



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:20 PM UTC

PDB ID : 3KR4 / pdb_00003kr4
Title : Structure of a protease 3
Authors : McGowan, S.; Whisstock, J.C.
Deposited on : 2009-11-17
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

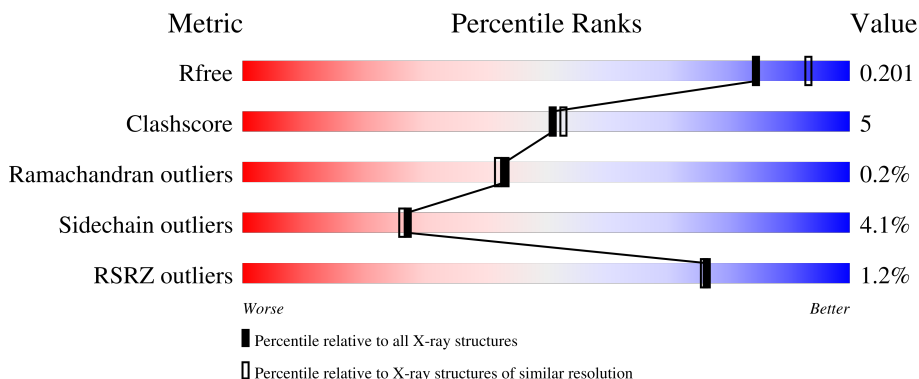
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	528	 89% 8% .
1	B	528	 86% 10% ..
1	C	528	 85% 12% ..
1	D	528	 86% 10% ..
1	E	528	 84% 11% ..

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Mol	Chain	Length	Quality of chain	
1	F	528	% 82%	13% ..
1	G	528	% 87%	9% ..
1	H	528	2% 84%	10% ..
1	I	528	% 86%	10% ..
1	J	528	% 85%	10% ..
1	K	528	% 86%	9% ..
1	L	528	2% 83%	13% ..

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
6	SO4	L	25	-	-	X	-
7	1PE	B	61	-	-	X	-
7	1PE	B	62	-	-	-	X
7	1PE	L	612	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 53016 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 M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	518	3983	2558	639	766	20	3	1	0
1	B	518	3936	2531	637	748	20	0	0	0
1	C	518	3955	2545	638	753	19	0	1	0
1	D	516	3946	2541	638	747	20	0	0	0
1	E	510	3896	2509	626	743	18	0	0	0
1	F	510	3873	2492	623	739	19	0	0	0
1	G	516	3996	2564	650	762	20	0	0	0
1	H	509	3943	2534	641	749	19	0	1	0
1	I	518	4008	2570	652	767	19	0	1	0
1	J	513	3963	2545	641	757	20	0	1	0
1	K	509	3935	2528	638	750	19	0	1	0
1	L	513	3944	2532	635	758	19	0	1	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP Q8IL11
A	515	GLN	ASN	engineered mutation	UNP Q8IL11
A	546	GLN	ASN	engineered mutation	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11
A	607	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11

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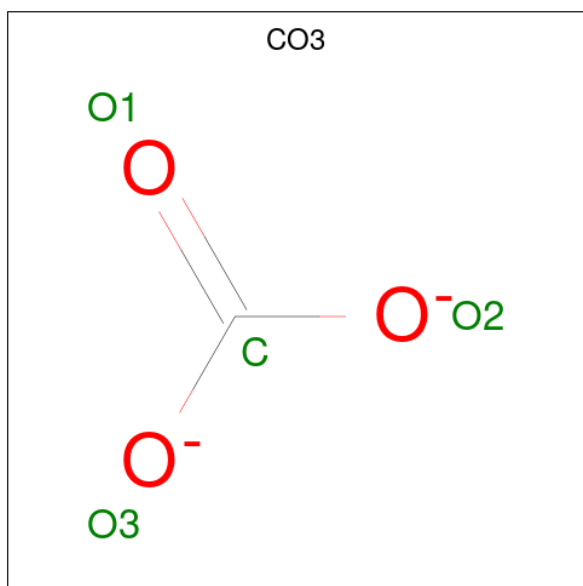
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	606	HIS	-	expression tag	UNP Q8IL11
G	607	HIS	-	expression tag	UNP Q8IL11
G	608	HIS	-	expression tag	UNP Q8IL11
G	609	HIS	-	expression tag	UNP Q8IL11
G	610	HIS	-	expression tag	UNP Q8IL11
G	611	HIS	-	expression tag	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	606	HIS	-	expression tag	UNP Q8IL11
H	607	HIS	-	expression tag	UNP Q8IL11
H	608	HIS	-	expression tag	UNP Q8IL11
H	609	HIS	-	expression tag	UNP Q8IL11
H	610	HIS	-	expression tag	UNP Q8IL11
H	611	HIS	-	expression tag	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	606	HIS	-	expression tag	UNP Q8IL11
I	607	HIS	-	expression tag	UNP Q8IL11
I	608	HIS	-	expression tag	UNP Q8IL11
I	609	HIS	-	expression tag	UNP Q8IL11
I	610	HIS	-	expression tag	UNP Q8IL11
I	611	HIS	-	expression tag	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	606	HIS	-	expression tag	UNP Q8IL11
J	607	HIS	-	expression tag	UNP Q8IL11
J	608	HIS	-	expression tag	UNP Q8IL11
J	609	HIS	-	expression tag	UNP Q8IL11
J	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	expression tag	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	606	HIS	-	expression tag	UNP Q8IL11
K	607	HIS	-	expression tag	UNP Q8IL11
K	608	HIS	-	expression tag	UNP Q8IL11
K	609	HIS	-	expression tag	UNP Q8IL11
K	610	HIS	-	expression tag	UNP Q8IL11
K	611	HIS	-	expression tag	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	606	HIS	-	expression tag	UNP Q8IL11
L	607	HIS	-	expression tag	UNP Q8IL11
L	608	HIS	-	expression tag	UNP Q8IL11
L	609	HIS	-	expression tag	UNP Q8IL11
L	610	HIS	-	expression tag	UNP Q8IL11
L	611	HIS	-	expression tag	UNP Q8IL11

- Molecule 2 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		

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

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

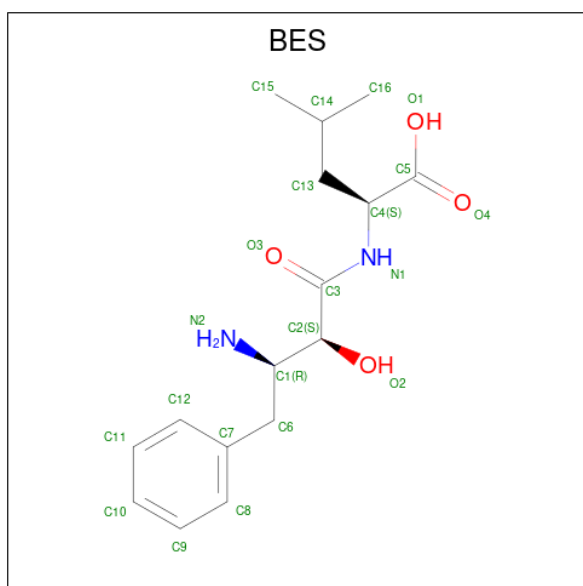
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	G	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	I	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Zn 1 1	0	0
3	K	1	Total Zn 1 1	0	0
3	L	1	Total Zn 1 1	0	0

- Molecule 4 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (CCD ID: BES) (formula: $C_{16}H_{24}N_2O_4$).



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

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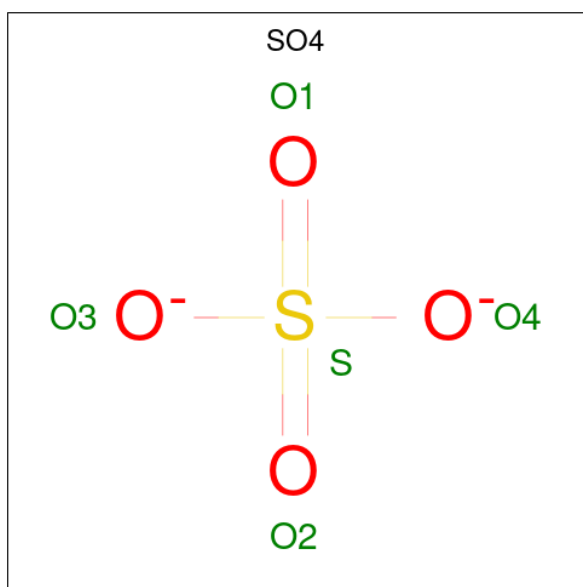
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	1	Total	C	N	O	0	0
			22	16	2	4		
4	J	1	Total	C	N	O	0	0
			22	16	2	4		
4	K	1	Total	C	N	O	0	0
			22	16	2	4		
4	L	1	Total	C	N	O	0	0
			22	16	2	4		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

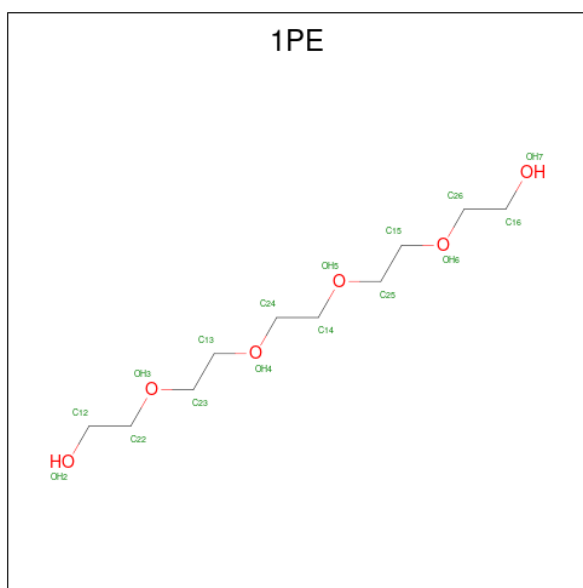
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	L	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	6	3		
7	A	1	Total	C	O	0	0
			12	8	4		
7	B	1	Total	C	O	0	0
			10	7	3		
7	B	1	Total	C	O	0	0
			10	7	3		
7	B	1	Total	C	O	0	0
			10	7	3		
7	C	1	Total	C	O	0	0
			13	9	4		
7	C	1	Total	C	O	0	0
			9	6	3		
7	D	1	Total	C	O	0	0
			10	7	3		
7	D	1	Total	C	O	0	0
			11	8	3		
7	D	1	Total	C	O	0	0
			10	7	3		
7	D	1	Total	C	O	0	0
			7	5	2		
7	E	1	Total	C	O	0	0
			12	8	4		
7	E	1	Total	C	O	0	0
			12	8	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	E	1	8	5	3	0	0
7	F	1	10	6	4	0	0
7	F	1	10	6	4	0	0
7	F	1	10	6	4	0	0
7	G	1	9	6	3	0	0
7	G	1	7	4	3	0	0
7	G	1	6	4	2	0	0
7	G	1	6	4	2	0	0
7	G	1	15	10	5	0	0
7	H	1	10	7	3	0	0
7	H	1	10	7	3	0	0
7	I	1	15	10	5	0	0
7	I	1	11	8	3	0	0
7	I	1	7	5	2	0	0
7	J	1	11	7	4	0	0
7	J	1	10	6	4	0	0
7	J	1	10	7	3	0	0
7	K	1	12	8	4	0	0
7	K	1	12	8	4	0	0
7	K	1	11	7	4	0	0
7	K	1	6	4	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			10	6	4		
7	L	1	Total	C	O	0	0
			12	8	4		
7	L	1	Total	C	O	0	0
			11	7	4		

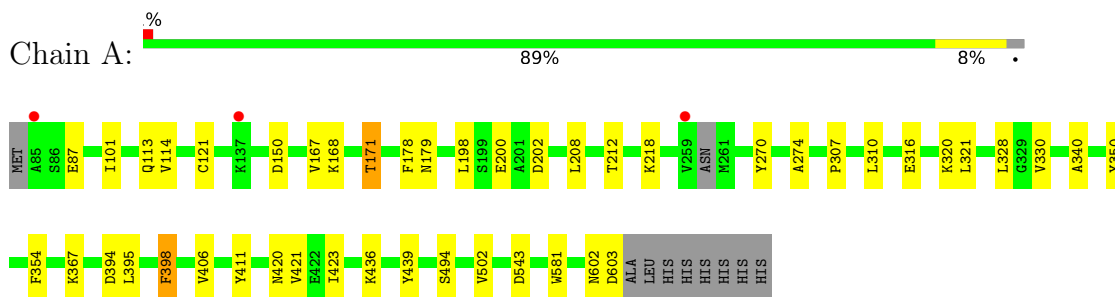
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	423	Total	O	0	0
			423	423		
8	B	361	Total	O	0	0
			361	361		
8	C	427	Total	O	0	0
			427	427		
8	D	411	Total	O	0	0
			411	411		
8	E	442	Total	O	0	0
			442	442		
8	F	373	Total	O	0	0
			373	373		
8	G	421	Total	O	0	0
			421	421		
8	H	389	Total	O	0	0
			389	389		
8	I	414	Total	O	0	0
			414	414		
8	J	403	Total	O	0	0
			403	403		
8	K	438	Total	O	0	0
			438	438		
8	L	356	Total	O	0	0
			356	356		

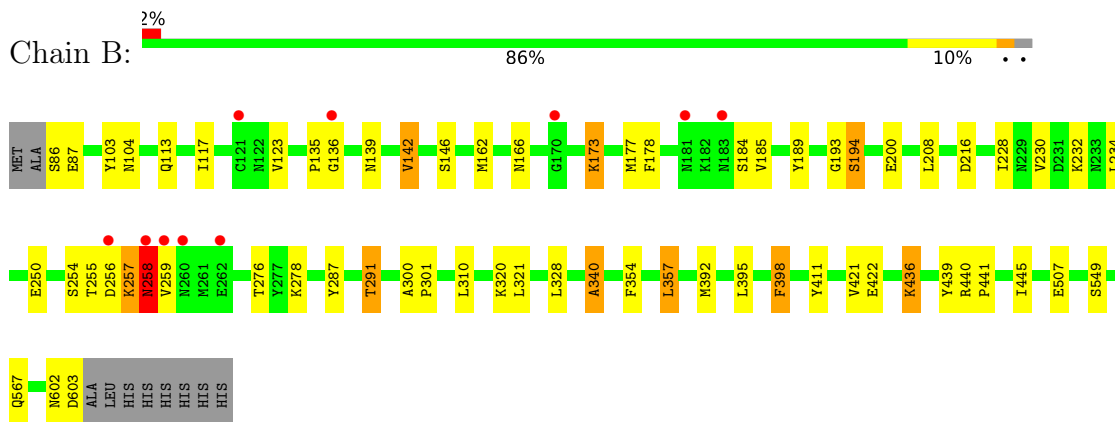
3 Residue-property plots [i](#)

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.

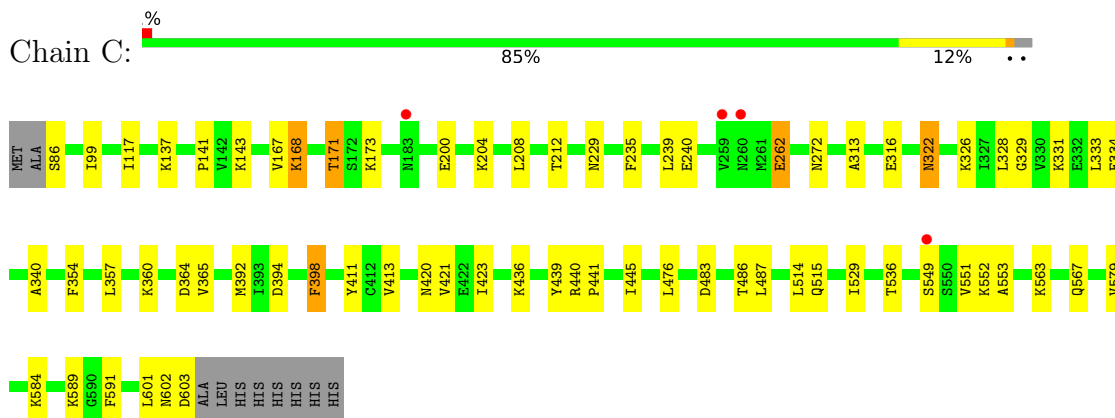
- Molecule 1: M17 leucyl aminopeptidase



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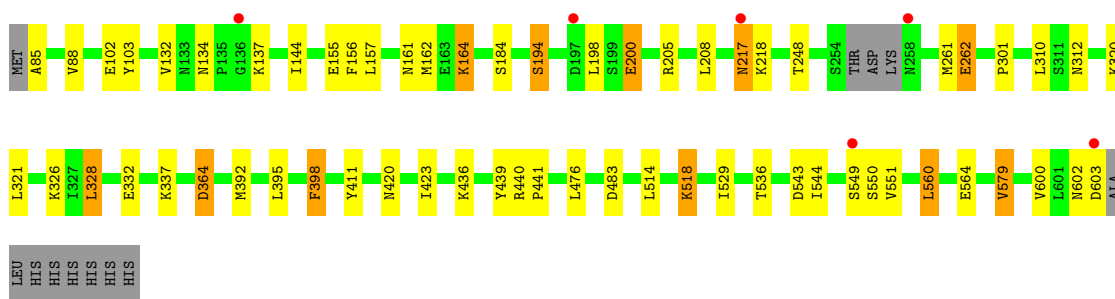


- Molecule 1: M17 leucyl aminopeptidase



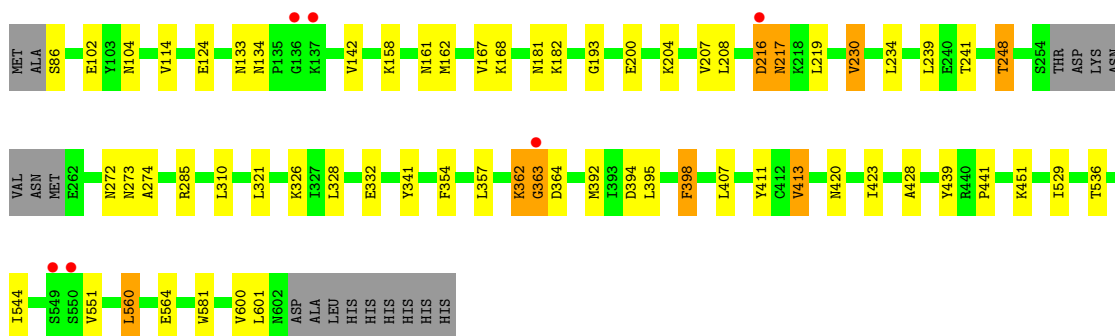
- Molecule 1: M17 leucyl aminopeptidase

Chain D: 86% 10% ..



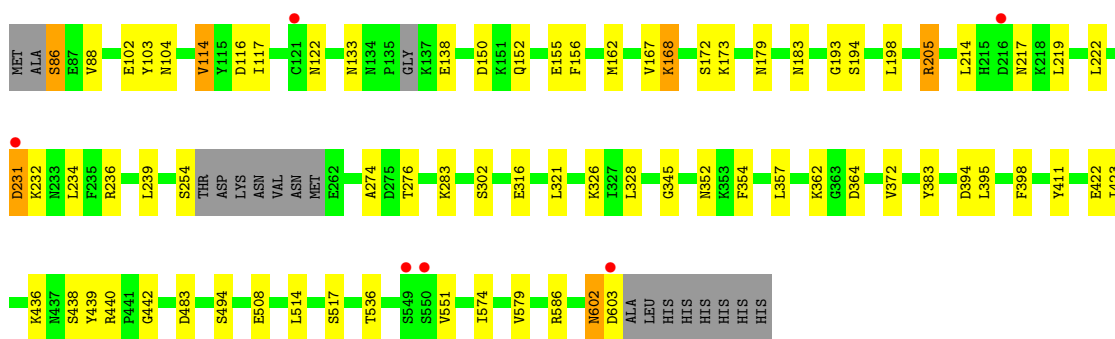
- Molecule 1: M17 leucyl aminopeptidase

Chain E: 84% 11% ..



- Molecule 1: M17 leucyl aminopeptidase

Chain F: 82% 13% ..



- Molecule 1: M17 leucyl aminopeptidase

Chain G: 87% 9% ..



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.56Å 178.12Å 230.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.15 – 2.00 43.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (43.15-2.00) 98.3 (43.15-2.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.192 , 0.242 (Not available) , 0.201	Depositor DCC
R_{free} test set	23578 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtrriage
Anisotropy	0.457	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53016	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0558e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CO3, SO4, ZN, BES, 1PE

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	1.01	4/4063 (0.1%)	0.97	2/5508 (0.0%)
1	B	0.98	5/4014 (0.1%)	1.01	4/5450 (0.1%)
1	C	1.01	3/4036 (0.1%)	0.97	7/5477 (0.1%)
1	D	1.02	1/4023 (0.0%)	1.00	3/5454 (0.1%)
1	E	1.04	2/3973 (0.1%)	1.00	3/5392 (0.1%)
1	F	1.00	2/3949 (0.1%)	1.03	3/5364 (0.1%)
1	G	1.01	2/4073 (0.0%)	0.98	4/5513 (0.1%)
1	H	0.96	1/4022 (0.0%)	1.01	10/5445 (0.2%)
1	I	0.99	3/4089 (0.1%)	0.98	6/5539 (0.1%)
1	J	1.03	2/4043 (0.0%)	1.01	8/5476 (0.1%)
1	K	1.05	2/4014 (0.0%)	1.02	10/5438 (0.2%)
1	L	1.02	4/4024 (0.1%)	1.04	8/5460 (0.1%)
All	All	1.01	31/48323 (0.1%)	1.00	68/65516 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	G	0	1
All	All	0	2

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	362	LYS	C-O	-6.71	1.15	1.24
1	B	421	VAL	C-O	-6.56	1.17	1.24
1	D	184	SER	C-O	-6.56	1.16	1.23
1	L	602	ASN	C-O	-6.50	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	123	VAL	C-O	-6.43	1.17	1.24

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	124	GLU	N-CA-C	9.21	130.43	110.80
1	G	136	GLY	CA-C-N	8.19	134.40	122.36
1	G	136	GLY	C-N-CA	8.19	134.40	122.36
1	D	579	VAL	N-CA-CB	-7.28	102.30	112.35
1	C	440	ARG	NE-CZ-NH2	-7.21	112.71	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	257	LYS	Peptide
1	G	136	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3983	0	3917	26	0
1	B	3936	0	3843	50	0
1	C	3955	0	3881	39	0
1	D	3946	0	3888	47	0
1	E	3896	0	3819	53	0
1	F	3873	0	3771	47	0
1	G	3996	0	3988	37	0
1	H	3943	0	3937	37	0
1	I	4008	0	3985	38	0
1	J	3963	0	3940	50	0
1	K	3935	0	3907	42	0
1	L	3944	0	3874	45	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	22	0	22	1	0
4	B	22	0	22	3	0
4	C	22	0	22	4	0
4	D	22	0	22	3	0
4	E	22	0	22	4	0
4	F	22	0	22	0	0
4	G	22	0	22	0	0
4	H	22	0	22	3	0
4	I	22	0	22	2	0
4	J	22	0	22	2	0
4	K	22	0	22	5	0
4	L	22	0	22	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	15	0	0	0	0
6	B	5	0	0	0	0
6	D	10	0	0	1	0
6	E	5	0	0	0	0
6	F	5	0	0	0	0
6	G	10	0	0	0	0
6	J	10	0	0	1	0
6	K	5	0	0	0	0
6	L	5	0	0	2	0
7	A	21	0	22	2	0
7	B	30	0	30	7	0
7	C	22	0	24	5	0
7	D	38	0	38	6	0
7	E	32	0	36	3	0
7	F	30	0	39	3	0
7	G	43	0	47	5	0
7	H	20	0	20	4	0
7	I	33	0	37	8	0
7	J	31	0	36	10	0
7	K	41	0	44	1	0
7	L	33	0	40	11	0
8	A	423	0	0	3	0
8	B	361	0	0	8	0
8	C	427	0	0	9	0
8	D	411	0	0	13	0
8	E	442	0	0	13	0
8	F	373	0	0	12	0
8	G	421	0	0	5	0
8	H	389	0	0	5	0
8	I	414	0	0	11	0
8	J	403	0	0	12	0
8	K	438	0	0	10	0
8	L	356	0	0	7	0
All	All	53016	0	47427	497	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 5.

The worst 5 of 497 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:104:ASN:HB2	8:B:3372:HOH:O	1.37	1.21
1:B:257:LYS:CB	1:B:258:ASN:HB3	1.71	1.18
1:F:316:GLU:HG3	7:F:32:1PE:H141	1.28	1.12
1:J:518:LYS:HE2	8:J:2650:HOH:O	1.50	1.08
1:D:320:LYS:HZ1	7:D:63:1PE:H142	1.16	1.06

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	515/528 (98%)	503 (98%)	12 (2%)	0	100	100
1	B	516/528 (98%)	502 (97%)	11 (2%)	3 (1%)	21	17
1	C	517/528 (98%)	509 (98%)	8 (2%)	0	100	100
1	D	512/528 (97%)	492 (96%)	18 (4%)	2 (0%)	30	27
1	E	506/528 (96%)	493 (97%)	10 (2%)	3 (1%)	21	17
1	F	504/528 (96%)	487 (97%)	17 (3%)	0	100	100
1	G	512/528 (97%)	500 (98%)	11 (2%)	1 (0%)	43	42
1	H	504/528 (96%)	493 (98%)	10 (2%)	1 (0%)	43	42
1	I	517/528 (98%)	507 (98%)	10 (2%)	0	100	100
1	J	510/528 (97%)	496 (97%)	14 (3%)	0	100	100
1	K	504/528 (96%)	495 (98%)	9 (2%)	0	100	100
1	L	510/528 (97%)	501 (98%)	9 (2%)	0	100	100
All	All	6127/6336 (97%)	5978 (98%)	139 (2%)	10 (0%)	43	42

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	124	GLU

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Mol	Chain	Res	Type
1	B	136	GLY
1	B	258	ASN
1	B	259	VAL
1	E	362	LYS

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	427/455 (94%)	417 (98%)	10 (2%)	44	49
1	B	414/455 (91%)	395 (95%)	19 (5%)	24	22
1	C	419/455 (92%)	404 (96%)	15 (4%)	31	31
1	D	418/455 (92%)	398 (95%)	20 (5%)	23	21
1	E	413/455 (91%)	399 (97%)	14 (3%)	32	33
1	F	409/455 (90%)	392 (96%)	17 (4%)	26	25
1	G	437/455 (96%)	422 (97%)	15 (3%)	32	33
1	H	431/455 (95%)	406 (94%)	25 (6%)	18	15
1	I	437/455 (96%)	416 (95%)	21 (5%)	23	21
1	J	432/455 (95%)	414 (96%)	18 (4%)	26	25
1	K	428/455 (94%)	414 (97%)	14 (3%)	33	34
1	L	424/455 (93%)	402 (95%)	22 (5%)	21	18
All	All	5089/5460 (93%)	4879 (96%)	210 (4%)	27	26

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	194	SER
1	I	230	VAL
1	L	310	LEU
1	H	291	THR
1	H	518	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	183	ASN
1	L	217	ASN
1	J	420	ASN
1	L	161	ASN
1	E	134	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 99 ligands modelled in this entry, 24 are monoatomic - leaving 75 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CO3	K	1002	-	3,3,3	0.43	0	2,3,3	0.94	0
7	1PE	E	43	-	7,7,15	0.54	0	6,6,14	0.29	0
4	BES	A	1003	3,5	22,22,22	0.87	0	26,29,29	1.58	4 (15%)
7	1PE	C	17	-	12,12,15	0.56	0	11,11,14	0.49	0
6	SO4	A	2	-	4,4,4	0.30	0	6,6,6	0.27	0
7	1PE	E	8	-	11,11,15	0.39	0	10,10,14	0.52	0
4	BES	B	1003	3,5	22,22,22	0.73	0	26,29,29	1.65	9 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	1PE	E	7	-	11,11,15	0.54	0	10,10,14	0.43	0
4	BES	L	1003	3,5	22,22,22	0.80	0	26,29,29	1.53	6 (23%)
6	SO4	J	20	-	4,4,4	0.18	0	6,6,6	0.21	0
7	1PE	B	61	-	9,9,15	0.64	0	8,8,14	0.83	0
6	SO4	J	18	-	4,4,4	0.43	0	6,6,6	0.57	0
7	1PE	G	47	-	5,5,15	0.51	0	4,4,14	0.50	0
2	CO3	A	1002	-	3,3,3	0.48	0	2,3,3	1.39	0
7	1PE	L	1	-	9,9,15	0.32	0	8,8,14	0.52	0
7	1PE	L	612	-	11,11,15	0.45	0	10,10,14	0.50	0
6	SO4	G	23	-	4,4,4	0.30	0	6,6,6	0.32	0
7	1PE	F	31	-	9,9,15	0.37	0	8,8,14	0.61	0
7	1PE	G	30	-	6,6,15	0.49	0	5,5,14	0.32	0
4	BES	I	1003	3,5	22,22,22	0.97	0	26,29,29	1.72	6 (23%)
2	CO3	D	1002	-	3,3,3	1.35	1 (33%)	2,3,3	1.62	1 (50%)
6	SO4	A	1	-	4,4,4	0.29	0	6,6,6	0.35	0
6	SO4	E	22	-	4,4,4	0.23	0	6,6,6	0.23	0
7	1PE	K	50	-	5,5,15	0.61	0	4,4,14	0.33	0
4	BES	H	1003	3,5	22,22,22	0.79	0	26,29,29	1.45	4 (15%)
2	CO3	G	1002	-	3,3,3	0.80	0	2,3,3	0.76	0
7	1PE	D	67	-	6,6,15	0.50	0	5,5,14	0.29	0
4	BES	C	1003	3,5	22,22,22	0.91	0	26,29,29	1.47	2 (7%)
6	SO4	F	21	-	4,4,4	0.27	0	6,6,6	0.17	0
7	1PE	B	60	-	9,9,15	0.44	0	8,8,14	0.56	0
7	1PE	G	48	-	5,5,15	0.64	0	4,4,14	0.78	0
2	CO3	F	1002	-	3,3,3	1.25	0	2,3,3	1.55	0
6	SO4	D	5	-	4,4,4	0.20	0	6,6,6	0.23	0
7	1PE	D	63	-	9,9,15	0.75	0	8,8,14	0.80	0
4	BES	D	1003	3,5	22,22,22	0.85	0	26,29,29	1.14	3 (11%)
6	SO4	K	19	-	4,4,4	0.32	0	6,6,6	0.21	0
7	1PE	I	66	-	6,6,15	0.60	0	5,5,14	0.33	0
6	SO4	B	3	-	4,4,4	0.41	0	6,6,6	0.41	0
6	SO4	D	7	-	4,4,4	0.38	0	6,6,6	0.52	0
4	BES	E	1003	3,5	22,22,22	0.90	1 (4%)	26,29,29	1.42	2 (7%)
2	CO3	J	1002	-	3,3,3	0.67	0	2,3,3	1.64	0
7	1PE	B	62	-	9,9,15	0.61	0	8,8,14	0.40	0
4	BES	F	1003	3,5	22,22,22	0.81	0	26,29,29	1.60	5 (19%)
7	1PE	H	64	-	9,9,15	0.53	0	8,8,14	0.55	0
7	1PE	H	65	-	9,9,15	0.64	0	8,8,14	0.73	0
7	1PE	K	5	-	11,11,15	0.44	0	10,10,14	0.63	0
7	1PE	L	56	-	10,10,15	0.56	0	9,9,14	0.28	0
2	CO3	L	1002	-	3,3,3	0.38	0	2,3,3	1.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BES	K	1003	3,5	22,22,22	0.92	0	26,29,29	1.61	4 (15%)
7	1PE	A	19	-	8,8,15	0.51	0	7,7,14	0.24	0
7	1PE	J	3	-	9,9,15	0.54	0	8,8,14	0.49	0
2	CO3	C	1002	-	3,3,3	0.90	0	2,3,3	1.14	0
7	1PE	G	58	-	14,14,15	0.71	0	13,13,14	0.54	0
4	BES	G	1003	3,5	22,22,22	0.99	2 (9%)	26,29,29	1.68	3 (11%)
4	BES	J	1003	3,5	22,22,22	0.97	1 (4%)	26,29,29	1.63	4 (15%)
7	1PE	C	18	-	8,8,15	0.54	0	7,7,14	0.41	0
6	SO4	A	24	-	4,4,4	0.29	0	6,6,6	0.14	0
7	1PE	D	9	-	9,9,15	0.46	0	8,8,14	0.30	0
7	1PE	D	44	-	10,10,15	0.73	0	9,9,14	0.65	0
2	CO3	I	1002	-	3,3,3	1.14	0	2,3,3	1.30	0
7	1PE	I	21	-	14,14,15	0.67	0	13,13,14	0.76	0
7	1PE	I	22	-	10,10,15	0.50	0	9,9,14	0.34	0
7	1PE	J	2	-	10,10,15	0.41	0	9,9,14	0.58	0
7	1PE	K	4	-	11,11,15	0.57	0	10,10,14	0.37	0
6	SO4	L	25	-	4,4,4	0.31	0	6,6,6	0.34	0
2	CO3	H	1002	-	3,3,3	0.68	0	2,3,3	1.24	0
6	SO4	G	17	-	4,4,4	0.20	0	6,6,6	0.39	0
7	1PE	F	33	-	9,9,15	0.55	0	8,8,14	0.32	0
2	CO3	E	1002	-	3,3,3	0.97	0	2,3,3	0.94	0
7	1PE	A	20	-	11,11,15	0.62	0	10,10,14	0.53	0
7	1PE	F	32	-	9,9,15	0.57	0	8,8,14	0.39	0
7	1PE	J	45	-	9,9,15	0.52	0	8,8,14	0.36	0
7	1PE	K	42	-	10,10,15	0.58	0	9,9,14	0.40	0
2	CO3	B	1002	-	3,3,3	0.50	0	2,3,3	2.24	2 (100%)
7	1PE	G	12	-	8,8,15	0.58	0	7,7,14	0.38	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
7	1PE	E	43	-	-	2/5/5/13	-
4	BES	A	1003	3,5	-	2/24/24/24	0/1/1/1
7	1PE	C	17	-	-	2/10/10/13	-
7	1PE	E	8	-	-	0/9/9/13	-
4	BES	B	1003	3,5	-	5/24/24/24	0/1/1/1
7	1PE	E	7	-	-	3/9/9/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BES	L	1003	3,5	-	6/24/24/24	0/1/1/1
7	1PE	B	61	-	-	7/7/7/13	-
7	1PE	G	47	-	-	3/3/3/13	-
7	1PE	L	1	-	-	5/7/7/13	-
7	1PE	L	612	-	-	5/9/9/13	-
7	1PE	F	31	-	-	0/7/7/13	-
7	1PE	G	30	-	-	3/4/4/13	-
4	BES	I	1003	3,5	-	7/24/24/24	0/1/1/1
7	1PE	K	50	-	-	3/3/3/13	-
4	BES	H	1003	3,5	-	6/24/24/24	0/1/1/1
7	1PE	D	67	-	-	3/4/4/13	-
4	BES	C	1003	3,5	-	7/24/24/24	0/1/1/1
7	1PE	B	60	-	-	3/7/7/13	-
7	1PE	G	48	-	-	2/3/3/13	-
7	1PE	D	63	-	-	3/7/7/13	-
4	BES	D	1003	3,5	-	6/24/24/24	0/1/1/1
7	1PE	I	66	-	-	2/4/4/13	-
7	1PE	H	64	-	-	2/7/7/13	-
7	1PE	K	5	-	-	2/9/9/13	-
4	BES	E	1003	3,5	-	6/24/24/24	0/1/1/1
7	1PE	B	62	-	-	1/7/7/13	-
7	1PE	L	56	-	-	1/8/8/13	-
4	BES	F	1003	3,5	-	11/24/24/24	0/1/1/1
7	1PE	H	65	-	-	3/7/7/13	-
4	BES	K	1003	3,5	-	9/24/24/24	0/1/1/1
7	1PE	A	19	-	-	2/6/6/13	-
7	1PE	J	3	-	-	4/7/7/13	-
7	1PE	G	58	-	-	6/12/12/13	-
4	BES	G	1003	3,5	-	7/24/24/24	0/1/1/1
4	BES	J	1003	3,5	-	5/24/24/24	0/1/1/1
7	1PE	C	18	-	-	4/6/6/13	-
7	1PE	D	9	-	-	6/7/7/13	-
7	1PE	D	44	-	-	3/8/8/13	-
7	1PE	I	21	-	-	4/12/12/13	-
7	1PE	K	4	-	-	1/9/9/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	I	22	-	-	5/8/8/13	-
7	1PE	J	2	-	-	6/8/8/13	-
7	1PE	F	33	-	-	4/7/7/13	-
7	1PE	K	42	-	-	4/8/8/13	-
7	1PE	A	20	-	-	4/9/9/13	-
7	1PE	F	32	-	-	3/7/7/13	-
7	1PE	J	45	-	-	4/7/7/13	-
7	1PE	G	12	-	-	6/6/6/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1003	BES	O4-C5	2.19	1.28	1.22
4	E	1003	BES	C2-C3	-2.19	1.48	1.52
4	J	1003	BES	O2-C2	2.16	1.46	1.42
2	D	1002	CO3	O1-C	2.12	1.33	1.25
4	G	1003	BES	C2-C1	2.10	1.56	1.54

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1003	BES	O2-C2-C1	5.53	121.01	109.64
4	G	1003	BES	O2-C2-C1	5.23	120.41	109.64
4	G	1003	BES	O2-C2-C3	-4.75	100.69	110.63
4	F	1003	BES	O2-C2-C1	4.75	119.42	109.64
4	K	1003	BES	O2-C2-C3	-4.57	101.08	110.63

There are no chirality outliers.

5 of 198 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	BES	O2-C2-C3-O3
4	A	1003	BES	O2-C2-C3-N1
4	B	1003	BES	O2-C2-C3-O3
4	B	1003	BES	O2-C2-C3-N1
4	C	1003	BES	N2-C1-C2-C3

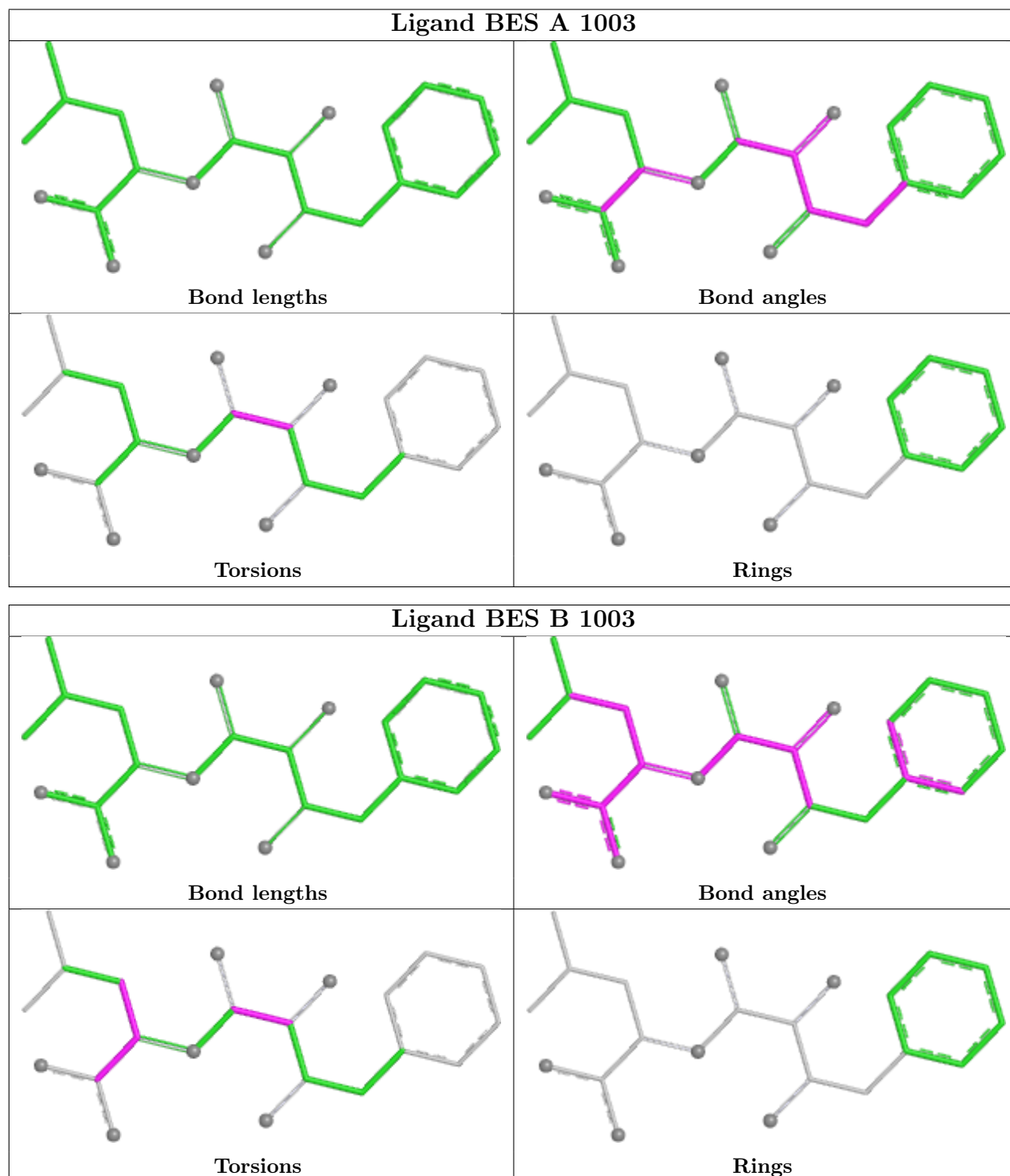
There are no ring outliers.

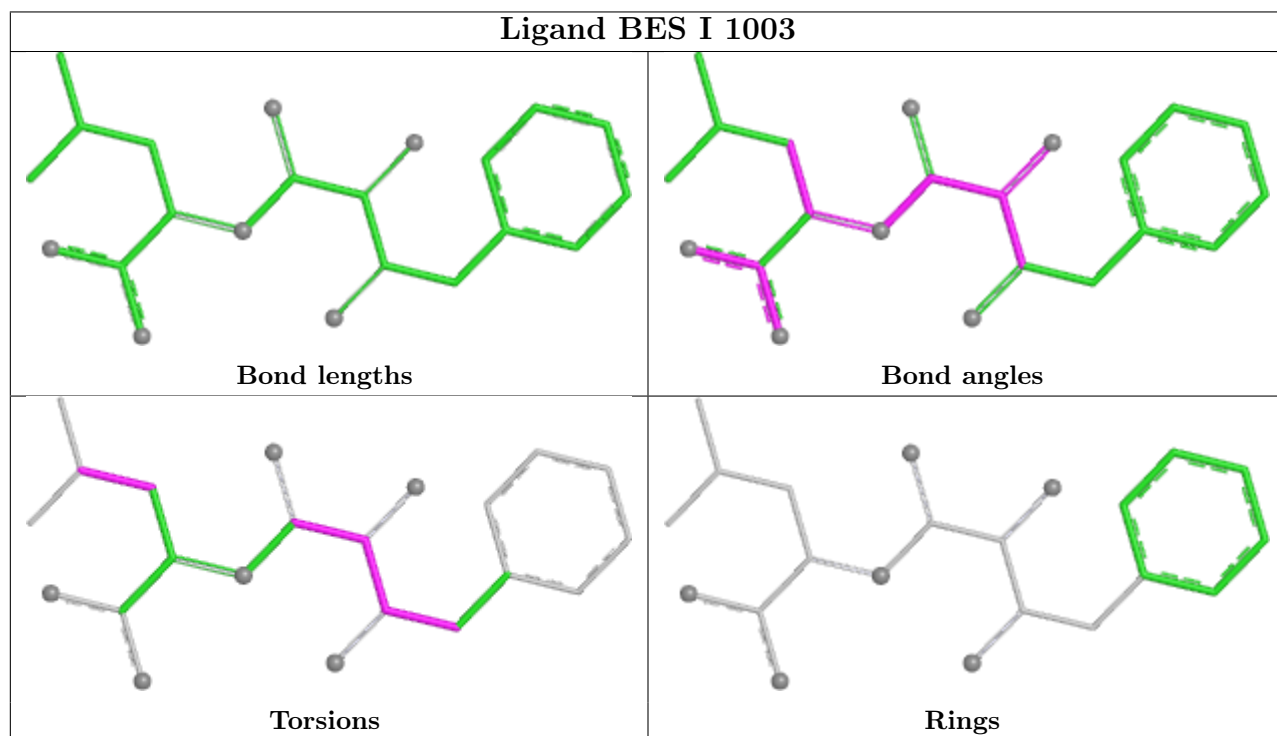
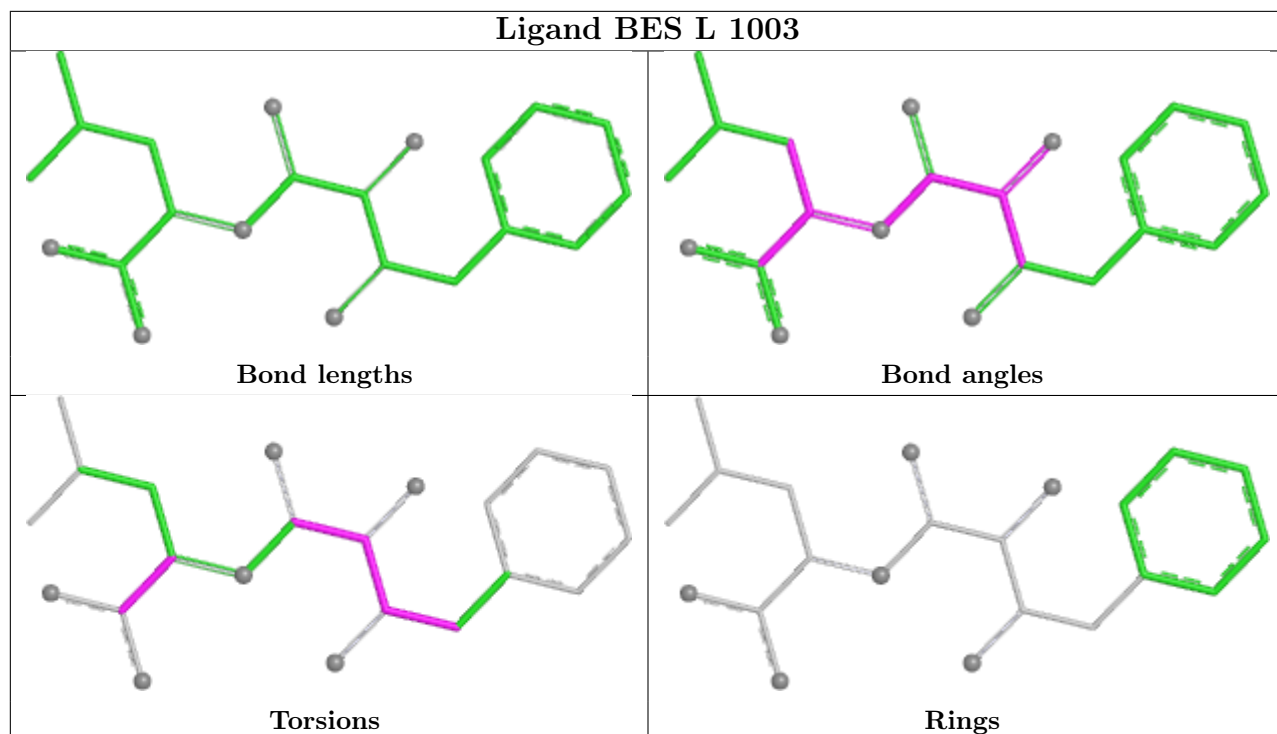
35 monomers are involved in 96 short contacts:

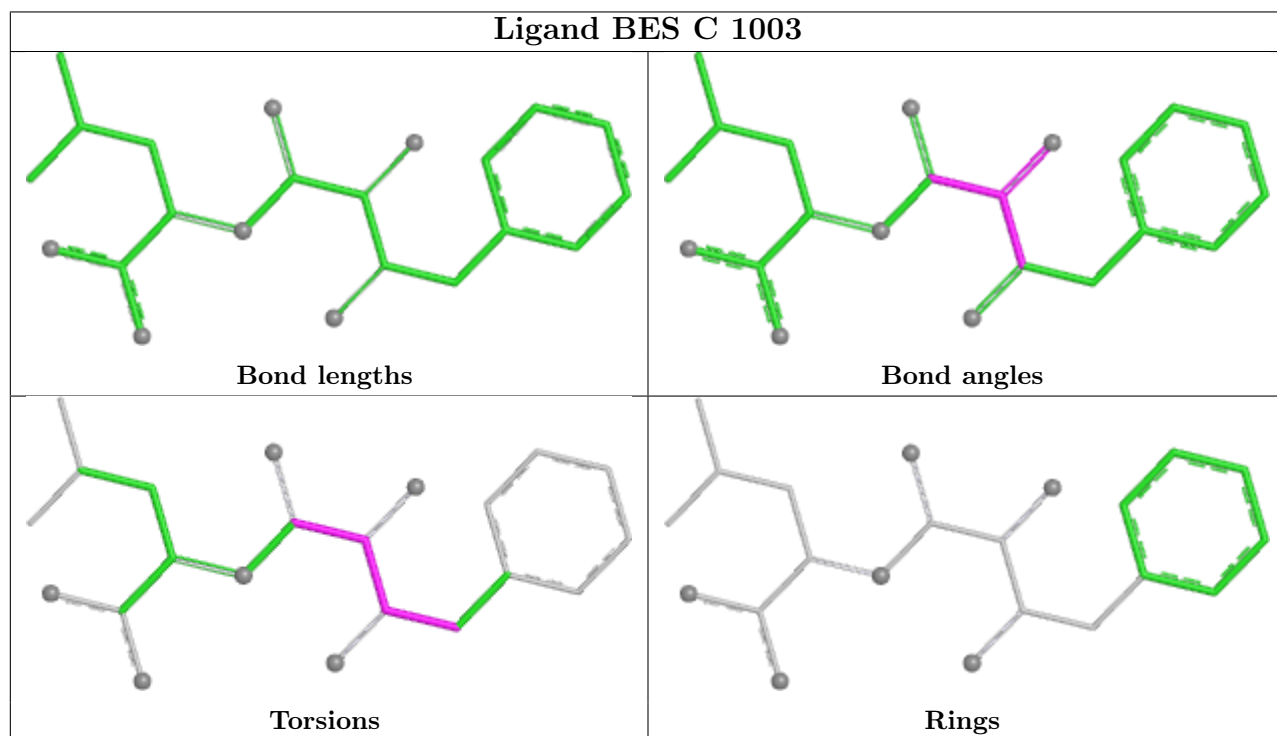
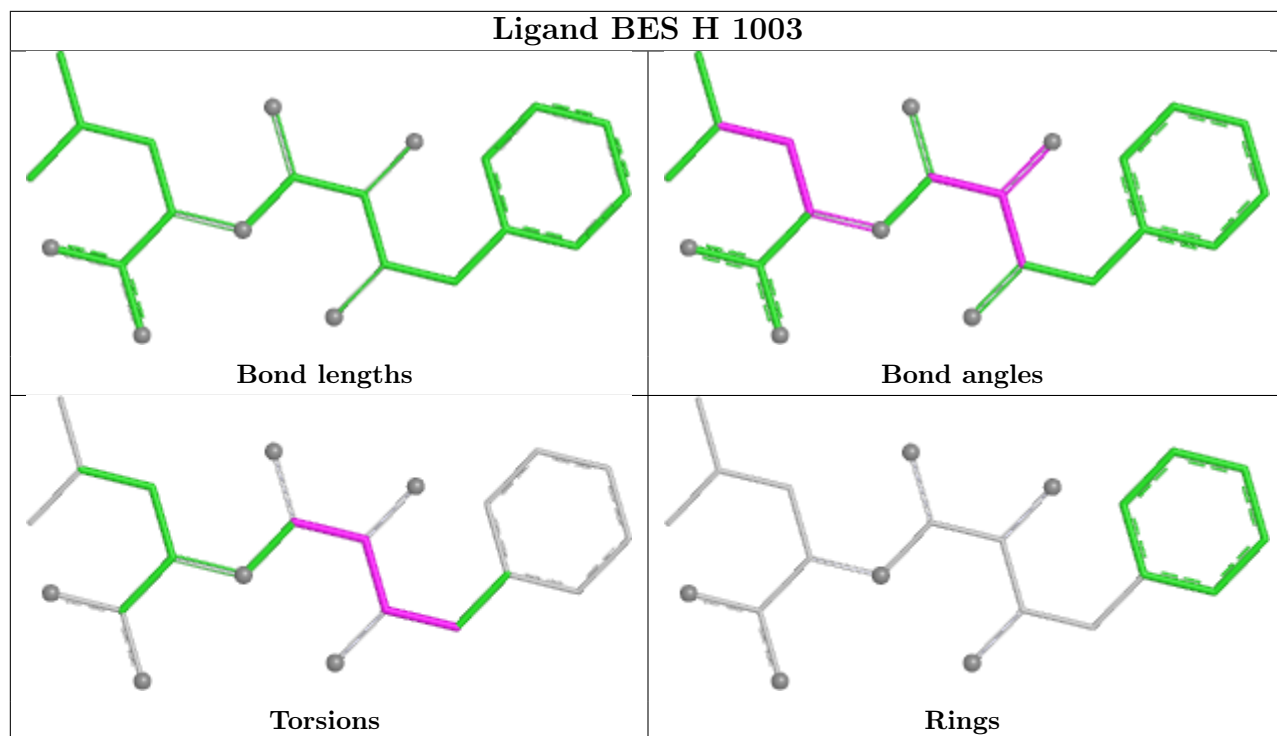
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	43	1PE	3	0
4	A	1003	BES	1	0
7	C	17	1PE	1	0
4	B	1003	BES	3	0
6	J	20	SO4	1	0
7	B	61	1PE	7	0
7	L	1	1PE	3	0
7	L	612	1PE	8	0
4	I	1003	BES	2	0
4	H	1003	BES	3	0
7	D	67	1PE	1	0
4	C	1003	BES	4	0
7	D	63	1PE	2	0
4	D	1003	BES	3	0
6	D	7	SO4	1	0
4	E	1003	BES	4	0
7	H	64	1PE	1	0
7	H	65	1PE	3	0
4	K	1003	BES	5	0
7	A	19	1PE	1	0
7	J	3	1PE	6	0
7	G	58	1PE	4	0
4	J	1003	BES	2	0
7	C	18	1PE	4	0
7	D	9	1PE	1	0
7	D	44	1PE	2	0
7	I	21	1PE	3	0
7	I	22	1PE	5	0
7	J	2	1PE	2	0
6	L	25	SO4	2	0
7	A	20	1PE	1	0
7	F	32	1PE	3	0
7	J	45	1PE	2	0
7	K	42	1PE	1	0
7	G	12	1PE	1	0

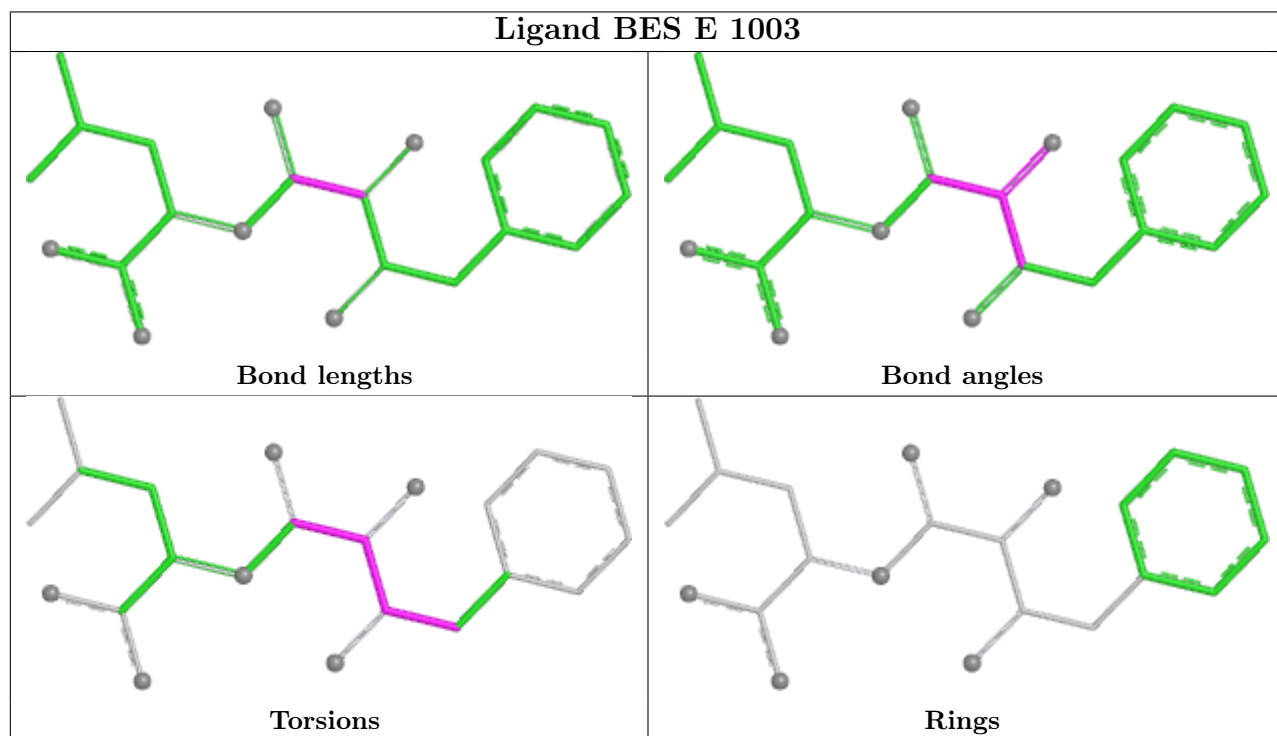
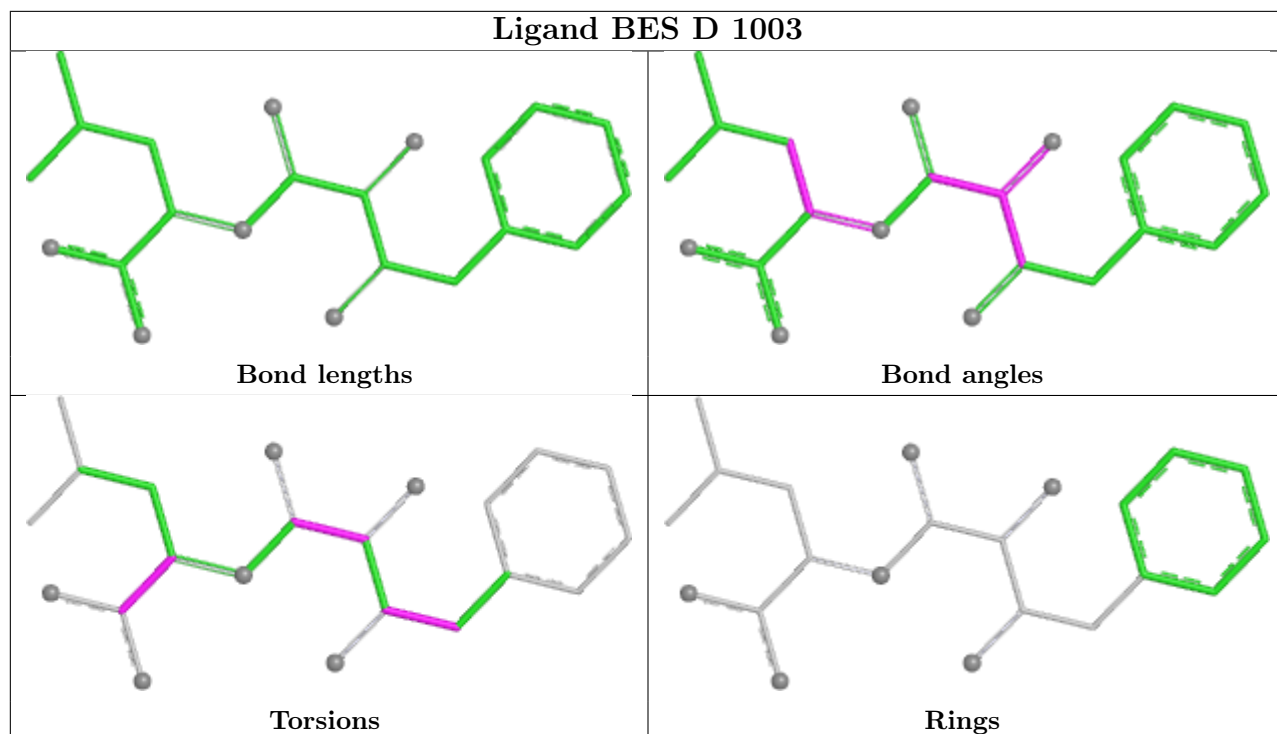
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

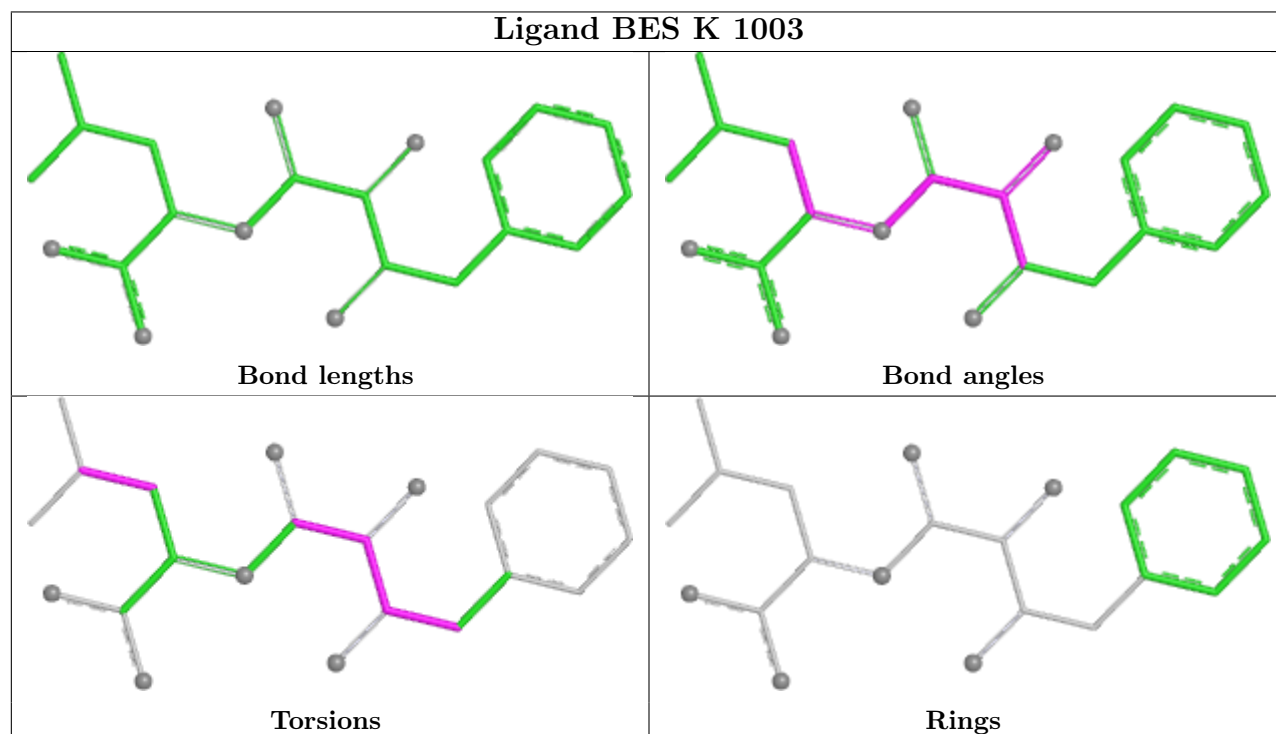
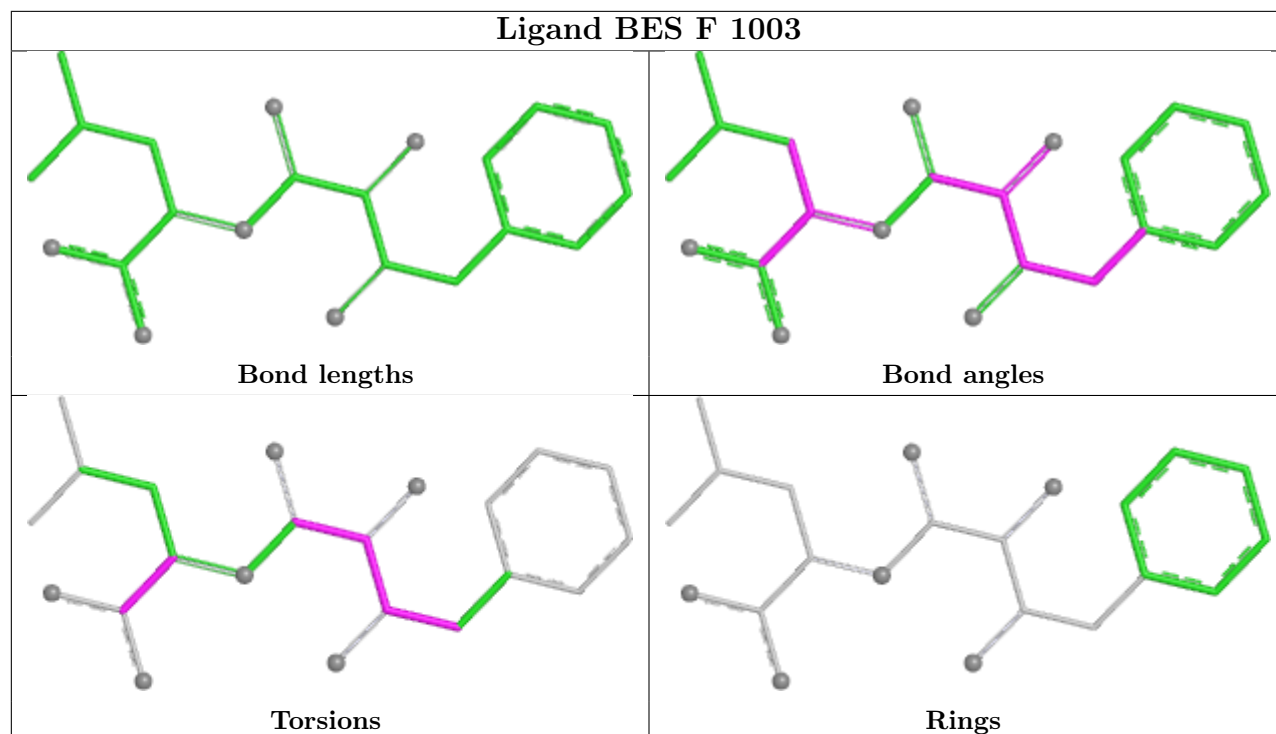
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

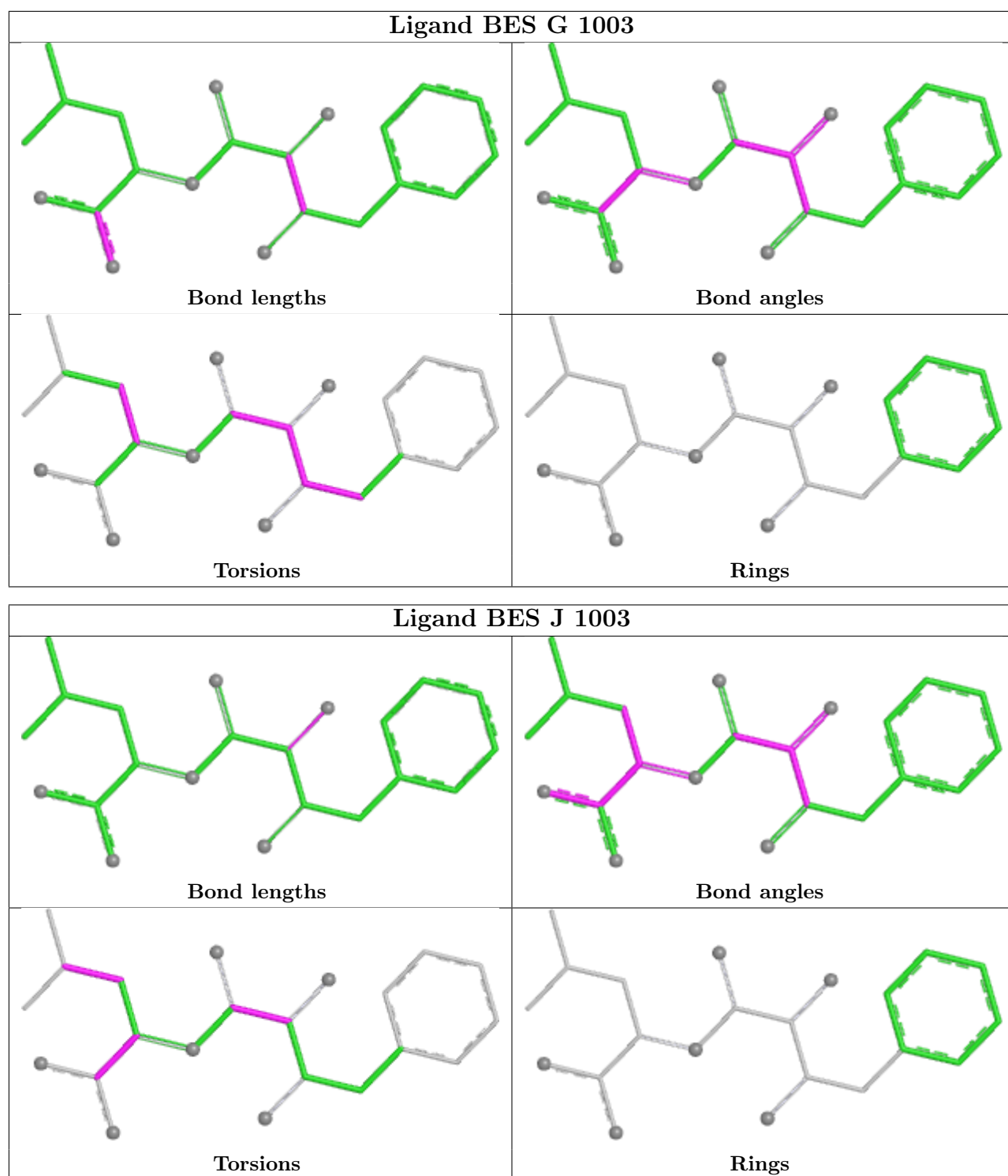












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	518/528 (98%)	-0.54	3 (0%) 85 85	5, 14, 29, 39	1 (0%)
1	B	518/528 (98%)	-0.30	10 (1%) 66 66	7, 16, 42, 51	0
1	C	518/528 (98%)	-0.50	4 (0%) 82 82	7, 15, 31, 42	1 (0%)
1	D	516/528 (97%)	-0.51	6 (1%) 76 76	8, 15, 29, 39	0
1	E	510/528 (96%)	-0.57	6 (1%) 76 76	8, 14, 25, 37	0
1	F	510/528 (96%)	-0.36	6 (1%) 76 76	8, 17, 37, 46	0
1	G	516/528 (97%)	-0.52	4 (0%) 82 82	7, 14, 28, 40	0
1	H	509/528 (96%)	-0.32	9 (1%) 67 67	7, 16, 42, 52	1 (0%)
1	I	518/528 (98%)	-0.49	3 (0%) 85 85	7, 14, 31, 41	1 (0%)
1	J	513/528 (97%)	-0.51	7 (1%) 73 73	8, 15, 29, 40	1 (0%)
1	K	509/528 (96%)	-0.56	4 (0%) 82 82	8, 14, 25, 38	1 (0%)
1	L	513/528 (97%)	-0.37	9 (1%) 67 67	8, 16, 40, 46	1 (0%)
All	All	6168/6336 (97%)	-0.46	71 (1%) 76 76	5, 15, 34, 52	7 (0%)

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	217	ASN	4.8
1	E	216	ASP	4.8
1	D	136	GLY	4.7
1	J	136	GLY	4.4
1	B	136	GLY	4.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	1PE	B	62	10/16	0.28	0.44	91,95,97,98	0
7	1PE	K	50	6/16	0.66	0.20	37,40,45,46	0
7	1PE	D	44	11/16	0.70	0.19	36,38,43,44	0
7	1PE	D	63	10/16	0.75	0.17	22,30,33,36	0
7	1PE	B	61	10/16	0.75	0.16	38,40,42,43	0
7	1PE	I	66	7/16	0.78	0.16	30,32,34,34	0
7	1PE	H	65	10/16	0.78	0.15	32,40,41,41	0
7	1PE	A	20	12/16	0.79	0.19	40,43,46,47	0
7	1PE	J	45	10/16	0.81	0.18	44,48,51,51	0
5	MG	D	1004	1/1	0.82	0.35	28,28,28,28	0
7	1PE	C	17	13/16	0.82	0.13	22,36,38,38	0
7	1PE	D	67	7/16	0.82	0.17	29,33,41,41	0
7	1PE	G	58	15/16	0.82	0.17	37,42,52,53	0
7	1PE	K	42	11/16	0.83	0.14	33,42,47,47	0
7	1PE	L	56	11/16	0.83	0.14	43,45,48,50	0
7	1PE	K	4	12/16	0.84	0.12	31,32,34,35	0
7	1PE	E	43	8/16	0.84	0.13	33,35,35,39	0
7	1PE	E	7	12/16	0.85	0.13	32,34,36,36	0
6	SO4	A	24	5/5	0.85	0.13	52,55,56,57	0
7	1PE	I	21	15/16	0.85	0.13	26,33,46,47	0
5	MG	L	1004	1/1	0.86	0.28	33,33,33,33	0
5	MG	A	1004	1/1	0.86	0.34	24,24,24,24	0
7	1PE	J	3	10/16	0.87	0.13	36,37,40,41	0
7	1PE	G	12	9/16	0.87	0.12	27,28,32,32	0
4	BES	B	1003	22/22	0.88	0.12	17,30,39,45	0
7	1PE	L	612	12/16	0.88	0.11	22,36,39,40	0
5	MG	J	1004	1/1	0.88	0.48	22,22,22,22	0
5	MG	H	1004	1/1	0.89	0.34	40,40,40,40	0
7	1PE	F	32	10/16	0.89	0.11	37,39,39,39	0
7	1PE	D	9	10/16	0.89	0.12	21,25,35,37	0
6	SO4	L	25	5/5	0.89	0.13	56,59,59,60	0
4	BES	F	1003	22/22	0.89	0.12	13,27,36,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BES	G	1003	22/22	0.89	0.12	13,28,34,39	0
6	SO4	A	2	5/5	0.89	0.13	45,46,50,51	0
4	BES	H	1003	22/22	0.90	0.11	15,25,34,37	0
4	BES	I	1003	22/22	0.90	0.10	11,27,30,32	0
7	1PE	J	2	11/16	0.90	0.10	23,26,37,42	0
4	BES	K	1003	22/22	0.90	0.11	16,26,32,39	0
4	BES	A	1003	22/22	0.90	0.11	20,29,35,40	0
5	MG	C	1004	1/1	0.90	0.26	27,27,27,27	0
7	1PE	G	30	7/16	0.90	0.11	35,38,42,43	0
7	1PE	G	48	6/16	0.90	0.12	25,31,33,36	0
4	BES	C	1003	22/22	0.90	0.11	22,27,36,36	0
7	1PE	A	19	9/16	0.90	0.10	20,24,28,31	0
4	BES	E	1003	22/22	0.91	0.10	19,29,35,39	0
7	1PE	G	47	6/16	0.91	0.10	30,31,32,35	0
7	1PE	I	22	11/16	0.91	0.10	18,23,36,38	0
7	1PE	F	33	10/16	0.91	0.10	21,29,31,34	0
4	BES	D	1003	22/22	0.91	0.10	13,28,32,33	0
7	1PE	H	64	10/16	0.91	0.10	19,26,34,35	0
5	MG	F	1004	1/1	0.92	0.23	37,37,37,37	0
7	1PE	B	60	10/16	0.92	0.10	23,28,33,35	0
5	MG	B	1004	1/1	0.92	0.40	16,16,16,16	0
6	SO4	E	22	5/5	0.92	0.20	44,45,47,48	0
7	1PE	K	5	12/16	0.92	0.10	25,27,38,38	0
6	SO4	J	20	5/5	0.92	0.11	60,62,62,62	0
7	1PE	C	18	9/16	0.92	0.09	20,21,26,29	0
4	BES	L	1003	22/22	0.92	0.09	12,26,33,34	0
4	BES	J	1003	22/22	0.92	0.11	11,28,37,40	0
6	SO4	K	19	5/5	0.93	0.10	52,53,54,54	0
5	MG	E	1004	1/1	0.93	0.30	26,26,26,26	0
6	SO4	D	5	5/5	0.93	0.11	53,53,56,56	0
6	SO4	A	1	5/5	0.93	0.15	50,51,53,53	0
6	SO4	G	23	5/5	0.93	0.17	46,49,50,50	0
2	CO3	A	1002	4/4	0.93	0.10	13,14,14,17	0
5	MG	I	1004	1/1	0.94	0.37	15,15,15,15	0
7	1PE	E	8	12/16	0.94	0.09	20,23,35,35	0
5	MG	G	1004	1/1	0.94	0.22	23,23,23,23	0
7	1PE	L	1	10/16	0.94	0.08	25,27,32,38	0
7	1PE	F	31	10/16	0.94	0.08	26,27,29,29	0
6	SO4	F	21	5/5	0.94	0.10	56,59,59,59	0
2	CO3	B	1002	4/4	0.95	0.06	11,12,12,16	0
2	CO3	J	1002	4/4	0.95	0.06	12,14,15,16	0
5	MG	K	1004	1/1	0.95	0.26	23,23,23,23	0

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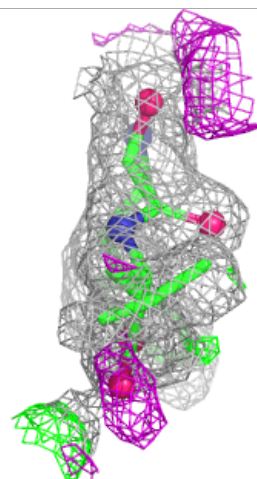
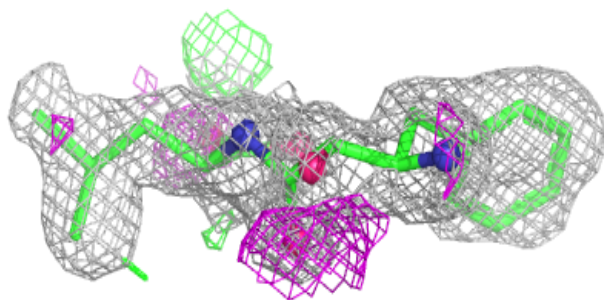
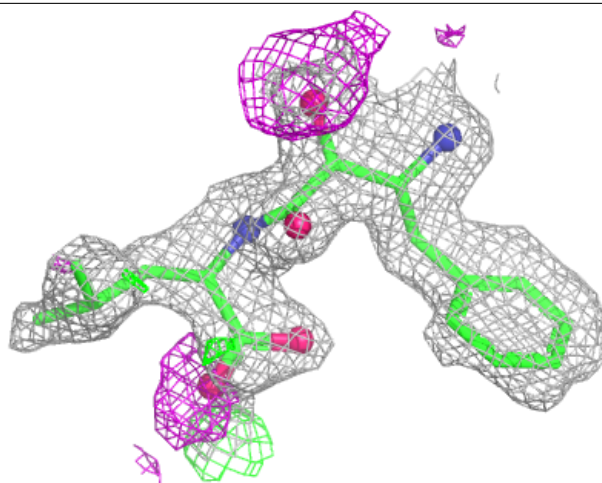
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CO3	E	1002	4/4	0.96	0.07	16,17,18,19	0
2	CO3	G	1002	4/4	0.97	0.05	11,12,12,15	0
2	CO3	H	1002	4/4	0.97	0.04	10,10,11,14	0
2	CO3	I	1002	4/4	0.97	0.05	14,15,15,18	0
2	CO3	C	1002	4/4	0.97	0.05	12,13,13,16	0
2	CO3	K	1002	4/4	0.97	0.05	13,14,14,18	0
2	CO3	L	1002	4/4	0.97	0.05	14,15,15,16	0
2	CO3	F	1002	4/4	0.97	0.05	12,12,13,15	0
3	ZN	F	1001	1/1	0.98	0.09	40,40,40,40	0
2	CO3	D	1002	4/4	0.98	0.05	11,12,12,16	0
3	ZN	I	1001	1/1	0.99	0.10	36,36,36,36	0
3	ZN	J	1001	1/1	0.99	0.07	38,38,38,38	0
3	ZN	K	1001	1/1	0.99	0.11	37,37,37,37	0
3	ZN	L	1001	1/1	0.99	0.10	37,37,37,37	0
6	SO4	B	3	5/5	0.99	0.03	8,9,10,10	0
3	ZN	B	1001	1/1	0.99	0.10	37,37,37,37	0
6	SO4	D	7	5/5	0.99	0.03	8,11,11,12	0
3	ZN	C	1001	1/1	0.99	0.11	39,39,39,39	0
3	ZN	E	1001	1/1	0.99	0.07	38,38,38,38	0
6	SO4	G	17	5/5	0.99	0.03	10,11,13,14	0
3	ZN	A	1001	1/1	0.99	0.09	39,39,39,39	0
6	SO4	J	18	5/5	0.99	0.03	11,11,12,14	0
3	ZN	G	1001	1/1	0.99	0.09	38,38,38,38	0
3	ZN	H	1001	1/1	1.00	0.11	34,34,34,34	0
3	ZN	D	1001	1/1	1.00	0.07	34,34,34,34	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.

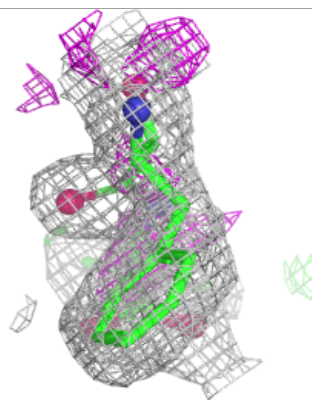
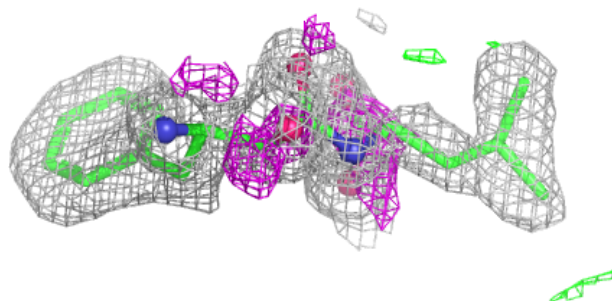
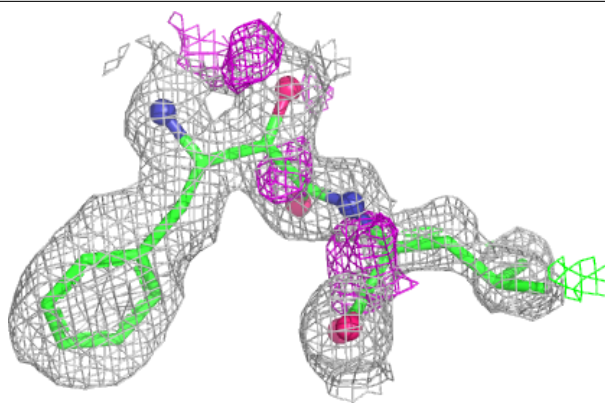
Electron density around BES B 1003:

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

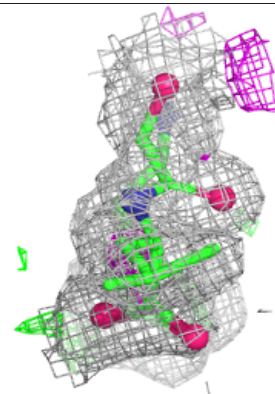
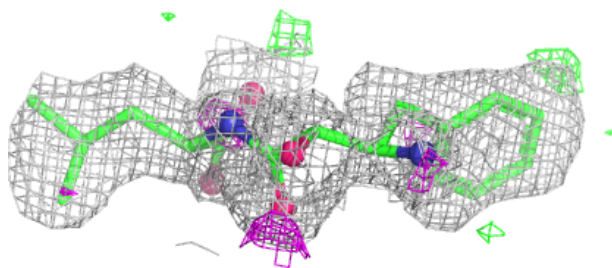
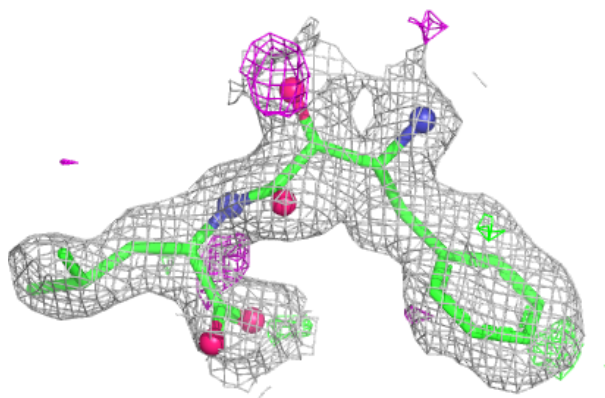


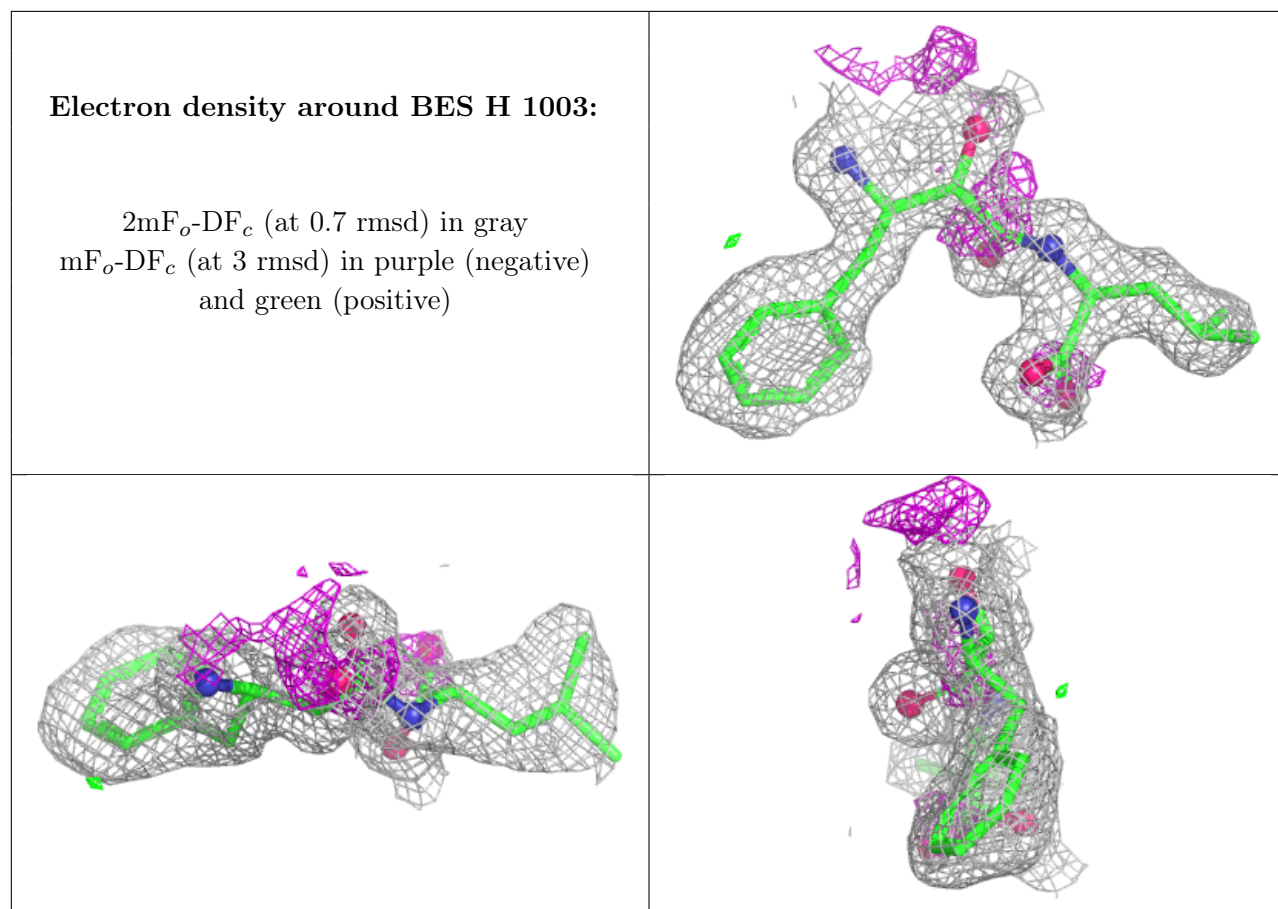
Electron density around BES F 1003:

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

**Electron density around BES G 1003:**

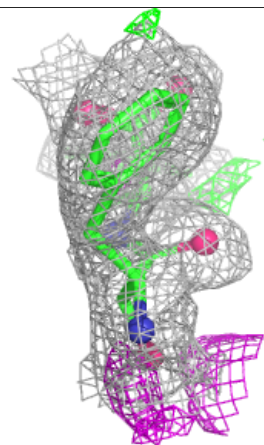
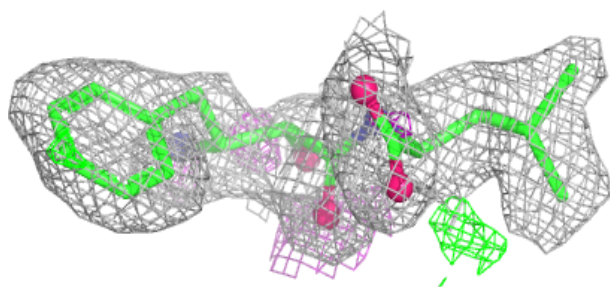
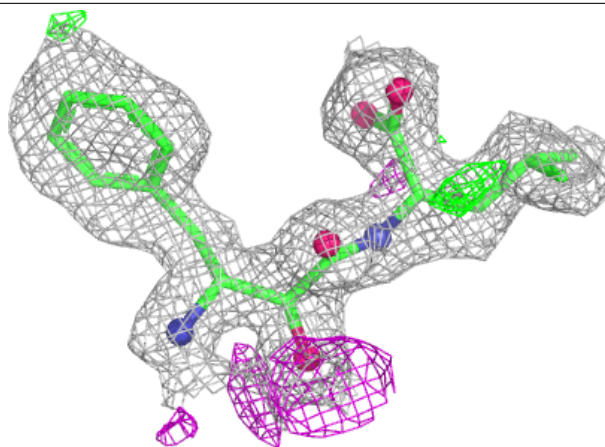
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





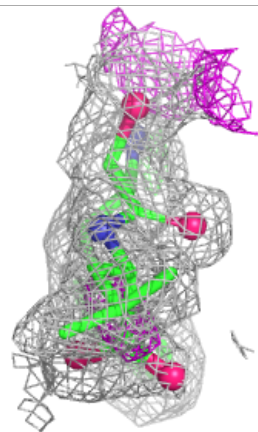
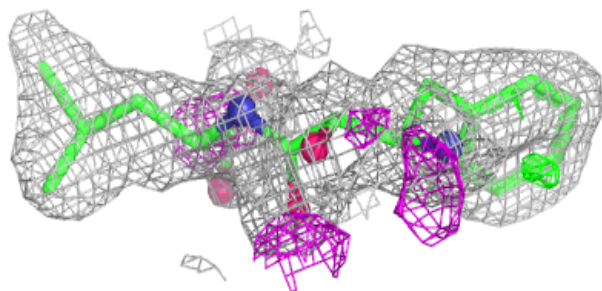
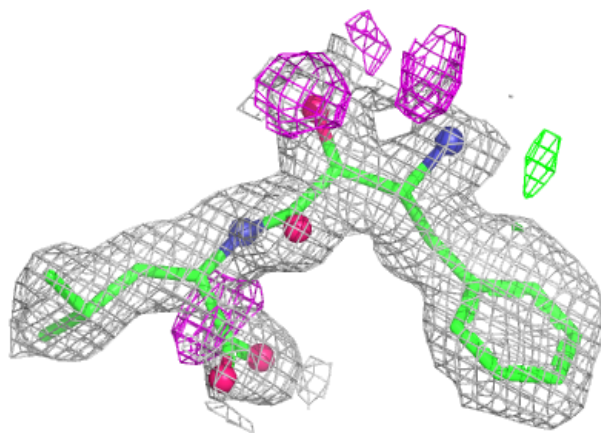
Electron density around BES I 1003:

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



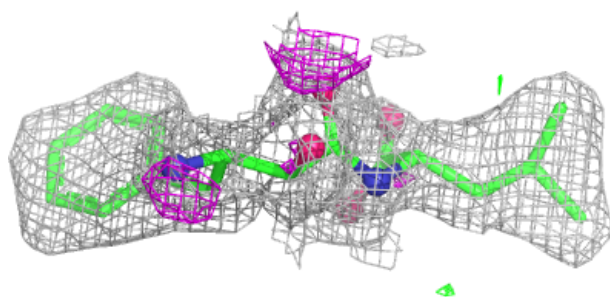
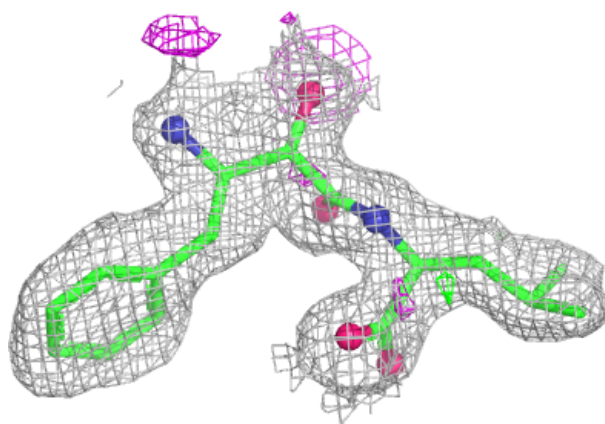
Electron density around BES K 1003:

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



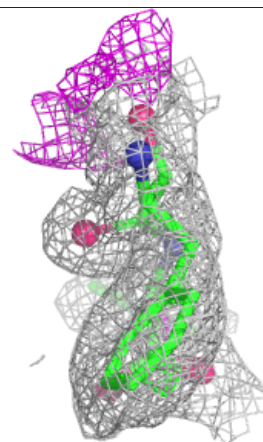
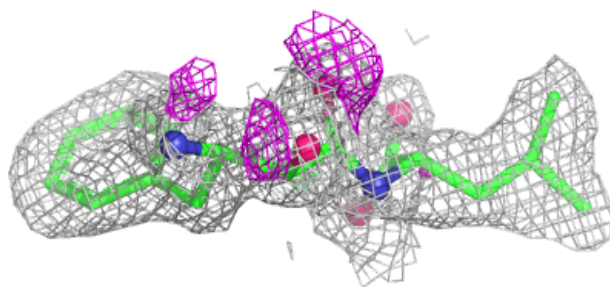
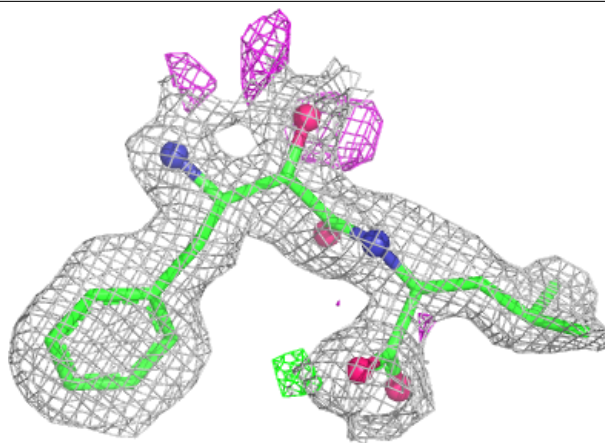
Electron density around BES A 1003:

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



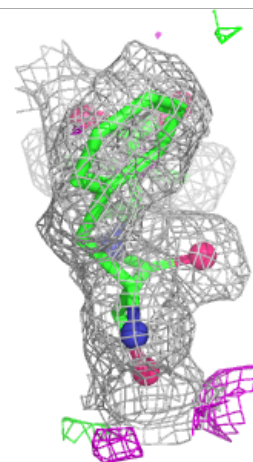
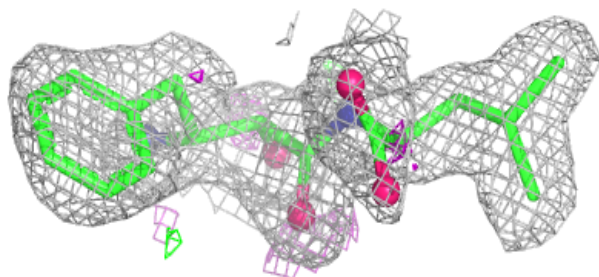
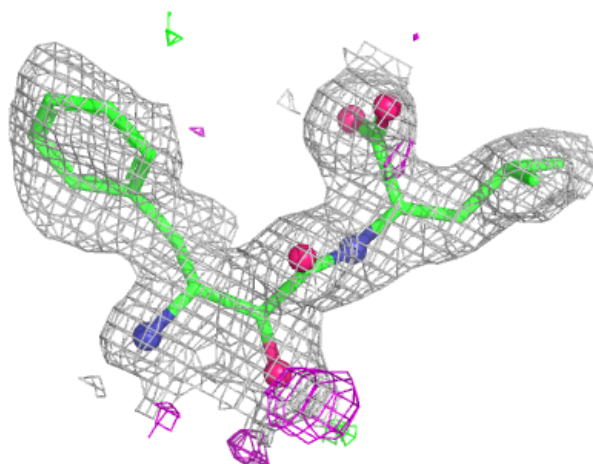
Electron density around BES C 1003:

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



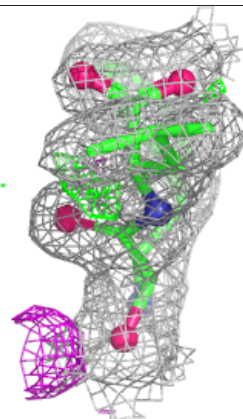
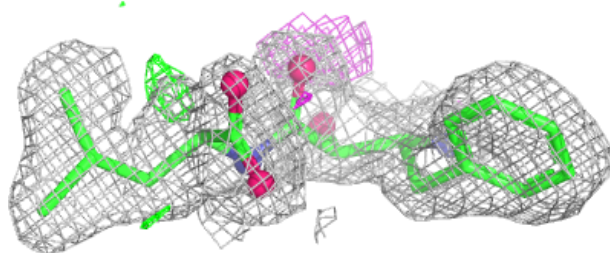
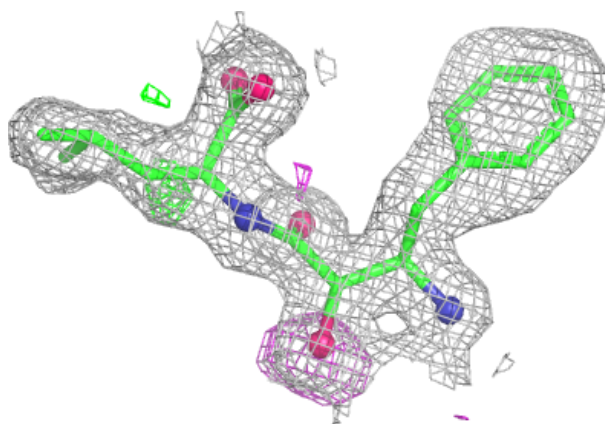
Electron density around BES E 1003:

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

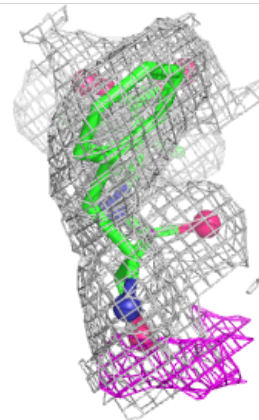
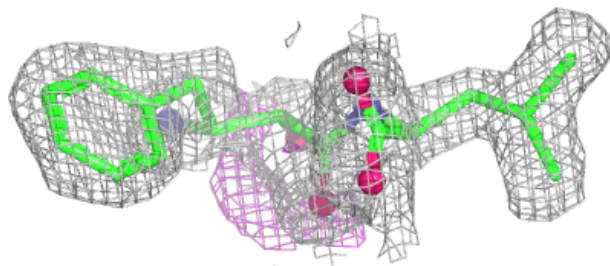
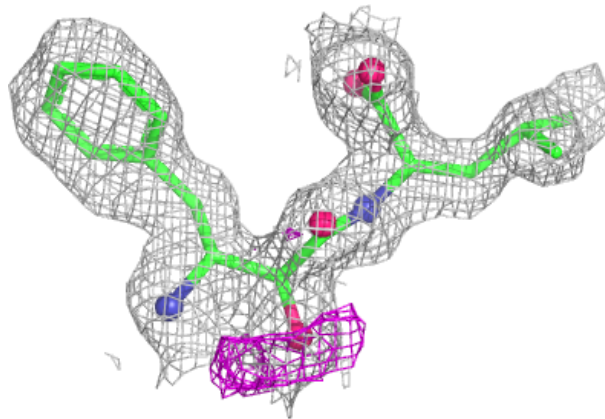


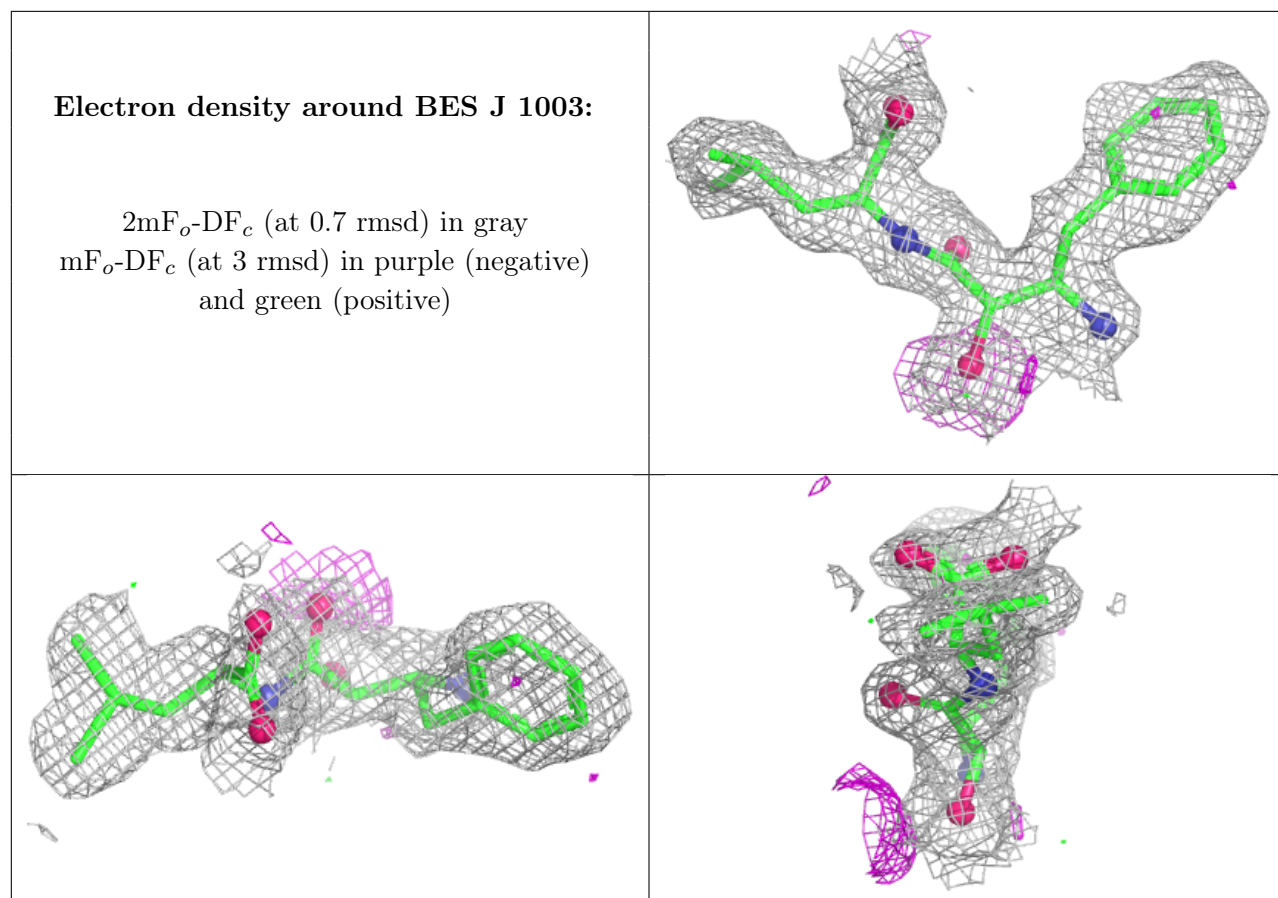
Electron density around BES D 1003:

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

**Electron density around BES L 1003:**

$2mF_o-DF_c$ (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.