



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:33 PM UTC

PDB ID : 9OZS / pdb_00009ozs
Title : Structure of phospholipase D BetaIB1i from Sicarius terrosus venom, H47N mutant bound to substrate sphingolipids at 2.60 Å resolution
Authors : Sundman, A.K.; Montfort, W.R.; Binford, G.J.; Cordes, M.H.
Deposited on : 2025-06-05
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

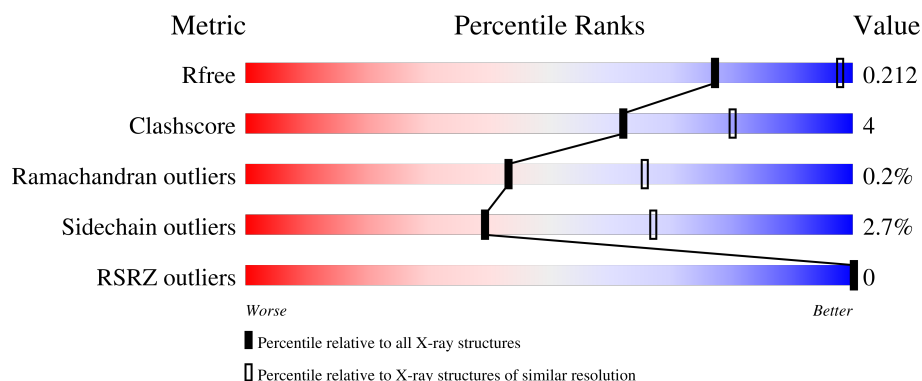
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	301	
1	B	301	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5431 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	0	0
			2238	1407	389	435	7			
1	B	278	Total	C	N	O	S	0	1	0
			2246	1411	390	438	7			

There are 46 discrepancies between the modelled and reference sequences:

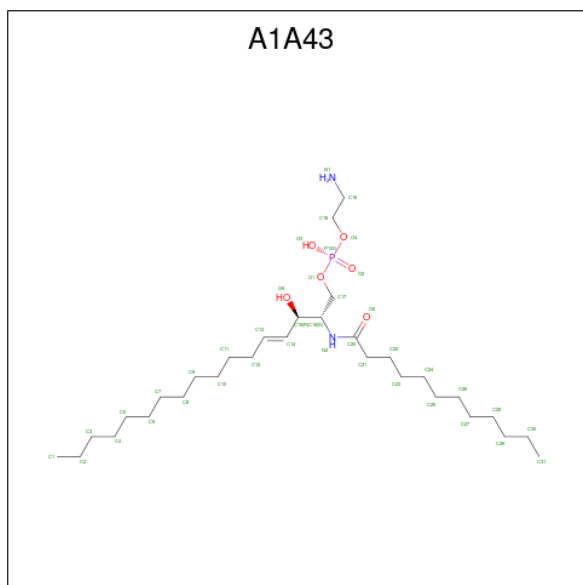
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP A0A0D4WV12
A	-21	LYS	-	expression tag	UNP A0A0D4WV12
A	-20	HIS	-	expression tag	UNP A0A0D4WV12
A	-19	HIS	-	expression tag	UNP A0A0D4WV12
A	-18	HIS	-	expression tag	UNP A0A0D4WV12
A	-17	HIS	-	expression tag	UNP A0A0D4WV12
A	-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	-	expression tag	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	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		
2	B	1	Total	C	N	O	P	0	0
			40	31	2	6	1		

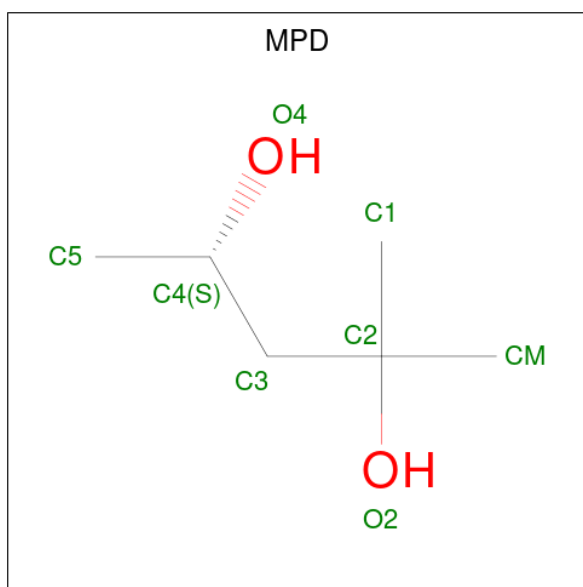
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

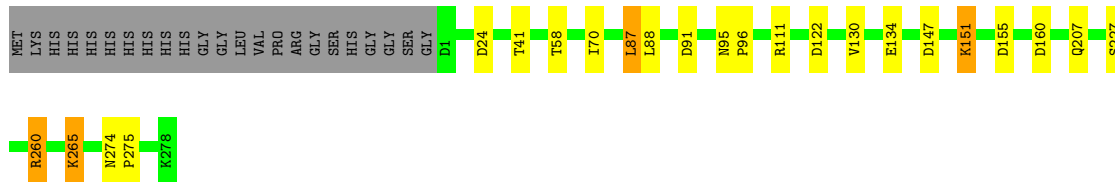
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	333	Total	O	0	0
			333	333		
6	B	354	Total	O	0	1
			354	354		

- Molecule 1: Dermonecrotic toxin StSicTox-betaIB1i

D147	D148	D149	D150	D151	D152	D153	D154	D155	D156	D157	D158	D159	D160	D161	D162	D163	D164	D165	D166	D167	D168	D169	D170	D171	D172	D173	D174	D175	D176	D177	D178	D179	D180	D181	D182	D183	D184	D185	D186	D187	D188	D189	D190	D191	D192	D193	D194	D195	D196	D197	D198	D199	D200	D201	D202	D203	D204	D205	D206	D207	D208	D209	D210	D211	D212	D213	D214	D215	D216	D217	D218	D219	D220	D221	D222	D223	D224	D225	D226	D227	D228	D229	D230	D231	D232	D233	D234	D235	D236	D237	D238	D239	D240	D241	D242	D243	D244	D245	D246	D247	D248	D249	D250	D251	D252	D253	D254	D255	D256	D257	D258	D259	D260	D261	D262	D263	D264	D265	D266	D267	D268	D269	D270	D271	D272	D273	D274	D275	D276	D277	D278	D279	D280	D281	D282	D283	D284	D285	D286	D287	D288	D289	D290	D291	D292	D293	D294	D295	D296	D297	D298	D299	D300	D301	D302	D303	D304	D305	D306	D307	D308	D309	D310	D311	D312	D313	D314	D315	D316	D317	D318	D319	D320	D321	D322	D323	D324	D325	D326	D327	D328	D329	D330	D331	D332	D333	D334	D335	D336	D337	D338	D339	D340	D341	D342	D343	D344	D345	D346	D347	D348	D349	D350	D351	D352	D353	D354	D355	D356	D357	D358	D359	D360	D361	D362	D363	D364	D365	D366	D367	D368	D369	D370	D371	D372	D373	D374	D375	D376	D377	D378	D379	D380	D381	D382	D383	D384	D385	D386	D387	D388	D389	D390	D391	D392	D393	D394	D395	D396	D397	D398	D399	D400	D401	D402	D403	D404	D405	D406	D407	D408	D409	D410	D411	D412	D413	D414	D415	D416	D417	D418	D419	D420	D421	D422	D423	D424	D425	D426	D427	D428	D429	D430	D431	D432	D433	D434	D435	D436	D437	D438	D439	D440	D441	D442	D443	D444	D445	D446	D447	D448	D449	D450	D451	D452	D453	D454	D455	D456	D457	D458	D459	D460	D461	D462	D463	D464	D465	D466	D467	D468	D469	D470	D471	D472	D473	D474	D475	D476	D477	D478	D479	D480	D481	D482	D483	D484	D485	D486	D487	D488	D489	D490	D491	D492	D493	D494	D495	D496	D497	D498	D499	D500	D501	D502	D503	D504	D505	D506	D507	D508	D509	D510	D511	D512	D513	D514	D515	D516	D517	D518	D519	D520	D521	D522	D523	D524	D525	D526	D527	D528	D529	D530	D531	D532	D533	D534	D535	D536	D537	D538	D539	D540	D541	D542	D543	D544	D545	D546	D547	D548	D549	D550	D551	D552	D553	D554	D555	D556	D557	D558	D559	D560	D561	D562	D563	D564	D565	D566	D567	D568	D569	D570	D571	D572	D573	D574	D575	D576	D577	D578	D579	D580	D581	D582	D583	D584	D585	D586	D587	D588	D589	D590	D591	D592	D593	D594	D595	D596	D597	D598	D599	D600
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Chain B: 85% 6% • 8%



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.79Å 105.85Å 109.11Å 90.00° 93.62° 90.00°	Depositor
Resolution (Å)	24.41 – 2.60 24.41 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.41-2.60) 99.8 (24.41-2.60)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.149 , 0.209 (Not available) , 0.212	Depositor DCC
R_{free} test set	1528 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5431	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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: NA, A1A43, MPD, MG

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	0.62	0/2284	1.16	6/3087 (0.2%)
1	B	0.64	0/2292	1.15	8/3098 (0.3%)
All	All	0.63	0/4576	1.15	14/6185 (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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	ASP	CA-CB-CG	7.76	120.36	112.60
1	B	265	LYS	CB-CA-C	7.26	124.88	110.42
1	B	265	LYS	N-CA-CB	-6.00	100.36	110.49
1	B	151	LYS	CB-CA-C	5.76	121.28	110.63
1	B	207	GLN	CB-CA-C	-5.73	101.88	110.88
1	A	122	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	24	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	147	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	91	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	147	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	160	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	122	ASP	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	115	ASP	CA-CB-CG	5.07	117.67	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	TRP	Peptide
1	B	260	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	2238	0	2177	19	0
1	B	2246	0	2178	10	0
2	A	120	0	0	5	0
2	B	120	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	16	0	28	2	0
6	A	333	0	0	11	1
6	B	354	0	0	3	1
All	All	5431	0	4383	35	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 4.

All (35) 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)
2:B:303:A1A43:P1	2:B:303:A1A43:O6	2.46	0.73
1:A:61:GLU:OE1	6:A:401:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:303:A1A43:P1	2:A:303:A1A43:O6	2.52	0.68
2:A:303:A1A43:O6	2:A:303:A1A43:O2	2.17	0.62
1:B:111:ARG:HD3	6:B:503:HOH:O	1.99	0.61
1:B:70:ILE:HG21	1:B:88:LEU:HD11	1.85	0.58
1:B:274:ASN:HD22	1:B:275:PRO:HD2	1.69	0.58
1:A:159:TYR:OH	1:A:186:GLU:OE1	2.13	0.58
2:B:303:A1A43:O6	2:B:303:A1A43:O2	2.20	0.57
1:A:20:ASP:HB2	6:A:411:HOH:O	2.05	0.56
1:A:160:ASP:HB2	6:A:593:HOH:O	2.07	0.54
1:A:21:GLU:OE2	2:A:302:A1A43:N1	2.41	0.54
1:B:95:ASN:N	1:B:96:PRO:HD3	2.25	0.51
1:A:96:PRO:HB3	1:B:58:THR:HB	1.92	0.50
1:A:124:LYS:HE2	6:A:679:HOH:O	2.12	0.49
1:B:95:ASN:N	1:B:96:PRO:CD	2.76	0.48
1:A:213:TYR:OH	6:A:402:HOH:O	2.17	0.48
5:A:307:MPD:H51	6:A:553:HOH:O	2.13	0.48
1:B:41:THR:HG23	6:B:512:HOH:O	2.13	0.48
1:A:9:ILE:O	1:A:246:MET:HA	2.18	0.43
2:A:302:A1A43:C31	6:A:625:HOH:O	2.65	0.43
1:A:58:THR:HB	1:B:96:PRO:HB3	1.99	0.43
1:A:61:GLU:OE2	6:A:403:HOH:O	2.21	0.43
1:A:170:GLU:OE1	6:A:404:HOH:O	2.21	0.43
1:A:70:ILE:HG21	1:A:88:LEU:HD21	2.00	0.43
1:B:87:LEU:HD11	1:B:130:VAL:HG23	2.00	0.43
1:A:212:ARG:HD3	1:A:212:ARG:C	2.43	0.43
1:A:95:ASN:N	1:A:96:PRO:CD	2.81	0.43
1:B:155:ASP:HB2	6:B:663:HOH:O	2.19	0.43
1:A:185:ARG:HD2	1:A:219:TYR:OH	2.18	0.43
5:A:306:MPD:H11	5:A:306:MPD:H53	2.00	0.43
2:A:302:A1A43:C30	6:A:733:HOH:O	2.67	0.42
1:A:33:ASP:CG	6:A:407:HOH:O	2.63	0.41
1:A:95:ASN:N	1:A:96:PRO:HD3	2.35	0.41
1:A:16:LEU:HD22	1:A:69:TYR:CD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:526:HOH:O	6:B:625:HOH:O[4_555]	2.18	0.02

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	276/301 (92%)	265 (96%)	11 (4%)	0	100	100
1	B	277/301 (92%)	267 (96%)	9 (3%)	1 (0%)	30	51
All	All	553/602 (92%)	532 (96%)	20 (4%)	1 (0%)	43	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	GLU

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	242/259 (93%)	235 (97%)	7 (3%)	37	65
1	B	243/259 (94%)	236 (97%)	7 (3%)	37	65
All	All	485/518 (94%)	471 (97%)	14 (3%)	39	65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	21	GLU
1	A	50	PRO
1	A	80	LYS
1	A	88	LEU

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Mol	Chain	Res	Type
1	A	136	ILE
1	A	172	LEU
1	B	87	LEU
1	B	91[A]	ASP
1	B	91[B]	ASP
1	B	151	LYS
1	B	227	SER
1	B	260	ARG
1	B	265	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	203	ASN
1	B	47	ASN
1	B	72	GLN
1	B	119	GLN
1	B	274	ASN

5.3.3 RNA [i](#)

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 12 ligands modelled in this entry, 4 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
2	A1A43	A	303	4	38,39,39	0.54	0	41,44,44	0.98	2 (4%)
2	A1A43	B	301	-	38,39,39	0.39	0	41,44,44	0.68	1 (2%)
2	A1A43	B	303	4	38,39,39	0.54	0	41,44,44	1.14	4 (9%)
2	A1A43	A	301	-	38,39,39	0.46	0	41,44,44	0.70	1 (2%)
2	A1A43	B	302	-	38,39,39	0.58	0	41,44,44	1.07	3 (7%)
5	MPD	A	306	-	7,7,7	0.30	0	9,10,10	0.90	0
5	MPD	A	307	-	7,7,7	0.14	0	9,10,10	0.51	0
2	A1A43	A	302	-	38,39,39	0.44	0	41,44,44	0.99	4 (9%)

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
2	A1A43	A	303	4	-	26/44/44/44	-
2	A1A43	B	301	-	-	13/44/44/44	-
2	A1A43	B	303	4	-	19/44/44/44	-
2	A1A43	A	301	-	-	8/44/44/44	-
2	A1A43	B	302	-	-	25/44/44/44	-
5	MPD	A	306	-	-	2/5/5/5	-
5	MPD	A	307	-	-	2/5/5/5	-
2	A1A43	A	302	-	-	23/44/44/44	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	303	A1A43	C16-N2-C20	3.82	129.77	123.40
2	B	302	A1A43	C16-N2-C20	3.66	129.50	123.40
2	B	303	A1A43	O4-C18-C19	3.63	122.44	109.17
2	A	303	A1A43	O4-C18-C19	3.45	121.81	109.17
2	A	303	A1A43	C16-N2-C20	3.22	128.77	123.40
2	B	301	A1A43	C16-N2-C20	3.15	128.65	123.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	A1A43	C16-N2-C20	3.04	128.47	123.40
2	B	303	A1A43	C17-C16-C15	-2.92	106.37	112.90
2	A	302	A1A43	C15-C14-C13	2.91	130.72	124.69
2	A	302	A1A43	O6-C15-C16	2.51	114.48	107.85
2	A	302	A1A43	C15-C16-N2	2.31	113.57	109.66
2	B	303	A1A43	C17-C16-N2	2.30	112.93	109.66
2	B	302	A1A43	O6-C15-C14	-2.23	105.11	110.88
2	A	302	A1A43	C16-N2-C20	2.14	126.97	123.40
2	B	302	A1A43	C15-C16-N2	2.10	113.22	109.66

There are no chirality outliers.

All (118) torsion outliers are listed below:

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	C17-O1-P1-O2
2	A	302	A1A43	C17-O1-P1-O4
2	A	302	A1A43	C18-O4-P1-O2
2	A	302	A1A43	C18-O4-P1-O3
2	A	302	A1A43	O4-C18-C19-N1
2	A	303	A1A43	N2-C16-C17-O1
2	A	303	A1A43	C16-C17-O1-P1
2	A	303	A1A43	C17-O1-P1-O2
2	A	303	A1A43	C17-O1-P1-O3
2	A	303	A1A43	C17-O1-P1-O4
2	B	302	A1A43	C15-C16-C17-O1
2	B	302	A1A43	N2-C16-C17-O1
2	B	302	A1A43	C17-O1-P1-O3
2	B	302	A1A43	C17-O1-P1-O4
2	B	302	A1A43	O4-C18-C19-N1
2	B	303	A1A43	N2-C16-C17-O1
2	B	303	A1A43	C16-C17-O1-P1
2	B	303	A1A43	C17-O1-P1-O3
2	B	303	A1A43	C17-O1-P1-O4
2	B	303	A1A43	O4-C18-C19-N1
5	A	307	MPD	C2-C3-C4-O4
5	A	307	MPD	C2-C3-C4-C5
2	B	301	A1A43	C3-C4-C5-C6
2	B	301	A1A43	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	A	303	A1A43	C22-C23-C24-C25
2	A	301	A1A43	C6-C7-C8-C9
2	A	303	A1A43	C27-C28-C29-C30
2	B	303	A1A43	C25-C26-C27-C28
2	B	301	A1A43	C5-C6-C7-C8
2	B	302	A1A43	C7-C8-C9-C10
2	A	303	A1A43	C24-C25-C26-C27
2	B	301	A1A43	C28-C29-C30-C31
2	B	303	A1A43	C9-C10-C11-C12
2	B	303	A1A43	C26-C27-C28-C29
2	B	303	A1A43	C4-C5-C6-C7
2	B	302	A1A43	C1-C2-C3-C4
2	B	302	A1A43	C21-C22-C23-C24
2	A	303	A1A43	C10-C11-C12-C13
2	A	301	A1A43	C11-C10-C9-C8
2	B	302	A1A43	C28-C29-C30-C31
2	A	301	A1A43	C2-C3-C4-C5
2	A	302	A1A43	C2-C3-C4-C5
2	B	302	A1A43	C3-C4-C5-C6
2	A	302	A1A43	C27-C28-C29-C30
2	A	303	A1A43	C11-C10-C9-C8
2	A	302	A1A43	C24-C25-C26-C27
2	B	303	A1A43	C3-C4-C5-C6
2	B	302	A1A43	C23-C24-C25-C26
2	B	301	A1A43	C22-C23-C24-C25
2	A	301	A1A43	C27-C28-C29-C30
2	B	302	A1A43	C25-C26-C27-C28
2	A	301	A1A43	C10-C11-C12-C13
2	B	303	A1A43	C10-C11-C12-C13
2	A	303	A1A43	C9-C10-C11-C12
2	B	301	A1A43	C24-C25-C26-C27
2	B	302	A1A43	C2-C3-C4-C5
2	B	302	A1A43	C11-C10-C9-C8
2	A	302	A1A43	C28-C29-C30-C31
2	B	301	A1A43	C1-C2-C3-C4
2	B	302	A1A43	C9-C10-C11-C12
2	A	303	A1A43	C28-C29-C30-C31
2	B	302	A1A43	C22-C23-C24-C25
2	B	303	A1A43	C23-C24-C25-C26
2	B	301	A1A43	C7-C8-C9-C10
2	A	303	A1A43	C1-C2-C3-C4
2	B	302	A1A43	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
2	B	303	A1A43	C2-C3-C4-C5
2	A	302	A1A43	C6-C7-C8-C9
2	A	302	A1A43	C7-C8-C9-C10
2	A	303	A1A43	C14-C15-C16-C17
2	A	303	A1A43	O6-C15-C16-C17
2	B	302	A1A43	C14-C15-C16-C17
2	B	302	A1A43	O6-C15-C16-C17
2	B	303	A1A43	C11-C10-C9-C8
5	A	306	MPD	C1-C2-C3-C4
5	A	306	MPD	CM-C2-C3-C4
2	A	303	A1A43	C13-C14-C15-O6
2	A	303	A1A43	C23-C24-C25-C26
2	B	303	A1A43	C15-C16-C17-O1
2	A	301	A1A43	C25-C26-C27-C28
2	A	302	A1A43	C18-O4-P1-O1
2	B	302	A1A43	C18-O4-P1-O1
2	B	302	A1A43	C18-O4-P1-O2
2	B	302	A1A43	C18-O4-P1-O3
2	A	303	A1A43	C6-C7-C8-C9
2	A	302	A1A43	C25-C26-C27-C28
2	B	301	A1A43	C27-C28-C29-C30
2	A	302	A1A43	C3-C4-C5-C6
2	B	301	A1A43	C10-C11-C12-C13
2	A	303	A1A43	C7-C8-C9-C10
2	B	302	A1A43	C6-C7-C8-C9
2	A	303	A1A43	C20-C21-C22-C23
2	A	302	A1A43	C23-C24-C25-C26
2	B	302	A1A43	C24-C25-C26-C27
2	A	301	A1A43	C22-C23-C24-C25
2	A	302	A1A43	C1-C2-C3-C4
2	A	301	A1A43	C3-C4-C5-C6
2	A	303	A1A43	C21-C22-C23-C24
2	A	303	A1A43	C13-C14-C15-C16
2	B	303	A1A43	C5-C6-C7-C8
2	B	302	A1A43	O5-C20-C21-C22
2	A	303	A1A43	O6-C15-C16-N2
2	A	303	A1A43	C11-C12-C13-C14
2	B	301	A1A43	C25-C26-C27-C28
2	A	302	A1A43	C26-C27-C28-C29
2	A	302	A1A43	C11-C12-C13-C14
2	A	303	A1A43	C4-C5-C6-C7
2	B	303	A1A43	O6-C15-C16-C17

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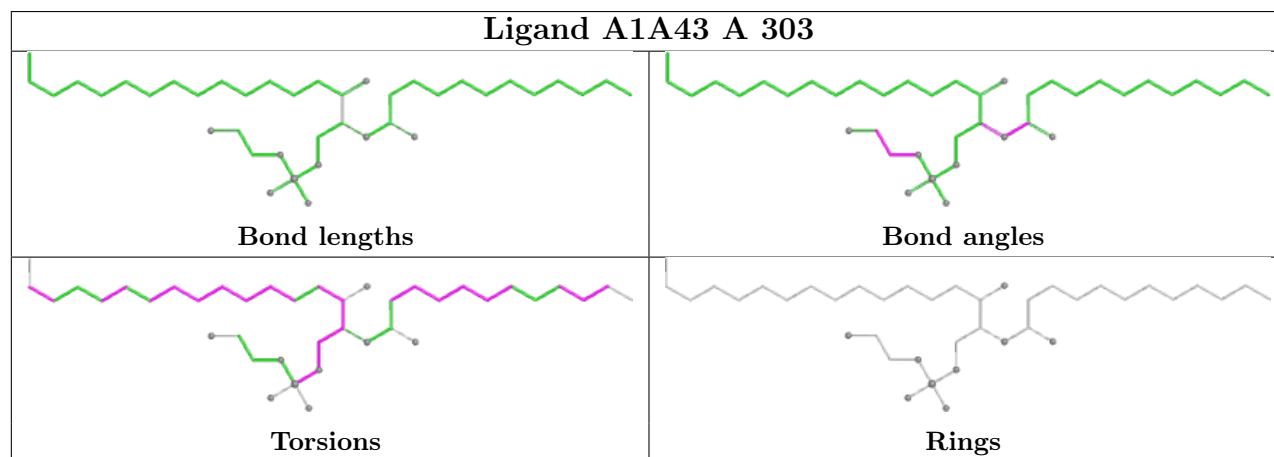
Mol	Chain	Res	Type	Atoms
2	B	303	A1A43	C24-C25-C26-C27
2	B	301	A1A43	C2-C3-C4-C5
2	B	303	A1A43	C11-C12-C13-C14
2	B	301	A1A43	C21-C22-C23-C24
2	A	302	A1A43	C22-C23-C24-C25
2	A	303	A1A43	C15-C16-C17-O1

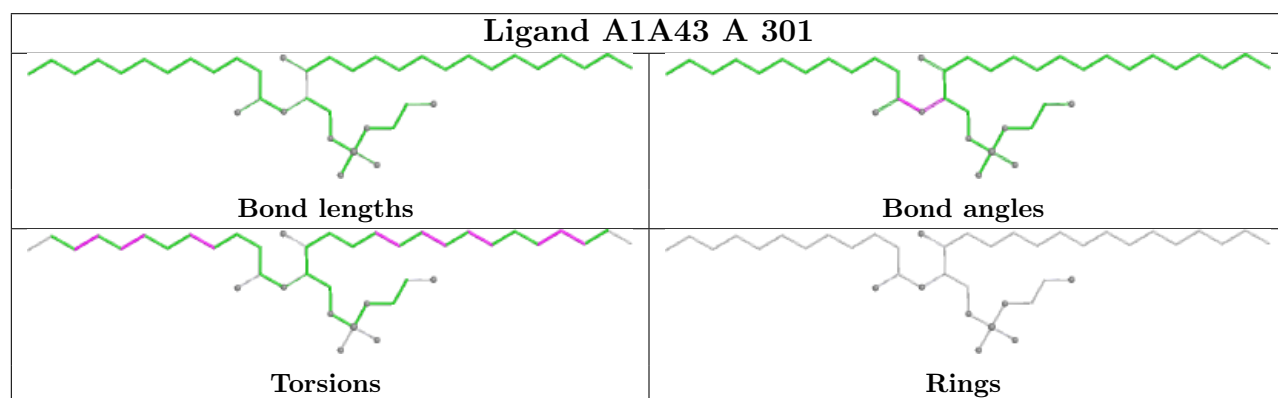
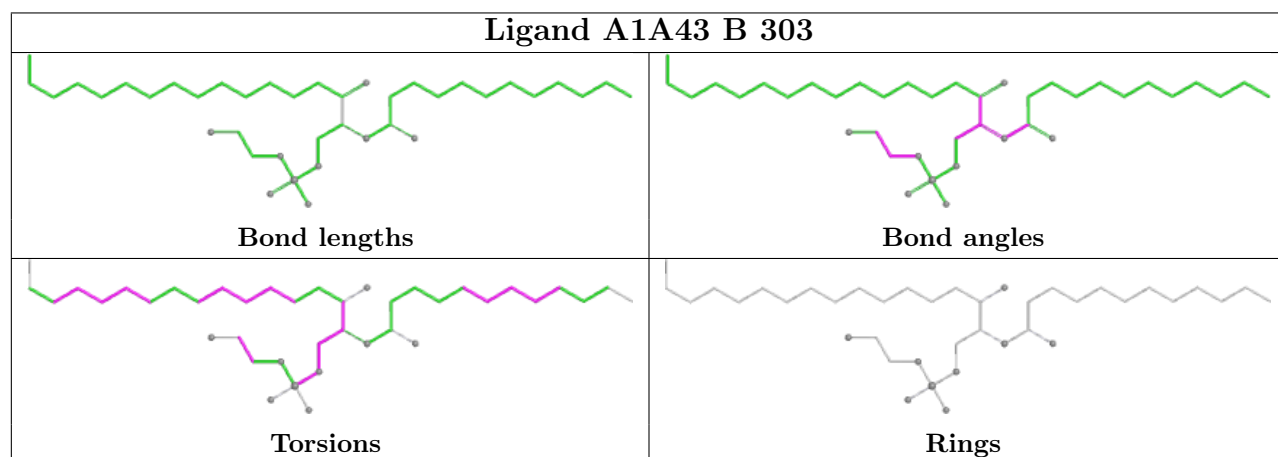
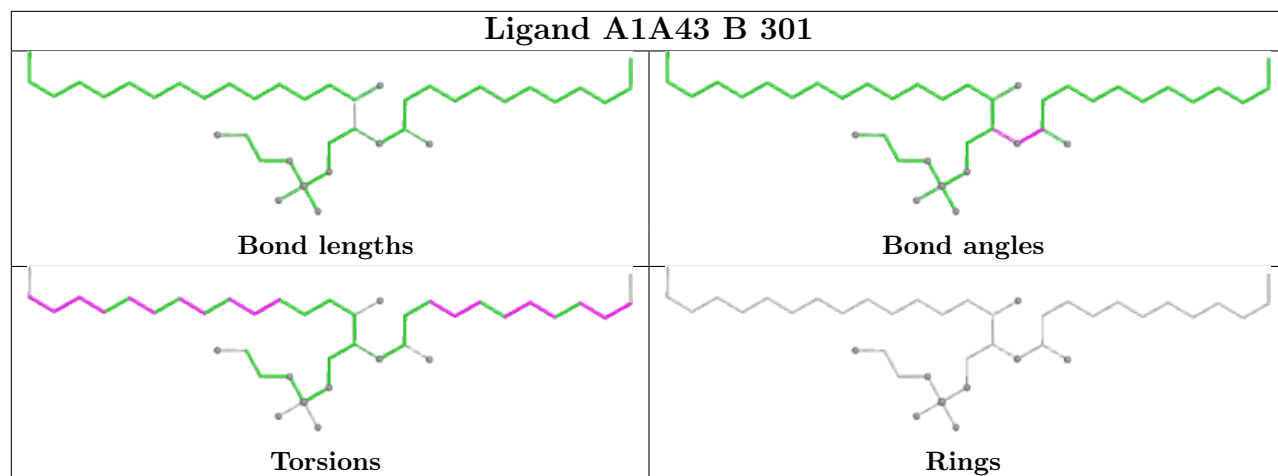
There are no ring outliers.

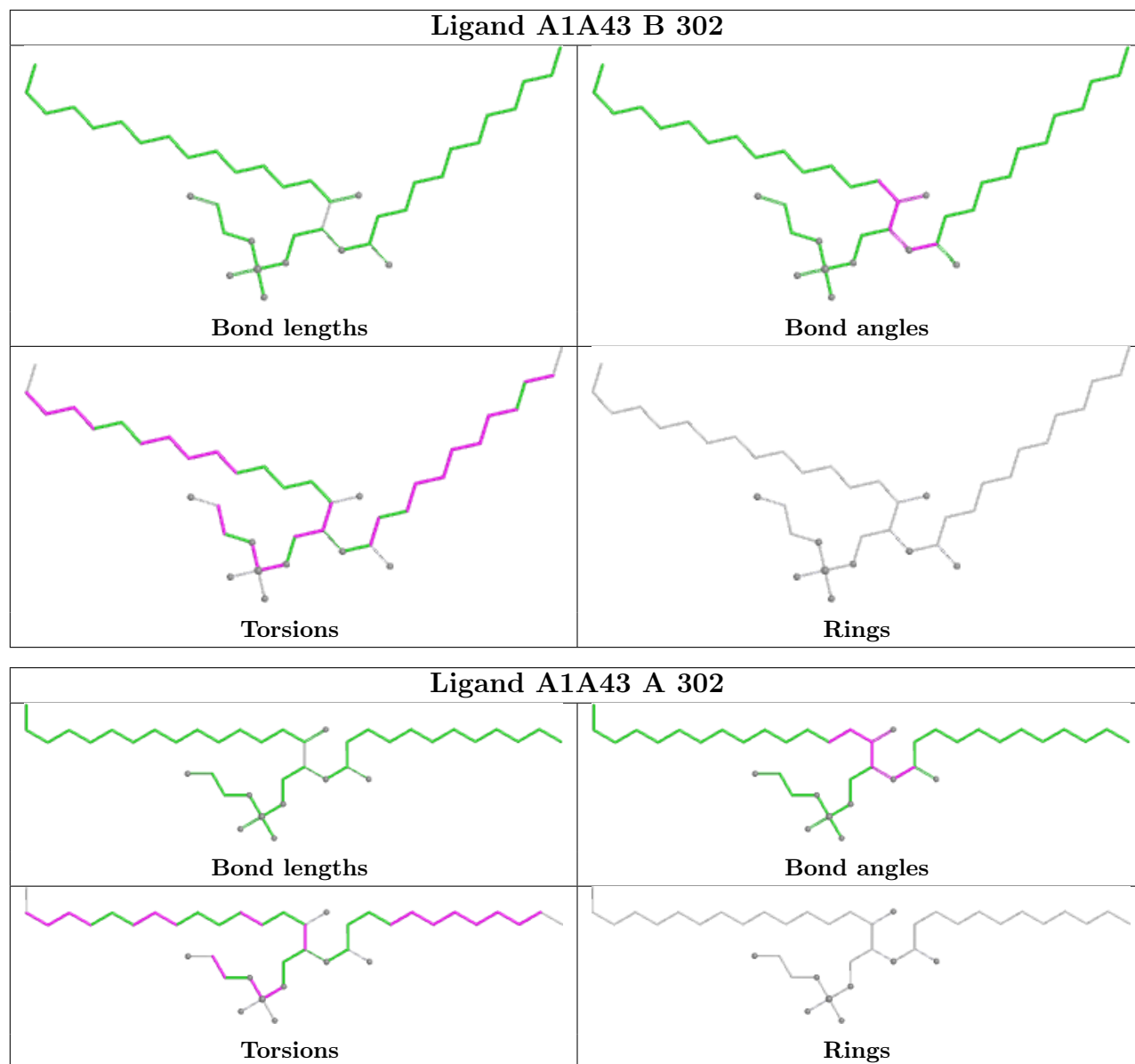
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	303	A1A43	2	0
2	B	303	A1A43	2	0
5	A	306	MPD	1	0
5	A	307	MPD	1	0
2	A	302	A1A43	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	278/301 (92%)	-0.54	0 100 100	9, 16, 34, 54	0
1	B	278/301 (92%)	-0.57	0 100 100	5, 15, 33, 63	1 (0%)
All	All	556/602 (92%)	-0.56	0 100 100	5, 16, 34, 63	1 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	A1A43	B	302	40/40	0.76	0.29	46,92,111,112	0
2	A1A43	A	302	40/40	0.77	0.25	63,84,109,117	0
5	MPD	A	307	8/8	0.85	0.21	59,63,70,73	0
2	A1A43	B	303	40/40	0.88	0.17	33,50,111,115	0
2	A1A43	A	303	40/40	0.89	0.15	35,48,95,97	0
5	MPD	A	306	8/8	0.90	0.16	44,52,68,70	0
3	NA	B	304	1/1	0.93	0.11	32,32,32,32	0

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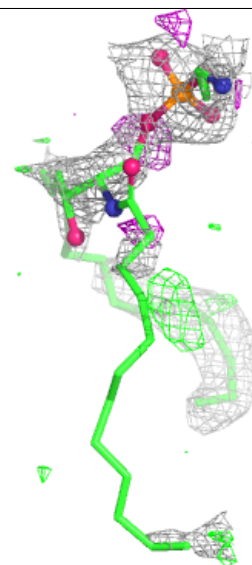
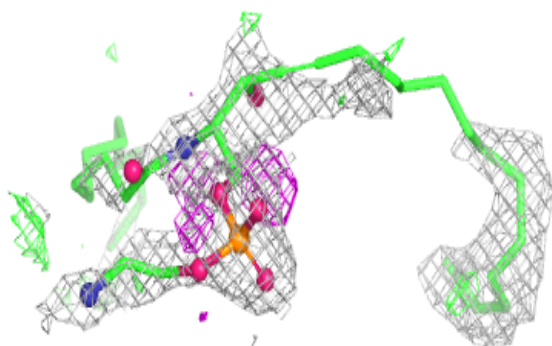
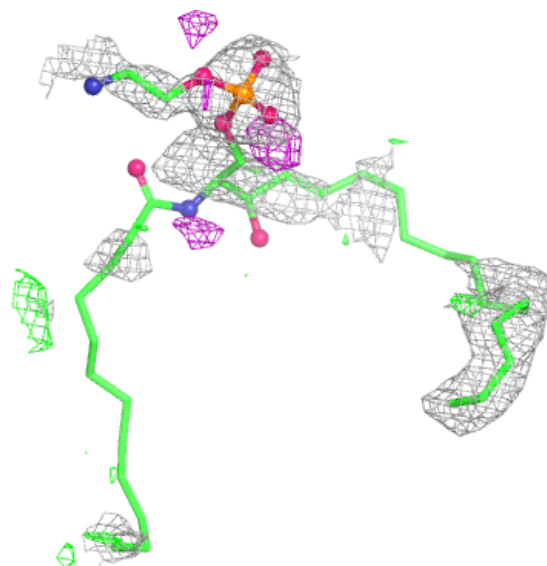
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1A43	B	301	40/40	0.94	0.16	15,43,110,120	0
2	A1A43	A	301	40/40	0.95	0.13	15,37,89,95	0
3	NA	A	304	1/1	0.96	0.10	33,33,33,33	0
4	MG	A	305	1/1	1.00	0.07	4,4,4,4	0
4	MG	B	305	1/1	1.00	0.08	4,4,4,4	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.

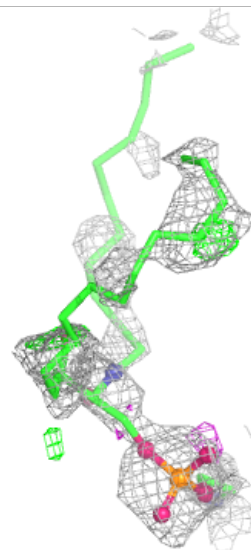
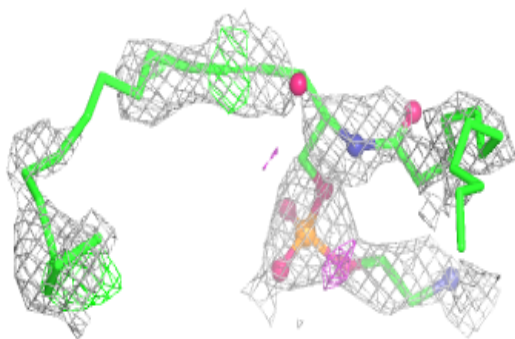
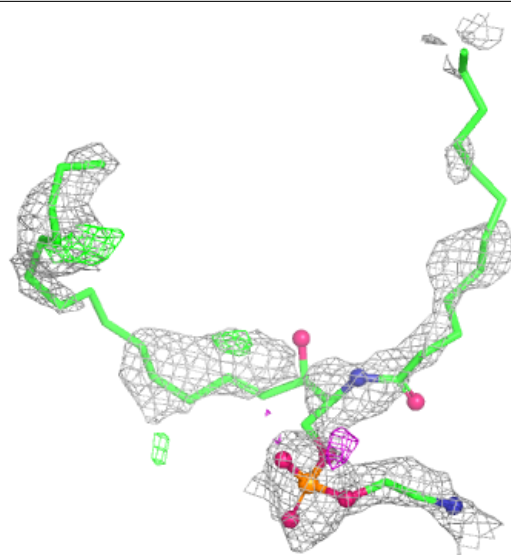
Electron density around A1A43 B 302:

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



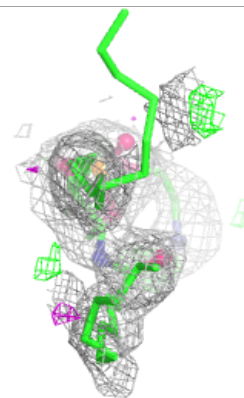
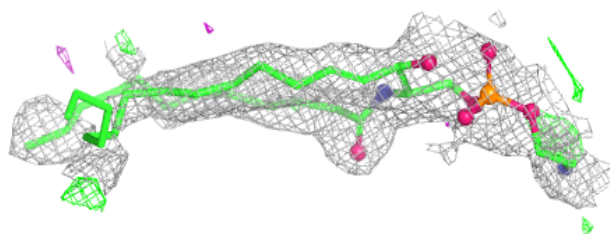
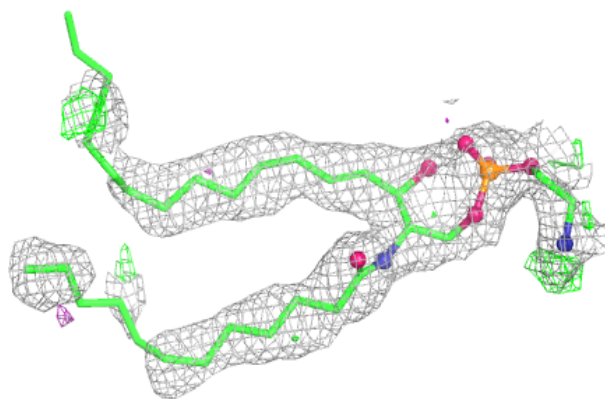
Electron density around A1A43 A 302:

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

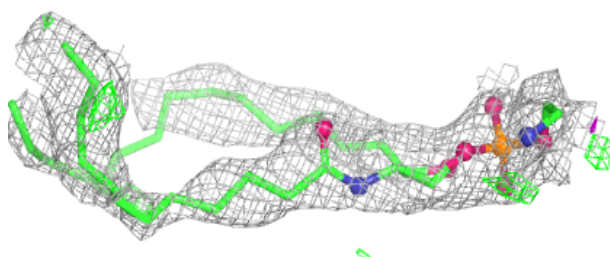
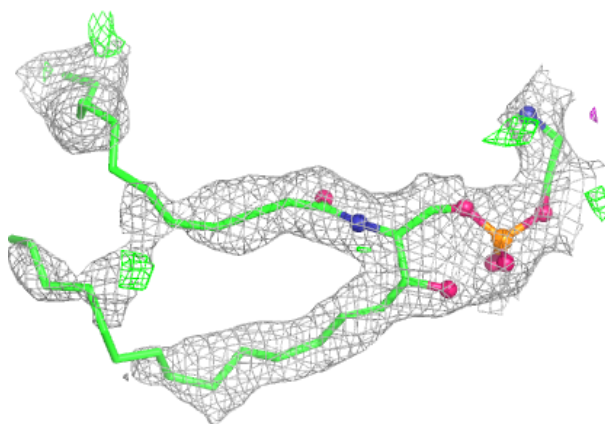


Electron density around A1A43 B 303:

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

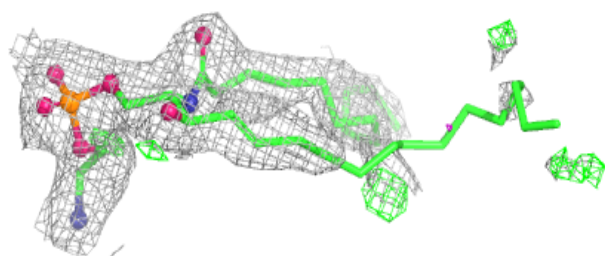
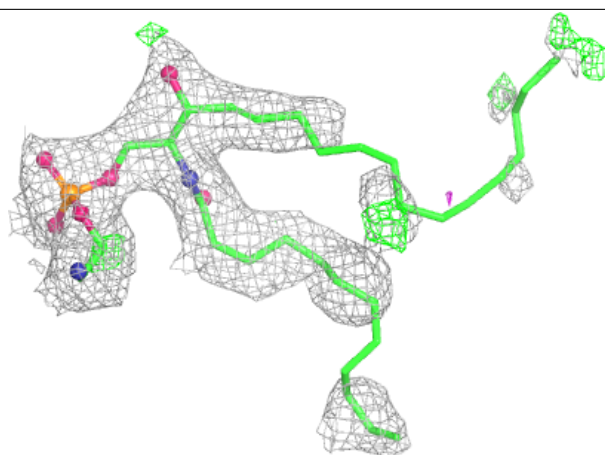
**Electron density around A1A43 A 303:**

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

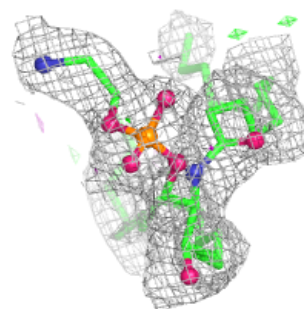
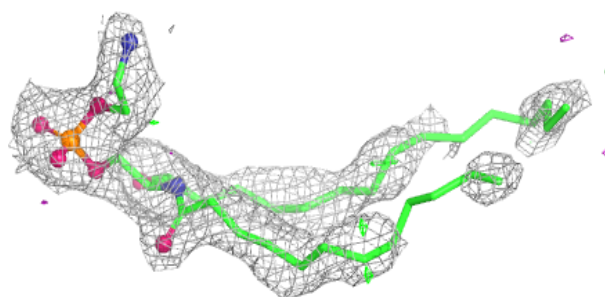
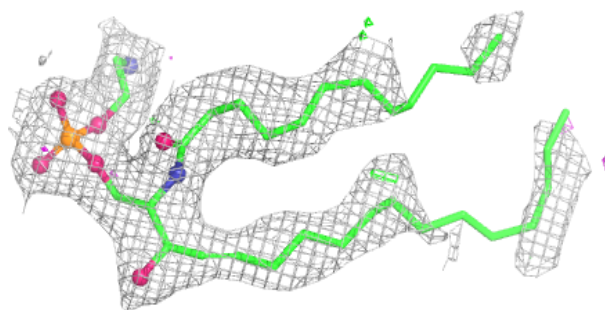


Electron density around A1A43 B 301:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.