



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:14 PM BST

PDB ID : 4HOD
Title : Crystal structure of LeuT-E290S with bound Cl
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Deposited on : 2012-10-22
Resolution : 3.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

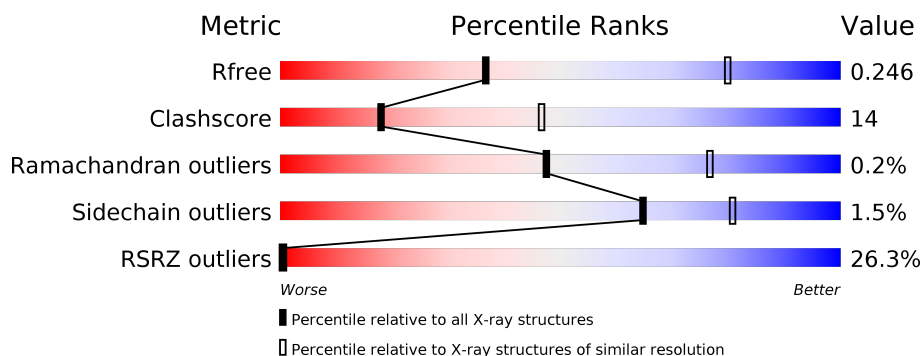
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	515	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BOG	A	605	-	-	-	X
5	BOG	A	606	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BOG	A	607	-	-	-	X
5	BOG	A	609	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4153 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.

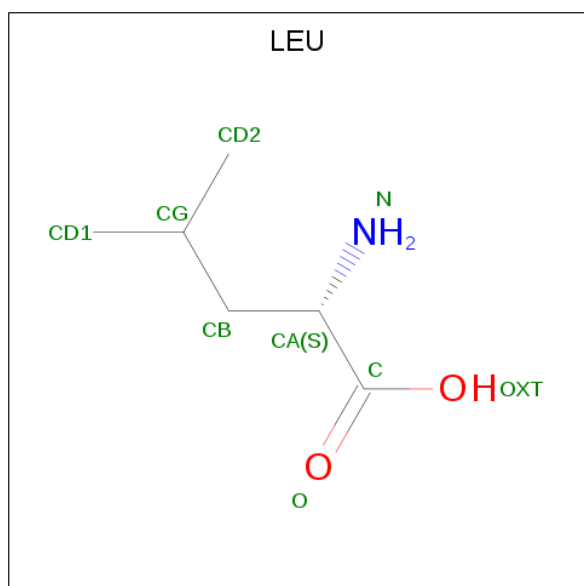
- Molecule 1 is a protein called Transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	509	4041	2736	634	659	12	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	SER	GLU	engineered mutation	UNP O67854
A	514	GLY	-	expression tag	UNP O67854
A	515	THR	-	expression tag	UNP O67854

- Molecule 2 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	9	6	1	2	0	0

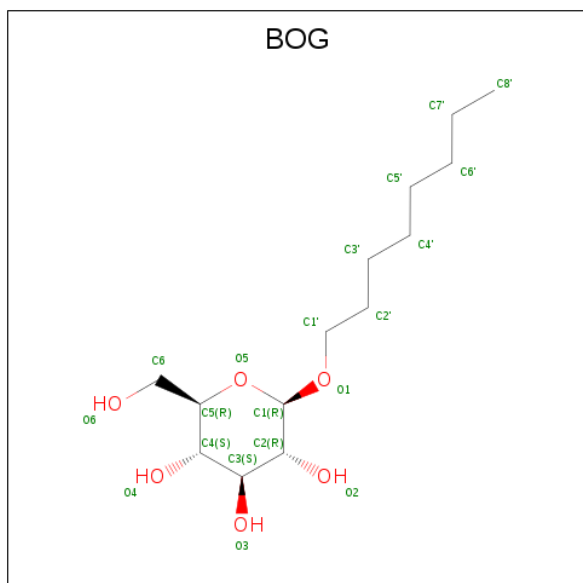
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



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

3 Residue-property plots [i](#)

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

• Molecule 1: Transporter



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.58Å 87.48Å 80.86Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	47.62 – 3.30 47.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.62-3.30) 98.3 (47.62-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.190 , 0.254 0.192 , 0.246	Depositor DCC
R_{free} test set	682 reflections (7.50%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 91.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4153	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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, CL, 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	0.30	0/4168	0.45	0/5677

There are no bond length outliers.

There are no bond angle outliers.

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	4041	0	4129	110	0
2	A	9	0	10	1	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	100	0	140	12	0
All	All	4153	0	4279	114	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 14.

All (114) 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:11:ARG:NH2	1:A:274:ASP:OD2	2.08	0.86
1:A:42:ALA:HB2	1:A:234:ASP:HB3	1.61	0.82
1:A:47:TYR:OH	1:A:287:GLU:OE1	1.99	0.80
1:A:392:LEU:CD1	5:A:608:BOG:H8'1	2.12	0.79
5:A:608:BOG:H8'3	5:A:609:BOG:H8'2	1.65	0.78
1:A:395:PHE:HB3	5:A:609:BOG:H5'2	1.65	0.75
1:A:287:GLU:O	1:A:291:VAL:HG22	1.90	0.72
1:A:45:ILE:HB	1:A:46:PRO:HD3	1.72	0.72
1:A:472:ILE:N	1:A:473:PRO:HD2	2.06	0.70
1:A:505:GLU:HG3	1:A:506:ARG:NH1	2.08	0.69
1:A:392:LEU:HD12	5:A:608:BOG:H8'1	1.75	0.68
1:A:166:LEU:HD23	5:A:606:BOG:H1'2	1.75	0.68
1:A:245:ILE:HG12	1:A:463:LEU:HD12	1.78	0.66
1:A:331:PHE:O	1:A:337:GLY:HA3	1.96	0.65
1:A:51:PHE:CZ	1:A:56:ILE:HD11	2.32	0.65
1:A:8:TRP:CD1	1:A:14:LEU:HD13	2.32	0.64
1:A:239:LYS:N	1:A:239:LYS:HD2	2.14	0.62
1:A:11:ARG:O	1:A:15:ILE:HG12	2.00	0.62
1:A:238:LEU:O	1:A:244:TRP:NE1	2.27	0.62
1:A:392:LEU:HD13	5:A:608:BOG:H8'1	1.81	0.62
1:A:110:TYR:CZ	1:A:394:MET:HG2	2.34	0.61
1:A:111:ILE:HD11	1:A:400:LEU:HD11	1.82	0.61
1:A:61:ILE:O	1:A:65:MET:HG3	2.00	0.61
1:A:161:ILE:HD12	5:A:609:BOG:H5'1	1.83	0.60
1:A:471:TYR:C	1:A:473:PRO:HD2	2.23	0.59
1:A:241:PRO:O	1:A:245:ILE:HG13	2.03	0.58
1:A:310:ASN:O	1:A:314:ILE:HG13	2.05	0.57
1:A:51:PHE:CE1	1:A:287:GLU:HG3	2.39	0.57
1:A:77:THR:OG1	1:A:97:GLY:HA3	2.05	0.57
1:A:245:ILE:HG12	1:A:463:LEU:CD1	2.33	0.57
1:A:46:PRO:HG2	1:A:243:VAL:HG12	1.87	0.57
1:A:423:PHE:CE2	1:A:432:ALA:HB1	2.40	0.56
5:A:608:BOG:H6'2	5:A:609:BOG:H6'1	1.86	0.56
5:A:608:BOG:H8'3	5:A:609:BOG:C8'	2.35	0.56
1:A:256:SER:HG	2:A:601:LEU:N	2.04	0.56
1:A:130:PRO:HG3	1:A:144:PHE:HE2	1.70	0.56
1:A:245:ILE:HA	1:A:463:LEU:HD11	1.87	0.55
1:A:155:PRO:HD3	1:A:162:LEU:HD23	1.88	0.55
1:A:56:ILE:N	1:A:57:PRO:HD2	2.21	0.55
1:A:167:PHE:HE1	5:A:606:BOG:H6'2	1.72	0.55
1:A:396:LEU:HB3	1:A:399:SER:HB2	1.89	0.54
1:A:31:PHE:HB3	1:A:32:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LYS:HA	1:A:193:ARG:HG3	1.90	0.54
1:A:472:ILE:N	1:A:473:PRO:CD	2.71	0.53
1:A:170:ILE:O	1:A:174:ILE:HG13	2.09	0.53
1:A:110:TYR:CE1	1:A:394:MET:HG2	2.43	0.53
1:A:128:PRO:HD3	1:A:147:PHE:CD1	2.44	0.52
1:A:117:GLY:HA3	1:A:151:TYR:OH	2.09	0.52
1:A:77:THR:O	1:A:81:PHE:HB2	2.09	0.52
1:A:416:GLY:O	1:A:419:GLU:HG2	2.10	0.51
1:A:5:ARG:HH22	1:A:369:ASP:CG	2.13	0.51
1:A:327:LEU:HD23	1:A:344:TRP:CE2	2.45	0.51
1:A:145:LYS:HA	1:A:325:ILE:HD13	1.93	0.51
1:A:255:LEU:HD23	1:A:286:ASN:ND2	2.26	0.50
1:A:361:GLN:N	1:A:362:PRO:CD	2.75	0.50
1:A:305:PHE:CE1	1:A:330:ILE:HG23	2.47	0.49
1:A:461:ALA:O	1:A:465:VAL:HG23	2.13	0.49
1:A:199:MET:HB2	1:A:200:PRO:HD3	1.93	0.48
1:A:37:GLU:HG2	1:A:316:LYS:HG2	1.93	0.48
1:A:167:PHE:CE1	5:A:606:BOG:H6'2	2.48	0.48
1:A:76:THR:HG21	1:A:98:LEU:HD21	1.96	0.48
1:A:401:ASP:OD1	1:A:401:ASP:N	2.45	0.48
1:A:423:PHE:O	1:A:427:PHE:HB3	2.14	0.48
1:A:167:PHE:O	1:A:171:VAL:HG23	2.14	0.48
1:A:299:ILE:HB	1:A:300:PRO:HD3	1.95	0.48
1:A:432:ALA:O	1:A:436:ILE:HG13	2.14	0.47
1:A:18:MET:CE	1:A:265:TYR:HB3	2.44	0.47
1:A:358:ALA:O	1:A:362:PRO:HD3	2.14	0.47
1:A:259:PHE:CZ	1:A:412:VAL:HG11	2.50	0.47
1:A:59:MET:O	1:A:63:TRP:HD1	1.98	0.46
1:A:30:ARG:O	1:A:34:GLN:HG2	2.15	0.46
1:A:487:ARG:O	1:A:491:ILE:HG13	2.15	0.46
1:A:277:LEU:HD13	1:A:442:ILE:HD13	1.97	0.46
1:A:237:LYS:O	1:A:239:LYS:N	2.49	0.46
1:A:240:ASP:HB3	1:A:243:VAL:HG23	1.97	0.46
1:A:136:ASP:O	1:A:140:ILE:HG13	2.16	0.45
1:A:235:PHE:HD1	1:A:238:LEU:HD11	1.82	0.45
1:A:289:ALA:O	1:A:293:LEU:HB2	2.17	0.45
5:A:607:BOG:H2'1	5:A:608:BOG:H1'2	1.99	0.44
1:A:43:PHE:CE1	1:A:247:ALA:HA	2.53	0.44
1:A:58:LEU:O	1:A:62:GLU:HG3	2.17	0.44
1:A:127:VAL:HB	1:A:128:PRO:HD2	1.98	0.44
1:A:78:PRO:HD3	1:A:94:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:SER:C	1:A:300:PRO:HG2	2.39	0.43
1:A:61:ILE:HG23	1:A:423:PHE:CD2	2.54	0.43
1:A:65:MET:HE1	1:A:81:PHE:HE1	1.83	0.43
1:A:65:MET:HE2	1:A:84:LEU:HD11	1.99	0.43
1:A:356:SER:HA	1:A:359:ILE:HG12	2.00	0.43
1:A:44:MET:O	1:A:48:ILE:HG13	2.19	0.42
1:A:131:PRO:HA	1:A:132:PRO:HD3	1.87	0.42
1:A:57:PRO:O	1:A:61:ILE:HG13	2.18	0.42
1:A:16:LEU:HD23	1:A:16:LEU:HA	1.88	0.42
1:A:77:THR:N	1:A:78:PRO:CD	2.83	0.42
1:A:130:PRO:HG3	1:A:144:PHE:CE2	2.52	0.42
1:A:412:VAL:HG23	1:A:413:VAL:N	2.35	0.42
1:A:66:GLY:O	1:A:267:SER:HA	2.20	0.42
1:A:339:PHE:O	1:A:342:PHE:N	2.52	0.42
1:A:226:GLY:HA3	1:A:300:PRO:HA	2.02	0.42
1:A:76:THR:CG2	1:A:98:LEU:HD21	2.50	0.41
1:A:456:THR:N	1:A:457:PRO:HD2	2.34	0.41
1:A:456:THR:HB	1:A:457:PRO:HD3	2.01	0.41
1:A:24:GLY:HA2	1:A:351:ALA:O	2.21	0.41
1:A:11:ARG:CZ	1:A:278:SER:OG	2.67	0.41
1:A:11:ARG:HH22	1:A:274:ASP:CG	2.19	0.41
1:A:206:ALA:O	1:A:210:VAL:HG23	2.19	0.41
1:A:479:THR:HB	1:A:483:VAL:HG11	2.03	0.41
1:A:66:GLY:HA3	1:A:266:ALA:HB3	2.02	0.41
1:A:298:SER:HB3	1:A:322:LEU:HD21	2.02	0.41
1:A:11:ARG:NH2	1:A:278:SER:OG	2.53	0.41
1:A:280:LEU:HD12	1:A:280:LEU:O	2.21	0.41
1:A:421:ILE:O	1:A:425:TRP:HB2	2.20	0.41
1:A:100:ILE:N	1:A:101:PRO:HD2	2.37	0.40
1:A:269:VAL:CG1	1:A:273:GLN:HB3	2.51	0.40
1:A:505:GLU:HG3	1:A:506:ARG:HH11	1.83	0.40

There are no symmetry-related clashes.

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	505/515 (98%)	476 (94%)	28 (6%)	1 (0%)	47 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	LEU

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	411/416 (99%)	405 (98%)	6 (2%)	65 81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	LYS
1	A	274	ASP
1	A	401	ASP
1	A	424	PHE
1	A	448	TYR
1	A	467	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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$
5	BOG	A	605	-	20,20,20	1.36	2 (10%)	25,25,25	2.06	10 (40%)
5	BOG	A	608	-	20,20,20	1.37	3 (15%)	25,25,25	2.07	9 (36%)
5	BOG	A	609	-	20,20,20	1.36	2 (10%)	25,25,25	1.82	7 (28%)
5	BOG	A	606	-	20,20,20	1.39	2 (10%)	25,25,25	1.92	9 (36%)
5	BOG	A	607	-	20,20,20	1.37	2 (10%)	25,25,25	2.10	8 (32%)

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
5	BOG	A	605	-	-	2/11/31/31	0/1/1/1
5	BOG	A	608	-	-	2/11/31/31	0/1/1/1
5	BOG	A	609	-	-	5/11/31/31	0/1/1/1
5	BOG	A	606	-	-	8/11/31/31	0/1/1/1
5	BOG	A	607	-	-	4/11/31/31	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606	BOG	O5-C1	4.73	1.53	1.41
5	A	607	BOG	O5-C1	4.70	1.53	1.41
5	A	609	BOG	O5-C1	4.63	1.53	1.41
5	A	608	BOG	O5-C1	4.50	1.53	1.41
5	A	605	BOG	O5-C1	4.50	1.53	1.41
5	A	609	BOG	O2-C2	2.27	1.48	1.43
5	A	607	BOG	O2-C2	2.22	1.48	1.43
5	A	606	BOG	O2-C2	2.16	1.48	1.43
5	A	608	BOG	O2-C2	2.16	1.48	1.43
5	A	605	BOG	O2-C2	2.11	1.47	1.43
5	A	608	BOG	C3-C2	-2.10	1.47	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	607	BOG	C1'-O1-C1	4.82	121.83	113.84
5	A	609	BOG	C1'-O1-C1	4.72	121.67	113.84
5	A	608	BOG	O5-C5-C4	4.66	118.17	109.69
5	A	607	BOG	O5-C5-C4	4.45	117.78	109.69
5	A	605	BOG	O5-C5-C4	4.44	117.75	109.69
5	A	606	BOG	O5-C5-C4	4.04	117.04	109.69
5	A	607	BOG	C4-C3-C2	3.81	117.47	110.82
5	A	605	BOG	O5-C1-C2	3.73	118.24	110.35
5	A	606	BOG	C1'-O1-C1	3.64	119.88	113.84
5	A	608	BOG	C1'-O1-C1	3.62	119.85	113.84
5	A	607	BOG	C1-O5-C5	3.54	120.63	113.69
5	A	608	BOG	C1-O5-C5	3.37	120.30	113.69
5	A	605	BOG	C1-O5-C5	3.35	120.27	113.69
5	A	609	BOG	O5-C5-C4	3.32	115.73	109.69
5	A	608	BOG	O6-C6-C5	3.26	122.49	111.29
5	A	605	BOG	C4-C3-C2	3.21	116.43	110.82
5	A	608	BOG	O5-C1-C2	3.20	117.12	110.35
5	A	606	BOG	O5-C1-C2	3.17	117.07	110.35
5	A	607	BOG	O6-C6-C5	3.13	122.02	111.29
5	A	606	BOG	O6-C6-C5	3.10	121.92	111.29
5	A	607	BOG	O5-C1-C2	2.97	116.64	110.35
5	A	608	BOG	C4-C3-C2	2.95	115.98	110.82
5	A	605	BOG	O6-C6-C5	2.89	121.21	111.29
5	A	605	BOG	C1'-O1-C1	2.87	118.60	113.84
5	A	609	BOG	O6-C6-C5	2.82	120.97	111.29
5	A	606	BOG	C4-C3-C2	2.77	115.67	110.82
5	A	605	BOG	C1-C2-C3	2.67	115.55	110.00
5	A	609	BOG	C4-C3-C2	2.66	115.47	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	BOG	O5-C5-C6	2.65	113.02	106.44
5	A	606	BOG	C1-O5-C5	2.64	118.86	113.69
5	A	605	BOG	C3-C4-C5	2.57	114.81	110.24
5	A	607	BOG	C3-C4-C5	2.56	114.80	110.24
5	A	609	BOG	C1-C2-C3	2.29	114.76	110.00
5	A	606	BOG	O1-C1'-C2'	2.28	117.54	109.56
5	A	605	BOG	O1-C1'-C2'	2.26	117.49	109.56
5	A	607	BOG	C1-C2-C3	2.25	114.69	110.00
5	A	608	BOG	O1-C1-C2	2.18	111.71	108.30
5	A	605	BOG	O1-C1-C2	2.15	111.66	108.30
5	A	608	BOG	C3-C4-C5	2.08	113.95	110.24
5	A	606	BOG	C3-C4-C5	2.08	113.94	110.24
5	A	609	BOG	O5-C5-C6	2.07	111.59	106.44
5	A	609	BOG	O5-C1-C2	2.06	114.70	110.35
5	A	608	BOG	O1-C1'-C2'	2.00	116.58	109.56

There are no chirality outliers.

All (21) torsion outliers are listed below:

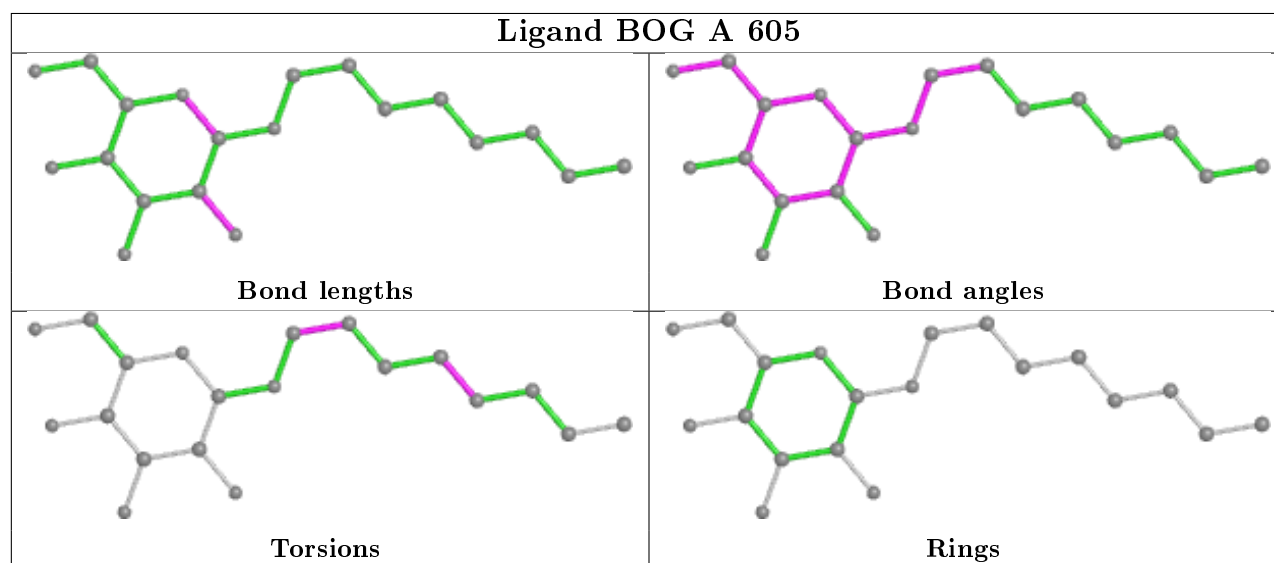
Mol	Chain	Res	Type	Atoms
5	A	607	BOG	C3'-C4'-C5'-C6'
5	A	606	BOG	C4-C5-C6-O6
5	A	607	BOG	O5-C5-C6-O6
5	A	608	BOG	O1-C1'-C2'-C3'
5	A	606	BOG	O1-C1'-C2'-C3'
5	A	605	BOG	C3'-C4'-C5'-C6'
5	A	609	BOG	C2-C1-O1-C1'
5	A	607	BOG	C4-C5-C6-O6
5	A	608	BOG	C3'-C4'-C5'-C6'
5	A	609	BOG	C2'-C1'-O1-C1
5	A	609	BOG	C1'-C2'-C3'-C4'
5	A	606	BOG	C2'-C3'-C4'-C5'
5	A	606	BOG	O5-C5-C6-O6
5	A	609	BOG	C5'-C6'-C7'-C8'
5	A	606	BOG	C3'-C4'-C5'-C6'
5	A	606	BOG	C1'-C2'-C3'-C4'
5	A	609	BOG	O5-C1-O1-C1'
5	A	607	BOG	C2-C1-O1-C1'
5	A	605	BOG	O1-C1'-C2'-C3'
5	A	606	BOG	C4'-C5'-C6'-C7'
5	A	606	BOG	C2'-C1'-O1-C1

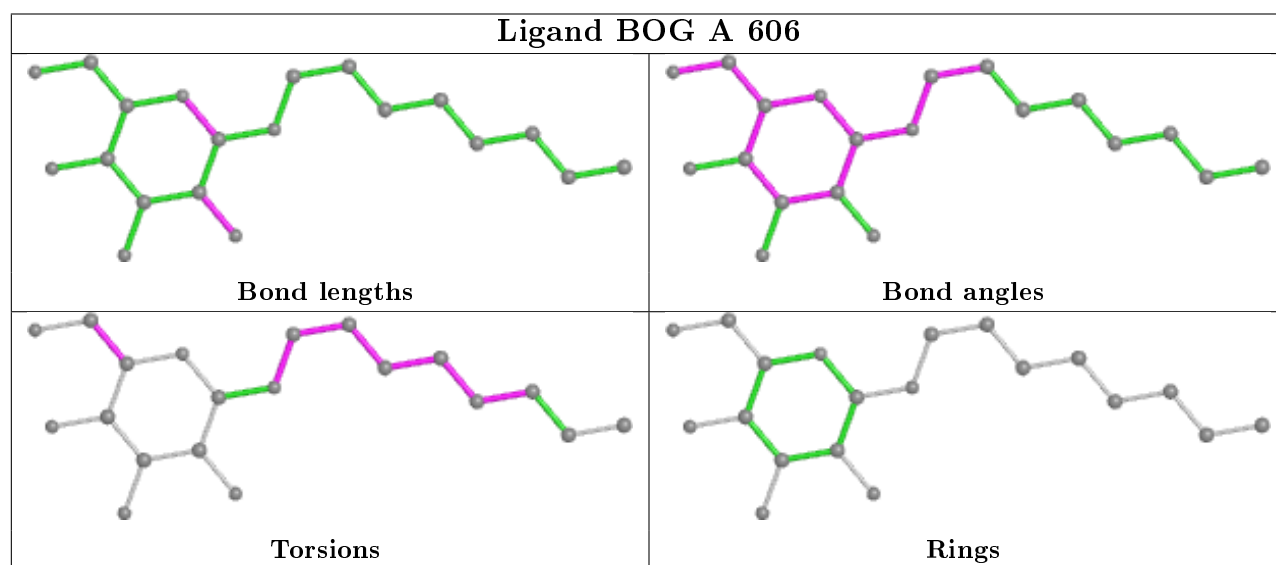
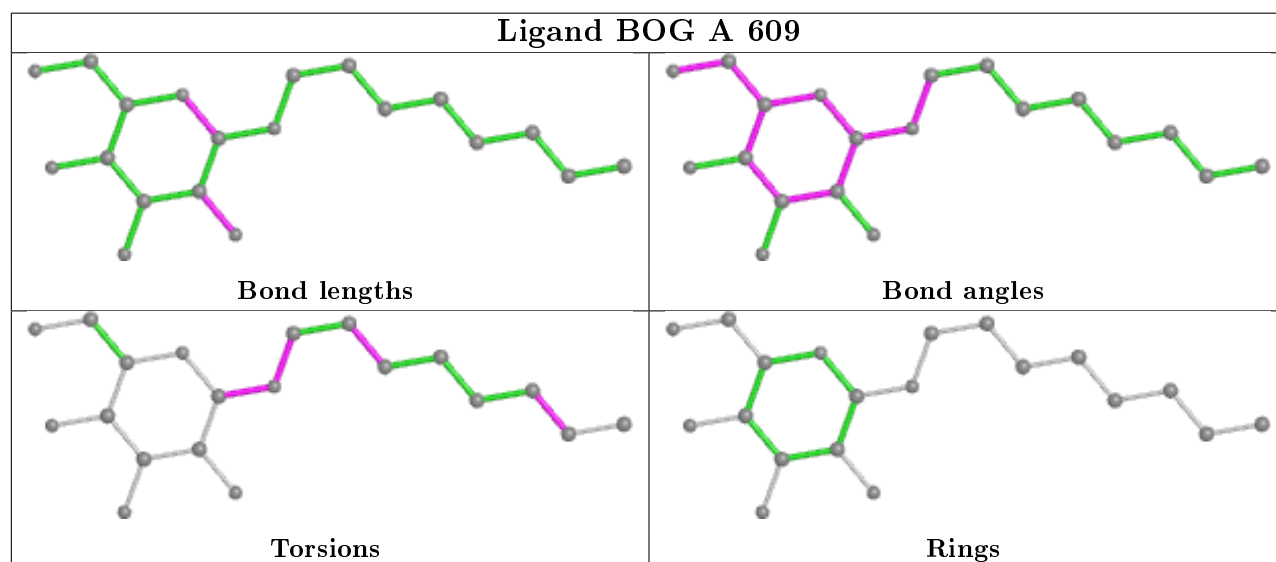
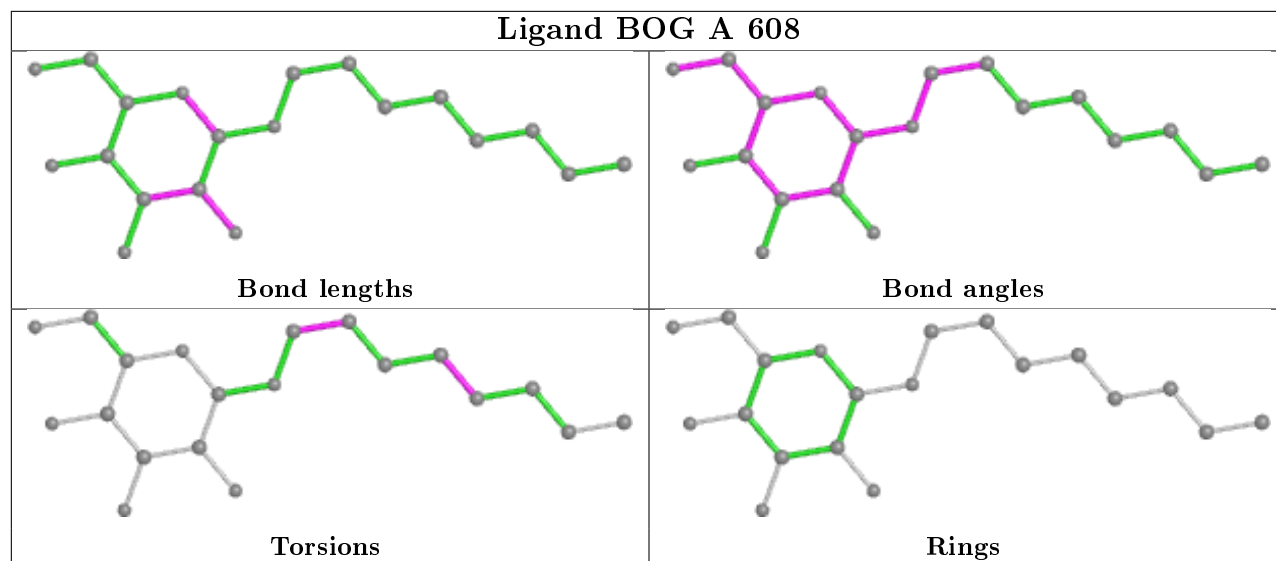
There are no ring outliers.

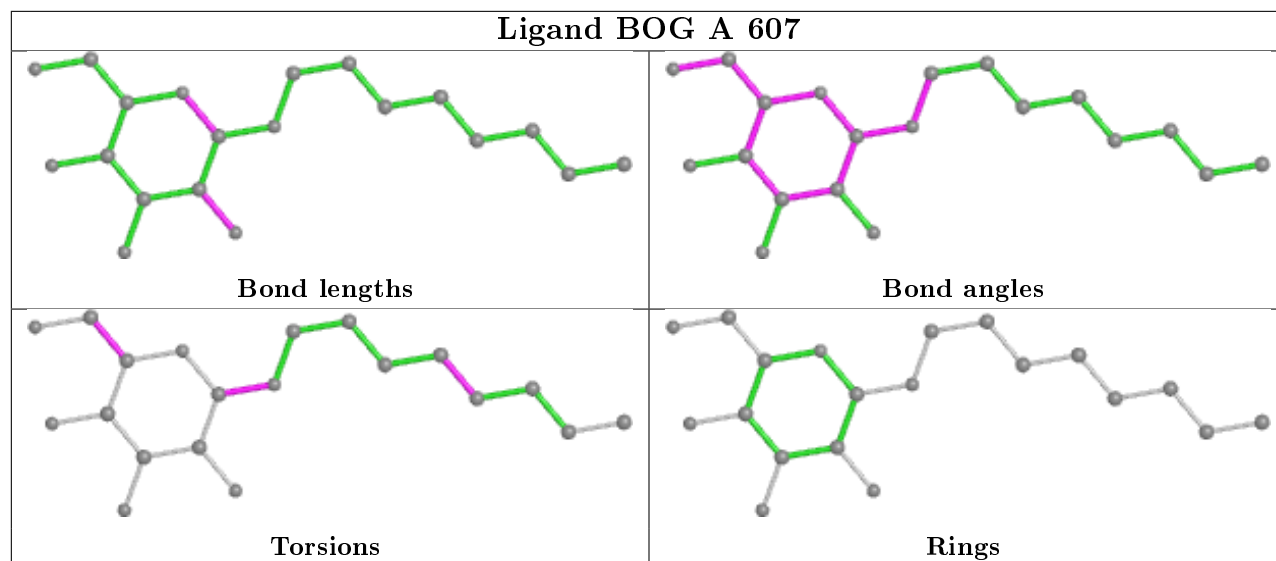
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	608	BOG	7	0
5	A	609	BOG	5	0
5	A	606	BOG	3	0
5	A	607	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	509/515 (98%)	1.25	134 (26%) 0 0	73, 93, 137, 166	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	ALA	9.3
1	A	310	ASN	8.0
1	A	296	SER	7.8
1	A	317	ALA	7.6
1	A	46	PRO	7.5
1	A	216	LEU	7.1
1	A	451	VAL	7.0
1	A	241	PRO	6.6
1	A	321	ASN	6.6
1	A	511	GLU	6.1
1	A	158	ASP	5.8
1	A	223	ALA	5.6
1	A	138	ASP	5.6
1	A	318	GLY	5.3
1	A	428	GLY	5.3
1	A	267	SER	5.3
1	A	217	GLU	5.2
1	A	463	LEU	5.2
1	A	507	ARG	5.0
1	A	50	ALA	5.0
1	A	468	ALA	4.9
1	A	314	ILE	4.7
1	A	232	THR	4.7
1	A	228	ASN	4.7
1	A	48	ILE	4.7
1	A	196	LYS	4.6
1	A	181	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	44	MET	4.5
1	A	308	VAL	4.4
1	A	226	GLY	4.4
1	A	512	SER	4.3
1	A	464	LEU	4.2
1	A	222	THR	4.2
1	A	45	ILE	4.2
1	A	322	LEU	4.1
1	A	6	GLU	4.0
1	A	42	ALA	4.0
1	A	214	PHE	3.9
1	A	309	ALA	3.9
1	A	140	ILE	3.8
1	A	450	TYR	3.7
1	A	87	ASN	3.7
1	A	313	ALA	3.7
1	A	319	ALA	3.6
1	A	509	ASN	3.6
1	A	515	THR	3.6
1	A	195	ALA	3.6
1	A	299	ILE	3.5
1	A	461	ALA	3.5
1	A	229	PHE	3.5
1	A	304	ALA	3.5
1	A	330	ILE	3.5
1	A	513	ALA	3.4
1	A	141	LEU	3.3
1	A	119	ALA	3.3
1	A	131	PRO	3.3
1	A	171	VAL	3.3
1	A	53	LEU	3.3
1	A	469	ARG	3.3
1	A	213	VAL	3.3
1	A	9	ALA	3.2
1	A	307	GLY	3.1
1	A	230	LEU	3.1
1	A	132	PRO	3.1
1	A	452	MET	3.1
1	A	192	GLU	3.1
1	A	220	ASN	3.1
1	A	315	ALA	3.1
1	A	300	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	185	ARG	3.0
1	A	233	PRO	3.0
1	A	429	ALA	3.0
1	A	37	GLU	2.9
1	A	514	GLY	2.9
1	A	326	THR	2.9
1	A	221	GLY	2.9
1	A	303	VAL	2.9
1	A	34	GLN	2.9
1	A	245	ILE	2.9
1	A	340	LEU	2.9
1	A	231	TRP	2.9
1	A	244	TRP	2.8
1	A	193	ARG	2.8
1	A	38	ASN	2.8
1	A	238	LEU	2.8
1	A	312	VAL	2.8
1	A	410	ILE	2.8
1	A	234	ASP	2.8
1	A	225	ASP	2.8
1	A	295	GLY	2.7
1	A	32	PRO	2.7
1	A	210	VAL	2.7
1	A	218	THR	2.7
1	A	177	PHE	2.7
1	A	297	ILE	2.7
1	A	325	ILE	2.7
1	A	137	PRO	2.7
1	A	447	ILE	2.7
1	A	40	GLY	2.6
1	A	369	ASP	2.6
1	A	250	GLN	2.6
1	A	180	VAL	2.6
1	A	89	PHE	2.6
1	A	136	ASP	2.6
1	A	174	ILE	2.5
1	A	425	TRP	2.5
1	A	266	ALA	2.5
1	A	43	PHE	2.5
1	A	186	GLY	2.5
1	A	465	VAL	2.5
1	A	467	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	200	PRO	2.3
1	A	506	ARG	2.3
1	A	139	SER	2.3
1	A	224	ALA	2.3
1	A	419	GLU	2.3
1	A	239	LYS	2.3
1	A	49	ILE	2.3
1	A	86	ARG	2.2
1	A	82	TYR	2.2
1	A	194	PHE	2.1
1	A	460	LEU	2.1
1	A	459	PHE	2.1
1	A	155	PRO	2.1
1	A	298	SER	2.1
1	A	260	GLY	2.1
1	A	235	PHE	2.1
1	A	454	TYR	2.1
1	A	480	HIS	2.1
1	A	472	ILE	2.1
1	A	316	LYS	2.0
1	A	10	THR	2.0
1	A	123	LEU	2.0
1	A	431	LYS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

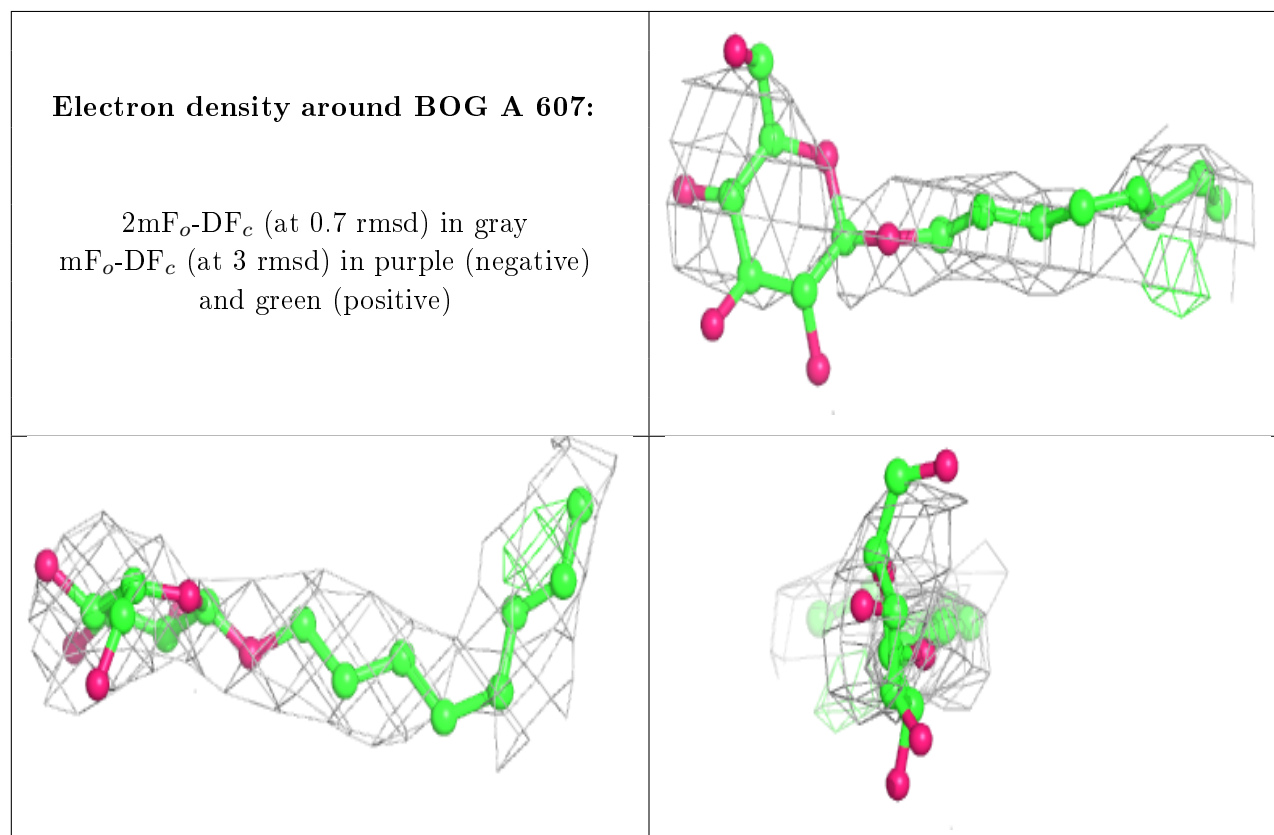
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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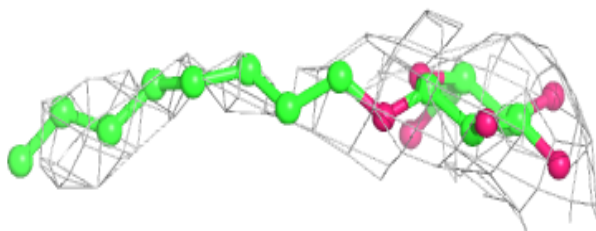
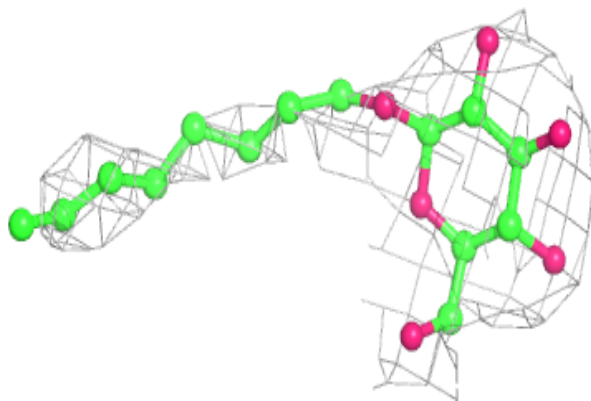
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	A	602	1/1	0.55	0.17	96,96,96,96	0
5	BOG	A	607	20/20	0.60	0.48	97,109,129,133	0
5	BOG	A	606	20/20	0.61	0.44	81,123,144,144	0
5	BOG	A	605	20/20	0.68	0.47	87,122,130,138	0
5	BOG	A	609	20/20	0.77	0.46	90,115,127,133	0
4	CL	A	604	1/1	0.77	0.30	118,118,118,118	0
5	BOG	A	608	20/20	0.80	0.34	86,114,128,132	0
2	LEU	A	601	9/9	0.83	0.36	86,91,95,96	0
3	NA	A	603	1/1	0.98	0.21	84,84,84,84	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.

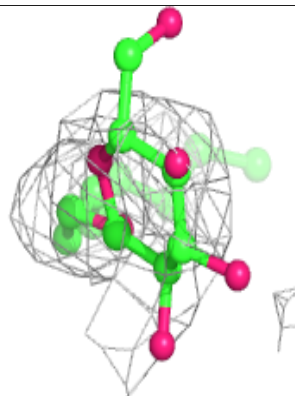
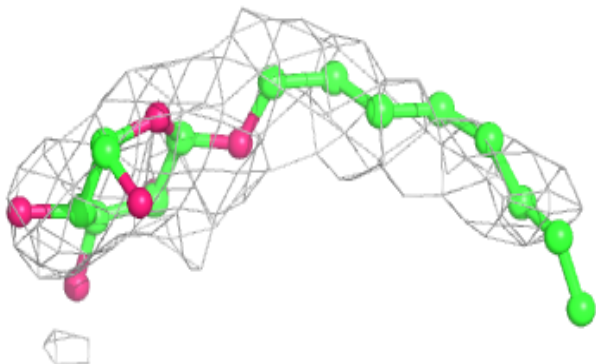
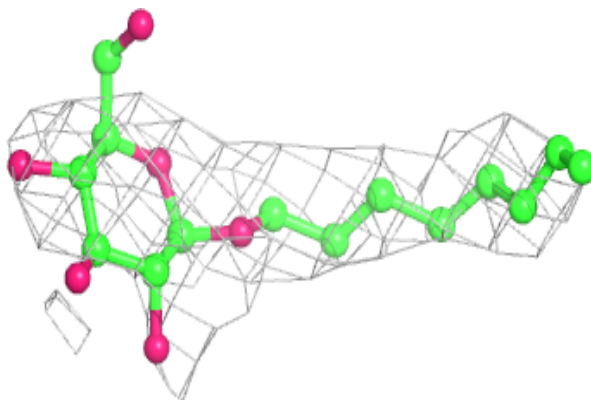


Electron density around BOG A 606:

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

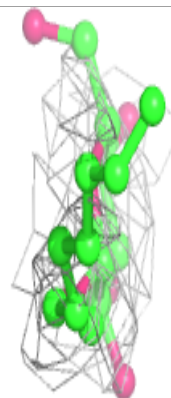
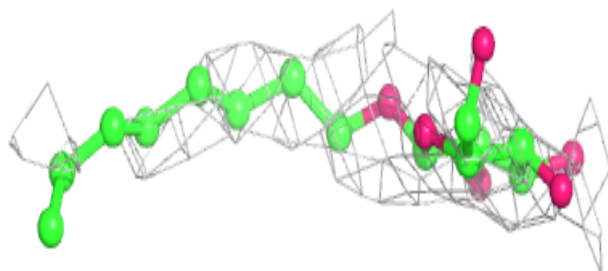
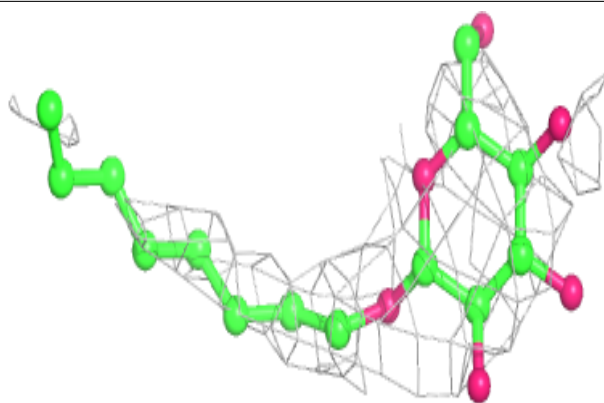
**Electron density around BOG A 605:**

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

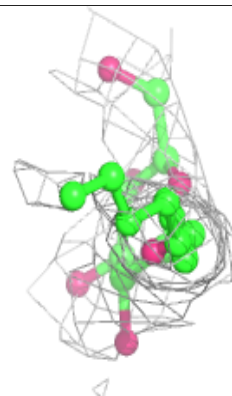
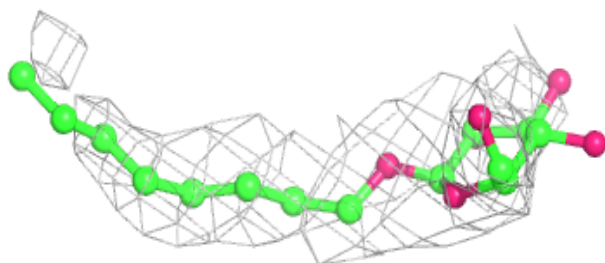
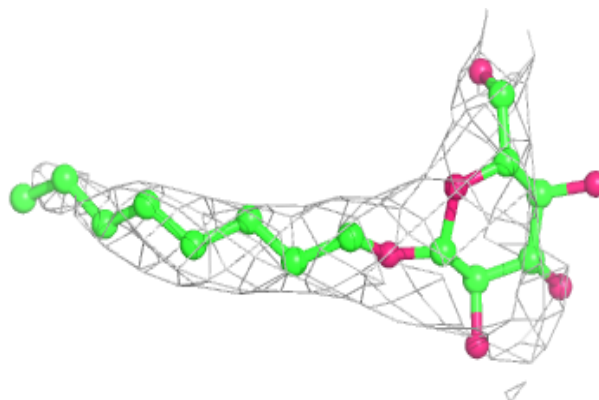


Electron density around BOG A 609:

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

**Electron density around BOG A 608:**

$2mF_o-DF_c$ (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.