



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:34 PM EDT

PDB ID : 6II8 / pdb_00006ii8
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:

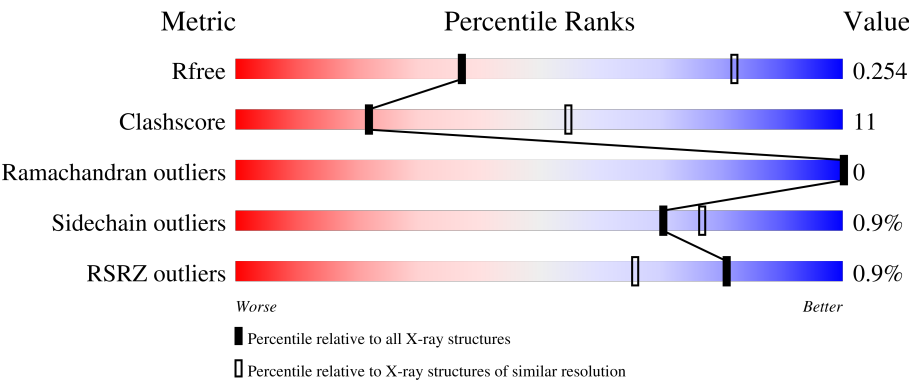
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (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 $\leq 5\%$. 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	316	77%22%.
1	C	316	77%22%
1	E	316	77%23%
2	B	172	76%23%.
2	D	172	%65%34%.

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[illegible]

2 Entry composition

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.

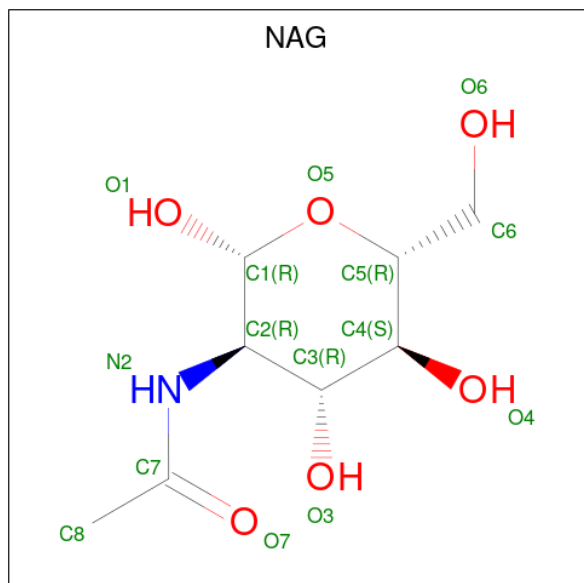
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	100	Total	C	N	O	S	0	0	0
			758	463	128	164	3			

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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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

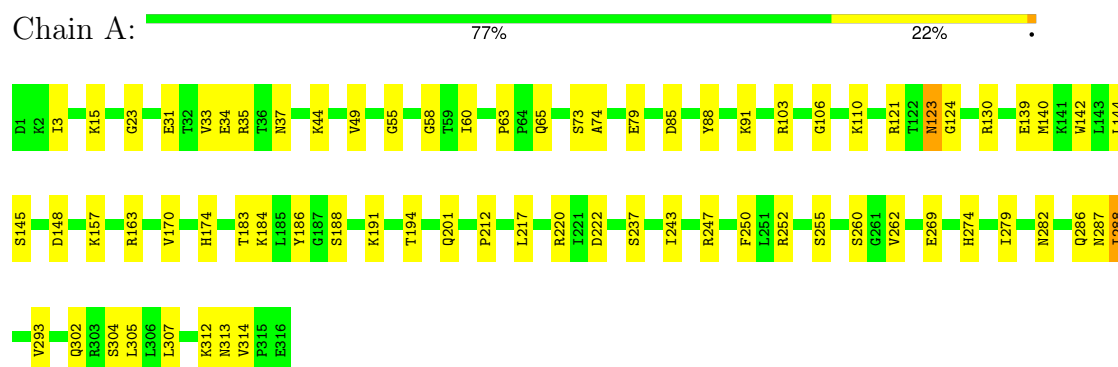


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1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

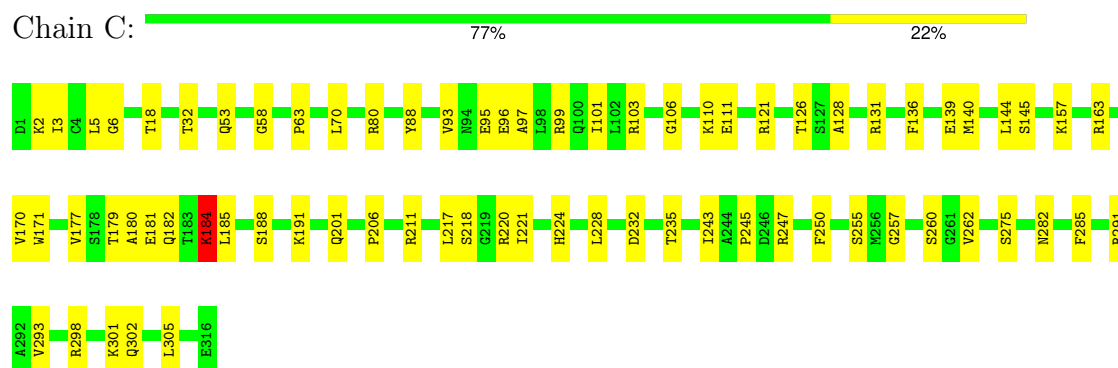
3 Residue-property plots

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

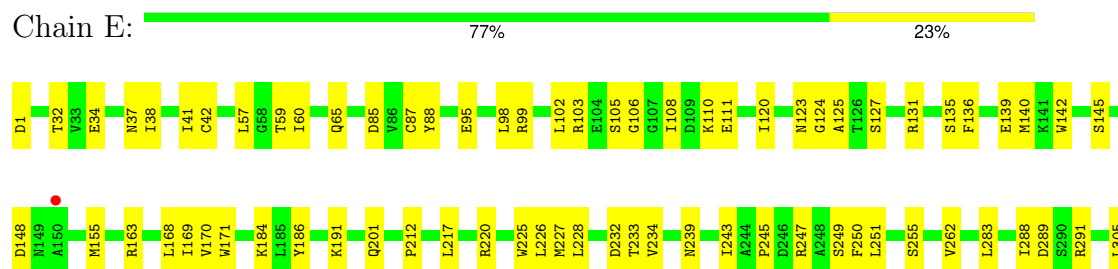
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

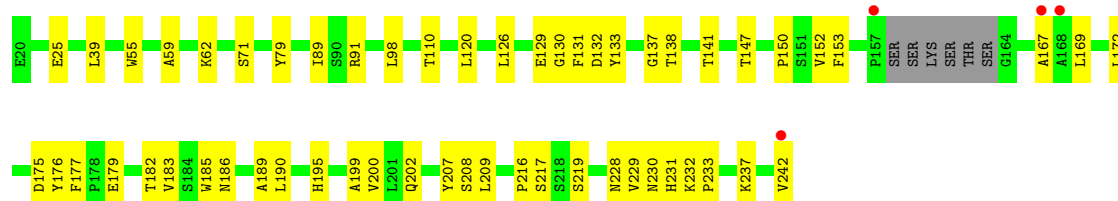


• Molecule 1: Hemagglutinin

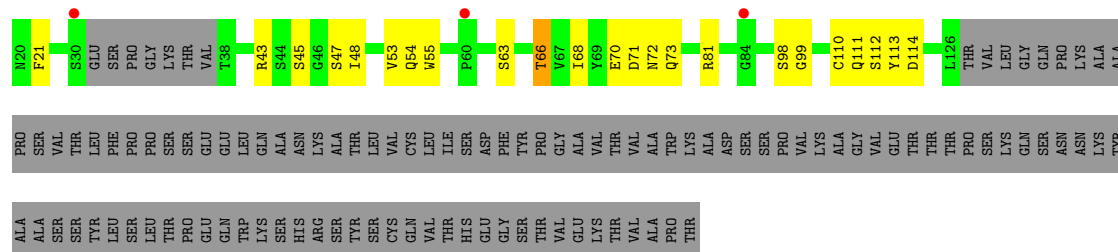
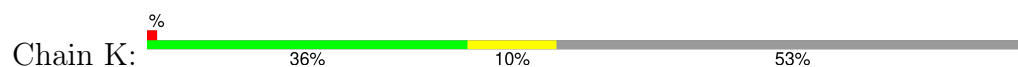




• Molecule 3: Heavy chain of L4B-18 Fab



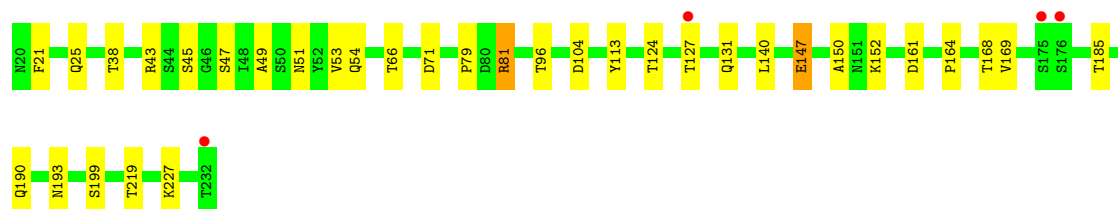
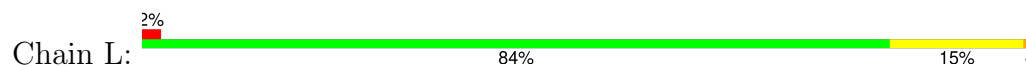
• Molecule 4: Light chain of L4B-18 Fab



• Molecule 4: Light chain of L4B-18 Fab



• Molecule 4: Light chain of L4B-18 Fab



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.203 , 0.251 0.207 , 0.254	Depositor DCC
R_{free} test set	3009 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	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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	0.49	4/2458 (0.2%)	0.54	2/3322 (0.1%)
1	C	0.62	4/2458 (0.2%)	0.54	0/3322
1	E	0.31	0/2458	0.46	0/3322
2	B	0.60	0/1420	0.54	0/1913
2	D	0.84	6/1420 (0.4%)	0.63	1/1913 (0.1%)
2	F	0.62	1/1411 (0.1%)	0.55	2/1901 (0.1%)
3	G	0.34	0/1701	0.41	0/2314
3	H	0.23	0/1660	0.36	0/2258
3	J	0.20	0/937	0.40	0/1266
4	I	0.37	0/1639	0.46	0/2238
4	K	0.32	0/773	0.50	0/1049
4	L	0.26	0/1639	0.44	0/2238
All	All	0.48	15/19974 (0.1%)	0.49	5/27056 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	ILE	CA-CB	-9.55	1.45	1.55
1	C	182	GLN	C-O	-6.81	1.16	1.24
2	D	417	ALA	C-O	-5.95	1.17	1.24
2	D	416	ASN	C-O	-5.94	1.17	1.24
1	A	286	GLN	C-O	-5.71	1.16	1.23
1	A	288	ILE	C-O	-5.52	1.17	1.23
1	C	53	GLN	C-O	-5.39	1.17	1.24
2	D	414	SER	C-O	-5.36	1.17	1.24
2	D	384	PHE	C-O	-5.31	1.17	1.23
1	C	184	LYS	C-O	-5.26	1.17	1.24
2	D	416	ASN	CA-C	-5.22	1.46	1.52
2	D	383	GLN	CA-C	-5.21	1.46	1.52
1	A	287	ASN	C-O	-5.20	1.19	1.24
2	F	486	GLU	CA-C	-5.16	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	ALA	CA-C	-5.07	1.45	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ILE	CB-CA-C	-8.43	101.85	111.80
1	A	288	ILE	N-CA-C	8.36	119.61	111.67
2	F	447	LEU	N-CA-C	-6.54	98.53	108.67
2	F	486	GLU	CB-CA-C	-5.24	102.66	110.88
2	D	415	TYR	N-CA-C	-5.06	105.84	111.36

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	55	0
2	B	1396	0	1296	37	0
2	D	1396	0	1296	59	0
2	F	1387	0	1288	31	0
3	G	1661	0	1621	32	0
3	H	1621	0	1580	41	0
3	J	916	0	875	31	0
4	I	1601	0	1532	41	0
4	K	758	0	699	19	0
4	L	1601	0	1532	24	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	412	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 11.

All (412) 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)
2:D:343:TYR:HD1	2:D:436:MET:HE3	1.43	0.83
2:D:343:TYR:CD1	2:D:436:MET:HE3	2.17	0.80
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
2:D:347:HIS:HB2	2:D:470:MET:HE3	1.70	0.74
1:A:124:GLY:HA3	1:A:142:TRP:HB3	1.69	0.74
2:B:372:LYS:NZ	2:B:424:GLU:OE1	2.20	0.73
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
3:J:25:GLU:H	3:J:136:GLN:HE22	1.40	0.70
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:102:MET:HE2	3:G:105:LEU:HD21	1.80	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: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
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
2:D:463:HIS:NE2	2:D:478:TYR:OH	2.31	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:6:GLY:C	2:D:436:MET:HE1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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
1:E:168:LEU:HB2	1:E:227:MET:HE3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:163:ARG:HD3	1:A:250:PHE:CZ	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:25:GLU:CD	3:H:137:GLY:H	2.20	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
1:A:110:LYS:NZ	1:A:139:GLU:OE2	2.35	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
1:E:65:GLN:CD	1:E:65:GLN:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:301:LYS:HD2	2:F:382:GLN:NE2	2.28	0.47
2:D:447:LEU:O	2:D:448:ARG:C	2.57	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
2:D:435:GLU:OE2	2:D:438:LYS:NZ	2.39	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
1:E:140:MET:HE1	1:E:171:TRP:HA	1.97	0.46
2:B:440:TYR:OH	2:B:453:GLU:OE2	2.34	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
1:E:289:ASP:OD1	1:E:289:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:174:LYS:NZ	4:I:154:THR:OG1	2.28	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
4:I:185:THR:HG1	4:I:198:SER:H	1.59	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:OE2	1:A:35:ARG:N	2.52	0.43
1:A:123:ASN:O	1:A:124:GLY:C	2.57	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: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
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
3:J:25:GLU:CD	3:J:137:GLY:H	2.27	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: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
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
3:H:207:TYR:C	3:H:208:SER:HG	2.27	0.42
2:B:386:LEU:HD23	2:B:386:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:140:MET:HE1	1:C:171:TRP:HA	2.02	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: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
4:K:81:ARG:HB3	4:K:98:SER:O	2.21	0.41
4:L:79:PRO:C	4:L:81:ARG:H	2.28	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
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:A:140:MET:HE3	1:A:243:ILE:HG22	2.03	0.41
2:B:435:GLU:OE2	2:B:438:LYS:NZ	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

5.3.1 Protein backbone

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
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 ⓘ

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%)	264 (100%)	1 (0%)	84	83
1	C	265/265 (100%)	262 (99%)	3 (1%)	65	74
1	E	265/265 (100%)	265 (100%)	0	100	100
2	B	147/147 (100%)	145 (99%)	2 (1%)	59	72
2	D	147/147 (100%)	142 (97%)	5 (3%)	32	59
2	F	146/147 (99%)	143 (98%)	3 (2%)	47	66
3	G	184/184 (100%)	183 (100%)	1 (0%)	81	82
3	H	178/184 (97%)	178 (100%)	0	100	100
3	J	95/184 (52%)	95 (100%)	0	100	100
4	I	186/186 (100%)	185 (100%)	1 (0%)	81	82
4	K	89/186 (48%)	88 (99%)	1 (1%)	65	74
4	L	186/186 (100%)	184 (99%)	2 (1%)	65	74
All	All	2153/2346 (92%)	2134 (99%)	19 (1%)	70	77

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
2	B	323	LEU
2	B	453	GLU
1	C	179	THR
1	C	184	LYS
1	C	188	SER
2	D	348	GLN
2	D	380	THR
2	D	381	ASN
2	D	447	LEU
2	D	450	ASN
2	F	447	LEU
2	F	484	ARG
2	F	488	MET

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Mol	Chain	Res	Type
4	K	66	THR
3	G	23	LEU
4	I	57	GLN
4	L	81	ARG
4	L	147	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
2	B	446	GLN
2	B	490	ASN
2	D	383	GLN
1	E	146	ASN
1	E	287	ASN
2	F	374	ASN
2	F	397	GLN
3	J	136	GLN
4	K	20	ASN
3	H	186	ASN
4	I	20	ASN
4	I	117	ASN
4	L	131	GLN
4	L	211	HIS
4	L	217	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	0.47	0	17,19,21	0.54	0
5	NAG	A	601	1	14,14,15	0.30	0	17,19,21	0.56	0
5	NAG	A	602	1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	D	501	2	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	C	601	1	14,14,15	0.28	0	17,19,21	0.56	0
5	NAG	C	602	1	14,14,15	0.54	0	17,19,21	0.51	0
5	NAG	F	501	2	14,14,15	0.65	0	17,19,21	0.61	0
5	NAG	E	601	1	14,14,15	0.29	0	17,19,21	0.57	0
5	NAG	E	602	1	14,14,15	0.36	0	17,19,21	0.52	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	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	602	1	-	2/6/23/26	0/1/1/1
5	NAG	D	501	2	-	0/6/23/26	0/1/1/1
5	NAG	C	601	1	-	2/6/23/26	0/1/1/1
5	NAG	C	602	1	-	0/6/23/26	0/1/1/1
5	NAG	F	501	2	-	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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

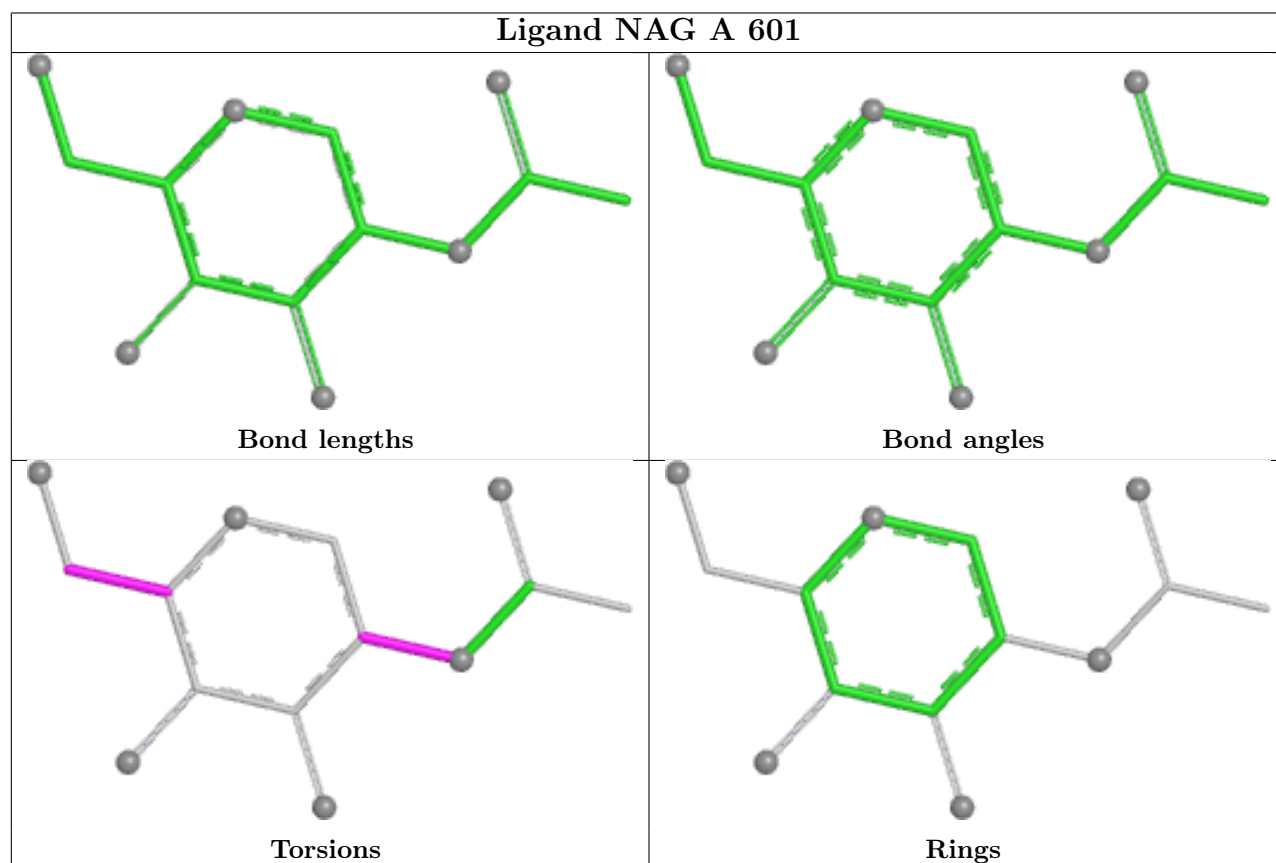
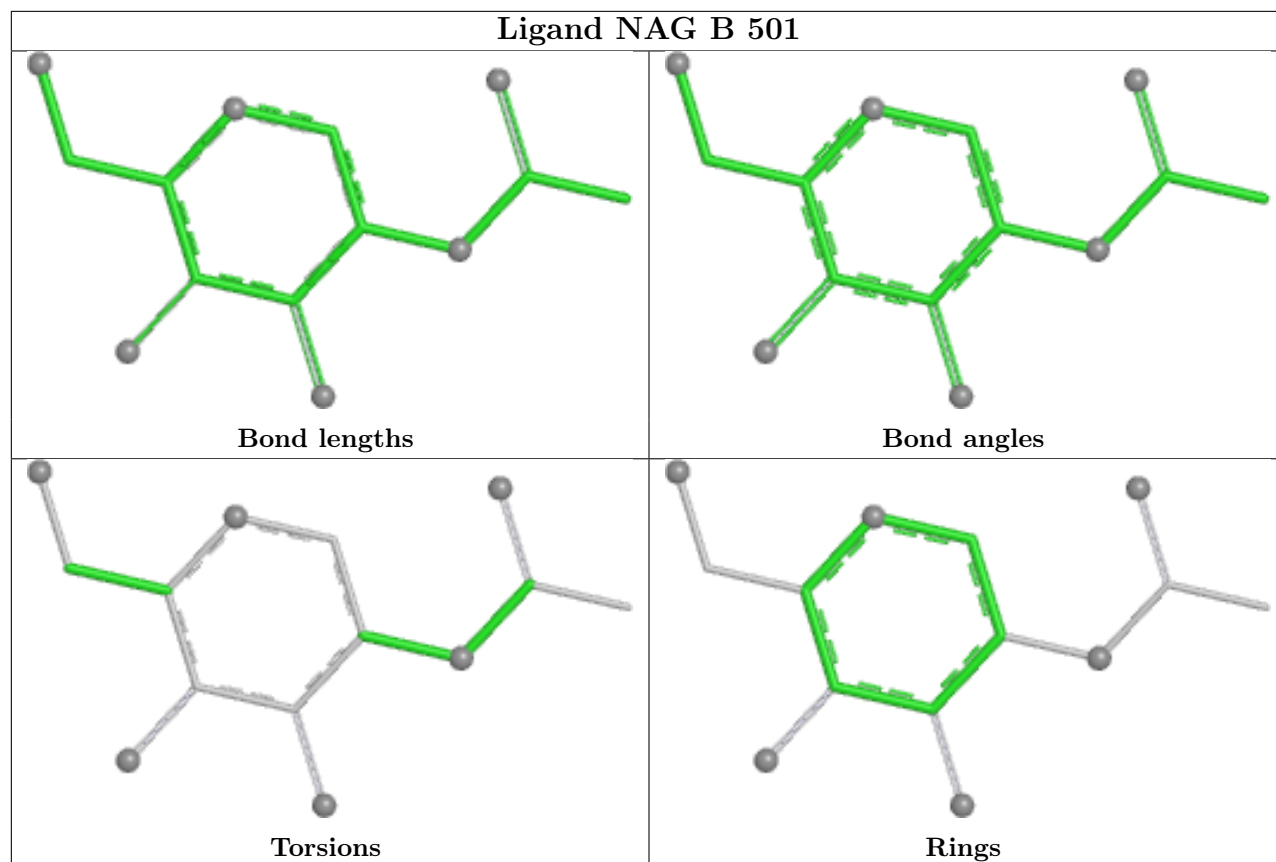
All (10) torsion outliers are listed below:

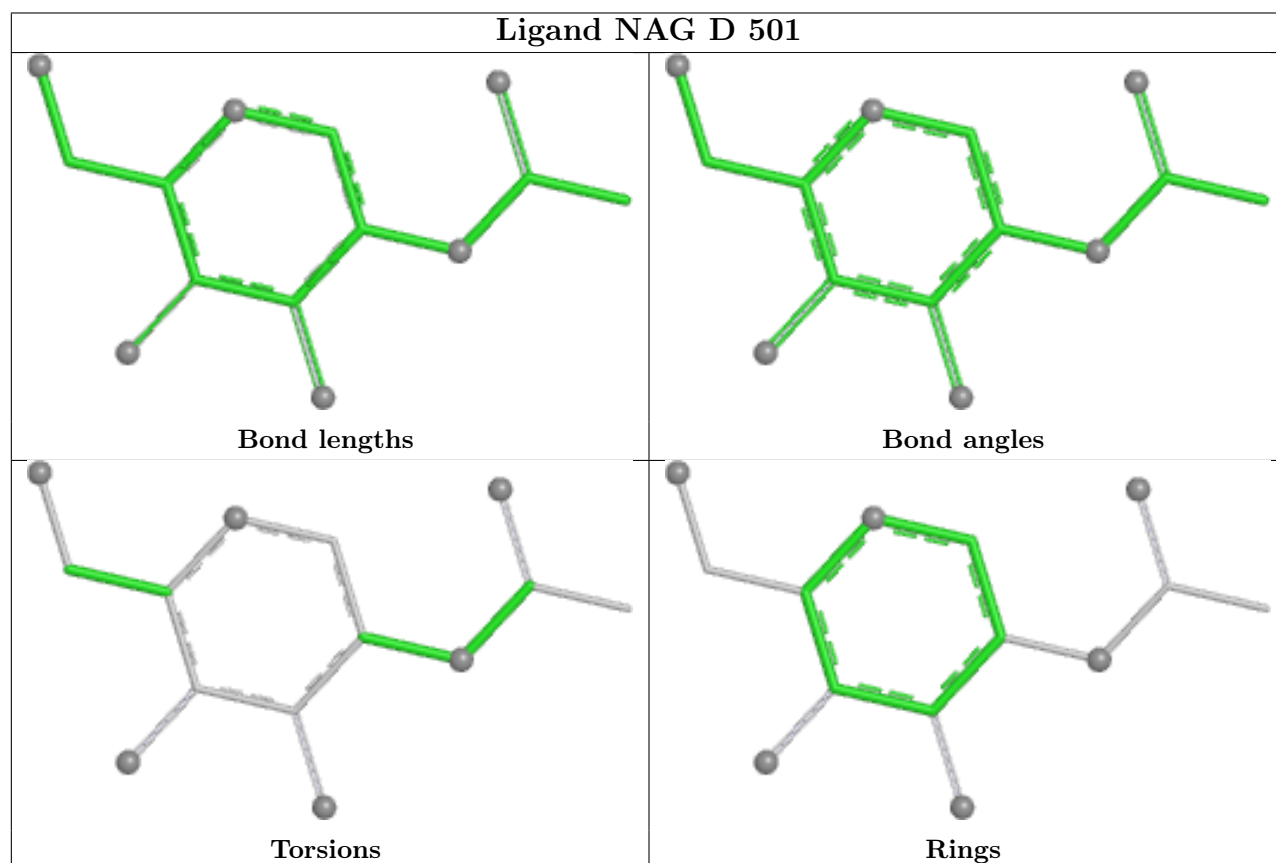
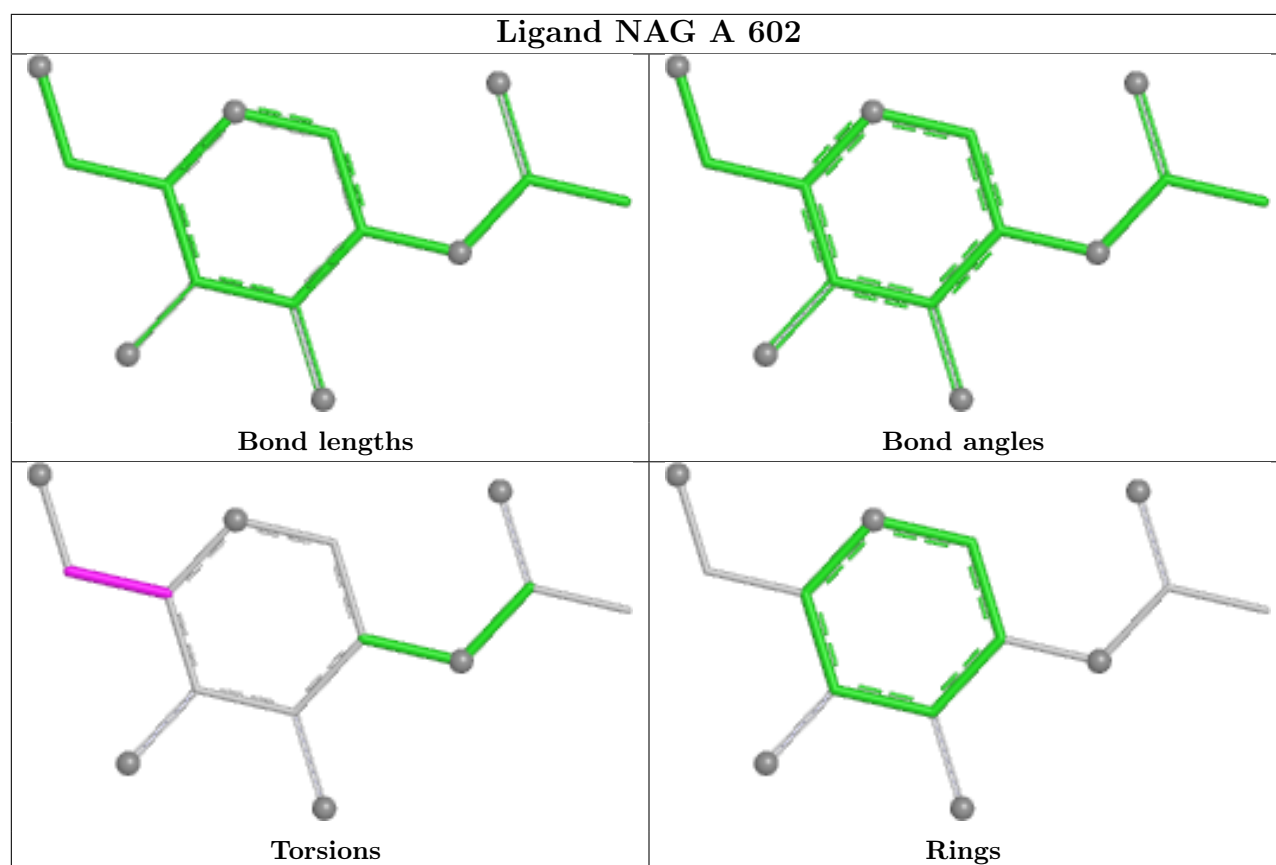
Mol	Chain	Res	Type	Atoms
5	E	601	NAG	O5-C5-C6-O6
5	A	602	NAG	O5-C5-C6-O6
5	E	602	NAG	O5-C5-C6-O6
5	E	601	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	A	602	NAG	C4-C5-C6-O6
5	E	602	NAG	C4-C5-C6-O6
5	C	601	NAG	C4-C5-C6-O6
5	A	601	NAG	C1-C2-N2-C7
5	C	601	NAG	O5-C5-C6-O6

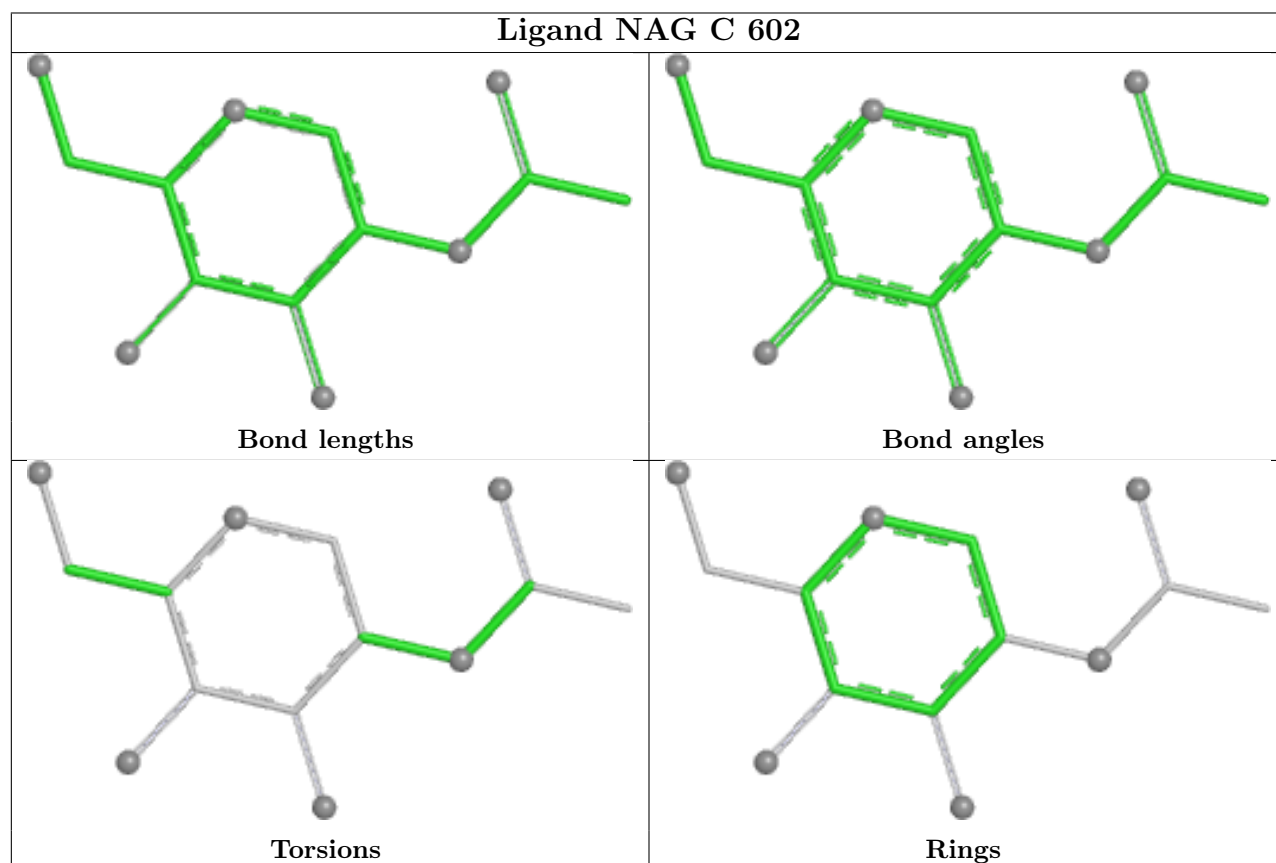
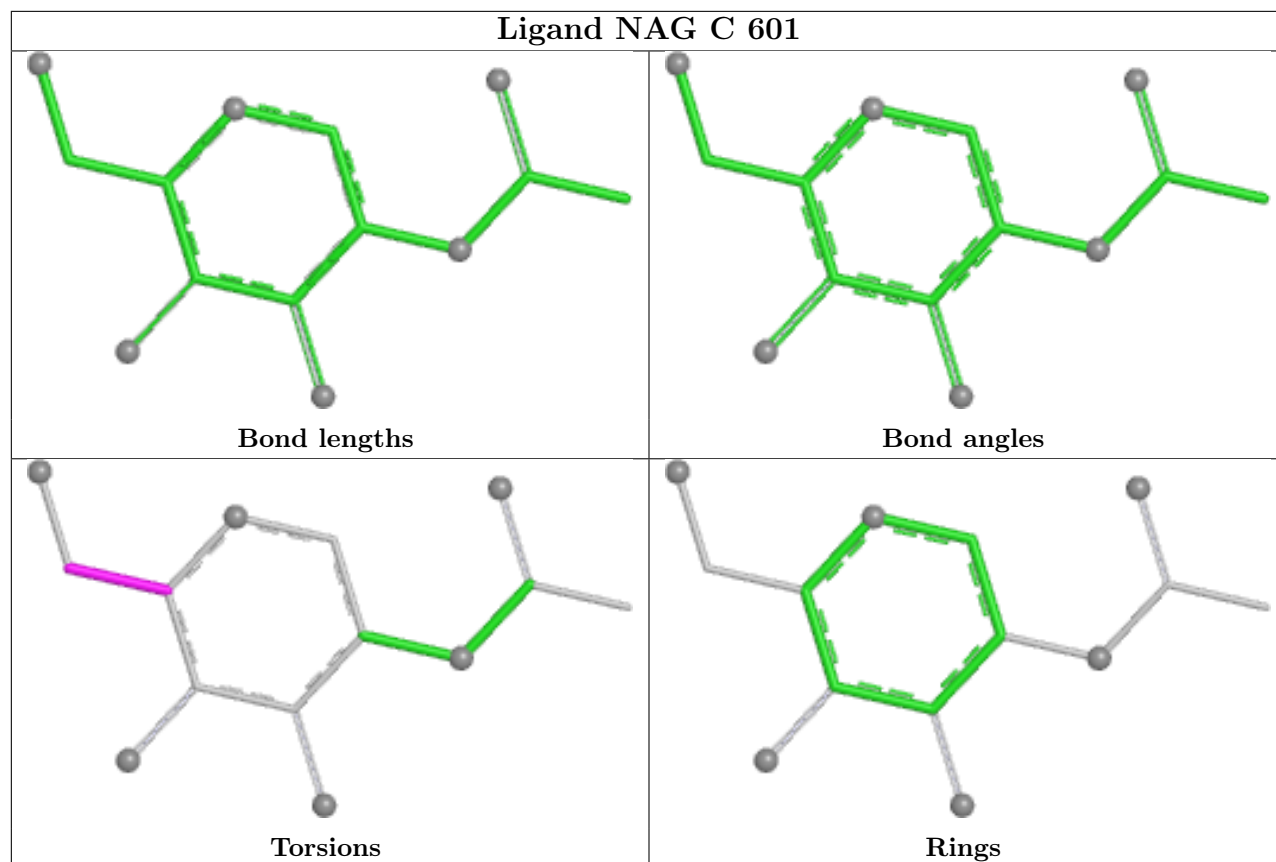
There are no ring outliers.

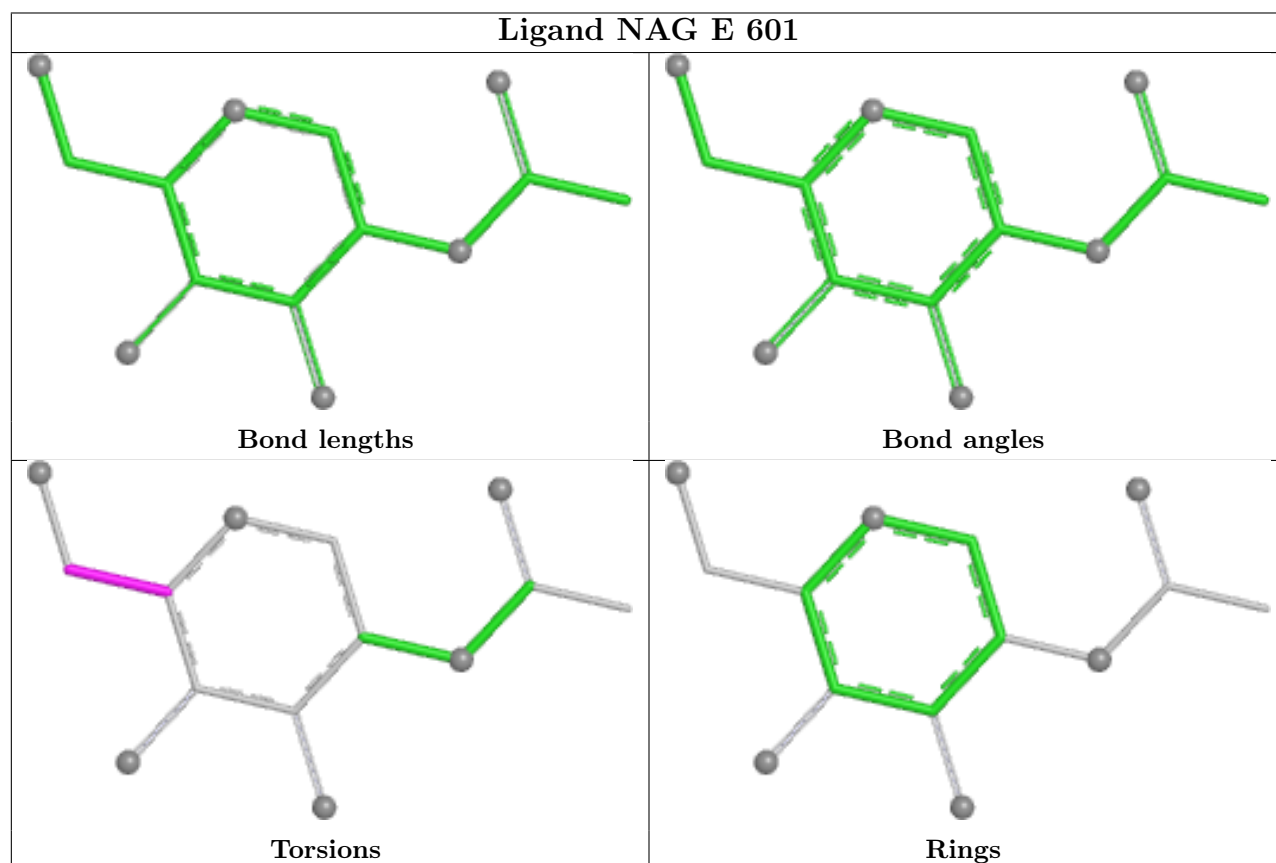
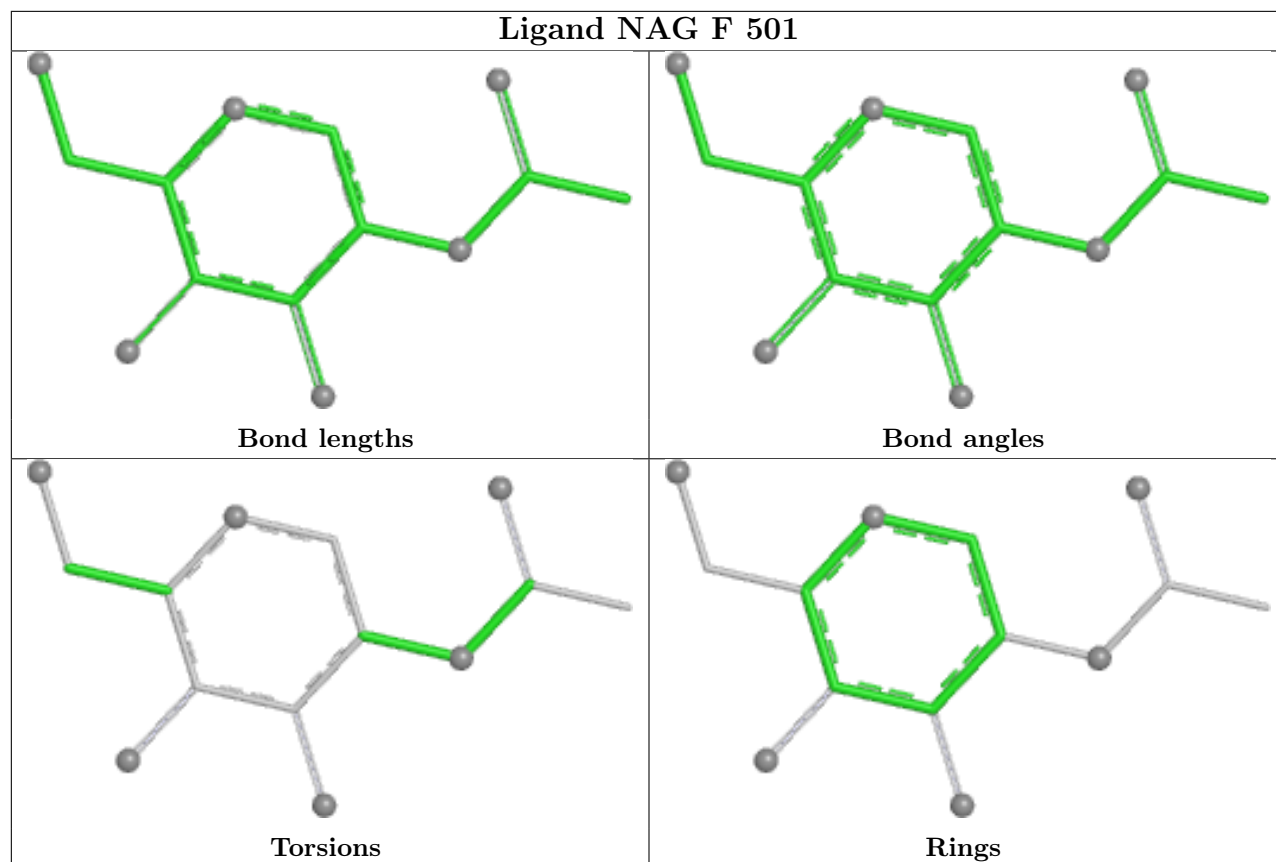
No monomer is involved in short contacts.

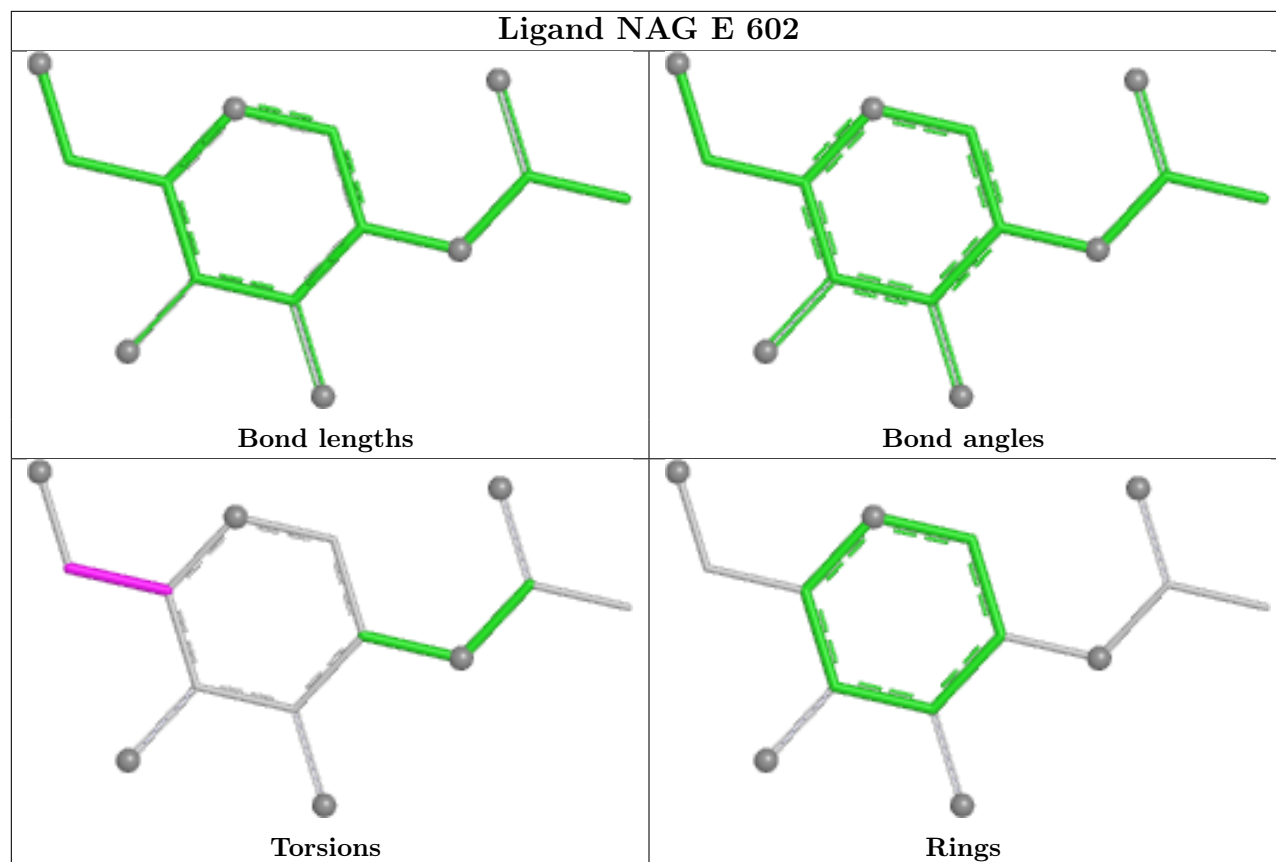
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	316/316 (100%)	-0.30	0 100 100	35, 54, 75, 95	0
1	C	316/316 (100%)	-0.28	0 100 100	37, 54, 72, 92	0
1	E	316/316 (100%)	-0.28	1 (0%) 90 82	34, 55, 74, 95	0
2	B	172/172 (100%)	-0.07	0 100 100	37, 68, 89, 99	0
2	D	172/172 (100%)	-0.08	2 (1%) 76 58	37, 63, 86, 100	0
2	F	171/172 (99%)	-0.09	1 (0%) 85 73	37, 61, 83, 94	0
3	G	223/223 (100%)	0.07	1 (0%) 88 79	49, 84, 111, 127	0
3	H	217/223 (97%)	0.26	4 (1%) 67 49	45, 83, 141, 151	0
3	J	118/223 (52%)	0.73	7 (5%) 28 19	64, 114, 137, 145	0
4	I	213/213 (100%)	-0.01	0 100 100	60, 75, 102, 114	0
4	K	100/213 (46%)	0.48	3 (3%) 52 35	75, 103, 126, 131	0
4	L	213/213 (100%)	0.04	4 (1%) 66 47	56, 77, 102, 117	0
All	All	2547/2772 (91%)	-0.04	23 (0%) 81 66	34, 67, 118, 151	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	322	GLY	5.7
3	J	132	ASP	3.6
3	H	242	VAL	3.1
3	H	167	ALA	3.0
3	G	132	ASP	2.9
4	L	176	SER	2.8
4	K	84	GLY	2.7
3	H	157	PRO	2.7
4	L	175	SER	2.7
3	J	112	VAL	2.6
4	K	60	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	168	ALA	2.4
4	K	30	SER	2.3
3	J	113	TYR	2.3
2	F	492	ILE	2.3
4	L	127	THR	2.2
2	D	379	LYS	2.2
3	J	140	VAL	2.2
3	J	33	PRO	2.1
1	E	150	ALA	2.0
4	L	232	THR	2.0
3	J	30	LEU	2.0
3	J	37	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

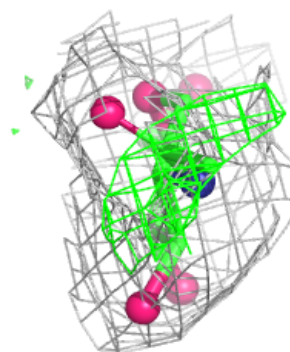
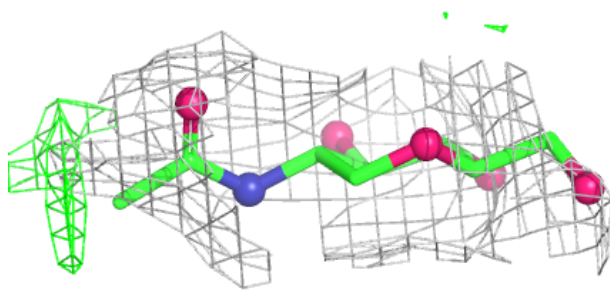
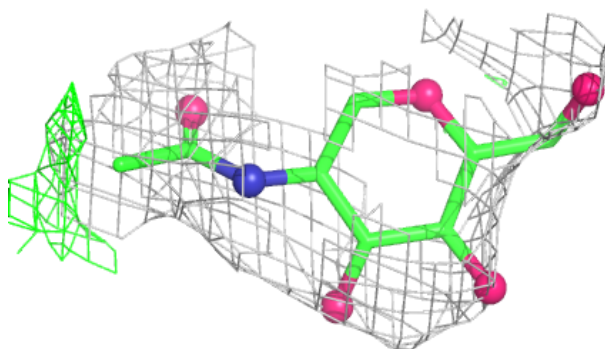
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	C	601	14/15	0.58	0.14	74,84,93,97	0
5	NAG	E	602	14/15	0.60	0.12	75,93,100,101	0
5	NAG	A	601	14/15	0.67	0.12	69,78,89,92	0
5	NAG	A	602	14/15	0.69	0.11	81,98,106,106	0
5	NAG	C	602	14/15	0.71	0.12	89,106,113,121	0
5	NAG	E	601	14/15	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.

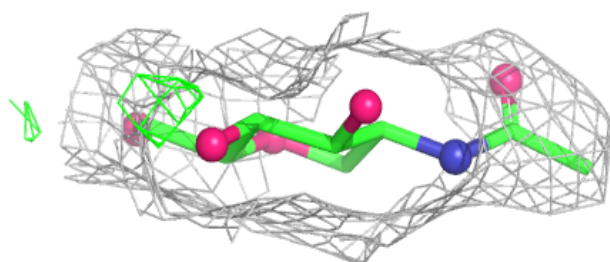
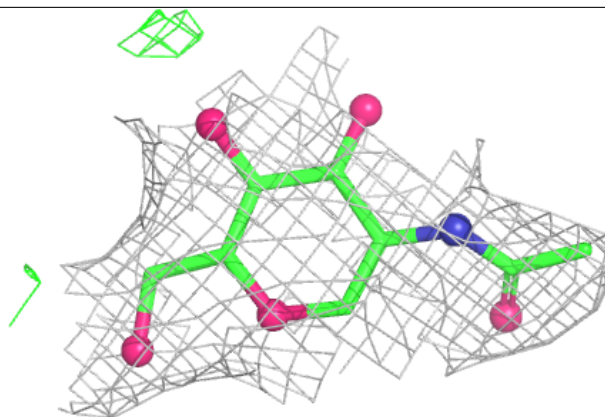
Electron density around NAG C 601:

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

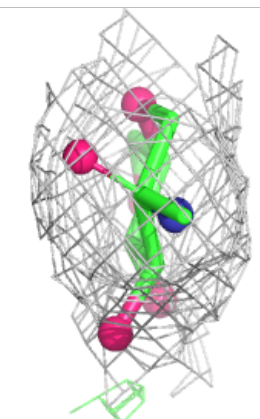
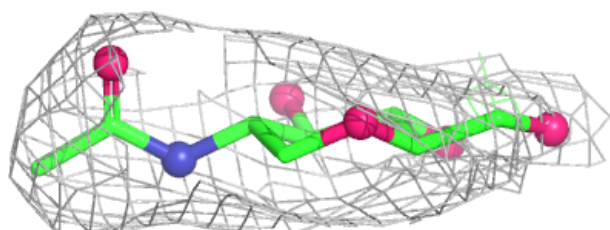
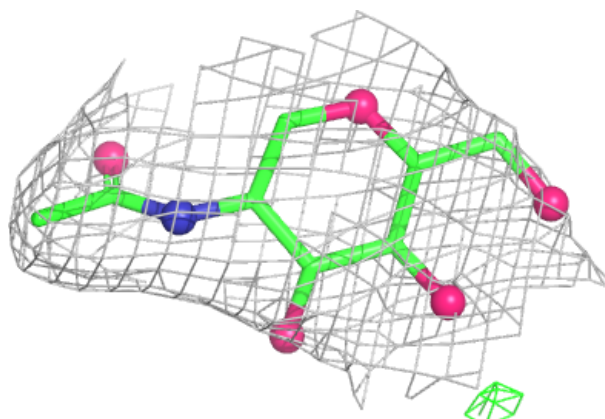


Electron density around NAG E 602:

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

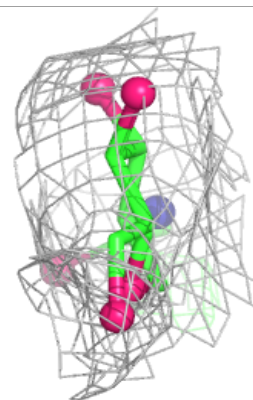
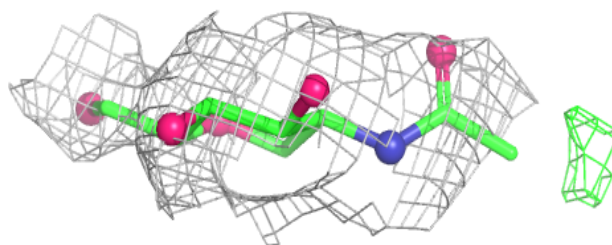
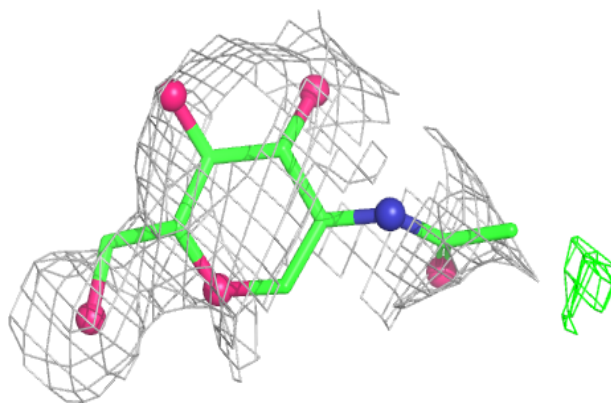
**Electron density around NAG A 601:**

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

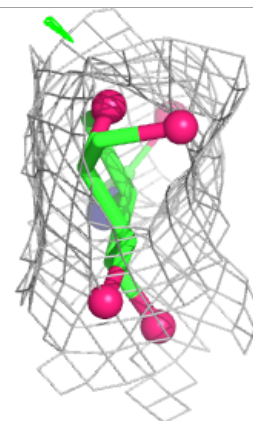
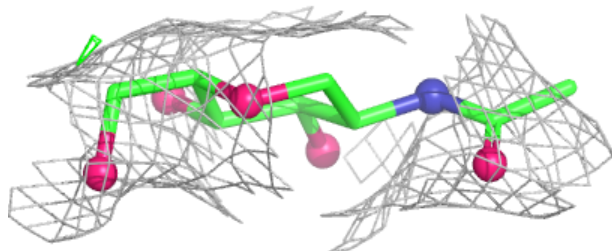
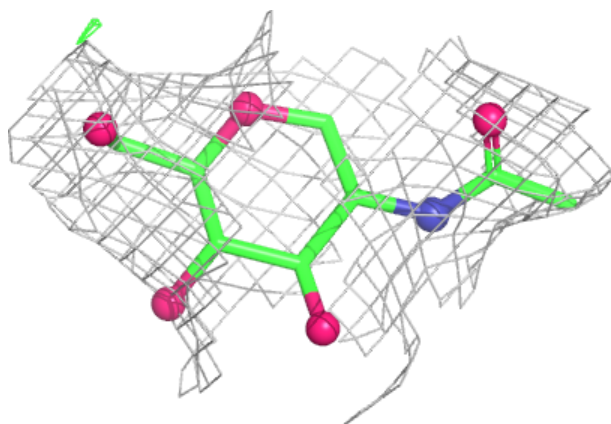


Electron density around NAG A 602:

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

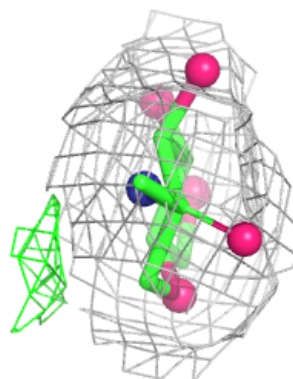
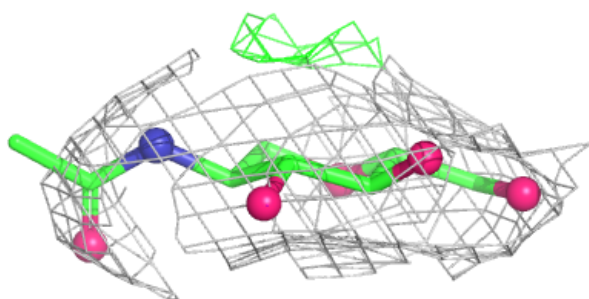
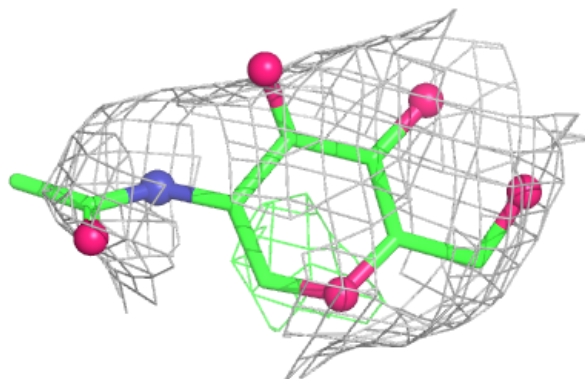
**Electron density around NAG C 602:**

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

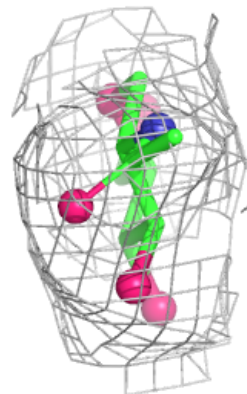
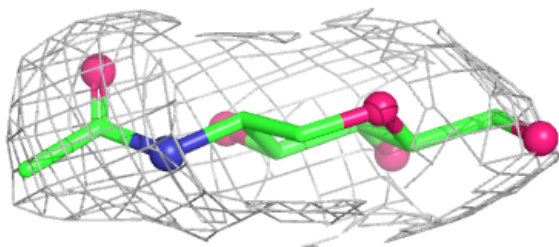
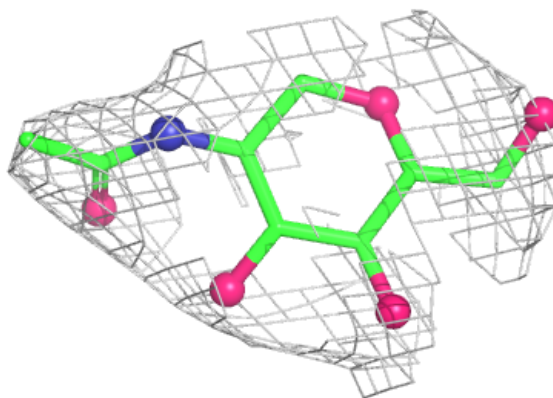


Electron density around NAG E 601:

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

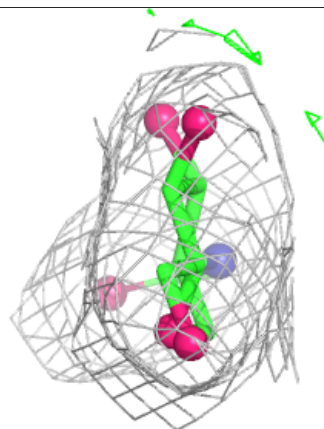
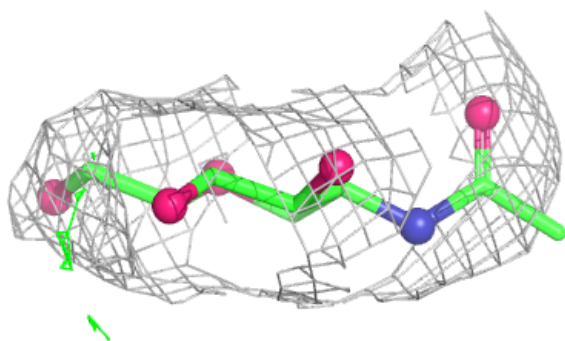
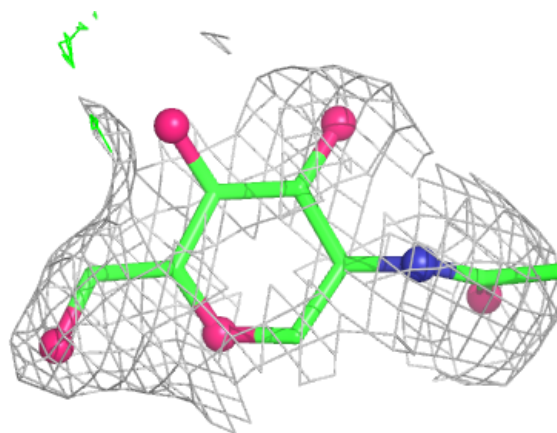
**Electron density around NAG F 501:**

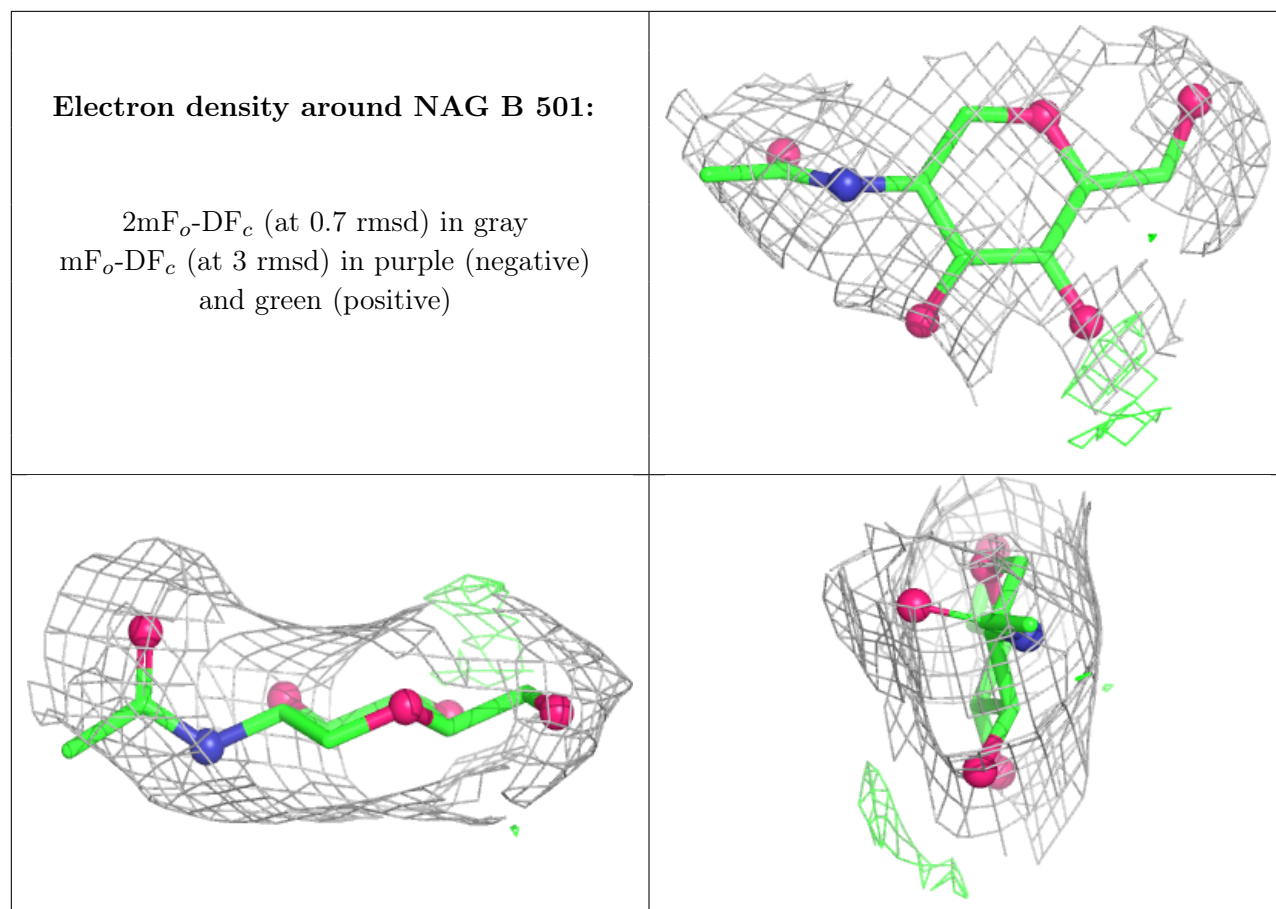
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.