



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:08 PM UTC

PDB ID : 6KSI / pdb_00006ksi
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 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)
Xtriage (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

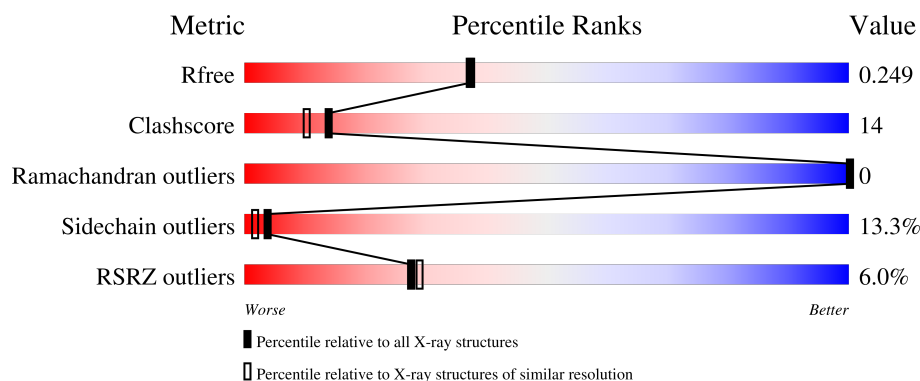
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (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 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	408	3% 59% 26% 7% • 6%
1	B	408	9% 63% 21% 8% • 6%

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
8	PLM	A	408	-	-	-	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

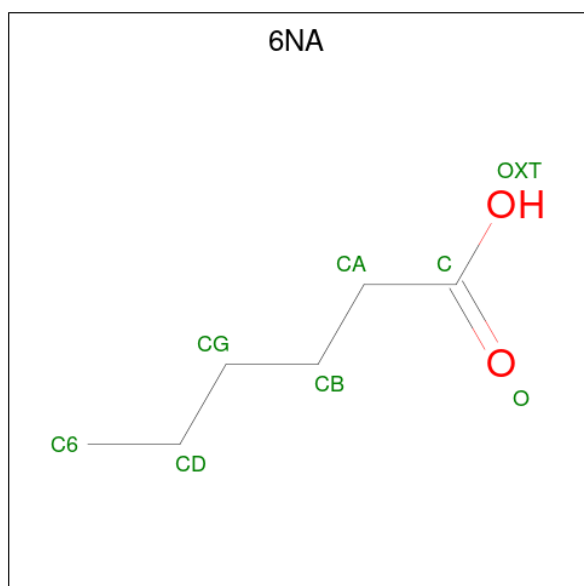
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is HEXANOIC ACID (CCD ID: 6NA) (formula: C₆H₁₂O₂) (labeled as "Ligand of Interest" by depositor).



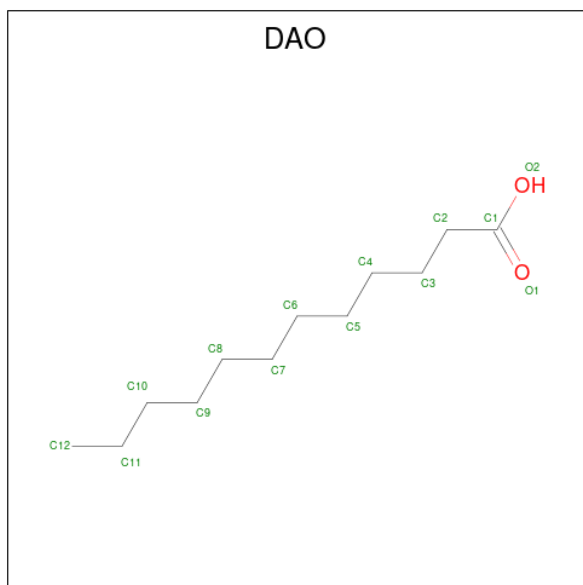
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0

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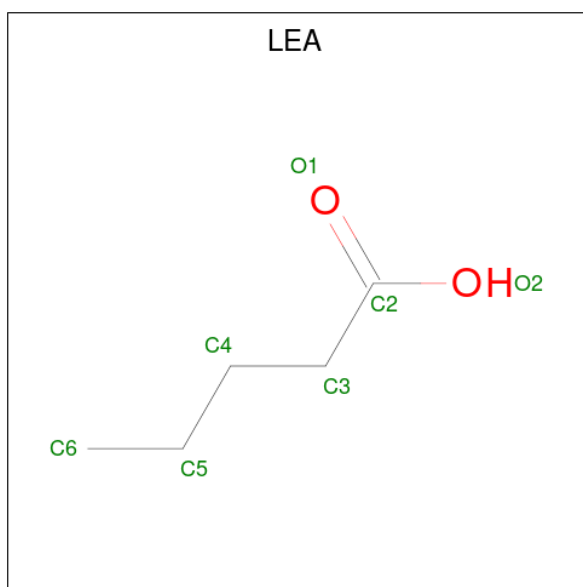
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$) (labeled as "Ligand of Interest" by depositor).



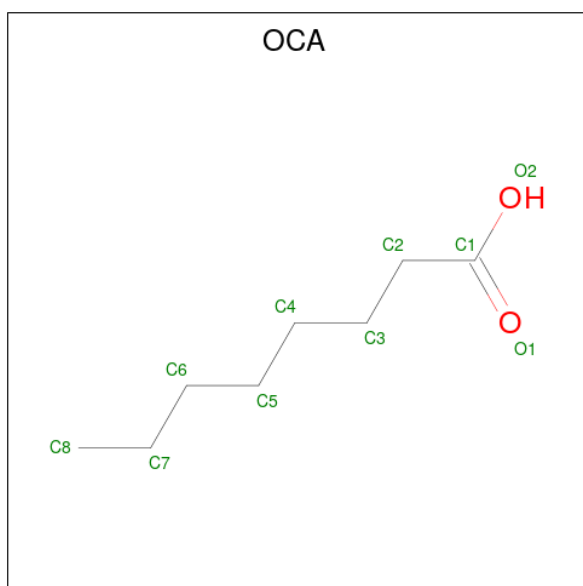
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	12	2		
5	A	1	Total	C	O	0	0
			14	12	2		
5	B	1	Total	C	O	0	0
			14	12	2		

- Molecule 6 is PENTANOIC ACID (CCD ID: LEA) (formula: $C_5H_{10}O_2$) (labeled as "Ligand of Interest" by depositor).



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) (CCD ID: OCA) (formula: $C_8H_{16}O_2$) (labeled as "Ligand of Interest" by depositor).



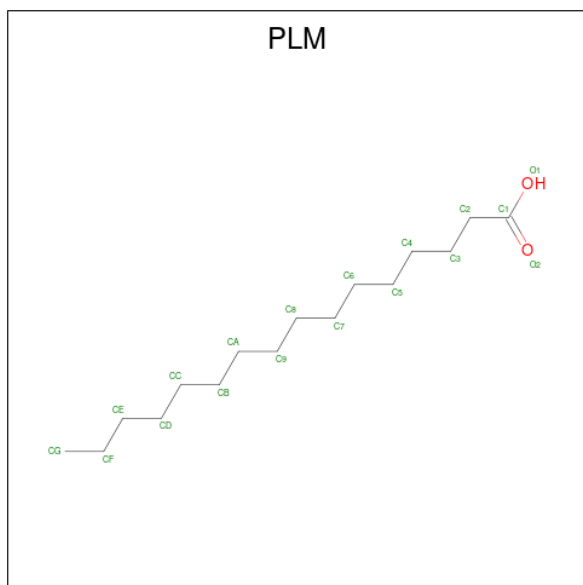
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	8	2		

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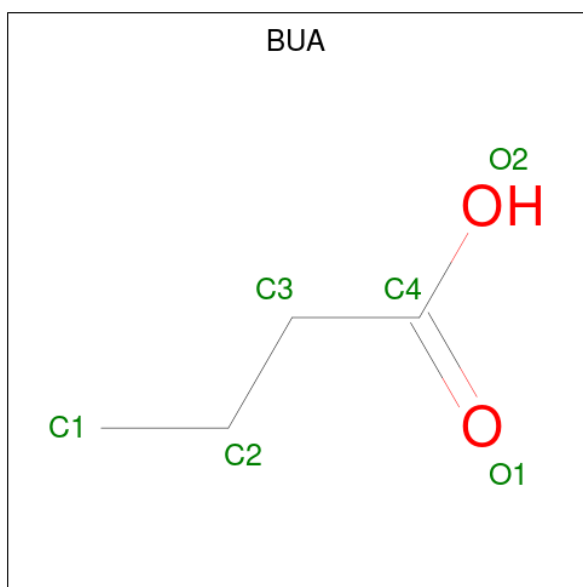
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	8	2		

- Molecule 8 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is butanoic acid (CCD ID: BUA) (formula: $C_4H_8O_2$) (labeled as "Ligand of Interest" by depositor).



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		

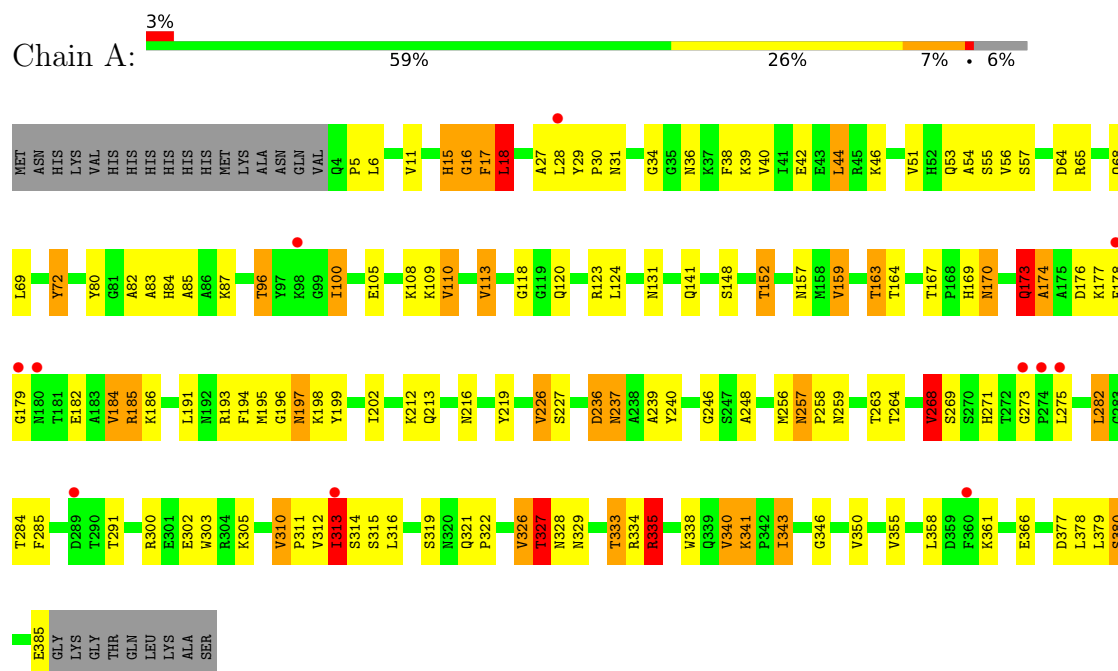
- Molecule 10 is water.

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

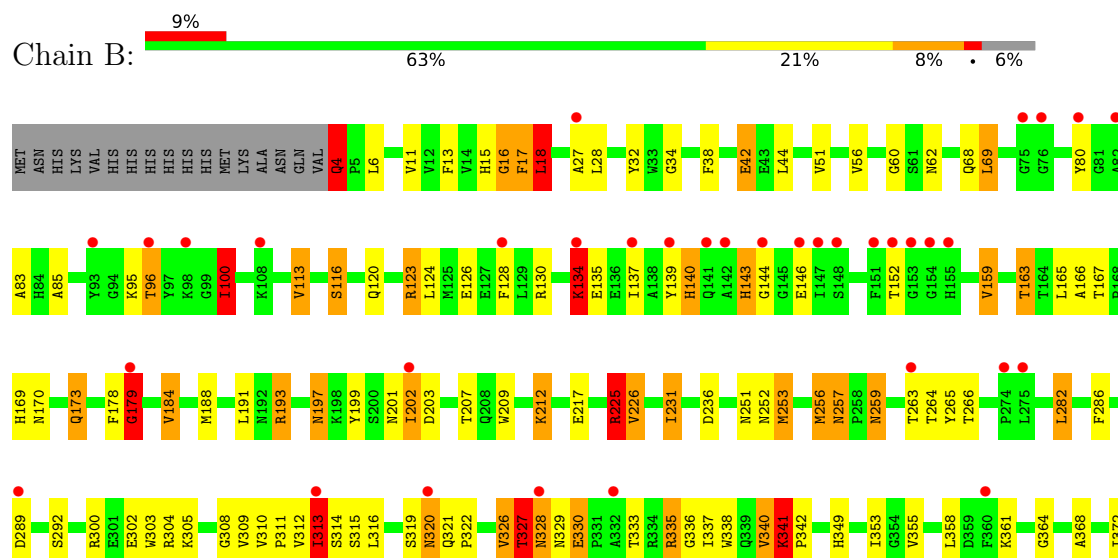
3 Residue-property plots

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: Lipase 2



• Molecule 1: Lipase 2



L378	L379	E386	GLY	LYS	GLY	THR	GLN	LEU	LYS	ALA	SER
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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 0.229 , 0.249	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 , 32.9	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	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LEA, BUA, ZN, CA, DAO, OCA, 6NA, PLM

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	1.87	40/3106 (1.3%)	1.76	63/4212 (1.5%)
1	B	1.75	38/3106 (1.2%)	1.75	63/4212 (1.5%)
All	All	1.81	78/6212 (1.3%)	1.75	126/8424 (1.5%)

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 (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	LEU	N-CA	29.51	1.80	1.46
1	B	18	LEU	N-CA	25.88	1.76	1.46
1	A	17	PHE	C-O	13.14	1.39	1.24
1	A	236	ASP	CG-OD2	11.11	1.46	1.25
1	B	328	ASN	CG-ND2	9.54	1.53	1.33
1	B	225	ARG	CD-NE	-9.10	1.33	1.46
1	B	179	GLY	N-CA	8.63	1.57	1.45
1	A	291	THR	CA-C	8.27	1.63	1.52
1	B	17	PHE	N-CA	-8.20	1.36	1.46
1	A	170	ASN	CA-CB	8.05	1.65	1.53
1	A	300	ARG	CD-NE	8.03	1.57	1.46
1	A	313	ILE	CB-CG1	7.24	1.68	1.53
1	B	203	ASP	C-O	-7.10	1.15	1.24
1	A	85	ALA	N-CA	7.06	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	GLU	C-O	7.04	1.32	1.24
1	A	196	GLY	CA-C	6.63	1.60	1.51
1	B	17	PHE	CA-C	-6.62	1.44	1.52
1	B	300	ARG	CD-NE	6.62	1.55	1.46
1	B	312	VAL	CA-CB	6.58	1.61	1.54
1	A	64	ASP	CG-OD1	6.57	1.37	1.25
1	B	341	LYS	CA-CB	-6.57	1.43	1.53
1	A	194	PHE	N-CA	-6.52	1.38	1.46
1	A	55	SER	CA-CB	6.33	1.63	1.53
1	A	31	ASN	CA-C	6.25	1.60	1.52
1	B	236	ASP	CG-OD2	6.22	1.37	1.25
1	B	266	THR	C-O	6.18	1.31	1.23
1	A	65	ARG	CZ-NH1	6.13	1.41	1.32
1	B	328	ASN	N-CA	6.11	1.53	1.46
1	A	313	ILE	CG1-CD1	6.10	1.75	1.51
1	B	310	VAL	N-CA	6.04	1.50	1.45
1	B	337	ILE	C-O	6.02	1.30	1.23
1	B	143	HIS	CE1-NE2	5.92	1.38	1.32
1	A	236	ASP	CA-CB	5.88	1.59	1.52
1	A	310	VAL	CA-C	5.87	1.56	1.52
1	A	237	ASN	N-CA	5.86	1.53	1.45
1	A	29	TYR	C-N	5.81	1.41	1.33
1	A	176	ASP	CA-CB	5.79	1.62	1.53
1	A	269	SER	C-O	5.77	1.29	1.24
1	B	60	GLY	N-CA	5.69	1.52	1.45
1	A	84	HIS	CA-C	5.67	1.60	1.52
1	B	62	ASN	C-O	5.60	1.30	1.24
1	A	118	GLY	N-CA	5.59	1.53	1.45
1	A	30	PRO	C-O	-5.59	1.17	1.23
1	A	334	ARG	CA-C	5.58	1.60	1.52
1	B	314	SER	N-CA	5.53	1.53	1.46
1	B	178	PHE	N-CA	-5.48	1.39	1.46
1	B	178	PHE	C-N	-5.42	1.25	1.33
1	A	174	ALA	N-CA	5.41	1.53	1.46
1	B	364	GLY	C-O	5.39	1.30	1.23
1	B	286	PHE	CA-C	5.38	1.60	1.52
1	B	193	ARG	C-O	5.38	1.30	1.24
1	B	143	HIS	CG-CD2	5.37	1.41	1.35
1	B	188	MET	CA-C	5.35	1.59	1.52
1	B	361	LYS	N-CA	5.31	1.53	1.46
1	B	85	ALA	N-CA	5.29	1.52	1.46
1	A	343	ILE	N-CA	-5.29	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	ARG	C-O	5.27	1.30	1.24
1	B	128	PHE	CA-CB	5.26	1.61	1.53
1	B	355	VAL	N-CA	5.24	1.53	1.46
1	A	246	GLY	N-CA	5.20	1.52	1.45
1	A	72	TYR	CG-CD1	5.18	1.50	1.39
1	A	305	LYS	C-O	5.18	1.29	1.23
1	B	120	GLN	C-O	5.18	1.30	1.24
1	B	212	LYS	C-O	-5.17	1.18	1.23
1	A	346	GLY	C-O	-5.16	1.16	1.24
1	B	140	HIS	CG-ND1	-5.14	1.32	1.38
1	A	57	SER	CA-C	5.14	1.58	1.52
1	A	82	ALA	CA-CB	5.14	1.61	1.53
1	A	83	ALA	CA-CB	5.13	1.61	1.53
1	A	271	HIS	N-CA	5.12	1.52	1.45
1	B	178	PHE	C-O	5.10	1.29	1.23
1	B	166	ALA	CA-CB	5.09	1.61	1.53
1	A	5	PRO	N-CA	5.09	1.53	1.47
1	A	170	ASN	CG-OD1	5.08	1.33	1.23
1	B	116	SER	CA-C	5.07	1.57	1.52
1	B	231	ILE	C-O	-5.07	1.18	1.24
1	A	105	GLU	C-N	5.02	1.39	1.33
1	A	131	ASN	N-CA	5.01	1.52	1.45

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	PHE	CA-C-N	-24.44	83.39	122.73
1	A	17	PHE	C-N-CA	-24.44	83.39	122.73
1	B	17	PHE	CA-C-N	-23.08	85.57	122.73
1	B	17	PHE	C-N-CA	-23.08	85.57	122.73
1	B	178	PHE	CA-C-N	-15.80	90.45	121.41
1	B	178	PHE	C-N-CA	-15.80	90.45	121.41
1	B	225	ARG	NE-CZ-NH2	-15.11	105.60	119.20
1	B	225	ARG	NE-CZ-NH1	11.70	133.20	121.50
1	A	313	ILE	CB-CG1-CD1	10.93	136.76	113.80
1	B	17	PHE	O-C-N	-10.64	111.11	122.07
1	A	335	ARG	NE-CZ-NH2	10.21	128.39	119.20
1	B	178	PHE	O-C-N	-10.06	109.55	123.34
1	B	225	ARG	CD-NE-CZ	9.34	137.47	124.40
1	A	268	VAL	CB-CA-C	-9.30	95.80	110.69
1	B	335	ARG	NE-CZ-NH2	8.30	126.67	119.20
1	B	4	GLN	CA-C-N	-8.05	112.06	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	GLN	C-N-CA	-8.05	112.06	120.03
1	A	335	ARG	NE-CZ-NH1	-8.03	113.47	121.50
1	B	18	LEU	CA-C-N	-7.98	113.77	122.38
1	B	18	LEU	C-N-CA	-7.98	113.77	122.38
1	B	83	ALA	N-CA-C	-7.95	102.70	111.36
1	A	152	THR	N-CA-CB	-7.83	99.03	110.47
1	A	273	GLY	CA-C-N	-7.78	111.78	119.87
1	A	273	GLY	C-N-CA	-7.78	111.78	119.87
1	B	313	ILE	CB-CA-C	-7.67	97.15	111.79
1	A	17	PHE	O-C-N	-7.62	113.86	122.09
1	B	327	THR	N-CA-CB	-7.59	98.91	110.45
1	B	178	PHE	CA-C-O	7.27	130.07	120.11
1	A	227	SER	N-CA-C	-7.18	104.39	113.01
1	B	330	GLU	CA-C-N	-7.08	112.47	119.76
1	B	330	GLU	C-N-CA	-7.08	112.47	119.76
1	B	225	ARG	CG-CD-NE	-7.03	96.53	112.00
1	A	226	VAL	CG1-CB-CG2	6.98	126.16	110.80
1	A	326	VAL	CG1-CB-CG2	6.92	126.02	110.80
1	A	53	GLN	N-CA-CB	-6.90	99.75	110.65
1	A	64	ASP	N-CA-C	-6.85	103.89	111.36
1	A	100	ILE	CA-CB-CG2	6.68	121.86	110.50
1	B	256	MET	CG-SD-CE	-6.65	86.26	100.90
1	A	313	ILE	CG1-CB-CG2	6.56	130.38	110.70
1	B	69	LEU	N-CA-C	-6.54	104.24	111.36
1	B	134	LYS	CA-CB-CG	6.43	126.96	114.10
1	A	163	THR	CB-CA-C	6.38	121.38	109.71
1	A	328	ASN	N-CA-C	6.36	119.19	111.82
1	B	134	LYS	CB-CG-CD	6.32	125.84	111.30
1	B	207	THR	N-CA-C	-6.31	104.50	111.82
1	B	95	LYS	CA-C-N	-6.21	114.23	122.99
1	B	95	LYS	C-N-CA	-6.21	114.23	122.99
1	A	310	VAL	CB-CA-C	6.20	116.14	110.13
1	A	18	LEU	CA-CB-CG	6.17	137.90	116.30
1	A	335	ARG	CD-NE-CZ	6.14	133.00	124.40
1	A	248	ALA	N-CA-C	-6.13	104.71	111.82
1	A	340	VAL	CB-CA-C	6.12	118.37	110.96
1	A	110	VAL	N-CA-CB	-6.12	101.40	111.44
1	B	305	LYS	CD-CE-NZ	6.10	131.43	111.90
1	B	326	VAL	CB-CA-C	6.10	120.44	110.69
1	A	83	ALA	N-CA-C	-6.04	104.62	111.14
1	A	177	LYS	N-CA-C	6.02	120.76	113.17
1	B	313	ILE	CA-CB-CG2	6.02	120.73	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	GLY	N-CA-C	-6.01	105.31	115.34
1	B	100	ILE	CB-CA-C	6.01	119.51	111.94
1	A	148	SER	CA-C-N	-6.00	113.94	119.82
1	A	148	SER	C-N-CA	-6.00	113.94	119.82
1	A	327	THR	N-CA-CB	-6.00	101.32	110.45
1	A	333	THR	N-CA-CB	-6.00	101.85	110.80
1	B	313	ILE	N-CA-C	-5.99	103.26	111.89
1	B	236	ASP	CB-CG-OD2	5.99	132.17	118.40
1	B	202	ILE	N-CA-C	5.98	117.20	108.53
1	B	42	GLU	N-CA-CB	-5.98	101.31	110.16
1	B	342	PRO	CA-C-N	5.95	128.54	120.63
1	B	342	PRO	C-N-CA	5.95	128.54	120.63
1	B	159	VAL	CB-CA-C	5.93	119.20	110.77
1	B	16	GLY	CA-C-N	5.89	128.10	120.44
1	B	16	GLY	C-N-CA	5.89	128.10	120.44
1	B	212	LYS	N-CA-C	-5.82	98.60	108.26
1	A	310	VAL	CA-CB-CG1	5.80	120.26	110.40
1	B	201	ASN	N-CA-C	-5.80	106.25	113.38
1	B	326	VAL	CA-CB-CG1	5.75	120.17	110.40
1	A	53	GLN	N-CA-C	-5.75	97.96	108.02
1	A	152	THR	CA-CB-CG2	5.74	120.27	110.50
1	B	282	LEU	CA-C-N	-5.72	110.20	121.41
1	B	282	LEU	C-N-CA	-5.72	110.20	121.41
1	B	137	ILE	N-CA-C	-5.70	104.97	110.72
1	A	305	LYS	CD-CE-NZ	5.66	130.00	111.90
1	A	335	ARG	CB-CG-CD	5.65	124.30	111.30
1	B	96	THR	CB-CA-C	5.64	120.03	109.71
1	A	282	LEU	CA-C-N	-5.58	114.31	122.46
1	A	282	LEU	C-N-CA	-5.58	114.31	122.46
1	B	146	GLU	N-CA-C	5.58	118.81	109.95
1	B	100	ILE	CA-CB-CG2	5.56	119.95	110.50
1	A	310	VAL	N-CA-CB	5.55	118.25	112.37
1	B	340	VAL	CB-CA-C	5.50	118.24	111.25
1	A	380	SER	CB-CA-C	-5.50	101.66	110.79
1	B	337	ILE	N-CA-C	-5.46	101.14	108.35
1	B	236	ASP	CB-CG-OD1	-5.45	105.87	118.40
1	B	282	LEU	N-CA-C	-5.41	102.62	110.24
1	A	236	ASP	N-CA-C	-5.40	102.34	110.70
1	A	185	ARG	CG-CD-NE	-5.38	100.16	112.00
1	A	159	VAL	CG1-CB-CG2	5.38	122.64	110.80
1	A	326	VAL	N-CA-CB	-5.37	103.46	112.47
1	A	15	HIS	N-CA-C	-5.36	103.32	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	VAL	CA-CB-CG2	5.35	119.50	110.40
1	A	31	ASN	N-CA-CB	-5.34	101.17	109.87
1	A	113	VAL	N-CA-C	5.32	115.51	107.75
1	B	336	GLY	N-CA-C	5.31	122.94	115.30
1	A	16	GLY	N-CA-C	5.29	119.22	112.13
1	A	310	VAL	N-CA-C	5.29	113.90	107.61
1	B	18	LEU	CA-CB-CG	5.26	134.71	116.30
1	A	216	ASN	N-CA-C	5.25	119.00	112.59
1	A	380	SER	CA-CB-OG	-5.24	100.63	111.10
1	B	313	ILE	N-CA-CB	5.20	121.08	110.78
1	B	341	LYS	CB-CG-CD	5.20	123.27	111.30
1	A	113	VAL	CG1-CB-CG2	5.18	122.20	110.80
1	A	36	ASN	N-CA-C	5.17	119.23	113.02
1	A	18	LEU	N-CA-C	5.17	118.61	112.72
1	A	326	VAL	CA-CB-CG1	5.17	119.18	110.40
1	B	304	ARG	N-CA-C	5.15	119.45	112.04
1	A	120	GLN	CB-CG-CD	-5.14	103.87	112.60
1	A	236	ASP	CB-CG-OD2	5.13	130.21	118.40
1	B	252	ASN	CA-C-N	-5.13	114.44	122.49
1	B	252	ASN	C-N-CA	-5.13	114.44	122.49
1	A	173	GLN	N-CA-C	-5.13	106.29	112.54
1	A	96	THR	CB-CA-C	5.10	119.12	109.37
1	A	159	VAL	N-CA-C	5.08	115.29	107.77
1	A	186	LYS	CA-CB-CG	-5.06	103.97	114.10
1	B	326	VAL	N-CA-CB	-5.04	102.62	111.93
1	B	226	VAL	CG1-CB-CG2	5.03	121.86	110.80

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	91	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	175	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 (175) 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:CD1	1:A:313:ILE:CG1	1.75	1.61
1:B:18:LEU:CA	1:B:18:LEU:N	1.76	1.48
1:A:18:LEU:N	1:A:18:LEU:CA	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:17:PHE:C	1:A:18:LEU:CA	2.10	1.22
1:B:17:PHE:C	1:B:18:LEU:CA	2.09	1.22
1:A:179:GLY:HA2	1:A:184:VAL:CG2	1.72	1.18
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:HD13	1:B:313:ILE:H	1.14	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:219:TYR:H	5:A:405:DAO:H52	1.26	1.00
1:A:17:PHE:C	1:A:18:LEU:HA	1.79	0.97
1:B:313:ILE:HD13	1:B:313:ILE:N	1.79	0.97
1:B:173:GLN:HE21	1:B:173:GLN:H	1.01	0.97
1:B:313:ILE:H	1:B:313:ILE:CD1	1.77	0.96
1:B:256:MET:HE1	1:B:321:GLN:HB3	1.49	0.94
1:A:173:GLN:HE21	1:A:173:GLN:H	1.08	0.91
1:A:195:MET:HE2	1:A:202:ILE:HD11	1.52	0.89
1:A:256:MET:HE3	1:A:321:GLN:HB3	1.53	0.88
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:256:MET:HE3	1:A:322:PRO:HD2	1.56	0.85
1:B:17:PHE:C	1:B:18:LEU:HA	1.85	0.85
1:B:256:MET:HE3	1:B:322:PRO:HD2	1.59	0.84
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:313:ILE:CD1	1:A:313:ILE:H	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:256:MET:HE1	1:A:321:GLN:HB3	1.66	0.78
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
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:173:GLN:H	1:B:173:GLN:NE2	1.85	0.69
1:B:15:HIS:HE1	1:B:56:VAL:H	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:THR:CG2	1:B:329:ASN:H	2.06	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:HE21	1:A:173:GLN:N	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:253:MET:O	1:B:253:MET:HE3	1.97	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:179:GLY:C	1:A:184:VAL:HG22	2.26	0.60
1:A:257:ASN:HD22	1:A:257:ASN:C	2.09	0.60
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: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
1:B:257:ASN:ND2	1:B:259:ASN:HB2	2.19	0.57
1:B:257:ASN:HD22	1:B:257:ASN:C	2.13	0.56
1:B:173:GLN:HE22	1:B:311:PRO:HG3	1.71	0.56
1:A:327:THR:CG2	1:A:329:ASN:H	2.19	0.55
1:B:173:GLN:HE21	1:B:173:GLN:N	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:256:MET:HE1	1:A:321:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:256:MET:HE3	1:B:321:GLN:HB3	1.82	0.53
1:A:34:GLY:HA3	1:A:38:PHE:O	2.09	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:195:MET:HE2	1:A:202:ILE:CD1	2.31	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:A:264:THR:O	1:A:341:LYS:HB2	2.10	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:A:17:PHE:O	1:A:18:LEU:C	2.51	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:B:256:MET:HE3	1:B:322:PRO:CD	2.35	0.49
1:A:313:ILE:CD1	1:A:313:ILE:HG12	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:284:THR:O	1:A:285:PHE:C	2.60	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:197:ASN:HD22	1:A:197:ASN:C	2.26	0.44
1:B:256:MET:HE1	1:B:321:GLN:CB	2.34	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:68:GLN:NE2	1:B:80:TYR:OH	2.46	0.43
1:B:193:ARG:NH1	5:B:404:DAO:H22	2.27	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:256:MET:CE	1:B:322:PRO:HD2	2.39	0.42
1:B:116:SER:HG	1:B:349:HIS:CE1	2.37	0.42
1:B:256:MET:HE1	1:B:338:TRP:HE1	1.83	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:O1	5:A:405:DAO:H41	2.20	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
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:256:MET:HE1	1:A:338:TRP:HE1	1.86	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: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 sym-

metry 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%)	277 (87%)	42 (13%)	4	2
1	B	319/341 (94%)	276 (86%)	43 (14%)	4	2
All	All	638/682 (94%)	553 (87%)	85 (13%)	4	2

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU

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Mol	Chain	Res	Type
1	A	18	LEU
1	A	28	LEU
1	A	39	LYS
1	A	44	LEU
1	A	69	LEU
1	A	87	LYS
1	A	96	THR
1	A	100	ILE
1	A	108	LYS
1	A	110	VAL
1	A	113	VAL
1	A	124	LEU
1	A	141	GLN
1	A	152	THR
1	A	159	VAL
1	A	163	THR
1	A	173	GLN
1	A	184	VAL
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	310	VAL
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
1	A	361	LYS
1	A	378	LEU
1	A	379	LEU
1	A	385	GLU
1	B	4	GLN

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Mol	Chain	Res	Type
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	113	VAL
1	B	124	LEU
1	B	134	LYS
1	B	152	THR
1	B	159	VAL
1	B	163	THR
1	B	165	LEU
1	B	173	GLN
1	B	184	VAL
1	B	191	LEU
1	B	197	ASN
1	B	202	ILE
1	B	212	LYS
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	309	VAL
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	340	VAL
1	B	341	LYS
1	B	358	LEU
1	B	378	LEU
1	B	379	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	31	ASN
1	A	47	GLN
1	A	52	HIS
1	A	143	HIS
1	A	156	ASN
1	A	157	ASN
1	A	169	HIS
1	A	170	ASN
1	A	173	GLN
1	A	180	ASN
1	A	197	ASN
1	A	213	GLN
1	A	237	ASN
1	A	257	ASN
1	A	259	ASN
1	A	345	GLN
1	A	369	ASN
1	B	15	HIS
1	B	31	ASN
1	B	120	GLN
1	B	141	GLN
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	369	ASN

5.3.3 RNA ⓘ

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 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	-	7,7,7	0.99	0	7,7,7	1.39	2 (28%)
7	OCA	B	406	-	9,9,9	1.16	0	9,9,9	0.93	1 (11%)
8	PLM	A	408	-	17,17,17	0.77	0	17,17,17	1.13	1 (5%)
7	OCA	A	407	-	9,9,9	1.15	1 (11%)	9,9,9	1.32	2 (22%)
5	DAO	A	405	-	13,13,13	0.93	1 (7%)	13,13,13	1.60	2 (15%)
6	LEA	B	405	-	6,6,6	0.80	0	6,6,6	1.83	2 (33%)
5	DAO	B	404	-	13,13,13	0.76	0	13,13,13	1.19	2 (15%)
5	DAO	A	404	-	13,13,13	0.81	0	13,13,13	1.34	2 (15%)
6	LEA	A	406	-	6,6,6	0.86	0	6,6,6	1.41	1 (16%)
9	BUA	B	407	-	5,5,5	1.11	0	5,5,5	1.50	1 (20%)
4	6NA	B	403	-	7,7,7	1.19	0	7,7,7	0.95	1 (14%)
9	BUA	A	409	-	5,5,5	1.08	0	5,5,5	1.39	1 (20%)

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	-	-	2/5/5/5	-
7	OCA	B	406	-	-	2/7/7/7	-
8	PLM	A	408	-	-	8/15/15/15	-
7	OCA	A	407	-	-	3/7/7/7	-
5	DAO	A	405	-	-	7/11/11/11	-
6	LEA	B	405	-	-	2/4/4/4	-
5	DAO	B	404	-	-	4/11/11/11	-
5	DAO	A	404	-	-	6/11/11/11	-
6	LEA	A	406	-	-	4/4/4/4	-
9	BUA	B	407	-	-	2/3/3/3	-
4	6NA	B	403	-	-	2/5/5/5	-
9	BUA	A	409	-	-	2/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	DAO	C2-C1	2.14	1.55	1.50
7	A	407	OCA	C2-C1	2.08	1.55	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	DAO	O2-C1-C2	3.46	124.93	114.00
5	A	404	DAO	C5-C4-C3	-3.36	97.36	114.37
8	A	408	PLM	CC-CB-CA	-3.24	97.97	114.37
6	B	405	LEA	O2-C2-C3	3.19	124.07	114.00
5	A	405	DAO	C4-C3-C2	-3.03	101.98	113.13
5	B	404	DAO	C5-C4-C3	-2.95	99.45	114.37
7	A	407	OCA	O2-C1-O1	-2.95	115.74	123.33
6	B	405	LEA	O1-C2-C3	-2.90	113.89	123.09
6	A	406	LEA	O2-C2-C3	2.61	122.25	114.00
9	B	407	BUA	O2-C4-C3	2.56	122.09	114.00
5	A	404	DAO	C4-C3-C2	2.51	122.35	113.13
7	A	407	OCA	O2-C1-C2	2.45	121.73	114.00
9	A	409	BUA	O2-C4-C3	2.25	121.10	114.00
7	B	406	OCA	O2-C1-O1	-2.21	117.64	123.33
4	A	403	6NA	CG-CB-CA	2.19	121.17	113.13
4	B	403	6NA	OXT-C-O	-2.11	117.91	123.33
5	B	404	DAO	O1-C1-C2	-2.07	116.51	123.09
4	A	403	6NA	OXT-C-CA	2.01	120.35	114.00

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	406	LEA	C2-C3-C4-C5
7	A	407	OCA	C1-C2-C3-C4
8	A	408	PLM	C1-C2-C3-C4
5	A	404	DAO	C3-C4-C5-C6
5	A	405	DAO	C6-C7-C8-C9
5	A	405	DAO	C4-C5-C6-C7
8	A	408	PLM	C2-C3-C4-C5
5	B	404	DAO	C3-C4-C5-C6
9	B	407	BUA	C1-C2-C3-C4
8	A	408	PLM	C7-C8-C9-CA
4	A	403	6NA	C-CA-CB-CG
6	B	405	LEA	C2-C3-C4-C5
5	A	404	DAO	C7-C8-C9-C10
8	A	408	PLM	CC-CD-CE-CF
8	A	408	PLM	CA-CB-CC-CD
5	B	404	DAO	C6-C7-C8-C9
8	A	408	PLM	C4-C5-C6-C7
5	B	404	DAO	C7-C8-C9-C10
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
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
7	B	406	OCA	O1-C1-C2-C3
5	A	405	DAO	C5-C6-C7-C8
6	A	406	LEA	O2-C2-C3-C4
7	B	406	OCA	O2-C1-C2-C3
9	A	409	BUA	C2-C3-C4-O2
6	A	406	LEA	O1-C2-C3-C4
9	A	409	BUA	C2-C3-C4-O1
6	A	406	LEA	C3-C4-C5-C6
7	A	407	OCA	O1-C1-C2-C3

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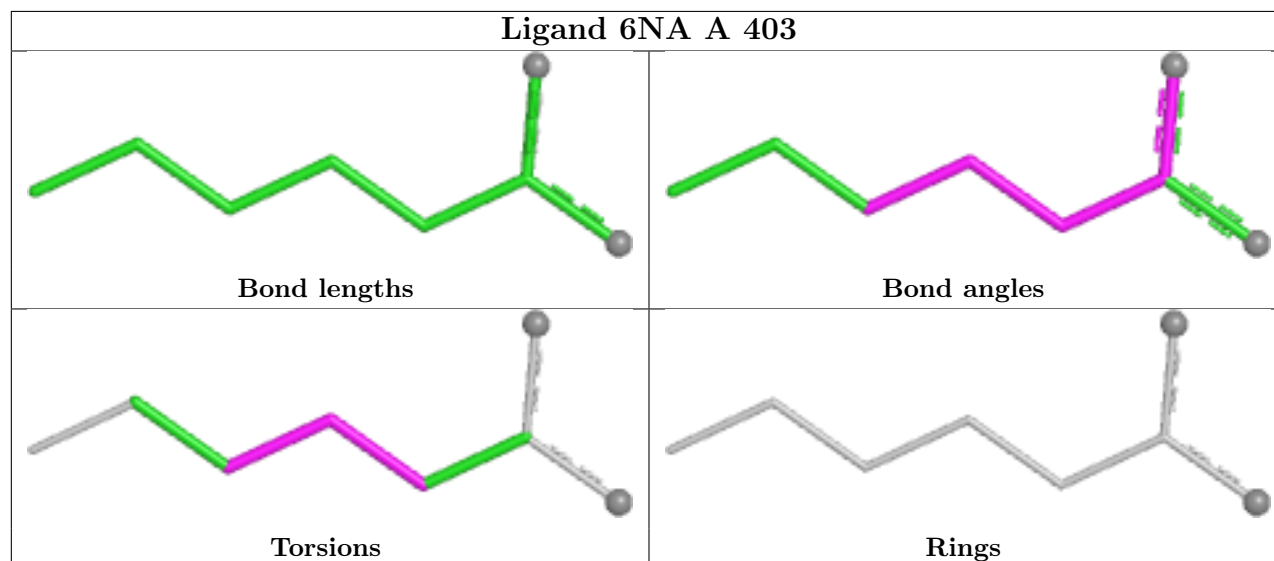
Mol	Chain	Res	Type	Atoms
7	A	407	OCA	O2-C1-C2-C3
4	B	403	6NA	OXT-C-CA-CB
9	B	407	BUA	C2-C3-C4-O2
4	B	403	6NA	O-C-CA-CB

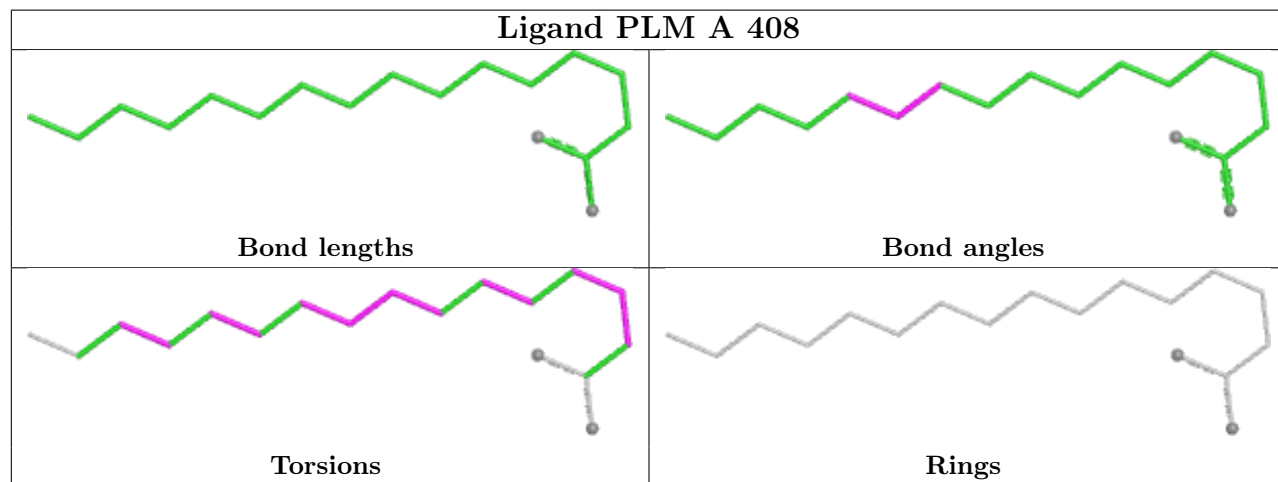
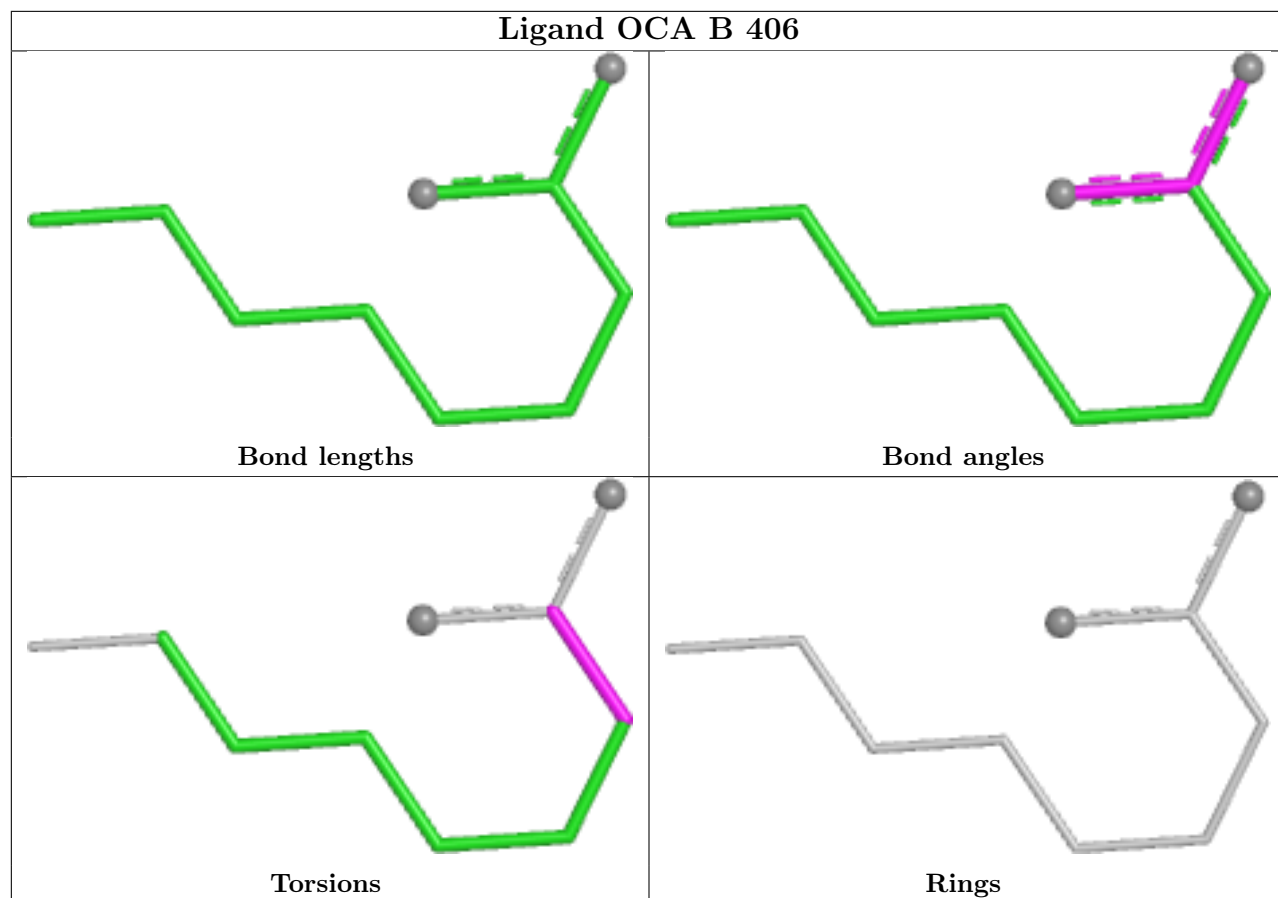
There are no ring outliers.

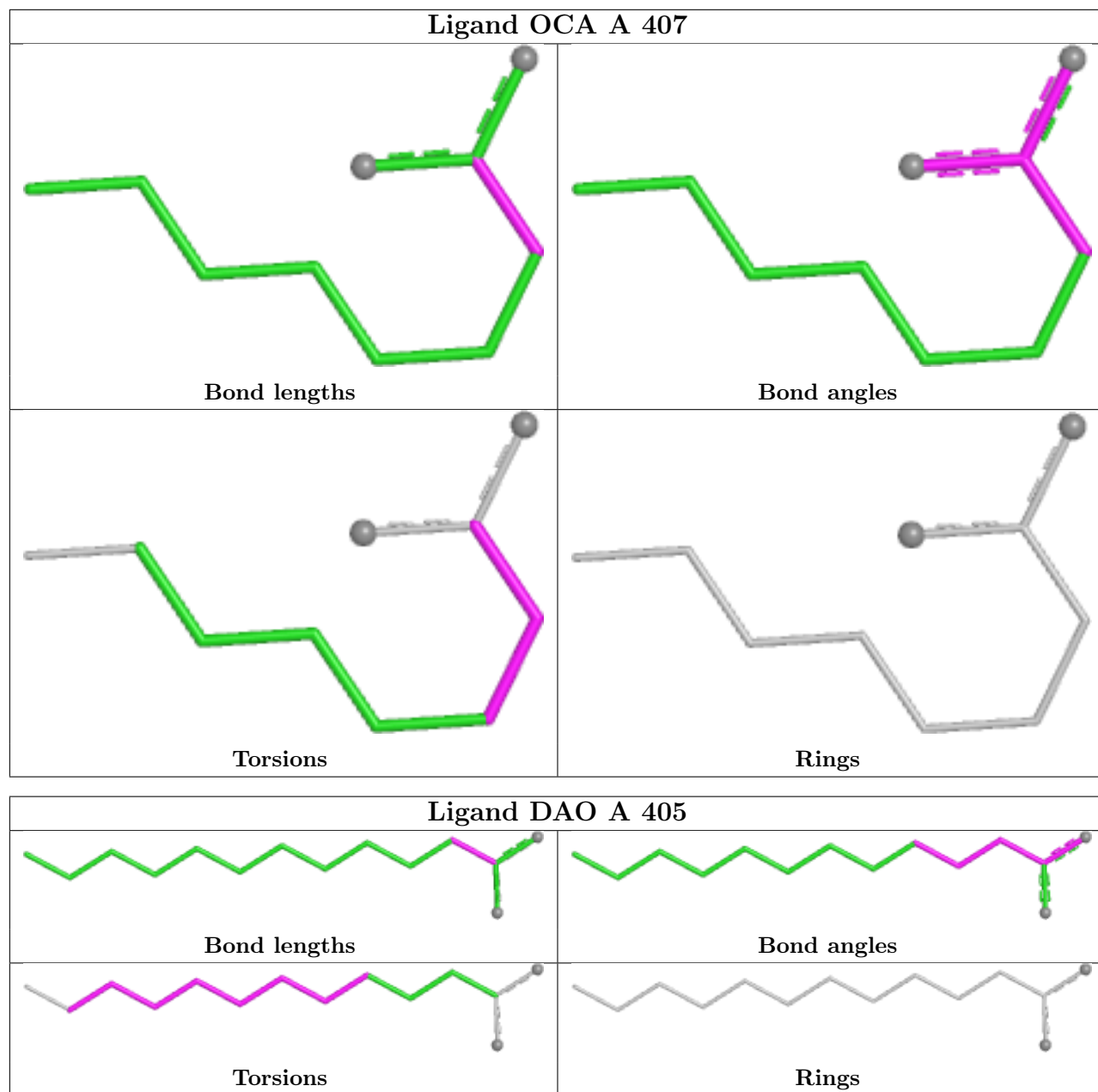
5 monomers are involved in 13 short contacts:

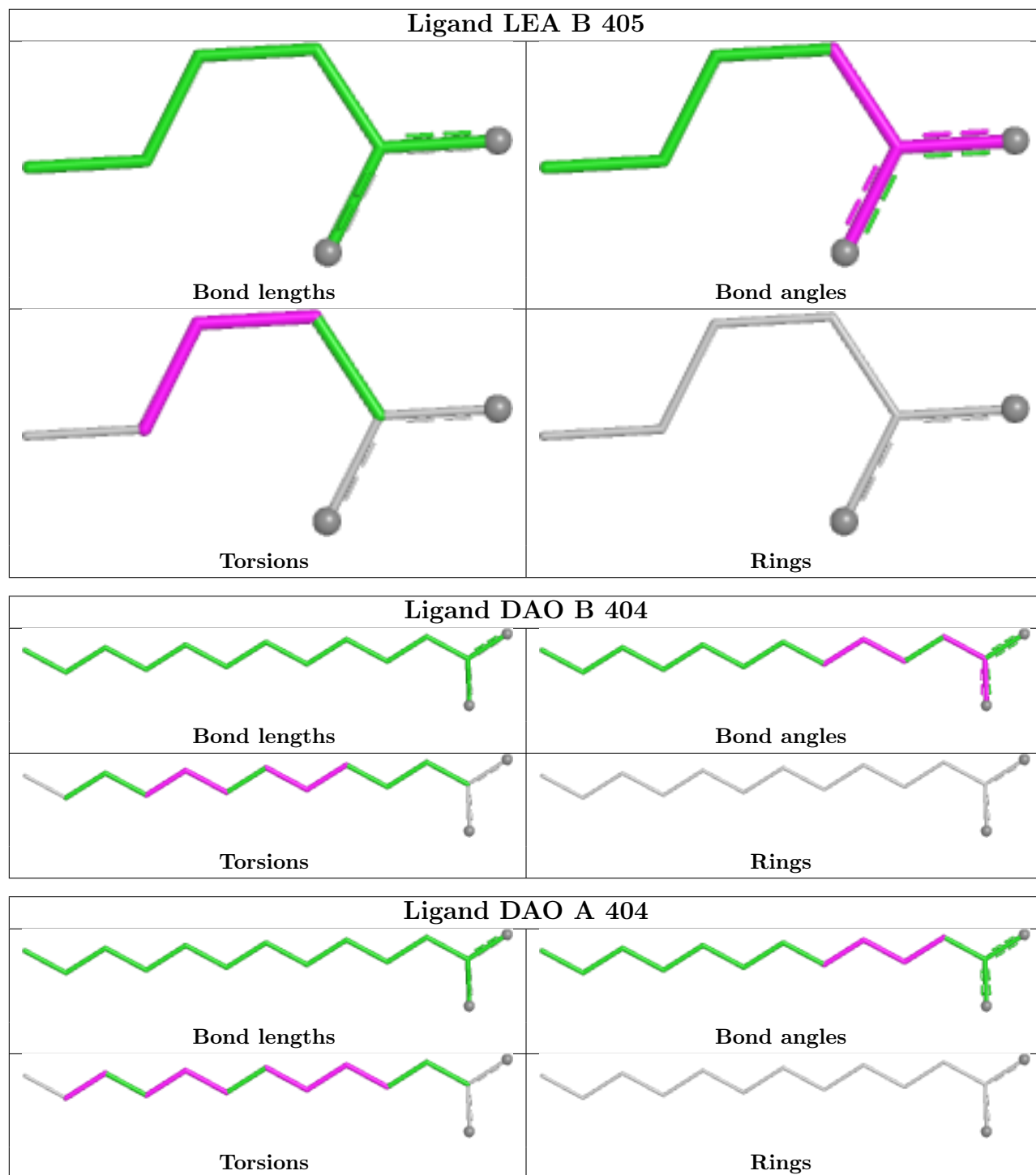
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	DAO	5	0
5	B	404	DAO	4	0
5	A	404	DAO	3	0
9	B	407	BUA	1	0
4	B	403	6NA	1	0

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

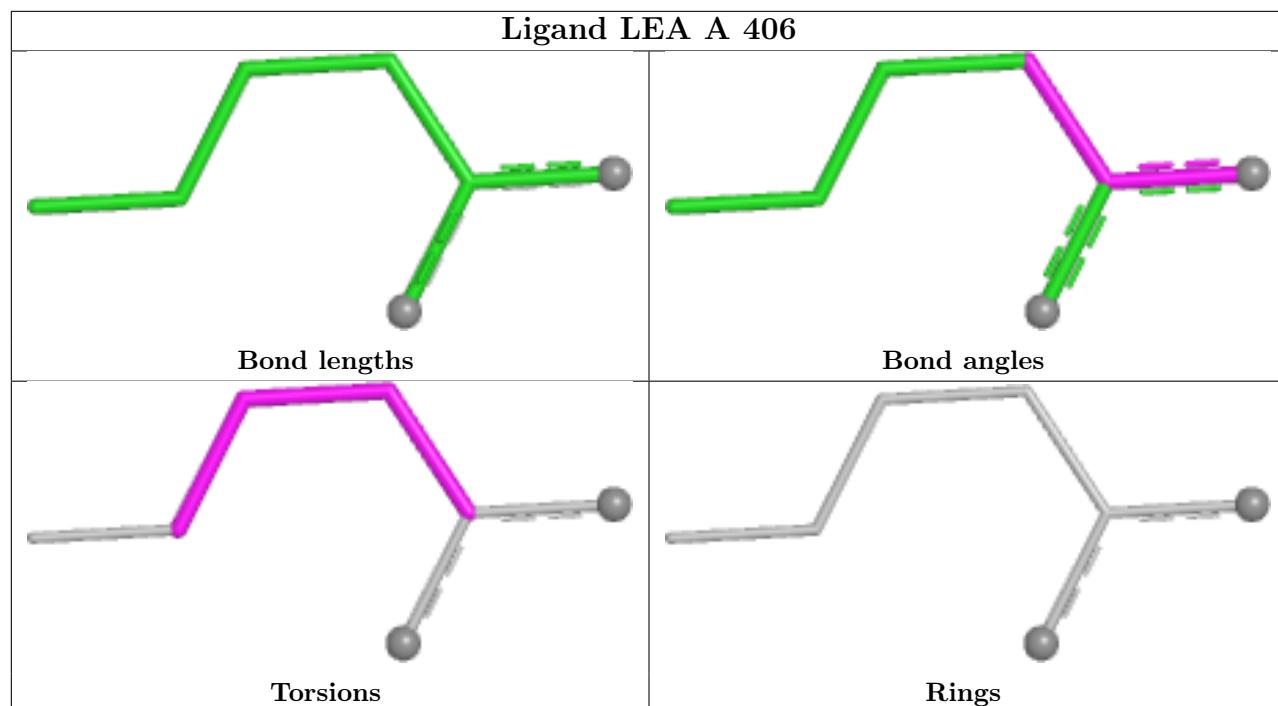




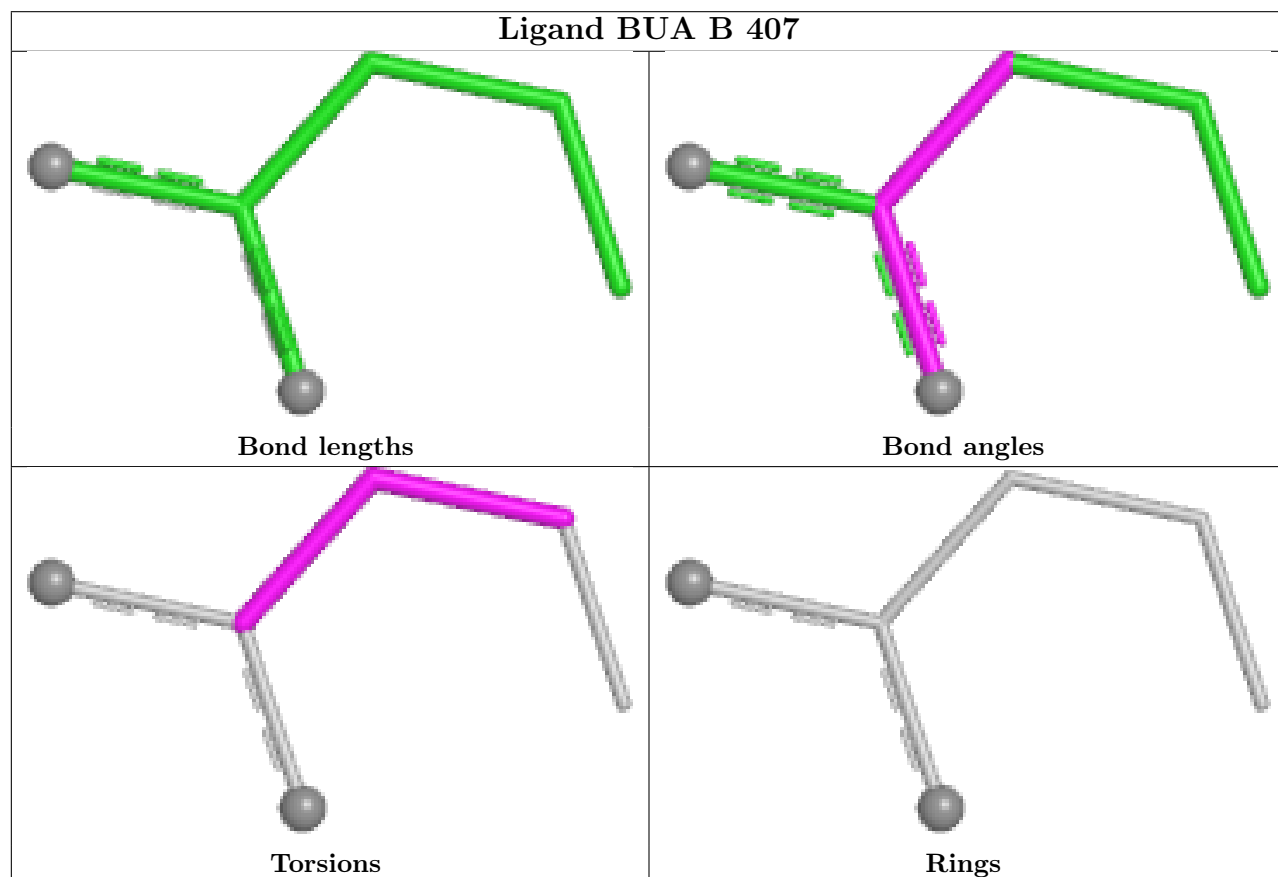


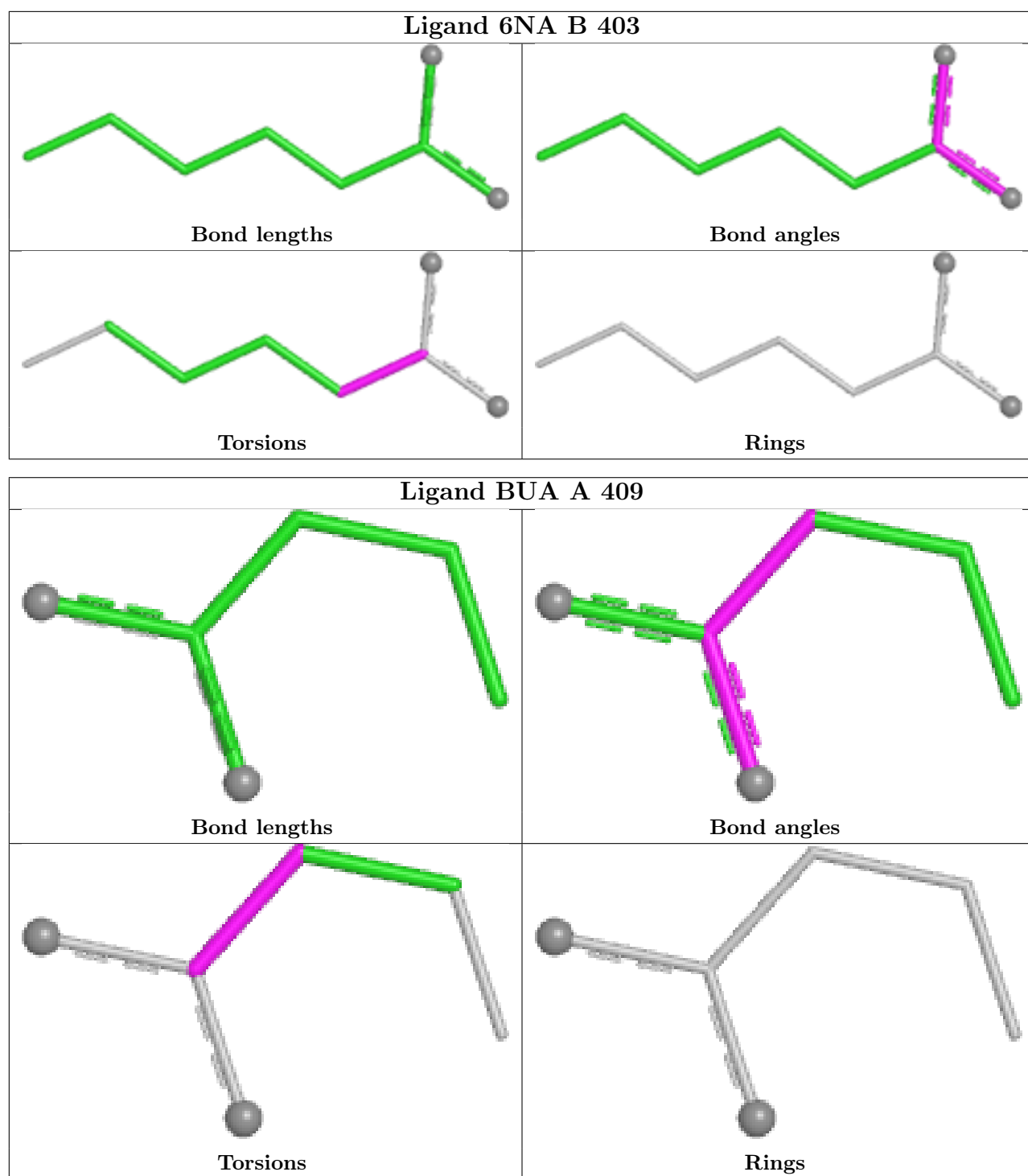


Ligand LEA A 406



Ligand BUA B 407





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

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%)	0.12	11 (2%) 53 56	34, 42, 57, 83	0
1	B	382/408 (93%)	0.60	35 (9%) 14 15	37, 47, 65, 79	0
All	All	764/816 (93%)	0.36	46 (6%) 27 29	34, 45, 63, 83	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	GLY	9.2
1	A	178	PHE	5.3
1	B	139	TYR	4.6
1	A	360	PHE	4.6
1	B	27	ALA	4.6
1	A	274	PRO	4.6
1	A	180	ASN	4.0
1	A	313	ILE	3.8
1	B	141	GLN	3.4
1	B	134	LYS	3.3
1	B	275	LEU	3.3
1	B	142	ALA	3.2
1	B	93	TYR	3.0
1	B	179	GLY	3.0
1	A	289	ASP	3.0
1	B	274	PRO	3.0
1	B	128	PHE	2.9
1	A	28	LEU	2.8
1	B	137	ILE	2.8
1	B	313	ILE	2.8
1	A	98	LYS	2.8
1	B	332	ALA	2.7
1	B	289	ASP	2.7
1	B	108	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	147	ILE	2.6
1	A	275	LEU	2.6
1	B	96	THR	2.6
1	A	273	GLY	2.5
1	B	328	ASN	2.5
1	B	155	HIS	2.4
1	B	146	GLU	2.4
1	B	148	SER	2.4
1	B	202	ILE	2.3
1	B	144	GLY	2.3
1	B	98	LYS	2.3
1	B	151	PHE	2.3
1	B	360	PHE	2.2
1	B	153	GLY	2.1
1	B	80	TYR	2.1
1	B	320	ASN	2.1
1	B	75	GLY	2.1
1	B	152	THR	2.1
1	B	263	THR	2.1
1	B	76	GLY	2.0
1	B	154	GLY	2.0
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 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.

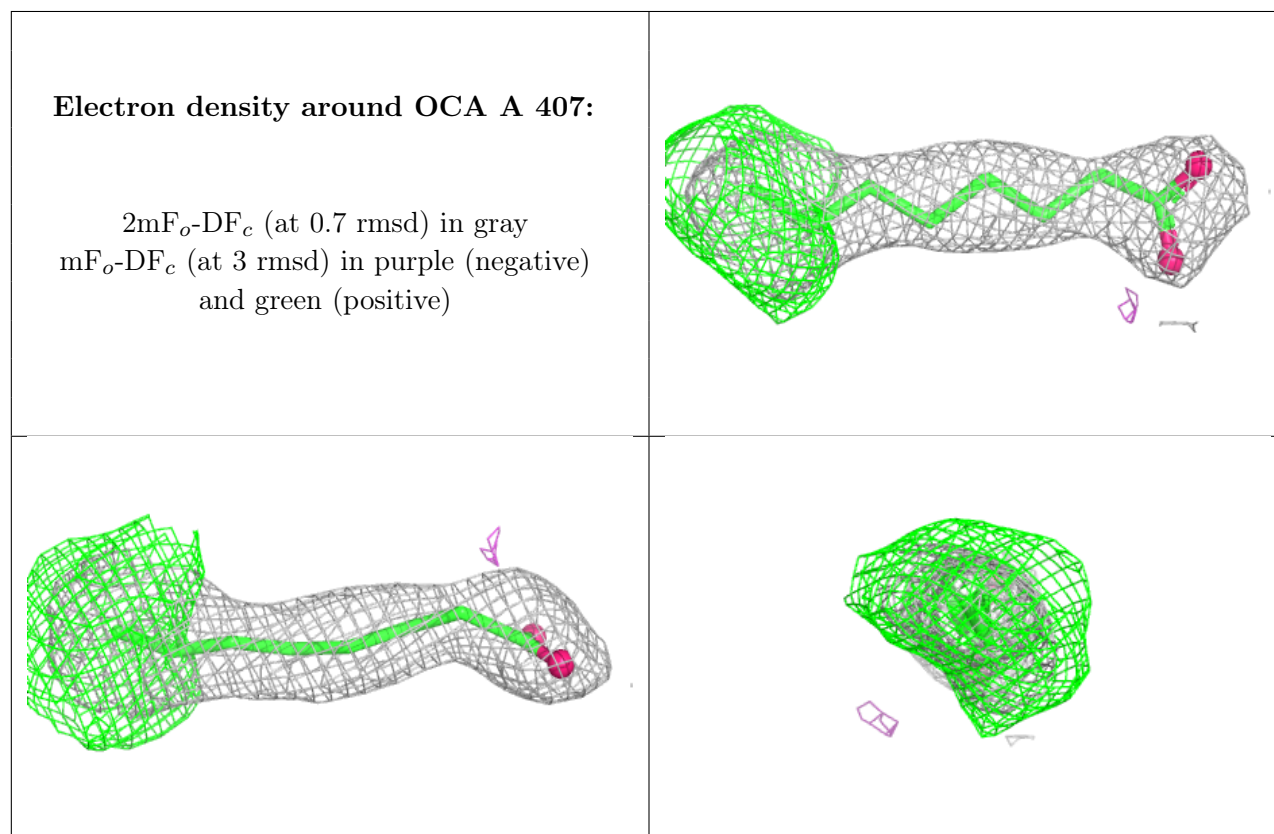
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	OCA	A	407	10/10	0.79	0.35	66,76,78,78	0

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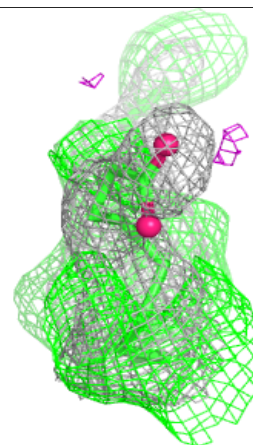
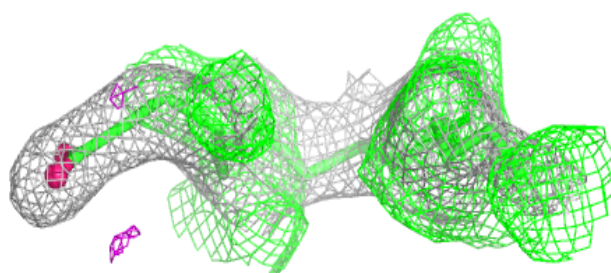
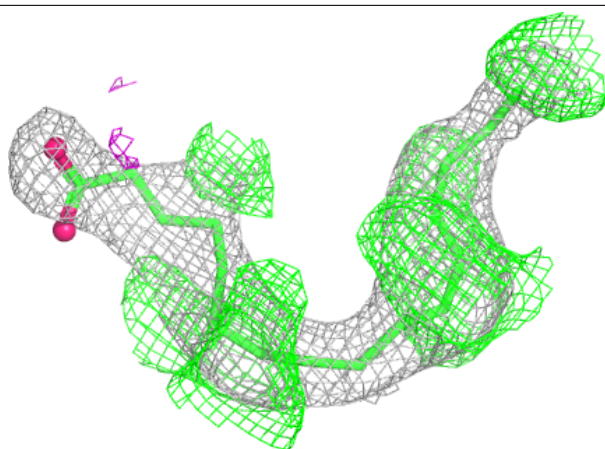
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	PLM	A	408	18/18	0.79	0.41	49,84,99,104	0
5	DAO	A	405	14/14	0.81	0.36	51,80,90,97	0
4	6NA	B	403	8/8	0.84	0.34	78,90,93,112	0
6	LEA	A	406	7/7	0.89	0.32	74,83,108,127	0
7	OCA	B	406	10/10	0.89	0.28	71,75,85,92	0
6	LEA	B	405	7/7	0.89	0.29	70,76,90,94	0
9	BUA	B	407	6/6	0.91	0.25	72,85,94,100	0
4	6NA	A	403	8/8	0.92	0.25	68,75,90,108	0
9	BUA	A	409	6/6	0.93	0.24	82,96,103,109	0
5	DAO	B	404	14/14	0.93	0.21	47,68,82,86	0
5	DAO	A	404	14/14	0.94	0.22	55,73,79,85	0
3	CA	A	402	1/1	0.96	0.09	66,66,66,66	0
3	CA	B	402	1/1	0.98	0.14	61,61,61,61	0
2	ZN	B	401	1/1	0.99	0.07	63,63,63,63	0
2	ZN	A	401	1/1	1.00	0.05	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.



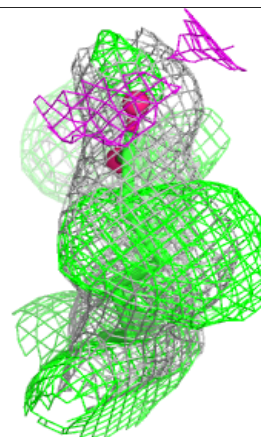
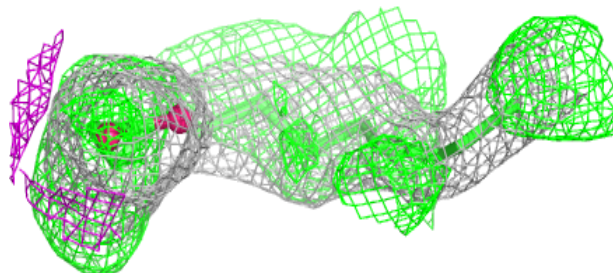
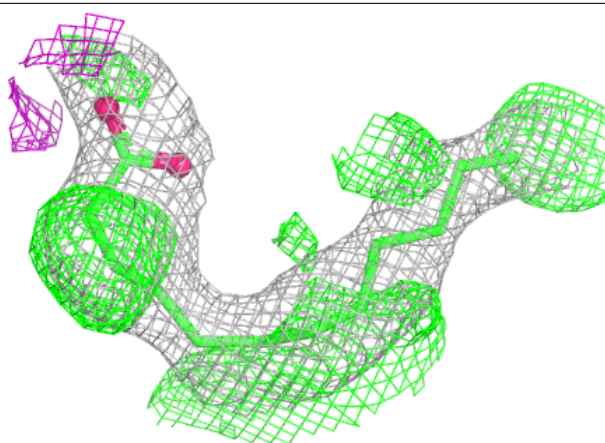
Electron density around PLM A 408:

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

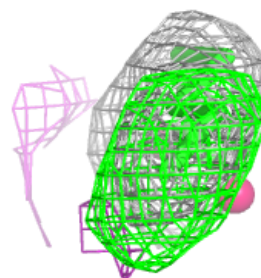
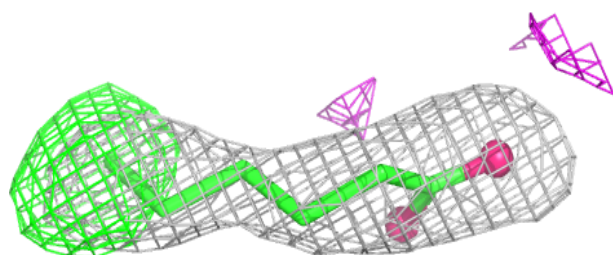
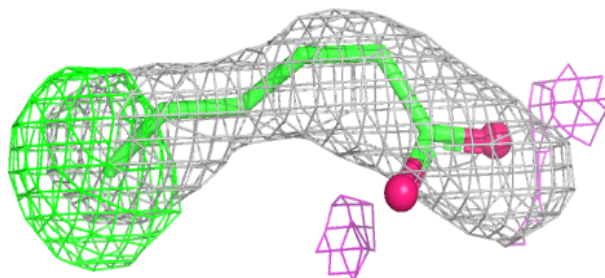


Electron density around DAO A 405:

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

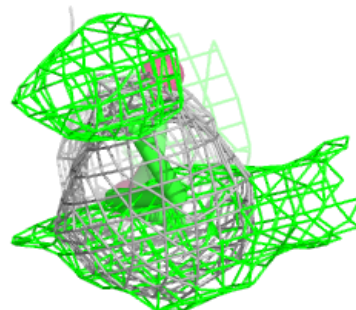
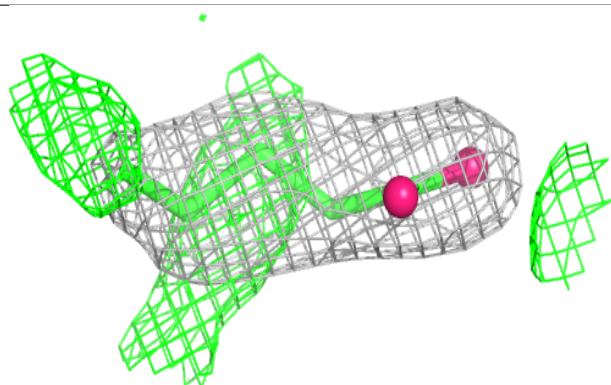
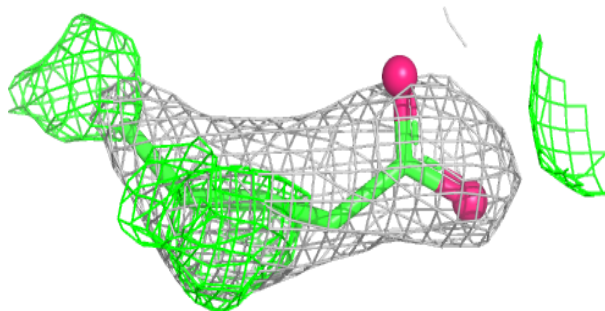
**Electron density around 6NA B 403:**

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

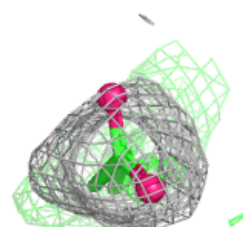
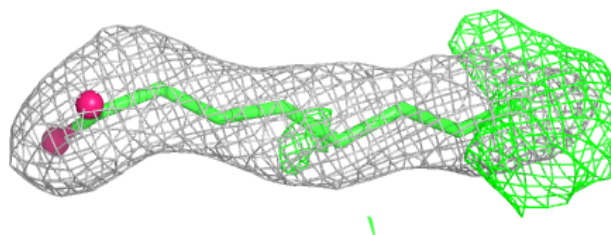
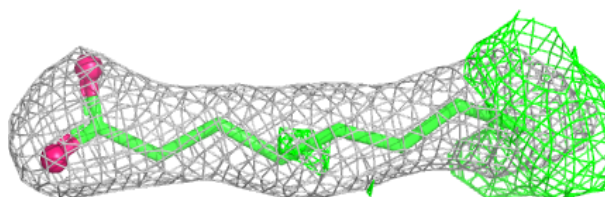


Electron density around LEA A 406:

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

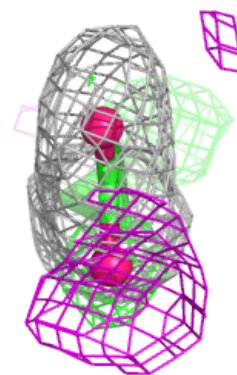
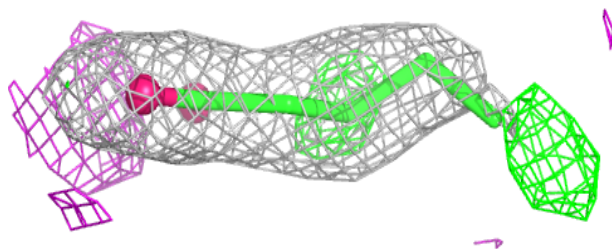
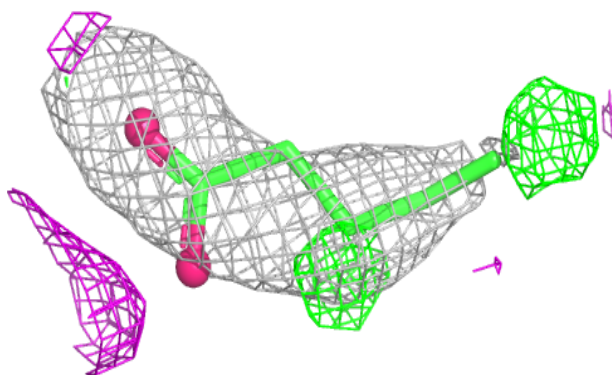
**Electron density around OCA B 406:**

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

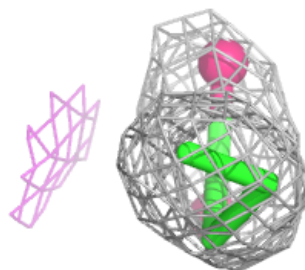
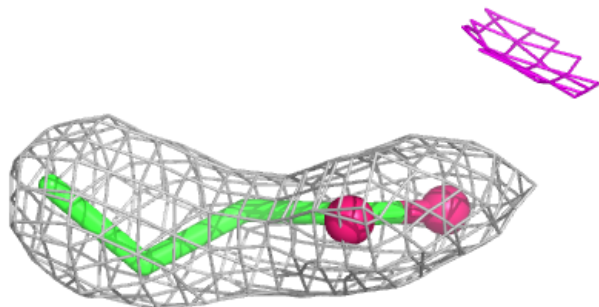
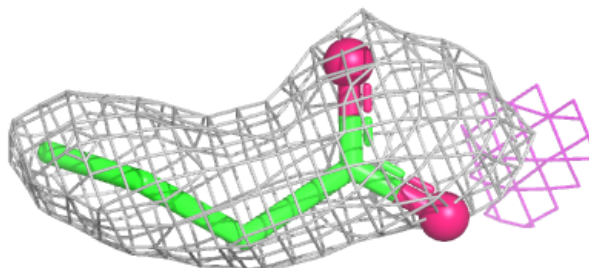


Electron density around LEA B 405:

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

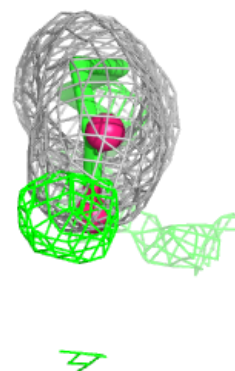
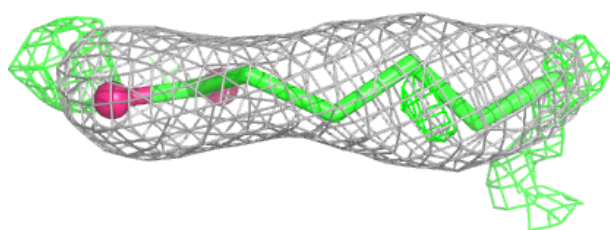
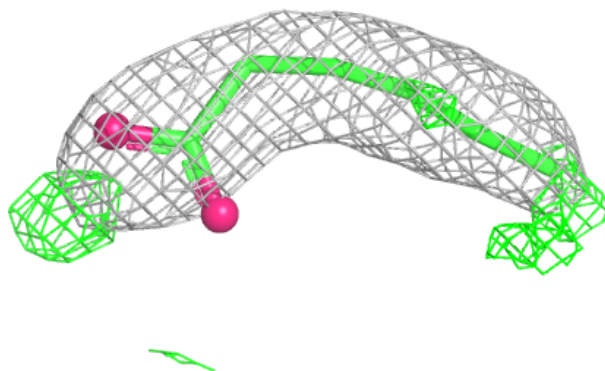
**Electron density around BUA B 407:**

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



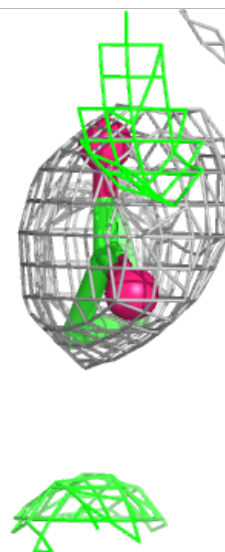
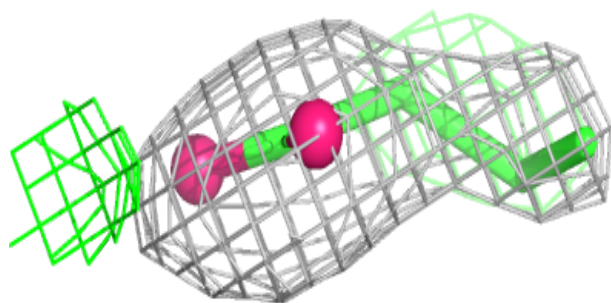
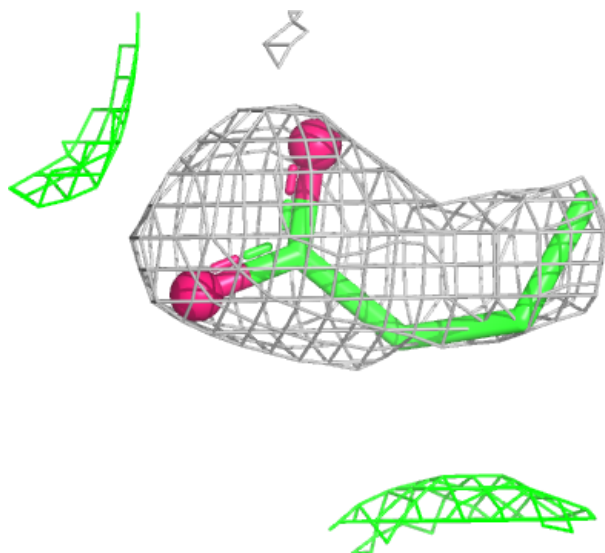
Electron density around 6NA A 403:

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



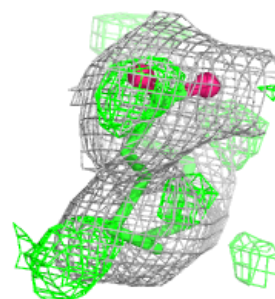
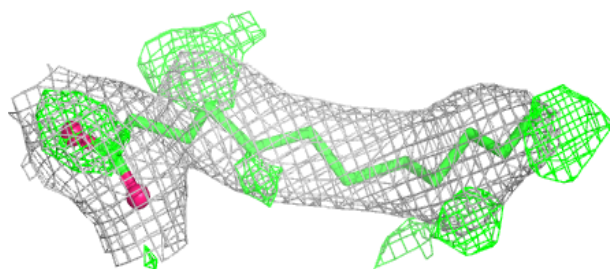
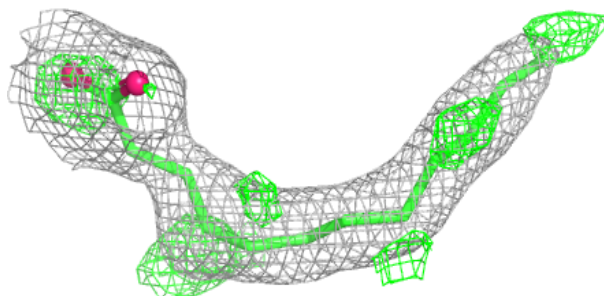
Electron density around BUA A 409:

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

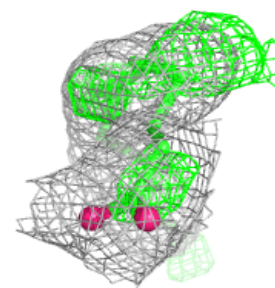
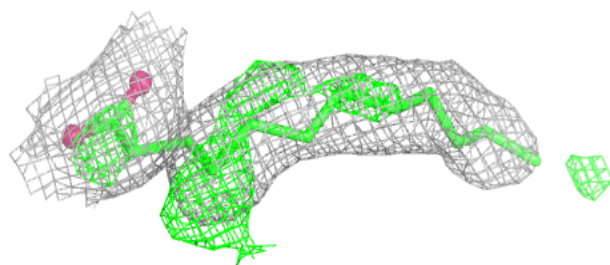
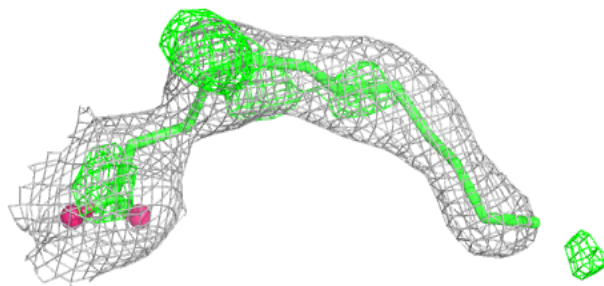


Electron density around DAO B 404:

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

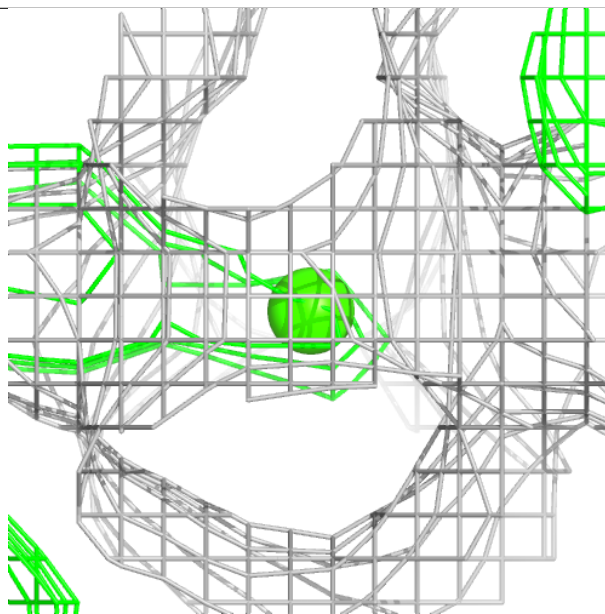
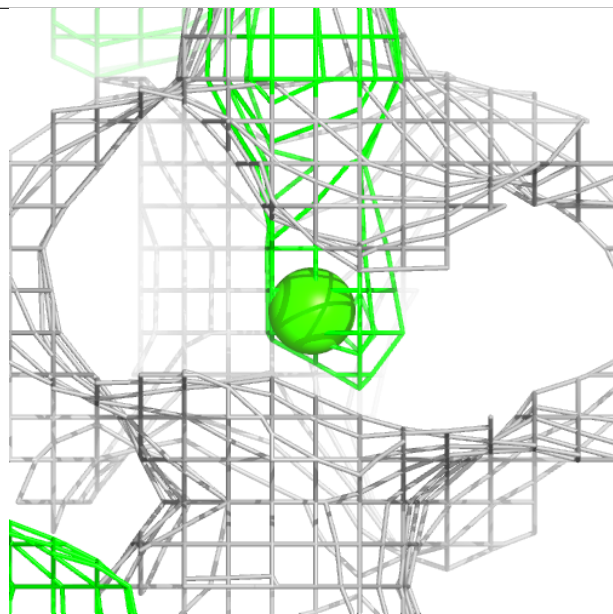
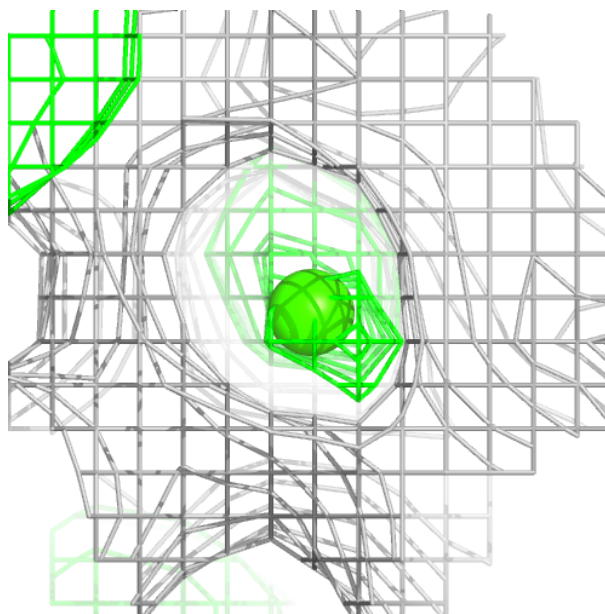
**Electron density around DAO A 404:**

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



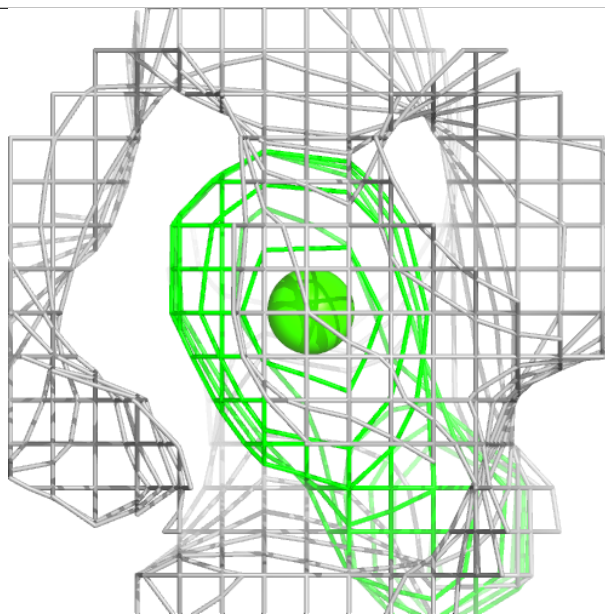
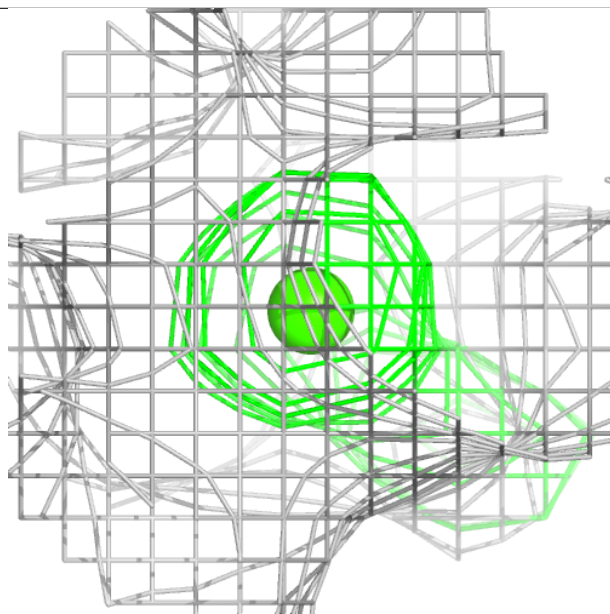
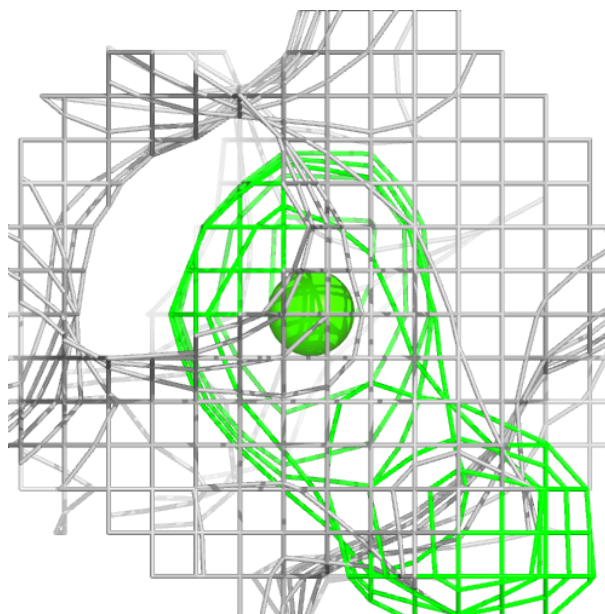
Electron density around CA A 402:

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



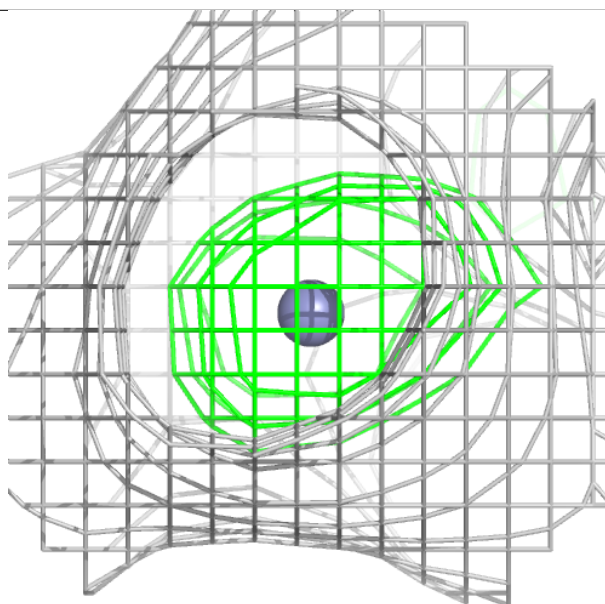
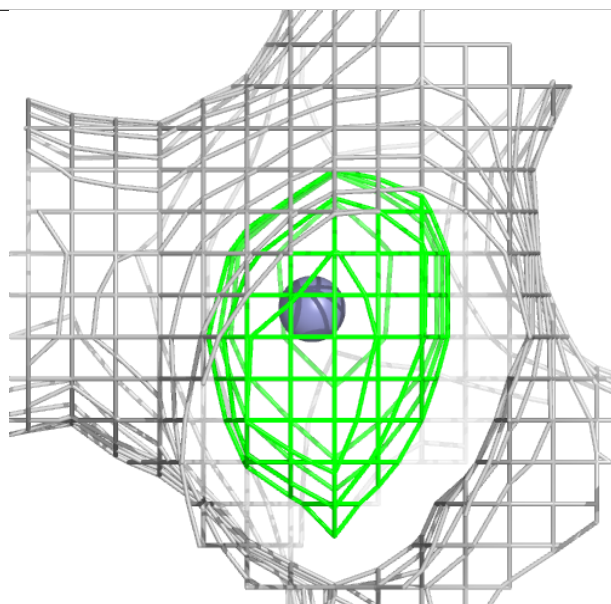
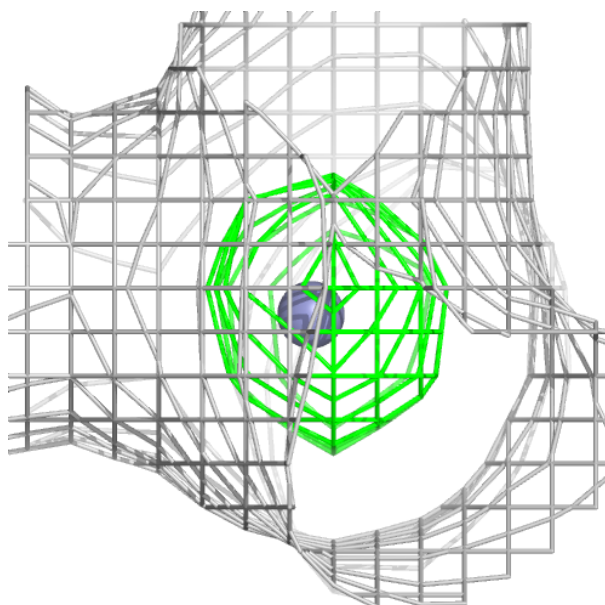
Electron density around CA B 402:

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



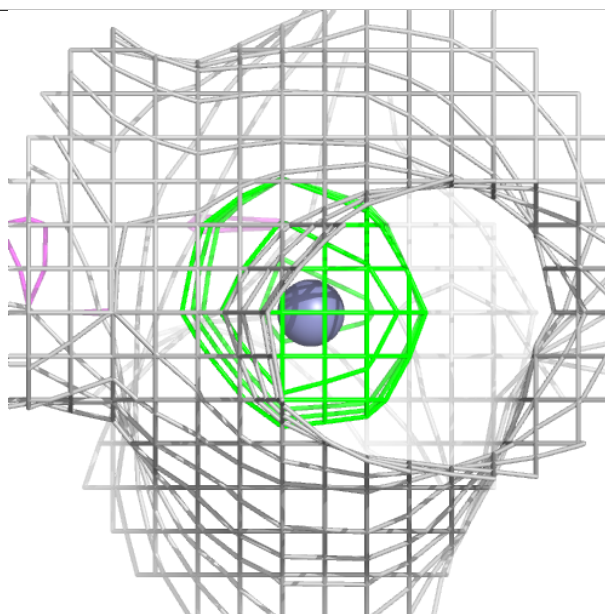
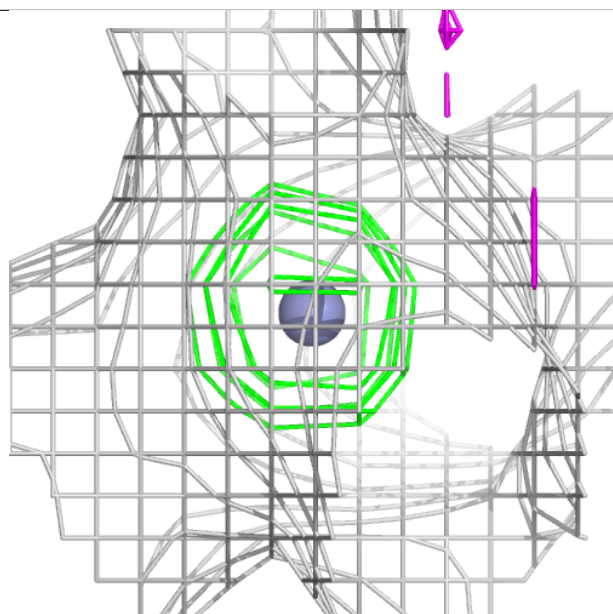
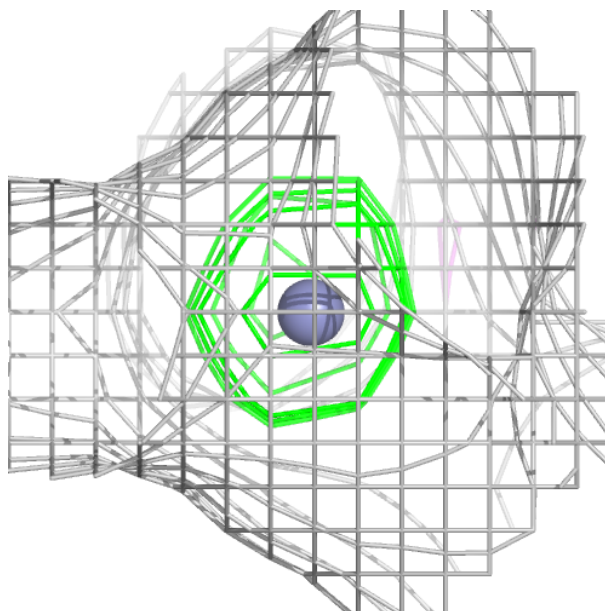
Electron density around ZN B 401:

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



Electron density around ZN A 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.