



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:42 PM UTC

PDB ID : 8YIB / pdb_00008yib
Title : Staphylococcus aureus lipase -PSA complex - covalent bonding state
Authors : Kitadokoro, J.; Kamitani, S.; Kitadokoro, K.
Deposited on : 2024-02-29
Resolution : 2.27 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

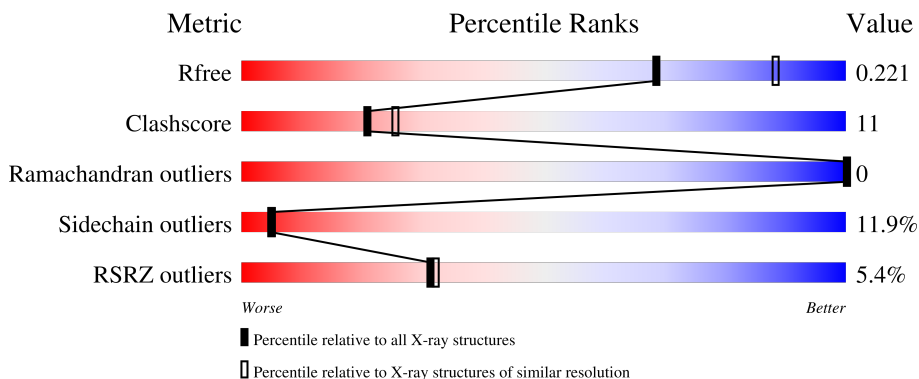
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	408	 3% 75% 15% 6%
1	B	408	 7% 72% 16% 5% 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
11	MG	A	411	-	-	-	X
2	FMT	A	416	-	-	X	-
2	FMT	B	402	-	-	X	-
2	FMT	B	414	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 6438 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:

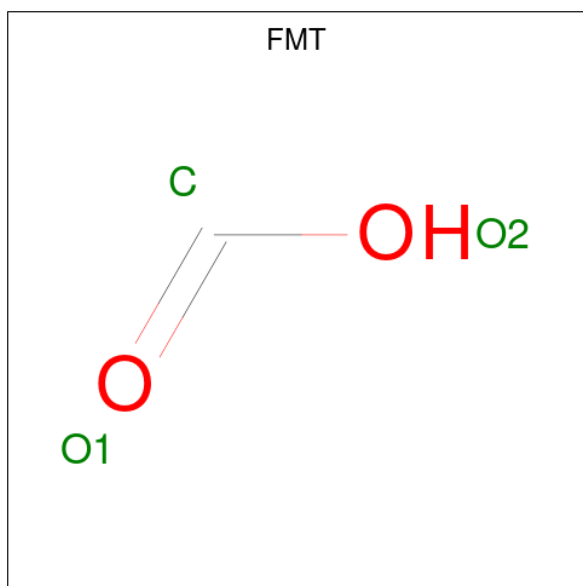
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A0U1MWF9
A	-12	ASN	-	expression tag	UNP A0A0U1MWF9
A	-11	HIS	-	expression tag	UNP A0A0U1MWF9
A	-10	LYS	-	expression tag	UNP A0A0U1MWF9
A	-9	VAL	-	expression tag	UNP A0A0U1MWF9
A	-8	HIS	-	expression tag	UNP A0A0U1MWF9
A	-7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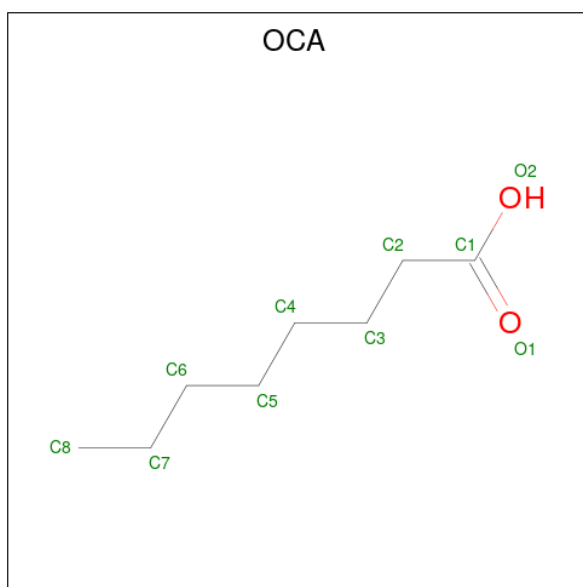
Chain	Residue	Modelled	Actual	Comment	Reference
B	68	GLN	GLU	conflict	UNP A0A0U1MWF9

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



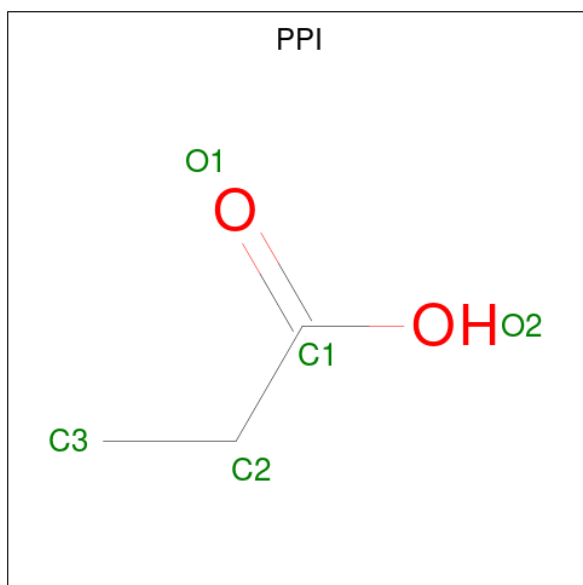
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		
2	A	1	Total	C	O	0	0
			3	1	2		
2	A	1	Total	C	O	0	0
			3	1	2		
2	A	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula: $\text{C}_8\text{H}_{16}\text{O}_2$).



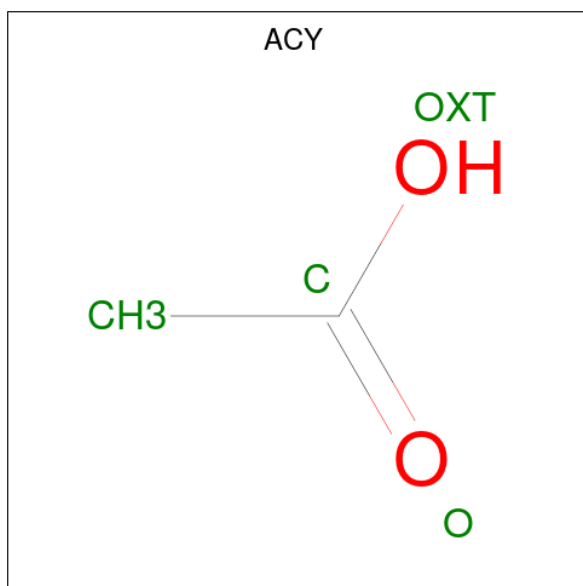
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	8	2		
3	A	1	Total	C	O	0	0
			10	8	2		
3	B	1	Total	C	O	0	0
			10	8	2		
3	B	1	Total	C	O	0	0
			10	8	2		

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



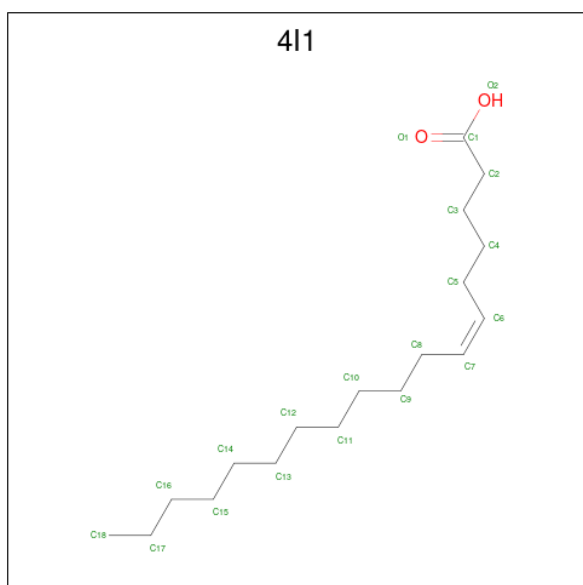
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



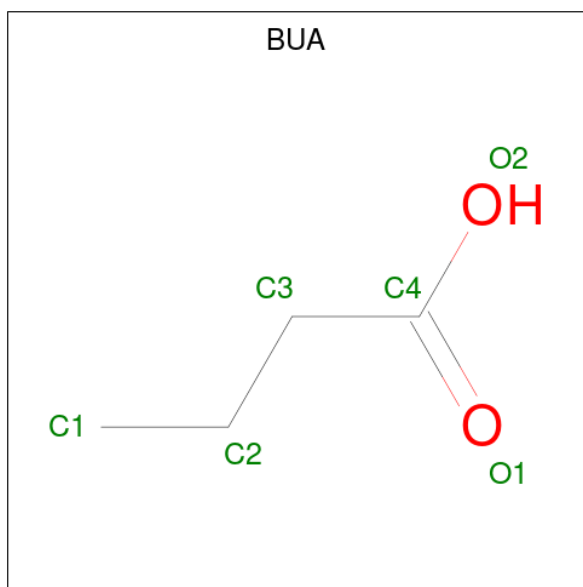
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is Petroselinic acid (CCD ID: 4I1) (formula: $C_{18}H_{34}O_2$) (labeled as "Ligand of Interest" by depositor).



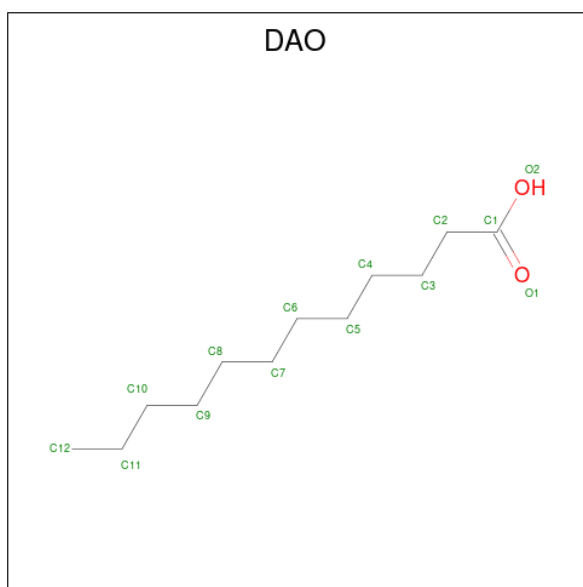
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	18	2		
6	B	1	Total	C	O	0	0
			20	18	2		

- 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	0	0
			6	4	2		
7	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 8 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

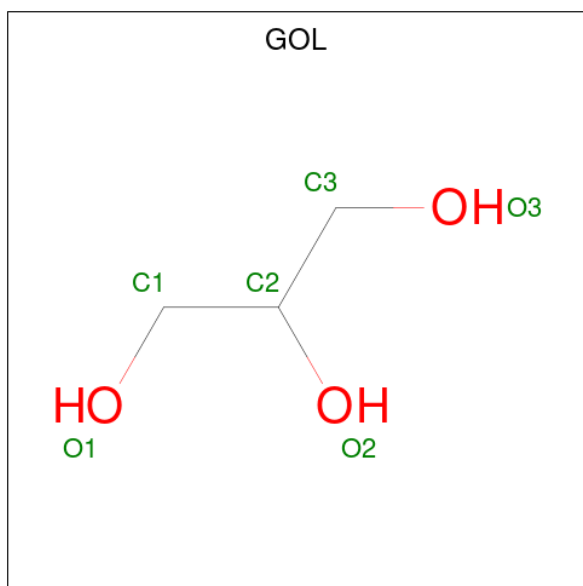
- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

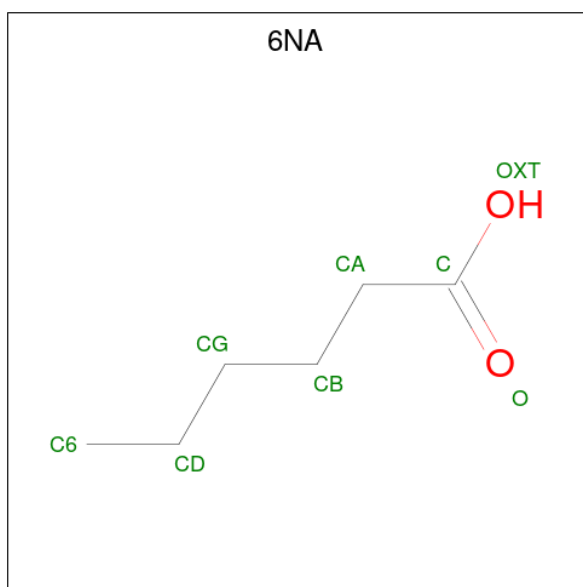
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Mg	0	0
			1	1		

- Molecule 12 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 8 6 2	0	0
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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	2	Total Cl 2 2	0	0
14	B	2	Total Cl 2 2	0	0

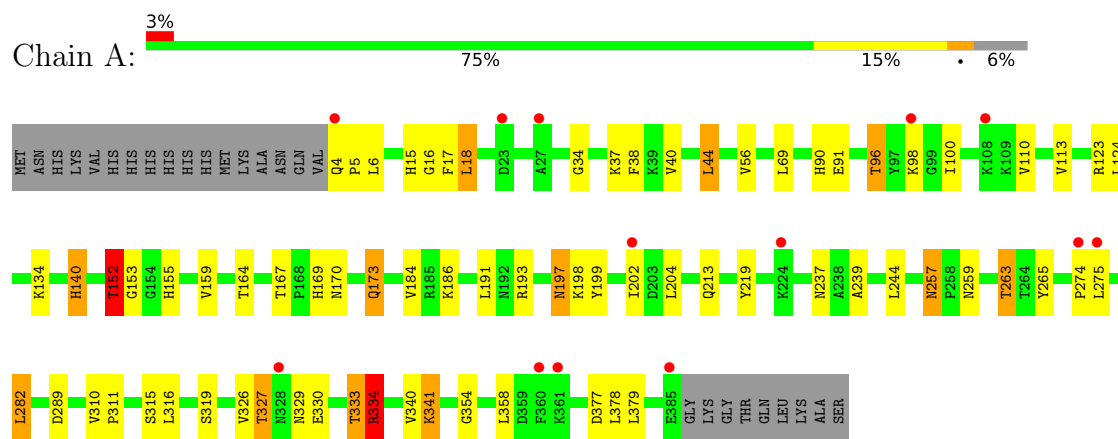
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	89	Total O 89 89	0	0
15	B	51	Total O 51 51	0	0

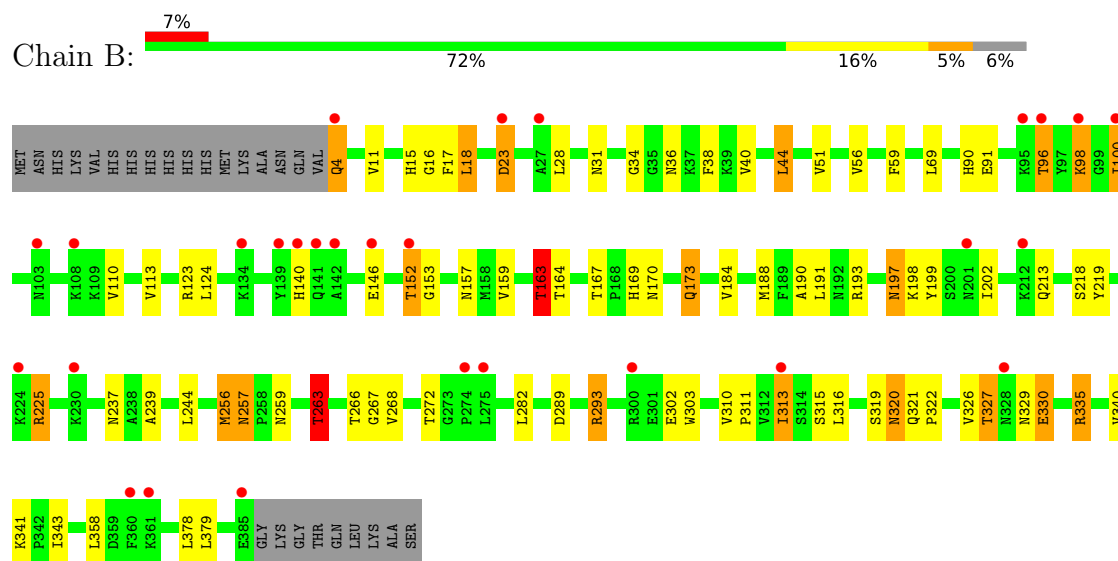
3 Residue-property plots [i](#)

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



• Molecule 1: Lipase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	132.55Å 132.55Å 249.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 2.27 48.29 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.29-2.27) 99.8 (48.29-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.197 , 0.221 0.197 , 0.221	Depositor DCC
R_{free} test set	5125 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6438	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: 4I1, BUA, DAO, PPI, ACY, OCA, CA, 6NA, ZN, GOL, MG, FMT, CL

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	0.58	0/3106	1.13	6/4212 (0.1%)
1	B	0.57	1/3106 (0.0%)	1.15	9/4212 (0.2%)
All	All	0.58	1/6212 (0.0%)	1.14	15/8424 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	310	VAL	N-CA	5.05	1.49	1.45

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	THR	CA-CB-OG1	-8.85	96.33	109.60
1	B	225	ARG	CB-CG-CD	-7.62	93.77	111.30
1	B	163	THR	CB-CA-C	7.58	123.58	109.71
1	B	335	ARG	CB-CG-CD	7.41	128.34	111.30
1	B	282	LEU	CA-C-N	-7.34	114.70	123.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	225	ARG	Sidechain
1	B	293	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3024	0	2918	56	0
1	B	3024	0	2918	78	0
2	A	15	0	10	3	0
2	B	15	0	10	8	0
3	A	20	0	30	1	0
3	B	20	0	30	0	0
4	A	5	0	5	0	0
5	A	4	0	3	0	0
6	A	20	0	0	0	0
6	B	20	0	0	1	0
7	A	6	0	7	0	0
7	B	6	0	7	0	0
8	A	28	0	46	5	0
8	B	28	0	46	6	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	1	0	0	0	0
12	A	12	0	16	2	0
12	B	18	0	24	1	0
13	A	8	0	11	0	0
13	B	16	0	22	0	0
14	A	2	0	0	1	0
14	B	2	0	0	0	0
15	A	89	0	0	4	1
15	B	51	0	0	1	0
All	All	6438	0	6103	137	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 11.

The worst 5 of 137 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)
14:A:421:CL:CL	15:A:580:HOH:O	1.90	1.21
1:B:313:ILE:H	1:B:313:ILE:HD13	0.96	1.11
1:A:327:THR:HG23	1:A:329:ASN:H	1.21	1.06
1:B:256:MET:CE	1:B:321:GLN:HB3	1.87	1.04
1:B:313:ILE:H	1:B:313:ILE:CD1	1.76	0.96

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)
15:A:575:HOH:O	15:A:575:HOH:O[5_555]	2.19	0.01

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%)	370 (97%)	10 (3%)	0	100	100
1	B	380/408 (93%)	371 (98%)	9 (2%)	0	100	100
All	All	760/816 (93%)	741 (98%)	19 (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%)	283 (89%)	36 (11%)	5	6
1	B	319/341 (94%)	279 (88%)	40 (12%)	4	4
All	All	638/682 (94%)	562 (88%)	76 (12%)	5	5

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	ASN
1	B	340	VAL
1	B	244	LEU
1	B	313	ILE
1	B	379	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	213	GLN
1	B	237	ASN
1	B	320	ASN
1	A	197	ASN
1	A	180	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 41 ligands modelled in this entry, 9 are monoatomic - leaving 32 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$
2	FMT	A	416	-	2,2,2	1.72	1 (50%)	1,1,1	0.17	0
2	FMT	A	417	-	2,2,2	1.16	0	1,1,1	0.18	0
3	OCA	A	402	-	9,9,9	0.87	0	9,9,9	1.18	1 (11%)
8	DAO	A	419	-	13,13,13	0.76	0	13,13,13	0.69	0
12	GOL	B	411	-	5,5,5	0.20	0	5,5,5	0.53	0
2	FMT	B	417	-	2,2,2	2.23	1 (50%)	1,1,1	0.29	0
12	GOL	B	412	-	5,5,5	0.13	0	5,5,5	0.41	0
6	4I1	A	405	1	19,19,19	0.94	0	19,19,19	1.53	3 (15%)
5	ACY	A	404	-	3,3,3	1.35	0	3,3,3	0.75	0
3	OCA	A	406	-	9,9,9	0.80	0	9,9,9	0.75	0
4	PPI	A	403	-	4,4,4	0.93	0	4,4,4	0.84	0
12	GOL	B	413	-	5,5,5	0.18	0	5,5,5	0.52	0
2	FMT	B	402	-	2,2,2	2.12	1 (50%)	1,1,1	0.29	0
8	DAO	A	408	-	13,13,13	0.57	0	13,13,13	0.75	0
7	BUA	A	407	-	5,5,5	1.05	0	5,5,5	1.02	0
8	DAO	B	418	-	13,13,13	0.72	0	13,13,13	0.80	0
2	FMT	B	414	-	2,2,2	1.97	1 (50%)	1,1,1	0.28	0
13	6NA	B	403	-	7,7,7	1.02	0	7,7,7	0.77	0
6	4I1	B	407	1	19,19,19	0.90	0	19,19,19	1.59	2 (10%)
2	FMT	A	415	-	2,2,2	1.98	1 (50%)	1,1,1	0.15	0
12	GOL	A	412	-	5,5,5	0.25	0	5,5,5	0.31	0
2	FMT	A	401	-	2,2,2	1.37	0	1,1,1	0.17	0
7	BUA	B	404	-	5,5,5	1.08	0	5,5,5	1.02	0
2	FMT	A	418	-	2,2,2	1.29	0	1,1,1	0.21	0
12	GOL	A	413	-	5,5,5	0.19	0	5,5,5	0.52	0
3	OCA	B	405	-	9,9,9	0.85	0	9,9,9	1.08	0
2	FMT	B	415	-	2,2,2	1.18	0	1,1,1	0.18	0
2	FMT	B	416	-	2,2,2	1.14	0	1,1,1	0.16	0
8	DAO	B	408	-	13,13,13	0.62	0	13,13,13	0.82	0
3	OCA	B	406	-	9,9,9	1.11	1 (11%)	9,9,9	1.03	0
13	6NA	B	401	-	7,7,7	0.79	0	7,7,7	1.17	1 (14%)
13	6NA	A	414	-	7,7,7	0.63	0	7,7,7	1.06	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
3	OCA	A	402	-	-	5/7/7/7	-
8	DAO	A	419	-	-	6/11/11/11	-
12	GOL	B	411	-	-	4/4/4/4	-
12	GOL	B	412	-	-	2/4/4/4	-
6	4I1	A	405	1	-	8/17/17/17	-
3	OCA	A	406	-	-	5/7/7/7	-
4	PPI	A	403	-	-	0/2/2/2	-
12	GOL	B	413	-	-	0/4/4/4	-
8	DAO	A	408	-	-	4/11/11/11	-
8	DAO	B	418	-	-	6/11/11/11	-
7	BUA	A	407	-	-	1/3/3/3	-
13	6NA	B	403	-	-	2/5/5/5	-
6	4I1	B	407	1	-	9/17/17/17	-
12	GOL	A	412	-	-	2/4/4/4	-
7	BUA	B	404	-	-	2/3/3/3	-
12	GOL	A	413	-	-	0/4/4/4	-
3	OCA	B	405	-	-	5/7/7/7	-
8	DAO	B	408	-	-	9/11/11/11	-
3	OCA	B	406	-	-	2/7/7/7	-
13	6NA	B	401	-	-	1/5/5/5	-
13	6NA	A	414	-	-	2/5/5/5	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	417	FMT	O2-C	3.13	1.44	1.28
2	B	402	FMT	O2-C	2.98	1.43	1.28
2	A	415	FMT	O2-C	2.78	1.42	1.28
2	B	414	FMT	O2-C	2.77	1.42	1.28
2	A	416	FMT	O2-C	2.41	1.41	1.28

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	407	4I1	C3-C2-C1	4.52	126.31	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	405	4I1	C3-C2-C1	4.08	125.17	114.51
6	B	407	4I1	C12-C11-C10	3.42	131.66	114.37
6	A	405	4I1	C12-C11-C10	2.99	129.46	114.37
6	A	405	4I1	C15-C14-C13	2.32	126.11	114.37

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	411	GOL	O1-C1-C2-C3
12	B	412	GOL	O1-C1-C2-C3
8	A	419	DAO	C3-C4-C5-C6
8	B	418	DAO	C3-C4-C5-C6
6	B	407	4I1	C9-C10-C11-C12

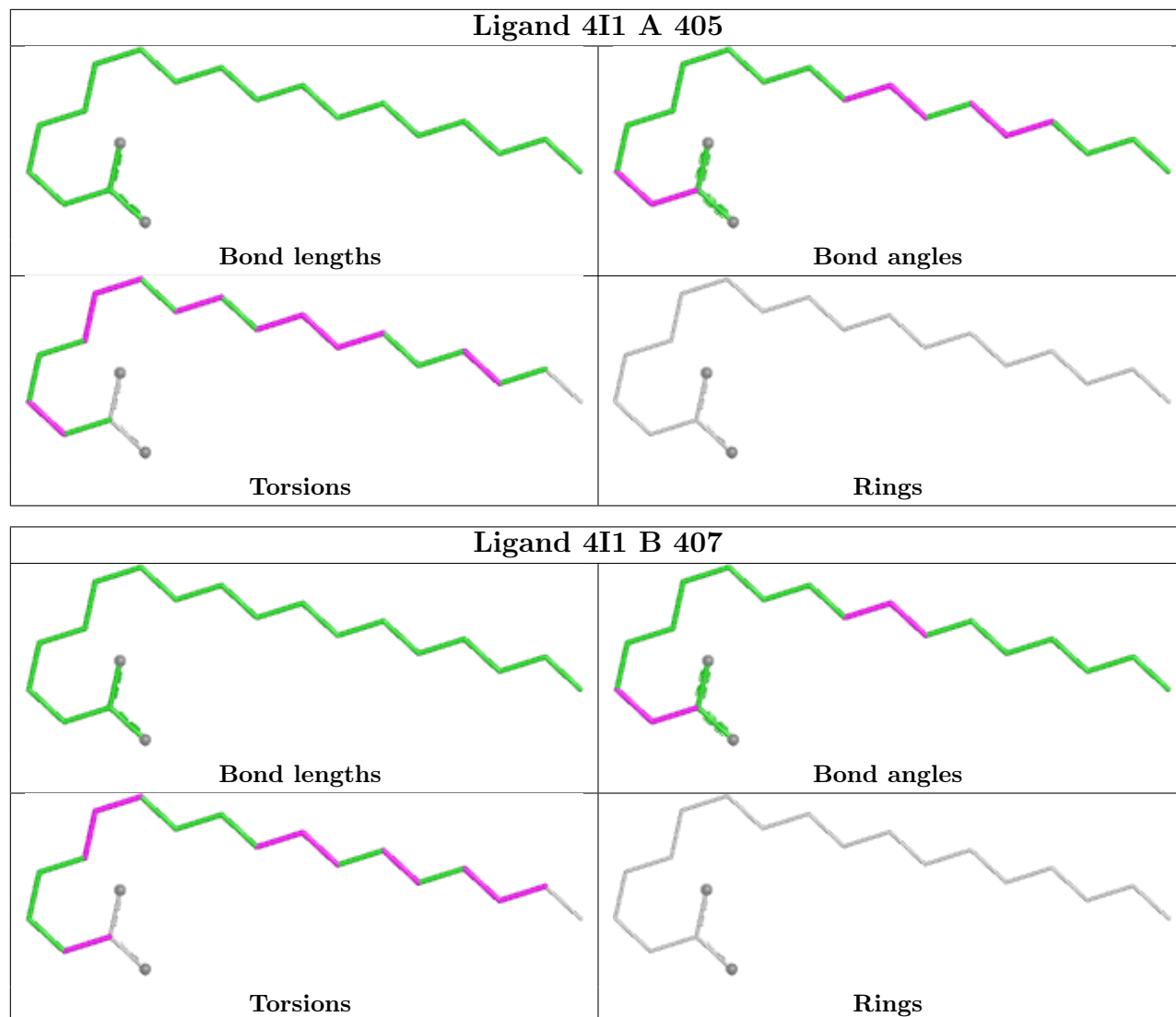
There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	416	FMT	3	0
3	A	402	OCA	1	0
8	A	419	DAO	3	0
12	B	412	GOL	1	0
2	B	402	FMT	7	0
8	A	408	DAO	2	0
8	B	418	DAO	3	0
2	B	414	FMT	1	0
6	B	407	4I1	1	0
12	A	412	GOL	2	0
8	B	408	DAO	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.02	13 (3%) 48 50	45, 57, 83, 133	0
1	B	382/408 (93%)	0.28	28 (7%) 21 22	48, 64, 92, 120	0
All	All	764/816 (93%)	0.13	41 (5%) 31 32	45, 60, 89, 133	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	5.4
1	A	274	PRO	5.3
1	B	27	ALA	5.0
1	B	360	PHE	4.4
1	B	274	PRO	4.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

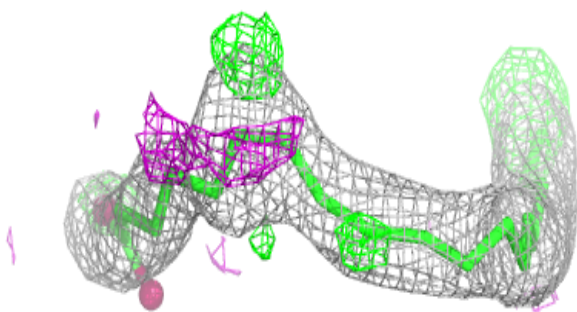
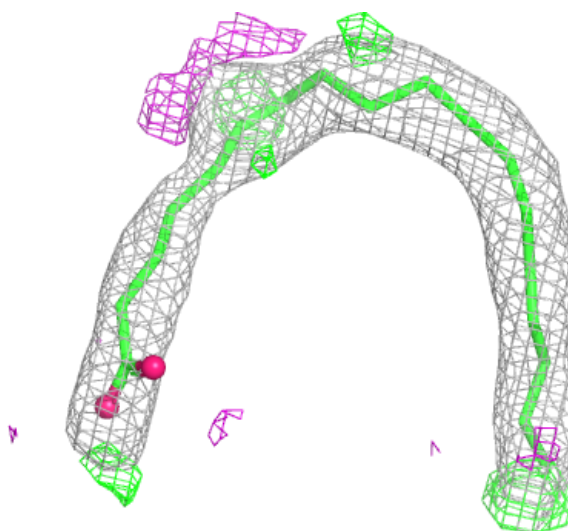
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	MG	A	411	1/1	0.67	0.69	101,101,101,101	0
2	FMT	B	415	3/3	0.70	0.23	98,98,136,137	0
2	FMT	B	414	3/3	0.77	0.44	64,64,79,113	0
2	FMT	A	415	3/3	0.78	0.39	74,74,76,122	0
5	ACY	A	404	4/4	0.78	0.30	87,97,98,106	0
7	BUA	A	407	6/6	0.78	0.37	87,109,124,128	0
2	FMT	A	401	3/3	0.78	0.28	72,72,97,107	0
12	GOL	B	412	6/6	0.82	0.23	93,116,122,128	0
13	6NA	B	403	8/8	0.82	0.26	85,100,109,109	0
3	OCA	A	406	10/10	0.83	0.32	88,114,134,136	0
12	GOL	B	411	6/6	0.83	0.30	85,92,112,115	0
12	GOL	A	412	6/6	0.84	0.24	69,101,109,112	0
3	OCA	B	406	10/10	0.84	0.26	68,77,87,94	0
2	FMT	A	417	3/3	0.85	0.37	72,72,79,96	0
4	PPI	A	403	5/5	0.87	0.23	79,86,102,108	0
2	FMT	A	418	3/3	0.87	0.31	76,76,89,98	0
13	6NA	B	401	8/8	0.88	0.24	71,83,97,100	0
2	FMT	B	402	3/3	0.89	0.38	58,58,67,102	0
7	BUA	B	404	6/6	0.89	0.26	77,101,111,116	0
8	DAO	B	408	14/14	0.89	0.25	68,89,118,119	0
14	CL	B	420	1/1	0.89	0.35	95,95,95,95	0
8	DAO	A	408	14/14	0.90	0.21	80,91,111,113	0
3	OCA	B	405	10/10	0.90	0.23	68,82,108,121	0
13	6NA	A	414	8/8	0.90	0.21	66,86,91,92	0
3	OCA	A	402	10/10	0.90	0.20	64,80,109,124	0
2	FMT	A	416	3/3	0.90	0.34	61,61,66,90	0
12	GOL	A	413	6/6	0.90	0.24	84,89,93,103	0
2	FMT	B	417	3/3	0.92	0.26	58,58,62,100	0
6	4I1	A	405	20/20	0.92	0.19	57,69,97,123	0
6	4I1	B	407	20/20	0.92	0.20	48,70,94,119	0
2	FMT	B	416	3/3	0.92	0.25	79,79,84,92	0
8	DAO	A	419	14/14	0.93	0.16	56,74,82,86	0
12	GOL	B	413	6/6	0.93	0.20	75,89,100,108	0
8	DAO	B	418	14/14	0.93	0.16	50,69,87,93	0
14	CL	B	419	1/1	0.97	0.35	81,81,81,81	0
14	CL	A	421	1/1	0.97	0.17	81,81,81,81	0
14	CL	A	420	1/1	0.98	0.31	75,75,75,75	0
9	ZN	B	409	1/1	1.00	0.01	63,63,63,63	0
10	CA	A	410	1/1	1.00	0.03	62,62,62,62	0
10	CA	B	410	1/1	1.00	0.02	57,57,57,57	0
9	ZN	A	409	1/1	1.00	0.01	52,52,52,52	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.

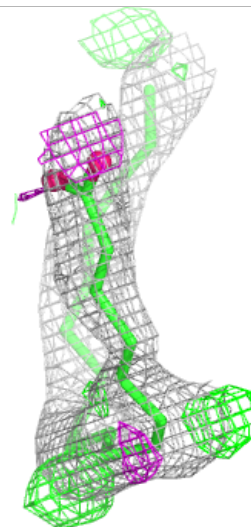
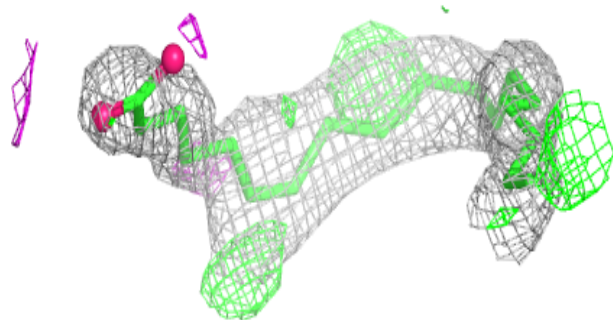
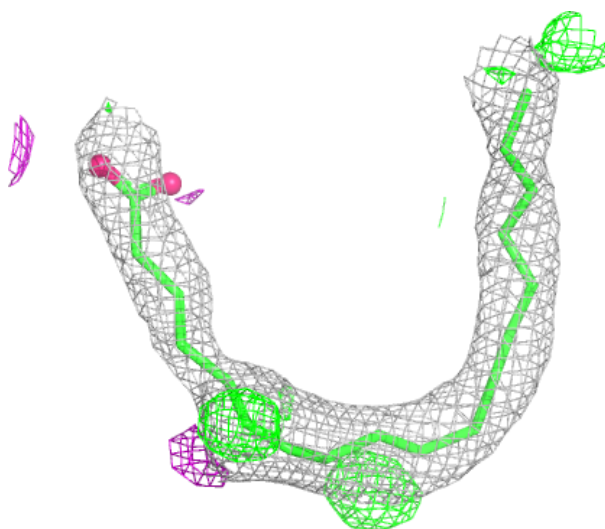
Electron density around 4I1 A 405:

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



Electron density around 4I1 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.