



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 6IDD / pdb_00006idd
Title : Crystal structure of H7 hemagglutinin mutant SH1-AVPL (S138A, G186V, T221P, Q226L) from the influenza virus A/Shanghai/1/2013 (H7N9)
Authors : Gao, G.F.; Xu, Y.; Qi, J.X.
Deposited on : 2018-09-09
Resolution : 2.38 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 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

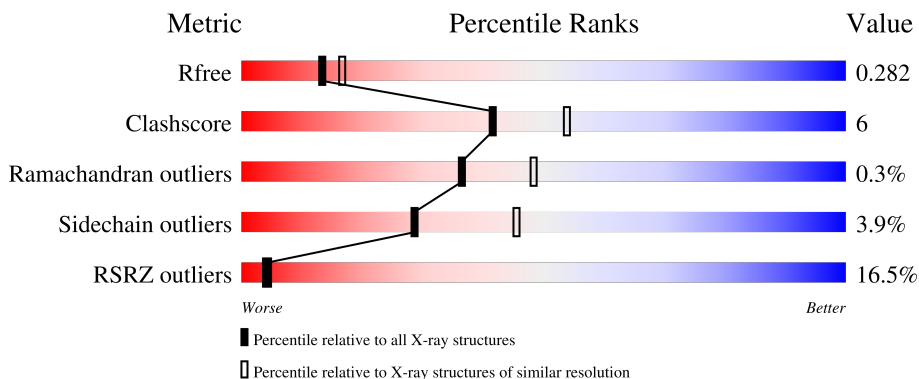
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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.



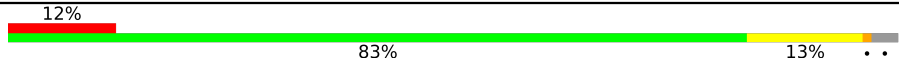
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	498	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">9% 81% 16% ..</p>
1	C	498	<div style="display: flex; align-items: center;"> <div style="width: 22%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">22% 75% 21% ..</p>
1	E	498	<div style="display: flex; align-items: center;"> <div style="width: 21%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">21% 81% 15% ..</p>
1	G	498	<div style="display: flex; align-items: center;"> <div style="width: 20%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">20% 80% 16% ..</p>
1	I	498	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">12% 77% 18% ..</p>

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Mol	Chain	Length	Quality of chain
1	K	498	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '12%', a large green segment in the middle labeled '83%', and a yellow segment on the right labeled '13%'. At the far right end of the bar, there are two small black dots.</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23265 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	485	3783	2347	670	744	22	0	0	0
1	C	484	3772	2339	669	742	22	0	0	0
1	E	484	3779	2345	669	743	22	0	0	0
1	G	484	3775	2343	669	741	22	0	0	0
1	I	484	3776	2344	668	742	22	0	0	0
1	K	484	3775	2342	668	743	22	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

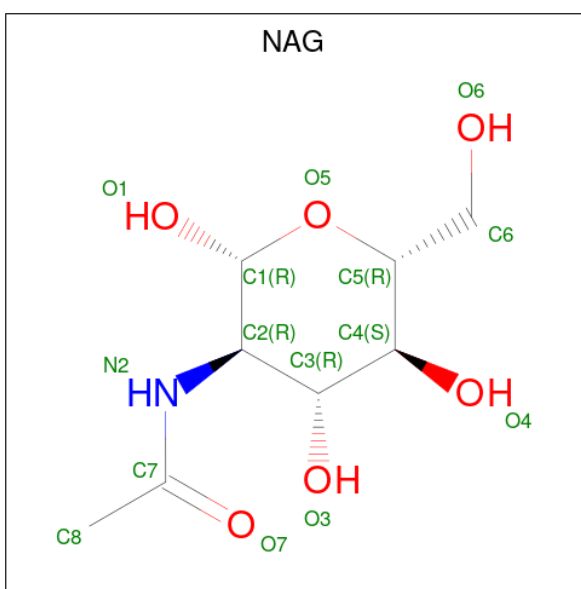
Chain	Residue	Modelled	Actual	Comment	Reference
A	165	ASN	SER	engineered mutation	UNP A0A088BEK2
A	267	ASP	ASN	engineered mutation	UNP A0A088BEK2
A	274	TYR	HIS	engineered mutation	UNP A0A088BEK2
A	392	THR	ASN	engineered mutation	UNP A0A088BEK2
C	165	ASN	SER	engineered mutation	UNP A0A088BEK2
C	267	ASP	ASN	engineered mutation	UNP A0A088BEK2
C	274	TYR	HIS	engineered mutation	UNP A0A088BEK2
C	392	THR	ASN	engineered mutation	UNP A0A088BEK2
E	165	ASN	SER	engineered mutation	UNP A0A088BEK2
E	267	ASP	ASN	engineered mutation	UNP A0A088BEK2
E	274	TYR	HIS	engineered mutation	UNP A0A088BEK2
E	392	THR	ASN	engineered mutation	UNP A0A088BEK2
G	165	ASN	SER	engineered mutation	UNP A0A088BEK2
G	267	ASP	ASN	engineered mutation	UNP A0A088BEK2
G	274	TYR	HIS	engineered mutation	UNP A0A088BEK2
G	392	THR	ASN	engineered mutation	UNP A0A088BEK2
I	165	ASN	SER	engineered mutation	UNP A0A088BEK2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	267	ASP	ASN	engineered mutation	UNP A0A088BEK2
I	274	TYR	HIS	engineered mutation	UNP A0A088BEK2
I	392	THR	ASN	engineered mutation	UNP A0A088BEK2
K	165	ASN	SER	engineered mutation	UNP A0A088BEK2
K	267	ASP	ASN	engineered mutation	UNP A0A088BEK2
K	274	TYR	HIS	engineered mutation	UNP A0A088BEK2
K	392	THR	ASN	engineered mutation	UNP A0A088BEK2

- Molecule 2 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
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		

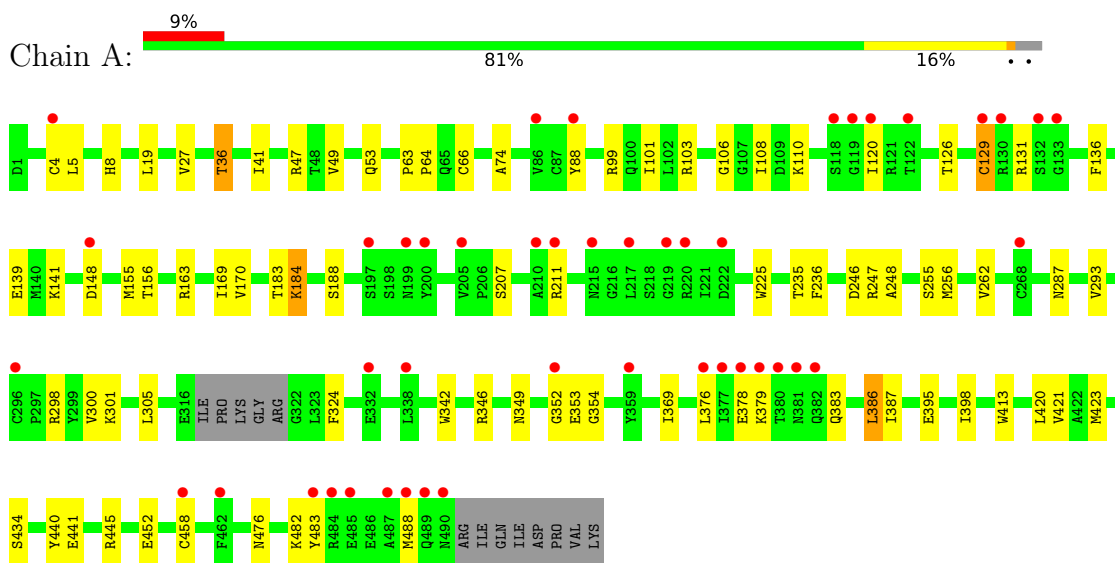
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	0	0
			111	111		
3	C	84	Total	O	0	0
			84	84		
3	E	65	Total	O	0	0
			65	65		
3	G	71	Total	O	0	0
			71	71		
3	I	89	Total	O	0	0
			89	89		
3	K	59	Total	O	0	0
			59	59		

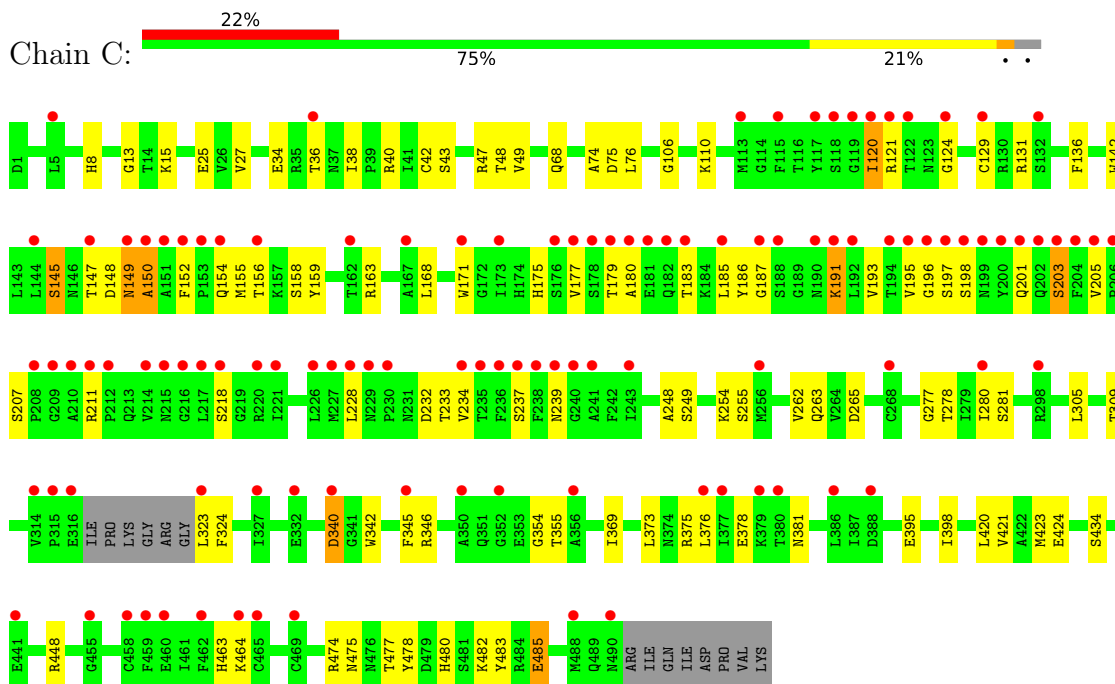
3 Residue-property plots [i](#)

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

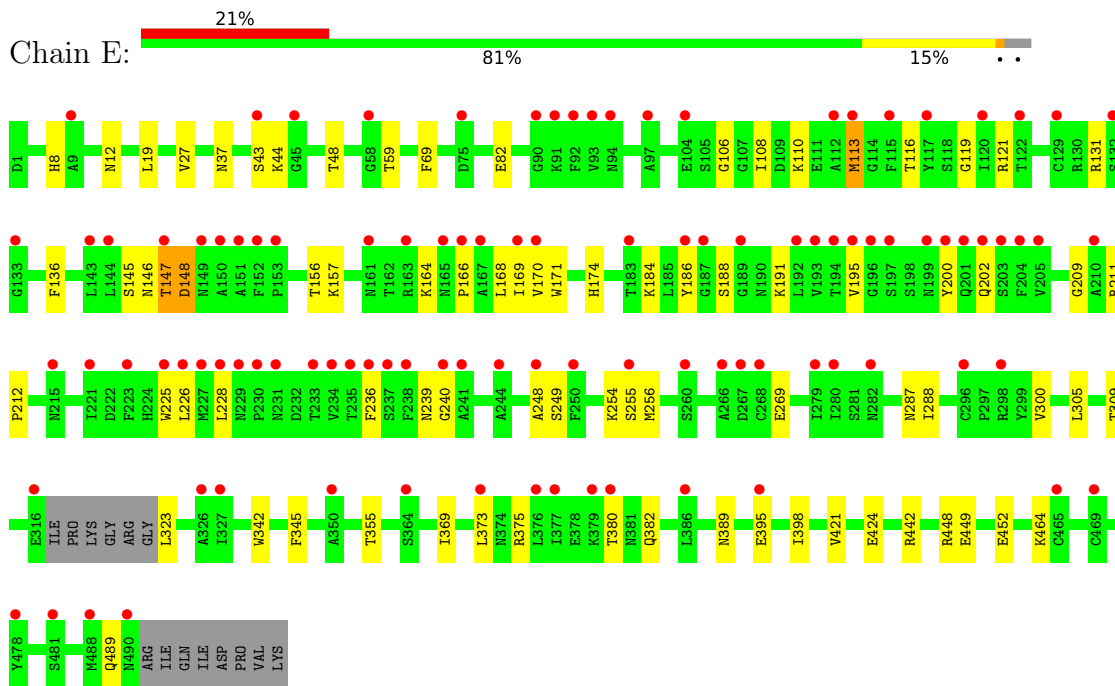
- Molecule 1: Hemagglutinin



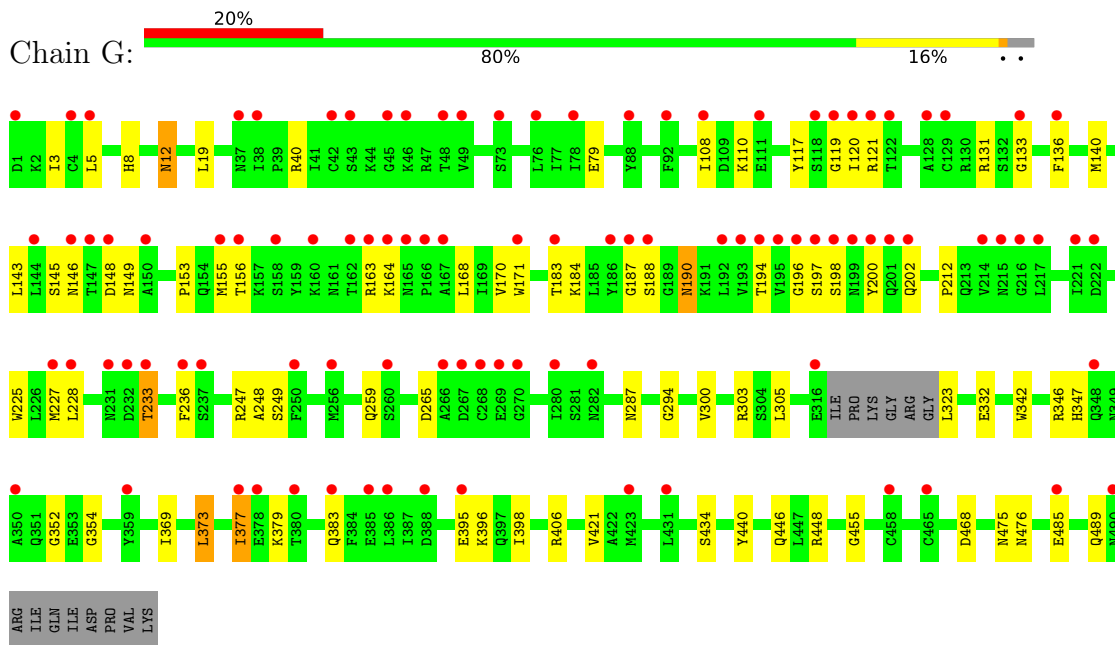
- Molecule 1: Hemagglutinin



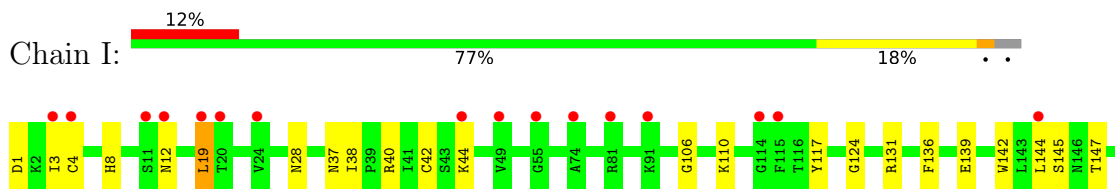
• Molecule 1: Hemagglutinin

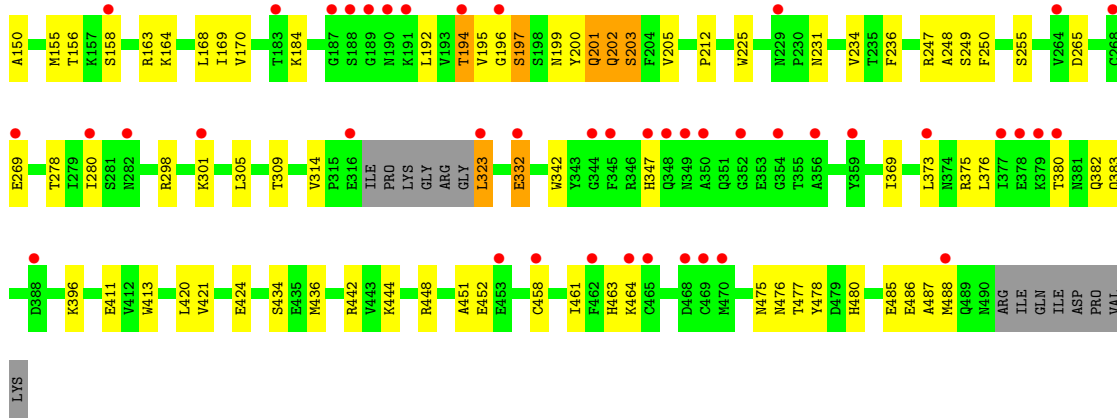


• Molecule 1: Hemagglutinin

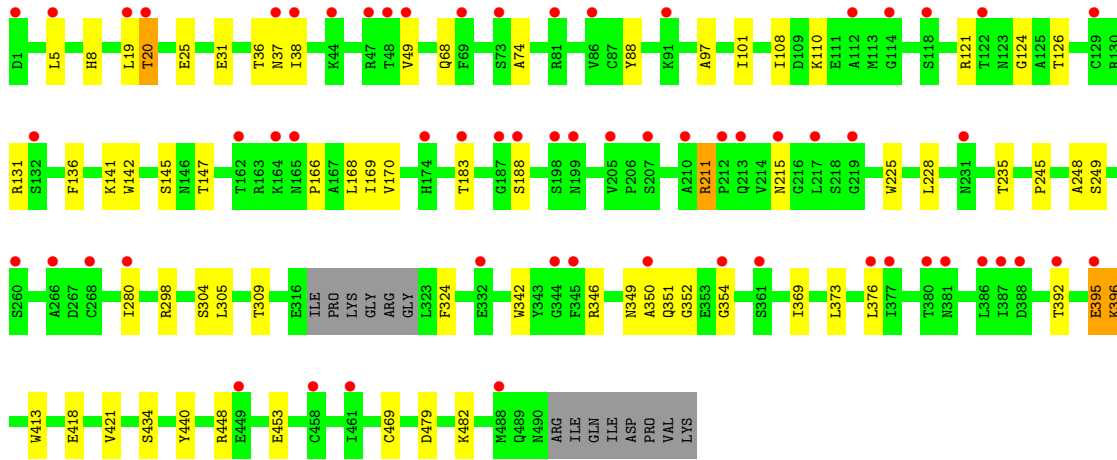
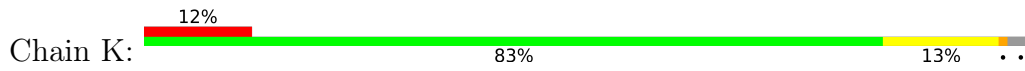


• Molecule 1: Hemagglutinin





• Molecule 1: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.18Å 226.27Å 116.78Å 90.00° 96.65° 90.00°	Depositor
Resolution (Å)	40.55 – 2.38 40.55 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.55-2.38) 97.8 (40.55-2.38)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.253 , 0.282 0.254 , 0.282	Depositor DCC
R_{free} test set	7463 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtrriage
Anisotropy	0.643	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23265	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.09	0/3853	0.29	0/5203
1	C	0.10	0/3841	0.29	0/5187
1	E	0.10	0/3849	0.29	0/5198
1	G	0.11	0/3845	0.31	0/5193
1	I	0.09	0/3846	0.30	0/5194
1	K	0.09	0/3845	0.27	0/5194
All	All	0.10	0/23079	0.29	0/31169

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 [i](#)

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	3783	0	3639	47	0
1	C	3772	0	3629	67	0
1	E	3779	0	3637	49	0
1	G	3775	0	3632	46	0
1	I	3776	0	3633	54	0
1	K	3775	0	3626	43	0
2	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	26	0	0
2	E	14	0	13	0	0
2	G	28	0	26	0	0
2	I	14	0	13	0	0
2	K	14	0	13	1	0
3	A	111	0	0	3	0
3	C	84	0	0	13	0
3	E	65	0	0	6	0
3	G	71	0	0	4	0
3	I	89	0	0	4	0
3	K	59	0	0	5	0
All	All	23265	0	21913	287	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 (287) 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:C:48:THR:HG22	1:C:76:LEU:HB3	1.65	0.78
1:G:119:GLY:O	1:G:146:ASN:ND2	2.13	0.78
1:C:8:HIS:HD2	1:C:342:TRP:HA	1.54	0.73
1:C:149:ASN:OD1	3:C:701:HOH:O	2.08	0.72
1:G:121:ARG:NH1	1:G:145:SER:O	2.24	0.71
1:C:239:ASN:O	3:C:702:HOH:O	2.08	0.71
1:I:194:THR:HA	1:I:203:SER:HA	1.74	0.70
1:A:8:HIS:CD2	1:A:342:TRP:HA	2.27	0.70
1:C:186:TYR:O	3:C:702:HOH:O	2.10	0.69
1:K:469:CYS:SG	3:K:640:HOH:O	2.49	0.69
1:E:148:ASP:OD1	1:E:184:LYS:NZ	2.25	0.69
1:C:8:HIS:CD2	1:C:342:TRP:HA	2.28	0.68
1:I:451:ALA:HB2	1:I:461:ILE:HD12	1.75	0.68
1:A:488:MET:SD	3:A:776:HOH:O	2.52	0.67
1:G:485:GLU:O	3:G:701:HOH:O	2.12	0.66
1:C:121:ARG:NH1	1:C:145:SER:O	2.28	0.66
1:E:200:TYR:CZ	1:E:202:GLN:HG3	2.31	0.66
1:C:485:GLU:O	3:C:703:HOH:O	2.11	0.66
1:C:193:VAL:O	1:C:203:SER:HA	1.96	0.66
1:A:8:HIS:HD2	1:A:342:TRP:HA	1.60	0.66
1:I:380:THR:HG22	1:I:382:GLN:H	1.61	0.65
1:C:150:ALA:O	3:C:701:HOH:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:375:ARG:NH2	1:I:424:GLU:OE2	2.30	0.65
1:E:131:ARG:NH1	1:E:136:PHE:O	2.31	0.64
1:G:148:ASP:OD1	1:G:184:LYS:NZ	2.31	0.63
1:I:411:GLU:OE1	1:K:298:ARG:NH1	2.32	0.62
1:K:131:ARG:NH1	1:K:136:PHE:O	2.31	0.62
1:E:43:SER:OG	3:E:601:HOH:O	2.16	0.62
1:E:323:LEU:O	1:G:434:SER:OG	2.17	0.62
1:E:166:PRO:HA	1:E:228:LEU:O	2.00	0.62
1:I:4:CYS:HA	1:I:458:CYS:HA	1.82	0.62
1:A:207:SER:O	1:A:211:ARG:NH2	2.32	0.62
1:G:131:ARG:NH1	1:G:136:PHE:O	2.29	0.61
1:C:120:ILE:HG12	1:C:155:MET:HE1	1.82	0.61
1:G:5:LEU:HD11	1:G:440:TYR:HA	1.83	0.61
1:G:168:LEU:HB3	1:G:249:SER:HB2	1.83	0.61
1:A:305:LEU:HB3	1:A:421:VAL:HG21	1.84	0.60
1:K:305:LEU:HB3	1:K:421:VAL:HG21	1.82	0.60
1:C:43:SER:HB2	1:C:48:THR:HG21	1.83	0.59
1:K:352:GLY:O	3:K:601:HOH:O	2.15	0.59
1:C:211:ARG:NH1	1:C:218:SER:O	2.34	0.59
1:E:200:TYR:CG	1:E:226:LEU:HD11	2.37	0.59
1:G:117:TYR:HD2	1:G:155:MET:HE1	1.67	0.59
1:G:489:GLN:N	3:G:701:HOH:O	2.32	0.59
1:A:131:ARG:NH1	1:A:136:PHE:O	2.36	0.58
1:E:59:THR:OG1	1:E:69:PHE:O	2.21	0.58
1:G:197:SER:O	1:G:198:SER:OG	2.16	0.58
1:A:287:ASN:ND2	1:A:300:VAL:O	2.32	0.58
1:A:445:ARG:HG2	1:G:455:GLY:HA2	1.86	0.58
1:E:110:LYS:HA	1:E:248:ALA:O	2.04	0.58
1:A:101:ILE:HD11	1:G:396:LYS:HG2	1.86	0.57
1:A:183:THR:HG22	1:A:188:SER:HA	1.86	0.57
1:G:287:ASN:ND2	1:G:300:VAL:O	2.36	0.57
1:A:47:ARG:NH2	3:A:714:HOH:O	2.37	0.57
1:A:434:SER:OG	1:G:323:LEU:O	2.22	0.57
1:C:158:SER:HA	1:C:234:VAL:O	2.05	0.57
1:G:305:LEU:HB3	1:G:421:VAL:HG21	1.87	0.56
1:I:8:HIS:HD1	1:I:342:TRP:HA	1.70	0.56
1:A:256:MET:SD	1:A:383:GLN:NE2	2.79	0.56
1:I:305:LEU:HB3	1:I:421:VAL:HG21	1.87	0.56
1:A:120:ILE:HD13	1:A:155:MET:HE1	1.86	0.56
1:A:235:THR:HB	1:G:212:PRO:HD3	1.87	0.56
1:E:108:ILE:HD12	1:E:110:LYS:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:38:ILE:HD12	1:K:280:ILE:HD12	1.88	0.55
1:K:124:GLY:HA3	1:K:142:TRP:HB3	1.89	0.55
1:G:190:ASN:OD1	1:G:190:ASN:N	2.36	0.55
1:I:298:ARG:HG2	1:I:413:TRP:CD2	2.42	0.55
1:A:378:GLU:HG3	1:A:379:LYS:H	1.72	0.55
1:E:287:ASN:ND2	1:E:300:VAL:O	2.38	0.55
1:E:170:VAL:HG22	1:E:225:TRP:HB3	1.89	0.54
1:C:124:GLY:HA3	1:C:142:TRP:HB3	1.90	0.54
1:C:346:ARG:HA	1:C:354:GLY:O	2.08	0.54
1:E:211:ARG:HG3	1:G:196:GLY:HA3	1.88	0.54
1:I:231:ASN:ND2	3:I:611:HOH:O	2.40	0.54
1:C:309:THR:HG22	1:C:373:LEU:HD11	1.89	0.54
1:K:298:ARG:NH1	3:K:612:HOH:O	2.41	0.54
1:C:323:LEU:O	1:I:434:SER:OG	2.22	0.54
1:A:395:GLU:HB3	1:A:398:ILE:HG22	1.90	0.54
1:C:180:ALA:O	1:C:183:THR:OG1	2.22	0.53
1:C:197:SER:OG	1:C:198:SER:N	2.39	0.53
1:E:389:ASN:ND2	3:E:604:HOH:O	2.41	0.53
1:C:34:GLU:OE2	1:C:36:THR:HB	2.07	0.53
1:C:40:ARG:HD2	1:C:265:ASP:HB2	1.89	0.53
1:I:396:LYS:HB3	1:K:97:ALA:HB1	1.90	0.53
1:C:131:ARG:NH1	1:C:136:PHE:O	2.36	0.53
1:G:346:ARG:HA	1:G:354:GLY:O	2.09	0.53
1:I:342:TRP:HH2	1:I:369:ILE:HD12	1.73	0.53
1:E:106:GLY:HA2	1:E:255:SER:HB3	1.91	0.53
1:E:147:THR:N	3:E:603:HOH:O	2.41	0.53
1:K:5:LEU:HD11	1:K:440:TYR:HA	1.90	0.53
1:E:156:THR:HA	1:E:236:PHE:O	2.09	0.52
1:I:131:ARG:NH1	1:I:136:PHE:O	2.38	0.52
1:K:169:ILE:O	1:K:225:TRP:HA	2.09	0.52
1:K:298:ARG:HG2	1:K:413:TRP:CE2	2.45	0.52
1:A:106:GLY:HA2	1:A:255:SER:HB3	1.91	0.52
1:E:188:SER:O	1:E:191:LYS:NZ	2.36	0.52
1:C:13:GLY:N	3:C:716:HOH:O	2.39	0.52
1:I:28:ASN:ND2	3:I:616:HOH:O	2.43	0.52
1:I:475:ASN:ND2	3:I:613:HOH:O	2.41	0.52
1:K:396:LYS:HD3	2:K:501:NAG:H81	1.91	0.52
1:C:38:ILE:HG13	1:C:280:ILE:HD12	1.92	0.52
1:A:169:ILE:O	1:A:225:TRP:HA	2.10	0.51
1:C:106:GLY:HA2	1:C:255:SER:HB3	1.93	0.51
1:E:395:GLU:HB3	1:E:398:ILE:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:LYS:HA	1:G:248:ALA:O	2.10	0.51
1:C:463:HIS:NE2	1:C:478:TYR:OH	2.42	0.51
1:C:340:ASP:OD1	1:C:340:ASP:N	2.40	0.51
1:E:171:TRP:HZ3	1:E:226:LEU:HB2	1.75	0.51
1:I:196:GLY:O	1:I:197:SER:HB3	2.11	0.50
1:I:156:THR:HA	1:I:236:PHE:O	2.12	0.50
1:I:168:LEU:HB3	1:I:249:SER:HB2	1.93	0.50
1:K:298:ARG:HG2	1:K:413:TRP:CD2	2.47	0.50
1:A:170:VAL:HG22	1:A:225:TRP:HB3	1.94	0.50
1:C:8:HIS:HE1	1:C:27:VAL:HG11	1.76	0.50
1:E:305:LEU:HB3	1:E:421:VAL:HG21	1.92	0.50
1:C:49:VAL:HG23	1:C:74:ALA:HB2	1.94	0.50
1:C:196:GLY:HA3	1:K:211:ARG:HB3	1.94	0.50
1:C:381:ASN:ND2	3:C:713:HOH:O	2.36	0.49
1:G:156:THR:HA	1:G:236:PHE:O	2.12	0.49
1:C:228:LEU:HD22	1:C:232:ASP:HB3	1.94	0.49
1:C:342:TRP:HH2	1:C:369:ILE:HD12	1.78	0.49
1:C:159:TYR:O	1:C:233:THR:HA	2.12	0.49
1:K:346:ARG:HA	1:K:354:GLY:O	2.12	0.49
1:I:3:ILE:HA	1:I:347:HIS:HA	1.94	0.49
1:C:395:GLU:HB3	1:C:398:ILE:HG22	1.94	0.49
1:E:191:LYS:HD2	1:E:240:GLY:HA3	1.95	0.49
1:I:376:LEU:HD22	1:I:420:LEU:HD21	1.93	0.49
1:I:463:HIS:HB3	1:I:487:ALA:HB2	1.94	0.49
1:C:110:LYS:HA	1:C:248:ALA:O	2.14	0.48
1:E:116:THR:O	1:E:157:LYS:NZ	2.42	0.48
1:K:349:ASN:C	1:K:351:GLN:H	2.22	0.48
1:A:4:CYS:HA	1:A:458:CYS:HA	1.95	0.48
1:E:37:ASN:HB3	1:E:288:ILE:HD13	1.95	0.48
1:G:108:ILE:HD12	1:G:110:LYS:HE3	1.96	0.48
1:G:110:LYS:HB2	1:G:247:ARG:HH21	1.78	0.48
1:I:139:GLU:OE1	1:I:247:ARG:HD3	2.12	0.48
1:I:44:LYS:HE2	1:I:269:GLU:HB2	1.96	0.48
1:K:350:ALA:N	3:K:601:HOH:O	2.47	0.48
1:I:145:SER:HB3	1:I:150:ALA:HB3	1.95	0.47
1:A:346:ARG:HA	1:A:354:GLY:O	2.14	0.47
1:E:309:THR:HG22	1:E:373:LEU:HD11	1.96	0.47
1:C:8:HIS:CE1	1:C:27:VAL:HG11	2.48	0.47
1:E:168:LEU:HB3	1:E:249:SER:HB2	1.96	0.47
1:I:298:ARG:HG2	1:I:413:TRP:CE2	2.49	0.47
1:G:170:VAL:HG22	1:G:225:TRP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:HIS:ND1	1:I:342:TRP:HA	2.29	0.47
1:A:148:ASP:OD1	1:A:184:LYS:HD2	2.15	0.47
1:E:191:LYS:HD3	1:E:239:ASN:ND2	2.30	0.47
1:I:42:CYS:HB2	1:I:278:THR:HG21	1.97	0.47
1:E:212:PRO:HG3	1:G:233:THR:O	2.15	0.47
1:I:201:GLN:NE2	3:I:621:HOH:O	2.48	0.47
1:A:110:LYS:HA	1:A:248:ALA:O	2.15	0.47
1:C:475:ASN:OD1	1:C:477:THR:OG1	2.30	0.47
1:E:119:GLY:O	1:E:146:ASN:ND2	2.48	0.47
1:E:209:GLY:HA3	1:G:194:THR:HG21	1.97	0.47
1:K:342:TRP:HH2	1:K:369:ILE:HD12	1.79	0.47
1:C:34:GLU:OE1	1:C:281:SER:OG	2.29	0.47
1:E:200:TYR:CD1	1:E:226:LEU:HD11	2.50	0.47
1:I:40:ARG:NE	1:I:265:ASP:OD2	2.46	0.47
1:G:406:ARG:NH2	3:G:720:HOH:O	2.42	0.46
1:C:448:ARG:HD3	1:K:453:GLU:O	2.15	0.46
1:G:395:GLU:HB3	1:G:398:ILE:HG22	1.97	0.46
1:I:323:LEU:O	1:K:434:SER:OG	2.28	0.46
1:G:79:GLU:HB2	1:G:259:GLN:HG2	1.97	0.46
1:K:20:THR:O	1:K:20:THR:OG1	2.33	0.46
1:K:309:THR:HG22	1:K:373:LEU:HD11	1.97	0.46
1:A:108:ILE:HD12	1:A:110:LYS:HE3	1.98	0.46
1:I:442:ARG:HH11	1:I:476:ASN:HB2	1.81	0.46
1:I:332:GLU:CD	1:I:332:GLU:H	2.22	0.46
1:I:309:THR:HG22	1:I:373:LEU:HD11	1.96	0.46
1:K:170:VAL:HG22	1:K:225:TRP:HB3	1.98	0.46
1:G:446:GLN:NE2	1:G:476:ASN:HA	2.31	0.45
1:K:110:LYS:HA	1:K:248:ALA:O	2.16	0.45
1:E:226:LEU:HD12	1:E:226:LEU:HA	1.70	0.45
1:I:124:GLY:HA3	1:I:142:TRP:HB3	1.96	0.45
1:I:396:LYS:HG2	1:K:101:ILE:HD11	1.99	0.45
1:A:5:LEU:HD22	1:A:440:TYR:HA	1.99	0.45
1:C:345:PHE:CD1	1:C:474:ARG:HG2	2.52	0.45
1:A:8:HIS:CE1	1:A:27:VAL:HG11	2.51	0.45
1:K:215:ASN:ND2	3:K:609:HOH:O	2.37	0.45
1:I:110:LYS:HA	1:I:248:ALA:O	2.16	0.45
1:I:169:ILE:O	1:I:225:TRP:HA	2.17	0.45
1:K:479:ASP:HB3	1:K:482:LYS:HG3	1.99	0.45
1:C:355:THR:N	3:C:729:HOH:O	2.48	0.45
1:G:140:MET:HE1	1:G:171:TRP:HA	1.99	0.45
1:A:293:VAL:HG11	1:A:386:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:464:LYS:HD3	1:E:464:LYS:HA	1.88	0.45
1:E:442:ARG:NH2	3:E:621:HOH:O	2.50	0.44
1:G:183:THR:HA	1:G:187:GLY:O	2.18	0.44
1:C:175:HIS:HD2	1:C:207:SER:H	1.64	0.44
1:C:482:LYS:HD2	1:C:483:TYR:CZ	2.52	0.44
1:C:324:PHE:CE2	1:C:434:SER:HB2	2.53	0.44
1:G:40:ARG:HD2	1:G:265:ASP:HB2	1.99	0.44
1:G:183:THR:HG22	1:G:188:SER:HA	2.00	0.44
1:I:38:ILE:C	1:I:40:ARG:H	2.26	0.44
1:I:192:LEU:HD11	1:I:203:SER:HB2	1.98	0.44
1:I:195:VAL:O	1:I:201:GLN:HA	2.18	0.44
1:C:171:TRP:CE2	1:C:195:VAL:HG21	2.53	0.44
1:A:64:PRO:HD3	1:A:129:CYS:SG	2.57	0.44
1:C:345:PHE:O	1:C:355:THR:HA	2.17	0.44
1:E:191:LYS:HA	1:E:239:ASN:HD21	1.83	0.44
1:G:373:LEU:O	1:G:377:ILE:HG12	2.18	0.44
1:A:126:THR:HG23	1:A:129:CYS:H	1.82	0.44
1:C:191:LYS:NZ	3:C:702:HOH:O	2.46	0.43
1:C:305:LEU:HB3	1:C:421:VAL:HG21	2.00	0.43
1:E:174:HIS:ND1	1:E:186:TYR:OH	2.44	0.43
1:I:117:TYR:HD2	1:I:155:MET:HE1	1.82	0.43
1:K:31:GLU:OE1	1:K:304:SER:OG	2.36	0.43
1:G:12:ASN:O	1:G:12:ASN:ND2	2.51	0.43
1:G:342:TRP:HH2	1:G:369:ILE:HD12	1.82	0.43
1:E:164:LYS:HE3	1:E:164:LYS:HB2	1.85	0.43
1:K:324:PHE:CE2	1:K:434:SER:HB2	2.53	0.43
1:A:342:TRP:HH2	1:A:369:ILE:HD12	1.83	0.43
1:E:380:THR:HG22	1:E:382:GLN:H	1.83	0.43
1:I:106:GLY:HA2	1:I:255:SER:HB3	2.00	0.43
1:K:183:THR:HG22	1:K:188:SER:HA	2.00	0.43
1:G:198:SER:C	1:G:200:TYR:H	2.27	0.43
1:K:168:LEU:HB3	1:K:249:SER:HB2	1.99	0.43
1:A:298:ARG:HG2	1:A:413:TRP:CD2	2.53	0.43
1:E:8:HIS:NE2	1:E:27:VAL:HG11	2.34	0.43
1:A:324:PHE:CE2	1:A:434:SER:HB2	2.54	0.42
1:C:378:GLU:N	3:C:718:HOH:O	2.41	0.42
1:G:120:ILE:HD12	1:G:143:LEU:HB3	1.99	0.42
1:G:352:GLY:O	3:G:702:HOH:O	2.21	0.42
1:K:395:GLU:HG2	1:K:396:LYS:N	2.33	0.42
1:C:448:ARG:HG3	1:C:480:HIS:CG	2.54	0.42
1:E:452:GLU:OE2	3:E:602:HOH:O	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:463:HIS:NE2	1:I:478:TYR:OH	2.51	0.42
1:A:452:GLU:OE1	1:E:448:ARG:NH2	2.52	0.42
1:I:110:LYS:HB2	1:I:247:ARG:NH2	2.33	0.42
1:K:88:TYR:HD1	1:K:126:THR:HG21	1.83	0.42
1:K:166:PRO:HA	1:K:228:LEU:O	2.20	0.42
1:A:156:THR:HA	1:A:236:PHE:O	2.19	0.42
1:E:113:MET:HE3	1:E:169:ILE:HD12	2.01	0.42
1:A:36:THR:HG23	1:C:36:THR:HG23	2.00	0.42
1:G:228:LEU:HD23	1:G:228:LEU:HA	1.90	0.42
1:C:15:LYS:HG3	1:C:25:GLU:HG2	2.01	0.42
1:A:423:MET:SD	3:A:779:HOH:O	2.62	0.42
1:E:121:ARG:HG3	1:E:145:SER:C	2.45	0.41
1:K:49:VAL:HG23	1:K:74:ALA:HB2	2.02	0.41
1:K:121:ARG:HD3	1:K:145:SER:O	2.20	0.41
1:C:145:SER:HB2	3:C:711:HOH:O	2.20	0.41
1:A:141:LYS:HE2	1:A:246:ASP:OD1	2.20	0.41
1:C:175:HIS:CD2	1:C:207:SER:H	2.37	0.41
1:C:262:VAL:HG21	1:C:277:GLY:HA2	2.02	0.41
1:G:448:ARG:HE	1:G:448:ARG:HB3	1.64	0.41
1:I:158:SER:HA	1:I:234:VAL:O	2.21	0.41
1:C:375:ARG:HH22	1:C:424:GLU:CD	2.28	0.41
1:A:376:LEU:HD22	1:A:420:LEU:HD21	2.02	0.41
1:C:42:CYS:HB2	1:C:278:THR:HG21	2.03	0.41
1:G:294:GLY:HA2	1:G:383:GLN:HG3	2.02	0.41
1:I:448:ARG:HG3	1:I:480:HIS:CD2	2.56	0.41
1:I:19:LEU:HD12	1:I:19:LEU:HA	1.91	0.41
1:I:170:VAL:HG22	1:I:225:TRP:HB3	2.02	0.41
1:I:200:TYR:OH	1:I:202:GLN:HG3	2.19	0.41
1:A:349:ASN:H	1:A:352:GLY:HA2	1.84	0.41
1:C:423:MET:SD	3:C:762:HOH:O	2.63	0.41
1:E:345:PHE:O	1:E:355:THR:HA	2.20	0.41
1:I:212:PRO:HD3	1:K:235:THR:HB	2.02	0.41
1:G:120:ILE:HG22	1:G:153:PRO:HD2	2.03	0.41
1:K:170:VAL:O	1:K:245:PRO:HB3	2.20	0.41
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.21	0.41
1:C:68:GLN:OE1	1:C:68:GLN:N	2.46	0.41
1:C:376:LEU:HD22	1:C:420:LEU:HD21	2.03	0.41
1:E:44:LYS:HD3	1:E:269:GLU:HB2	2.02	0.41
1:E:342:TRP:HH2	1:E:369:ILE:HD12	1.86	0.41
1:G:347:HIS:NE2	1:G:354:GLY:HA3	2.36	0.41
1:K:68:GLN:OE1	1:K:68:GLN:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HG23	1:A:74:ALA:HB2	2.03	0.41
1:C:179:THR:O	1:C:183:THR:HG23	2.21	0.41
1:E:171:TRP:CE2	1:E:195:VAL:HG21	2.56	0.41
1:E:449:GLU:HG3	3:E:632:HOH:O	2.20	0.41
1:I:163:ARG:HD3	1:I:250:PHE:CZ	2.56	0.41
1:A:482:LYS:NZ	1:A:483:TYR:OH	2.54	0.40
1:C:177:VAL:HG22	1:C:218:SER:HB2	2.03	0.40
1:C:187:GLY:HA2	3:C:701:HOH:O	2.20	0.40
1:I:452:GLU:OE1	1:K:448:ARG:NH2	2.54	0.40
1:E:375:ARG:HH22	1:E:424:GLU:CD	2.28	0.40
1:A:41:ILE:HG12	1:A:262:VAL:HG23	2.03	0.40
1:A:88:TYR:HD1	1:A:126:THR:HG21	1.86	0.40
1:C:47:ARG:NH1	1:C:75:ASP:OD1	2.54	0.40
1:C:168:LEU:HB3	1:C:249:SER:HB2	2.04	0.40
1:K:108:ILE:HD12	1:K:110:LYS:HE3	2.03	0.40
1:K:342:TRP:CH2	1:K:369:ILE:HD12	2.56	0.40
1:A:63:PRO:HD2	1:A:66:CYS:HB2	2.04	0.40
1:A:99:ARG:O	1:A:103:ARG:HG3	2.22	0.40
1:I:164:LYS:HE3	1:I:164:LYS:HB2	1.87	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	A	481/498 (97%)	460 (96%)	20 (4%)	1 (0%)	43 56
1	C	480/498 (96%)	439 (92%)	37 (8%)	4 (1%)	16 23
1	E	480/498 (96%)	446 (93%)	34 (7%)	0	100 100
1	G	480/498 (96%)	451 (94%)	27 (6%)	2 (0%)	30 40
1	I	480/498 (96%)	453 (94%)	25 (5%)	2 (0%)	30 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	480/498 (96%)	452 (94%)	28 (6%)	0	100	100
All	All	2881/2988 (96%)	2701 (94%)	171 (6%)	9 (0%)	36	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	149	ASN
1	C	203	SER
1	I	197	SER
1	A	353	GLU
1	C	154	GLN
1	I	203	SER
1	C	150	ALA
1	G	377	ILE
1	G	133	GLY

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	409/421 (97%)	398 (97%)	11 (3%)	39	59
1	C	408/421 (97%)	390 (96%)	18 (4%)	25	40
1	E	409/421 (97%)	399 (98%)	10 (2%)	43	63
1	G	408/421 (97%)	391 (96%)	17 (4%)	26	42
1	I	408/421 (97%)	383 (94%)	25 (6%)	17	27
1	K	408/421 (97%)	394 (97%)	14 (3%)	32	51
All	All	2450/2526 (97%)	2355 (96%)	95 (4%)	28	45

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	36	THR

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Mol	Chain	Res	Type
1	A	53	GLN
1	A	129	CYS
1	A	163	ARG
1	A	184	LYS
1	A	301	LYS
1	A	386	LEU
1	A	387	ILE
1	A	441	GLU
1	A	476	ASN
1	C	120	ILE
1	C	129	CYS
1	C	145	SER
1	C	147	THR
1	C	148	ASP
1	C	152	PHE
1	C	156	THR
1	C	163	ARG
1	C	185	LEU
1	C	191	LYS
1	C	201	GLN
1	C	205	VAL
1	C	237	SER
1	C	254	LYS
1	C	263	GLN
1	C	340	ASP
1	C	464	LYS
1	C	485	GLU
1	E	12	ASN
1	E	19	LEU
1	E	48	THR
1	E	82	GLU
1	E	113	MET
1	E	147	THR
1	E	148	ASP
1	E	254	LYS
1	E	256	MET
1	E	489	GLN
1	G	3	ILE
1	G	8	HIS
1	G	12	ASN
1	G	19	LEU
1	G	149	ASN

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Mol	Chain	Res	Type
1	G	163	ARG
1	G	164	LYS
1	G	190	ASN
1	G	202	GLN
1	G	227	MET
1	G	233	THR
1	G	303	ARG
1	G	332	GLU
1	G	373	LEU
1	G	379	LYS
1	G	468	ASP
1	G	475	ASN
1	I	1	ASP
1	I	12	ASN
1	I	19	LEU
1	I	37	ASN
1	I	144	LEU
1	I	147	THR
1	I	184	LYS
1	I	194	THR
1	I	199	ASN
1	I	201	GLN
1	I	202	GLN
1	I	205	VAL
1	I	280	ILE
1	I	301	LYS
1	I	314	VAL
1	I	323	LEU
1	I	332	GLU
1	I	383	GLN
1	I	436	MET
1	I	444	LYS
1	I	464	LYS
1	I	477	THR
1	I	485	GLU
1	I	486	GLU
1	I	488	MET
1	K	8	HIS
1	K	19	LEU
1	K	20	THR
1	K	25	GLU
1	K	36	THR

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Mol	Chain	Res	Type
1	K	37	ASN
1	K	141	LYS
1	K	147	THR
1	K	211	ARG
1	K	376	LEU
1	K	392	THR
1	K	395	GLU
1	K	396	LYS
1	K	418	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	201	GLN
1	A	282	ASN
1	A	490	ASN
1	C	8	HIS
1	C	123	ASN
1	C	224	HIS
1	C	239	ASN
1	C	351	GLN
1	C	382	GLN
1	C	480	HIS
1	E	149	ASN
1	E	201	GLN
1	E	383	GLN
1	E	446	GLN
1	E	476	ASN
1	E	490	ASN
1	G	17	ASN
1	G	37	ASN
1	G	202	GLN
1	G	490	ASN
1	I	7	HIS
1	I	202	GLN
1	I	263	GLN
1	I	374	ASN
1	K	37	ASN
1	K	53	GLN
1	K	229	ASN
1	K	263	GLN

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Mol	Chain	Res	Type
1	K	383	GLN
1	K	446	GLN
1	K	480	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	602	1	14,14,15	0.25	0	17,19,21	0.46	0
2	NAG	G	601	1	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	C	601	1	14,14,15	0.26	0	17,19,21	0.50	0
2	NAG	I	501	1	14,14,15	0.26	0	17,19,21	0.43	0
2	NAG	E	501	1	14,14,15	0.26	0	17,19,21	0.46	0
2	NAG	A	601	1	14,14,15	0.25	0	17,19,21	0.50	0
2	NAG	K	501	1	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	G	602	1	14,14,15	0.28	0	17,19,21	0.46	0
2	NAG	A	602	1	14,14,15	0.29	0	17,19,21	0.47	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
2	NAG	C	602	1	-	0/6/23/26	0/1/1/1
2	NAG	G	601	1	-	1/6/23/26	0/1/1/1
2	NAG	C	601	1	-	1/6/23/26	0/1/1/1
2	NAG	I	501	1	-	0/6/23/26	0/1/1/1
2	NAG	E	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
2	NAG	K	501	1	-	0/6/23/26	0/1/1/1
2	NAG	G	602	1	-	1/6/23/26	0/1/1/1
2	NAG	A	602	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 (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAG	O5-C5-C6-O6
2	A	601	NAG	C4-C5-C6-O6
2	G	601	NAG	O5-C5-C6-O6
2	G	602	NAG	O5-C5-C6-O6
2	C	601	NAG	O5-C5-C6-O6

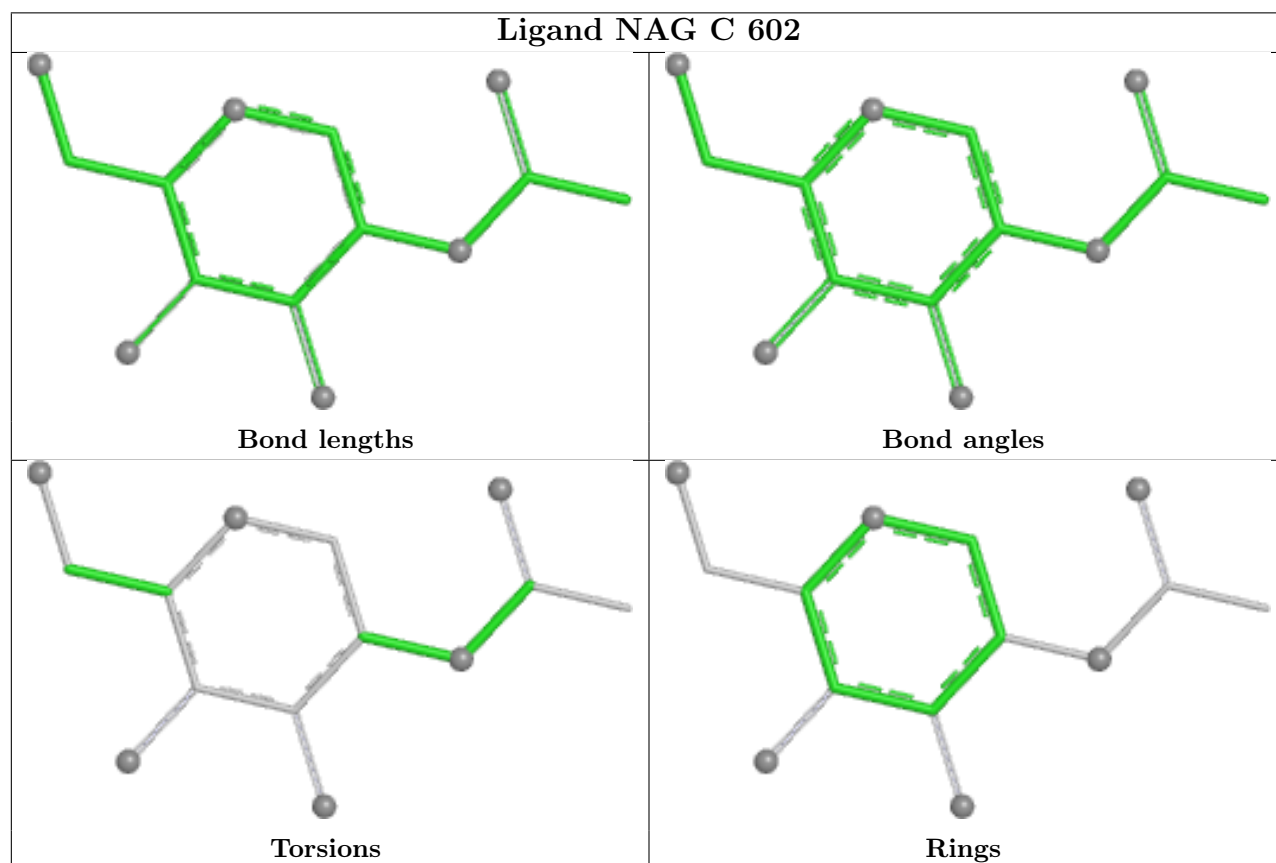
There are no ring outliers.

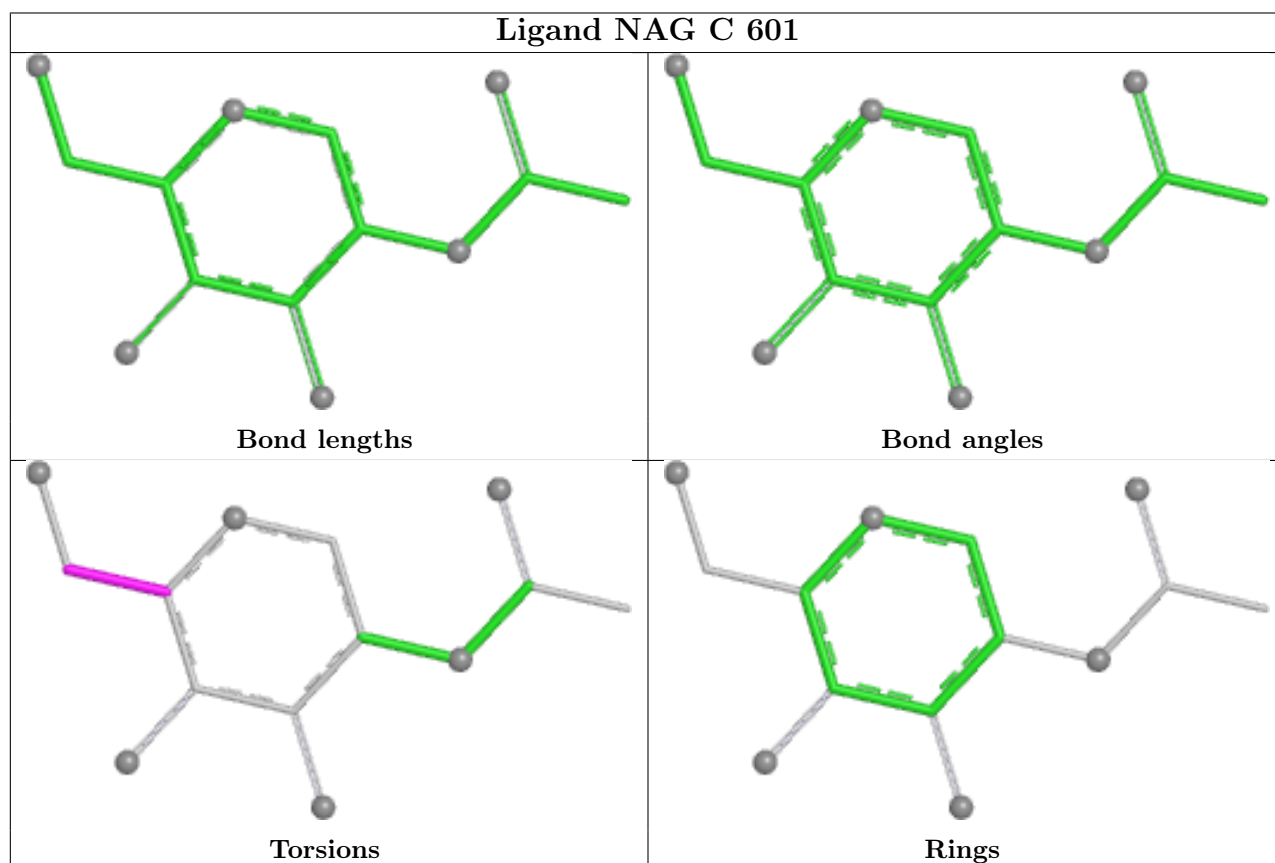
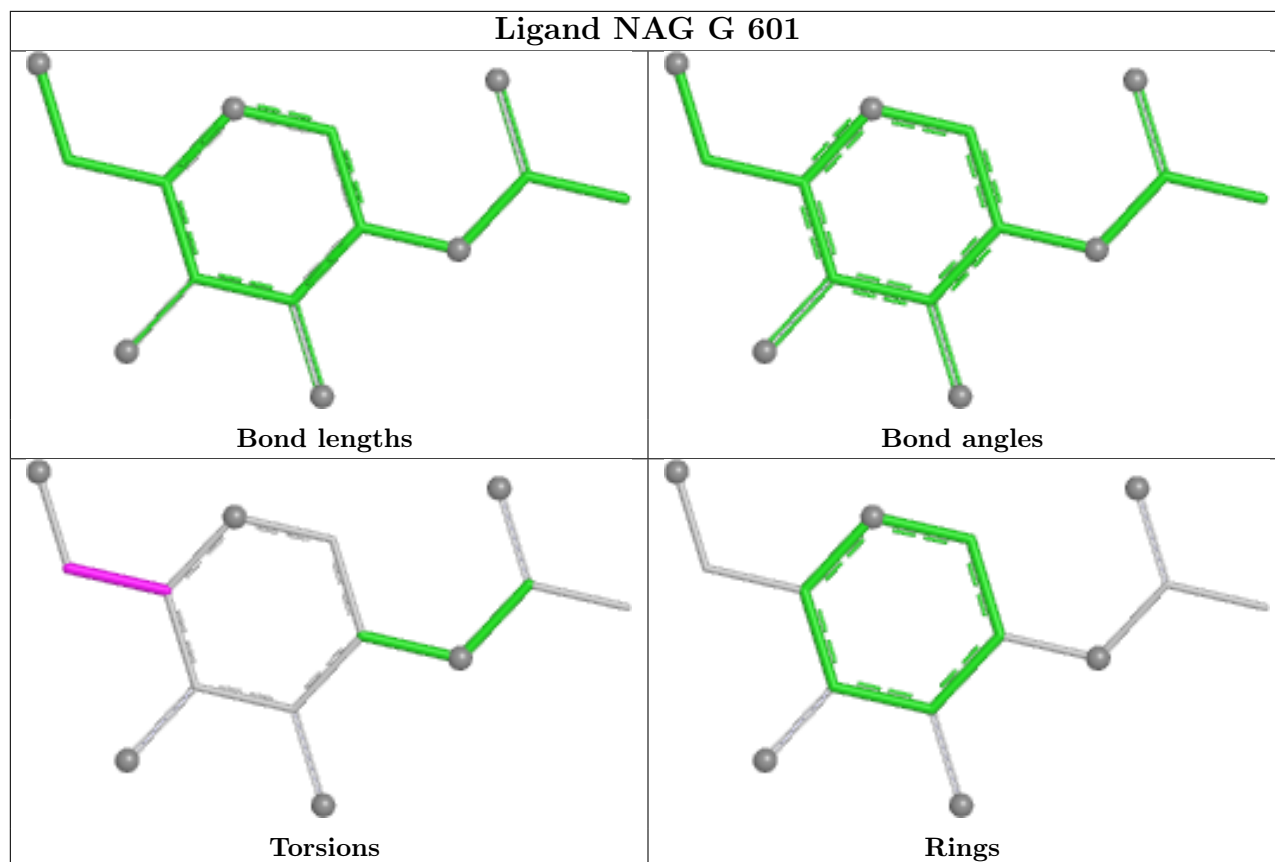
1 monomer is involved in 1 short contact:

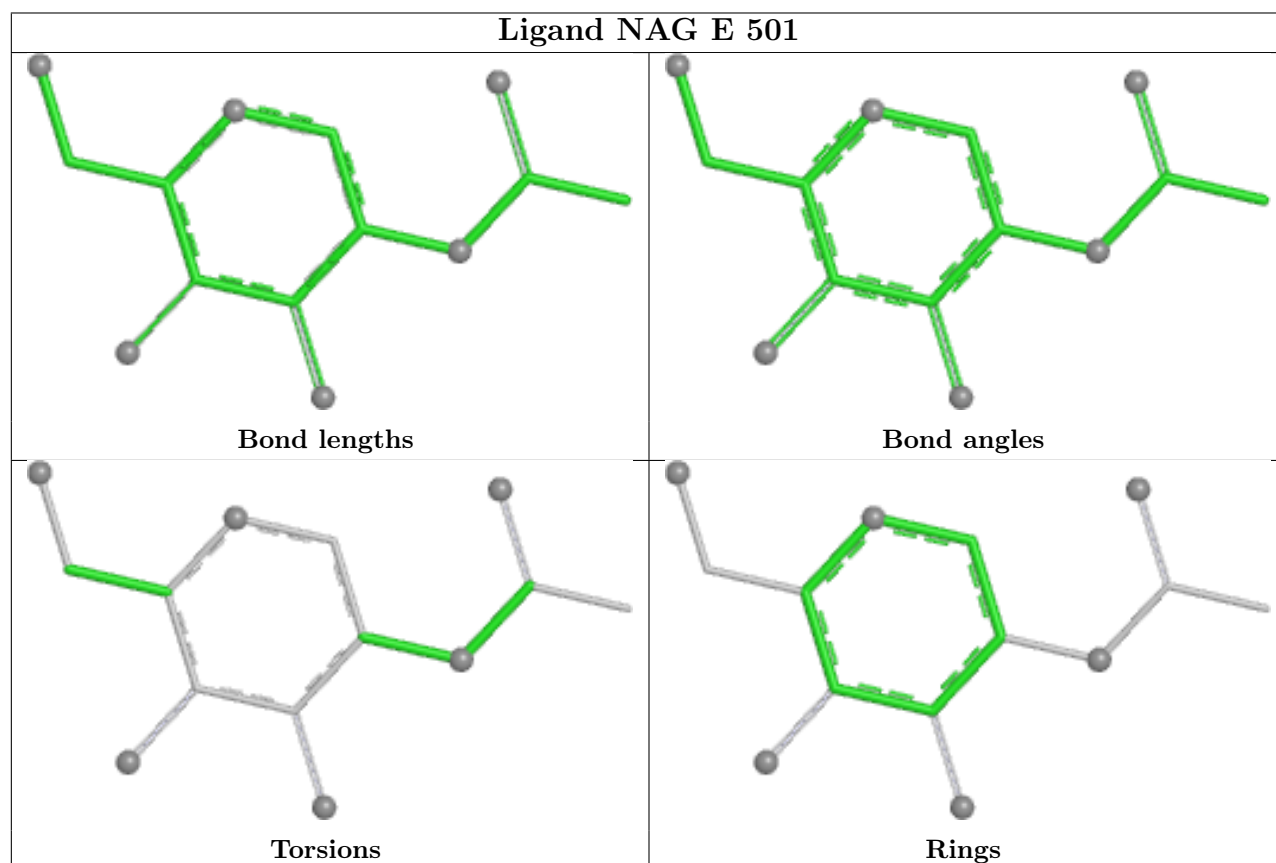
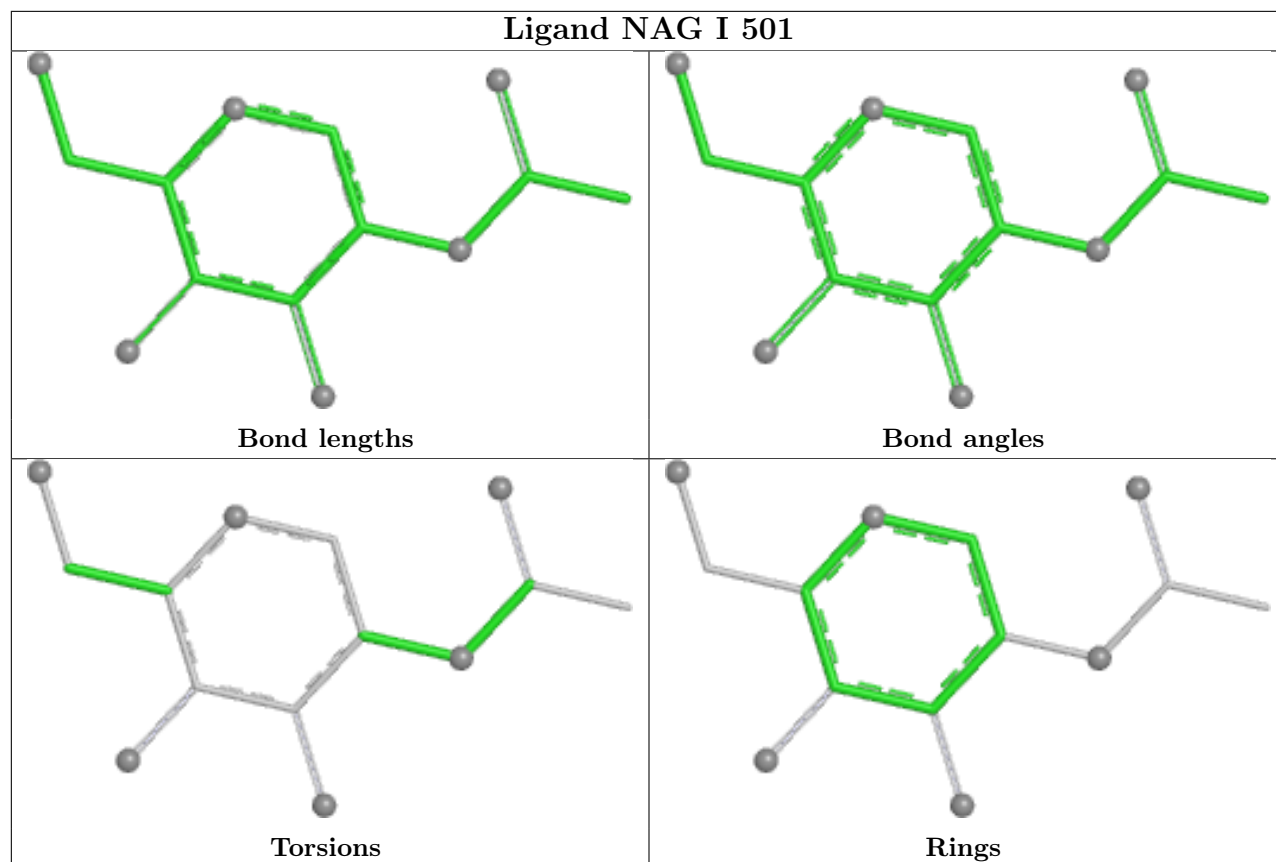
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	501	NAG	1	0

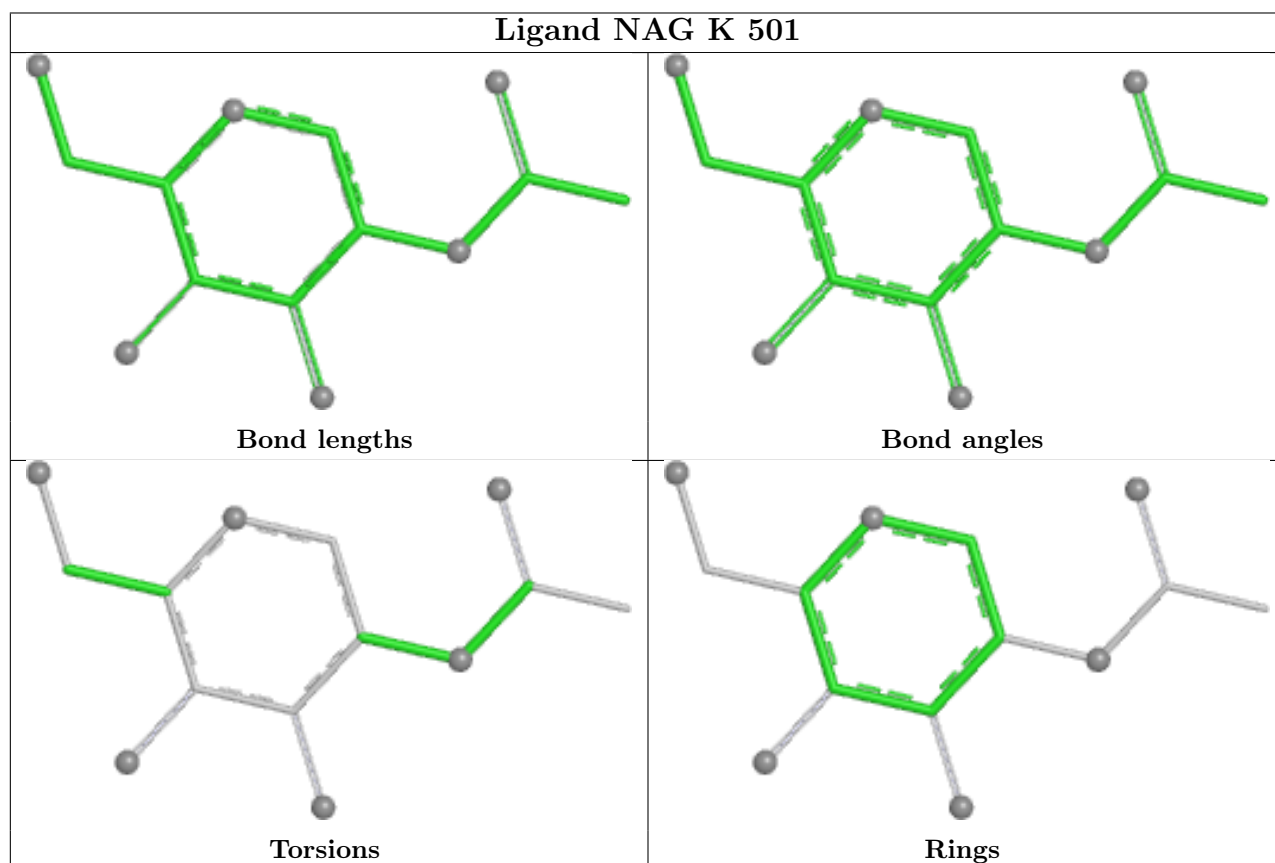
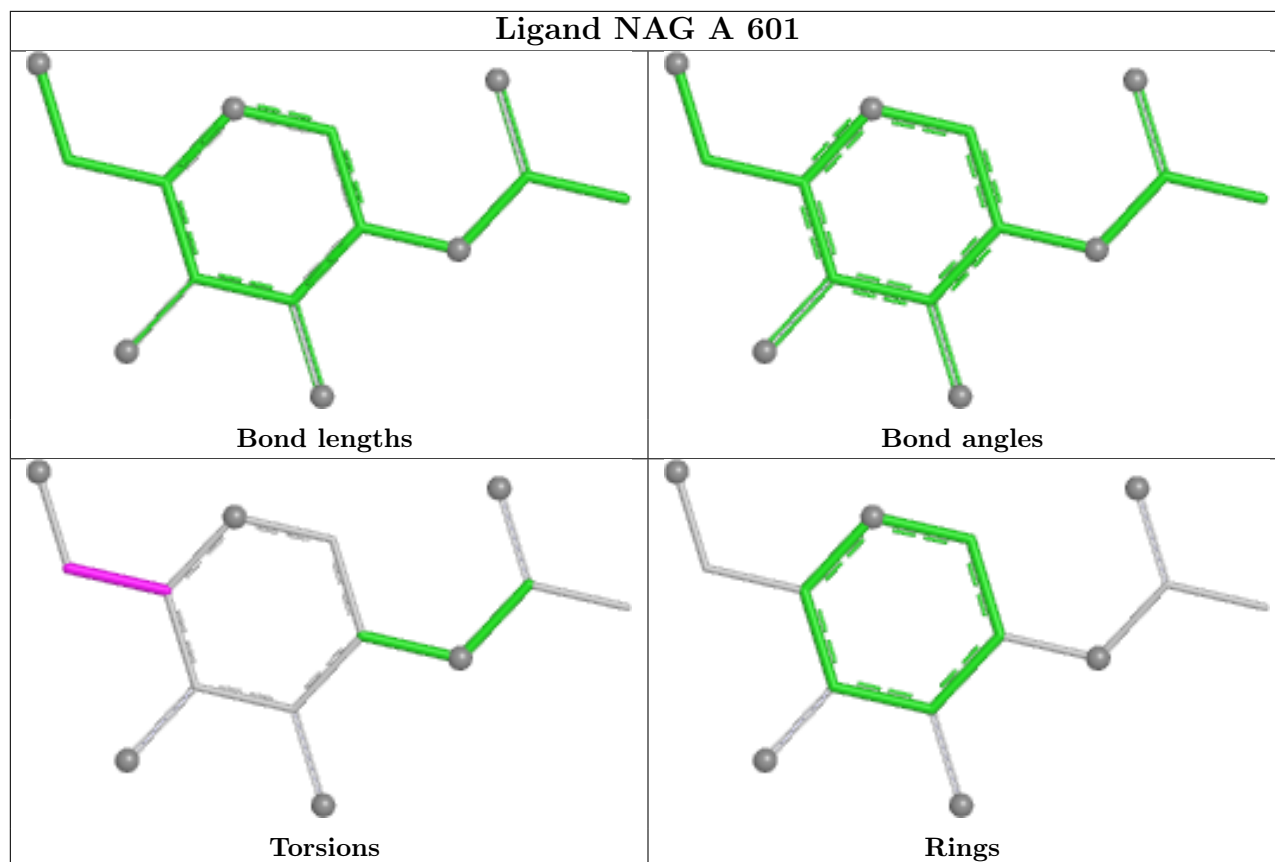
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

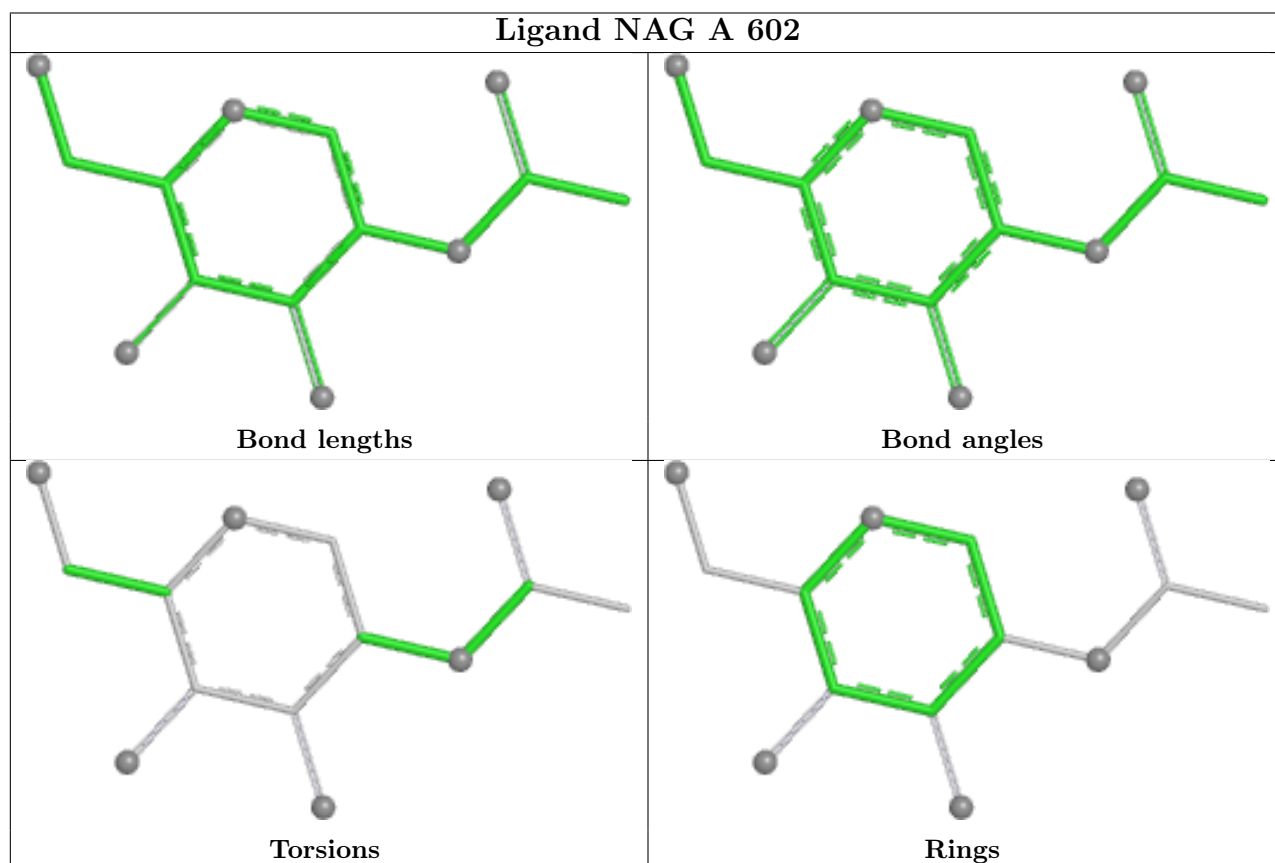
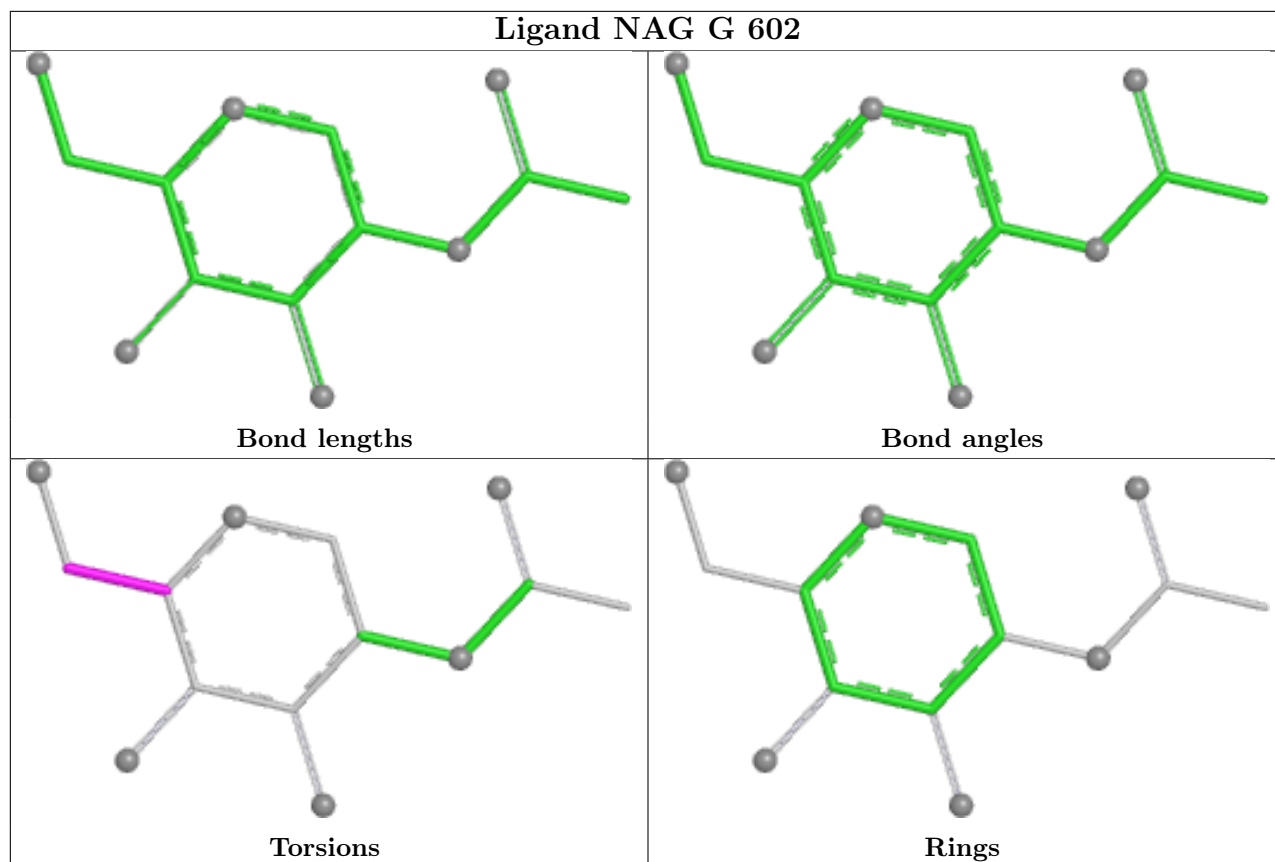
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	485/498 (97%)	0.76	45 (9%) 14 13	29, 48, 77, 120	0
1	C	484/498 (97%)	1.34	111 (22%) 2 1	29, 59, 101, 131	0
1	E	484/498 (97%)	1.31	103 (21%) 2 2	35, 60, 101, 130	0
1	G	484/498 (97%)	1.29	99 (20%) 2 2	33, 59, 93, 140	0
1	I	484/498 (97%)	0.97	60 (12%) 8 7	32, 54, 92, 183	0
1	K	484/498 (97%)	0.94	62 (12%) 7 7	32, 55, 85, 146	0
All	All	2905/2988 (97%)	1.10	480 (16%) 4 4	29, 55, 93, 183	0

All (480) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	187	GLY	7.7
1	C	192	LEU	7.2
1	C	199	ASN	6.8
1	C	194	THR	6.8
1	C	215	ASN	6.7
1	C	195	VAL	6.7
1	G	150	ALA	6.5
1	C	185	LEU	6.5
1	G	194	THR	6.3
1	E	240	GLY	6.1
1	G	167	ALA	6.1
1	C	201	GLN	5.9
1	I	188	SER	5.6
1	C	183	THR	5.6
1	I	190	ASN	5.5
1	C	200	TYR	5.5
1	C	214	VAL	5.4
1	G	199	ASN	5.2
1	C	465	CYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	G	200	TYR	5.1
1	G	201	GLN	5.1
1	E	201	GLN	4.9
1	E	386	LEU	4.9
1	A	487	ALA	4.7
1	G	120	ILE	4.7
1	G	221	ILE	4.6
1	C	152	PHE	4.5
1	E	200	TYR	4.5
1	C	212	PRO	4.4
1	G	147	THR	4.4
1	E	377	ILE	4.4
1	E	204	PHE	4.4
1	C	237	SER	4.4
1	I	316	GLU	4.3
1	C	350	ALA	4.3
1	G	270	GLY	4.3
1	K	162	THR	4.3
1	C	229	ASN	4.2
1	G	43	SER	4.2
1	C	196	GLY	4.2
1	C	178	SER	4.2
1	E	192	LEU	4.2
1	C	240	GLY	4.2
1	C	149	ASN	4.1
1	G	316	GLU	4.1
1	E	234	VAL	4.1
1	A	352	GLY	4.1
1	E	203	SER	4.1
1	K	212	PRO	4.1
1	E	150	ALA	4.0
1	C	228	LEU	4.0
1	I	196	GLY	4.0
1	G	198	SER	4.0
1	I	377	ILE	4.0
1	C	469	CYS	4.0
1	I	469	CYS	4.0
1	C	156	THR	4.0
1	G	166	PRO	3.9
1	E	186	TYR	3.9
1	C	154	GLN	3.9
1	E	202	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	199	ASN	3.9
1	A	377	ILE	3.9
1	G	195	VAL	3.9
1	C	179	THR	3.9
1	C	198	SER	3.8
1	C	120	ILE	3.8
1	G	49	VAL	3.8
1	G	37	ASN	3.8
1	G	128	ALA	3.8
1	I	356	ALA	3.8
1	E	147	THR	3.7
1	E	194	THR	3.7
1	G	490	ASN	3.7
1	I	470	MET	3.7
1	G	122	THR	3.7
1	A	197	SER	3.7
1	C	209	GLY	3.7
1	C	202	GLN	3.7
1	G	165	ASN	3.7
1	G	118	SER	3.7
1	E	268	CYS	3.7
1	K	164	LYS	3.7
1	C	380	THR	3.6
1	G	377	ILE	3.6
1	K	377	ILE	3.6
1	G	129	CYS	3.6
1	G	268	CYS	3.6
1	I	268	CYS	3.6
1	G	197	SER	3.6
1	C	352	GLY	3.6
1	G	386	LEU	3.6
1	K	122	THR	3.6
1	E	167	ALA	3.6
1	E	266	ALA	3.6
1	E	350	ALA	3.6
1	C	197	SER	3.5
1	E	237	SER	3.5
1	C	238	PHE	3.5
1	E	236	PHE	3.5
1	C	217	LEU	3.5
1	I	388	ASP	3.5
1	E	113	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	37	ASN	3.5
1	C	129	CYS	3.5
1	E	241	ALA	3.5
1	C	203	SER	3.5
1	G	119	GLY	3.5
1	A	122	THR	3.4
1	E	117	TYR	3.4
1	A	489	GLN	3.4
1	E	395	GLU	3.4
1	G	133	GLY	3.4
1	A	376	LEU	3.4
1	E	120	ILE	3.4
1	E	226	LEU	3.4
1	I	349	ASN	3.4
1	C	210	ALA	3.4
1	K	207	SER	3.4
1	E	478	TYR	3.3
1	E	197	SER	3.3
1	E	45	GLY	3.3
1	E	94	ASN	3.3
1	I	347	HIS	3.3
1	C	182	GLN	3.3
1	C	314	VAL	3.3
1	E	196	GLY	3.3
1	E	228	LEU	3.3
1	I	323	LEU	3.3
1	A	268	CYS	3.3
1	K	387	ILE	3.3
1	I	380	THR	3.3
1	G	237	SER	3.3
1	A	490	ASN	3.2
1	E	152	PHE	3.2
1	C	226	LEU	3.2
1	G	228	LEU	3.2
1	E	380	THR	3.2
1	I	194	THR	3.2
1	I	352	GLY	3.2
1	A	148	ASP	3.2
1	A	332	GLU	3.2
1	C	315	PRO	3.2
1	C	327	ILE	3.2
1	G	78	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	204	PHE	3.2
1	C	180	ALA	3.2
1	I	12	ASN	3.2
1	K	199	ASN	3.2
1	C	153	PRO	3.2
1	E	280	ILE	3.2
1	K	380	THR	3.2
1	K	392	THR	3.2
1	C	462	PHE	3.1
1	C	124	GLY	3.1
1	G	187	GLY	3.1
1	I	19	LEU	3.1
1	C	316	GLU	3.1
1	G	146	ASN	3.1
1	E	144	LEU	3.1
1	E	233	THR	3.1
1	G	380	THR	3.1
1	C	118	SER	3.1
1	C	241	ALA	3.1
1	C	386	LEU	3.1
1	C	379	LYS	3.1
1	E	225	TRP	3.1
1	K	449	GLU	3.1
1	C	147	THR	3.1
1	C	345	PHE	3.1
1	C	150	ALA	3.1
1	K	266	ALA	3.1
1	C	234	VAL	3.1
1	I	464	LYS	3.1
1	C	323	LEU	3.1
1	G	48	THR	3.0
1	I	183	THR	3.0
1	C	176	SER	3.0
1	E	282	ASN	3.0
1	G	217	LEU	3.0
1	I	488	MET	3.0
1	E	260	SER	3.0
1	K	361	SER	3.0
1	A	219	GLY	3.0
1	I	354	GLY	3.0
1	C	236	PHE	3.0
1	C	205	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	376	LEU	3.0
1	G	378	GLU	3.0
1	G	156	THR	3.0
1	G	231	ASN	3.0
1	K	458	CYS	3.0
1	C	119	GLY	3.0
1	E	223	PHE	2.9
1	G	280	ILE	2.9
1	E	199	ASN	2.9
1	G	76	LEU	2.9
1	K	386	LEU	2.9
1	K	38	ILE	2.9
1	C	190	ASN	2.9
1	E	58	GLY	2.9
1	K	47	ARG	2.9
1	I	280	ILE	2.9
1	E	161	ASN	2.9
1	G	5	LEU	2.9
1	C	177	VAL	2.9
1	K	86	VAL	2.9
1	E	490	ASN	2.9
1	G	216	GLY	2.8
1	K	187	GLY	2.8
1	G	202	GLN	2.8
1	A	129	CYS	2.8
1	A	211	ARG	2.8
1	I	11	SER	2.8
1	C	208	PRO	2.8
1	A	379	LYS	2.8
1	E	465	CYS	2.8
1	K	268	CYS	2.8
1	A	133	GLY	2.8
1	E	132	SER	2.8
1	I	144	LEU	2.8
1	G	111	GLU	2.8
1	K	395	GLU	2.8
1	K	350	ALA	2.8
1	C	227	MET	2.8
1	I	115	PHE	2.8
1	E	195	VAL	2.8
1	A	130	ARG	2.8
1	C	220	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	215	ASN	2.8
1	G	465	CYS	2.8
1	G	348	GLN	2.8
1	E	91	LYS	2.8
1	I	350	ALA	2.8
1	K	49	VAL	2.8
1	C	162	THR	2.7
1	E	149	ASN	2.7
1	E	279	ILE	2.7
1	A	118	SER	2.7
1	E	43	SER	2.7
1	E	133	GLY	2.7
1	A	205	VAL	2.7
1	E	193	VAL	2.7
1	I	24	VAL	2.7
1	K	213	GLN	2.7
1	K	280	ILE	2.7
1	G	164	LYS	2.7
1	E	248	ALA	2.7
1	G	236	PHE	2.7
1	G	215	ASN	2.7
1	E	379	LYS	2.7
1	I	348	GLN	2.7
1	I	462	PHE	2.7
1	G	214	VAL	2.7
1	C	173	ILE	2.7
1	K	344	GLY	2.7
1	K	260	SER	2.7
1	G	458	CYS	2.7
1	E	97	ALA	2.6
1	I	269	GLU	2.6
1	E	205	VAL	2.6
1	I	465	CYS	2.6
1	K	19	LEU	2.6
1	G	196	GLY	2.6
1	I	3	ILE	2.6
1	K	132	SER	2.6
1	K	231	ASN	2.6
1	K	388	ASP	2.6
1	G	183	THR	2.6
1	G	233	THR	2.6
1	K	20	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	73	SER	2.6
1	G	266	ALA	2.6
1	C	239	ASN	2.6
1	K	1	ASP	2.6
1	E	227	MET	2.6
1	E	153	PRO	2.6
1	E	364	SER	2.6
1	K	44	LYS	2.6
1	G	485	GLU	2.5
1	E	92	PHE	2.5
1	E	115	PHE	2.5
1	G	250	PHE	2.5
1	G	158	SER	2.5
1	E	316	GLU	2.5
1	G	269	GLU	2.5
1	C	211	ARG	2.5
1	E	143	LEU	2.5
1	G	256	MET	2.5
1	G	1	ASP	2.5
1	G	388	ASP	2.5
1	I	189	GLY	2.5
1	C	122	THR	2.5
1	G	162	THR	2.5
1	E	250	PHE	2.5
1	G	383	GLN	2.5
1	G	163	ARG	2.5
1	A	462	PHE	2.5
1	E	170	VAL	2.5
1	K	118	SER	2.5
1	A	200	TYR	2.5
1	I	91	LYS	2.5
1	E	231	ASN	2.5
1	G	222	ASP	2.5
1	E	163	ARG	2.4
1	G	385	GLU	2.4
1	C	218	SER	2.4
1	G	73	SER	2.4
1	I	345	PHE	2.4
1	A	217	LEU	2.4
1	C	5	LEU	2.4
1	G	192	LEU	2.4
1	I	379	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	216	GLY	2.4
1	E	166	PRO	2.4
1	C	132	SER	2.4
1	C	458	CYS	2.4
1	A	86	VAL	2.4
1	K	69	PHE	2.4
1	C	117	TYR	2.4
1	C	388	ASP	2.4
1	I	229	ASN	2.4
1	C	441	GLU	2.4
1	E	481	SER	2.4
1	G	188	SER	2.4
1	K	198	SER	2.4
1	C	464	LYS	2.4
1	E	169	ILE	2.4
1	E	238	PHE	2.4
1	G	38	ILE	2.4
1	G	186	TYR	2.4
1	K	174	HIS	2.4
1	K	165	ASN	2.4
1	E	112	ALA	2.4
1	K	210	ALA	2.4
1	G	46	LYS	2.4
1	A	4	CYS	2.4
1	A	488	MET	2.4
1	E	488	MET	2.4
1	K	129	CYS	2.4
1	K	345	PHE	2.4
1	A	338	LEU	2.4
1	E	376	LEU	2.4
1	E	230	PRO	2.3
1	C	191	LYS	2.3
1	K	114	GLY	2.3
1	C	356	ALA	2.3
1	G	260	SER	2.3
1	C	115	PHE	2.3
1	C	144	LEU	2.3
1	G	359	TYR	2.3
1	I	344	GLY	2.3
1	G	350	ALA	2.3
1	I	74	ALA	2.3
1	A	380	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	5	LEU	2.3
1	A	381	ASN	2.3
1	A	119	GLY	2.3
1	I	114	GLY	2.3
1	G	395	GLU	2.3
1	K	91	LYS	2.3
1	K	217	LEU	2.3
1	I	458	CYS	2.3
1	G	267	ASP	2.3
1	C	455	GLY	2.3
1	A	483	TYR	2.3
1	C	167	ALA	2.3
1	E	235	THR	2.3
1	A	120	ILE	2.3
1	C	280	ILE	2.3
1	C	377	ILE	2.3
1	G	193	VAL	2.3
1	I	49	VAL	2.3
1	K	205	VAL	2.3
1	C	268	CYS	2.2
1	E	129	CYS	2.2
1	E	469	CYS	2.2
1	I	282	ASN	2.2
1	C	460	GLU	2.2
1	I	20	THR	2.2
1	G	108	ILE	2.2
1	G	144	LEU	2.2
1	A	484	ARG	2.2
1	E	298	ARG	2.2
1	G	227	MET	2.2
1	E	187	GLY	2.2
1	C	332	GLU	2.2
1	K	332	GLU	2.2
1	I	301	LYS	2.2
1	K	48	THR	2.2
1	A	132	SER	2.2
1	A	215	ASN	2.2
1	C	298	ARG	2.2
1	G	232	ASP	2.2
1	K	381	ASN	2.2
1	C	206	PRO	2.2
1	A	296	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	45	GLY	2.2
1	I	4	CYS	2.2
1	K	219	GLY	2.2
1	E	104	GLU	2.2
1	I	378	GLU	2.2
1	E	9	ALA	2.2
1	E	183	THR	2.2
1	K	183	THR	2.2
1	A	88	TYR	2.2
1	A	359	TYR	2.2
1	G	88	TYR	2.2
1	K	81	ARG	2.2
1	G	92	PHE	2.2
1	K	488	MET	2.2
1	C	187	GLY	2.2
1	C	36	THR	2.2
1	E	151	ALA	2.2
1	I	158	SER	2.2
1	I	81	ARG	2.1
1	G	171	TRP	2.1
1	E	165	ASN	2.1
1	E	229	ASN	2.1
1	G	282	ASN	2.1
1	K	215	ASN	2.1
1	G	136	PHE	2.1
1	A	210	ALA	2.1
1	C	188	SER	2.1
1	E	244	ALA	2.1
1	K	112	ALA	2.1
1	C	256	MET	2.1
1	I	359	TYR	2.1
1	G	431	LEU	2.1
1	A	222	ASP	2.1
1	C	181	GLU	2.1
1	I	468	ASP	2.1
1	G	4	CYS	2.1
1	E	122	THR	2.1
1	C	488	MET	2.1
1	I	44	LYS	2.1
1	C	221	ILE	2.1
1	C	490	ASN	2.1
1	E	327	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	354	GLY	2.1
1	E	255	SER	2.1
1	G	42	CYS	2.1
1	C	151	ALA	2.1
1	I	191	LYS	2.1
1	G	155	MET	2.1
1	A	485	GLU	2.1
1	I	332	GLU	2.1
1	C	340	ASP	2.1
1	G	148	ASP	2.1
1	E	93	VAL	2.1
1	I	264	VAL	2.1
1	C	459	PHE	2.1
1	I	55	GLY	2.1
1	C	235	THR	2.0
1	K	188	SER	2.0
1	A	378	GLU	2.0
1	A	458	CYS	2.0
1	E	210	ALA	2.0
1	G	423	MET	2.0
1	A	382	GLN	2.0
1	E	75	ASP	2.0
1	E	373	LEU	2.0
1	K	376	LEU	2.0
1	K	461	ILE	2.0
1	C	230	PRO	2.0
1	C	121	ARG	2.0
1	E	90	GLY	2.0
1	E	189	GLY	2.0
1	G	160	LYS	2.0
1	C	171	TRP	2.0
1	C	113	MET	2.0
1	I	453	GLU	2.0
1	E	326	ALA	2.0
1	E	296	CYS	2.0
1	E	267	ASP	2.0
1	I	373	LEU	2.0
1	A	220	ARG	2.0
1	C	243	ILE	2.0
1	E	221	ILE	2.0
1	G	121	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

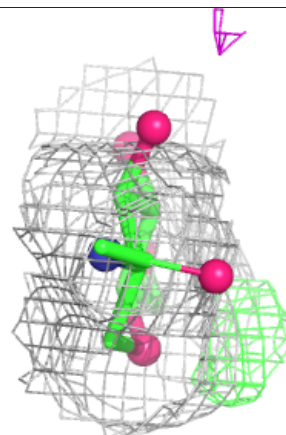
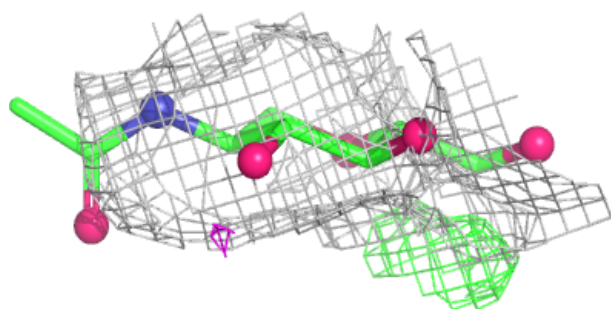
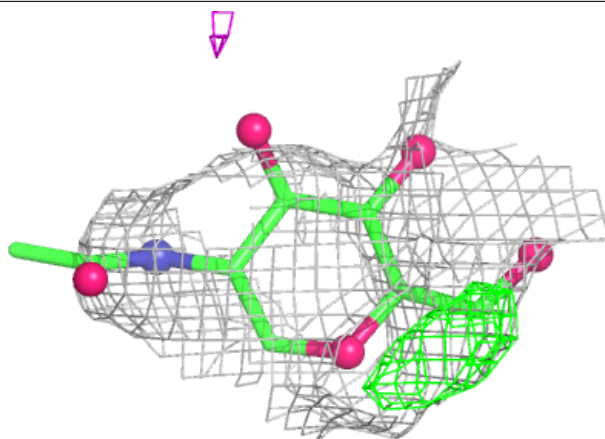
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	G	601	14/15	0.49	0.24	127,135,142,143	0
2	NAG	C	601	14/15	0.73	0.16	74,80,90,94	0
2	NAG	A	601	14/15	0.74	0.17	81,92,95,97	0
2	NAG	K	501	14/15	0.77	0.18	75,93,99,109	0
2	NAG	A	602	14/15	0.78	0.16	56,79,88,91	0
2	NAG	G	602	14/15	0.83	0.12	44,69,90,94	0
2	NAG	C	602	14/15	0.84	0.14	48,77,105,110	0
2	NAG	I	501	14/15	0.86	0.12	60,70,78,85	0
2	NAG	E	501	14/15	0.86	0.14	56,75,82,82	0

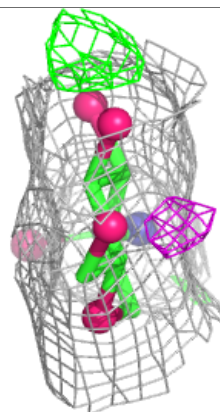
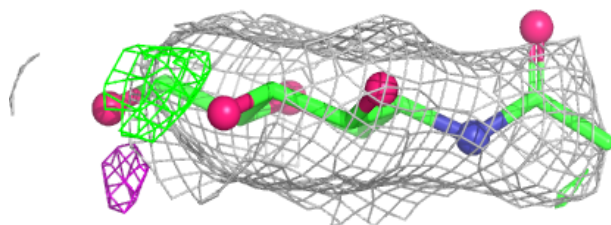
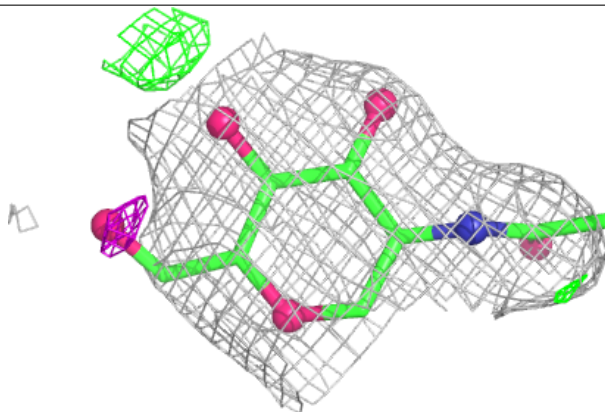
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG G 601:

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

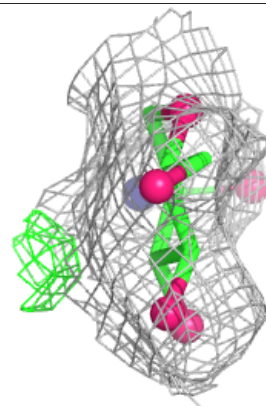
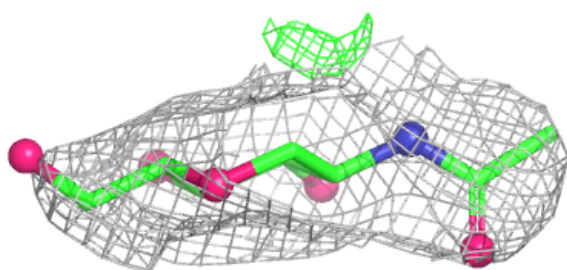
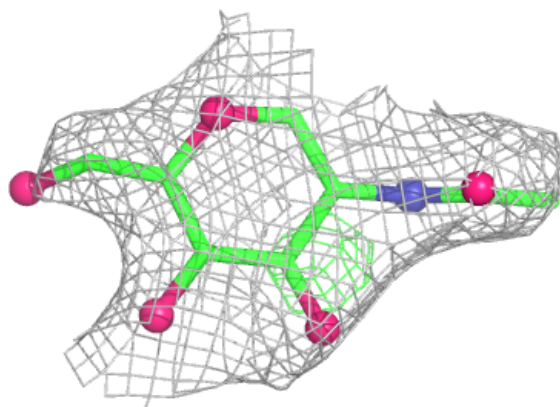
**Electron density around NAG C 601:**

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

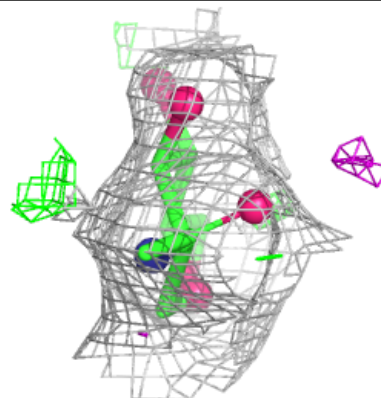
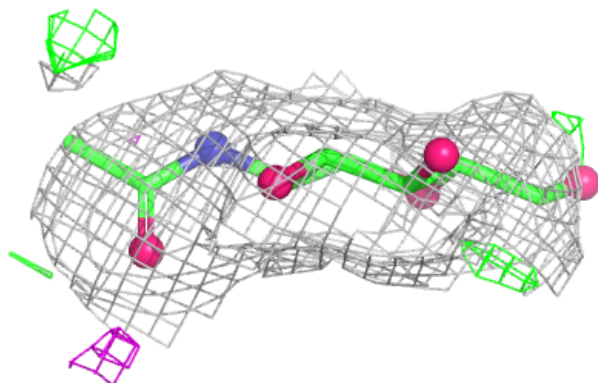
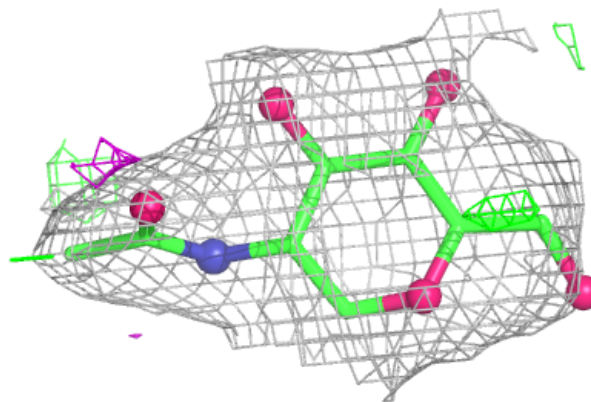


Electron density around NAG A 601:

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

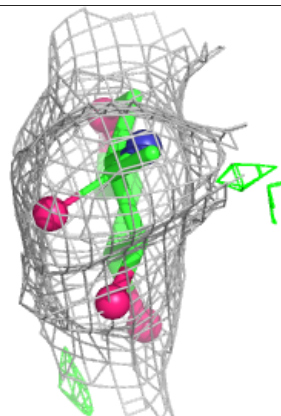
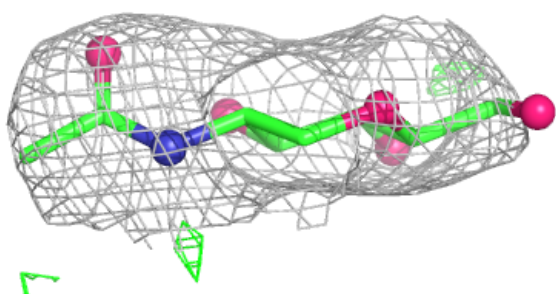
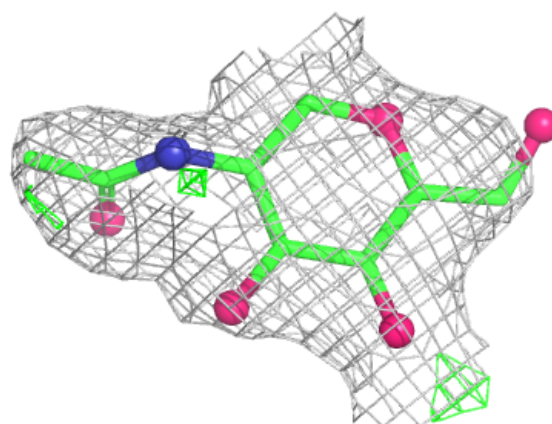
**Electron density around NAG K 501:**

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



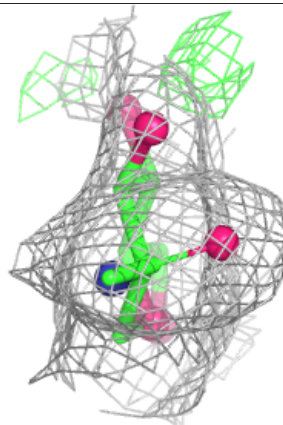
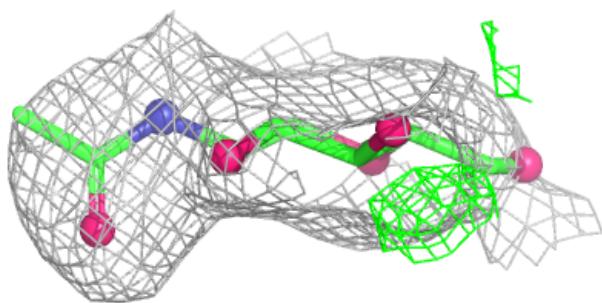
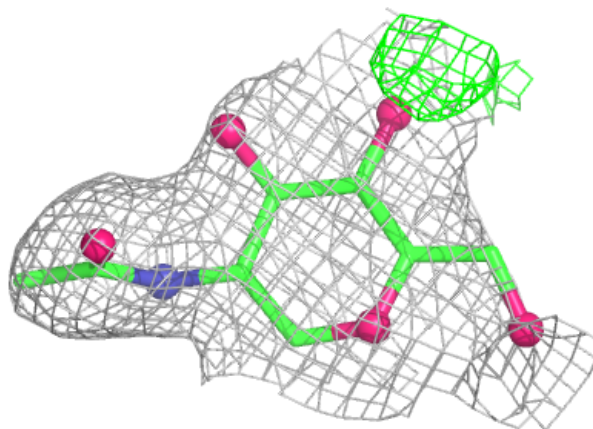
Electron density around NAG A 602:

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

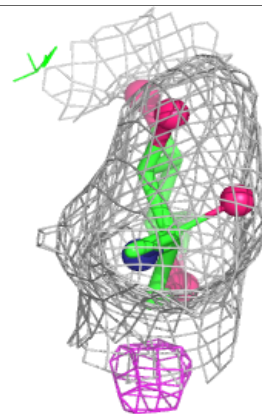
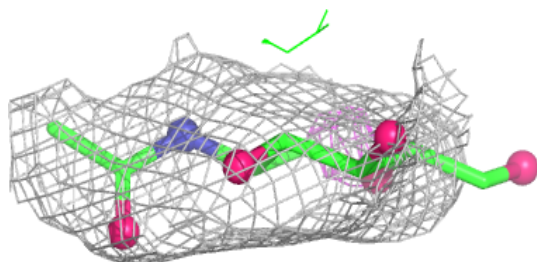
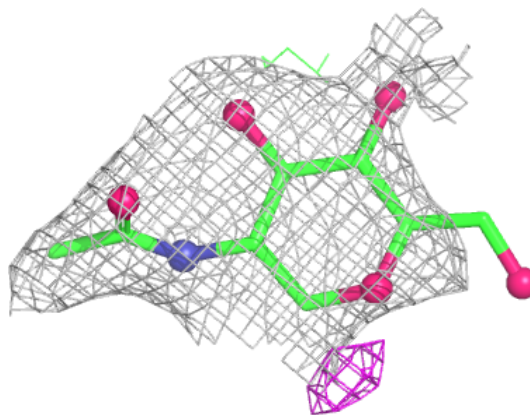


Electron density around NAG G 602:

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

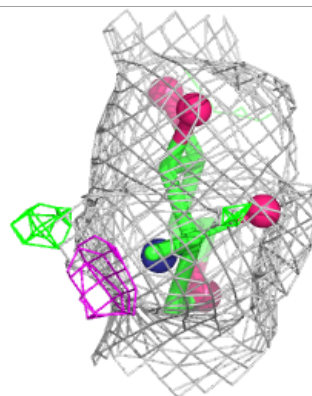
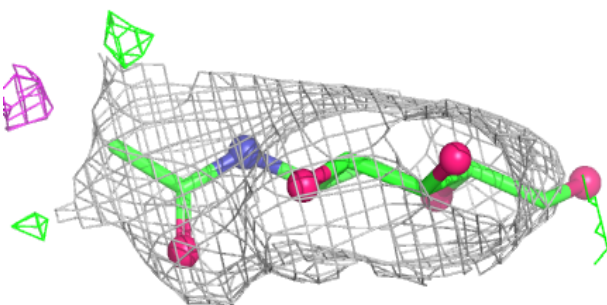
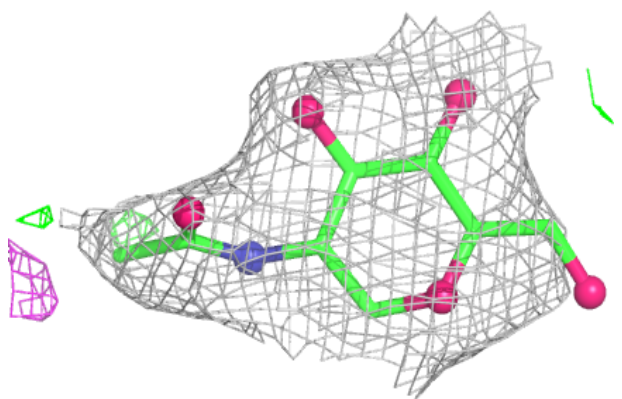
**Electron density around NAG C 602:**

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

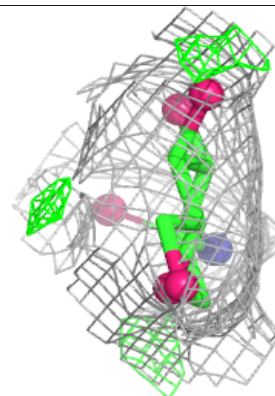
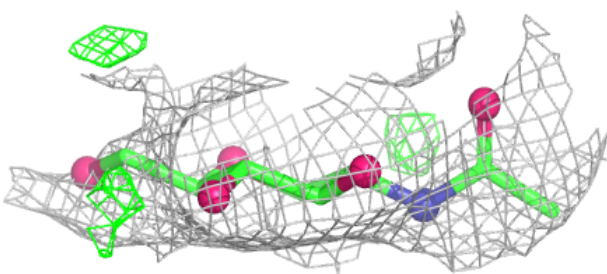
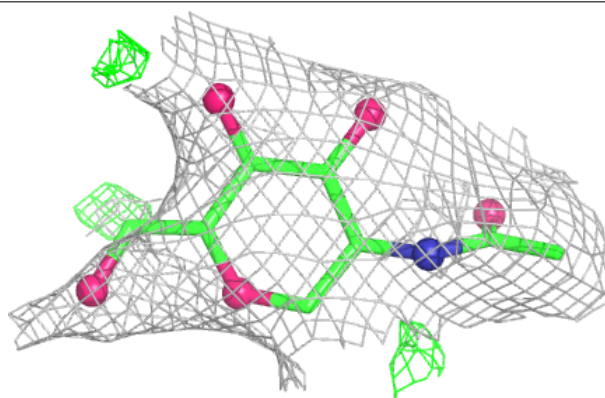


Electron density around NAG I 501:

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

**Electron density around NAG E 501:**

$2mF_o-DF_c$ (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.