



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

PDB ID : 5JAE / pdb_00005jae
Title : LeuT in the outward-oriented, Na⁺-free return state, P21 form at pH 6.5
Authors : Malinauskaite, L.; Sahin, C.; Said, S.; Grouleff, J.; Shahsavar, A.; Bjerregaard, H.; Noer, P.; Severinsen, K.; Boesen, T.; Schiott, B.; Sinning, S.; Nissen, P.
Deposited on : 2016-04-12
Resolution : 2.50 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

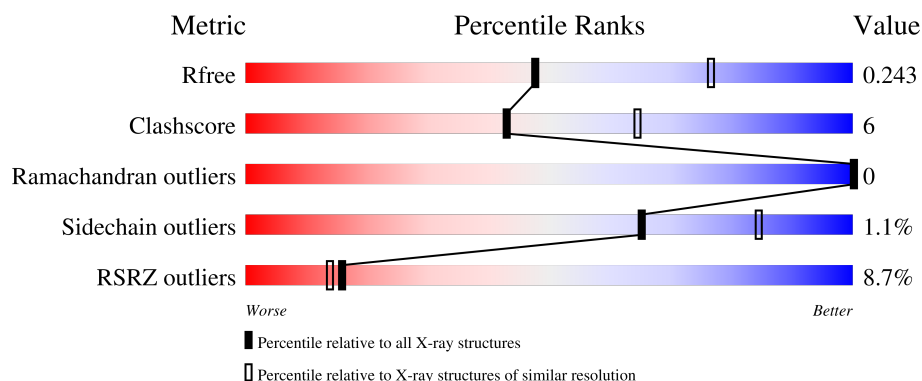
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	519	9% 82% 15% ..
1	B	519	8% 79% 18% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8224 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.

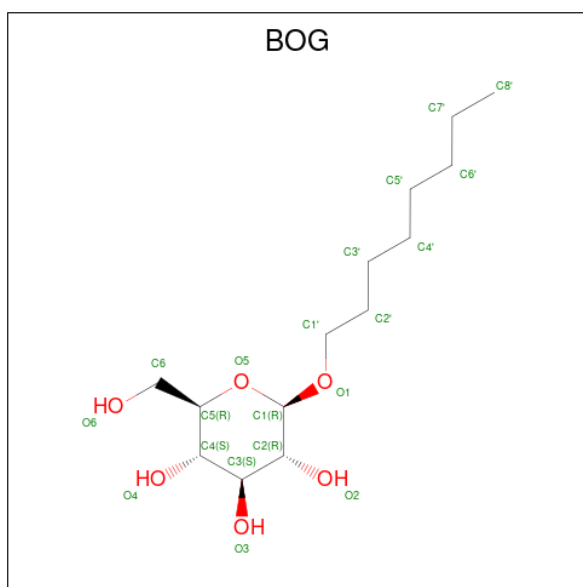
- Molecule 1 is a protein called Transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4002	2714	626	650	12			
1	B	503	Total	C	N	O	S	0	0	0
			3969	2692	625	641	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	514	GLY	-	expression tag	UNP O67854
A	515	THR	-	expression tag	UNP O67854
A	516	LEU	-	expression tag	UNP O67854
A	517	VAL	-	expression tag	UNP O67854
A	518	PRO	-	expression tag	UNP O67854
A	519	ARG	-	expression tag	UNP O67854
B	514	GLY	-	expression tag	UNP O67854
B	515	THR	-	expression tag	UNP O67854
B	516	LEU	-	expression tag	UNP O67854
B	517	VAL	-	expression tag	UNP O67854
B	518	PRO	-	expression tag	UNP O67854
B	519	ARG	-	expression tag	UNP O67854

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			9	8	1		
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		

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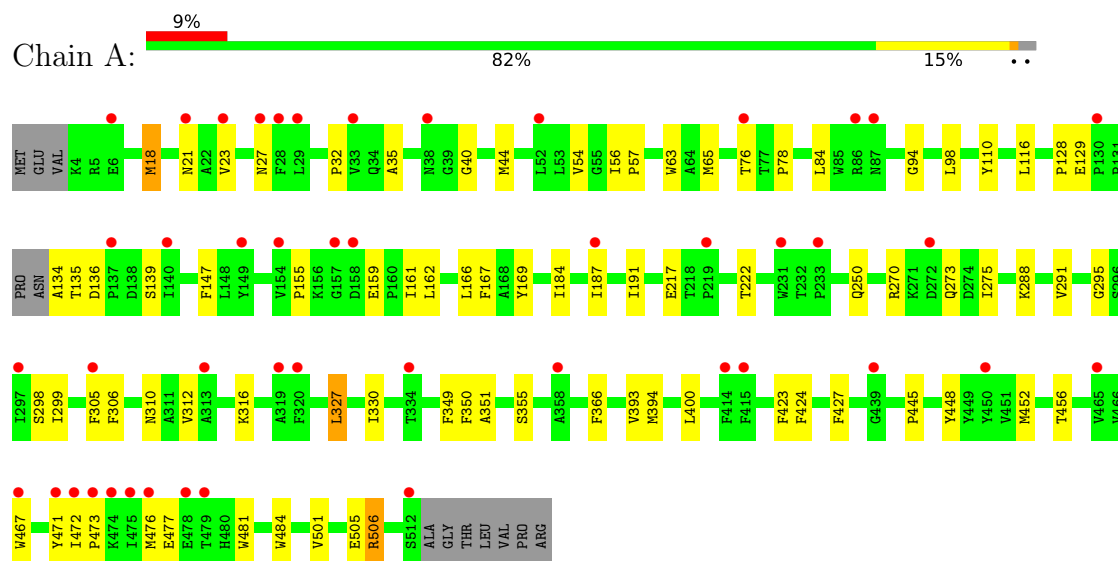
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	21	Total	O	0	0
			21	21		

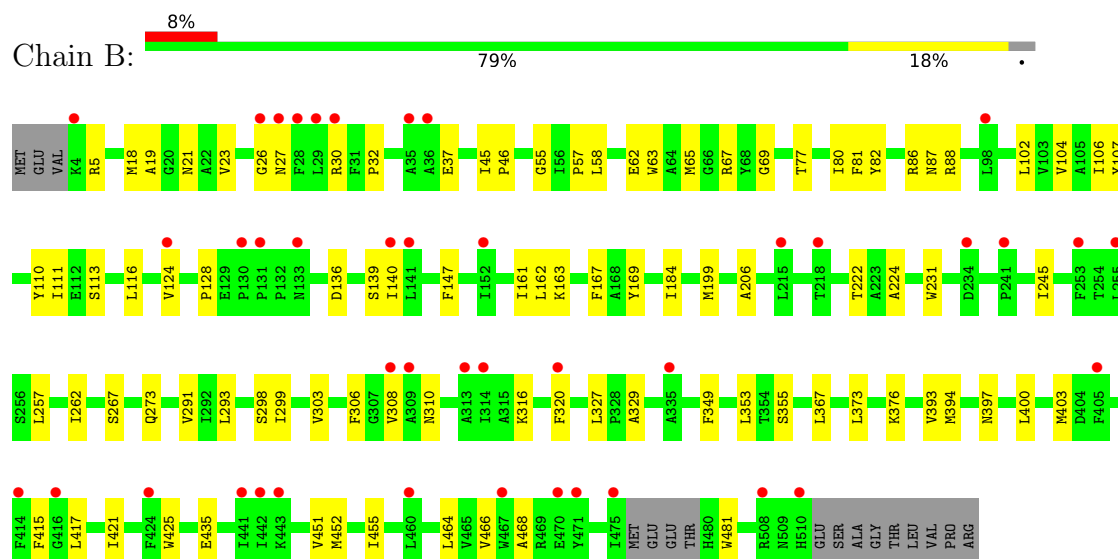
3 Residue-property plots

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: Transporter



• Molecule 1: Transporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.57Å 92.08Å 92.47Å 90.00° 95.18° 90.00°	Depositor
Resolution (Å)	46.05 – 2.50 46.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.05-2.50) 99.0 (46.05-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.51Å)	Xtriage
Refinement program	PHENIX (dev_2283: ???)	Depositor
R, R_{free}	0.223 , 0.245 0.227 , 0.243	Depositor DCC
R_{free} test set	1001 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8224	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BOG

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	0.19	0/4128	0.36	1/5627 (0.0%)
1	B	0.21	0/4096	0.37	0/5586
All	All	0.20	0/8224	0.36	1/11213 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	ILE	N-CA-C	-5.42	108.22	113.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4002	0	4069	50	0
1	B	3969	0	4027	54	0
2	A	80	0	112	4	0
2	B	129	0	184	4	0
3	A	23	0	0	1	0
3	B	21	0	0	1	0
All	All	8224	0	8392	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (102) 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:76:THR:HG22	1:A:78:PRO:HD2	1.46	0.95
1:B:77:THR:HG21	1:B:415:PHE:HZ	1.56	0.70
2:B:603:BOG:H1'1	2:B:607:BOG:H5	1.73	0.69
1:A:166:LEU:HD13	2:A:601:BOG:H61	1.75	0.69
1:A:18:MET:HG2	1:A:63:TRP:CZ2	2.28	0.68
1:B:32:PRO:HB3	1:B:299:ILE:HG12	1.76	0.66
1:A:167:PHE:HD1	2:A:604:BOG:H2'1	1.63	0.63
1:A:136:ASP:HB3	1:A:139:SER:HB3	1.80	0.62
1:B:140:ILE:HG22	1:B:329:ALA:HB1	1.81	0.62
1:A:477:GLU:O	2:A:602:BOG:O4	2.16	0.62
1:A:250:GLN:NE2	3:A:701:HOH:O	2.32	0.61
1:A:35:ALA:HB1	1:A:40:GLY:HA2	1.84	0.59
1:B:113:SER:OG	3:B:701:HOH:O	2.17	0.59
1:A:472:ILE:HB	1:A:473:PRO:HD3	1.85	0.58
1:A:161:ILE:HD11	1:B:481:TRP:CE3	2.39	0.57
1:A:270:ARG:HB2	1:A:273:GLN:HG3	1.87	0.56
1:B:55:GLY:HA2	1:B:257:LEU:HD11	1.86	0.56
1:A:481:TRP:CE3	1:B:161:ILE:HD11	2.40	0.56
1:A:128:PRO:HG2	1:A:147:PHE:HB2	1.88	0.56
1:B:231:TRP:HH2	1:B:291:VAL:HG13	1.72	0.55
1:B:303:VAL:HG13	1:B:308:VAL:HA	1.87	0.55
1:A:155:PRO:HD3	1:A:162:LEU:HD23	1.90	0.53
1:A:110:TYR:CZ	1:A:394:MET:HG2	2.44	0.52
1:A:393:VAL:HG13	1:A:400:LEU:HB2	1.91	0.52
1:B:222:THR:HG22	1:B:224:ALA:H	1.75	0.52
1:B:184:ILE:HD11	1:B:376:LYS:HA	1.92	0.52
1:B:111:ILE:HD13	1:B:320:PHE:HZ	1.74	0.51
1:A:32:PRO:HG3	1:A:295:GLY:HA2	1.91	0.51
1:A:217:GLU:HG3	1:A:222:THR:HG22	1.92	0.51
1:A:32:PRO:HB3	1:A:299:ILE:HG12	1.92	0.50
1:B:26:GLY:HA3	1:B:30:ARG:HG3	1.94	0.50
1:B:107:TYR:HD1	1:B:403:MET:HE3	1.75	0.50
1:B:45:ILE:HB	1:B:46:PRO:HD3	1.94	0.50
1:B:5:ARG:NH1	1:B:267:SER:OG	2.45	0.50
1:B:298:SER:HB3	1:B:327:LEU:HD11	1.92	0.50
1:B:102:LEU:O	1:B:106:ILE:HG13	2.11	0.49
1:B:451:VAL:HA	1:B:455:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:PHE:O	1:A:310:ASN:HB2	2.13	0.49
1:B:67:ARG:NH2	1:B:435:GLU:O	2.46	0.49
1:B:167:PHE:HD1	2:B:603:BOG:H2'2	1.76	0.49
1:A:159:GLU:HG3	1:A:161:ILE:H	1.78	0.49
1:B:87:ASN:OD1	1:B:88:ARG:N	2.47	0.48
1:A:57:PRO:HB3	1:A:452:MET:HG2	1.95	0.47
1:B:18:MET:HG3	1:B:63:TRP:CZ2	2.49	0.47
1:B:393:VAL:HG13	1:B:400:LEU:HB2	1.95	0.47
1:A:98:LEU:HD11	1:A:366:PHE:CG	2.49	0.47
1:B:107:TYR:HB3	1:B:403:MET:HE2	1.96	0.47
1:A:78:PRO:HD3	1:A:94:GLY:O	2.15	0.47
1:B:124:VAL:HG21	2:B:607:BOG:H2'1	1.96	0.47
1:A:18:MET:HG2	1:A:63:TRP:HZ2	1.76	0.47
1:A:305:PHE:CD1	1:A:330:ILE:HG23	2.50	0.47
1:B:37:GLU:HG2	1:B:316:LYS:HG3	1.97	0.47
1:B:65:MET:HE1	1:B:81:PHE:HE1	1.80	0.47
1:A:65:MET:HG2	1:A:84:LEU:HD11	1.95	0.47
1:A:505:GLU:OE2	1:A:506:ARG:NH2	2.48	0.47
1:B:136:ASP:HB2	1:B:139:SER:HB3	1.96	0.46
1:B:104:VAL:HA	1:B:107:TYR:CE1	2.51	0.46
1:B:367:LEU:HB3	1:B:373:LEU:HD22	1.97	0.46
1:A:187:ILE:HD13	1:A:191:ILE:HD12	1.98	0.46
1:B:82:TYR:CZ	1:B:86:ARG:HD3	2.51	0.45
1:B:110:TYR:O	1:B:113:SER:HB3	2.16	0.45
1:B:162:LEU:HG	1:B:397:ASN:HA	1.97	0.45
1:B:67:ARG:NH1	1:B:273:GLN:O	2.50	0.45
1:B:306:PHE:O	1:B:310:ASN:HB2	2.16	0.45
1:A:169:TYR:CD1	1:A:394:MET:HE1	2.51	0.45
1:A:134:ALA:HA	1:A:135:THR:HA	1.54	0.45
1:A:501:VAL:O	1:A:505:GLU:HG3	2.17	0.45
1:A:23:VAL:HG12	1:A:351:ALA:HB1	2.00	0.44
1:B:19:ALA:O	1:B:23:VAL:HG23	2.18	0.44
1:B:58:LEU:HD12	1:B:58:LEU:HA	1.89	0.44
1:A:169:TYR:CE1	1:A:394:MET:HE1	2.53	0.44
1:A:445:PRO:HD2	1:A:448:TYR:HD2	1.82	0.44
1:A:44:MET:HE1	1:A:291:VAL:HG11	2.00	0.43
1:B:23:VAL:HG21	1:B:199:MET:HE1	2.00	0.43
1:B:116:LEU:HB2	1:B:349:PHE:CE1	2.54	0.42
1:B:128:PRO:HD3	1:B:147:PHE:CD1	2.54	0.42
1:A:129:GLU:N	1:A:129:GLU:OE2	2.52	0.42
1:B:57:PRO:HB3	1:B:452:MET:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ILE:HD12	1:B:425:TRP:CE3	2.54	0.42
1:A:116:LEU:HB2	1:A:349:PHE:CD1	2.54	0.42
1:A:155:PRO:HB2	1:A:159:GLU:HB3	2.00	0.42
1:A:423:PHE:O	1:A:427:PHE:HB3	2.19	0.42
1:B:169:TYR:HE1	1:B:394:MET:HE1	1.84	0.42
1:A:54:VAL:HA	1:A:456:THR:HG23	2.01	0.42
1:B:23:VAL:O	1:B:27:ASN:HB3	2.20	0.42
1:A:56:ILE:HB	1:A:57:PRO:HD3	2.01	0.41
1:B:62:GLU:OE1	1:B:262:ILE:HD12	2.20	0.41
1:A:484:TRP:CZ2	2:B:602:BOG:H1'2	2.55	0.41
1:B:21:ASN:HA	1:B:355:SER:HA	2.02	0.41
1:B:417:LEU:O	1:B:421:ILE:HG12	2.20	0.41
1:A:288:LYS:HD3	1:A:288:LYS:HA	1.90	0.41
2:A:602:BOG:H2'1	1:B:161:ILE:HG21	2.03	0.41
1:B:69:GLY:HA3	1:B:80:ILE:HG12	2.03	0.41
1:A:481:TRP:CZ3	1:B:161:ILE:HD11	2.56	0.41
1:B:464:LEU:O	1:B:468:ALA:N	2.50	0.41
1:A:467:TRP:O	1:A:471:TYR:HB2	2.21	0.41
1:A:21:ASN:O	1:A:355:SER:OG	2.39	0.40
1:B:206:ALA:HB1	1:B:293:LEU:HB3	2.02	0.40
1:B:245:ILE:HG13	1:B:466:VAL:HG11	2.02	0.40
1:A:312:VAL:HG12	1:A:316:LYS:HE3	2.04	0.40
1:A:298:SER:HA	1:A:327:LEU:HD11	2.04	0.40
1:A:472:ILE:O	1:A:476:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	503/519 (97%)	488 (97%)	15 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	499/519 (96%)	492 (99%)	7 (1%)	0	100	100
All	All	1002/1038 (96%)	980 (98%)	22 (2%)	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	402/420 (96%)	395 (98%)	7 (2%)	53	78
1	B	397/420 (94%)	395 (100%)	2 (0%)	81	92
All	All	799/840 (95%)	790 (99%)	9 (1%)	65	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	27	ASN
1	A	184	ILE
1	A	327	LEU
1	A	350	PHE
1	A	424	PHE
1	A	506	ARG
1	B	163	LYS
1	B	353	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	179	ASN
1	A	273	GLN
1	B	179	ASN

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Mol	Chain	Res	Type
1	B	480	HIS

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 ⓘ

11 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	$\# Z > 2$
2	BOG	B	601	-	20,20,20	1.09	1 (5%)	25,25,25	0.83	0
2	BOG	A	602	-	20,20,20	1.12	2 (10%)	25,25,25	0.97	0
2	BOG	B	604	-	20,20,20	1.06	1 (5%)	25,25,25	1.25	2 (8%)
2	BOG	A	603	-	20,20,20	1.08	1 (5%)	25,25,25	1.04	2 (8%)
2	BOG	A	601	-	20,20,20	1.08	1 (5%)	25,25,25	0.94	0
2	BOG	B	606	-	20,20,20	1.07	1 (5%)	25,25,25	0.89	0
2	BOG	B	602	-	20,20,20	1.10	1 (5%)	25,25,25	0.80	0
2	BOG	B	607	-	20,20,20	1.10	1 (5%)	25,25,25	0.81	0
2	BOG	B	603	-	20,20,20	1.08	1 (5%)	25,25,25	0.95	0
2	BOG	A	604	-	20,20,20	1.08	1 (5%)	25,25,25	0.87	0
2	BOG	B	605	-	8,8,20	0.34	0	7,7,25	0.65	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
2	BOG	B	601	-	-	6/11/31/31	0/1/1/1
2	BOG	A	602	-	-	5/11/31/31	0/1/1/1
2	BOG	B	604	-	-	6/11/31/31	0/1/1/1
2	BOG	A	603	-	-	7/11/31/31	0/1/1/1
2	BOG	A	601	-	-	4/11/31/31	0/1/1/1
2	BOG	B	606	-	-	6/11/31/31	0/1/1/1
2	BOG	B	602	-	-	7/11/31/31	0/1/1/1
2	BOG	B	607	-	-	4/11/31/31	0/1/1/1
2	BOG	B	603	-	-	6/11/31/31	0/1/1/1
2	BOG	A	604	-	-	3/11/31/31	0/1/1/1
2	BOG	B	605	-	-	1/6/6/31	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	607	BOG	O5-C1	3.71	1.51	1.41
2	A	604	BOG	O5-C1	3.61	1.51	1.41
2	B	603	BOG	O5-C1	3.60	1.51	1.41
2	B	602	BOG	O5-C1	3.60	1.51	1.41
2	B	601	BOG	O5-C1	3.57	1.51	1.41
2	A	602	BOG	O5-C1	3.55	1.51	1.41
2	A	601	BOG	O5-C1	3.52	1.50	1.41
2	B	606	BOG	O5-C1	3.51	1.50	1.41
2	B	604	BOG	O5-C1	3.49	1.50	1.41
2	A	603	BOG	O5-C1	3.34	1.50	1.41
2	A	602	BOG	O1-C1	-2.09	1.36	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	604	BOG	O1-C1-C2	3.65	113.82	108.27
2	B	604	BOG	C3-C4-C5	3.00	115.66	110.23
2	A	603	BOG	O5-C5-C4	2.79	114.73	109.70
2	A	603	BOG	C6-C5-C4	-2.45	107.01	113.02

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	BOG	C2-C1-O1-C1'
2	A	602	BOG	O5-C1-O1-C1'
2	B	604	BOG	C2'-C1'-O1-C1
2	B	603	BOG	O5-C5-C6-O6
2	B	604	BOG	O5-C5-C6-O6
2	B	602	BOG	O5-C5-C6-O6
2	B	603	BOG	C4-C5-C6-O6
2	B	603	BOG	O5-C1-O1-C1'
2	B	604	BOG	C4-C5-C6-O6
2	A	601	BOG	O5-C5-C6-O6
2	B	603	BOG	C2-C1-O1-C1'
2	B	602	BOG	C4-C5-C6-O6
2	B	604	BOG	O1-C1'-C2'-C3'
2	B	606	BOG	O1-C1'-C2'-C3'
2	A	602	BOG	O5-C5-C6-O6
2	B	606	BOG	O5-C1-O1-C1'
2	A	601	BOG	O1-C1'-C2'-C3'
2	A	603	BOG	C1'-C2'-C3'-C4'
2	A	601	BOG	C4-C5-C6-O6
2	B	606	BOG	C2'-C3'-C4'-C5'
2	B	603	BOG	C2'-C1'-O1-C1
2	B	604	BOG	C2'-C3'-C4'-C5'
2	B	607	BOG	C4'-C5'-C6'-C7'
2	A	604	BOG	C2'-C3'-C4'-C5'
2	B	606	BOG	C3'-C4'-C5'-C6'
2	B	607	BOG	C2-C1-O1-C1'
2	A	602	BOG	C2'-C3'-C4'-C5'
2	A	602	BOG	C3'-C4'-C5'-C6'
2	A	603	BOG	O5-C5-C6-O6
2	B	601	BOG	O1-C1'-C2'-C3'
2	B	606	BOG	C4'-C5'-C6'-C7'
2	A	604	BOG	C4-C5-C6-O6
2	B	602	BOG	O1-C1'-C2'-C3'
2	B	606	BOG	O5-C5-C6-O6
2	B	604	BOG	C5'-C6'-C7'-C8'
2	B	602	BOG	C4'-C5'-C6'-C7'
2	A	601	BOG	C3'-C4'-C5'-C6'
2	B	601	BOG	C2'-C1'-O1-C1
2	B	602	BOG	C2'-C1'-O1-C1
2	A	603	BOG	C2-C1-O1-C1'
2	B	601	BOG	C5'-C6'-C7'-C8'
2	B	601	BOG	O5-C1-O1-C1'

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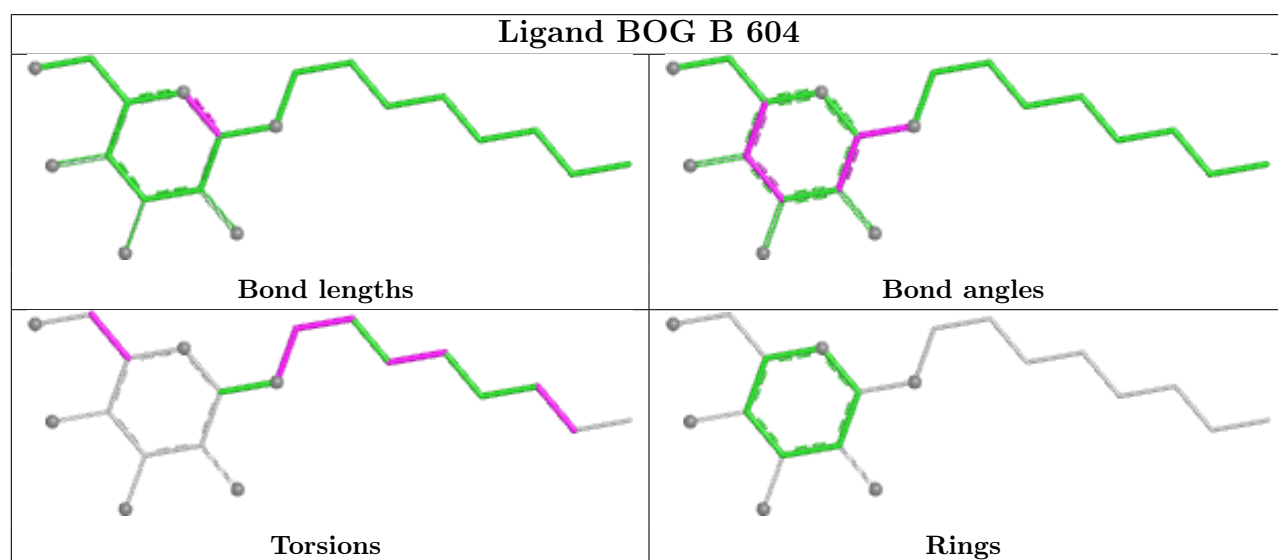
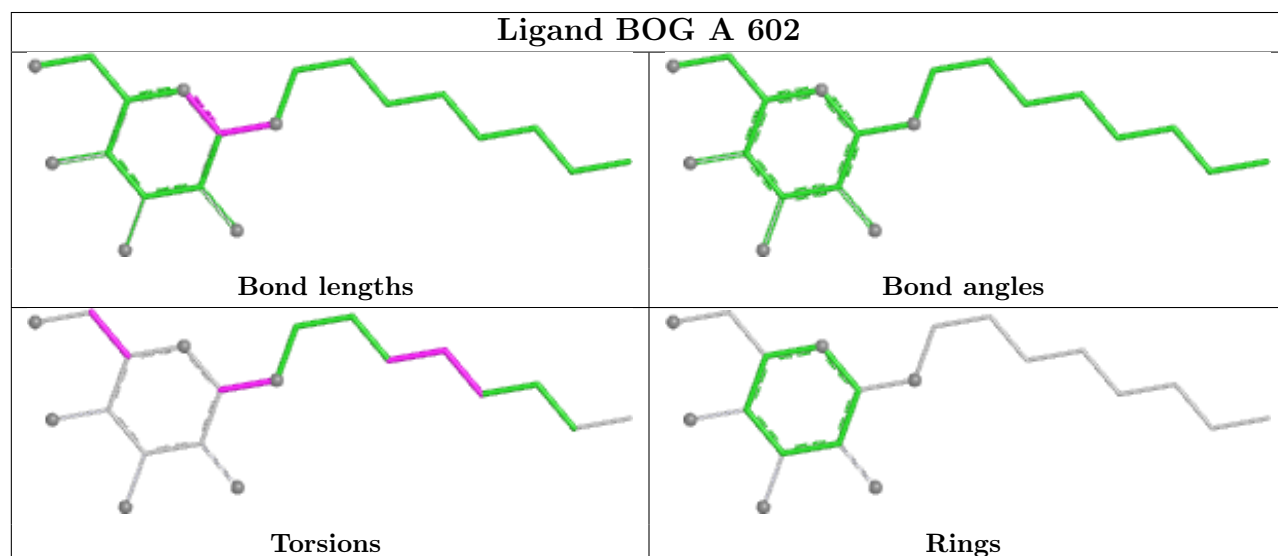
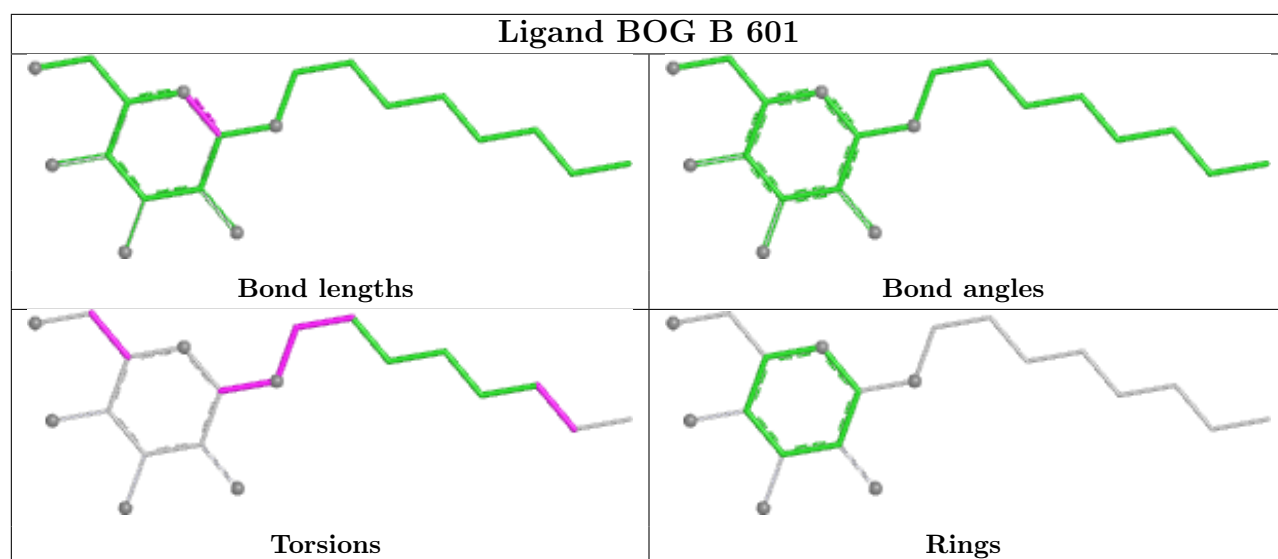
Mol	Chain	Res	Type	Atoms
2	A	603	BOG	C2'-C3'-C4'-C5'
2	B	607	BOG	C3'-C4'-C5'-C6'
2	A	603	BOG	O5-C1-O1-C1'
2	B	601	BOG	C4-C5-C6-O6
2	A	603	BOG	C2'-C1'-O1-C1
2	A	604	BOG	O5-C5-C6-O6
2	B	601	BOG	O5-C5-C6-O6
2	B	603	BOG	C1'-C2'-C3'-C4'
2	B	605	BOG	C4'-C5'-C6'-C7'
2	B	602	BOG	C1'-C2'-C3'-C4'
2	A	603	BOG	O1-C1'-C2'-C3'
2	B	602	BOG	C3'-C4'-C5'-C6'
2	B	607	BOG	C5'-C6'-C7'-C8'

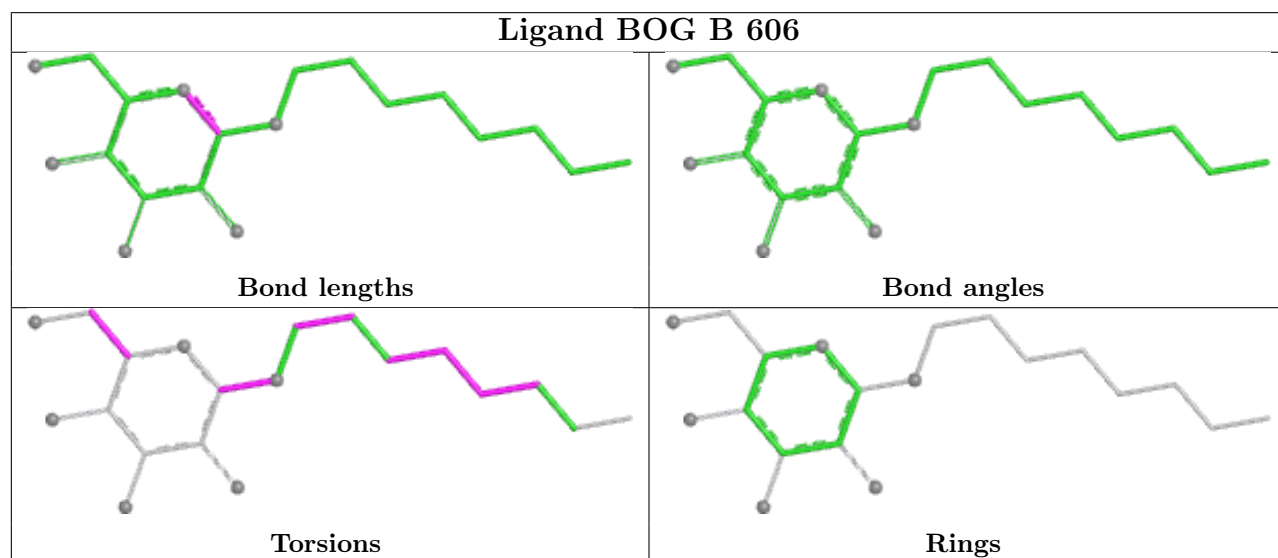
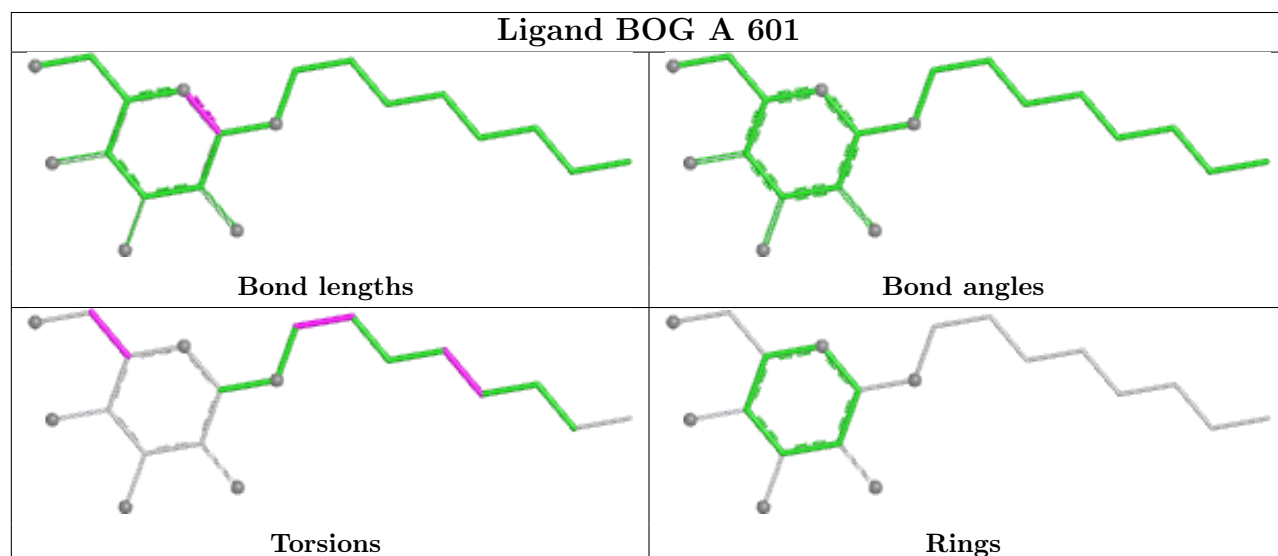
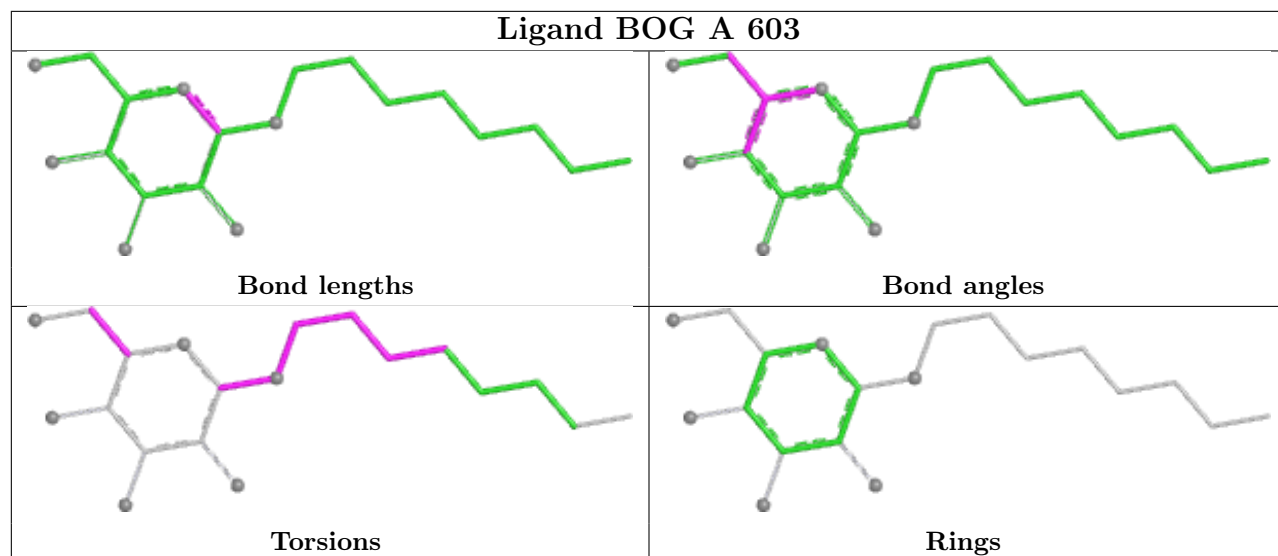
There are no ring outliers.

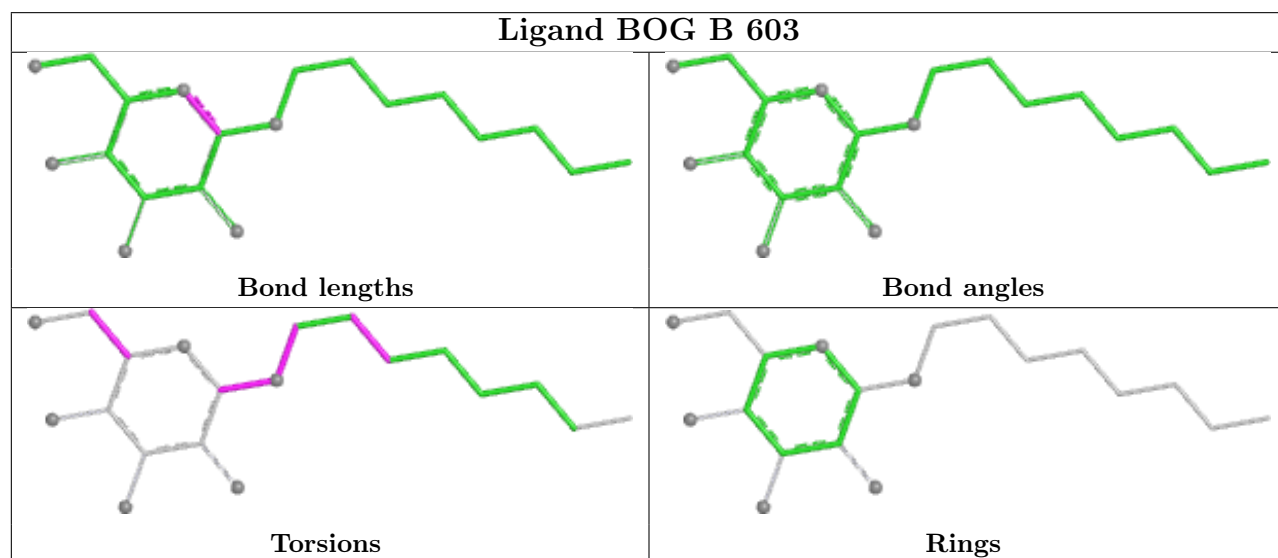
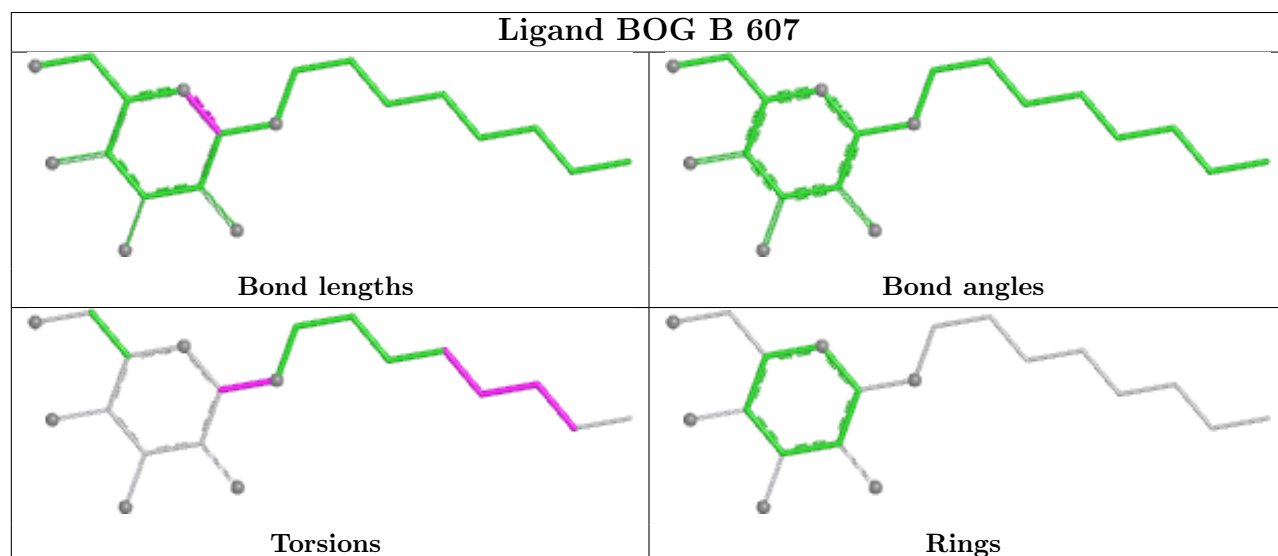
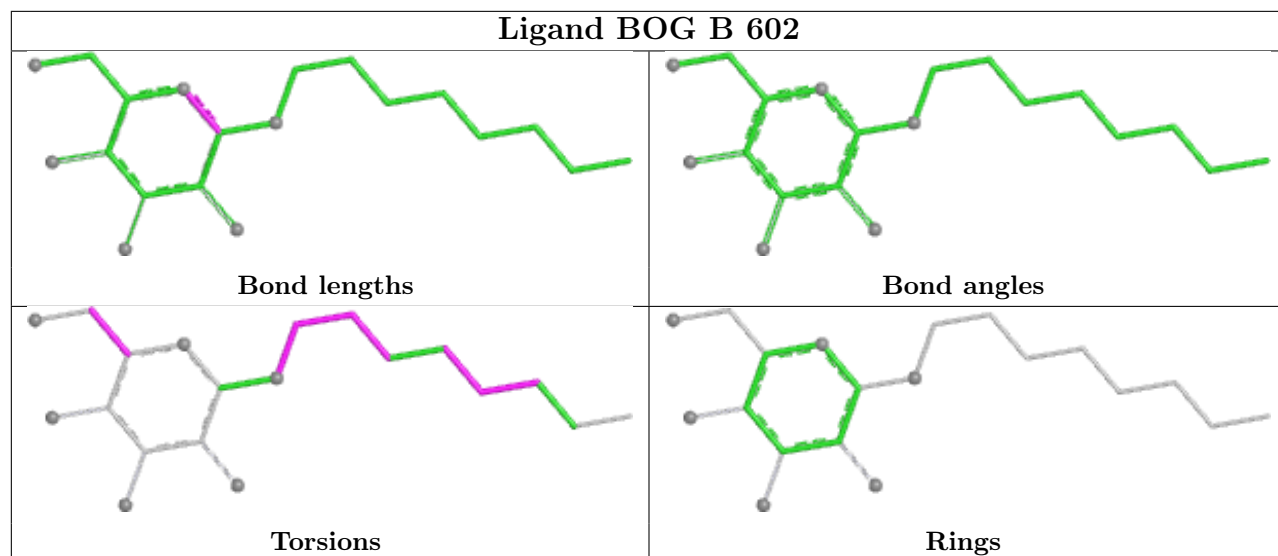
6 monomers are involved in 8 short contacts:

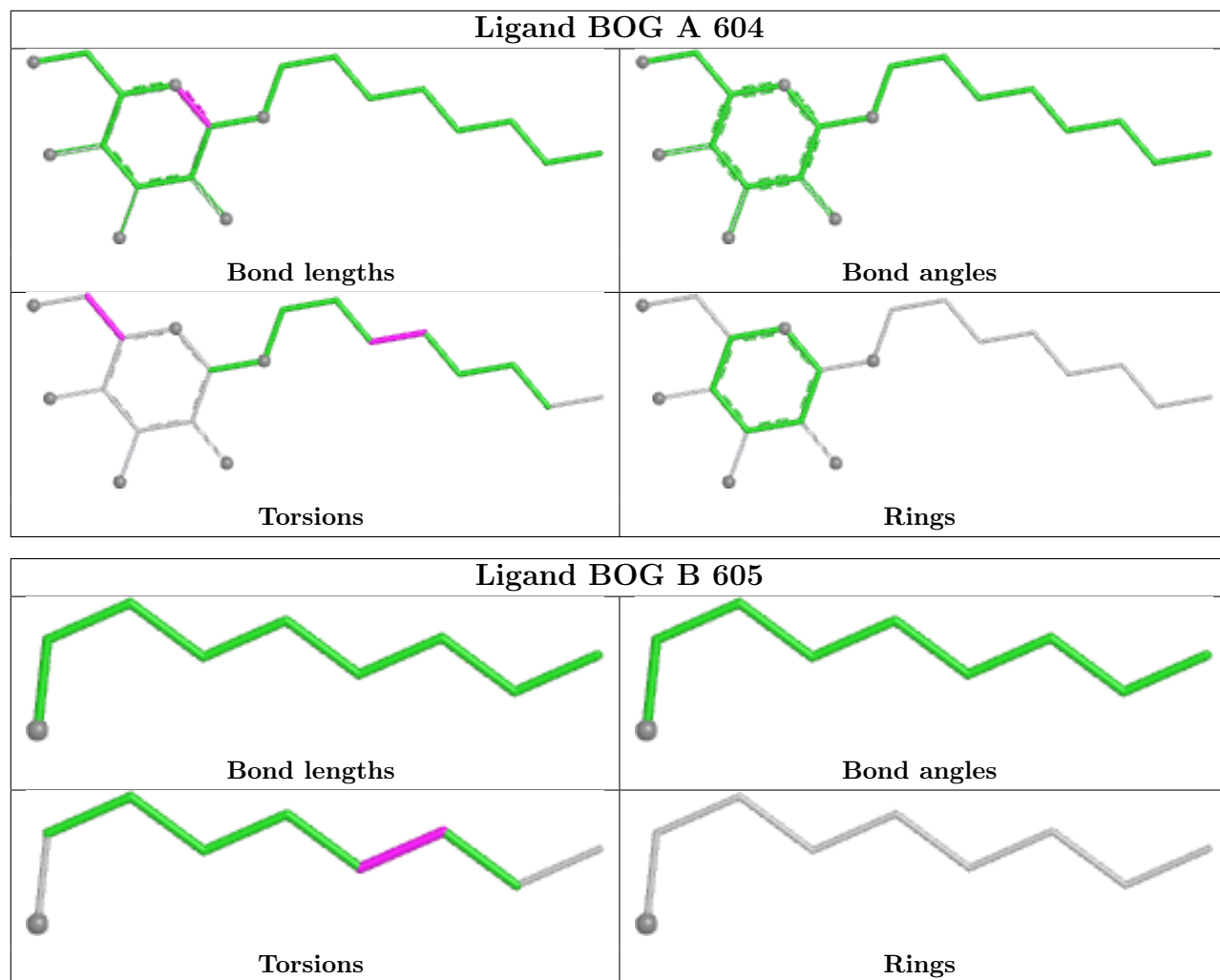
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	BOG	2	0
2	A	601	BOG	1	0
2	B	602	BOG	1	0
2	B	607	BOG	2	0
2	B	603	BOG	2	0
2	A	604	BOG	1	0

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	507/519 (97%)	0.67	46 (9%)	15 13	50, 86, 166, 225	0
1	B	503/519 (96%)	0.73	42 (8%)	17 15	50, 88, 170, 236	0
All	All	1010/1038 (97%)	0.70	88 (8%)	16 14	50, 87, 170, 236	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	ILE	6.8
1	B	320	PHE	5.7
1	B	471	TYR	5.2
1	A	476	MET	4.6
1	B	416	GLY	4.2
1	A	475	ILE	4.1
1	B	442	ILE	3.9
1	B	28	PHE	3.8
1	B	234	ASP	3.8
1	A	512	SER	3.7
1	B	470	GLU	3.7
1	B	475	ILE	3.6
1	B	36	ALA	3.6
1	A	334	THR	3.5
1	B	29	LEU	3.4
1	A	320	PHE	3.4
1	A	414	PHE	3.4
1	A	21	ASN	3.4
1	B	460	LEU	3.4
1	B	131	PRO	3.3
1	B	241	PRO	3.3
1	B	441	ILE	3.3
1	B	308	VAL	3.2
1	B	27	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	29	LEU	3.2
1	B	133	ASN	3.1
1	A	479	THR	3.1
1	A	478	GLU	3.1
1	B	335	ALA	3.0
1	A	415	PHE	3.0
1	A	471	TYR	2.9
1	B	414	PHE	2.9
1	B	314	ILE	2.8
1	A	154	VAL	2.8
1	B	30	ARG	2.8
1	A	137	PRO	2.7
1	A	86	ARG	2.7
1	A	473	PRO	2.7
1	A	6	GLU	2.7
1	B	35	ALA	2.6
1	A	467	TRP	2.6
1	A	130	PRO	2.6
1	B	443	LYS	2.6
1	A	187	ILE	2.6
1	A	28	PHE	2.6
1	B	253	PHE	2.6
1	A	157	GLY	2.5
1	A	272	ASP	2.5
1	A	439	GLY	2.5
1	A	23	VAL	2.5
1	A	87	ASN	2.5
1	B	405	PHE	2.5
1	A	38	ASN	2.5
1	A	76	THR	2.5
1	B	255	LEU	2.5
1	A	27	ASN	2.4
1	A	358	ALA	2.4
1	B	124	VAL	2.4
1	B	508	ARG	2.4
1	A	313	ALA	2.4
1	B	218	THR	2.3
1	B	130	PRO	2.3
1	B	152	ILE	2.3
1	A	450	TYR	2.3
1	B	510	HIS	2.2
1	B	26	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	231	TRP	2.2
1	A	233	PRO	2.2
1	B	309	ALA	2.2
1	B	467	TRP	2.2
1	B	98	LEU	2.1
1	A	149	TYR	2.1
1	A	52	LEU	2.1
1	B	140	ILE	2.1
1	A	219	PRO	2.1
1	A	305	PHE	2.1
1	A	33	VAL	2.1
1	A	319	ALA	2.1
1	A	297	ILE	2.1
1	A	465	VAL	2.1
1	B	424	PHE	2.0
1	B	313	ALA	2.0
1	B	141	LEU	2.0
1	B	215	LEU	2.0
1	A	474	LYS	2.0
1	B	4	LYS	2.0
1	A	158	ASP	2.0
1	A	140	ILE	2.0

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.

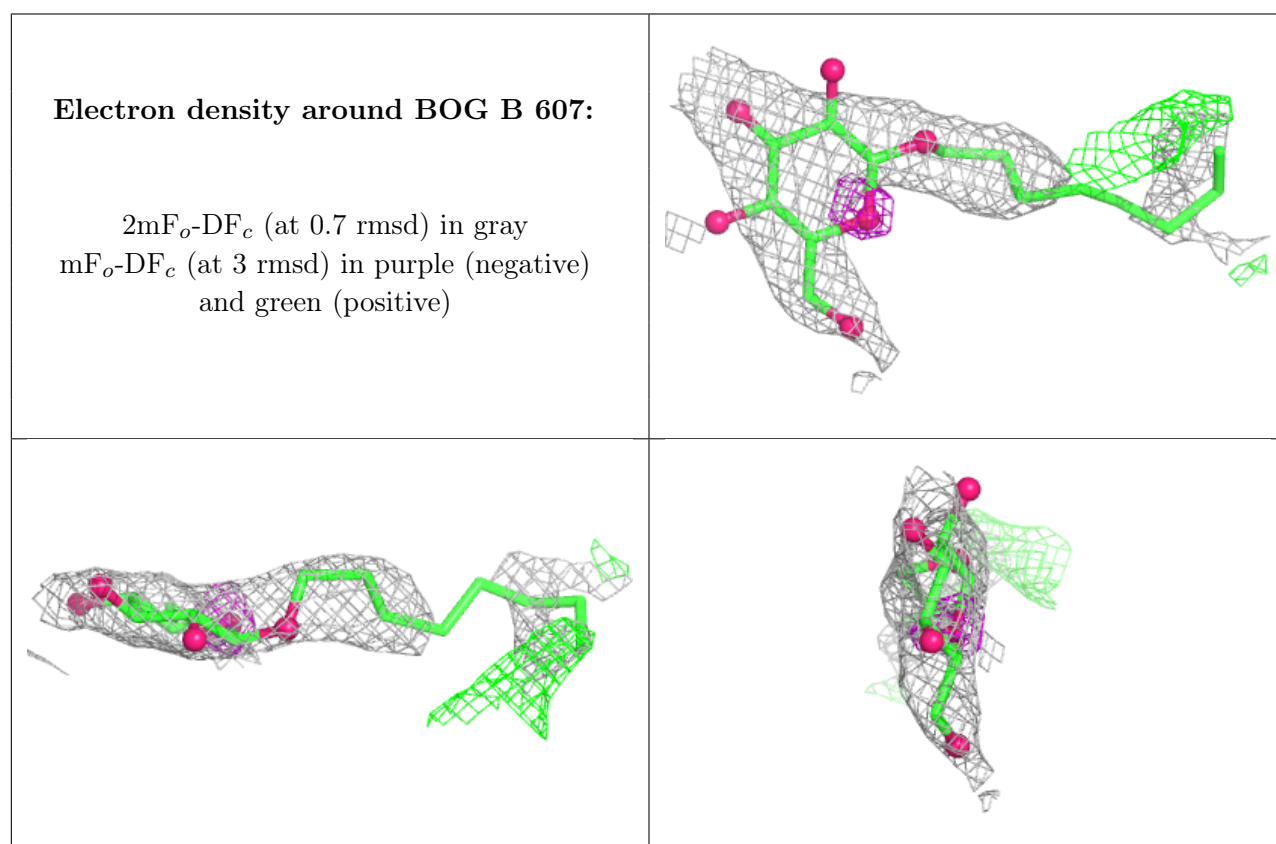
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BOG	B	607	20/20	0.66	0.20	120,131,132,132	0

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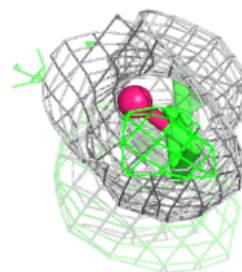
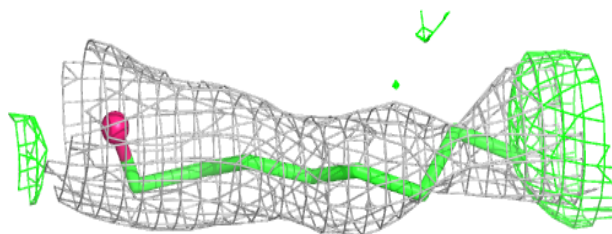
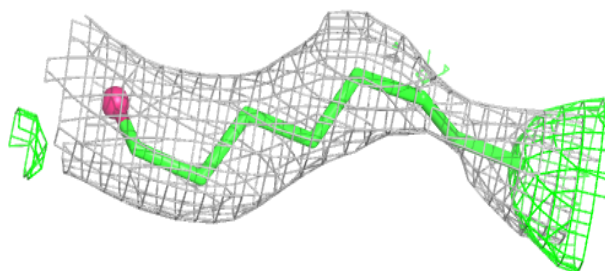
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BOG	B	605	9/20	0.75	0.21	86,88,92,93	0
2	BOG	B	606	20/20	0.75	0.20	116,135,140,140	0
2	BOG	B	603	20/20	0.75	0.17	107,123,126,126	0
2	BOG	A	604	20/20	0.81	0.18	111,131,135,135	0
2	BOG	B	604	20/20	0.82	0.19	92,113,118,121	0
2	BOG	B	602	20/20	0.84	0.16	75,108,114,115	0
2	BOG	A	603	20/20	0.84	0.16	117,127,131,131	0
2	BOG	A	601	20/20	0.84	0.16	109,122,124,124	0
2	BOG	A	602	20/20	0.86	0.13	80,115,122,125	0
2	BOG	B	601	20/20	0.86	0.17	97,107,110,111	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.

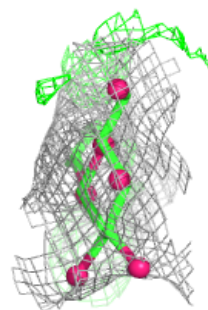
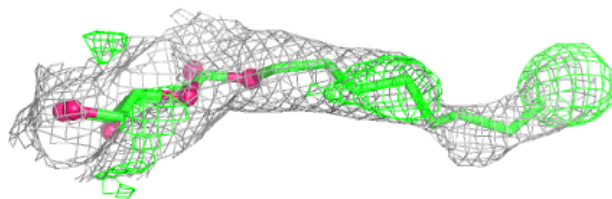
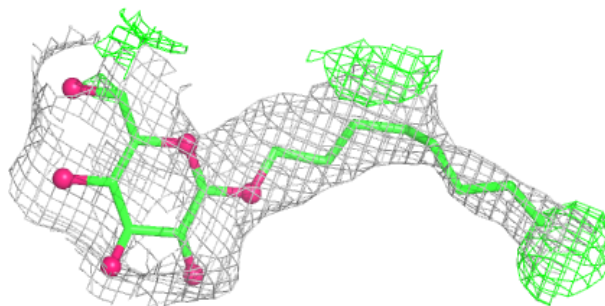


Electron density around BOG B 605:

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

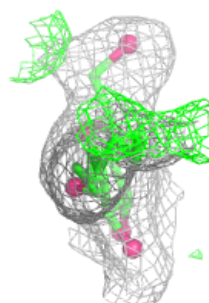
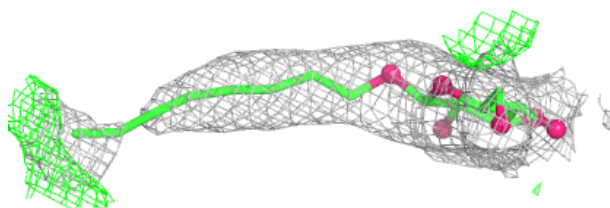
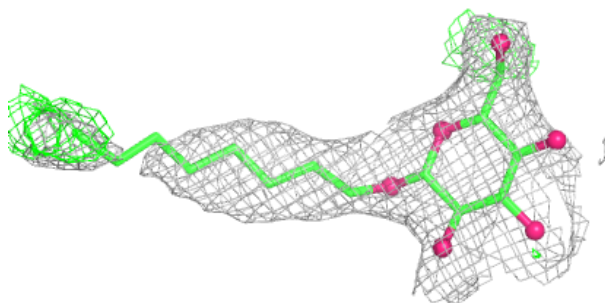
**Electron density around BOG B 606:**

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

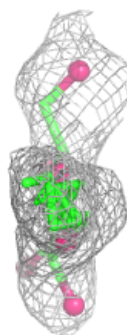
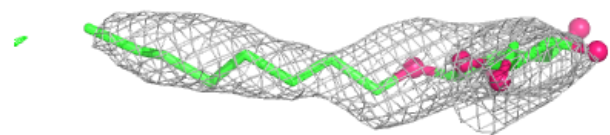
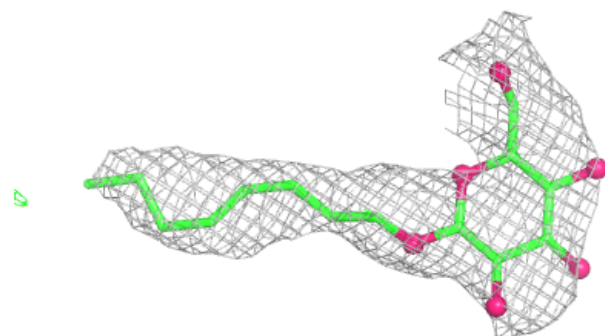


Electron density around BOG B 603:

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

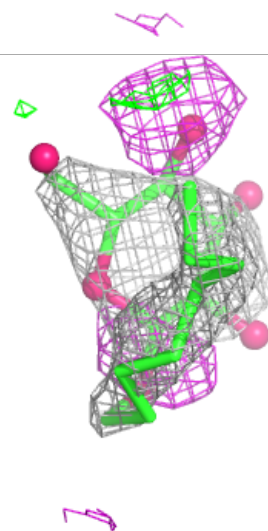
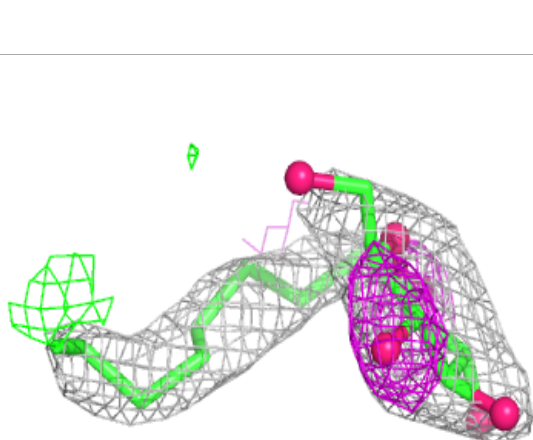
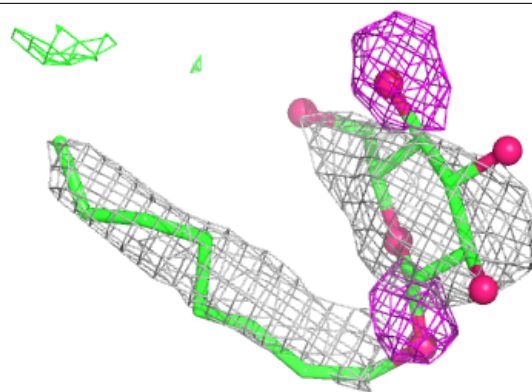
**Electron density around BOG A 604:**

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



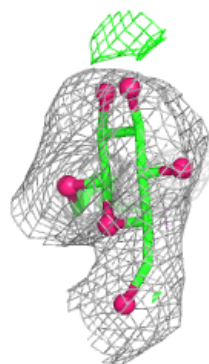
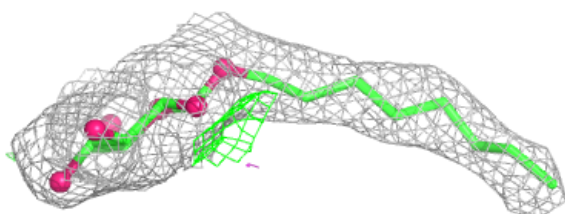
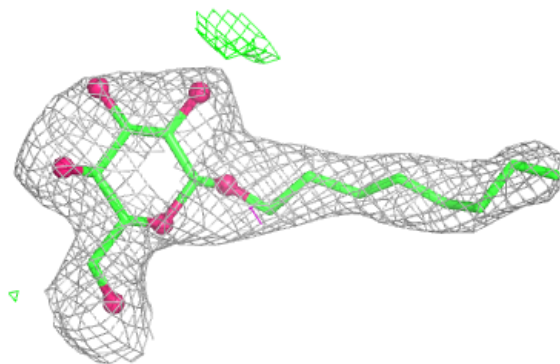
Electron density around BOG B 604:

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

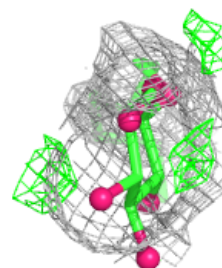
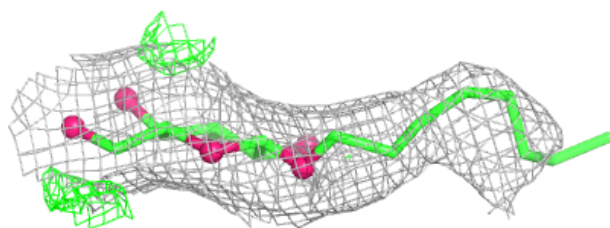
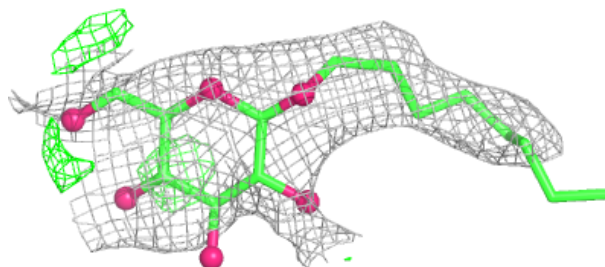


Electron density around BOG B 602:

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

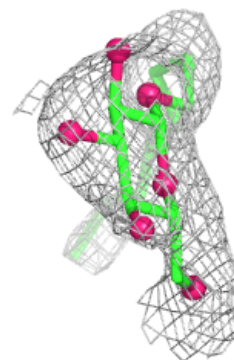
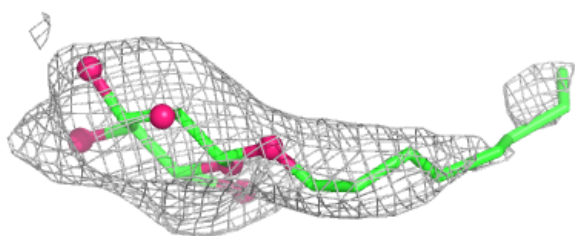
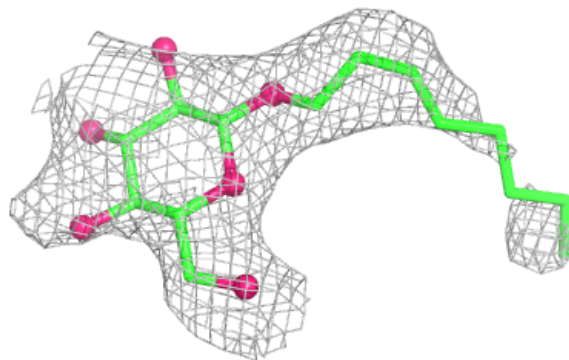
**Electron density around BOG A 603:**

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

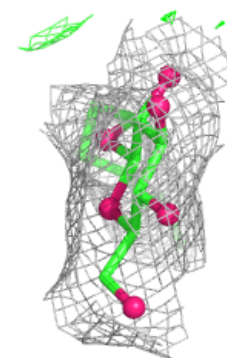
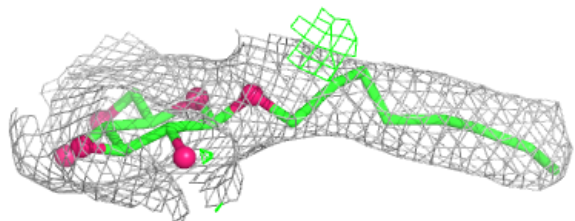
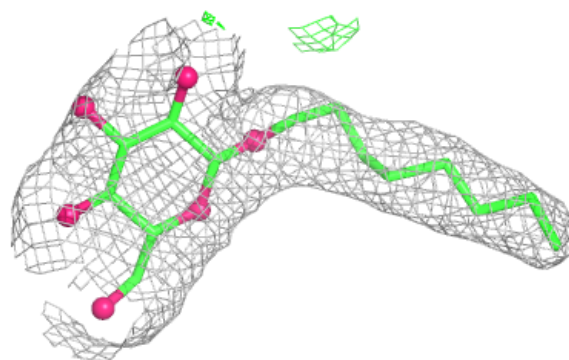


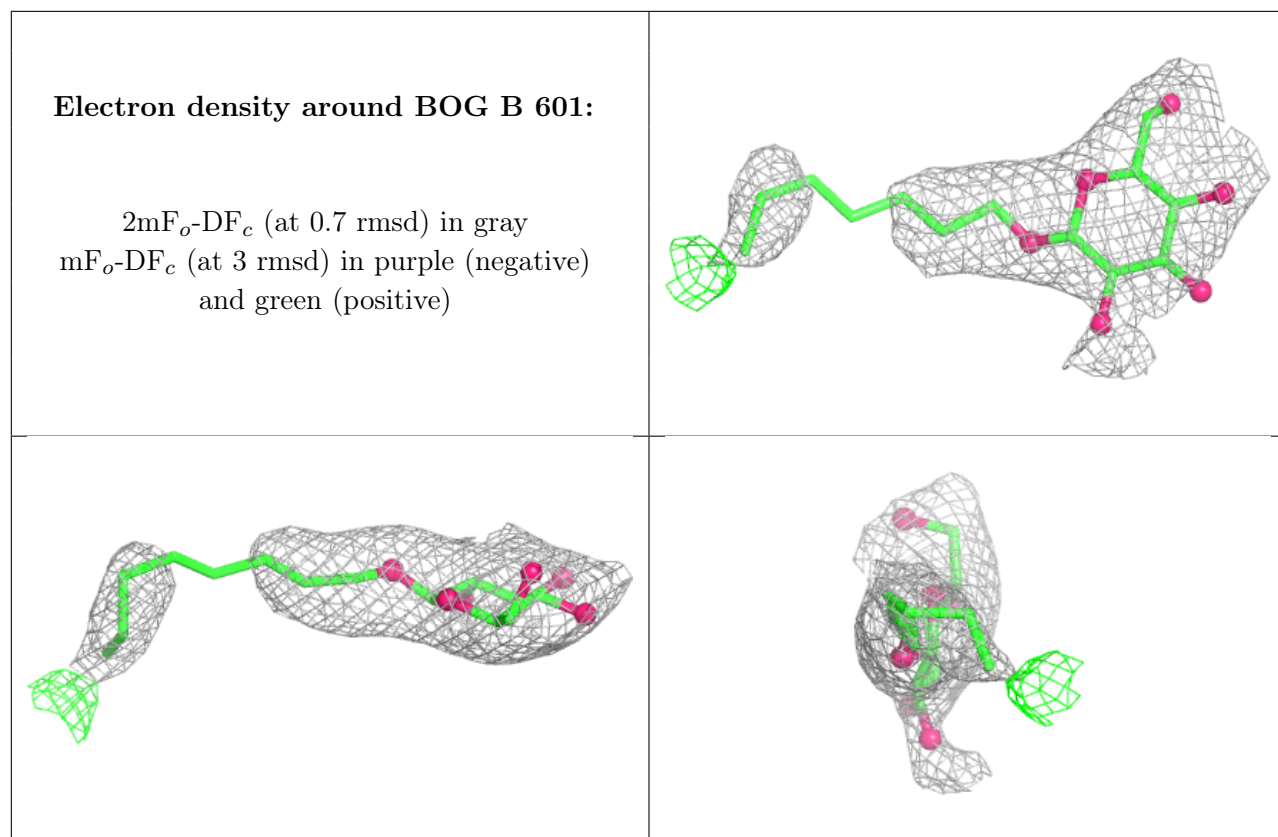
Electron density around BOG A 601:

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

**Electron density around BOG A 602:**

$2mF_o-DF_c$ (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.