



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:07 am BST

PDB ID : 6KSI
Title : Staphylococcus aureus lipase - native
Authors : Kitadokoro, K.; Tanaka, M.; Kamitani, S.
Deposited on : 2019-08-24
Resolution : 2.08 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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

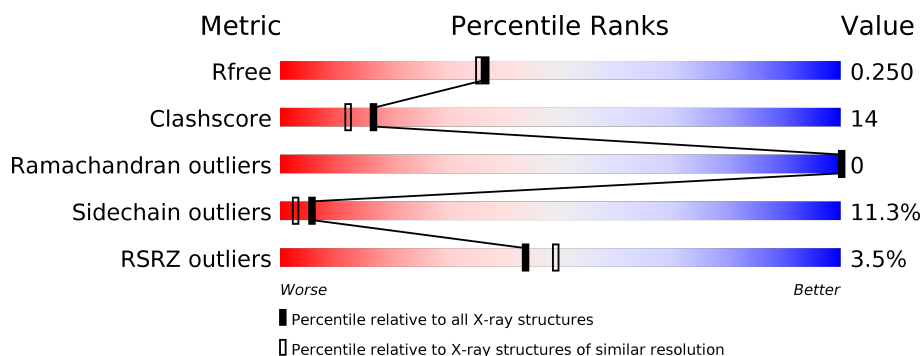
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 ≥ 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	408	
1	B	408	

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
4	6NA	B	403	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6250 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 Lipase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3024	1925	527	563	9			
1	B	382	Total	C	N	O	S	0	0	0
			3024	1925	527	563	9			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A0U1MWF9
A	-12	ASN	-	expression tag	UNP A0A0U1MWF9
A	-11	HIS	-	expression tag	UNP A0A0U1MWF9
A	-10	LYS	-	expression tag	UNP A0A0U1MWF9
A	-9	VAL	-	expression tag	UNP A0A0U1MWF9
A	-8	HIS	-	expression tag	UNP A0A0U1MWF9
A	-7	HIS	-	expression tag	UNP A0A0U1MWF9
A	-6	HIS	-	expression tag	UNP A0A0U1MWF9
A	-5	HIS	-	expression tag	UNP A0A0U1MWF9
A	-4	HIS	-	expression tag	UNP A0A0U1MWF9
A	-3	HIS	-	expression tag	UNP A0A0U1MWF9
A	-2	MET	-	expression tag	UNP A0A0U1MWF9
A	68	GLN	GLU	variant	UNP A0A0U1MWF9
B	-13	MET	-	expression tag	UNP A0A0U1MWF9
B	-12	ASN	-	expression tag	UNP A0A0U1MWF9
B	-11	HIS	-	expression tag	UNP A0A0U1MWF9
B	-10	LYS	-	expression tag	UNP A0A0U1MWF9
B	-9	VAL	-	expression tag	UNP A0A0U1MWF9
B	-8	HIS	-	expression tag	UNP A0A0U1MWF9
B	-7	HIS	-	expression tag	UNP A0A0U1MWF9
B	-6	HIS	-	expression tag	UNP A0A0U1MWF9
B	-5	HIS	-	expression tag	UNP A0A0U1MWF9
B	-4	HIS	-	expression tag	UNP A0A0U1MWF9
B	-3	HIS	-	expression tag	UNP A0A0U1MWF9
B	-2	MET	-	expression tag	UNP A0A0U1MWF9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	68	GLN	GLU	variant	UNP A0A0U1MWF9

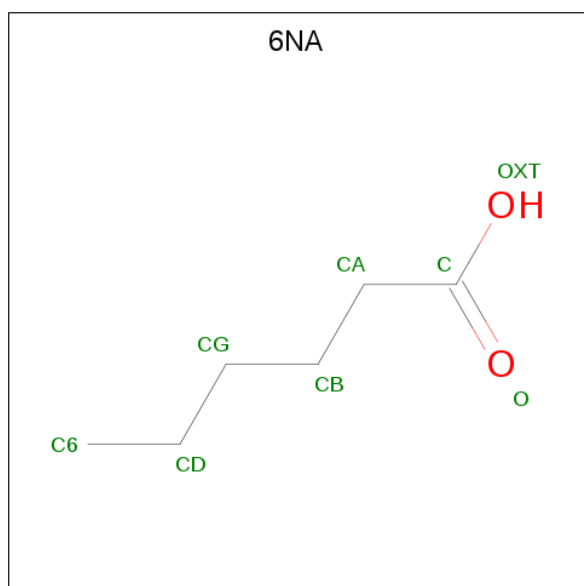
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is HEXANOIC ACID (three-letter code: 6NA) (formula: C₆H₁₂O₂) (labeled as "Ligand of Interest" by author).



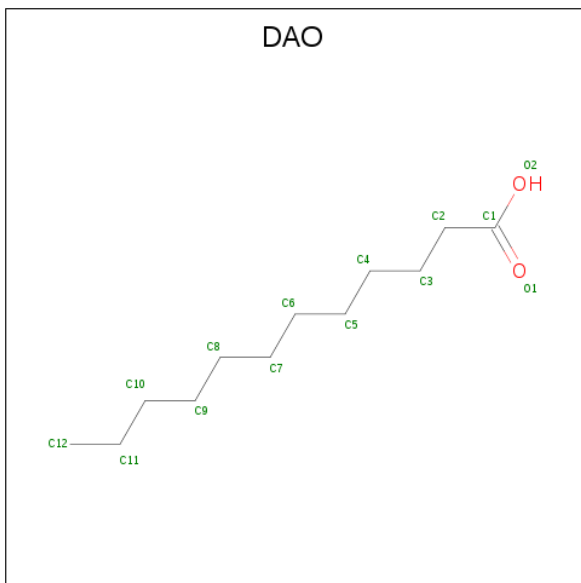
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0

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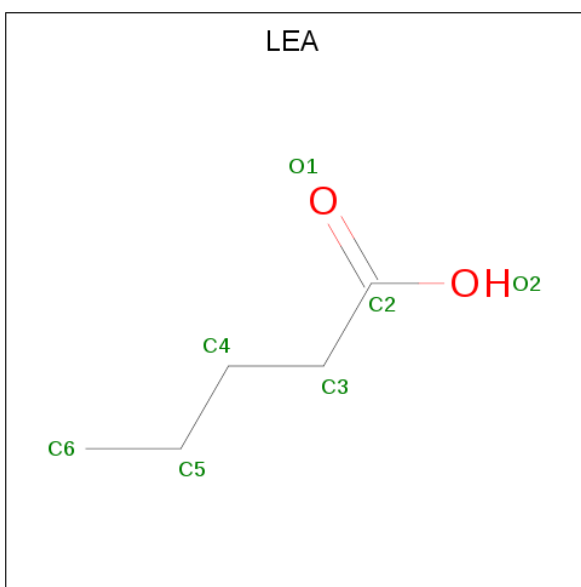
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$) (labeled as "Ligand of Interest" by author).



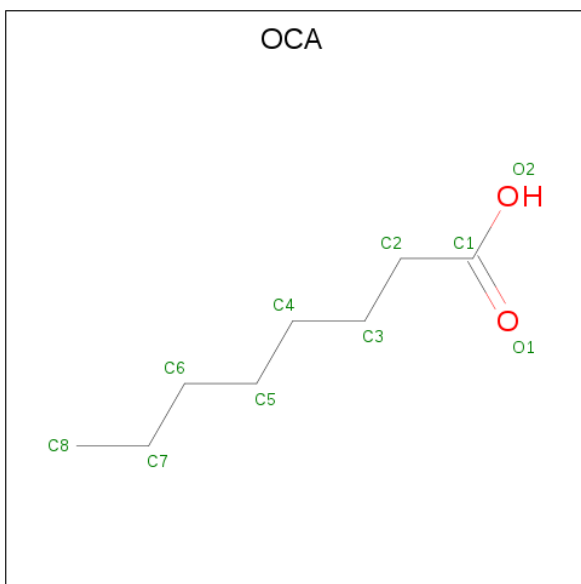
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	12	2		
5	A	1	Total	C	O	0	0
			14	12	2		
5	B	1	Total	C	O	0	0
			14	12	2		

- Molecule 6 is PENTANOIC ACID (three-letter code: LEA) (formula: $C_5H_{10}O_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	5	2		
6	B	1	Total	C	O	0	0
			7	5	2		

- Molecule 7 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula: $C_8H_{16}O_2$) (labeled as "Ligand of Interest" by author).



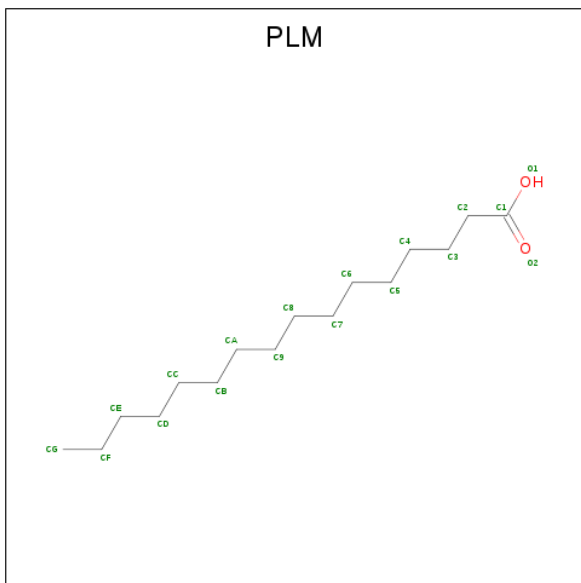
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	8	2		

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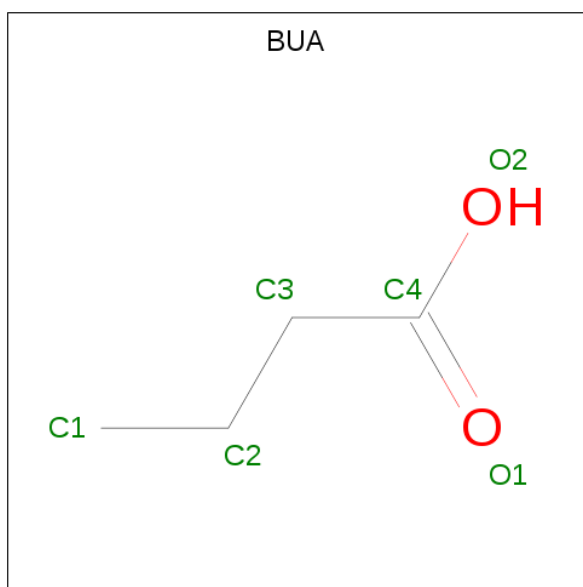
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	8	2		

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 9 is BUTANOIC ACID (three-letter code: BUA) (formula: $C_4H_8O_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	4	2		
9	B	1	Total	C	O	0	0
			6	4	2		

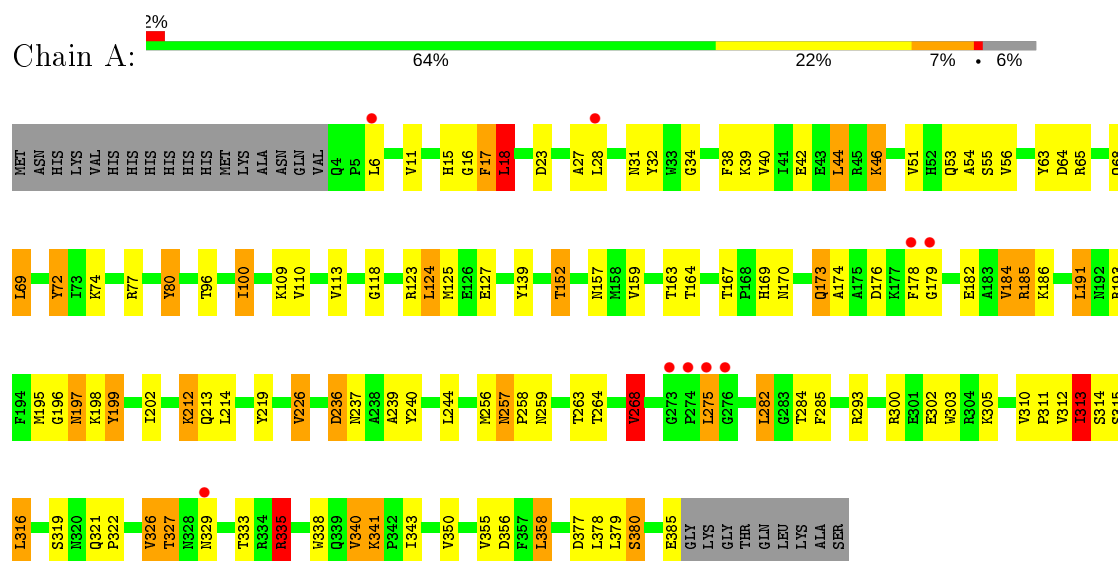
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	59	Total	O	0	0
			59	59		
10	B	17	Total	O	0	0
			17	17		

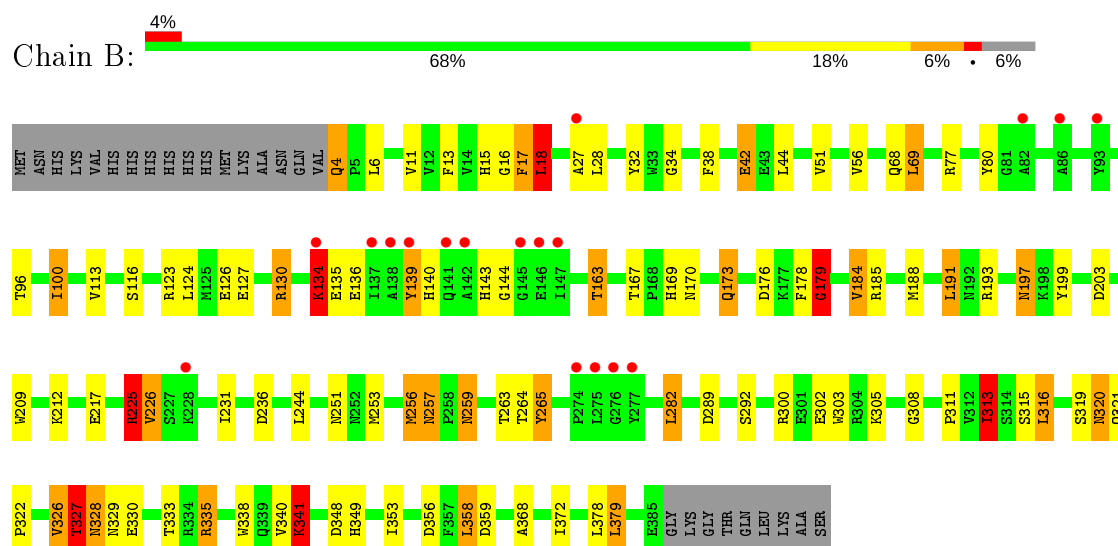
3 Residue-property plots [i](#)

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: Lipase 2



• Molecule 1: Lipase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.91Å 129.91Å 251.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.74 – 2.08 47.74 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.74-2.08) 99.9 (47.74-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.231 , 0.250 0.230 , 0.250	Depositor DCC
R_{free} test set	6444 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.5	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	0.95	EDS
Total number of atoms	6250	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: LEA, ZN, 6NA, OCA, CA, DAO, PLM, BUA

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	1.50	22/3106 (0.7%)	1.49	55/4212 (1.3%)
1	B	1.39	11/3106 (0.4%)	1.55	48/4212 (1.1%)
All	All	1.45	33/6212 (0.5%)	1.52	103/8424 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
All	All	0	5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	LEU	N-CA	17.25	1.80	1.46
1	B	18	LEU	N-CA	15.11	1.76	1.46
1	A	236	ASP	CG-OD2	9.18	1.46	1.25
1	A	72	TYR	CG-CD1	8.52	1.50	1.39
1	A	17	PHE	C-O	8.42	1.39	1.23
1	B	328	ASN	CG-ND2	8.17	1.53	1.32
1	A	63	TYR	CG-CD1	8.17	1.49	1.39
1	B	139	TYR	CE1-CZ	8.13	1.49	1.38
1	B	179	GLY	N-CA	7.89	1.57	1.46
1	B	225	ARG	CD-NE	-7.61	1.33	1.46
1	A	80	TYR	CE1-CZ	7.57	1.48	1.38
1	A	55	SER	CA-CB	6.92	1.63	1.52
1	A	32	TYR	CB-CG	6.54	1.61	1.51
1	A	300	ARG	CD-NE	6.50	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	ARG	CZ-NH1	6.37	1.41	1.33
1	A	127	GLU	CG-CD	6.19	1.61	1.51
1	B	127	GLU	CD-OE1	6.04	1.32	1.25
1	B	265	TYR	CG-CD1	5.89	1.46	1.39
1	A	380	SER	CB-OG	-5.79	1.34	1.42
1	A	127	GLU	CD-OE2	-5.62	1.19	1.25
1	A	63	TYR	CE1-CZ	5.62	1.45	1.38
1	A	196	GLY	CA-C	5.56	1.60	1.51
1	A	64	ASP	CG-OD1	5.43	1.37	1.25
1	A	139	TYR	CE1-CZ	5.36	1.45	1.38
1	B	139	TYR	CG-CD1	5.36	1.46	1.39
1	B	300	ARG	CD-NE	5.34	1.55	1.46
1	B	136	GLU	CD-OE1	5.23	1.31	1.25
1	A	118	GLY	N-CA	5.19	1.53	1.46
1	B	236	ASP	CG-OD2	5.14	1.37	1.25
1	A	72	TYR	CE1-CZ	5.08	1.45	1.38
1	A	305	LYS	CE-NZ	5.08	1.61	1.49
1	A	338	TRP	CE3-CZ3	5.04	1.47	1.38
1	A	199	TYR	CD2-CE2	5.01	1.46	1.39

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ARG	NE-CZ-NH2	-29.40	105.60	120.30
1	B	225	ARG	NE-CZ-NH1	25.80	133.20	120.30
1	A	335	ARG	NE-CZ-NH2	16.18	128.39	120.30
1	B	236	ASP	CB-CG-OD2	15.41	132.17	118.30
1	A	17	PHE	C-N-CA	-15.32	83.39	121.70
1	B	178	PHE	C-N-CA	-15.17	90.45	122.30
1	B	17	PHE	C-N-CA	-14.45	85.57	121.70
1	B	236	ASP	CB-CG-OD1	-13.81	105.87	118.30
1	A	335	ARG	NE-CZ-NH1	-13.65	113.47	120.30
1	A	236	ASP	CB-CG-OD2	13.23	130.21	118.30
1	B	335	ARG	NE-CZ-NH2	12.74	126.67	120.30
1	A	64	ASP	CB-CG-OD1	10.15	127.43	118.30
1	B	225	ARG	CD-NE-CZ	9.91	137.47	123.60
1	A	18	LEU	CA-CB-CG	9.83	137.90	115.30
1	A	226	VAL	CG1-CB-CG2	9.54	126.16	110.90
1	A	326	VAL	CG1-CB-CG2	9.45	126.02	110.90
1	A	65	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	130	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	77	ARG	NE-CZ-NH2	-8.72	115.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	MET	CG-SD-CE	-8.71	86.26	100.20
1	B	77	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	A	313	ILE	CG1-CB-CG2	8.63	130.38	111.40
1	B	305	LYS	CD-CE-NZ	8.58	131.43	111.70
1	B	18	LEU	CA-CB-CG	8.44	134.71	115.30
1	A	268	VAL	CB-CA-C	-8.21	95.80	111.40
1	A	313	ILE	CB-CG1-CD1	8.16	136.76	113.90
1	A	356	ASP	CB-CG-OD1	8.06	125.55	118.30
1	B	178	PHE	O-C-N	-8.03	109.55	123.20
1	A	316	LEU	CB-CG-CD2	8.01	124.62	111.00
1	A	305	LYS	CD-CE-NZ	7.95	130.00	111.70
1	B	191	LEU	CB-CG-CD2	7.54	123.82	111.00
1	B	335	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	B	359	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	A	64	ASP	CB-CG-OD2	-7.47	111.57	118.30
1	A	124	LEU	CB-CG-CD2	7.44	123.65	111.00
1	B	359	ASP	CB-CG-OD1	7.43	124.99	118.30
1	A	159	VAL	CG1-CB-CG2	7.33	122.64	110.90
1	B	225	ARG	CG-CD-NE	-7.27	96.53	111.80
1	B	17	PHE	O-C-N	-7.24	111.11	122.70
1	B	313	ILE	CB-CA-C	-7.23	97.15	111.60
1	B	185	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	113	VAL	CG1-CB-CG2	7.06	122.20	110.90
1	A	244	LEU	CB-CG-CD2	7.03	122.96	111.00
1	A	212	LYS	CD-CE-NZ	7.01	127.81	111.70
1	A	125	MET	CG-SD-CE	6.85	111.16	100.20
1	B	226	VAL	CG1-CB-CG2	6.85	121.86	110.90
1	A	340	VAL	CG1-CB-CG2	6.80	121.78	110.90
1	A	293	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	A	335	ARG	CD-NE-CZ	6.71	133.00	123.60
1	A	282	LEU	CA-CB-CG	6.71	130.73	115.30
1	B	326	VAL	CG1-CB-CG2	6.66	121.56	110.90
1	B	188	MET	CG-SD-CE	6.59	110.74	100.20
1	B	358	LEU	CB-CG-CD1	6.58	122.18	111.00
1	A	185	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	236	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	A	358	LEU	CB-CG-CD1	6.45	121.96	111.00
1	B	130	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	184	VAL	CG1-CB-CG2	6.31	121.00	110.90
1	B	184	VAL	CG1-CB-CG2	6.26	120.92	110.90
1	A	310	VAL	CA-CB-CG1	6.24	120.26	110.90
1	A	127	GLU	OE1-CD-OE2	-6.24	115.81	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	356	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	B	326	VAL	CA-CB-CG1	6.18	120.17	110.90
1	B	134	LYS	CA-CB-CG	6.16	126.96	113.40
1	A	23	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	176	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	53	GLN	N-CA-CB	-6.03	99.75	110.60
1	B	327	THR	N-CA-CB	-6.00	98.91	110.30
1	A	69	LEU	CB-CG-CD2	5.94	121.09	111.00
1	A	152	THR	N-CA-CB	-5.93	99.03	110.30
1	A	191	LEU	CB-CG-CD1	5.92	121.07	111.00
1	B	282	LEU	C-N-CA	-5.76	110.20	122.30
1	A	268	VAL	CA-CB-CG2	5.73	119.50	110.90
1	A	268	VAL	CG1-CB-CG2	5.69	120.01	110.90
1	B	341	LYS	CD-CE-NZ	5.67	124.75	111.70
1	B	316	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	282	LEU	CB-CG-CD1	5.63	120.57	111.00
1	B	313	ILE	CG1-CB-CG2	5.63	123.79	111.40
1	A	152	THR	CA-CB-CG2	5.62	120.27	112.40
1	A	310	VAL	CG1-CB-CG2	5.62	119.89	110.90
1	A	185	ARG	CG-CD-NE	-5.54	100.16	111.80
1	B	69	LEU	CB-CG-CD2	5.53	120.41	111.00
1	A	17	PHE	O-C-N	-5.52	113.86	122.70
1	A	326	VAL	CA-CB-CG1	5.52	119.18	110.90
1	A	214	LEU	CB-CG-CD2	5.51	120.37	111.00
1	A	100	ILE	CA-CB-CG2	5.48	121.86	110.90
1	B	134	LYS	CB-CG-CD	5.47	125.84	111.60
1	A	275	LEU	CA-CB-CG	5.46	127.86	115.30
1	B	356	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	340	VAL	CG1-CB-CG2	5.34	119.45	110.90
1	B	300	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	186	LYS	CD-CE-NZ	-5.32	99.46	111.70
1	B	203	ASP	CB-CG-OD1	5.29	123.07	118.30
1	A	31	ASN	N-CA-CB	-5.24	101.17	110.60
1	B	17	PHE	CA-C-N	5.17	128.57	117.20
1	A	139	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	B	42	GLU	N-CA-CB	-5.16	101.31	110.60
1	A	113	VAL	CA-CB-CG2	5.13	118.59	110.90
1	B	244	LEU	CB-CG-CD2	5.10	119.67	111.00
1	A	184	VAL	CA-CB-CG2	5.03	118.45	110.90
1	A	74	LYS	CD-CE-NZ	-5.02	100.16	111.70
1	B	335	ARG	CD-NE-CZ	5.00	130.60	123.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	LEU	Peptide
1	B	179	GLY	Peptide
1	B	18	LEU	Peptide
1	B	225	ARG	Sidechain
1	B	4	GLN	Peptide

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	3024	0	2919	89	0
1	B	3024	0	2919	82	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	11	0	0
4	B	8	0	11	1	0
5	A	28	0	46	8	0
5	B	14	0	23	4	0
6	A	7	0	9	0	0
6	B	7	0	9	0	0
7	A	10	0	15	0	0
7	B	10	0	15	0	0
8	A	18	0	31	0	0
9	A	6	0	7	0	0
9	B	6	0	7	1	0
10	A	59	0	0	1	1
10	B	17	0	0	1	0
All	All	6250	0	6022	173	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 14.

All (173) 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:A:313:ILE:CG1	1:A:313:ILE:CD1	1.75	1.61
1:B:18:LEU:N	1:B:18:LEU:CA	1.76	1.48
1:A:18:LEU:CA	1:A:18:LEU:N	1.80	1.43
1:B:17:PHE:O	1:B:18:LEU:CA	1.70	1.38
1:A:17:PHE:O	1:A:18:LEU:CA	1.75	1.34
1:A:179:GLY:HA2	1:A:184:VAL:CG2	1.72	1.18
1:A:17:PHE:C	1:A:18:LEU:CA	2.10	1.18
1:B:17:PHE:C	1:B:18:LEU:CA	2.09	1.17
1:A:17:PHE:O	1:A:18:LEU:HA	0.96	1.13
1:B:17:PHE:O	1:B:18:LEU:HA	0.97	1.12
1:B:256:MET:CE	1:B:321:GLN:HB3	1.81	1.10
1:B:313:ILE:H	1:B:313:ILE:HD13	1.14	1.09
1:B:27:ALA:HB3	10:B:513:HOH:O	1.53	1.06
1:A:256:MET:CE	1:A:321:GLN:HB3	1.88	1.03
1:A:179:GLY:HA2	1:A:184:VAL:HG22	1.40	1.03
1:A:179:GLY:HA2	1:A:184:VAL:HG21	1.41	1.01
1:A:256:MET:HE3	1:A:321:GLN:HB3	1.40	1.01
1:A:219:TYR:H	5:A:405:DAO:H52	1.26	1.00
1:B:313:ILE:HD13	1:B:313:ILE:N	1.79	0.97
1:B:173:GLN:H	1:B:173:GLN:HE21	1.01	0.97
1:B:313:ILE:H	1:B:313:ILE:CD1	1.77	0.96
1:A:17:PHE:C	1:A:18:LEU:HA	1.79	0.93
1:A:173:GLN:H	1:A:173:GLN:HE21	1.08	0.91
1:B:256:MET:HE1	1:B:321:GLN:HB3	1.52	0.90
1:B:320:ASN:H	1:B:320:ASN:HD22	1.21	0.86
1:B:179:GLY:HA2	1:B:184:VAL:HG22	1.58	0.86
1:A:15:HIS:HE1	1:A:56:VAL:H	1.21	0.84
1:A:179:GLY:CA	1:A:184:VAL:HG22	2.07	0.84
1:A:193:ARG:HH11	5:A:404:DAO:C2	1.91	0.82
1:A:256:MET:HE2	1:A:322:PRO:HD2	1.61	0.82
1:B:17:PHE:C	1:B:18:LEU:HA	1.85	0.80
1:A:313:ILE:H	1:A:313:ILE:CD1	1.93	0.80
1:A:197:ASN:HD22	1:A:199:TYR:H	1.30	0.79
1:B:179:GLY:HA2	1:B:184:VAL:CG2	2.12	0.79
1:A:174:ALA:O	1:A:178:PHE:O	2.02	0.78
1:A:313:ILE:H	1:A:313:ILE:HD13	1.49	0.78
1:A:302:GLU:O	1:A:313:ILE:HG13	1.84	0.77
1:B:193:ARG:HH11	5:B:404:DAO:C2	1.97	0.77
1:B:264:THR:O	1:B:341:LYS:HB2	1.84	0.77
1:A:257:ASN:HD22	1:A:259:ASN:H	1.31	0.76
1:B:197:ASN:HD22	1:B:199:TYR:H	1.33	0.75
1:A:257:ASN:ND2	1:A:259:ASN:H	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASN:HD21	1:B:319:SER:H	1.34	0.74
1:A:179:GLY:CA	1:A:184:VAL:CG2	2.60	0.74
1:B:193:ARG:HH11	5:B:404:DAO:H22	1.53	0.72
1:B:257:ASN:HD22	1:B:259:ASN:H	1.38	0.72
1:A:193:ARG:HH11	5:A:404:DAO:H21	1.56	0.71
1:B:265:TYR:CE1	1:B:341:LYS:HG2	2.27	0.70
1:B:256:MET:HE3	1:B:322:PRO:HD2	1.74	0.69
1:B:173:GLN:NE2	1:B:173:GLN:H	1.85	0.69
1:B:327:THR:CG2	1:B:329:ASN:H	2.06	0.69
1:B:15:HIS:HE1	1:B:56:VAL:H	1.41	0.69
1:B:257:ASN:HD21	1:B:259:ASN:HB2	1.57	0.69
1:A:327:THR:HG22	1:A:329:ASN:N	2.07	0.69
1:B:134:LYS:HE2	1:B:135:GLU:H	1.58	0.68
1:A:173:GLN:N	1:A:173:GLN:HE21	1.88	0.68
1:A:237:ASN:HD22	1:A:239:ALA:H	1.40	0.67
1:A:173:GLN:H	1:A:173:GLN:NE2	1.87	0.67
1:A:197:ASN:ND2	1:A:199:TYR:H	1.94	0.66
1:A:15:HIS:CE1	1:A:56:VAL:H	2.10	0.66
1:A:193:ARG:HH11	5:A:404:DAO:H22	1.58	0.65
1:B:256:MET:HE3	1:B:321:GLN:HB3	1.76	0.65
1:A:123:ARG:HH11	1:A:169:HIS:HD2	1.42	0.65
1:B:134:LYS:HE3	1:B:135:GLU:HG3	1.80	0.64
1:B:327:THR:HG22	1:B:330:GLU:H	1.63	0.64
1:B:368:ALA:O	1:B:372:ILE:HG12	1.98	0.64
1:B:197:ASN:ND2	1:B:199:TYR:H	1.95	0.64
1:A:256:MET:CE	1:A:321:GLN:CB	2.73	0.64
1:B:257:ASN:ND2	1:B:259:ASN:H	1.97	0.63
1:B:15:HIS:HD2	1:B:16:GLY:O	1.83	0.62
1:B:313:ILE:N	1:B:313:ILE:CD1	2.48	0.62
1:A:236:ASP:OD2	2:A:401:ZN:ZN	1.47	0.61
1:A:327:THR:HG22	1:A:329:ASN:H	1.66	0.60
1:A:256:MET:HE2	1:A:321:GLN:HB3	1.82	0.59
1:A:179:GLY:O	1:A:184:VAL:HG22	2.01	0.59
1:B:15:HIS:CE1	1:B:56:VAL:H	2.19	0.59
1:B:327:THR:HG23	1:B:329:ASN:H	1.68	0.58
1:A:170:ASN:HD21	1:A:319:SER:H	1.52	0.58
1:B:327:THR:HG22	1:B:329:ASN:N	2.18	0.58
1:A:256:MET:HE1	1:A:321:GLN:CD	2.24	0.58
1:A:198:LYS:H	1:A:213:GLN:NE2	2.02	0.58
1:A:42:GLU:O	1:A:46:LYS:HD3	2.04	0.57
1:B:311:PRO:HB2	1:B:313:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASN:ND2	1:B:259:ASN:HB2	2.19	0.57
1:B:173:GLN:HE22	1:B:311:PRO:HG3	1.71	0.56
1:A:179:GLY:C	1:A:184:VAL:HG22	2.26	0.56
1:A:327:THR:CG2	1:A:329:ASN:H	2.19	0.55
1:A:257:ASN:HD22	1:A:257:ASN:C	2.09	0.55
1:B:173:GLN:N	1:B:173:GLN:HE21	1.86	0.54
1:B:320:ASN:HD22	1:B:320:ASN:N	1.94	0.54
1:B:217:GLU:OE2	1:B:225:ARG:HD3	2.07	0.54
1:B:303:TRP:HA	1:B:313:ILE:HD11	1.90	0.54
1:A:219:TYR:HB2	5:A:405:DAO:H72	1.89	0.54
1:A:15:HIS:HD2	1:A:16:GLY:O	1.91	0.54
1:A:303:TRP:HA	1:A:313:ILE:HG13	1.89	0.54
1:A:237:ASN:HD22	1:A:239:ALA:N	2.04	0.54
1:A:123:ARG:NH1	1:A:169:HIS:HD2	2.05	0.53
1:B:134:LYS:HE2	1:B:135:GLU:N	2.23	0.53
1:A:34:GLY:HA3	1:A:38:PHE:O	2.09	0.53
1:B:256:MET:HE1	1:B:321:GLN:CB	2.34	0.53
1:A:219:TYR:N	5:A:405:DAO:H52	2.10	0.53
1:A:198:LYS:HE3	5:A:405:DAO:H71	1.90	0.53
1:B:11:VAL:HB	1:B:51:VAL:HG12	1.90	0.52
1:A:109:LYS:HE2	1:A:157:ASN:HD22	1.74	0.52
1:A:173:GLN:HE22	1:A:311:PRO:HG3	1.75	0.52
1:A:182:GLU:OE2	1:A:185:ARG:NH2	2.41	0.52
1:B:256:MET:CE	1:B:322:PRO:HD2	2.39	0.52
1:A:264:THR:O	1:A:341:LYS:HB2	2.10	0.52
1:B:257:ASN:C	1:B:257:ASN:HD22	2.13	0.52
1:B:170:ASN:HD21	1:B:319:SER:N	2.05	0.51
1:B:123:ARG:HH11	1:B:169:HIS:HD2	1.57	0.51
1:A:302:GLU:O	1:A:313:ILE:CG1	2.56	0.51
1:A:27:ALA:HB3	10:A:537:HOH:O	2.10	0.51
1:B:311:PRO:HB2	1:B:313:ILE:CD1	2.41	0.51
1:B:327:THR:CG2	1:B:329:ASN:N	2.73	0.51
1:A:313:ILE:CD1	1:A:313:ILE:HG13	2.18	0.50
1:B:302:GLU:O	1:B:313:ILE:HD12	2.12	0.50
1:A:11:VAL:HB	1:A:51:VAL:HG12	1.93	0.50
1:B:167:THR:O	1:B:315:SER:HA	2.12	0.49
1:A:17:PHE:CZ	1:A:18:LEU:HD13	2.47	0.49
1:A:313:ILE:HG12	1:A:313:ILE:CD1	2.18	0.49
1:A:198:LYS:H	1:A:213:GLN:HE21	1.59	0.49
1:B:193:ARG:HH11	5:B:404:DAO:H21	1.77	0.48
1:B:327:THR:HG22	1:B:329:ASN:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLN:NE2	1:A:80:TYR:OH	2.38	0.48
1:B:100:ILE:HD12	1:B:100:ILE:HA	1.66	0.48
1:A:377:ASP:O	1:A:380:SER:HB2	2.13	0.47
1:B:123:ARG:NH1	1:B:169:HIS:HD2	2.12	0.47
1:A:268:VAL:HG22	1:A:343:ILE:CG2	2.44	0.47
1:B:320:ASN:H	1:B:320:ASN:ND2	2.00	0.47
1:A:195:MET:CE	1:A:202:ILE:HD11	2.45	0.47
1:B:256:MET:HE1	1:B:321:GLN:OE1	2.14	0.46
1:A:17:PHE:O	1:A:18:LEU:C	2.51	0.46
1:A:197:ASN:HD21	1:A:199:TYR:HB2	1.80	0.46
1:B:140:HIS:O	1:B:144:GLY:N	2.50	0.45
1:B:179:GLY:HA2	1:B:184:VAL:HG21	1.94	0.45
4:B:403:6NA:OXT	9:B:407:BUA:H13	2.17	0.45
1:B:256:MET:HE3	1:B:322:PRO:CD	2.45	0.45
1:A:237:ASN:ND2	1:A:240:TYR:H	2.15	0.45
1:B:292:SER:HB2	1:B:308:GLY:HA2	1.99	0.45
1:A:167:THR:O	1:A:315:SER:HA	2.16	0.44
1:A:350:VAL:HB	1:A:355:VAL:HG22	2.00	0.43
1:A:54:ALA:HA	1:A:72:TYR:CZ	2.53	0.43
1:A:170:ASN:ND2	1:A:319:SER:H	2.15	0.43
1:B:193:ARG:NH1	5:B:404:DAO:H22	2.27	0.43
1:B:68:GLN:NE2	1:B:80:TYR:OH	2.46	0.43
1:A:312:VAL:N	1:A:313:ILE:HD13	2.34	0.43
1:A:198:LYS:N	1:A:213:GLN:HE21	2.16	0.43
1:B:134:LYS:CE	1:B:135:GLU:HG3	2.47	0.43
1:B:379:LEU:HD12	1:B:379:LEU:HA	1.91	0.43
1:B:126:GLU:OE1	1:B:130:ARG:NH1	2.52	0.43
1:B:116:SER:HG	1:B:349:HIS:CE1	2.37	0.42
1:B:256:MET:CE	1:B:321:GLN:CB	2.74	0.42
1:A:164:THR:HB	1:A:167:THR:OG1	2.19	0.42
1:B:139:TYR:CE2	1:B:143:HIS:CD2	3.08	0.42
1:B:13:PHE:CD1	1:B:113:VAL:HG22	2.54	0.42
1:B:209:TRP:CE2	1:B:231:ILE:HD13	2.55	0.42
1:A:268:VAL:HG22	1:A:343:ILE:HG21	2.01	0.41
5:A:405:DAO:H41	5:A:405:DAO:O1	2.20	0.41
1:B:256:MET:HE1	1:B:338:TRP:HE1	1.86	0.41
1:A:237:ASN:ND2	1:A:239:ALA:N	2.68	0.41
1:B:34:GLY:HA3	1:B:38:PHE:O	2.20	0.41
1:B:32:TYR:O	1:B:353:ILE:HB	2.21	0.41
1:A:40:VAL:HG13	1:A:44:LEU:HD22	2.03	0.41
1:B:251:ASN:HB3	1:B:320:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:HIS:HB2	1:A:314:SER:O	2.20	0.41
1:B:113:VAL:HA	1:B:163:THR:O	2.21	0.41
1:A:170:ASN:HD21	1:A:319:SER:N	2.17	0.40
1:A:195:MET:HE2	1:A:202:ILE:HD11	2.03	0.40
1:A:257:ASN:HD22	1:A:258:PRO:N	2.18	0.40
1:A:258:PRO:O	1:A:335:ARG:HB3	2.21	0.40
1:A:284:THR:O	1:A:285:PHE:C	2.60	0.40
1:A:311:PRO:HB2	1:A:313:ILE:HG12	2.03	0.40

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)
10:A:537:HOH:O	10:A:537:HOH:O[7_554]	1.54	0.66

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	380/408 (93%)	367 (97%)	13 (3%)	0	100	100
1	B	380/408 (93%)	372 (98%)	8 (2%)	0	100	100
All	All	760/816 (93%)	739 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	319/341 (94%)	283 (89%)	36 (11%)	6	3
1	B	319/341 (94%)	283 (89%)	36 (11%)	6	3
All	All	638/682 (94%)	566 (89%)	72 (11%)	6	3

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	18	LEU
1	A	28	LEU
1	A	39	LYS
1	A	44	LEU
1	A	46	LYS
1	A	69	LEU
1	A	96	THR
1	A	100	ILE
1	A	110	VAL
1	A	124	LEU
1	A	152	THR
1	A	163	THR
1	A	173	GLN
1	A	176	ASP
1	A	191	LEU
1	A	197	ASN
1	A	212	LYS
1	A	226	VAL
1	A	257	ASN
1	A	263	THR
1	A	268	VAL
1	A	275	LEU
1	A	282	LEU
1	A	313	ILE
1	A	316	LEU
1	A	326	VAL
1	A	327	THR
1	A	333	THR
1	A	335	ARG
1	A	340	VAL
1	A	341	LYS
1	A	358	LEU

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Mol	Chain	Res	Type
1	A	378	LEU
1	A	379	LEU
1	A	385	GLU
1	B	4	GLN
1	B	6	LEU
1	B	18	LEU
1	B	28	LEU
1	B	42	GLU
1	B	44	LEU
1	B	69	LEU
1	B	96	THR
1	B	100	ILE
1	B	124	LEU
1	B	134	LYS
1	B	163	THR
1	B	173	GLN
1	B	191	LEU
1	B	197	ASN
1	B	212	LYS
1	B	225	ARG
1	B	226	VAL
1	B	253	MET
1	B	257	ASN
1	B	259	ASN
1	B	263	THR
1	B	282	LEU
1	B	289	ASP
1	B	313	ILE
1	B	316	LEU
1	B	320	ASN
1	B	326	VAL
1	B	327	THR
1	B	328	ASN
1	B	333	THR
1	B	335	ARG
1	B	341	LYS
1	B	358	LEU
1	B	378	LEU
1	B	379	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	52	HIS
1	A	143	HIS
1	A	157	ASN
1	A	169	HIS
1	A	170	ASN
1	A	173	GLN
1	A	197	ASN
1	A	213	GLN
1	A	237	ASN
1	A	257	ASN
1	A	259	ASN
1	A	369	ASN
1	B	15	HIS
1	B	143	HIS
1	B	169	HIS
1	B	170	ASN
1	B	173	GLN
1	B	197	ASN
1	B	213	GLN
1	B	237	ASN
1	B	257	ASN
1	B	259	ASN
1	B	297	HIS
1	B	320	ASN
1	B	328	ASN
1	B	369	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
4	6NA	A	403	-	4,7,7	0.38	0	3,7,7	1.19	0
7	OCA	A	407	-	6,9,9	0.59	0	5,9,9	0.37	0
5	DAO	B	404	-	10,13,13	0.65	0	9,13,13	1.08	1 (11%)
5	DAO	A	404	-	10,13,13	0.63	0	9,13,13	1.42	2 (22%)
8	PLM	A	408	-	14,17,17	0.52	0	13,17,17	1.02	1 (7%)
6	LEA	A	406	-	3,6,6	0.26	0	2,6,6	0.45	0
7	OCA	B	406	-	6,9,9	0.58	0	5,9,9	0.43	0
6	LEA	B	405	-	3,6,6	0.55	0	2,6,6	0.70	0
9	BUA	A	409	-	2,5,5	0.56	0	2,5,5	1.17	0
4	6NA	B	403	-	4,7,7	0.57	0	3,7,7	0.15	0
5	DAO	A	405	-	10,13,13	0.69	0	9,13,13	1.19	1 (11%)
9	BUA	B	407	-	2,5,5	0.40	0	2,5,5	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
4	6NA	A	403	-	-	2/3/5/5	-
7	OCA	A	407	-	-	1/5/7/7	-
5	DAO	B	404	-	-	4/9/11/11	-
5	DAO	A	404	-	-	6/9/11/11	-
8	PLM	A	408	-	-	8/13/15/15	-
6	LEA	A	406	-	-	2/2/4/4	-
7	OCA	B	406	-	-	0/5/7/7	-
6	LEA	B	405	-	-	2/2/4/4	-
9	BUA	A	409	-	-	0/1/3/3	-
4	6NA	B	403	-	-	1/3/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DAO	A	405	-	-	8/9/11/11	-
9	BUA	B	407	-	-	1/1/3/3	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	DAO	C5-C4-C3	-3.36	97.36	114.42
8	A	408	PLM	CC-CB-CA	-3.24	97.97	114.42
5	A	405	DAO	C4-C3-C2	-3.03	101.98	113.76
5	B	404	DAO	C5-C4-C3	-2.95	99.45	114.42
5	A	404	DAO	C4-C3-C2	2.21	122.35	113.76

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	6NA	C-CA-CB-CG
7	A	407	OCA	C1-C2-C3-C4
8	A	408	PLM	C1-C2-C3-C4
6	A	406	LEA	C2-C3-C4-C5
6	B	405	LEA	C2-C3-C4-C5
9	B	407	BUA	C1-C2-C3-C4
5	A	405	DAO	C6-C7-C8-C9
5	A	404	DAO	C3-C4-C5-C6
5	A	405	DAO	C4-C5-C6-C7
8	A	408	PLM	C2-C3-C4-C5
5	B	404	DAO	C3-C4-C5-C6
8	A	408	PLM	C7-C8-C9-CA
5	A	404	DAO	C7-C8-C9-C10
8	A	408	PLM	CC-CD-CE-CF
5	B	404	DAO	C6-C7-C8-C9
8	A	408	PLM	CA-CB-CC-CD
5	B	404	DAO	C7-C8-C9-C10
8	A	408	PLM	C4-C5-C6-C7
5	A	404	DAO	C4-C5-C6-C7
6	B	405	LEA	C3-C4-C5-C6
5	A	404	DAO	C6-C7-C8-C9
5	B	404	DAO	C4-C5-C6-C7
5	A	405	DAO	C3-C4-C5-C6
5	A	405	DAO	C7-C8-C9-C10

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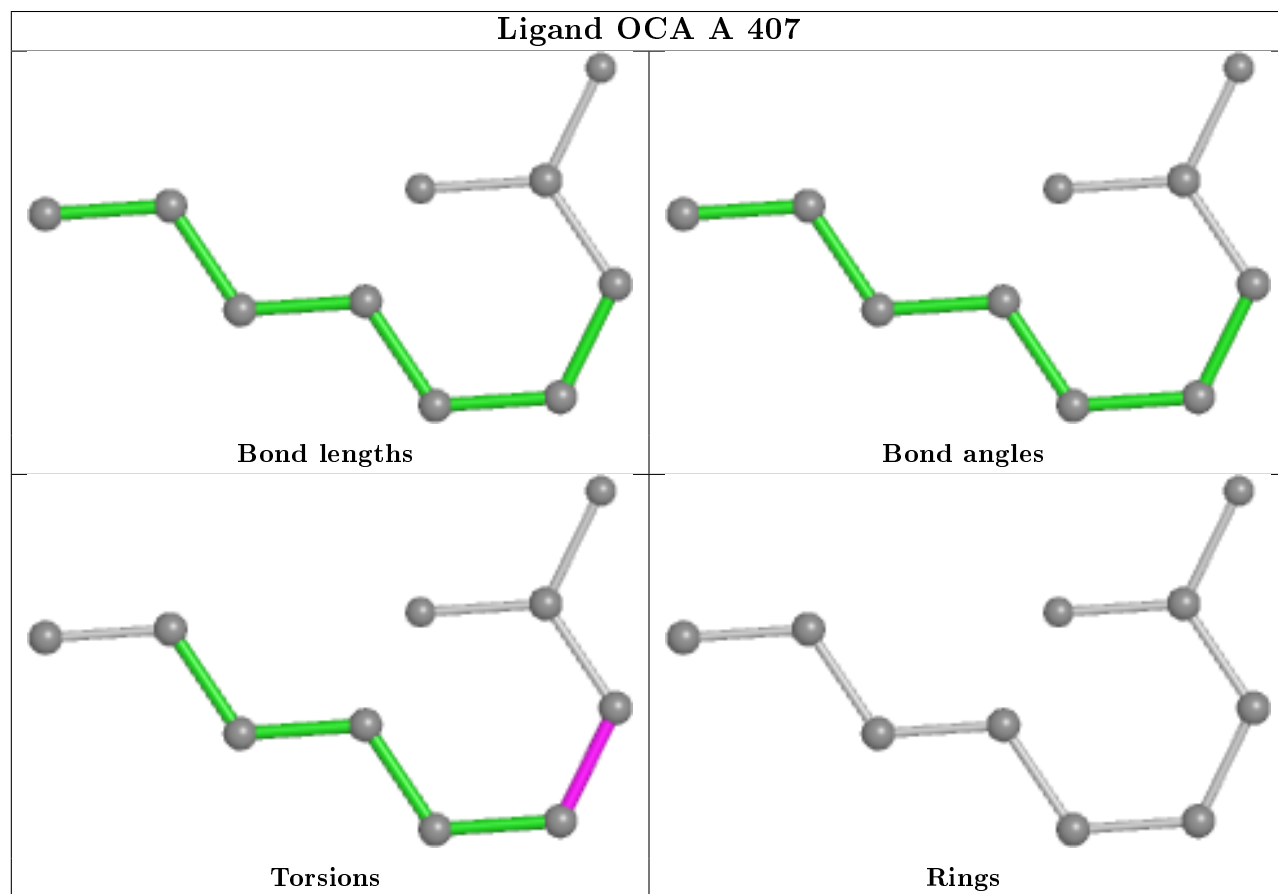
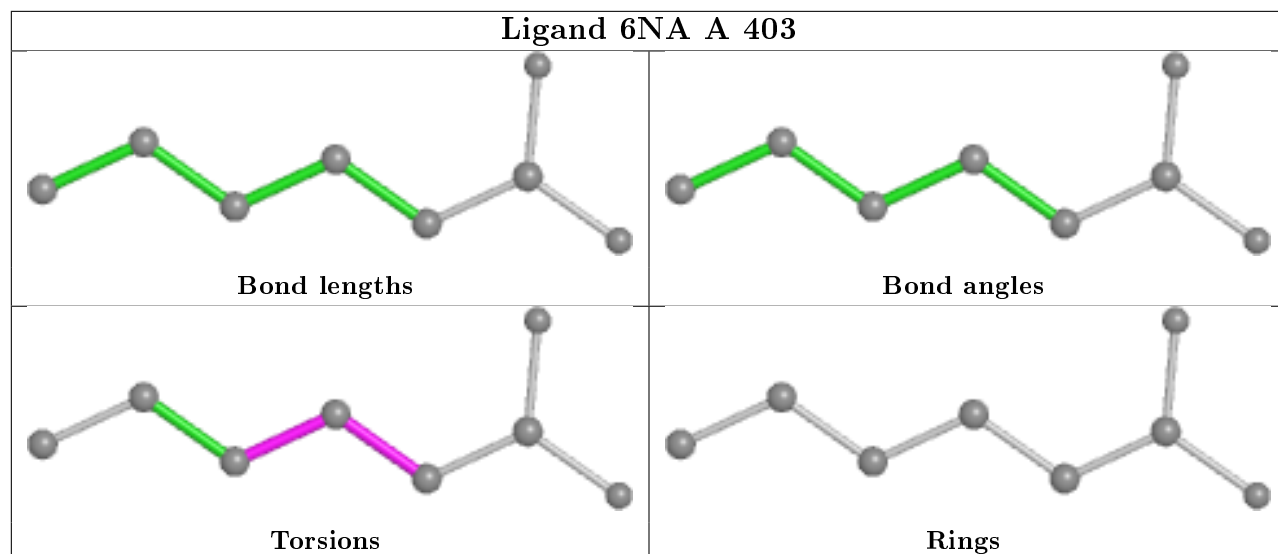
Mol	Chain	Res	Type	Atoms
5	A	405	DAO	C9-C10-C11-C12
5	A	404	DAO	C9-C10-C11-C12
5	A	405	DAO	C11-C10-C9-C8
8	A	408	PLM	C8-C9-CA-CB
5	A	404	DAO	C2-C3-C4-C5
8	A	408	PLM	C6-C7-C8-C9
4	A	403	6NA	CA-CB-CG-CD
5	A	405	DAO	C5-C6-C7-C8
6	A	406	LEA	C3-C4-C5-C6
4	B	403	6NA	C-CA-CB-CG
5	A	405	DAO	C1-C2-C3-C4

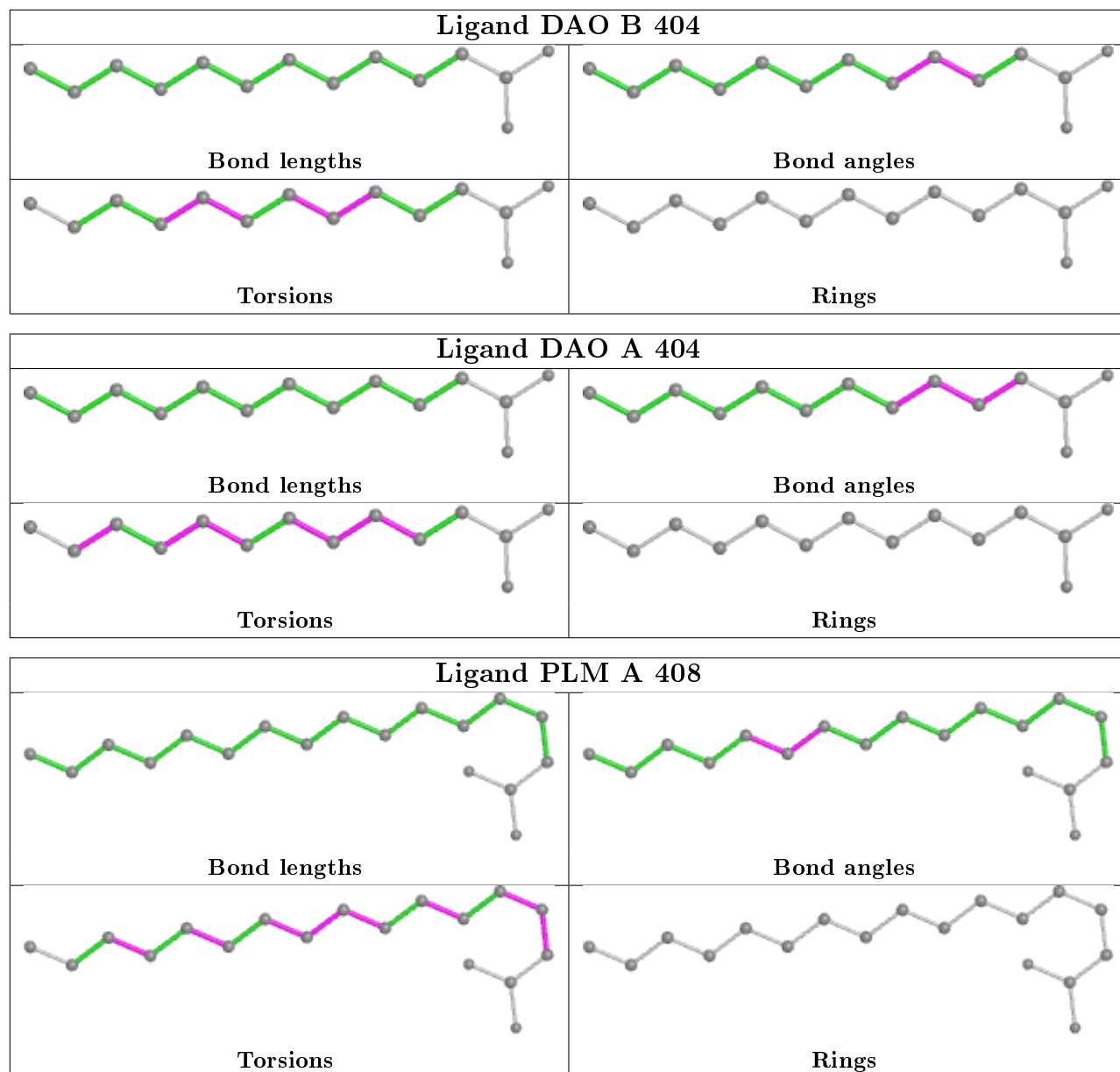
There are no ring outliers.

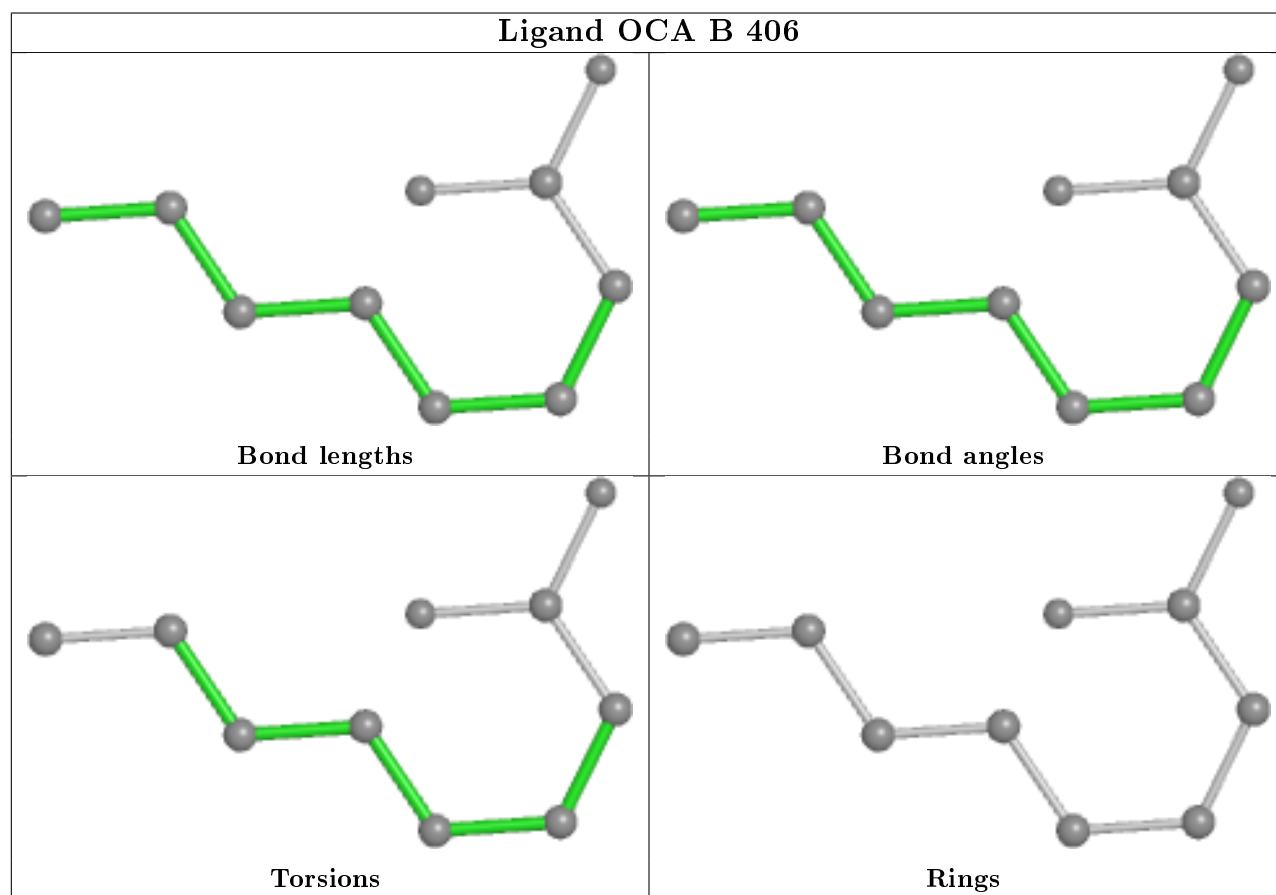
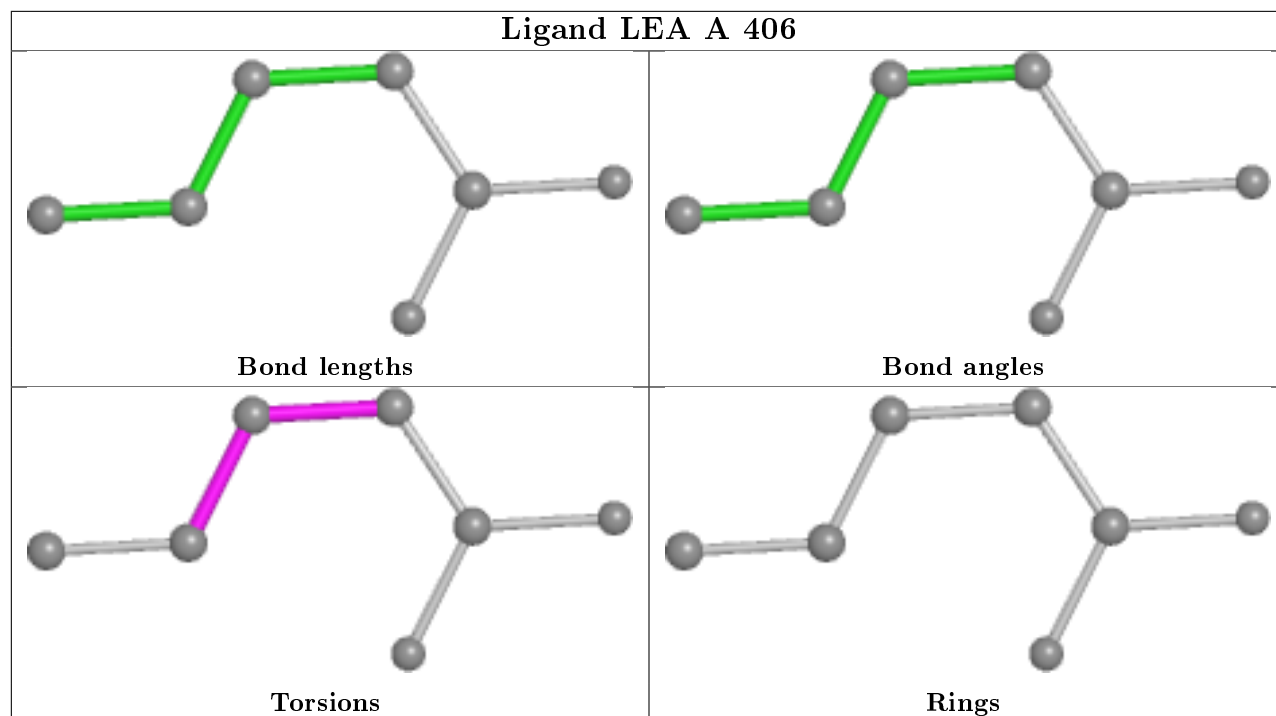
5 monomers are involved in 13 short contacts:

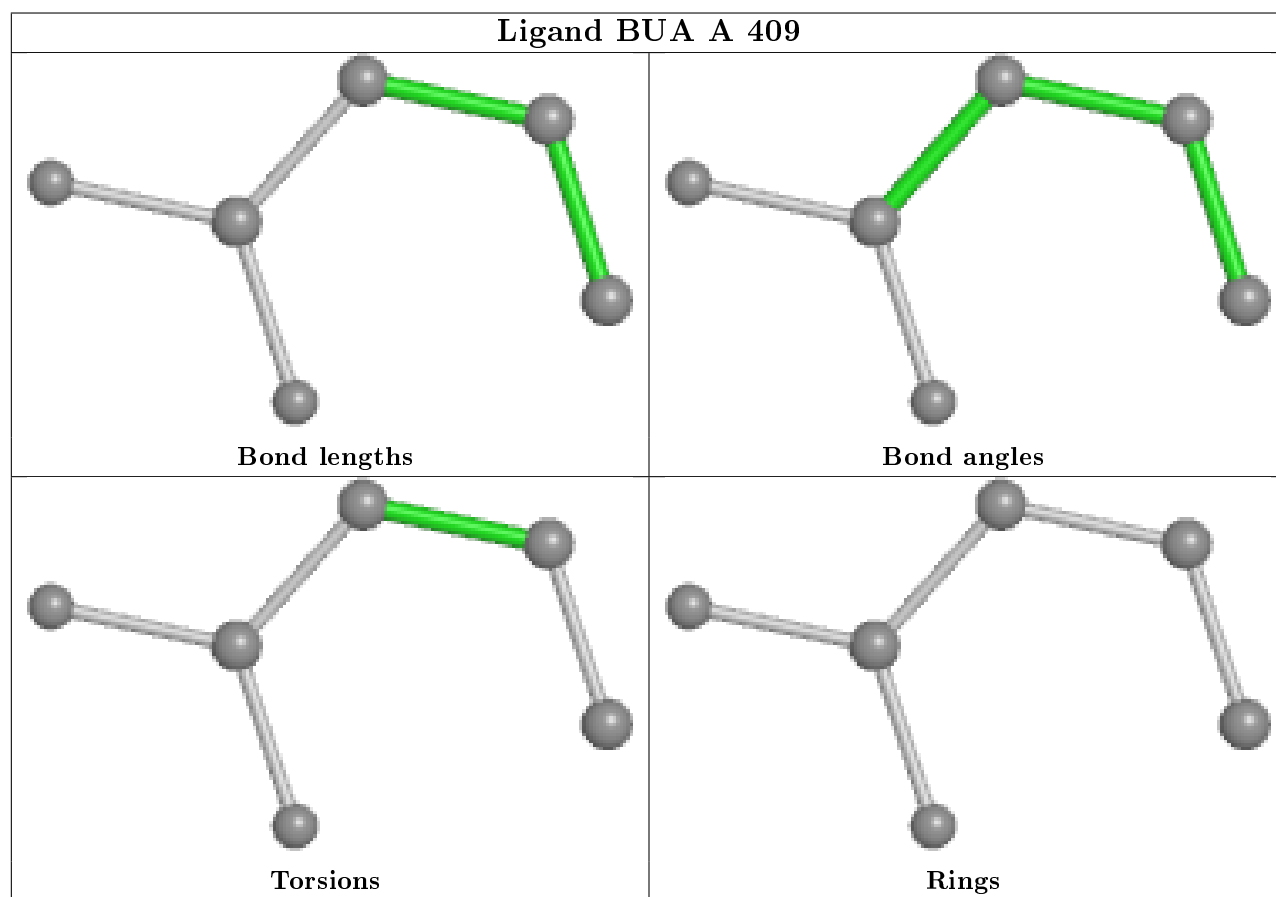
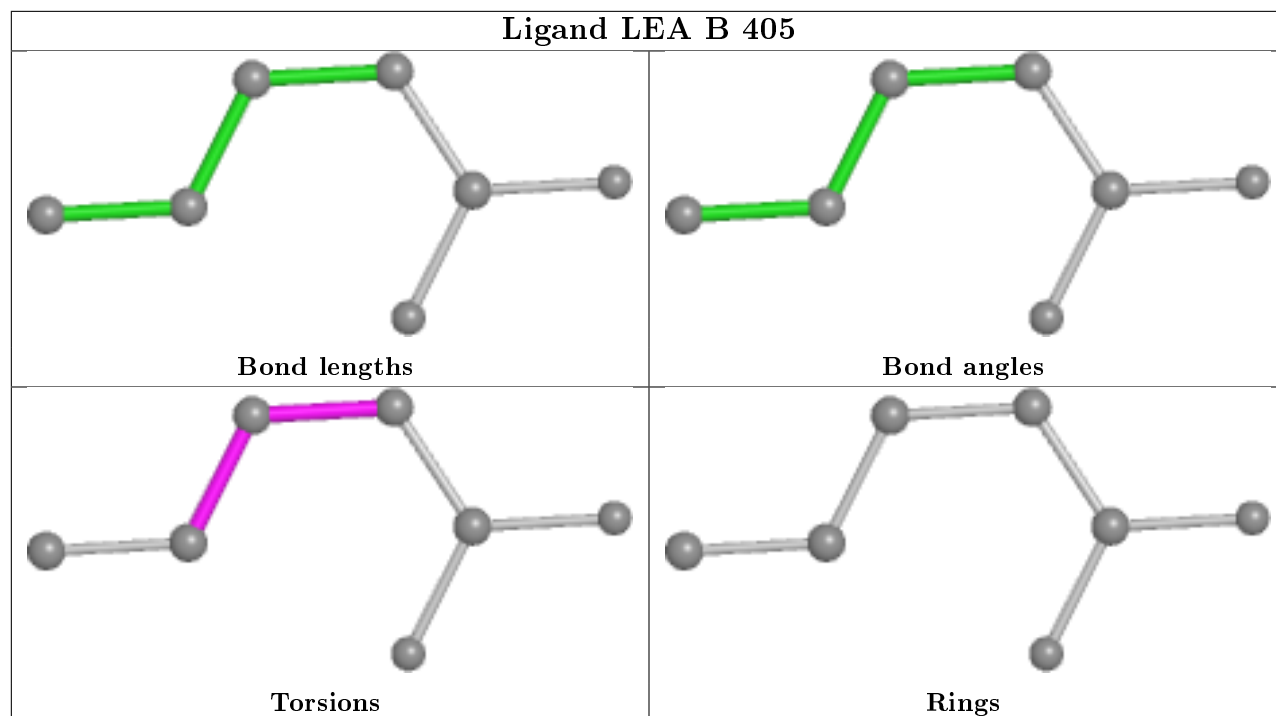
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	404	DAO	4	0
5	A	404	DAO	3	0
4	B	403	6NA	1	0
5	A	405	DAO	5	0
9	B	407	BUA	1	0

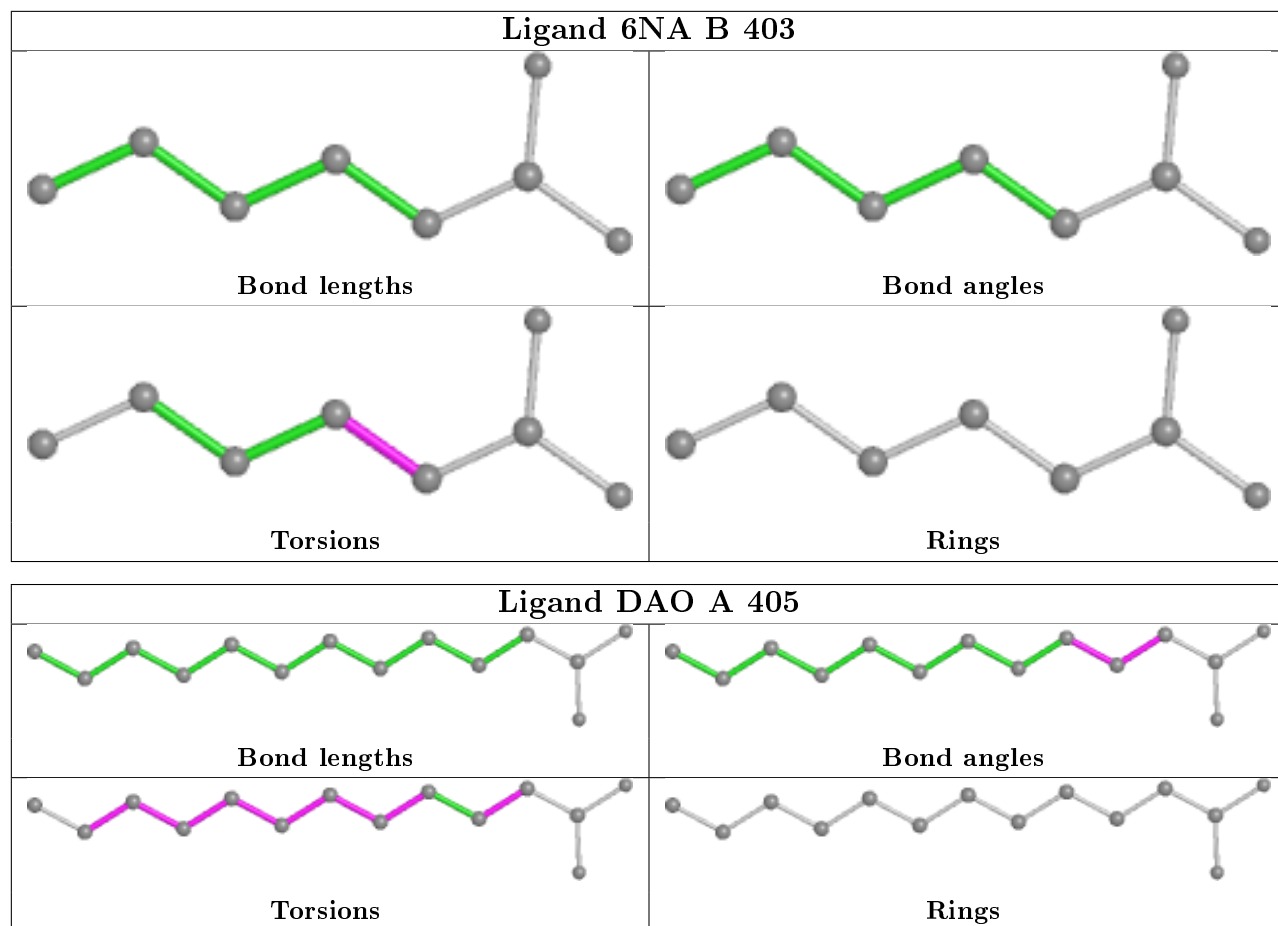
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

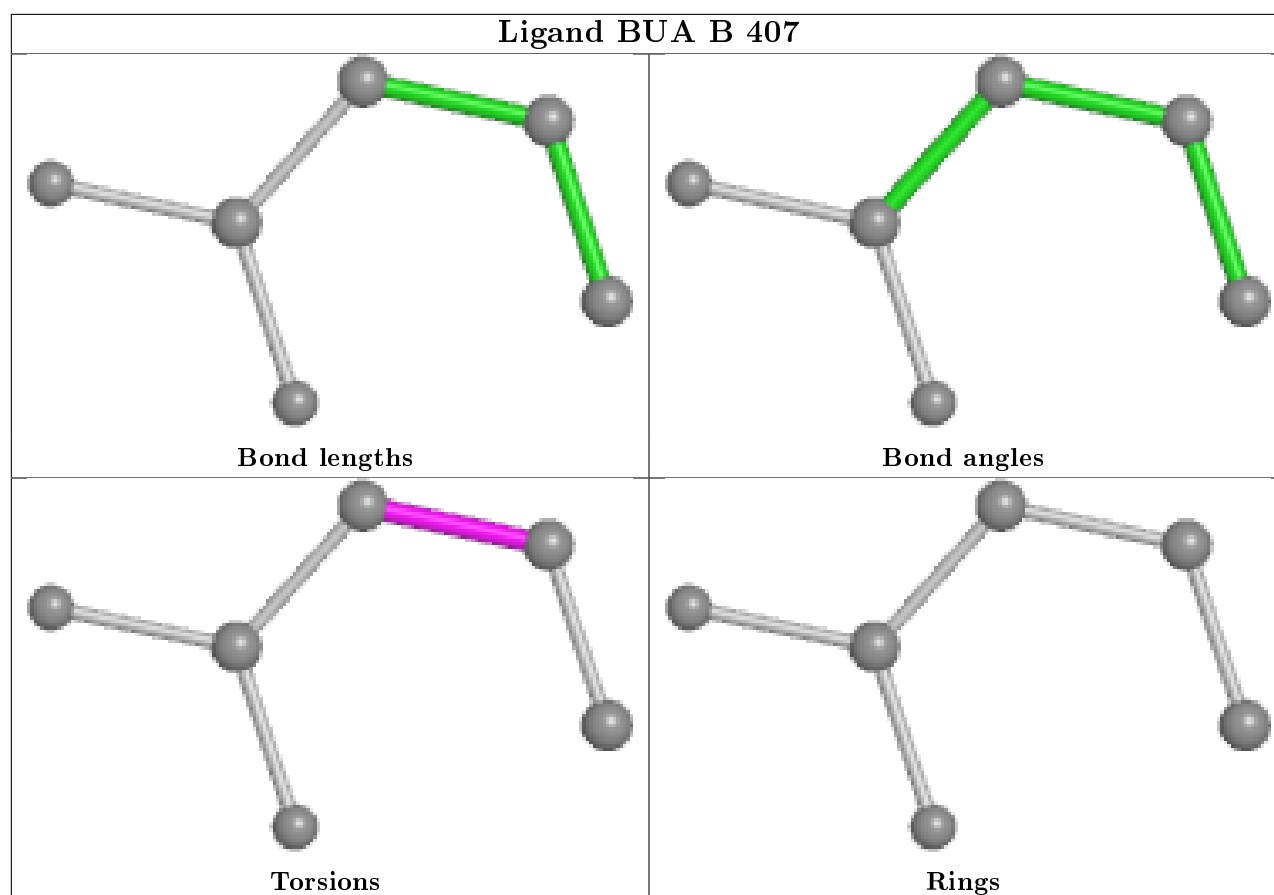












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	382/408 (93%)	0.07	9 (2%) 59 63	34, 42, 57, 83	0
1	B	382/408 (93%)	0.20	18 (4%) 31 36	37, 47, 65, 79	0
All	All	764/816 (93%)	0.13	27 (3%) 44 49	34, 45, 63, 83	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	GLY	4.4
1	B	141	GLN	4.3
1	B	137	ILE	4.2
1	A	274	PRO	4.0
1	B	142	ALA	3.9
1	B	274	PRO	3.6
1	B	275	LEU	3.6
1	A	275	LEU	3.2
1	B	145	GLY	3.1
1	B	93	TYR	3.0
1	B	139	TYR	2.9
1	A	6	LEU	2.8
1	B	276	GLY	2.8
1	B	86	ALA	2.7
1	B	147	ILE	2.7
1	B	146	GLU	2.7
1	B	134	LYS	2.6
1	B	277	TYR	2.6
1	B	27	ALA	2.5
1	A	273	GLY	2.4
1	A	329	ASN	2.4
1	B	138	ALA	2.3
1	A	178	PHE	2.3
1	A	276	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	228	LYS	2.2
1	A	28	LEU	2.1
1	B	82	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

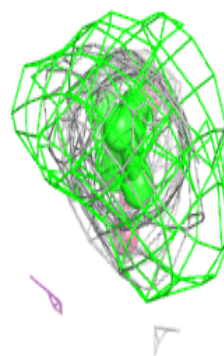
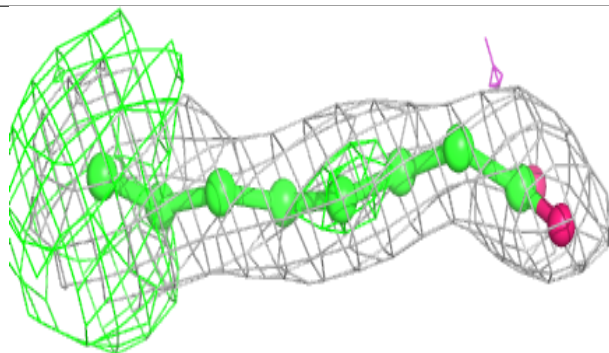
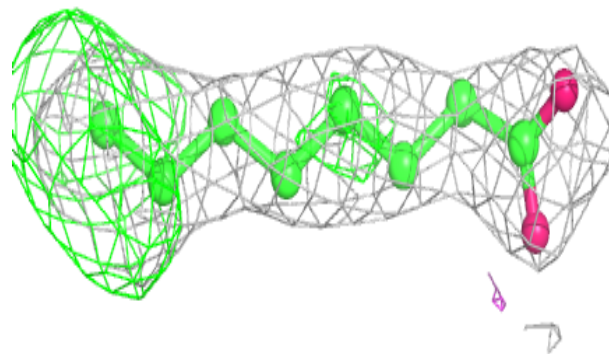
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	OCA	A	407	10/10	0.64	0.39	66,76,78,78	0
6	LEA	B	405	7/7	0.66	0.35	70,76,90,94	0
4	6NA	B	403	8/8	0.72	0.44	78,90,93,112	0
9	BUA	B	407	6/6	0.74	0.32	72,85,94,100	0
5	DAO	A	405	14/14	0.76	0.37	51,80,90,97	0
6	LEA	A	406	7/7	0.77	0.39	74,83,108,127	0
8	PLM	A	408	18/18	0.82	0.35	49,84,99,104	0
7	OCA	B	406	10/10	0.87	0.41	71,75,85,92	0
4	6NA	A	403	8/8	0.87	0.26	68,75,90,108	0
9	BUA	A	409	6/6	0.87	0.22	82,96,103,109	0
5	DAO	B	404	14/14	0.88	0.32	47,68,82,86	0
5	DAO	A	404	14/14	0.89	0.34	55,73,79,85	0
3	CA	A	402	1/1	0.95	0.14	66,66,66,66	0
2	ZN	B	401	1/1	0.98	0.18	63,63,63,63	0
3	CA	B	402	1/1	0.98	0.24	61,61,61,61	0
2	ZN	A	401	1/1	1.00	0.18	55,55,55,55	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.

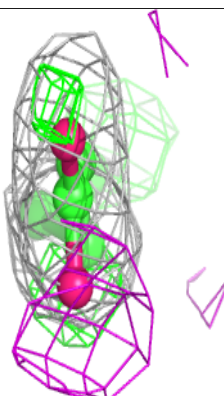
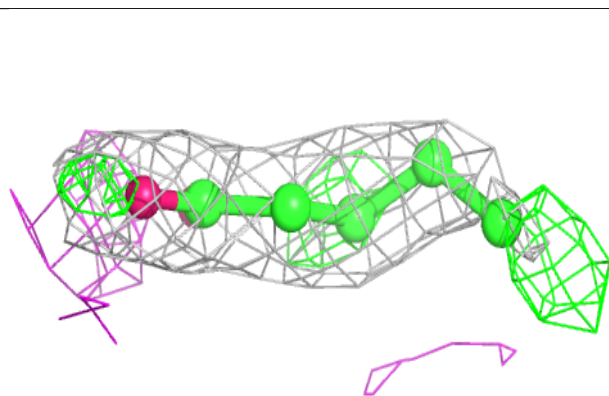
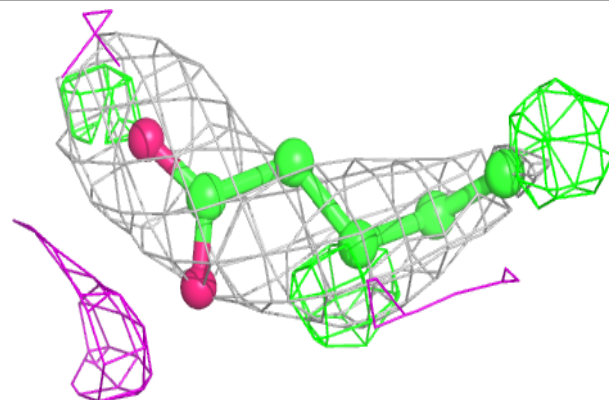
Electron density around OCA A 407:

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



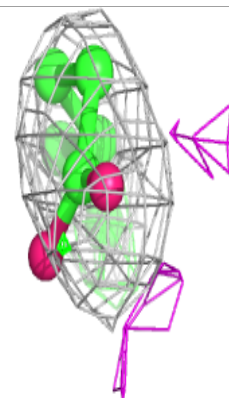
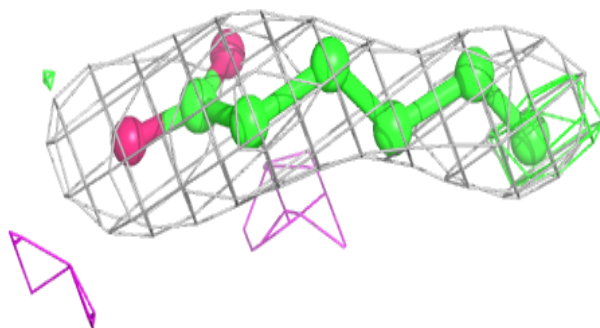
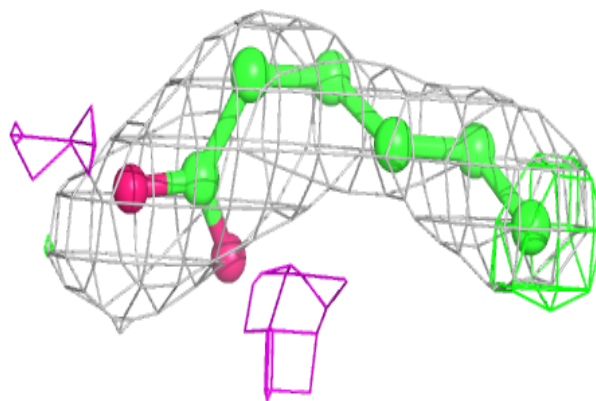
Electron density around LEA B 405:

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

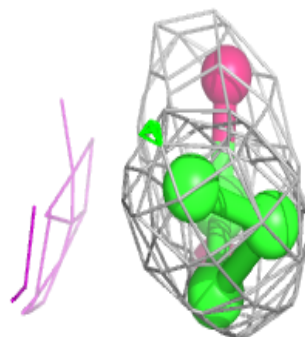
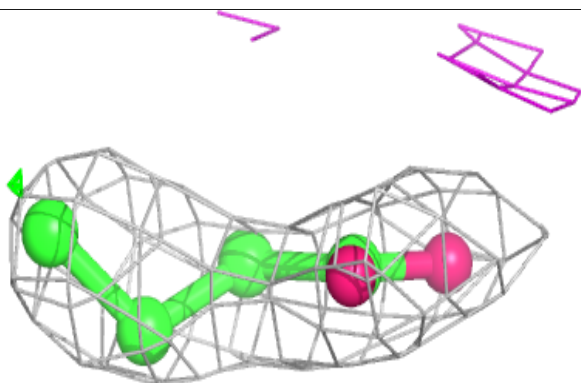
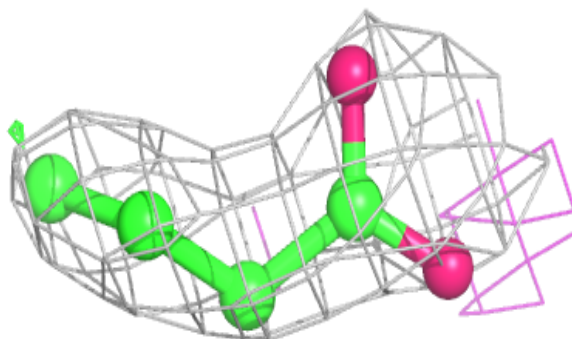


Electron density around 6NA B 403:

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

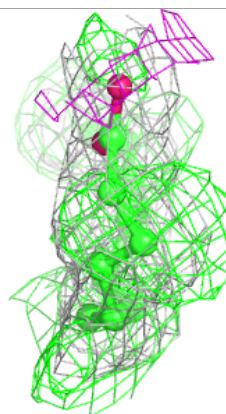
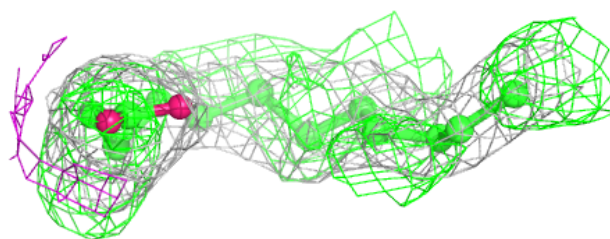
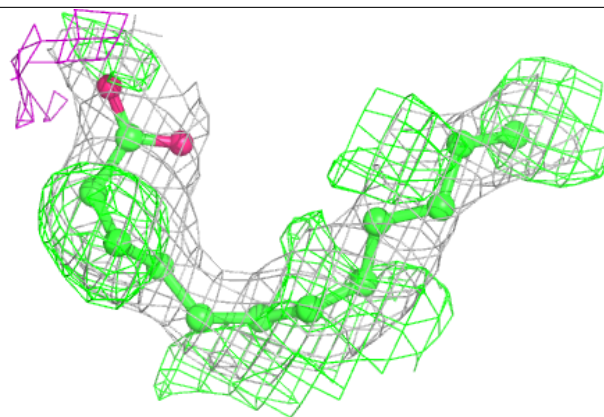
**Electron density around BUA B 407:**

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

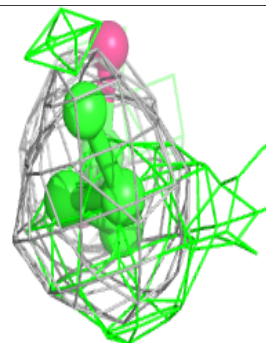
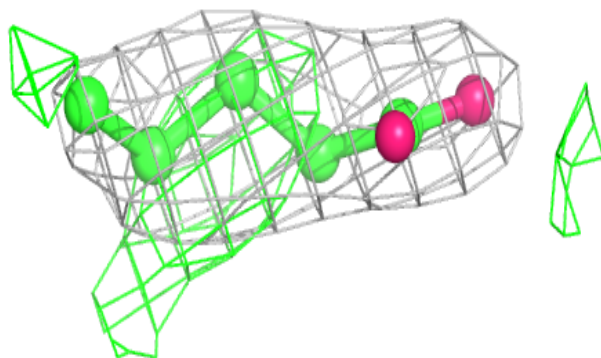
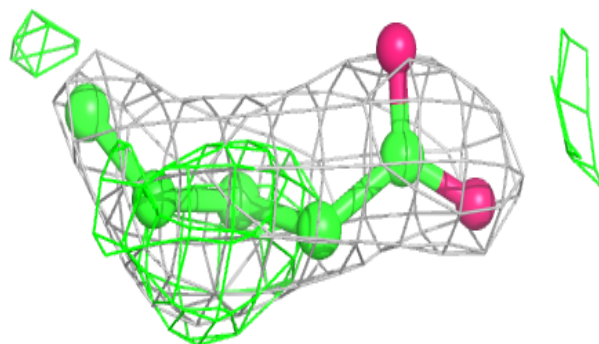


Electron density around DAO A 405:

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

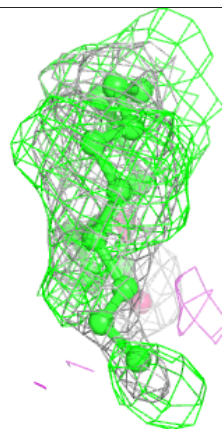
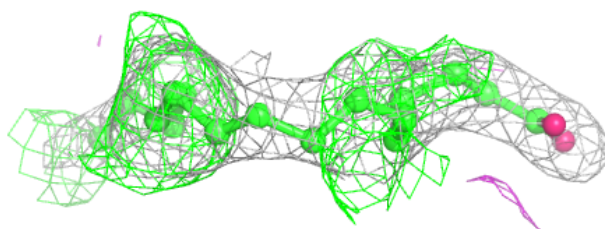
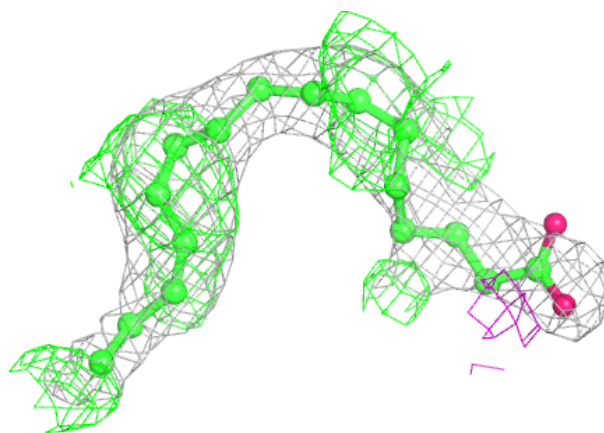
**Electron density around LEA A 406:**

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

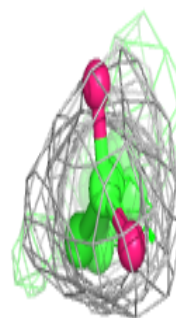
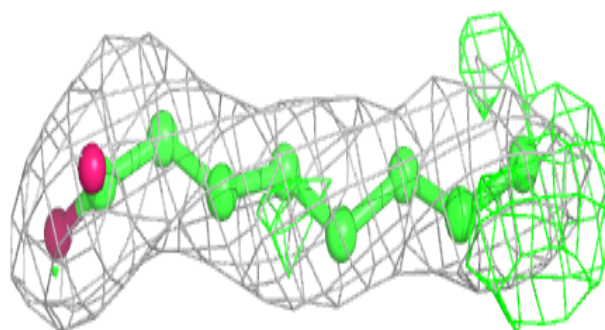
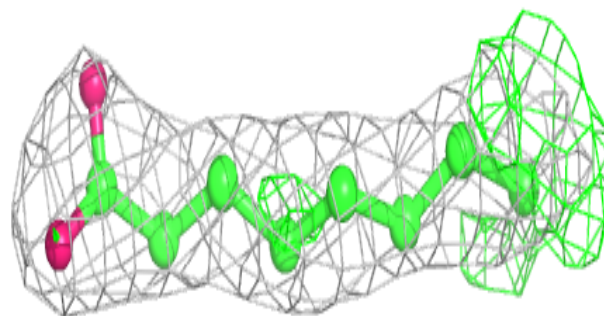


Electron density around PLM A 408:

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

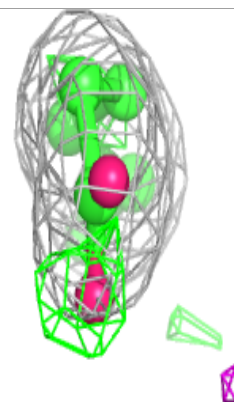
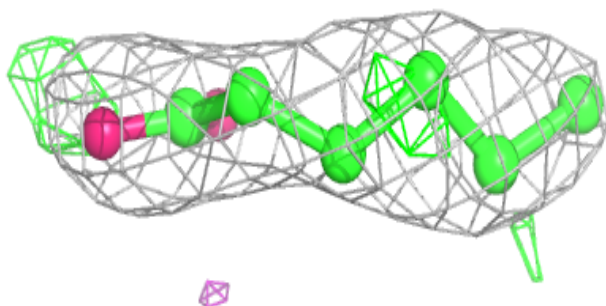
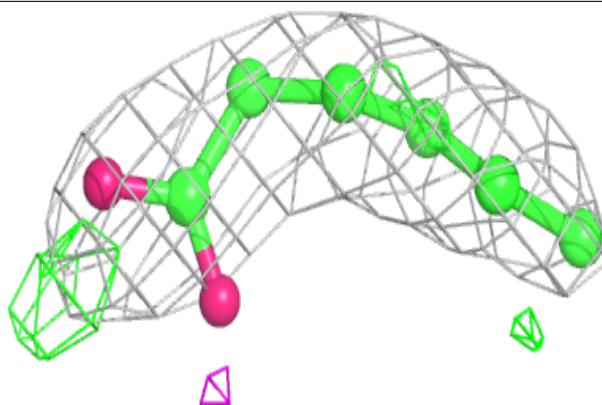
**Electron density around OCA B 406:**

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



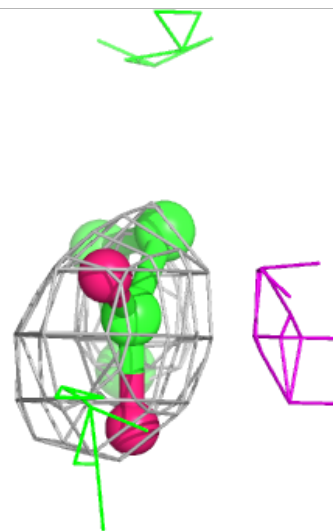
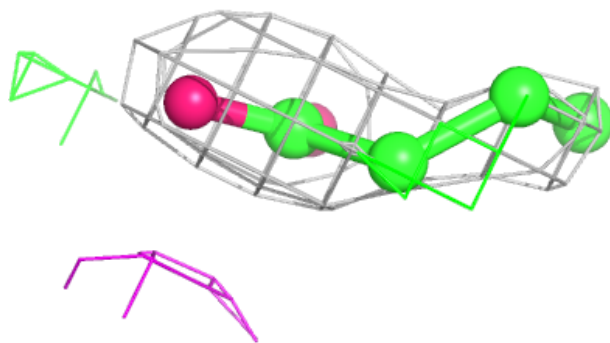
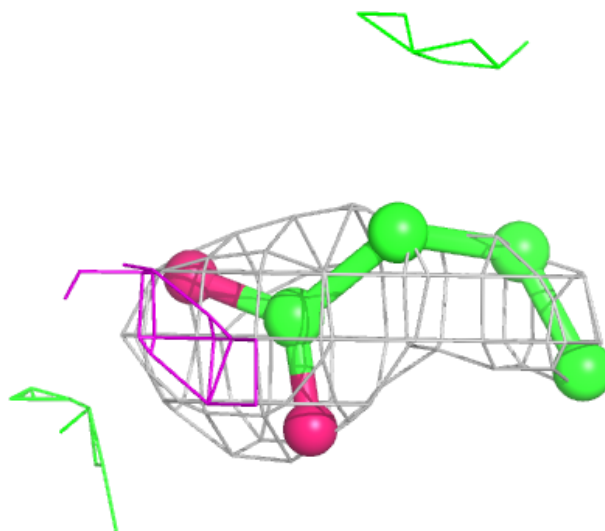
Electron density around 6NA A 403:

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



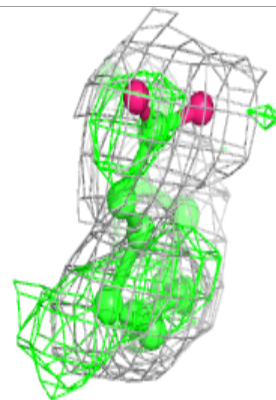
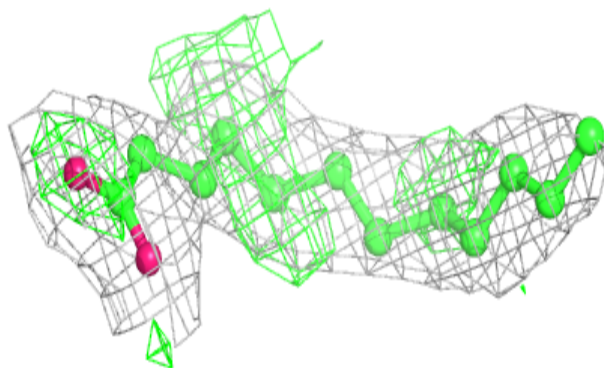
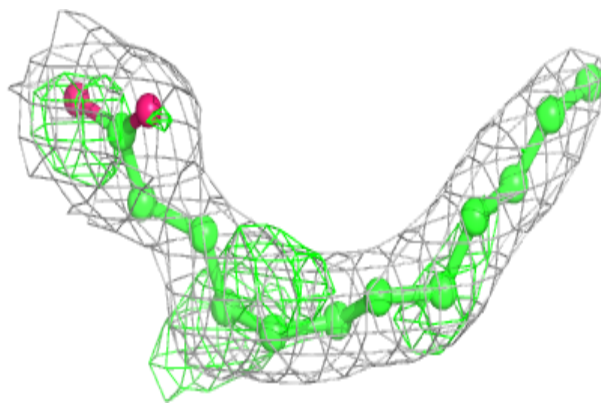
Electron density around BUA A 409:

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

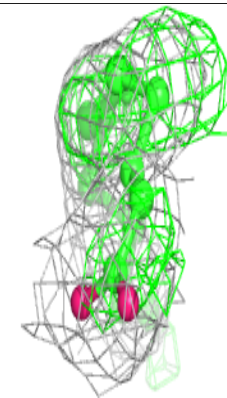
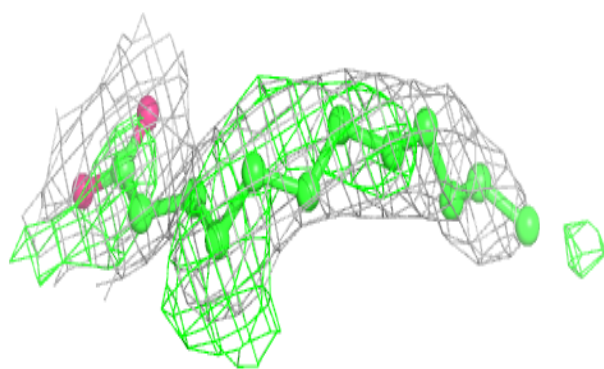
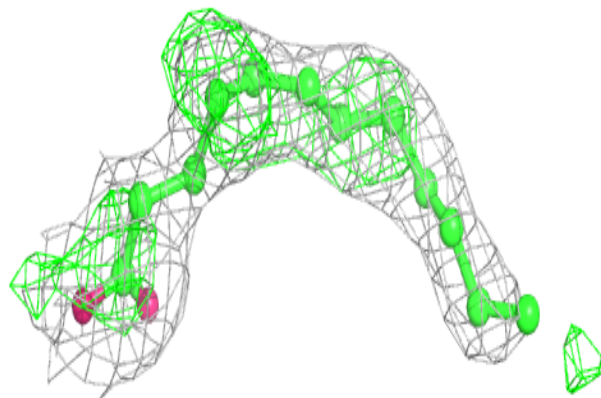


Electron density around DAO B 404:

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

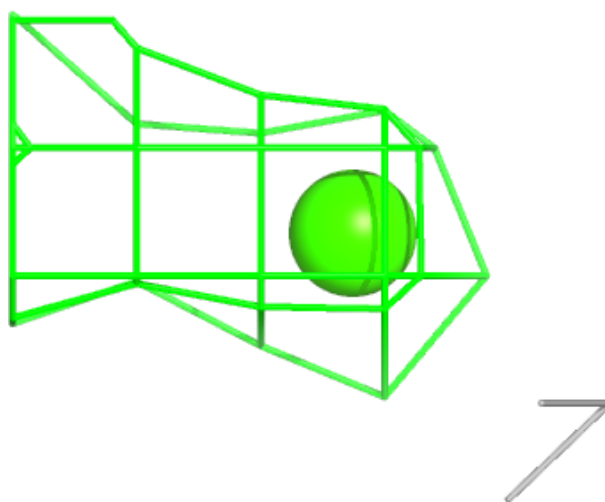
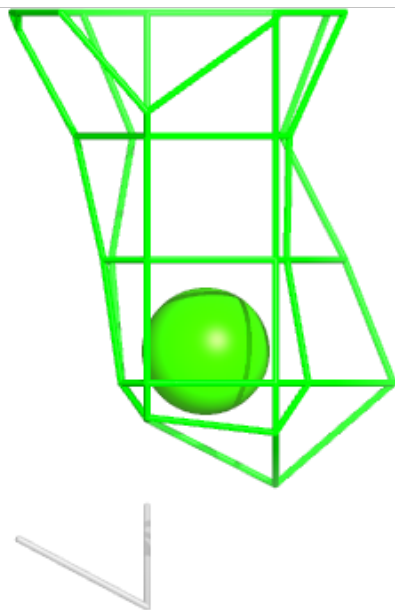
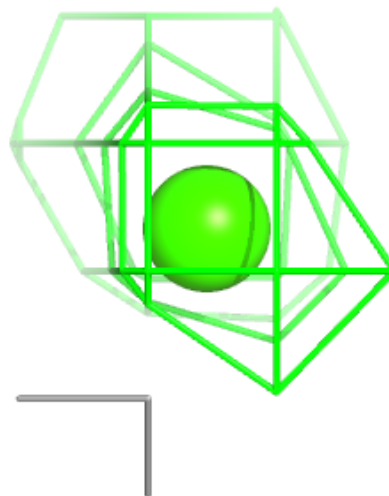
**Electron density around DAO A 404:**

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



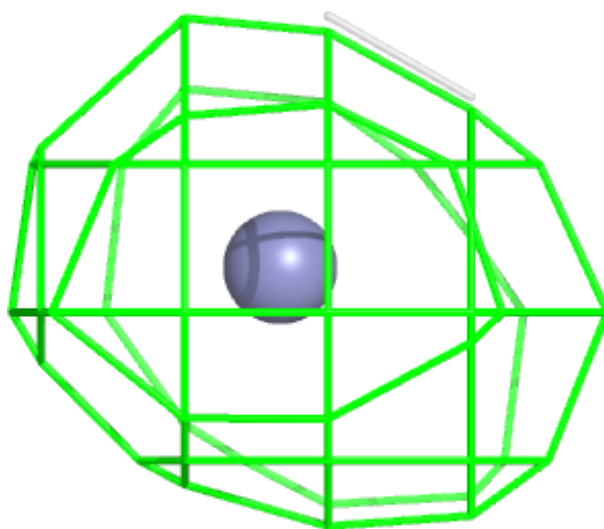
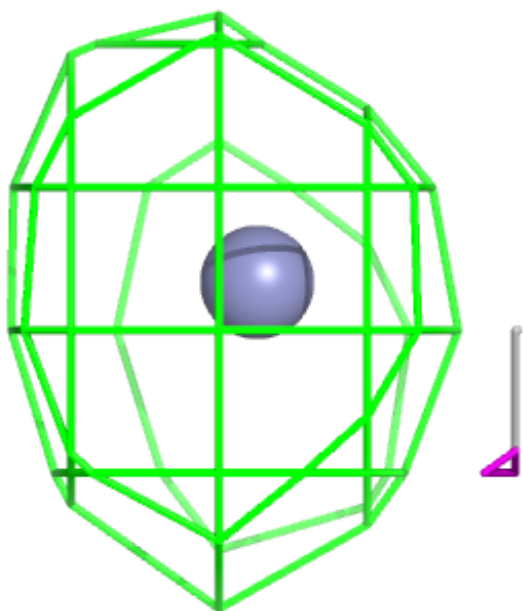
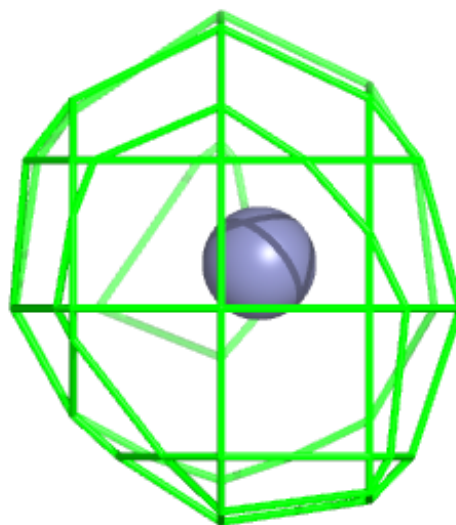
Electron density around CA A 402:

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



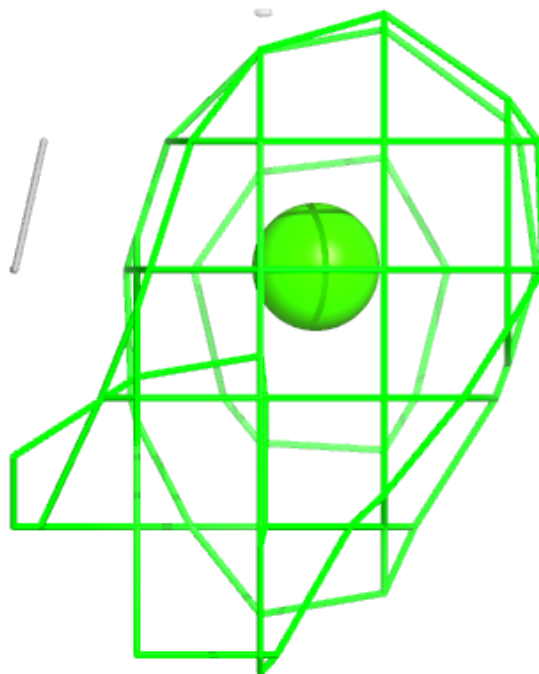
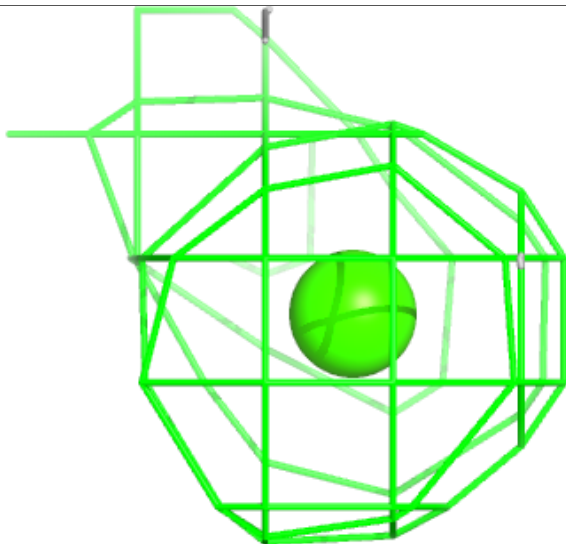
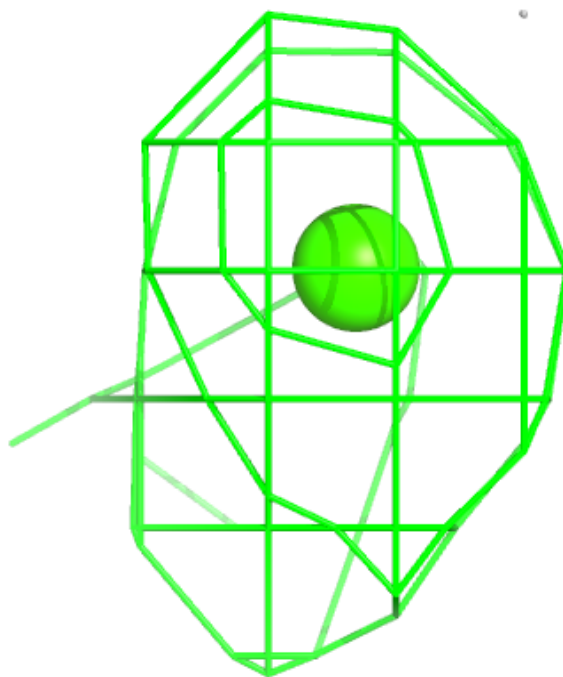
Electron density around ZN B 401:

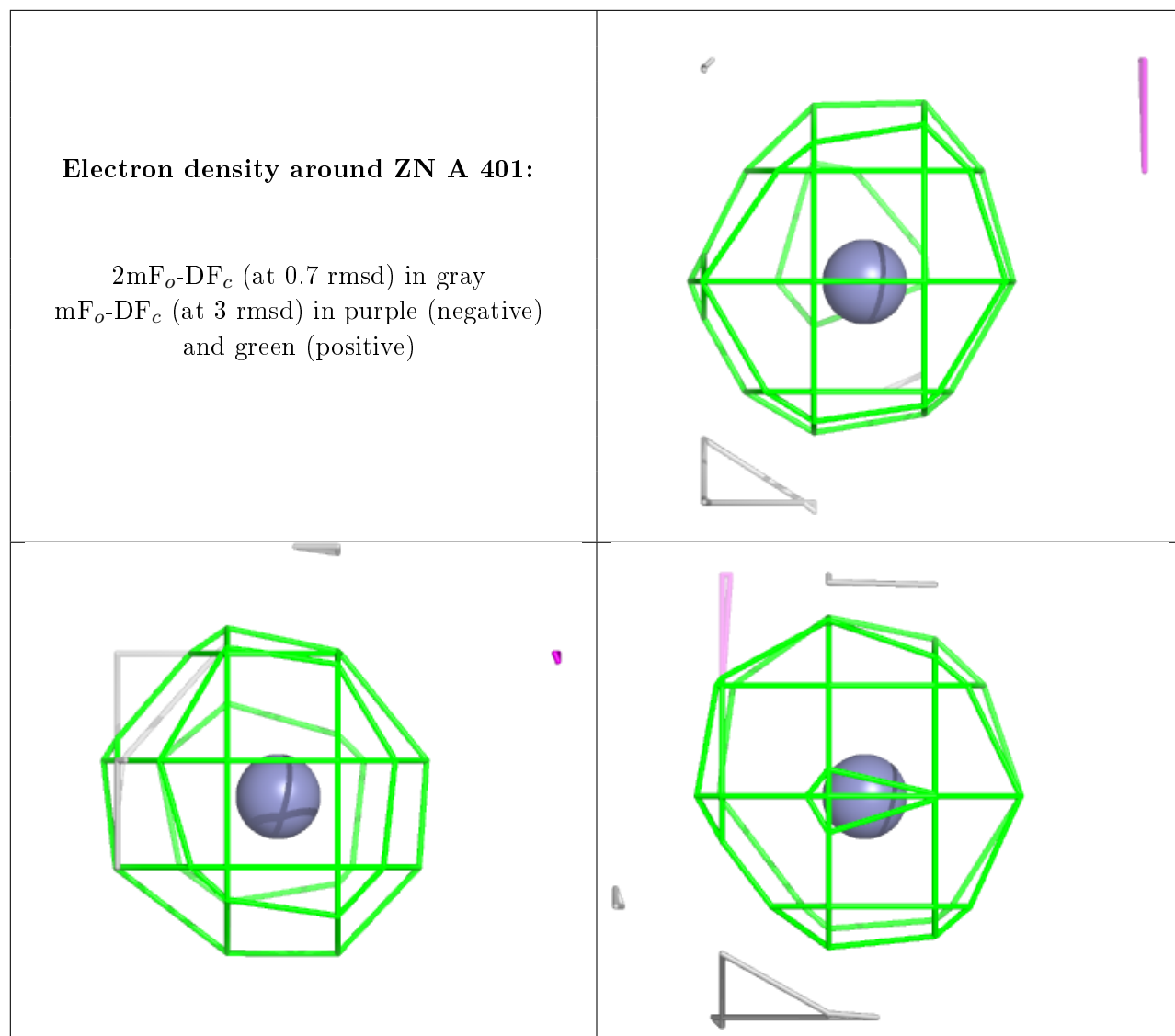
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 402:

$2mF_o-DF_c$ (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.