Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 12:22 AM JST

PDB ID	:	6II8
Title	:	Crystal structure of H7 hemagglutinin from A/Anhui/1/2013 in complex with a human neutralizing antibody L4B-18
Authors	:	Jiang, H.H.; Shi, Y.; Qi, J.; Gao, G.F.
Deposited on	:	2018-10-03
Resolution	:	3.32 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:

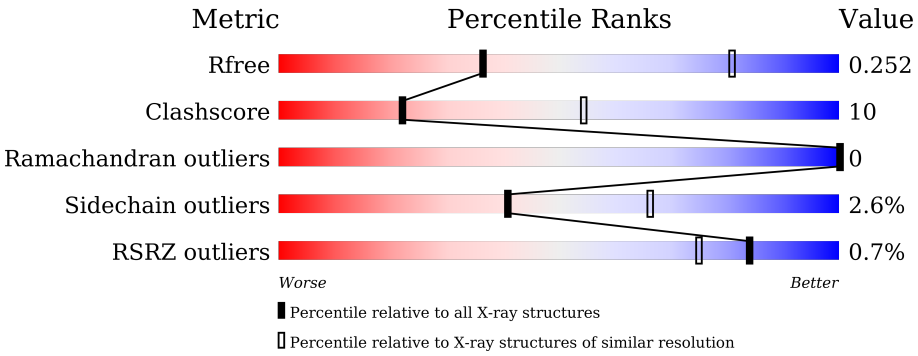
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1066 (3.34-3.30)
Clashscore	180529	1111 (3.34-3.30)
Ramachandran outliers	177936	1109 (3.34-3.30)
Sidechain outliers	177891	1108 (3.34-3.30)
RSRZ outliers	164620	1066 (3.34-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	316	76% 24%
1	C	316	77% 22% .
1	E	316	76% 23% .
2	B	172	75% 23% .
2	D	172	% 68% 30% .
2	F	172	% 79% 19% ..

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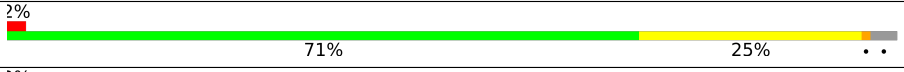
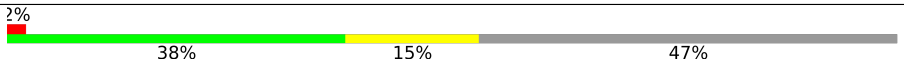
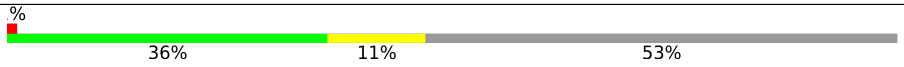
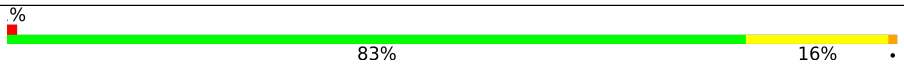
Mol	Chain	Length	Quality of chain
3	G	223	
3	H	223	
3	J	223	
4	I	213	
4	K	213	
4	L	213	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19699 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	316	Total	C	N	O	S	0	0	0
			2412	1498	436	463	15			
1	C	316	Total	C	N	O	S	0	0	0
			2412	1498	436	463	15			
1	E	316	Total	C	N	O	S	0	0	0
			2412	1498	436	463	15			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1396	862	244	283	7			
2	D	172	Total	C	N	O	S	0	0	0
			1396	862	244	283	7			
2	F	171	Total	C	N	O	S	0	0	0
			1387	857	242	281	7			

- Molecule 3 is a protein called Heavy chain of L4B-18 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	118	Total	C	N	O	S	0	0	0
			916	585	152	175	4			
3	G	223	Total	C	N	O	S	0	0	0
			1661	1053	275	327	6			
3	H	217	Total	C	N	O	S	0	0	0
			1621	1031	268	316	6			

- Molecule 4 is a protein called Light chain of L4B-18 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	100	Total	C	N	O	S	0	0	0
			758	463	128	164	3			

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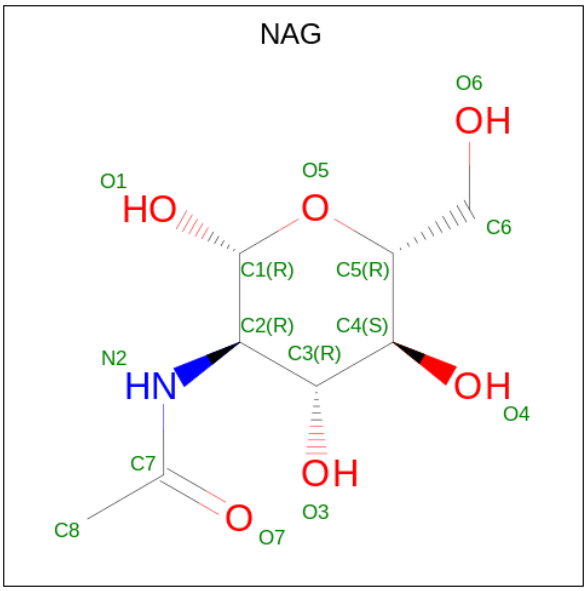
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	213	Total	C	N	O	S	0	0	0
			1601	993	267	336	5			
4	L	213	Total	C	N	O	S	0	0	0
			1601	993	267	336	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



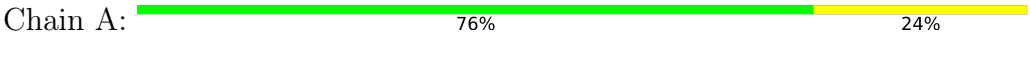
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	B	1	Total	C	N	O		0	0
			14	8	1	5			
5	C	1	Total	C	N	O		0	0
			14	8	1	5			
5	C	1	Total	C	N	O		0	0
			14	8	1	5			
5	D	1	Total	C	N	O		0	0
			14	8	1	5			
5	E	1	Total	C	N	O		0	0
			14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

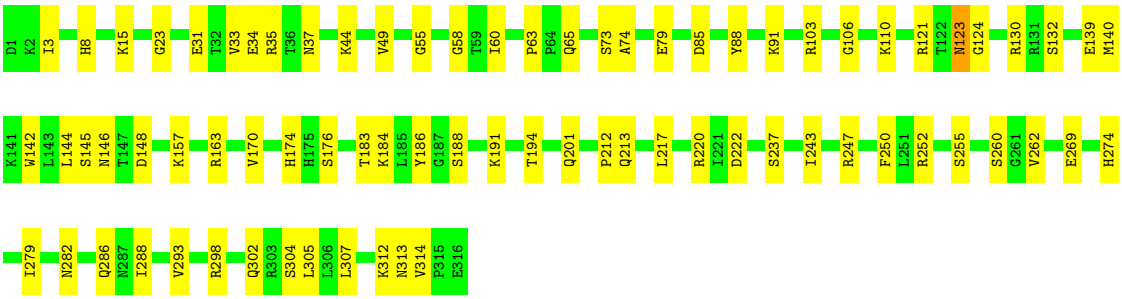
3 Residue-property plots (i)

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

Chain A:



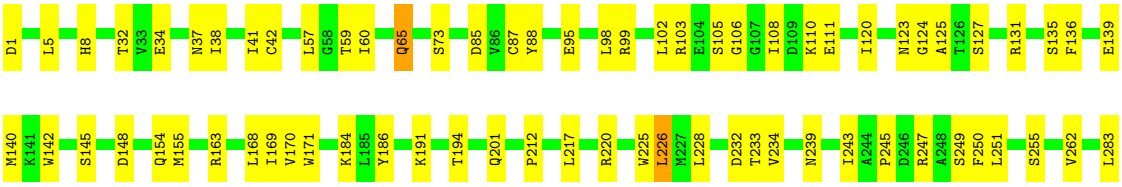


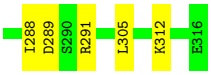
• Molecule 1: Hemagglutinin

Chain C:

• Molecule 1: Hemagglutinin

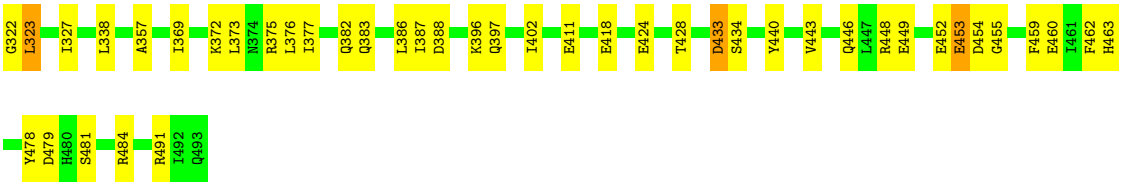
Chain E:





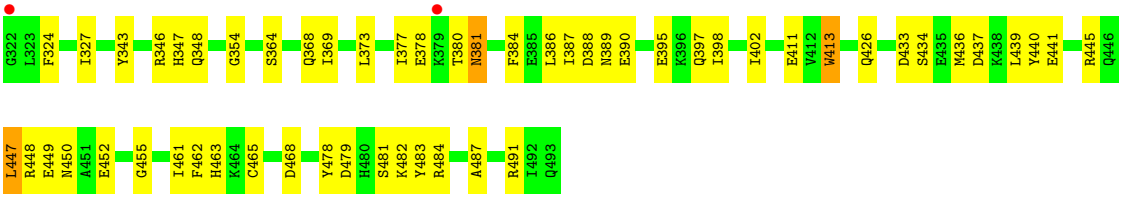
• Molecule 2: Hemagglutinin

Chain B:



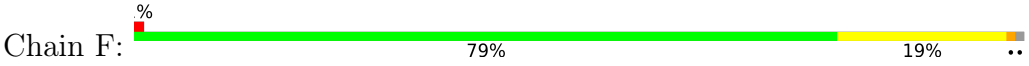
• Molecule 2: Hemagglutinin

Chain D:



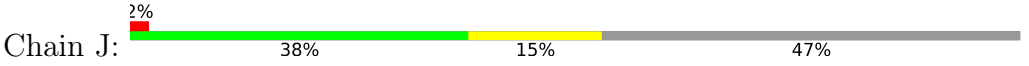
• Molecule 2: Hemagglutinin

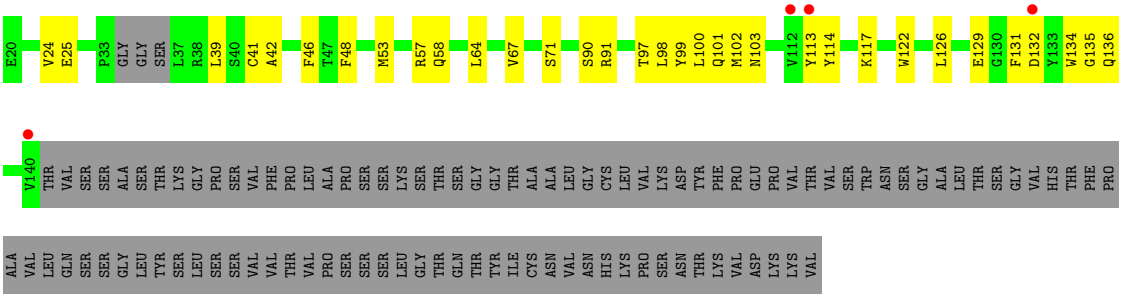
Chain F:



• Molecule 3: Heavy chain of L4B-18 Fab

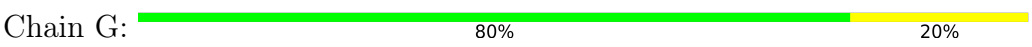
Chain J:

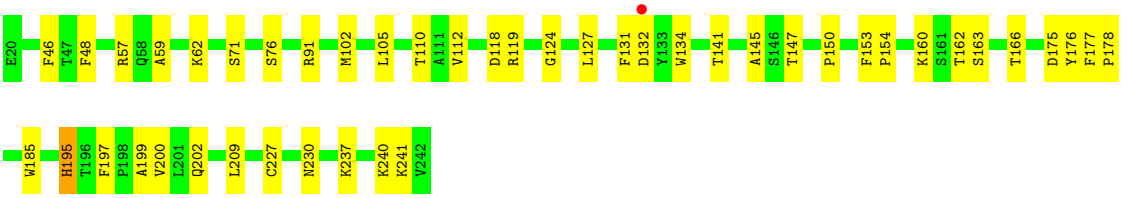




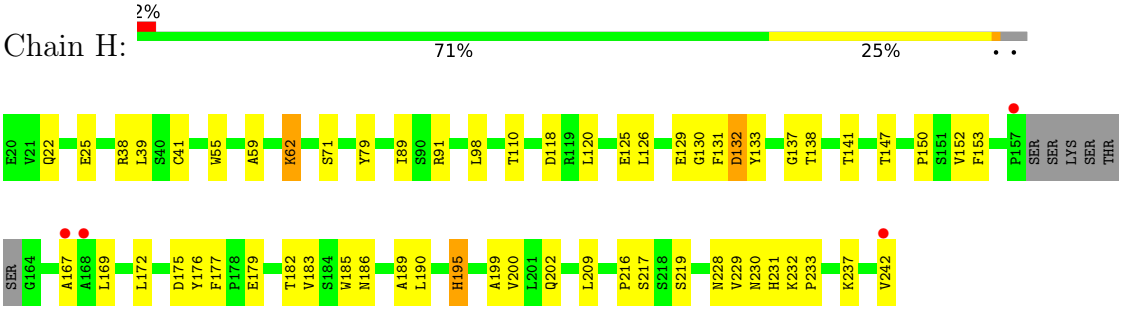
• Molecule 3: Heavy chain of L4B-18 Fab

Chain G:

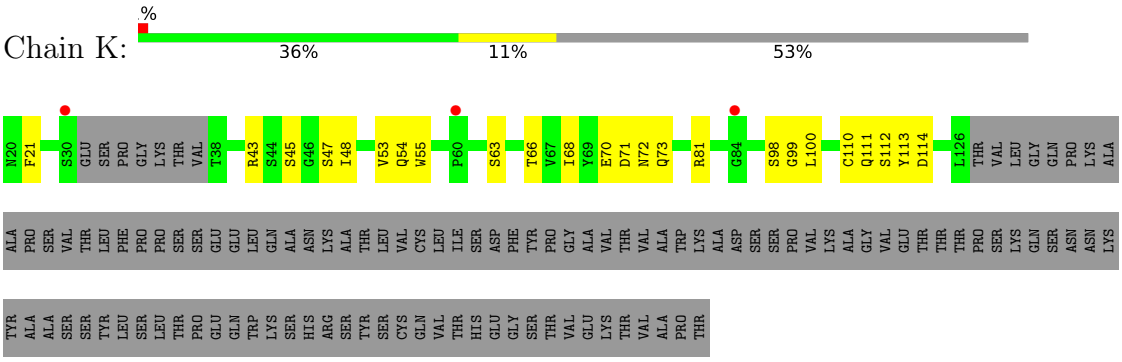




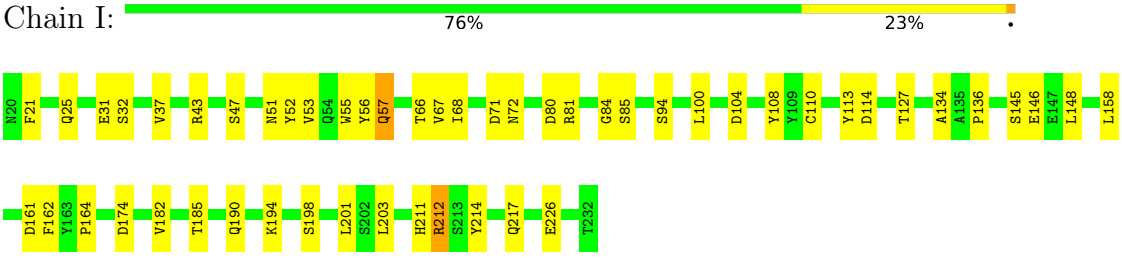
• Molecule 3: Heavy chain of L4B-18 Fab



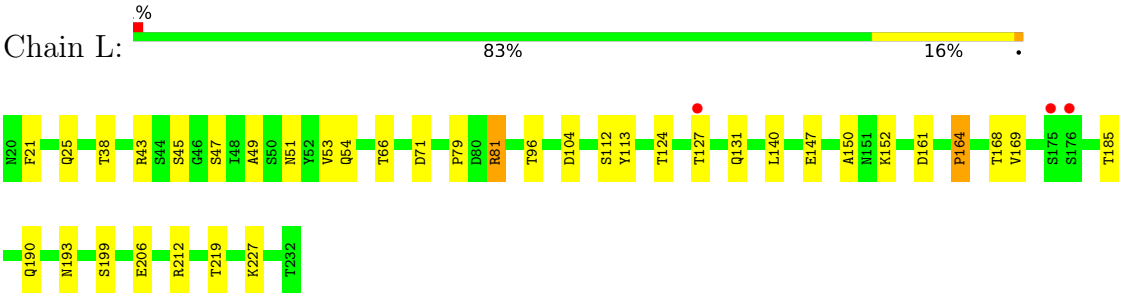
• Molecule 4: Light chain of L4B-18 Fab



• Molecule 4: Light chain of L4B-18 Fab



• Molecule 4: Light chain of L4B-18 Fab



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	203.41Å 116.06Å 185.21Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	49.49 – 3.32 49.49 – 3.32	Depositor EDS
% Data completeness (in resolution range)	94.4 (49.49-3.32) 94.4 (49.49-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.203 , 0.251 0.204 , 0.252	Depositor DCC
R_{free} test set	3007 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	72.4	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.035 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.042 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19699	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.47	0/2458	0.55	0/3322
1	C	0.56	0/2458	0.57	0/3322
1	E	0.40	0/2458	0.53	0/3322
2	B	0.54	0/1420	0.54	0/1913
2	D	0.67	0/1420	0.57	0/1913
2	F	0.53	0/1411	0.54	0/1901
3	G	0.37	0/1701	0.53	1/2314 (0.0%)
3	H	0.33	0/1660	0.51	1/2258 (0.0%)
3	J	0.30	0/937	0.51	1/1266 (0.1%)
4	I	0.40	0/1639	0.52	0/2238
4	K	0.35	0/773	0.52	0/1049
4	L	0.36	0/1639	0.49	0/2238
All	All	0.46	0/19974	0.53	3/27056 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	132	ASP	CB-CG-OD2	5.21	122.99	118.30
3	J	132	ASP	CB-CG-OD2	5.21	122.99	118.30
3	H	132	ASP	CB-CG-OD2	5.21	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2412	0	2372	54	0
1	C	2412	0	2372	59	0
1	E	2412	0	2372	53	0
2	B	1396	0	1296	38	0
2	D	1396	0	1296	56	0
2	F	1387	0	1288	32	0
3	G	1661	0	1621	31	0
3	H	1621	0	1580	41	0
3	J	916	0	875	30	0
4	I	1601	0	1532	40	0
4	K	758	0	699	19	0
4	L	1601	0	1532	23	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0
5	C	28	0	26	0	0
5	D	14	0	13	0	0
5	E	28	0	26	0	0
5	F	14	0	13	0	0
All	All	19699	0	18952	405	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 10.

All (405) 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)
3:J:97:THR:CG2	3:J:99:TYR:HE1	1.97	0.77
1:C:293:VAL:HG11	2:D:386:LEU:HG	1.67	0.76
4:L:38:THR:HG22	4:L:96:THR:HG23	1.67	0.76
2:B:396:LYS:HE2	1:C:101:ILE:HD11	1.68	0.74
4:L:131:GLN:NE2	4:L:193:ASN:O	2.20	0.74
1:A:124:GLY:HA3	1:A:142:TRP:HB3	1.69	0.74
2:F:447:LEU:H	2:F:447:LEU:HD23	1.52	0.73
1:C:211:ARG:NH1	1:C:218:SER:O	2.21	0.72
2:D:445:ARG:HH21	2:D:445:ARG:HG3	1.55	0.72
4:K:55:TRP:HB2	4:K:68:ILE:HB	1.72	0.72
1:A:184:LYS:NZ	4:I:71:ASP:OD2	2.22	0.71
1:E:125:ALA:O	3:J:126:LEU:HD13	1.91	0.71
2:B:411:GLU:OE2	1:C:298:ARG:NH1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:25:GLU:H	3:J:136:GLN:HE22	1.40	0.70
2:B:372:LYS:NZ	2:B:424:GLU:OE1	2.20	0.69
1:C:70:LEU:O	1:C:110:LYS:NZ	2.24	0.69
1:A:312:LYS:NZ	1:A:313:ASN:O	2.26	0.69
1:C:298:ARG:HD3	2:D:413:TRP:CE2	2.28	0.69
3:J:97:THR:CG2	3:J:99:TYR:CE1	2.76	0.68
1:E:289:ASP:OD1	1:E:291:ARG:N	2.27	0.68
3:J:97:THR:HG21	3:J:99:TYR:HE1	1.55	0.68
1:C:282:ASN:HB3	2:D:378:GLU:HB3	1.76	0.68
2:D:395:GLU:OE2	2:D:397:GLN:N	2.22	0.68
2:D:343:TYR:HD1	2:D:436:MET:HE1	1.59	0.68
2:D:452:GLU:OE1	2:F:448:ARG:NH2	2.26	0.67
4:L:79:PRO:HB2	4:L:81:ARG:HG3	1.75	0.67
4:L:81:ARG:NH1	4:L:104:ASP:OD2	2.21	0.67
3:H:230:ASN:HD22	3:H:237:LYS:HD3	1.59	0.67
2:B:449:GLU:OE1	2:B:491:ARG:NH2	2.27	0.66
4:L:168:THR:HB	4:L:219:THR:HB	1.78	0.65
1:E:37:ASN:HB2	1:E:288:ILE:HD13	1.79	0.65
1:C:291:ARG:NH2	2:D:388:ASP:HB3	2.11	0.65
2:D:381:ASN:OD1	2:D:381:ASN:N	2.29	0.65
4:I:37:VAL:HG13	4:I:100:LEU:HD11	1.79	0.65
1:C:177:VAL:HG23	1:C:181:GLU:OE1	1.96	0.65
1:C:184:LYS:HD2	4:L:49:ALA:O	1.96	0.65
3:J:101:GLN:NE2	3:J:103:ASN:OD1	2.30	0.64
1:A:212:PRO:O	1:A:220:ARG:NH2	2.24	0.64
3:H:150:PRO:HB3	3:H:176:TYR:HB3	1.78	0.64
1:E:106:GLY:HA2	1:E:255:SER:HB3	1.78	0.64
1:E:169:ILE:HB	1:E:226:LEU:CD2	2.28	0.64
2:F:447:LEU:HD23	2:F:447:LEU:N	2.14	0.63
4:K:21:PHE:HE1	4:K:114:ASP:HB2	1.62	0.63
4:I:146:GLU:N	4:I:146:GLU:OE1	2.31	0.62
1:A:121:ARG:HG3	1:A:123:ASN:OD1	1.99	0.62
2:D:387:ILE:HD13	2:D:402:ILE:HG21	1.82	0.62
3:J:71:SER:O	3:J:91:ARG:NH1	2.33	0.62
3:G:230:ASN:HD22	3:G:237:LYS:HD3	1.63	0.62
2:D:463:HIS:NE2	2:D:478:TYR:OH	2.31	0.62
2:D:343:TYR:HD1	2:D:436:MET:CE	2.13	0.61
1:C:5:LEU:HD22	2:D:439:LEU:HD22	1.82	0.61
1:C:131:ARG:NH1	1:C:136:PHE:O	2.32	0.61
1:E:171:TRP:HZ3	1:E:226:LEU:HD22	1.66	0.61
1:A:121:ARG:NH1	1:A:145:SER:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:462:PHE:CD2	2:D:491:ARG:HG2	2.36	0.61
3:G:124:GLY:HA2	4:I:113:TYR:OH	2.00	0.61
4:I:53:VAL:N	4:I:71:ASP:OD1	2.30	0.61
1:E:38:ILE:HD11	1:E:42:CYS:SG	2.40	0.60
3:H:153:PHE:CD2	4:L:147:GLU:HG3	2.36	0.60
3:H:179:GLU:OE2	3:H:199:ALA:HB3	2.02	0.60
2:F:375:ARG:NH2	2:F:424:GLU:OE1	2.34	0.60
1:C:291:ARG:HH22	2:D:388:ASP:HB3	1.66	0.60
3:G:175:ASP:OD1	3:G:202:GLN:NE2	2.35	0.59
1:A:44:LYS:HE2	1:A:269:GLU:HB2	1.85	0.59
1:C:58:GLY:O	1:C:63:PRO:HD2	2.02	0.59
4:I:161:ASP:OD1	4:I:190:GLN:NE2	2.35	0.59
4:K:81:ARG:NH1	4:K:99:GLY:O	2.36	0.58
1:A:279:ILE:CD1	1:A:288:ILE:HD12	2.33	0.58
2:D:449:GLU:HG3	2:D:491:ARG:NH1	2.18	0.58
3:J:136:GLN:HA	4:K:63:SER:HB3	1.83	0.58
1:C:298:ARG:HD3	2:D:413:TRP:NE1	2.19	0.58
1:A:49:VAL:HG23	1:A:74:ALA:HB2	1.87	0.57
1:C:121:ARG:HB3	1:C:144:LEU:HB2	1.85	0.57
1:C:103:ARG:HB3	1:C:257:GLY:HA3	1.85	0.57
1:C:3:ILE:HA	2:D:347:HIS:HA	1.85	0.56
2:F:484:ARG:HD2	2:F:484:ARG:O	2.05	0.56
3:G:102:MET:HE2	3:G:105:LEU:HD21	1.87	0.56
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.05	0.56
3:J:97:THR:HG22	3:J:99:TYR:CE1	2.40	0.56
2:B:369:ILE:HD11	2:B:428:THR:HG23	1.86	0.56
1:C:32:THR:HG22	1:C:285:PHE:HD2	1.71	0.56
1:C:220:ARG:HG3	1:E:201:GLN:HG2	1.87	0.56
3:G:230:ASN:HA	3:G:237:LYS:HG2	1.88	0.56
3:H:175:ASP:OD1	3:H:202:GLN:NE2	2.39	0.56
1:E:131:ARG:NH1	1:E:135:SER:OG	2.38	0.56
2:D:387:ILE:HD12	2:D:388:ASP:N	2.21	0.56
1:E:228:LEU:HD21	1:E:234:VAL:HB	1.87	0.56
2:B:443:VAL:HA	2:B:446:GLN:HG3	1.86	0.56
2:D:346:ARG:O	2:D:346:ARG:HG2	2.05	0.56
1:C:106:GLY:HA2	1:C:255:SER:HB3	1.88	0.56
4:I:185:THR:HG1	4:I:198:SER:H	1.51	0.56
1:C:5:LEU:HD11	2:D:440:TYR:HD1	1.71	0.56
2:F:447:LEU:HD12	2:F:451:ALA:CB	2.35	0.56
1:C:298:ARG:HH12	2:D:384:PHE:HE2	1.54	0.55
1:A:212:PRO:HD3	1:C:235:THR:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASN:OD1	1:A:123:ASN:N	2.34	0.55
3:G:163:SER:OG	3:G:166:THR:OG1	2.24	0.55
1:A:110:LYS:NZ	1:A:139:GLU:OE2	2.35	0.55
1:A:279:ILE:HD13	1:A:288:ILE:HD12	1.88	0.55
3:J:39:LEU:HB2	3:J:100:LEU:HB3	1.88	0.55
3:J:100:LEU:HG	3:J:102:MET:HG2	1.89	0.55
3:G:59:ALA:HB3	3:G:62:LYS:HB2	1.89	0.55
1:E:169:ILE:HB	1:E:226:LEU:HD23	1.88	0.55
2:F:340:ASP:HB3	2:F:357:ALA:HB2	1.88	0.55
3:J:41:CYS:HB3	3:J:98:LEU:HB3	1.89	0.55
2:D:447:LEU:N	2:D:447:LEU:HD23	2.22	0.55
4:I:55:TRP:HB2	4:I:68:ILE:HB	1.89	0.55
3:J:25:GLU:OE2	3:J:25:GLU:N	2.40	0.55
3:G:147:THR:HG23	3:G:178:PRO:HD3	1.89	0.55
4:I:127:THR:HG21	4:I:164:PRO:HB3	1.89	0.54
3:G:110:THR:HG23	3:G:141:THR:HA	1.90	0.54
1:C:96:GLU:OE1	2:D:389:ASN:ND2	2.34	0.54
3:J:24:VAL:HB	3:J:42:ALA:HB3	1.88	0.54
4:I:217:GLN:HG2	4:I:226:GLU:HG2	1.90	0.54
1:A:302:GLN:HG2	1:A:305:LEU:HD21	1.90	0.54
1:C:221:ILE:HD13	1:C:243:ILE:HG13	1.89	0.54
2:D:373:LEU:O	2:D:377:ILE:HG22	2.07	0.54
3:H:132:ASP:OD1	3:H:133:TYR:N	2.40	0.54
3:G:71:SER:O	3:G:91:ARG:NH1	2.42	0.53
1:A:302:GLN:NE2	2:B:418:GLU:HB2	2.23	0.53
1:C:103:ARG:O	1:C:255:SER:OG	2.26	0.53
1:E:85:ASP:OD2	1:E:99:ARG:NH2	2.41	0.53
1:E:145:SER:OG	1:E:186:TYR:HA	2.09	0.53
2:D:445:ARG:HG3	2:D:445:ARG:NH2	2.21	0.53
3:J:58:GLN:HB2	3:J:64:LEU:HD23	1.91	0.53
4:K:55:TRP:CH2	4:K:110:CYS:HB3	2.43	0.53
1:A:307:LEU:HD22	2:B:376:LEU:HD12	1.90	0.53
2:D:411:GLU:OE2	2:F:382:GLN:HG3	2.08	0.53
1:E:139:GLU:OE1	1:E:247:ARG:HD3	2.09	0.53
1:E:170:VAL:HG22	1:E:225:TRP:HB3	1.91	0.52
4:K:53:VAL:N	4:K:71:ASP:OD1	2.31	0.52
1:C:139:GLU:OE1	1:C:247:ARG:HD3	2.09	0.52
4:I:81:ARG:NH1	4:I:104:ASP:OD2	2.43	0.52
2:B:449:GLU:HB3	2:B:491:ARG:HH21	1.73	0.52
2:B:454:ASP:OD1	2:B:455:GLY:N	2.43	0.52
1:C:2:LYS:HA	2:D:461:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:HD3	1:A:250:PHE:CZ	2.44	0.52
2:B:434:SER:OG	2:F:323:LEU:O	2.24	0.52
3:J:53:MET:HB3	3:J:98:LEU:CD2	2.40	0.52
1:A:88:TYR:CD1	1:A:217:LEU:HD13	2.45	0.52
1:C:111:GLU:OE2	1:C:163:ARG:HD2	2.10	0.52
2:F:447:LEU:HD12	2:F:451:ALA:HB3	1.92	0.52
3:H:199:ALA:HB2	3:H:209:LEU:HD23	1.91	0.52
2:B:397:GLN:HB2	1:C:97:ALA:HB2	1.91	0.52
1:C:99:ARG:O	1:C:103:ARG:HG3	2.10	0.52
1:E:212:PRO:O	1:E:220:ARG:NH2	2.34	0.52
2:D:364:SER:O	2:D:368:GLN:HG3	2.10	0.52
2:B:460:GLU:OE1	2:D:448:ARG:NH2	2.43	0.52
1:C:18:THR:HB	2:D:426:GLN:OE1	2.10	0.52
2:D:413:TRP:HA	2:D:413:TRP:CE3	2.44	0.51
1:E:163:ARG:HD3	1:E:250:PHE:CZ	2.45	0.51
4:K:43:ARG:HB2	4:K:48:ILE:HD13	1.93	0.51
1:C:3:ILE:HG22	2:D:461:ILE:HD11	1.92	0.51
2:D:479:ASP:OD1	2:D:481:SER:OG	2.27	0.51
3:H:153:PHE:CE2	4:L:147:GLU:HG3	2.44	0.51
1:A:183:THR:HG22	1:A:188:SER:HA	1.91	0.51
1:A:79:GLU:OE2	1:A:103:ARG:NE	2.31	0.51
1:A:130:ARG:NH1	3:G:76:SER:OG	2.44	0.51
3:H:147:THR:HA	3:H:177:PHE:HD2	1.76	0.51
4:K:21:PHE:CE1	4:K:114:ASP:HB2	2.43	0.51
1:A:3:ILE:HG23	2:B:459:PHE:HB2	1.93	0.50
3:H:131:PHE:O	4:L:66:THR:HG21	2.11	0.50
4:I:182:VAL:HG12	4:I:201:LEU:HD13	1.94	0.50
2:B:387:ILE:HD12	2:B:388:ASP:N	2.25	0.50
2:B:484:ARG:NH2	2:F:452:GLU:OE2	2.31	0.50
4:I:145:SER:HA	4:I:148:LEU:HD12	1.92	0.50
2:B:479:ASP:OD1	2:B:481:SER:OG	2.27	0.50
1:E:111:GLU:OE2	1:E:163:ARG:HD2	2.11	0.50
2:F:322:GLY:HA2	2:F:433:ASP:OD2	2.12	0.50
3:G:131:PHE:O	4:I:66:THR:HG21	2.11	0.50
1:C:170:VAL:O	1:C:245:PRO:HB3	2.11	0.50
2:D:449:GLU:HG3	2:D:491:ARG:HH12	1.76	0.50
1:A:58:GLY:O	1:A:63:PRO:HD2	2.12	0.50
3:G:199:ALA:HB2	3:G:209:LEU:HD23	1.93	0.50
3:H:59:ALA:HB3	3:H:62:LYS:HB2	1.94	0.50
1:E:105:SER:HB2	1:E:251:LEU:HD22	1.94	0.49
3:H:216:PRO:O	3:H:219:SER:OG	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:54:GLN:NE2	4:K:111:GLN:OE1	2.43	0.49
1:A:121:ARG:HB3	1:A:144:LEU:HB2	1.93	0.49
3:H:89:ILE:HD11	3:H:98:LEU:HD11	1.94	0.49
1:E:99:ARG:O	1:E:103:ARG:HG3	2.13	0.49
2:F:420:LEU:O	2:F:424:GLU:HB2	2.12	0.49
2:D:369:ILE:O	2:D:373:LEU:HD12	2.12	0.49
3:J:46:PHE:CE1	3:J:117:LYS:HD2	2.48	0.49
3:H:167:ALA:N	3:H:217:SER:OG	2.46	0.49
3:H:230:ASN:HA	3:H:237:LYS:HG2	1.94	0.49
1:A:60:ILE:HG22	1:A:170:VAL:HG11	1.94	0.49
3:H:25:GLU:OE2	3:H:25:GLU:N	2.38	0.49
1:C:191:LYS:HB2	1:C:206:PRO:HG3	1.94	0.49
2:B:375:ARG:NH2	2:B:424:GLU:OE2	2.46	0.49
3:H:169:LEU:HD13	3:H:242:VAL:HG11	1.95	0.49
1:A:222:ASP:OD1	1:C:201:GLN:NE2	2.45	0.48
1:E:110:LYS:NZ	1:E:139:GLU:OE2	2.34	0.48
2:B:323:LEU:HD22	2:D:434:SER:CB	2.43	0.48
2:D:347:HIS:CE1	2:D:354:GLY:HA3	2.48	0.48
2:B:338:LEU:HD11	2:B:357:ALA:HB2	1.95	0.48
1:A:31:GLU:HG3	1:A:33:VAL:H	1.78	0.48
1:C:131:ARG:O	1:C:132:SER:OG	2.30	0.48
2:D:441:GLU:O	2:D:445:ARG:NH2	2.47	0.48
2:B:387:ILE:HD13	2:B:402:ILE:HG21	1.95	0.48
1:C:70:LEU:HD13	1:C:139:GLU:OE2	2.13	0.48
4:K:43:ARG:NE	4:K:45:SER:O	2.38	0.48
2:B:448:ARG:NH2	2:F:452:GLU:OE1	2.37	0.48
1:E:169:ILE:HB	1:E:226:LEU:HD21	1.96	0.48
1:A:194:THR:OG1	1:A:237:SER:HB2	2.14	0.48
1:A:314:VAL:HG21	2:B:327:ILE:O	2.14	0.48
1:E:124:GLY:HA3	1:E:142:TRP:HB3	1.95	0.48
3:G:150:PRO:HB3	3:G:176:TYR:HB3	1.96	0.48
2:F:450:ASN:HA	2:F:487:ALA:HB1	1.96	0.47
3:G:199:ALA:HA	3:G:209:LEU:HB3	1.96	0.47
1:E:191:LYS:HA	1:E:239:ASN:HD21	1.78	0.47
1:C:80:ARG:NH1	1:C:262:VAL:O	2.37	0.47
1:A:106:GLY:HA2	1:A:255:SER:HB3	1.96	0.47
3:J:129:GLU:OE2	4:K:70:GLU:OE2	2.33	0.47
3:J:48:PHE:O	3:J:91:ARG:NH2	2.47	0.47
3:G:227:CYS:SG	3:G:240:LYS:HB3	2.55	0.47
3:H:110:THR:HG23	3:H:141:THR:HA	1.97	0.47
2:B:455:GLY:HA2	2:D:445:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:LYS:HD2	2:F:382:GLN:NE2	2.28	0.47
3:J:134:TRP:HE1	4:K:66:THR:HG22	1.80	0.47
3:H:79:TYR:CE1	3:H:89:ILE:HG22	2.49	0.47
4:I:134:ALA:HB3	4:I:194:LYS:HE3	1.97	0.47
1:A:15:LYS:HB3	1:A:23:GLY:HA2	1.97	0.47
2:B:443:VAL:HA	2:B:446:GLN:HE21	1.80	0.47
4:I:136:PRO:HB3	4:I:162:PHE:HB3	1.97	0.47
1:E:135:SER:OG	1:E:136:PHE:N	2.48	0.46
2:D:463:HIS:CD2	2:D:483:TYR:HB3	2.50	0.46
1:A:282:ASN:HB3	2:B:377:ILE:HG22	1.97	0.46
2:B:322:GLY:HA3	2:B:433:ASP:OD2	2.14	0.46
1:C:106:GLY:H	1:C:255:SER:HB3	1.79	0.46
1:A:293:VAL:HG11	2:B:386:LEU:HG	1.96	0.46
2:D:324:PHE:HB2	2:D:433:ASP:OD1	2.15	0.46
2:D:395:GLU:HB3	2:D:398:ILE:HG22	1.96	0.46
1:E:1:ASP:HB2	2:F:348:GLN:O	2.15	0.46
2:D:487:ALA:O	2:D:491:ARG:HG3	2.15	0.46
1:C:191:LYS:O	1:C:206:PRO:HD2	2.16	0.46
4:I:25:GLN:OE1	4:I:110:CYS:SG	2.74	0.46
1:A:44:LYS:HB3	1:A:269:GLU:HB2	1.97	0.46
1:A:142:TRP:NE1	1:A:186:TYR:OH	2.37	0.46
1:E:95:GLU:OE1	1:E:99:ARG:NH1	2.49	0.46
1:E:127:SER:HB2	3:J:122:TRP:CD2	2.51	0.46
4:K:53:VAL:HG22	4:K:112:SER:HB2	1.98	0.46
1:A:35:ARG:NH1	1:A:304:SER:HB2	2.31	0.46
1:A:37:ASN:OD1	1:A:274:HIS:NE2	2.35	0.46
2:D:455:GLY:HA2	2:F:445:ARG:HD3	1.97	0.46
3:H:185:TRP:HB2	3:H:190:LEU:HB3	1.98	0.46
1:C:88:TYR:CE1	1:C:217:LEU:HD13	2.51	0.45
3:H:150:PRO:HD3	3:H:231:HIS:ND1	2.31	0.45
3:H:183:VAL:HG22	3:H:229:VAL:HG22	1.98	0.45
2:F:441:GLU:O	2:F:445:ARG:HG2	2.16	0.45
3:H:130:GLY:HA3	4:L:54:GLN:HG2	1.99	0.45
1:A:148:ASP:O	4:I:47:SER:HB2	2.17	0.45
1:C:145:SER:HB2	1:C:185:LEU:O	2.16	0.45
4:I:174:ASP:HB2	4:I:211:HIS:HB3	1.98	0.45
1:E:32:THR:HB	1:E:305:LEU:O	2.16	0.45
3:J:24:VAL:O	3:J:42:ALA:N	2.50	0.45
4:K:72:ASN:OD1	4:K:73:GLN:NE2	2.47	0.45
2:D:327:ILE:HG12	2:D:433:ASP:HA	1.99	0.45
2:F:447:LEU:H	2:F:447:LEU:CD2	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:58:GLN:HE21	3:J:114:TYR:HE2	1.65	0.45
3:H:230:ASN:HD22	3:H:237:LYS:CD	2.28	0.45
2:D:482:LYS:HA	2:D:482:LYS:HD2	1.72	0.45
4:I:72:ASN:HA	4:I:84:GLY:HA3	1.98	0.45
1:A:55:GLY:HA3	1:A:85:ASP:OD1	2.17	0.45
1:C:126:THR:OG1	3:H:125:GLU:OE2	2.22	0.45
1:E:37:ASN:OD1	1:E:38:ILE:N	2.50	0.45
3:H:25:GLU:OE1	3:H:137:GLY:N	2.46	0.45
4:I:21:PHE:CE2	4:I:114:ASP:HB2	2.52	0.45
4:L:169:VAL:HG11	4:L:199:SER:OG	2.16	0.45
2:B:462:PHE:CD2	2:B:491:ARG:HG2	2.51	0.45
1:E:34:GLU:HB2	1:E:283:LEU:HD12	1.98	0.45
4:L:51:ASN:HD21	4:L:113:TYR:HD2	1.65	0.45
2:B:373:LEU:O	2:B:377:ILE:HG12	2.18	0.44
3:J:131:PHE:O	4:K:66:THR:HG21	2.16	0.44
3:H:25:GLU:CD	3:H:137:GLY:H	2.20	0.44
4:I:43:ARG:NH1	4:I:47:SER:O	2.50	0.44
2:B:443:VAL:O	2:B:446:GLN:HG3	2.17	0.44
1:C:275:SER:HB3	2:D:390:GLU:OE2	2.18	0.44
1:E:98:LEU:HD11	1:E:168:LEU:HD21	1.98	0.44
3:J:90:SER:O	3:J:98:LEU:HD12	2.16	0.44
3:G:57:ARG:HA	3:G:112:VAL:O	2.18	0.44
4:I:212:ARG:HB3	4:I:212:ARG:NH1	2.32	0.44
2:B:462:PHE:HD2	2:B:491:ARG:HG2	1.83	0.44
1:E:65:GLN:CD	1:E:65:GLN:H	2.20	0.44
1:E:123:ASN:O	1:E:123:ASN:ND2	2.50	0.44
4:K:112:SER:OG	4:K:113:TYR:N	2.48	0.44
3:H:195:HIS:NE2	4:L:190:GLN:OE1	2.46	0.44
1:E:312:LYS:HB2	2:F:327:ILE:HG21	2.00	0.44
3:G:145:ALA:HB1	3:G:177:PHE:CE2	2.52	0.44
1:E:170:VAL:O	1:E:245:PRO:HB3	2.17	0.44
3:G:162:THR:OG1	3:G:166:THR:O	2.34	0.44
3:G:195:HIS:NE2	4:I:190:GLN:OE1	2.47	0.44
3:H:182:THR:OG1	3:H:230:ASN:HB3	2.18	0.44
1:E:41:ILE:HG12	1:E:262:VAL:HG23	1.99	0.44
1:E:88:TYR:CE2	1:E:217:LEU:HD13	2.53	0.44
2:F:330:PHE:HB2	2:F:455:GLY:O	2.18	0.44
4:I:21:PHE:HE2	4:I:114:ASP:HB2	1.82	0.44
4:I:31:GLU:OE2	4:I:32:SER:N	2.33	0.44
2:B:323:LEU:HD23	2:B:323:LEU:HA	1.77	0.44
1:E:60:ILE:HG21	1:E:170:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:323:LEU:HG	2:F:430:ASP:OD2	2.17	0.44
3:J:57:ARG:HD3	3:J:67:VAL:HG22	1.99	0.44
3:G:185:TRP:CZ3	3:G:227:CYS:HB3	2.52	0.44
3:H:152:VAL:HA	3:H:172:LEU:O	2.18	0.44
1:A:201:GLN:OE1	1:E:220:ARG:HD2	2.18	0.43
1:C:302:GLN:HG2	1:C:305:LEU:HD21	1.99	0.43
1:A:157:LYS:HA	1:A:157:LYS:HD3	1.74	0.43
2:F:389:ASN:OD1	2:F:391:PHE:N	2.51	0.43
3:J:135:GLY:O	4:K:63:SER:HB2	2.18	0.43
4:I:25:GLN:OE1	4:I:110:CYS:N	2.40	0.43
1:A:191:LYS:HD3	1:A:191:LYS:HA	1.76	0.43
2:D:452:GLU:HB2	2:F:448:ARG:NH2	2.33	0.43
3:G:154:PRO:HG3	3:G:240:LYS:HD2	2.00	0.43
3:G:200:VAL:HB	4:I:185:THR:HG23	2.00	0.43
3:H:55:TRP:HD1	3:H:89:ILE:HD12	1.83	0.43
3:H:147:THR:HA	3:H:177:PHE:CD2	2.53	0.43
4:L:43:ARG:NH1	4:L:47:SER:O	2.52	0.43
1:A:34:GLU:OE2	1:A:35:ARG:N	2.52	0.43
2:D:445:ARG:NH2	2:D:445:ARG:CG	2.79	0.43
2:B:452:GLU:OE2	2:D:484:ARG:NH2	2.52	0.43
3:G:127:LEU:HD12	3:G:127:LEU:HA	1.82	0.43
1:C:106:GLY:CA	1:C:255:SER:HB3	2.49	0.43
1:E:103:ARG:O	1:E:255:SER:OG	2.37	0.43
3:H:120:LEU:HD21	3:H:129:GLU:OE1	2.18	0.43
3:J:57:ARG:HD2	3:J:113:TYR:CZ	2.53	0.43
3:H:230:ASN:ND2	3:H:237:LYS:HD3	2.32	0.43
4:I:57:GLN:OE1	4:I:108:TYR:CZ	2.71	0.43
4:L:25:GLN:NE2	4:L:124:THR:OG1	2.46	0.43
1:E:232:ASP:OD1	1:E:233:THR:N	2.51	0.43
2:F:443:VAL:HG12	2:F:447:LEU:HD21	2.01	0.43
3:G:160:LYS:HB3	3:G:160:LYS:HE2	1.76	0.43
4:L:53:VAL:N	4:L:71:ASP:OD1	2.30	0.43
4:L:161:ASP:OD1	4:L:190:GLN:NE2	2.43	0.43
2:B:463:HIS:HE2	2:B:478:TYR:HH	1.63	0.42
2:D:441:GLU:O	2:D:445:ARG:HG3	2.19	0.42
1:E:140:MET:HB3	1:E:243:ILE:HG22	2.01	0.42
2:F:379:LYS:HD2	2:F:379:LYS:HA	1.70	0.42
3:H:186:ASN:HB2	3:H:189:ALA:HB3	2.01	0.42
1:E:59:THR:HB	1:E:108:ILE:HD11	2.01	0.42
3:H:71:SER:O	3:H:91:ARG:NH1	2.52	0.42
4:I:134:ALA:CB	4:I:194:LYS:HE3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:GLN:HB2	2:F:411:GLU:OE2	2.19	0.42
1:C:93:VAL:HG21	1:C:224:HIS:CE1	2.55	0.42
1:E:148:ASP:O	4:K:47:SER:HB2	2.19	0.42
4:I:185:THR:OG1	4:I:198:SER:N	2.35	0.42
1:A:91:LYS:HB2	1:A:91:LYS:HE3	1.80	0.42
1:C:95:GLU:HB2	1:C:99:ARG:NH1	2.33	0.42
1:C:228:LEU:HD22	1:C:232:ASP:HB3	2.00	0.42
2:D:343:TYR:CD1	2:D:436:MET:CE	3.00	0.42
2:D:347:HIS:CE1	2:D:354:GLY:CA	3.03	0.42
2:F:444:LYS:O	2:F:447:LEU:O	2.37	0.42
4:L:140:LEU:HB3	4:L:227:LYS:HG3	2.01	0.42
1:A:288:ILE:O	1:A:288:ILE:HG22	2.16	0.42
2:D:447:LEU:O	2:D:448:ARG:C	2.57	0.42
3:G:118:ASP:OD1	3:G:119:ARG:N	2.52	0.42
1:A:73:SER:HB2	1:A:252:ARG:HD2	2.01	0.42
1:E:168:LEU:HB3	1:E:249:SER:HB2	2.01	0.42
2:B:386:LEU:HD23	2:B:386:LEU:HA	1.87	0.42
2:D:437:ASP:OD1	2:D:441:GLU:HG3	2.19	0.42
3:G:134:TRP:HE1	4:I:66:THR:HG22	1.85	0.42
4:L:21:PHE:CD2	4:L:43:ARG:HG3	2.54	0.42
1:E:120:ILE:HD13	1:E:155:MET:SD	2.60	0.42
2:F:326:ALA:O	2:F:327:ILE:HD12	2.20	0.42
3:J:53:MET:CB	3:J:98:LEU:HD22	2.50	0.42
3:H:39:LEU:HD22	3:H:138:THR:HG21	2.01	0.42
4:I:67:VAL:HG23	4:I:68:ILE:HG12	2.00	0.42
1:C:163:ARG:HD3	1:C:250:PHE:CZ	2.54	0.41
1:E:184:LYS:HA	1:E:184:LYS:HD3	1.92	0.41
3:G:46:PHE:CE2	3:G:48:PHE:HA	2.55	0.41
1:A:304:SER:O	1:A:305:LEU:HD23	2.20	0.41
1:C:144:LEU:HD21	3:H:126:LEU:HG	2.02	0.41
3:J:25:GLU:N	3:J:136:GLN:HE22	2.13	0.41
1:A:63:PRO:HB2	1:A:65:GLN:OE1	2.21	0.41
1:A:123:ASN:O	1:A:124:GLY:C	2.57	0.41
1:E:57:LEU:HD23	1:E:102:LEU:HD12	2.02	0.41
1:E:99:ARG:HH12	2:F:392:ASN:HD22	1.68	0.41
1:E:289:ASP:OD1	1:E:289:ASP:C	2.59	0.41
4:K:81:ARG:HB3	4:K:98:SER:O	2.21	0.41
1:A:140:MET:HE3	1:A:243:ILE:HG22	2.03	0.41
3:H:232:LYS:HB2	3:H:233:PRO:HD3	2.01	0.41
1:A:260:SER:OG	1:A:262:VAL:HG22	2.21	0.41
1:C:126:THR:HG23	1:C:128:ALA:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:TRP:CZ3	1:E:226:LEU:HD22	2.52	0.41
3:G:153:PHE:HA	3:G:154:PRO:HD3	1.91	0.41
1:C:106:GLY:N	1:C:255:SER:HB3	2.36	0.41
4:L:127:THR:HG21	4:L:164:PRO:HB3	2.03	0.41
1:C:157:LYS:HA	1:C:157:LYS:HD3	1.88	0.41
1:E:87:CYS:SG	1:E:88:TYR:N	2.94	0.41
4:I:51:ASN:ND2	4:I:113:TYR:HD2	2.19	0.41
4:L:21:PHE:HB3	4:L:45:SER:HB3	2.03	0.41
1:C:260:SER:OG	1:C:262:VAL:HG22	2.21	0.41
4:I:80:ASP:OD1	4:I:80:ASP:N	2.53	0.41
3:G:241:LYS:HE3	3:G:241:LYS:HB2	1.94	0.40
1:A:174:HIS:ND1	1:A:186:TYR:OH	2.37	0.40
3:H:200:VAL:HB	4:L:185:THR:HG22	2.03	0.40
4:I:203:LEU:HD11	4:I:214:TYR:CE2	2.56	0.40
1:A:184:LYS:HG3	4:I:52:TYR:CE1	2.56	0.40
2:F:368:GLN:OE1	2:F:431:LEU:HD11	2.20	0.40
3:G:197:PHE:CD2	4:I:158:LEU:HD22	2.56	0.40
3:H:183:VAL:HA	3:H:228:ASN:O	2.21	0.40
4:I:56:TYR:CD1	4:I:66:THR:HG22	2.56	0.40
2:B:440:TYR:OH	2:B:453:GLU:OE2	2.34	0.40
1:C:171:TRP:CE2	1:C:224:HIS:HB2	2.55	0.40
4:I:85:SER:OG	4:I:94:SER:O	2.32	0.40
4:L:150:ALA:O	4:L:152:LYS:HG2	2.21	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	314/316 (99%)	302 (96%)	12 (4%)	0	100	100
1	C	314/316 (99%)	303 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	314/316 (99%)	302 (96%)	12 (4%)	0	100	100
2	B	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
2	D	170/172 (99%)	157 (92%)	13 (8%)	0	100	100
2	F	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
3	G	221/223 (99%)	212 (96%)	9 (4%)	0	100	100
3	H	213/223 (96%)	205 (96%)	8 (4%)	0	100	100
3	J	114/223 (51%)	112 (98%)	2 (2%)	0	100	100
4	I	211/213 (99%)	199 (94%)	12 (6%)	0	100	100
4	K	96/213 (45%)	86 (90%)	10 (10%)	0	100	100
4	L	211/213 (99%)	196 (93%)	15 (7%)	0	100	100
All	All	2517/2772 (91%)	2395 (95%)	122 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	265/265 (100%)	257 (97%)	8 (3%)	36	63
1	C	265/265 (100%)	255 (96%)	10 (4%)	28	56
1	E	265/265 (100%)	258 (97%)	7 (3%)	41	66
2	B	147/147 (100%)	143 (97%)	4 (3%)	40	66
2	D	147/147 (100%)	139 (95%)	8 (5%)	18	46
2	F	146/147 (99%)	142 (97%)	4 (3%)	40	66
3	G	184/184 (100%)	183 (100%)	1 (0%)	86	91
3	H	178/184 (97%)	172 (97%)	6 (3%)	32	59
3	J	95/184 (52%)	95 (100%)	0	100	100
4	I	186/186 (100%)	184 (99%)	2 (1%)	70	82
4	K	89/186 (48%)	88 (99%)	1 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	L	186/186 (100%)	181 (97%)	5 (3%)	40 66
All	All	2153/2346 (92%)	2097 (97%)	56 (3%)	41 66

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	123	ASN
1	A	132	SER
1	A	146	ASN
1	A	176	SER
1	A	213	GLN
1	A	286	GLN
1	A	298	ARG
2	B	323	LEU
2	B	383	GLN
2	B	433	ASP
2	B	453	GLU
1	C	8	HIS
1	C	73	SER
1	C	145	SER
1	C	148	ASP
1	C	158	SER
1	C	179	THR
1	C	184	LYS
1	C	188	SER
1	C	291	ARG
1	C	298	ARG
2	D	348	GLN
2	D	380	THR
2	D	381	ASN
2	D	413	TRP
2	D	447	LEU
2	D	450	ASN
2	D	465	CYS
2	D	468	ASP
1	E	5	LEU
1	E	8	HIS
1	E	65	GLN
1	E	73	SER
1	E	154	GLN
1	E	194	THR

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Mol	Chain	Res	Type
1	E	226	LEU
2	F	447	LEU
2	F	454	ASP
2	F	484	ARG
2	F	488	MET
4	K	100	LEU
3	G	195	HIS
3	H	22	GLN
3	H	38	ARG
3	H	41	CYS
3	H	62	LYS
3	H	118	ASP
3	H	195	HIS
4	I	57	GLN
4	I	212	ARG
4	L	81	ARG
4	L	112	SER
4	L	164	PRO
4	L	206	GLU
4	L	212	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	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 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	$\#\|Z\| > 2$
5	NAG	B	501	2	14,14,15	0.48	0	17,19,21	0.52	0
5	NAG	F	501	2	14,14,15	0.64	0	17,19,21	0.59	0
5	NAG	C	602	1	14,14,15	0.52	0	17,19,21	0.50	0
5	NAG	E	601	1	14,14,15	0.29	0	17,19,21	0.62	0
5	NAG	E	602	1	14,14,15	0.35	0	17,19,21	0.50	0
5	NAG	A	601	1	14,14,15	0.31	0	17,19,21	0.62	0
5	NAG	D	501	2	14,14,15	0.29	0	17,19,21	0.62	0
5	NAG	A	602	1	14,14,15	0.28	0	17,19,21	0.47	0
5	NAG	C	601	1	14,14,15	0.28	0	17,19,21	0.61	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
5	NAG	B	501	2	-	0/6/23/26	0/1/1/1
5	NAG	F	501	2	-	0/6/23/26	0/1/1/1
5	NAG	C	602	1	-	0/6/23/26	0/1/1/1
5	NAG	E	601	1	-	2/6/23/26	0/1/1/1
5	NAG	E	602	1	-	2/6/23/26	0/1/1/1
5	NAG	A	601	1	-	1/6/23/26	0/1/1/1
5	NAG	D	501	2	-	0/6/23/26	0/1/1/1
5	NAG	A	602	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

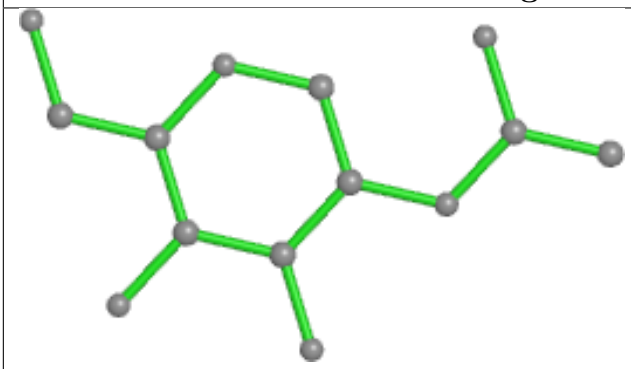
Mol	Chain	Res	Type	Atoms
5	E	601	NAG	O5-C5-C6-O6
5	A	602	NAG	O5-C5-C6-O6
5	E	602	NAG	O5-C5-C6-O6
5	E	601	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	A	602	NAG	C4-C5-C6-O6
5	E	602	NAG	C4-C5-C6-O6
5	C	601	NAG	C4-C5-C6-O6
5	C	601	NAG	O5-C5-C6-O6

There are no ring outliers.

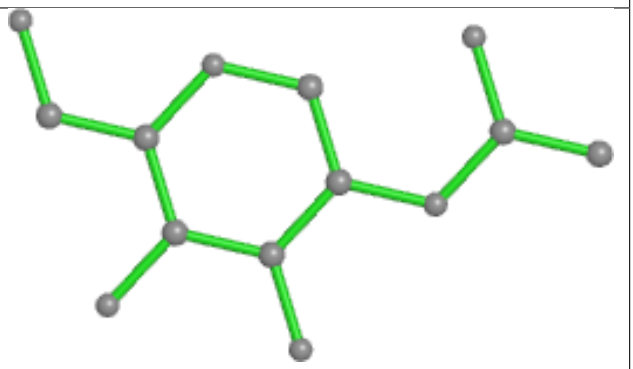
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

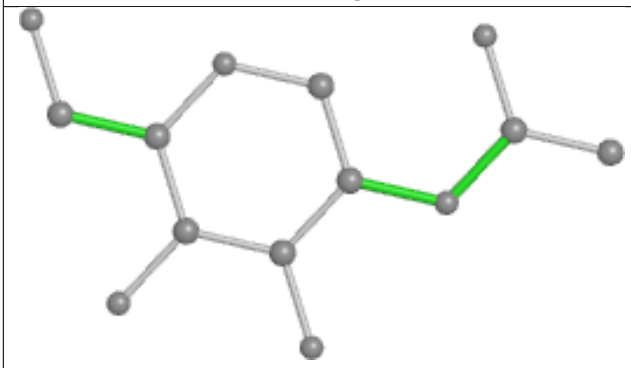
Ligand NAG B 501



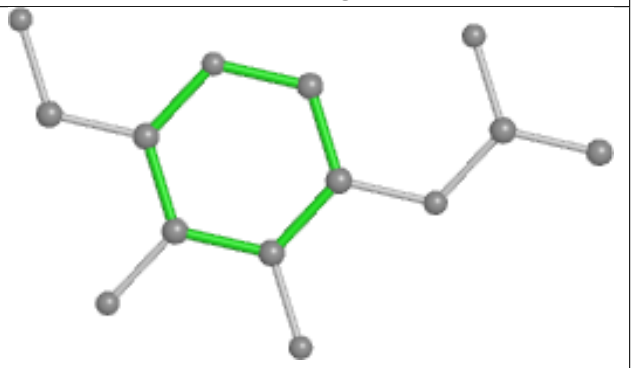
Bond lengths



Bond angles

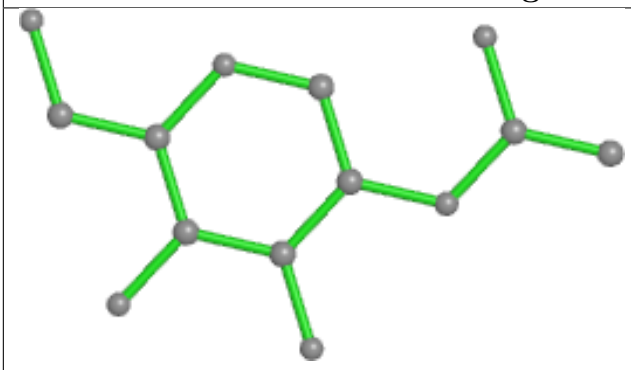


Torsions

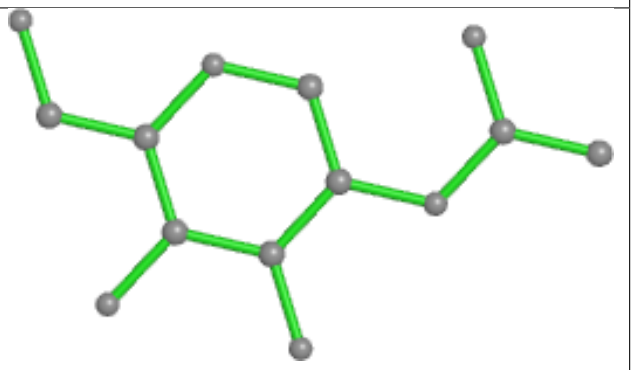


Rings

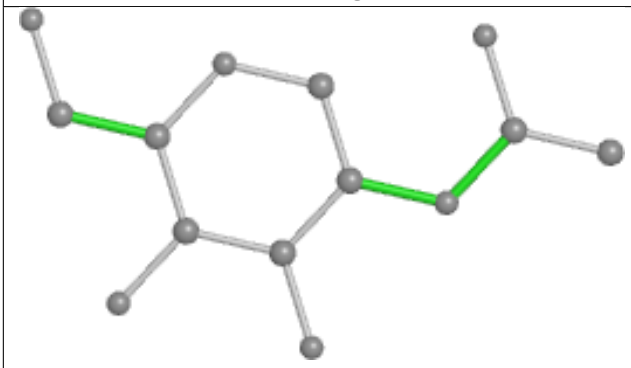
Ligand NAG F 501



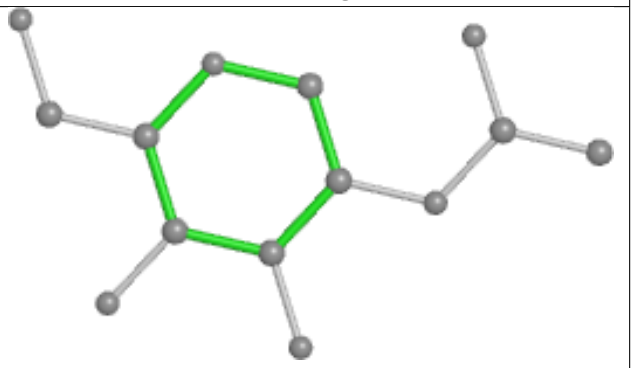
Bond lengths



Bond angles

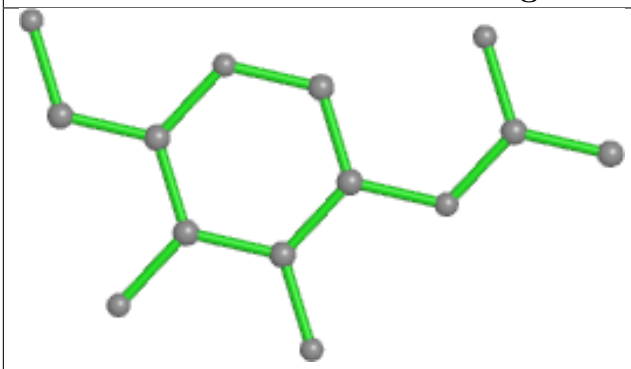


Torsions

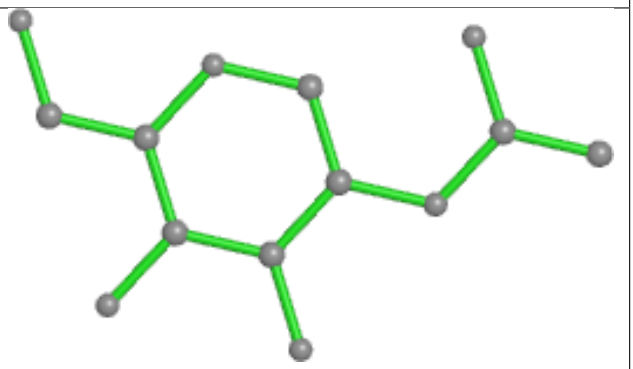


Rings

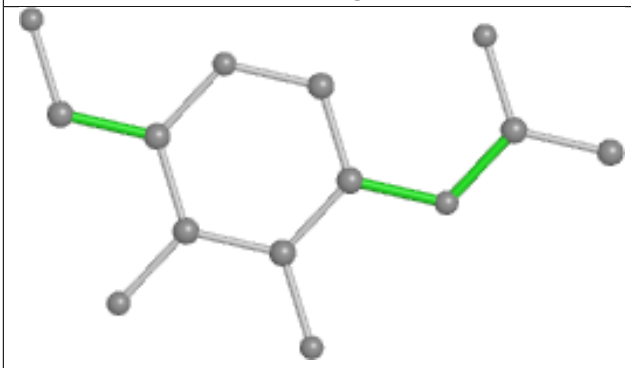
Ligand NAG C 602



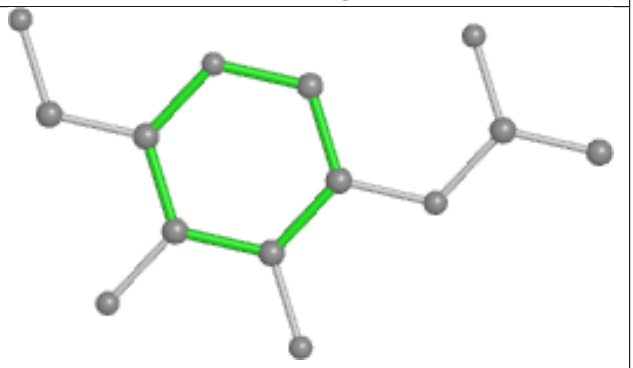
Bond lengths



Bond angles

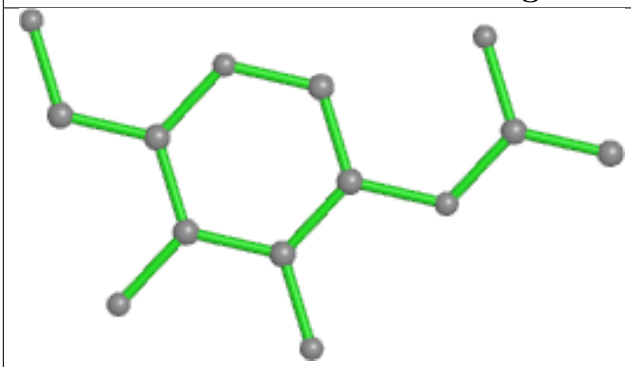


Torsions

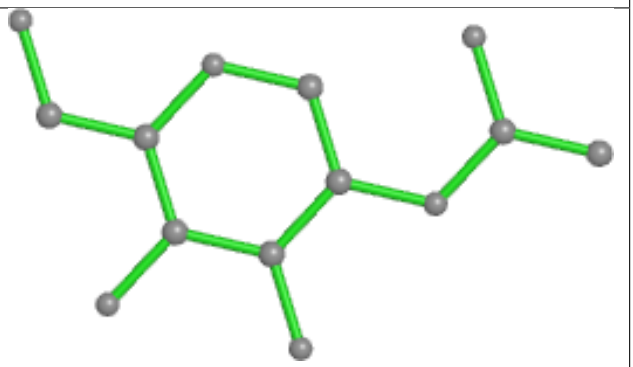


Rings

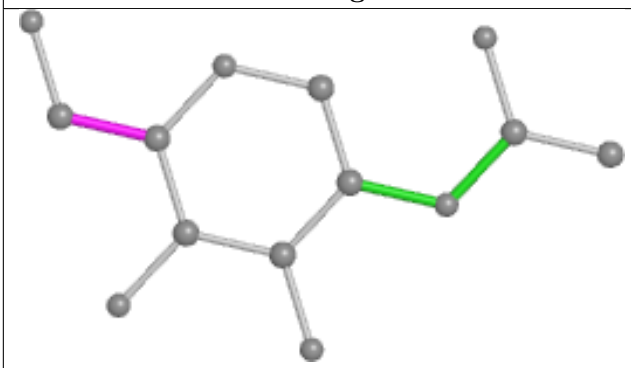
Ligand NAG E 601



Bond lengths



Bond angles



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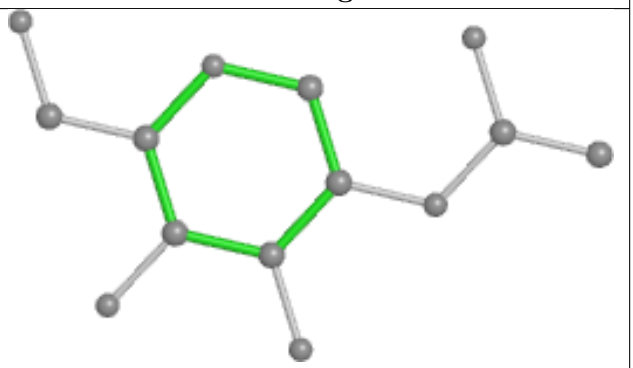
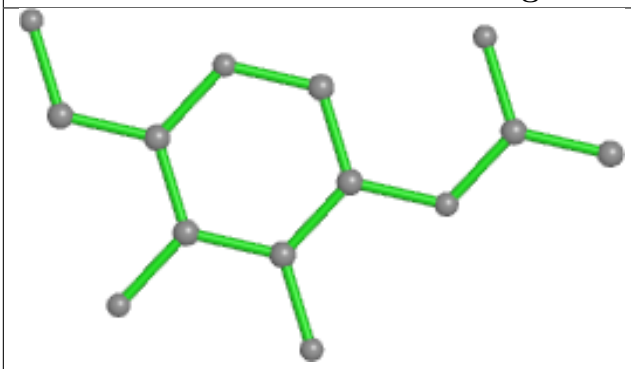
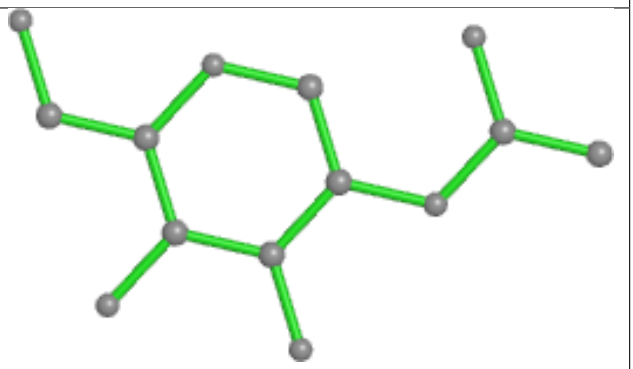


Rings

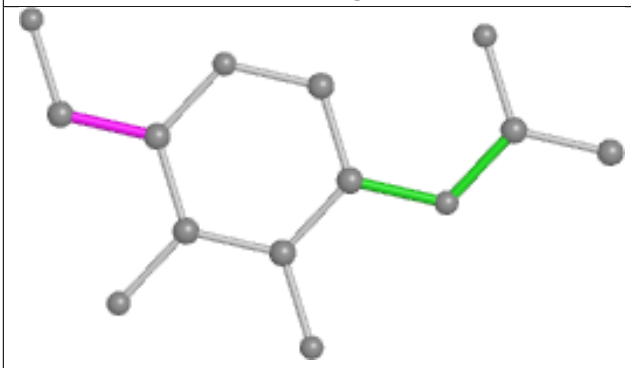
Ligand NAG E 602



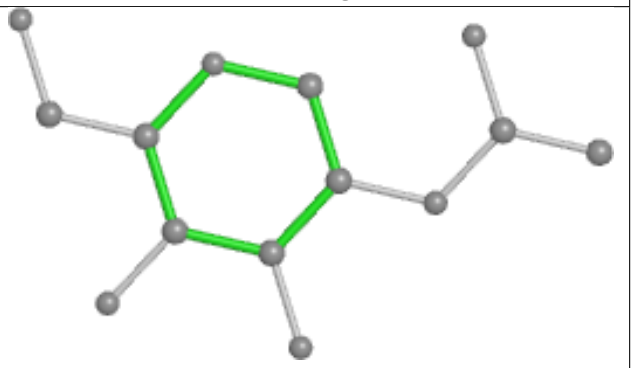
Bond lengths



Bond angles

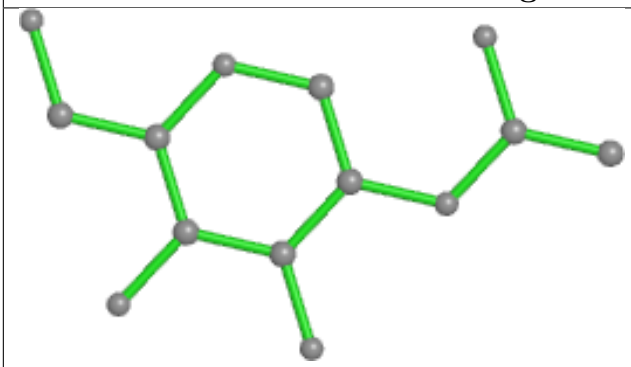


Torsions

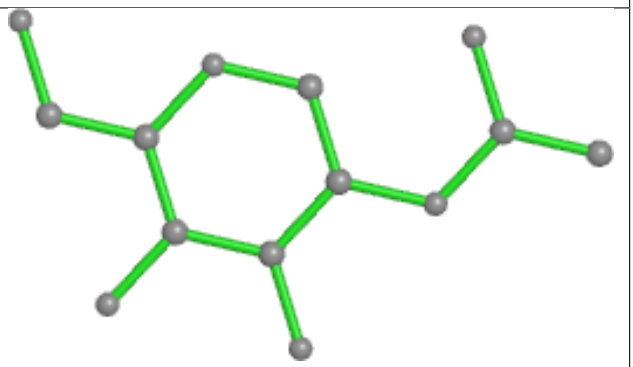


Rings

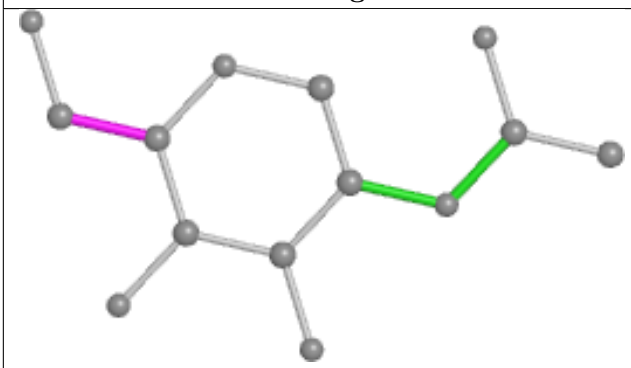
Ligand NAG A 601



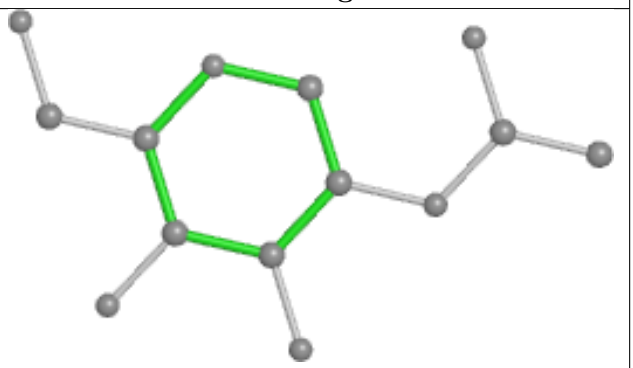
Bond lengths



Bond angles

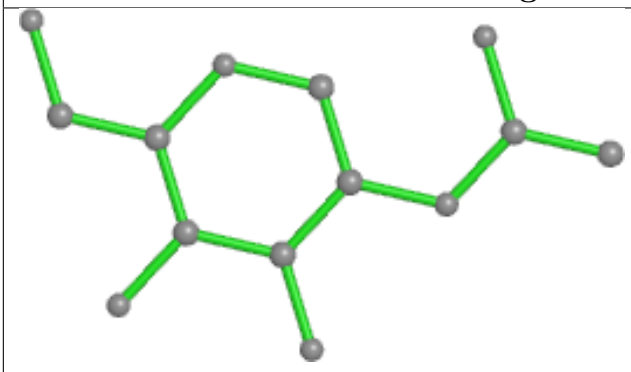


Torsions

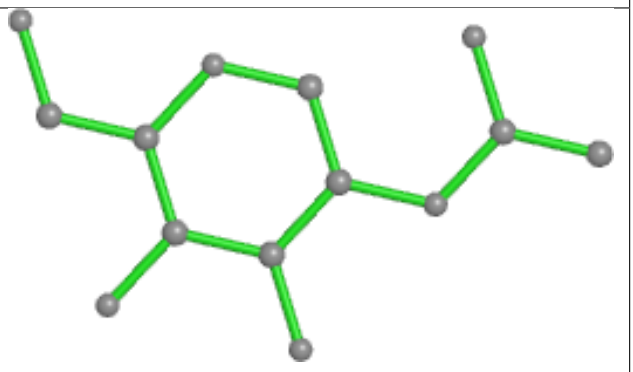


Rings

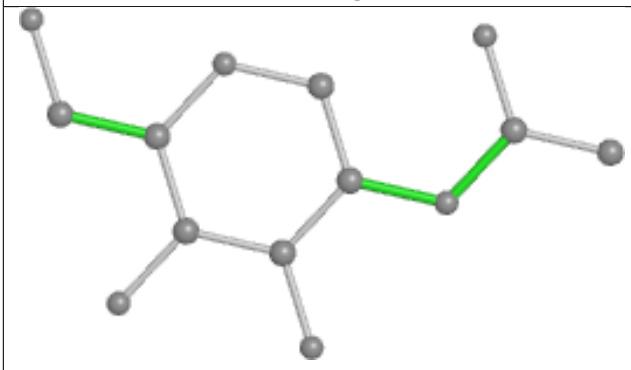
Ligand NAG D 501



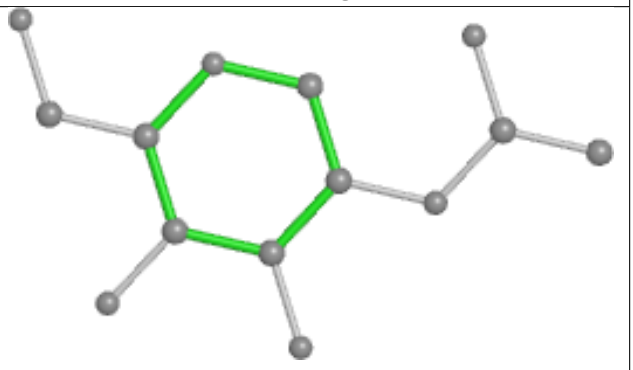
Bond lengths



Bond angles

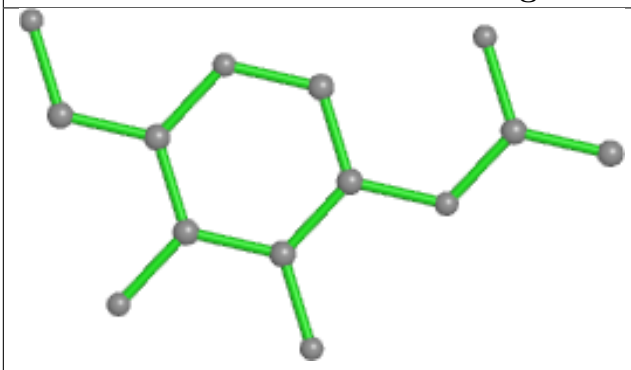


Torsions

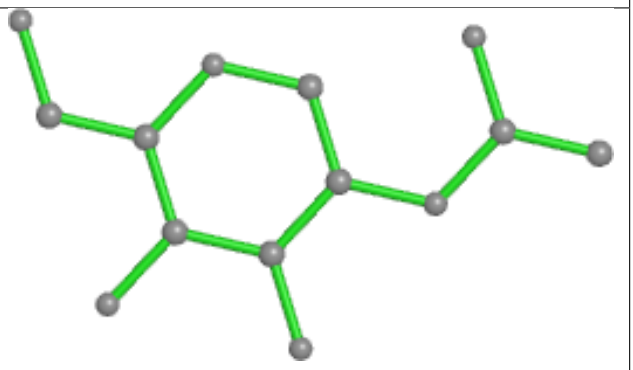


Rings

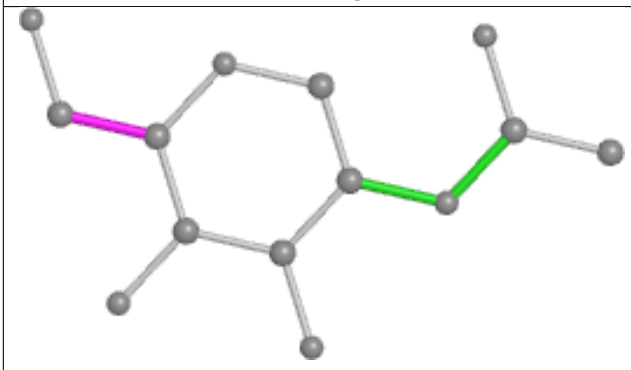
Ligand NAG A 602



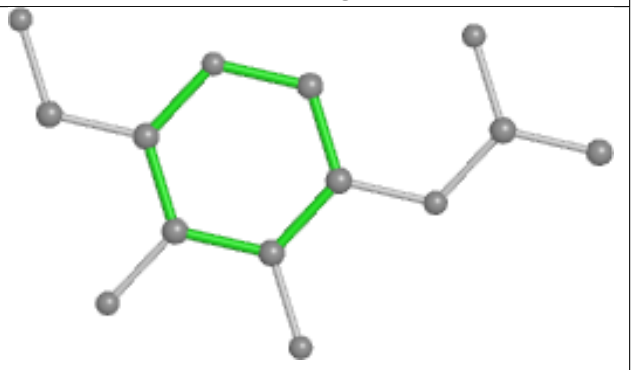
Bond lengths



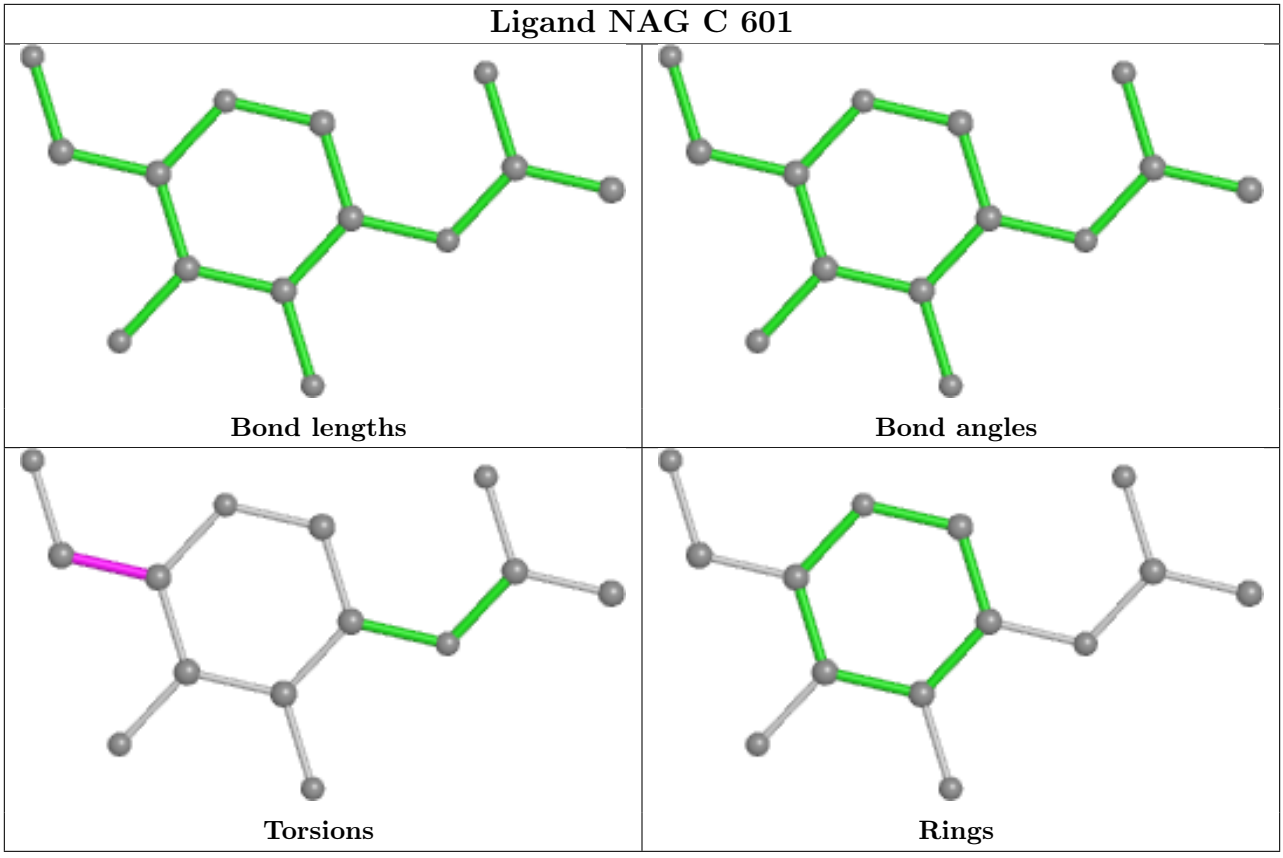
Bond angles



Torsions



Rings



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, 95^{th} 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	316/316 (100%)	-0.45	0 100 100	35, 54, 75, 95	0
1	C	316/316 (100%)	-0.43	0 100 100	37, 54, 72, 92	0
1	E	316/316 (100%)	-0.43	0 100 100	34, 55, 74, 95	0
2	B	172/172 (100%)	-0.22	0 100 100	37, 68, 89, 99	0
2	D	172/172 (100%)	-0.23	2 (1%) 76 64	37, 63, 86, 100	0
2	F	171/172 (99%)	-0.24	1 (0%) 85 78	37, 61, 83, 94	0
3	G	223/223 (100%)	-0.08	1 (0%) 89 83	49, 84, 111, 127	0
3	H	217/223 (97%)	0.11	4 (1%) 67 53	45, 83, 141, 151	0
3	J	118/223 (52%)	0.58	4 (3%) 48 35	64, 114, 137, 145	0
4	I	213/213 (100%)	-0.16	0 100 100	60, 75, 102, 114	0
4	K	100/213 (46%)	0.33	3 (3%) 52 38	75, 103, 126, 131	0
4	L	213/213 (100%)	-0.11	3 (1%) 73 60	56, 77, 102, 117	0
All	All	2547/2772 (91%)	-0.19	18 (0%) 84 75	34, 67, 118, 151	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	322	GLY	5.5
3	J	132	ASP	3.4
3	H	242	VAL	2.9
3	H	167	ALA	2.8
3	G	132	ASP	2.7
4	K	84	GLY	2.6
4	L	176	SER	2.6
3	H	157	PRO	2.5
4	L	175	SER	2.5
3	J	112	VAL	2.4
4	K	60	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	H	168	ALA	2.3
4	K	30	SER	2.1
2	F	492	ILE	2.1
3	J	113	TYR	2.1
2	D	379	LYS	2.1
4	L	127	THR	2.1
3	J	140	VAL	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)

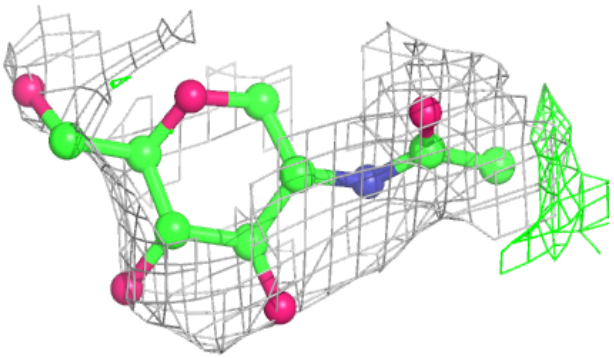
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

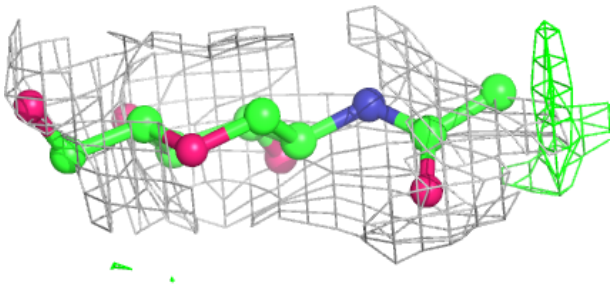
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	C	601	14/15	0.58	0.14	74,84,93,97	0
5	NAG	E	602	14/15	0.60	0.12	75,93,100,101	0
5	NAG	A	601	14/15	0.67	0.12	69,78,89,92	0
5	NAG	A	602	14/15	0.69	0.11	81,98,106,106	0
5	NAG	C	602	14/15	0.71	0.12	89,106,113,121	0
5	NAG	E	601	14/15	0.77	0.12	79,86,94,96	0
5	NAG	F	501	14/15	0.88	0.09	61,65,73,81	0
5	NAG	D	501	14/15	0.91	0.09	64,71,78,80	0
5	NAG	B	501	14/15	0.91	0.09	52,58,68,72	0

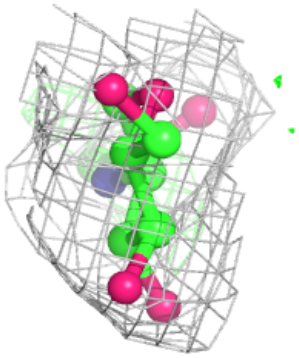
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

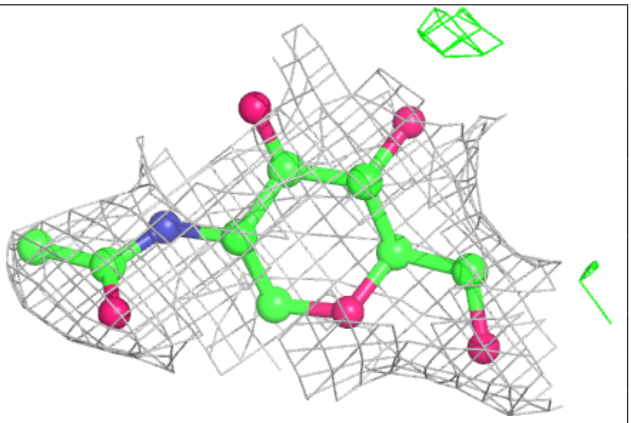


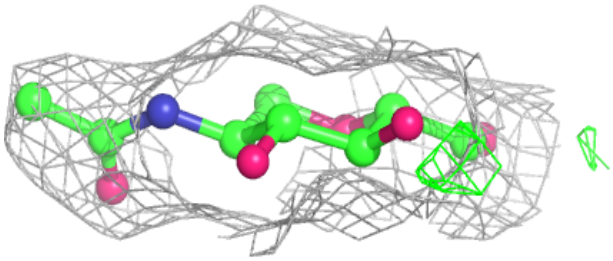


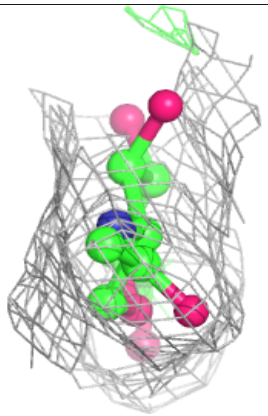


Electron density around NAG E 602:

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

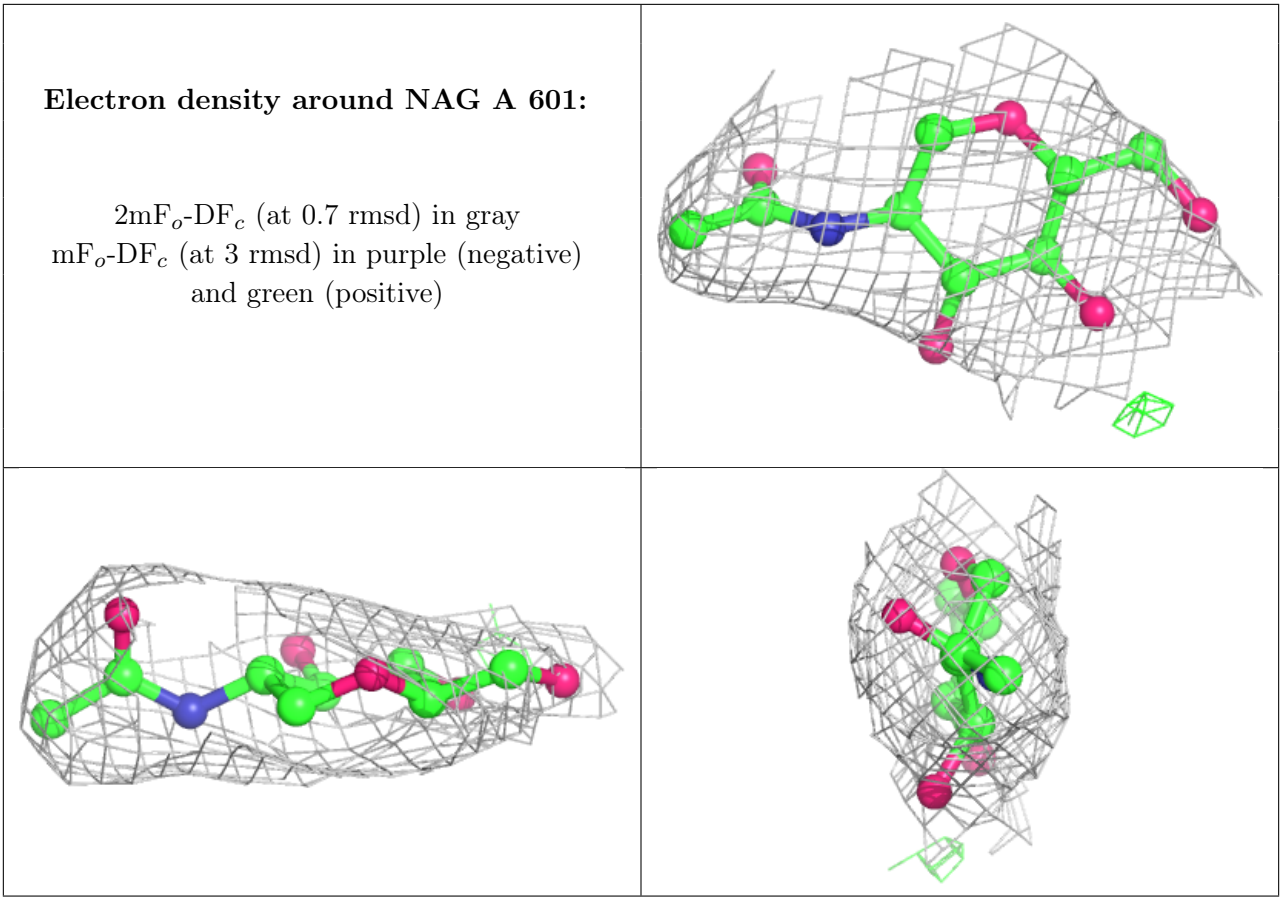






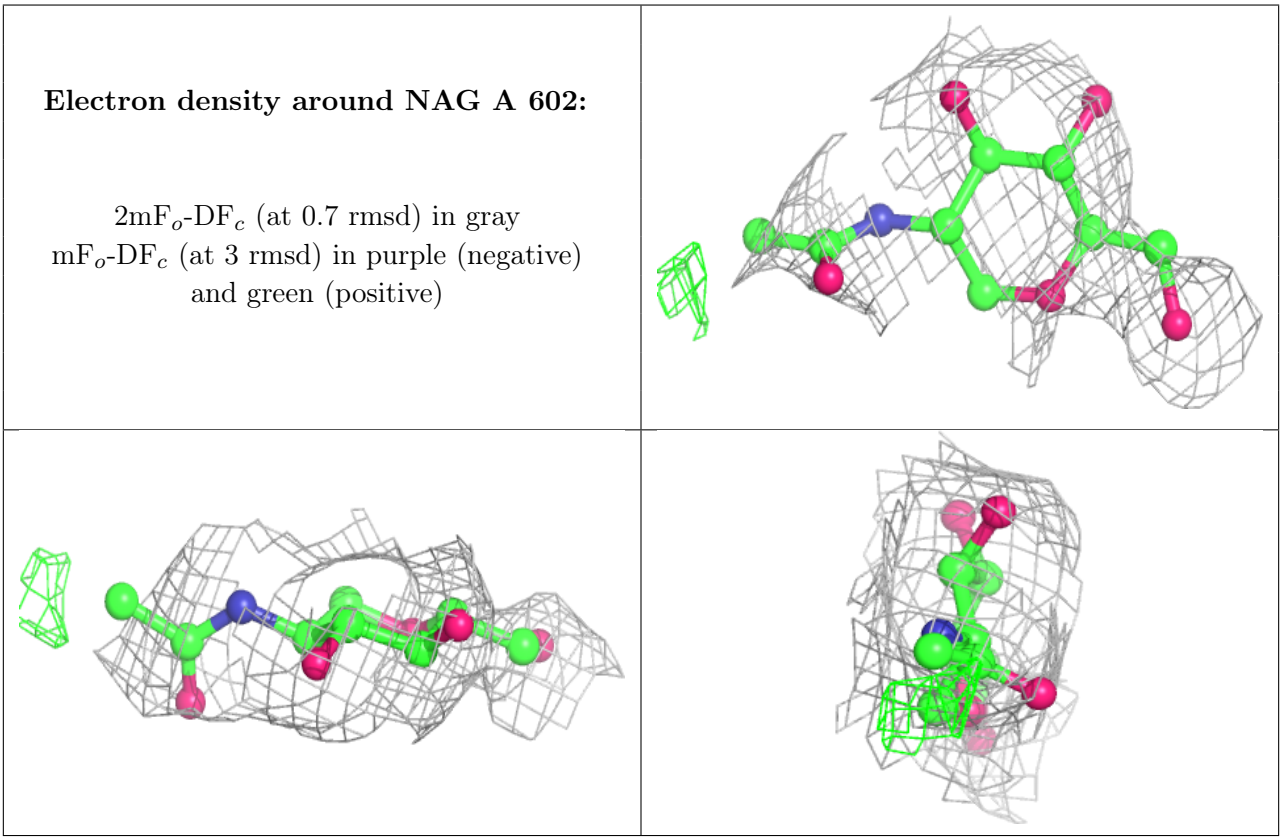
Electron density around NAG A 601:

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



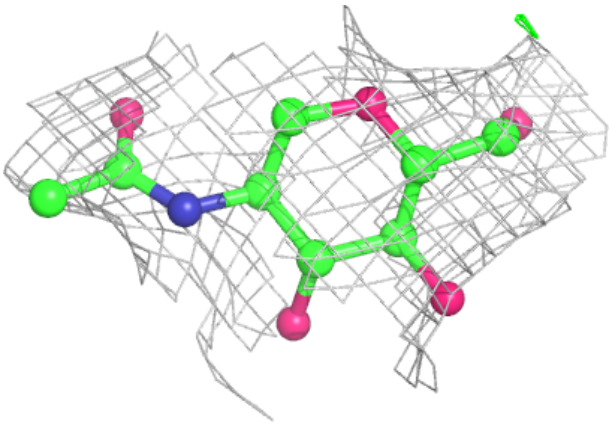
Electron density around NAG A 602:

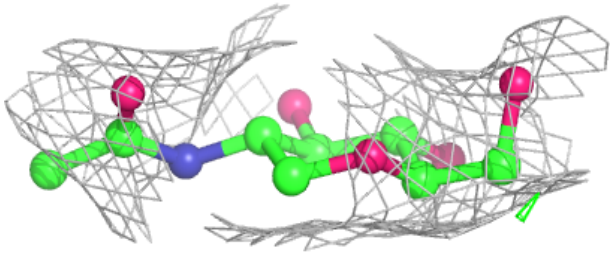
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

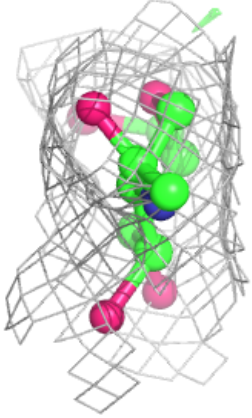


Electron density around NAG C 602:

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

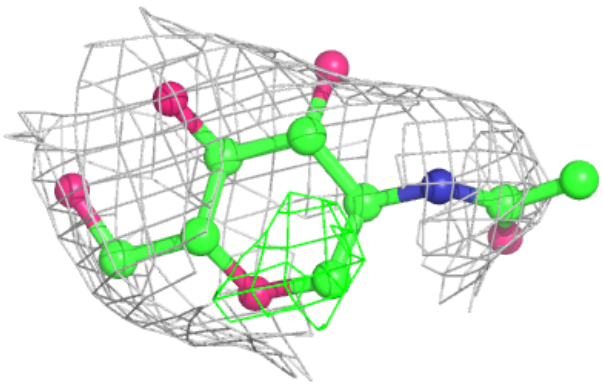


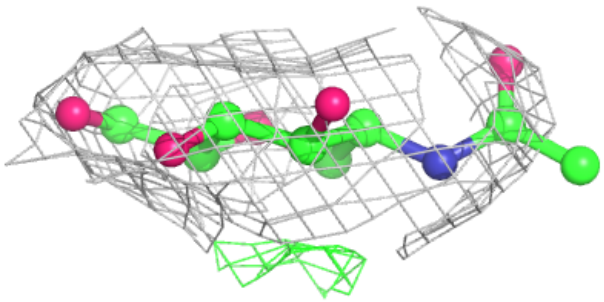


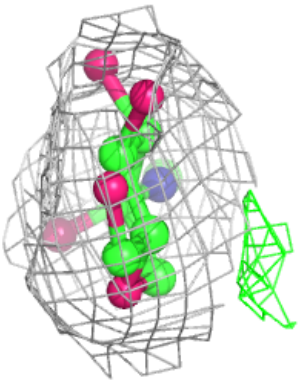


Electron density around NAG E 601:

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

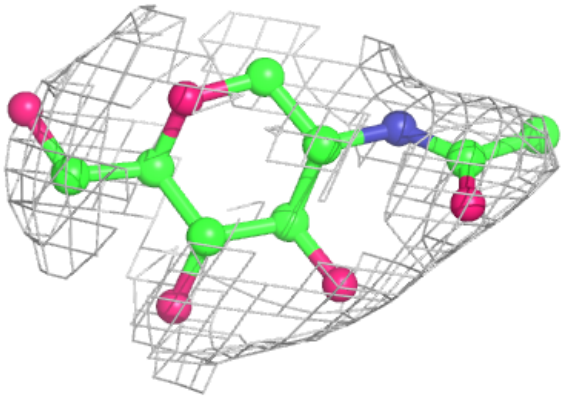


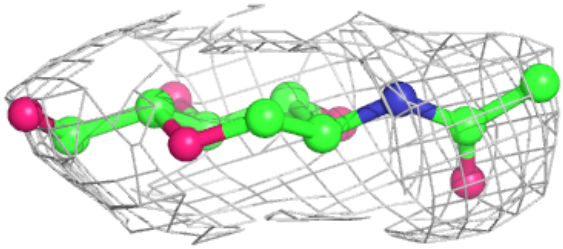


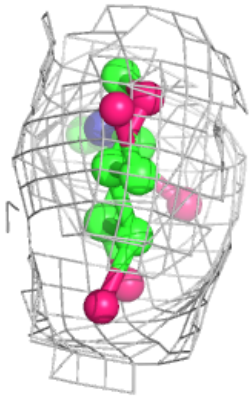


Electron density around NAG F 501:

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

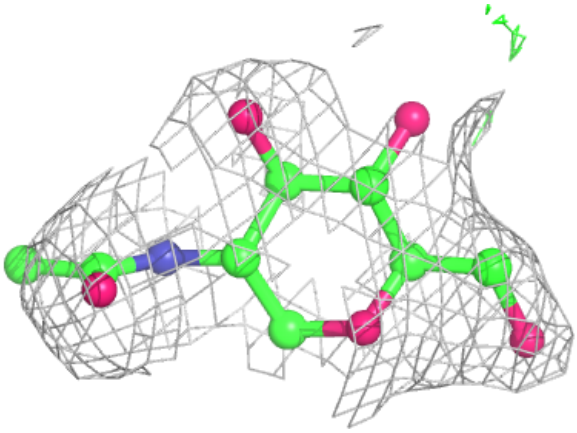


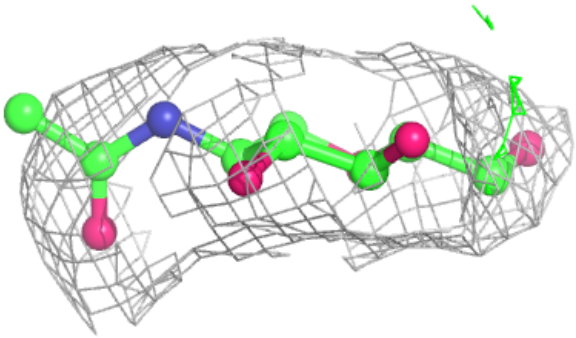


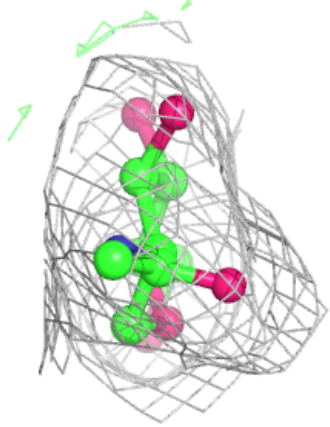


Electron density around NAG D 501:

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

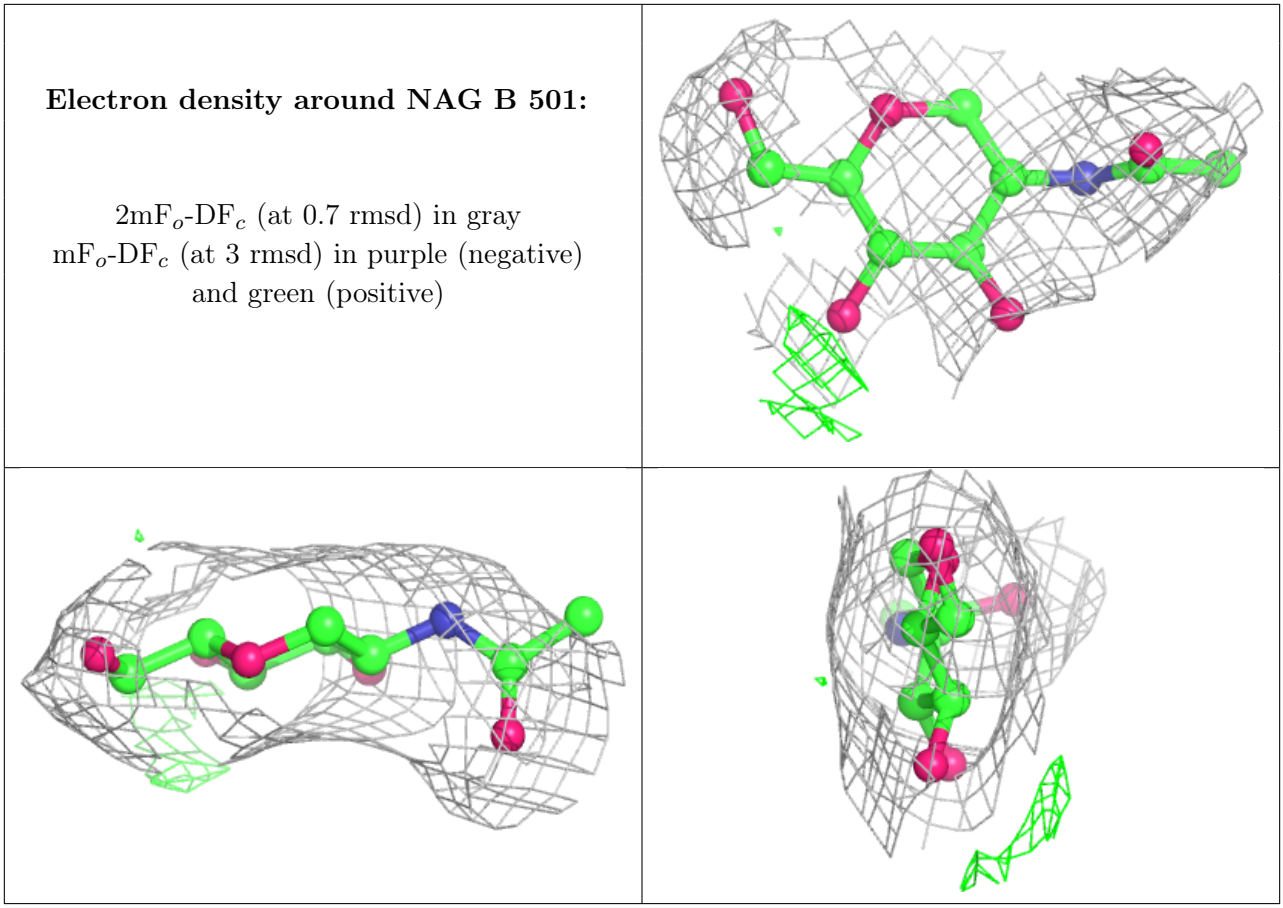






Electron density around NAG B 501:

$2mF_o$-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

There are no such residues in this entry.