



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 02:46 PM BST

PDB ID : 1YAE  
Title : Structure of the Kainate Receptor Subunit GluR6 Agonist Binding Domain  
Complexed with Domoic Acid  
Authors : Nanao, M.H.; Green, T.; Stern-Bach, Y.; Heinemann, S.F.; Choe, S.  
Deposited on : 2004-12-17  
Resolution : 3.11 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

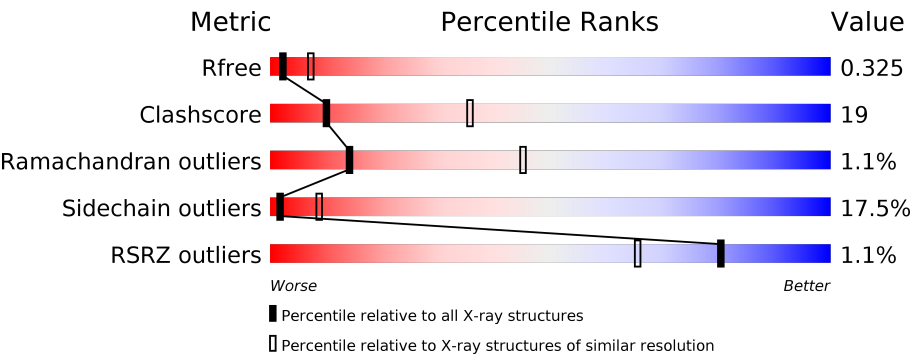
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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  $\geq 3$ , 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	312	
1	B	312	
1	C	312	
1	D	312	
1	E	312	
1	F	312	

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Mol	Chain	Length	Quality of chain
2	G	2	 100%

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
2	NAG	G	1	X	-	-	-
4	NAG	C	1302	X	-	-	-
4	NAG	D	1401	X	-	-	-
4	NAG	D	1402	X	-	-	-
4	NAG	E	1502	X	-	-	X
4	NAG	F	1601	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12512 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 Glutamate receptor, ionotropic kainate 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2079	1324	346	397	12			
1	B	261	Total	C	N	O	S	0	0	0
			2082	1325	347	398	12			
1	C	257	Total	C	N	O	S	0	0	0
			2053	1309	341	392	11			
1	D	259	Total	C	N	O	S	0	0	0
			2067	1316	344	395	12			
1	E	257	Total	C	N	O	S	0	0	0
			2056	1312	341	392	11			
1	F	226	Total	C	N	O	S	0	0	0
			1815	1163	297	344	11			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	653	GLY	-	linker	GB 56280
A	654	GLY	-	linker	GB 56280
A	655	SER	-	linker	GB 56280
A	656	LEU	-	linker	GB 56280
A	657	VAL	-	linker	GB 56280
A	658	PRO	-	linker	GB 56280
A	659	ARG	-	linker	GB 56280
A	660	GLY	-	linker	GB 56280
A	661	SER	-	linker	GB 56280
B	653	GLY	-	linker	GB 56280
B	654	GLY	-	linker	GB 56280
B	655	SER	-	linker	GB 56280
B	656	LEU	-	linker	GB 56280
B	657	VAL	-	linker	GB 56280
B	658	PRO	-	linker	GB 56280
B	659	ARG	-	linker	GB 56280
B	660	GLY	-	linker	GB 56280

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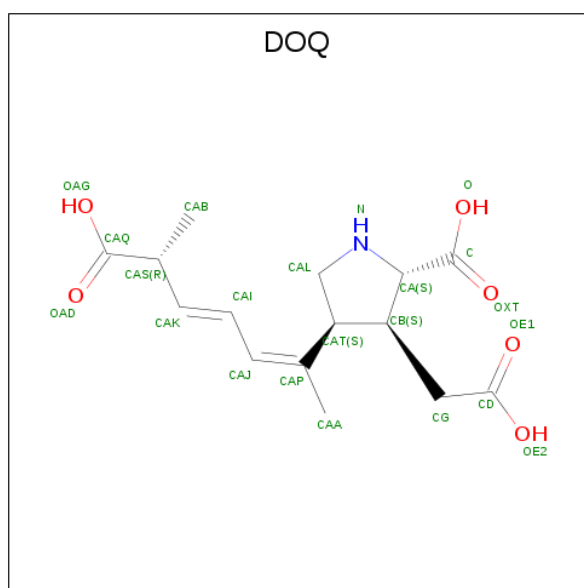
Chain	Residue	Modelled	Actual	Comment	Reference
B	661	SER	-	linker	GB 56280
C	653	GLY	-	linker	GB 56280
C	654	GLY	-	linker	GB 56280
C	655	SER	-	linker	GB 56280
C	656	LEU	-	linker	GB 56280
C	657	VAL	-	linker	GB 56280
C	658	PRO	-	linker	GB 56280
C	659	ARG	-	linker	GB 56280
C	660	GLY	-	linker	GB 56280
C	661	SER	-	linker	GB 56280
D	653	GLY	-	linker	GB 56280
D	654	GLY	-	linker	GB 56280
D	655	SER	-	linker	GB 56280
D	656	LEU	-	linker	GB 56280
D	657	VAL	-	linker	GB 56280
D	658	PRO	-	linker	GB 56280
D	659	ARG	-	linker	GB 56280
D	660	GLY	-	linker	GB 56280
D	661	SER	-	linker	GB 56280
E	653	GLY	-	linker	GB 56280
E	654	GLY	-	linker	GB 56280
E	655	SER	-	linker	GB 56280
E	656	LEU	-	linker	GB 56280
E	657	VAL	-	linker	GB 56280
E	658	PRO	-	linker	GB 56280
E	659	ARG	-	linker	GB 56280
E	660	GLY	-	linker	GB 56280
E	661	SER	-	linker	GB 56280
F	653	GLY	-	linker	GB 56280
F	654	GLY	-	linker	GB 56280
F	655	SER	-	linker	GB 56280
F	656	LEU	-	linker	GB 56280
F	657	VAL	-	linker	GB 56280
F	658	PRO	-	linker	GB 56280
F	659	ARG	-	linker	GB 56280
F	660	GLY	-	linker	GB 56280
F	661	SER	-	linker	GB 56280

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 3 is (2S,3S,4S)-2-CARBOXY-4-[(1Z,3E,5R)-5-CARBOXY-1-METHYL-1,3-HEXADIENYL]-3-PYRROLIDINEACETIC ACID (three-letter code: DOQ) (formula: C<sub>15</sub>H<sub>21</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	15	1	6		
3	B	1	Total	C	N	O	0	0
			22	15	1	6		
3	C	1	Total	C	N	O	0	0
			22	15	1	6		
3	D	1	Total	C	N	O	0	0
			22	15	1	6		
3	E	1	Total	C	N	O	0	0
			22	15	1	6		
3	F	1	Total	C	N	O	0	0
			22	15	1	6		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	19	Total	O	0	0
			19	19		
5	C	14	Total	O	0	0
			14	14		

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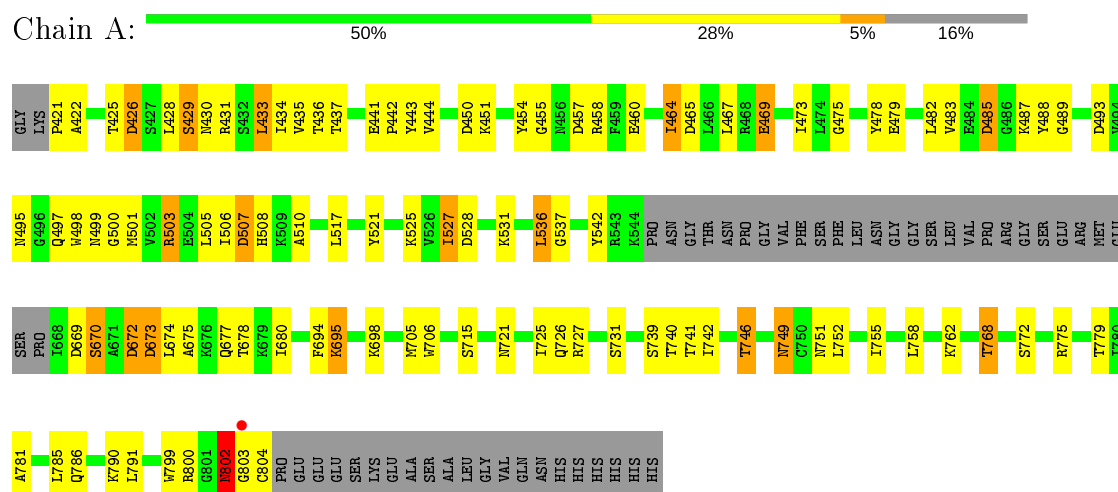
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	16	Total 16	O 16	0	0
5	E	9	Total 9	O 9	0	0
5	F	7	Total 7	O 7	0	0



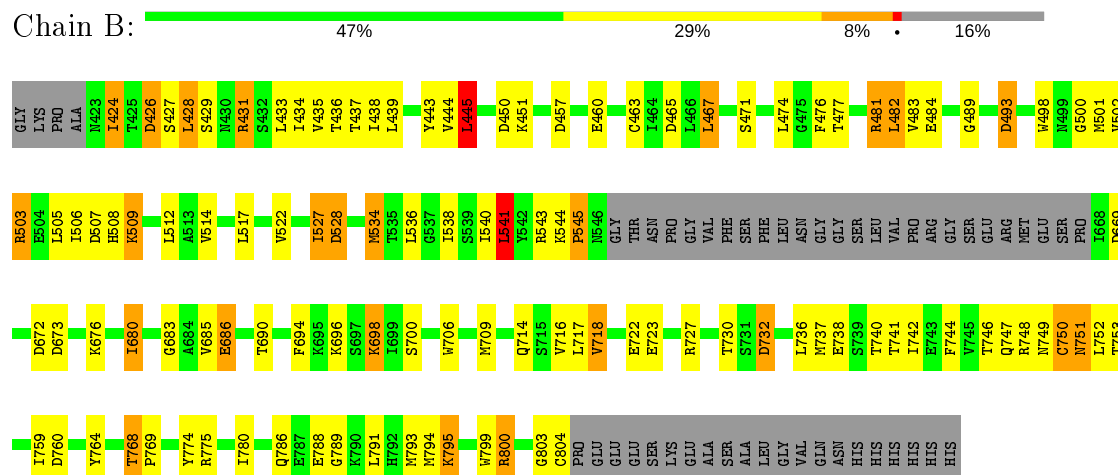
### 3 Residue-property plots

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

- Molecule 1: Glutamate receptor, ionotropic kainate 2

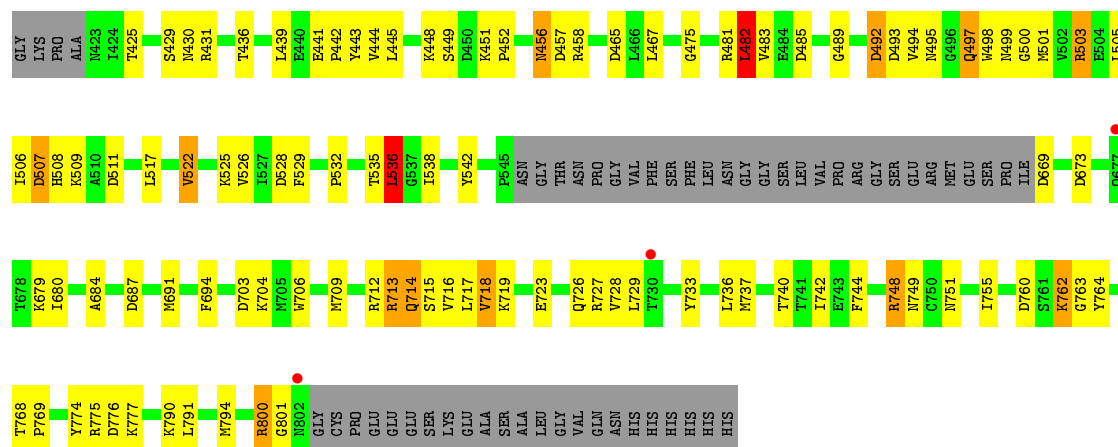


- Molecule 1: Glutamate receptor, ionotropic kainate 2

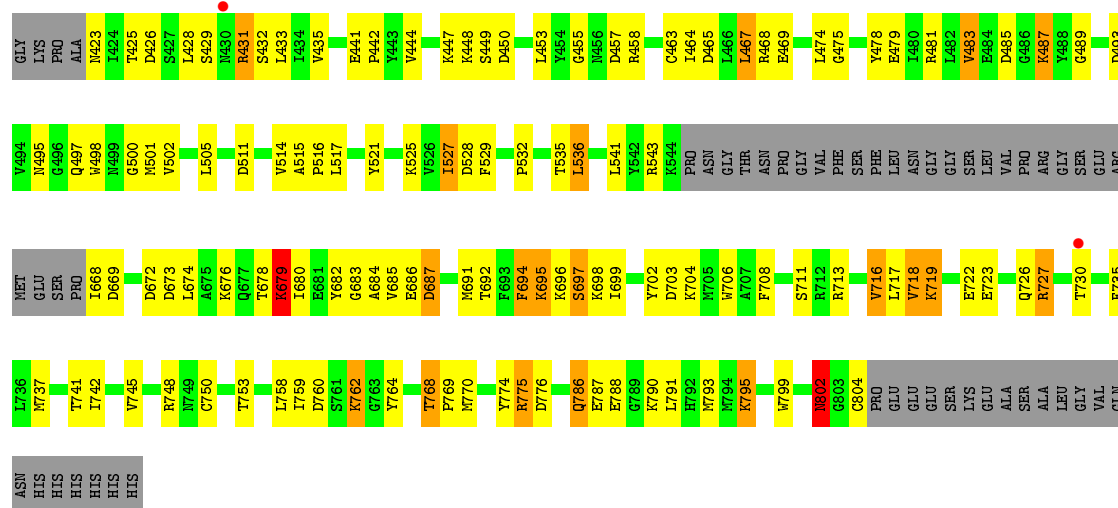
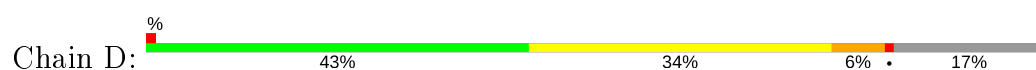


- Molecule 1: Glutamate receptor, ionotropic kainate 2

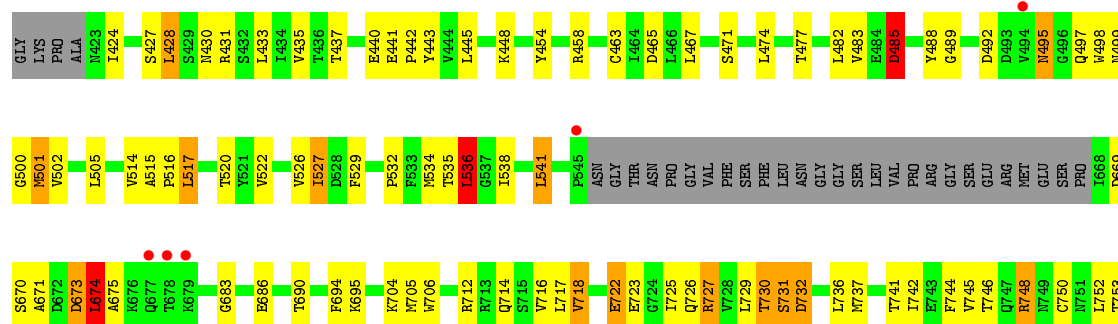




- Molecule 1: Glutamate receptor, ionotropic kainate 2

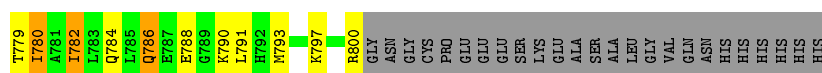
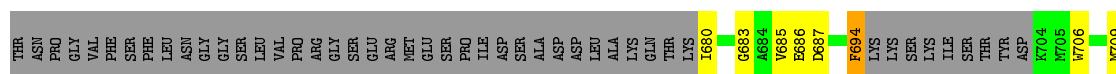
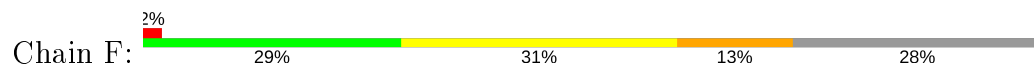


- Molecule 1: Glutamate receptor, ionotropic kainate 2





- Molecule 1: Glutamate receptor, ionotropic kainate 2



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	246.36Å 106.57Å 172.69Å 90.00° 133.19° 90.00°	Depositor
Resolution (Å)	45.00 – 3.11 44.49 – 3.11	Depositor EDS
% Data completeness (in resolution range)	94.3 (45.00-3.11) 94.4 (44.49-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.275 , 0.334 0.269 , 0.325	Depositor DCC
$R_{free}$ test set	2819 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.4	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.006 for h+2*l,k,-h-l 0.008 for h,-k,-h-l 0.021 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	12512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: DOQ, NAG, FUC

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	0.47	0/2116	0.83	6/2850 (0.2%)
1	B	0.46	0/2119	0.87	10/2855 (0.4%)
1	C	0.46	0/2090	0.85	10/2816 (0.4%)
1	D	0.58	2/2103 (0.1%)	0.87	11/2832 (0.4%)
1	E	0.51	0/2093	0.85	8/2820 (0.3%)
1	F	0.63	0/1845	0.86	4/2482 (0.2%)
All	All	0.52	2/12366 (0.0%)	0.86	49/16655 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	697	SER	CB-OG	-11.88	1.26	1.42
1	D	696	LYS	CB-CG	7.02	1.71	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	545	PRO	CA-N-CD	-12.18	94.44	111.50
1	B	732	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	493	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	694	PHE	CB-CG-CD1	-6.05	116.57	120.80
1	D	750	CYS	CA-CB-SG	-5.97	103.25	114.00

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	2079	0	2084	66	0
1	B	2082	0	2082	90	0
1	C	2053	0	2054	57	0
1	D	2067	0	2069	71	0
1	E	2056	0	2065	79	0
1	F	1815	0	1809	121	0
2	G	24	0	22	1	0
3	A	22	0	18	2	0
3	B	22	0	18	2	0
3	C	22	0	18	0	0
3	D	22	0	18	1	0
3	E	22	0	18	1	0
3	F	22	0	18	2	0
4	B	28	0	26	3	0
4	C	28	0	26	0	0
4	D	28	0	26	2	0
4	E	28	0	26	0	0
4	F	14	0	13	1	0
5	A	13	0	0	0	0
5	B	19	0	0	0	0
5	C	14	0	0	1	0
5	D	16	0	0	1	0
5	E	9	0	0	1	0
5	F	7	0	0	3	0
All	All	12512	0	12410	473	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 19.

The worst 5 of 473 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:F:498:TRP:CE3	1:F:502:VAL:HG11	1.66	1.28
1:F:506:ILE:HD13	1:F:506:ILE:C	1.67	1.11
1:E:727:ARG:HG2	1:E:727:ARG:HH11	1.18	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:498:TRP:HE3	1:F:502:VAL:HG11	0.99	1.08
1:F:447:LYS:HG2	1:F:460:GLU:HG3	1.40	1.01

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	257/312 (82%)	234 (91%)	21 (8%)	2 (1%)	19	53
1	B	257/312 (82%)	239 (93%)	17 (7%)	1 (0%)	34	68
1	C	253/312 (81%)	239 (94%)	13 (5%)	1 (0%)	34	68
1	D	255/312 (82%)	235 (92%)	17 (7%)	3 (1%)	13	43
1	E	253/312 (81%)	230 (91%)	21 (8%)	2 (1%)	19	53
1	F	214/312 (69%)	186 (87%)	21 (10%)	7 (3%)	4	20
All	All	1489/1872 (80%)	1363 (92%)	110 (7%)	16 (1%)	14	45

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	802	ASN
1	F	430	ASN
1	E	771	GLY
1	F	427	SER
1	F	429	SER

### 5.3.2 Protein sidechains [i](#)

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	228/270 (84%)	197 (86%)	31 (14%)	3	16
1	B	229/270 (85%)	190 (83%)	39 (17%)	2	9
1	C	225/270 (83%)	193 (86%)	32 (14%)	3	14
1	D	227/270 (84%)	186 (82%)	41 (18%)	1	8
1	E	226/270 (84%)	185 (82%)	41 (18%)	1	8
1	F	199/270 (74%)	149 (75%)	50 (25%)	0	2
All	All	1334/1620 (82%)	1100 (82%)	234 (18%)	2	9

5 of 234 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	433	LEU
1	D	719	LYS
1	F	687	ASP
1	D	467	LEU
1	D	672	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	491	GLN
1	C	714	GLN
1	F	491	GLN
1	C	456	ASN
1	F	497	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

2 monosaccharides 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	NAG	G	1	1,2	14,14,15	0.53	0	17,19,21	1.38	1 (5%)
2	FUC	G	2	2	10,10,11	0.78	0	14,14,16	1.88	5 (35%)

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	NAG	G	1	1,2	1/1/5/7	4/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-O5-C5	4.71	118.58	112.19
2	G	2	FUC	C1-C2-C3	4.20	114.83	109.67
2	G	2	FUC	O5-C5-C4	2.76	114.47	109.52
2	G	2	FUC	C2-C3-C4	2.71	115.58	110.89
2	G	2	FUC	C3-C4-C5	2.59	113.81	109.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NAG	C1

All (4) torsion outliers are listed below:

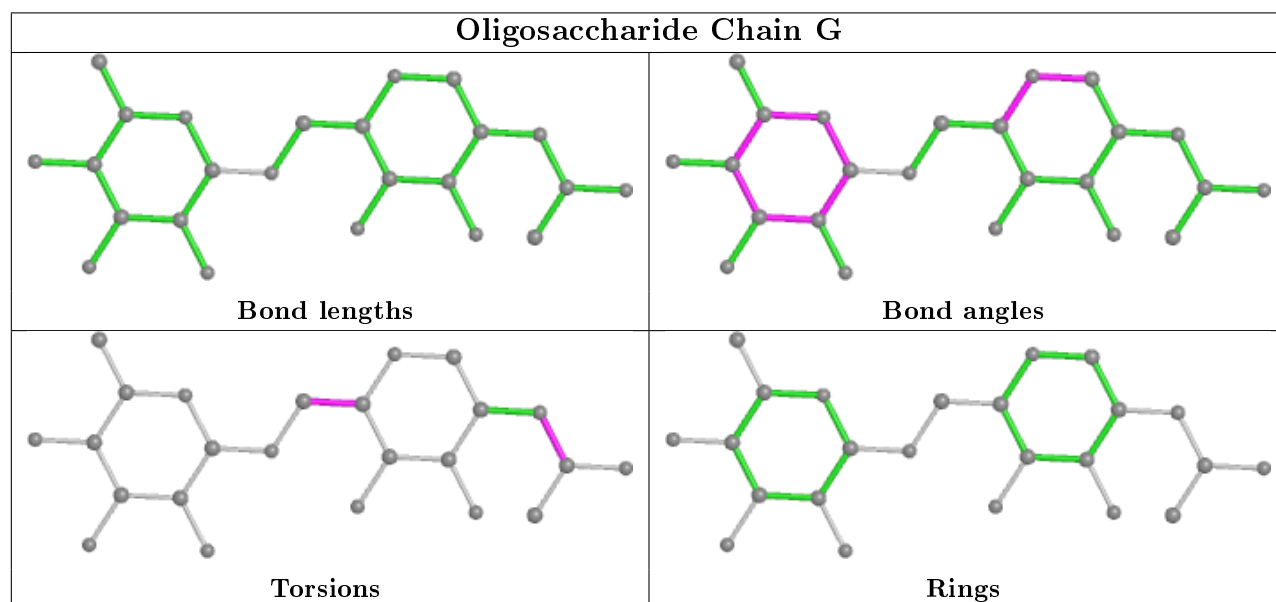
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	FUC	1	0
2	G	1	NAG	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 oligosaccharide.



## 5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DOQ	C	1303	-	10,22,22	2.82	3 (30%)	11,30,30	1.79	2 (18%)
3	DOQ	B	1203	-	10,22,22	2.32	2 (20%)	11,30,30	2.35	4 (36%)
3	DOQ	E	1503	-	10,22,22	2.57	4 (40%)	11,30,30	2.29	4 (36%)
3	DOQ	D	1403	-	10,22,22	2.78	3 (30%)	11,30,30	2.29	3 (27%)
4	NAG	B	1202	1	14,14,15	0.57	0	17,19,21	1.75	2 (11%)
4	NAG	C	1302	1	14,14,15	0.71	1 (7%)	17,19,21	1.46	4 (23%)
3	DOQ	F	1603	-	10,22,22	2.48	3 (30%)	11,30,30	2.19	5 (45%)
4	NAG	D	1402	1	14,14,15	0.68	0	17,19,21	1.29	1 (5%)
4	NAG	E	1501	1	14,14,15	0.70	0	17,19,21	1.58	4 (23%)
4	NAG	D	1401	1	14,14,15	0.54	0	17,19,21	1.60	3 (17%)
3	DOQ	A	1103	-	10,22,22	2.28	2 (20%)	11,30,30	2.22	5 (45%)
4	NAG	B	1201	1	14,14,15	0.80	1 (7%)	17,19,21	1.52	3 (17%)
4	NAG	E	1502	1	14,14,15	0.86	0	17,19,21	1.51	3 (17%)
4	NAG	C	1301	1	14,14,15	0.73	0	17,19,21	2.10	4 (23%)
4	NAG	F	1601	1	14,14,15	0.54	0	17,19,21	1.23	1 (5%)

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
4	NAG	B	1202	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1201	1	-	2/6/23/26	0/1/1/1
3	DOQ	C	1303	-	-	7/12/35/35	0/1/1/1
3	DOQ	B	1203	-	-	2/12/35/35	0/1/1/1
3	DOQ	E	1503	-	-	2/12/35/35	0/1/1/1
3	DOQ	D	1403	-	-	2/12/35/35	0/1/1/1
4	NAG	D	1402	1	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	E	1502	1	1/1/5/7	5/6/23/26	0/1/1/1
3	DOQ	F	1603	-	-	7/12/35/35	0/1/1/1
4	NAG	D	1401	1	1/1/5/7	4/6/23/26	0/1/1/1
3	DOQ	A	1103	-	-	5/12/35/35	0/1/1/1
4	NAG	F	1601	1	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	C	1302	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1501	1	-	4/6/23/26	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1403	DOQ	CAJ-CAP	7.74	1.40	1.33
3	C	1303	DOQ	CAJ-CAP	7.70	1.40	1.33
3	E	1503	DOQ	CAJ-CAP	6.79	1.40	1.33
3	B	1203	DOQ	CAJ-CAP	6.57	1.39	1.33
3	F	1603	DOQ	CAJ-CAP	6.48	1.39	1.33

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1202	NAG	C1-O5-C5	5.86	120.13	112.19
3	D	1403	DOQ	CAA-CAP-CAJ	-5.65	117.05	124.03
3	E	1503	DOQ	CAA-CAP-CAJ	-4.67	118.27	124.03
3	B	1203	DOQ	CAA-CAP-CAJ	-4.57	118.39	124.03
3	E	1503	DOQ	CAI-CAJ-CAP	-4.46	120.77	127.32

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	1302	NAG	C1
4	D	1402	NAG	C1
4	D	1401	NAG	C1
4	E	1502	NAG	C1
4	F	1601	NAG	C1

5 of 57 torsion outliers are listed below:

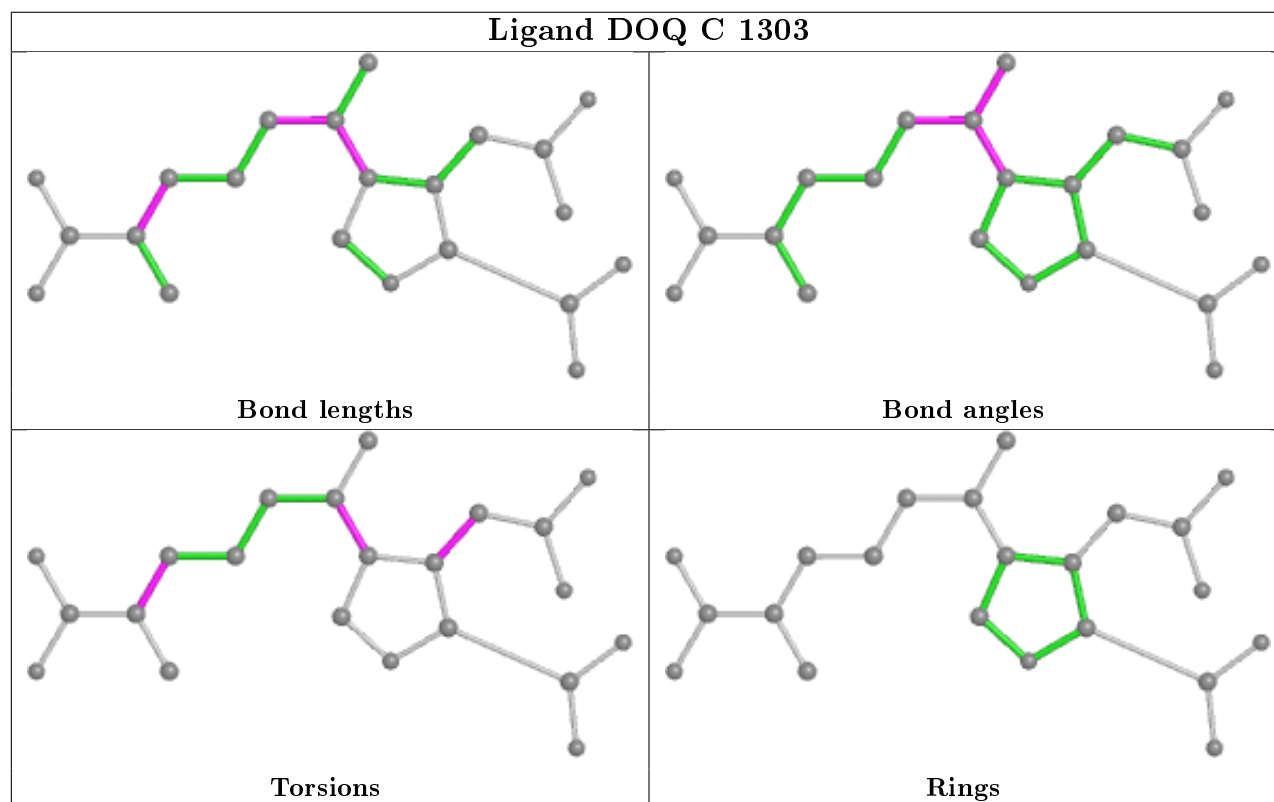
Mol	Chain	Res	Type	Atoms
3	F	1603	DOQ	CAT-CB-CG-CD
3	F	1603	DOQ	CA-CB-CG-CD
3	C	1303	DOQ	CAT-CB-CG-CD
3	C	1303	DOQ	CA-CB-CG-CD
3	A	1103	DOQ	CAI-CAK-CAS-CAB

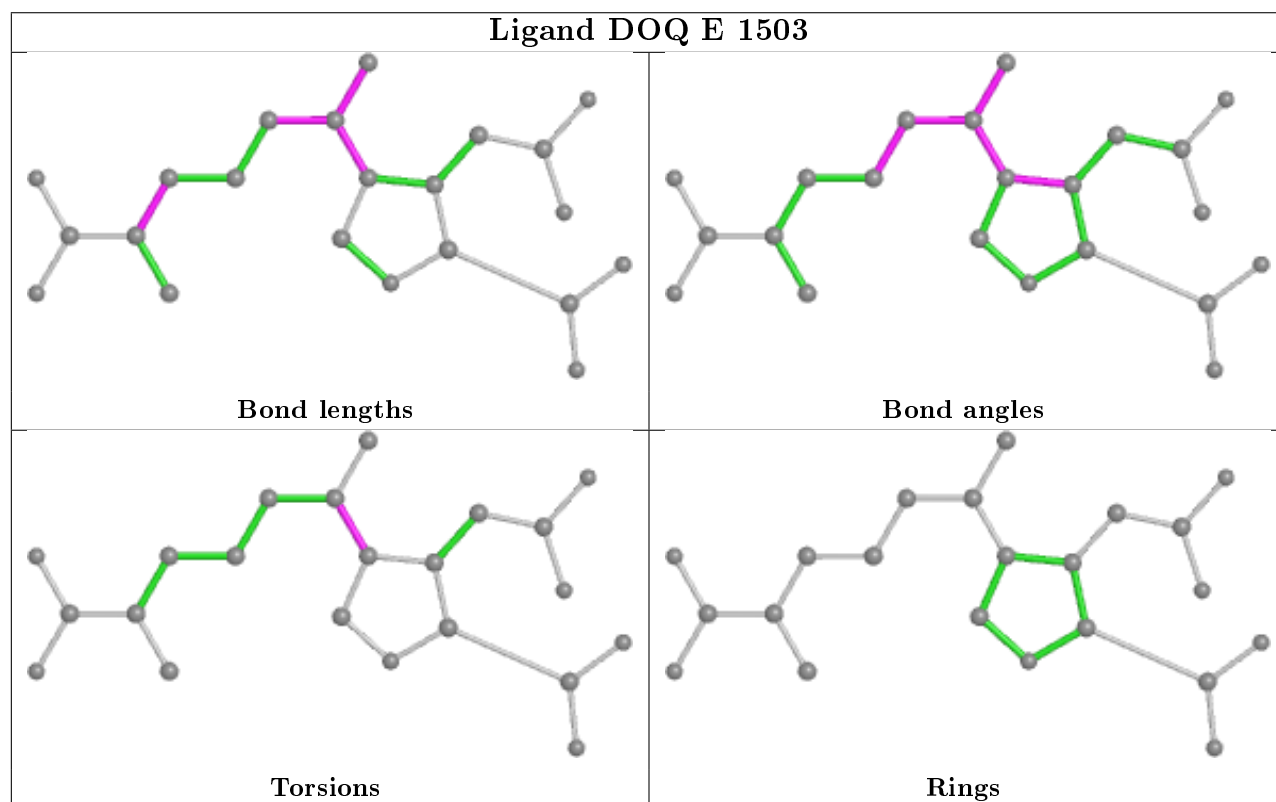
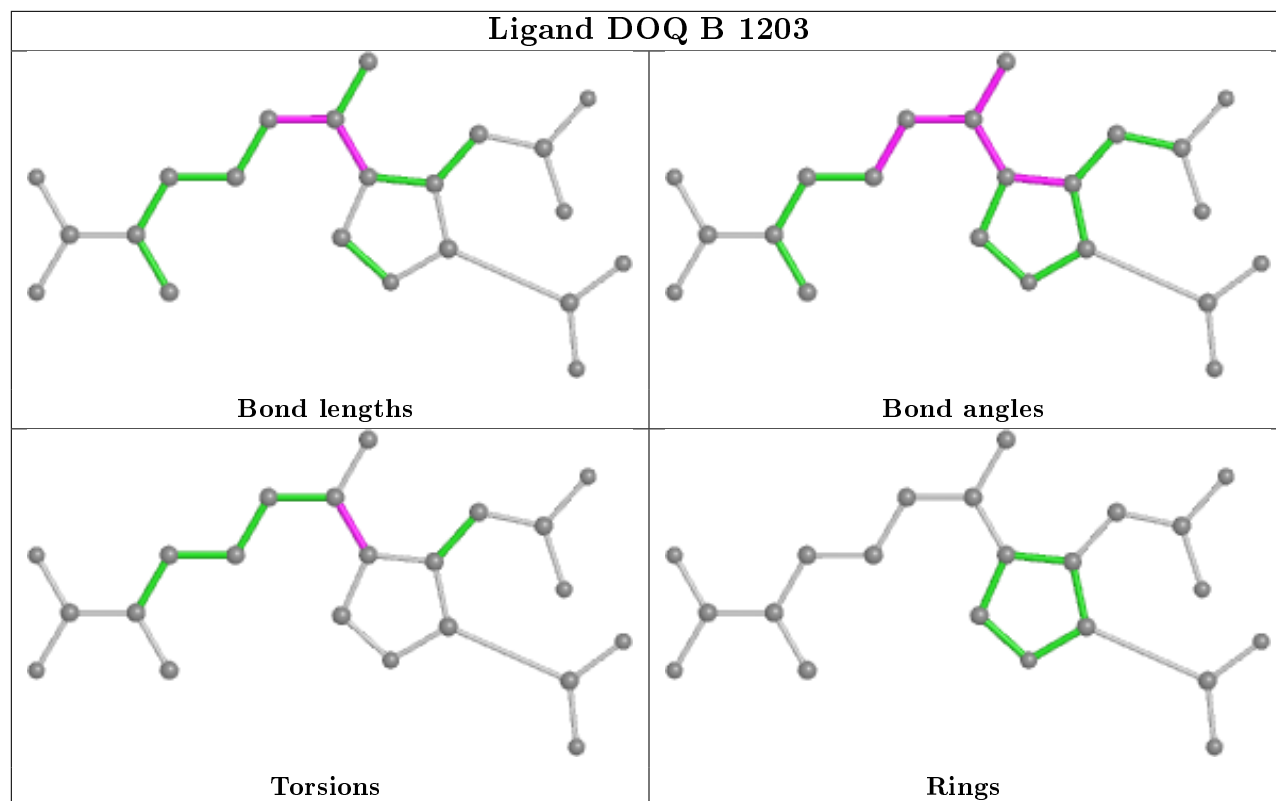
There are no ring outliers.

8 monomers are involved in 14 short contacts:

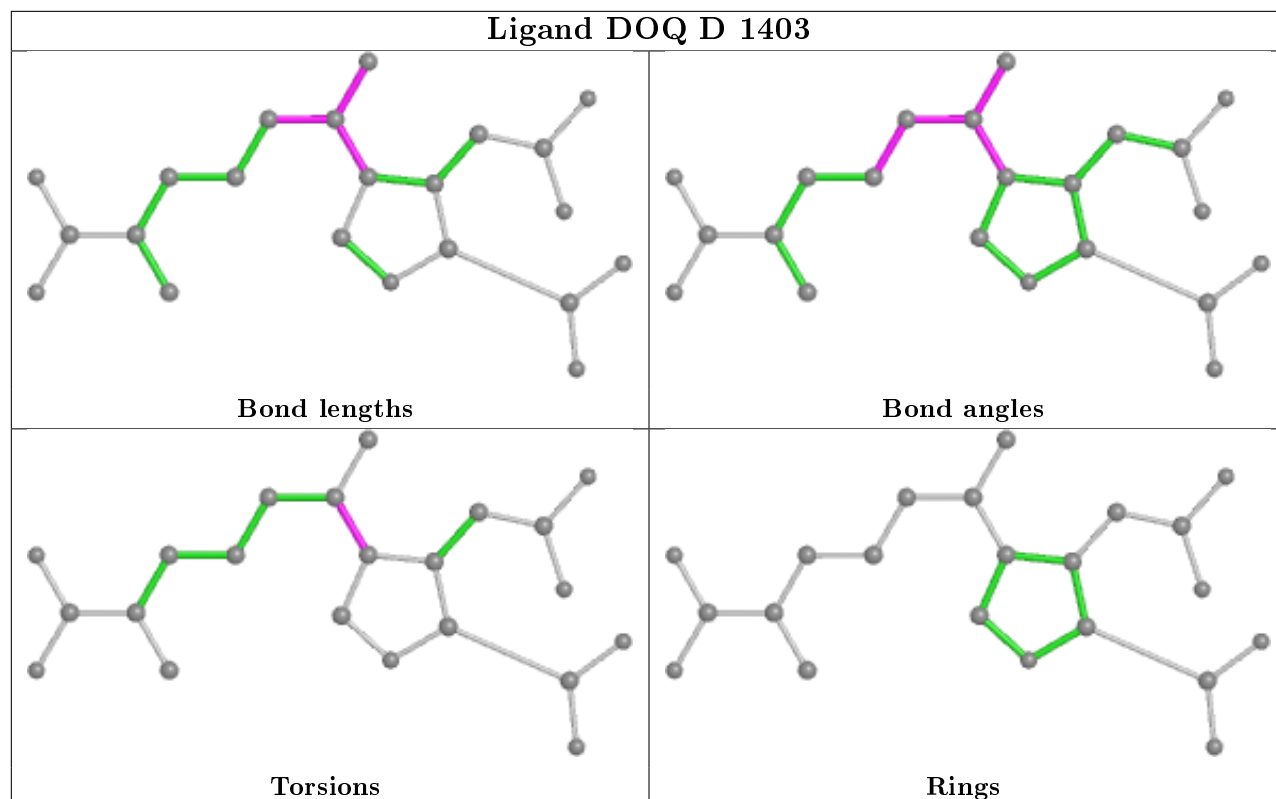
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1203	DOQ	2	0
3	E	1503	DOQ	1	0
3	D	1403	DOQ	1	0
4	B	1202	NAG	3	0
3	F	1603	DOQ	2	0
4	D	1402	NAG	2	0
3	A	1103	DOQ	2	0
4	F	1601	NAG	1	0

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.

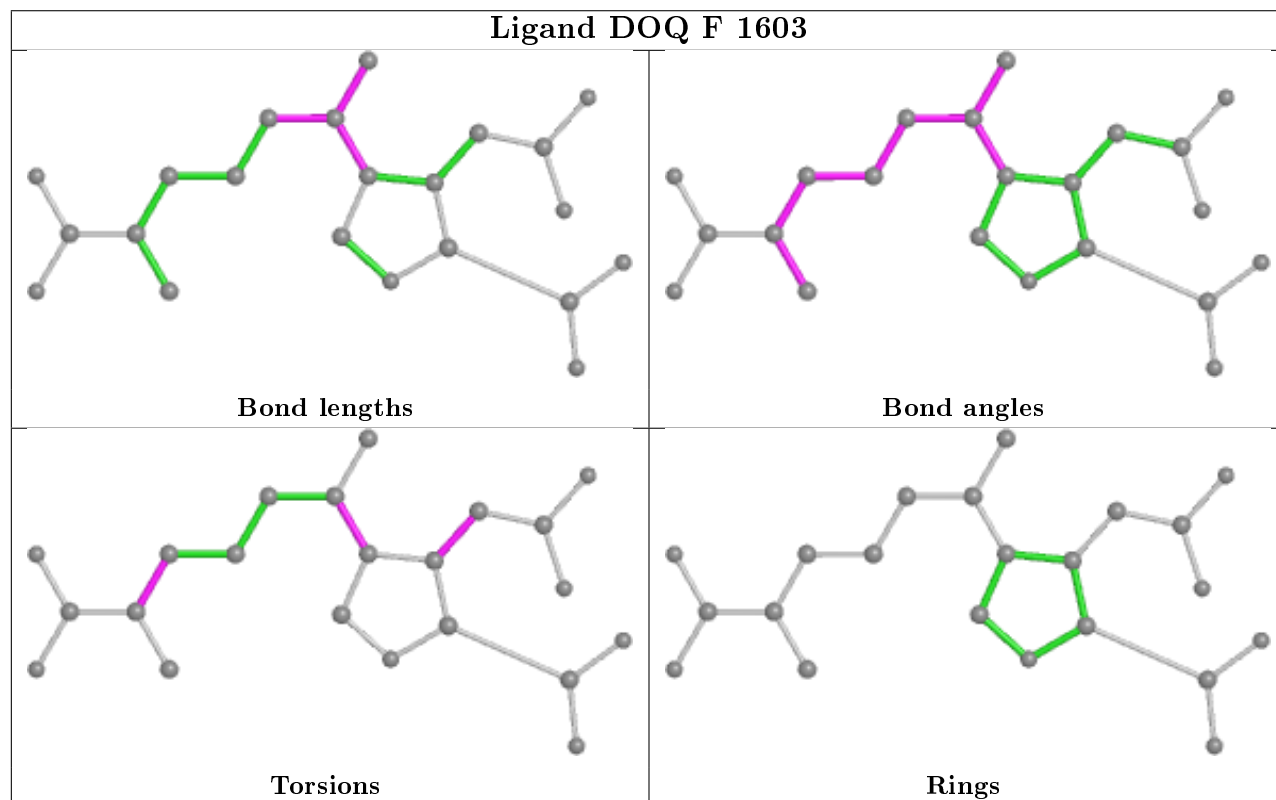


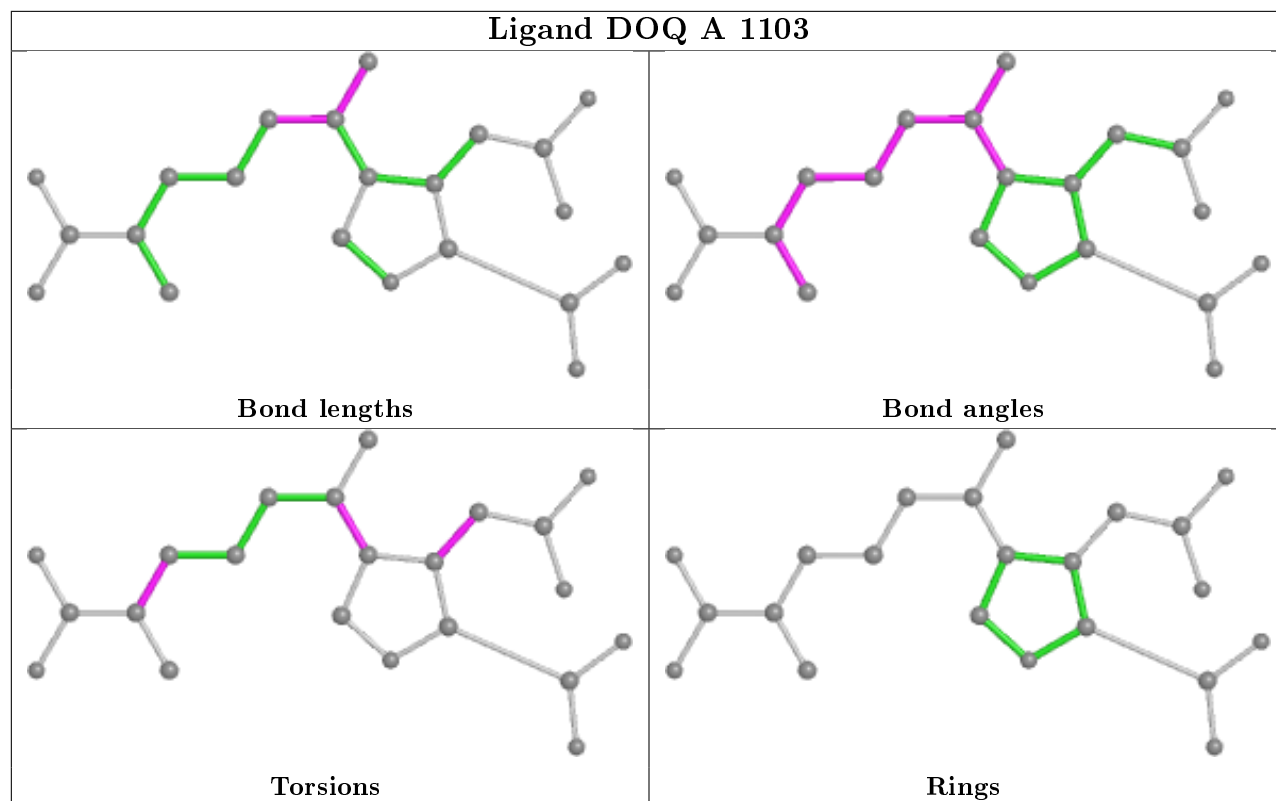


## Ligand DOQ D 1403



## Ligand DOQ F 1603





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	261/312 (83%)	-0.08	1 (0%) 92 85	24, 58, 73, 77	0
1	B	261/312 (83%)	-0.06	0 100 100	24, 57, 74, 79	0
1	C	257/312 (82%)	-0.05	3 (1%) 79 63	26, 58, 77, 86	0
1	D	259/312 (83%)	-0.05	2 (0%) 86 74	25, 58, 73, 79	0
1	E	257/312 (82%)	0.03	6 (2%) 60 39	26, 58, 81, 93	0
1	F	226/312 (72%)	0.06	5 (2%) 62 41	46, 58, 74, 79	0
All	All	1521/1872 (81%)	-0.03	17 (1%) 80 65	24, 58, 75, 93	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	677	GLN	3.2
1	E	678	THR	3.1
1	E	545	PRO	3.0
1	C	730	THR	2.7
1	E	679	LYS	2.6

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

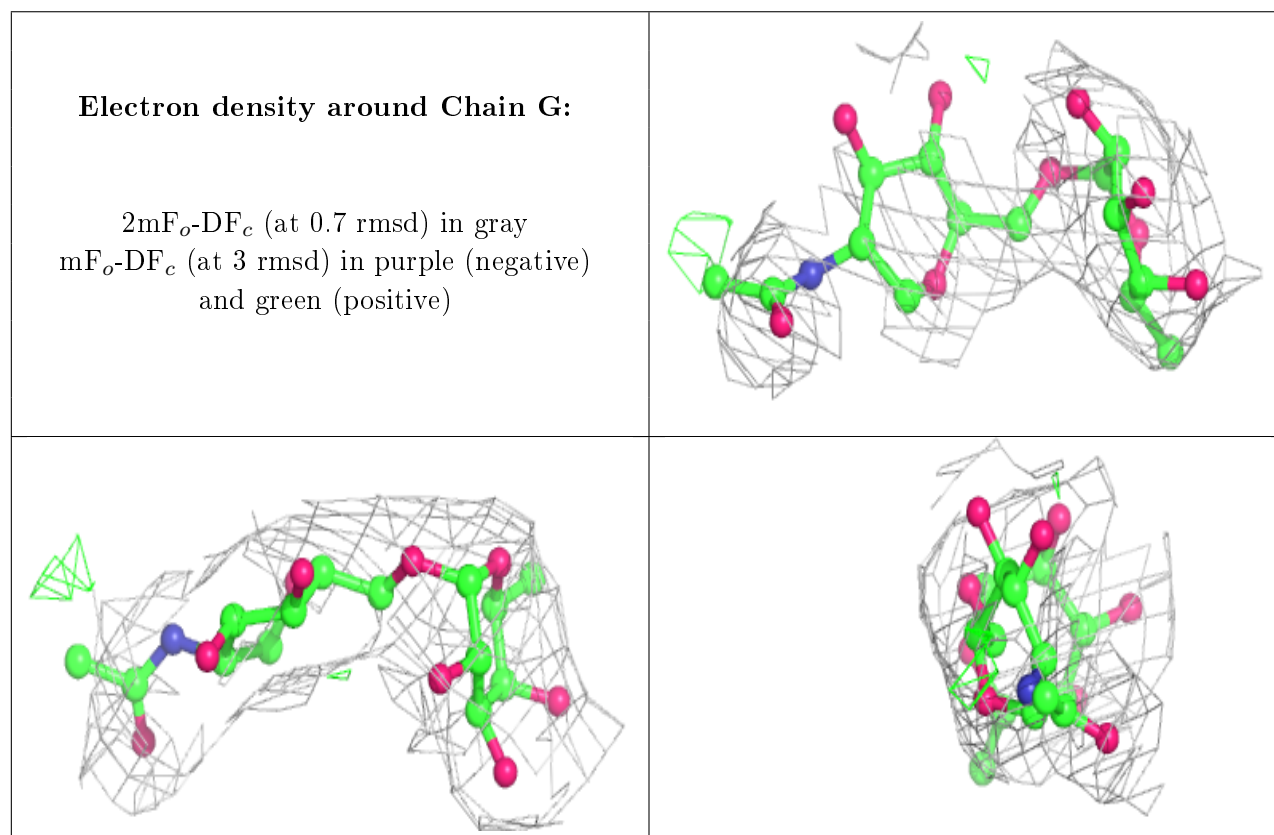
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	G	1	14/15	0.83	0.18	78,79,80,80	0
2	FUC	G	2	10/11	0.89	0.30	81,82,82,82	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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.

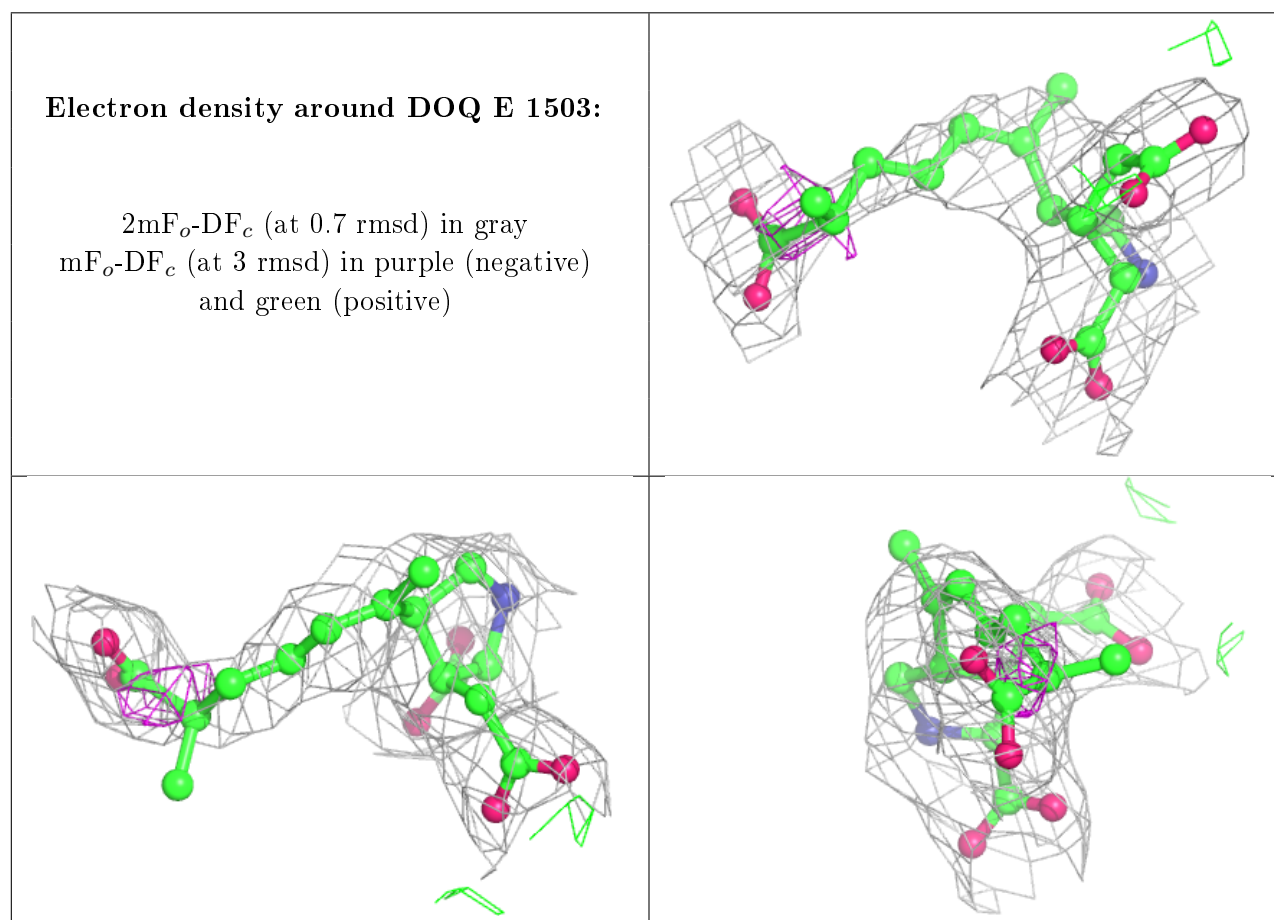
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	E	1501	14/15	0.69	0.33	85,87,88,88	0
4	NAG	E	1502	14/15	0.72	0.44	84,86,88,88	0
4	NAG	C	1301	14/15	0.78	0.22	82,84,85,85	0
4	NAG	F	1601	14/15	0.80	0.31	88,90,91,92	0
4	NAG	C	1302	14/15	0.81	0.36	85,88,89,90	0
4	NAG	D	1401	14/15	0.81	0.34	84,87,87,88	0
4	NAG	B	1202	14/15	0.81	0.37	81,82,85,85	0

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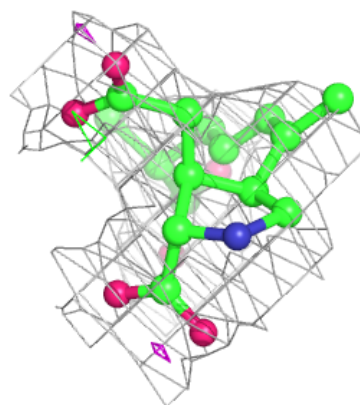
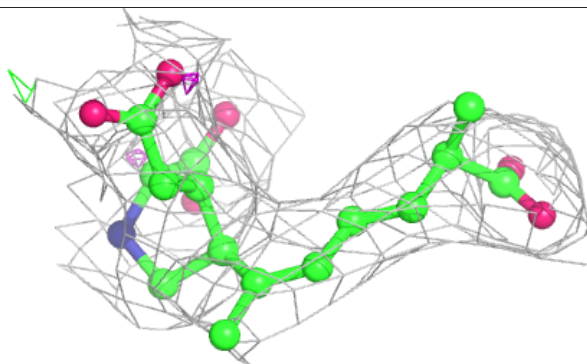
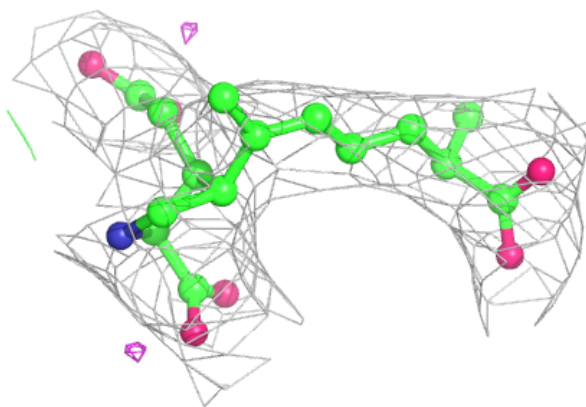
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	1201	14/15	0.82	0.26	79,80,81,81	0
4	NAG	D	1402	14/15	0.83	0.34	83,85,87,87	0
3	DOQ	E	1503	22/22	0.88	0.27	50,53,58,59	0
3	DOQ	D	1403	22/22	0.92	0.20	41,42,44,44	0
3	DOQ	F	1603	22/22	0.93	0.20	59,60,62,64	0
3	DOQ	B	1203	22/22	0.95	0.21	33,35,37,38	0
3	DOQ	C	1303	22/22	0.95	0.19	42,44,48,49	0
3	DOQ	A	1103	22/22	0.96	0.20	35,36,41,42	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.



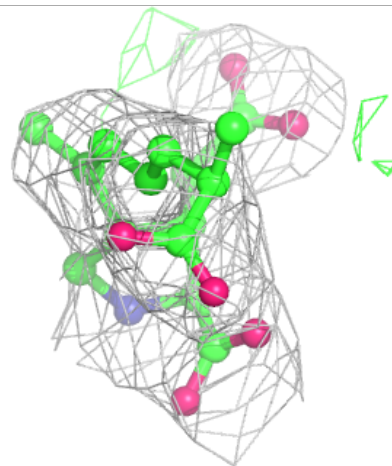
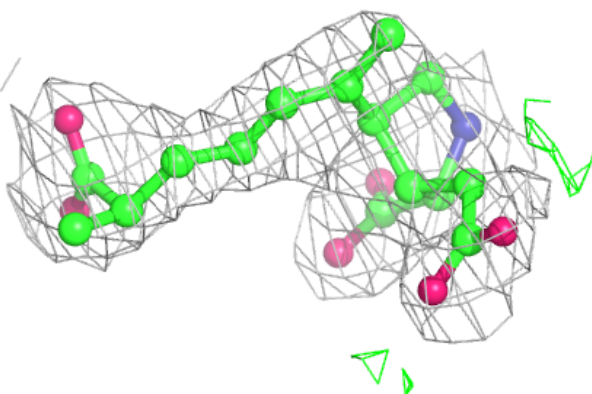
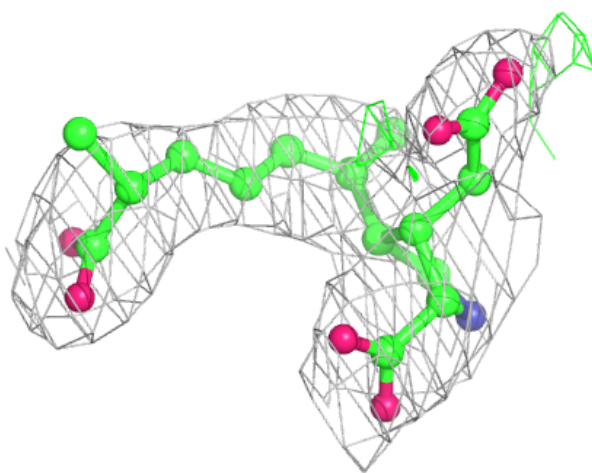
**Electron density around DOQ D 1403:**

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



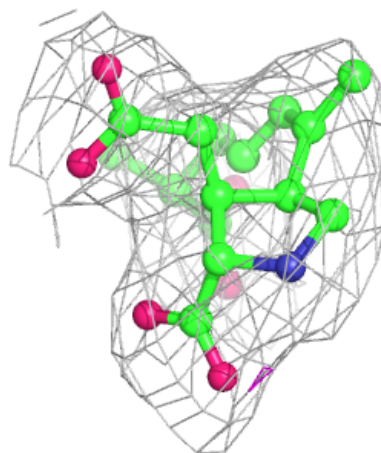
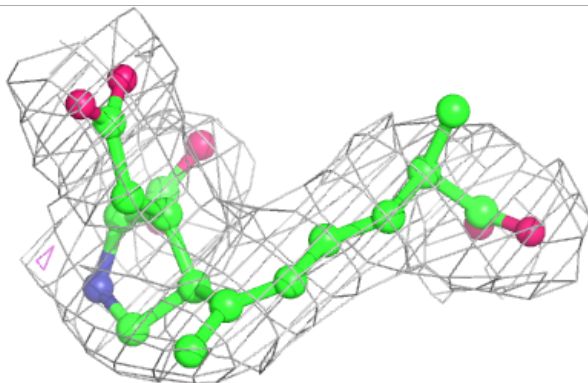
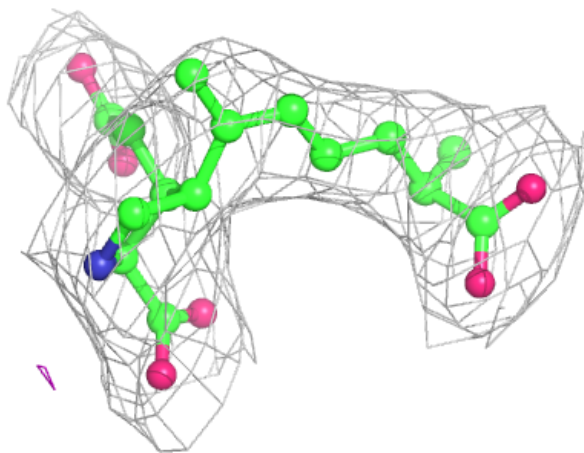
**Electron density around DOQ F 1603:**

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



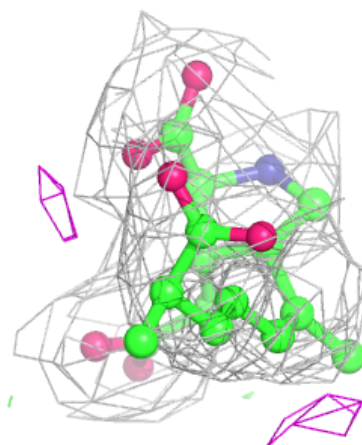
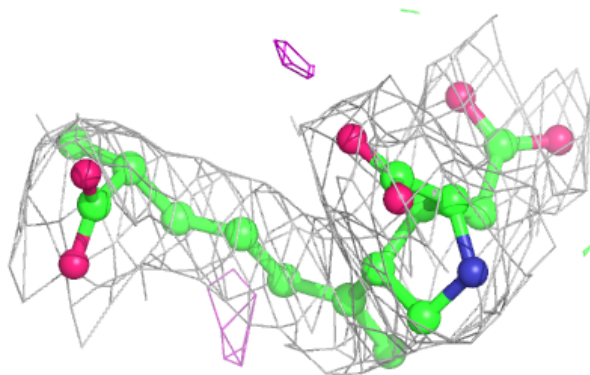
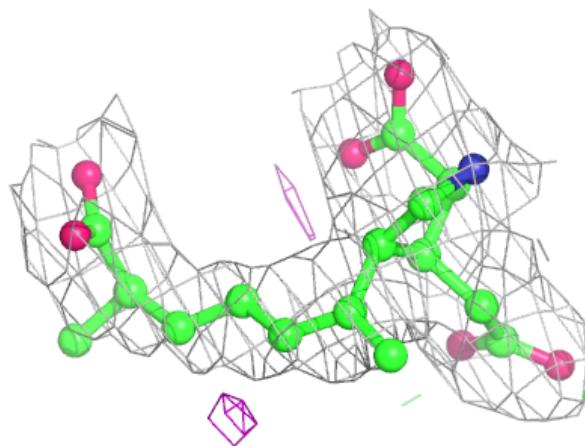
**Electron density around DOQ B 1203:**

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



**Electron density around DOQ C 1303:**

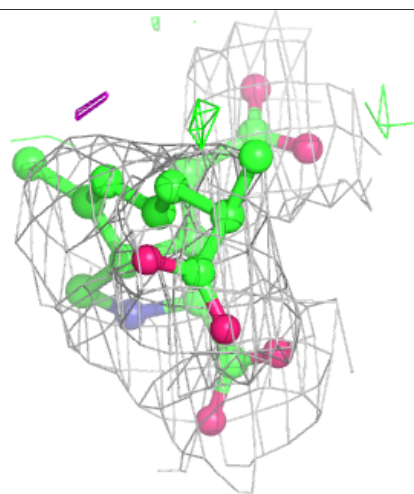
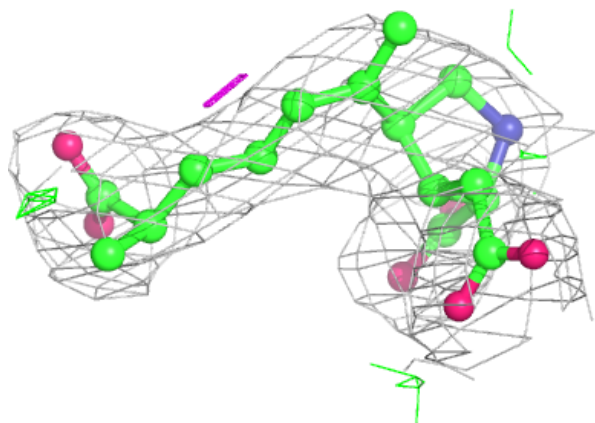
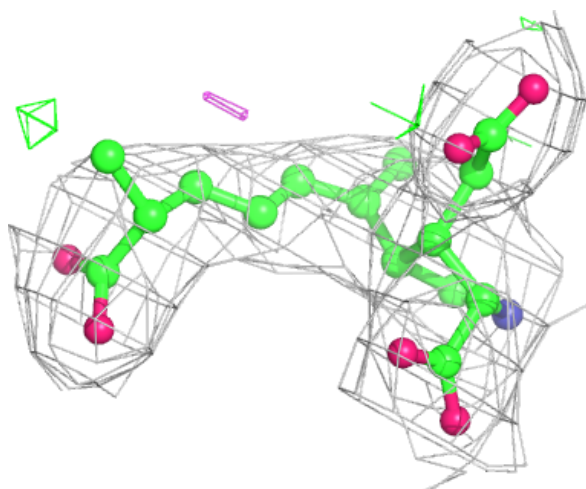
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around DOQ A 1103:**

$2mF_o-DF_c$  (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.