



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:31 PM UTC

PDB ID : 9DIE / pdb\_00009die  
Title : Structure of phospholipase D BetaIB1i from Sicarius terrosus venom, H47N mutant bound to product and substrate sphingolipids at 1.85 Å resolution  
Authors : Sundman, A.K.; Montfort, W.R.; Binford, G.J.; Cordes, M.H.  
Deposited on : 2024-09-05  
Resolution : 1.85 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](mailto: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>.

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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

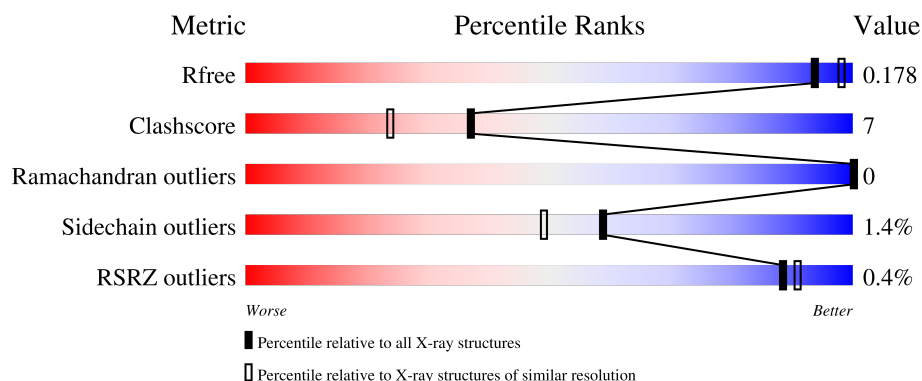
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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  $\geq 3$ , 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	301	 81% 10% • 8%
1	B	301	 81% 10% • 8%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5866 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 Dermonecrotic toxin StSicTox-betaIB1i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	21	0
			2367	1489	404	466	8			
1	B	278	Total	C	N	O	S	0	21	0
			2361	1489	401	463	8			

There are 46 discrepancies between the modelled and reference sequences:

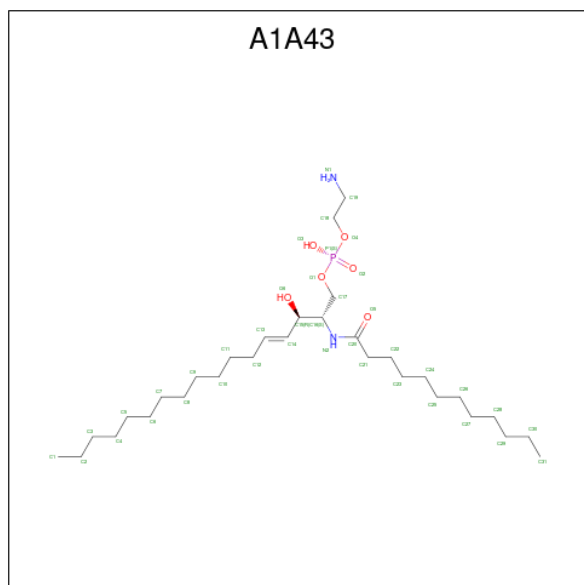
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP A0A0D4WV12
A	-21	LYS	-	expression tag	UNP A0A0D4WV12
A	-20	HIS	-	expression tag	UNP A0A0D4WV12
A	-19	HIS	-	expression tag	UNP A0A0D4WV12
A	-18	HIS	-	expression tag	UNP A0A0D4WV12
A	-17	HIS	-	expression tag	UNP A0A0D4WV12
A	-16	HIS	-	expression tag	UNP A0A0D4WV12
A	-15	HIS	-	expression tag	UNP A0A0D4WV12
A	-14	HIS	-	expression tag	UNP A0A0D4WV12
A	-13	HIS	-	expression tag	UNP A0A0D4WV12
A	-12	GLY	-	expression tag	UNP A0A0D4WV12
A	-11	GLY	-	expression tag	UNP A0A0D4WV12
A	-10	LEU	-	expression tag	UNP A0A0D4WV12
A	-9	VAL	-	expression tag	UNP A0A0D4WV12
A	-8	PRO	-	expression tag	UNP A0A0D4WV12
A	-7	ARG	-	expression tag	UNP A0A0D4WV12
A	-6	GLY	-	expression tag	UNP A0A0D4WV12
A	-5	SER	-	expression tag	UNP A0A0D4WV12
A	-4	HIS	-	expression tag	UNP A0A0D4WV12
A	-3	GLY	-	expression tag	UNP A0A0D4WV12
A	-2	GLY	-	expression tag	UNP A0A0D4WV12
A	-1	SER	-	expression tag	UNP A0A0D4WV12
A	47	ASN	HIS	engineered mutation	UNP A0A0D4WV12
B	-22	MET	-	initiating methionine	UNP A0A0D4WV12
B	-21	LYS	-	expression tag	UNP A0A0D4WV12

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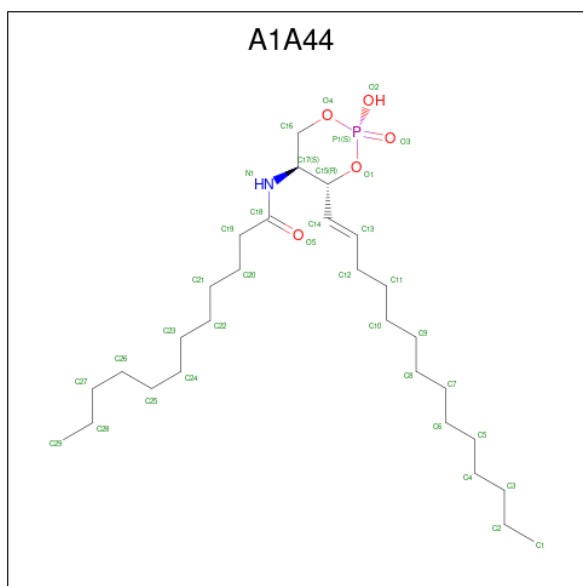
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP A0A0D4WV12
B	-19	HIS	-	expression tag	UNP A0A0D4WV12
B	-18	HIS	-	expression tag	UNP A0A0D4WV12
B	-17	HIS	-	expression tag	UNP A0A0D4WV12
B	-16	HIS	-	expression tag	UNP A0A0D4WV12
B	-15	HIS	-	expression tag	UNP A0A0D4WV12
B	-14	HIS	-	expression tag	UNP A0A0D4WV12
B	-13	HIS	-	expression tag	UNP A0A0D4WV12
B	-12	GLY	-	expression tag	UNP A0A0D4WV12
B	-11	GLY	-	expression tag	UNP A0A0D4WV12
B	-10	LEU	-	expression tag	UNP A0A0D4WV12
B	-9	VAL	-	expression tag	UNP A0A0D4WV12
B	-8	PRO	-	expression tag	UNP A0A0D4WV12
B	-7	ARG	-	expression tag	UNP A0A0D4WV12
B	-6	GLY	-	expression tag	UNP A0A0D4WV12
B	-5	SER	-	expression tag	UNP A0A0D4WV12
B	-4	HIS	-	expression tag	UNP A0A0D4WV12
B	-3	GLY	-	expression tag	UNP A0A0D4WV12
B	-2	GLY	-	expression tag	UNP A0A0D4WV12
B	-1	SER	-	expression tag	UNP A0A0D4WV12
B	47	ASN	HIS	engineered mutation	UNP A0A0D4WV12

- Molecule 2 is 2-aminoethyl (2S,3R,4E)-2-dodecanamido-3-hydroxyheptadec-4-en-1-yl hydrogen (S)-phosphate (CCD ID: A1A43) (formula:  $C_{31}H_{63}N_2O_6P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			40	31	2	6	1		
2	A	1	Total	C	N	O	P	0	0
			40	31	2	6	1		
2	B	1	Total	C	N	O	P	0	0
			40	31	2	6	1		
2	B	1	Total	C	N	O	P	0	0
			40	31	2	6	1		

- Molecule 3 is N-{(2S,4R,5S)-2-hydroxy-2-oxo-4-[(1E,7Z)-tetradeca-1,7-dien-1-yl]-1,3,2lambda 5 -dioxaphosphinan-5-yl}dodecanamide (CCD ID: A1A44) (formula: C<sub>29</sub>H<sub>56</sub>NO<sub>5</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	29	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			36	29	1	5	1		

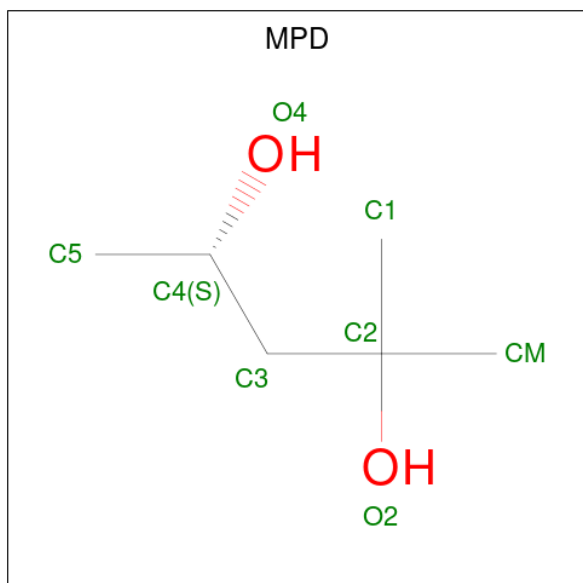
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0
4	B	2	Total Na 2 2	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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


- Molecule 7 is water.

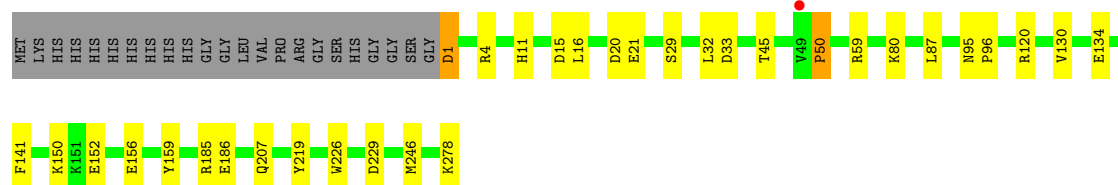
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	442	Total	O	0	20
			442	442		
7	B	442	Total	O	0	10
			442	442		

### 3 Residue-property plots


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

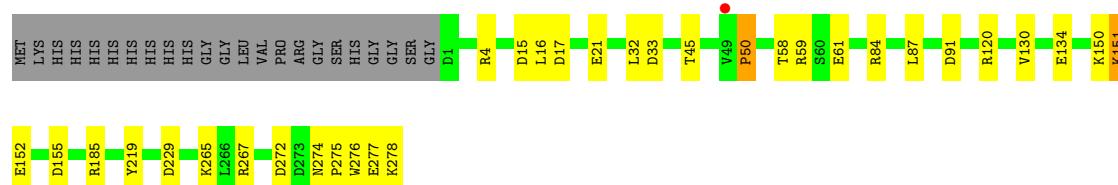
- Molecule 1: Dermonecrotic toxin StSicTox-betaIB1i

Chain A: 



- Molecule 1: Dermonecrotic toxin StSicTox-betaIB1i

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.00Å 105.33Å 108.41Å 90.00° 93.83° 90.00°	Depositor
Resolution (Å)	24.43 – 1.85 24.43 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.43-1.85) 99.9 (24.43-1.85)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.119 , 0.167 0.149 , 0.178	Depositor DCC
$R_{free}$ test set	3751 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, MPD, MG, A1A44, A1A43

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	0.61	0/2455	0.95	2/3314 (0.1%)
1	B	0.63	0/2455	0.97	2/3314 (0.1%)
All	All	0.62	0/4910	0.96	4/6628 (0.1%)

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	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ASP	CA-CB-CG	7.41	120.01	112.60
1	A	156	GLU	CB-CG-CD	6.10	122.97	112.60
1	B	59	ARG	CA-CB-CG	-6.03	102.03	114.10
1	A	278	LYS	CB-CA-C	-5.64	99.37	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	267	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	2367	0	2319	30	0
1	B	2361	0	2325	36	0
2	A	80	0	0	1	0
2	B	80	0	0	1	0
3	A	36	0	0	3	0
3	B	36	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	16	0	28	1	0
7	A	442	0	0	16	3
7	B	442	0	0	19	2
All	All	5866	0	4672	69	3

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 7.

All (69) 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:150[B]:LYS:HE3	7:A:715[B]:HOH:O	1.68	0.93
1:B:84[B]:ARG:HD3	7:B:696[B]:HOH:O	1.72	0.89
1:B:150[B]:LYS:HZ2	1:B:155[B]:ASP:CG	1.84	0.84
1:B:84[B]:ARG:HD2	7:B:600:HOH:O	1.76	0.84
1:A:21[A]:GLU:OE1	2:A:302:A1A43:N1	2.13	0.81
1:A:1:ASP:HA	7:A:687:HOH:O	1.79	0.81
1:B:4:ARG:HD3	7:B:703:HOH:O	1.82	0.78
1:A:150[B]:LYS:CE	7:A:715[B]:HOH:O	2.31	0.76
1:B:134[A]:GLU:OE1	7:B:404[A]:HOH:O	2.06	0.73
1:B:120:ARG:HH12	1:B:152[B]:GLU:HG2	1.55	0.71
1:A:229:ASP:OD1	7:A:402:HOH:O	2.09	0.70
1:A:226:TRP:HB2	1:A:246[B]:MET:HE2	1.73	0.70
1:B:84[B]:ARG:CD	7:B:696[B]:HOH:O	2.34	0.70
1:B:229:ASP:OD1	7:B:405:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:307:MPD:H53	6:A:307:MPD:H11	1.75	0.67
1:A:152[A]:GLU:OE2	7:A:403[A]:HOH:O	2.14	0.66
1:B:134[A]:GLU:HG3	7:B:635[A]:HOH:O	1.96	0.65
1:B:21:GLU:HG3	7:B:527:HOH:O	1.96	0.64
1:B:274[B]:ASN:OD1	1:B:277[B]:GLU:HG3	1.97	0.63
1:A:80:LYS:HE3	7:A:578:HOH:O	1.97	0.62
1:A:246[B]:MET:HE1	7:A:734:HOH:O	1.98	0.62
3:A:303:A1A44:C26	7:A:816:HOH:O	2.48	0.61
3:A:303:A1A44:C27	7:A:816:HOH:O	2.47	0.61
1:A:11:HIS:CD2	1:A:246[B]:MET:HE3	2.36	0.61
1:A:4:ARG:NH2	7:A:401:HOH:O	2.32	0.61
1:A:87[A]:LEU:HD11	1:A:130:VAL:HG23	1.84	0.58
1:B:151[A]:LYS:NZ	7:B:413:HOH:O	2.37	0.57
1:A:29[B]:SER:HB3	1:A:87[B]:LEU:HB3	1.87	0.56
1:B:4:ARG:NH2	7:B:403:HOH:O	2.39	0.55
1:A:207[B]:GLN:NE2	7:A:407:HOH:O	2.40	0.55
1:B:151[B]:LYS:HG3	7:B:628:HOH:O	2.08	0.53
1:B:150[B]:LYS:NZ	1:B:155[B]:ASP:OD1	2.41	0.53
1:A:50:PRO:HD3	1:B:50:PRO:HD3	1.91	0.52
1:A:150[B]:LYS:HG3	7:A:715[B]:HOH:O	2.09	0.52
1:B:274[B]:ASN:CG	1:B:277[B]:GLU:HG3	2.34	0.51
1:A:120:ARG:NH1	1:A:152[B]:GLU:OE1	2.42	0.50
1:B:120:ARG:HH12	1:B:152[B]:GLU:CG	2.22	0.50
1:B:87[A]:LEU:HD11	1:B:130:VAL:HG23	1.94	0.50
1:B:33:ASP:O	1:B:45:THR:HA	2.12	0.49
1:B:274[B]:ASN:HD22	1:B:275:PRO:HD2	1.78	0.48
1:B:185:ARG:HD2	1:B:219:TYR:OH	2.13	0.47
1:B:274[B]:ASN:ND2	1:B:276:TRP:H	2.12	0.47
1:A:33:ASP:O	1:A:45:THR:HA	2.14	0.47
1:A:134[A]:GLU:CG	7:A:611[A]:HOH:O	2.64	0.46
1:A:15:ASP:OD2	1:A:59[B]:ARG:NH2	2.49	0.46
3:A:303:A1A44:C28	7:A:816:HOH:O	2.64	0.46
1:A:185:ARG:HD2	1:A:219:TYR:OH	2.16	0.45
1:A:16:LEU:O	1:A:20[A]:ASP:OD2	2.35	0.45
1:B:272[B]:ASP:OD1	7:B:406:HOH:O	2.21	0.45
1:B:278:LYS:C	7:B:415:HOH:O	2.59	0.45
1:B:120:ARG:NH1	1:B:152[B]:GLU:HG2	2.29	0.44
1:B:84[B]:ARG:NH1	7:B:434:HOH:O	2.51	0.43
1:B:134[A]:GLU:CG	7:B:635[A]:HOH:O	2.62	0.43
1:A:141:PHE:CD1	1:A:141:PHE:C	2.96	0.42
2:B:302:A1A43:C1	7:B:709:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TRP:CB	1:A:246[B]:MET:HE2	2.46	0.42
1:B:17:ASP:O	1:B:21:GLU:HG3	2.20	0.42
1:B:84[B]:ARG:NH2	7:B:442:HOH:O	2.52	0.41
1:A:59[B]:ARG:HD3	7:A:705:HOH:O	2.19	0.41
1:A:134[A]:GLU:HG2	7:A:611[A]:HOH:O	2.20	0.41
1:A:96:PRO:HB3	1:B:58:THR:HB	2.03	0.41
1:B:21:GLU:CG	7:B:527:HOH:O	2.61	0.41
1:B:120:ARG:NH2	1:B:152[B]:GLU:OE1	2.47	0.41
1:A:11:HIS:HD2	1:A:246[B]:MET:HE3	1.85	0.41
1:B:151[A]:LYS:HE3	1:B:151[A]:LYS:HB2	1.83	0.40
1:A:95:ASN:N	1:A:96:PRO:CD	2.84	0.40
1:B:91[B]:ASP:CG	7:B:512[B]:HOH:O	2.65	0.40
1:A:159:TYR:OH	1:A:186:GLU:OE1	2.38	0.40
1:B:16:LEU:HG	1:B:61[A]:GLU:OE2	2.22	0.40

All (3) 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)
7:A:496:HOH:O	7:A:651:HOH:O[2_556]	1.95	0.25
7:A:422:HOH:O	7:B:468:HOH:O[4_555]	2.10	0.10
7:A:783:HOH:O	7:B:758:HOH:O[4_455]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	297/301 (99%)	287 (97%)	10 (3%)	0	100	100
1	B	297/301 (99%)	288 (97%)	9 (3%)	0	100	100
All	All	594/602 (99%)	575 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/259 (102%)	260 (99%)	3 (1%)	65	57
1	B	263/259 (102%)	258 (98%)	5 (2%)	50	38
All	All	526/518 (102%)	518 (98%)	8 (2%)	59	47

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	32	LEU
1	A	50	PRO
1	B	32	LEU
1	B	50	PRO
1	B	151[A]	LYS
1	B	151[B]	LYS
1	B	265	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	203	ASN
1	B	203	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 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\# Z  > 2$
3	A1A44	B	303	5	35,36,36	0.82	2 (5%)	36,42,42	1.24	3 (8%)
2	A1A43	B	301	-	38,39,39	0.41	0	41,44,44	0.66	1 (2%)
6	MPD	A	307	-	7,7,7	0.28	0	9,10,10	0.79	0
2	A1A43	B	302	-	38,39,39	0.44	0	41,44,44	1.07	4 (9%)
2	A1A43	A	302	-	38,39,39	0.49	0	41,44,44	1.14	3 (7%)
3	A1A44	A	303	5	35,36,36	0.92	3 (8%)	36,42,42	1.31	6 (16%)
2	A1A43	A	301	-	38,39,39	0.46	0	41,44,44	0.61	0
6	MPD	A	308	-	7,7,7	0.26	0	9,10,10	0.37	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	A1A44	B	303	5	-	14/29/44/44	0/1/1/1
2	A1A43	B	301	-	-	11/44/44/44	-
6	MPD	A	307	-	-	4/5/5/5	-
2	A1A43	B	302	-	-	19/44/44/44	-
2	A1A43	A	302	-	-	21/44/44/44	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1A44	A	303	5	-	14/29/44/44	0/1/1/1
2	A1A43	A	301	-	-	8/44/44/44	-
6	MPD	A	308	-	-	4/5/5/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	A1A44	P1-O4	3.24	1.61	1.57
3	A	303	A1A44	P1-O4	3.17	1.61	1.57
3	B	303	A1A44	P1-O1	2.72	1.62	1.57
3	A	303	A1A44	P1-O1	2.49	1.61	1.57
3	A	303	A1A44	O1-C15	-2.19	1.43	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	A1A44	O1-C15-C17	5.01	117.56	109.53
2	A	302	A1A43	C15-C16-N2	4.38	117.07	109.66
2	B	302	A1A43	C15-C16-N2	3.47	115.53	109.66
3	A	303	A1A44	O2-P1-O3	3.32	118.78	108.56
3	A	303	A1A44	O1-C15-C17	2.92	114.22	109.53
3	A	303	A1A44	C17-N1-C18	2.82	128.10	123.40
3	B	303	A1A44	C17-N1-C18	2.70	127.91	123.40
3	A	303	A1A44	C19-C18-N1	-2.69	111.13	115.86
2	A	302	A1A43	C16-N2-C20	2.67	127.86	123.40
3	B	303	A1A44	O2-P1-O3	2.63	116.65	108.56
3	A	303	A1A44	O2-P1-O1	2.50	112.86	107.04
2	A	302	A1A43	C17-C16-C15	-2.49	107.34	112.90
2	B	302	A1A43	C16-N2-C20	2.30	127.23	123.40
3	A	303	A1A44	O5-C18-N1	2.22	126.71	122.95
2	B	302	A1A43	O3-P1-O1	2.20	117.56	107.57
2	B	301	A1A43	C15-C14-C13	-2.14	120.25	124.69
2	B	302	A1A43	C17-C16-N2	-2.06	106.73	109.66

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	A1A43	C13-C14-C15-C16
2	A	302	A1A43	C13-C14-C15-O6

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Mol	Chain	Res	Type	Atoms
2	A	302	A1A43	C14-C15-C16-C17
2	A	302	A1A43	C14-C15-C16-N2
2	A	302	A1A43	O6-C15-C16-C17
2	A	302	A1A43	O6-C15-C16-N2
2	A	302	A1A43	C15-C16-N2-C20
2	A	302	A1A43	C17-C16-N2-C20
2	A	302	A1A43	O4-C18-C19-N1
2	B	302	A1A43	C14-C15-C16-C17
2	B	302	A1A43	C14-C15-C16-N2
2	B	302	A1A43	O6-C15-C16-C17
2	B	302	A1A43	O6-C15-C16-N2
2	B	302	A1A43	C18-O4-P1-O1
2	B	302	A1A43	C18-O4-P1-O2
6	A	307	MPD	C1-C2-C3-C4
6	A	308	MPD	C2-C3-C4-O4
6	A	308	MPD	C2-C3-C4-C5
2	A	302	A1A43	C20-C21-C22-C23
2	B	301	A1A43	C6-C7-C8-C9
3	A	303	A1A44	C6-C7-C8-C9
2	B	301	A1A43	C24-C25-C26-C27
2	B	302	A1A43	C13-C14-C15-O6
3	B	303	A1A44	C25-C26-C27-C28
2	A	301	A1A43	C27-C28-C29-C30
2	B	302	A1A43	C7-C8-C9-C10
2	A	301	A1A43	C4-C5-C6-C7
2	A	301	A1A43	C7-C8-C9-C10
2	A	302	A1A43	C3-C4-C5-C6
3	A	303	A1A44	C2-C3-C4-C5
2	A	302	A1A43	C4-C5-C6-C7
3	B	303	A1A44	C7-C8-C9-C10
2	A	301	A1A43	C11-C10-C9-C8
2	A	302	A1A43	C25-C26-C27-C28
3	B	303	A1A44	C22-C23-C24-C25
3	A	303	A1A44	C4-C5-C6-C7
2	B	301	A1A43	C10-C11-C12-C13
2	B	301	A1A43	C22-C23-C24-C25
2	B	301	A1A43	C27-C28-C29-C30
2	B	302	A1A43	C6-C7-C8-C9
3	B	303	A1A44	C4-C5-C6-C7
2	B	301	A1A43	C11-C10-C9-C8
2	B	302	A1A43	C4-C5-C6-C7
3	A	303	A1A44	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	B	302	A1A43	C22-C23-C24-C25
3	B	303	A1A44	C23-C24-C25-C26
2	A	302	A1A43	C11-C10-C9-C8
3	A	303	A1A44	C25-C26-C27-C28
2	B	301	A1A43	C4-C5-C6-C7
2	B	301	A1A43	C2-C3-C4-C5
3	B	303	A1A44	C6-C7-C8-C9
3	B	303	A1A44	C3-C4-C5-C6
2	B	301	A1A43	C23-C24-C25-C26
2	B	302	A1A43	C11-C10-C9-C8
2	B	302	A1A43	C25-C26-C27-C28
3	A	303	A1A44	C26-C27-C28-C29
3	B	303	A1A44	C26-C27-C28-C29
3	B	303	A1A44	C24-C25-C26-C27
2	B	301	A1A43	C5-C6-C7-C8
3	B	303	A1A44	C11-C10-C9-C8
2	A	302	A1A43	C7-C8-C9-C10
2	B	302	A1A43	C27-C28-C29-C30
2	B	302	A1A43	C23-C24-C25-C26
2	B	302	A1A43	C3-C4-C5-C6
3	A	303	A1A44	C18-C19-C20-C21
3	A	303	A1A44	C13-C14-C15-C17
2	A	301	A1A43	C22-C23-C24-C25
2	A	302	A1A43	C24-C25-C26-C27
6	A	307	MPD	CM-C2-C3-C4
2	B	301	A1A43	C28-C29-C30-C31
2	B	302	A1A43	C18-O4-P1-O3
6	A	307	MPD	C2-C3-C4-C5
3	A	303	A1A44	C19-C20-C21-C22
2	B	302	A1A43	C5-C6-C7-C8
2	A	302	A1A43	C1-C2-C3-C4
3	A	303	A1A44	C1-C2-C3-C4
3	B	303	A1A44	C2-C3-C4-C5
3	A	303	A1A44	C24-C25-C26-C27
2	A	302	A1A43	C27-C28-C29-C30
2	A	302	A1A43	O5-C20-C21-C22
2	A	301	A1A43	C2-C3-C4-C5
2	A	301	A1A43	C23-C24-C25-C26
3	A	303	A1A44	C13-C14-C15-O1
2	A	302	A1A43	N2-C20-C21-C22
3	B	303	A1A44	C13-C14-C15-C17
2	A	301	A1A43	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
3	A	303	A1A44	C3-C4-C5-C6
3	A	303	A1A44	C19-C18-N1-C17
6	A	307	MPD	O2-C2-C3-C4
2	A	302	A1A43	C21-C22-C23-C24
6	A	308	MPD	C1-C2-C3-C4
6	A	308	MPD	CM-C2-C3-C4
3	B	303	A1A44	C5-C6-C7-C8
3	B	303	A1A44	C9-C10-C11-C12
2	B	302	A1A43	O5-C20-C21-C22

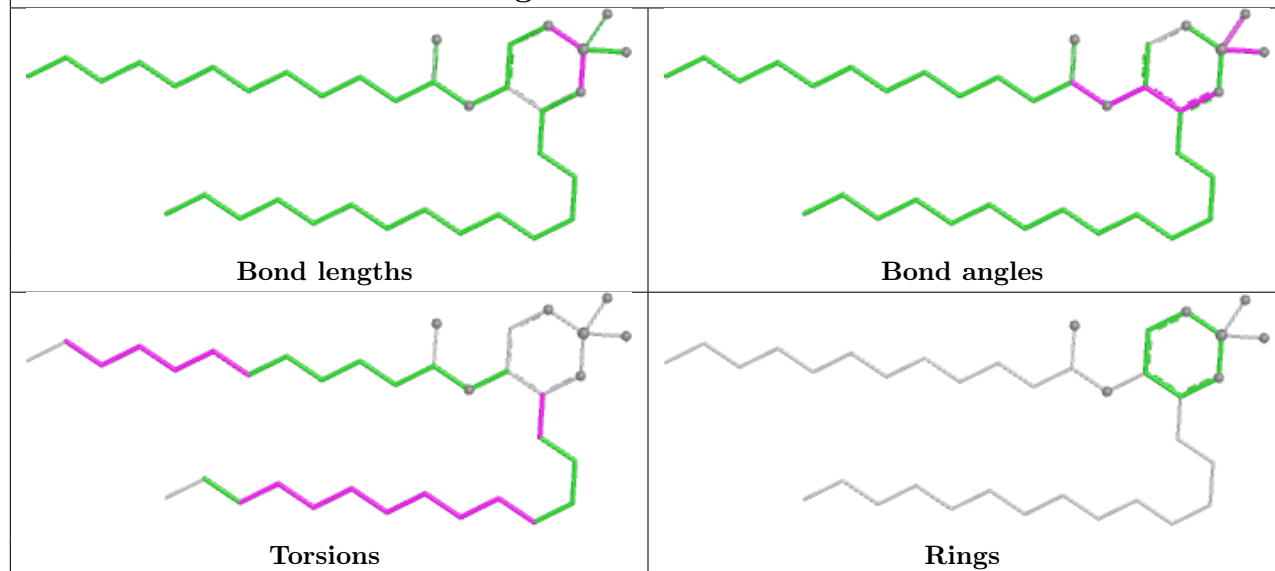
There are no ring outliers.

4 monomers are involved in 6 short contacts:

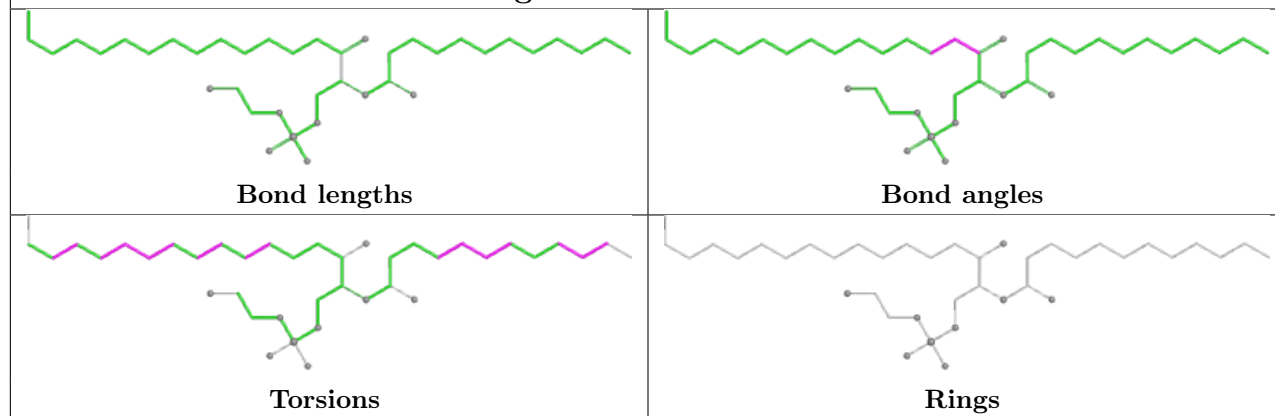
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	307	MPD	1	0
2	B	302	A1A43	1	0
2	A	302	A1A43	1	0
3	A	303	A1A44	3	0

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.

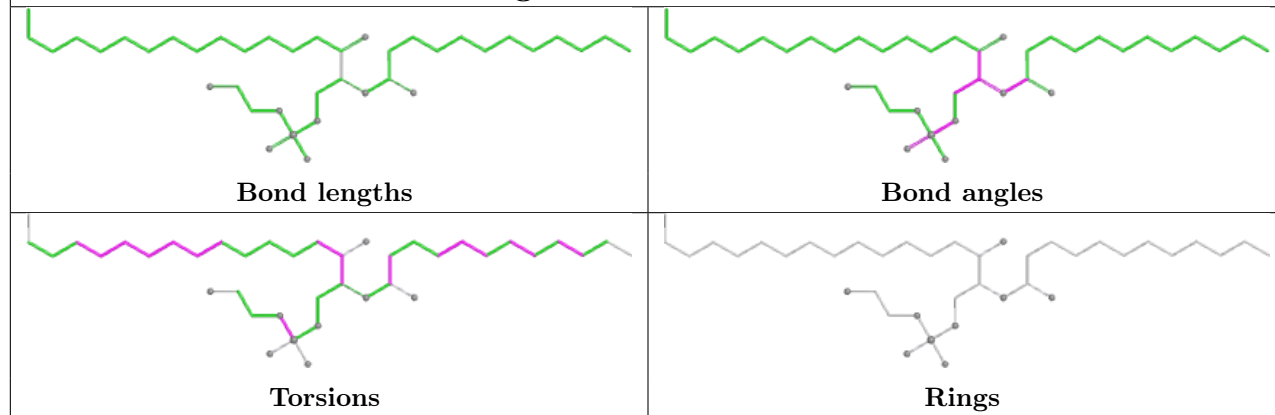
## Ligand A1A44 B 303

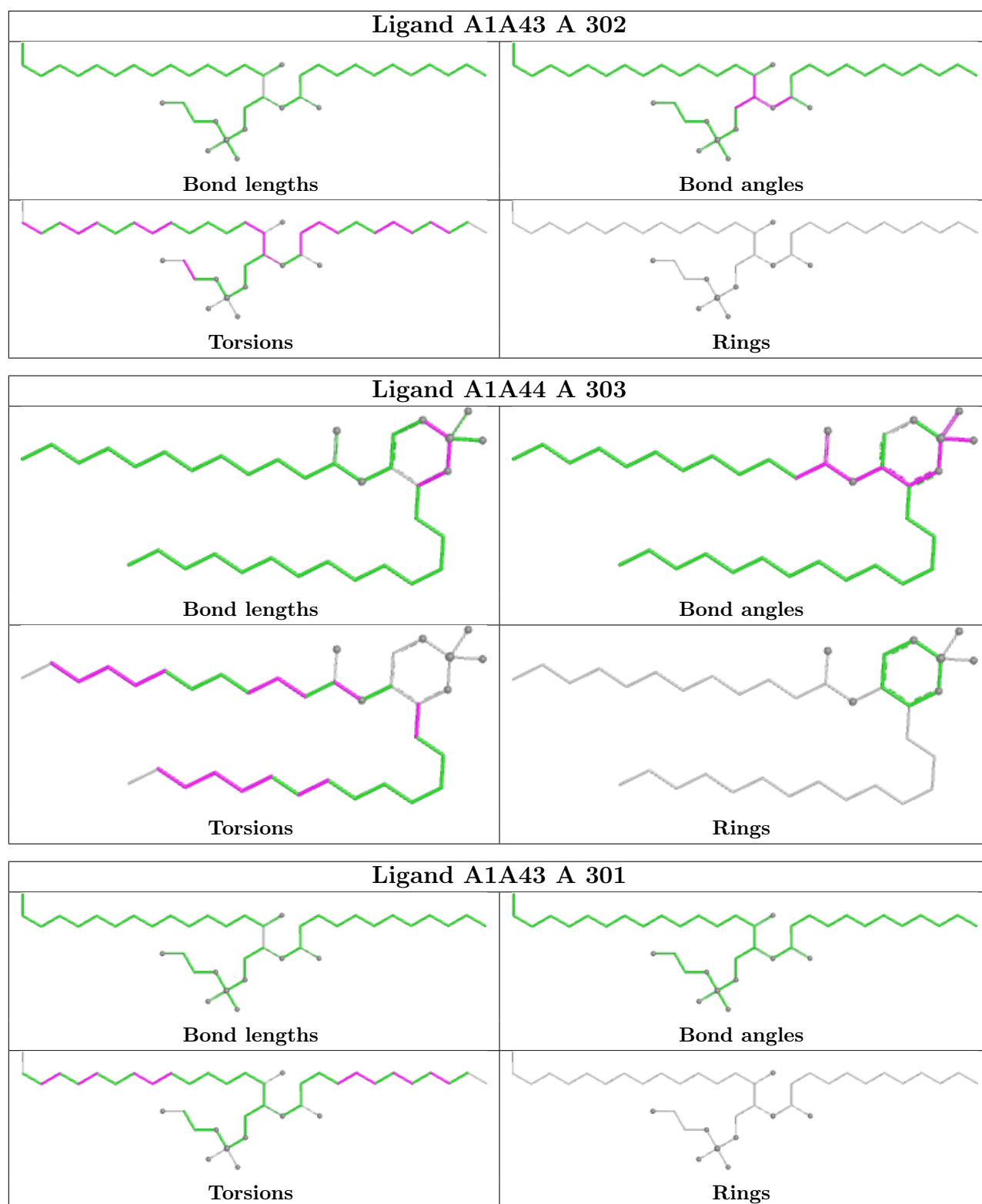


## Ligand A1A43 B 301



## Ligand A1A43 B 302





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	278/301 (92%)	-0.52	1 (0%) 88 91	5, 14, 27, 51	21 (7%)
1	B	278/301 (92%)	-0.55	1 (0%) 88 91	5, 14, 26, 46	21 (7%)
All	All	556/602 (92%)	-0.54	2 (0%) 88 91	5, 14, 26, 51	42 (7%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	VAL	2.6
1	A	49	VAL	2.5

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	A1A43	A	302	40/40	0.70	0.30	23,96,114,119	0
6	MPD	A	308	8/8	0.74	0.26	58,66,68,69	0
2	A1A43	B	302	40/40	0.76	0.29	24,92,110,112	0

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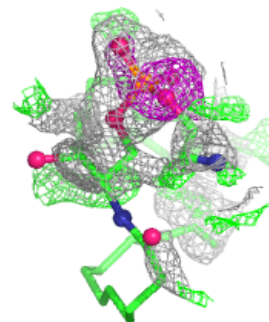
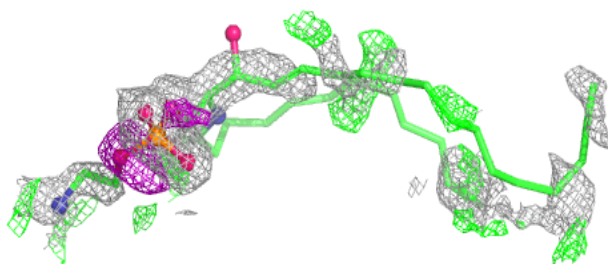
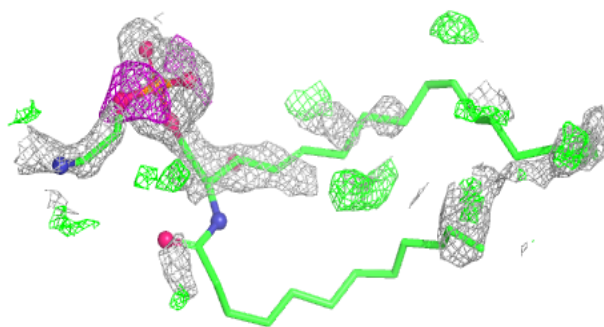
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MPD	A	307	8/8	0.82	0.22	53,61,71,76	0
4	NA	B	305	1/1	0.82	0.20	49,49,49,49	0
4	NA	A	305	1/1	0.86	0.22	52,52,52,52	0
3	A1A44	A	303	36/36	0.86	0.17	22,40,75,79	0
3	A1A44	B	303	36/36	0.90	0.16	21,36,109,113	0
2	A1A43	A	301	40/40	0.96	0.13	12,27,103,105	0
4	NA	A	304	1/1	0.97	0.08	25,25,25,25	0
2	A1A43	B	301	40/40	0.97	0.13	11,31,101,106	0
4	NA	B	304	1/1	0.97	0.07	25,25,25,25	0
5	MG	A	306	1/1	0.99	0.04	6,6,6,6	0
5	MG	B	306	1/1	0.99	0.03	8,8,8,8	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.

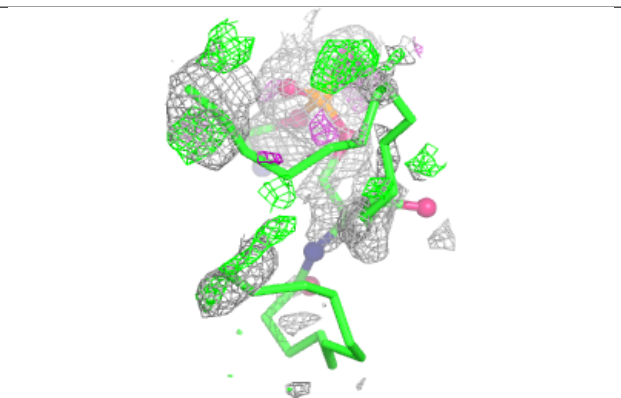
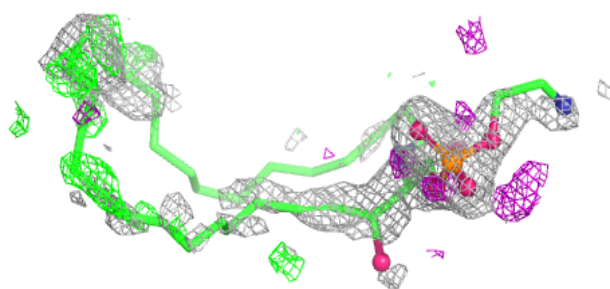
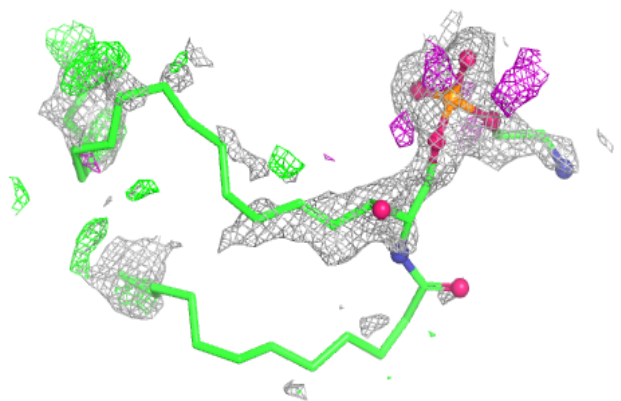
**Electron density around A1A43 A 302:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

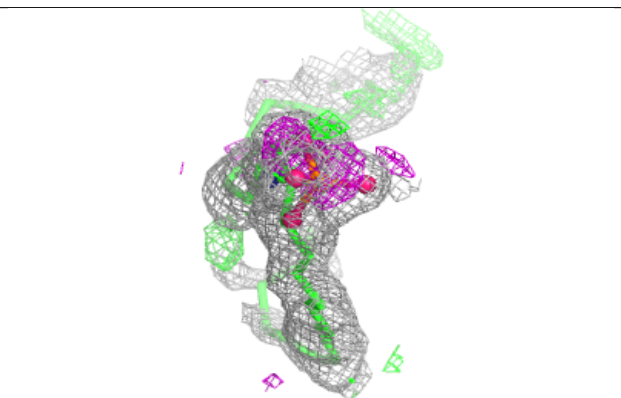
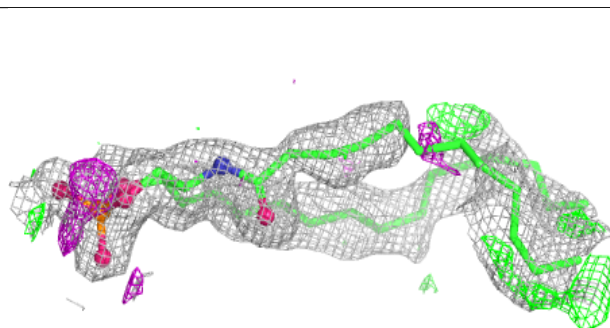
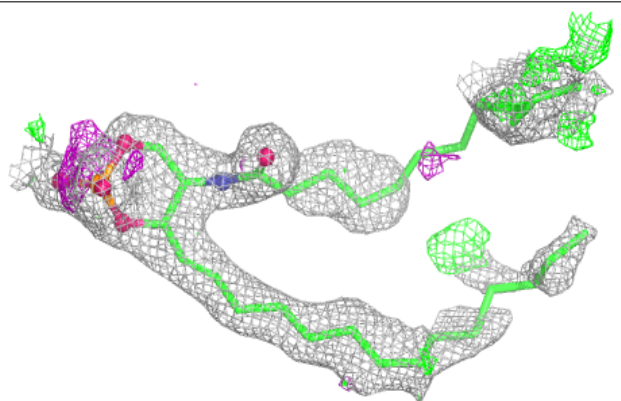


**Electron density around A1A43 B 302:**

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

**Electron density around A1A44 A 303:**

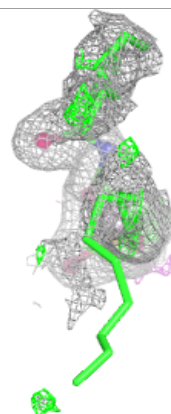
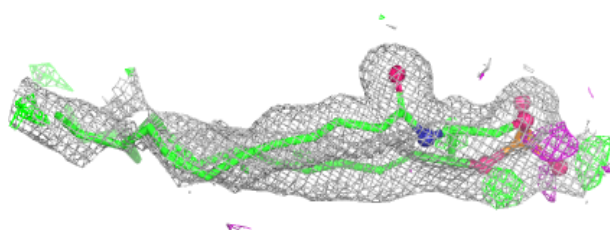
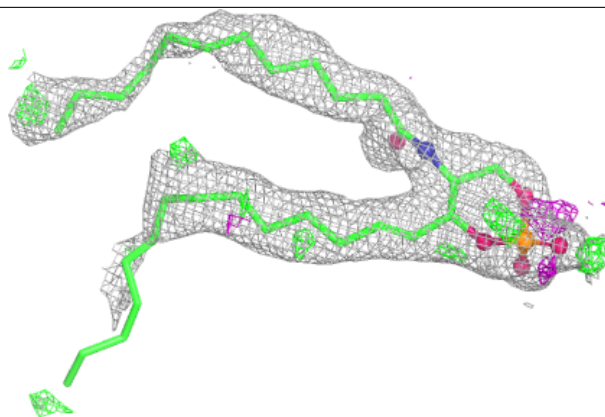
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



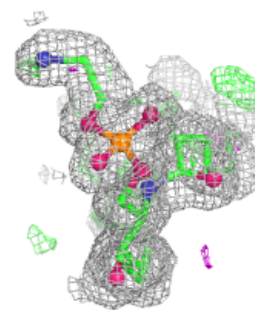
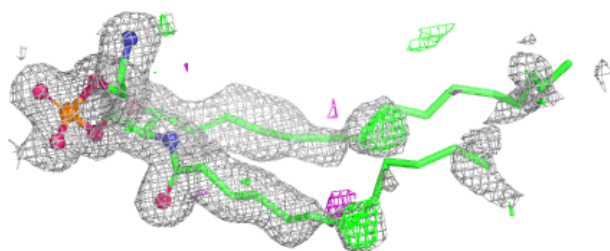
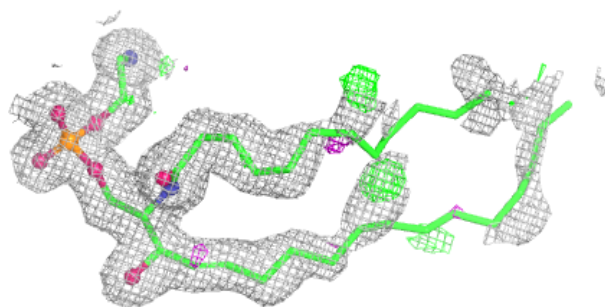


**Electron density around A1A44 B 303:**

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

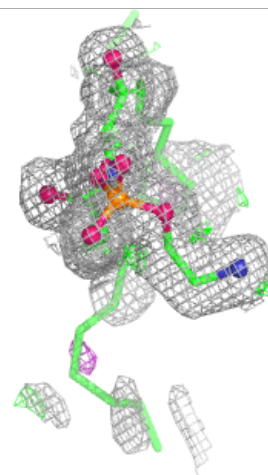
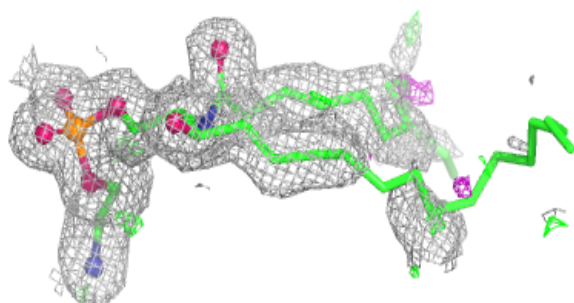
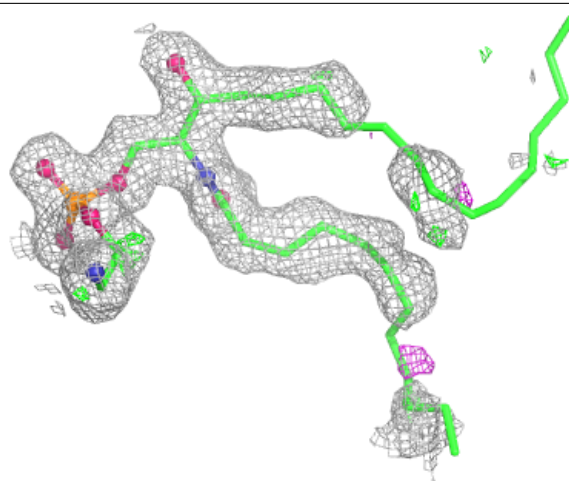
**Electron density around A1A43 A 301:**

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



**Electron density around A1A43 B 301:**

$2mF_o-DF_c$  (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.