



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2025 – 06:40 PM JST

PDB ID : 9LU3 / pdb_00009lu3
Title : LN1F9 Fab bound to Nipah Virus attachment (G) glycoprotein head domain
Authors : Deng, Z.; Kuang, W.
Deposited on : 2025-02-07
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

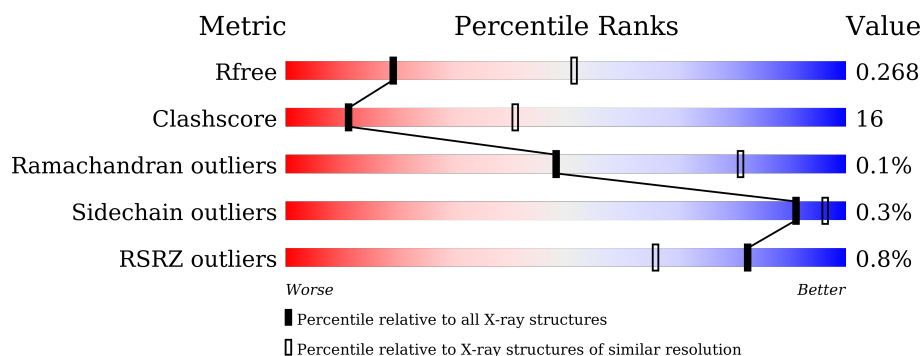
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	441	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>32%</div> <div>5%</div> </div> </div>
1	B	441	<div> <div></div> <div>62%</div> <div>32%</div> <div>5%</div> </div>
2	D	234	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>5%</div> </div> </div>
2	H	234	<div> <div></div> <div>68%</div> <div>26%</div> <div>• 5%</div> </div>
3	E	214	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>34%</div> <div>•</div> </div> </div>
3	L	214	<div> <div></div> <div>63%</div> <div>37%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13333 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 Glycoprotein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3294	2104	555	614	21			
1	B	418	Total	C	N	O	S	0	0	0
			3303	2108	557	617	21			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	HIS	-	expression tag	UNP Q9IH62
A	163	HIS	-	expression tag	UNP Q9IH62
A	164	HIS	-	expression tag	UNP Q9IH62
A	165	HIS	-	expression tag	UNP Q9IH62
A	166	HIS	-	expression tag	UNP Q9IH62
A	167	HIS	-	expression tag	UNP Q9IH62
A	168	LEU	-	expression tag	UNP Q9IH62
A	169	GLU	-	expression tag	UNP Q9IH62
A	170	VAL	-	expression tag	UNP Q9IH62
A	171	LEU	-	expression tag	UNP Q9IH62
A	172	PHE	-	expression tag	UNP Q9IH62
A	173	GLN	-	expression tag	UNP Q9IH62
A	174	GLY	-	expression tag	UNP Q9IH62
A	175	PRO	-	expression tag	UNP Q9IH62
B	162	HIS	-	expression tag	UNP Q9IH62
B	163	HIS	-	expression tag	UNP Q9IH62
B	164	HIS	-	expression tag	UNP Q9IH62
B	165	HIS	-	expression tag	UNP Q9IH62
B	166	HIS	-	expression tag	UNP Q9IH62
B	167	HIS	-	expression tag	UNP Q9IH62
B	168	LEU	-	expression tag	UNP Q9IH62
B	169	GLU	-	expression tag	UNP Q9IH62
B	170	VAL	-	expression tag	UNP Q9IH62
B	171	LEU	-	expression tag	UNP Q9IH62
B	172	PHE	-	expression tag	UNP Q9IH62

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Chain	Residue	Modelled	Actual	Comment	Reference
B	173	GLN	-	expression tag	UNP Q9IH62
B	174	GLY	-	expression tag	UNP Q9IH62
B	175	PRO	-	expression tag	UNP Q9IH62

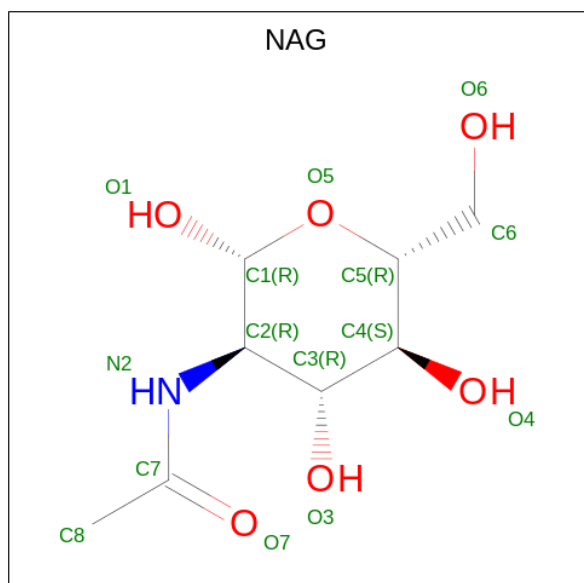
- Molecule 2 is a protein called mAb LN1F9 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	223	Total	C	N	O	S	0	0	0
			1677	1063	277	330	7			
2	D	222	Total	C	N	O	S	0	0	0
			1668	1057	275	329	7			

- Molecule 3 is a protein called mAb LN1F9 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1644	1029	276	335	4			
3	E	209	Total	C	N	O	S	0	0	0
			1607	1009	267	327	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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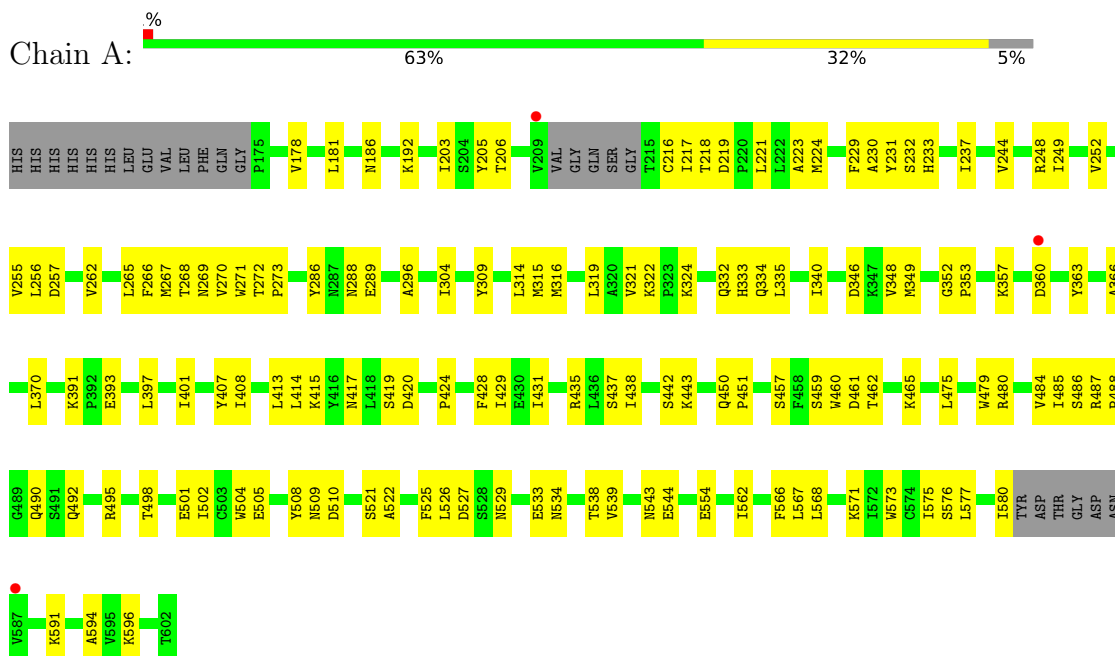
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
	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

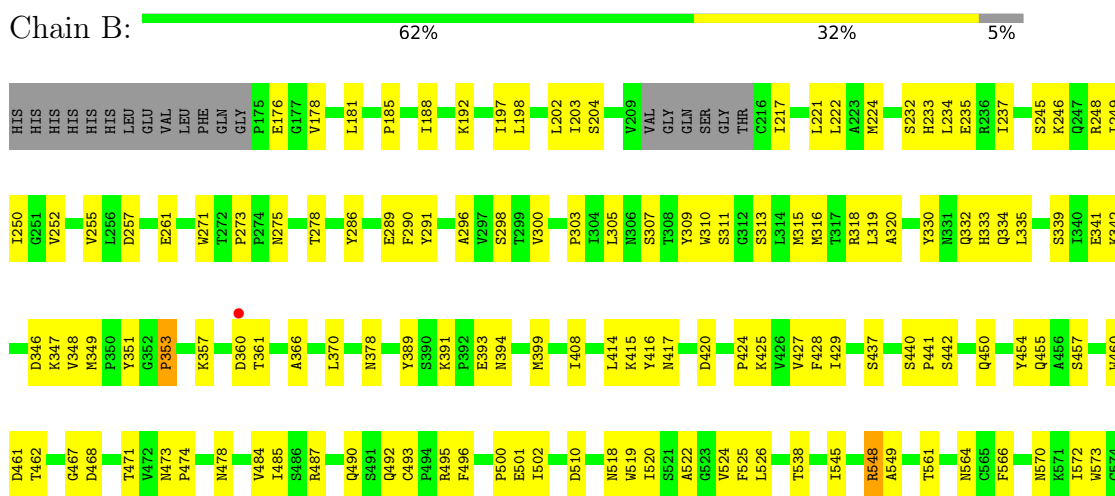
3 Residue-property plots

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: Glycoprotein G



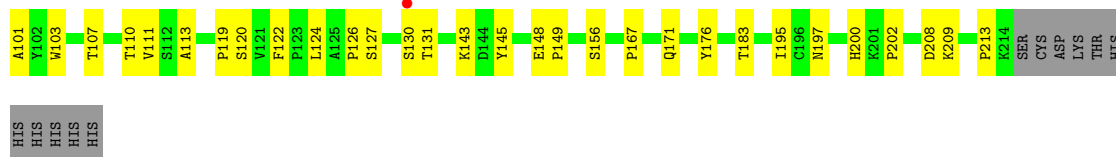
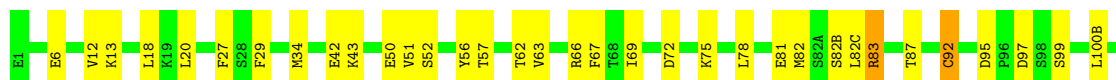
• Molecule 1: Glycoprotein G





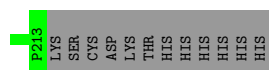
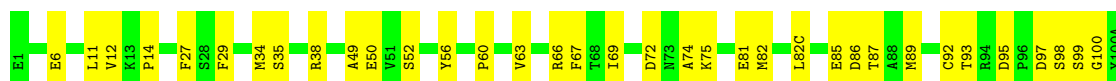
- Molecule 2: mAb LN1F9 Fab heavy chain

Chain H: 68% 26% 5%



- Molecule 2: mAb LN1F9 Fab heavy chain

Chain D: 65% 30% 5%



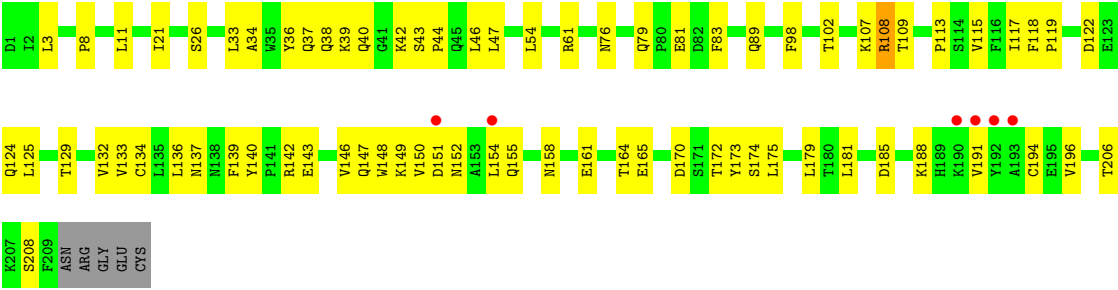
- Molecule 3: mAb LN1F9 Fab light chain

Chain L: 63% 37%



- Molecule 3: mAb LN1F9 Fab light chain

Chain E: 3% 63% 34%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.42Å 125.16Å 152.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.44 – 3.00 20.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.44-3.00) 98.4 (20.44-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.219 , 0.269 0.221 , 0.268	Depositor DCC
R_{free} test set	2408 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13333	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3993e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	A	0.51	0/3373	0.76	0/4586
1	B	0.51	0/3382	0.75	0/4598
2	D	0.47	0/1711	0.73	0/2331
2	H	0.47	0/1720	0.73	0/2342
3	E	0.49	0/1642	0.80	1/2231 (0.0%)
3	L	0.47	0/1679	0.73	0/2280
All	All	0.49	0/13507	0.75	1/18368 (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	B	0	1
2	D	0	2
2	H	0	1
3	E	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	149	LYS	CA-CB-CG	5.21	124.51	114.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	548	ARG	Sidechain
2	D	130	SER	Peptide
2	D	205	THR	Peptide
3	E	108	ARG	Sidechain
2	H	83	ARG	Sidechain

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	3294	0	3252	104	1
1	B	3303	0	3253	117	1
2	D	1668	0	1628	53	0
2	H	1677	0	1641	55	0
3	E	1607	0	1562	61	1
3	L	1644	0	1592	60	1
4	A	70	0	65	1	0
4	B	70	0	65	1	0
All	All	13333	0	13058	421	2

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 16.

All (421) 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:B:501:GLU:OE2	2:D:98:SER:OG	1.84	0.94
1:B:224:MET:HE1	1:B:575:ILE:HB	1.53	0.91
1:A:186:ASN:HD22	1:A:571:LYS:HE3	1.38	0.87
3:E:115:VAL:HG21	3:E:196:VAL:HG21	1.55	0.86
2:H:82:MET:HE2	2:H:82(C):LEU:HD21	1.59	0.84
2:H:50:GLU:OE2	2:H:95:ASP:OD2	1.96	0.83
1:B:307:SER:O	1:B:347:LYS:NZ	2.11	0.83
2:D:119:PRO:HB3	2:D:145:TYR:HB3	1.62	0.81
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.62	0.81
1:B:316:MET:HG2	1:B:335:LEU:HD12	1.62	0.79
3:L:151:ASP:OD2	3:L:189:HIS:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ILE:HD11	1:B:246:LYS:HD3	1.63	0.77
1:B:391:LYS:NZ	2:D:100:GLY:O	2.17	0.76
1:B:296:ALA:HB2	1:B:349:MET:HG3	1.66	0.76
2:H:6:GLU:OE2	2:H:92:CYS:N	2.15	0.76
1:B:351:TYR:CZ	1:B:441:PRO:HD3	2.21	0.75
1:A:420:ASP:HB3	1:A:424:PRO:HB3	1.69	0.74
3:E:152:ASN:O	3:E:152:ASN:ND2	2.20	0.74
1:A:571:LYS:HD3	1:A:596:LYS:HZ1	1.52	0.73
3:E:136:LEU:HB2	3:E:175:LEU:HB3	1.71	0.72
1:B:351:TYR:CE2	1:B:441:PRO:HD3	2.24	0.72
1:B:351:TYR:HE2	1:B:440:SER:HA	1.55	0.72
3:E:143:GLU:N	3:E:143:GLU:OE1	2.22	0.71
1:B:222:LEU:HD21	1:B:224:MET:HE2	1.71	0.71
2:H:130:SER:HA	3:L:116:PHE:HD1	1.54	0.71
3:E:21:ILE:HD12	3:E:102:THR:HG21	1.73	0.70
1:A:203:ILE:HD13	1:A:594:ALA:HB2	1.74	0.70
2:D:66:ARG:NH2	2:D:86:ASP:OD2	2.26	0.69
3:L:8:PRO:HG2	3:L:11:LEU:HD13	1.75	0.68
3:E:40:GLN:NE2	3:E:83:PHE:HE2	1.92	0.68
1:A:580:ILE:HD12	1:A:591:LYS:HD3	1.76	0.68
1:B:417:ASN:HB3	1:B:420:ASP:HB2	1.74	0.68
1:A:566:PHE:HE1	1:A:575:ILE:HG13	1.59	0.68
1:A:495:ARG:HE	1:A:529:ASN:HA	1.59	0.67
2:H:156:SER:H	2:H:197:ASN:HD21	1.42	0.67
2:H:12:VAL:HG11	2:H:18:LEU:HG	1.76	0.67
2:D:87:THR:HG23	2:D:110:THR:HA	1.75	0.67
2:H:103:TRP:HB2	3:L:43:SER:HB2	1.76	0.67
1:B:275:ASN:HB3	1:B:278:THR:HG22	1.76	0.67
3:E:40:GLN:HG3	3:E:165:GLU:HG3	1.77	0.66
2:H:66:ARG:NH1	2:H:83:ARG:NH1	2.43	0.66
1:A:333:HIS:CE1	1:A:335:LEU:HD23	2.31	0.66
2:H:42:GLU:N	2:H:42:GLU:OE1	2.29	0.66
3:L:192:TYR:HB2	3:L:209:PHE:CE1	2.31	0.65
1:A:363:TYR:HE1	1:A:415:LYS:HD2	1.61	0.65
3:E:108:ARG:NH1	3:E:109:THR:O	2.28	0.65
1:B:315:MET:HE2	1:B:334:GLN:HE22	1.61	0.65
1:B:224:MET:HE3	1:B:564:ASN:HB2	1.79	0.65
3:E:161:GLU:HG2	3:E:175:LEU:HD11	1.79	0.65
3:L:118:PHE:HB2	3:L:133:VAL:HB	1.78	0.64
1:A:248:ARG:HB3	1:A:273:PRO:HD2	1.79	0.64
3:L:132:VAL:HB	3:L:179:LEU:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:HB3	1:B:427:VAL:HG22	1.80	0.63
2:D:89:MET:HE3	2:D:107:THR:N	2.14	0.63
3:L:124:GLN:NE2	3:L:129:THR:O	2.31	0.63
3:L:131:SER:OG	3:L:180:THR:HG22	1.99	0.63
1:A:484:VAL:HG23	1:A:485:ILE:HG12	1.81	0.62
1:B:351:TYR:CE1	1:B:441:PRO:HG3	2.34	0.62
2:D:72:ASP:OD2	2:D:75:LYS:HG3	1.98	0.62
2:D:138:LEU:HD21	2:D:194:TYR:CD2	2.34	0.62
1:B:333:HIS:ND1	1:B:335:LEU:HD23	2.15	0.62
1:A:457:SER:HB3	1:A:461:ASP:O	2.00	0.62
1:A:484:VAL:HG13	1:A:543:ASN:HA	1.83	0.61
3:E:185:ASP:HA	3:E:188:LYS:HD2	1.82	0.61
3:L:115:VAL:HG21	3:L:196:VAL:HG11	1.82	0.61
1:A:571:LYS:HD3	1:A:596:LYS:NZ	2.14	0.61
2:D:11:LEU:HD23	2:D:116:THR:HG22	1.82	0.61
3:L:145:LYS:HB2	3:L:197:THR:HB	1.83	0.60
3:L:22:THR:HG22	3:L:72:SER:HB3	1.82	0.60
3:E:122:ASP:HA	3:E:125:LEU:HD12	1.82	0.60
2:D:89:MET:HE3	2:D:106:GLY:C	2.27	0.60
2:H:122:PHE:CE2	3:L:124:GLN:HG3	2.37	0.60
1:B:315:MET:CE	1:B:334:GLN:HE22	2.14	0.60
1:A:363:TYR:CE1	1:A:415:LYS:HD2	2.37	0.60
1:A:257:ASP:HB2	1:A:568:LEU:HD11	1.82	0.59
2:D:183:THR:HG21	3:E:137:ASN:ND2	2.17	0.59
2:D:60:PRO:HG2	2:D:63:VAL:HG22	1.85	0.59
2:H:6:GLU:HB3	2:H:107:THR:HB	1.85	0.59
3:E:155:GLN:HE21	3:E:158:ASN:ND2	1.99	0.59
2:H:87:THR:HG23	2:H:110:THR:HA	1.84	0.59
3:L:151:ASP:HA	3:L:191:VAL:HB	1.85	0.58
3:E:152:ASN:HD22	3:E:152:ASN:C	2.11	0.58
2:D:200:HIS:NE2	2:D:202:PRO:HG2	2.17	0.58
2:H:195:ILE:HD11	2:H:208:ASP:C	2.28	0.58
1:A:249:ILE:HD13	1:A:272:THR:HG22	1.84	0.58
1:B:303:PRO:HB2	1:B:349:MET:HE1	1.85	0.58
3:L:33:LEU:HD11	3:L:88:CYS:HB2	1.84	0.58
1:A:218:THR:HG22	1:A:219:ASP:H	1.68	0.58
3:L:41:GLY:O	3:L:42:LYS:HG2	2.03	0.58
1:B:495:ARG:HG2	1:B:496:PHE:CD2	2.39	0.58
1:B:351:TYR:CZ	1:B:441:PRO:HG3	2.39	0.58
1:B:351:TYR:CE2	1:B:440:SER:C	2.82	0.58
1:B:351:TYR:CE2	1:B:441:PRO:CD	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:PHE:CE1	1:A:575:ILE:HG13	2.39	0.57
1:A:486:SER:OG	1:A:487:ARG:N	2.36	0.57
2:H:124:LEU:HB3	3:L:118:PHE:CD2	2.38	0.57
1:B:393:GLU:HG3	2:D:100(B):LEU:HD11	1.86	0.57
2:H:72:ASP:OD2	2:H:75:LYS:HD2	2.04	0.57
1:B:351:TYR:CE2	1:B:440:SER:HA	2.39	0.57
1:A:256:LEU:HD12	1:A:266:PHE:CD2	2.39	0.57
1:B:188:ILE:HA	1:B:599:GLU:HA	1.85	0.57
2:H:62:THR:HG23	2:H:63:VAL:HG13	1.86	0.56
3:E:136:LEU:HD22	3:E:175:LEU:HD23	1.87	0.56
1:A:352:GLY:HA3	1:A:442:SER:O	2.04	0.56
2:H:120:SER:HB3	2:H:122:PHE:CZ	2.40	0.56
3:E:117:ILE:HD13	3:E:208:SER:HA	1.86	0.56
1:A:492:GLN:HE21	1:A:501:GLU:CG	2.18	0.56
1:B:234:LEU:HD11	1:B:245:SER:HB3	1.86	0.56
1:B:290:PHE:CG	1:B:318:ARG:HD2	2.40	0.56
2:H:156:SER:HA	2:H:197:ASN:ND2	2.21	0.56
1:B:457:SER:HB3	1:B:461:ASP:O	2.06	0.56
2:D:122:PHE:CE2	3:E:124:GLN:HG3	2.41	0.56
1:B:518:ASN:HB2	1:B:520:ILE:HD12	1.87	0.56
2:H:126:PRO:HG2	2:H:213:PRO:HA	1.87	0.55
1:A:186:ASN:ND2	1:A:571:LYS:HE3	2.15	0.55
1:A:221:LEU:HB3	1:A:232:SER:HB3	1.89	0.55
1:A:304:ILE:HD11	1:A:349:MET:HE1	1.89	0.55
1:B:286:TYR:O	1:B:357:LYS:HD3	2.06	0.55
3:L:37:GLN:HG3	3:L:86:TYR:CZ	2.42	0.55
1:B:252:VAL:HG13	1:B:319:LEU:HD12	1.89	0.55
3:E:170:ASP:OD1	3:E:172:THR:OG1	2.20	0.55
2:D:183:THR:HG21	3:E:137:ASN:HD21	1.72	0.55
1:B:351:TYR:CZ	1:B:441:PRO:CD	2.89	0.54
3:E:33:LEU:HG	3:E:34:ALA:N	2.22	0.54
3:E:39:LYS:HE2	3:E:81:GLU:O	2.07	0.54
1:B:333:HIS:CE1	1:B:335:LEU:HD23	2.43	0.54
3:L:142:ARG:HB2	3:L:173:TYR:CE2	2.42	0.54
1:B:181:LEU:HD11	1:B:572:ILE:CD1	2.37	0.54
1:B:275:ASN:HB3	1:B:278:THR:CG2	2.37	0.54
1:B:275:ASN:O	1:B:278:THR:HG22	2.08	0.54
1:B:492:GLN:HE21	1:B:501:GLU:HG2	1.72	0.54
1:A:319:LEU:CD2	1:A:332:GLN:HG2	2.38	0.54
1:A:487:ARG:HD2	1:A:488:PRO:O	2.07	0.54
1:A:502:ILE:HB	2:H:99:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:GLU:HG3	2:D:99:SER:OG	2.08	0.54
3:E:37:GLN:HB2	3:E:47:LEU:HD11	1.89	0.54
2:H:183:THR:HG21	3:L:137:ASN:ND2	2.23	0.54
1:B:204:SER:OG	1:B:592:LEU:N	2.37	0.54
1:B:580:ILE:HG13	1:B:591:LYS:HD3	1.88	0.54
2:H:12:VAL:HG21	2:H:82(C):LEU:HD13	1.89	0.53
1:B:203:ILE:HD13	1:B:594:ALA:HB2	1.89	0.53
1:B:391:LYS:HG2	1:B:394:ASN:OD1	2.07	0.53
3:E:164:THR:HB	3:E:174:SER:H	1.73	0.53
1:A:316:MET:HG2	1:A:335:LEU:HD12	1.90	0.53
1:B:178:VAL:HG21	1:B:255:VAL:HG12	1.89	0.53
1:B:198:LEU:HB2	1:B:549:ALA:HB2	1.90	0.53
1:A:393:GLU:HG3	2:H:100(B):LEU:HD11	1.90	0.53
1:B:440:SER:OG	1:B:455:GLN:HG2	2.08	0.53
1:A:221:LEU:HD13	1:A:353:PRO:HA	1.91	0.53
3:L:89:GLN:HB2	3:L:98:PHE:CD2	2.43	0.53
1:B:492:GLN:HE21	1:B:501:GLU:CG	2.21	0.53
3:E:164:THR:HG22	3:E:165:GLU:O	2.09	0.53
1:B:250:ILE:HD12	1:B:271:TRP:CZ3	2.44	0.52
1:B:339:SER:HB2	1:B:425:LYS:HB3	1.92	0.52
1:A:413:LEU:HG	1:A:475:LEU:HD22	1.91	0.52
2:H:156:SER:N	2:H:197:ASN:HD21	2.06	0.52
3:L:33:LEU:HD22	3:L:71:PHE:CB	2.40	0.52
1:A:314:LEU:HD12	1:A:340:ILE:HD13	1.90	0.52
3:L:19:VAL:HG21	3:L:78:LEU:HD22	1.90	0.52
3:E:118:PHE:HB2	3:E:133:VAL:HB	1.91	0.52
3:L:166:GLN:HG2	3:L:171:SER:HA	1.92	0.52
1:B:319:LEU:CD2	1:B:332:GLN:HG2	2.40	0.52
1:A:360:ASP:OD1	1:A:360:ASP:N	2.41	0.52
1:A:417:ASN:HB3	1:A:420:ASP:HB2	1.91	0.52
3:L:184:ALA:O	3:L:188:LYS:HG2	2.09	0.52
1:A:522:ALA:HA	1:A:538:THR:O	2.10	0.51
1:B:370:LEU:HB3	1:B:408:ILE:HG13	1.92	0.51
3:E:89:GLN:HB2	3:E:98:PHE:CD2	2.45	0.51
1:A:391:LYS:NZ	2:H:97:ASP:OD2	2.39	0.51
2:H:124:LEU:HD21	3:L:133:VAL:HG21	1.91	0.51
1:B:197:ILE:HD12	1:B:598:PRO:HG2	1.92	0.51
1:A:218:THR:HG22	1:A:219:ASP:N	2.25	0.51
1:A:393:GLU:HG3	2:H:100(B):LEU:CD1	2.41	0.51
1:B:524:VAL:HG12	1:B:561:THR:HG21	1.91	0.51
3:E:3:LEU:HB3	3:E:26:SER:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:PRO:HA	1:B:570:ASN:OD1	2.10	0.51
1:A:333:HIS:ND1	1:A:335:LEU:HD23	2.25	0.51
2:H:167:PRO:O	3:L:162:SER:OG	2.27	0.50
2:H:143:LYS:NZ	2:H:171:GLN:OE1	2.43	0.50
2:H:195:ILE:HD12	2:H:209:LYS:O	2.11	0.50
3:E:8:PRO:O	3:E:102:THR:HG23	2.11	0.50
3:E:132:VAL:CG1	3:E:179:LEU:HB3	2.41	0.50
3:L:148:TRP:HB2	3:L:155:GLN:HB2	1.93	0.50
1:B:176:GLU:OE1	1:B:176:GLU:HA	2.12	0.50
1:B:351:TYR:CD2	1:B:440:SER:C	2.90	0.50
1:B:429:ILE:HD13	1:B:473:ASN:CG	2.35	0.50
3:E:151:ASP:HA	3:E:191:VAL:HB	1.94	0.50
1:A:348:VAL:HG11	1:A:428:PHE:HB2	1.94	0.50
1:B:468:ASP:OD1	1:B:519:TRP:HZ2	1.94	0.50
3:L:143:GLU:N	3:L:143:GLU:OE1	2.45	0.50
2:D:170:LEU:HB2	2:D:176:TYR:HE1	1.76	0.50
1:A:413:LEU:HB2	1:A:429:ILE:HB	1.92	0.50
1:A:437:SER:HB3	1:A:465:LYS:NZ	2.27	0.50
1:B:393:GLU:HG3	2:D:100(B):LEU:CD1	2.42	0.50
2:H:42:GLU:C	2:H:43:LYS:HD3	2.37	0.49
2:H:145:TYR:CE1	2:H:176:TYR:HB2	2.47	0.49
1:B:353:PRO:HD2	1:B:442:SER:O	2.12	0.49
1:B:416:TYR:OH	1:B:424:PRO:HD2	2.12	0.49
2:D:200:HIS:CD2	2:D:202:PRO:HG2	2.47	0.49
2:H:27:PHE:CE2	2:H:29:PHE:HA	2.48	0.49
2:H:67:PHE:HA	2:H:81:GLU:O	2.12	0.49
1:A:309:TYR:CD2	4:A:704:NAG:H5	2.48	0.49
3:L:40:GLN:HB2	3:L:165:GLU:OE1	2.12	0.49
3:E:107:LYS:HA	3:E:140:TYR:OH	2.13	0.49
2:H:69:ILE:HD11	2:H:78:LEU:HD11	1.95	0.49
3:L:11:LEU:HD23	3:L:104:LEU:HD13	1.95	0.49
1:A:205:TYR:CE1	1:A:206:THR:HG22	2.49	0.48
3:L:195:GLU:HG3	3:L:206:THR:HG22	1.94	0.48
1:B:221:LEU:HD23	1:B:221:LEU:C	2.39	0.48
1:A:366:ALA:CB	1:A:414:LEU:HG	2.44	0.48
1:A:450:GLN:HG2	1:A:451:PRO:CD	2.44	0.48
2:H:51:VAL:HG23	2:H:57:THR:HG22	1.95	0.48
2:D:171:GLN:NE2	2:D:177:SER:HB2	2.29	0.48
3:E:132:VAL:HG13	3:E:179:LEU:HB3	1.96	0.48
1:A:401:ILE:HG22	1:A:504:TRP:CD2	2.48	0.48
1:B:348:VAL:HG11	1:B:428:PHE:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:HD12	1:A:244:VAL:HB	1.96	0.48
1:A:322:LYS:O	1:A:324:LYS:NZ	2.41	0.48
1:B:311:SER:OG	1:B:313:SER:OG	2.21	0.48
1:A:324:LYS:HE2	1:B:289:GLU:OE2	2.14	0.47
3:E:150:VAL:HG23	3:E:155:GLN:HG2	1.96	0.47
3:E:155:GLN:HG3	3:E:158:ASN:HD21	1.79	0.47
1:A:296:ALA:HA	1:A:314:LEU:HD23	1.95	0.47
1:B:342:LYS:NZ	1:B:346:ASP:O	2.34	0.47
1:A:508:TYR:CZ	1:A:510:ASP:HB3	2.49	0.47
2:H:183:THR:HG21	3:L:137:ASN:HD21	1.79	0.47
3:L:124:GLN:HE22	3:L:131:SER:N	2.12	0.47
1:B:351:TYR:CE2	1:B:440:SER:CA	2.97	0.47
3:E:38:GLN:HG3	3:E:44:PRO:HA	1.96	0.47
1:A:262:VAL:HG22	1:A:573:TRP:CH2	2.49	0.47
1:B:462:THR:HG22	1:B:487:ARG:NH2	2.29	0.47
1:B:399:MET:HE1	1:B:437:SER:C	2.39	0.47
2:D:6:GLU:HB3	2:D:107:THR:HB	1.96	0.47
3:E:108:ARG:HH11	3:E:108:ARG:HG3	1.80	0.47
3:L:107:LYS:HA	3:L:140:TYR:OH	2.13	0.47
1:B:389:TYR:O	2:D:97:ASP:HB2	2.14	0.47
1:A:224:MET:HE1	1:A:566:PHE:CE1	2.50	0.47
1:A:573:TRP:CE2	1:A:596:LYS:HB2	2.49	0.47
3:E:113:PRO:HB3	3:E:139:PHE:HB3	1.96	0.47
1:A:490:GLN:HB2	1:A:505:GLU:CD	2.39	0.46
2:H:127:SER:O	2:H:131:THR:HG23	2.15	0.46
1:B:471:THR:OG1	1:B:474:PRO:O	2.32	0.46
1:A:267:MET:HE3	1:A:270:VAL:HG22	1.96	0.46
1:A:366:ALA:HB2	1:A:414:LEU:HG	1.96	0.46
1:A:460:TRP:H	1:A:460:TRP:CD1	2.32	0.46
1:A:508:TYR:CE1	1:A:510:ASP:HB3	2.50	0.46
1:B:303:PRO:HB2	1:B:349:MET:CE	2.45	0.46
3:L:33:LEU:HG	3:L:34:ALA:N	2.30	0.46
1:B:351:TYR:OH	1:B:441:PRO:HD3	2.16	0.46
1:B:233:HIS:C	1:B:233:HIS:CD2	2.93	0.46
3:L:61:ARG:CZ	3:L:79:GLN:HG3	2.46	0.46
1:A:229:PHE:CD1	1:A:229:PHE:C	2.93	0.46
3:L:22:THR:CG2	3:L:72:SER:HB3	2.46	0.46
1:B:484:VAL:HG23	1:B:485:ILE:HG12	1.97	0.46
2:D:121:VAL:O	2:D:209:LYS:HG3	2.15	0.46
1:B:548:ARG:HG2	1:B:548:ARG:HH11	1.80	0.46
1:A:252:VAL:HG22	1:A:269:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:SER:HA	1:B:249:ILE:O	2.17	0.45
1:A:271:TRP:HH2	1:A:315:MET:HE1	1.81	0.45
1:A:286:TYR:O	1:A:357:LYS:HD3	2.15	0.45
3:L:190:LYS:O	3:L:210:ASN:HA	2.16	0.45
3:L:196:VAL:HG12	3:L:205:VAL:O	2.15	0.45
3:E:42:LYS:HE3	3:E:42:LYS:HB3	1.73	0.45
1:A:431:ILE:HA	1:A:475:LEU:HB3	1.98	0.45
2:H:82(B):SER:O	2:H:82(B):SER:OG	2.35	0.45
1:B:310:TRP:O	1:B:347:LYS:HE2	2.15	0.45
2:D:207:VAL:HG12	2:D:208:ASP:N	2.31	0.45
1:A:562:ILE:O	1:A:576:SER:HA	2.17	0.45
1:B:221:LEU:HB3	1:B:232:SER:HB3	1.99	0.45
1:B:351:TYR:HE2	1:B:440:SER:CA	2.26	0.45
1:A:192:LYS:NZ	1:A:544:GLU:HG3	2.32	0.45
3:L:2:ILE:HD13	3:L:27:GLU:HG2	1.99	0.45
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.51	0.45
3:L:155:GLN:HE21	3:L:158:ASN:HD21	1.65	0.45
2:D:35:SER:HA	2:D:49:ALA:O	2.17	0.45
3:E:142:ARG:HB2	3:E:173:TYR:CE2	2.52	0.45
2:H:83:ARG:O	2:H:111:VAL:HG11	2.16	0.45
1:B:525:PHE:C	1:B:526:LEU:HD23	2.42	0.45
3:E:40:GLN:CD	3:E:40:GLN:N	2.75	0.45
1:A:233:HIS:CD2	1:A:233:HIS:C	2.95	0.45
2:H:12:VAL:HG11	2:H:18:LEU:CG	2.45	0.45
2:H:13:LYS:HE3	2:H:113:ALA:O	2.17	0.45
1:B:351:TYR:CZ	1:B:441:PRO:CG	3.00	0.45
3:E:108:ARG:HG2	3:E:140:TYR:CG	2.52	0.45
1:A:206:THR:OG1	1:A:265:LEU:O	2.28	0.45
3:E:61:ARG:HB2	3:E:76:ASN:O	2.17	0.45
3:E:158:ASN:HD22	3:E:181:LEU:HD21	1.82	0.45
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.79	0.44
1:A:443:LYS:HD3	1:A:508:TYR:OH	2.17	0.44
1:B:300:VAL:HG21	1:B:309:TYR:O	2.17	0.44
1:B:378:ASN:HD22	4:B:705:NAG:H83	1.82	0.44
2:D:93:THR:HB	2:D:100(E):PHE:HB3	1.99	0.44
3:L:118:PHE:HA	3:L:119:PRO:HD3	1.88	0.44
1:A:296:ALA:HB2	1:A:349:MET:HG3	1.98	0.44
1:A:480:ARG:HD2	1:A:480:ARG:HA	1.73	0.44
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.00	0.44
2:D:50:GLU:OE1	2:D:95:ASP:OD2	2.35	0.44
2:H:124:LEU:HD22	3:L:118:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:103:TRP:CB	3:L:43:SER:HB2	2.45	0.44
1:B:319:LEU:HD23	1:B:332:GLN:HG2	1.98	0.44
3:E:8:PRO:HG3	3:E:11:LEU:HD13	1.99	0.44
1:A:485:ILE:HD12	1:A:525:PHE:CE2	2.53	0.44
1:A:577:LEU:C	1:A:577:LEU:HD23	2.43	0.44
2:H:101:ALA:HA	3:L:46:LEU:HD22	1.98	0.44
1:B:298:SER:HB2	1:B:310:TRP:CD1	2.52	0.44
2:D:52:SER:HB3	2:D:56:TYR:HB2	2.00	0.44
2:D:148:GLU:CD	2:D:149:PRO:HA	2.42	0.44
2:H:148:GLU:OE1	2:H:149:PRO:HA	2.18	0.44
3:L:46:LEU:HD11	3:L:49:TYR:HB3	2.00	0.44
1:B:485:ILE:HD12	1:B:525:PHE:CD2	2.52	0.44
3:E:158:ASN:ND2	3:E:179:LEU:HD11	2.33	0.44
1:A:268:THR:OG1	1:A:321:VAL:O	2.31	0.43
1:A:360:ASP:OD2	1:A:419:SER:OG	2.32	0.43
2:H:34:MET:HE3	2:H:34:MET:HB3	1.76	0.43
2:H:130:SER:HB3	3:L:116:PHE:HB3	1.99	0.43
1:B:490:GLN:OE1	1:B:490:GLN:HA	2.18	0.43
2:D:67:PHE:CD2	2:D:82:MET:HG2	2.53	0.43
2:D:162:GLY:C	2:D:182:VAL:HG23	2.43	0.43
2:D:163:VAL:HG22	2:D:182:VAL:HB	2.00	0.43
3:E:118:PHE:HA	3:E:119:PRO:HD3	1.88	0.43
3:E:118:PHE:O	3:E:132:VAL:HG23	2.18	0.43
1:A:346:ASP:OD2	1:A:407:TYR:OH	2.24	0.43
3:L:117:ILE:HD12	3:L:194:CYS:HB2	2.00	0.43
3:L:120:PRO:HD3	3:L:132:VAL:HG22	2.01	0.43
2:D:12:VAL:HG11	2:D:82(C):LEU:HD12	2.01	0.43
3:E:147:GLN:CD	3:E:154:LEU:HD11	2.44	0.43
1:B:460:TRP:CD2	1:B:500:PRO:HA	2.53	0.43
1:B:502:ILE:HB	2:D:99:SER:HB3	2.00	0.43
1:A:502:ILE:HD13	1:A:502:ILE:HG21	1.85	0.42
1:A:527:ASP:HB3	1:A:534:ASN:HD22	1.84	0.42
1:B:566:PHE:CZ	1:B:575:ILE:HG13	2.54	0.42
3:L:185:ASP:HA	3:L:188:LYS:HG3	2.00	0.42
1:B:467:GLY:HA3	1:B:478:ASN:O	2.18	0.42
2:D:85:GLU:OE1	2:D:85:GLU:N	2.51	0.42
2:D:144:ASP:HB3	2:D:175:LEU:HD22	2.02	0.42
2:D:67:PHE:HA	2:D:81:GLU:O	2.19	0.42
2:D:121:VAL:HG12	2:D:142:VAL:HG13	2.01	0.42
2:D:193:THR:HB	2:D:210:LYS:HE2	2.01	0.42
3:E:194:CYS:O	3:E:206:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TRP:CH2	1:A:315:MET:HE1	2.55	0.42
2:H:20:LEU:N	2:H:20:LEU:HD23	2.34	0.42
3:L:89:GLN:HG2	3:L:90:HIS:N	2.33	0.42
2:D:34:MET:HE3	2:D:34:MET:HB3	1.95	0.42
1:A:229:PHE:CE2	1:A:265:LEU:HB3	2.53	0.42
3:L:210:ASN:O	3:L:213:GLU:HG3	2.19	0.42
1:B:573:TRP:CE2	1:B:596:LYS:HB2	2.54	0.42
1:A:498:THR:O	1:A:498:THR:HG22	2.18	0.42
2:H:52:SER:HB3	2:H:56:TYR:HB2	2.02	0.42
3:L:146:VAL:HA	3:L:195:GLU:O	2.19	0.42
1:B:192:LYS:HD2	1:B:545:ILE:O	2.20	0.42
2:D:148:GLU:HG2	2:D:176:TYR:CD2	2.55	0.42
3:E:134:CYS:HB2	3:E:148:TRP:CZ2	2.55	0.42
1:A:178:VAL:HG21	1:A:255:VAL:HG12	2.01	0.42
1:A:438:ILE:HG22	1:A:459:SER:HB2	2.02	0.42
1:B:361:THR:HG23	1:B:417:ASN:HA	2.02	0.42
2:D:27:PHE:CE2	2:D:29:PHE:HA	2.54	0.42
2:D:49:ALA:HB1	2:D:69:ILE:HB	2.02	0.42
2:D:103:TRP:HB2	3:E:43:SER:HB2	2.02	0.42
3:E:40:GLN:HE21	3:E:83:PHE:HE2	1.67	0.42
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.65	0.42
1:B:454:TYR:CE1	1:B:510:ASP:HA	2.54	0.42
3:E:36:TYR:CD2	3:E:46:LEU:HA	2.55	0.42
3:E:151:ASP:OD1	3:E:191:VAL:N	2.53	0.42
1:A:216:CYS:SG	1:A:217:ILE:N	2.93	0.42
1:A:435:ARG:HB3	1:A:479:TRP:CD1	2.54	0.42
1:A:462:THR:HG22	1:A:487:ARG:NH2	2.34	0.42
3:L:164:THR:OG1	3:L:174:SER:N	2.52	0.42
3:E:146:VAL:HG12	3:E:161:GLU:OE2	2.19	0.41
1:A:370:LEU:HB3	1:A:408:ILE:HG13	2.01	0.41
2:H:156:SER:CA	2:H:197:ASN:HD21	2.33	0.41
1:B:181:LEU:HD11	1:B:572:ILE:HD13	2.02	0.41
3:E:113:PRO:HB3	3:E:139:PHE:CD1	2.55	0.41
1:A:271:TRP:CZ2	1:A:334:GLN:NE2	2.88	0.41
1:A:490:GLN:HA	1:A:490:GLN:OE1	2.20	0.41
2:H:200:HIS:ND1	2:H:202:PRO:HD2	2.36	0.41
1:B:320:ALA:HB2	1:B:330:TYR:O	2.21	0.41
1:B:414:LEU:HD23	1:B:414:LEU:HA	1.83	0.41
1:B:454:TYR:CZ	1:B:510:ASP:HA	2.55	0.41
1:B:588:ILE:HD12	1:B:588:ILE:H	1.85	0.41
1:A:221:LEU:O	1:A:231:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:HB3	1:A:230:ALA:HB3	2.02	0.41
2:D:72:ASP:OD1	2:D:74:ALA:N	2.51	0.41
1:A:393:GLU:O	1:A:397:LEU:HG	2.21	0.41
2:H:103:TRP:CD1	2:H:103:TRP:N	2.88	0.41
1:B:248:ARG:O	1:B:273:PRO:HD2	2.20	0.41
1:B:522:ALA:HA	1:B:538:THR:O	2.21	0.41
2:D:67:PHE:CE2	2:D:82:MET:HG2	2.54	0.41
1:A:249:ILE:HD13	1:A:249:ILE:HA	1.98	0.41
2:D:67:PHE:CE2	2:D:82:MET:HE3	2.56	0.41
3:E:118:PHE:N	3:E:133:VAL:O	2.45	0.41
1:B:460:TRP:HA	1:B:493:CYS:SG	2.60	0.41
1:B:460:TRP:CG	1:B:500:PRO:HA	2.56	0.41
3:E:151:ASP:H	3:E:191:VAL:HB	1.85	0.41
1:A:521:SER:O	1:A:539:VAL:HA	2.20	0.41
3:L:125:LEU:O	3:L:183:LYS:HE3	2.21	0.41
1:B:181:LEU:HD12	1:B:181:LEU:HA	1.65	0.41
1:B:366:ALA:CB	1:B:414:LEU:HG	2.50	0.41
3:E:54:LEU:HA	3:E:54:LEU:HD23	1.61	0.41
1:A:288:ASN:O	1:A:289:GLU:HG2	2.20	0.41
1:A:509:ASN:HD21	1:A:526:LEU:HG	1.85	0.41
1:A:181:LEU:HA	1:A:567:LEU:HD13	2.03	0.40
1:A:533:GLU:HG3	1:A:554:GLU:O	2.21	0.40
2:H:156:SER:HA	2:H:197:ASN:HD21	1.85	0.40
1:B:202:LEU:HA	1:B:202:LEU:HD22	1.84	0.40
1:B:252:VAL:HG11	1:B:291:TYR:HB2	2.03	0.40
1:A:218:THR:CG2	1:A:219:ASP:H	2.34	0.40
1:A:319:LEU:HD22	1:A:332:GLN:HG2	2.03	0.40
3:L:140:TYR:CG	3:L:141:PRO:HA	2.57	0.40
1:B:250:ILE:HD12	1:B:271:TRP:HZ3	1.84	0.40
2:D:170:LEU:HB2	2:D:176:TYR:CE1	2.55	0.40
1:B:217:ILE:CD1	1:B:235:GLU:HB2	2.52	0.40
2:D:103:TRP:N	2:D:103:TRP:CD1	2.89	0.40
2:D:119:PRO:CB	2:D:145:TYR:HB3	2.43	0.40
3:L:194:CYS:O	3:L:206:THR:HA	2.21	0.40
1:B:250:ILE:HD12	1:B:271:TRP:CE3	2.57	0.40
1:B:257:ASP:OD2	1:B:261:GLU:HA	2.20	0.40
1:B:573:TRP:CZ2	1:B:596:LYS:HB2	2.56	0.40
2:D:38:ARG:HA	2:D:89:MET:O	2.21	0.40
3:E:124:GLN:HG2	3:E:129:THR:O	2.22	0.40
1:B:450:GLN:OE1	1:B:468:ASP:HB3	2.21	0.40
2:D:103:TRP:CE3	3:E:44:PRO:HD2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ASP:OD2	3:E:79:GLN:NE2[3_544]	1.77	0.43
3:L:79:GLN:OE1	1:B:360:ASP:OD2[3_545]	1.82	0.38

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	411/441 (93%)	379 (92%)	32 (8%)	0	100	100
1	B	412/441 (93%)	380 (92%)	31 (8%)	1 (0%)	44	77
2	D	220/234 (94%)	207 (94%)	12 (6%)	1 (0%)	25	61
2	H	221/234 (94%)	211 (96%)	10 (4%)	0	100	100
3	E	207/214 (97%)	190 (92%)	17 (8%)	0	100	100
3	L	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
All	All	1683/1778 (95%)	1566 (93%)	115 (7%)	2 (0%)	48	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	14	PRO
1	B	353	PRO

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	375/395 (95%)	375 (100%)	0	100	100
1	B	376/395 (95%)	375 (100%)	1 (0%)	91	96
2	D	186/198 (94%)	184 (99%)	2 (1%)	70	87
2	H	187/198 (94%)	186 (100%)	1 (0%)	86	94
3	E	183/187 (98%)	183 (100%)	0	100	100
3	L	186/187 (100%)	186 (100%)	0	100	100
All	All	1493/1560 (96%)	1489 (100%)	4 (0%)	91	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	92	CYS
1	B	415	LYS
2	D	92	CYS
2	D	196	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	A	326	ASN
1	A	333	HIS
1	A	381	ASN
1	A	492	GLN
1	A	509	ASN
1	A	530	GLN
1	A	534	ASN
1	A	570	ASN
2	H	39	GLN
2	H	164	HIS
2	H	197	ASN
2	H	200	HIS
3	L	38	GLN
3	L	124	GLN
3	L	137	ASN
3	L	155	GLN
1	B	195	ASN
1	B	334	GLN
1	B	358	GLN
1	B	406	HIS

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Mol	Chain	Res	Type
1	B	497	ASN
3	E	155	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	$\# Z > 2$
4	NAG	A	705	1	14,14,15	0.87	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	A	704	1	14,14,15	0.41	0	17,19,21	0.53	0
4	NAG	A	702	1	14,14,15	1.16	2 (14%)	17,19,21	0.57	0
4	NAG	B	701	1	14,14,15	0.80	0	17,19,21	1.05	1 (5%)
4	NAG	B	705	1	14,14,15	0.77	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	A	701	1	14,14,15	0.31	0	17,19,21	0.92	1 (5%)
4	NAG	B	703	1	14,14,15	0.46	0	17,19,21	0.49	0
4	NAG	B	704	1	14,14,15	0.57	0	17,19,21	0.71	0
4	NAG	A	703	1	14,14,15	0.44	0	17,19,21	0.81	1 (5%)
4	NAG	B	702	1	14,14,15	1.04	1 (7%)	17,19,21	1.06	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	A	705	1	-	4/6/23/26	0/1/1/1
4	NAG	A	704	1	-	2/6/23/26	0/1/1/1
4	NAG	A	702	1	-	2/6/23/26	0/1/1/1
4	NAG	B	701	1	-	1/6/23/26	0/1/1/1
4	NAG	B	705	1	-	2/6/23/26	0/1/1/1
4	NAG	A	701	1	-	4/6/23/26	0/1/1/1
4	NAG	B	703	1	-	3/6/23/26	0/1/1/1
4	NAG	B	704	1	-	2/6/23/26	0/1/1/1
4	NAG	A	703	1	-	1/6/23/26	0/1/1/1
4	NAG	B	702	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	NAG	O5-C1	3.21	1.48	1.43
4	B	702	NAG	C1-C2	3.16	1.57	1.52
4	A	705	NAG	O5-C1	3.05	1.48	1.43
4	B	705	NAG	O5-C1	2.79	1.48	1.43
4	A	702	NAG	C1-C2	2.73	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	NAG	C1-O5-C5	3.55	117.01	112.19
4	B	702	NAG	C2-N2-C7	3.50	127.88	122.90
4	A	701	NAG	C1-O5-C5	3.29	116.66	112.19
4	B	705	NAG	C1-O5-C5	2.79	115.97	112.19
4	A	703	NAG	C1-O5-C5	2.53	115.62	112.19
4	A	705	NAG	C1-O5-C5	2.25	115.24	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	702	NAG	C3-C2-N2-C7
4	A	702	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	702	NAG	O5-C5-C6-O6
4	A	705	NAG	C4-C5-C6-O6
4	A	701	NAG	O5-C5-C6-O6
4	B	704	NAG	O5-C5-C6-O6
4	A	705	NAG	O5-C5-C6-O6
4	B	702	NAG	C4-C5-C6-O6
4	A	702	NAG	C4-C5-C6-O6
4	A	701	NAG	C4-C5-C6-O6
4	A	701	NAG	C8-C7-N2-C2
4	A	701	NAG	O7-C7-N2-C2
4	A	704	NAG	C8-C7-N2-C2
4	A	704	NAG	O7-C7-N2-C2
4	A	705	NAG	C8-C7-N2-C2
4	A	705	NAG	O7-C7-N2-C2
4	B	703	NAG	C8-C7-N2-C2
4	B	703	NAG	O7-C7-N2-C2
4	B	705	NAG	C8-C7-N2-C2
4	B	705	NAG	O7-C7-N2-C2
4	B	704	NAG	C4-C5-C6-O6
4	A	703	NAG	O5-C5-C6-O6
4	B	703	NAG	O5-C5-C6-O6
4	B	702	NAG	C1-C2-N2-C7
4	B	701	NAG	O5-C5-C6-O6

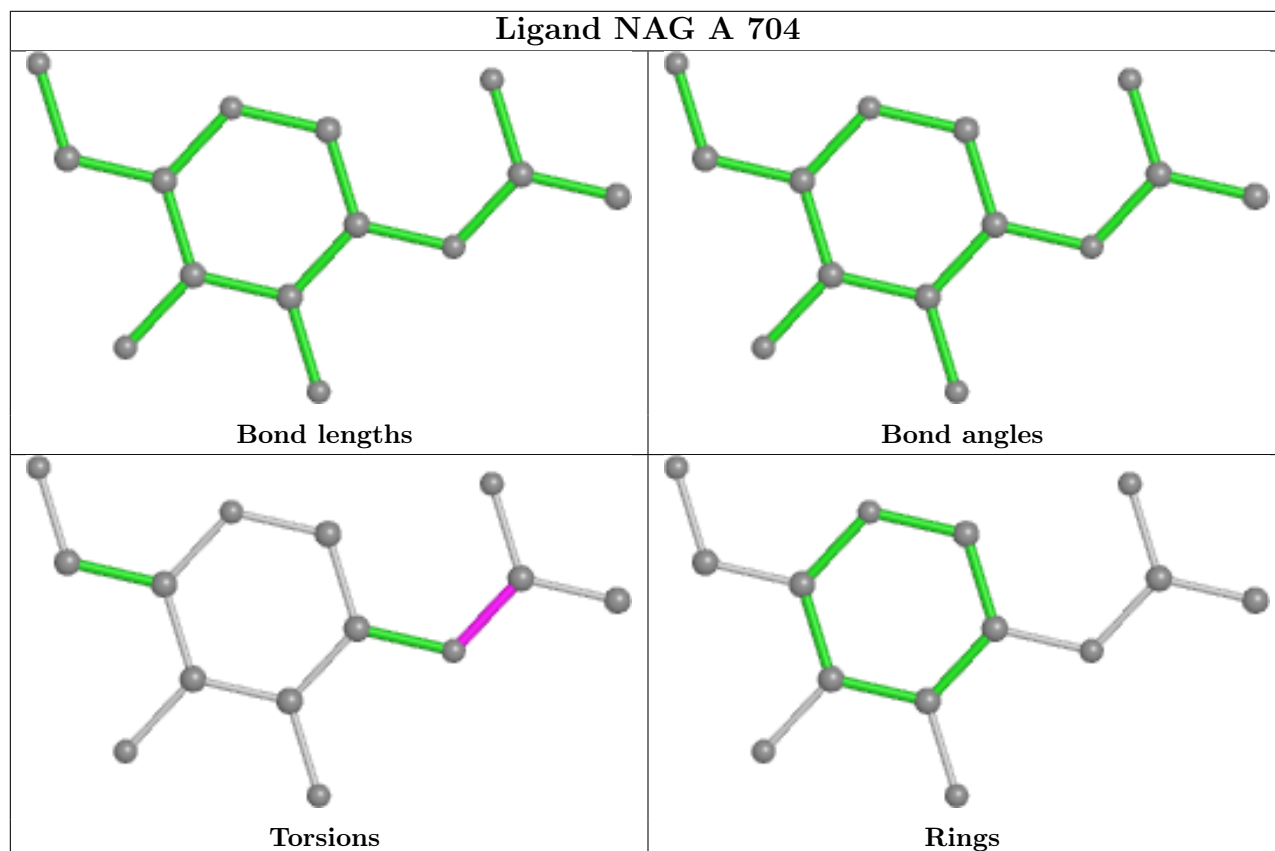
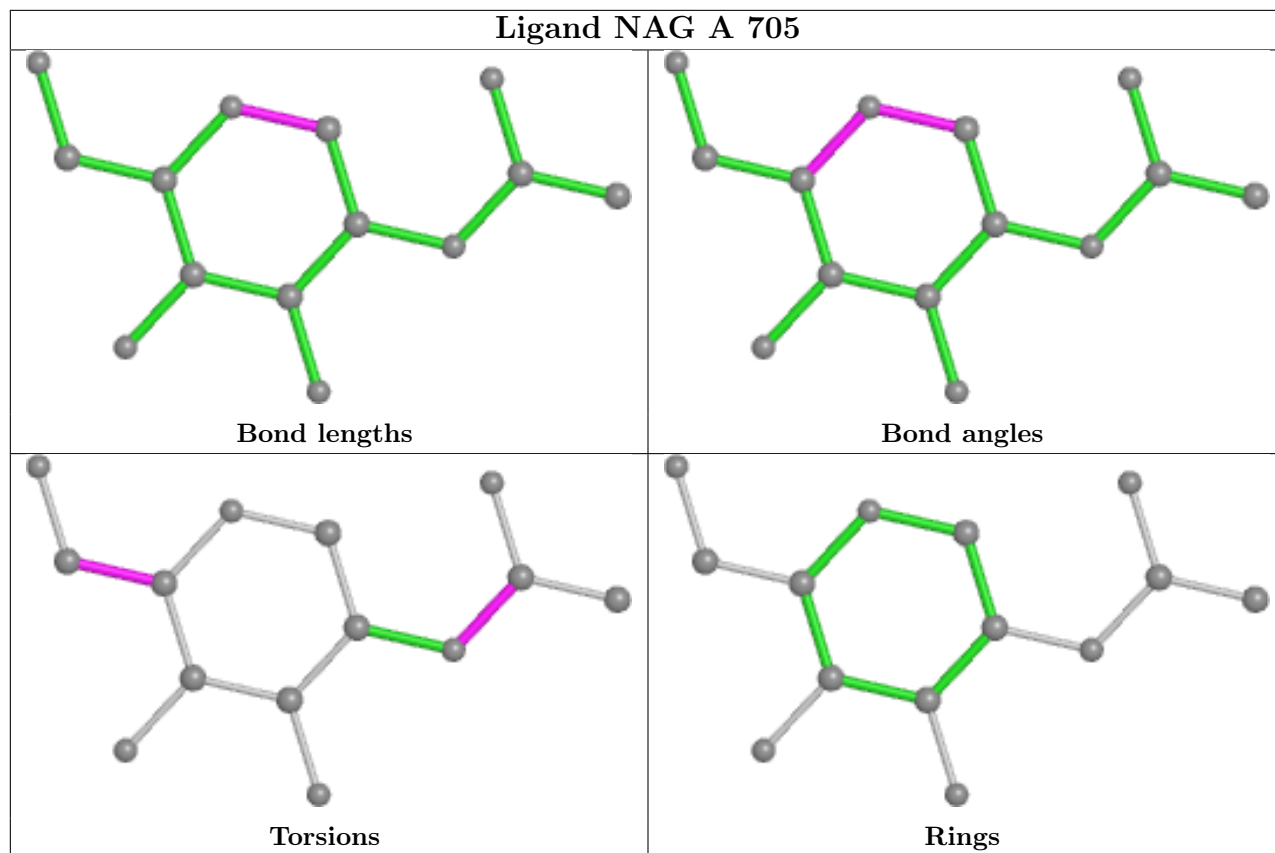
There are no ring outliers.

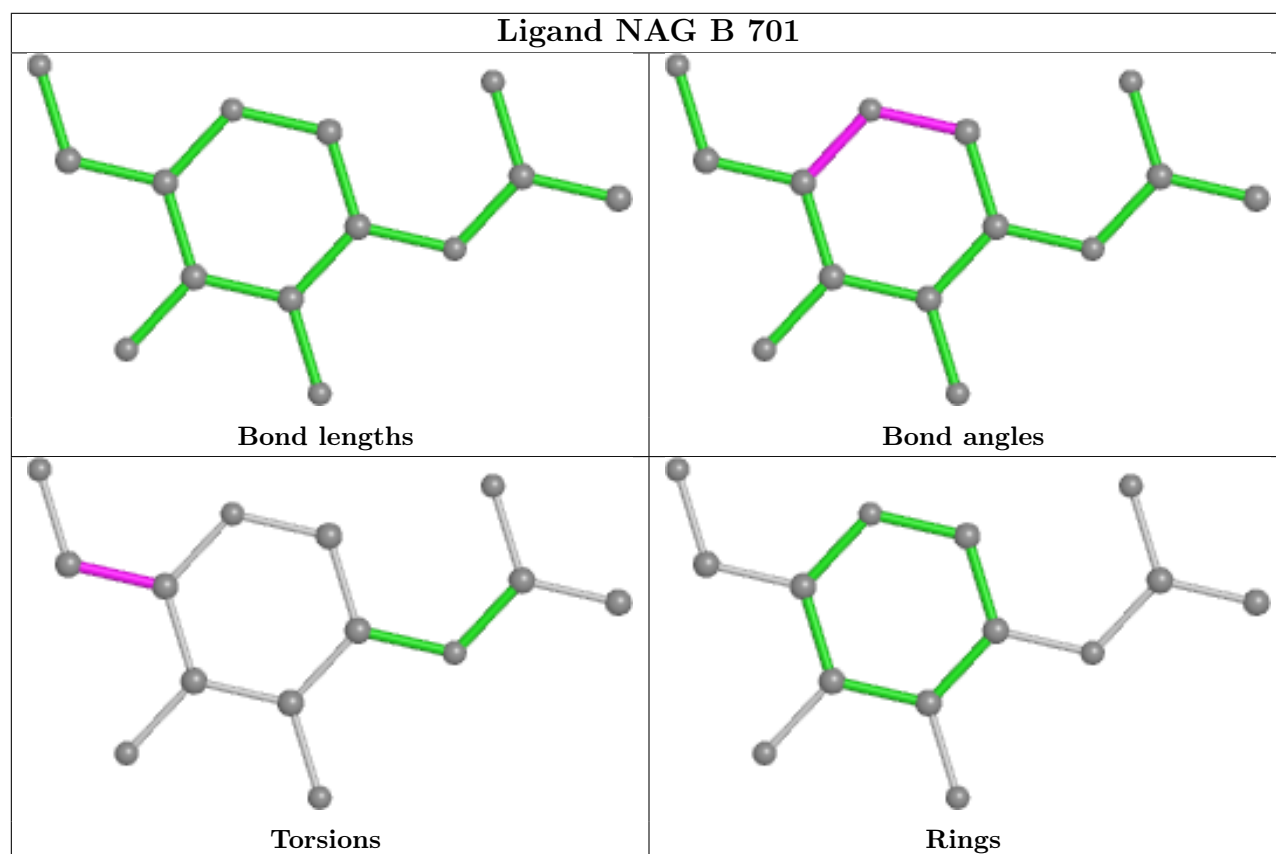
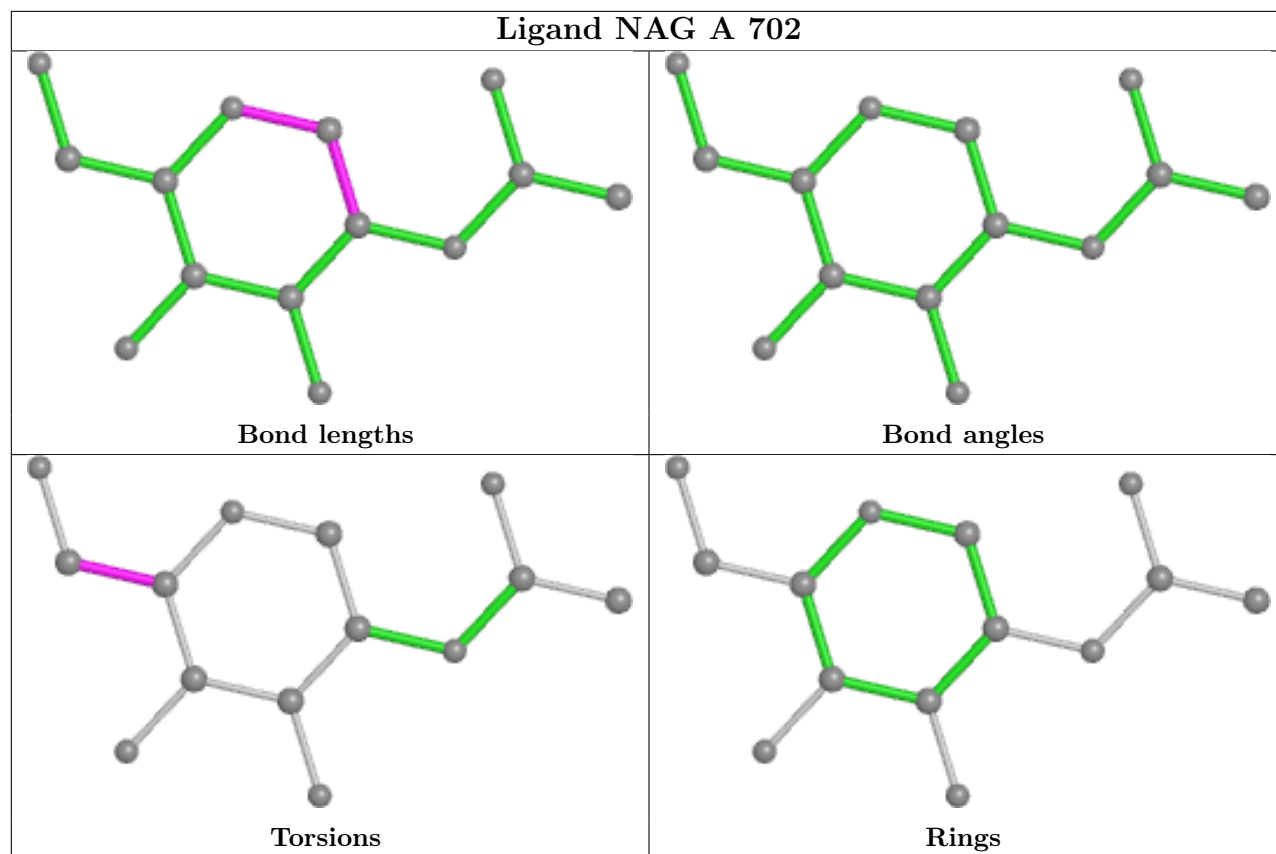
2 monomers are involved in 2 short contacts:

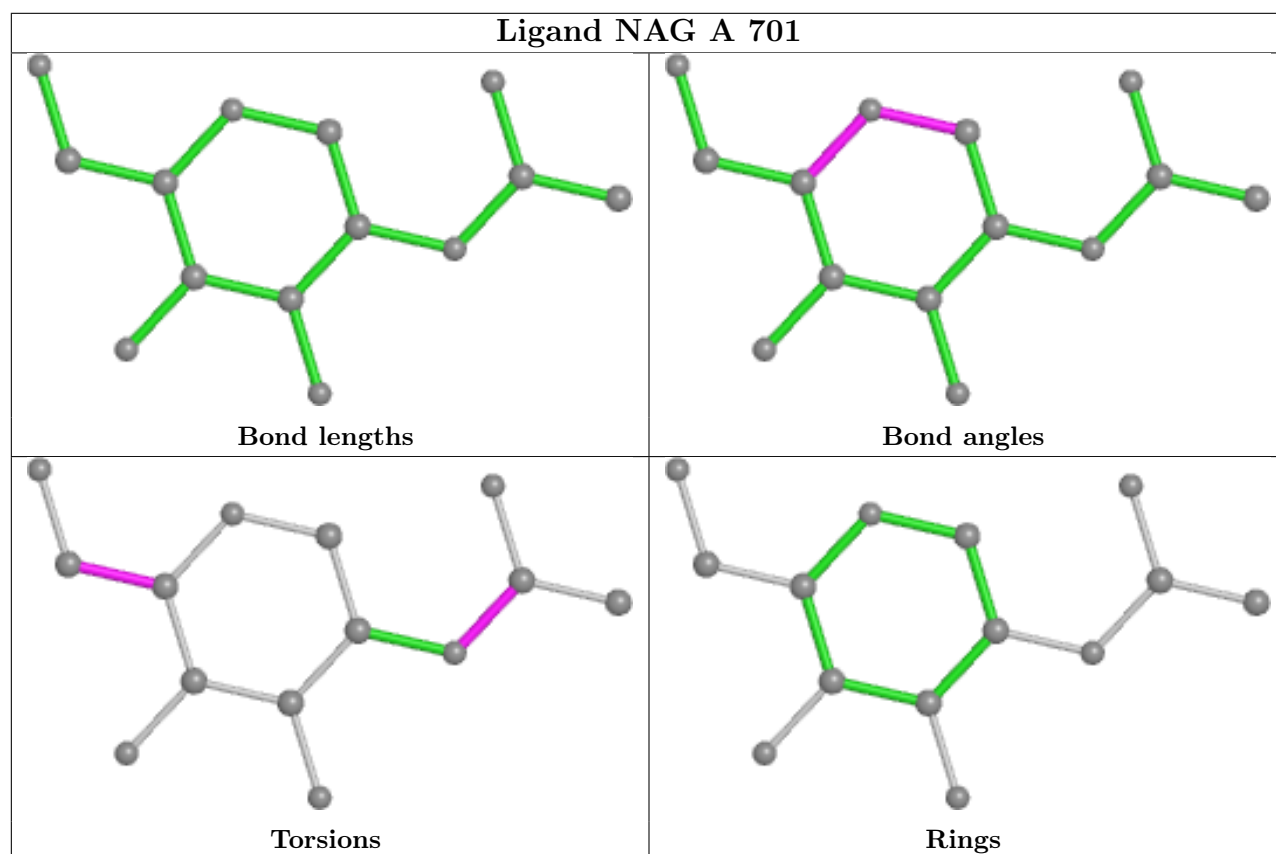
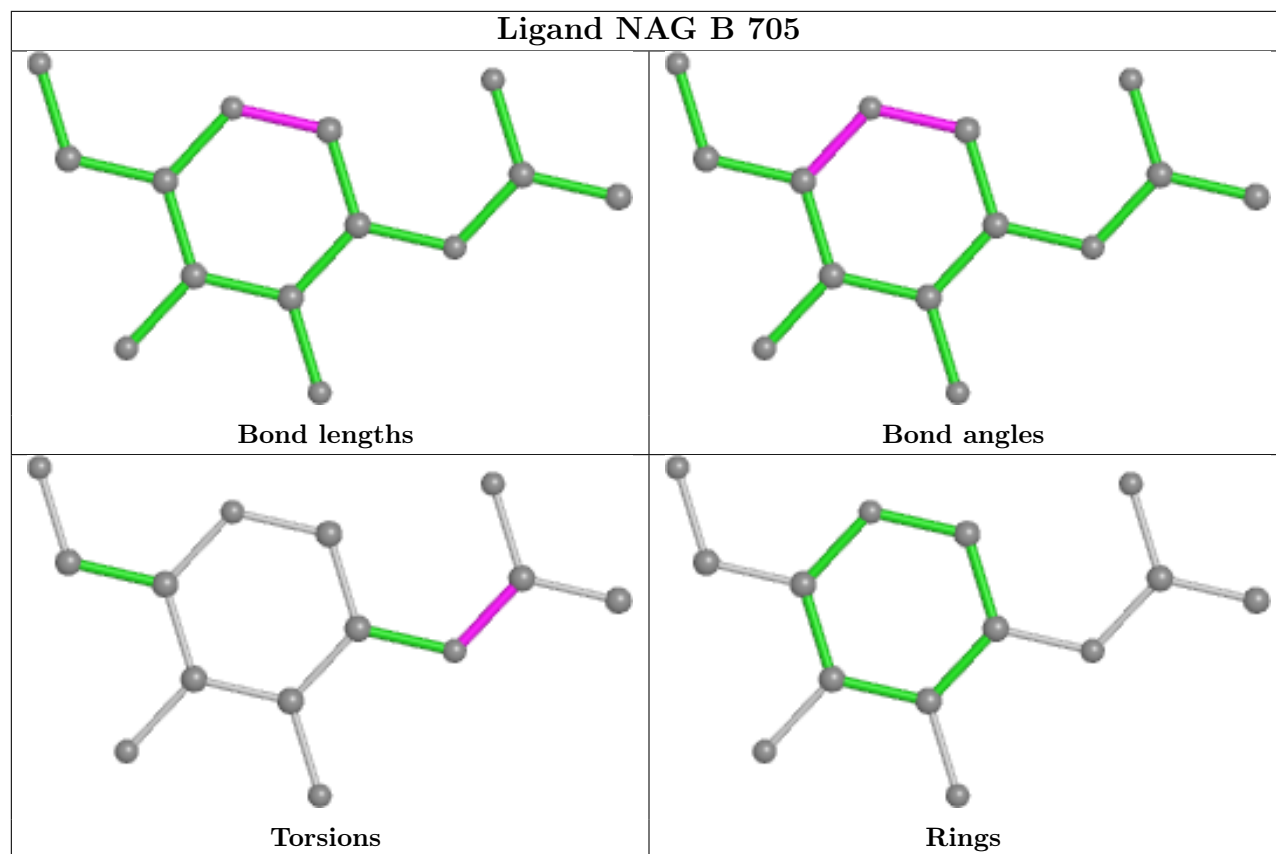
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	704	NAG	1	0
4	B	705	NAG	1	0

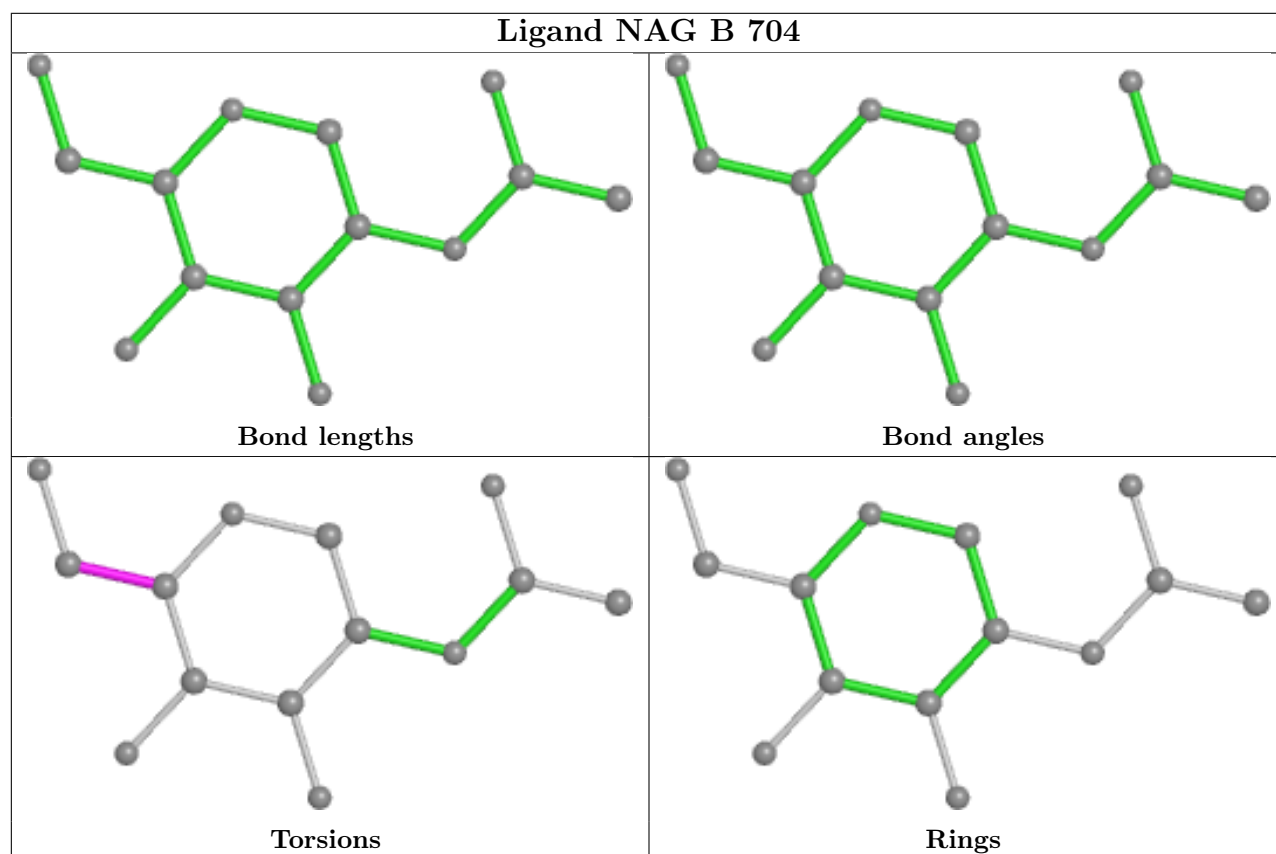
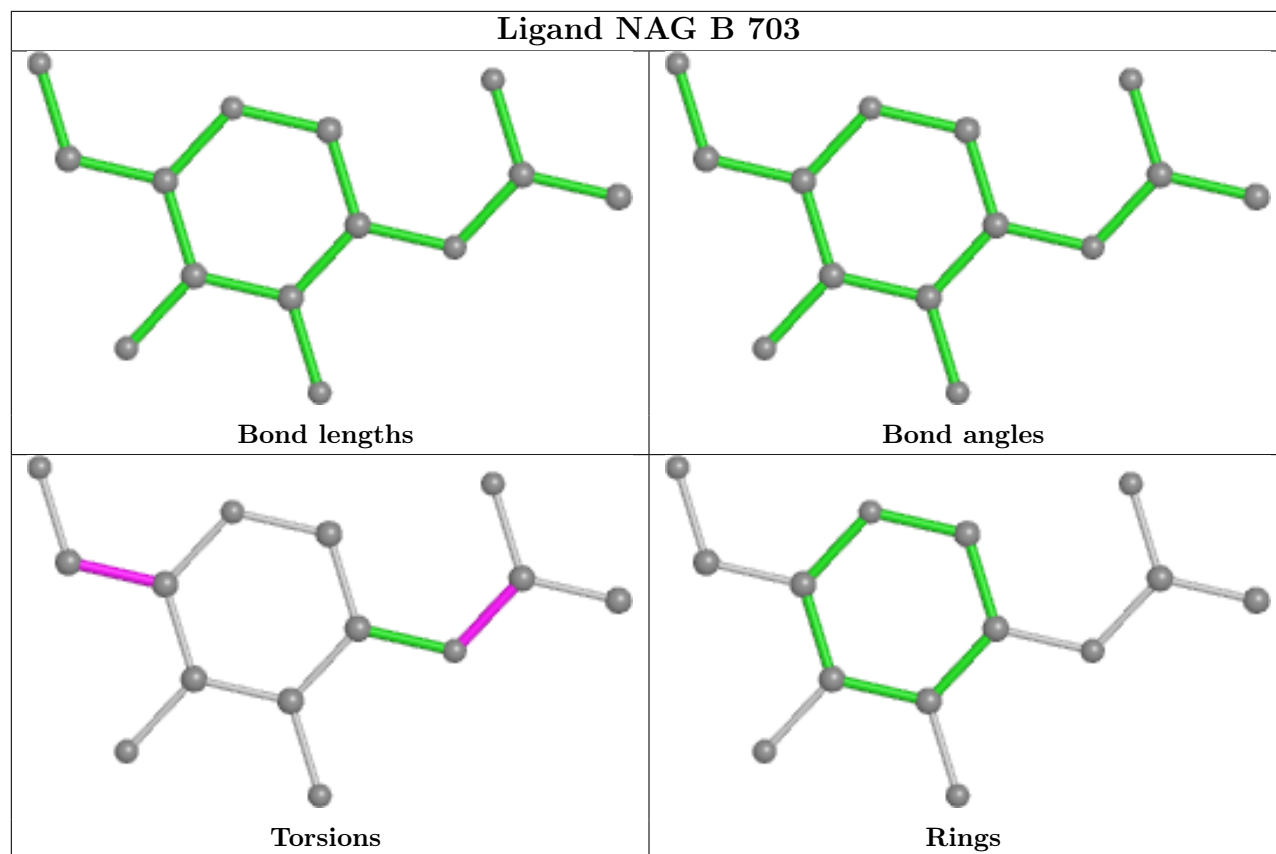
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

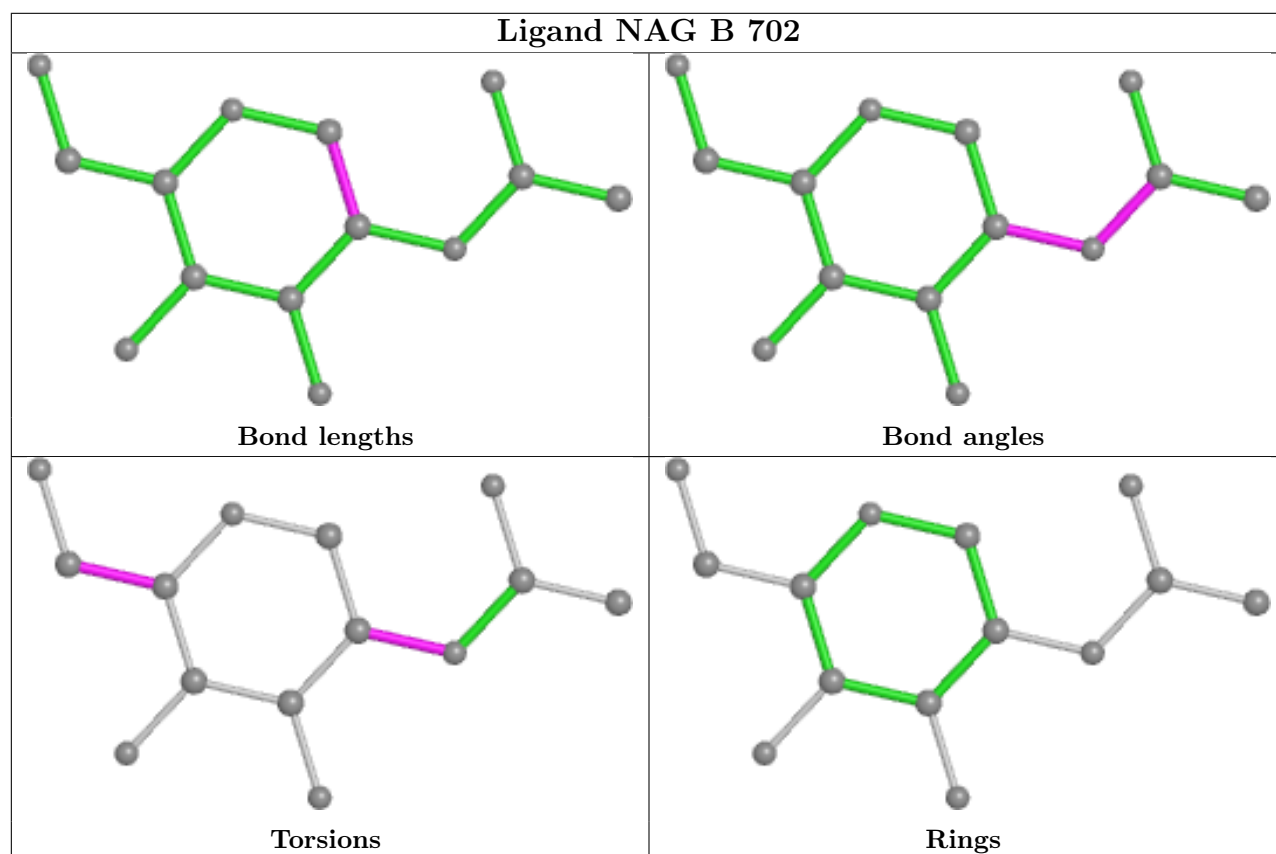
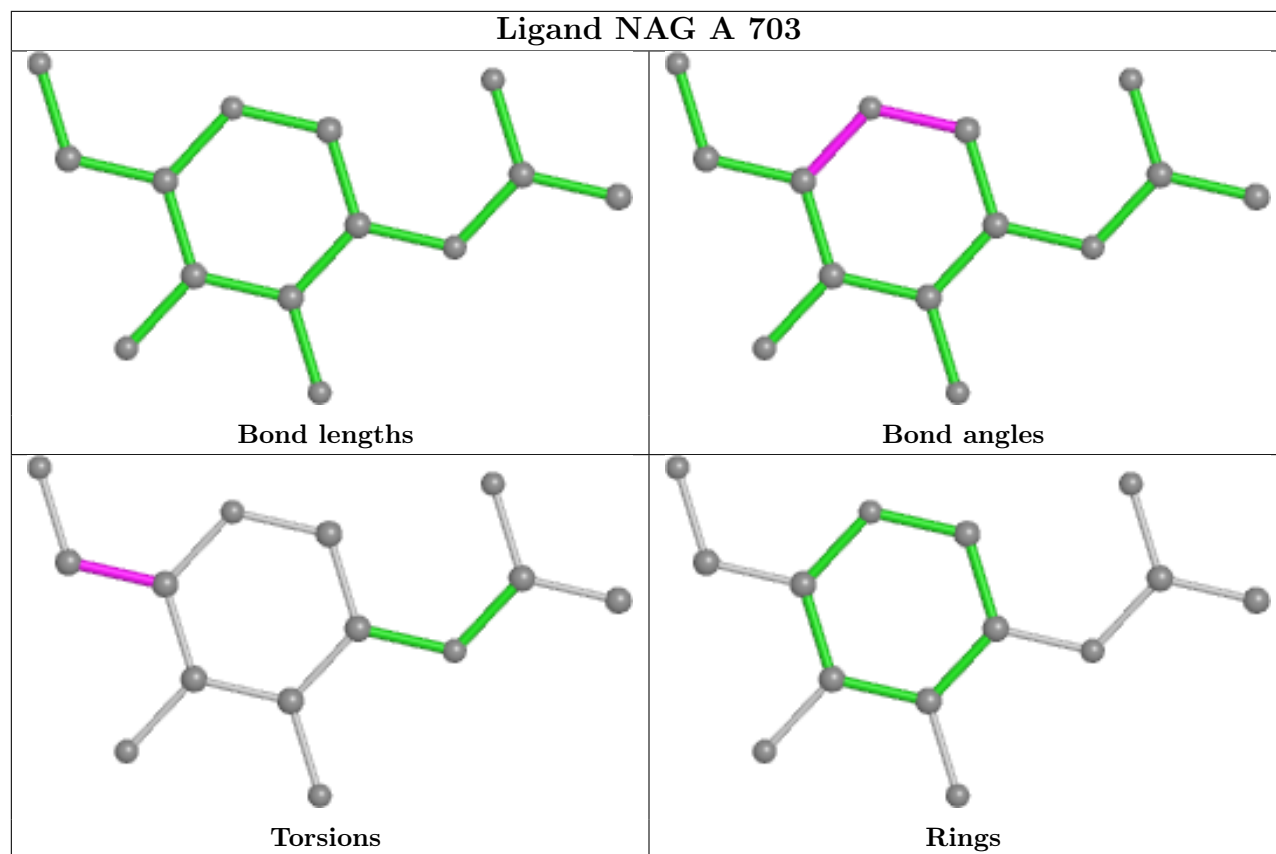
equivalents in the CSD to analyse the geometry.











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	417/441 (94%)	-0.40	3 (0%) 84 68	37, 52, 82, 102	0
1	B	418/441 (94%)	-0.30	1 (0%) 92 84	41, 53, 82, 107	0
2	D	222/234 (94%)	-0.16	2 (0%) 81 63	47, 63, 84, 110	0
2	H	223/234 (95%)	-0.18	1 (0%) 89 77	46, 63, 83, 100	0
3	E	209/214 (97%)	0.07	6 (2%) 54 32	39, 61, 104, 113	0
3	L	214/214 (100%)	-0.17	1 (0%) 87 75	40, 60, 92, 101	0
All	All	1703/1778 (95%)	-0.23	14 (0%) 82 66	37, 56, 89, 113	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	151	ASP	3.5
2	D	133	GLY	3.0
2	H	130	SER	2.9
1	B	360	ASP	2.8
3	E	154	LEU	2.7
1	A	209	VAL	2.6
1	A	360	ASP	2.5
3	E	192	TYR	2.5
2	D	130	SER	2.3
1	A	587	VAL	2.3
3	L	214	CYS	2.3
3	E	190	LYS	2.2
3	E	193	ALA	2.1
3	E	191	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

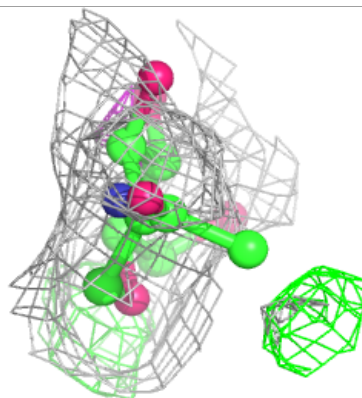
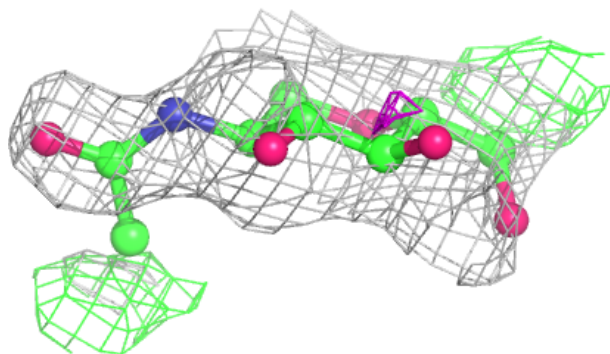
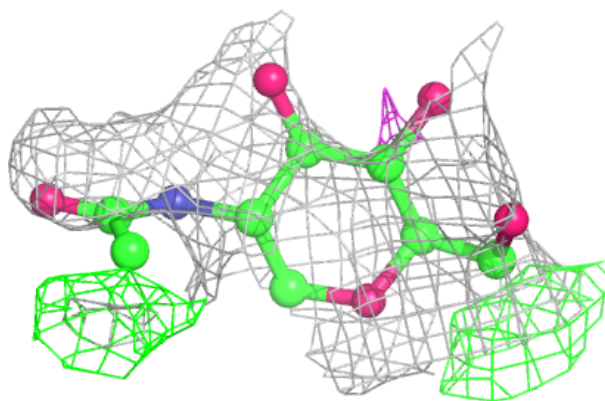
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	705	14/15	0.31	0.18	80,88,97,97	0
4	NAG	B	702	14/15	0.41	0.18	108,125,130,133	0
4	NAG	A	702	14/15	0.62	0.15	94,109,119,121	0
4	NAG	B	705	14/15	0.65	0.12	73,85,92,106	0
4	NAG	B	704	14/15	0.66	0.16	81,91,98,103	0
4	NAG	A	704	14/15	0.74	0.11	76,86,93,99	0
4	NAG	B	703	14/15	0.84	0.11	61,68,72,77	0
4	NAG	A	701	14/15	0.86	0.11	53,62,69,69	0
4	NAG	B	701	14/15	0.89	0.11	53,61,71,75	0
4	NAG	A	703	14/15	0.91	0.08	67,74,77,82	0

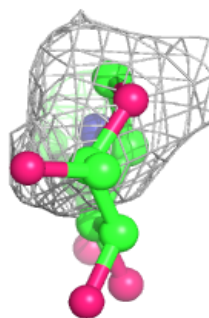
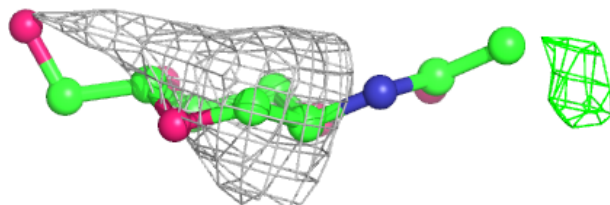
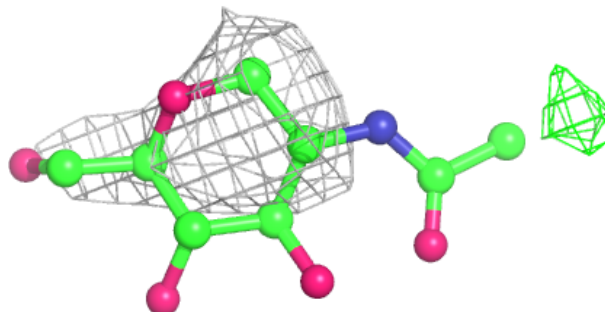
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG A 705:

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

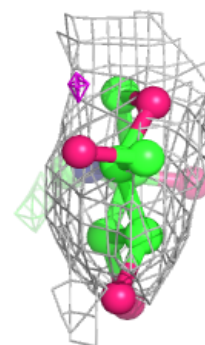
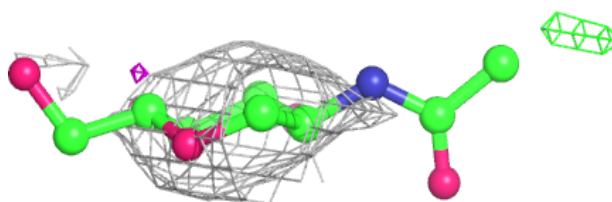
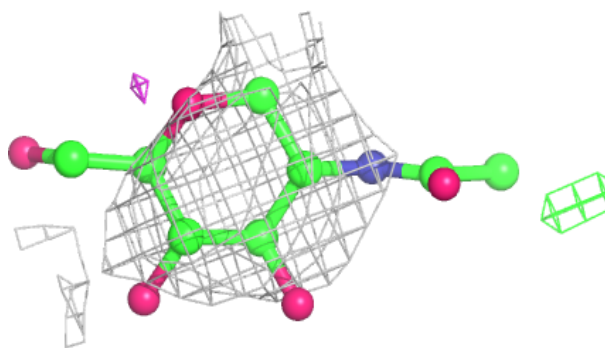
**Electron density around NAG B 702:**

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

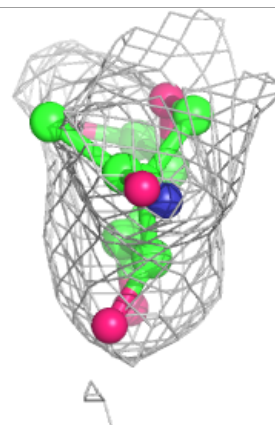
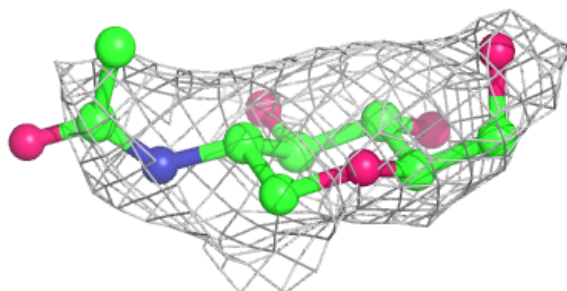
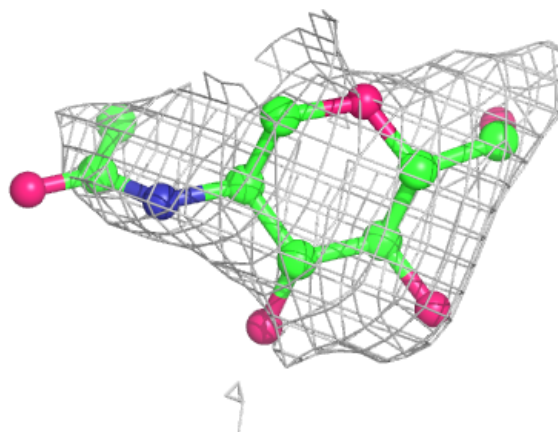


Electron density around NAG A 702:

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

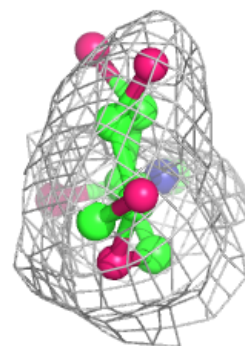
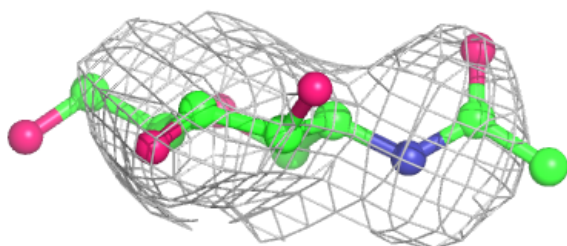
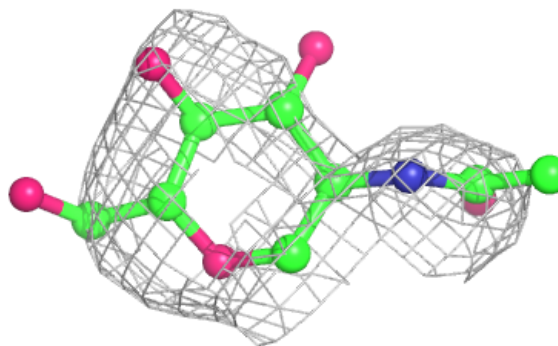
**Electron density around NAG B 705:**

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

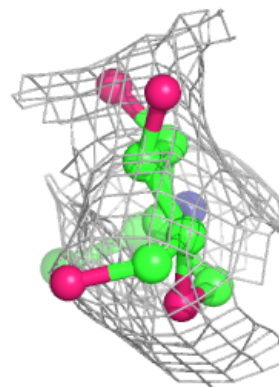
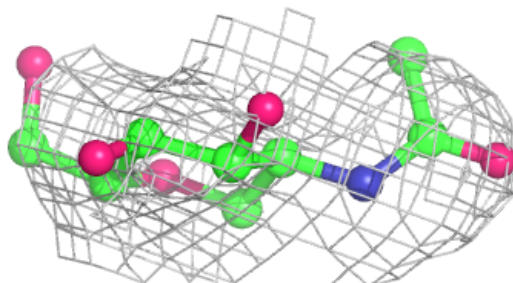
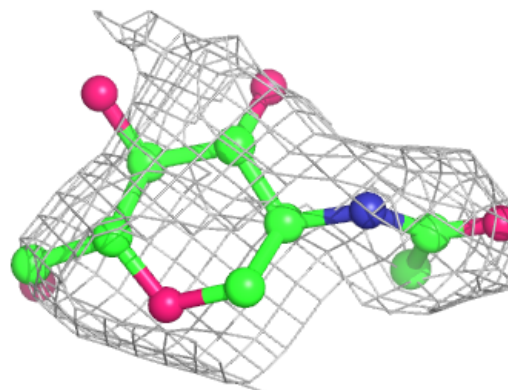


Electron density around NAG B 704:

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

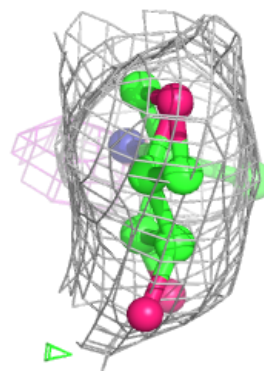
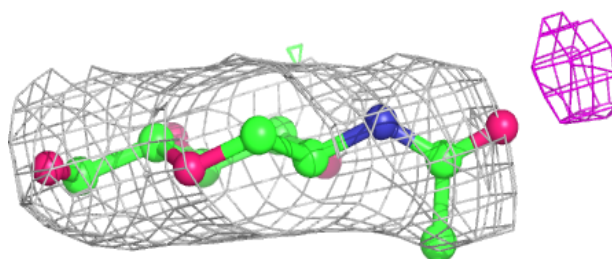
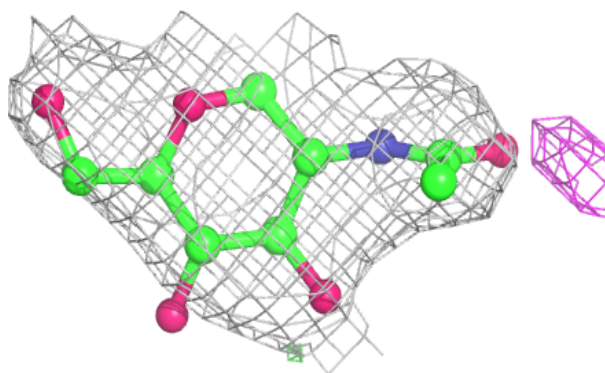
**Electron density around NAG A 704:**

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

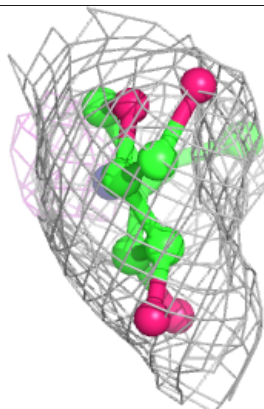
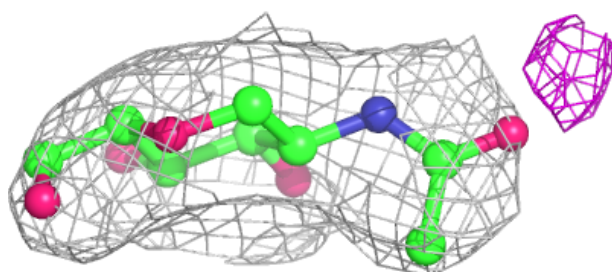
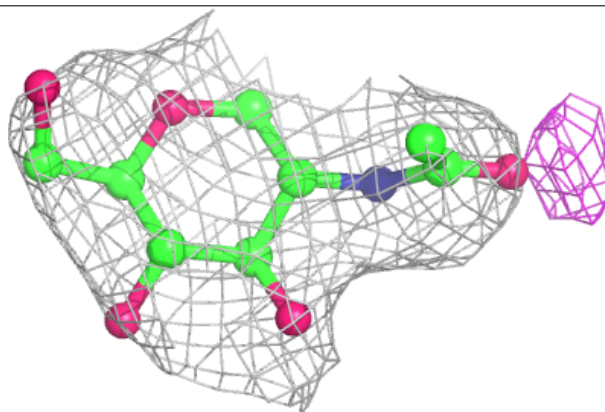


Electron density around NAG B 703:

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

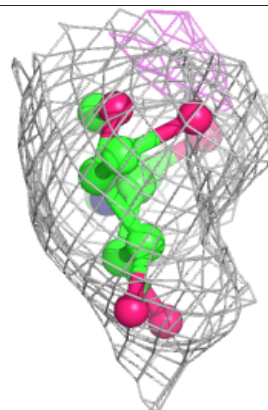
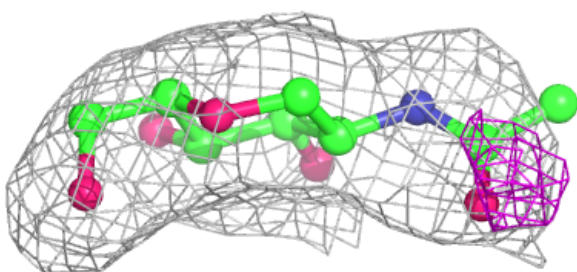
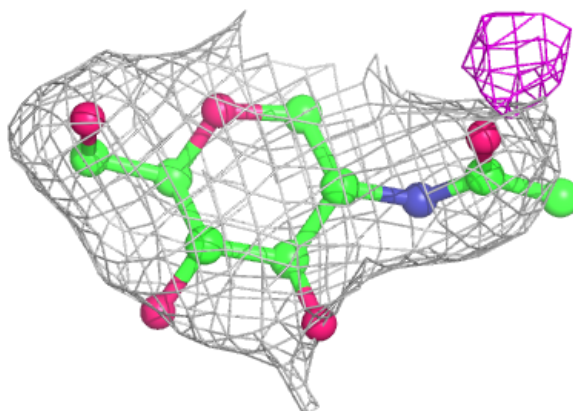
**Electron density around NAG A 701:**

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

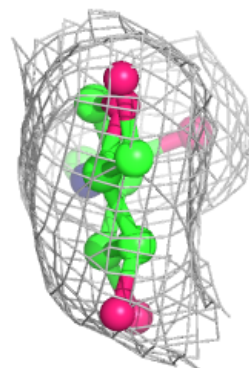
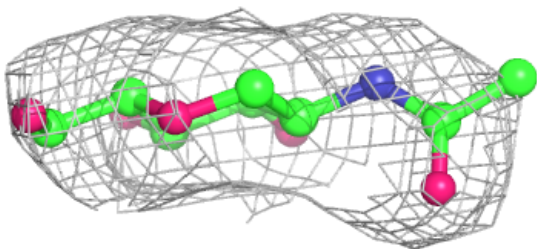
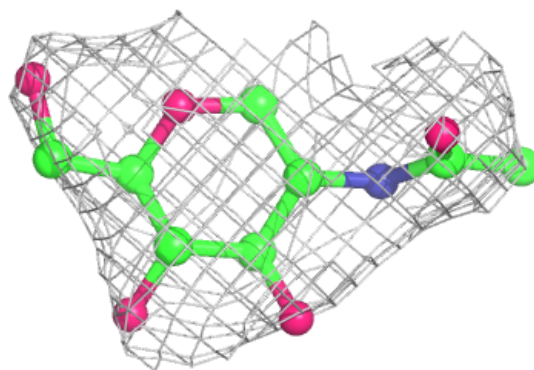


Electron density around NAG B 701:

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

**Electron density around NAG A 703:**

$2mF_o-DF_c$ (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.