



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 09:20 PM JST

PDB ID : 6LD0
Title : Structure of Bifidobacterium dentium beta-glucuronidase complexed with C6-hexyl uronic isofagomine
Authors : Lin, H.-Y.; Hsieh, T.-J.; Lin, C.-H.
Deposited on : 2019-11-20
Resolution : 1.90 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 : 2.23.1
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) : 2.23.1

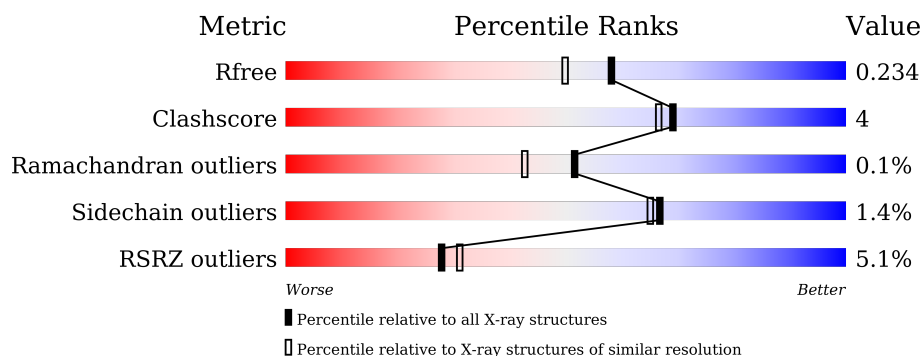
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	670	<div> <div>3%</div> <div>84% 8% 7%</div> </div>
1	B	670	<div> <div>4%</div> <div>85% 7% 7%</div> </div>
1	C	670	<div> <div>6%</div> <div>82% 10% 7%</div> </div>
1	D	670	<div> <div>5%</div> <div>84% 8% 7%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21312 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.

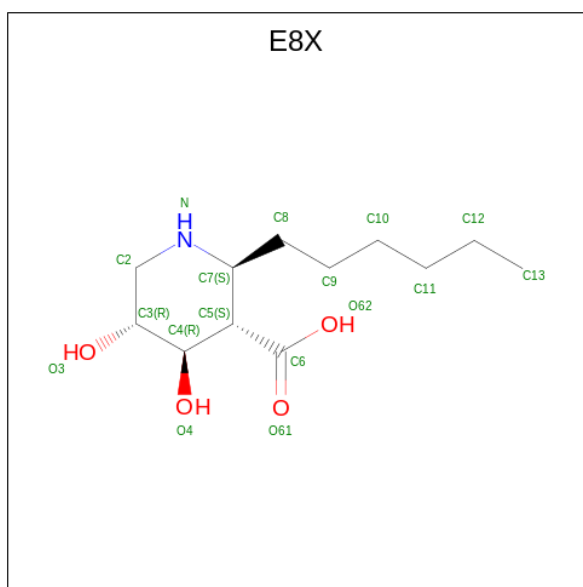
- Molecule 1 is a protein called LacZ1 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	0
			4909	3113	856	921	19			
1	B	620	Total	C	N	O	S	0	0	0
			4909	3113	856	921	19			
1	C	620	Total	C	N	O	S	0	0	0
			4909	3113	856	921	19			
1	D	620	Total	C	N	O	S	0	0	0
			4909	3113	856	921	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP D2Q7B1
A	0	GLY	-	expression tag	UNP D2Q7B1
B	-1	ASN	-	expression tag	UNP D2Q7B1
B	0	GLY	-	expression tag	UNP D2Q7B1
C	-1	ASN	-	expression tag	UNP D2Q7B1
C	0	GLY	-	expression tag	UNP D2Q7B1
D	-1	ASN	-	expression tag	UNP D2Q7B1
D	0	GLY	-	expression tag	UNP D2Q7B1

- Molecule 2 is (2 {S},3 {S},4 {R},5 {R})-2-hexyl-4,5-bis(oxidanyl)piperidine-3-carboxylic acid (three-letter code: E8X) (formula: C₁₂H₂₃NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	12	1	4		
2	B	1	Total	C	N	O	0	0
			17	12	1	4		
2	C	1	Total	C	N	O	0	0
			17	12	1	4		
2	D	1	Total	C	N	O	0	0
			17	12	1	4		

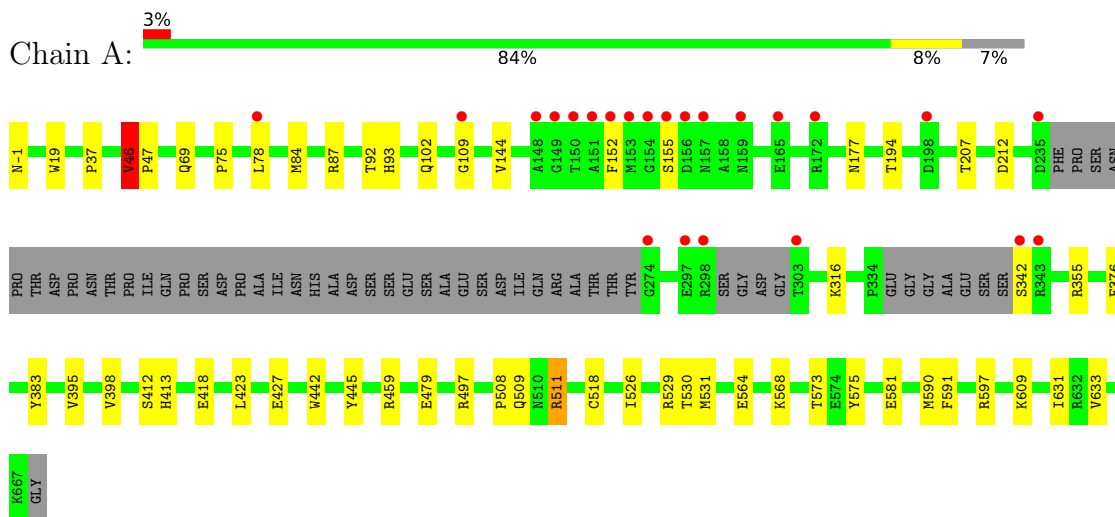
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	498	Total	O	0	0
			498	498		
3	B	466	Total	O	0	0
			466	466		
3	C	339	Total	O	0	0
			339	339		
3	D	305	Total	O	0	0
			305	305		

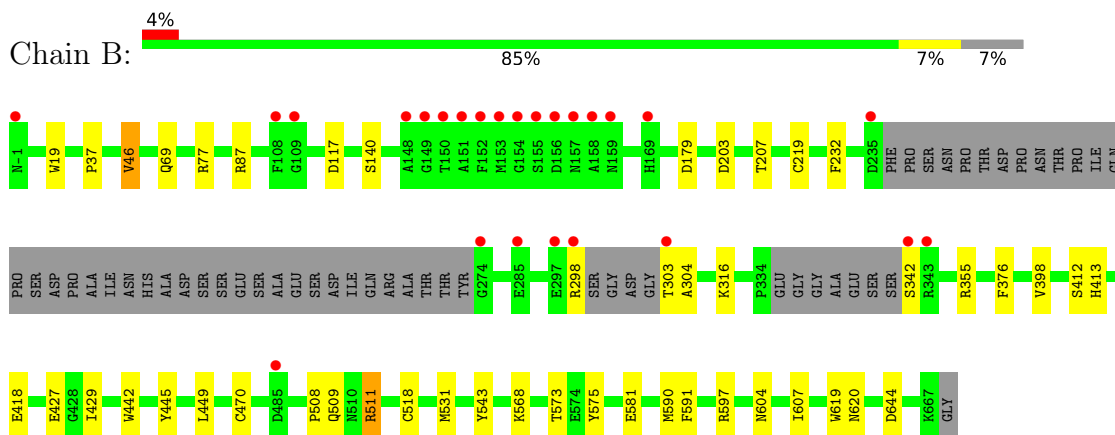
3 Residue-property plots [i](#)

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.

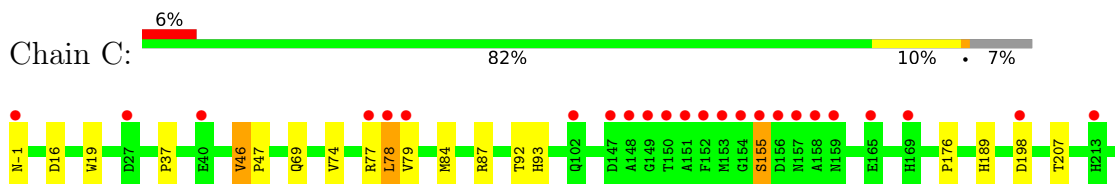
• Molecule 1: LacZ1 Beta-galactosidase

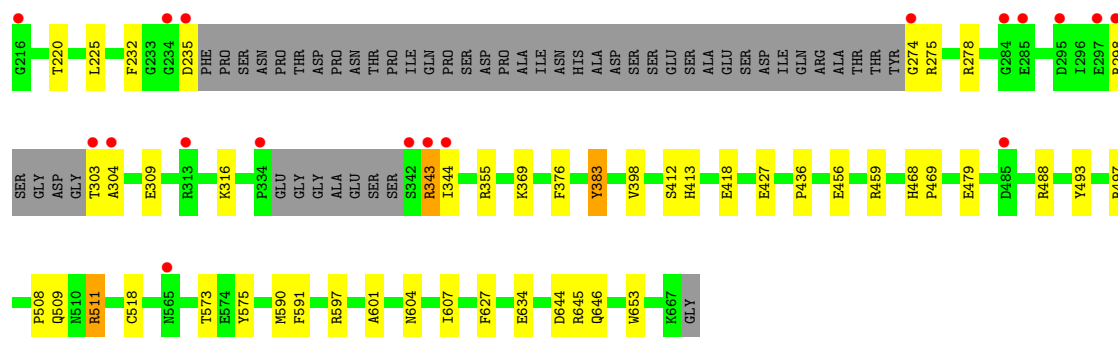


• Molecule 1: LacZ1 Beta-galactosidase

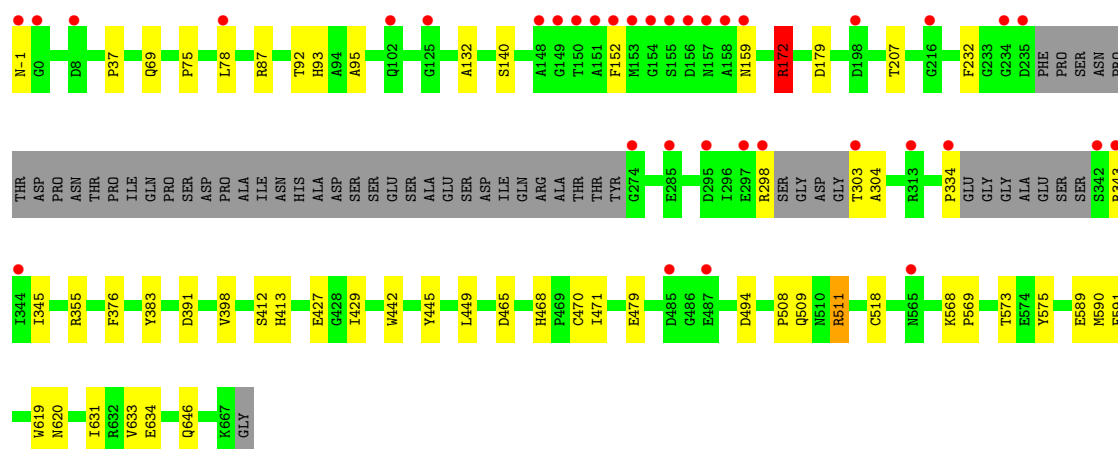
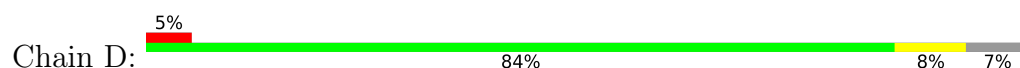


• Molecule 1: LacZ1 Beta-galactosidase





● Molecule 1: LacZ1 Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.91Å 105.39Å 162.29Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	20.19 – 1.90 20.19 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.2 (20.19-1.90) 87.9 (20.19-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.201 , 0.235 0.201 , 0.234	Depositor DCC
R_{free} test set	1992 reflections (0.83%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21312	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: E8X

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	0.29	0/5040	0.51	0/6857
1	B	0.29	0/5040	0.51	0/6857
1	C	0.27	0/5040	0.50	0/6857
1	D	0.27	0/5040	0.50	1/6857 (0.0%)
All	All	0.28	0/20160	0.50	1/27428 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	172	ARG	NE-CZ-NH1	6.71	123.66	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	VAL	Peptide
1	B	46	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	C	46	VAL	Peptide

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	4909	0	4659	36	0
1	B	4909	0	4659	30	0
1	C	4909	0	4659	45	0
1	D	4909	0	4659	36	0
2	A	17	0	0	0	0
2	B	17	0	0	1	0
2	C	17	0	0	0	0
2	D	17	0	0	0	0
3	A	498	0	0	16	0
3	B	466	0	0	11	0
3	C	339	0	0	12	0
3	D	305	0	0	9	0
All	All	21312	0	18636	143	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 4.

All (143) 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:526:ILE:O	3:A:801:HOH:O	1.97	0.81
1:C:456:GLU:O	3:C:801:HOH:O	2.02	0.77
1:A:530:THR:HG23	3:A:801:HOH:O	1.88	0.74
1:C:459:ARG:N	3:C:801:HOH:O	2.21	0.74
1:D:159:ASN:ND2	3:D:805:HOH:O	2.20	0.73
1:A:342:SER:N	3:A:805:HOH:O	2.22	0.73
1:A:383:TYR:O	3:A:802:HOH:O	2.09	0.70
1:B:219:CYS:SG	3:B:809:HOH:O	2.49	0.70
1:A:564:GLU:OE2	3:A:803:HOH:O	2.10	0.69
1:B:219:CYS:SG	3:B:1257:HOH:O	2.52	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ARG:NH1	1:B:303:THR:OG1	2.28	0.66
1:D:383:TYR:O	3:D:801:HOH:O	2.12	0.66
1:C:274:GLY:N	3:C:808:HOH:O	2.27	0.66
1:B:342:SER:N	3:B:807:HOH:O	2.28	0.66
1:D:646:GLN:OE1	3:D:802:HOH:O	2.14	0.66
1:A:597:ARG:NH1	3:A:813:HOH:O	2.29	0.66
1:A:316:LYS:NZ	3:A:812:HOH:O	2.28	0.65
1:C:646:GLN:OE1	3:C:802:HOH:O	2.15	0.65
1:D:-1:ASN:ND2	3:D:816:HOH:O	2.30	0.64
1:B:518:CYS:SG	3:B:1217:HOH:O	2.56	0.63
1:D:172:ARG:CG	1:D:172:ARG:HH11	2.13	0.62
1:C:369:LYS:NZ	3:C:810:HOH:O	2.29	0.61
1:C:597:ARG:NH1	3:C:813:HOH:O	2.32	0.60
1:C:343:ARG:HD3	1:C:344:ILE:H	1.66	0.60
1:B:568:LYS:NZ	3:B:815:HOH:O	2.35	0.60
1:B:597:ARG:NH1	3:B:814:HOH:O	2.34	0.60
1:C:-1:ASN:N	3:C:815:HOH:O	2.34	0.60
1:A:75:PRO:HD2	1:A:78:LEU:HD12	1.85	0.58
1:D:207:THR:HG21	1:D:508:PRO:HB2	1.85	0.58
1:D:509:GLN:HB3	1:D:511:ARG:HD2	1.86	0.57
1:D:298:ARG:NH1	1:D:303:THR:OG1	2.36	0.57
1:C:383:TYR:O	3:C:803:HOH:O	2.17	0.57
1:D:334:PRO:HB3	1:D:345:ILE:HD11	1.87	0.56
1:A:87:ARG:NH2	1:A:418:GLU:OE2	2.40	0.55
1:C:398:VAL:HG11	1:C:427:GLU:HG3	1.86	0.55
1:C:176:PRO:HG3	1:C:627:PHE:CD2	2.42	0.55
1:D:334:PRO:HG3	1:D:343:ARG:HG3	1.89	0.55
1:D:634:GLU:OE1	3:D:804:HOH:O	2.18	0.54
1:C:488:ARG:NH1	3:C:820:HOH:O	2.40	0.54
1:B:203:ASP:OD2	3:B:801:HOH:O	2.18	0.54
1:C:220:THR:HG22	1:C:316:LYS:HD3	1.90	0.54
1:D:391:ASP:OD1	3:D:803:HOH:O	2.18	0.53
1:A:-1:ASN:ND2	3:A:823:HOH:O	2.40	0.53
1:D:87:ARG:NH1	3:D:820:HOH:O	2.39	0.53
1:B:398:VAL:HG11	1:B:427:GLU:HG3	1.91	0.53
1:A:509:GLN:HB3	1:A:511:ARG:HD2	1.90	0.53
1:B:207:THR:HG21	1:B:508:PRO:HB2	1.90	0.53
1:A:207:THR:HG21	1:A:508:PRO:HB2	1.91	0.52
1:A:144:VAL:HG12	1:A:177:ASN:HD22	1.72	0.52
1:A:398:VAL:HG11	1:A:427:GLU:HG3	1.90	0.52
1:A:459:ARG:NH1	3:A:815:HOH:O	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:GLU:OE2	3:B:802:HOH:O	2.19	0.52
1:D:172:ARG:HH11	1:D:172:ARG:HG3	1.73	0.52
1:A:609:LYS:NZ	3:A:827:HOH:O	2.43	0.52
1:C:74:VAL:HB	1:C:78:LEU:HD21	1.91	0.51
1:D:398:VAL:HG11	1:D:427:GLU:HG3	1.93	0.51
1:D:568:LYS:HG3	1:D:569:PRO:HD2	1.92	0.51
1:B:509:GLN:HB3	1:B:511:ARG:HD2	1.93	0.51
1:A:531:MET:O	1:A:568:LYS:HE3	2.11	0.51
1:C:87:ARG:NH2	1:C:418:GLU:OE2	2.45	0.49
1:C:468:HIS:O	1:C:511:ARG:NH2	2.46	0.48
1:A:212:ASP:OD1	3:A:804:HOH:O	2.20	0.48
1:A:442:TRP:HA	1:A:445:TYR:CD2	2.49	0.48
1:C:74:VAL:HB	1:C:78:LEU:CD2	2.43	0.48
1:B:87:ARG:NH2	1:B:418:GLU:OE2	2.46	0.48
1:D:334:PRO:HG3	1:D:343:ARG:CG	2.43	0.48
1:A:497:ARG:NH1	3:A:809:HOH:O	2.26	0.47
1:C:343:ARG:CD	1:C:344:ILE:H	2.28	0.47
1:A:102:GLN:NE2	3:A:834:HOH:O	2.46	0.47
1:D:590:MET:O	1:D:591:PHE:HB2	2.14	0.47
1:B:531:MET:O	1:B:568:LYS:HE3	2.15	0.47
1:C:225:LEU:HD11	1:C:309:GLU:HB3	1.97	0.46
1:A:590:MET:O	1:A:591:PHE:HB2	2.16	0.46
1:A:479:GLU:HB3	1:A:518:CYS:HB3	1.96	0.46
1:C:176:PRO:HG3	1:C:627:PHE:CE2	2.50	0.46
1:A:631:ILE:HG22	1:D:631:ILE:HG22	1.97	0.46
1:D:152:PHE:HD2	1:D:179:ASP:HB2	1.81	0.46
1:B:442:TRP:HA	1:B:445:TYR:CD2	2.51	0.45
1:B:590:MET:O	1:B:591:PHE:HB2	2.16	0.45
1:D:494:ASP:OD2	3:D:806:HOH:O	2.21	0.45
1:A:529:ARG:HG2	3:A:801:HOH:O	2.16	0.45
1:D:468:HIS:O	1:D:511:ARG:NH2	2.50	0.45
1:B:604:ASN:HA	1:B:607:ILE:HG12	1.98	0.45
1:C:590:MET:O	1:C:591:PHE:HB2	2.16	0.45
1:C:207:THR:HG21	1:C:508:PRO:HB2	1.98	0.45
1:D:465:ASP:HB3	1:D:471:ILE:CD1	2.47	0.45
1:C:278:ARG:NH2	1:C:344:ILE:HD11	2.32	0.45
1:C:298:ARG:NH1	1:C:303:THR:OG1	2.49	0.45
1:A:84:MET:SD	1:A:194:THR:HG22	2.57	0.45
1:C:456:GLU:C	3:C:801:HOH:O	2.53	0.45
1:C:16:ASP:OD2	1:C:189:HIS:ND1	2.28	0.44
1:A:19:TRP:CD1	1:A:46:VAL:HG13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLY:HA3	3:A:1237:HOH:O	2.16	0.44
1:A:412:SER:HA	1:A:413:HIS:HA	1.68	0.44
1:C:479:GLU:HB3	1:C:518:CYS:HB3	1.99	0.44
1:D:75:PRO:HD2	1:D:78:LEU:HD12	2.00	0.44
1:C:601:ALA:HA	1:C:653:TRP:CH2	2.53	0.43
1:D:92:THR:HA	1:D:93:HIS:HA	1.71	0.43
1:C:644:ASP:OD1	3:C:804:HOH:O	2.21	0.43
1:D:232:PHE:HB2	1:D:304:ALA:HB3	2.00	0.43
1:C:37:PRO:HA	1:C:69:GLN:OE1	2.19	0.43
1:D:412:SER:HA	1:D:413:HIS:HA	1.67	0.43
1:C:509:GLN:HB3	1:C:511:ARG:HD2	2.01	0.43
1:B:117:ASP:OD2	3:B:804:HOH:O	2.21	0.43
1:B:140:SER:HB3	1:B:449:LEU:HD23	2.01	0.43
1:B:543:TYR:O	1:C:155:SER:HB2	2.19	0.43
1:A:207:THR:CG2	1:A:508:PRO:HB2	2.48	0.43
1:B:644:ASP:OD1	3:B:803:HOH:O	2.21	0.43
1:C:413:HIS:O	1:C:436:PRO:HA	2.19	0.43
1:D:479:GLU:HB3	1:D:518:CYS:HB3	2.00	0.43
1:D:429:ILE:O	1:D:470:CYS:HB2	2.19	0.42
1:C:79:VAL:HG23	1:C:84:MET:HG3	2.01	0.42
1:D:37:PRO:HA	1:D:69:GLN:OE1	2.19	0.42
1:B:412:SER:HA	1:B:413:HIS:HA	1.69	0.42
1:D:589:GLU:OE2	3:D:807:HOH:O	2.22	0.42
1:C:19:TRP:CD1	1:C:46:VAL:HG13	2.53	0.42
1:B:619:TRP:HA	1:B:620:ASN:HA	1.78	0.42
1:C:412:SER:HA	1:C:413:HIS:HA	1.67	0.42
1:B:19:TRP:CD1	1:B:46:VAL:HG13	2.54	0.42
1:C:92:THR:HA	1:C:93:HIS:HA	1.69	0.42
1:C:604:ASN:HA	1:C:607:ILE:HG12	2.01	0.42
1:C:343:ARG:HD3	1:C:343:ARG:HA	1.84	0.42
1:C:232:PHE:HB2	1:C:304:ALA:HB3	2.03	0.41
1:A:37:PRO:HA	1:A:69:GLN:OE1	2.20	0.41
1:A:581:GLU:OE2	3:A:806:HOH:O	2.22	0.41
1:B:37:PRO:HA	1:B:69:GLN:OE1	2.20	0.41
1:B:232:PHE:HB2	1:B:304:ALA:HB3	2.03	0.41
1:D:140:SER:HB2	1:D:449:LEU:HD23	2.03	0.41
1:A:395:VAL:HA	1:A:423:LEU:HD21	2.01	0.41
1:D:442:TRP:HA	1:D:445:TYR:CD2	2.56	0.41
1:A:92:THR:HA	1:A:93:HIS:HA	1.66	0.41
1:A:633:VAL:HG21	1:D:633:VAL:HG21	2.02	0.41
1:C:468:HIS:HA	1:C:469:PRO:HD2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ASP:OD2	2:B:701:E8X:O4	2.39	0.41
1:C:634:GLU:OE1	3:C:805:HOH:O	2.22	0.41
1:C:198:ASP:O	1:C:235:ASP:N	2.53	0.40
1:C:493:TYR:CZ	1:C:497:ARG:HG3	2.56	0.40
1:B:429:ILE:O	1:B:470:CYS:HB2	2.21	0.40
1:A:78:LEU:HA	1:B:77:ARG:HH12	1.86	0.40
1:B:316:LYS:NZ	3:B:809:HOH:O	2.29	0.40
1:C:275:ARG:HD2	1:C:275:ARG:HA	1.83	0.40
1:D:619:TRP:HA	1:D:620:ASN:HA	1.78	0.40
1:D:95:ALA:HA	1:D:132:ALA:O	2.20	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	612/670 (91%)	595 (97%)	16 (3%)	1 (0%)	47	38
1	B	612/670 (91%)	595 (97%)	17 (3%)	0	100	100
1	C	612/670 (91%)	594 (97%)	16 (3%)	2 (0%)	41	31
1	D	612/670 (91%)	595 (97%)	17 (3%)	0	100	100
All	All	2448/2680 (91%)	2379 (97%)	66 (3%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	383	TYR
1	C	47	PRO
1	A	47	PRO

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	503/543 (93%)	495 (98%)	8 (2%)	62	60
1	B	503/543 (93%)	498 (99%)	5 (1%)	76	76
1	C	503/543 (93%)	493 (98%)	10 (2%)	55	51
1	D	503/543 (93%)	497 (99%)	6 (1%)	71	70
All	All	2012/2172 (93%)	1983 (99%)	29 (1%)	67	65

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	VAL
1	A	152	PHE
1	A	155	SER
1	A	355	ARG
1	A	376	PHE
1	A	511	ARG
1	A	573	THR
1	A	575	TYR
1	B	355	ARG
1	B	376	PHE
1	B	511	ARG
1	B	573	THR
1	B	575	TYR
1	C	77	ARG
1	C	78	LEU
1	C	155	SER
1	C	343	ARG
1	C	355	ARG
1	C	376	PHE
1	C	511	ARG
1	C	573	THR
1	C	575	TYR
1	C	645	ARG
1	D	172	ARG

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Mol	Chain	Res	Type
1	D	355	ARG
1	D	376	PHE
1	D	511	ARG
1	D	573	THR
1	D	575	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	177	ASN
1	C	169	HIS
1	D	82	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	E8X	A	701	-	14,17,17	0.61	0	12,22,22	1.73	1 (8%)
2	E8X	D	701	-	14,17,17	0.65	0	12,22,22	1.62	2 (16%)
2	E8X	C	701	-	14,17,17	0.65	0	12,22,22	1.62	2 (16%)
2	E8X	B	701	-	14,17,17	0.58	0	12,22,22	1.67	1 (8%)

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	E8X	A	701	-	-	2/6/27/27	0/1/1/1
2	E8X	D	701	-	-	2/6/27/27	0/1/1/1
2	E8X	C	701	-	-	1/6/27/27	0/1/1/1
2	E8X	B	701	-	-	2/6/27/27	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	E8X	C2-N-C7	5.43	121.36	109.61
2	B	701	E8X	C2-N-C7	5.21	120.89	109.61
2	C	701	E8X	C2-N-C7	4.93	120.27	109.61
2	D	701	E8X	C2-N-C7	4.91	120.22	109.61
2	C	701	E8X	C9-C8-C7	-2.22	109.41	113.93
2	D	701	E8X	C9-C8-C7	-2.05	109.74	113.93

There are no chirality outliers.

All (7) torsion outliers are listed below:

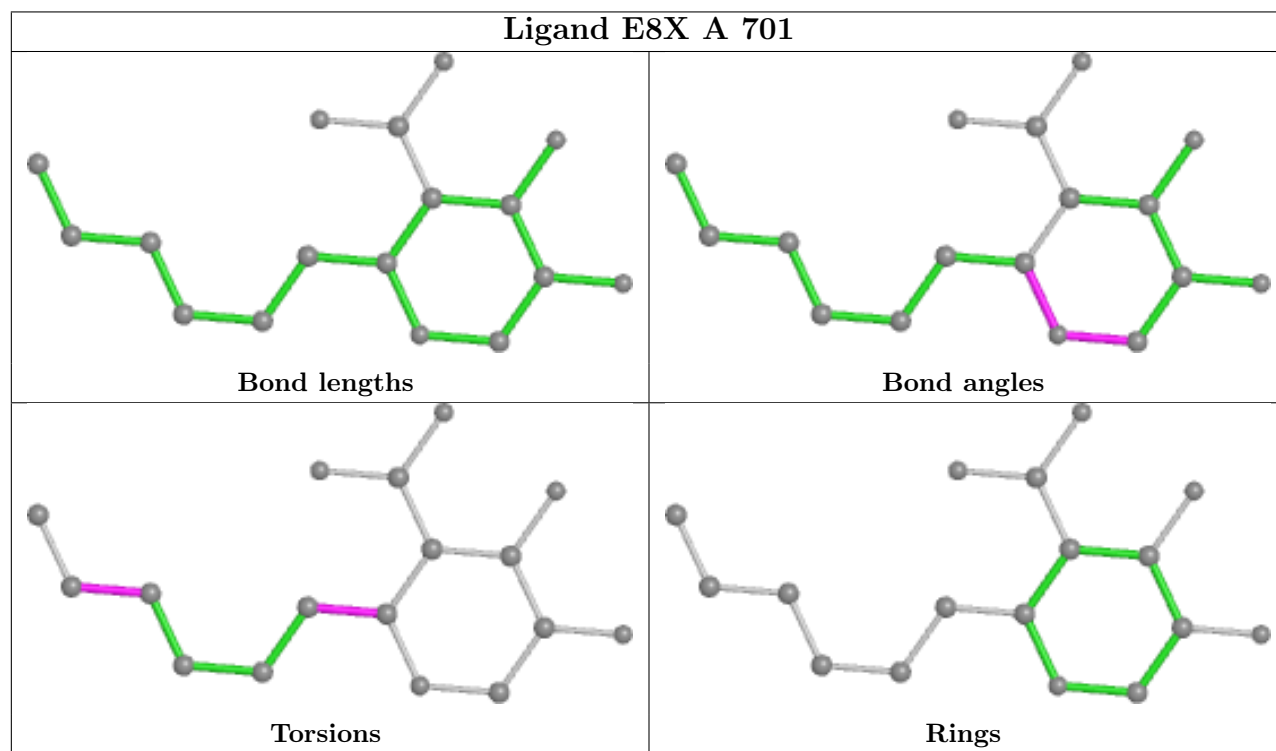
Mol	Chain	Res	Type	Atoms
2	C	701	E8X	N-C7-C8-C9
2	D	701	E8X	N-C7-C8-C9
2	A	701	E8X	N-C7-C8-C9
2	B	701	E8X	N-C7-C8-C9
2	B	701	E8X	C10-C11-C12-C13
2	D	701	E8X	C5-C7-C8-C9
2	A	701	E8X	C10-C11-C12-C13

There are no ring outliers.

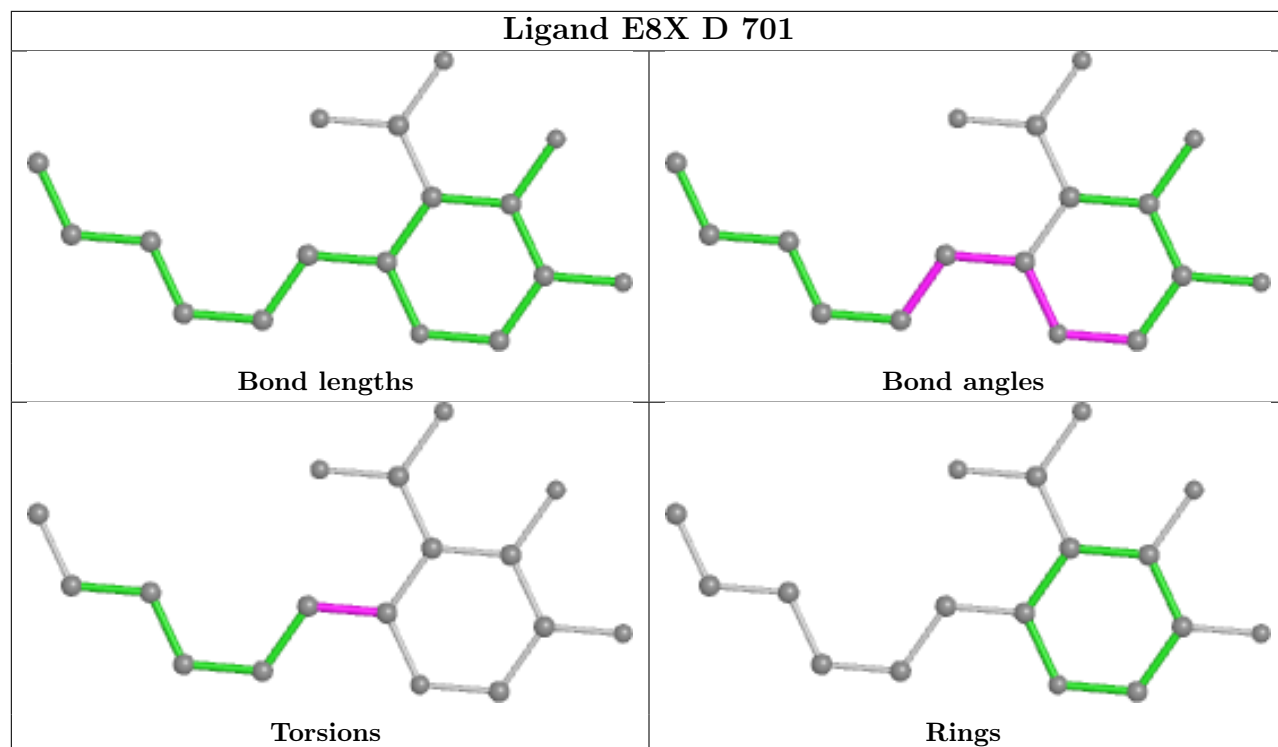
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	E8X	1	0

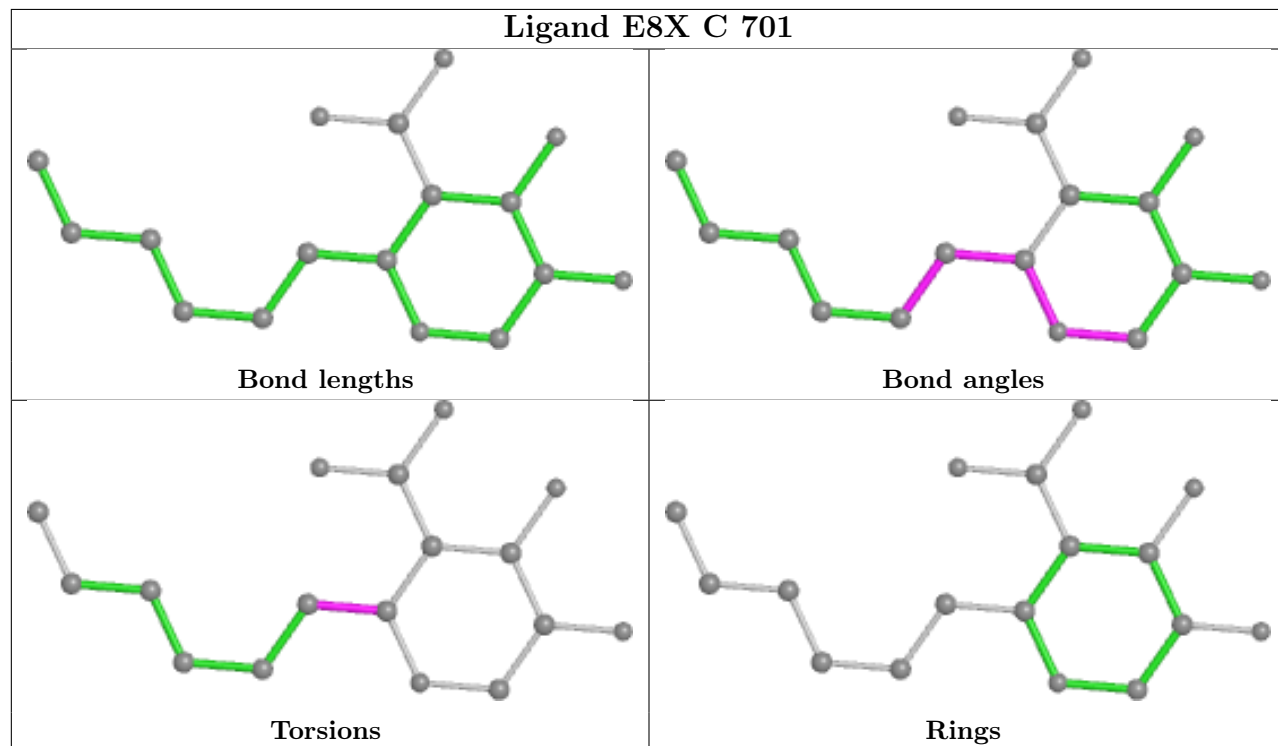
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

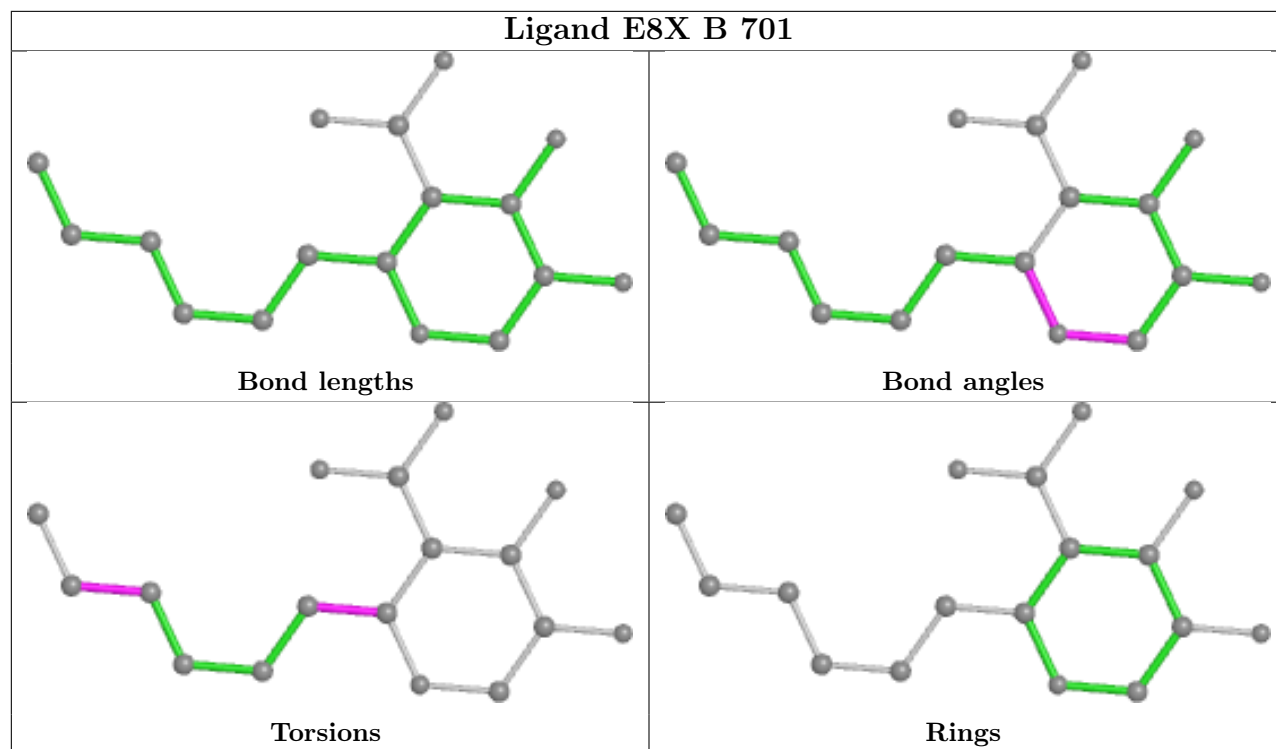


Ligand E8X D 701



Ligand E8X C 701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	620/670 (92%)	-0.09	23 (3%)	41	44	10, 20, 46, 140	0
1	B	620/670 (92%)	-0.02	25 (4%)	38	41	11, 21, 47, 134	0
1	C	620/670 (92%)	0.18	42 (6%)	17	19	14, 30, 59, 153	0
1	D	620/670 (92%)	0.20	36 (5%)	23	25	13, 32, 60, 124	0
All	All	2480/2680 (92%)	0.07	126 (5%)	28	31	10, 26, 54, 153	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	152	PHE	14.2
1	B	154	GLY	12.7
1	B	152	PHE	12.0
1	C	151	ALA	11.9
1	B	149	GLY	10.0
1	B	151	ALA	10.0
1	D	154	GLY	9.9
1	C	148	ALA	9.6
1	C	153	MET	9.6
1	D	149	GLY	9.2
1	D	148	ALA	8.9
1	D	150	THR	8.7
1	B	150	THR	8.6
1	B	157	ASN	8.4
1	A	151	ALA	8.0
1	A	148	ALA	8.0
1	C	154	GLY	7.9
1	A	152	PHE	7.4
1	C	150	THR	7.4
1	D	155	SER	7.1
1	A	150	THR	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLY	6.4
1	A	303	THR	6.4
1	C	303	THR	6.4
1	D	153	MET	6.2
1	B	148	ALA	6.0
1	B	155	SER	6.0
1	D	152	PHE	5.8
1	B	153	MET	5.7
1	D	151	ALA	5.7
1	C	343	ARG	5.7
1	D	-1	ASN	5.6
1	D	343	ARG	5.6
1	C	155	SER	5.4
1	C	149	GLY	5.3
1	B	159	ASN	5.1
1	B	303	THR	5.1
1	A	154	GLY	5.1
1	B	156	ASP	5.0
1	A	274	GLY	5.0
1	D	156	ASP	5.0
1	A	155	SER	4.7
1	A	156	ASP	4.7
1	C	158	ALA	4.7
1	C	298	ARG	4.5
1	D	303	THR	4.4
1	D	274	GLY	4.4
1	D	298	ARG	4.4
1	A	153	MET	4.4
1	D	159	ASN	4.3
1	B	158	ALA	4.2
1	C	274	GLY	4.2
1	B	342	SER	4.2
1	C	156	ASP	4.1
1	C	342	SER	4.0
1	C	157	ASN	4.0
1	D	342	SER	3.9
1	D	216	GLY	3.8
1	D	297	GLU	3.8
1	B	298	ARG	3.8
1	C	159	ASN	3.7
1	A	157	ASN	3.6
1	D	158	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	157	ASN	3.6
1	C	285	GLU	3.5
1	C	235	ASP	3.4
1	A	298	ARG	3.4
1	C	-1	ASN	3.4
1	C	198	ASP	3.4
1	C	234	GLY	3.3
1	A	343	ARG	3.3
1	A	159	ASN	3.3
1	D	78	LEU	3.3
1	C	297	GLU	3.2
1	D	285	GLU	3.2
1	D	235	ASP	3.2
1	D	234	GLY	3.2
1	D	313	ARG	3.2
1	C	216	GLY	3.2
1	B	343	ARG	3.1
1	D	295	ASP	3.0
1	B	235	ASP	3.0
1	D	334	PRO	3.0
1	D	487	GLU	2.9
1	D	8	ASP	2.8
1	B	109	GLY	2.8
1	A	297	GLU	2.8
1	C	79	VAL	2.8
1	C	77	ARG	2.7
1	D	0	GLY	2.7
1	A	109	GLY	2.7
1	B	274	GLY	2.7
1	C	78	LEU	2.7
1	C	27	ASP	2.6
1	C	169	HIS	2.6
1	A	78	LEU	2.6
1	A	342	SER	2.6
1	D	565	ASN	2.6
1	C	295	ASP	2.6
1	B	169	HIS	2.6
1	C	485	ASP	2.6
1	B	-1	ASN	2.5
1	D	485	ASP	2.5
1	C	565	ASN	2.4
1	B	297	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	125	GLY	2.3
1	A	235	ASP	2.3
1	C	334	PRO	2.3
1	C	313	ARG	2.3
1	A	165	GLU	2.2
1	B	108	PHE	2.2
1	B	485	ASP	2.2
1	C	147	ASP	2.2
1	C	40	GLU	2.2
1	C	102	GLN	2.2
1	A	198	ASP	2.2
1	C	165	GLU	2.1
1	C	344	ILE	2.1
1	D	102	GLN	2.1
1	C	304	ALA	2.1
1	C	213	HIS	2.1
1	C	284	GLY	2.1
1	D	198	ASP	2.1
1	A	172	ARG	2.0
1	D	344	ILE	2.0
1	B	285	GLU	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	E8X	C	701	17/17	0.94	0.12	20,23,40,41	0
2	E8X	B	701	17/17	0.95	0.12	13,21,37,38	0

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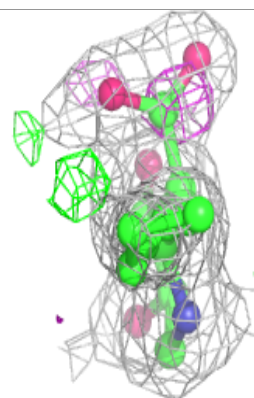
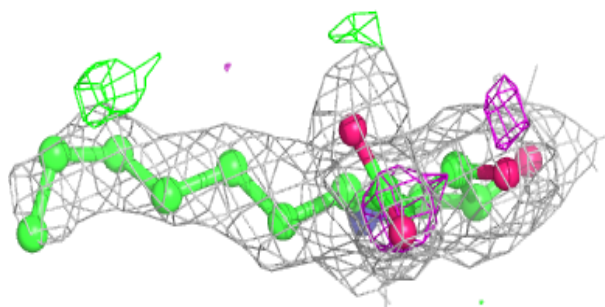
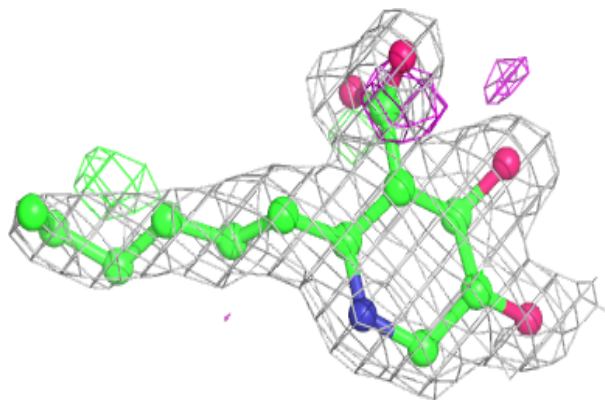
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	E8X	D	701	17/17	0.95	0.12	20,24,33,34	0
2	E8X	A	701	17/17	0.96	0.11	16,22,33,36	0

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.

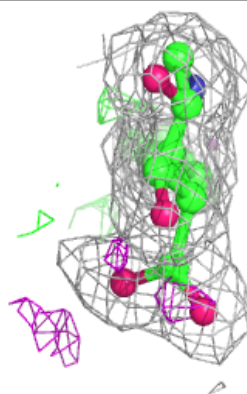
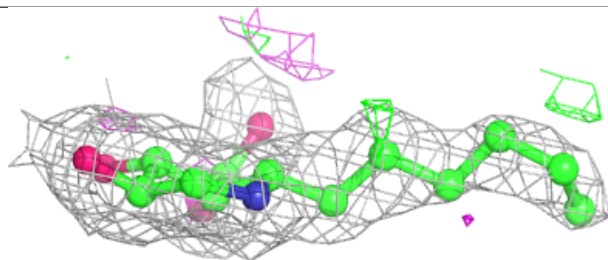
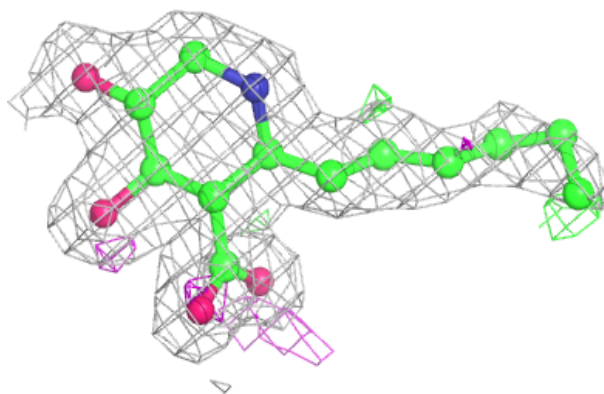
Electron density around E8X C 701:

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

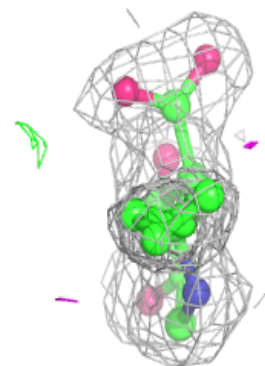
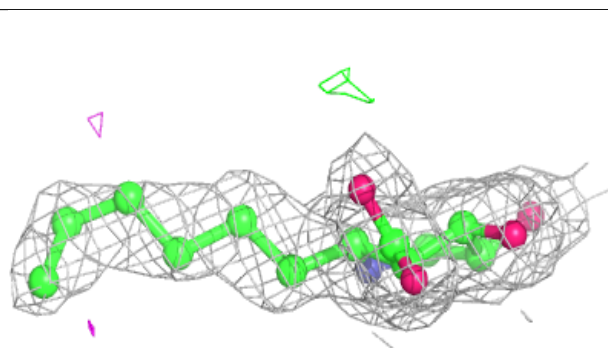
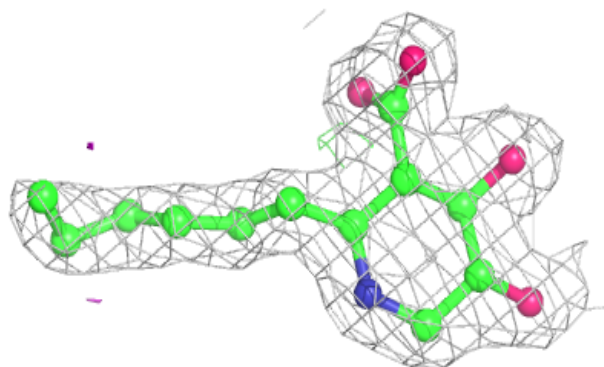


Electron density around E8X B 701:

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

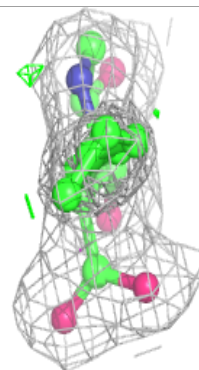
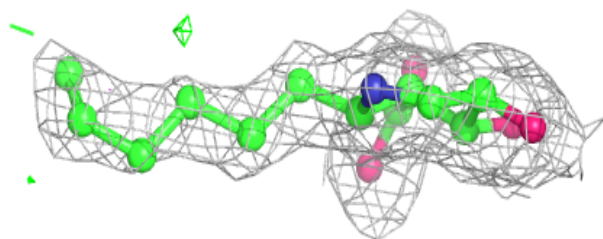
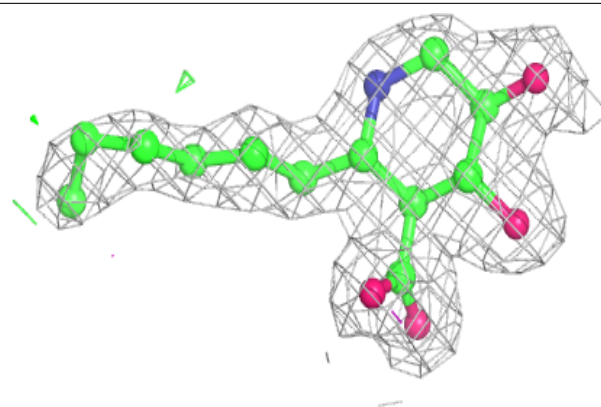
**Electron density around E8X D 701:**

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



Electron density around E8X A 701:

$2mF_o-DF_c$ (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.