



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:58 PM UTC

PDB ID : 4PSE / pdb_00004pse
Title : Trichoderma reesei cutinase in complex with a C11Y4 phosphonate inhibitor
Authors : Roussel, A.; Amara, S.; Nyysola, A.; Mateos-Diaz, E.; Blangy, S.; Kontkanen, H.; Westerholm-Parvinen, A.; Carriere, F.; Cambillau, C.
Deposited on : 2014-03-07
Resolution : 1.71 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

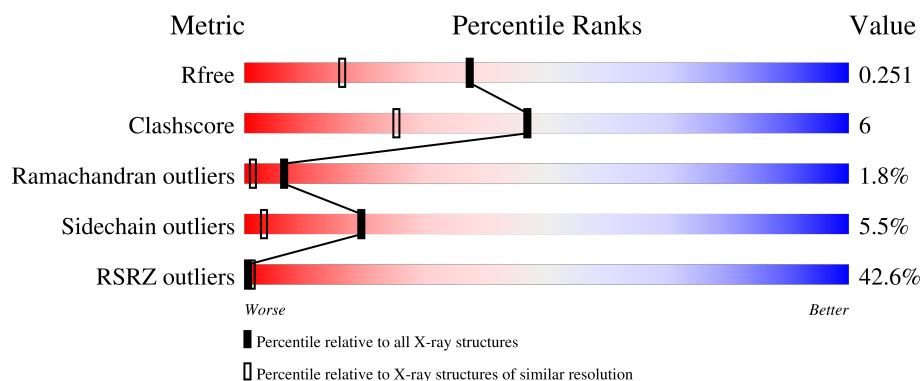
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	254	<div> <div>12%</div> <div>77%</div> <div>8%</div> <div>••</div> <div>13%</div> </div>
1	B	254	<div> <div>62%</div> <div>70%</div> <div>13%</div> <div>•</div> <div>14%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3459 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 Carbohydrate esterase family 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1595	1009	261	315	10			
1	B	219	Total	C	N	O	S	0	1	0
			1595	1008	263	314	10			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP G0RH85
A	2	ARG	-	expression tag	UNP G0RH85
A	3	SER	-	expression tag	UNP G0RH85
A	4	LEU	-	expression tag	UNP G0RH85
A	5	ALA	-	expression tag	UNP G0RH85
A	6	ILE	-	expression tag	UNP G0RH85
A	7	LEU	-	expression tag	UNP G0RH85
A	8	THR	-	expression tag	UNP G0RH85
A	9	THR	-	expression tag	UNP G0RH85
A	10	LEU	-	expression tag	UNP G0RH85
A	11	LEU	-	expression tag	UNP G0RH85
A	12	ALA	-	expression tag	UNP G0RH85
A	13	GLY	-	expression tag	UNP G0RH85
A	14	HIS	-	expression tag	UNP G0RH85
A	15	ALA	-	expression tag	UNP G0RH85
A	16	PHE	-	expression tag	UNP G0RH85
A	17	ALA	-	expression tag	UNP G0RH85
A	18	TYR	-	expression tag	UNP G0RH85
A	19	PRO	-	expression tag	UNP G0RH85
A	20	LYS	-	expression tag	UNP G0RH85
A	21	PRO	-	expression tag	UNP G0RH85
A	22	ALA	-	expression tag	UNP G0RH85
A	23	PRO	-	expression tag	UNP G0RH85
A	24	GLN	-	expression tag	UNP G0RH85
A	25	SER	-	expression tag	UNP G0RH85

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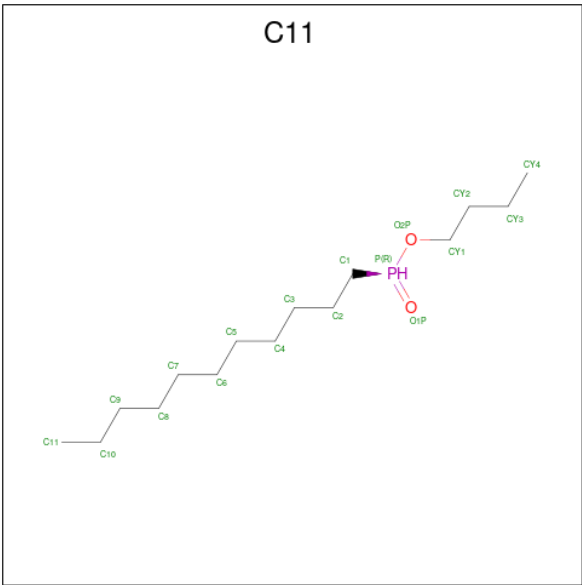
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	VAL	-	expression tag	UNP G0RH85
A	27	ASN	-	expression tag	UNP G0RH85
A	28	ARG	-	expression tag	UNP G0RH85
A	29	ARG	-	expression tag	UNP G0RH85
A	30	ASP	-	expression tag	UNP G0RH85
A	31	TRP	-	expression tag	UNP G0RH85
A	32	PRO	-	expression tag	UNP G0RH85
A	33	SER	-	expression tag	UNP G0RH85
A	34	ILE	-	expression tag	UNP G0RH85
A	35	ASN	-	expression tag	UNP G0RH85
A	36	GLU	-	expression tag	UNP G0RH85
A	37	PHE	-	expression tag	UNP G0RH85
A	38	LEU	-	expression tag	UNP G0RH85
A	39	SER	-	expression tag	UNP G0RH85
A	40	GLU	-	expression tag	UNP G0RH85
A	41	LEU	-	expression tag	UNP G0RH85
A	42	ALA	-	expression tag	UNP G0RH85
A	43	LYS	-	expression tag	UNP G0RH85
A	44	VAL	-	expression tag	UNP G0RH85
A	249	HIS	-	expression tag	UNP G0RH85
A	250	HIS	-	expression tag	UNP G0RH85
A	251	HIS	-	expression tag	UNP G0RH85
A	252	HIS	-	expression tag	UNP G0RH85
A	253	HIS	-	expression tag	UNP G0RH85
A	254	HIS	-	expression tag	UNP G0RH85
B	1	MET	-	initiating methionine	UNP G0RH85
B	2	ARG	-	expression tag	UNP G0RH85
B	3	SER	-	expression tag	UNP G0RH85
B	4	LEU	-	expression tag	UNP G0RH85
B	5	ALA	-	expression tag	UNP G0RH85
B	6	ILE	-	expression tag	UNP G0RH85
B	7	LEU	-	expression tag	UNP G0RH85
B	8	THR	-	expression tag	UNP G0RH85
B	9	THR	-	expression tag	UNP G0RH85
B	10	LEU	-	expression tag	UNP G0RH85
B	11	LEU	-	expression tag	UNP G0RH85
B	12	ALA	-	expression tag	UNP G0RH85
B	13	GLY	-	expression tag	UNP G0RH85
B	14	HIS	-	expression tag	UNP G0RH85
B	15	ALA	-	expression tag	UNP G0RH85
B	16	PHE	-	expression tag	UNP G0RH85
B	17	ALA	-	expression tag	UNP G0RH85

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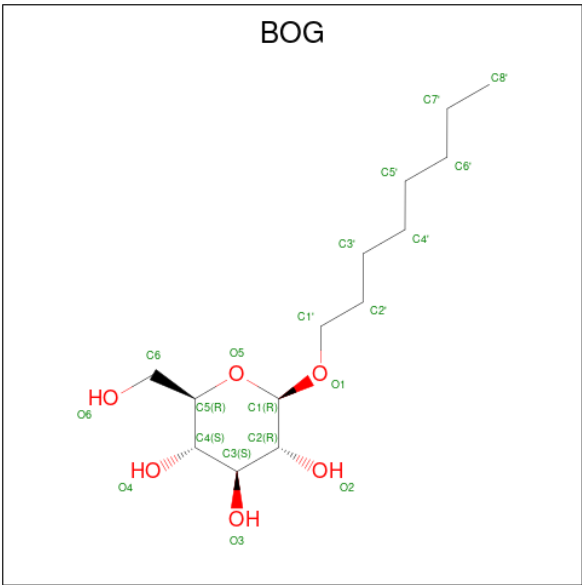
Chain	Residue	Modelled	Actual	Comment	Reference
B	18	TYR	-	expression tag	UNP G0RH85
B	19	PRO	-	expression tag	UNP G0RH85
B	20	LYS	-	expression tag	UNP G0RH85
B	21	PRO	-	expression tag	UNP G0RH85
B	22	ALA	-	expression tag	UNP G0RH85
B	23	PRO	-	expression tag	UNP G0RH85
B	24	GLN	-	expression tag	UNP G0RH85
B	25	SER	-	expression tag	UNP G0RH85
B	26	VAL	-	expression tag	UNP G0RH85
B	27	ASN	-	expression tag	UNP G0RH85
B	28	ARG	-	expression tag	UNP G0RH85
B	29	ARG	-	expression tag	UNP G0RH85
B	30	ASP	-	expression tag	UNP G0RH85
B	31	TRP	-	expression tag	UNP G0RH85
B	32	PRO	-	expression tag	UNP G0RH85
B	33	SER	-	expression tag	UNP G0RH85
B	34	ILE	-	expression tag	UNP G0RH85
B	35	ASN	-	expression tag	UNP G0RH85
B	36	GLU	-	expression tag	UNP G0RH85
B	37	PHE	-	expression tag	UNP G0RH85
B	38	LEU	-	expression tag	UNP G0RH85
B	39	SER	-	expression tag	UNP G0RH85
B	40	GLU	-	expression tag	UNP G0RH85
B	41	LEU	-	expression tag	UNP G0RH85
B	42	ALA	-	expression tag	UNP G0RH85
B	43	LYS	-	expression tag	UNP G0RH85
B	44	VAL	-	expression tag	UNP G0RH85
B	249	HIS	-	expression tag	UNP G0RH85
B	250	HIS	-	expression tag	UNP G0RH85
B	251	HIS	-	expression tag	UNP G0RH85
B	252	HIS	-	expression tag	UNP G0RH85
B	253	HIS	-	expression tag	UNP G0RH85
B	254	HIS	-	expression tag	UNP G0RH85

- Molecule 2 is UNDECYL-PHOSPHINIC ACID BUTYL ESTER (CCD ID: C11) (formula: $C_{15}H_{33}O_2P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			18	15	2	1		
2	B	1	Total	C	O	P	0	0
			17	14	2	1		

- Molecule 3 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		

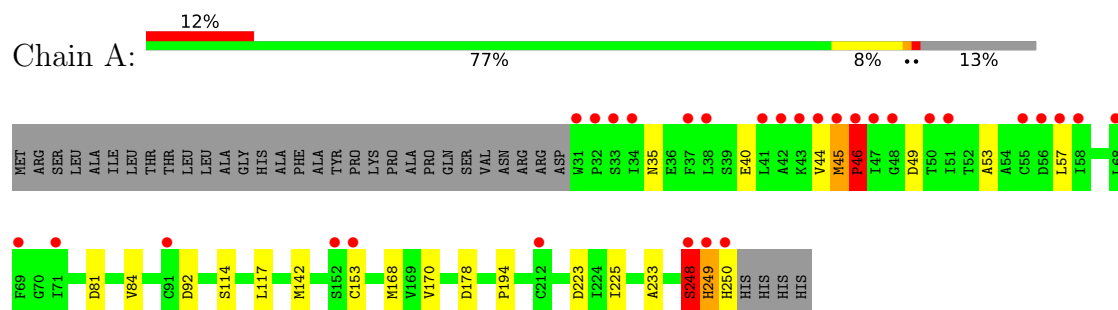
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total 167	O 167	0	0
4	B	27	Total 27	O 27	0	0

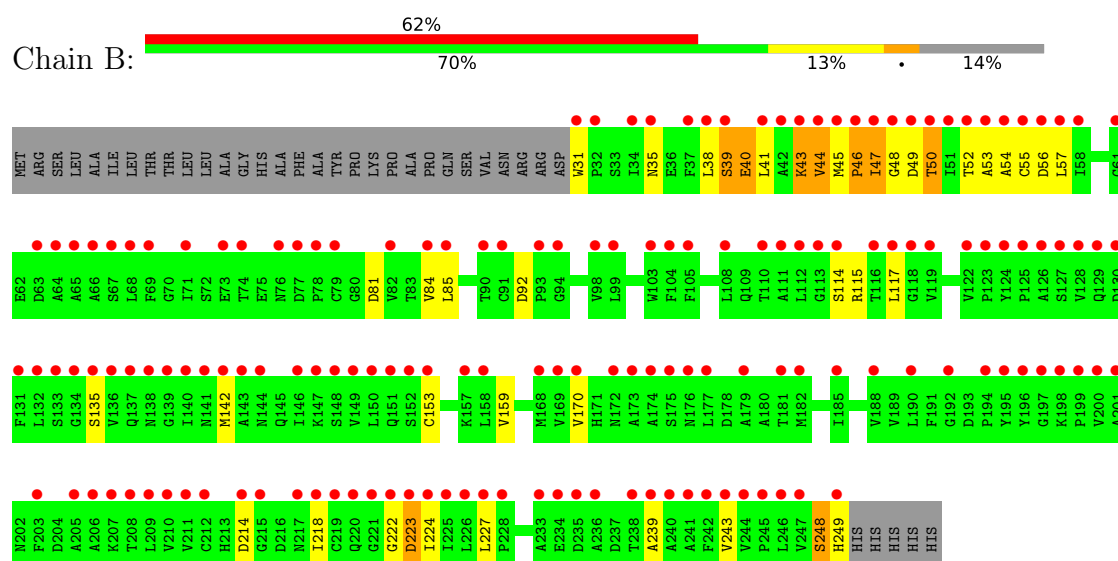
3 Residue-property plots

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: Carbohydrate esterase family 5



• Molecule 1: Carbohydrate esterase family 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.04Å 37.54Å 133.01Å 90.00° 97.38° 90.00°	Depositor
Resolution (Å)	47.66 – 1.71 47.66 – 1.71	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.66-1.71) 97.4 (47.66-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.65Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.220 , 0.234 (Not available) , 0.251	Depositor DCC
R_{free} test set	2858 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3459	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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: BOG, C11

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	0.79	0/1628	1.23	15/2226 (0.7%)
1	B	0.75	0/1631	1.29	10/2229 (0.4%)
All	All	0.77	0/3259	1.26	25/4455 (0.6%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	SER	CA-C-N	8.01	136.12	121.70
1	A	248	SER	C-N-CA	8.01	136.12	121.70
1	B	248	SER	N-CA-C	7.11	120.51	109.07
1	B	92	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	249	HIS	CA-C-N	6.88	134.09	121.70
1	A	249	HIS	C-N-CA	6.88	134.09	121.70
1	A	92	ASP	CA-CB-CG	6.68	119.28	112.60
1	B	50	THR	N-CA-C	-6.45	103.94	110.97
1	B	223	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	178	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	248	SER	N-CA-C	5.82	123.19	110.80
1	B	81	ASP	N-CA-C	-5.67	105.09	111.28
1	B	40	GLU	CB-CG-CD	5.66	122.22	112.60
1	A	249	HIS	N-CA-C	5.56	126.56	111.00
1	A	46	PRO	CA-C-N	5.35	128.92	120.47
1	A	46	PRO	C-N-CA	5.35	128.92	120.47
1	B	248	SER	CA-C-N	5.32	131.28	121.70
1	B	248	SER	C-N-CA	5.32	131.28	121.70
1	A	49	ASP	CA-C-N	5.21	127.22	120.44
1	A	49	ASP	C-N-CA	5.21	127.22	120.44
1	B	54	ALA	CA-C-N	5.20	127.67	120.29
1	B	54	ALA	C-N-CA	5.20	127.67	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ALA	CA-C-N	5.10	127.07	120.44
1	A	53	ALA	C-N-CA	5.10	127.07	120.44
1	A	81	ASP	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1595	0	1541	21	1
1	B	1595	0	1543	16	0
2	A	18	0	32	0	0
2	B	17	0	27	1	0
3	A	40	0	56	3	0
4	A	167	0	0	0	1
4	B	27	0	0	0	0
All	All	3459	0	3199	37	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 6.

All (37) 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:248:SER:HB3	1:A:249:HIS:O	1.51	1.11
1:A:45:MET:N	1:A:46:PRO:HD3	1.96	0.81
1:A:248:SER:CB	1:A:249:HIS:O	2.31	0.78
1:B:115[A]:ARG:NH2	1:B:248:SER:OG	2.23	0.72
1:A:249:HIS:HA	1:A:250:HIS:ND1	2.08	0.68
1:A:248:SER:HB3	1:A:249:HIS:C	2.19	0.68
1:A:44:VAL:C	1:A:46:PRO:HD3	2.21	0.66
1:B:44:VAL:C	1:B:46:PRO:HD3	2.21	0.66
1:B:49:ASP:HA	1:B:52:THR:HB	1.81	0.61
1:B:47:ILE:O	1:B:50:THR:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:HG23	1:A:117:LEU:HD11	1.90	0.54
1:B:52:THR:O	1:B:55:CYS:N	2.38	0.54
1:B:84:VAL:HG23	1:B:117:LEU:HD11	1.91	0.53
1:B:218:ILE:HD12	2:B:301:C11:HY21	1.92	0.52
1:A:45:MET:N	1:A:46:PRO:CD	2.73	0.50
1:B:39:SER:O	1:B:43:LYS:HD3	2.13	0.49
1:B:239:ALA:O	1:B:243:VAL:HG23	2.13	0.48
1:A:249:HIS:CB	1:A:250:HIS:HB2	2.43	0.48
1:A:249:HIS:HA	1:A:250:HIS:HB2	1.95	0.48
1:A:249:HIS:CA	1:A:250:HIS:HB2	2.43	0.48
1:A:249:HIS:HA	1:A:250:HIS:CG	2.48	0.47
1:A:249:HIS:HA	1:A:250:HIS:CB	2.44	0.47
1:A:44:VAL:HB	1:A:46:PRO:HG3	1.97	0.45
1:A:248:SER:HB3	1:A:249:HIS:CA	2.48	0.44
1:A:233:ALA:O	3:A:303:BOG:H61	2.19	0.43
1:A:35:ASN:ND2	1:A:223:ASP:OD2	2.43	0.43
1:B:31:TRP:CG	1:B:222:GLY:HA2	2.54	0.42
1:B:41:LEU:HA	1:B:44:VAL:HG23	2.01	0.42
1:A:35:ASN:HD21	1:A:223:ASP:CG	2.27	0.42
1:B:142:MET:HE1	1:B:170:VAL:HG22	2.02	0.42
1:B:35:ASN:HD21	1:B:223:ASP:CG	2.27	0.42
3:A:302:BOG:H8'1	1:B:224:ILE:HA	2.02	0.42
1:A:225:ILE:HB	3:A:302:BOG:H1'2	2.01	0.42
1:A:142:MET:HE1	1:A:170:VAL:HG22	2.01	0.41
1:A:168:MET:HG3	1:A:194:PRO:HG2	2.03	0.41
1:B:84:VAL:HG22	1:B:159:VAL:HB	2.02	0.40
1:B:50:THR:C	1:B:52:THR:H	2.29	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)
1:A:250:HIS:O	4:A:463:HOH:O[2_546]	1.97	0.23

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	218/254 (86%)	207 (95%)	8 (4%)	3 (1%)	9	2
1	B	218/254 (86%)	206 (94%)	7 (3%)	5 (2%)	5	1
All	All	436/508 (86%)	413 (95%)	15 (3%)	8 (2%)	6	1

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PRO
1	A	248	SER
1	B	45	MET
1	B	46	PRO
1	B	47	ILE
1	B	48	GLY
1	B	53	ALA
1	A	45	MET

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	172/204 (84%)	167 (97%)	5 (3%)	37	14
1	B	172/204 (84%)	158 (92%)	14 (8%)	11	1
All	All	344/408 (84%)	325 (94%)	19 (6%)	19	3

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	57	LEU
1	A	114	SER
1	A	153	CYS

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Mol	Chain	Res	Type
1	A	248	SER
1	B	38	LEU
1	B	39	SER
1	B	40	GLU
1	B	43	LYS
1	B	44	VAL
1	B	56	ASP
1	B	57	LEU
1	B	85	LEU
1	B	114	SER
1	B	135	SER
1	B	153	CYS
1	B	214	ASP
1	B	227	LEU
1	B	249	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	138	ASN
1	A	145	GLN
1	B	35	ASN
1	B	145	GLN
1	B	176	ASN
1	B	202	ASN
1	B	220	GLN

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

4 ligands are modelled in this entry.

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	BOG	A	303	-	20,20,20	0.22	0	25,25,25	0.84	1 (4%)
3	BOG	A	302	-	20,20,20	0.23	0	25,25,25	0.27	0
2	C11	B	301	1	13,16,17	0.31	0	11,16,17	0.74	0
2	C11	A	301	1	14,17,17	0.32	0	12,17,17	0.89	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	BOG	A	303	-	-	7/11/31/31	0/1/1/1
3	BOG	A	302	-	-	4/11/31/31	0/1/1/1
2	C11	B	301	1	-	4/11/15/16	-
2	C11	A	301	1	-	4/12/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	BOG	C1-O5-C5	2.02	117.66	113.72

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	BOG	C3'-C4'-C5'-C6'
3	A	302	BOG	O1-C1'-C2'-C3'
2	A	301	C11	C5-C6-C7-C8

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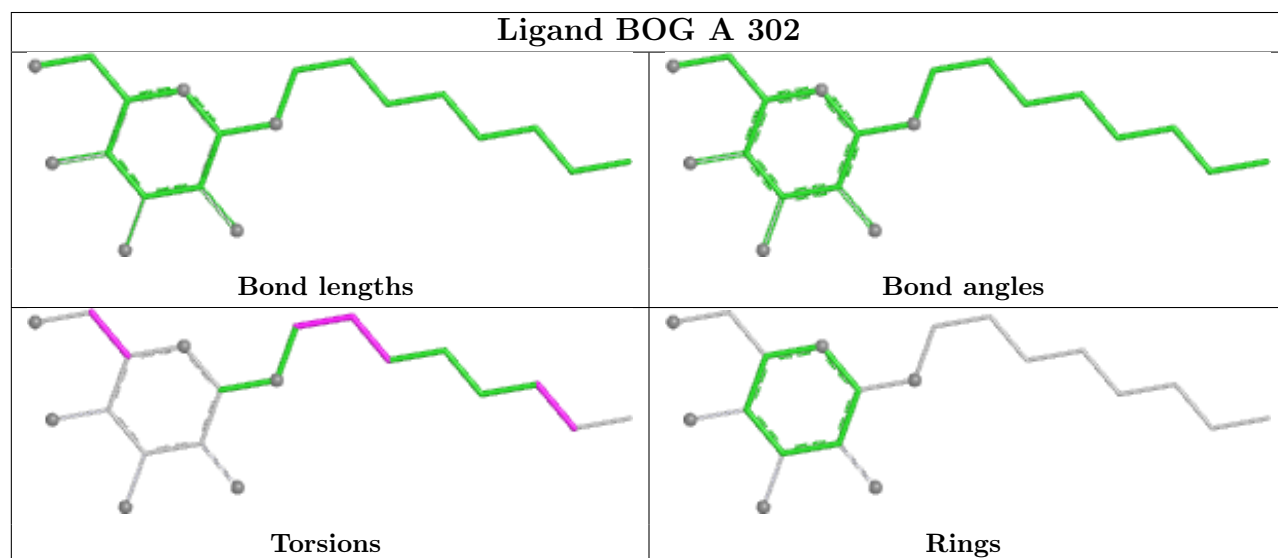
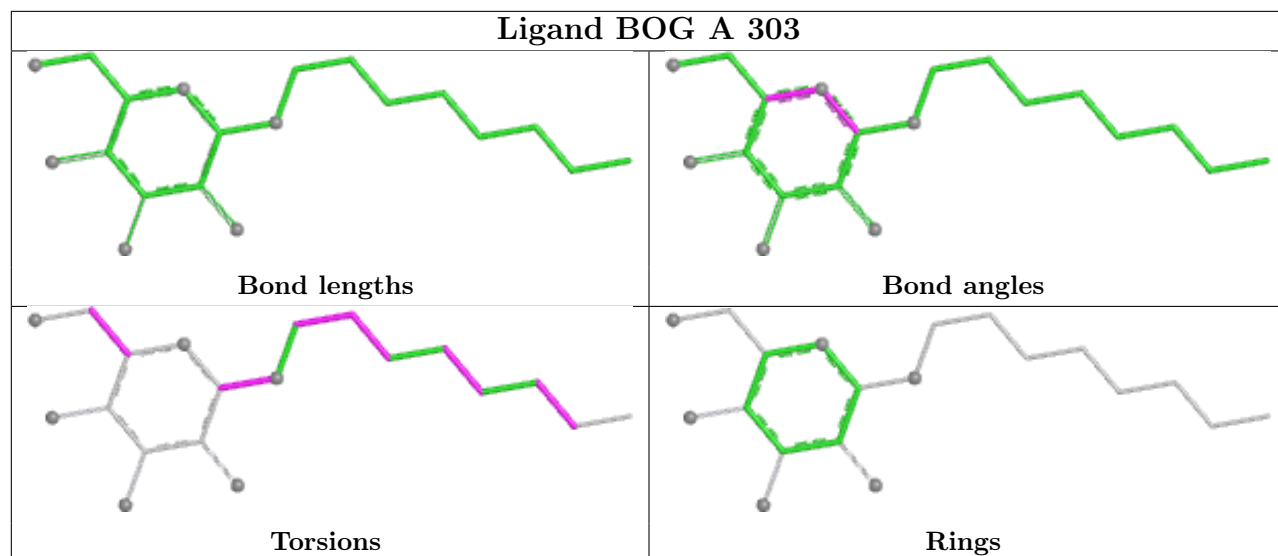
Mol	Chain	Res	Type	Atoms
3	A	302	BOG	O5-C5-C6-O6
3	A	302	BOG	C1'-C2'-C3'-C4'
3	A	303	BOG	O5-C1-O1-C1'
3	A	303	BOG	C1'-C2'-C3'-C4'
3	A	303	BOG	O1-C1'-C2'-C3'
2	B	301	C11	C4-C5-C6-C7
3	A	303	BOG	C5'-C6'-C7'-C8'
3	A	303	BOG	C2-C1-O1-C1'
2	B	301	C11	C7-C8-C9-C10
2	A	301	C11	C3-C4-C5-C6
2	B	301	C11	C3-C4-C5-C6
3	A	302	BOG	C5'-C6'-C7'-C8'
2	A	301	C11	C6-C7-C8-C9
3	A	303	BOG	C4-C5-C6-O6
2	B	301	C11	C2-C3-C4-C5
2	A	301	C11	C11-C10-C9-C8

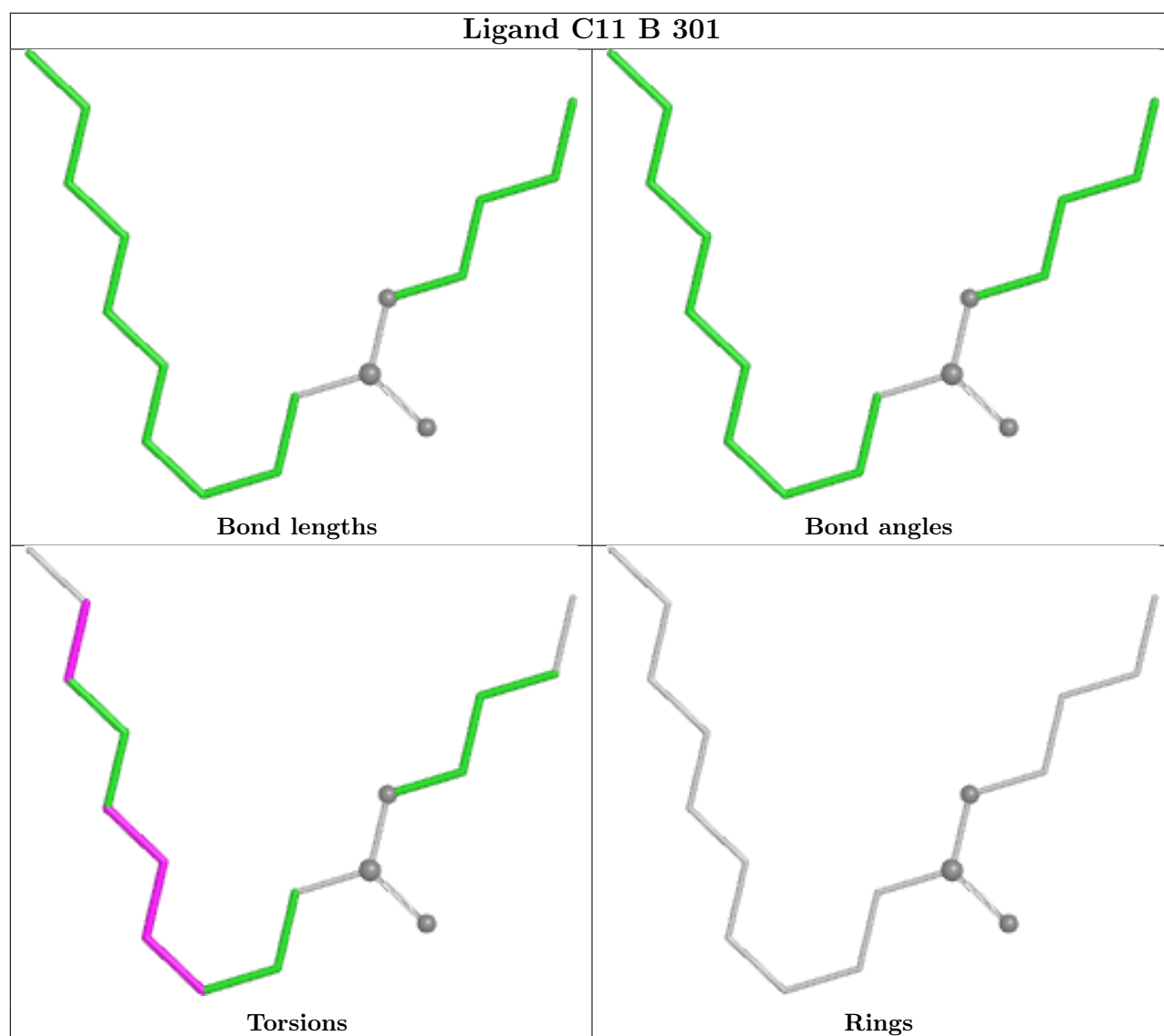
There are no ring outliers.

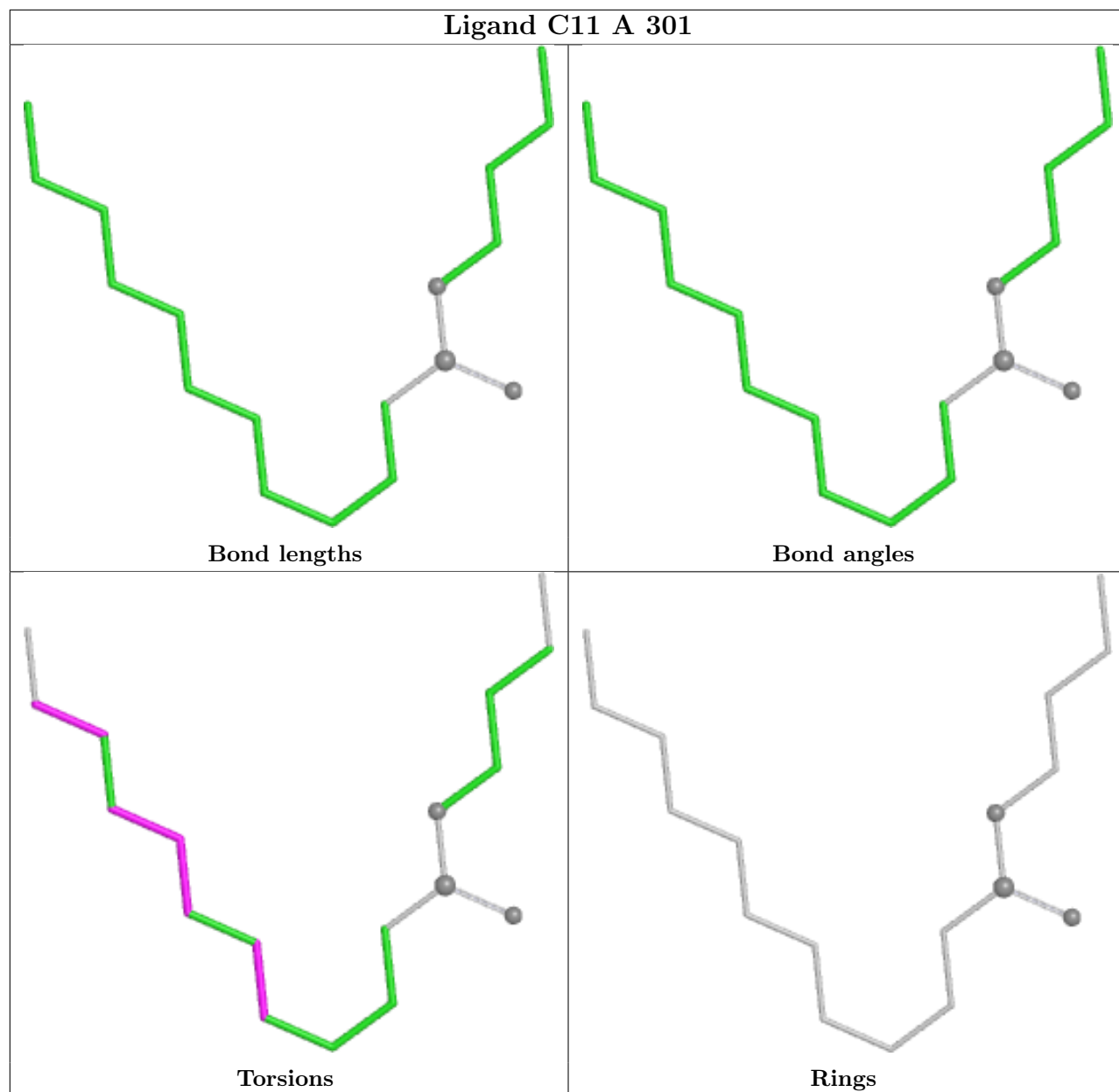
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	BOG	1	0
3	A	302	BOG	2	0
2	B	301	C11	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	220/254 (86%)	0.70	30 (13%)	7 10	16, 28, 60, 83	0
1	B	219/254 (86%)	2.65	157 (71%)	0 0	32, 64, 90, 96	2 (0%)
All	All	439/508 (86%)	1.67	187 (42%)	0 1	16, 46, 84, 96	2 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	PRO	7.9
1	A	44	VAL	7.2
1	B	44	VAL	7.0
1	B	201	ALA	5.7
1	B	131	PHE	5.7
1	B	51	ILE	5.6
1	B	136	VAL	5.5
1	B	68	LEU	5.3
1	B	140	ILE	5.2
1	B	57	LEU	5.2
1	B	37	PHE	5.0
1	B	200	VAL	5.0
1	A	31	TRP	5.0
1	B	71	ILE	4.9
1	B	34	ILE	4.8
1	B	244	VAL	4.8
1	B	132	LEU	4.8
1	B	45	MET	4.7
1	B	31	TRP	4.6
1	B	38	LEU	4.5
1	B	128	VAL	4.4
1	B	169	VAL	4.4
1	B	239	ALA	4.3
1	B	144	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	41	LEU	4.3
1	B	211	VAL	4.2
1	B	79	CYS	4.2
1	B	49	ASP	4.2
1	B	124	TYR	4.1
1	B	153	CYS	4.1
1	A	250	HIS	3.9
1	A	248	SER	3.9
1	B	236	ALA	3.9
1	A	46	PRO	3.9
1	B	197	GLY	3.9
1	A	47	ILE	3.8
1	B	234	GLU	3.8
1	B	112	LEU	3.8
1	B	150	LEU	3.8
1	B	214	ASP	3.8
1	B	32	PRO	3.7
1	B	218	ILE	3.7
1	B	209	LEU	3.7
1	B	240	ALA	3.7
1	B	104	PHE	3.6
1	B	246	LEU	3.6
1	B	55	CYS	3.6
1	B	42	ALA	3.6
1	B	249	HIS	3.6
1	B	94	GLY	3.5
1	B	142	MET	3.5
1	B	108	LEU	3.5
1	B	53	ALA	3.4
1	A	51	ILE	3.4
1	B	242	PHE	3.4
1	B	98	VAL	3.4
1	B	48	GLY	3.4
1	B	46	PRO	3.4
1	B	198	LYS	3.4
1	B	139	GLY	3.4
1	B	223	ASP	3.4
1	B	125	PRO	3.4
1	B	210	VAL	3.3
1	B	235	ASP	3.3
1	B	215	GLY	3.3
1	B	219	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	122	VAL	3.3
1	B	147	LYS	3.3
1	B	207	LYS	3.3
1	B	117	LEU	3.3
1	B	177	LEU	3.3
1	B	245	PRO	3.3
1	B	52	THR	3.2
1	B	35	ASN	3.2
1	B	126	ALA	3.2
1	B	247	VAL	3.2
1	B	138	ASN	3.2
1	B	137	GLN	3.2
1	B	134	GLY	3.2
1	B	69	PHE	3.2
1	B	196	TYR	3.1
1	B	243	VAL	3.1
1	B	135	SER	3.1
1	B	64	ALA	3.1
1	B	73	GLU	3.1
1	B	212	CYS	3.0
1	B	149	VAL	3.0
1	A	68	LEU	3.0
1	B	146	ILE	3.0
1	B	203	PHE	3.0
1	B	143	ALA	3.0
1	B	50	THR	2.9
1	B	241	ALA	2.9
1	B	47	ILE	2.9
1	B	133	SER	2.9
1	B	174	ALA	2.9
1	B	222	GLY	2.9
1	B	65	ALA	2.9
1	B	224	ILE	2.9
1	B	82	VAL	2.8
1	B	78	PRO	2.8
1	B	148	SER	2.8
1	B	225	ILE	2.8
1	B	74	THR	2.8
1	B	90	THR	2.8
1	B	190	LEU	2.8
1	B	227	LEU	2.8
1	B	66	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	116	THR	2.8
1	B	170	VAL	2.7
1	B	220	GLN	2.7
1	B	54	ALA	2.7
1	A	43	LYS	2.7
1	A	152	SER	2.7
1	B	76	ASN	2.7
1	A	45	MET	2.7
1	B	205	ALA	2.7
1	B	111	ALA	2.7
1	A	41	LEU	2.6
1	A	57	LEU	2.6
1	B	195	TYR	2.6
1	A	42	ALA	2.6
1	B	127	SER	2.6
1	A	48	GLY	2.6
1	B	208	THR	2.6
1	A	58	ILE	2.6
1	A	71	ILE	2.6
1	B	58	ILE	2.6
1	B	233	ALA	2.6
1	B	181	THR	2.6
1	B	93	PRO	2.6
1	B	206	ALA	2.5
1	B	118	GLY	2.5
1	B	103	TRP	2.5
1	B	141	ASN	2.5
1	A	55	CYS	2.5
1	A	34	ILE	2.5
1	B	151	GLN	2.5
1	B	168	MET	2.5
1	B	175	SER	2.5
1	B	130	ASP	2.4
1	B	85	LEU	2.4
1	B	123	PRO	2.4
1	A	33	SER	2.4
1	B	172	ASN	2.4
1	B	61	GLY	2.4
1	B	114	SER	2.4
1	A	38	LEU	2.4
1	A	50	THR	2.4
1	B	105	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	56	ASP	2.4
1	B	157	LYS	2.4
1	A	249	HIS	2.4
1	B	119	VAL	2.3
1	B	67	SER	2.3
1	B	173	ALA	2.3
1	A	69	PHE	2.3
1	B	194	PRO	2.3
1	A	153	CYS	2.3
1	B	129	GLN	2.3
1	B	39	SER	2.3
1	B	91	CYS	2.2
1	B	152	SER	2.2
1	B	110	THR	2.2
1	B	176	ASN	2.2
1	B	226	LEU	2.2
1	B	185	ILE	2.2
1	B	238	THR	2.2
1	B	188	VAL	2.2
1	B	99	LEU	2.2
1	B	158	LEU	2.2
1	B	192	GLY	2.2
1	A	37	PHE	2.2
1	B	228	PRO	2.2
1	B	56	ASP	2.1
1	B	63	ASP	2.1
1	B	217	ASN	2.1
1	B	199	PRO	2.1
1	B	84	VAL	2.1
1	B	179	ALA	2.1
1	B	43	LYS	2.1
1	A	91	CYS	2.1
1	A	212	CYS	2.1
1	B	77	ASP	2.1
1	B	113	GLY	2.0
1	B	182	MET	2.0
1	B	221	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

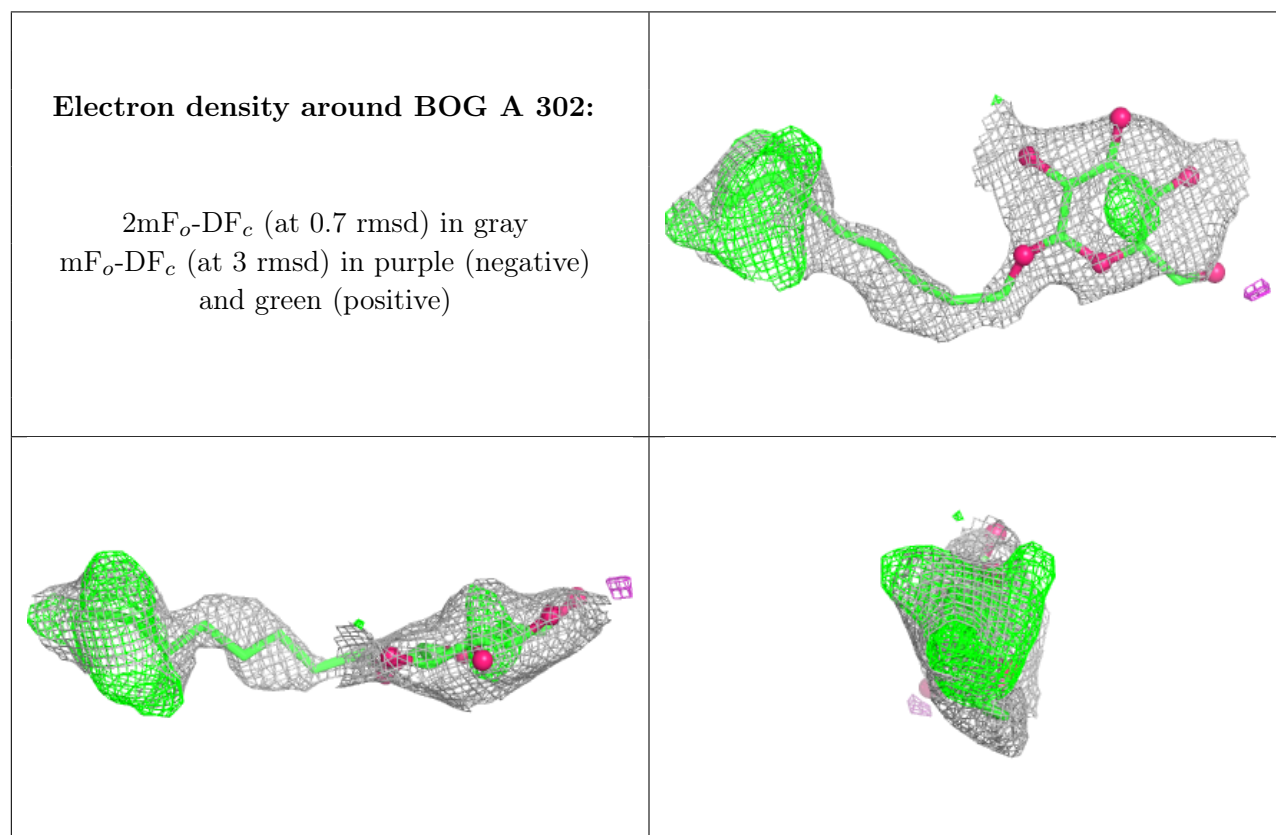
There are no oligosaccharides in this entry.

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.

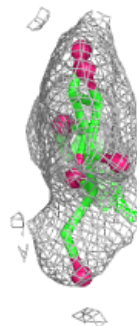
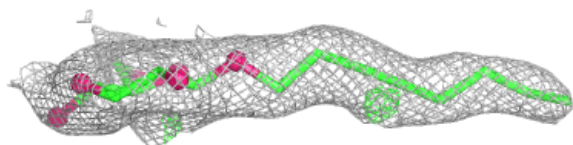
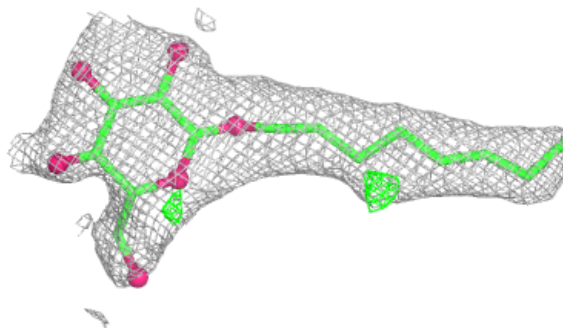
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BOG	A	302	20/20	0.60	0.29	67,81,83,83	0
3	BOG	A	303	20/20	0.82	0.15	52,62,67,68	0
2	C11	B	301	17/18	0.91	0.15	40,48,59,59	0
2	C11	A	301	18/18	0.96	0.12	21,34,64,64	0

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.

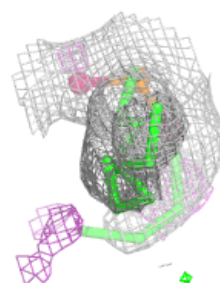
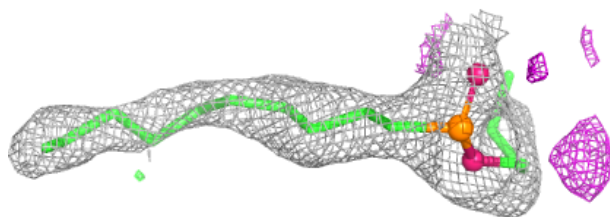
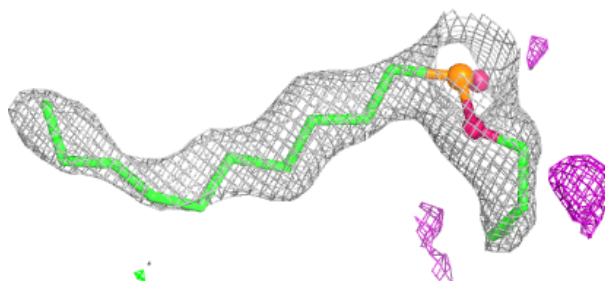


Electron density around BOG A 303:

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

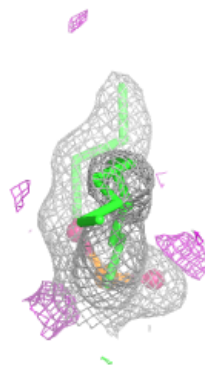
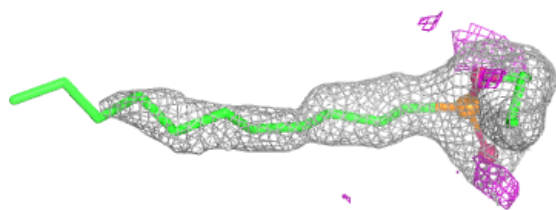
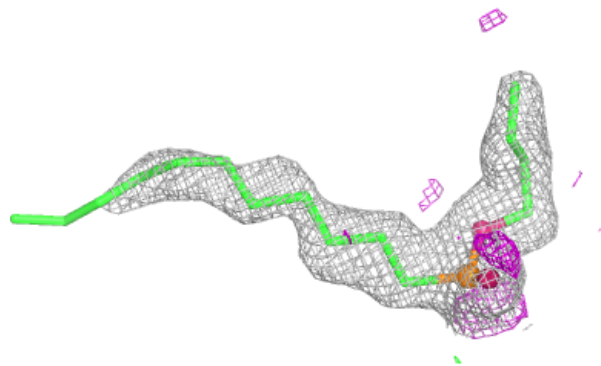
**Electron density around C11 B 301:**

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



Electron density around C11 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 ⓘ

There are no such residues in this entry.