



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2021 – 10:02 PM EST

PDB ID : 6UYG
Title : Structure of Hepatitis C Virus Envelope Glycoprotein E2c3 core from genotype 6a bound to broadly neutralizing antibody AR3A and non neutralizing antibody E1
Authors : Tzarum, N.; Wilson, I.A.; Zhu, J.
Deposited on : 2019-11-13
Resolution : 3.38 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 : 2.17.1
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) : 2.17.1

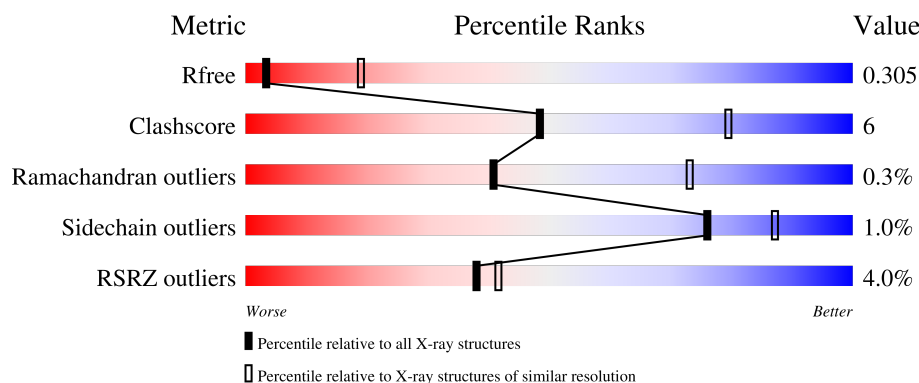
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	E	189	
2	H	232	
3	L	214	
4	A	227	
5	B	219	

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Mol	Chain	Length	Quality of chain
6	G	61	
7	C	2	

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
8	NAG	E	704	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7733 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 Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	146	Total	C	N	O	S	0	0	0
			1160	744	197	207	12			

- Molecule 2 is a protein called Fab AR3A heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	204	Total	C	N	O	S	0	0	0
			1551	988	257	298	8			

- Molecule 3 is a protein called Fab AR3A light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	190	Total	C	N	O	S	0	0	0
			1462	916	251	292	3			

- Molecule 4 is a protein called Fab E1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	195	Total	C	N	O	S	0	0	0
			1455	923	239	285	8			

- Molecule 5 is a protein called Fab E1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	209	Total	C	N	O	S	0	0	0
			1609	1009	274	321	5			

- Molecule 6 is a protein called Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	57	Total	C	N	O	0	0	0
			440	277	69	94			

There is a discrepancy between the modelled and reference sequences:

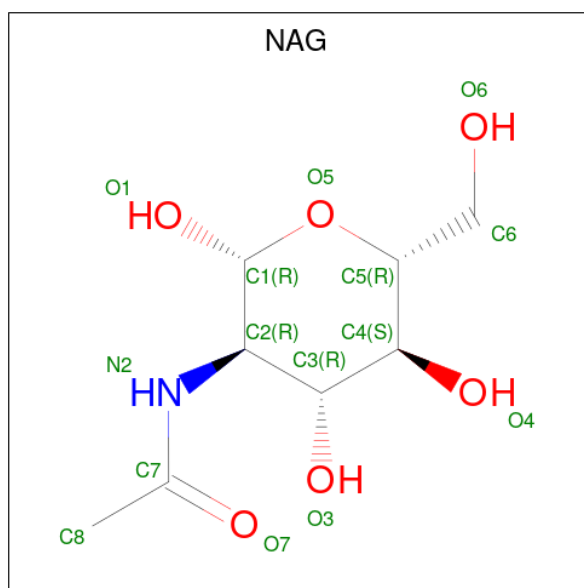
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP P19909

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

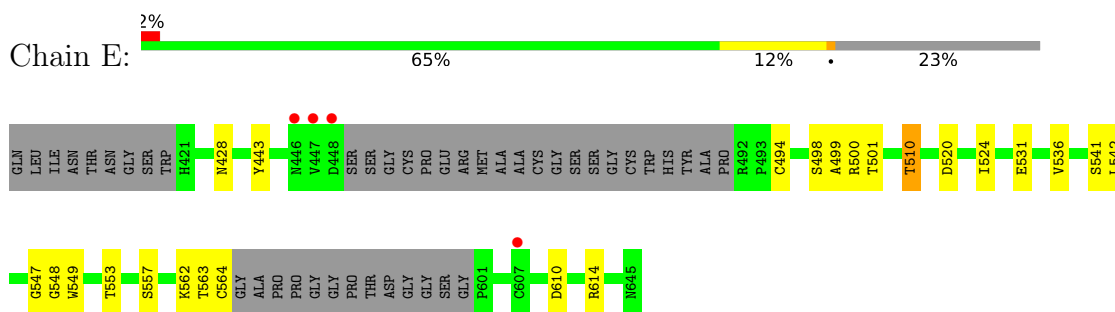


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		

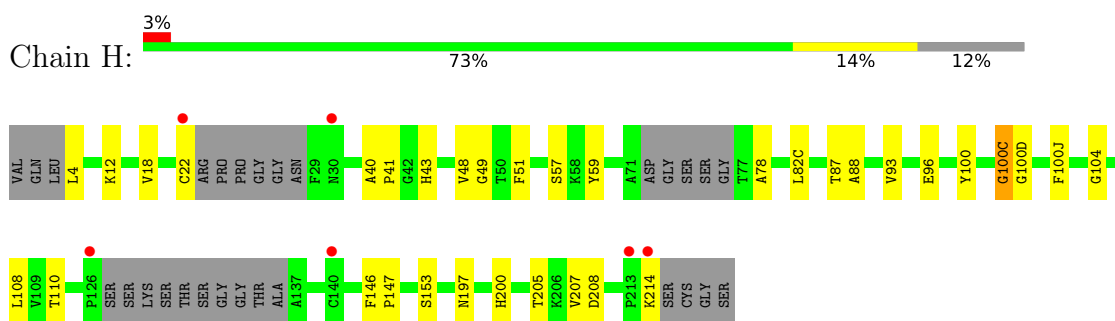
3 Residue-property plots

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.

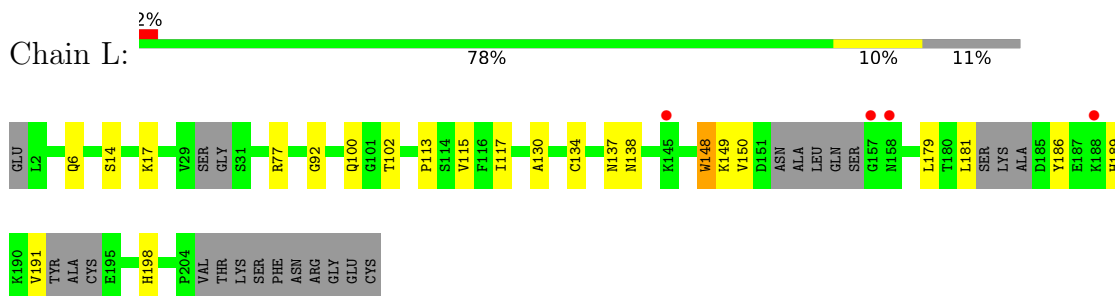
- Molecule 1: Envelope glycoprotein E2



- Molecule 2: Fab AR3A heavy chain

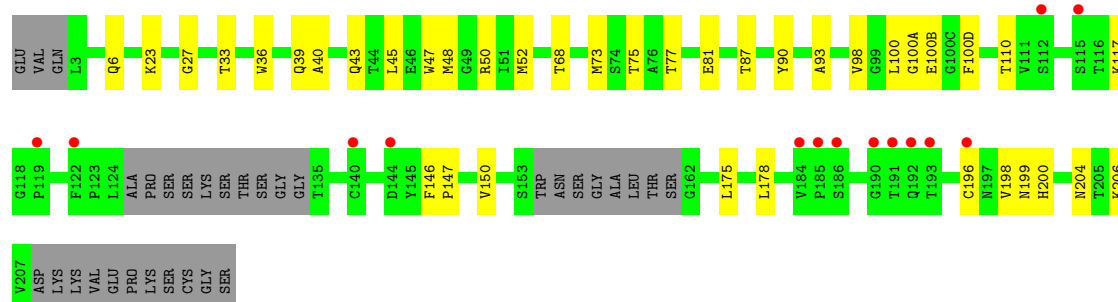


- Molecule 3: Fab AR3A light chain

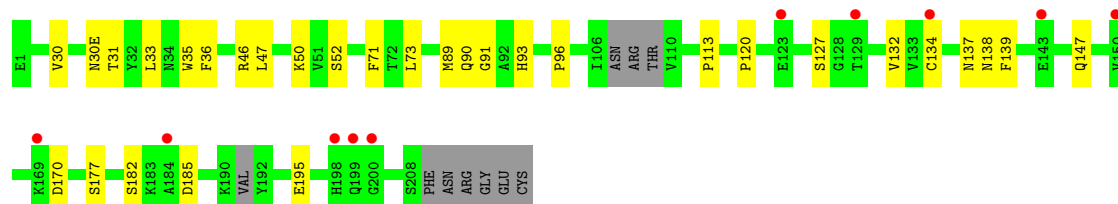
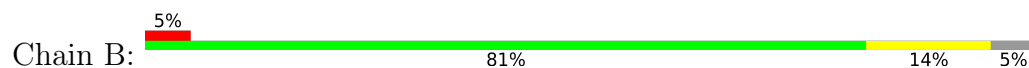


- Molecule 4: Fab E1 heavy chain

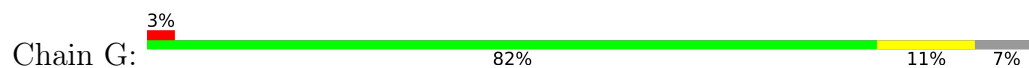




- Molecule 5: Fab E1 light chain



- Molecule 6: Immunoglobulin G-binding protein G



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	209.82Å 209.82Å 139.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.60 – 3.38 29.60 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.60-3.38) 99.5 (29.60-3.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.254 , 0.305 0.255 , 0.305	Depositor DCC
R_{free} test set	1265 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	100.5	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7733	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: NAG

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	E	0.27	0/1197	0.49	0/1635
2	H	0.25	0/1592	0.44	0/2168
3	L	0.25	0/1492	0.44	0/2022
4	A	0.25	0/1487	0.45	0/2023
5	B	0.24	0/1645	0.43	0/2234
6	G	0.23	0/446	0.44	0/606
All	All	0.25	0/7859	0.45	0/10688

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	E	1160	0	1097	15	0
2	H	1551	0	1493	21	0
3	L	1462	0	1420	13	0
4	A	1455	0	1441	25	0
5	B	1609	0	1561	20	0
6	G	440	0	428	4	0
7	C	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	28	0	26	0	0
All	All	7733	0	7491	91	0

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

All (91) 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)
5:B:36:PHE:HE2	5:B:89:MET:HG2	1.10	1.16
5:B:36:PHE:CE2	5:B:89:MET:HG2	2.00	0.96
5:B:36:PHE:HE2	5:B:89:MET:CG	1.90	0.85
2:H:4:LEU:HB2	2:H:104:GLY:HA2	1.71	0.73
4:A:100(A):GLY:HA2	5:B:91:GLY:HA3	1.72	0.71
2:H:197:ASN:ND2	2:H:208:ASP:OD2	2.26	0.68
1:E:562:LYS:NZ	7:C:1:NAG:O6	2.28	0.66
4:A:199:ASN:HB2	4:A:206:LYS:HE3	1.77	0.66
4:A:68:THR:HB	4:A:81:GLU:HB3	1.79	0.65
1:E:553:THR:HG22	1:E:563:THR:HG22	1.80	0.64
3:L:6:GLN:NE2	3:L:102:THR:OG1	2.32	0.62
4:A:100(B):GLU:O	5:B:46:ARG:NH1	2.33	0.62
4:A:100:LEU:HD23	5:B:96:PRO:HG3	1.82	0.61
6:G:13:ASN:HB2	6:G:60:THR:HG22	1.82	0.61
3:L:6:GLN:NE2	3:L:100:GLN:O	2.34	0.61
2:H:12:LYS:HG3	2:H:18:VAL:HG22	1.84	0.60
2:H:22:CYS:HB3	2:H:78:ALA:HB3	1.83	0.59
1:E:510:THR:HG22	1:E:549:TRP:HB3	1.84	0.59
4:A:87:THR:HG23	4:A:110:THR:HA	1.83	0.59
1:E:443:TYR:OH	2:H:96:GLU:O	2.21	0.58
2:H:51:PHE:HD1	2:H:57:SER:HB3	1.68	0.58
4:A:23:LYS:NZ	4:A:27:GLY:HA2	2.18	0.57
6:G:25:ALA:HB3	6:G:31:ALA:HB2	1.86	0.57
1:E:610:ASP:HA	1:E:614:ARG:HD3	1.86	0.57
1:E:428:ASN:ND2	1:E:499:ALA:O	2.38	0.56
3:L:137:ASN:ND2	3:L:138:ASN:OD1	2.39	0.56
5:B:147:GLN:HB2	5:B:195:GLU:HB3	1.86	0.56
4:A:33:THR:HG22	4:A:52:MET:HG2	1.88	0.55
2:H:18:VAL:HG23	2:H:82(C):LEU:HD11	1.89	0.54
2:H:48:VAL:HG12	2:H:49:GLY:H	1.72	0.54
4:A:200:HIS:O	4:A:204:ASN:N	2.40	0.54
2:H:49:GLY:HA3	2:H:59:TYR:HD1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:115:VAL:HG12	3:L:117:ILE:HG13	1.90	0.53
5:B:113:PRO:HB3	5:B:139:PHE:HB3	1.91	0.52
2:H:153:SER:O	2:H:197:ASN:N	2.42	0.52
3:L:148:TRP:CZ2	3:L:179:LEU:HB2	2.45	0.52
4:A:117:LYS:HD3	4:A:175:LEU:HD11	1.91	0.51
3:L:130:ALA:HB3	3:L:181:LEU:HB3	1.91	0.51
3:L:14:SER:H	3:L:17:LYS:HD3	1.76	0.50
5:B:33:LEU:HD22	5:B:71:PHE:CG	2.47	0.50
1:E:500:ARG:NH2	1:E:531:GLU:O	2.43	0.49
1:E:541:SER:HB3	1:E:548:GLY:H	1.77	0.49
2:H:41:PRO:HD3	2:H:88:ALA:HA	1.95	0.49
5:B:30:VAL:HA	5:B:31:THR:HG22	1.95	0.49
1:E:520:ASP:OD1	1:E:524:ILE:N	2.45	0.48
4:A:6:GLN:NE2	4:A:90:TYR:O	2.46	0.48
4:A:93:ALA:HB1	4:A:100(D):PHE:HB3	1.96	0.48
1:E:501:THR:O	1:E:557:SER:N	2.46	0.48
2:H:93:VAL:HG11	2:H:100(J):PHE:HB3	1.94	0.48
5:B:30(E):ASN:HB3	5:B:50:LYS:HD3	1.95	0.48
6:G:15:LYS:HG3	6:G:16:THR:HG23	1.95	0.48
5:B:90:GLN:NE2	5:B:93:HIS:O	2.43	0.47
2:H:100:TYR:OH	3:L:92:GLY:O	2.29	0.47
4:A:147:PRO:O	4:A:200:HIS:NE2	2.31	0.47
4:A:47:TRP:HZ2	4:A:50:ARG:HB2	1.80	0.47
4:A:23:LYS:HB2	4:A:77:THR:HG22	1.96	0.46
5:B:120:PRO:HD3	5:B:132:VAL:HG22	1.97	0.46
5:B:137:ASN:OD1	5:B:138:ASN:ND2	2.49	0.46
2:H:40:ALA:HB3	2:H:43:HIS:HB2	1.97	0.46
4:A:150:VAL:HB	4:A:178:LEU:HD21	1.98	0.46
2:H:146:PHE:HA	2:H:147:PRO:HA	1.79	0.46
1:E:542:LEU:HD12	4:A:98:VAL:HG12	1.98	0.45
5:B:170:ASP:N	5:B:170:ASP:OD1	2.47	0.45
5:B:50:LYS:O	5:B:52:SER:N	2.49	0.45
2:H:205:THR:HG22	2:H:207:VAL:HG23	2.00	0.44
4:A:73:MET:C	4:A:75:THR:H	2.21	0.44
3:L:148:TRP:N	3:L:148:TRP:CD1	2.86	0.43
2:H:100(C):GLY:HA2	2:H:100(D):GLY:HA2	1.56	0.43
3:L:148:TRP:O	3:L:150:VAL:HG23	2.19	0.43
1:E:494:CYS:HA	1:E:564:CYS:HB2	2.00	0.43
4:A:23:LYS:HZ2	4:A:27:GLY:HA2	1.82	0.43
1:E:498:SER:HA	1:E:536:VAL:HG12	2.00	0.43
3:L:113:PRO:HD3	3:L:198:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:35:TRP:CE2	5:B:73:LEU:HB2	2.53	0.43
5:B:182:SER:OG	5:B:185:ASP:OD1	2.36	0.43
1:E:542:LEU:O	1:E:547:GLY:HA3	2.19	0.42
4:A:146:PHE:HA	4:A:147:PRO:HA	1.86	0.42
2:H:87:THR:HG23	2:H:110:THR:HA	2.01	0.42
1:E:557:SER:OG	7:C:1:NAG:H82	2.19	0.42
4:A:39:GLN:HB2	4:A:45:LEU:HD23	2.01	0.42
5:B:147:GLN:O	5:B:195:GLU:N	2.44	0.42
3:L:149:LYS:HB2	3:L:149:LYS:HE3	1.85	0.42
4:A:150:VAL:HG13	4:A:198:VAL:HG13	2.01	0.42
2:H:205:THR:HG23	6:G:21:THR:HB	2.02	0.41
2:H:49:GLY:HA3	2:H:59:TYR:CD1	2.55	0.41
4:A:48:MET:HE1	4:A:90:TYR:HD2	1.86	0.41
3:L:134:CYS:HB2	3:L:148:TRP:CE3	2.55	0.41
2:H:200:HIS:HB3	2:H:205:THR:HB	2.03	0.41
4:A:40:ALA:HB3	4:A:43:GLN:HB2	2.03	0.41
5:B:134:CYS:HB3	5:B:177:SER:HB3	2.04	0.40
4:A:36:TRP:HB3	4:A:48:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	140/189 (74%)	131 (94%)	8 (6%)	1 (1%)	22	56
2	H	196/232 (84%)	183 (93%)	12 (6%)	1 (0%)	29	63
3	L	180/214 (84%)	166 (92%)	14 (8%)	0	100	100
4	A	189/227 (83%)	182 (96%)	7 (4%)	0	100	100
5	B	203/219 (93%)	190 (94%)	12 (6%)	1 (0%)	29	63
6	G	55/61 (90%)	53 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	963/1142 (84%)	905 (94%)	55 (6%)	3 (0%)	41 73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	100(C)	GLY
5	B	127	SER
1	E	510	THR

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	E	130/159 (82%)	130 (100%)	0	100 100
2	H	174/195 (89%)	172 (99%)	2 (1%)	73 86
3	L	165/184 (90%)	160 (97%)	5 (3%)	41 69
4	A	164/190 (86%)	163 (99%)	1 (1%)	86 93
5	B	183/192 (95%)	182 (100%)	1 (0%)	88 94
6	G	47/50 (94%)	47 (100%)	0	100 100
All	All	863/970 (89%)	854 (99%)	9 (1%)	76 87

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

Mol	Chain	Res	Type
2	H	108	LEU
2	H	214	LYS
3	L	77	ARG
3	L	148	TRP
3	L	186	TYR
3	L	189	HIS
3	L	191	VAL
4	A	196	CYS
5	B	47	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	197	ASN
3	L	6	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	$\# Z > 2$
7	NAG	C	1	1,7	14,14,15	0.37	0	17,19,21	0.55	0
7	NAG	C	2	7	14,14,15	0.27	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	C	2	7	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1	NAG	C4-C5-C6-O6
7	C	1	NAG	O5-C5-C6-O6
7	C	2	NAG	C4-C5-C6-O6
7	C	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1	NAG	2	0

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
8	NAG	E	701	1	14,14,15	0.24	0	17,19,21	0.46	0
8	NAG	E	704	1	14,14,15	0.23	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	E	701	1	-	2/6/23/26	0/1/1/1
8	NAG	E	704	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

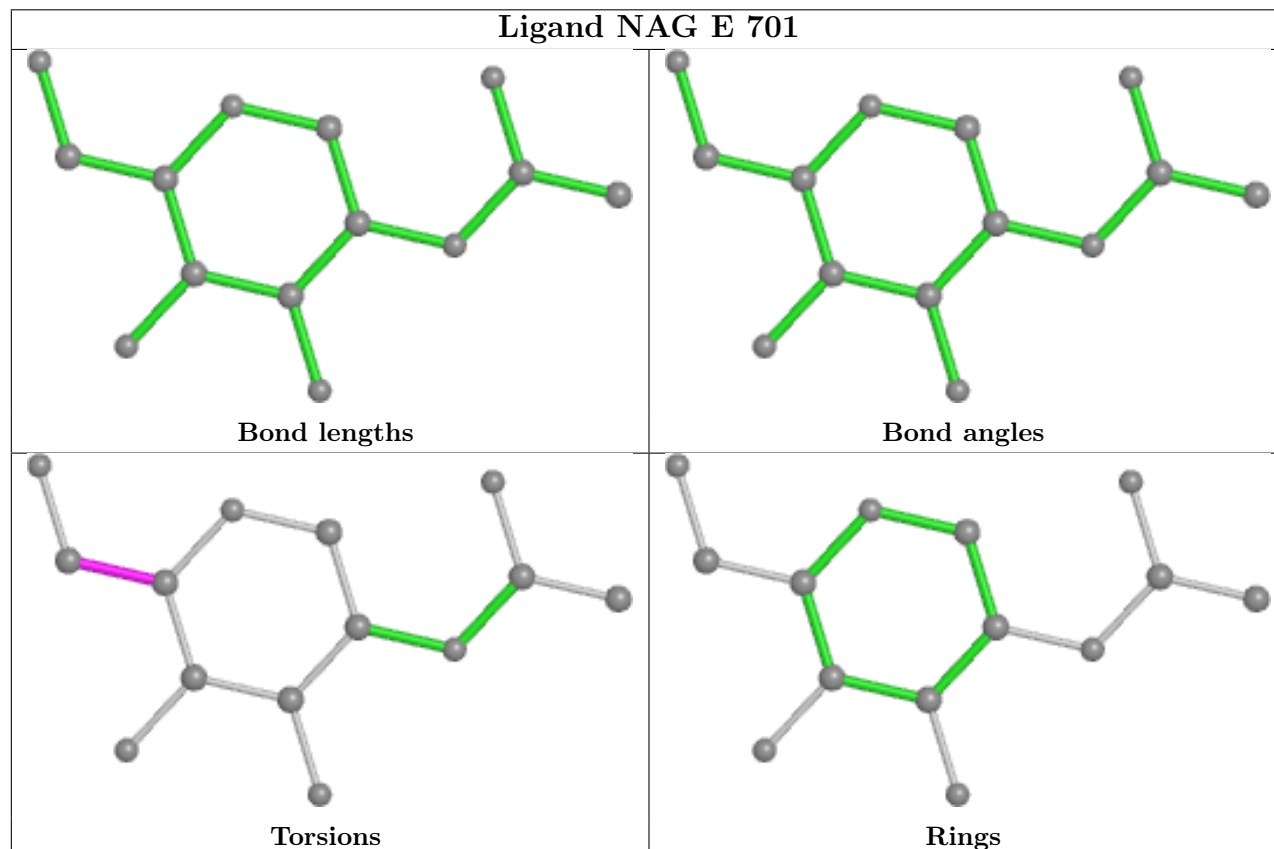
All (2) torsion outliers are listed below:

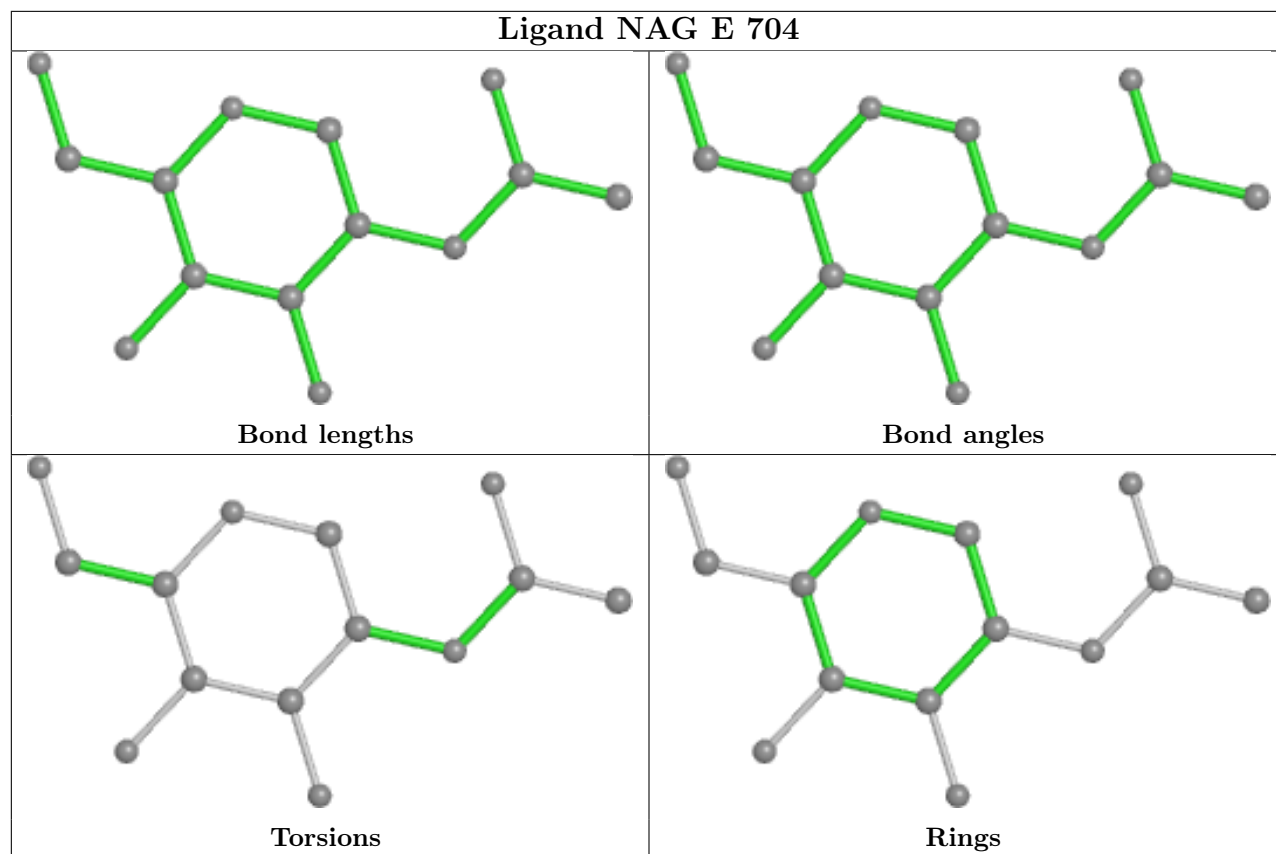
Mol	Chain	Res	Type	Atoms
8	E	701	NAG	O5-C5-C6-O6
8	E	701	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	E	146/189 (77%)	-0.03	4 (2%) 54 58	49, 77, 112, 158	0
2	H	204/232 (87%)	0.16	6 (2%) 51 55	57, 103, 140, 160	0
3	L	190/214 (88%)	0.04	4 (2%) 63 67	53, 95, 144, 156	0
4	A	195/227 (85%)	0.21	14 (7%) 15 19	55, 104, 161, 179	0
5	B	209/219 (95%)	0.38	10 (4%) 30 34	45, 111, 160, 177	0
6	G	57/61 (93%)	0.35	2 (3%) 44 47	98, 129, 147, 156	0
All	All	1001/1142 (87%)	0.17	40 (3%) 38 41	45, 102, 150, 179	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	191	THR	4.1
4	A	112	SER	4.0
4	A	186	SER	4.0
4	A	193	THR	3.8
4	A	140	CYS	3.7
5	B	143	GLU	3.6
2	H	140	CYS	3.5
1	E	448	ASP	3.5
1	E	447	VAL	3.5
4	A	185	PRO	3.5
5	B	199	GLN	3.3
5	B	169	LYS	3.3
5	B	198	HIS	3.1
3	L	157	GLY	3.0
5	B	123	GLU	2.9
6	G	26	VAL	2.9
2	H	213	PRO	2.8
4	A	184	VAL	2.8
4	A	119	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
5	B	184	ALA	2.8
5	B	129	THR	2.8
1	E	607	CYS	2.5
3	L	158	ASN	2.5
2	H	214	LYS	2.4
2	H	126	PRO	2.4
4	A	144	ASP	2.4
4	A	115	SER	2.4
4	A	192	GLN	2.3
4	A	122	PHE	2.3
5	B	150	VAL	2.3
1	E	446	ASN	2.2
2	H	30	ASN	2.2
2	H	22	CYS	2.2
4	A	196	CYS	2.2
4	A	190	GLY	2.1
3	L	145	LYS	2.1
6	G	56	THR	2.0
5	B	200	GLY	2.0
3	L	188	LYS	2.0
5	B	134	CYS	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](#)

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
7	NAG	C	2	14/15	0.85	0.31	101,124,139,146	0
7	NAG	C	1	14/15	0.92	0.14	67,78,88,121	0

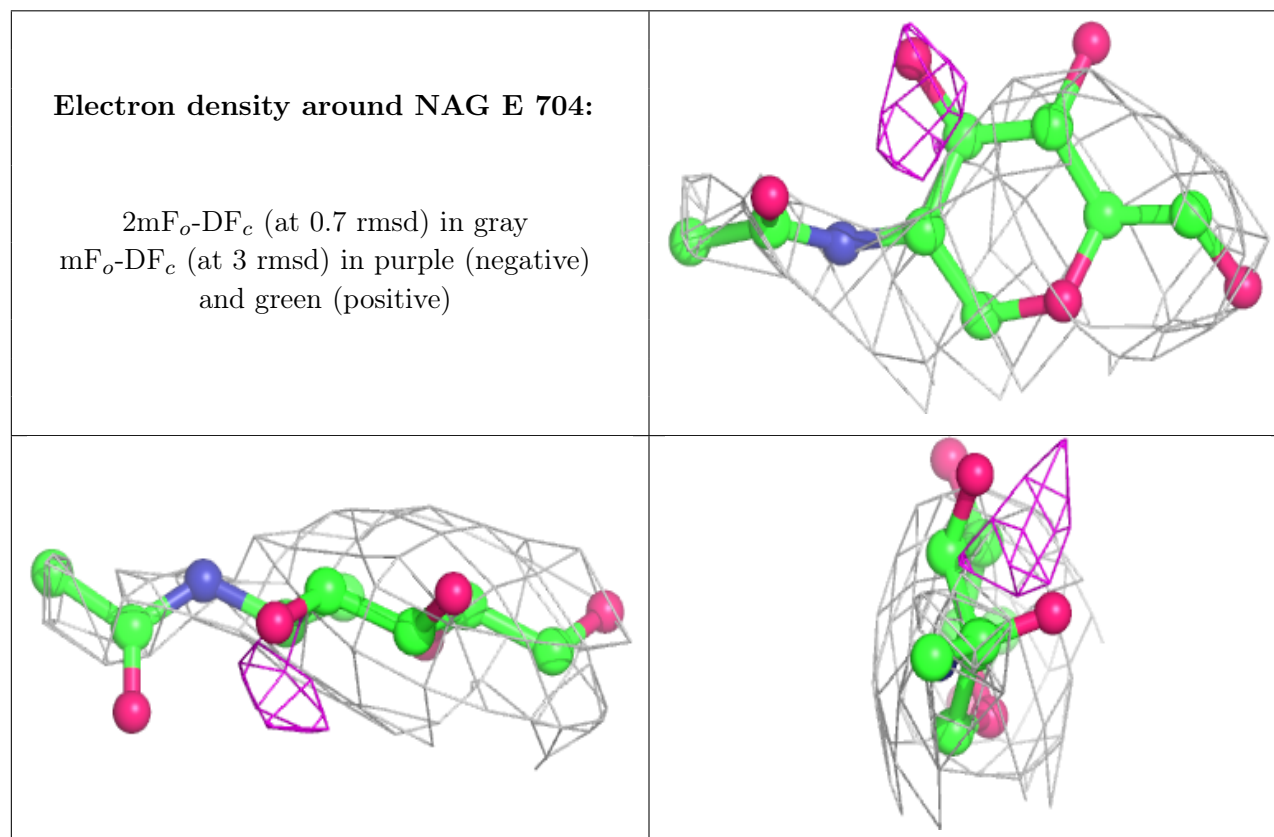
6.4 Ligands [i](#)

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.

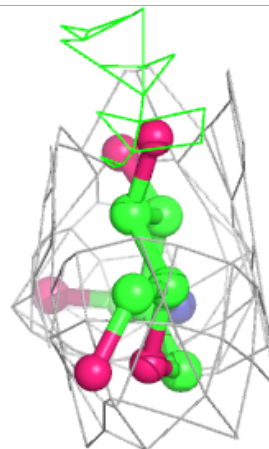
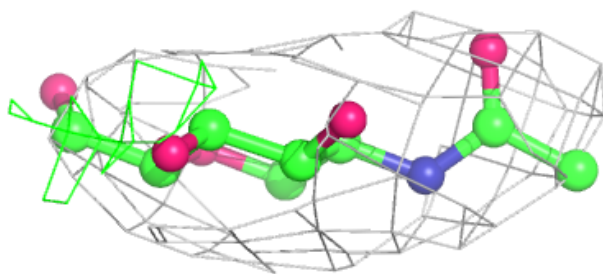
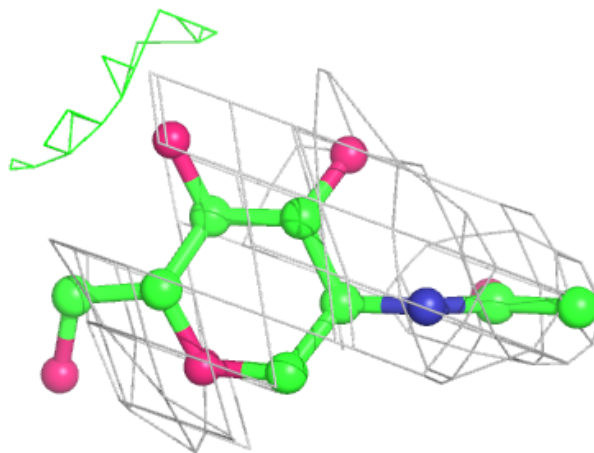
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	E	704	14/15	0.70	0.65	121,154,170,185	0
8	NAG	E	701	14/15	0.90	0.22	87,100,121,126	0

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 NAG E 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.