



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2026 – 01:09 am BST

PDB ID : 9SUR / pdb_00009sur
Title : Crystal Structure of the NlpC/P60 Peptidase YkfC from *Bacillus subtilis* with Covalently Bound Dipeptide
Authors : Voelpel, S.V.; Reiter, O.M.; Stehle, T.
Deposited on : 2025-09-29
Resolution : 2.34 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 Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

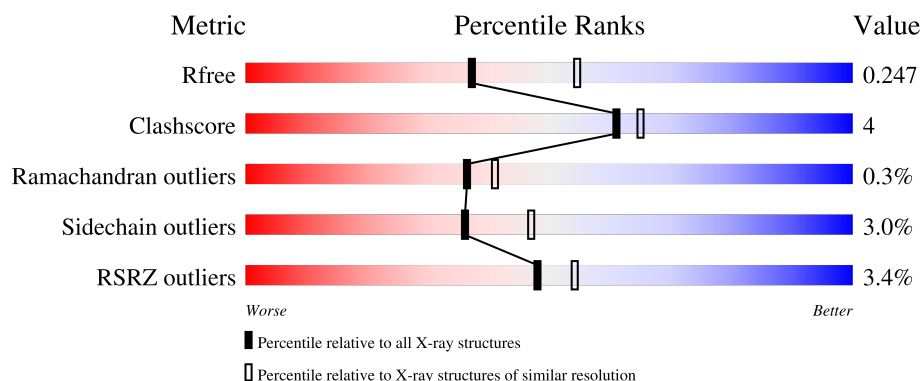
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

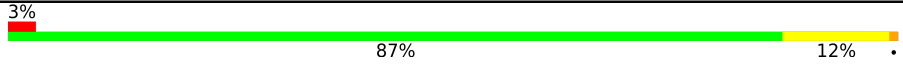
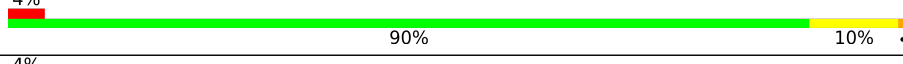
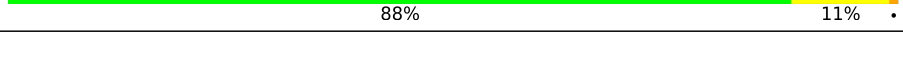
The reported resolution of this entry is 2.34 Å.

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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	AAA	304	
1	BBB	304	
1	CCC	304	
1	DDD	304	

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
7	DGL	CCC	405	-	X	-	-
7	DGL	DDD	406	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9961 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 Gamma-D-glutamyl-L-lysine dipeptidyl-peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BBB	304	Total	C	N	O	S	0	0	0
			2391	1535	406	437	13			
1	AAA	304	Total	C	N	O	S	0	0	0
			2393	1536	405	439	13			
1	CCC	304	Total	C	N	O	S	0	0	0
			2376	1525	402	436	13			
1	DDD	304	Total	C	N	O	S	0	0	0
			2390	1534	406	437	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	297	LEU	-	expression tag	UNP O35010
BBB	298	GLU	-	expression tag	UNP O35010
BBB	299	HIS	-	expression tag	UNP O35010
BBB	300	HIS	-	expression tag	UNP O35010
BBB	301	HIS	-	expression tag	UNP O35010
BBB	302	HIS	-	expression tag	UNP O35010
BBB	303	HIS	-	expression tag	UNP O35010
BBB	304	HIS	-	expression tag	UNP O35010
AAA	297	LEU	-	expression tag	UNP O35010
AAA	298	GLU	-	expression tag	UNP O35010
AAA	299	HIS	-	expression tag	UNP O35010
AAA	300	HIS	-	expression tag	UNP O35010
AAA	301	HIS	-	expression tag	UNP O35010
AAA	302	HIS	-	expression tag	UNP O35010
AAA	303	HIS	-	expression tag	UNP O35010
AAA	304	HIS	-	expression tag	UNP O35010
CCC	297	LEU	-	expression tag	UNP O35010
CCC	298	GLU	-	expression tag	UNP O35010
CCC	299	HIS	-	expression tag	UNP O35010
CCC	300	HIS	-	expression tag	UNP O35010
CCC	301	HIS	-	expression tag	UNP O35010

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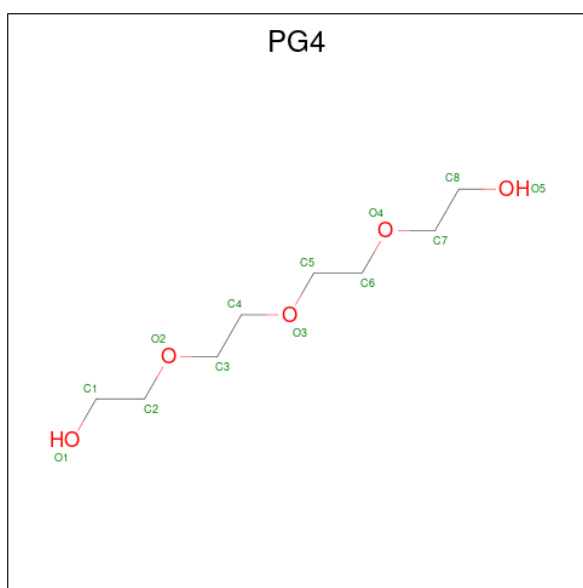
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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	302	HIS	-	expression tag	UNP O35010
CCC	303	HIS	-	expression tag	UNP O35010
CCC	304	HIS	-	expression tag	UNP O35010
DDD	297	LEU	-	expression tag	UNP O35010
DDD	298	GLU	-	expression tag	UNP O35010
DDD	299	HIS	-	expression tag	UNP O35010
DDD	300	HIS	-	expression tag	UNP O35010
DDD	301	HIS	-	expression tag	UNP O35010
DDD	302	HIS	-	expression tag	UNP O35010
DDD	303	HIS	-	expression tag	UNP O35010
DDD	304	HIS	-	expression tag	UNP O35010

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

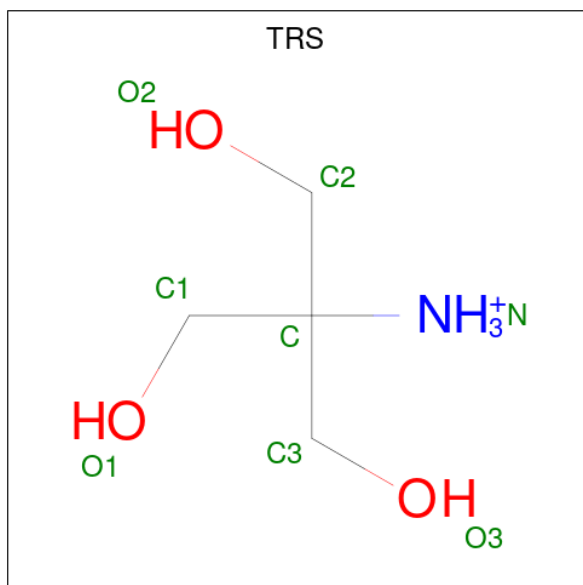
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BBB	2	Total Zn 2 2	0	0
2	AAA	2	Total Zn 2 2	0	0
2	CCC	2	Total Zn 2 2	0	0
2	DDD	2	Total Zn 2 2	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



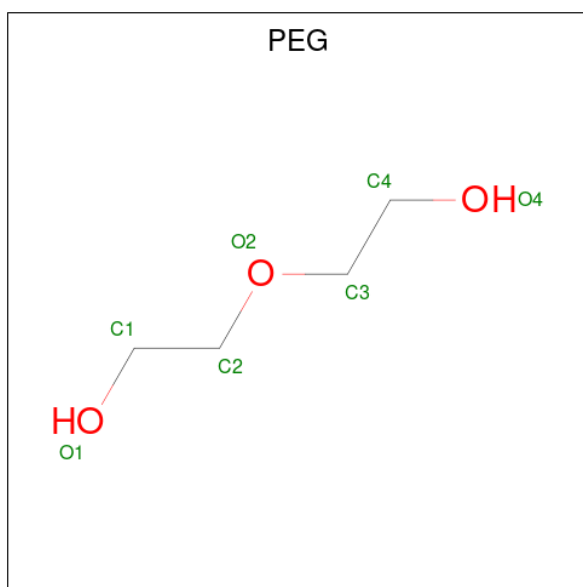
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	O	0	0
			13	8	5		
3	AAA	1	Total	C	O	0	0
			13	8	5		
3	DDD	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



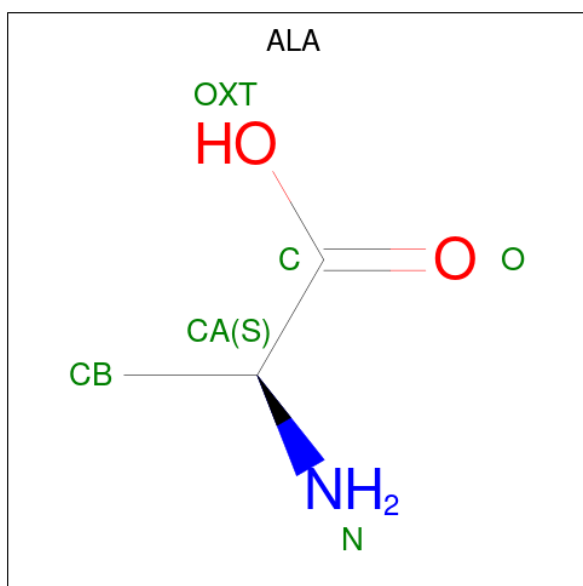
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	BBB	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



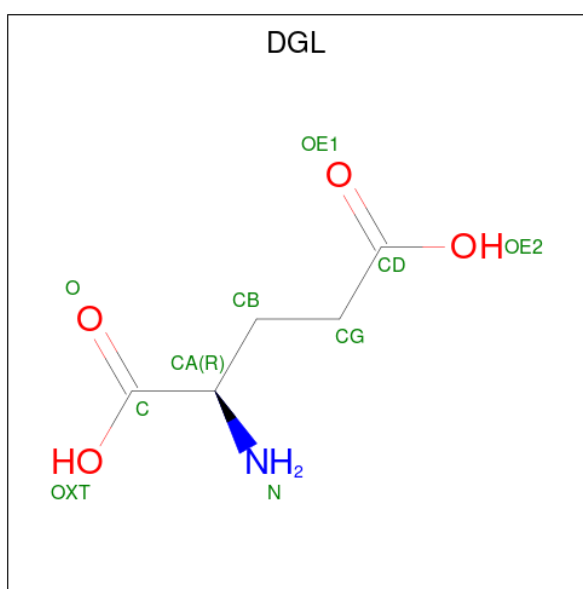
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	BBB	1	Total	C	O	0	0
			7	4	3		
5	AAA	1	Total	C	O	0	0
			7	4	3		
5	DDD	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$) (labeled as "Ligand of Interest" by depositor).



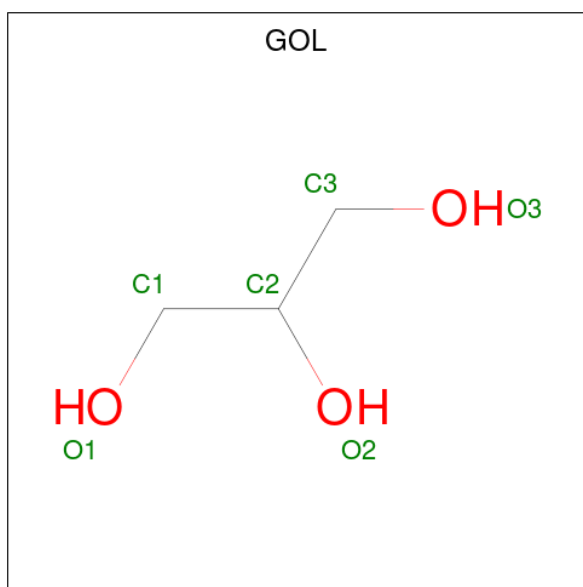
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	BBB	1	Total	C	N	O	0	0
			5	3	1	1		
6	AAA	1	Total	C	N	O	0	0
			5	3	1	1		
6	CCC	1	Total	C	N	O	0	0
			5	3	1	1		
6	DDD	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 7 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	BBB	1	Total	C	N	O	0	0
			9	5	1	3		
7	AAA	1	Total	C	N	O	0	0
			9	5	1	3		
7	CCC	1	Total	C	N	O	0	0
			9	5	1	3		
7	DDD	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	C	O	0	0
			6	3	3		
8	CCC	1	Total	C	O	0	0
			6	3	3		

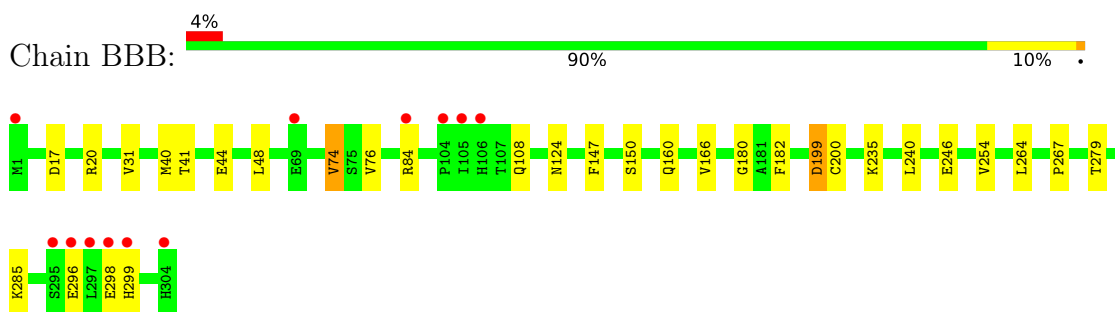
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	BBB	66	Total	O	0	0
			66	66		
9	AAA	77	Total	O	0	0
			77	77		
9	CCC	54	Total	O	0	0
			54	54		
9	DDD	70	Total	O	0	0
			70	70		

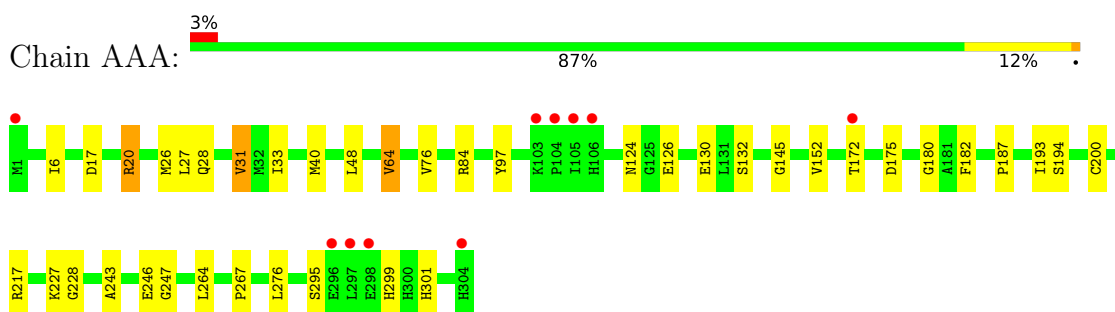
3 Residue-property plots [i](#)

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.

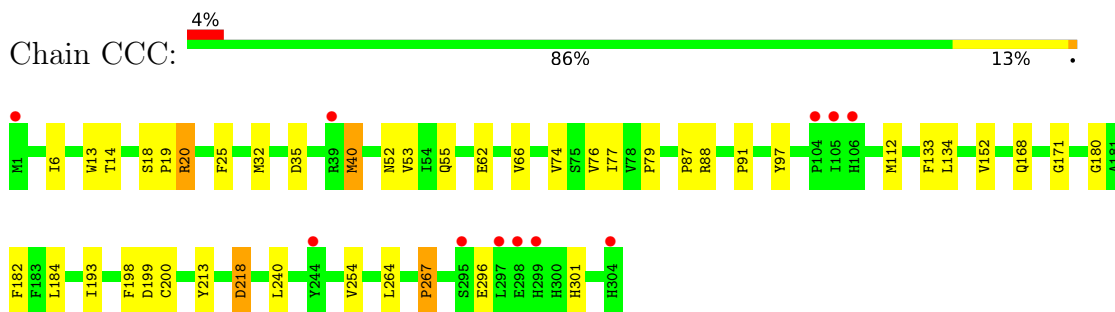
- Molecule 1: Gamma-D-glutamyl-L-lysine dipeptidyl-peptidase



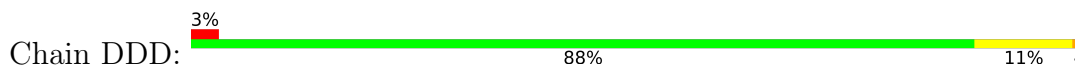
- Molecule 1: Gamma-D-glutamyl-L-lysine dipeptidyl-peptidase

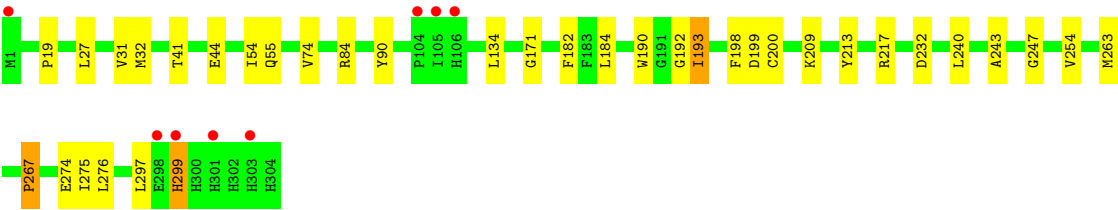


- Molecule 1: Gamma-D-glutamyl-L-lysine dipeptidyl-peptidase



- Molecule 1: Gamma-D-glutamyl-L-lysine dipeptidyl-peptidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.25Å 161.38Å 75.39Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	47.69 – 2.34 47.69 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.69-2.34) 98.7 (47.69-2.34)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.204 , 0.246 0.206 , 0.247	Depositor DCC
R_{free} test set	1555 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9961	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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: PG4, DGL, TRS, PEG, ZN, GOL

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	AAA	1.00	0/2456	1.40	7/3323 (0.2%)
1	BBB	1.01	0/2455	1.37	9/3323 (0.3%)
1	CCC	1.05	0/2440	1.39	12/3307 (0.4%)
1	DDD	1.01	0/2454	1.39	4/3322 (0.1%)
All	All	1.02	0/9805	1.39	32/13275 (0.2%)

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	182	PHE	CB-CA-C	-11.52	86.02	110.32
1	CCC	182	PHE	CB-CA-C	-10.42	91.35	110.63
1	DDD	182	PHE	CA-CB-CG	7.78	121.58	113.80
1	BBB	299	HIS	N-CA-C	6.69	118.72	108.42
1	DDD	267	PRO	N-CA-C	6.57	126.00	112.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2393	0	2357	17	0
1	BBB	2391	0	2349	16	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	2376	0	2312	28	0
1	DDD	2390	0	2347	20	1
2	AAA	2	0	0	0	0
2	BBB	2	0	0	0	0
2	CCC	2	0	0	0	0
2	DDD	2	0	0	0	0
3	AAA	13	0	18	0	0
3	BBB	13	0	18	1	0
3	DDD	13	0	18	0	0
4	BBB	8	0	12	0	0
5	AAA	7	0	10	0	0
5	BBB	7	0	10	0	0
5	DDD	7	0	10	0	0
6	AAA	5	0	4	0	0
6	BBB	5	0	4	0	0
6	CCC	5	0	4	3	0
6	DDD	5	0	4	0	0
7	AAA	9	0	5	1	0
7	BBB	9	0	5	2	0
7	CCC	9	0	6	2	0
7	DDD	9	0	6	4	0
8	AAA	6	0	8	0	0
8	CCC	6	0	8	0	0
9	AAA	77	0	0	3	0
9	BBB	66	0	0	1	0
9	CCC	54	0	0	5	0
9	DDD	70	0	0	2	0
All	All	9961	0	9515	80	1

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 4.

The worst 5 of 80 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:CCC:53:VAL:O	9:CCC:501:HOH:O	1.62	1.14
1:CCC:13:TRP:HA	9:CCC:501:HOH:O	1.79	0.82
1:CCC:87:PRO:HD3	9:CCC:526:HOH:O	1.85	0.77
1:AAA:200:CYS:H	7:AAA:407:DGL:CD	1.99	0.74
1:CCC:14:THR:HG21	1:CCC:52:ASN:O	1.91	0.70

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:84:ARG:NH2	1:DDD:84:ARG:NE[1_554]	2.01	0.19

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	AAA	302/304 (99%)	283 (94%)	18 (6%)	1 (0%)	36	41
1	BBB	302/304 (99%)	286 (95%)	15 (5%)	1 (0%)	36	41
1	CCC	302/304 (99%)	285 (94%)	16 (5%)	1 (0%)	36	41
1	DDD	302/304 (99%)	286 (95%)	15 (5%)	1 (0%)	36	41
All	All	1208/1216 (99%)	1140 (94%)	64 (5%)	4 (0%)	36	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	267	PRO
1	BBB	267	PRO
1	CCC	267	PRO
1	DDD	267	PRO

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	AAA	256/258 (99%)	245 (96%)	11 (4%)	26	33
1	BBB	255/258 (99%)	250 (98%)	5 (2%)	48	61
1	CCC	251/258 (97%)	244 (97%)	7 (3%)	38	50
1	DDD	255/258 (99%)	247 (97%)	8 (3%)	35	45
All	All	1017/1032 (98%)	986 (97%)	31 (3%)	36	47

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	295	SER
1	DDD	193	ILE
1	CCC	35	ASP
1	DDD	297	LEU
1	DDD	74	VAL

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

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 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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	$\# Z > 2$
8	GOL	AAA	405	-	5,5,5	0.18	0	5,5,5	0.34	0
6	ALA	BBB	406	7	3,4,5	0.77	0	2,4,6	2.32	1 (50%)
8	GOL	CCC	403	-	5,5,5	0.15	0	5,5,5	0.43	0
7	DGL	BBB	407	6	7,8,9	1.47	1 (14%)	7,9,11	2.61	4 (57%)
3	PG4	DDD	403	-	12,12,12	0.30	0	11,11,11	0.17	0
6	ALA	DDD	405	7	3,4,5	0.93	0	2,4,6	3.35	1 (50%)
3	PG4	AAA	403	-	12,12,12	0.32	0	11,11,11	0.18	0
4	TRS	BBB	404	-	7,7,7	0.23	0	9,9,9	0.36	0
6	ALA	CCC	404	7	3,4,5	1.00	0	2,4,6	2.71	1 (50%)
7	DGL	AAA	407	6	7,8,9	0.98	0	7,9,11	1.51	1 (14%)
5	PEG	AAA	404	-	6,6,6	0.41	0	5,5,5	0.31	0
7	DGL	DDD	406	6	7,8,9	1.73	2 (28%)	7,9,11	2.65	2 (28%)
5	PEG	DDD	404	-	6,6,6	0.37	0	5,5,5	0.24	0
6	ALA	AAA	406	7	3,4,5	0.81	0	2,4,6	1.42	0
5	PEG	BBB	405	-	6,6,6	0.30	0	5,5,5	0.20	0
3	PG4	BBB	403	-	12,12,12	0.29	0	11,11,11	0.16	0
7	DGL	CCC	405	6	7,8,9	1.20	1 (14%)	7,9,11	2.52	4 (57%)

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
8	GOL	AAA	405	-	-	2/4/4/4	-
6	ALA	BBB	406	7	-	0/0/2/4	-
8	GOL	CCC	403	-	-	1/4/4/4	-
7	DGL	BBB	407	6	-	3/7/8/9	-
3	PG4	DDD	403	-	-	4/10/10/10	-
6	ALA	DDD	405	7	-	0/0/2/4	-
3	PG4	AAA	403	-	-	8/10/10/10	-
4	TRS	BBB	404	-	-	4/9/9/9	-
6	ALA	CCC	404	7	-	0/0/2/4	-
7	DGL	AAA	407	6	-	0/7/8/9	-
5	PEG	AAA	404	-	-	1/4/4/4	-
7	DGL	DDD	406	6	-	4/7/8/9	-
5	PEG	DDD	404	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ALA	AAA	406	7	-	0/0/2/4	-
5	PEG	BBB	405	-	-	2/4/4/4	-
3	PG4	BBB	403	-	-	6/10/10/10	-
7	DGL	CCC	405	6	-	6/7/8/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	DDD	406	DGL	CB-CA	2.89	1.59	1.53
7	BBB	407	DGL	CB-CA	2.85	1.59	1.53
7	CCC	405	DGL	CB-CA	2.27	1.58	1.53
7	DDD	406	DGL	O-C	2.16	1.28	1.22

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	DDD	406	DGL	CB-CA-N	5.96	125.79	110.17
7	BBB	407	DGL	CB-CA-N	5.10	123.55	110.17
6	DDD	405	ALA	O-C-CA	-4.74	109.26	124.28
7	CCC	405	DGL	OXT-C-O	-4.03	114.94	124.09
6	CCC	404	ALA	O-C-CA	-3.35	113.66	124.28

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	404	TRS	N-C-C3-O3
7	BBB	407	DGL	C-CA-CB-CG
7	CCC	405	DGL	C-CA-CB-CG
7	DDD	406	DGL	C-CA-CB-CG
8	AAA	405	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 12 short contacts:

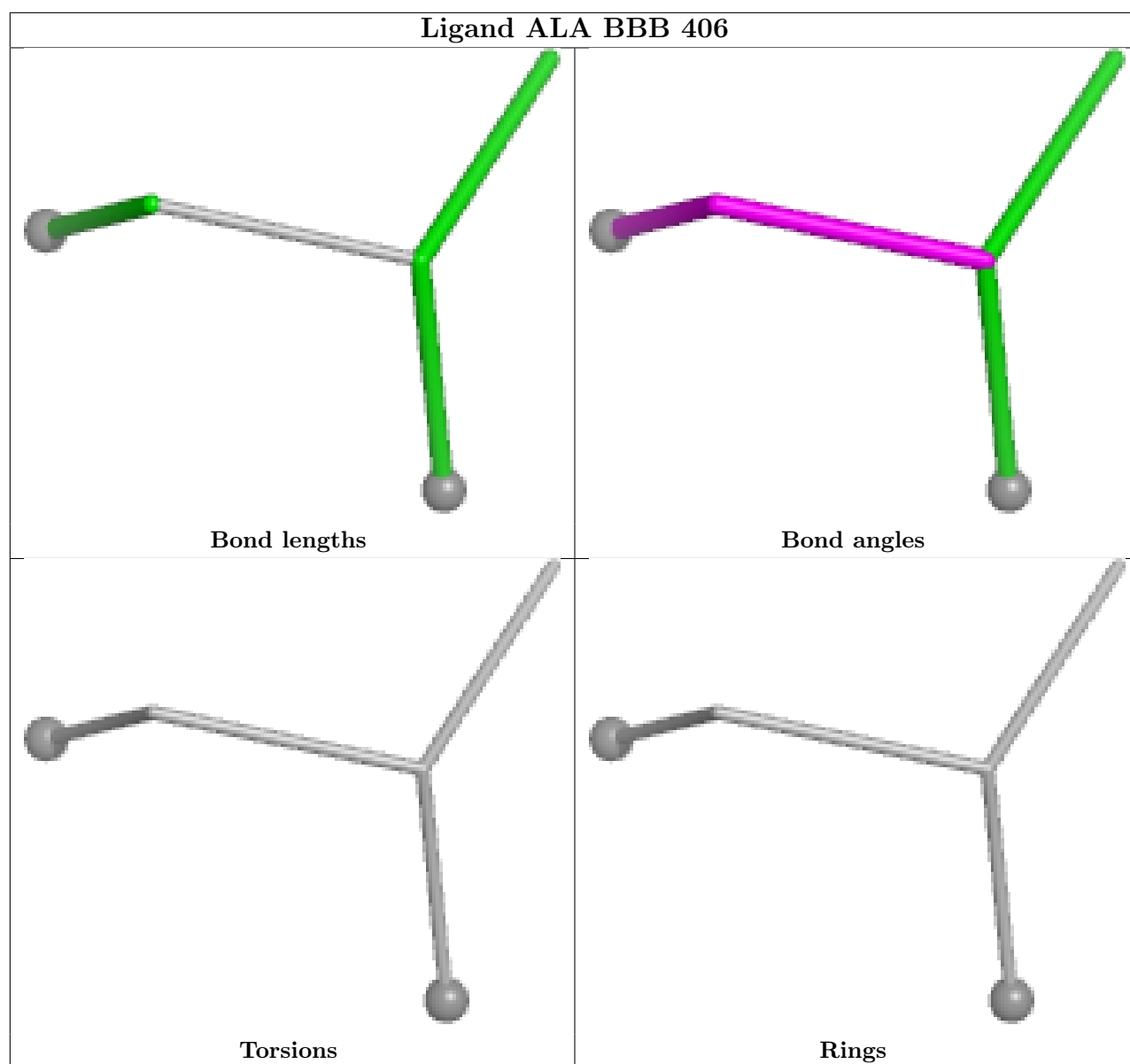
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	BBB	407	DGL	2	0
6	CCC	404	ALA	3	0
7	AAA	407	DGL	1	0
7	DDD	406	DGL	4	0

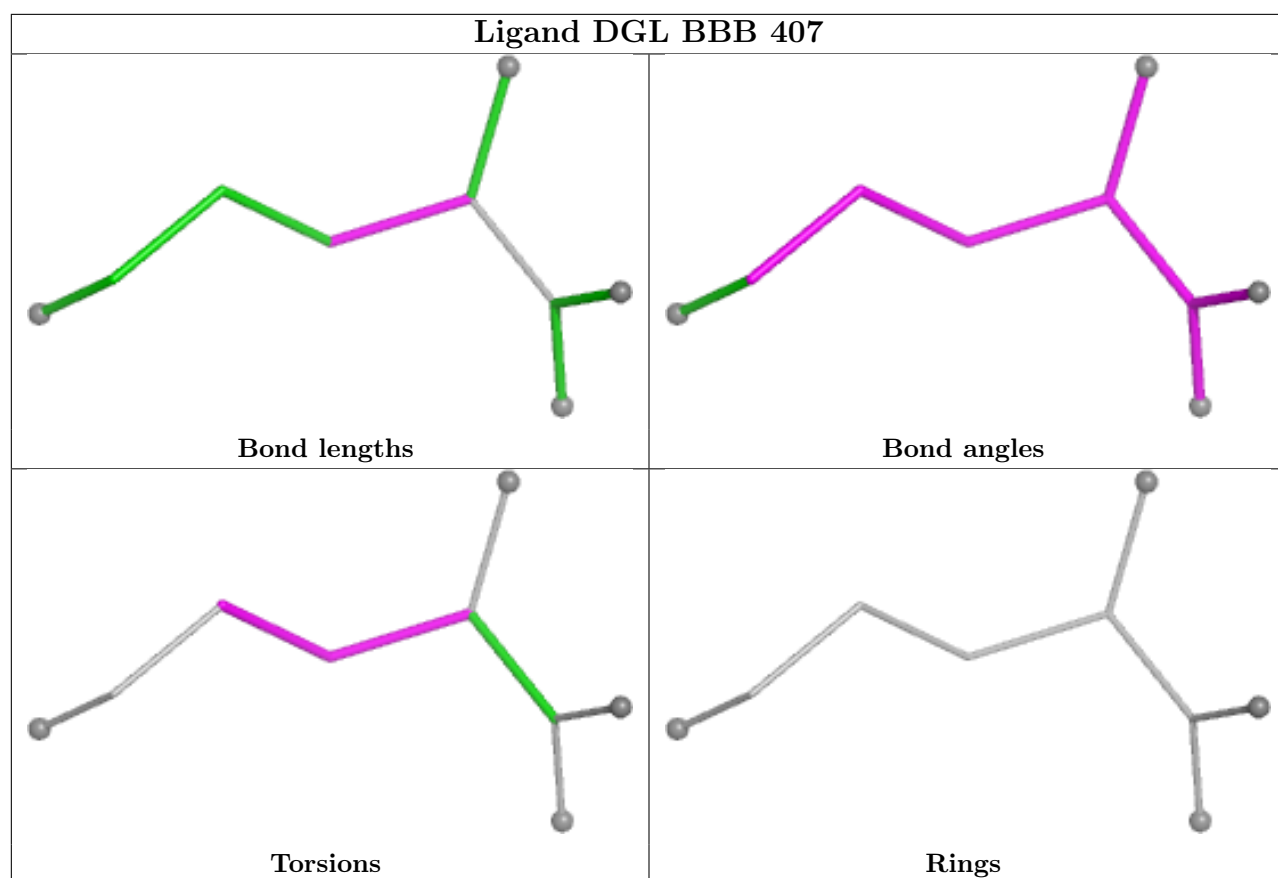
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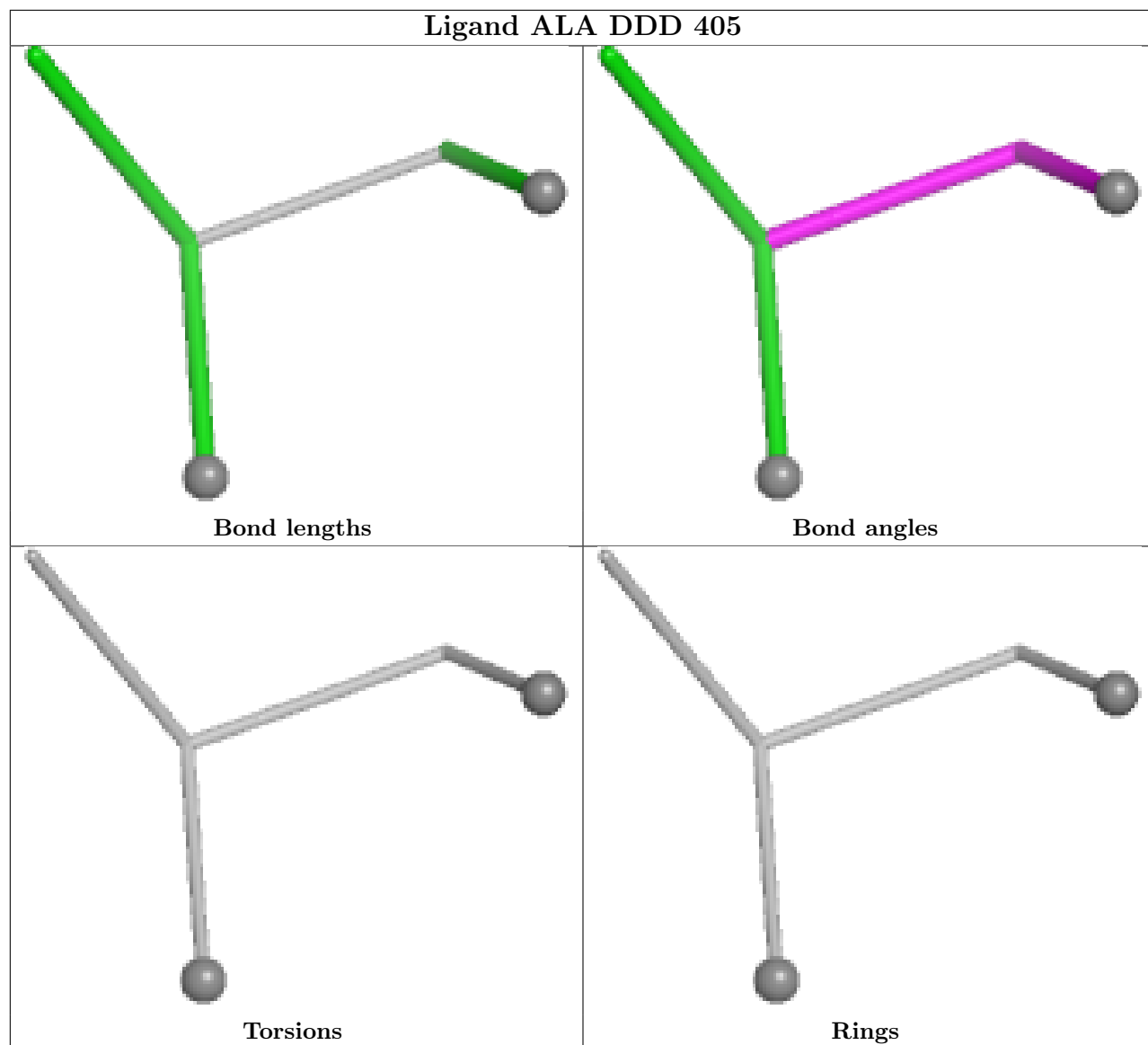
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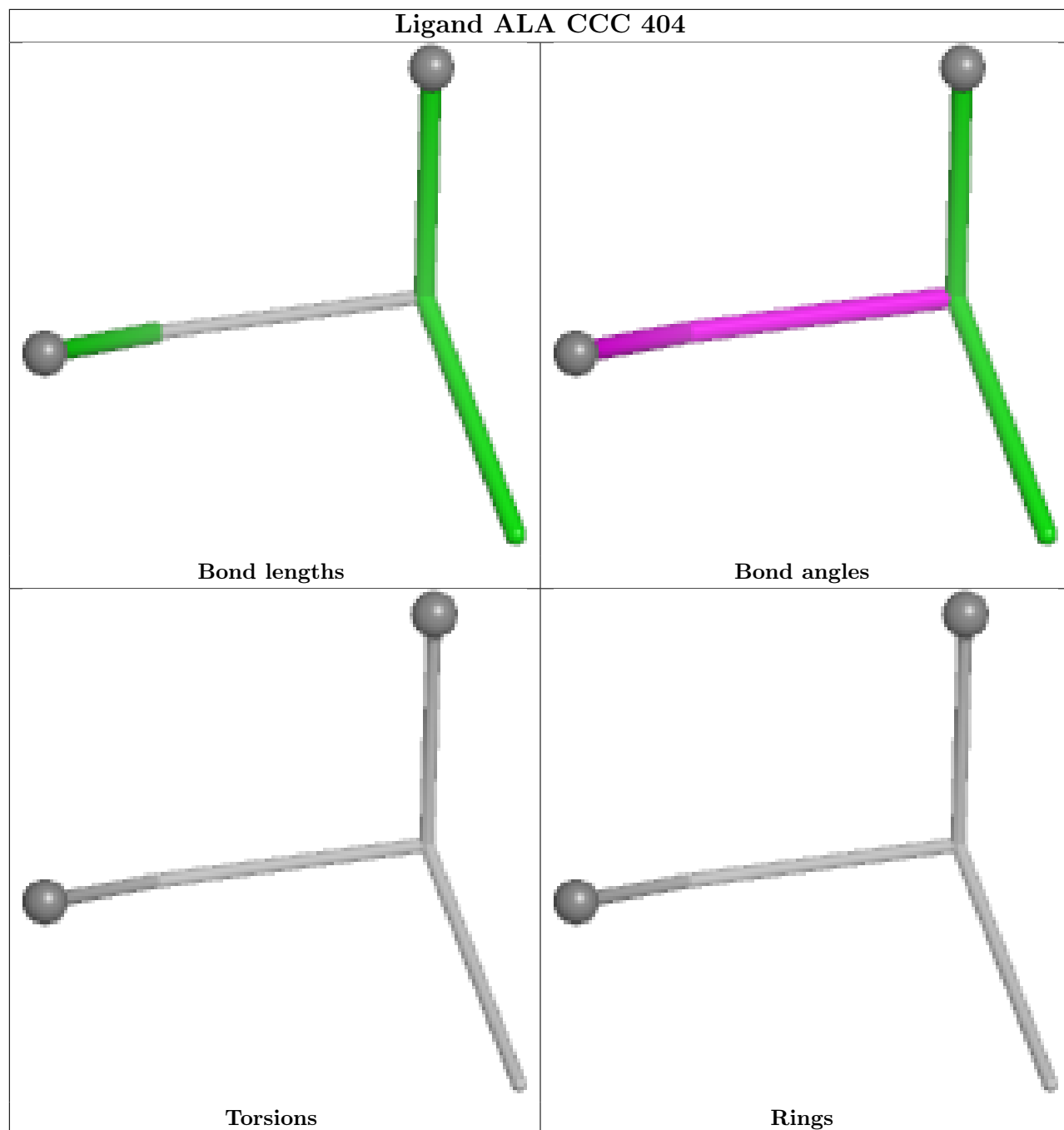
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	403	PG4	1	0
7	CCC	405	DGL	2	0

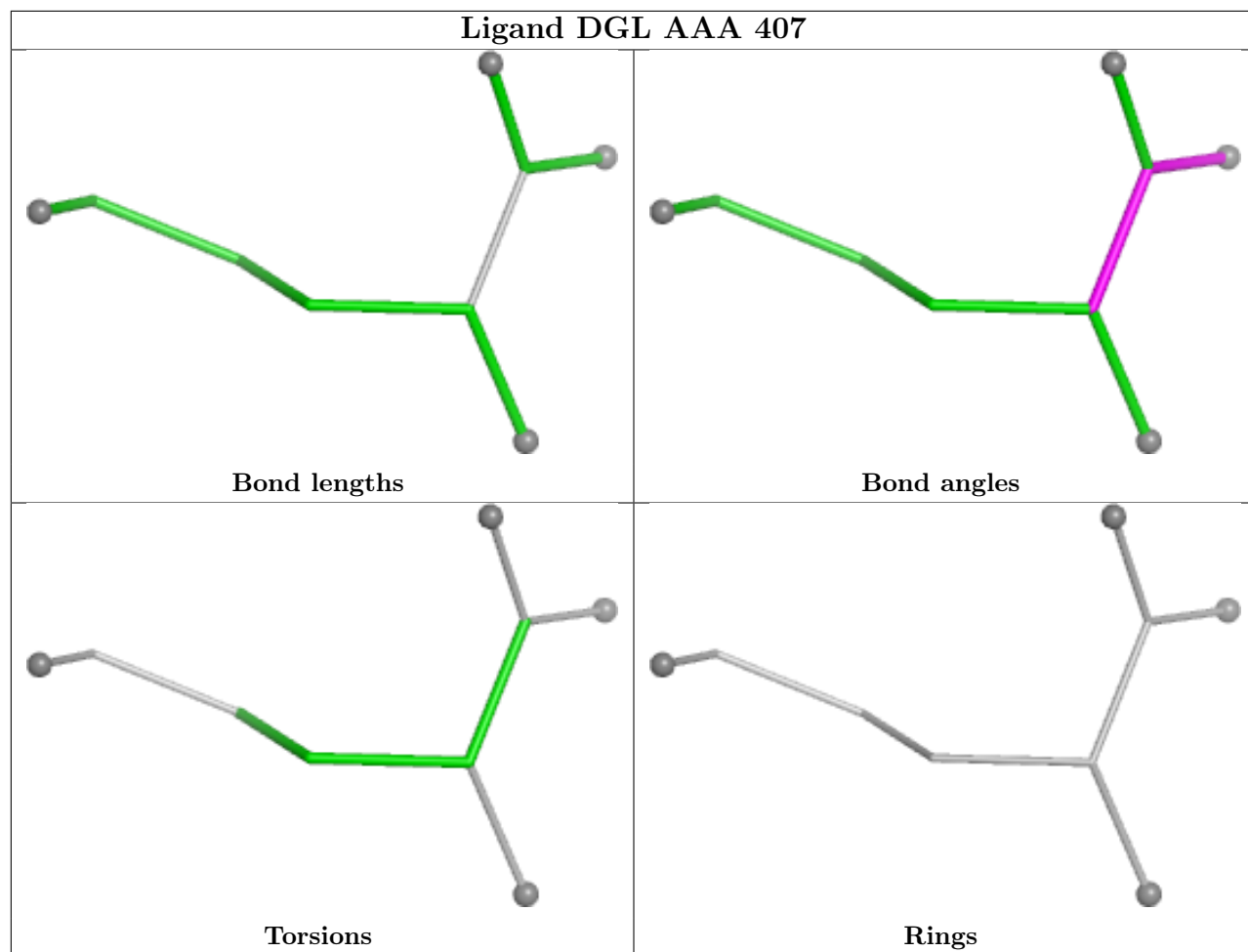
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

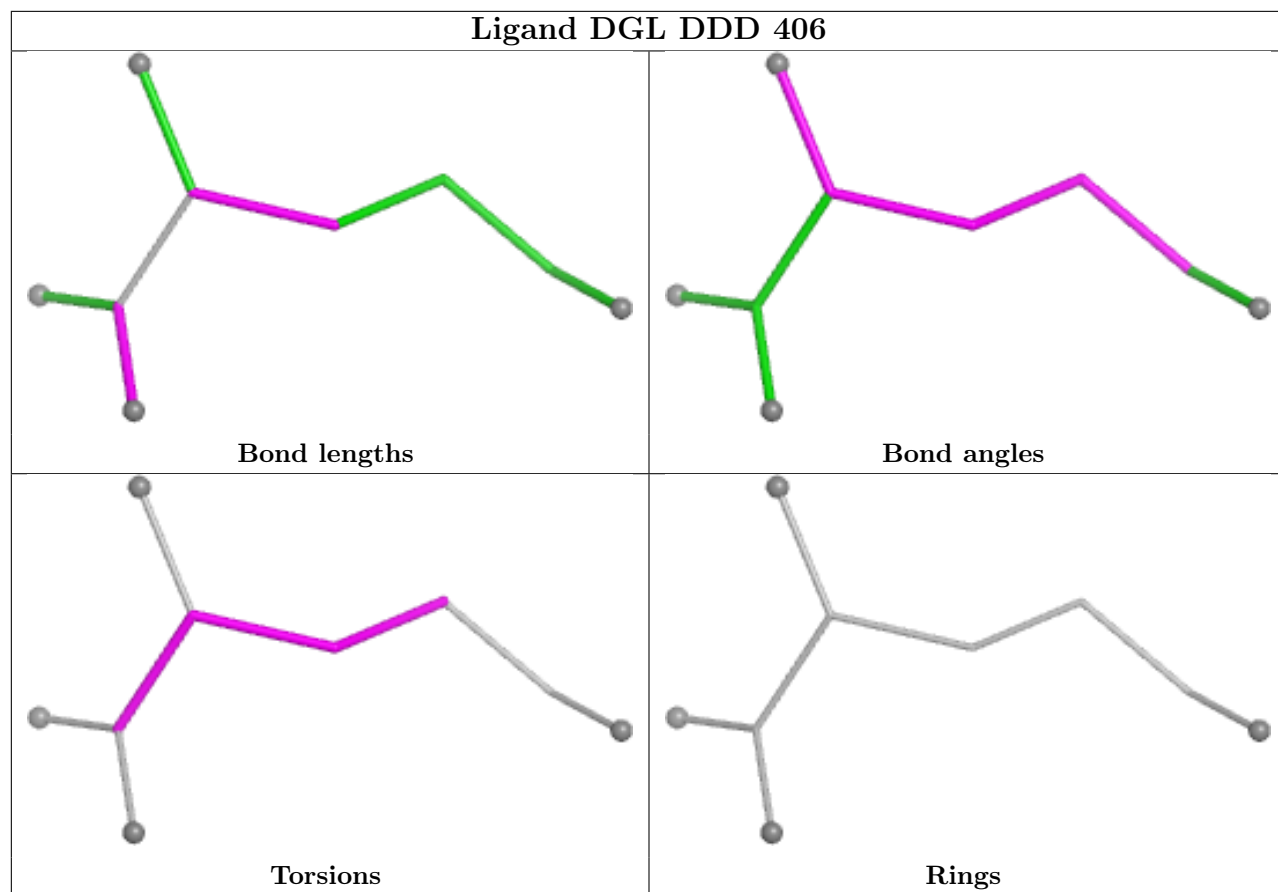


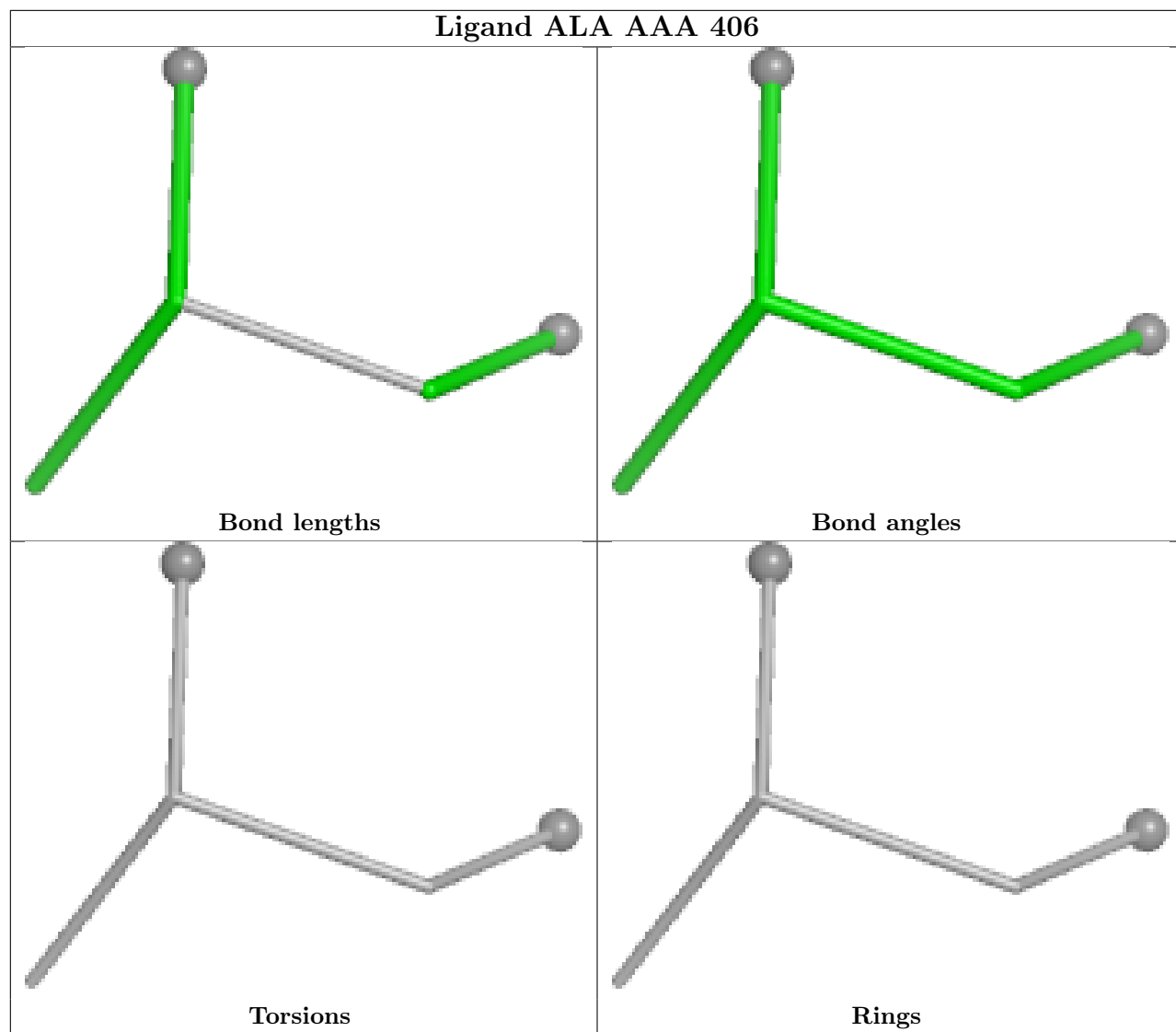


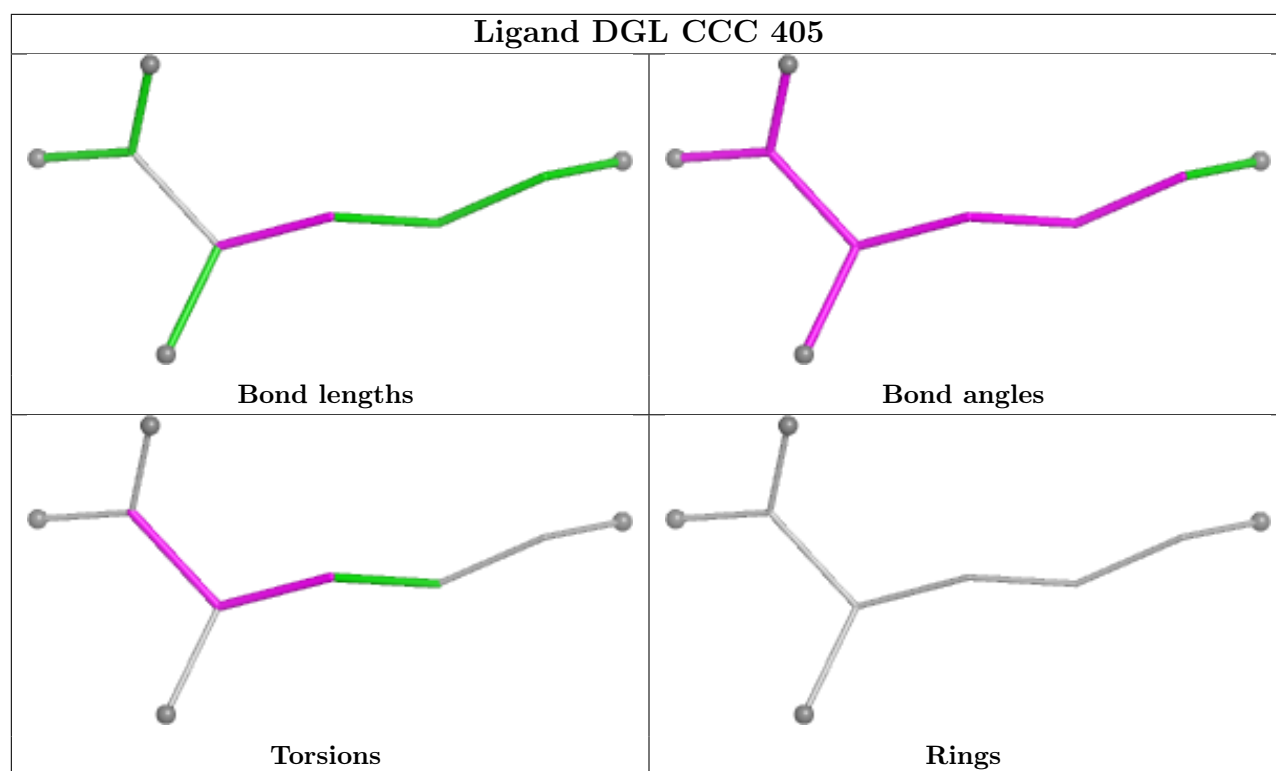












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AAA	304/304 (100%)	0.10	10 (3%)	49	55	34, 50, 79, 111	2 (0%)
1	BBB	304/304 (100%)	0.23	12 (3%)	43	49	36, 52, 83, 116	2 (0%)
1	CCC	304/304 (100%)	0.37	11 (3%)	46	52	35, 54, 83, 116	2 (0%)
1	DDD	304/304 (100%)	0.22	8 (2%)	57	63	36, 52, 82, 128	2 (0%)
All	All	1216/1216 (100%)	0.23	41 (3%)	48	54	34, 52, 83, 128	8 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	1	MET	4.8
1	CCC	1	MET	4.6
1	DDD	1	MET	4.6
1	BBB	1	MET	4.2
1	CCC	105	ILE	3.7

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

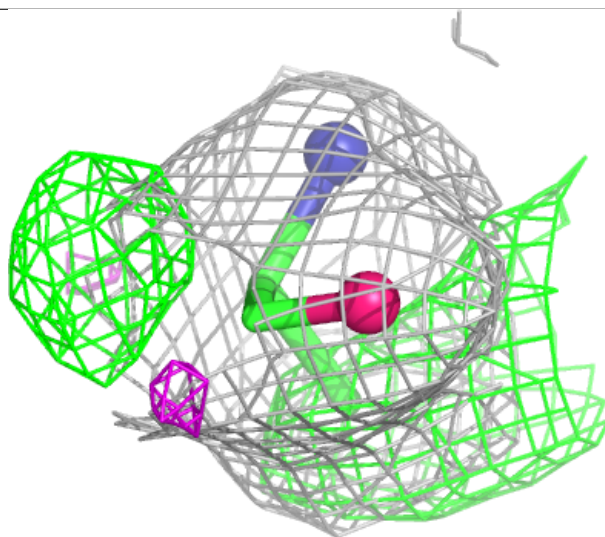
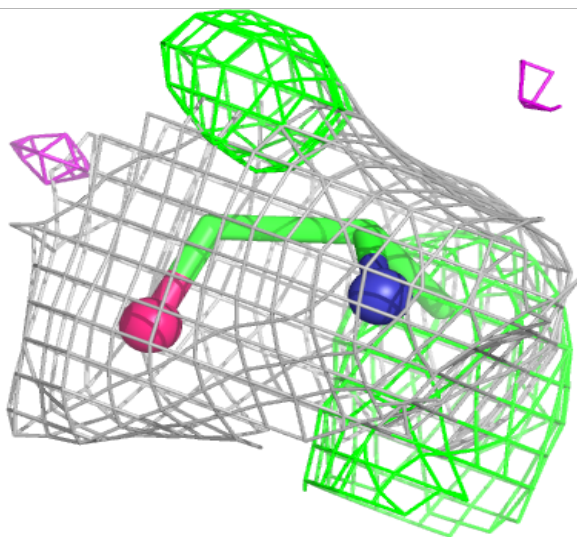
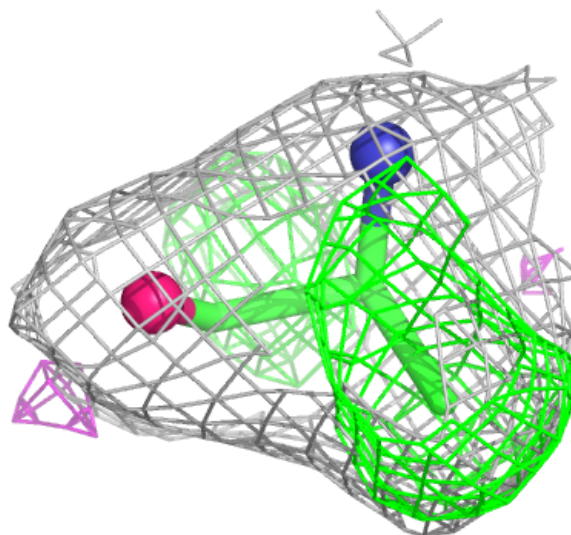
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ALA	BBB	406	5/6	0.78	0.17	47,56,57,67	0
6	ALA	AAA	406	5/6	0.79	0.18	45,46,58,62	0
4	TRS	BBB	404	8/8	0.80	0.17	74,88,91,92	0
6	ALA	DDD	405	5/6	0.84	0.16	46,48,56,59	0
8	GOL	AAA	405	6/6	0.84	0.32	96,102,114,117	0
7	DGL	DDD	406	9/10	0.85	0.15	60,69,79,82	0
5	PEG	BBB	405	7/7	0.85	0.20	71,81,109,112	0
7	DGL	CCC	405	9/10	0.86	0.15	52,59,75,83	0
3	PG4	AAA	403	13/13	0.87	0.20	74,92,105,105	0
7	DGL	BBB	407	9/10	0.88	0.12	51,61,73,76	0
3	PG4	BBB	403	13/13	0.88	0.21	82,93,103,105	0
3	PG4	DDD	403	13/13	0.89	0.17	70,79,89,90	0
7	DGL	AAA	407	9/10	0.90	0.12	49,66,76,78	0
6	ALA	CCC	404	5/6	0.90	0.11	48,49,53,58	0
8	GOL	CCC	403	6/6	0.91	0.16	84,89,90,95	0
5	PEG	AAA	404	7/7	0.92	0.17	64,69,78,78	0
2	ZN	AAA	402	1/1	0.93	0.06	42,42,42,42	0
5	PEG	DDD	404	7/7	0.93	0.15	60,66,74,80	0
2	ZN	CCC	402	1/1	0.95	0.06	43,43,43,43	0
2	ZN	DDD	402	1/1	0.96	0.06	39,39,39,39	0
2	ZN	BBB	402	1/1	0.96	0.07	43,43,43,43	0
2	ZN	AAA	401	1/1	0.98	0.06	69,69,69,69	0
2	ZN	DDD	401	1/1	0.98	0.08	70,70,70,70	0
2	ZN	BBB	401	1/1	0.98	0.05	68,68,68,68	0
2	ZN	CCC	401	1/1	0.98	0.08	70,70,70,70	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.

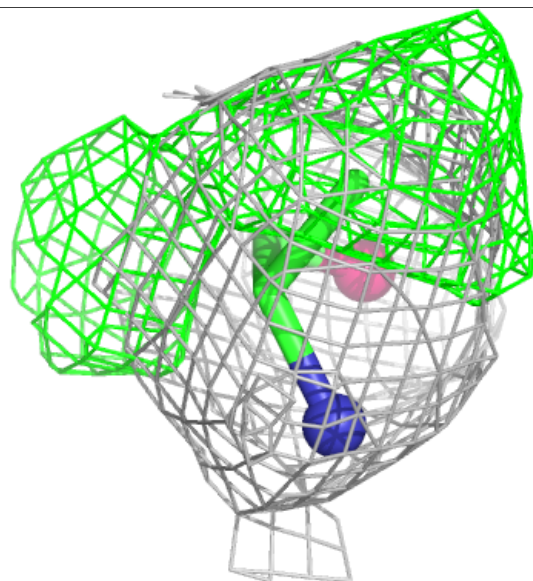
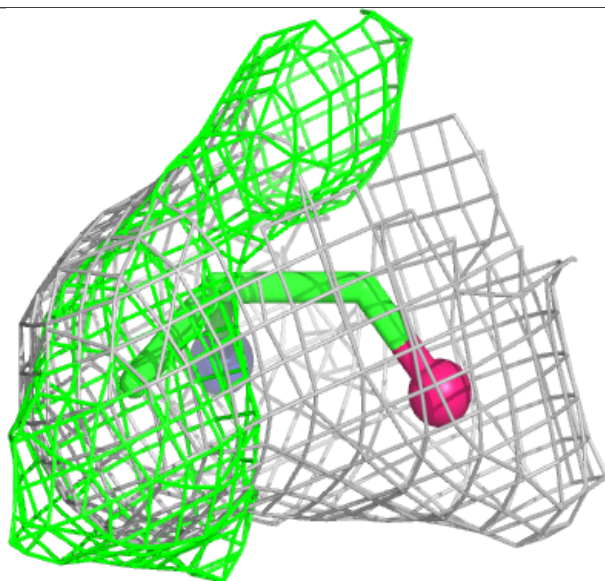
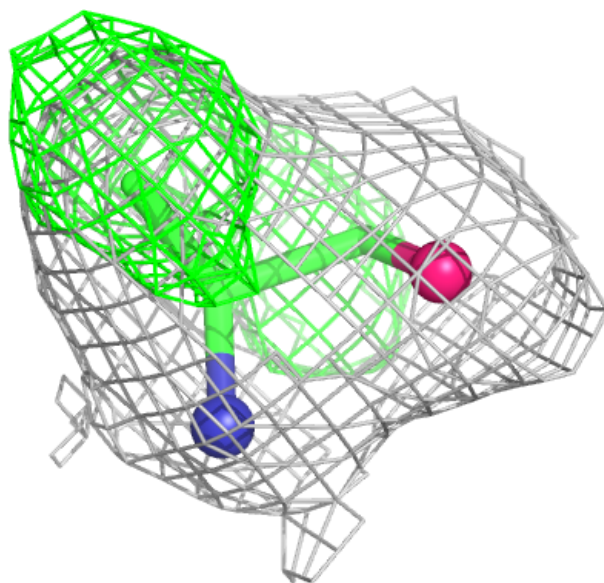
Electron density around ALA BBB 406:

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



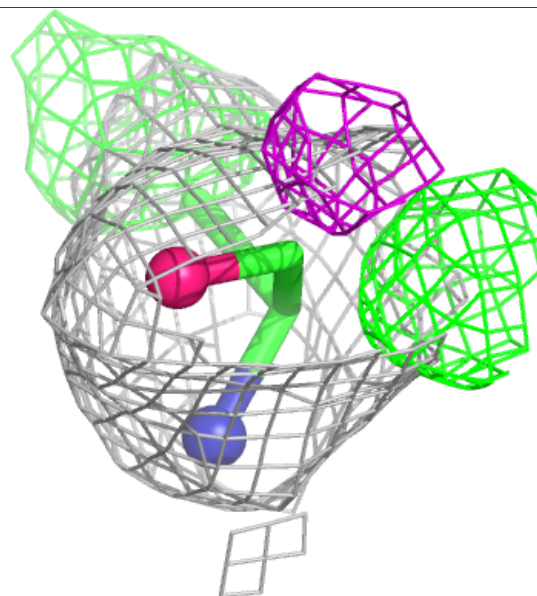
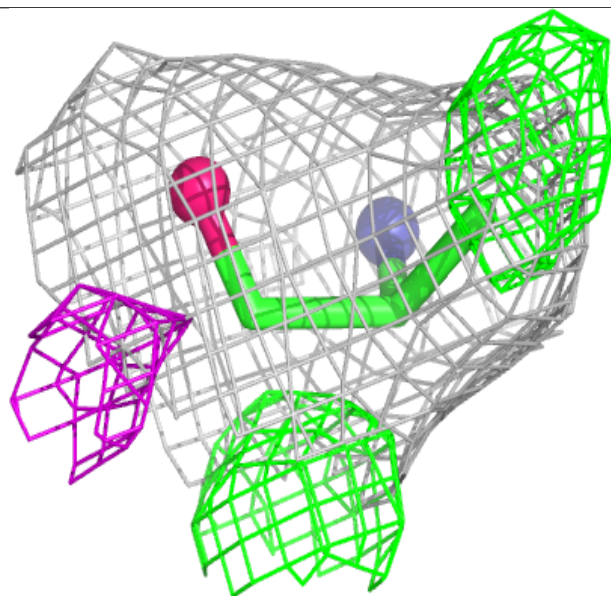
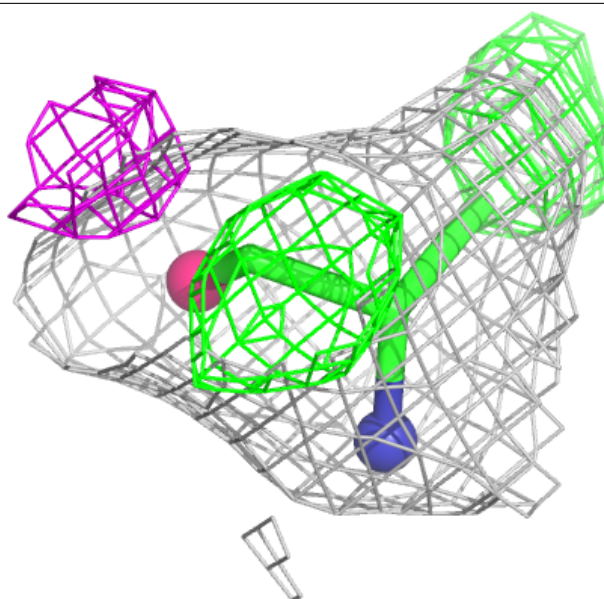
Electron density around ALA AAA 406:

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



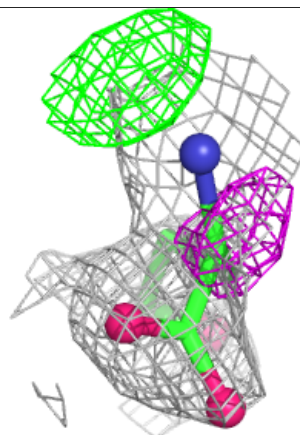
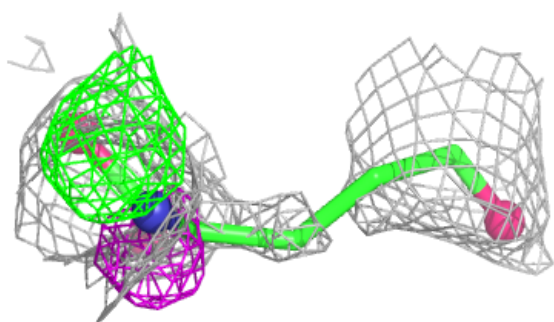
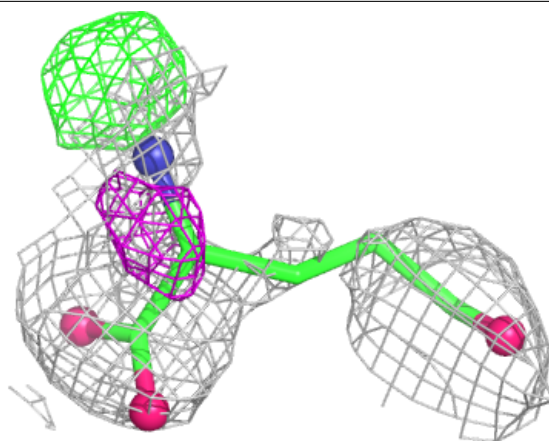
Electron density around ALA DDD 405:

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



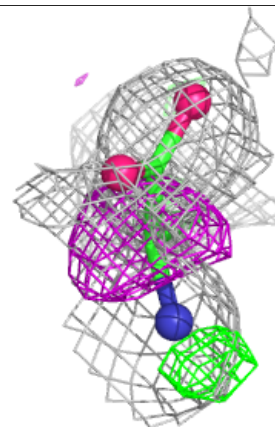
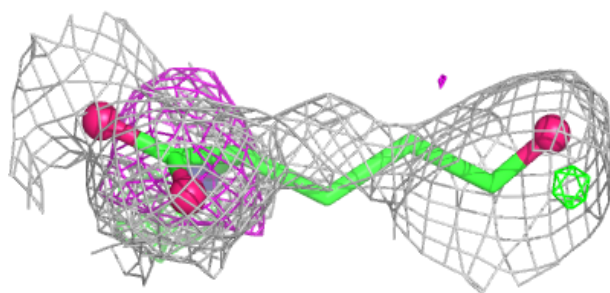
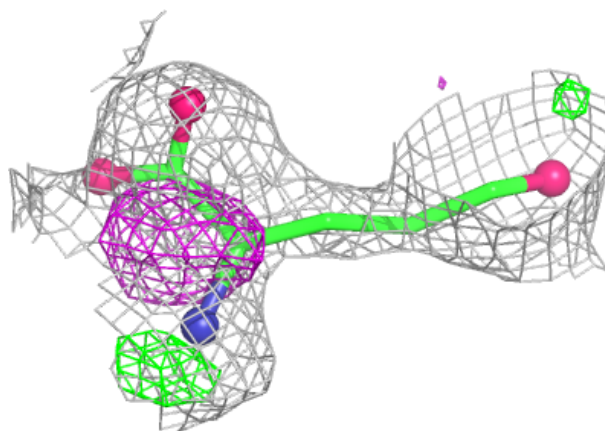
Electron density around DGL DDD 406:

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

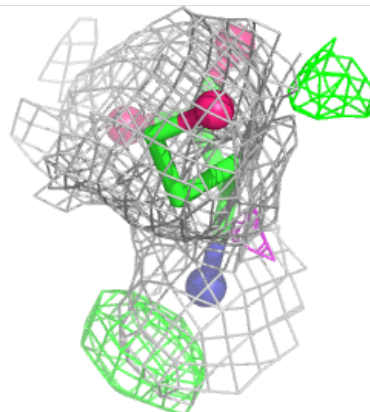
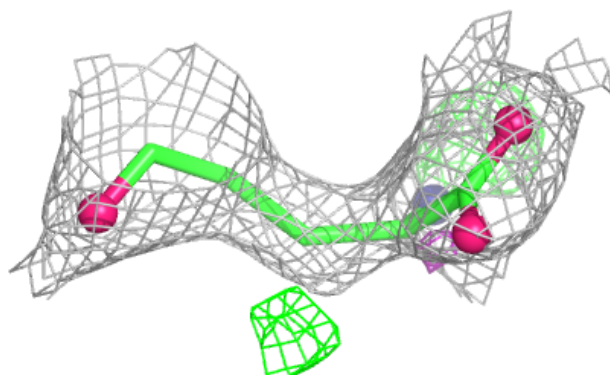
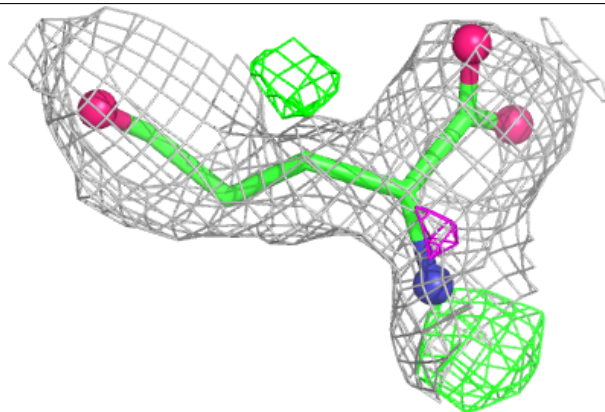


Electron density around DGL CCC 405:

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

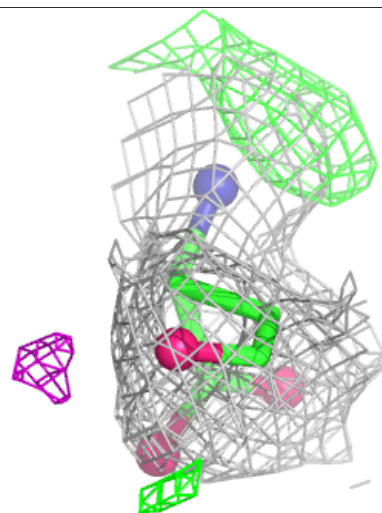
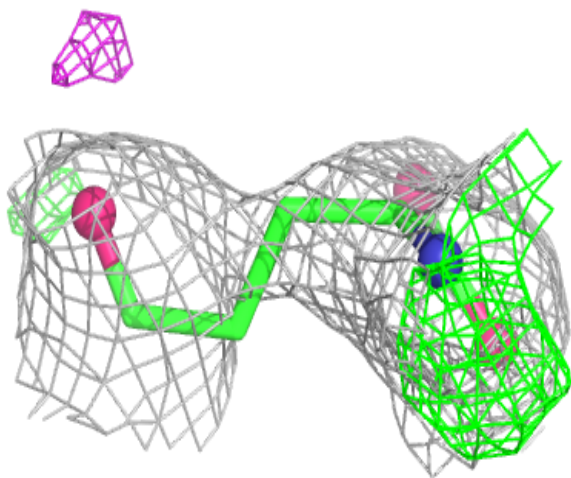
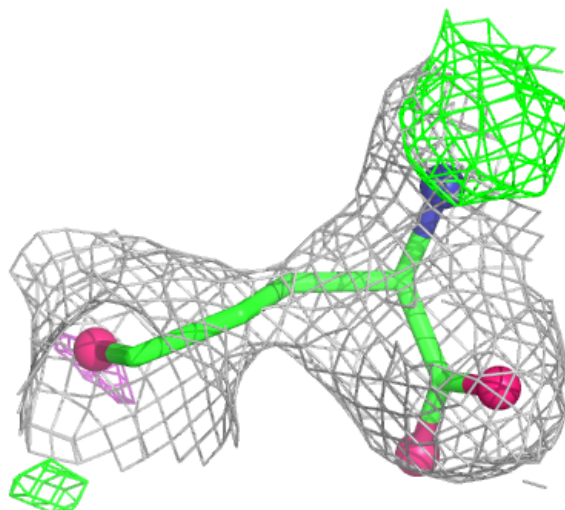
**Electron density around DGL BBB 407:**

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



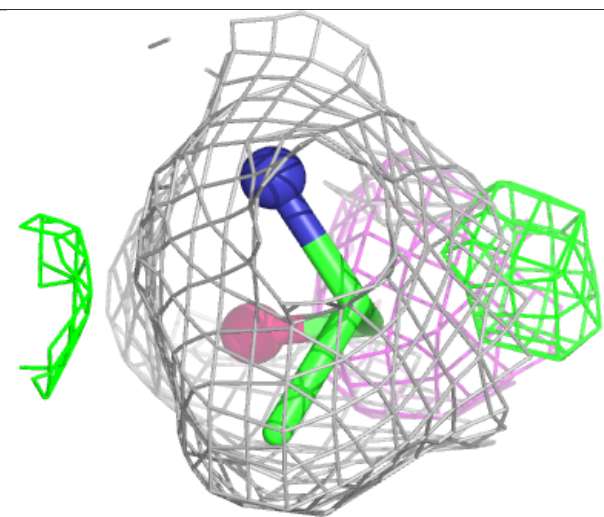
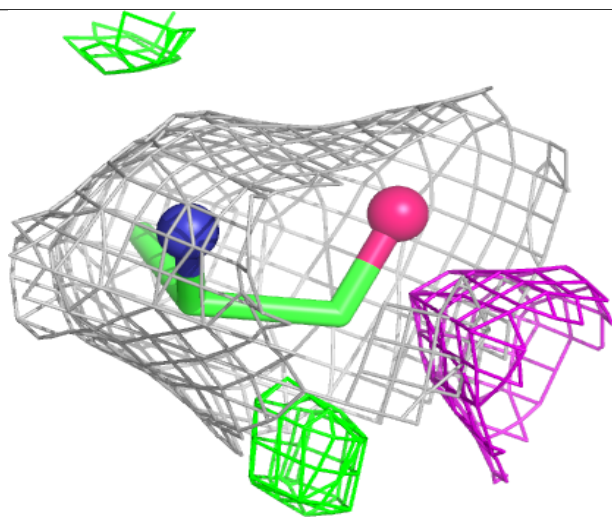
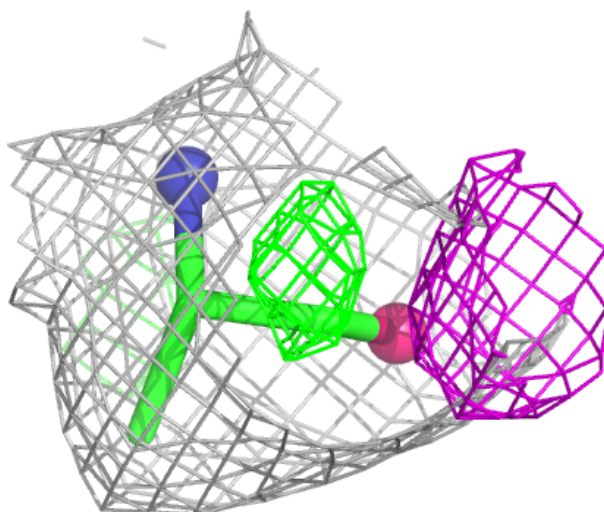
Electron density around DGL AAA 407:

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



Electron density around ALA CCC 404:

$2mF_o-DF_c$ (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.