Full wwPDB X-ray Structure Validation Report (i)

Apr 24, 2025 – 12:13 PM JST

PDB ID	:	9L3C / pdb_00009l3c
Title	:	Staphylococcus aureus lipase-Penfluridol complex (on the ground)
Authors	:	Kitadokoro, J.; Hirokawa, T.; Kamitani, S.; Kitadokoro, K.
Deposited on	:	2024-12-18
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 (i) 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 (i)) were used in the production of this report:

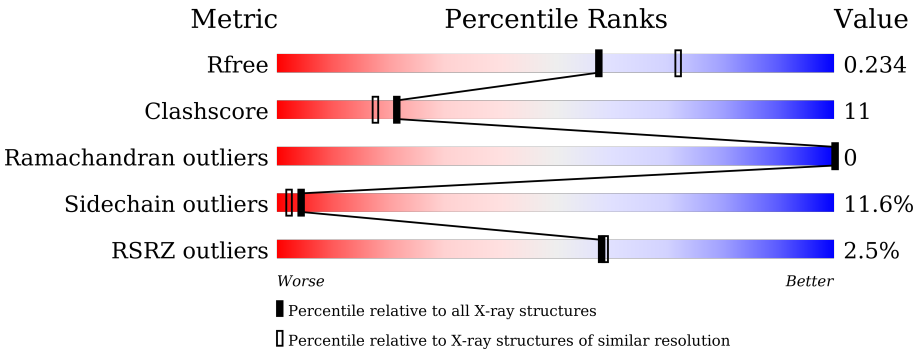
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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}	164625	3139 (2.26-2.22)
Clashscore	180529	3381 (2.26-2.22)
Ramachandran outliers	177936	3334 (2.26-2.22)
Sidechain outliers	177891	3335 (2.26-2.22)
RSRZ outliers	164620	3138 (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 <=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% 72% 18% · 6%
1	B	408	3% 72% 17% · 6%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 6328 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	conflict	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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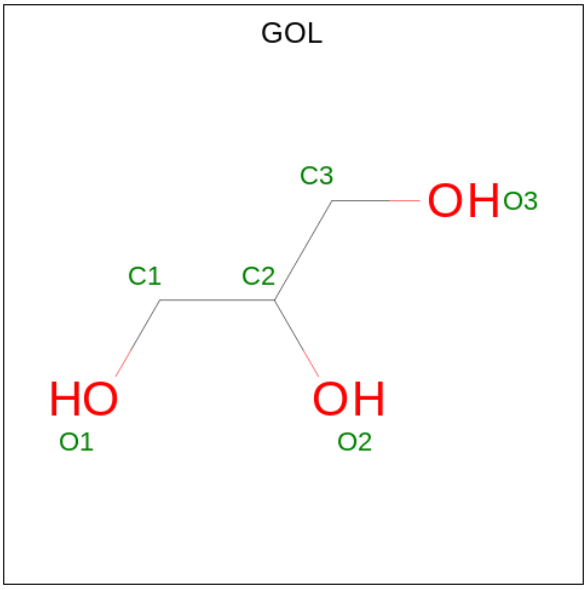
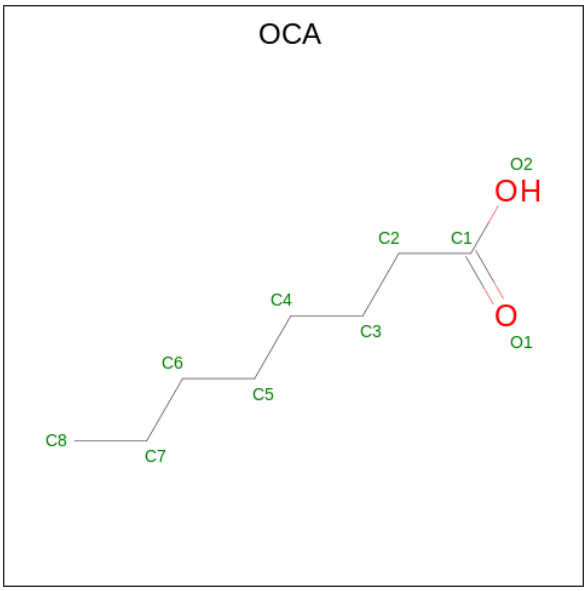
Chain	Residue	Modelled	Actual	Comment	Reference
B	68	GLN	GLU	conflict	UNP A0A0U1MWF9

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



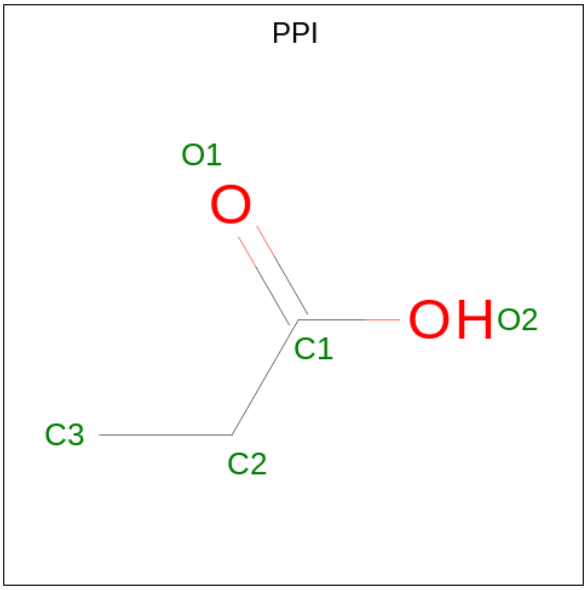
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula: $C_8H_{16}O_2$).



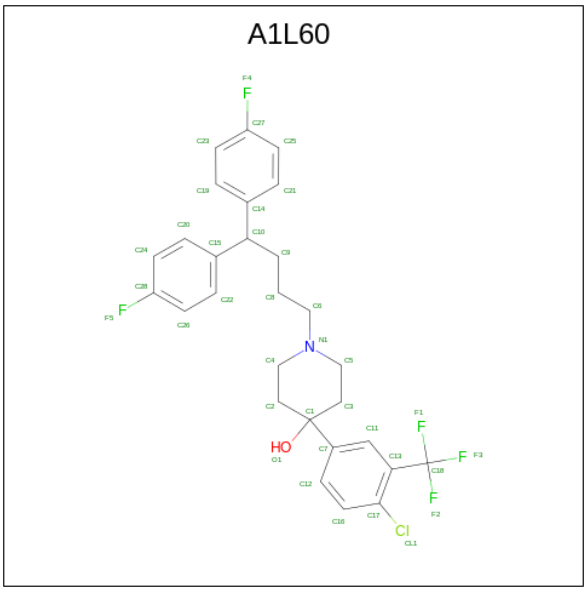
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 8 2	0	0
3	A	1	Total C O 10 8 2	0	0
3	A	1	Total C O 10 8 2	0	0

- Molecule 4 is PROPANOIC ACID (CCD ID: PPI) (formula: $C_3H_6O_2$).



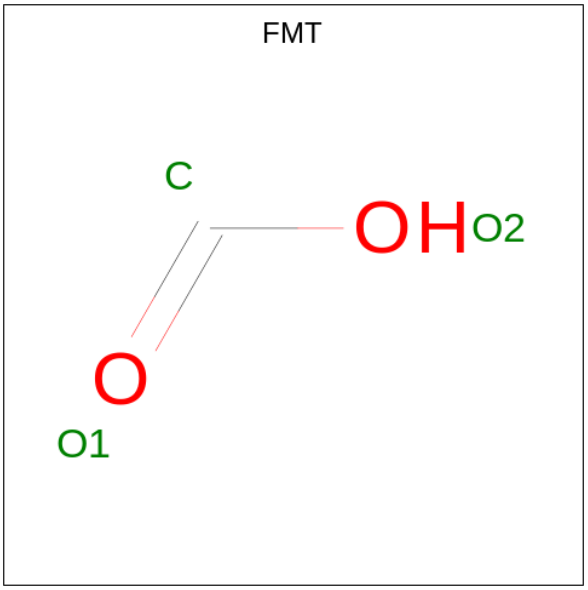
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 5 3 2	0	0
4	B	1	Total C O 5 3 2	0	0

- Molecule 5 is 1-[4,4-bis(4-fluorophenyl)butyl]-4-[4-chloranyl-3-(trifluoromethyl)phenyl]piperidin-4-ol (CCD ID: A1L60) (formula: $C_{28}H_{27}ClF_5NO$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Cl	F	N	O	0	0
			36	28	1	5	1	1		
5	B	1	Total	C	Cl	F	N	O	0	0
			36	28	1	5	1	1		

- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		

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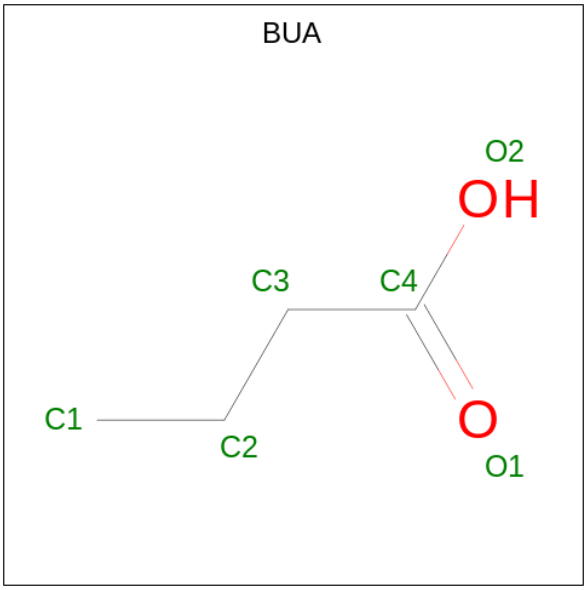
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0

- Molecule 7 is butanoic acid (CCD ID: BUA) (formula: $C_4H_8O_2$).



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

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

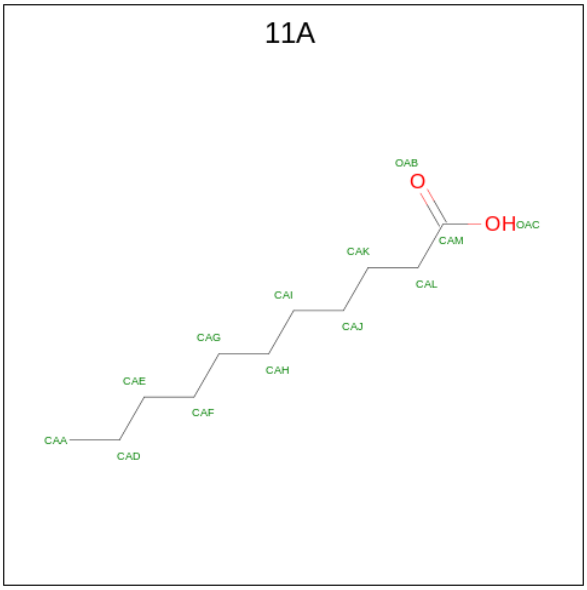
- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

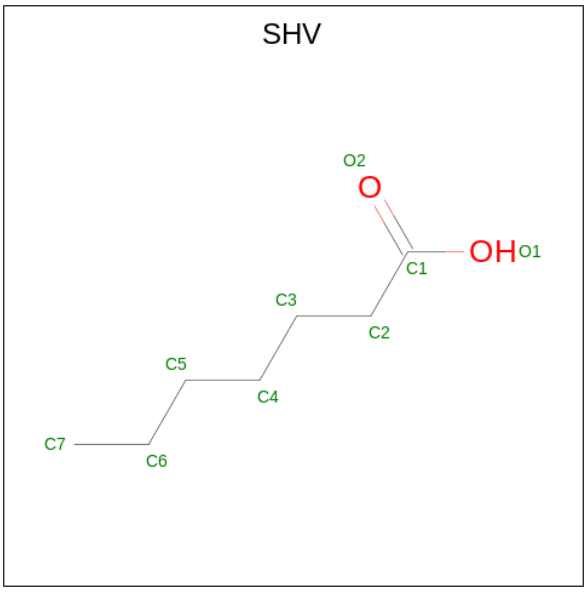
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total Cl 3 3	0	0
10	B	1	Total Cl 1 1	0	0

- Molecule 11 is UNDECANOIC ACID (CCD ID: 11A) (formula: $C_{11}H_{22}O_2$).



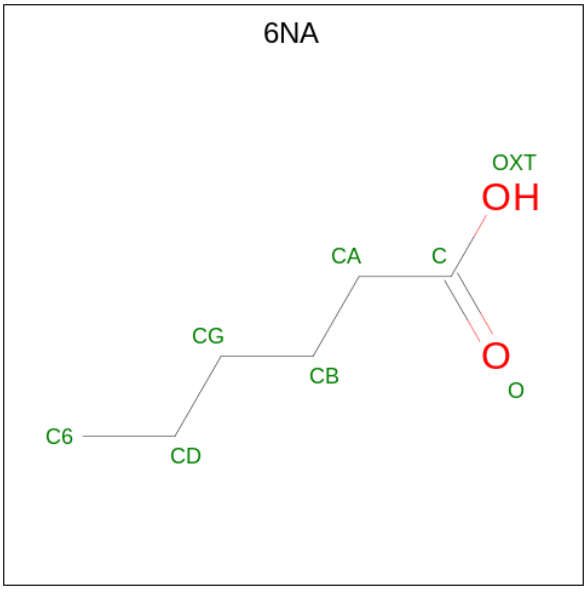
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C O 13 11 2	0	0
11	B	1	Total C O 13 11 2	0	0

- Molecule 12 is HEPTANOIC ACID (CCD ID: SHV) (formula: $C_7H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C O 9 7 2	0	0

- Molecule 13 is HEXANOIC ACID (CCD ID: 6NA) (formula: $C_6H_{12}O_2$).



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

- Molecule 14 is water.

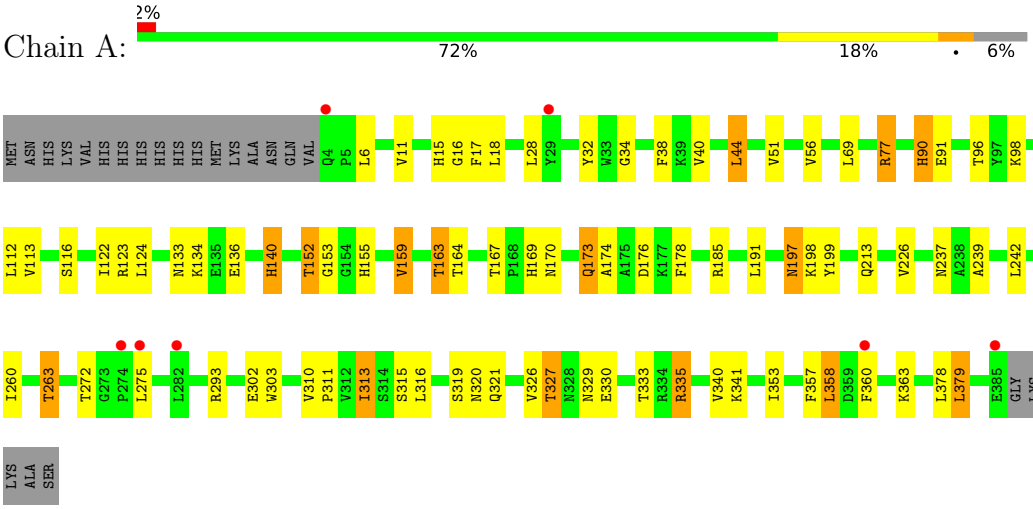
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	30	Total O 30 30	0	0
14	B	16	Total O 16 16	0	0

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.

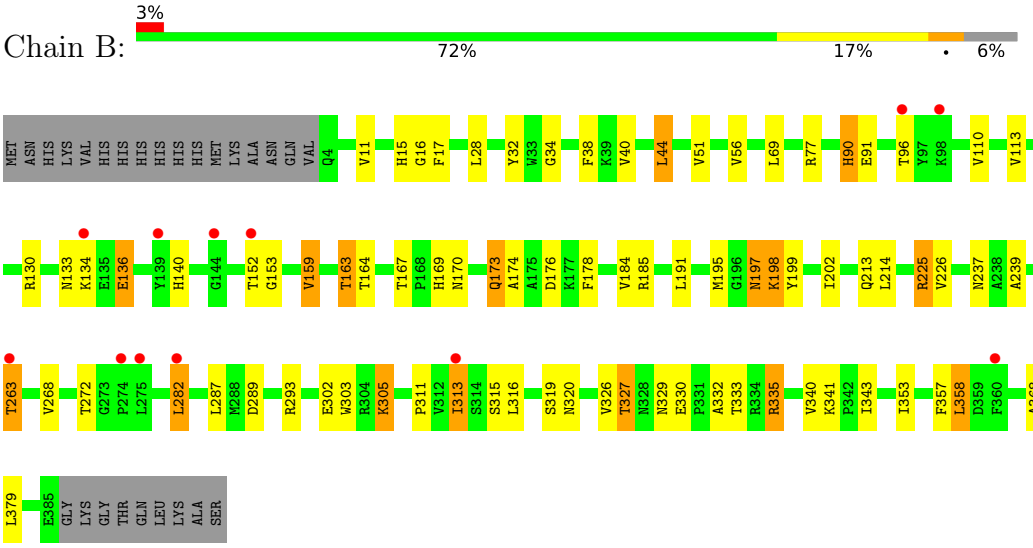
• Molecule 1: Lipase 2

Chain A:



• Molecule 1: Lipase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	127.47Å 127.47Å 252.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 2.23 47.00 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.00-2.23) 99.7 (47.00-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.190 , 0.224 0.202 , 0.234	Depositor DCC
R_{free} test set	5092 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	74.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 69.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6328	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, PPI, BUA, GOL, OCA, FMT, 11A, CL, A1L60, SHV, CA, 6NA

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	0.45	0/3106	0.80	2/4212 (0.0%)
1	B	0.45	1/3106 (0.0%)	0.77	0/4212
All	All	0.45	1/6212 (0.0%)	0.79	2/8424 (0.0%)

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	4
1	B	0	5
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	GLU	CD-OE1	6.88	1.33	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	ASN	CB-CA-C	6.37	123.14	110.40
1	A	152	THR	CA-CB-OG1	-5.21	98.07	109.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ARG	Sidechain
1	A	293	ARG	Sidechain
1	A	335	ARG	Sidechain
1	A	77	ARG	Sidechain
1	B	185	ARG	Sidechain
1	B	225	ARG	Sidechain
1	B	293	ARG	Sidechain
1	B	332	ALA	Peptide
1	B	335	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3024	0	2919	64	0
1	B	3024	0	2919	67	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	30	0	45	1	0
4	A	20	0	20	1	0
4	B	5	0	5	0	0
5	A	36	0	0	1	0
5	B	36	0	0	0	0
6	A	6	0	4	0	0
6	B	6	0	4	1	0
7	A	6	0	7	0	0
7	B	18	0	21	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	3	0	0	0	0
10	B	1	0	0	0	0
11	B	26	0	42	1	0
12	B	9	0	13	0	0
13	B	16	0	22	0	0
14	A	30	0	0	2	0
14	B	16	0	0	1	0
All	All	6328	0	6037	132	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 11.

All (132) 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:H	1:A:313:ILE:HD13	1.03	1.12
1:B:313:ILE:HD13	1:B:313:ILE:H	1.12	1.11
1:A:133:ASN:HD22	1:A:136:GLU:HG2	1.21	1.05
1:A:313:ILE:H	1:A:313:ILE:CD1	1.70	1.03
1:A:313:ILE:HD13	1:A:313:ILE:N	1.77	0.99
1:B:173:GLN:HE22	1:B:311:PRO:HG3	1.30	0.97
1:B:313:ILE:H	1:B:313:ILE:CD1	1.77	0.96
1:A:173:GLN:HE22	1:A:311:PRO:HG3	1.30	0.94
1:A:173:GLN:HE21	1:A:173:GLN:H	1.16	0.93
1:B:313:ILE:HD13	1:B:313:ILE:N	1.82	0.92
1:B:173:GLN:HE21	1:B:173:GLN:H	1.20	0.86
1:A:133:ASN:ND2	1:A:136:GLU:HG2	1.93	0.82
1:A:327:THR:HG22	1:A:330:GLU:H	1.44	0.82
1:B:197:ASN:HD22	1:B:199:TYR:H	1.26	0.81
1:A:257:ASN:HD22	1:A:259:ASN:H	1.29	0.79
1:A:256:MET:HE1	1:A:321:GLN:OE1	1.83	0.78
1:A:15:HIS:HE1	1:A:56:VAL:H	1.32	0.77
1:B:282:LEU:H	1:B:282:LEU:HD22	1.49	0.77
1:A:197:ASN:HD22	1:A:199:TYR:H	1.30	0.76
1:A:257:ASN:ND2	1:A:259:ASN:H	1.84	0.76
1:A:140:HIS:HB2	14:A:522:HOH:O	1.84	0.76
1:B:170:ASN:HD21	1:B:319:SER:H	1.34	0.75
1:B:268:VAL:HG23	1:B:343:ILE:HG21	1.68	0.74
1:A:197:ASN:ND2	1:A:199:TYR:H	1.85	0.74
1:B:133:ASN:ND2	1:B:136:GLU:HG2	2.04	0.73
1:B:327:THR:HG22	1:B:330:GLU:H	1.53	0.73
1:B:268:VAL:HG23	1:B:343:ILE:CG2	2.19	0.73
1:A:170:ASN:HD21	1:A:319:SER:H	1.37	0.72
1:B:197:ASN:ND2	1:B:199:TYR:H	1.87	0.72
1:B:15:HIS:HE1	1:B:56:VAL:H	1.35	0.71
1:A:173:GLN:HE22	1:A:311:PRO:CG	2.07	0.67
1:B:368:ALA:O	1:B:372:ILE:HG12	1.96	0.65
1:B:327:THR:CG2	1:B:329:ASN:H	2.10	0.64
1:B:303:TRP:HA	1:B:313:ILE:HD11	1.79	0.63
1:A:123:ARG:HH11	1:A:169:HIS:HD2	1.44	0.63
1:B:90:HIS:HD2	1:B:91:GLU:O	1.83	0.62
1:B:302:GLU:O	1:B:313:ILE:HD12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLY:HA3	1:B:38:PHE:O	2.02	0.60
1:B:173:GLN:HE22	1:B:311:PRO:CG	2.12	0.60
1:A:303:TRP:HA	1:A:313:ILE:HD11	1.85	0.59
1:B:163:THR:HB	1:B:263:THR:HG23	1.83	0.59
1:B:357:PHE:CE2	1:B:358:LEU:HD13	2.36	0.59
1:A:90:HIS:HD2	1:A:91:GLU:O	1.85	0.58
1:A:327:THR:CG2	1:A:329:ASN:H	2.17	0.57
1:B:123:ARG:HH11	1:B:169:HIS:HD2	1.52	0.57
1:B:268:VAL:CG2	1:B:343:ILE:HG21	2.34	0.57
1:B:133:ASN:HD22	1:B:136:GLU:HG2	1.69	0.56
1:B:198:LYS:HE2	11:B:405:11A:HAA1	1.87	0.56
1:B:15:HIS:HD2	1:B:16:GLY:O	1.88	0.56
1:A:257:ASN:HD22	1:A:257:ASN:C	2.08	0.55
1:A:34:GLY:HA3	1:A:38:PHE:O	2.06	0.55
1:A:163:THR:HB	1:A:263:THR:HG23	1.89	0.55
1:B:327:THR:HG22	1:B:329:ASN:H	1.72	0.55
1:A:173:GLN:H	1:A:173:GLN:NE2	1.97	0.55
1:B:170:ASN:HD21	1:B:319:SER:N	2.04	0.55
1:B:214:LEU:HG	1:B:225:ARG:HH12	1.72	0.54
1:A:15:HIS:CE1	1:A:56:VAL:H	2.20	0.54
1:A:155:HIS:HD2	14:A:508:HOH:O	1.90	0.54
1:A:327:THR:HG23	1:A:329:ASN:H	1.73	0.54
1:A:302:GLU:O	1:A:313:ILE:HD12	2.07	0.54
1:A:164:THR:HB	1:A:167:THR:OG1	2.08	0.53
1:B:164:THR:HB	1:B:167:THR:OG1	2.08	0.53
1:B:40:VAL:O	1:B:44:LEU:HB2	2.08	0.53
1:B:305:LYS:HE3	1:B:305:LYS:H	1.74	0.53
1:B:90:HIS:CD2	1:B:91:GLU:O	2.63	0.52
1:B:173:GLN:HE21	1:B:173:GLN:N	2.00	0.52
1:A:170:ASN:HD21	1:A:319:SER:N	2.05	0.52
1:B:126:GLU:OE1	1:B:130:ARG:NH1	2.44	0.51
1:A:357:PHE:CE2	1:A:358:LEU:HD13	2.46	0.50
1:B:159:VAL:O	1:B:260:ILE:HG12	2.11	0.50
1:B:173:GLN:H	1:B:173:GLN:NE2	1.99	0.50
1:A:173:GLN:HE21	1:A:173:GLN:N	1.97	0.50
1:A:15:HIS:HD2	1:A:16:GLY:O	1.95	0.49
1:B:15:HIS:CE1	1:B:56:VAL:H	2.22	0.49
1:B:195:MET:HE2	1:B:202:ILE:HG12	1.93	0.49
1:A:133:ASN:HD22	1:A:136:GLU:CG	2.08	0.49
1:A:123:ARG:NH1	1:A:169:HIS:HD2	2.10	0.49
1:A:152:THR:HG22	1:A:153:GLY:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:THR:HG23	1:B:329:ASN:H	1.78	0.49
1:B:302:GLU:O	1:B:313:ILE:CD1	2.61	0.48
1:A:90:HIS:CD2	1:A:91:GLU:O	2.65	0.47
1:A:197:ASN:HD22	1:A:197:ASN:C	2.18	0.47
1:B:357:PHE:CD2	1:B:358:LEU:HD13	2.49	0.47
1:B:173:GLN:NE2	1:B:311:PRO:HG3	2.12	0.47
1:A:17:PHE:CE2	1:A:18:LEU:HD13	2.50	0.47
1:A:302:GLU:O	1:A:313:ILE:CD1	2.63	0.47
1:B:32:TYR:O	1:B:353:ILE:HB	2.16	0.46
1:A:197:ASN:ND2	1:A:197:ASN:C	2.69	0.46
1:B:237:ASN:ND2	1:B:239:ALA:HB3	2.30	0.46
1:B:327:THR:HG22	1:B:329:ASN:N	2.31	0.46
1:B:197:ASN:HA	1:B:213:GLN:HE21	1.81	0.45
1:A:242:LEU:HD13	5:A:406:A1L60:CL1	2.54	0.45
1:A:173:GLN:NE2	1:A:311:PRO:HG3	2.13	0.45
1:B:11:VAL:HB	1:B:51:VAL:HG12	1.98	0.45
1:A:112:LEU:HD13	1:A:122:ILE:HG23	1.97	0.45
1:A:159:VAL:O	1:A:260:ILE:HG12	2.17	0.45
1:A:237:ASN:HD22	1:A:239:ALA:H	1.65	0.45
7:B:401:BUA:H11	14:B:514:HOH:O	2.16	0.45
1:B:167:THR:O	1:B:315:SER:HA	2.17	0.45
1:A:197:ASN:HD22	1:A:198:LYS:N	2.15	0.45
1:A:360:PHE:CZ	1:B:289:ASP:OD1	2.70	0.45
1:B:44:LEU:HD12	1:B:44:LEU:HA	1.82	0.45
1:B:197:ASN:HD22	1:B:197:ASN:C	2.19	0.45
1:B:123:ARG:NH1	1:B:169:HIS:HD2	2.13	0.44
1:B:237:ASN:HD21	1:B:239:ALA:HB3	1.83	0.44
1:B:130:ARG:NH2	1:B:255:SER:OG	2.50	0.44
1:A:167:THR:O	1:A:315:SER:HA	2.17	0.44
1:A:327:THR:HB	1:A:330:GLU:HG2	1.99	0.44
1:A:11:VAL:HB	1:A:51:VAL:HG12	1.99	0.43
1:B:152:THR:HG22	1:B:153:GLY:O	2.18	0.43
1:B:327:THR:HG22	1:B:330:GLU:N	2.26	0.43
1:A:174:ALA:O	1:A:178:PHE:HB3	2.19	0.42
1:A:116:SER:HA	1:A:167:THR:HA	2.01	0.42
1:A:379:LEU:HD12	1:A:379:LEU:HA	1.92	0.42
1:B:197:ASN:HD22	1:B:198:LYS:N	2.17	0.42
1:A:256:MET:CE	1:A:321:GLN:OE1	2.62	0.42
1:B:174:ALA:O	1:B:178:PHE:HB3	2.20	0.42
1:A:237:ASN:ND2	1:A:239:ALA:HB3	2.35	0.42
1:A:40:VAL:O	1:A:44:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:PHE:CD2	1:A:358:LEU:HD13	2.56	0.41
1:B:197:ASN:ND2	1:B:197:ASN:C	2.74	0.41
1:A:197:ASN:HA	1:A:213:GLN:HE21	1.84	0.41
1:A:257:ASN:HD22	1:A:259:ASN:N	2.07	0.41
1:A:32:TYR:O	1:A:353:ILE:HB	2.20	0.41
1:B:17:PHE:N	6:B:407:FMT:H	2.35	0.41
1:B:163:THR:HA	1:B:263:THR:O	2.21	0.41
3:A:402:OCA:H51	4:A:417:PPI:H22	2.02	0.40
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.89	0.40
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.87	0.40
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.93	0.40
1:A:17:PHE:CZ	1:A:18:LEU:HD13	2.56	0.40
1:B:197:ASN:HD22	1:B:199:TYR:N	2.07	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%)	373 (98%)	7 (2%)	0	100	100
1	B	380/408 (93%)	373 (98%)	7 (2%)	0	100	100
All	All	760/816 (93%)	746 (98%)	14 (2%)	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%)	281 (88%)	38 (12%)	4 2
1	B	319/341 (94%)	283 (89%)	36 (11%)	4 2
All	All	638/682 (94%)	564 (88%)	74 (12%)	4 2

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	28	LEU
1	A	44	LEU
1	A	69	LEU
1	A	77	ARG
1	A	90	HIS
1	A	96	THR
1	A	98	LYS
1	A	108	LYS
1	A	110	VAL
1	A	113	VAL
1	A	124	LEU
1	A	134	LYS
1	A	140	HIS
1	A	159	VAL
1	A	163	THR
1	A	173	GLN
1	A	176	ASP
1	A	191	LEU
1	A	197	ASN
1	A	226	VAL
1	A	257	ASN
1	A	263	THR
1	A	272	THR
1	A	275	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

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Mol	Chain	Res	Type
1	A	341	LYS
1	A	358	LEU
1	A	363	LYS
1	A	378	LEU
1	A	379	LEU
1	B	28	LEU
1	B	44	LEU
1	B	69	LEU
1	B	77	ARG
1	B	90	HIS
1	B	96	THR
1	B	110	VAL
1	B	113	VAL
1	B	124	LEU
1	B	134	LYS
1	B	140	HIS
1	B	159	VAL
1	B	163	THR
1	B	173	GLN
1	B	176	ASP
1	B	184	VAL
1	B	191	LEU
1	B	197	ASN
1	B	198	LYS
1	B	226	VAL
1	B	263	THR
1	B	272	THR
1	B	282	LEU
1	B	305	LYS
1	B	313	ILE
1	B	316	LEU
1	B	320	ASN
1	B	326	VAL
1	B	327	THR
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 (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	90	HIS
1	A	133	ASN
1	A	169	HIS
1	A	170	ASN
1	A	173	GLN
1	A	197	ASN
1	A	213	GLN
1	A	237	ASN
1	A	257	ASN
1	A	259	ASN
1	A	369	ASN
1	B	15	HIS
1	B	90	HIS
1	B	133	ASN
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	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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 33 ligands modelled in this entry, 8 are monoatomic - leaving 25 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	PPI	A	405	-	4,4,4	0.87	0	4,4,4	0.98	0
4	PPI	A	417	-	4,4,4	0.87	0	4,4,4	0.80	0
7	BUA	B	401	-	5,5,5	0.93	0	5,5,5	1.11	0
3	OCA	A	402	-	9,9,9	0.85	1 (11%)	9,9,9	0.80	0
5	A1L60	A	406	-	39,39,39	0.56	1 (2%)	56,57,57	1.50	10 (17%)
4	PPI	A	404	-	4,4,4	0.88	0	4,4,4	0.81	0
6	FMT	A	407	-	2,2,2	1.64	1 (50%)	1,1,1	0.06	0
7	BUA	A	409	-	5,5,5	1.44	1 (20%)	5,5,5	0.97	0
3	OCA	A	410	-	9,9,9	1.07	1 (11%)	9,9,9	0.98	1 (11%)
4	PPI	B	416	-	4,4,4	1.05	0	4,4,4	0.78	0
13	6NA	B	412	-	7,7,7	0.80	0	7,7,7	0.93	0
12	SHV	B	409	-	8,8,8	0.92	0	8,8,8	0.94	0
6	FMT	B	407	-	2,2,2	1.66	1 (50%)	1,1,1	0.05	0
7	BUA	B	403	-	5,5,5	1.08	0	5,5,5	0.94	0
13	6NA	B	413	-	7,7,7	0.78	0	7,7,7	0.86	0
2	GOL	A	401	-	5,5,5	0.17	0	5,5,5	0.45	0
11	11A	B	405	-	12,12,12	0.76	1 (8%)	12,12,12	0.88	0
6	FMT	A	408	-	2,2,2	1.57	1 (50%)	1,1,1	0.08	0
5	A1L60	B	406	-	39,39,39	0.50	0	56,57,57	1.38	8 (14%)
7	BUA	B	415	-	5,5,5	0.90	0	5,5,5	1.12	0
4	PPI	A	403	-	4,4,4	0.89	0	4,4,4	0.75	0
2	GOL	B	402	-	5,5,5	0.21	0	5,5,5	0.40	0
3	OCA	A	413	-	9,9,9	0.73	0	9,9,9	0.86	0
11	11A	B	404	-	12,12,12	0.52	0	12,12,12	0.72	0
6	FMT	B	408	-	2,2,2	1.85	1 (50%)	1,1,1	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PPI	A	405	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PPI	A	417	-	-	0/2/2/2	-
7	BUA	B	401	-	-	0/3/3/3	-
3	OCA	A	402	-	-	6/7/7/7	-
5	A1L60	A	406	-	-	12/26/38/38	0/4/4/4
4	PPI	A	404	-	-	0/2/2/2	-
7	BUA	A	409	-	-	2/3/3/3	-
3	OCA	A	410	-	-	4/7/7/7	-
4	PPI	B	416	-	-	2/2/2/2	-
13	6NA	B	412	-	-	1/5/5/5	-
12	SHV	B	409	-	-	4/6/6/6	-
7	BUA	B	403	-	-	3/3/3/3	-
13	6NA	B	413	-	-	2/5/5/5	-
2	GOL	A	401	-	-	0/4/4/4	-
11	11A	B	405	-	-	8/10/10/10	-
5	A1L60	B	406	-	-	5/26/38/38	0/4/4/4
7	BUA	B	415	-	-	2/3/3/3	-
4	PPI	A	403	-	-	0/2/2/2	-
2	GOL	B	402	-	-	4/4/4/4	-
3	OCA	A	413	-	-	1/7/7/7	-
11	11A	B	404	-	-	9/10/10/10	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	410	OCA	O1-C1	2.64	1.30	1.22
6	B	408	FMT	O2-C	2.60	1.41	1.28
6	B	407	FMT	O2-C	2.33	1.40	1.28
6	A	407	FMT	O2-C	2.31	1.40	1.28
6	A	408	FMT	O2-C	2.21	1.39	1.28
3	A	402	OCA	O1-C1	2.21	1.29	1.22
5	A	406	A1L60	C17-C13	2.19	1.43	1.39
7	A	409	BUA	O1-C4	2.12	1.29	1.22
11	B	405	11A	OAB-CAM	2.10	1.29	1.22

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	406	A1L60	C18-C13-C17	6.08	125.85	121.88
5	B	406	A1L60	C18-C13-C17	5.82	125.68	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	406	A1L60	O1-C1-C2	3.72	116.13	107.69
5	A	406	A1L60	C13-C17-CL1	2.80	124.89	121.68
5	B	406	A1L60	C16-C17-CL1	-2.73	112.92	118.41
5	B	406	A1L60	C3-C5-N1	-2.56	108.71	111.23
5	A	406	A1L60	C16-C17-CL1	-2.54	113.32	118.41
5	A	406	A1L60	C22-C15-C10	2.50	127.59	120.81
5	B	406	A1L60	C13-C17-CL1	2.48	124.53	121.68
5	A	406	A1L60	C20-C15-C10	-2.42	114.24	120.81
5	B	406	A1L60	C22-C15-C10	2.37	127.25	120.81
5	B	406	A1L60	C2-C4-N1	-2.36	108.90	111.23
5	A	406	A1L60	C9-C10-C14	2.30	119.02	112.44
5	B	406	A1L60	C20-C15-C10	-2.30	114.57	120.81
5	B	406	A1L60	O1-C1-C2	2.29	112.88	107.69
5	A	406	A1L60	F3-C18-F2	-2.27	97.39	105.72
5	A	406	A1L60	C3-C5-N1	-2.24	109.03	111.23
5	A	406	A1L60	C2-C1-C7	-2.19	106.66	111.06
3	A	410	OCA	O1-C1-C2	-2.09	116.37	123.08

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402	GOL	C1-C2-C3-O3
5	A	406	A1L60	C17-C13-C18-F1
5	A	406	A1L60	C17-C13-C18-F2
5	A	406	A1L60	C17-C13-C18-F3
5	A	406	A1L60	C14-C10-C9-C8
5	B	406	A1L60	C15-C10-C9-C8
5	B	406	A1L60	C14-C10-C9-C8
5	A	406	A1L60	C15-C10-C9-C8
5	B	406	A1L60	C8-C6-N1-C4
5	A	406	A1L60	C8-C6-N1-C4
5	A	406	A1L60	N1-C6-C8-C9
5	B	406	A1L60	N1-C6-C8-C9
3	A	402	OCA	C1-C2-C3-C4
13	B	413	6NA	C-CA-CB-CG
11	B	405	11A	CAF-CAG-CAH-CAI
5	B	406	A1L60	C8-C6-N1-C5
11	B	405	11A	CAI-CAJ-CAK-CAL
3	A	410	OCA	C4-C5-C6-C7
13	B	413	6NA	CA-CB-CG-CD
2	B	402	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	B	404	11A	CAG-CAH-CAI-CAJ
5	A	406	A1L60	C8-C6-N1-C5
11	B	405	11A	CAH-CAI-CAJ-CAK
2	B	402	GOL	O1-C1-C2-O2
2	B	402	GOL	O2-C2-C3-O3
11	B	404	11A	CAI-CAJ-CAK-CAL
7	B	403	BUA	C1-C2-C3-C4
3	A	413	OCA	C4-C5-C6-C7
11	B	405	11A	CAE-CAF-CAG-CAH
3	A	402	OCA	C2-C3-C4-C5
11	B	405	11A	CAJ-CAK-CAL-CAM
11	B	404	11A	CAJ-CAK-CAL-CAM
11	B	404	11A	CAD-CAE-CAF-CAG
3	A	402	OCA	C5-C6-C7-C8
11	B	404	11A	CAE-CAF-CAG-CAH
11	B	404	11A	CAA-CAD-CAE-CAF
13	B	412	6NA	C6-CD-CG-CB
12	B	409	SHV	C4-C5-C6-C7
4	B	416	PPI	O1-C1-C2-C3
4	B	416	PPI	O2-C1-C2-C3
5	A	406	A1L60	C11-C13-C18-F3
3	A	410	OCA	C2-C3-C4-C5
12	B	409	SHV	C1-C2-C3-C4
5	A	406	A1L60	C6-C8-C9-C10
12	B	409	SHV	O2-C1-C2-C3
3	A	410	OCA	O2-C1-C2-C3
7	B	403	BUA	C2-C3-C4-O1
12	B	409	SHV	O1-C1-C2-C3
7	B	403	BUA	C2-C3-C4-O2
5	A	406	A1L60	C11-C13-C18-F2
5	A	406	A1L60	C11-C13-C18-F1
7	A	409	BUA	C2-C3-C4-O2
7	B	415	BUA	C2-C3-C4-O2
3	A	410	OCA	O1-C1-C2-C3
11	B	404	11A	CAK-CAL-CAM-OAC
3	A	402	OCA	O2-C1-C2-C3
7	B	415	BUA	C2-C3-C4-O1
3	A	402	OCA	O1-C1-C2-C3
11	B	405	11A	CAG-CAH-CAI-CAJ
7	A	409	BUA	C2-C3-C4-O1
11	B	404	11A	CAH-CAI-CAJ-CAK
11	B	404	11A	CAK-CAL-CAM-OAB

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Mol	Chain	Res	Type	Atoms
3	A	402	OCA	C4-C5-C6-C7
11	B	405	11A	CAK-CAL-CAM-OAC
11	B	405	11A	CAK-CAL-CAM-OAB

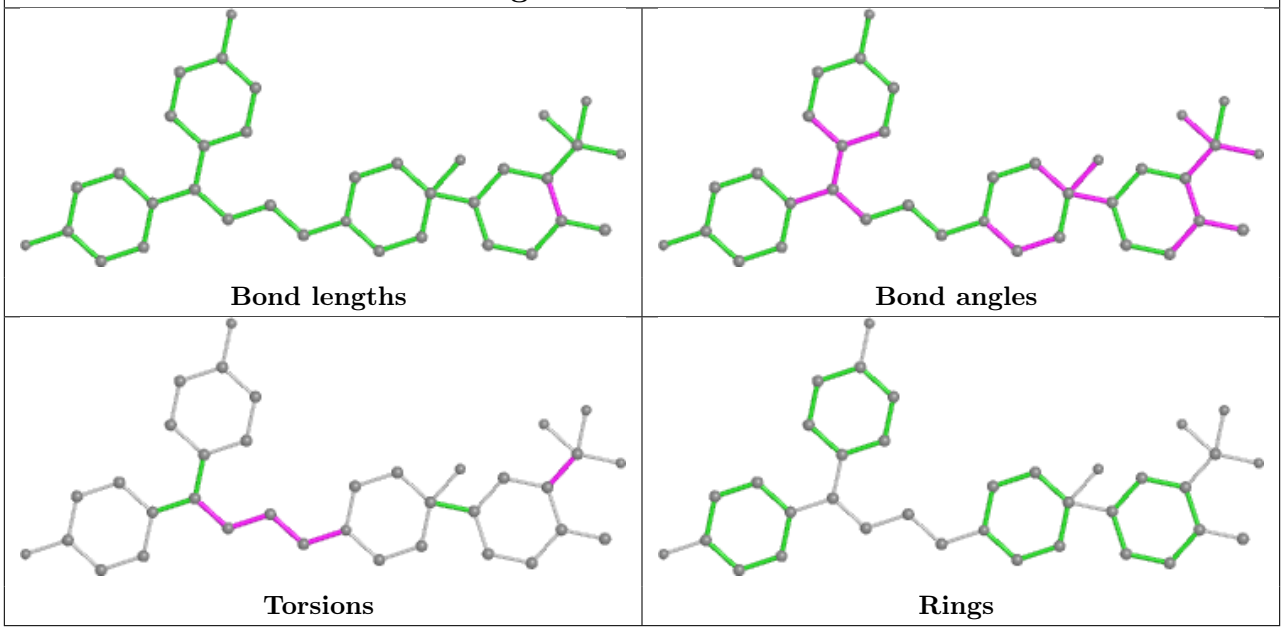
There are no ring outliers.

6 monomers are involved in 5 short contacts:

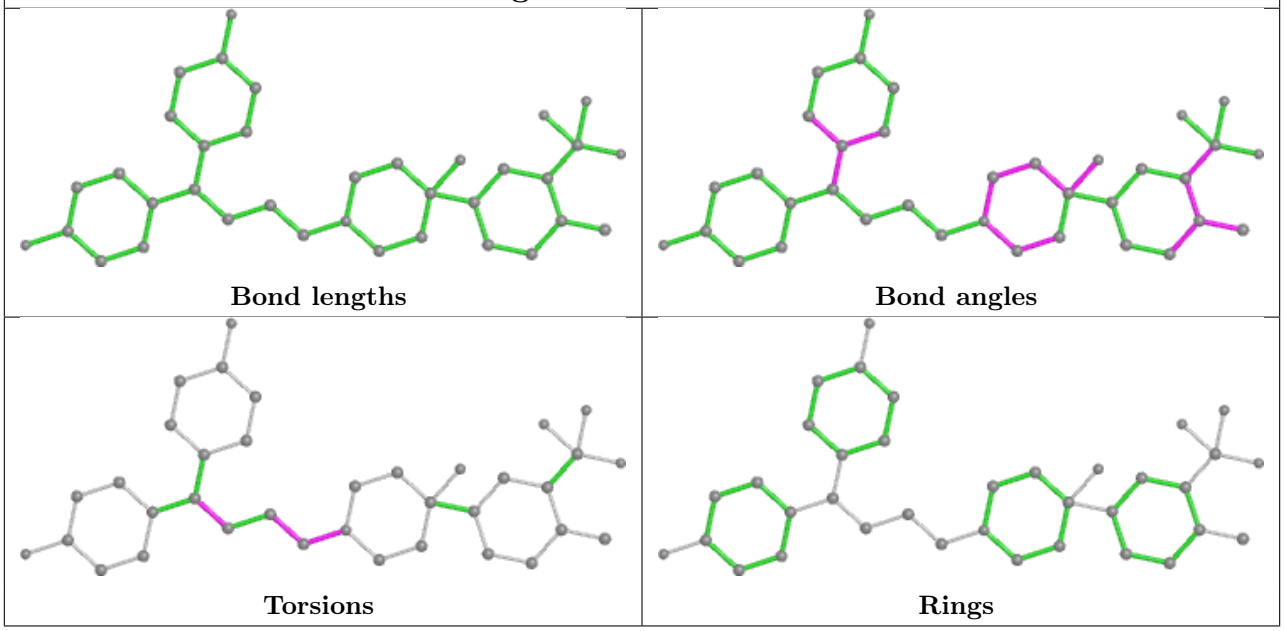
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	417	PPI	1	0
7	B	401	BUA	1	0
3	A	402	OCA	1	0
5	A	406	A1L60	1	0
6	B	407	FMT	1	0
11	B	405	11A	1	0

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 then 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 A1L60 A 406



Ligand A1L60 B 406



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, 95^{th} 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%)	-0.17	7 (1%)	67	68	43, 69, 99, 140	0
1	B	382/408 (93%)	0.06	12 (3%)	51	52	60, 79, 113, 135	0
All	All	764/816 (93%)	-0.05	19 (2%)	58	59	43, 74, 110, 140	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	PHE	7.8
1	B	360	PHE	4.9
1	B	134	LYS	4.7
1	A	274	PRO	4.1
1	B	282	LEU	4.0
1	A	282	LEU	3.5
1	A	29	TYR	3.3
1	B	139	TYR	3.2
1	B	152	THR	3.2
1	B	263	THR	2.9
1	B	96	THR	2.6
1	B	98	LYS	2.5
1	B	313	ILE	2.5
1	B	274	PRO	2.5
1	A	4	GLN	2.4
1	B	275	LEU	2.3
1	A	275	LEU	2.2
1	A	385	GLU	2.1
1	B	144	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 (i)

There are no monosaccharides 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, 95^{th} 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
4	PPI	A	403	5/5	0.76	0.29	117,119,123,124	0
4	PPI	A	405	5/5	0.78	0.36	122,127,161,162	0
4	PPI	B	416	5/5	0.79	0.27	104,118,133,140	0
13	6NA	B	413	8/8	0.79	0.37	134,148,163,163	0
7	BUA	B	403	6/6	0.83	0.36	112,141,152,164	0
4	PPI	A	417	5/5	0.84	0.26	126,136,145,149	0
13	6NA	B	412	8/8	0.84	0.33	81,106,125,129	0
4	PPI	A	404	5/5	0.84	0.29	105,110,122,131	0
3	OCA	A	413	10/10	0.87	0.23	86,94,103,106	0
12	SHV	B	409	9/9	0.87	0.25	87,102,107,112	0
11	11A	B	404	13/13	0.89	0.30	108,134,147,148	0
7	BUA	A	409	6/6	0.89	0.27	88,114,132,140	0
2	GOL	B	402	6/6	0.90	0.22	105,119,126,128	0
7	BUA	B	415	6/6	0.90	0.21	85,94,103,104	0
7	BUA	B	401	6/6	0.92	0.23	94,109,117,130	0
3	OCA	A	410	10/10	0.92	0.23	81,100,107,110	0
11	11A	B	405	13/13	0.92	0.21	84,105,118,120	0
3	OCA	A	402	10/10	0.94	0.20	82,108,112,113	0
2	GOL	A	401	6/6	0.94	0.13	101,127,130,131	0
5	A1L60	B	406	36/36	0.94	0.16	84,106,143,147	0
6	FMT	B	408	3/3	0.95	0.17	105,105,111,126	0
5	A1L60	A	406	36/36	0.95	0.14	80,105,131,150	0
6	FMT	A	408	3/3	0.96	0.17	107,107,114,125	0
6	FMT	B	407	3/3	0.97	0.16	84,84,87,100	0
6	FMT	A	407	3/3	0.97	0.11	77,77,78,93	0
10	CL	A	414	1/1	0.97	0.17	81,81,81,81	0
10	CL	A	415	1/1	0.97	0.18	106,106,106,106	0
10	CL	A	416	1/1	0.97	0.32	93,93,93,93	0
10	CL	B	414	1/1	0.98	0.18	87,87,87,87	0
9	CA	B	411	1/1	0.99	0.03	74,74,74,74	0
9	CA	A	412	1/1	0.99	0.03	82,82,82,82	0
8	ZN	B	410	1/1	1.00	0.02	78,78,78,78	0

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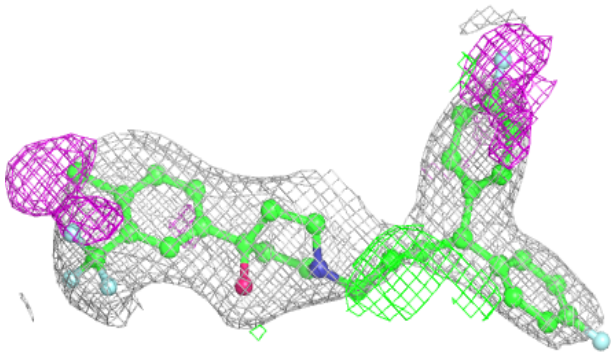
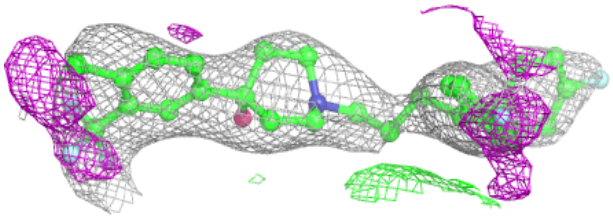
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	ZN	A	411	1/1	1.00	0.02	61,61,61,61	0

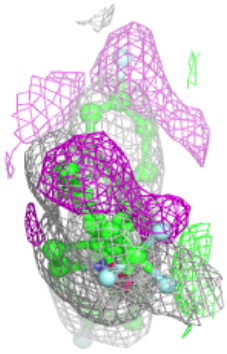
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1L60 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)

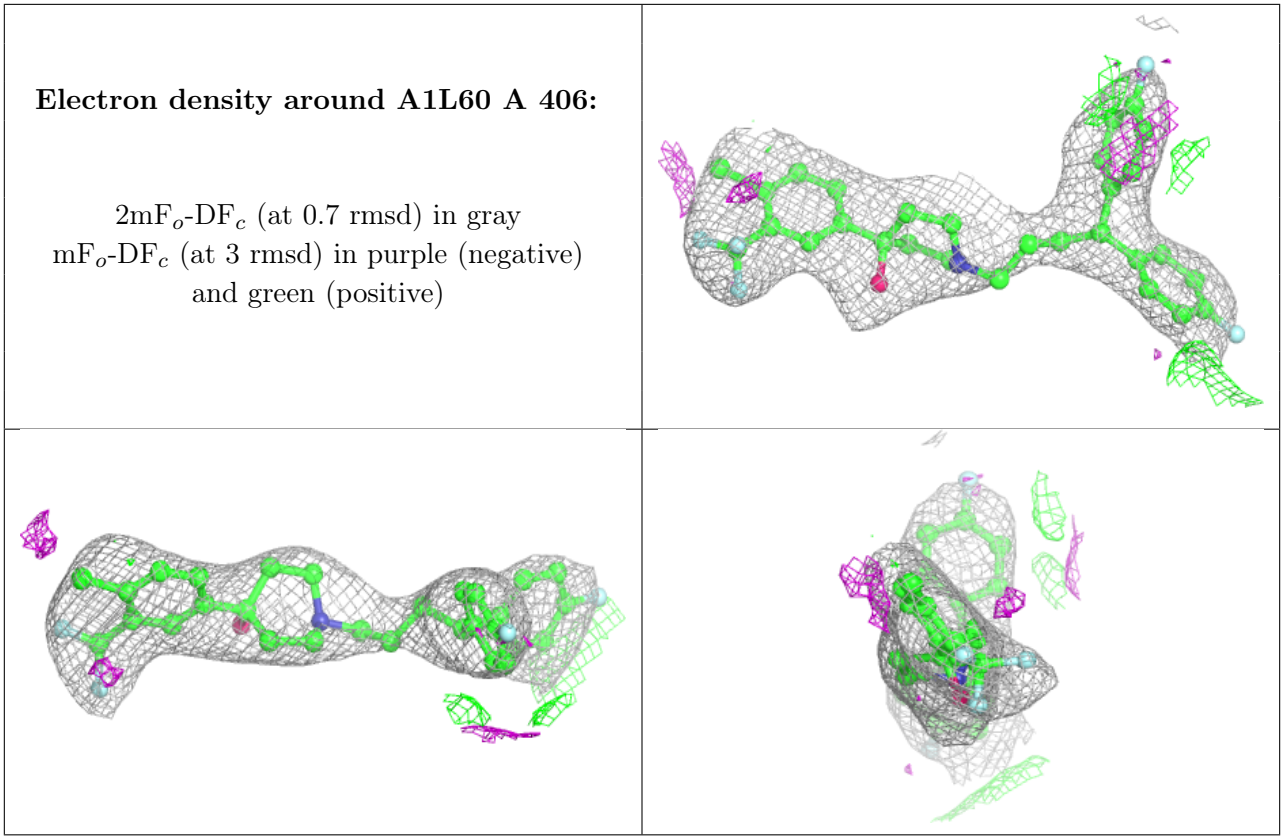






Electron density around A1L60 A 406:

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



6.5 Other polymers (i)

There are no such residues in this entry.