



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:40 am BST

PDB ID : 6KSL
Title : Staphylococcus aureus lipase - S116A inactive mutant
Authors : Kitadokoro, K.; Tanaka, M.; Kamitani, S.
Deposited on : 2019-08-24
Resolution : 2.59 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

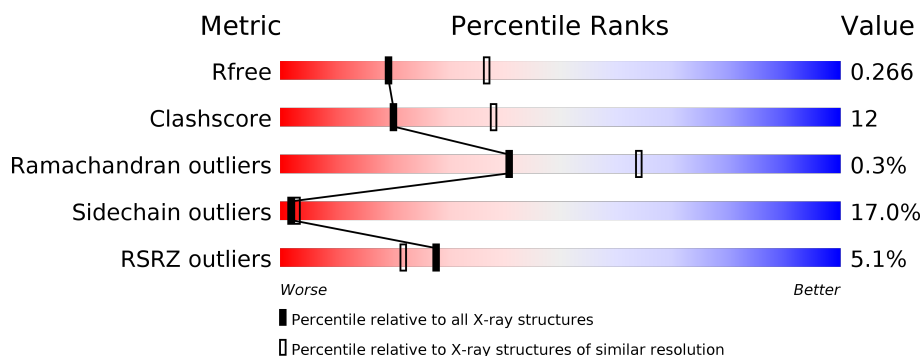
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>22%</div> <div>6%</div> <div>6%</div> </div> </div>
1	B	408	<div> <div>7%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>6%</div> <div>6%</div> </div> </div>

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	DAO	B	404	-	-	-	X
5	BUA	A	404	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6116 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
			3023	1925	527	562	9			
1	B	382	Total	C	N	O	S	0	0	0
			3023	1925	527	562	9			

There are 28 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
A	116	ALA	SER	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP A0A0U1MWF9
B	68	GLN	GLU	variant	UNP A0A0U1MWF9
B	116	ALA	SER	engineered mutation	UNP A0A0U1MWF9

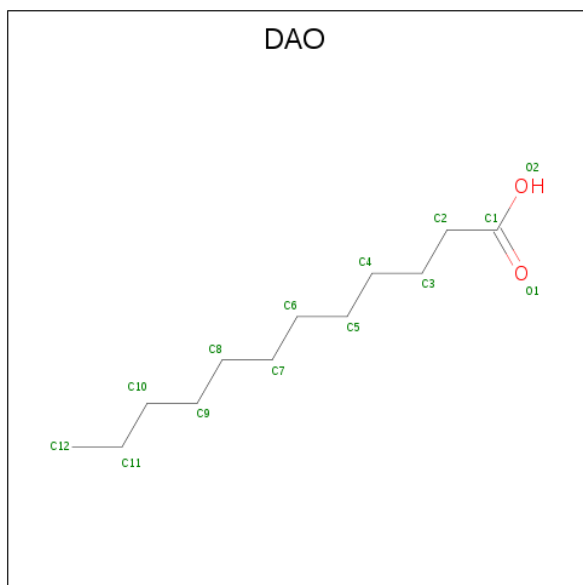
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

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).

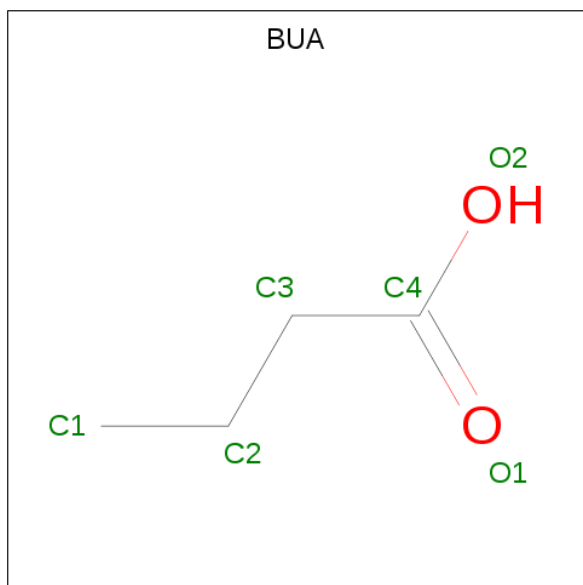
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is LAURIC ACID (three-letter code: DAO) (formula: C₁₂H₂₄O₂) (labeled as "Ligand of Interest" by author).



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

- Molecule 5 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
5	A	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		

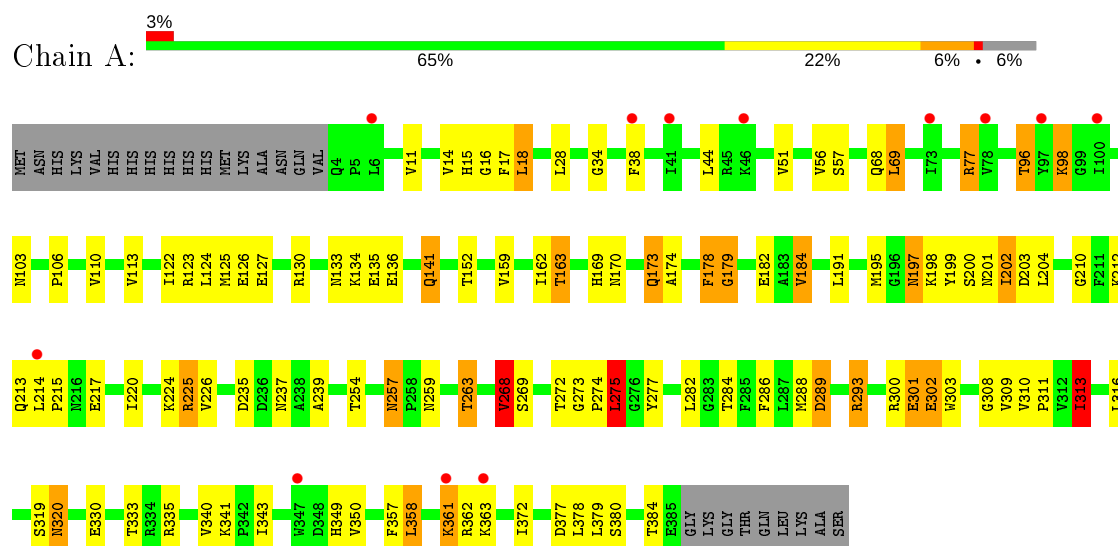
- Molecule 6 is water.

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

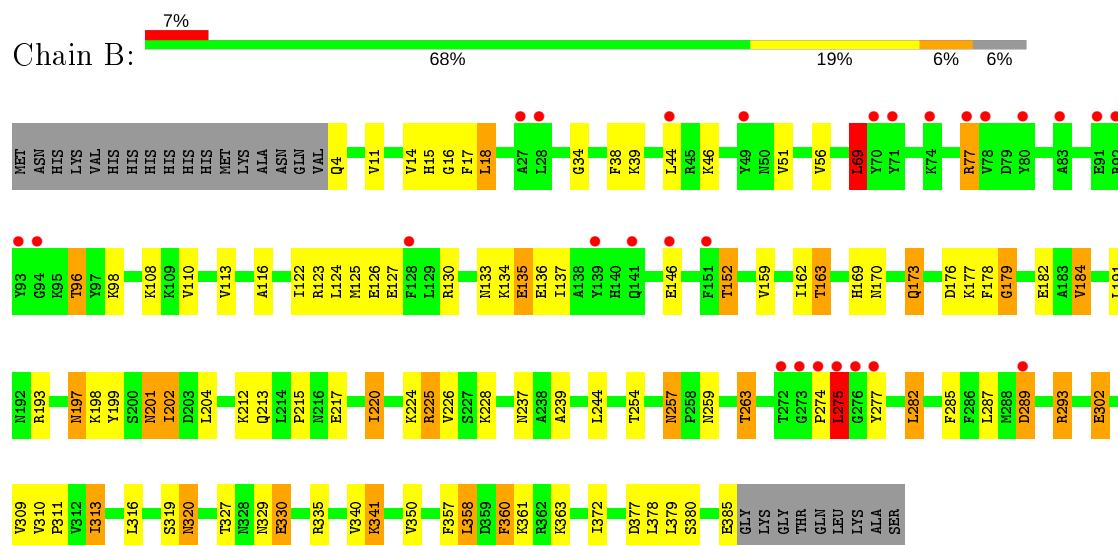
3 Residue-property plots [i](#)

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 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	164.21Å 164.21Å 233.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.81 – 2.59 48.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.81-2.59) 99.8 (48.81-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.249 , 0.268 0.246 , 0.266	Depositor DCC
R_{free} test set	2901 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	92.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6116	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: ZN, BUA, CA, DAO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.93	2/3105 (0.1%)	1.06	13/4211 (0.3%)
1	B	0.89	2/3105 (0.1%)	1.03	13/4211 (0.3%)
All	All	0.91	4/6210 (0.1%)	1.04	26/8422 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	GLY	N-CA	5.78	1.54	1.46
1	B	18	LEU	N-CA	5.36	1.57	1.46
1	B	179	GLY	N-CA	5.31	1.54	1.46
1	A	301	GLU	CG-CD	5.12	1.59	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	PHE	C-N-CA	-11.21	98.77	122.30
1	A	178	PHE	C-N-CA	-10.67	99.90	122.30
1	A	203	ASP	CB-CG-OD1	10.10	127.39	118.30
1	A	293	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	B	193	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	B	17	PHE	C-N-CA	-7.50	102.96	121.70
1	A	17	PHE	C-N-CA	-7.03	104.13	121.70
1	A	268	VAL	CB-CA-C	-6.31	99.41	111.40
1	A	275	LEU	CB-CG-CD2	6.25	121.63	111.00
1	B	220	ILE	CG1-CB-CG2	-6.02	98.16	111.40
1	A	225	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	225	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	293	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	B	293	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	B	177	LYS	CD-CE-NZ	-5.42	99.25	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	LEU	CB-CG-CD2	5.40	120.18	111.00
1	B	275	LEU	CB-CG-CD2	5.32	120.04	111.00
1	A	18	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	300	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	B	193	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	B	275	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	275	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	235	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	17	PHE	O-C-N	-5.13	114.49	122.70
1	A	313	ILE	CB-CA-C	-5.08	101.45	111.60
1	B	17	PHE	O-C-N	-5.05	114.63	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3023	0	2919	82	1
1	B	3023	0	2919	67	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	14	0	23	1	0
4	B	28	0	46	2	0
5	A	6	0	7	0	0
5	B	6	0	7	0	0
6	A	7	0	0	0	0
6	B	5	0	0	1	0
All	All	6116	0	5921	150	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 12.

All (150) 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:202:ILE:HD11	1:A:204:LEU:CD1	1.58	1.33
1:A:289:ASP:OD1	1:A:293:ARG:NH2	1.62	1.31
1:A:313:ILE:H	1:A:313:ILE:CD1	1.67	1.07
1:A:202:ILE:HD11	1:A:204:LEU:HD13	1.38	1.05
1:A:288:MET:CE	1:A:308:GLY:HA3	1.87	1.04
1:A:202:ILE:HD11	1:A:204:LEU:HD11	1.39	1.03
1:A:313:ILE:HD13	1:A:313:ILE:N	1.70	1.02
1:A:202:ILE:CD1	1:A:204:LEU:CD1	2.39	1.01
1:A:313:ILE:H	1:A:313:ILE:HD13	0.86	0.99
1:B:173:GLN:HE22	1:B:311:PRO:HG3	1.33	0.93
1:B:302:GLU:O	1:B:313:ILE:HD11	1.67	0.93
1:B:202:ILE:HD11	1:B:204:LEU:CD1	2.00	0.91
1:A:173:GLN:HE22	1:A:311:PRO:HG3	1.33	0.91
1:B:289:ASP:OD2	1:B:293:ARG:NH2	2.04	0.89
1:B:201:ASN:HA	6:B:502:HOH:O	1.72	0.89
1:A:173:GLN:HE21	1:A:173:GLN:H	1.22	0.87
1:B:198:LYS:H	1:B:213:GLN:HE21	1.23	0.85
1:B:173:GLN:H	1:B:173:GLN:HE21	1.21	0.85
1:B:327:THR:CG2	1:B:330:GLU:HG3	2.07	0.83
1:B:198:LYS:H	1:B:213:GLN:NE2	1.78	0.82
1:A:198:LYS:H	1:A:213:GLN:NE2	1.78	0.81
1:A:197:ASN:HD22	1:A:199:TYR:H	1.28	0.81
1:B:202:ILE:HD11	1:B:204:LEU:HD11	1.64	0.80
1:B:257:ASN:HD22	1:B:259:ASN:H	1.31	0.79
1:A:198:LYS:H	1:A:213:GLN:HE21	1.29	0.78
1:A:257:ASN:HD22	1:A:259:ASN:H	1.31	0.78
1:B:15:HIS:HE1	1:B:56:VAL:H	1.34	0.74
1:A:195:MET:HE2	1:A:202:ILE:HG12	1.70	0.73
1:B:327:THR:HG22	1:B:330:GLU:CG	2.19	0.73
1:A:202:ILE:CD1	1:A:204:LEU:HD13	2.11	0.72
1:A:15:HIS:HE1	1:A:56:VAL:H	1.35	0.71
1:A:197:ASN:ND2	1:A:199:TYR:H	1.88	0.71
1:A:14:VAL:HG21	1:A:122:ILE:HD11	1.72	0.71
1:A:195:MET:CE	1:A:202:ILE:HG12	2.21	0.71
1:A:288:MET:HE2	1:A:308:GLY:HA3	1.73	0.71
1:A:141:GLN:HA	1:A:141:GLN:HE21	1.54	0.71
1:B:123:ARG:HH11	1:B:169:HIS:HD2	1.40	0.70
1:A:57:SER:H	1:A:68:GLN:NE2	1.90	0.69
1:A:173:GLN:NE2	1:A:311:PRO:HG3	2.06	0.69
1:B:197:ASN:HD22	1:B:199:TYR:H	1.40	0.69
1:A:123:ARG:HH11	1:A:169:HIS:HD2	1.41	0.68
1:A:15:HIS:CE1	1:A:56:VAL:H	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:HIS:CE1	1:B:56:VAL:H	2.12	0.68
1:B:202:ILE:CD1	1:B:204:LEU:CD1	2.72	0.67
1:A:302:GLU:O	1:A:313:ILE:HD12	1.94	0.67
1:B:163:THR:HB	1:B:263:THR:HG23	1.76	0.66
1:B:173:GLN:NE2	1:B:311:PRO:HG3	2.06	0.66
1:A:275:LEU:HD23	1:A:277:TYR:H	1.61	0.66
1:A:163:THR:HB	1:A:263:THR:HG23	1.76	0.66
1:B:14:VAL:HG21	1:B:122:ILE:HD11	1.77	0.66
1:B:137:ILE:HD11	1:B:152:THR:HA	1.78	0.65
1:B:133:ASN:ND2	1:B:136:GLU:HG2	2.12	0.64
1:A:133:ASN:ND2	1:A:136:GLU:HG2	2.14	0.63
1:A:288:MET:HE3	1:A:308:GLY:HA3	1.80	0.62
1:B:198:LYS:N	1:B:213:GLN:HE21	1.95	0.62
1:B:127:GLU:HG3	1:B:254:THR:HG22	1.82	0.62
1:B:327:THR:CG2	1:B:330:GLU:CG	2.77	0.61
1:A:288:MET:CE	1:A:308:GLY:CA	2.73	0.61
1:A:170:ASN:HD21	1:A:319:SER:H	1.48	0.60
1:A:198:LYS:N	1:A:213:GLN:HE21	1.98	0.60
1:B:327:THR:HG23	1:B:330:GLU:HG3	1.80	0.60
1:A:127:GLU:HG3	1:A:254:THR:HG22	1.83	0.60
1:B:257:ASN:ND2	1:B:259:ASN:H	2.00	0.59
1:B:285:PHE:HE2	1:B:287:LEU:HD12	1.67	0.59
1:B:170:ASN:HD21	1:B:319:SER:H	1.50	0.59
1:A:257:ASN:ND2	1:A:259:ASN:H	1.99	0.59
1:B:134:LYS:CD	1:B:135:GLU:N	2.66	0.59
1:A:269:SER:OG	1:A:284:THR:OG1	2.20	0.58
1:A:302:GLU:O	1:A:313:ILE:CD1	2.50	0.58
1:B:202:ILE:HD11	1:B:204:LEU:HD13	1.84	0.58
1:B:302:GLU:O	1:B:313:ILE:CD1	2.49	0.58
1:A:77:ARG:HA	1:A:96:THR:HB	1.86	0.57
1:B:116:ALA:HB1	4:B:403:DAO:C1	2.36	0.56
1:A:320:ASN:H	1:A:320:ASN:HD22	1.53	0.55
1:B:275:LEU:HD23	1:B:277:TYR:H	1.72	0.54
1:B:77:ARG:HA	1:B:96:THR:HB	1.88	0.54
1:A:57:SER:H	1:A:68:GLN:HE22	1.55	0.54
1:A:123:ARG:NH1	1:A:169:HIS:HD2	2.06	0.53
1:A:349:HIS:NE2	4:A:403:DAO:O2	2.42	0.53
1:B:123:ARG:NH1	1:B:169:HIS:HD2	2.04	0.53
1:A:179:GLY:H	1:A:184:VAL:HG13	1.74	0.53
1:B:197:ASN:ND2	1:B:199:TYR:H	2.06	0.52
1:A:341:LYS:NZ	1:A:377:ASP:OD2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:HB2	1:A:68:GLN:HE22	1.74	0.52
1:A:288:MET:HE2	1:A:308:GLY:CA	2.39	0.51
1:A:14:VAL:CG2	1:A:122:ILE:HD11	2.40	0.51
1:B:34:GLY:HA3	1:B:38:PHE:O	2.10	0.51
1:A:173:GLN:NE2	1:A:173:GLN:H	2.01	0.51
1:A:34:GLY:HA3	1:A:38:PHE:O	2.11	0.51
4:B:404:DAO:H112	4:B:404:DAO:H52	1.92	0.51
1:B:327:THR:HG22	1:B:330:GLU:CD	2.32	0.50
1:B:341:LYS:NZ	1:B:377:ASP:OD2	2.45	0.50
1:A:217:GLU:OE1	1:A:225:ARG:NH1	2.46	0.49
1:B:134:LYS:HD3	1:B:135:GLU:N	2.26	0.49
1:B:217:GLU:OE1	1:B:225:ARG:NH1	2.45	0.49
1:B:14:VAL:CG2	1:B:122:ILE:HD11	2.42	0.49
1:B:179:GLY:H	1:B:184:VAL:HG13	1.77	0.49
1:A:361:LYS:HE2	1:A:362:ARG:HH22	1.78	0.48
1:B:320:ASN:H	1:B:320:ASN:HD22	1.63	0.47
1:A:202:ILE:CD1	1:A:204:LEU:HD12	2.41	0.47
1:B:15:HIS:HD2	1:B:16:GLY:O	1.97	0.47
1:B:173:GLN:NE2	1:B:173:GLN:H	2.01	0.47
1:A:214:LEU:HB3	1:A:215:PRO:HD3	1.96	0.47
1:A:320:ASN:HD22	1:A:320:ASN:N	2.12	0.47
1:B:11:VAL:HB	1:B:51:VAL:HG12	1.98	0.46
1:A:127:GLU:HG3	1:A:254:THR:HA	1.97	0.46
1:A:357:PHE:CE2	1:A:358:LEU:HD13	2.51	0.46
1:B:69:LEU:HD13	1:B:125:MET:SD	2.56	0.46
1:A:357:PHE:CD2	1:A:358:LEU:HD13	2.51	0.46
1:B:122:ILE:CG2	1:B:162:ILE:HG12	2.46	0.45
1:B:357:PHE:CD2	1:B:358:LEU:HD13	2.52	0.45
1:A:57:SER:CB	1:A:68:GLN:HE22	2.30	0.45
1:A:98:LYS:HD2	1:A:98:LYS:HA	1.72	0.45
1:B:134:LYS:CD	1:B:134:LYS:C	2.85	0.45
1:A:126:GLU:OE1	1:A:130:ARG:NH1	2.49	0.45
1:A:122:ILE:CG2	1:A:162:ILE:HG12	2.47	0.45
1:A:141:GLN:HA	1:A:141:GLN:NE2	2.28	0.44
1:A:272:THR:HG22	1:A:273:GLY:O	2.17	0.44
1:A:11:VAL:HB	1:A:51:VAL:HG12	1.98	0.44
1:B:127:GLU:HG3	1:B:254:THR:HA	1.99	0.44
1:A:288:MET:HE2	1:A:288:MET:HB3	1.57	0.44
1:A:288:MET:HE1	1:A:308:GLY:HA3	1.87	0.44
1:A:69:LEU:HD13	1:A:125:MET:SD	2.56	0.44
1:B:220:ILE:HD13	1:B:220:ILE:HG21	1.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASN:ND2	1:A:239:ALA:H	2.16	0.44
1:B:134:LYS:HD3	1:B:135:GLU:HA	2.00	0.44
1:A:15:HIS:HD2	1:A:16:GLY:O	2.01	0.44
1:A:274:PRO:HG2	1:A:275:LEU:HD13	1.99	0.44
1:B:282:LEU:HD22	1:B:282:LEU:HA	1.90	0.44
1:B:108:LYS:HE3	1:B:108:LYS:HB3	1.85	0.43
1:A:268:VAL:HG22	1:A:343:ILE:CG2	2.48	0.43
1:A:14:VAL:HG21	1:A:122:ILE:CD1	2.46	0.43
1:A:303:TRP:HA	1:A:313:ILE:HD11	1.99	0.43
1:B:372:ILE:HD12	1:B:372:ILE:HA	1.90	0.43
1:B:126:GLU:OE1	1:B:130:ARG:NH1	2.51	0.43
1:B:274:PRO:HG2	1:B:275:LEU:HD13	2.01	0.42
1:A:174:ALA:O	1:A:178:PHE:O	2.38	0.41
1:A:237:ASN:HD22	1:A:239:ALA:H	1.68	0.41
1:B:173:GLN:N	1:B:173:GLN:HE21	2.02	0.41
1:A:214:LEU:HB3	1:A:215:PRO:CD	2.50	0.41
1:A:210:GLY:O	1:A:225:ARG:NH2	2.54	0.41
1:A:195:MET:O	1:A:200:SER:OG	2.33	0.41
1:B:377:ASP:O	1:B:380:SER:HB2	2.21	0.41
1:B:197:ASN:ND2	1:B:197:ASN:C	2.75	0.40
1:B:237:ASN:HD22	1:B:239:ALA:H	1.70	0.40
1:B:134:LYS:HD2	1:B:135:GLU:N	2.35	0.40
1:B:134:LYS:HD3	1:B:134:LYS:C	2.41	0.40
1:B:237:ASN:ND2	1:B:239:ALA:H	2.19	0.40
1:A:333:THR:CG2	1:A:380:SER:HB3	2.51	0.40
1:A:257:ASN:HD22	1:A:259:ASN:N	2.08	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)
1:A:289:ASP:OD2	1:B:360:PHE:CZ[6_555]	2.05	0.15

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%)	366 (96%)	13 (3%)	1 (0%)	41	64
1	B	380/408 (93%)	365 (96%)	14 (4%)	1 (0%)	41	64
All	All	760/816 (93%)	731 (96%)	27 (4%)	2 (0%)	41	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	PHE
1	B	275	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/340 (94%)	265 (83%)	53 (17%)	2	3
1	B	318/340 (94%)	263 (83%)	55 (17%)	2	3
All	All	636/680 (94%)	528 (83%)	108 (17%)	2	3

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	28	LEU
1	A	44	LEU
1	A	69	LEU
1	A	77	ARG
1	A	96	THR
1	A	98	LYS
1	A	103	ASN
1	A	106	PRO
1	A	110	VAL
1	A	113	VAL

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Mol	Chain	Res	Type
1	A	124	LEU
1	A	134	LYS
1	A	135	GLU
1	A	141	GLN
1	A	152	THR
1	A	159	VAL
1	A	163	THR
1	A	173	GLN
1	A	182	GLU
1	A	184	VAL
1	A	191	LEU
1	A	197	ASN
1	A	201	ASN
1	A	202	ILE
1	A	212	LYS
1	A	220	ILE
1	A	224	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	289	ASP
1	A	301	GLU
1	A	302	GLU
1	A	309	VAL
1	A	310	VAL
1	A	313	ILE
1	A	316	LEU
1	A	320	ASN
1	A	330	GLU
1	A	335	ARG
1	A	340	VAL
1	A	350	VAL
1	A	358	LEU
1	A	361	LYS
1	A	363	LYS
1	A	372	ILE
1	A	378	LEU
1	A	379	LEU
1	A	384	THR

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Mol	Chain	Res	Type
1	B	4	GLN
1	B	18	LEU
1	B	39	LYS
1	B	44	LEU
1	B	46	LYS
1	B	69	LEU
1	B	77	ARG
1	B	96	THR
1	B	98	LYS
1	B	110	VAL
1	B	113	VAL
1	B	124	LEU
1	B	135	GLU
1	B	146	GLU
1	B	152	THR
1	B	159	VAL
1	B	163	THR
1	B	173	GLN
1	B	176	ASP
1	B	182	GLU
1	B	184	VAL
1	B	191	LEU
1	B	197	ASN
1	B	201	ASN
1	B	202	ILE
1	B	212	LYS
1	B	215	PRO
1	B	224	LYS
1	B	226	VAL
1	B	228	LYS
1	B	244	LEU
1	B	257	ASN
1	B	263	THR
1	B	275	LEU
1	B	282	LEU
1	B	289	ASP
1	B	302	GLU
1	B	309	VAL
1	B	310	VAL
1	B	313	ILE
1	B	316	LEU
1	B	320	ASN

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Mol	Chain	Res	Type
1	B	329	ASN
1	B	330	GLU
1	B	335	ARG
1	B	340	VAL
1	B	341	LYS
1	B	350	VAL
1	B	358	LEU
1	B	360	PHE
1	B	361	LYS
1	B	363	LYS
1	B	378	LEU
1	B	379	LEU
1	B	385	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	50	ASN
1	A	52	HIS
1	A	68	GLN
1	A	133	ASN
1	A	141	GLN
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	297	HIS
1	A	320	ASN
1	A	328	ASN
1	A	369	ASN
1	B	15	HIS
1	B	50	ASN
1	B	52	HIS
1	B	133	ASN
1	B	169	HIS
1	B	170	ASN
1	B	173	GLN
1	B	197	ASN

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Mol	Chain	Res	Type
1	B	213	GLN
1	B	237	ASN
1	B	257	ASN
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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
5	BUA	B	405	-	2,5,5	0.39	0	2,5,5	0.69	0
4	DAO	B	403	-	10,13,13	0.45	0	9,13,13	0.47	0
4	DAO	A	403	-	10,13,13	0.64	0	9,13,13	0.51	0
5	BUA	A	404	-	2,5,5	0.56	0	2,5,5	0.31	0
4	DAO	B	404	-	10,13,13	0.33	0	9,13,13	0.66	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
5	BUA	B	405	-	-	1/1/3/3	-
4	DAO	B	403	-	-	4/9/11/11	-
4	DAO	A	403	-	-	5/9/11/11	-
5	BUA	A	404	-	-	1/1/3/3	-
4	DAO	B	404	-	-	7/9/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

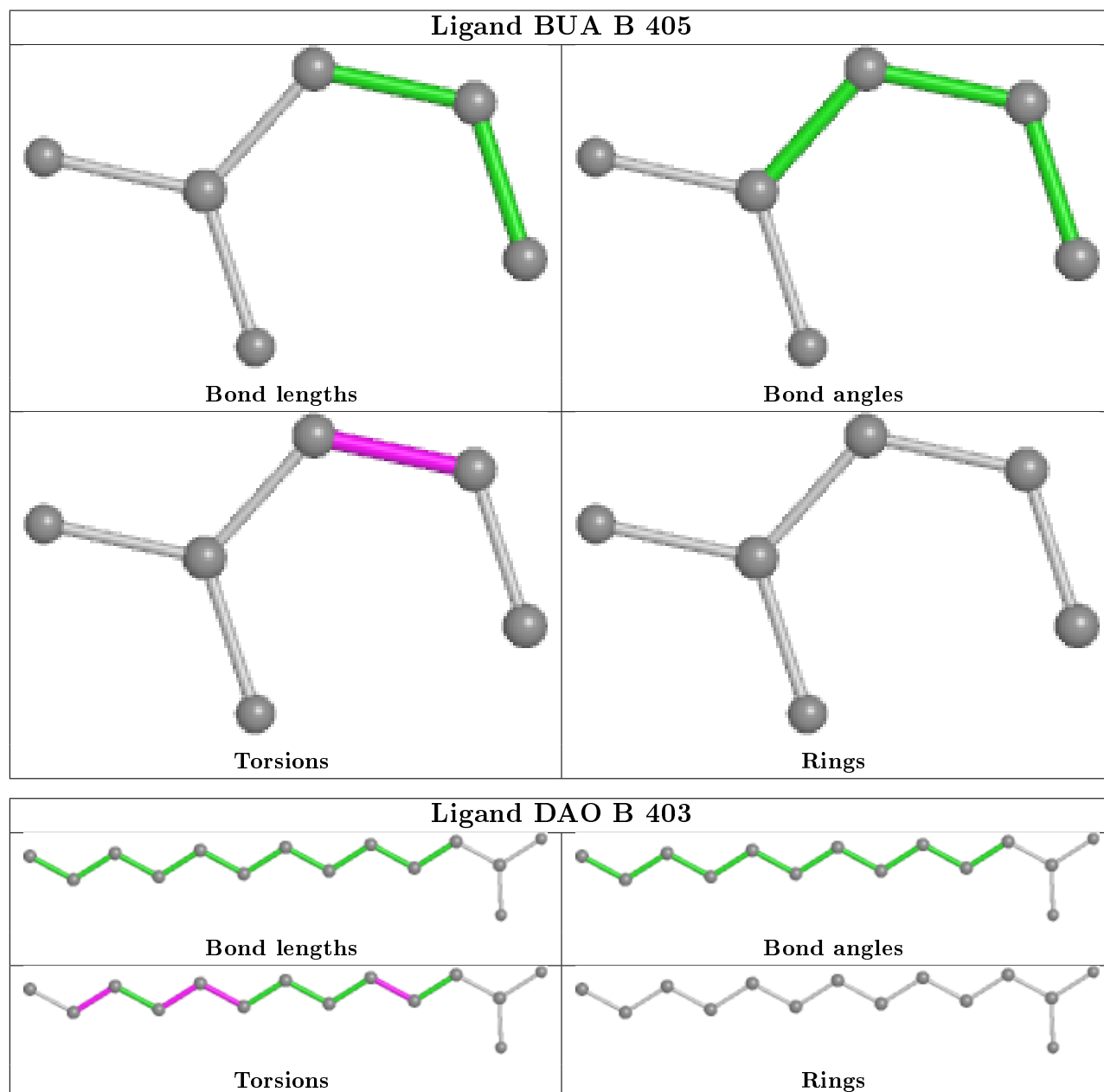
Mol	Chain	Res	Type	Atoms
4	A	403	DAO	C1-C2-C3-C4
5	B	405	BUA	C1-C2-C3-C4
4	B	404	DAO	C1-C2-C3-C4
5	A	404	BUA	C1-C2-C3-C4
4	B	403	DAO	C7-C8-C9-C10
4	B	403	DAO	C2-C3-C4-C5
4	B	403	DAO	C6-C7-C8-C9
4	A	403	DAO	C3-C4-C5-C6
4	A	403	DAO	C4-C5-C6-C7
4	B	404	DAO	C7-C8-C9-C10
4	A	403	DAO	C6-C7-C8-C9
4	B	404	DAO	C3-C4-C5-C6
4	B	404	DAO	C9-C10-C11-C12
4	B	404	DAO	C5-C6-C7-C8
4	B	404	DAO	C11-C10-C9-C8
4	B	404	DAO	C2-C3-C4-C5
4	A	403	DAO	C7-C8-C9-C10
4	B	403	DAO	C9-C10-C11-C12

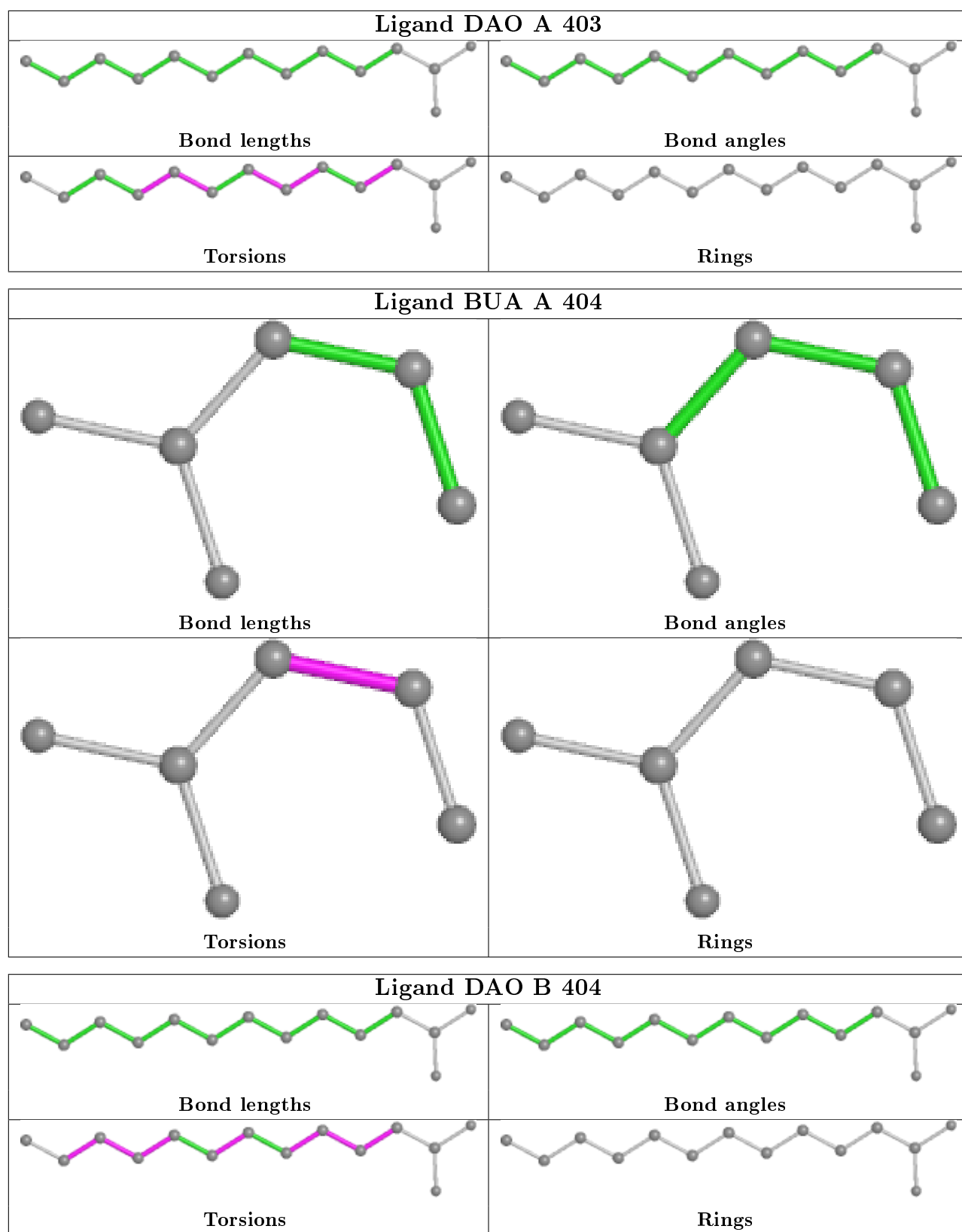
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	DAO	1	0
4	A	403	DAO	1	0
4	B	404	DAO	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 ⓘ

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%)	0.45	12 (3%) 49 42	44, 62, 85, 114	0
1	B	382/408 (93%)	0.62	27 (7%) 16 11	46, 63, 88, 122	0
All	All	764/816 (93%)	0.53	39 (5%) 28 22	44, 62, 86, 122	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	PRO	5.7
1	B	93	TYR	4.7
1	B	277	TYR	4.6
1	B	78	VAL	4.0
1	A	38	PHE	3.9
1	A	6	LEU	3.8
1	B	139	TYR	3.7
1	B	275	LEU	3.5
1	B	27	ALA	3.1
1	B	146	GLU	3.1
1	B	276	GLY	3.0
1	B	92	ARG	2.8
1	A	73	ILE	2.8
1	A	78	VAL	2.7
1	B	70	TYR	2.6
1	B	80	TYR	2.6
1	A	41	ILE	2.6
1	B	74	LYS	2.5
1	B	71	TYR	2.5
1	A	100	ILE	2.5
1	A	363	LYS	2.5
1	B	289	ASP	2.5
1	B	28	LEU	2.4
1	B	77	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	44	LEU	2.4
1	B	49	TYR	2.4
1	B	141	GLN	2.3
1	B	94	GLY	2.3
1	B	151	PHE	2.2
1	A	214	LEU	2.2
1	B	91	GLU	2.2
1	A	46	LYS	2.2
1	A	361	LYS	2.2
1	B	272	THR	2.1
1	B	83	ALA	2.1
1	B	128	PHE	2.1
1	A	97	TYR	2.1
1	B	273	GLY	2.1
1	A	347	TRP	2.1

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.

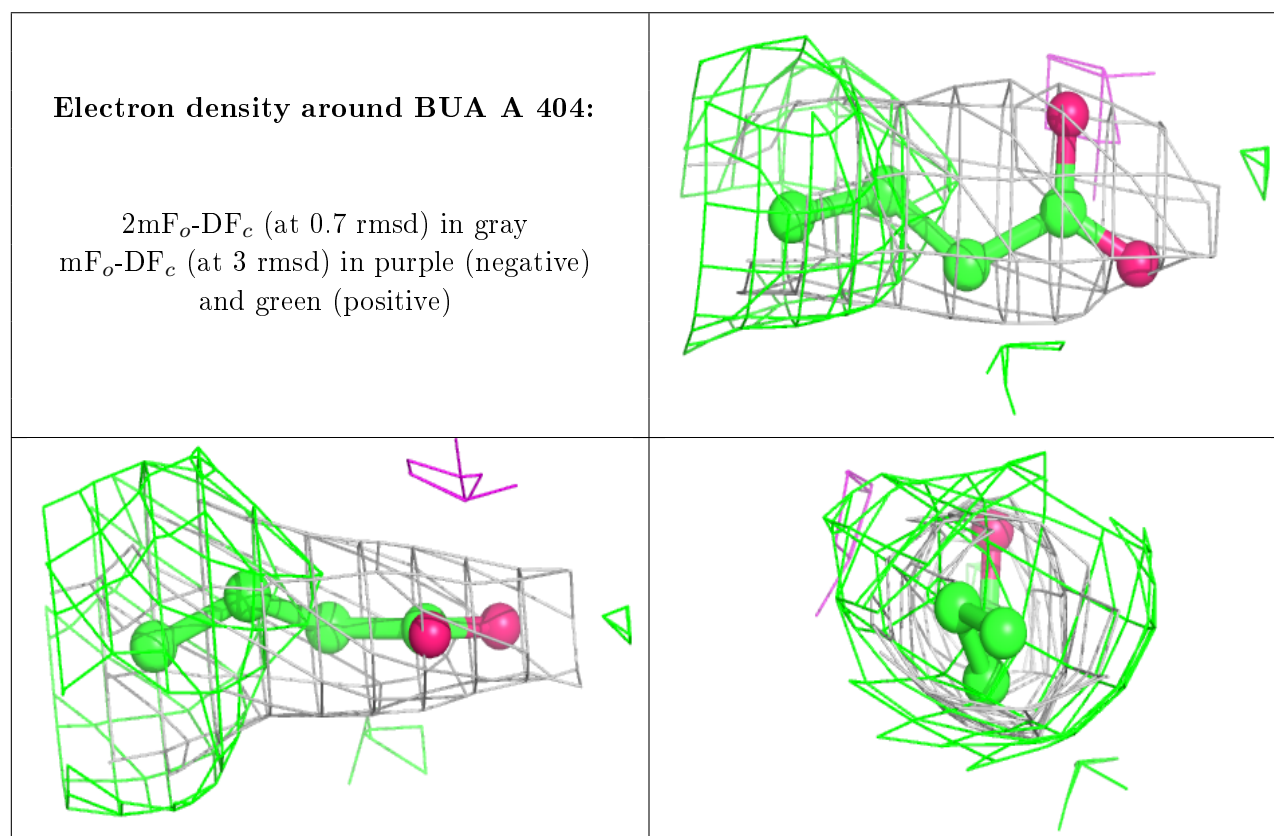
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BUA	A	404	6/6	0.61	0.49	95,113,121,124	0
3	CA	A	402	1/1	0.75	0.14	77,77,77,77	0
4	DAO	B	404	14/14	0.79	0.48	95,121,135,142	0
5	BUA	B	405	6/6	0.85	0.45	103,110,111,124	0
4	DAO	B	403	14/14	0.85	0.43	77,90,97,99	0
4	DAO	A	403	14/14	0.89	0.41	79,89,95,109	0
2	ZN	A	401	1/1	0.89	0.26	69,69,69,69	0
3	CA	B	402	1/1	0.93	0.17	79,79,79,79	0

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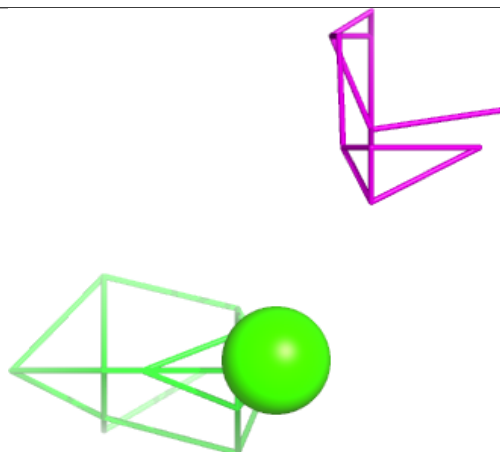
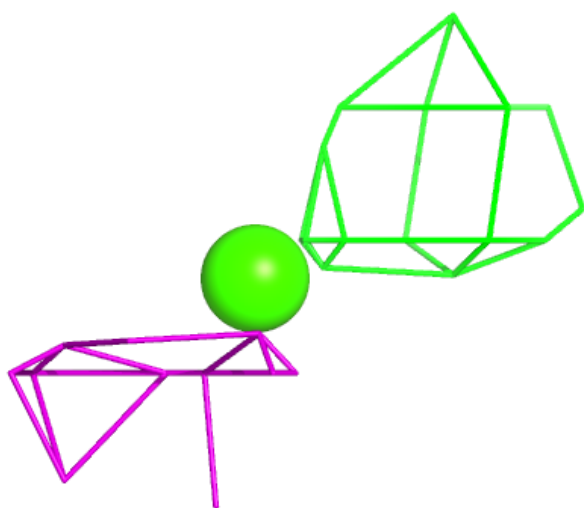
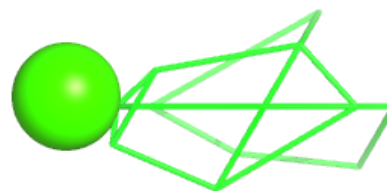
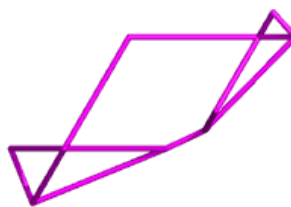
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	401	1/1	0.98	0.19	75,75,75,75	0

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.



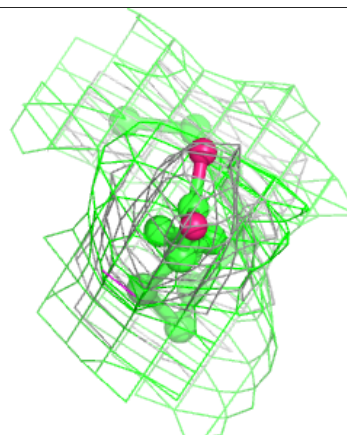
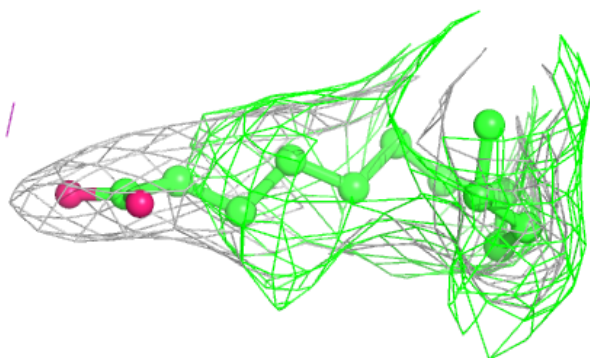
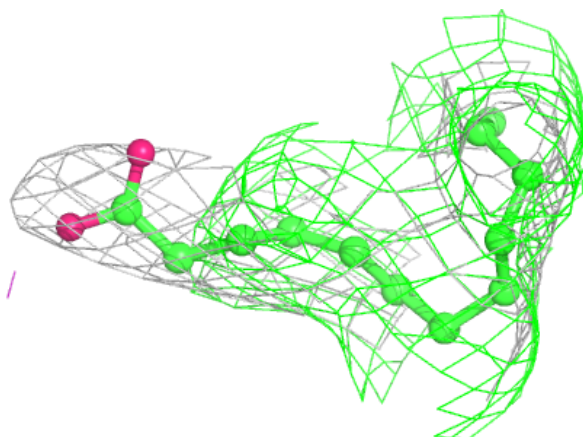
Electron density around CA A 402:

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

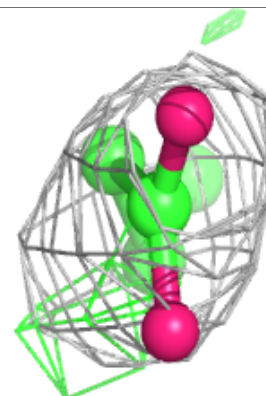
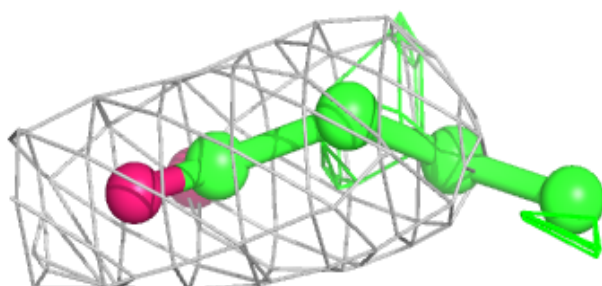
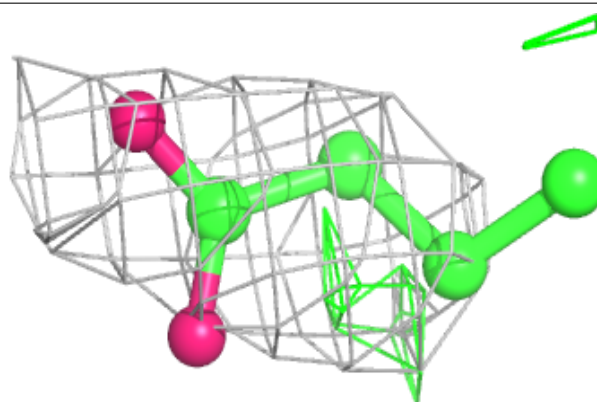


Electron density around DAO B 404:

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

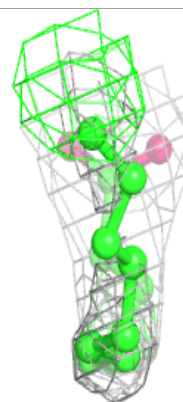
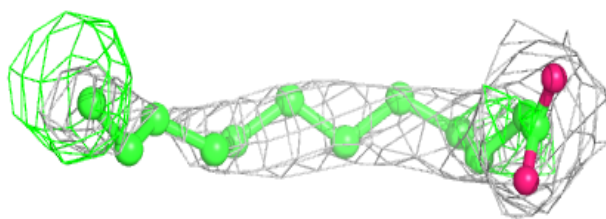
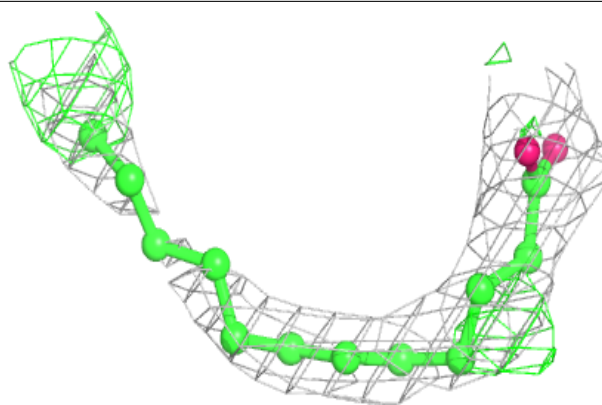
**Electron density around BUA B 405:**

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

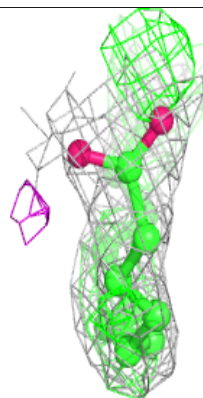
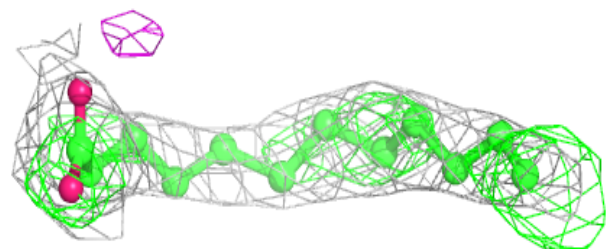
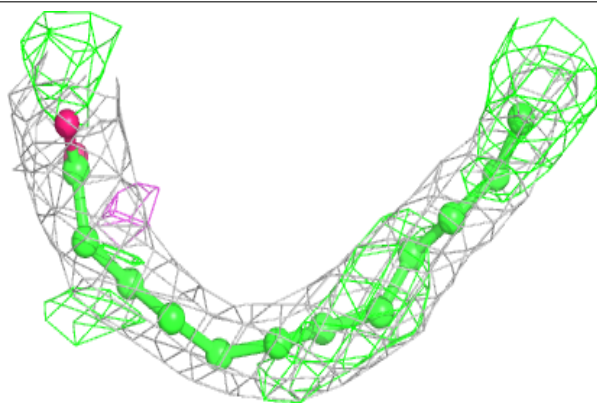


Electron density around DAO B 403:

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

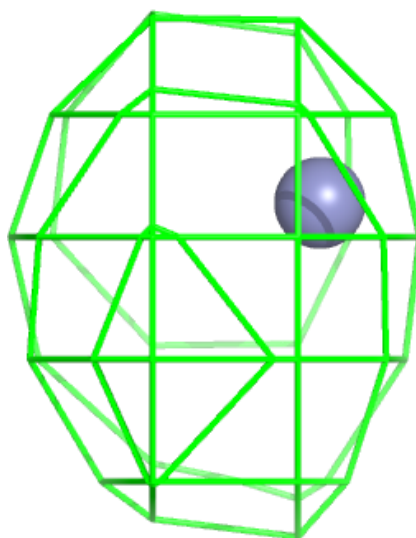
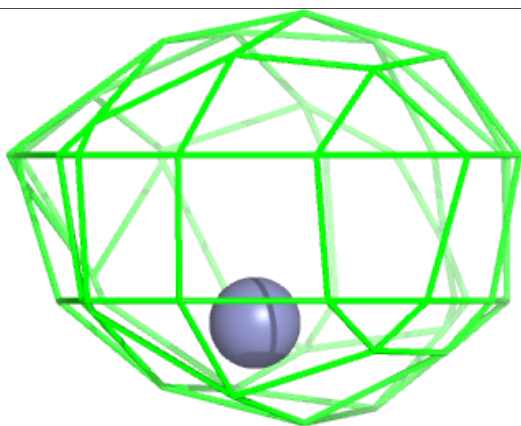
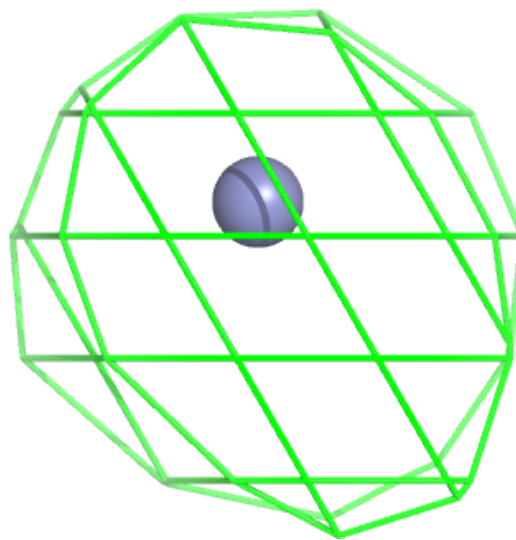
**Electron density around DAO A 403:**

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



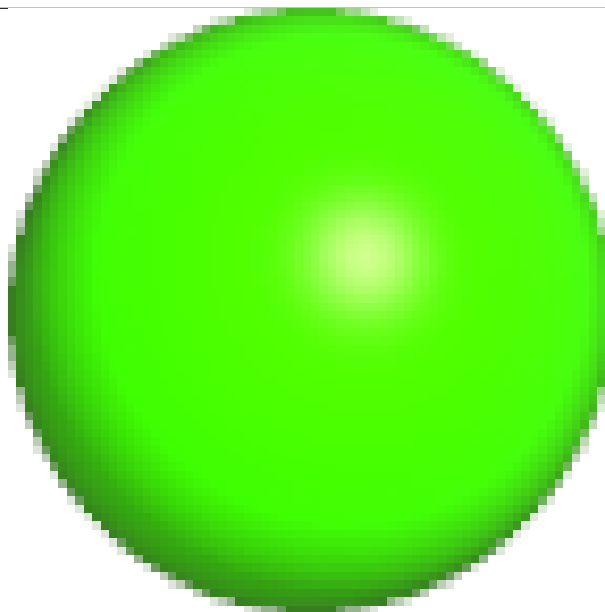
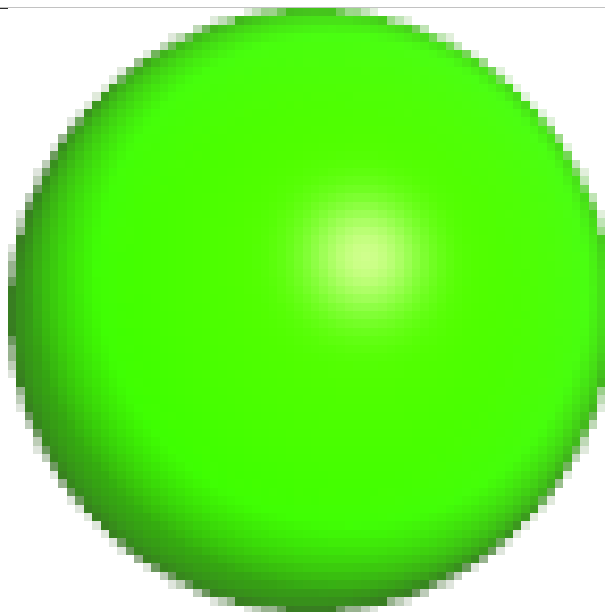
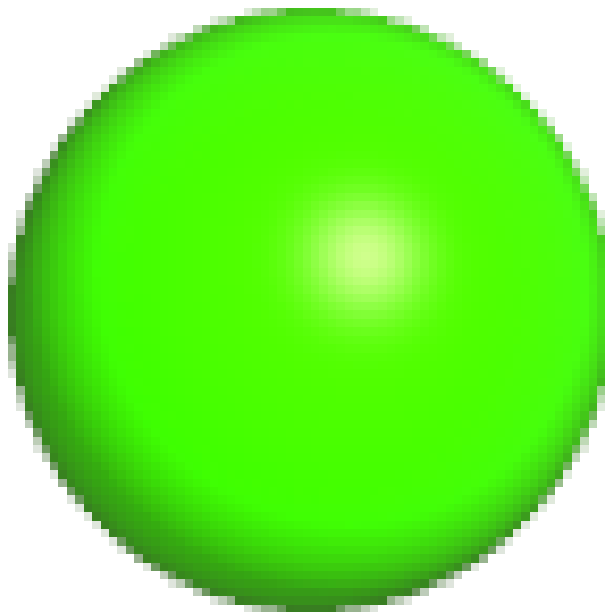
Electron density around ZN A 401:

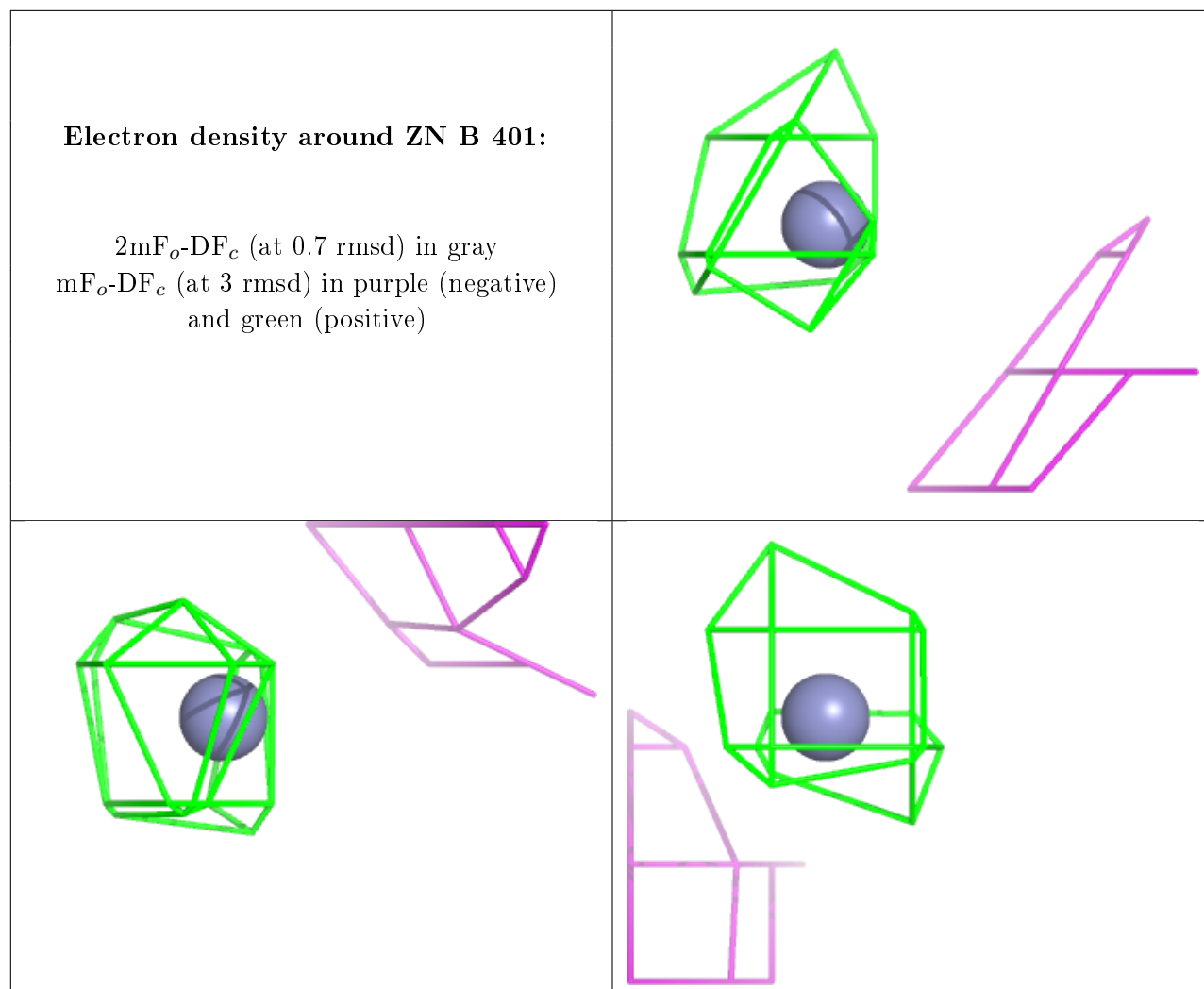
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

There are no such residues in this entry.