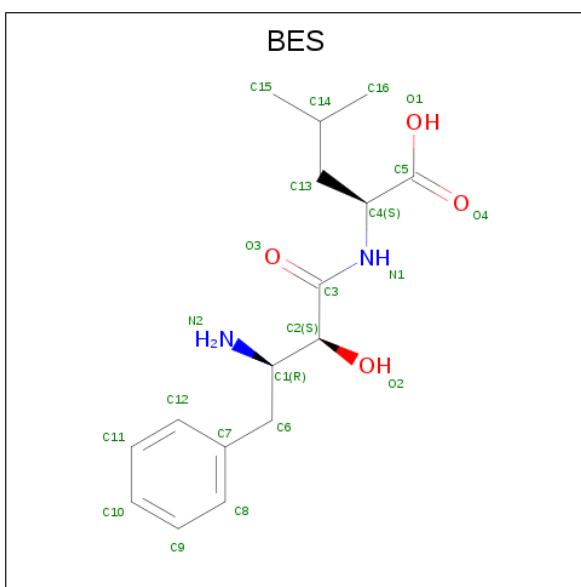
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Mn	0	0
			2	2		
4	J	2	Total	Mn	0	0
			2	2		
4	D	2	Total	Mn	0	0
			2	2		
4	K	2	Total	Mn	0	0
			2	2		
4	E	2	Total	Mn	0	0
			2	2		
4	H	2	Total	Mn	0	0
			2	2		
4	B	2	Total	Mn	0	0
			2	2		
4	I	2	Total	Mn	0	0
			2	2		
4	C	2	Total	Mn	0	0
			2	2		
4	A	2	Total	Mn	0	0
			2	2		
4	L	2	Total	Mn	0	0
			2	2		
4	F	2	Total	Mn	0	0
			2	2		

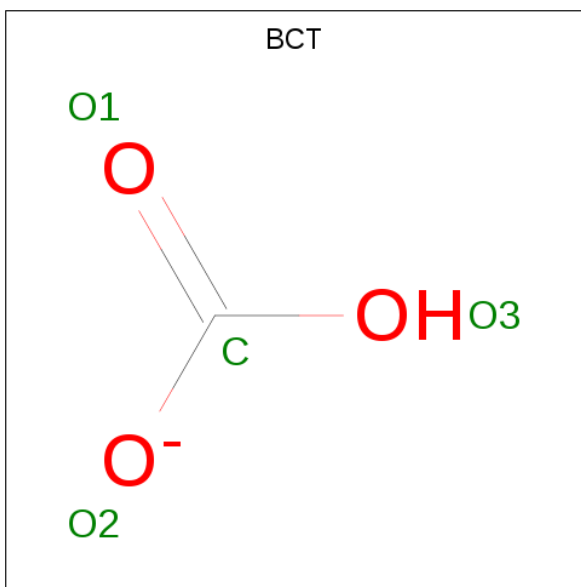
- Molecule 5 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (three-letter code: BES) (formula: C<sub>16</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			22	16	2	4		
5	B	1	Total	C	N	O	0	0
			22	16	2	4		
5	D	1	Total	C	N	O	0	0
			22	16	2	4		
5	C	1	Total	C	N	O	0	0
			22	16	2	4		
5	E	1	Total	C	N	O	0	0
			22	16	2	4		
5	F	1	Total	C	N	O	0	0
			22	16	2	4		
5	G	1	Total	C	N	O	0	0
			22	16	2	4		
5	H	1	Total	C	N	O	0	0
			22	16	2	4		
5	I	1	Total	C	N	O	0	0
			22	16	2	4		
5	J	1	Total	C	N	O	0	0
			22	16	2	4		
5	K	1	Total	C	N	O	0	0
			22	16	2	4		
5	L	1	Total	C	N	O	0	0
			22	16	2	4		

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	B	1	Total	C	O	0	0
			4	1	3		
6	D	1	Total	C	O	0	0
			4	1	3		
6	C	1	Total	C	O	0	0
			4	1	3		
6	E	1	Total	C	O	0	0
			4	1	3		
6	F	1	Total	C	O	0	0
			4	1	3		
6	G	1	Total	C	O	0	0
			4	1	3		
6	H	1	Total	C	O	0	0
			4	1	3		
6	I	1	Total	C	O	0	0
			4	1	3		
6	J	1	Total	C	O	0	0
			4	1	3		
6	K	1	Total	C	O	0	0
			4	1	3		
6	L	1	Total	C	O	0	0
			4	1	3		

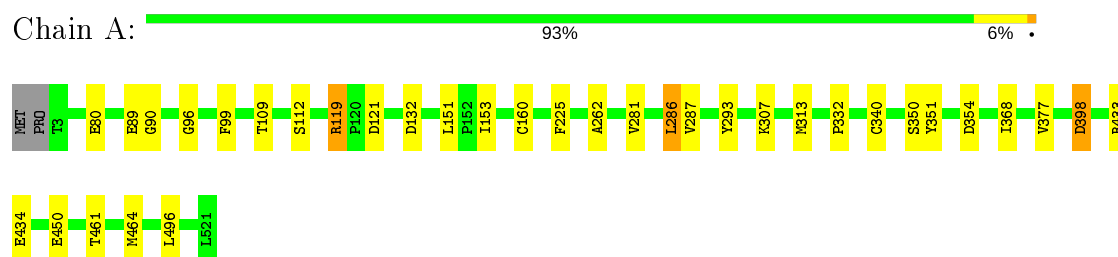
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	294	Total 294	O 294	0	0
7	B	222	Total 222	O 222	0	0
7	D	321	Total 321	O 321	0	0
7	C	235	Total 235	O 235	0	0
7	E	248	Total 248	O 248	0	0
7	F	220	Total 220	O 220	0	0
7	G	231	Total 231	O 231	0	0
7	H	212	Total 212	O 212	0	0
7	I	130	Total 130	O 130	0	0
7	J	251	Total 251	O 251	0	0
7	K	217	Total 217	O 217	0	0
7	L	217	Total 217	O 217	0	0

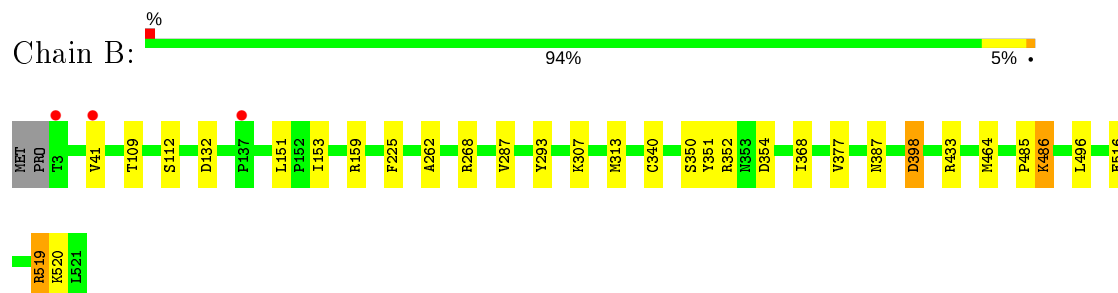
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

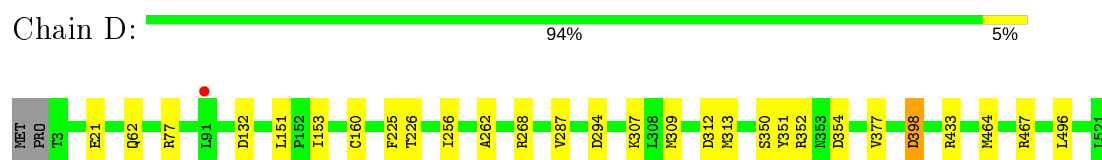
- Molecule 1: leucyl aminopeptidase



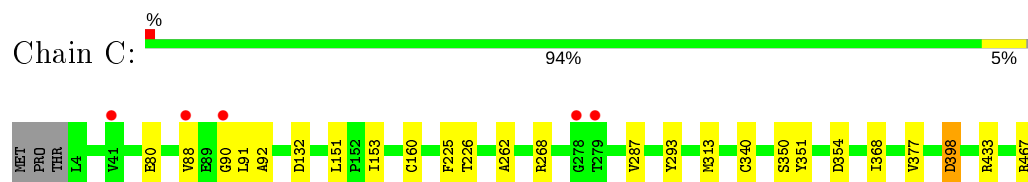
- Molecule 1: leucyl aminopeptidase



- Molecule 1: leucyl aminopeptidase

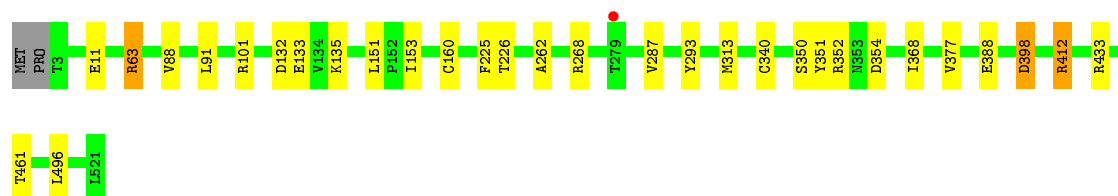


- Molecule 1: leucyl aminopeptidase



- Molecule 1: leucyl aminopeptidase





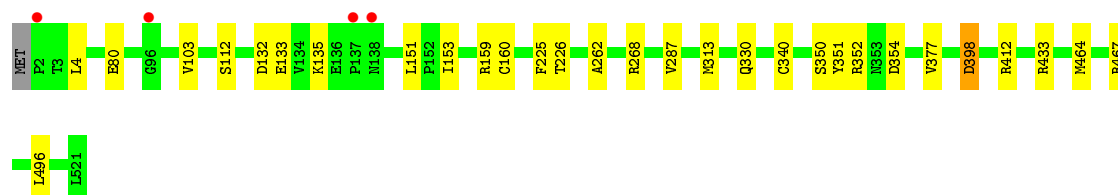
- Molecule 1: leucyl aminopeptidase

Chain F: 96%



- Molecule 1: leucyl aminopeptidase

Chain G: 94% 6%



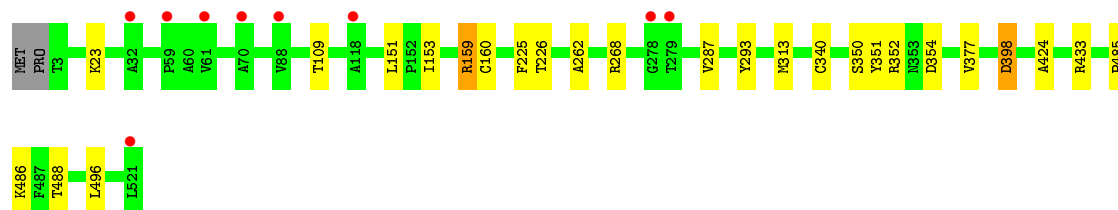
- Molecule 1: leucyl aminopeptidase

Chain H: 95%



- Molecule 1: leucyl aminopeptidase

Chain I: 95% 5% 2%

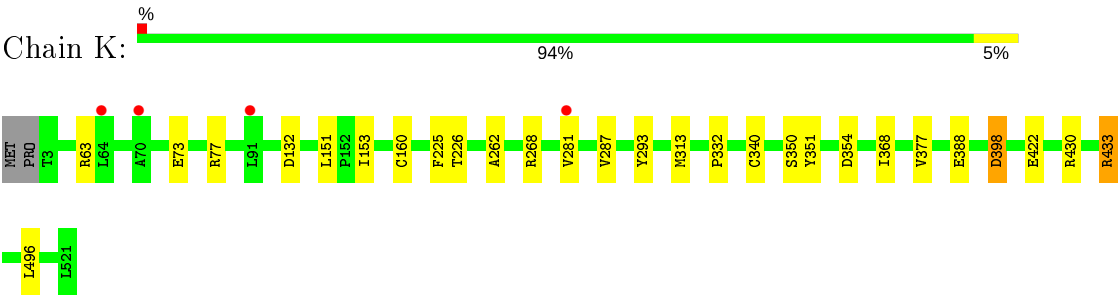


- Molecule 1: leucyl aminopeptidase

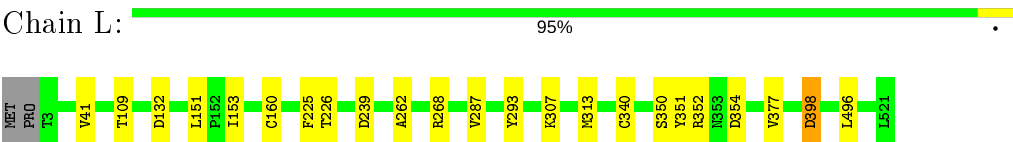
Chain J: 95% 5%



● Molecule 1: leucyl aminopeptidase



● Molecule 1: leucyl aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.26Å 143.45Å 268.03Å 90.00° 95.54° 90.00°	Depositor
Resolution (Å)	80.33 – 2.30 80.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (80.33-2.30) 99.7 (80.33-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.189 , 0.214 0.197 , 0.219	Depositor DCC
$R_{free}$ test set	14322 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	48865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, BES, MN, EPE, 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	0.77	2/3913 (0.1%)	0.83	8/5337 (0.1%)
1	B	0.72	1/3889 (0.0%)	0.80	5/5313 (0.1%)
1	C	0.71	0/3888	0.76	2/5307 (0.0%)
1	D	0.73	1/3887 (0.0%)	0.77	1/5305 (0.0%)
1	E	0.72	2/3890 (0.1%)	0.80	6/5311 (0.1%)
1	F	0.71	0/3886	0.76	1/5306 (0.0%)
1	G	0.73	2/3896 (0.1%)	0.77	2/5322 (0.0%)
1	H	0.76	0/3868	0.80	4/5285 (0.1%)
1	I	0.73	0/3866	0.76	2/5282 (0.0%)
1	J	0.73	2/3889 (0.1%)	0.78	3/5308 (0.1%)
1	K	0.73	0/3859	0.77	3/5272 (0.1%)
1	L	0.76	0/3859	0.76	1/5275 (0.0%)
All	All	0.73	10/46590 (0.0%)	0.78	38/63623 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	80	GLU	CD-OE1	-6.50	1.18	1.25
1	A	450	GLU	CD-OE2	-6.42	1.18	1.25
1	G	80	GLU	CD-OE1	-6.00	1.19	1.25
1	B	112	SER	CB-OG	5.56	1.49	1.42
1	D	21	GLU	CD-OE1	-5.52	1.19	1.25

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	H	433	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	E	433[A]	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	E	433[B]	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	B	433	ARG	NE-CZ-NH2	-7.47	116.56	120.30

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	3833	0	3758	21	0
1	B	3805	0	3695	15	0
1	C	3807	0	3717	17	0
1	D	3809	0	3726	16	0
1	E	3809	0	3717	14	0
1	F	3808	0	3715	8	0
1	G	3812	0	3703	13	0
1	H	3790	0	3681	13	0
1	I	3785	0	3680	17	0
1	J	3811	0	3726	11	0
1	K	3781	0	3677	14	0
1	L	3781	0	3655	10	0
2	A	15	0	17	1	0
2	E	15	0	17	0	0
2	L	15	0	18	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	22	0	21	0	0
5	B	22	0	21	0	0
5	C	22	0	21	0	0
5	D	22	0	21	0	0
5	E	22	0	21	0	0
5	F	22	0	21	0	0
5	G	22	0	21	0	0
5	H	22	0	21	0	0
5	I	22	0	21	0	0
5	J	22	0	21	0	0
5	K	22	0	21	0	0
5	L	22	0	21	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
6	E	4	0	1	0	0
6	F	4	0	0	0	0
6	G	4	0	0	0	0
6	H	4	0	0	0	0
6	I	4	0	0	0	0
6	J	4	0	0	0	0
6	K	4	0	0	0	0
6	L	4	0	0	0	0
7	A	294	0	0	4	0
7	B	222	0	0	2	0
7	C	235	0	0	1	0
7	D	321	0	0	3	0
7	E	248	0	0	2	0
7	F	220	0	0	0	0
7	G	231	0	0	5	0
7	H	212	0	0	3	0
7	I	130	0	0	2	0
7	J	251	0	0	0	0
7	K	217	0	0	4	0
7	L	217	0	0	0	0
All	All	48865	0	44755	144	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 2.

The worst 5 of 144 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:K:422:GLU:CB	7:K:896:HOH:O	2.11	0.98
1:C:92:ALA:CB	1:I:485:PRO:HB2	2.02	0.89
1:A:119:ARG:NH1	1:A:121:ASP:OD2	2.15	0.79
1:C:92:ALA:HB2	1:I:485:PRO:HB2	1.63	0.78
1:E:88:VAL:HG21	1:E:91:LEU:HD22	1.65	0.76

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/521 (99%)	509 (98%)	8 (2%)	1 (0%)	47	58
1	B	519/521 (100%)	509 (98%)	9 (2%)	1 (0%)	47	58
1	C	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	47	58
1	D	517/521 (99%)	507 (98%)	9 (2%)	1 (0%)	47	58
1	E	518/521 (99%)	509 (98%)	8 (2%)	1 (0%)	47	58
1	F	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	47	58
1	G	520/521 (100%)	510 (98%)	9 (2%)	1 (0%)	47	58
1	H	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	47	58
1	I	518/521 (99%)	507 (98%)	10 (2%)	1 (0%)	47	58
1	J	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	47	58
1	K	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	47	58
1	L	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	47	58
All	All	6212/6252 (99%)	6099 (98%)	101 (2%)	12 (0%)	47	58

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ASP
1	B	354	ASP
1	D	354	ASP
1	C	354	ASP
1	E	354	ASP

### 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	398/411 (97%)	387 (97%)	11 (3%)	43	60
1	B	391/411 (95%)	379 (97%)	12 (3%)	40	55
1	C	393/411 (96%)	384 (98%)	9 (2%)	50	67
1	D	393/411 (96%)	382 (97%)	11 (3%)	43	60
1	E	392/411 (95%)	383 (98%)	9 (2%)	50	67
1	F	393/411 (96%)	383 (98%)	10 (2%)	47	65
1	G	393/411 (96%)	383 (98%)	10 (2%)	47	65
1	H	389/411 (95%)	379 (97%)	10 (3%)	46	63
1	I	385/411 (94%)	375 (97%)	10 (3%)	46	63
1	J	394/411 (96%)	384 (98%)	10 (2%)	47	65
1	K	386/411 (94%)	377 (98%)	9 (2%)	50	67
1	L	386/411 (94%)	376 (97%)	10 (3%)	46	63
All	All	4693/4932 (95%)	4572 (97%)	121 (3%)	46	63

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	153	ILE
1	G	225	PHE
1	L	109	THR
1	F	160	CYS

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Mol	Chain	Res	Type
1	F	496	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	210	GLN
1	F	413	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 62 ligands modelled in this entry, 24 are monoatomic - leaving 38 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	$\# Z  > 2$
6	BCT	J	605	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BES	K	604	4	19,22,22	1.01	1 (5%)	23,29,29	1.71	6 (26%)
5	BES	B	604	4	19,22,22	0.81	1 (5%)	23,29,29	1.61	5 (21%)
6	BCT	C	605	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BCT	B	605	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	I	601	-	4,4,4	0.11	0	6,6,6	0.46	0
3	SO4	D	601	-	4,4,4	0.21	0	6,6,6	0.46	0
3	SO4	H	601	-	4,4,4	0.49	0	6,6,6	0.67	0
2	EPE	A	601	-	15,15,15	1.91	1 (6%)	18,20,20	1.79	2 (11%)
6	BCT	L	606	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BCT	I	605	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BCT	H	605	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BES	I	604	4	19,22,22	1.22	2 (10%)	23,29,29	1.74	4 (17%)
5	BES	L	605	4	19,22,22	0.73	0	23,29,29	1.74	6 (26%)
5	BES	C	604	4	19,22,22	0.79	1 (5%)	23,29,29	1.66	4 (17%)
5	BES	F	604	4	19,22,22	1.04	1 (5%)	23,29,29	1.73	5 (21%)
5	BES	E	604	4	19,22,22	0.92	1 (5%)	23,29,29	1.61	5 (21%)
2	EPE	E	601	-	15,15,15	2.10	1 (6%)	18,20,20	1.96	4 (22%)
3	SO4	B	601	-	4,4,4	0.28	0	6,6,6	0.35	0
3	SO4	G	601	-	4,4,4	0.28	0	6,6,6	0.39	0
5	BES	A	605	4	19,22,22	0.78	0	23,29,29	1.83	4 (17%)
3	SO4	C	601	-	4,4,4	0.38	0	6,6,6	0.98	1 (16%)
5	BES	D	604	4	19,22,22	0.86	1 (5%)	23,29,29	1.90	5 (21%)
2	EPE	L	601	-	15,15,15	1.77	1 (6%)	18,20,20	2.22	6 (33%)
3	SO4	L	602	-	4,4,4	0.28	0	6,6,6	0.13	0
5	BES	G	604	4	19,22,22	0.93	2 (10%)	23,29,29	1.71	4 (17%)
5	BES	J	604	4	19,22,22	1.20	2 (10%)	23,29,29	1.55	3 (13%)
6	BCT	K	605	-	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	J	601	-	4,4,4	0.32	0	6,6,6	0.54	0
3	SO4	F	601	-	4,4,4	0.26	0	6,6,6	0.35	0
3	SO4	A	602	-	4,4,4	0.33	0	6,6,6	0.42	0
6	BCT	D	605	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BCT	G	605	-	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	K	601	-	4,4,4	0.11	0	6,6,6	0.25	0
6	BCT	A	606	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BCT	F	605	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BCT	E	605	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BES	H	604	4	19,22,22	1.00	1 (5%)	23,29,29	1.62	5 (21%)

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
5	BES	J	604	4	-	9/20/24/24	0/1/1/1
5	BES	I	604	4	-	8/20/24/24	0/1/1/1
5	BES	K	604	4	-	6/20/24/24	0/1/1/1
5	BES	B	604	4	-	9/20/24/24	0/1/1/1
5	BES	D	604	4	-	10/20/24/24	0/1/1/1
5	BES	C	604	4	-	11/20/24/24	0/1/1/1
5	BES	F	604	4	-	6/20/24/24	0/1/1/1
5	BES	L	605	4	-	9/20/24/24	0/1/1/1
5	BES	E	604	4	-	7/20/24/24	0/1/1/1
2	EPE	E	601	-	-	1/9/19/19	0/1/1/1
2	EPE	A	601	-	-	1/9/19/19	0/1/1/1
5	BES	A	605	4	-	6/20/24/24	0/1/1/1
2	EPE	L	601	-	-	4/9/19/19	0/1/1/1
5	BES	H	604	4	-	9/20/24/24	0/1/1/1
5	BES	G	604	4	-	7/20/24/24	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	EPE	C10-S	-7.74	1.66	1.77
2	A	601	EPE	C10-S	-6.89	1.67	1.77
2	L	601	EPE	C10-S	-6.43	1.68	1.77
5	I	604	BES	C2-C1	-3.78	1.49	1.54
5	J	604	BES	O2-C2	3.01	1.48	1.42

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	EPE	O1S-S-C10	6.35	114.56	106.92
5	G	604	BES	O3-C3-N1	4.94	132.08	122.93
2	A	601	EPE	O2S-S-C10	4.86	112.76	106.92
5	D	604	BES	O3-C3-N1	4.70	131.63	122.93
5	H	604	BES	O3-C3-N1	4.56	131.38	122.93

There are no chirality outliers.

5 of 103 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	604	BES	N2-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	K	604	BES	N2-C1-C2-C3
5	B	604	BES	N2-C1-C2-C3
5	L	605	BES	N2-C1-C2-C3
5	L	605	BES	C6-C1-C2-C3

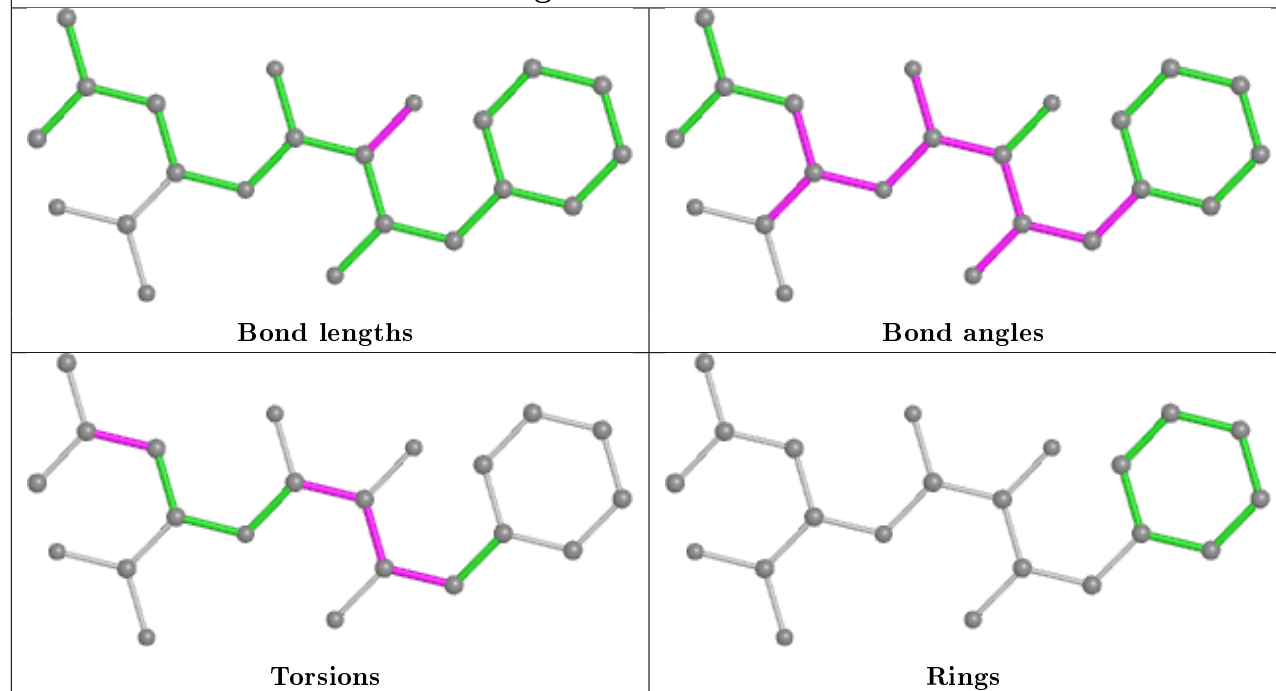
There are no ring outliers.

2 monomers are involved in 2 short contacts:

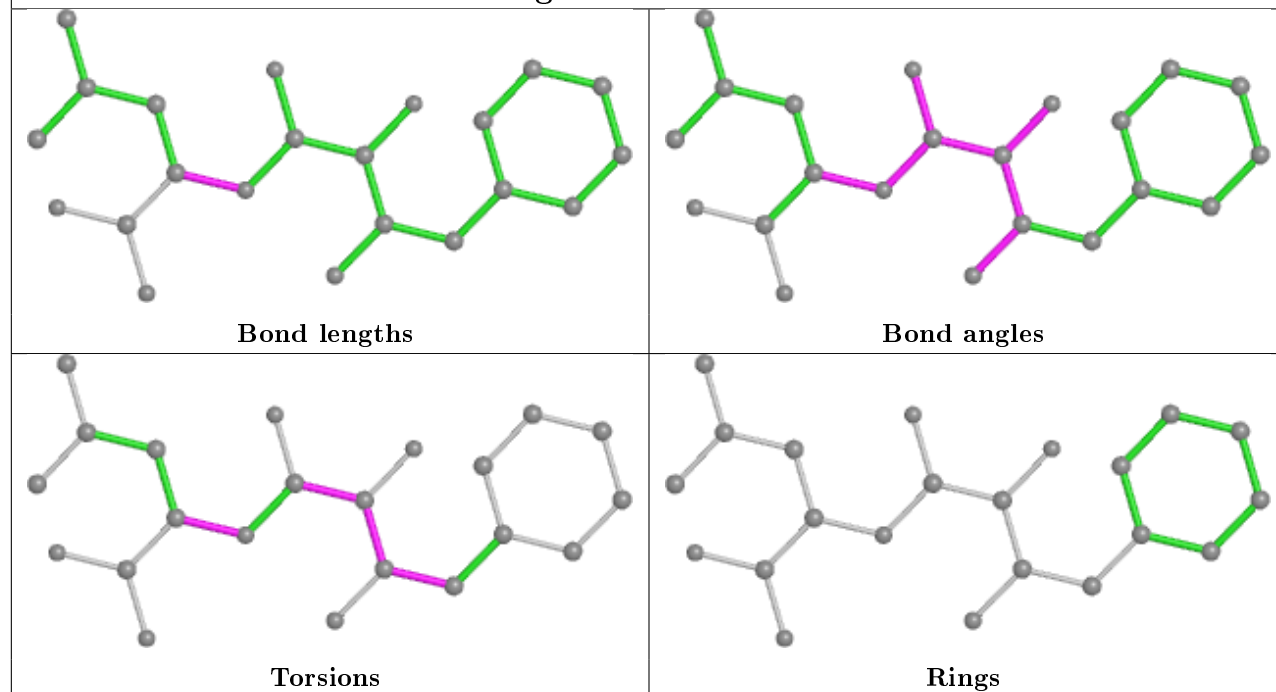
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	EPE	1	0
2	L	601	EPE	2	0

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

## Ligand BES K 604

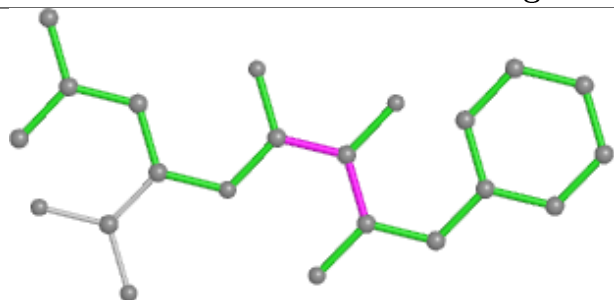


## Ligand BES B 604

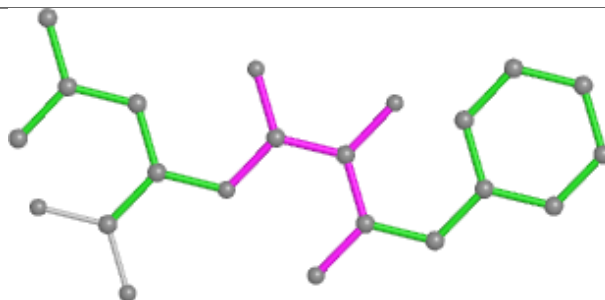




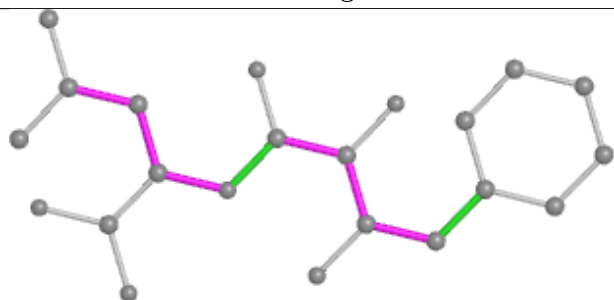
## Ligand BES I 604



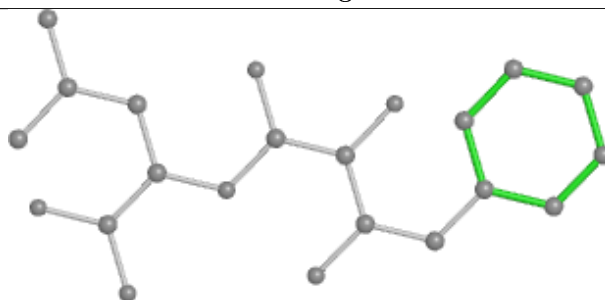
Bond lengths



Bond angles

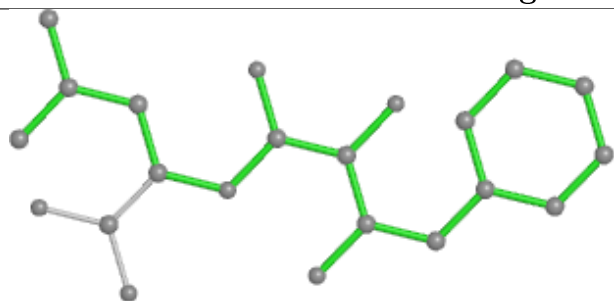


Torsions

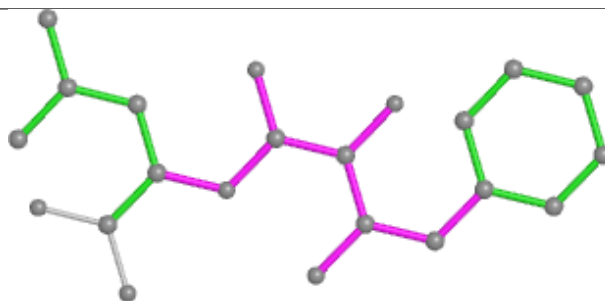


Rings

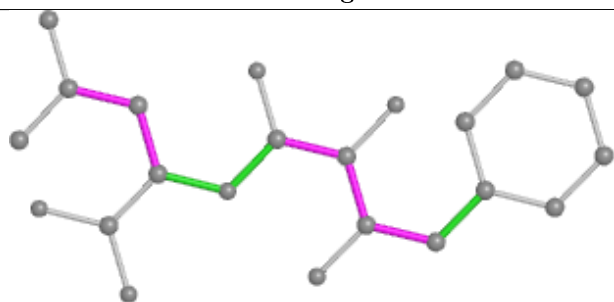
## Ligand BES L 605



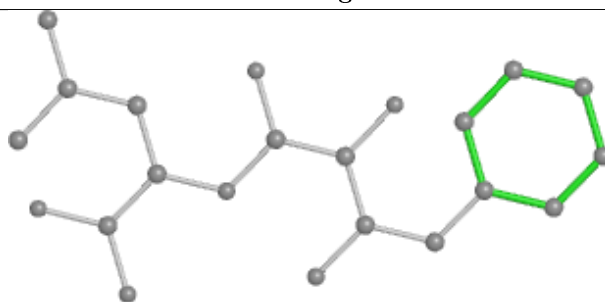
Bond lengths



Bond angles

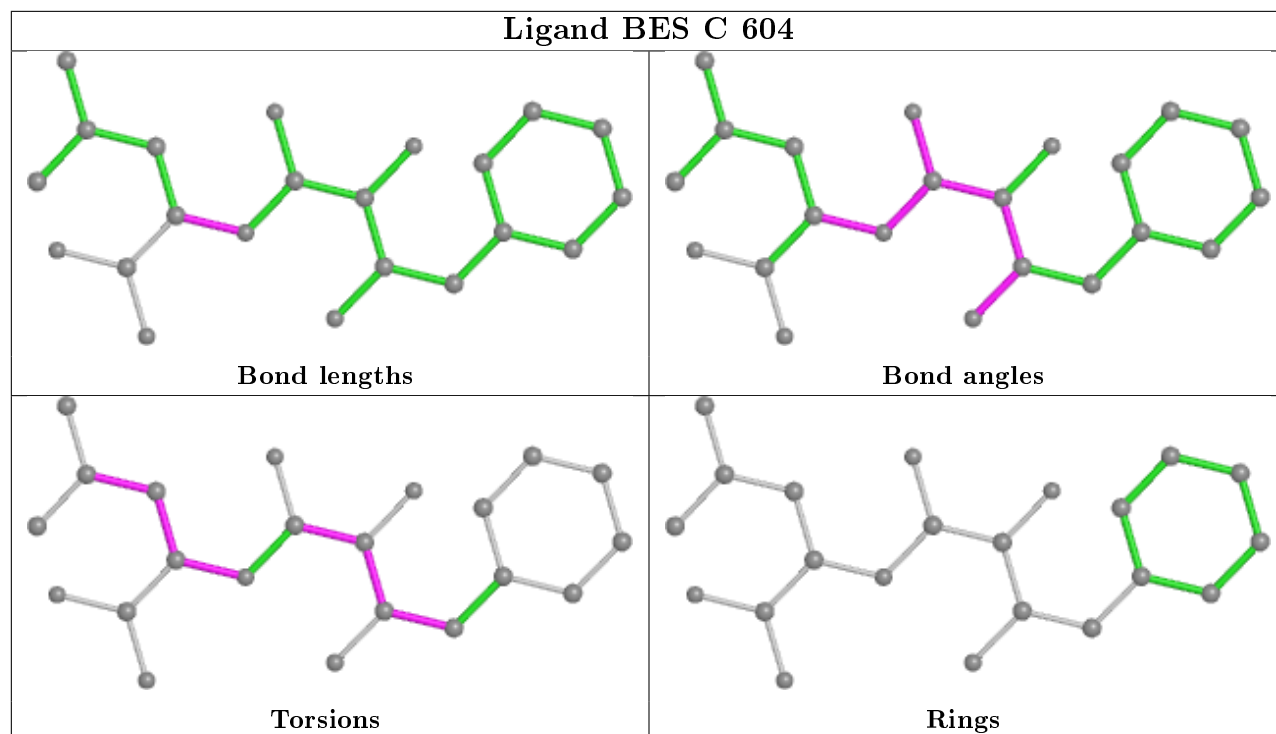


Torsions

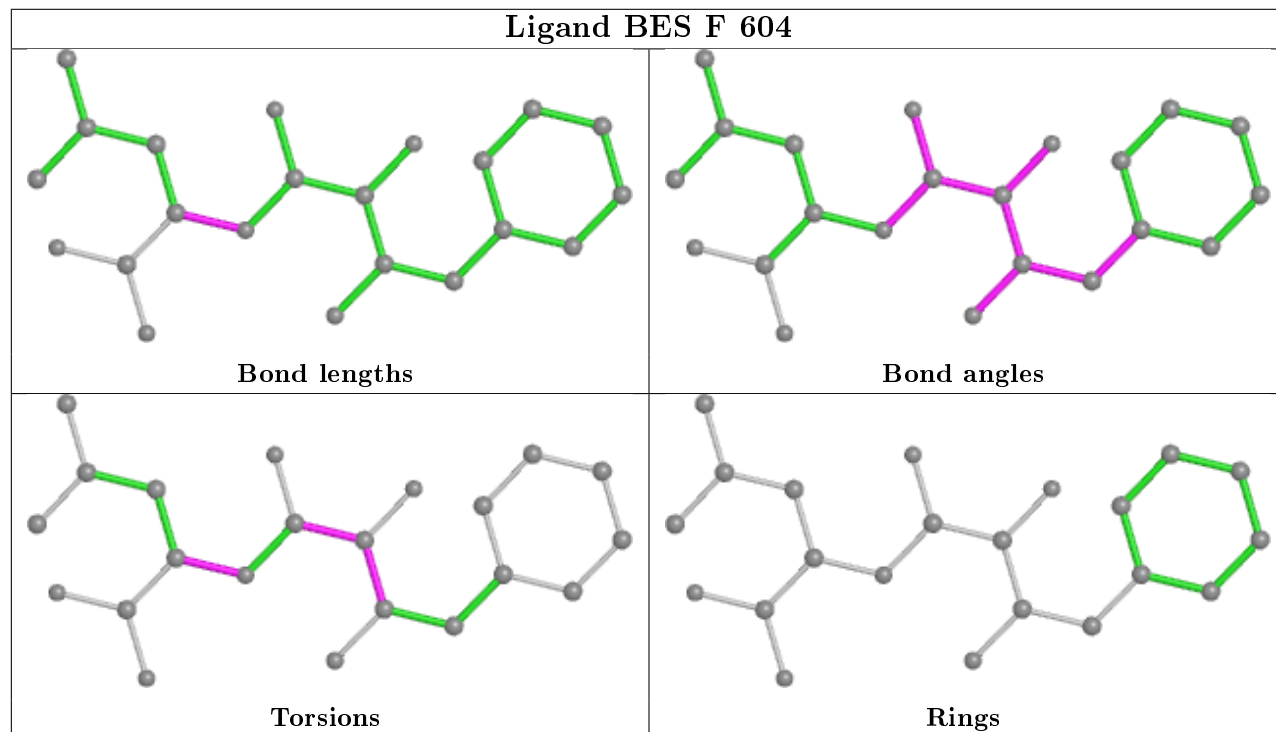


Rings

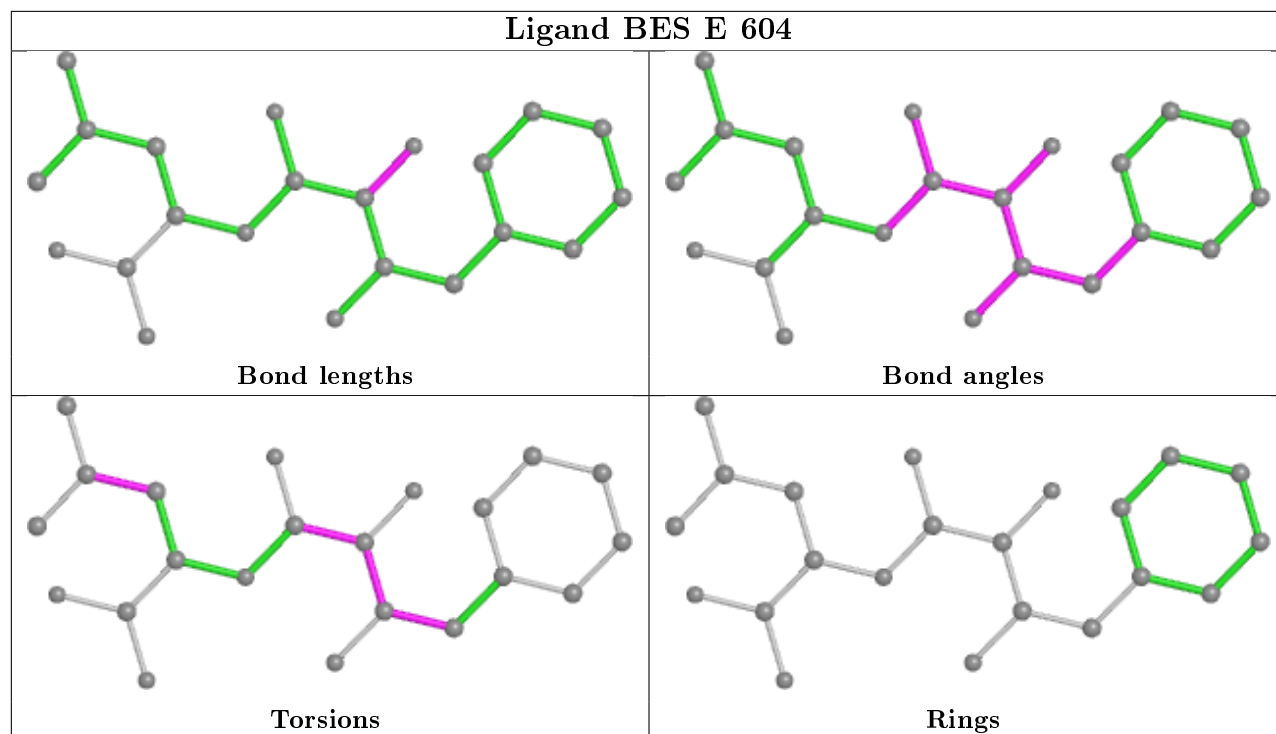
## Ligand BES C 604



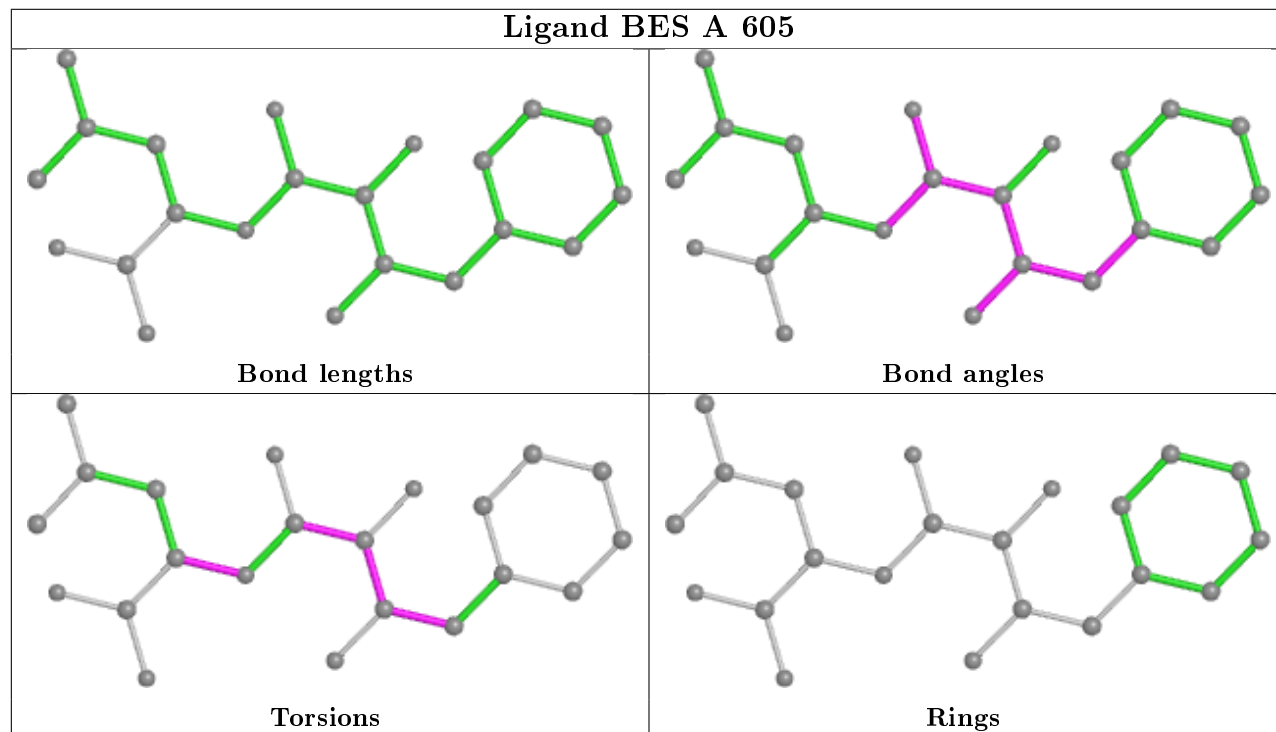
## Ligand BES F 604



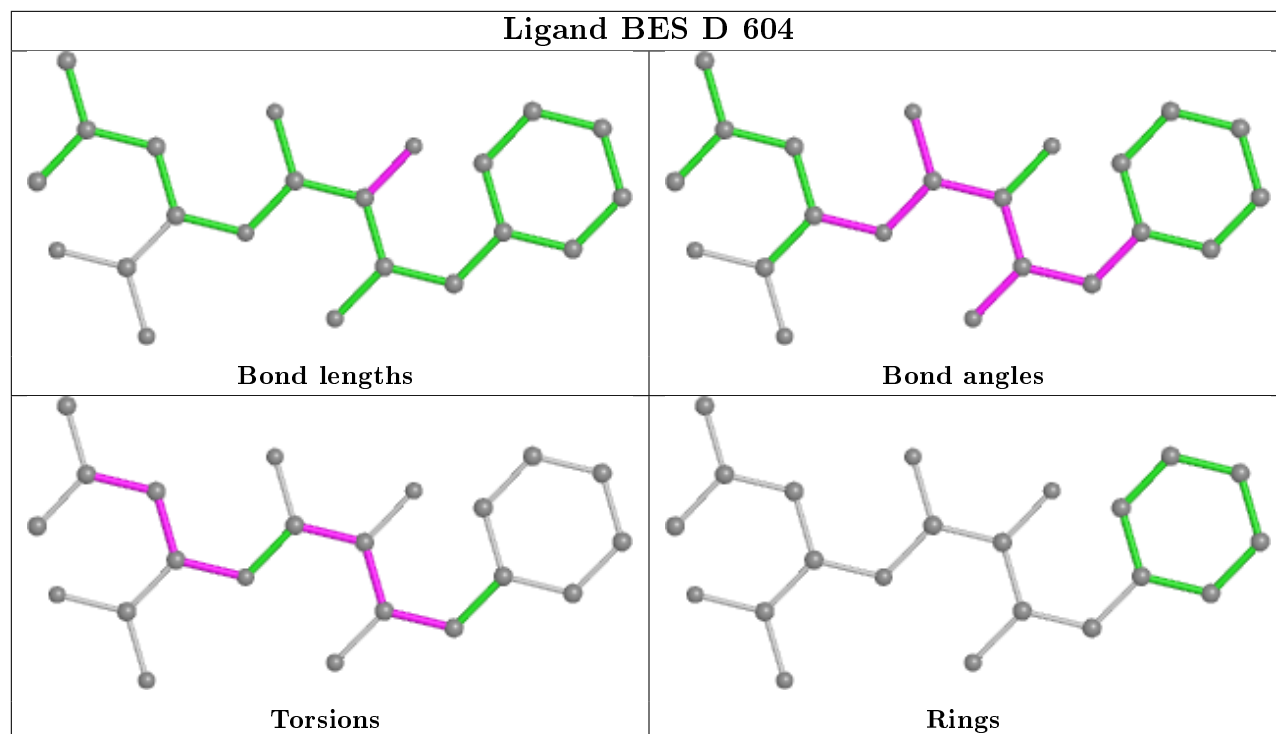
## Ligand BES E 604



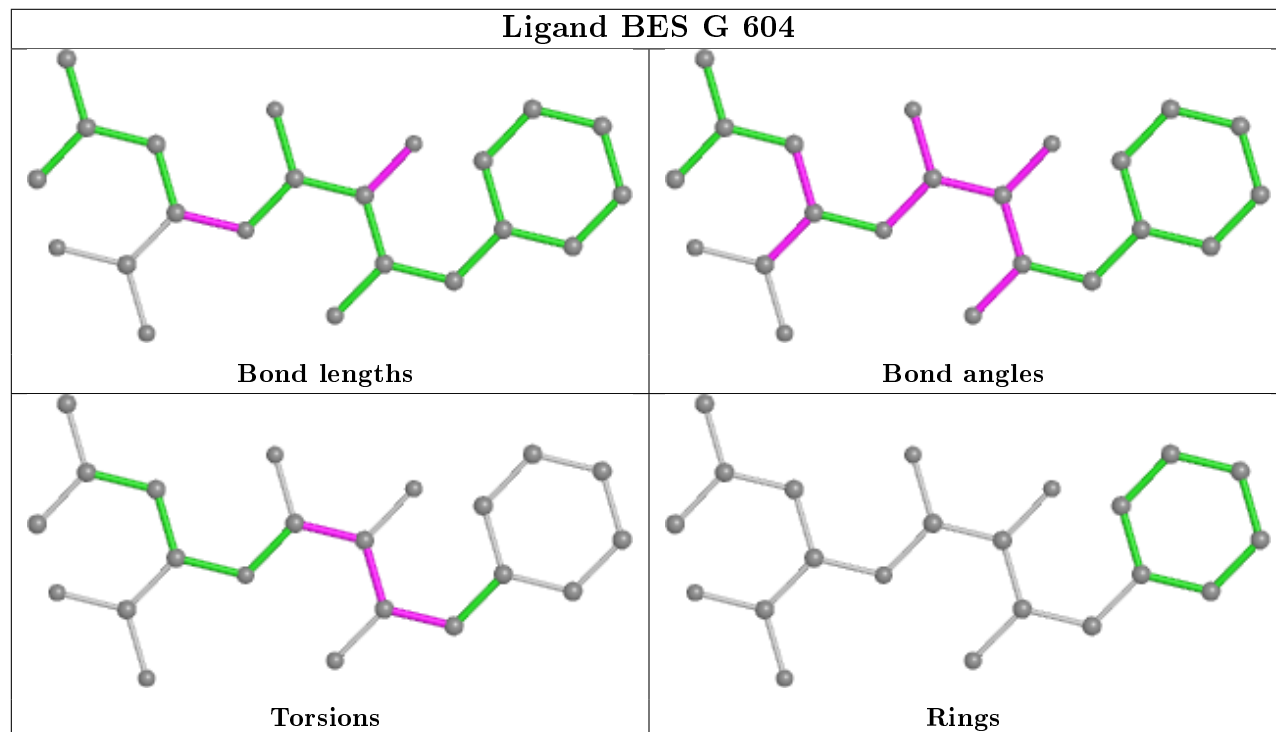
## Ligand BES A 605

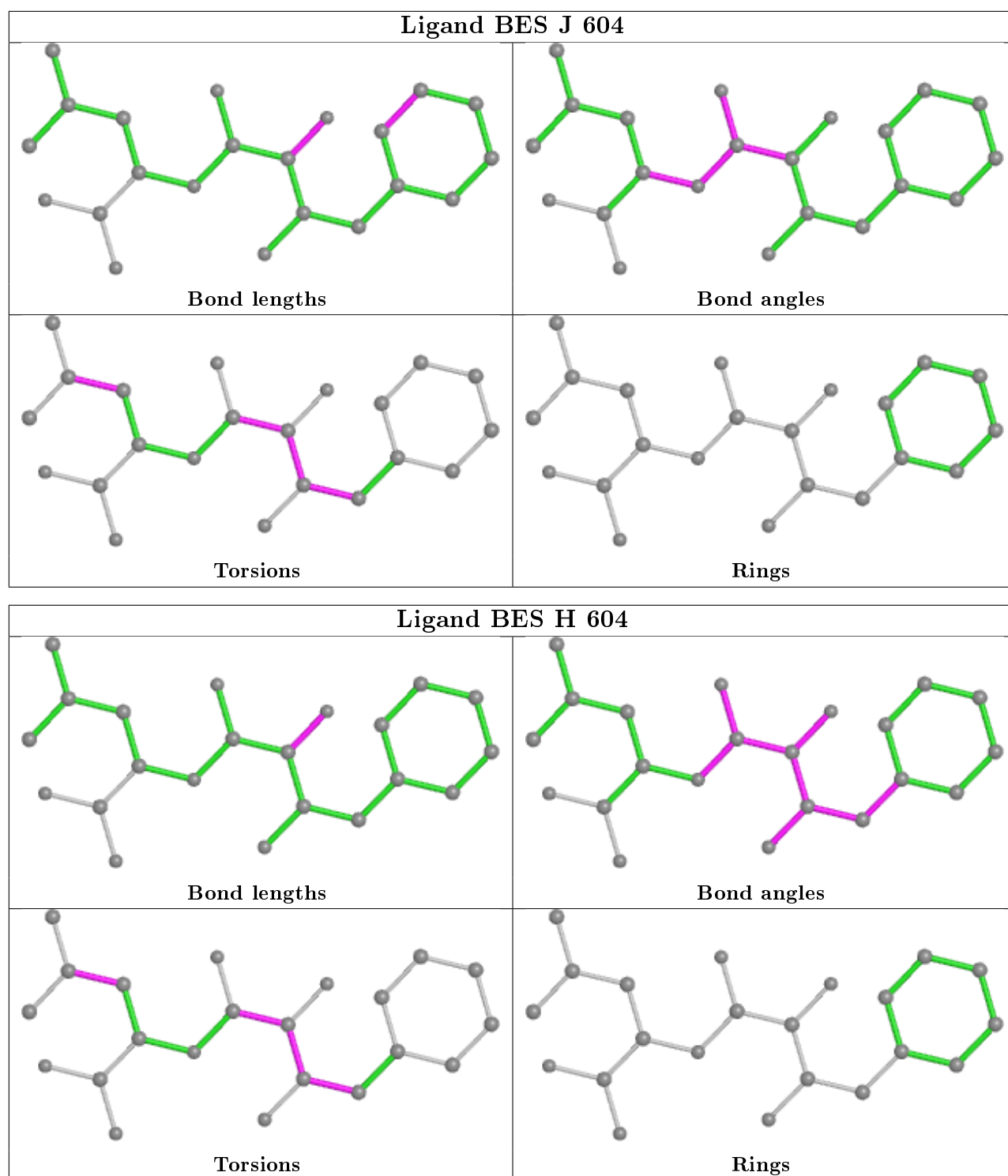


## Ligand BES D 604



## Ligand BES G 604





## 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 [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	519/521 (99%)	-0.34	0 <a href="#">100</a> <a href="#">100</a>	21, 27, 46, 78	0
1	B	519/521 (99%)	-0.23	3 (0%) <a href="#">89</a> <a href="#">92</a>	23, 31, 49, 71	0
1	C	518/521 (99%)	-0.24	5 (0%) <a href="#">82</a> <a href="#">86</a>	24, 33, 49, 76	0
1	D	519/521 (99%)	-0.32	1 (0%) <a href="#">95</a> <a href="#">96</a>	21, 29, 46, 72	0
1	E	519/521 (99%)	-0.37	1 (0%) <a href="#">95</a> <a href="#">96</a>	23, 31, 46, 70	0
1	F	519/521 (99%)	-0.26	1 (0%) <a href="#">95</a> <a href="#">96</a>	22, 31, 47, 81	0
1	G	520/521 (99%)	-0.42	4 (0%) <a href="#">86</a> <a href="#">89</a>	23, 30, 47, 81	0
1	H	519/521 (99%)	-0.24	1 (0%) <a href="#">95</a> <a href="#">96</a>	23, 32, 49, 80	0
1	I	519/521 (99%)	0.06	9 (1%) <a href="#">70</a> <a href="#">76</a>	27, 38, 53, 70	0
1	J	519/521 (99%)	-0.21	2 (0%) <a href="#">92</a> <a href="#">95</a>	23, 30, 49, 71	0
1	K	519/521 (99%)	-0.12	4 (0%) <a href="#">86</a> <a href="#">89</a>	24, 32, 51, 92	0
1	L	519/521 (99%)	-0.29	0 <a href="#">100</a> <a href="#">100</a>	23, 30, 45, 65	0
All	All	6228/6252 (99%)	-0.25	31 (0%) <a href="#">91</a> <a href="#">94</a>	21, 31, 49, 92	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	GLY	4.2
1	I	279	THR	3.6
1	I	61	VAL	2.9
1	B	137	PRO	2.8
1	G	96	GLY	2.7

### 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 ⓘ

There are no carbohydrates 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, 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(Å <sup>2</sup> )	Q<0.9
6	BCT	J	605	4/4	0.90	0.22	28,34,34,49	0
3	SO4	H	601	5/5	0.90	0.25	53,67,76,84	0
5	BES	H	604	22/22	0.91	0.14	40,45,51,55	0
6	BCT	G	605	4/4	0.92	0.22	32,40,42,55	0
2	EPE	L	601	15/15	0.92	0.23	58,71,91,95	0
6	BCT	K	605	4/4	0.92	0.24	28,36,38,51	0
6	BCT	A	606	4/4	0.92	0.18	31,41,43,49	0
5	BES	F	604	22/22	0.92	0.16	34,38,50,54	0
6	BCT	B	605	4/4	0.93	0.18	30,36,37,45	0
4	MN	I	603	1/1	0.93	0.05	43,43,43,43	0
6	BCT	E	605	4/4	0.93	0.18	30,36,38,47	0
5	BES	G	604	22/22	0.93	0.14	35,41,49,54	0
5	BES	J	604	22/22	0.93	0.16	37,38,46,52	0
6	BCT	L	606	4/4	0.93	0.20	34,40,42,52	0
5	BES	B	604	22/22	0.93	0.16	34,38,45,54	0
5	BES	E	604	22/22	0.93	0.15	37,40,50,54	0
6	BCT	D	605	4/4	0.94	0.15	33,37,39,39	0
5	BES	K	604	22/22	0.94	0.12	34,40,46,49	0
6	BCT	I	605	4/4	0.94	0.15	39,44,46,53	0
5	BES	D	604	22/22	0.94	0.16	32,34,42,44	0
6	BCT	H	605	4/4	0.94	0.18	28,36,38,49	0
5	BES	I	604	22/22	0.94	0.13	39,47,54,59	0
3	SO4	I	601	5/5	0.94	0.14	63,68,71,76	0
5	BES	L	605	22/22	0.94	0.13	39,44,49,53	0
5	BES	A	605	22/22	0.94	0.16	30,36,42,44	0
5	BES	C	604	22/22	0.95	0.13	37,43,47,53	0
3	SO4	L	602	5/5	0.95	0.15	76,77,80,88	0
3	SO4	F	601	5/5	0.95	0.14	54,65,72,73	0
2	EPE	E	601	15/15	0.95	0.16	52,81,93,94	0
6	BCT	C	605	4/4	0.95	0.20	37,39,41,53	0
2	EPE	A	601	15/15	0.96	0.17	46,66,74,76	0
3	SO4	C	601	5/5	0.96	0.12	50,57,64,65	0

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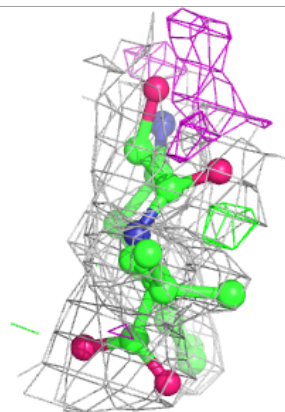
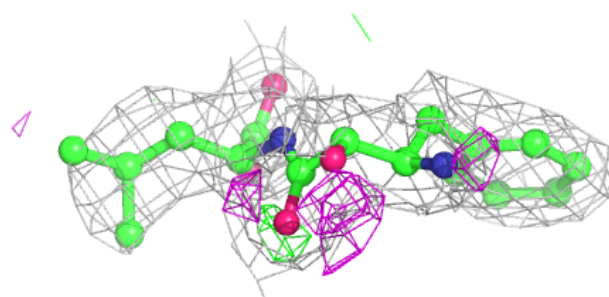
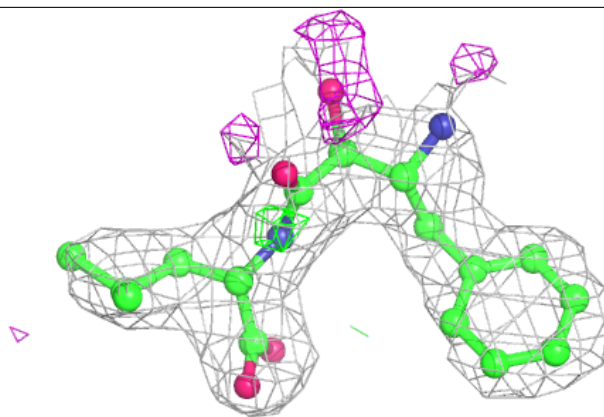
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BCT	F	605	4/4	0.96	0.17	31,37,42,47	0
4	MN	C	602	1/1	0.96	0.03	39,39,39,39	0
3	SO4	D	601	5/5	0.97	0.15	56,56,66,67	0
3	SO4	K	601	5/5	0.97	0.19	56,62,67,68	0
4	MN	B	603	1/1	0.97	0.09	29,29,29,29	0
3	SO4	A	602	5/5	0.97	0.11	54,57,59,62	0
3	SO4	G	601	5/5	0.97	0.14	52,62,67,73	0
4	MN	A	604	1/1	0.98	0.07	26,26,26,26	0
4	MN	B	602	1/1	0.98	0.06	33,33,33,33	0
3	SO4	B	601	5/5	0.98	0.09	63,63,67,71	0
4	MN	H	602	1/1	0.98	0.06	36,36,36,36	0
4	MN	K	602	1/1	0.98	0.06	33,33,33,33	0
4	MN	A	603	1/1	0.98	0.04	31,31,31,31	0
4	MN	E	602	1/1	0.98	0.04	35,35,35,35	0
4	MN	G	603	1/1	0.98	0.06	30,30,30,30	0
4	MN	F	603	1/1	0.98	0.07	31,31,31,31	0
3	SO4	J	601	5/5	0.98	0.12	54,54,63,64	0
4	MN	G	602	1/1	0.98	0.04	36,36,36,36	0
4	MN	I	602	1/1	0.99	0.05	43,43,43,43	0
4	MN	D	602	1/1	0.99	0.05	31,31,31,31	0
4	MN	E	603	1/1	0.99	0.06	32,32,32,32	0
4	MN	D	603	1/1	0.99	0.06	28,28,28,28	0
4	MN	K	603	1/1	0.99	0.06	30,30,30,30	0
4	MN	J	602	1/1	0.99	0.05	32,32,32,32	0
4	MN	C	603	1/1	0.99	0.06	32,32,32,32	0
4	MN	L	604	1/1	0.99	0.07	33,33,33,33	0
4	MN	H	603	1/1	0.99	0.05	34,34,34,34	0
4	MN	L	603	1/1	0.99	0.05	36,36,36,36	0
4	MN	J	603	1/1	0.99	0.07	31,31,31,31	0
4	MN	F	602	1/1	1.00	0.06	31,31,31,31	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.

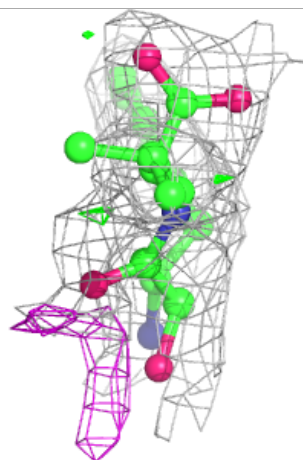
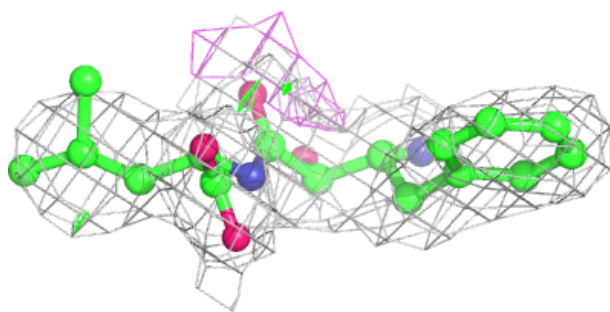
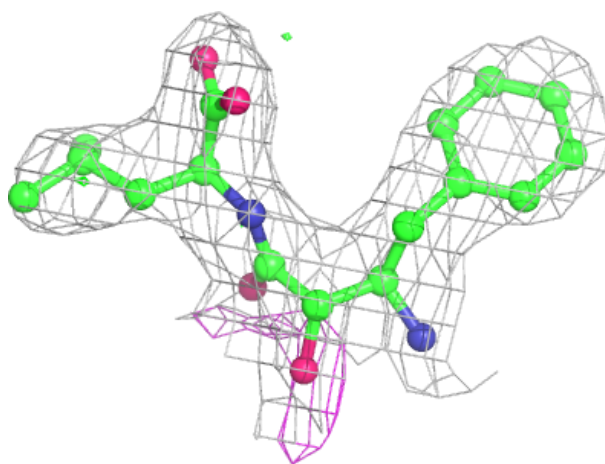
**Electron density around BES H 604:**

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



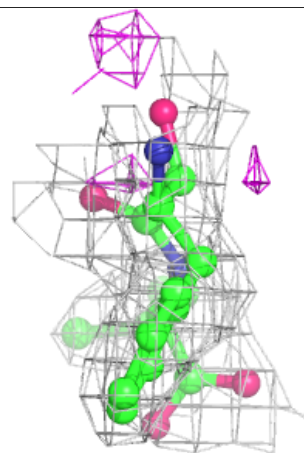
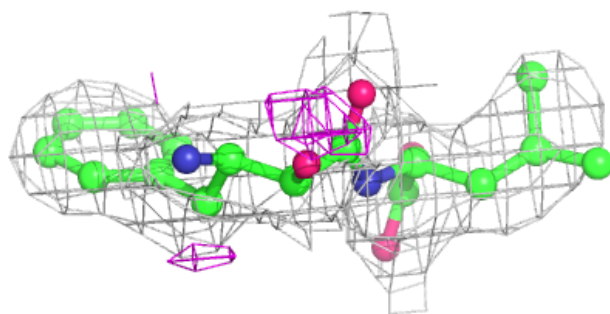
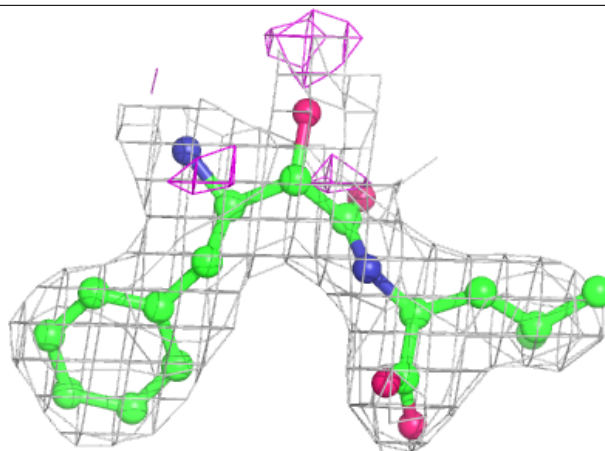
**Electron density around BES F 604:**

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

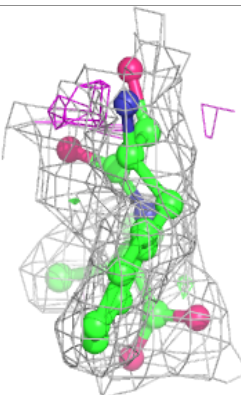
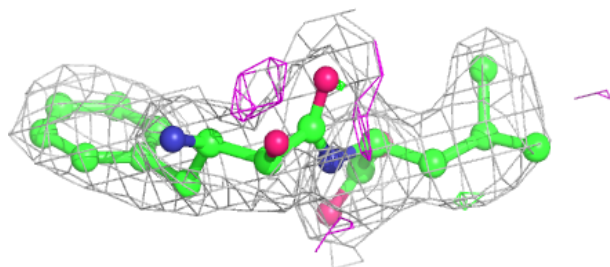
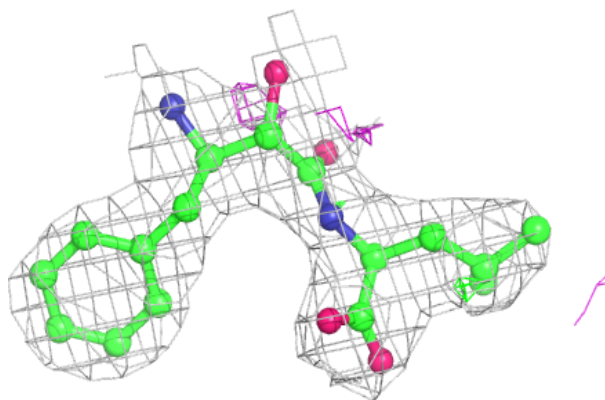


**Electron density around BES G 604:**

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

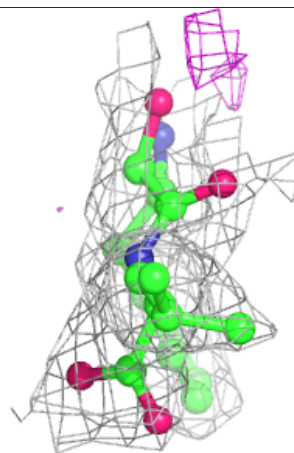
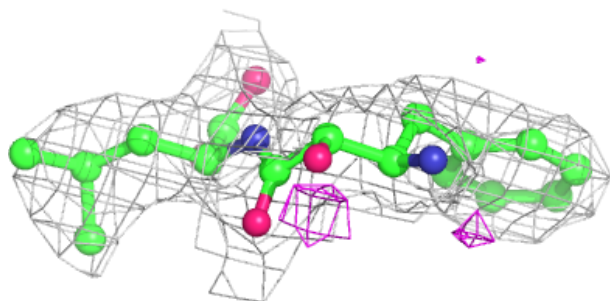
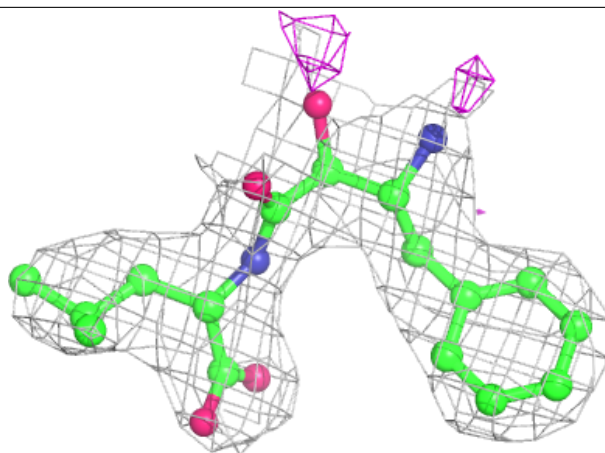
**Electron density around BES J 604:**

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



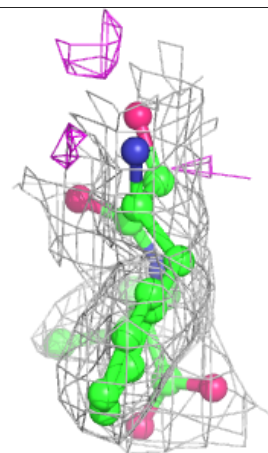
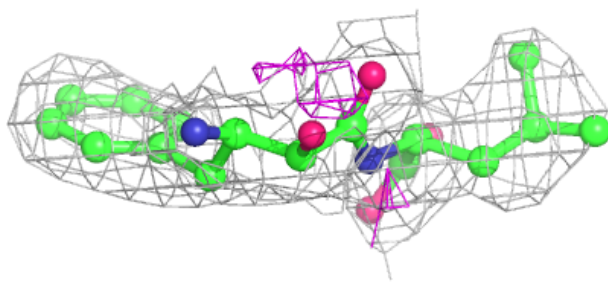
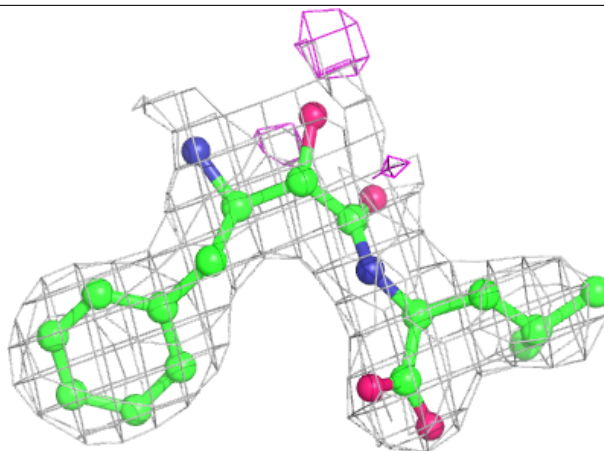
**Electron density around BES B 604:**

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



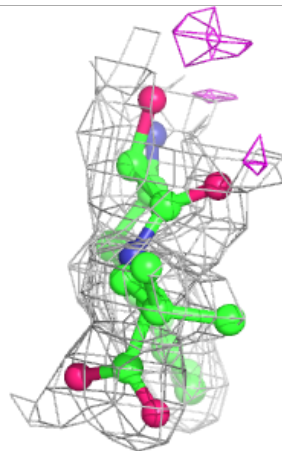
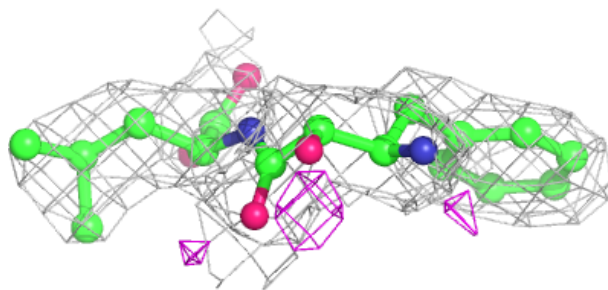
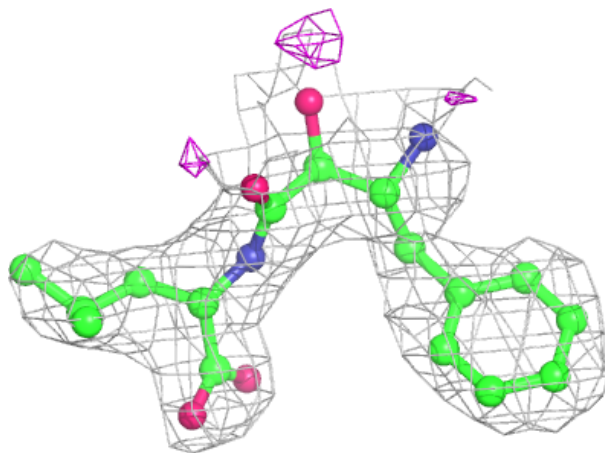
**Electron density around BES E 604:**

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



**Electron density around BES K 604:**

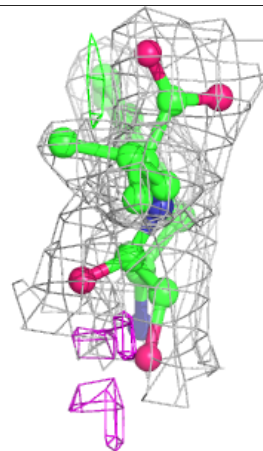
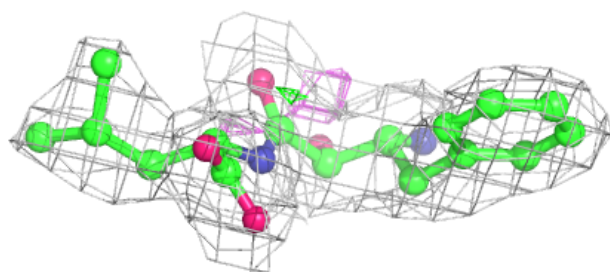
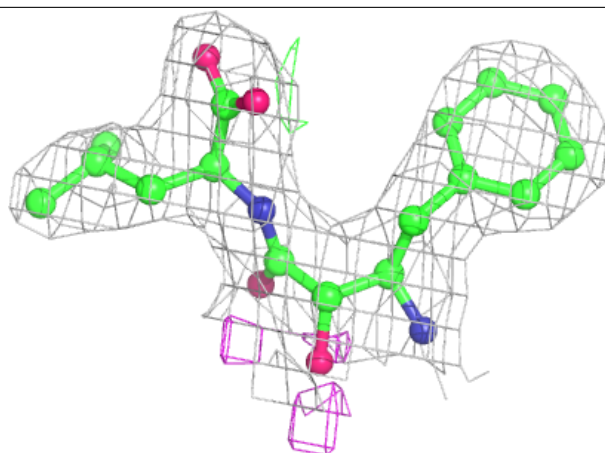
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around BES D 604:**

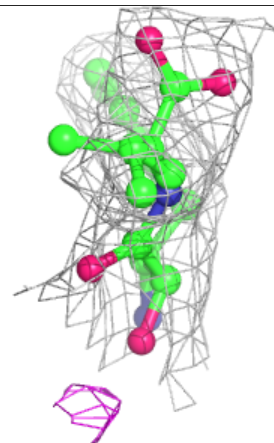
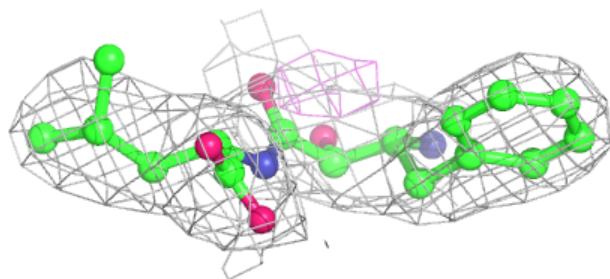
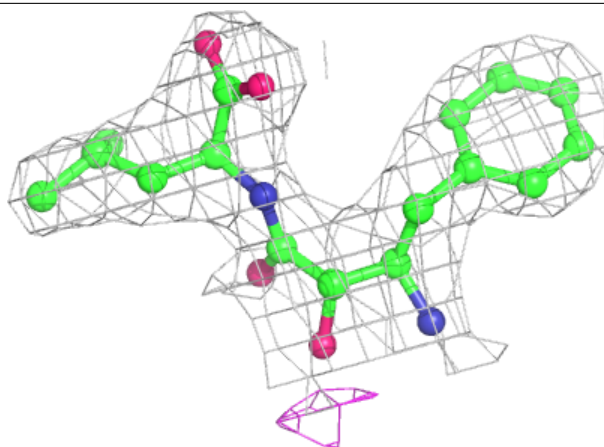
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





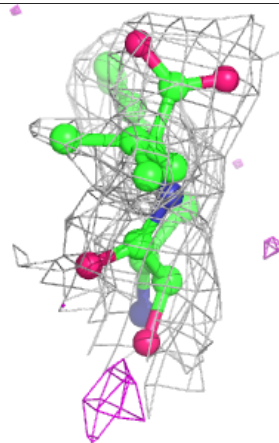
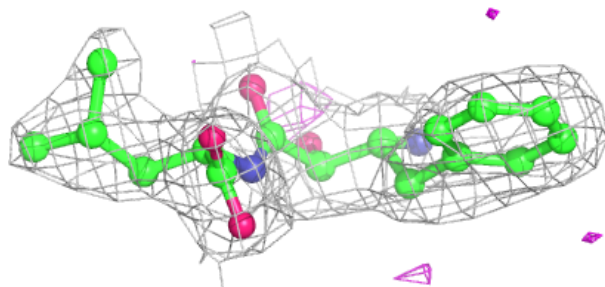
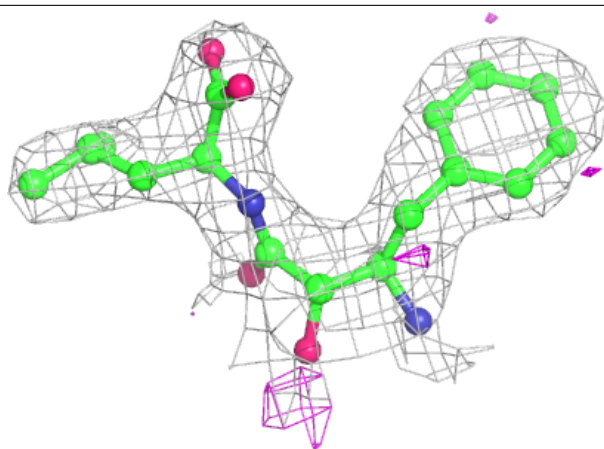
**Electron density around BES I 604:**

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



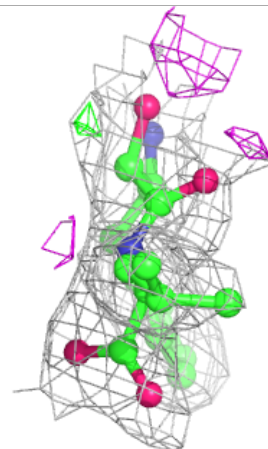
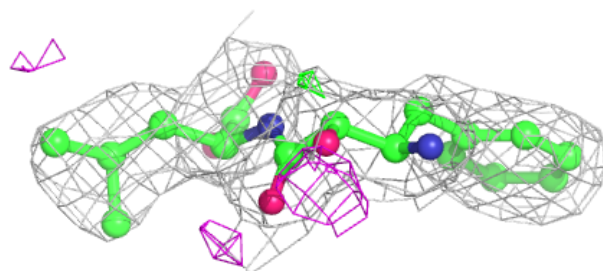
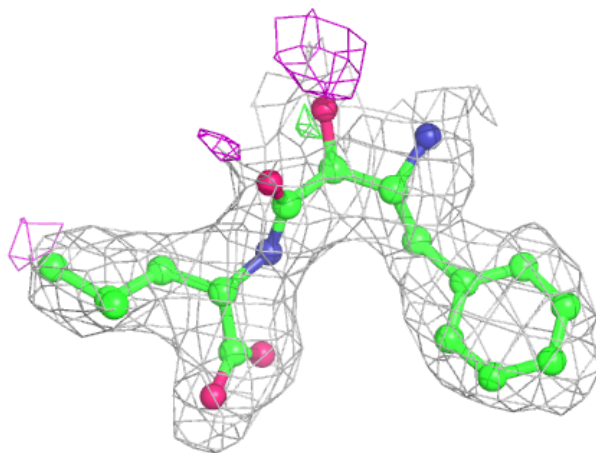
**Electron density around BES L 605:**

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



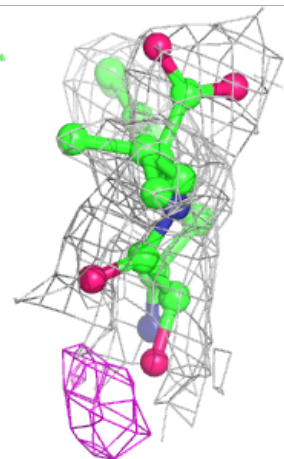
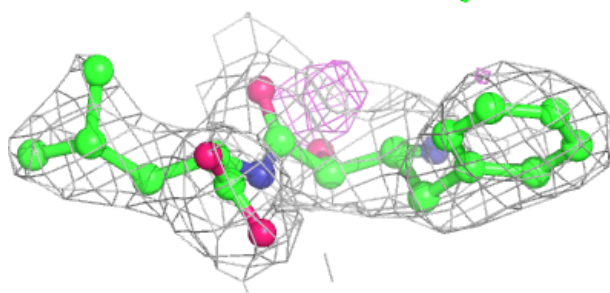
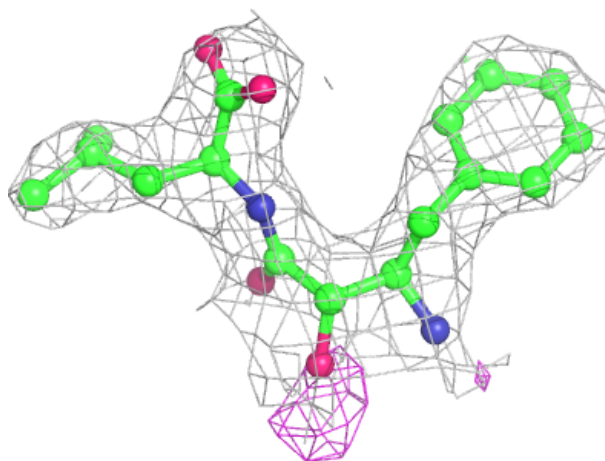
**Electron density around BES A 605:**

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



**Electron density around BES C 604:**

$2mF_o-DF_c$  (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.