



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:15 PM BST

PDB ID : 6IDD
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

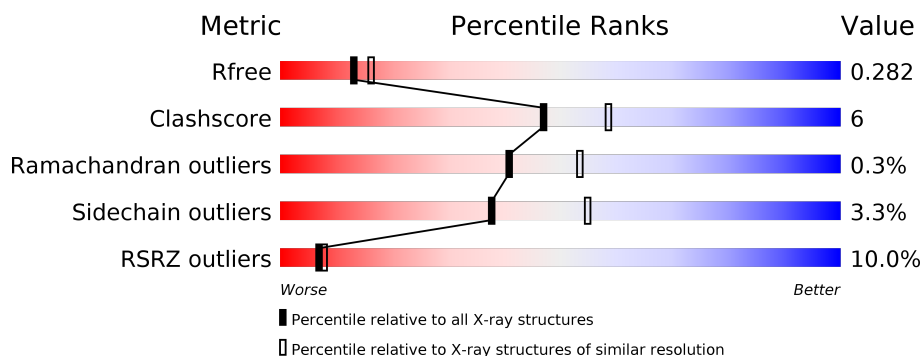
1 Overall quality at a glance

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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (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 on 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> <div>6%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>• •</div> </div> </div>
1	C	498	<div> <div>14%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>
1	E	498	<div> <div>15%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>• •</div> </div> </div>
1	G	498	<div> <div>12%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>• •</div> </div> </div>
1	I	498	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
1	K	498	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>•</div> </div> </div>

2 Entry composition

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

There are 24 discrepancies between the modelled and reference sequences:

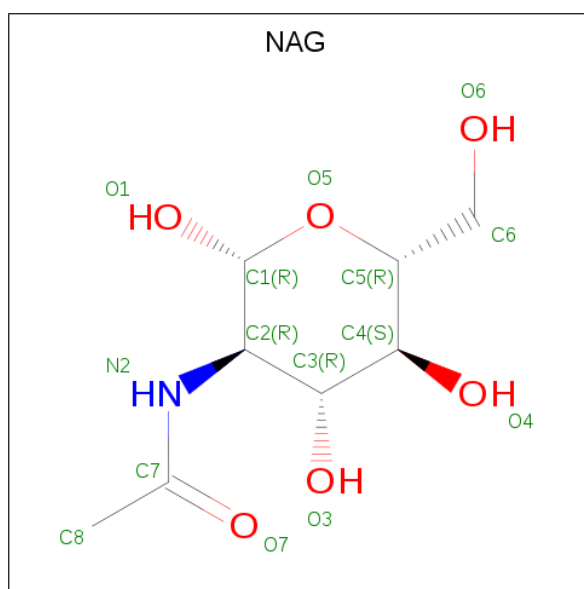
Chain	Residue	Modelled	Actual	Comment	Reference
A	165	ASN	SER	engineered mutation	UNP A0A088BEK2
A	267	ASP	ASN	engineered mutation	UNP A0A088BEK2
A	274	TYR	HIS	engineered mutation	UNP A0A088BEK2
A	392	THR	ASN	engineered mutation	UNP A0A088BEK2
C	165	ASN	SER	engineered mutation	UNP A0A088BEK2
C	267	ASP	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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by author).



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		

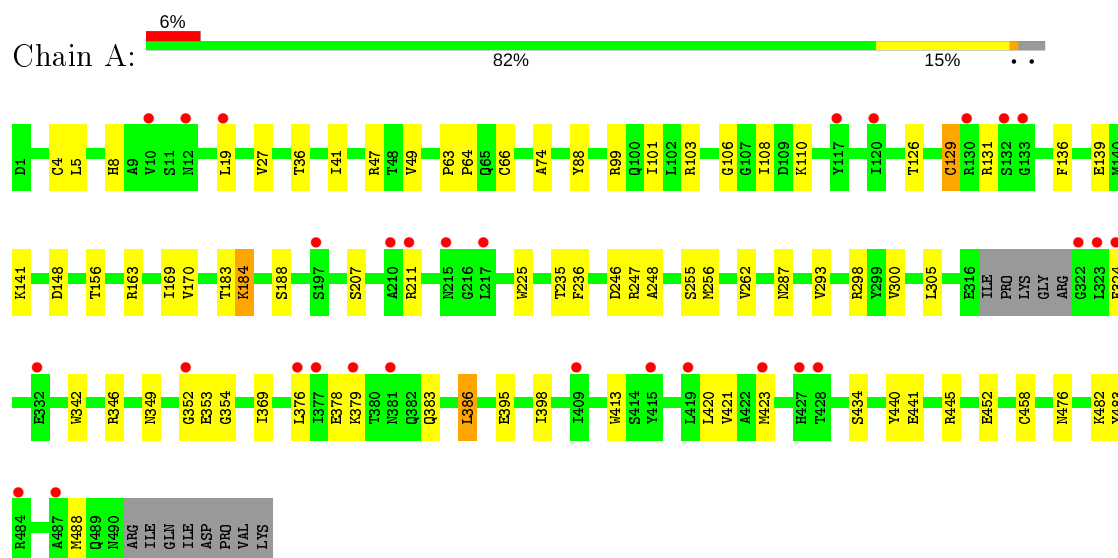
- Molecule 3 is water.

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		

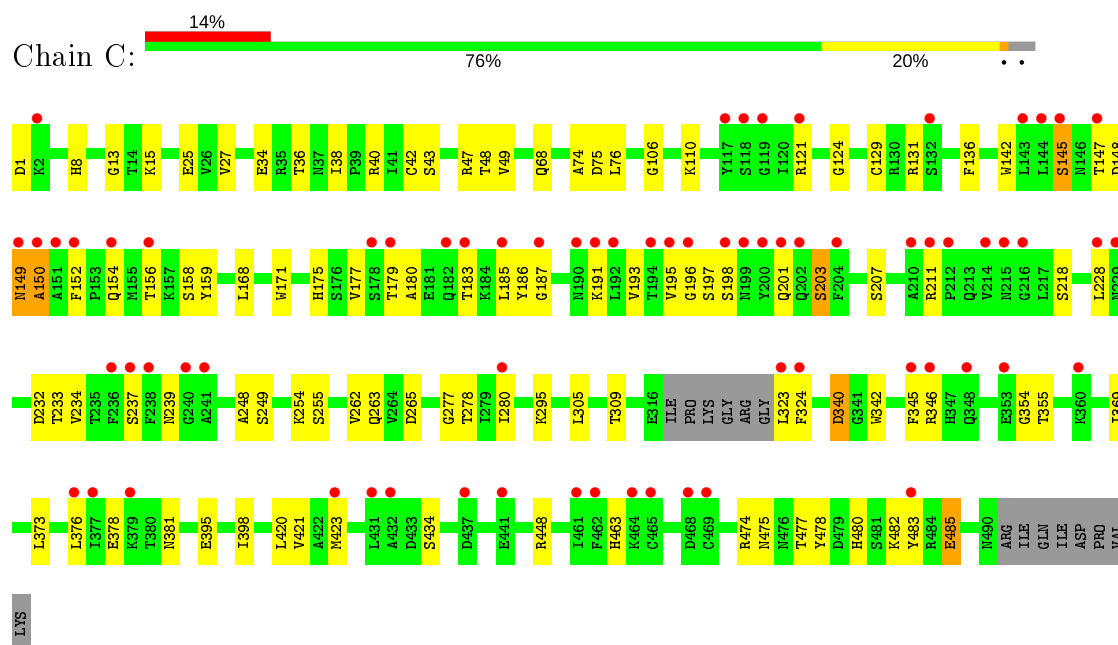
3 Residue-property plots [i](#)

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



Chain E:

15% 83% 14%

Polar Non-polar

Chain G:

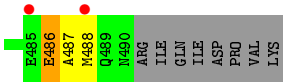
12% 81% 16%

D1 L5 H8 M12 L19 T36 R40 S43 K44 Q45 K46 R47 T48 V49 L76 I77 I78 E79 I108 D109 K110 Y117 S118 G119 I120 R121 A128 R131 S132 G133 F136 L143 I144 S145 M146 T147 D148 N149 A150 A151 F152 Q154 M155 T156 T162 R163 K164 H165 P166 A167 L168 L169 V170 T183 K184 L185 Y186 G187 G188 S189 M190 T194 V195 G196 S197 S198 M199 Q201 Q202 Q203 F204 P212 I221 W225 L226 M227 L228 F231 D232 T233 F236 R247 A248 S249 F250 Q259 V264 D265 A266 D267 C268 F269 A270 D271 I280 W287 G294 V300 R303 S304 L305 E316 ILE PRO LYS GLY ARG GLY L323 E332 W342 R346 H347 Q348 R349 A350 Q351 G352 F353 G354 T355 A356 I369 L373 I377 E378 R379 Q383 E395 K396 Q397 I398 R406 L420 V421 A422 W423 Q426 D430 L431 S434 Y440 Q446 L447 R448 G455 K464 D468 N475 N476 E485 Q489 R490 ARG ILE GLN ILE ASP PRO VAL LYS

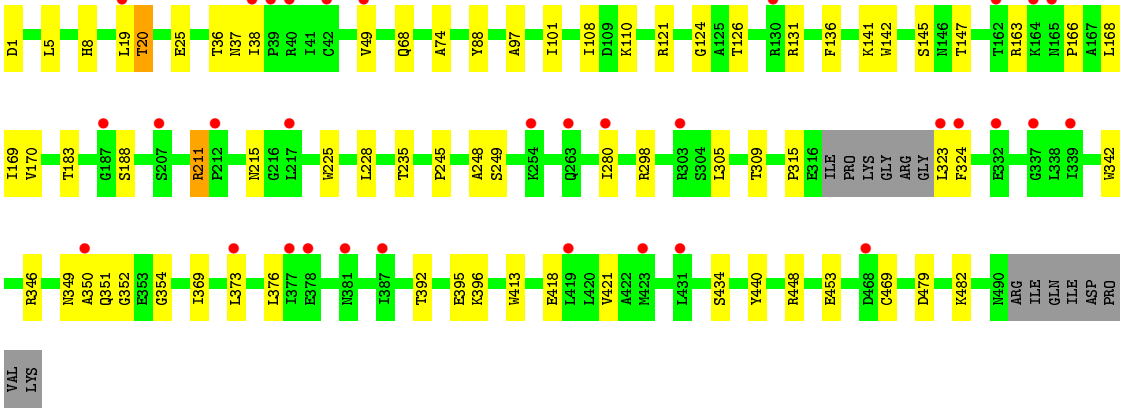
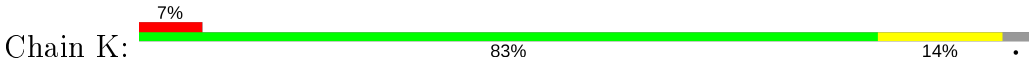
Chain I:

5% 79% 16%

D1 I3 C4 I12 L19 Y24 F115 T116 Y117 F136 E139 W142 L143 L144 S145 M146 T147 A150 T156 K157 S158 R163 K164 L168 I169 V170 V174 G187 S188 G189 M190 K191 L192 Y193 T194 V195 G196 A197 S198 M199 Y200 Q201 Q202 S203 P212 W225 W231 V234 T235 F236 R247 A248 S249 F250 S255 D265 E269 T278 R298 L305 T309 P315 E316 ILE P310 LYS GLY ANG G1Y L323 E332 W342 H347 Q348 H349 G354 T355 A356 L369 L373 N374 R375 L376 L377 N381 Q382 Q383 K386 E411 V412 W413 L420 V421 E424 S434 R442 R448 A451 E452 C458 I461 F462 H463 R464 C465 C469 M470 N475 M476 T477 Y478 D479 A480



● Molecule 1: Hemagglutinin



VAL
LYS

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 43.06 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.55-2.38) 97.9 (43.06-2.38)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.253 , 0.282 0.253 , 0.282	Depositor DCC
R_{free} test set	7463 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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	0.24	0/3853	0.43	0/5203
1	C	0.25	0/3841	0.43	0/5187
1	E	0.24	0/3849	0.43	0/5198
1	G	0.24	0/3845	0.43	0/5193
1	I	0.24	0/3846	0.43	0/5194
1	K	0.24	0/3845	0.43	0/5194
All	All	0.24	0/23079	0.43	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	46	0
1	C	3772	0	3629	65	0
1	E	3779	0	3637	46	0
1	G	3775	0	3632	44	0
1	I	3776	0	3633	55	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	279	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 (279) 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:187:GLY:H	1:I:191:LYS:HZ1	1.45	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: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:G:5:LEU:HD11	1:G:440:TYR:HA	1.83	0.61
1:E:43:SER:OG	3:E:601:HOH:O	2.16	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: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:E:110:LYS:HA	1:E:248:ALA:O	2.04	0.58
1:A:445:ARG:HG2	1:G:455:GLY:HA2	1.86	0.58
1:A:183:THR:HG22	1:A:188:SER:HA	1.86	0.57
1:A:101:ILE:HD11	1:G:396:LYS:HG2	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:C:158:SER:HA	1:C:234:VAL:O	2.05	0.57
1:A:434:SER:OG	1:G:323:LEU:O	2.22	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: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
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:N	1:G:190:ASN:OD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:295:LYS:NZ	3:C:713:HOH:O	2.40	0.55
1:E:170:VAL:HG22	1:E:225:TRP:HB3	1.89	0.54
1:E:323:LEU:O	1:G:434:SER:OG	2.17	0.54
1:G:117:TYR:HD2	1:G:155:MET:HE1	1.72	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:40:ARG:HD2	1:C:265:ASP:HB2	1.89	0.53
1:C:34:GLU:OE2	1:C:36:THR:HB	2.07	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:C:340:ASP:OD1	1:C:340:ASP:N	2.40	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:GLU:HB3	1:E:398:ILE:HG22	1.91	0.51
1:G:110:LYS:HA	1:G:248:ALA:O	2.10	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: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
1:I:8:HIS:ND1	1:I:342:TRP:HA	2.29	0.47
1:I:42:CYS:HB2	1:I:278:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:169:ILE:O	1:I:225:TRP:HA	2.17	0.45
1:I:110:LYS:HA	1:I:248:ALA:O	2.16	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:A:293:VAL:HG11	1:A:386:LEU:HD13	1.98	0.45
1:E:464:LYS:HA	1:E:464:LYS:HD3	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:I:323:LEU:O	1:K:434:SER:OG	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:434:SER:OG	1:K:323:LEU:O	2.25	0.44
1:C:171:TRP:CE2	1:C:195:VAL:HG21	2.53	0.44
1:E:174:HIS:ND1	1:E:186:TYR:OH	2.44	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:C:463:HIS:NE2	1:C:478:TYR:OH	2.42	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:305:LEU:HB3	1:C:421:VAL:HG21	2.00	0.43
1:K:349:ASN:C	1:K:351:GLN:H	2.22	0.43
1:G:12:ASN:ND2	1:G:12:ASN:O	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: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
1:I:463:HIS:NE2	1:I:478:TYR:OH	2.51	0.42
1:I:464:LYS:NZ	1:I:486:GLU:OE1	2.35	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:166:PRO:HA	1:K:228:LEU:O	2.20	0.42
1:K:88:TYR:HD1	1:K:126:THR:HG21	1.83	0.42
1:A:156:THR:HA	1:A:236:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:HG23	1:C:36:THR:HG23	2.00	0.42
1:G:228:LEU:HA	1:G:228:LEU:HD23	1.90	0.42
1:I:463:HIS:HE2	1:I:478:TYR:HH	1.63	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:K:121:ARG:HD3	1:K:145:SER:O	2.20	0.41
1:K:49:VAL:HG23	1:K:74:ALA:HB2	2.02	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: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:170:VAL:HG22	1:I:225:TRP:HB3	2.02	0.41
1:I:19:LEU:HA	1:I:19:LEU:HD12	1.91	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:E:44:LYS:HD3	1:E:269:GLU:HB2	2.02	0.41
1:K:68:GLN:OE1	1:K:68:GLN:N	2.49	0.41
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.21	0.41
1:C:376:LEU:HD22	1:C:420:LEU:HD21	2.03	0.41
1:C:68:GLN:N	1:C:68:GLN:OE1	2.46	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: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:187:GLY:HA2	3:C:701:HOH:O	2.20	0.40
1:C:177:VAL:HG22	1:C:218:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:332:GLU:CD	1:I:332:GLU:H	2.22	0.40
1:I:452:GLU:OE1	1:K:448:ARG:NH2	2.54	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:168:LEU:HB3	1:C:249:SER:HB2	2.04	0.40
1:C:47:ARG:NH1	1:C:75:ASP:OD1	2.54	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:HB2	1:I:164:LYS:HE3	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%)	47	61
1	C	480/498 (96%)	439 (92%)	37 (8%)	4 (1%)	19	27
1	E	480/498 (96%)	446 (93%)	34 (7%)	0	100	100
1	G	480/498 (96%)	451 (94%)	27 (6%)	2 (0%)	34	46
1	I	480/498 (96%)	453 (94%)	25 (5%)	2 (0%)	34	46
1	K	480/498 (96%)	452 (94%)	28 (6%)	0	100	100
All	All	2881/2988 (96%)	2701 (94%)	171 (6%)	9 (0%)	41	53

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	149	ASN

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Mol	Chain	Res	Type
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 ⓘ

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%)	402 (98%)	7 (2%)	60	76
1	C	408/421 (97%)	393 (96%)	15 (4%)	34	50
1	E	409/421 (97%)	400 (98%)	9 (2%)	52	69
1	G	408/421 (97%)	393 (96%)	15 (4%)	34	50
1	I	408/421 (97%)	389 (95%)	19 (5%)	26	39
1	K	408/421 (97%)	393 (96%)	15 (4%)	34	50
All	All	2450/2526 (97%)	2370 (97%)	80 (3%)	38	55

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	129	CYS
1	A	163	ARG
1	A	184	LYS
1	A	386	LEU
1	A	441	GLU
1	A	476	ASN
1	C	1	ASP
1	C	129	CYS
1	C	145	SER

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Mol	Chain	Res	Type
1	C	147	THR
1	C	148	ASP
1	C	152	PHE
1	C	156	THR
1	C	185	LEU
1	C	191	LYS
1	C	201	GLN
1	C	237	SER
1	C	254	LYS
1	C	263	GLN
1	C	340	ASP
1	C	485	GLU
1	E	12	ASN
1	E	37	ASN
1	E	48	THR
1	E	113	MET
1	E	130	ARG
1	E	147	THR
1	E	148	ASP
1	E	254	LYS
1	E	256	MET
1	G	1	ASP
1	G	8	HIS
1	G	12	ASN
1	G	19	LEU
1	G	149	ASN
1	G	163	ARG
1	G	190	ASN
1	G	201	GLN
1	G	202	GLN
1	G	227	MET
1	G	303	ARG
1	G	332	GLU
1	G	379	LYS
1	G	468	ASP
1	G	475	ASN
1	I	1	ASP
1	I	19	LEU
1	I	37	ASN
1	I	144	LEU
1	I	147	THR
1	I	184	LYS

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Mol	Chain	Res	Type
1	I	194	THR
1	I	199	ASN
1	I	201	GLN
1	I	202	GLN
1	I	298	ARG
1	I	315	PRO
1	I	323	LEU
1	I	332	GLU
1	I	383	GLN
1	I	464	LYS
1	I	477	THR
1	I	486	GLU
1	I	488	MET
1	K	1	ASP
1	K	8	HIS
1	K	19	LEU
1	K	20	THR
1	K	25	GLU
1	K	36	THR
1	K	37	ASN
1	K	141	LYS
1	K	147	THR
1	K	163	ARG
1	K	211	ARG
1	K	315	PRO
1	K	376	LEU
1	K	392	THR
1	K	418	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	C	8	HIS
1	E	446	GLN
1	I	199	ASN
1	I	263	GLN
1	K	53	GLN
1	K	383	GLN
1	K	446	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	602	1	14,14,15	0.28	0	17,19,21	0.45	0
2	NAG	K	501	1	14,14,15	0.24	0	17,19,21	0.43	0
2	NAG	C	601	1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	I	501	1	14,14,15	0.25	0	17,19,21	0.41	0
2	NAG	A	601	1	14,14,15	0.24	0	17,19,21	0.48	0
2	NAG	G	601	1	14,14,15	0.28	0	17,19,21	0.44	0
2	NAG	C	602	1	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	E	501	1	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	G	602	1	14,14,15	0.26	0	17,19,21	0.44	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	A	602	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	K	501	1	-	0/6/23/26	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	A	601	1	-	2/6/23/26	0/1/1/1
2	NAG	G	601	1	-	1/6/23/26	0/1/1/1
2	NAG	C	602	1	-	0/6/23/26	0/1/1/1
2	NAG	E	501	1	-	0/6/23/26	0/1/1/1
2	NAG	G	602	1	-	1/6/23/26	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:

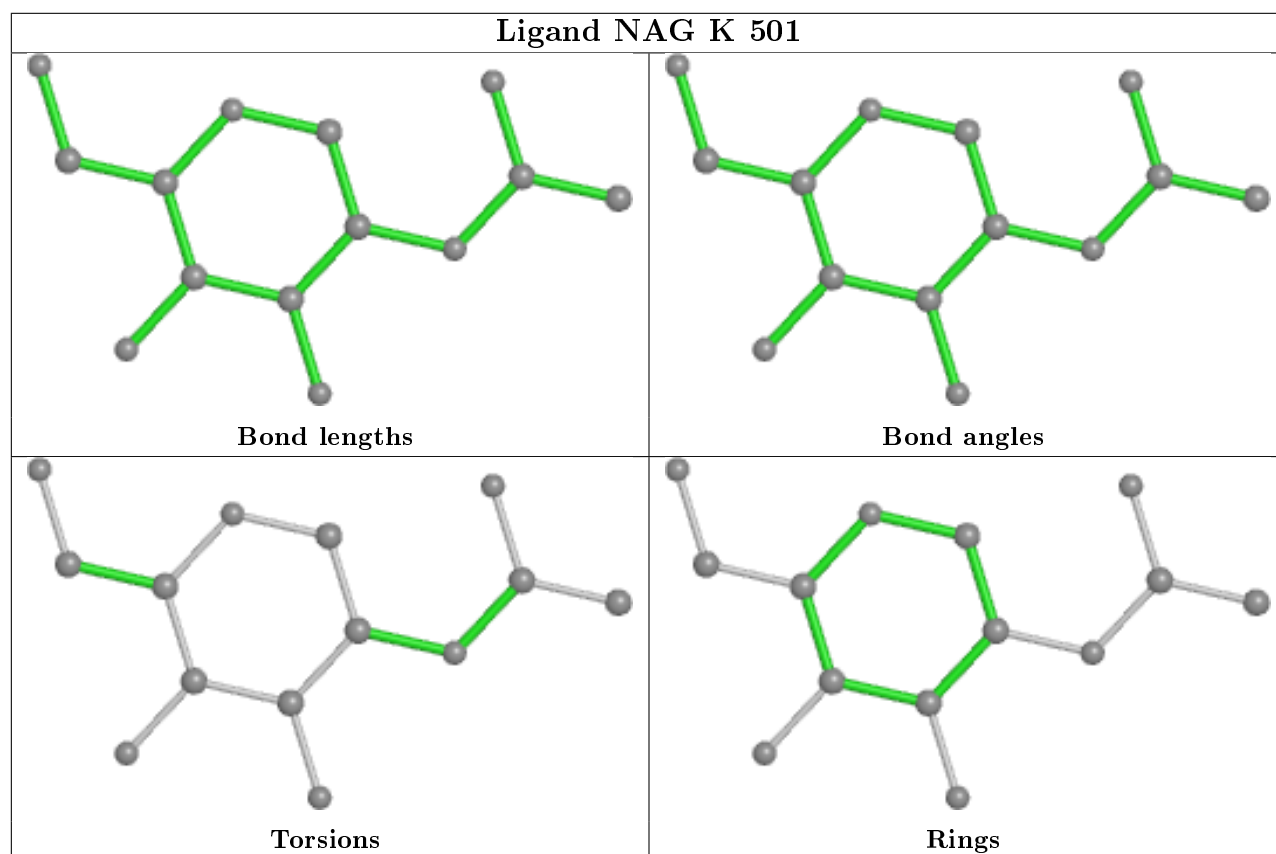
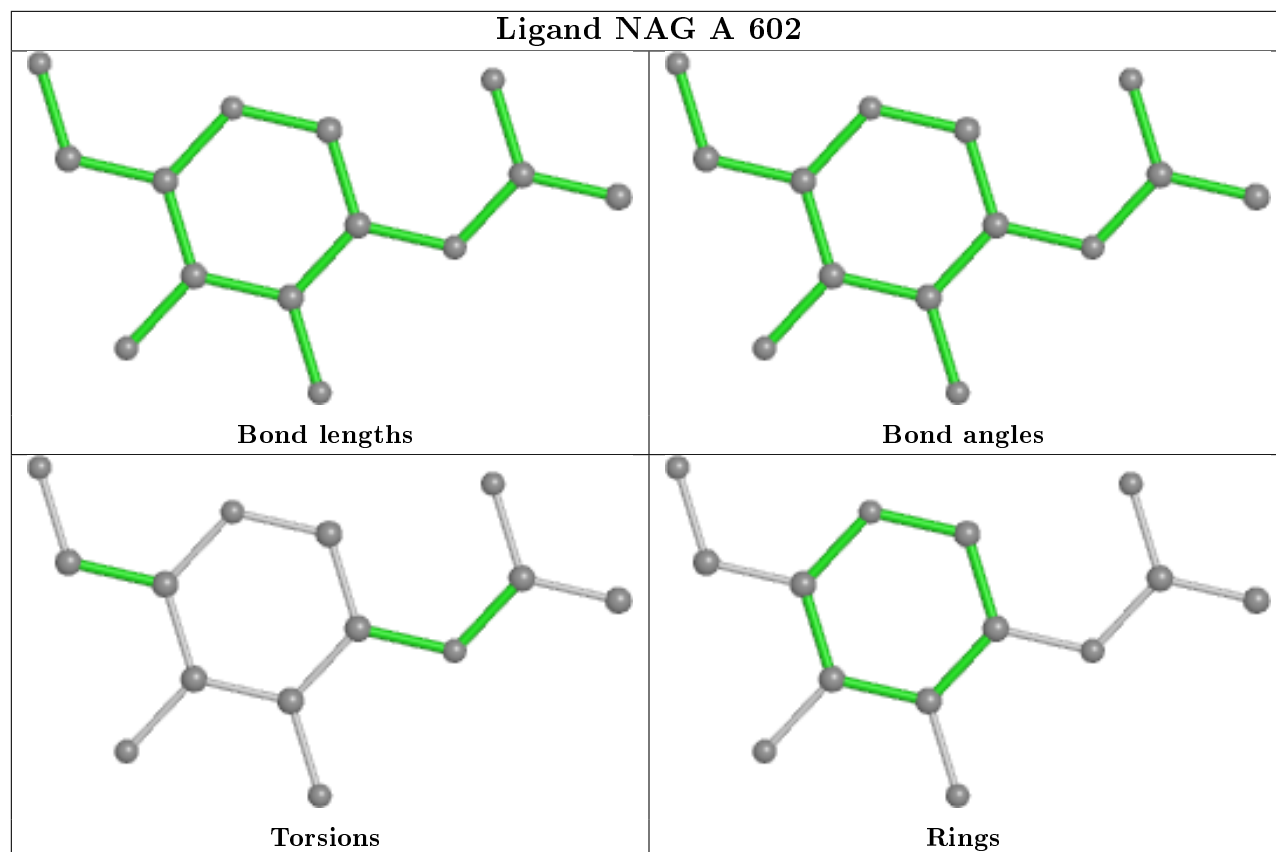
Mol	Chain	Res	Type	Atoms
2	A	601	NAG	O5-C5-C6-O6
2	A	601	NAG	C4-C5-C6-O6
2	G	601	NAG	O5-C5-C6-O6
2	G	602	NAG	O5-C5-C6-O6
2	C	601	NAG	O5-C5-C6-O6

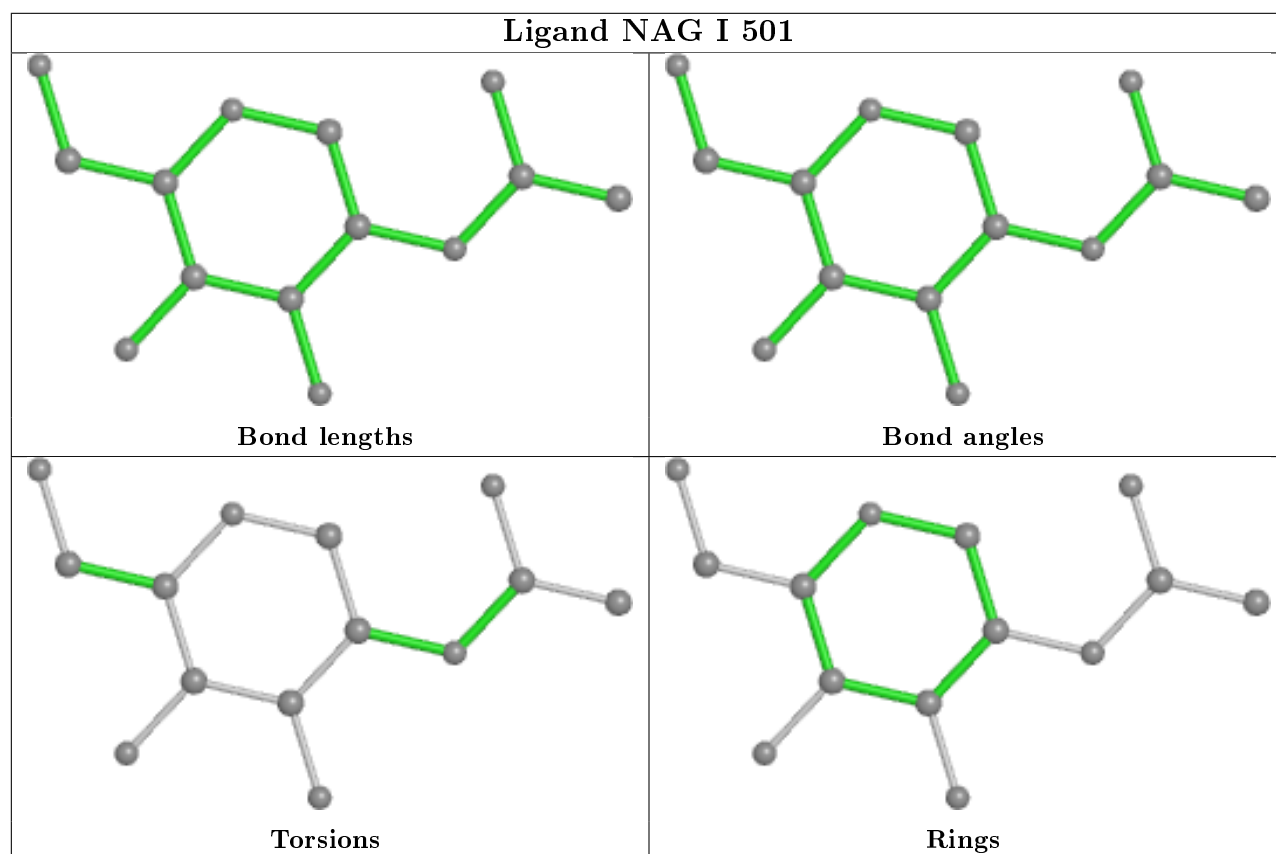
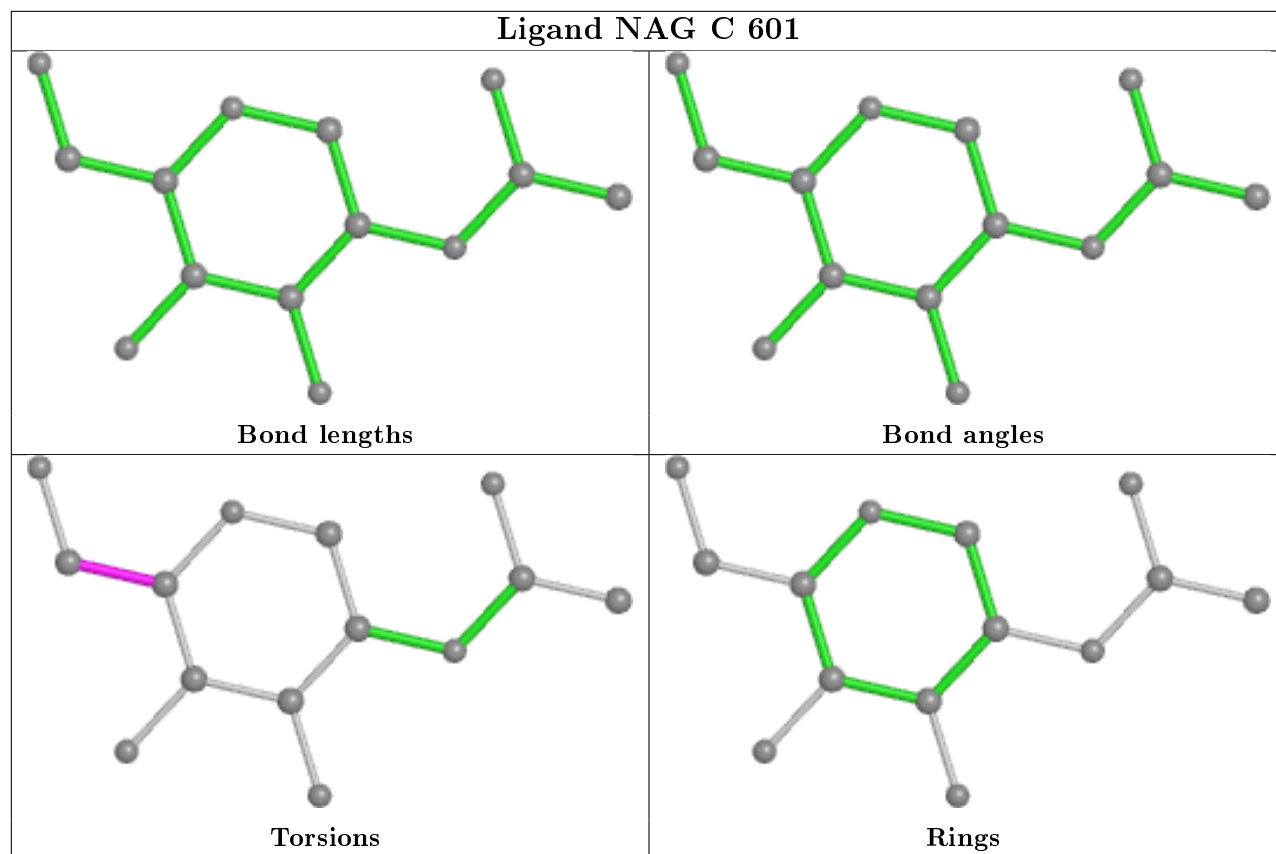
There are no ring outliers.

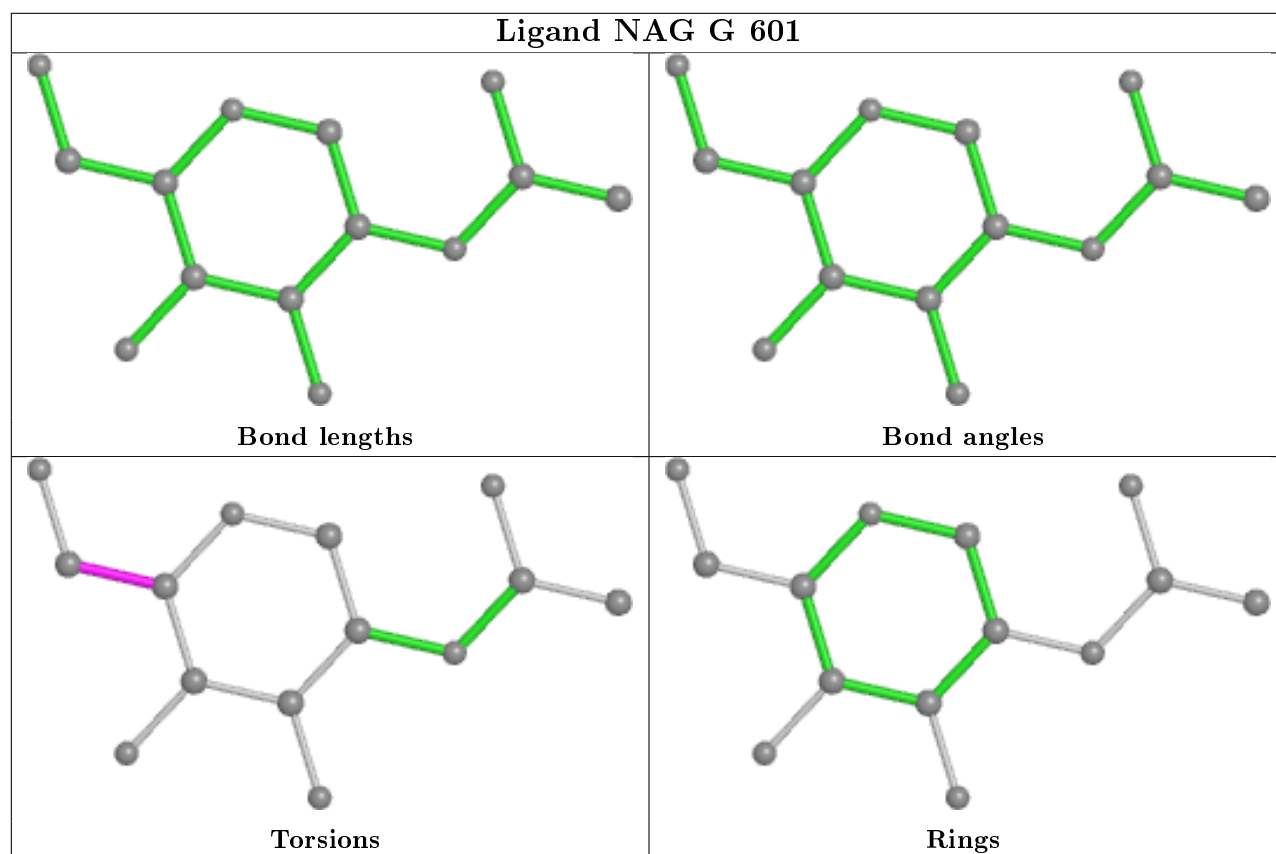
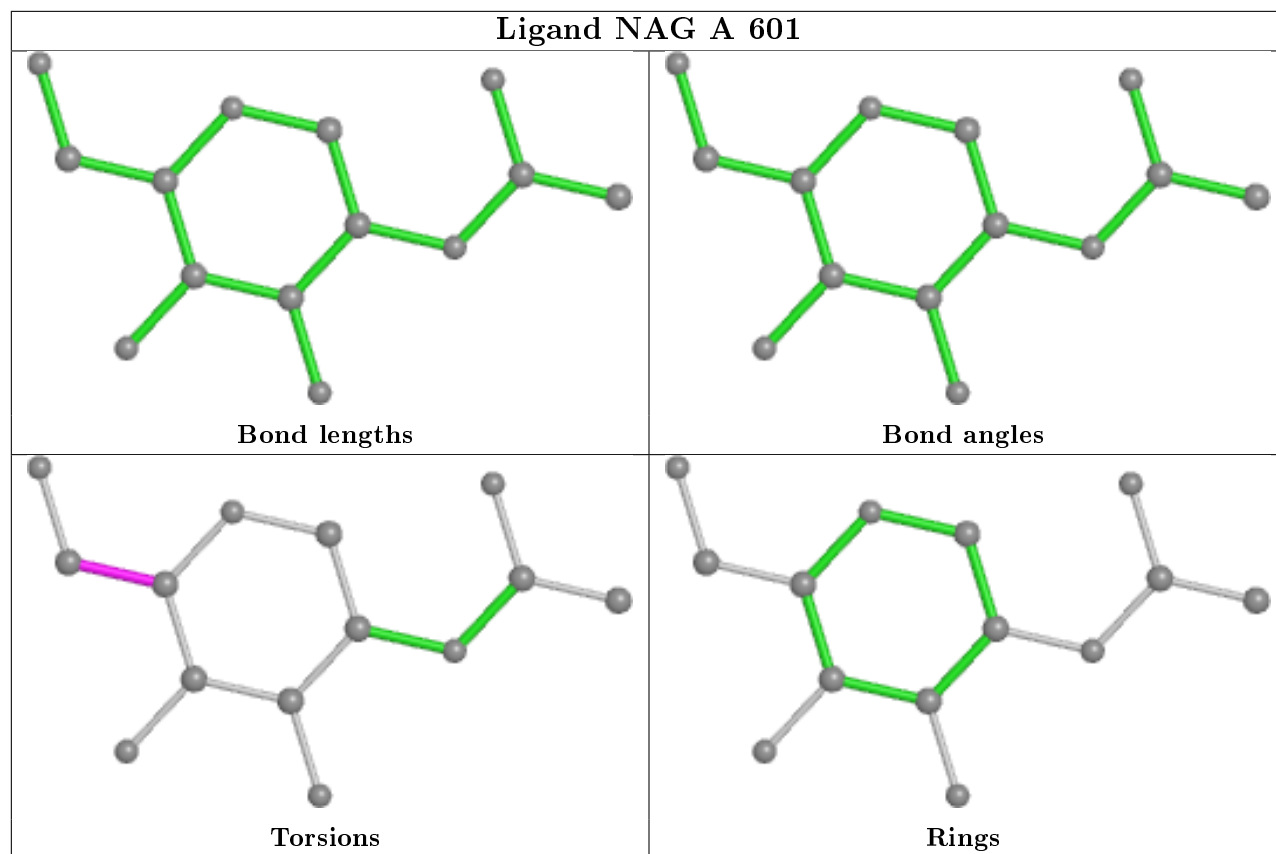
1 monomer is involved in 1 short contact:

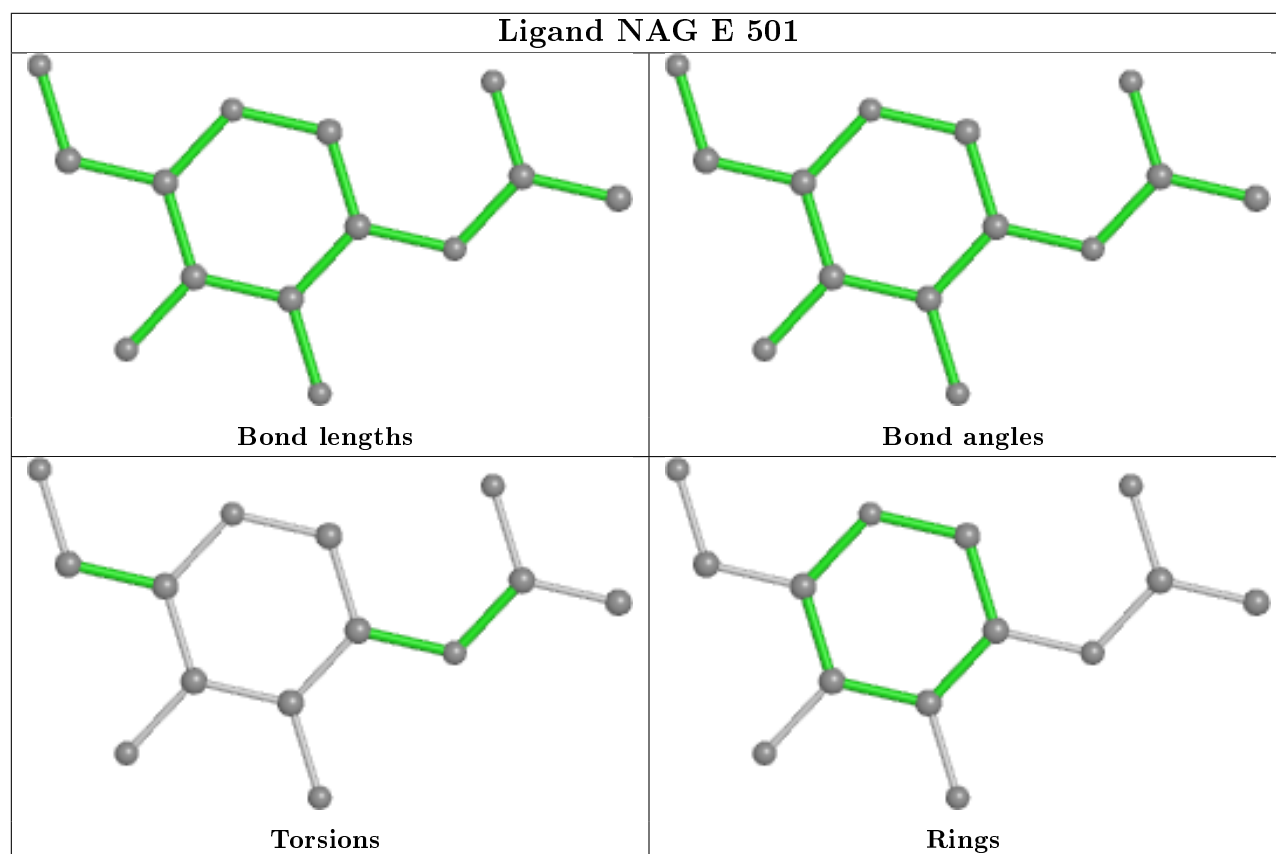
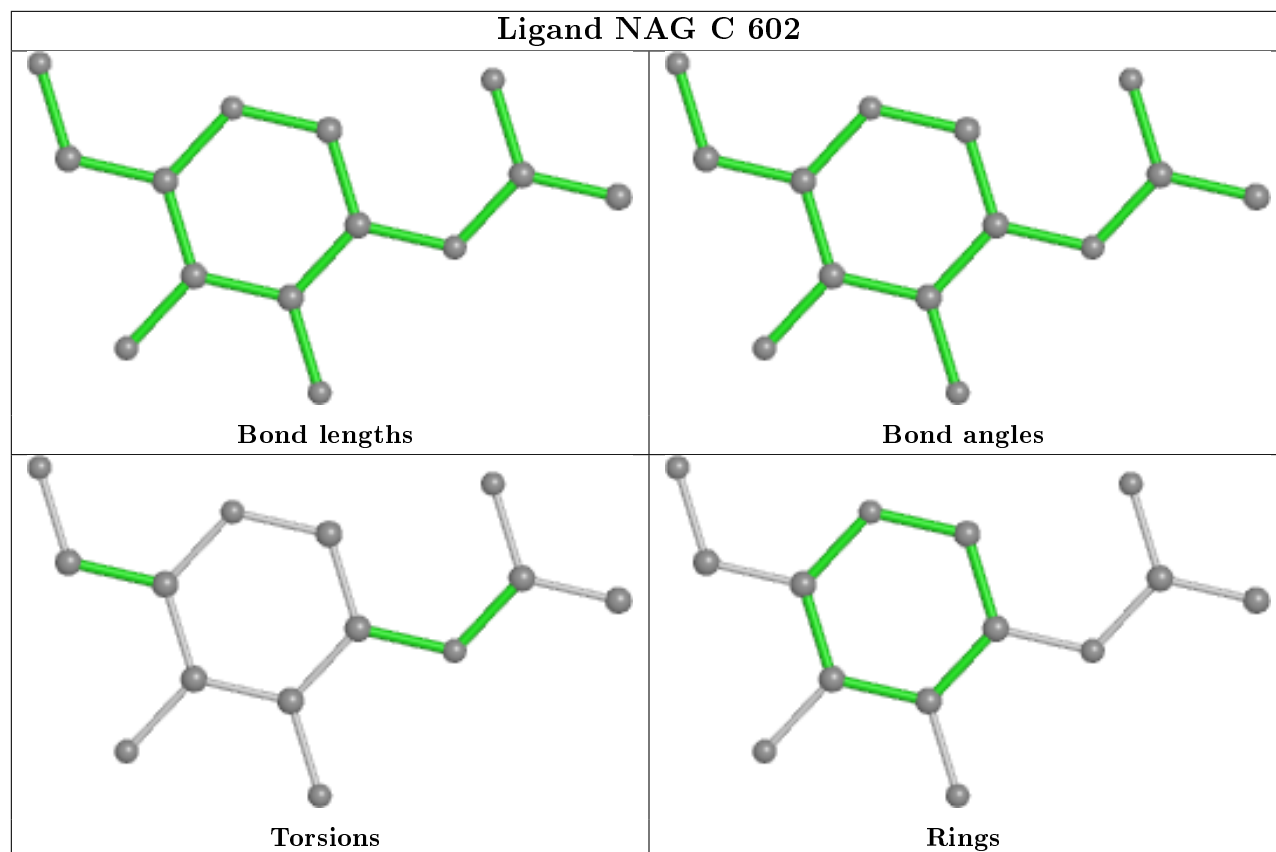
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	501	NAG	1	0

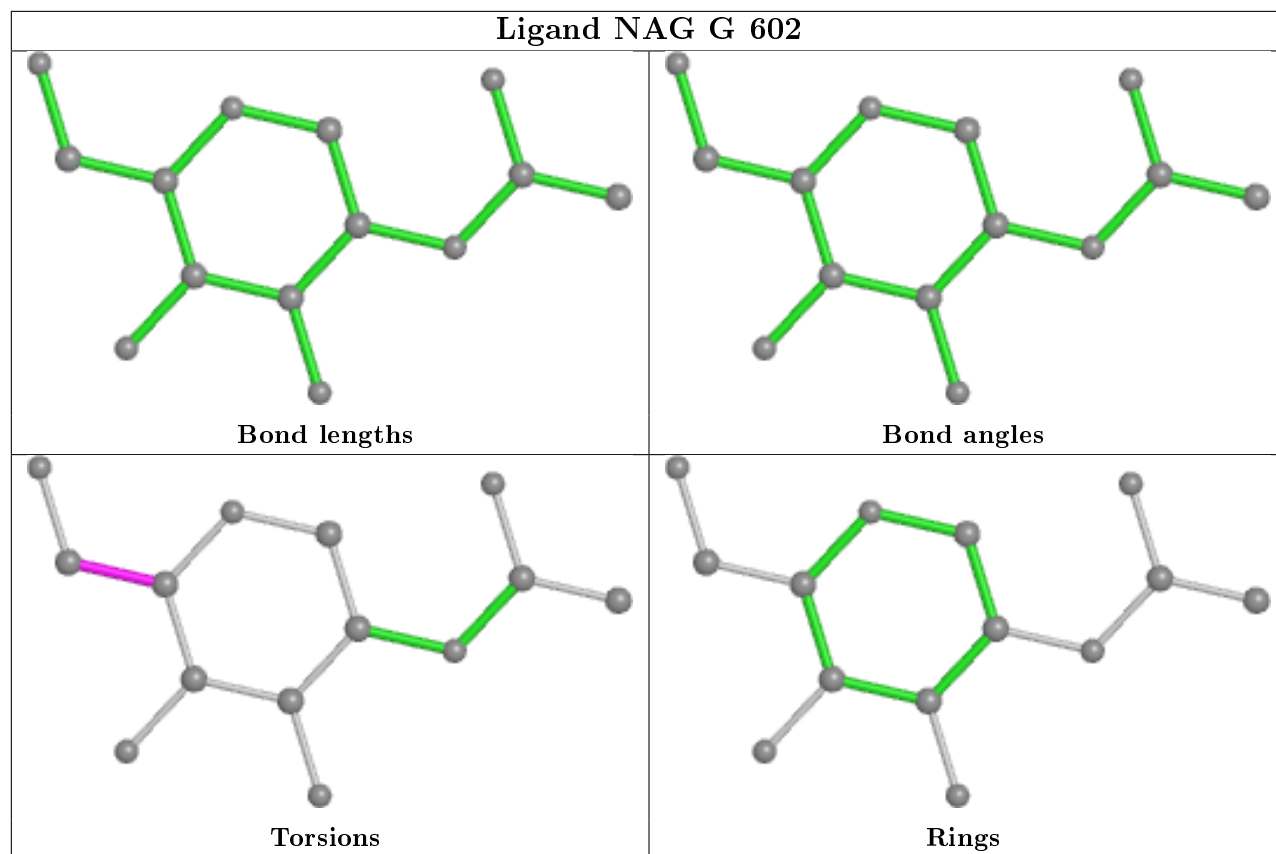
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	0.56	30 (6%)	20 22	29, 48, 77, 120	0
1	C	484/498 (97%)	0.93	70 (14%)	2 2	29, 59, 101, 131	0
1	E	484/498 (97%)	0.91	73 (15%)	2 2	35, 60, 101, 130	0
1	G	484/498 (97%)	0.88	58 (11%)	4 5	33, 59, 93, 140	0
1	I	484/498 (97%)	0.56	26 (5%)	25 28	32, 54, 92, 183	0
1	K	484/498 (97%)	0.64	33 (6%)	17 18	32, 55, 85, 146	0
All	All	2905/2988 (97%)	0.74	290 (9%)	7 8	29, 55, 93, 183	0

All (290) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	ASN	10.2
1	C	183	THR	7.4
1	I	190	ASN	7.1
1	C	214	VAL	6.8
1	G	150	ALA	6.5
1	C	212	PRO	6.0
1	E	379	LYS	5.8
1	C	240	GLY	5.7
1	C	185	LEU	5.6
1	G	120	ILE	5.6
1	G	280	ILE	5.6
1	E	120	ILE	5.2
1	A	487	ALA	4.8
1	G	199	ASN	4.8
1	C	118	SER	4.6
1	E	203	SER	4.5
1	E	260	SER	4.5
1	E	204	PHE	4.5
1	G	268	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	216	GLY	4.3
1	G	270	GLY	4.3
1	A	323	LEU	4.3
1	G	76	LEU	4.3
1	G	164	LYS	4.3
1	G	201	GLN	4.2
1	K	162	THR	4.2
1	G	200	TYR	4.2
1	E	200	TYR	4.2
1	C	323	LEU	4.1
1	C	462	PHE	4.1
1	G	194	THR	4.1
1	C	152	PHE	4.1
1	I	356	ALA	4.0
1	E	117	TYR	4.0
1	I	323	LEU	4.0
1	K	350	ALA	4.0
1	C	199	ASN	4.0
1	C	195	VAL	3.9
1	K	339	ILE	3.9
1	K	323	LEU	3.9
1	C	464	LYS	3.9
1	E	202	GLN	3.9
1	C	379	LYS	3.8
1	C	210	ALA	3.8
1	I	464	LYS	3.7
1	G	323	LEU	3.7
1	G	348	GLN	3.7
1	A	379	LYS	3.6
1	I	196	GLY	3.6
1	G	45	GLY	3.6
1	E	240	GLY	3.5
1	G	195	VAL	3.5
1	K	381	ASN	3.5
1	E	386	LEU	3.5
1	G	221	ILE	3.5
1	A	324	PHE	3.4
1	C	154	GLN	3.4
1	I	348	GLN	3.4
1	C	201	GLN	3.4
1	E	119	GLY	3.4
1	C	117	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	200	TYR	3.3
1	K	431	LEU	3.3
1	C	147	THR	3.3
1	I	354	GLY	3.3
1	E	215	ASN	3.3
1	G	167	ALA	3.3
1	G	377	ILE	3.3
1	C	194	THR	3.2
1	A	133	GLY	3.2
1	G	267	ASP	3.2
1	E	423	MET	3.2
1	C	469	CYS	3.2
1	I	461	ILE	3.2
1	E	9	ALA	3.2
1	C	149	ASN	3.2
1	C	187	GLY	3.2
1	E	280	ILE	3.1
1	E	48	THR	3.1
1	E	196	GLY	3.1
1	G	264	VAL	3.1
1	C	431	LEU	3.1
1	A	132	SER	3.1
1	I	188	SER	3.1
1	E	167	ALA	3.1
1	K	49	VAL	3.1
1	I	488	MET	3.1
1	C	465	CYS	3.1
1	E	323	LEU	3.1
1	A	12	ASN	3.0
1	E	234	VAL	3.0
1	A	322	GLY	3.0
1	K	39	PRO	3.0
1	C	182	GLN	3.0
1	E	144	LEU	3.0
1	K	164	LYS	3.0
1	C	202	GLN	3.0
1	A	215	ASN	3.0
1	G	431	LEU	2.9
1	G	423	MET	2.9
1	G	133	GLY	2.9
1	E	194	THR	2.9
1	G	202	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	350	ALA	2.9
1	G	43	SER	2.9
1	A	10	VAL	2.9
1	E	268	CYS	2.9
1	A	217	LEU	2.9
1	K	254	LYS	2.9
1	G	379	LYS	2.8
1	I	3	ILE	2.8
1	G	48	THR	2.8
1	K	38	ILE	2.8
1	K	387	ILE	2.8
1	G	162	THR	2.8
1	I	377	ILE	2.8
1	E	43	SER	2.8
1	I	485	GLU	2.8
1	G	151	ALA	2.8
1	I	470	MET	2.8
1	K	332	GLU	2.8
1	C	468	ASP	2.7
1	E	241	ALA	2.7
1	A	211	ARG	2.7
1	E	186	TYR	2.7
1	K	212	PRO	2.7
1	E	49	VAL	2.7
1	E	113	MET	2.7
1	G	36	THR	2.7
1	I	12	ASN	2.7
1	I	349	ASN	2.7
1	C	145	SER	2.7
1	C	237	SER	2.7
1	C	441	GLU	2.7
1	G	349	ASN	2.7
1	A	332	GLU	2.7
1	E	233	THR	2.7
1	G	269	GLU	2.7
1	C	236	PHE	2.7
1	C	238	PHE	2.7
1	I	117	TYR	2.6
1	C	150	ALA	2.6
1	E	377	ILE	2.6
1	K	40	ARG	2.6
1	A	19	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	115	PHE	2.6
1	G	197	SER	2.6
1	C	179	THR	2.6
1	I	19	LEU	2.6
1	I	462	PHE	2.6
1	E	40	ARG	2.6
1	E	121	ARG	2.6
1	C	377	ILE	2.6
1	E	114	GLY	2.6
1	E	250	PHE	2.6
1	A	117	TYR	2.6
1	E	339	ILE	2.6
1	C	2	LYS	2.6
1	E	78	ILE	2.6
1	K	280	ILE	2.6
1	E	205	VAL	2.5
1	C	437	ASP	2.5
1	C	151	ALA	2.5
1	C	198	SER	2.5
1	G	166	PRO	2.5
1	E	324	PHE	2.5
1	C	346	ARG	2.5
1	E	41	ILE	2.5
1	K	468	ASP	2.5
1	C	121	ARG	2.5
1	E	152	PHE	2.5
1	G	49	VAL	2.5
1	C	178	SER	2.5
1	K	378	GLU	2.5
1	E	201	GLN	2.5
1	C	345	PHE	2.5
1	G	204	PHE	2.5
1	E	478	TYR	2.5
1	E	169	ILE	2.5
1	E	75	ASP	2.5
1	G	188	SER	2.4
1	C	324	PHE	2.4
1	C	483	TYR	2.4
1	A	484	ARG	2.4
1	C	228	LEU	2.4
1	E	42	CYS	2.4
1	I	373	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	192	LEU	2.4
1	E	376	LEU	2.4
1	G	165	ASN	2.4
1	K	423	MET	2.4
1	C	204	PHE	2.4
1	E	237	SER	2.4
1	C	143	LEU	2.4
1	C	423	MET	2.4
1	C	229	ASN	2.4
1	G	78	ILE	2.4
1	G	108	ILE	2.4
1	K	377	ILE	2.4
1	C	211	ARG	2.4
1	K	19	LEU	2.4
1	E	488	MET	2.4
1	A	428	THR	2.4
1	A	130	ARG	2.3
1	C	241	ALA	2.3
1	C	348	GLN	2.3
1	E	482	LYS	2.3
1	E	199	ASN	2.3
1	A	427	HIS	2.3
1	E	258	ILE	2.3
1	I	469	CYS	2.3
1	A	210	ALA	2.3
1	A	381	ASN	2.3
1	E	373	LEU	2.3
1	A	352	GLY	2.3
1	G	250	PHE	2.3
1	K	324	PHE	2.3
1	E	263	GLN	2.3
1	G	378	GLU	2.3
1	A	419	LEU	2.3
1	A	423	MET	2.3
1	I	189	GLY	2.3
1	K	263	GLN	2.3
1	K	337	GLY	2.3
1	G	271	ASP	2.3
1	K	165	ASN	2.3
1	C	280	ILE	2.3
1	C	432	ALA	2.3
1	G	128	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	353	GLU	2.2
1	E	229	ASN	2.2
1	E	132	SER	2.2
1	E	434	SER	2.2
1	C	461	ILE	2.2
1	E	147	THR	2.2
1	C	144	LEU	2.2
1	E	226	LEU	2.2
1	K	187	GLY	2.2
1	A	415	TYR	2.2
1	A	377	ILE	2.2
1	E	380	THR	2.2
1	G	356	ALA	2.2
1	G	426	GLN	2.2
1	I	24	VAL	2.2
1	G	118	SER	2.2
1	G	430	ASP	2.2
1	K	207	SER	2.2
1	G	464	LYS	2.2
1	C	376	LEU	2.2
1	K	373	LEU	2.2
1	E	94	ASN	2.2
1	I	465	CYS	2.2
1	A	376	LEU	2.1
1	E	420	LEU	2.1
1	E	282	ASN	2.1
1	E	195	VAL	2.1
1	E	150	ALA	2.1
1	E	431	LEU	2.1
1	E	395	GLU	2.1
1	C	156	THR	2.1
1	E	264	VAL	2.1
1	G	44	LYS	2.1
1	K	42	CYS	2.1
1	E	74	ALA	2.1
1	G	186	TYR	2.1
1	E	490	ASN	2.1
1	G	236	PHE	2.1
1	K	130	ARG	2.1
1	K	303	ARG	2.1
1	C	190	ASN	2.1
1	A	120	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	76	LEU	2.1
1	G	420	LEU	2.1
1	K	217	LEU	2.1
1	I	347	HIS	2.1
1	G	231	ASN	2.1
1	C	191	LYS	2.1
1	G	46	LYS	2.1
1	C	196	GLY	2.1
1	K	419	LEU	2.0
1	E	235	THR	2.0
1	G	421	VAL	2.0
1	A	409	ILE	2.0
1	E	441	GLU	2.0
1	C	119	GLY	2.0
1	G	147	THR	2.0
1	A	197	SER	2.0
1	C	132	SER	2.0
1	E	427	HIS	2.0
1	C	360	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

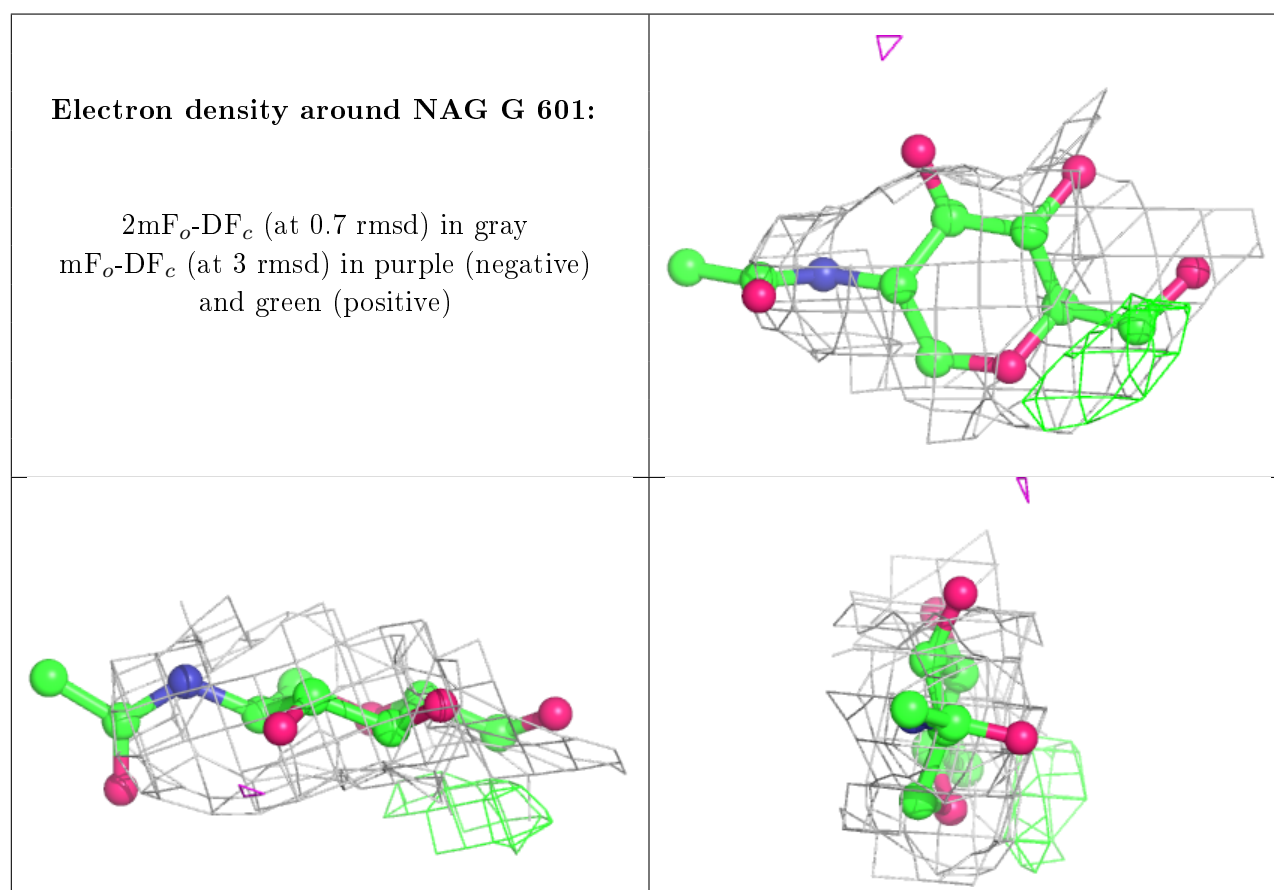
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	601	14/15	0.67	0.37	127,135,142,143	0
2	NAG	C	601	14/15	0.79	0.22	74,80,90,94	0
2	NAG	A	601	14/15	0.85	0.19	81,92,95,97	0
2	NAG	E	501	14/15	0.85	0.15	56,75,82,82	0

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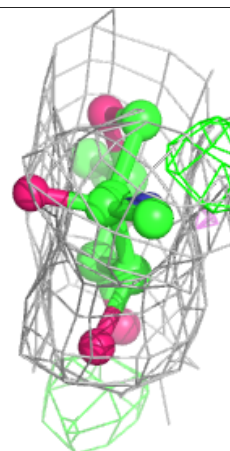
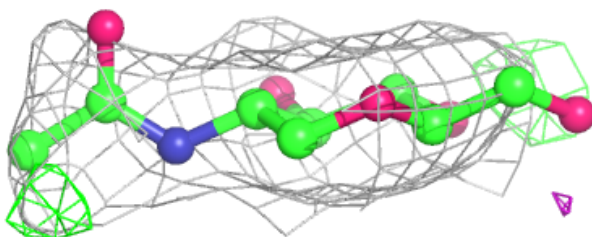
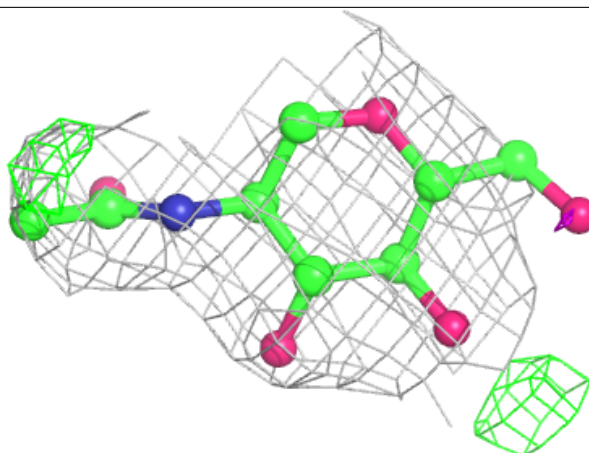
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	K	501	14/15	0.86	0.19	75,93,99,109	0
2	NAG	G	602	14/15	0.86	0.19	44,69,90,94	0
2	NAG	C	602	14/15	0.87	0.20	48,77,105,110	0
2	NAG	I	501	14/15	0.90	0.15	60,70,78,85	0
2	NAG	A	602	14/15	0.90	0.17	56,79,88,91	0

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.

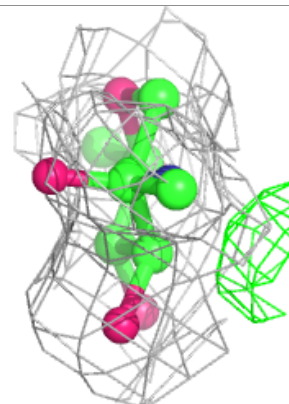
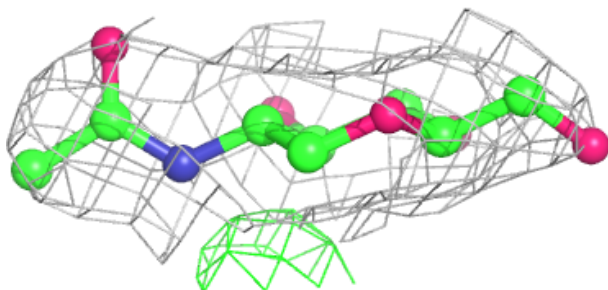
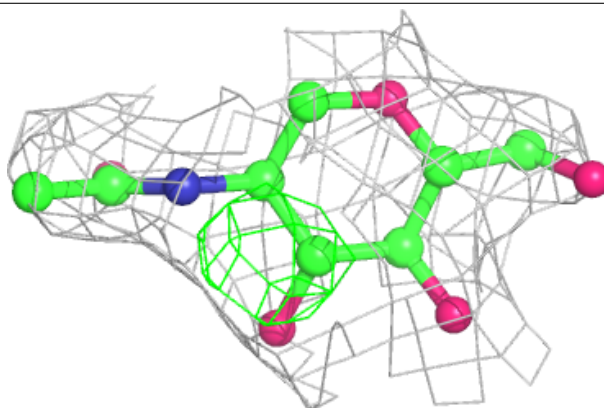


Electron density around NAG C 601:

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

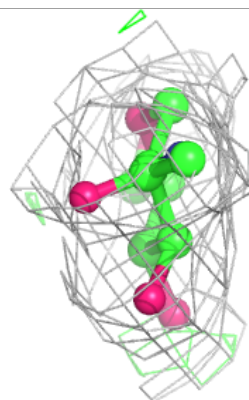
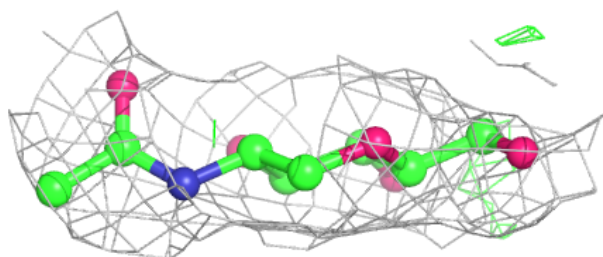
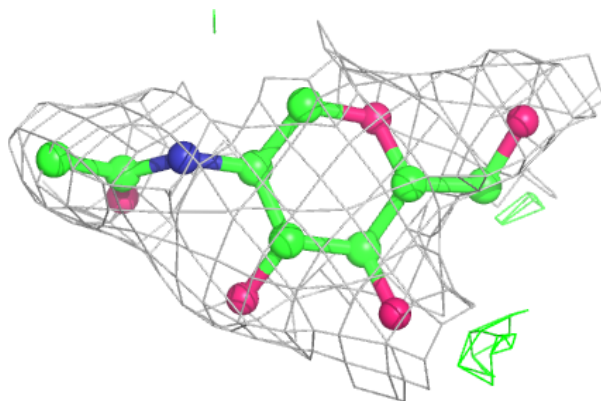
**Electron density around NAG A 601:**

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

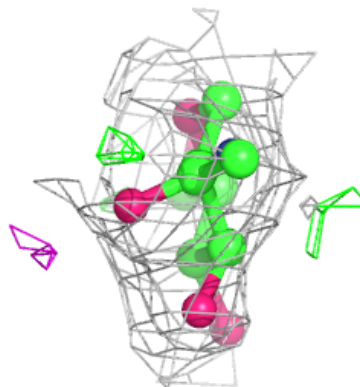
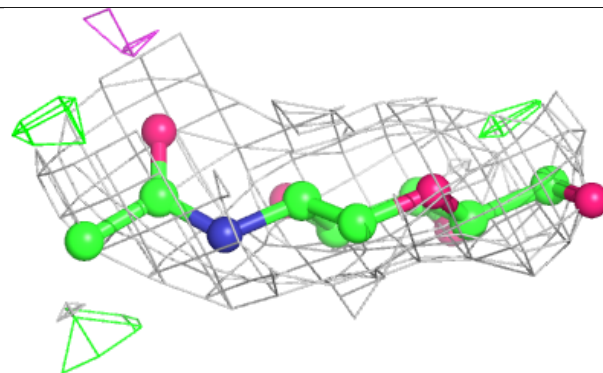
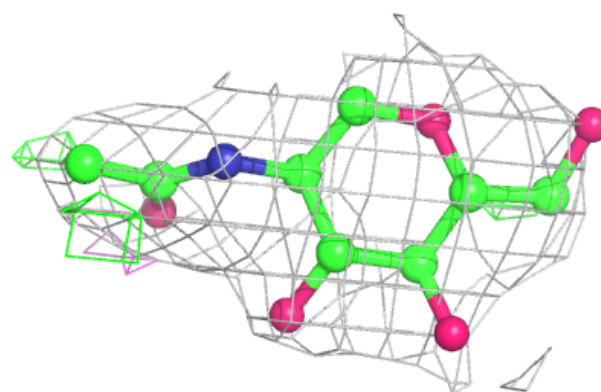


Electron density around NAG E 501:

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

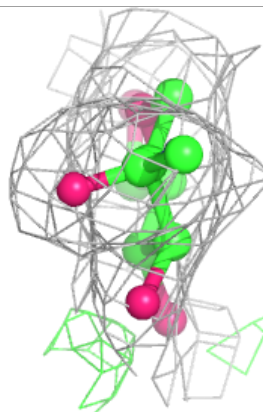
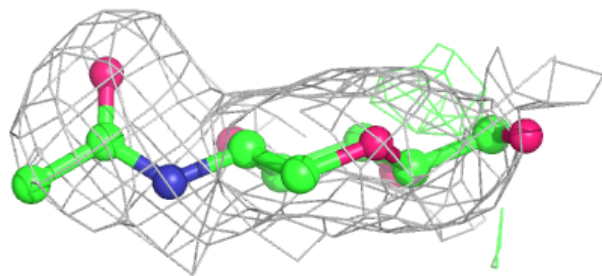
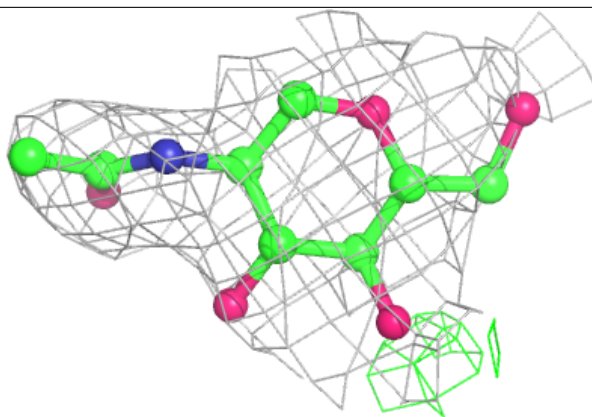
**Electron density around NAG K 501:**

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



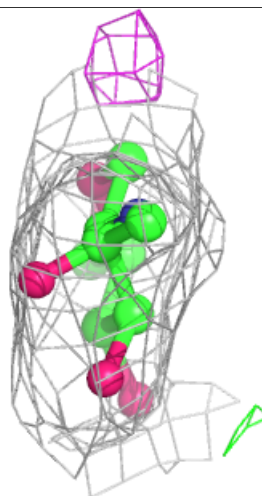
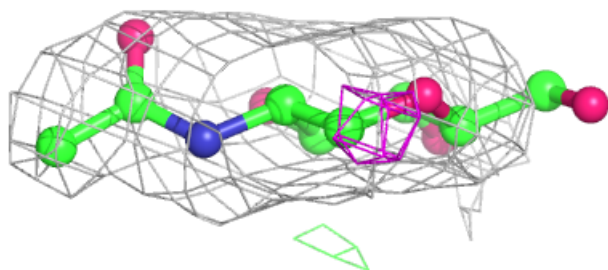
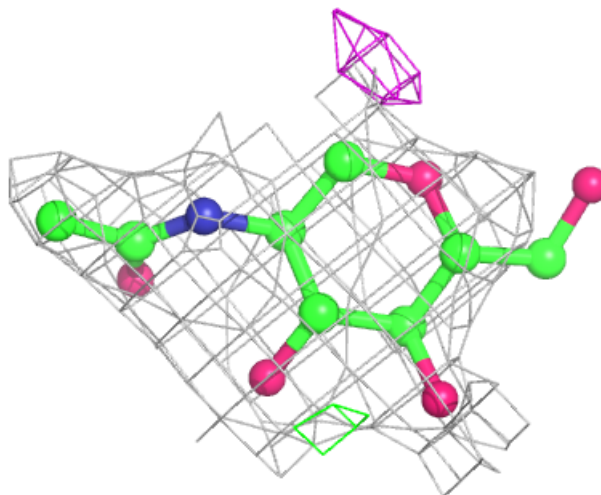
Electron density around NAG G 602:

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



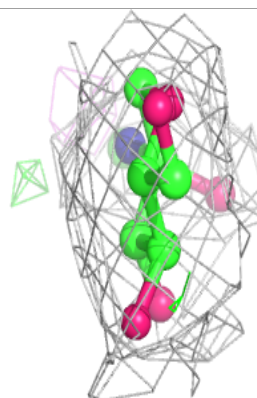
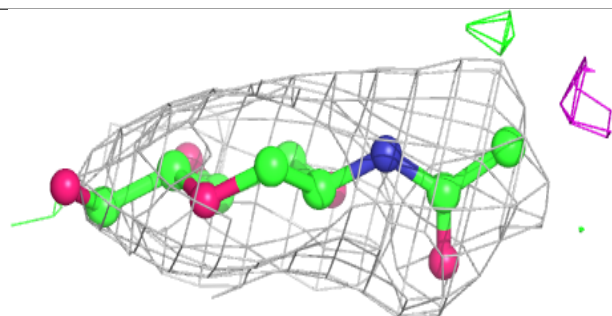
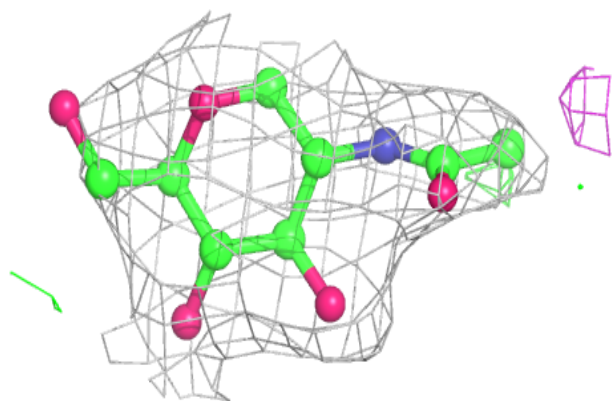
Electron density around NAG C 602:

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



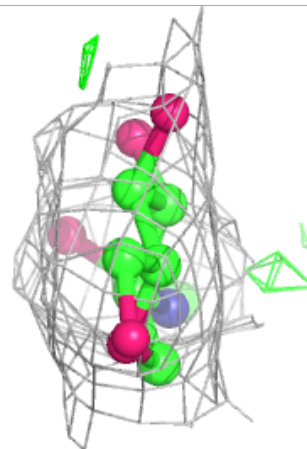
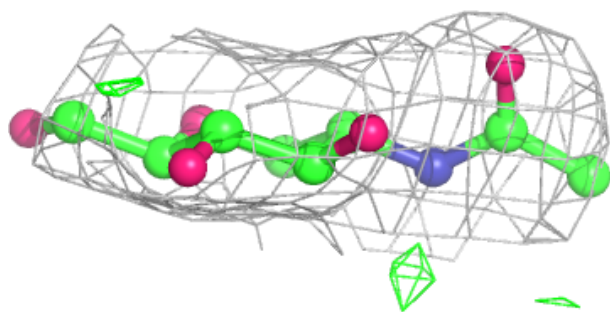
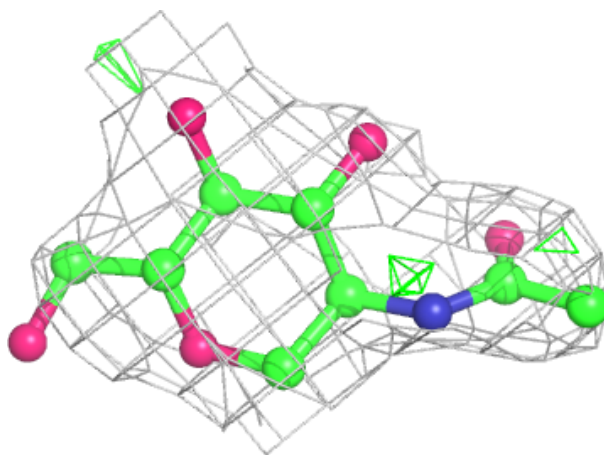
Electron density around NAG I 501:

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



Electron density around NAG 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.