



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:31 AM UTC

PDB ID : 6KSM / pdb_00006ksm
Title : Staphylococcus aureus lipase -Orlistat complex
Authors : Kitadokoro, K.; Tanaka, M.; Kamitani, S.
Deposited on : 2019-08-24
Resolution : 2.23 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

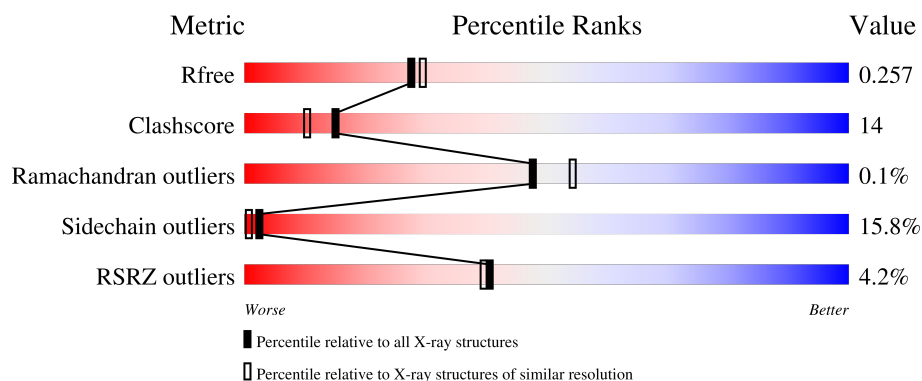
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	2% 61% 24% 8% 6%
1	B	408	5% 61% 25% 7% 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
5	DAO	A	405	-	-	-	X
5	DAO	B	405	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6264 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
			3020	1924	527	560	9			
1	B	382	Total	C	N	O	S	0	0	0
			3020	1924	527	560	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

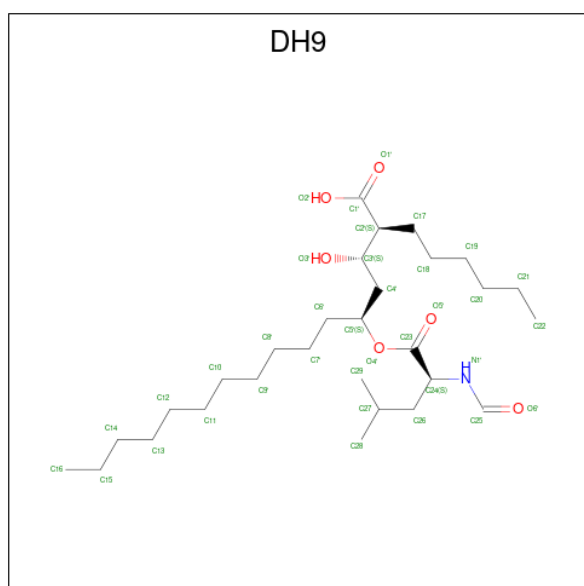
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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).

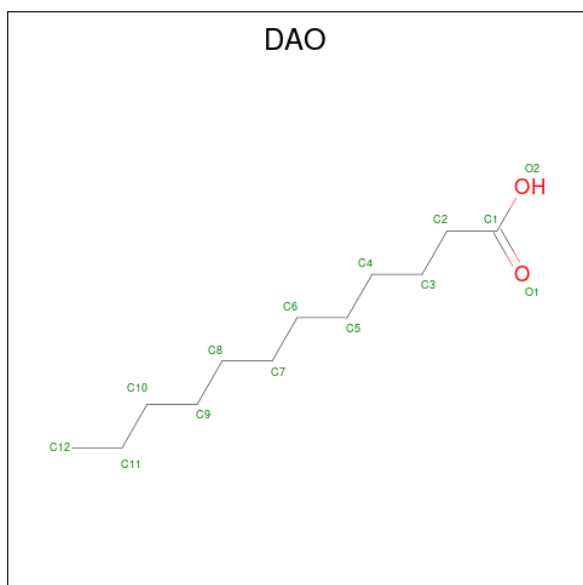
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is (2S,3S,5S)-5-[(N-FORMYL-L-LEUCYL)OXY]-2-HEXYL-3-HYDROXY HEXADECANOIC ACID (CCD ID: DH9) (formula: C₂₉H₅₅NO₆) (labeled as "Ligand of Interest" by depositor).



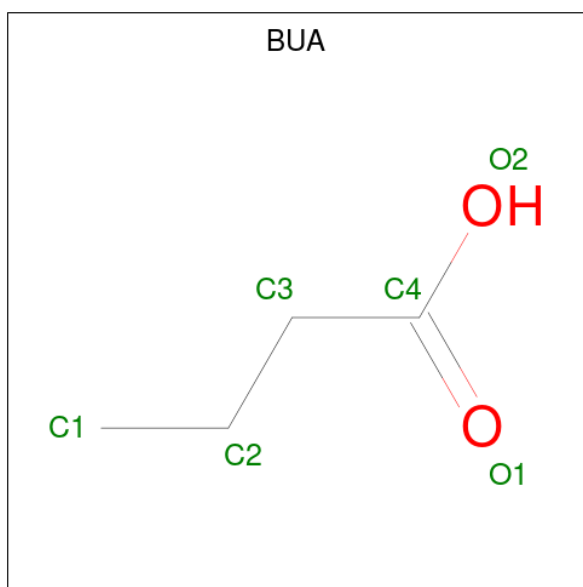
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			36	29	1	6		
4	B	1	Total	C	N	O	0	0
			36	29	1	6		

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



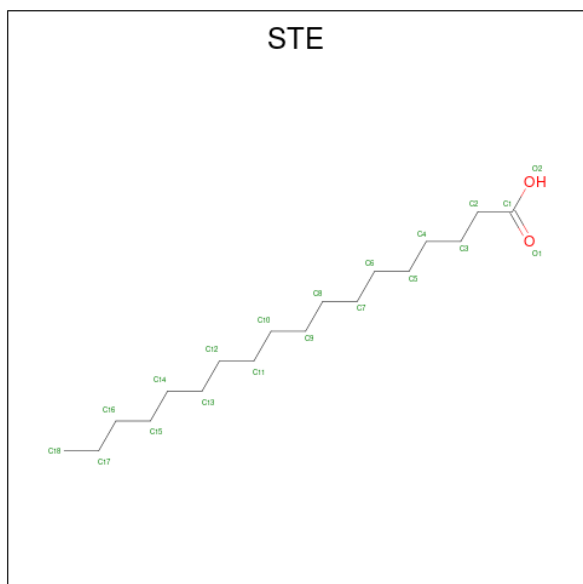
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	12	2		
5	A	1	Total	C	O	0	0
			14	12	2		
5	B	1	Total	C	O	0	0
			14	12	2		
5	B	1	Total	C	O	0	0
			14	12	2		

- Molecule 6 is butanoic acid (CCD ID: BUA) (formula: $C_4H_8O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			20	18	2		

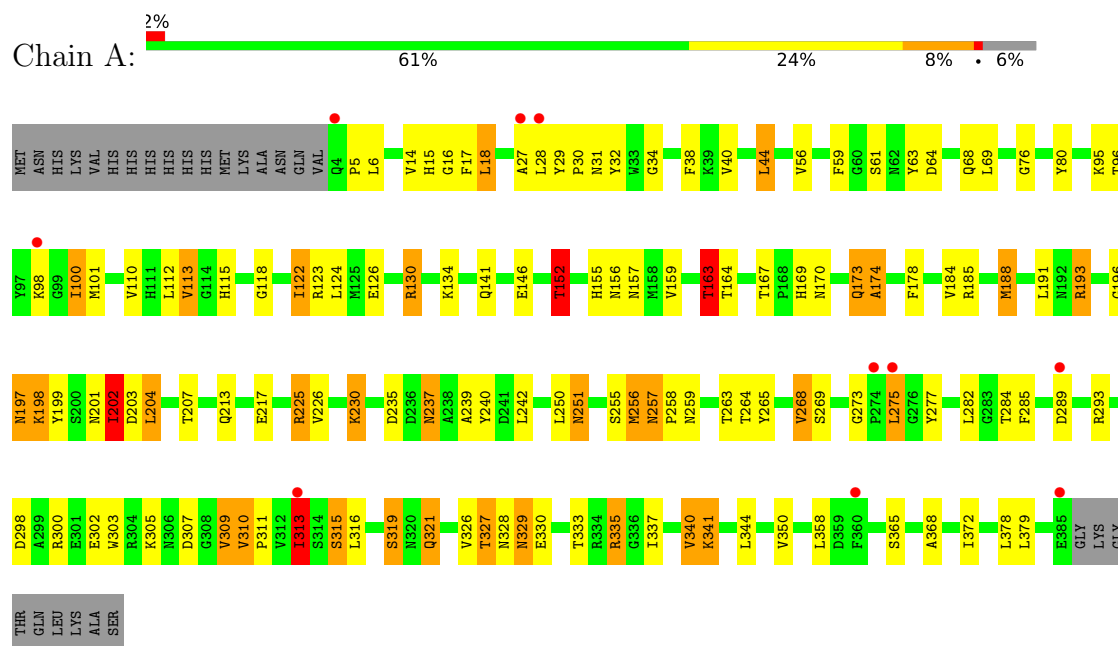
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	34	Total 34	O 34	0	0
8	B	26	Total 26	O 26	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lipase 2



E385
GLY
LYS
GLY
THR
GLN
LEU
LYS
ALA
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	132.51Å 132.51Å 248.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.18 – 2.23 48.18 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.18-2.23) 99.7 (48.18-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.226 , 0.259 0.223 , 0.257	Depositor DCC
R_{free} test set	5386 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.1	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	6264	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 2.68% 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: CA, DAO, DH9, BUA, ZN, STE

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	1.59	24/3102 (0.8%)	1.59	43/4207 (1.0%)
1	B	1.47	19/3102 (0.6%)	1.52	42/4207 (1.0%)
All	All	1.53	43/6204 (0.7%)	1.55	85/8414 (1.0%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	ILE	CB-CG1	7.05	1.67	1.53
1	A	300	ARG	CD-NE	7.00	1.56	1.46
1	A	27	ALA	CA-C	6.85	1.62	1.52
1	A	207	THR	N-CA	6.53	1.54	1.46
1	A	298	ASP	CA-C	6.51	1.61	1.52
1	A	240	TYR	C-O	6.34	1.31	1.24
1	A	196	GLY	CA-C	6.23	1.60	1.51
1	B	328	ASN	CG-ND2	6.13	1.46	1.33
1	A	5	PRO	N-CA	6.04	1.54	1.47
1	A	203	ASP	CA-C	6.00	1.60	1.52
1	B	345	GLN	CD-OE1	5.95	1.34	1.23
1	B	225	ARG	CD-NE	-5.94	1.38	1.46
1	B	96	THR	CA-C	5.90	1.59	1.52
1	A	250	LEU	CA-C	5.88	1.60	1.52
1	B	236	ASP	CG-OD2	5.87	1.36	1.25
1	A	313	ILE	CG1-CD1	5.85	1.74	1.51
1	A	269	SER	C-O	5.82	1.29	1.24
1	B	214	LEU	N-CA	5.78	1.53	1.45
1	A	300	ARG	CZ-NH1	5.74	1.40	1.32
1	B	111	HIS	N-CA	5.73	1.53	1.46
1	B	300	ARG	CD-NE	5.66	1.54	1.46
1	B	143	HIS	CG-CD2	5.60	1.42	1.35
1	A	174	ALA	CA-C	5.57	1.60	1.52
1	A	237	ASN	N-CA	5.56	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	ARG	CZ-NH2	-5.47	1.26	1.33
1	B	313	ILE	CG1-CD1	5.44	1.73	1.51
1	A	230	LYS	N-CA	5.43	1.53	1.46
1	A	31	ASN	CA-CB	-5.40	1.46	1.53
1	B	226	VAL	N-CA	5.34	1.52	1.46
1	A	76	GLY	C-O	5.33	1.28	1.23
1	A	185	ARG	CZ-NH1	5.32	1.40	1.32
1	B	91	GLU	C-O	5.30	1.30	1.23
1	B	168	PRO	CA-C	5.27	1.57	1.52
1	B	186	LYS	C-O	5.27	1.30	1.24
1	B	96	THR	CB-CG2	5.26	1.70	1.52
1	A	315	SER	CA-C	5.22	1.59	1.52
1	B	143	HIS	CE1-NE2	5.20	1.37	1.32
1	B	13	PHE	C-O	5.17	1.30	1.24
1	A	337	ILE	CA-CB	5.16	1.61	1.54
1	A	64	ASP	CG-OD1	5.08	1.34	1.25
1	B	184	VAL	CA-CB	5.07	1.61	1.54
1	A	251	ASN	N-CA	5.05	1.52	1.46
1	A	268	VAL	C-O	5.01	1.28	1.24

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ARG	NE-CZ-NH2	-12.39	108.05	119.20
1	A	225	ARG	NE-CZ-NH2	-9.73	110.44	119.20
1	A	273	GLY	CA-C-N	-9.34	110.15	119.87
1	A	273	GLY	C-N-CA	-9.34	110.15	119.87
1	A	313	ILE	CB-CG1-CD1	9.18	133.08	113.80
1	B	225	ARG	NE-CZ-NH1	8.77	130.27	121.50
1	A	225	ARG	CD-NE-CZ	8.29	136.01	124.40
1	A	268	VAL	CB-CA-C	-8.26	97.47	110.69
1	A	188	MET	CG-SD-CE	-8.25	82.74	100.90
1	B	282	LEU	CA-C-N	-8.18	110.92	122.86
1	B	282	LEU	C-N-CA	-8.18	110.92	122.86
1	B	100	ILE	CB-CA-C	8.09	120.85	111.55
1	A	130	ARG	NE-CZ-NH2	-8.06	111.95	119.20
1	A	310	VAL	N-CA-C	7.88	116.99	107.61
1	B	225	ARG	CG-CD-NE	-7.79	94.85	112.00
1	B	257	ASN	CA-C-N	-7.63	111.98	120.45
1	B	257	ASN	C-N-CA	-7.63	111.98	120.45
1	A	289	ASP	N-CA-CB	7.37	120.91	109.94
1	B	350	VAL	N-CA-CB	-7.32	100.95	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	THR	N-CA-CB	-7.30	99.81	110.47
1	B	313	ILE	CB-CG1-CD1	7.14	128.80	113.80
1	A	335	ARG	NE-CZ-NH2	7.07	125.56	119.20
1	A	130	ARG	CG-CD-NE	-6.98	96.65	112.00
1	A	225	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	A	122	ILE	CB-CA-C	-6.79	103.15	112.04
1	A	225	ARG	CG-CD-NE	-6.55	97.58	112.00
1	B	205	GLY	N-CA-C	6.54	125.15	115.08
1	B	341	LYS	CA-C-N	-6.52	113.26	119.85
1	B	341	LYS	C-N-CA	-6.52	113.26	119.85
1	A	328	ASN	N-CA-C	6.46	120.42	112.54
1	B	193	ARG	N-CA-C	-6.42	104.20	111.07
1	B	226	VAL	CG1-CB-CG2	6.32	124.70	110.80
1	B	326	VAL	N-CA-CB	-6.26	101.96	112.47
1	B	313	ILE	CG1-CB-CG2	6.20	129.31	110.70
1	A	130	ARG	CD-NE-CZ	6.15	133.01	124.40
1	A	235	ASP	CA-C-O	-6.12	111.90	119.18
1	A	335	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	B	95	LYS	CA-C-N	-6.09	114.40	122.99
1	B	95	LYS	C-N-CA	-6.09	114.40	122.99
1	B	333	THR	OG1-CB-CG2	6.07	121.44	109.30
1	A	202	ILE	CB-CG1-CD1	-6.05	101.09	113.80
1	A	64	ASP	N-CA-C	-5.93	104.81	111.28
1	B	289	ASP	N-CA-CB	5.91	118.74	109.94
1	B	67	VAL	N-CA-C	-5.88	105.00	110.53
1	B	335	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	B	236	ASP	CB-CG-OD1	-5.84	104.97	118.40
1	B	220	ILE	N-CA-C	5.83	116.48	110.36
1	A	313	ILE	CG1-CB-CG2	5.77	128.00	110.70
1	B	310	VAL	CB-CA-C	5.77	115.72	110.13
1	B	381	VAL	N-CA-C	-5.77	104.89	110.42
1	A	201	ASN	CA-CB-CG	-5.75	106.85	112.60
1	A	193	ARG	N-CA-C	-5.74	104.94	111.14
1	B	293	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	A	163	THR	CB-CA-C	5.73	120.20	109.71
1	B	301	GLU	N-CA-C	5.62	118.13	111.33
1	B	315	SER	N-CA-C	5.60	118.32	111.82
1	A	61	SER	N-CA-C	5.59	117.51	110.24
1	A	100	ILE	CA-CB-CG2	5.57	119.98	110.50
1	B	163	THR	CB-CA-C	5.53	119.71	109.70
1	A	256	MET	CG-SD-CE	-5.52	88.75	100.90
1	B	127	GLU	CB-CA-C	-5.50	101.33	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	LYS	CD-CE-NZ	-5.48	94.36	111.90
1	A	130	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	B	225	ARG	CD-NE-CZ	5.47	132.06	124.40
1	B	313	ILE	CB-CA-C	-5.47	103.67	112.16
1	A	340	VAL	N-CA-C	5.44	116.55	108.23
1	B	305	LYS	CD-CE-NZ	5.39	129.16	111.90
1	A	321	GLN	CB-CA-C	5.38	116.13	108.76
1	B	130	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	A	113	VAL	CB-CA-C	5.26	118.25	110.77
1	B	96	THR	CB-CA-C	5.26	119.33	109.71
1	A	319	SER	N-CA-C	5.25	117.84	110.23
1	B	284	THR	N-CA-C	-5.22	102.18	109.96
1	A	293	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	95	LYS	CA-C-N	-5.20	114.31	122.73
1	A	95	LYS	C-N-CA	-5.20	114.31	122.73
1	A	305	LYS	CB-CG-CD	5.19	123.24	111.30
1	A	310	VAL	CB-CA-C	5.18	115.16	110.13
1	A	101	MET	CB-CA-C	-5.17	102.61	111.15
1	B	273	GLY	CA-C-N	-5.14	114.37	119.56
1	B	273	GLY	C-N-CA	-5.14	114.37	119.56
1	B	330	GLU	N-CA-CB	5.10	119.02	109.68
1	B	310	VAL	N-CA-C	5.08	113.66	107.61
1	A	340	VAL	CA-CB-CG2	5.01	118.92	110.40
1	A	242	LEU	N-CA-C	-5.01	107.17	113.28

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	3020	0	2914	81	0
1	B	3020	0	2914	81	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	36	0	54	5	0
4	B	36	0	54	8	0
5	A	28	0	46	2	0
5	B	28	0	46	2	0
6	A	6	0	7	1	0
6	B	6	0	7	0	0
7	B	20	0	35	1	0
8	A	34	0	0	2	0
8	B	26	0	0	0	0
All	All	6264	0	6077	168	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (168) 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	1.74	1.60
1:B:116:SER:CB	4:B:403:DH9:O2'	1.79	1.30
1:B:195:MET:HE2	1:B:202:ILE:HD11	1.35	1.05
1:A:174:ALA:O	1:A:178:PHE:O	1.78	1.00
1:B:313:ILE:HD13	1:B:313:ILE:H	1.26	0.97
1:B:327:THR:HG22	1:B:329:ASN:H	1.29	0.97
1:B:313:ILE:H	1:B:313:ILE:CD1	1.81	0.90
1:B:173:GLN:HE21	1:B:173:GLN:H	1.15	0.89
1:A:313:ILE:CD1	1:A:313:ILE:H	1.87	0.88
1:B:115:HIS:HE1	4:B:403:DH9:H291	1.35	0.88
1:B:195:MET:HE2	1:B:202:ILE:CD1	2.03	0.88
1:A:313:ILE:H	1:A:313:ILE:HD13	1.38	0.87
1:A:173:GLN:HE21	1:A:173:GLN:H	1.19	0.85
1:B:115:HIS:CE1	4:B:403:DH9:H291	2.13	0.83
1:B:327:THR:CG2	1:B:329:ASN:H	1.91	0.83
1:A:257:ASN:ND2	1:A:259:ASN:H	1.77	0.82
1:B:116:SER:CB	4:B:403:DH9:C1'	2.58	0.82
1:A:15:HIS:HE1	1:A:56:VAL:H	1.28	0.81
1:B:170:ASN:HD21	1:B:319:SER:H	1.25	0.80
1:A:257:ASN:HD22	1:A:259:ASN:H	1.29	0.78
1:A:197:ASN:HD22	1:A:199:TYR:H	1.31	0.77
1:A:193:ARG:HH11	5:A:404:DAO:H21	1.49	0.77
1:A:115:HIS:HE1	4:A:403:DH9:H291	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASN:C	1:B:257:ASN:HD22	1.94	0.75
1:B:197:ASN:HD22	1:B:199:TYR:H	1.34	0.75
1:B:327:THR:HG22	1:B:329:ASN:N	2.03	0.74
1:A:198:LYS:H	1:A:213:GLN:NE2	1.85	0.74
1:A:327:THR:HG23	1:A:329:ASN:H	1.53	0.73
1:A:118:GLY:O	1:A:122:ILE:HG12	1.89	0.72
1:B:159:VAL:HG22	1:B:260:ILE:HD13	1.72	0.71
1:A:123:ARG:HH11	1:A:169:HIS:HD2	1.39	0.70
1:A:197:ASN:ND2	1:A:199:TYR:H	1.89	0.70
1:B:257:ASN:HD22	1:B:258:PRO:N	1.90	0.69
1:B:257:ASN:ND2	1:B:259:ASN:H	1.91	0.69
1:B:126:GLU:OE2	1:B:130:ARG:HD3	1.93	0.69
1:A:17:PHE:O	4:A:403:DH9:H262	1.93	0.68
4:B:403:DH9:H27	4:B:403:DH9:O3'	1.94	0.67
1:A:123:ARG:NH1	1:A:169:HIS:HD2	1.93	0.67
1:B:236:ASP:OD2	2:B:401:ZN:ZN	1.44	0.67
1:A:257:ASN:HD22	1:A:257:ASN:C	2.02	0.66
1:B:179:GLY:O	1:B:239:ALA:HB1	1.96	0.66
1:B:195:MET:CE	1:B:202:ILE:CD1	2.72	0.66
1:A:170:ASN:HD21	1:A:319:SER:H	1.42	0.66
1:A:256:MET:HE1	1:A:321:GLN:OE1	1.95	0.66
1:B:197:ASN:ND2	1:B:199:TYR:H	1.93	0.65
4:B:403:DH9:H192	4:B:403:DH9:H4'1	1.78	0.65
1:A:115:HIS:CE1	4:A:403:DH9:H291	2.32	0.64
1:B:180:ASN:ND2	1:B:243:THR:HG21	2.14	0.63
1:A:15:HIS:CE1	1:A:56:VAL:H	2.13	0.63
1:A:237:ASN:HD22	1:A:239:ALA:H	1.47	0.62
1:A:14:VAL:HG21	1:A:122:ILE:HD11	1.81	0.62
1:B:198:LYS:H	1:B:213:GLN:NE2	1.97	0.61
1:A:198:LYS:H	1:A:213:GLN:HE21	1.46	0.61
1:A:302:GLU:O	1:A:313:ILE:HG13	2.01	0.61
1:A:68:GLN:NE2	1:A:80:TYR:OH	2.33	0.60
1:A:163:THR:CG2	8:A:501:HOH:O	2.49	0.60
4:A:403:DH9:H27	4:A:403:DH9:O3'	2.02	0.60
1:B:15:HIS:HE1	1:B:56:VAL:H	1.50	0.60
1:A:193:ARG:HH11	5:A:404:DAO:C2	2.13	0.59
1:B:177:LYS:O	1:B:181:THR:HG23	2.03	0.59
1:A:34:GLY:HA3	1:A:38:PHE:O	2.03	0.59
1:A:173:GLN:H	1:A:173:GLN:NE2	1.95	0.59
1:B:170:ASN:ND2	1:B:319:SER:H	1.98	0.58
1:A:327:THR:HG22	1:A:330:GLU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:VAL:HG23	1:B:343:ILE:CG2	2.34	0.57
1:B:268:VAL:HG23	1:B:343:ILE:HG21	1.85	0.57
1:B:127:GLU:CG	1:B:254:THR:HG22	2.35	0.57
1:B:302:GLU:O	1:B:313:ILE:HG13	2.05	0.56
1:A:327:THR:HG22	1:A:330:GLU:HG2	1.86	0.56
1:B:127:GLU:HG2	1:B:254:THR:HG22	1.88	0.56
1:A:303:TRP:HA	1:A:313:ILE:HG13	1.88	0.56
1:A:17:PHE:O	1:A:18:LEU:HB2	2.07	0.55
1:A:156:ASN:O	1:A:157:ASN:HB2	2.06	0.55
1:B:15:HIS:CE1	1:B:56:VAL:H	2.24	0.54
1:B:173:GLN:HE22	1:B:311:PRO:HG3	1.72	0.54
1:A:275:LEU:H	1:A:275:LEU:HD22	1.73	0.54
1:B:17:PHE:O	1:B:18:LEU:HB2	2.07	0.54
1:B:123:ARG:NH1	1:B:169:HIS:HD2	2.06	0.53
1:B:173:GLN:H	1:B:173:GLN:NE2	1.95	0.53
1:A:329:ASN:H	1:A:329:ASN:HD22	1.55	0.53
1:B:123:ARG:HH11	1:B:169:HIS:HD2	1.55	0.53
1:B:313:ILE:HD13	1:B:313:ILE:N	2.09	0.53
1:A:170:ASN:ND2	1:A:319:SER:H	2.06	0.52
1:B:179:GLY:O	1:B:239:ALA:CB	2.57	0.52
1:B:112:LEU:HB3	1:B:122:ILE:HD13	1.92	0.52
1:B:198:LYS:H	1:B:213:GLN:HE21	1.57	0.52
1:A:264:THR:O	1:A:341:LYS:HB2	2.10	0.52
1:A:368:ALA:O	1:A:372:ILE:HG12	2.09	0.52
1:B:327:THR:HG22	1:B:330:GLU:H	1.74	0.51
1:A:32:TYR:OH	4:A:403:DH9:H282	2.10	0.51
1:B:47:GLN:OE1	1:B:372:ILE:HD11	2.11	0.51
1:A:197:ASN:ND2	1:A:197:ASN:C	2.68	0.51
1:A:15:HIS:HD2	1:A:16:GLY:O	1.93	0.51
1:A:327:THR:CG2	1:A:329:ASN:H	2.24	0.51
1:B:32:TYR:OH	4:B:403:DH9:H282	2.11	0.51
1:B:195:MET:CE	1:B:202:ILE:HD13	2.40	0.51
1:B:302:GLU:O	1:B:313:ILE:CD1	2.59	0.51
1:A:198:LYS:N	1:A:213:GLN:HE21	2.08	0.50
1:A:197:ASN:HD22	1:A:197:ASN:C	2.19	0.50
1:A:313:ILE:CD1	1:A:313:ILE:HG13	2.18	0.49
1:B:15:HIS:HD2	1:B:16:GLY:O	1.96	0.49
1:B:175:ALA:O	1:B:180:ASN:CB	2.60	0.49
1:A:29:TYR:CG	1:A:30:PRO:HD2	2.48	0.49
6:A:406:BUA:H11	5:B:405:DAO:H62	1.94	0.49
1:A:163:THR:HG23	8:A:501:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:MET:HE3	1:A:321:GLN:HB3	1.94	0.49
1:B:175:ALA:HA	1:B:178:PHE:O	2.12	0.49
1:B:11:VAL:HB	1:B:51:VAL:HG12	1.95	0.48
1:B:195:MET:CE	1:B:202:ILE:HD11	2.23	0.48
1:B:327:THR:HB	1:B:330:GLU:HG2	1.94	0.48
1:B:257:ASN:HD22	1:B:259:ASN:H	1.60	0.48
1:A:257:ASN:HD22	1:A:258:PRO:N	2.11	0.48
1:B:217:GLU:OE2	1:B:225:ARG:HD3	2.14	0.47
1:A:329:ASN:HD22	1:A:329:ASN:N	2.12	0.47
1:A:178:PHE:C	1:A:178:PHE:CD2	2.90	0.47
1:A:126:GLU:OE2	1:A:130:ARG:HD3	2.15	0.47
1:B:77:ARG:HA	1:B:96:THR:HB	1.96	0.47
1:B:181:THR:OG1	1:B:184:VAL:HG13	2.14	0.47
1:A:164:THR:HB	1:A:167:THR:OG1	2.15	0.46
1:B:268:VAL:CG2	1:B:343:ILE:HG21	2.45	0.46
4:B:403:DH9:H27	4:B:403:DH9:HO3'	1.81	0.46
1:A:197:ASN:HA	1:A:213:GLN:HE21	1.81	0.45
1:A:329:ASN:N	1:A:329:ASN:ND2	2.64	0.45
1:B:163:THR:HA	1:B:263:THR:O	2.16	0.45
1:A:178:PHE:O	1:A:178:PHE:CD2	2.70	0.45
1:A:112:LEU:HB3	1:A:122:ILE:HD12	1.98	0.44
1:B:175:ALA:O	1:B:180:ASN:HB2	2.17	0.44
1:B:130:ARG:NH2	1:B:255:SER:OG	2.49	0.44
1:B:170:ASN:HD21	1:B:319:SER:N	2.04	0.44
1:B:190:ALA:HB1	5:B:404:DAO:H22	1.99	0.44
1:B:237:ASN:HD21	1:B:239:ALA:HB3	1.83	0.44
1:A:313:ILE:HD13	1:A:313:ILE:N	2.17	0.44
1:B:320:ASN:H	1:B:320:ASN:HD22	1.64	0.44
1:A:59:PHE:HE2	1:A:188:MET:HG2	1.83	0.43
1:B:197:ASN:HA	1:B:213:GLN:HE21	1.83	0.43
1:A:63:TYR:CD1	1:A:63:TYR:C	2.96	0.43
7:B:406:STE:H101	7:B:406:STE:H151	2.01	0.43
1:A:152:THR:HG22	1:A:155:HIS:NE2	2.33	0.43
1:B:181:THR:HG1	1:B:184:VAL:HG13	1.84	0.43
1:A:40:VAL:HG13	1:A:44:LEU:HD22	2.01	0.42
1:A:170:ASN:ND2	1:A:251:ASN:HD21	2.17	0.42
1:B:127:GLU:HG3	1:B:254:THR:HG22	1.99	0.42
1:B:34:GLY:HA3	1:B:38:PHE:O	2.20	0.42
1:B:291:THR:O	1:B:295:ILE:HG13	2.19	0.42
1:A:202:ILE:HD11	1:A:204:LEU:CD1	2.50	0.42
1:A:265:TYR:CE2	1:A:341:LYS:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:THR:O	1:A:285:PHE:C	2.62	0.42
1:B:15:HIS:CD2	1:B:15:HIS:C	2.98	0.42
1:B:198:LYS:N	1:B:213:GLN:HE21	2.17	0.42
1:A:217:GLU:OE2	1:A:225:ARG:HD3	2.20	0.42
1:B:303:TRP:HA	1:B:313:ILE:HG13	2.01	0.42
1:A:167:THR:O	1:A:315:SER:HA	2.20	0.42
1:B:173:GLN:NE2	1:B:311:PRO:HG3	2.35	0.42
1:A:275:LEU:HD23	1:A:277:TYR:HB2	2.02	0.41
1:B:167:THR:O	1:B:315:SER:HA	2.20	0.41
1:B:357:PHE:CE2	1:B:358:LEU:HD13	2.55	0.41
1:A:307:ASP:C	1:A:307:ASP:OD1	2.63	0.41
1:A:302:GLU:O	1:A:313:ILE:CG1	2.67	0.41
1:B:173:GLN:HE21	1:B:173:GLN:N	1.98	0.41
1:A:202:ILE:CD1	1:A:204:LEU:HD13	2.51	0.41
1:A:173:GLN:HE22	1:A:311:PRO:HG3	1.84	0.41
1:A:170:ASN:HD22	1:A:251:ASN:HD21	1.69	0.41
1:B:302:GLU:O	1:B:313:ILE:CG1	2.68	0.41
1:A:14:VAL:CG2	1:A:122:ILE:HD11	2.50	0.40
1:A:130:ARG:NH2	1:A:255:SER:OG	2.39	0.40
1:A:237:ASN:HD22	1:A:239:ALA:N	2.16	0.40
1:B:20:LEU:HD13	1:B:26:PRO:HD3	2.03	0.40
1:B:84:HIS:NE2	1:B:236:ASP:OD2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/408 (93%)	367 (97%)	12 (3%)	1 (0%)	36	38
1	B	380/408 (93%)	370 (97%)	10 (3%)	0	100	100
All	All	760/816 (93%)	737 (97%)	22 (3%)	1 (0%)	48	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	VAL

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	317/341 (93%)	270 (85%)	47 (15%)	3	1
1	B	317/341 (93%)	264 (83%)	53 (17%)	2	0
All	All	634/682 (93%)	534 (84%)	100 (16%)	2	1

All (100) 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	44	LEU
1	A	69	LEU
1	A	96	THR
1	A	98	LYS
1	A	100	ILE
1	A	110	VAL
1	A	113	VAL
1	A	124	LEU
1	A	134	LYS
1	A	141	GLN
1	A	146	GLU
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	202	ILE

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Mol	Chain	Res	Type
1	A	204	LEU
1	A	226	VAL
1	A	230	LYS
1	A	257	ASN
1	A	263	THR
1	A	268	VAL
1	A	275	LEU
1	A	282	LEU
1	A	309	VAL
1	A	310	VAL
1	A	313	ILE
1	A	316	LEU
1	A	326	VAL
1	A	327	THR
1	A	329	ASN
1	A	333	THR
1	A	335	ARG
1	A	340	VAL
1	A	341	LYS
1	A	344	LEU
1	A	350	VAL
1	A	358	LEU
1	A	365	SER
1	A	378	LEU
1	A	379	LEU
1	B	4	GLN
1	B	6	LEU
1	B	18	LEU
1	B	28	LEU
1	B	44	LEU
1	B	46	LYS
1	B	69	LEU
1	B	87	LYS
1	B	95	LYS
1	B	96	THR
1	B	98	LYS
1	B	100	ILE
1	B	105	GLU
1	B	110	VAL
1	B	113	VAL
1	B	124	LEU
1	B	134	LYS

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Mol	Chain	Res	Type
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	204	LEU
1	B	226	VAL
1	B	230	LYS
1	B	244	LEU
1	B	257	ASN
1	B	263	THR
1	B	272	THR
1	B	275	LEU
1	B	282	LEU
1	B	302	GLU
1	B	309	VAL
1	B	310	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	350	VAL
1	B	358	LEU
1	B	378	LEU
1	B	379	LEU
1	B	385	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	31	ASN

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Mol	Chain	Res	Type
1	A	52	HIS
1	A	53	GLN
1	A	62	ASN
1	A	120	GLN
1	A	141	GLN
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	279	ASN
1	A	325	ASN
1	A	329	ASN
1	A	345	GLN
1	A	369	ASN
1	B	4	GLN
1	B	15	HIS
1	B	31	ASN
1	B	36	ASN
1	B	52	HIS
1	B	141	GLN
1	B	155	HIS
1	B	169	HIS
1	B	170	ASN
1	B	173	GLN
1	B	180	ASN
1	B	197	ASN
1	B	213	GLN
1	B	237	ASN
1	B	257	ASN
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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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$
6	BUA	A	406	-	5,5,5	1.21	0	5,5,5	0.98	0
4	DH9	B	403	-	35,35,35	0.97	3 (8%)	39,41,41	1.67	8 (20%)
5	DAO	B	405	-	13,13,13	0.84	0	13,13,13	1.19	2 (15%)
7	STE	B	406	-	19,19,19	0.67	0	19,19,19	0.88	1 (5%)
5	DAO	A	405	-	13,13,13	0.80	0	13,13,13	0.64	0
5	DAO	A	404	-	13,13,13	0.82	0	13,13,13	0.92	1 (7%)
4	DH9	A	403	1	35,35,35	1.10	3 (8%)	39,41,41	1.85	8 (20%)
5	DAO	B	404	-	13,13,13	0.70	0	13,13,13	0.77	0
6	BUA	B	407	-	5,5,5	1.09	0	5,5,5	1.37	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
6	BUA	A	406	-	-	1/3/3/3	-
4	DH9	B	403	-	-	19/44/44/44	-
5	DAO	B	405	-	-	8/11/11/11	-
7	STE	B	406	-	-	14/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DAO	A	405	-	-	8/11/11/11	-
5	DAO	A	404	-	-	4/11/11/11	-
4	DH9	A	403	1	-	16/44/44/44	-
5	DAO	B	404	-	-	8/11/11/11	-
6	BUA	B	407	-	-	2/3/3/3	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	DH9	O4'-C23	3.41	1.42	1.34
4	A	403	DH9	O4'-C5'	-3.37	1.38	1.46
4	A	403	DH9	O4'-C23	3.15	1.41	1.34
4	B	403	DH9	O4'-C5'	-2.72	1.40	1.46
4	A	403	DH9	O2'-C1'	-2.26	1.23	1.30
4	B	403	DH9	O2'-C1'	-2.04	1.24	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	DH9	O4'-C5'-C4'	-5.55	97.45	107.57
4	B	403	DH9	O4'-C5'-C4'	-5.06	98.34	107.57
4	A	403	DH9	O3'-C3'-C4'	4.62	118.39	109.15
4	B	403	DH9	C4'-C5'-C6'	-4.04	106.74	112.79
4	B	403	DH9	O6'-C25-N1'	-3.81	115.48	125.32
4	A	403	DH9	C5'-O4'-C23	3.65	123.46	117.72
4	A	403	DH9	C23-C24-N1'	3.54	119.71	110.59
4	B	403	DH9	C18-C17-C2'	-3.19	108.66	114.28
5	B	405	DAO	O2-C1-C2	3.07	123.69	114.00
4	A	403	DH9	C3'-C2'-C1'	2.73	114.14	109.37
4	A	403	DH9	O6'-C25-N1'	-2.70	118.33	125.32
7	B	406	STE	O2-C1-C2	2.70	122.54	114.00
4	B	403	DH9	C23-C24-N1'	2.70	117.56	110.59
4	A	403	DH9	O2'-C1'-O1'	-2.59	118.21	124.08
4	B	403	DH9	C5'-O4'-C23	2.48	121.62	117.72
5	B	405	DAO	O2-C1-O1	-2.47	116.98	123.33
6	B	407	BUA	O2-C4-C3	2.18	120.89	114.00
4	B	403	DH9	O4'-C5'-C6'	2.14	113.17	107.26
4	B	403	DH9	O4'-C23-O5'	-2.12	120.11	123.95
4	A	403	DH9	O1'-C1'-C2'	2.07	127.88	123.01
5	A	404	DAO	C6-C5-C4	2.02	124.56	114.37

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	DH9	C18-C17-C2'-C1'
4	A	403	DH9	C17-C2'-C3'-O3'
4	A	403	DH9	C17-C2'-C3'-C4'
4	A	403	DH9	C1'-C2'-C3'-O3'
4	A	403	DH9	C1'-C2'-C3'-C4'
4	A	403	DH9	C26-C24-N1'-C25
4	A	403	DH9	O6'-C25-N1'-C24
4	B	403	DH9	C18-C17-C2'-C1'
4	B	403	DH9	C17-C2'-C3'-O3'
4	B	403	DH9	C17-C2'-C3'-C4'
4	B	403	DH9	C1'-C2'-C3'-O3'
4	B	403	DH9	C1'-C2'-C3'-C4'
4	B	403	DH9	C23-C24-C26-C27
4	B	403	DH9	O6'-C25-N1'-C24
4	B	403	DH9	N1'-C24-C26-C27
5	B	405	DAO	C2-C3-C4-C5
4	A	403	DH9	N1'-C24-C26-C27
7	B	406	STE	C1-C2-C3-C4
7	B	406	STE	C12-C13-C14-C15
5	A	405	DAO	C1-C2-C3-C4
5	B	405	DAO	C1-C2-C3-C4
5	A	404	DAO	C1-C2-C3-C4
4	A	403	DH9	C11-C12-C13-C14
4	A	403	DH9	C23-C24-C26-C27
7	B	406	STE	C11-C12-C13-C14
5	A	404	DAO	C6-C7-C8-C9
5	A	405	DAO	C7-C8-C9-C10
5	A	405	DAO	C3-C4-C5-C6
4	A	403	DH9	C12-C13-C14-C15
7	B	406	STE	C2-C3-C4-C5
5	A	405	DAO	C6-C7-C8-C9
7	B	406	STE	C4-C5-C6-C7
5	B	404	DAO	C1-C2-C3-C4
5	A	405	DAO	C4-C5-C6-C7
7	B	406	STE	C10-C11-C12-C13
5	B	405	DAO	C6-C7-C8-C9
7	B	406	STE	C13-C14-C15-C16
4	A	403	DH9	C6'-C7'-C8'-C9'
4	B	403	DH9	C24-C26-C27-C29
4	A	403	DH9	C2'-C17-C18-C19

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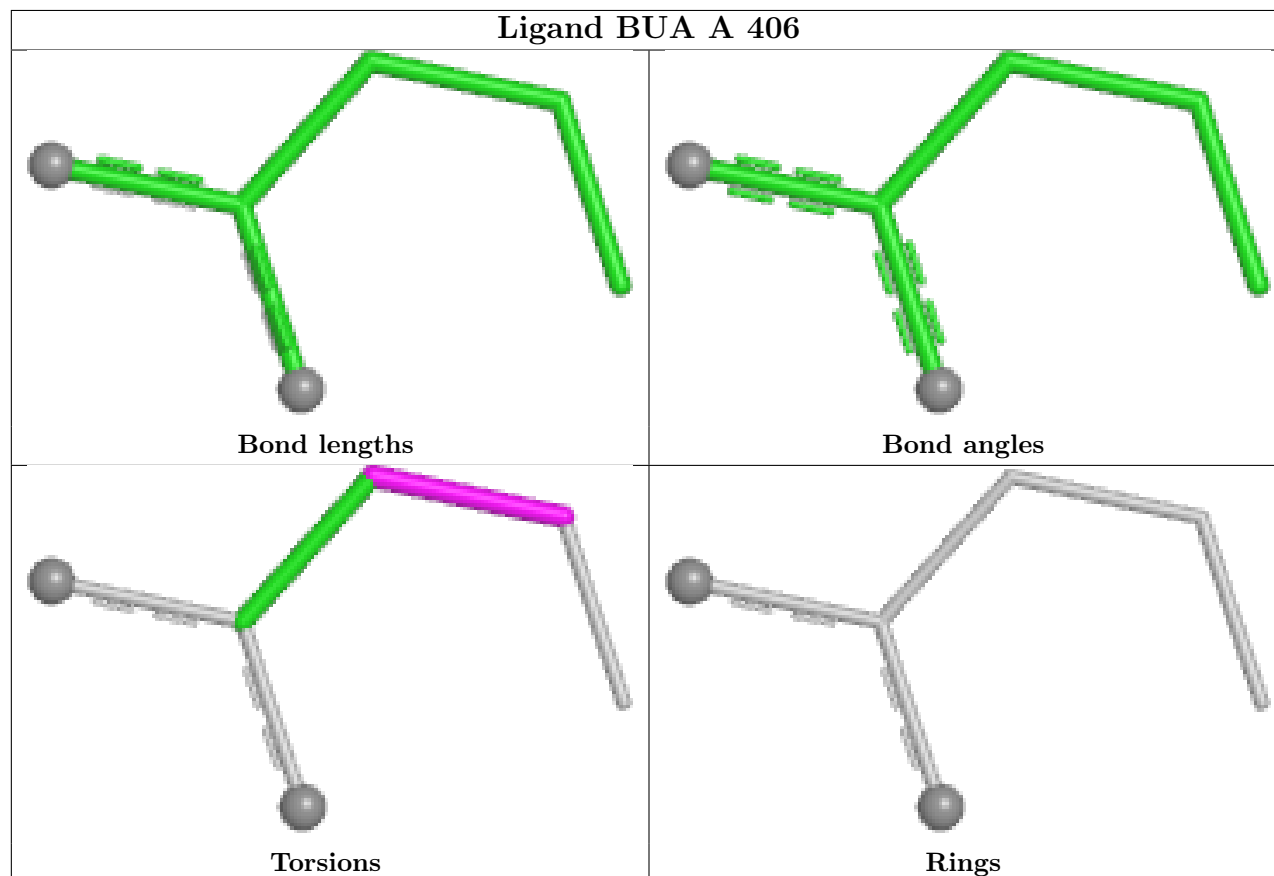
Mol	Chain	Res	Type	Atoms
5	B	404	DAO	C9-C10-C11-C12
4	B	403	DH9	C19-C20-C21-C22
7	B	406	STE	C7-C8-C9-C10
7	B	406	STE	C5-C6-C7-C8
5	B	404	DAO	C4-C5-C6-C7
5	A	404	DAO	C5-C6-C7-C8
5	B	405	DAO	C5-C6-C7-C8
4	B	403	DH9	C2'-C17-C18-C19
6	A	406	BUA	C1-C2-C3-C4
4	B	403	DH9	C24-C26-C27-C28
5	B	405	DAO	C4-C5-C6-C7
7	B	406	STE	C9-C10-C11-C12
7	B	406	STE	C14-C15-C16-C17
5	B	404	DAO	C11-C10-C9-C8
4	B	403	DH9	C26-C24-N1'-C25
4	B	403	DH9	C5'-C6'-C7'-C8'
5	B	405	DAO	C3-C4-C5-C6
4	A	403	DH9	C17-C18-C19-C20
7	B	406	STE	C11-C10-C9-C8
5	B	404	DAO	C7-C8-C9-C10
4	B	403	DH9	C6'-C7'-C8'-C9'
5	B	404	DAO	C2-C3-C4-C5
5	B	404	DAO	O2-C1-C2-C3
6	B	407	BUA	C2-C3-C4-O2
5	B	405	DAO	O2-C1-C2-C3
5	B	404	DAO	O1-C1-C2-C3
6	B	407	BUA	C2-C3-C4-O1
5	B	405	DAO	O1-C1-C2-C3
5	A	405	DAO	O2-C1-C2-C3
4	A	403	DH9	C9'-C10-C11-C12
5	A	405	DAO	O1-C1-C2-C3
7	B	406	STE	O1-C1-C2-C3
5	A	404	DAO	C3-C4-C5-C6
5	A	405	DAO	C9-C10-C11-C12
4	A	403	DH9	C18-C19-C20-C21
4	B	403	DH9	C11-C12-C13-C14
7	B	406	STE	O2-C1-C2-C3
4	B	403	DH9	O1'-C1'-C2'-C17
4	B	403	DH9	O2'-C1'-C2'-C17
4	B	403	DH9	C4'-C5'-C6'-C7'

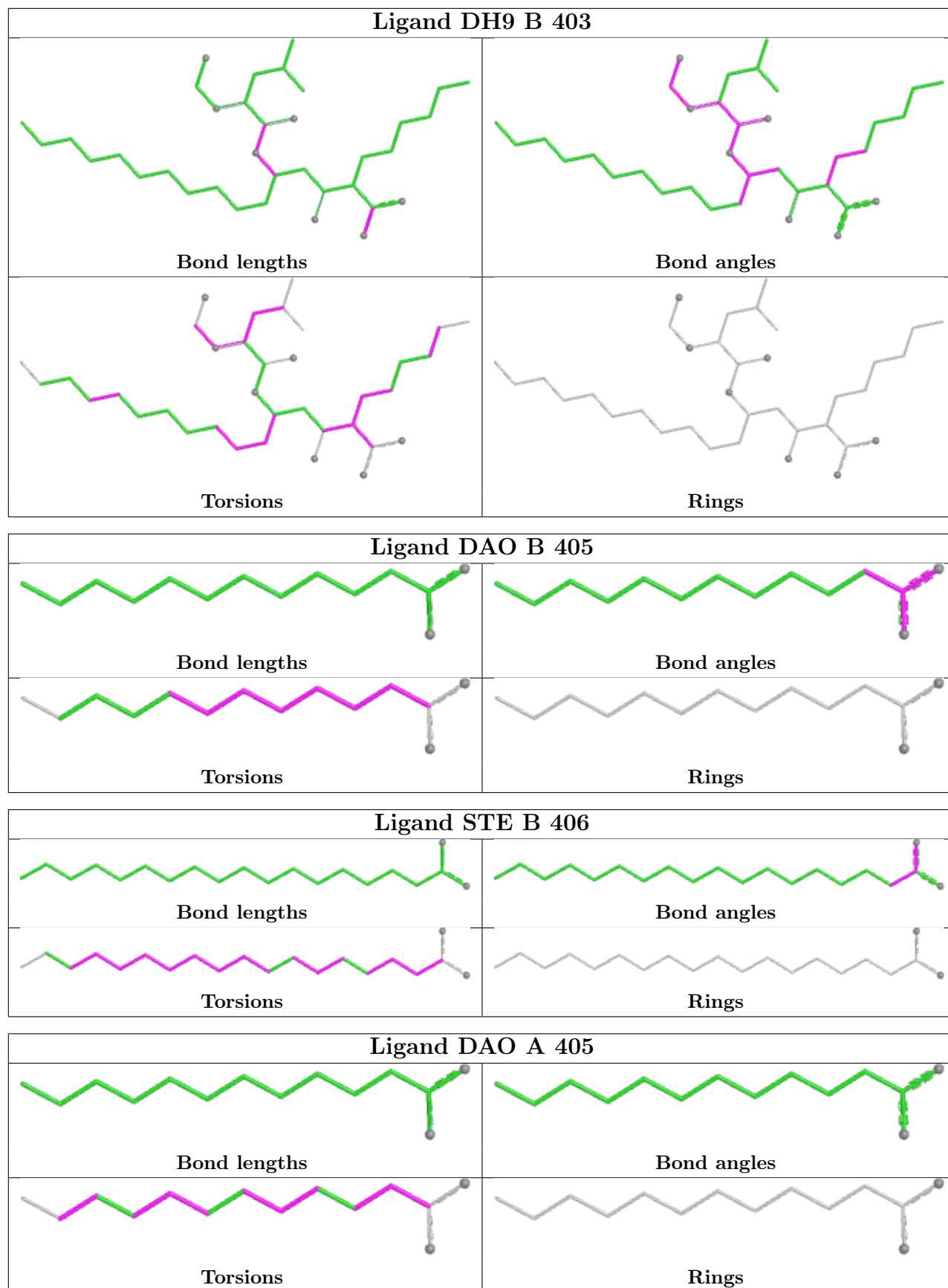
There are no ring outliers.

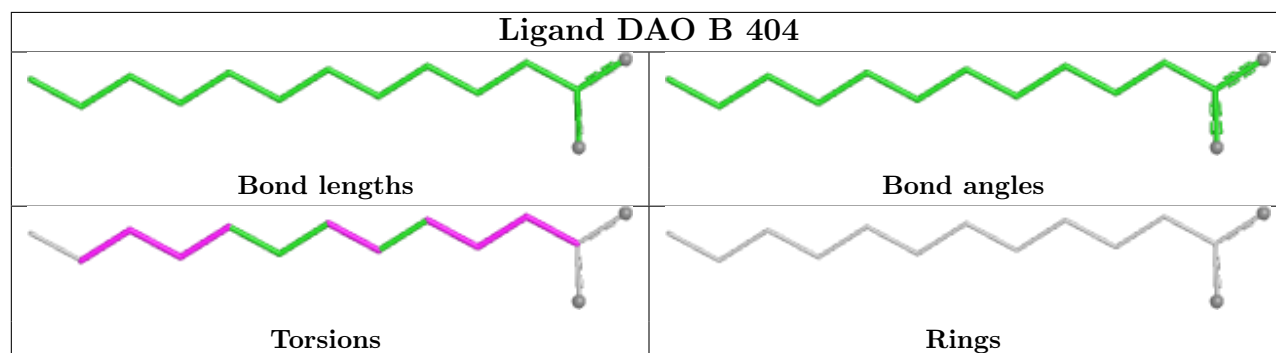
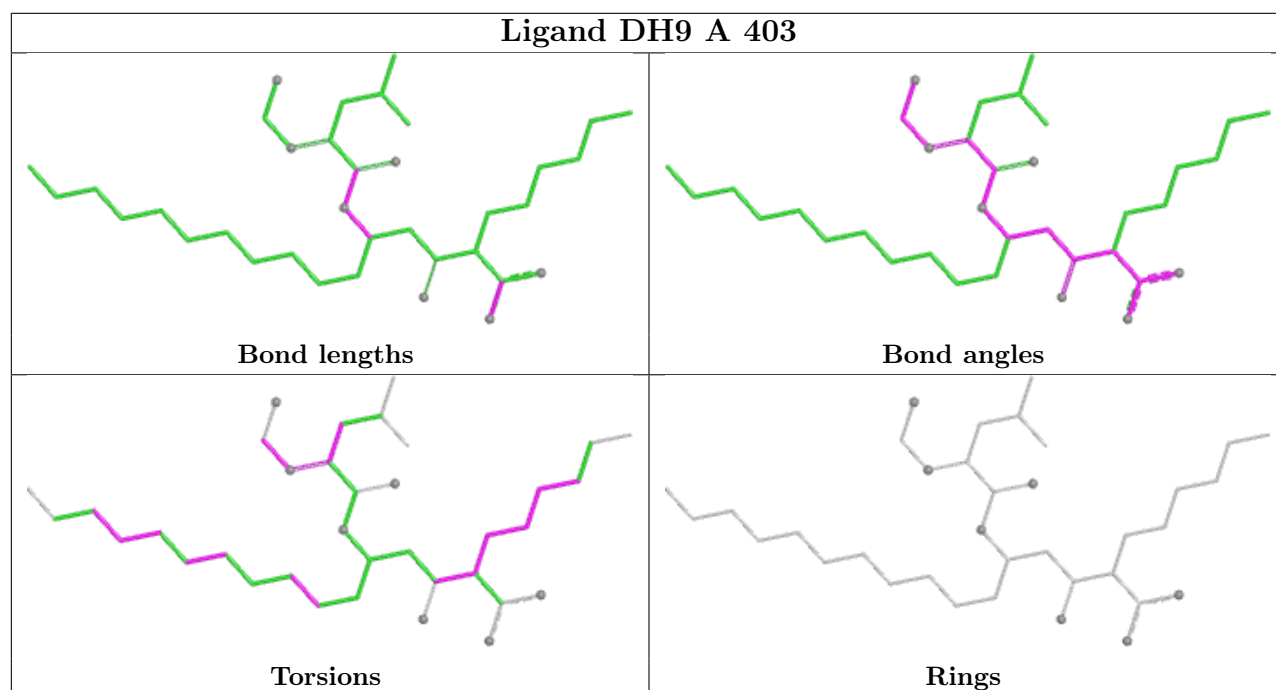
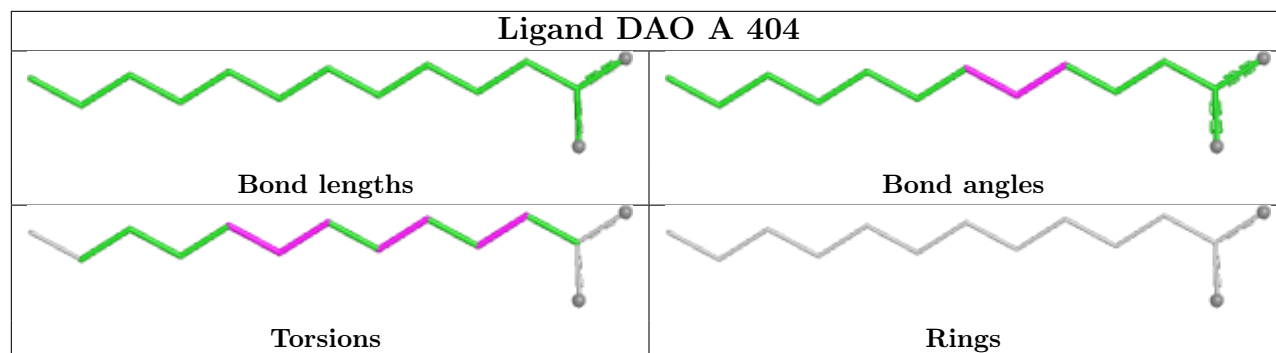
7 monomers are involved in 18 short contacts:

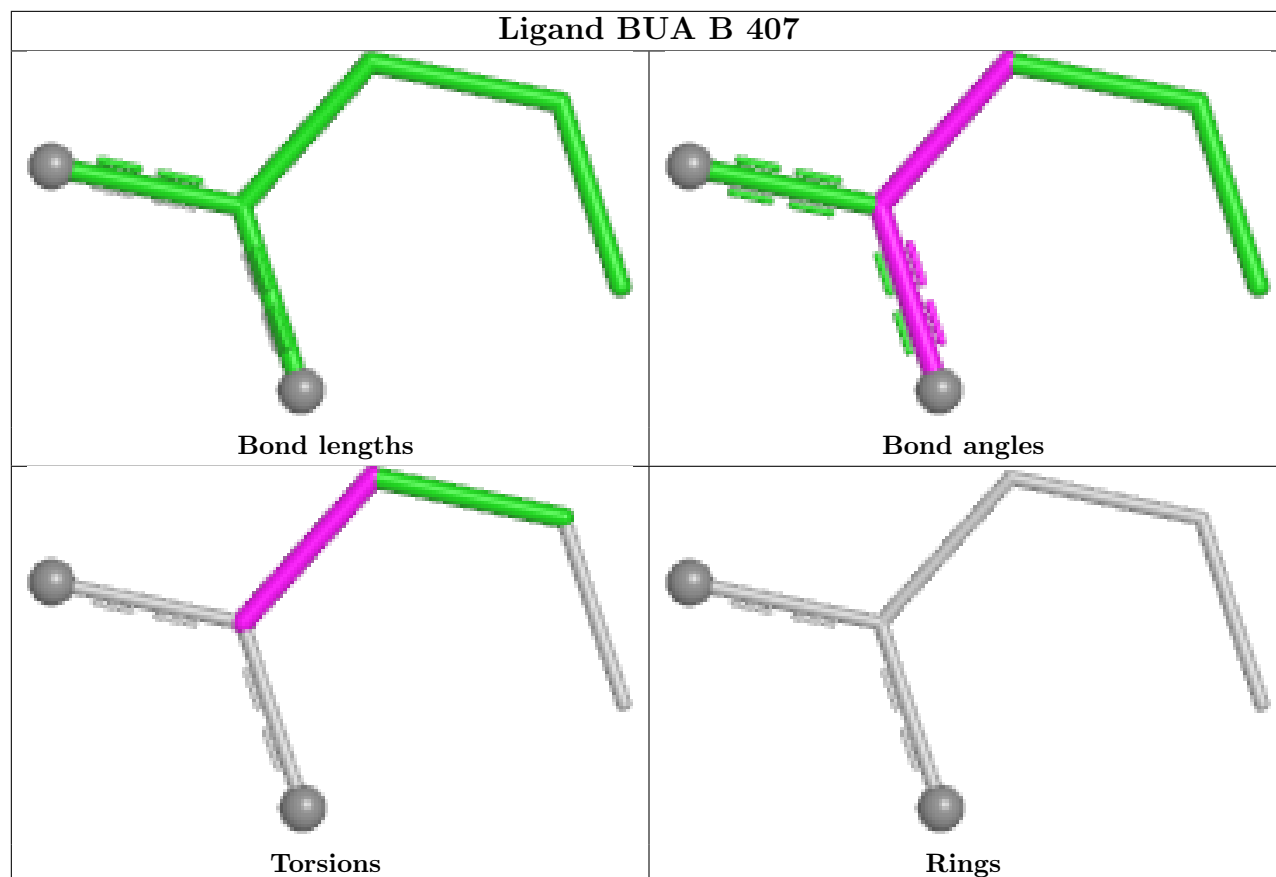
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	406	BUA	1	0
4	B	403	DH9	8	0
5	B	405	DAO	1	0
7	B	406	STE	1	0
5	A	404	DAO	2	0
4	A	403	DH9	5	0
5	B	404	DAO	1	0

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 [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%)	-0.20	10 (2%) 57 58	31, 39, 61, 86	0
1	B	382/408 (93%)	0.29	22 (5%) 29 27	35, 47, 66, 90	0
All	All	764/816 (93%)	0.04	32 (4%) 40 39	31, 44, 65, 90	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	GLY	10.3
1	B	178	PHE	8.2
1	A	275	LEU	4.4
1	B	274	PRO	4.4
1	B	180	ASN	4.2
1	B	139	TYR	4.2
1	A	274	PRO	4.1
1	B	275	LEU	3.8
1	B	385	GLU	3.7
1	B	177	LYS	3.7
1	B	4	GLN	3.6
1	B	141	GLN	3.4
1	A	385	GLU	3.2
1	A	360	PHE	3.1
1	B	95	LYS	3.1
1	B	134	LYS	2.8
1	B	140	HIS	2.8
1	B	27	ALA	2.8
1	B	28	LEU	2.8
1	B	144	GLY	2.6
1	A	27	ALA	2.6
1	A	4	GLN	2.6
1	A	98	LYS	2.6
1	B	142	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	289	ASP	2.4
1	B	360	PHE	2.4
1	A	28	LEU	2.3
1	B	313	ILE	2.3
1	B	328	ASN	2.2
1	A	313	ILE	2.2
1	B	143	HIS	2.2
1	B	145	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

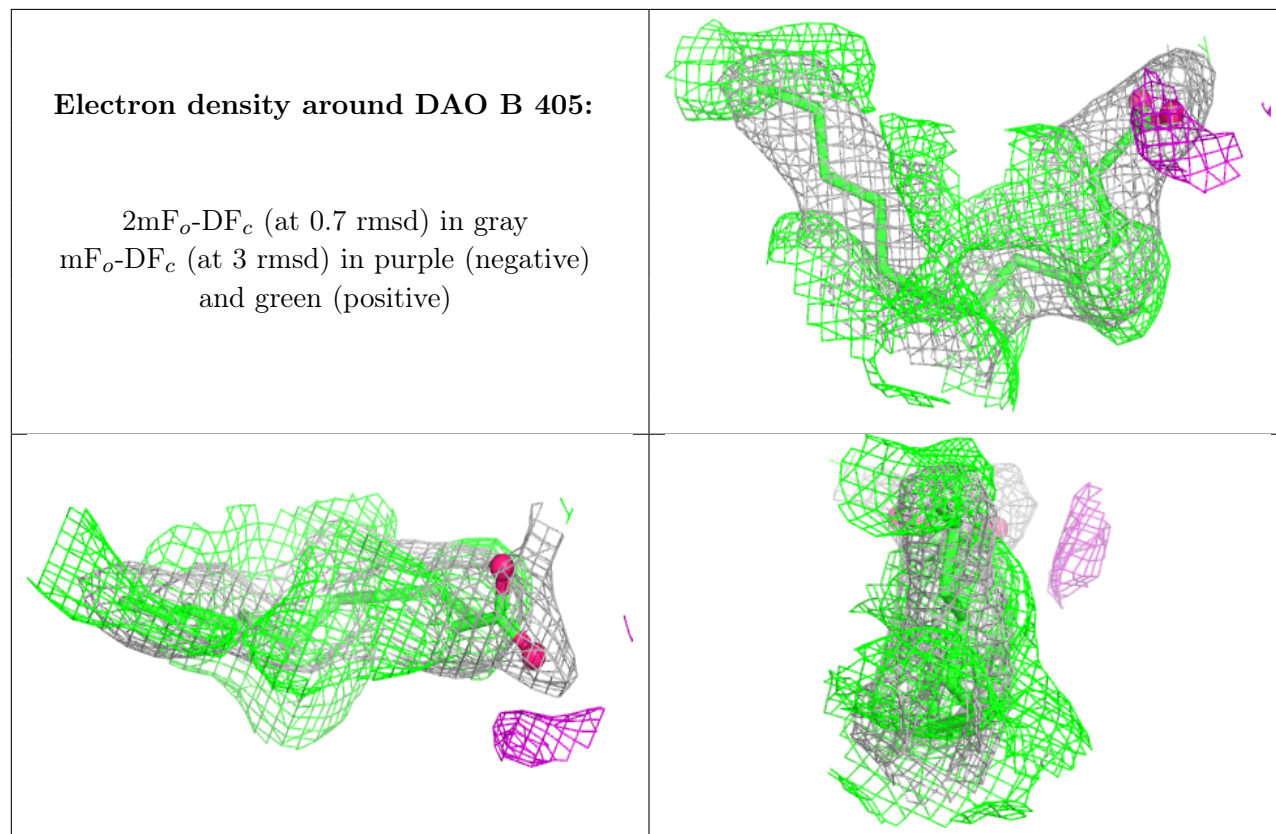
6.4 Ligands ⓘ

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	DAO	B	405	14/14	0.68	0.49	66,93,115,118	0
5	DAO	A	405	14/14	0.73	0.47	97,116,129,131	0
6	BUA	B	407	6/6	0.77	0.35	72,96,105,110	0
6	BUA	A	406	6/6	0.81	0.32	73,87,105,106	0
7	STE	B	406	20/20	0.85	0.35	71,108,126,127	0
5	DAO	B	404	14/14	0.86	0.32	56,97,122,122	0
4	DH9	A	403	36/36	0.88	0.25	49,67,98,109	0
5	DAO	A	404	14/14	0.88	0.31	59,92,106,109	0
4	DH9	B	403	36/36	0.96	0.18	48,68,94,99	0
3	CA	B	402	1/1	0.97	0.14	64,64,64,64	0
3	CA	A	402	1/1	0.97	0.09	75,75,75,75	0
2	ZN	A	401	1/1	0.98	0.15	68,68,68,68	0
2	ZN	B	401	1/1	1.00	0.07	69,69,69,69	0

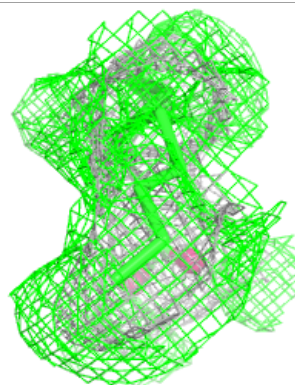
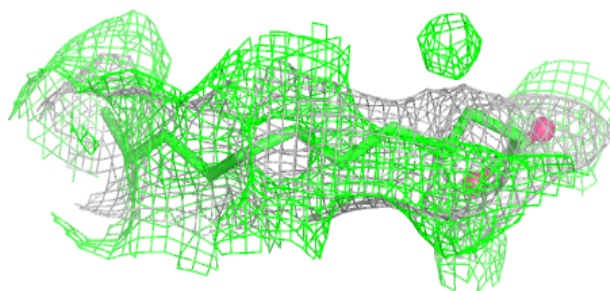
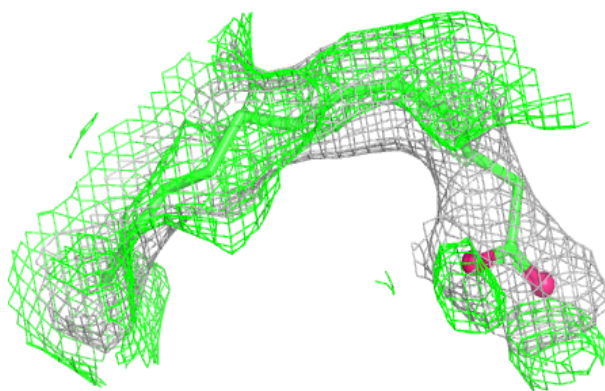
The following is a graphical depiction of the model fit to experimental electron density of all

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.

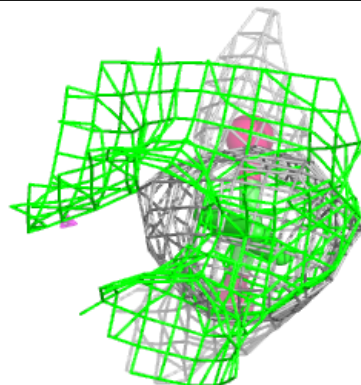
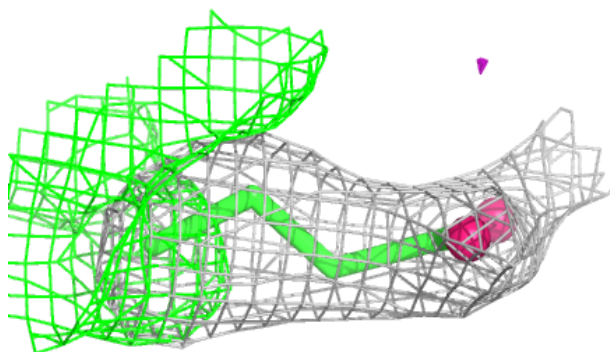
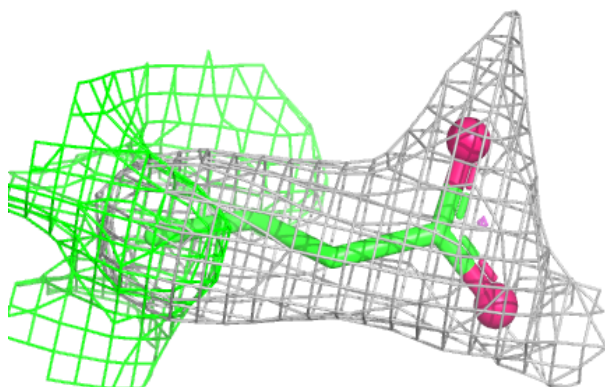


Electron density around DAO A 405:

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

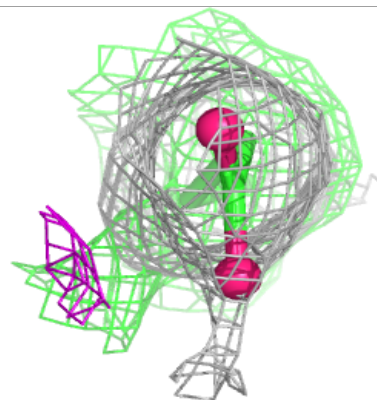
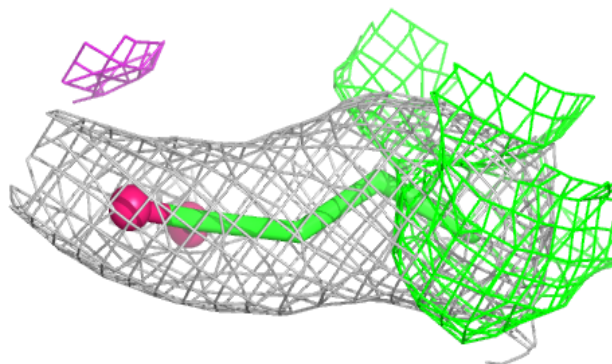
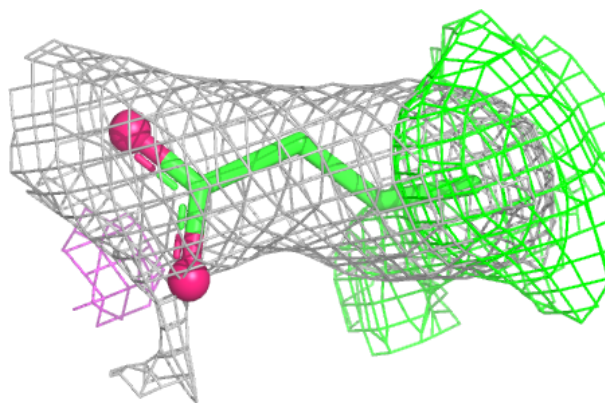
**Electron density around BUA B 407:**

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

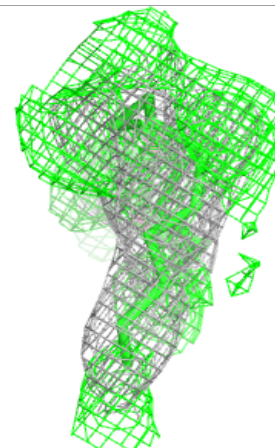
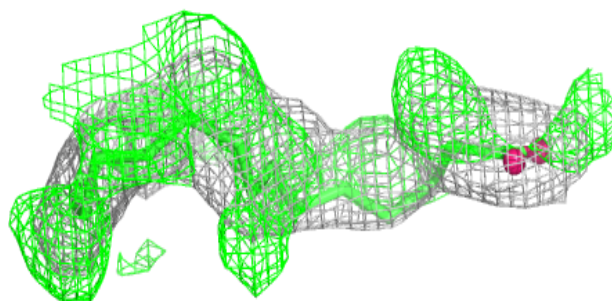
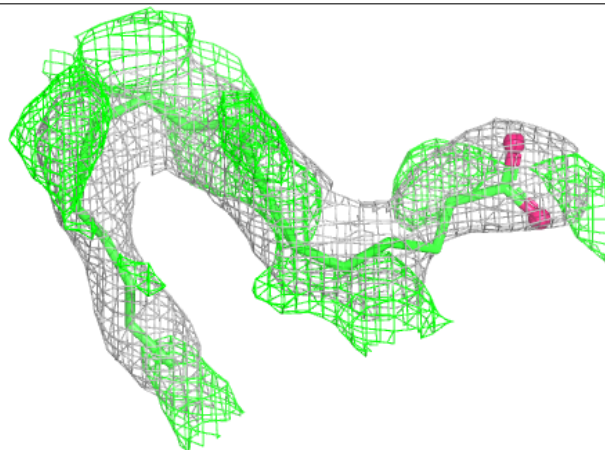


Electron density around BUA A 406:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

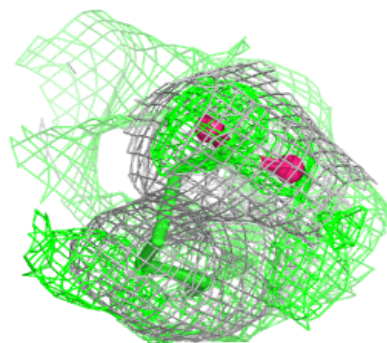
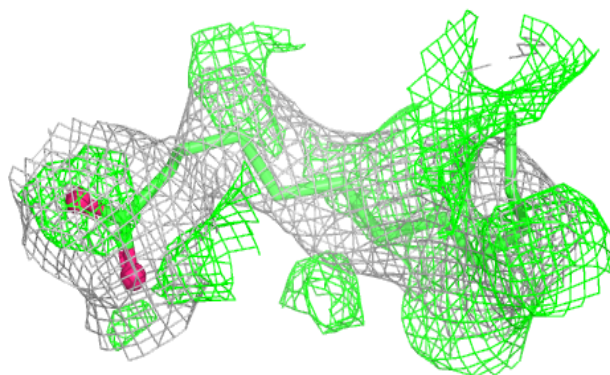
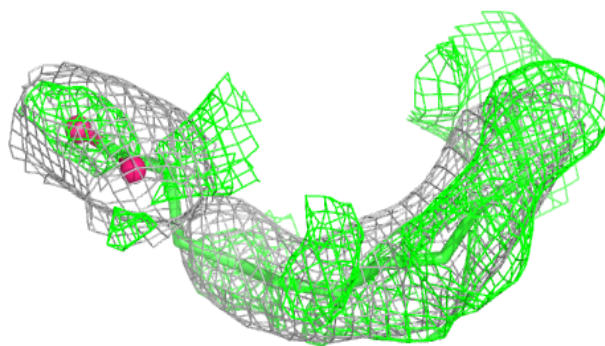
**Electron density around STE B 406:**

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



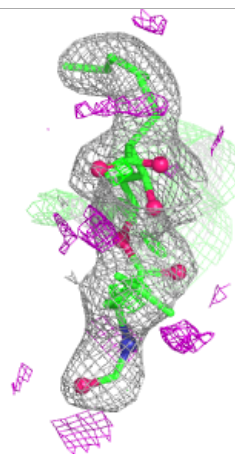
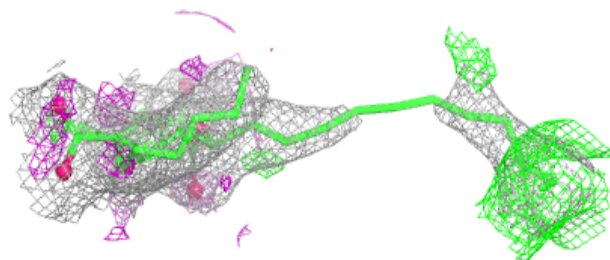
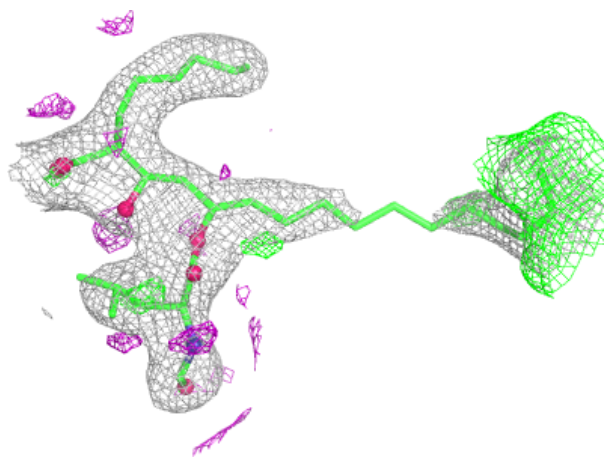
Electron density around DAO B 404:

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



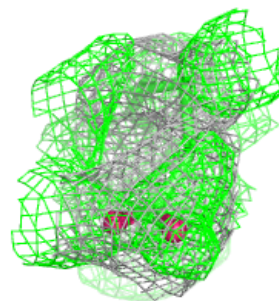
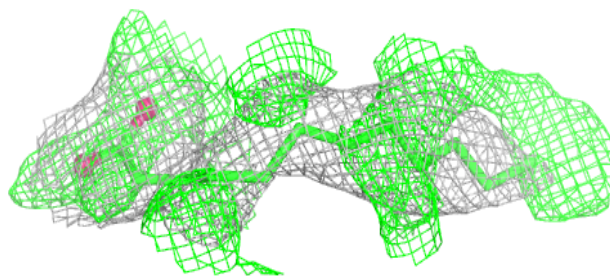
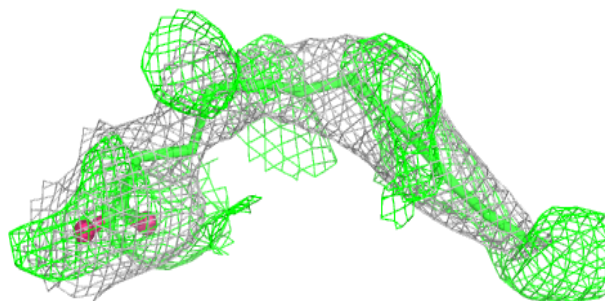
Electron density around DH9 A 403:

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and green (positive)

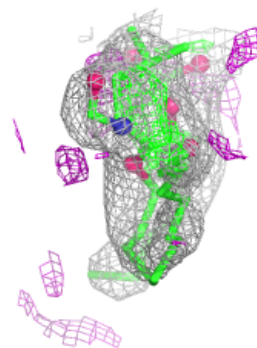
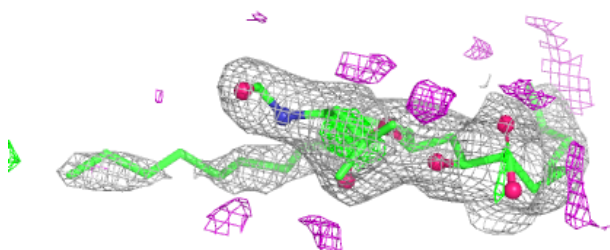
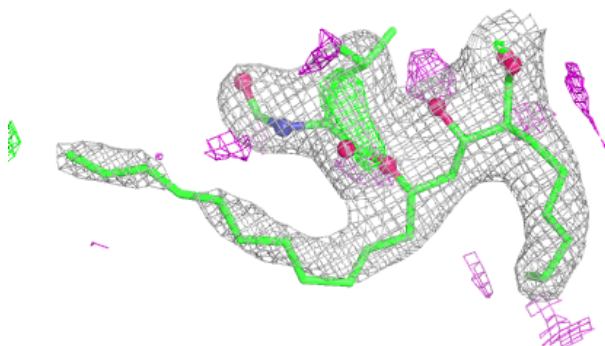


Electron density around DAO A 404:

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

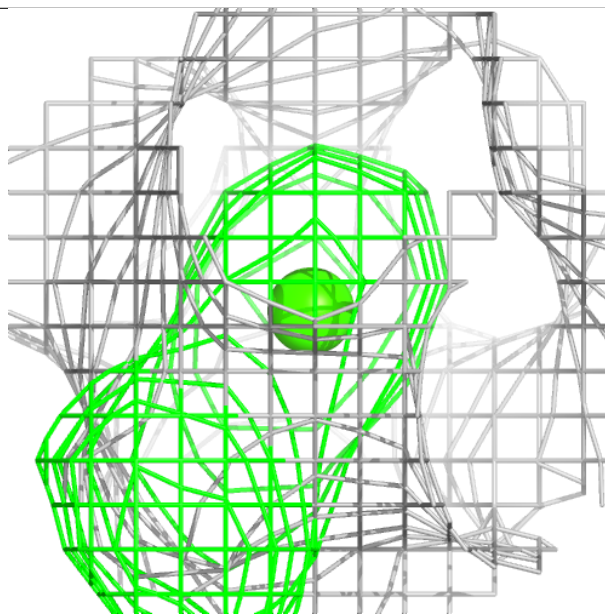
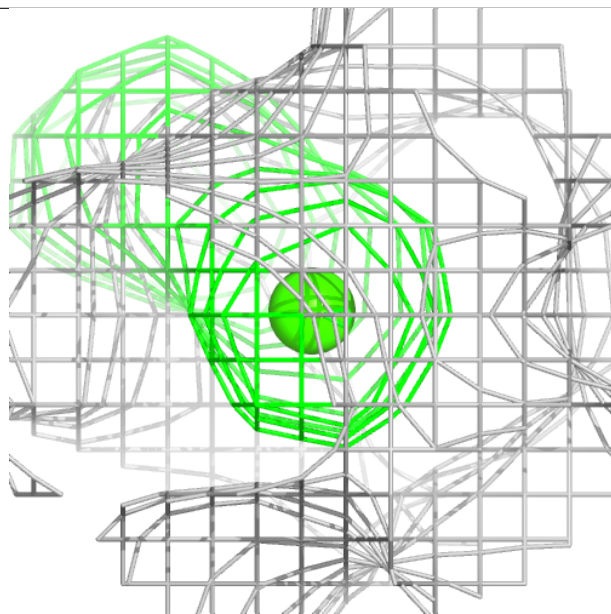
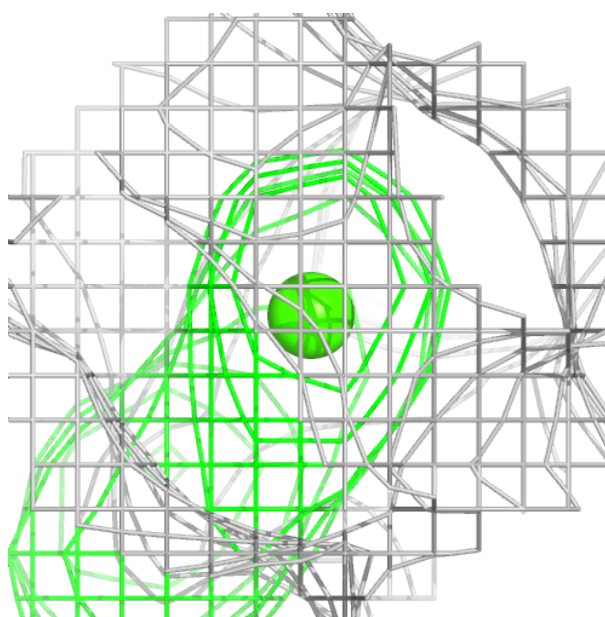
**Electron density around DH9 B 403:**

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



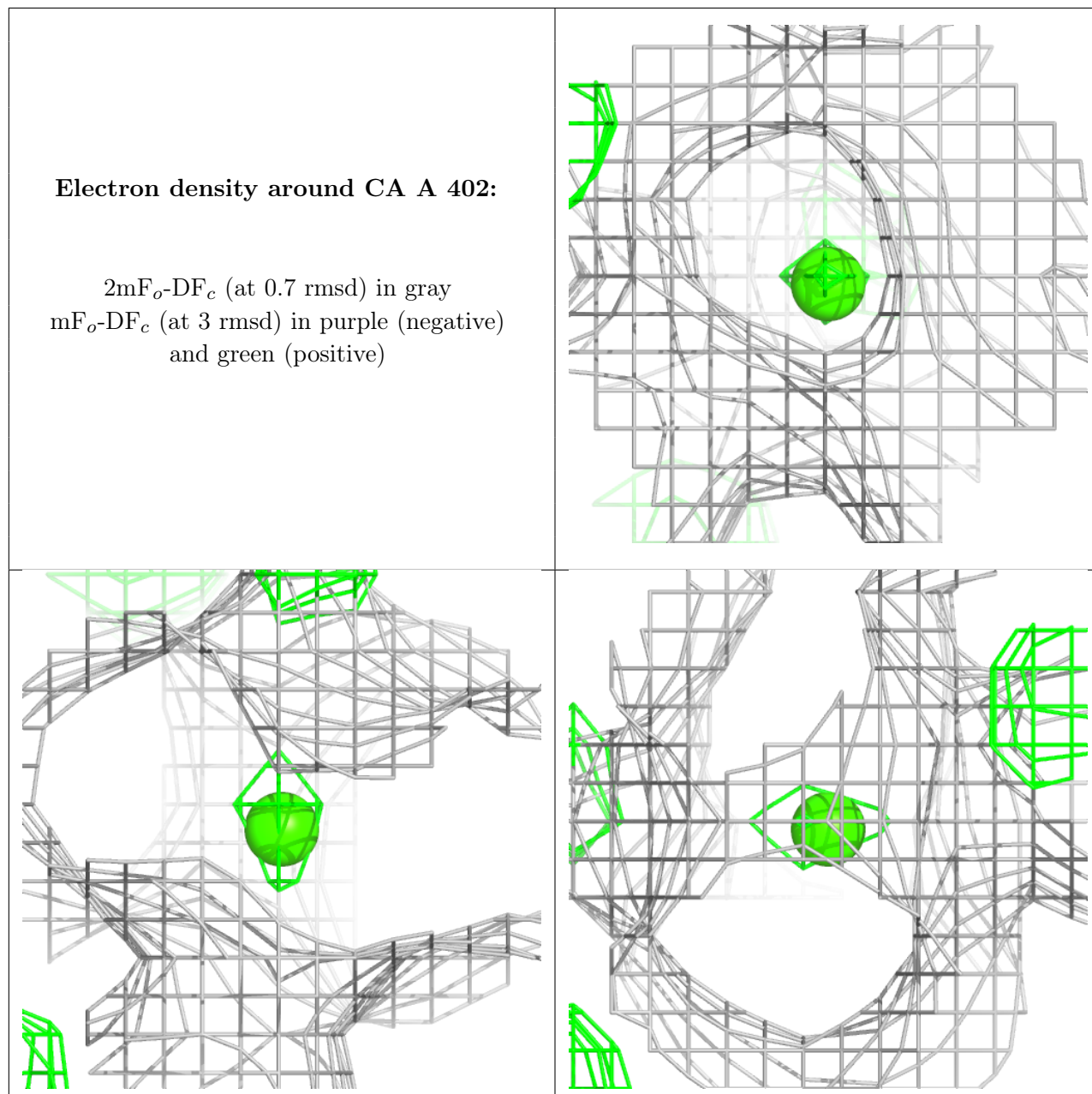
Electron density around CA B 402:

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



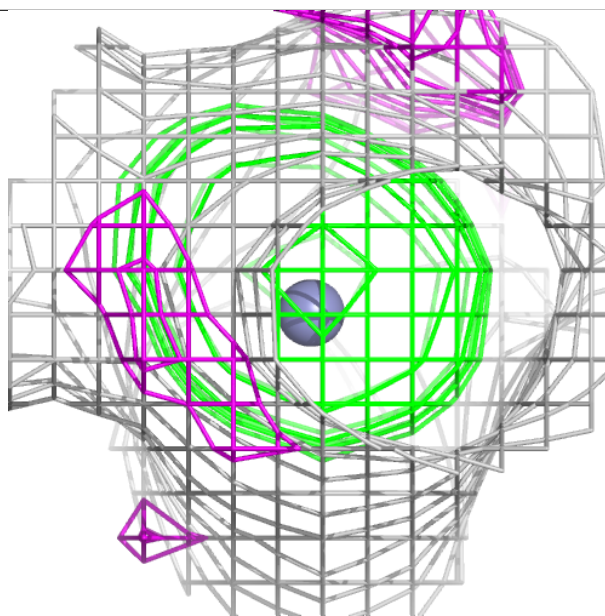
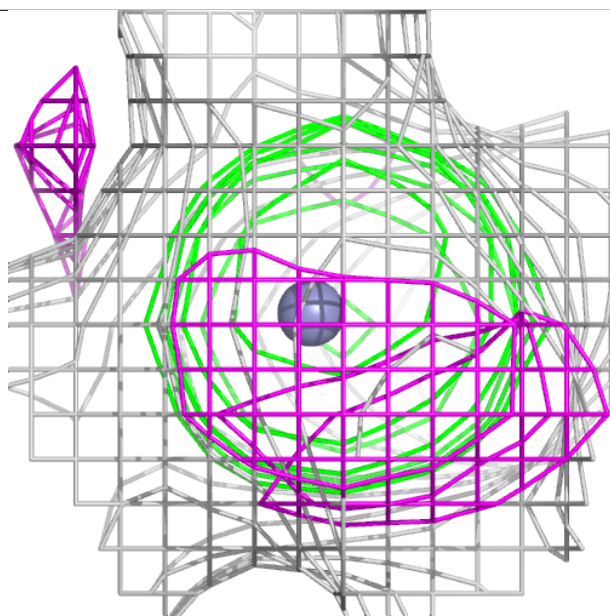
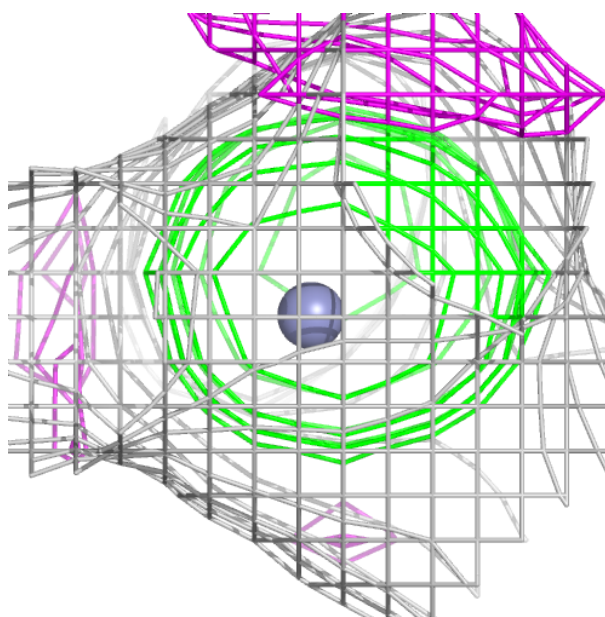
Electron density around CA A 402:

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



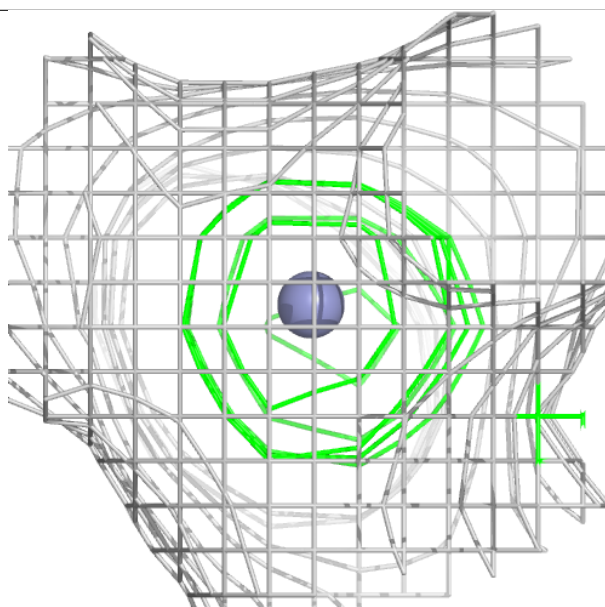
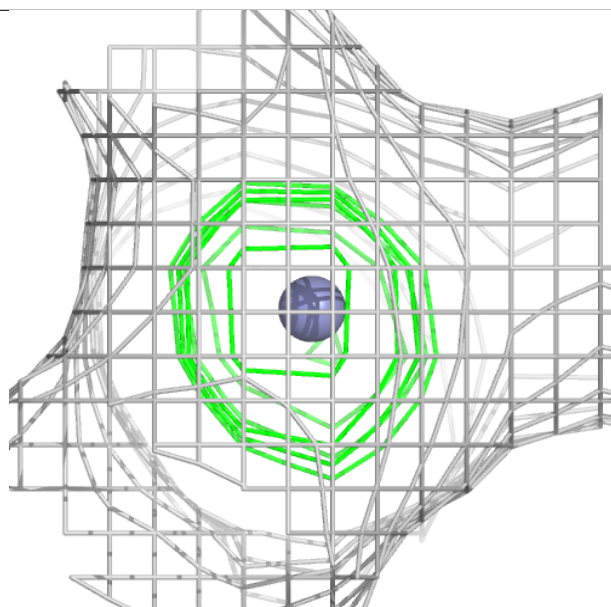
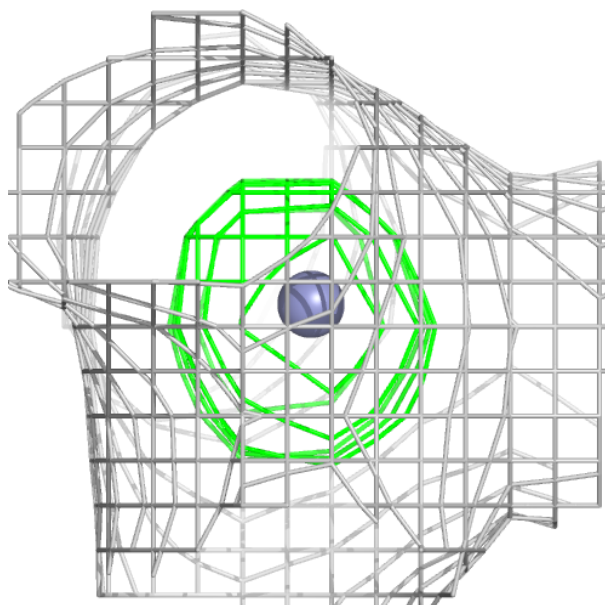
Electron density around ZN A 401:

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



Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.