



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2021 – 02:14 PM JST

PDB ID : 7DK2  
Title : Crystal structure of SARS-CoV-2 Spike RBD in complex with MW07 Fab  
Authors : Wang, J.; Jiao, S.; Wang, R.; Zhang, J.; Zhang, M.; Wang, M.; Chen, S.  
Deposited on : 2020-11-22  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

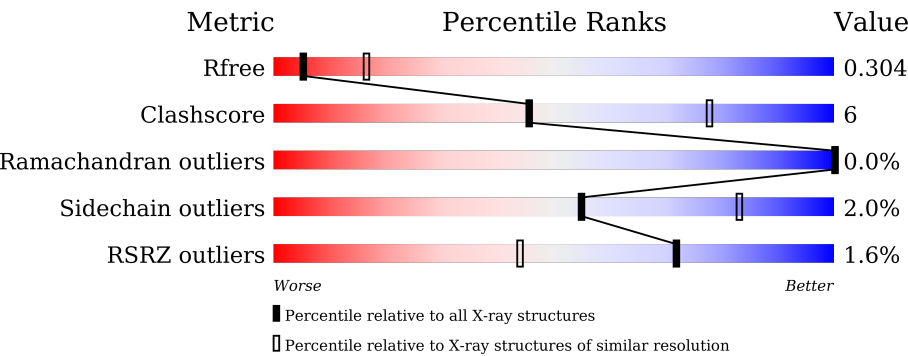
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	223	
1	D	223	
1	G	223	
1	J	223	
2	B	214	
2	E	214	

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Mol	Chain	Length	Quality of chain
2	H	214	 87% 13%
2	K	214	 81% 17%
3	C	223	 3% 70% 15% 14%
3	F	223	 4% 67% 18% 15%
3	I	223	 3% 66% 18% 15%
3	L	223	 3% 71% 14% 14%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19459 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 MW07 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1679	1065	280	327	7			
1	D	222	Total	C	N	O	S	0	0	0
			1673	1062	279	326	6			
1	G	221	Total	C	N	O	S	0	0	0
			1667	1059	278	324	6			
1	J	221	Total	C	N	O	S	0	0	0
			1667	1059	278	324	6			

- Molecule 2 is a protein called MW07 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1636	1021	275	334	6			
2	E	213	Total	C	N	O	S	0	0	0
			1630	1018	274	333	5			
2	H	214	Total	C	N	O	S	0	0	0
			1636	1021	275	334	6			
2	K	214	Total	C	N	O	S	0	0	0
			1636	1021	275	334	6			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	191	Total	C	N	O	S	0	0	0
			1513	970	252	283	8			
3	F	190	Total	C	N	O	S	0	0	0
			1509	968	251	282	8			
3	I	189	Total	C	N	O	S	0	0	0
			1503	965	250	281	7			
3	L	191	Total	C	N	O	S	0	0	0
			1513	970	252	283	8			

- Molecule 4 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
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	12	Total	O	0	0
			12	12		
5	C	2	Total	O	0	0
			2	2		
5	D	18	Total	O	0	0
			18	18		
5	E	14	Total	O	0	0
			14	14		
5	F	6	Total	O	0	0
			6	6		

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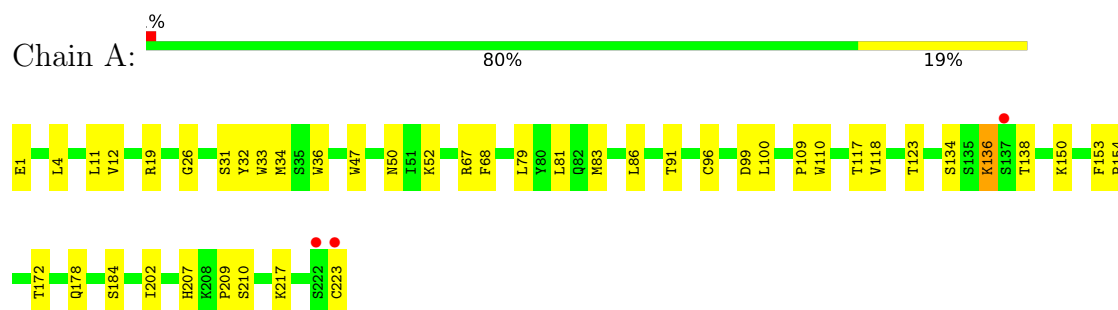
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	21	Total 21	O 21	0	0
5	H	13	Total 13	O 13	0	0
5	I	7	Total 7	O 7	0	0
5	J	19	Total 19	O 19	0	0
5	K	11	Total 11	O 11	0	0
5	L	5	Total 5	O 5	0	0

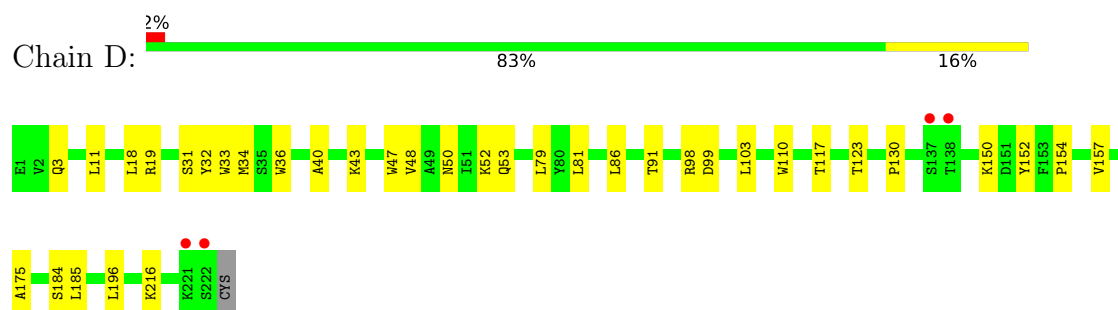
### 3 Residue-property plots [i](#)

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.

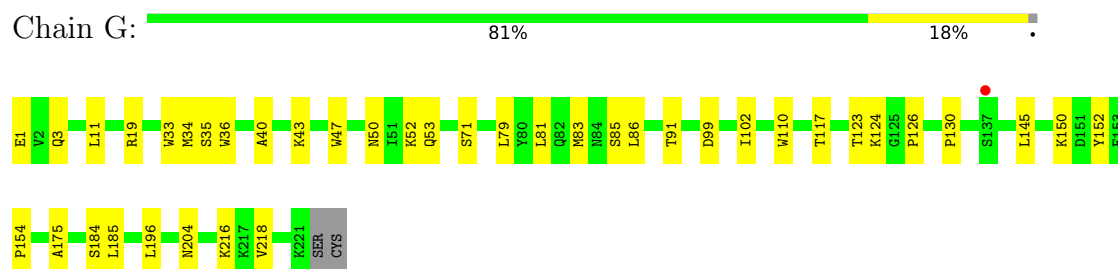
- Molecule 1: MW07 heavy chain



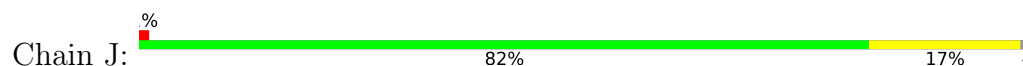
- Molecule 1: MW07 heavy chain

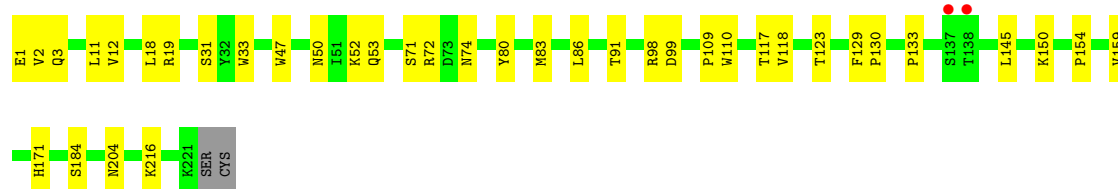


- Molecule 1: MW07 heavy chain



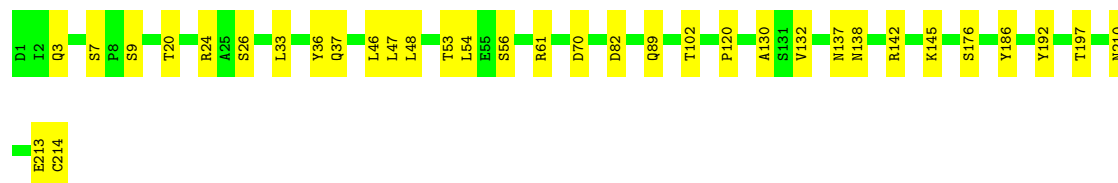
- Molecule 1: MW07 heavy chain





- Molecule 2: MW07 light chain

Chain B:   84% 16%



- Molecule 2: MW07 light chain

Chain E:   86% 13%



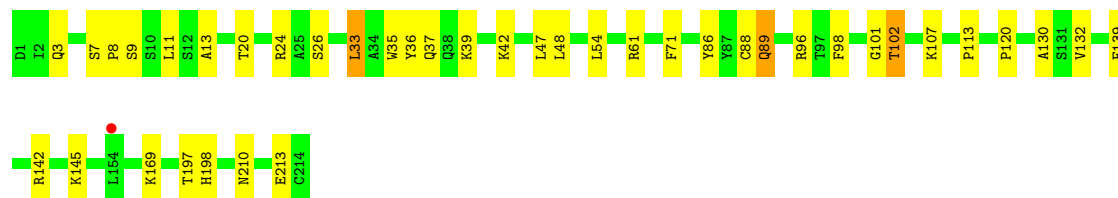
- Molecule 2: MW07 light chain

Chain H:   87% 13%



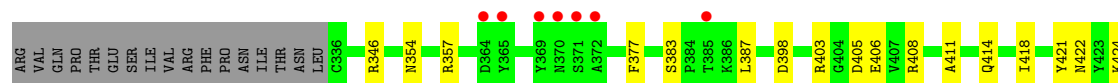
- Molecule 2: MW07 light chain

Chain K:   81% 17%



- Molecule 3: Spike protein S1

Chain C:     3% 70% 15% 14%



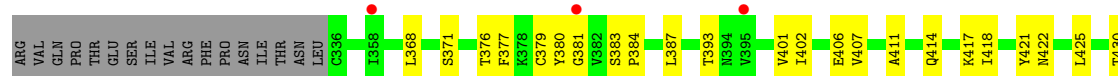




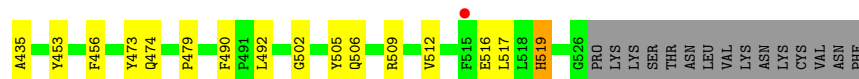
• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.73Å 102.81Å 163.42Å 90.00° 107.16° 90.00°	Depositor
Resolution (Å)	46.47 – 3.00 46.47 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.47-3.00) 97.8 (46.47-3.00)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.258 , 0.304 0.258 , 0.304	Depositor DCC
$R_{free}$ test set	3445 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 18.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	19459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5233e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.30	0/1721	0.54	0/2343
1	D	0.29	0/1715	0.53	0/2335
1	G	0.30	0/1709	0.54	0/2327
1	J	0.29	0/1709	0.53	0/2327
2	B	0.30	0/1670	0.53	0/2266
2	E	0.31	0/1664	0.52	0/2258
2	H	0.30	0/1670	0.52	0/2266
2	K	0.30	0/1670	0.53	0/2266
3	C	0.28	0/1556	0.44	0/2117
3	F	0.28	0/1552	0.45	0/2112
3	I	0.29	0/1546	0.46	0/2104
3	L	0.28	0/1556	0.45	0/2117
All	All	0.29	0/19738	0.51	0/26838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1679	0	1647	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1673	0	1643	22	0
1	G	1667	0	1638	23	0
1	J	1667	0	1638	23	0
2	B	1636	0	1591	20	0
2	E	1630	0	1587	17	0
2	H	1636	0	1592	19	0
2	K	1636	0	1592	24	0
3	C	1513	0	1428	19	0
3	F	1509	0	1425	23	0
3	I	1503	0	1422	24	0
3	L	1513	0	1428	18	0
4	C	14	0	13	0	0
4	F	14	0	13	1	0
4	I	14	0	13	0	0
4	L	14	0	13	0	0
5	A	13	0	0	1	0
5	B	12	0	0	0	0
5	C	2	0	0	0	0
5	D	18	0	0	0	0
5	E	14	0	0	0	0
5	F	6	0	0	0	0
5	G	21	0	0	0	0
5	H	13	0	0	2	0
5	I	7	0	0	0	0
5	J	19	0	0	1	0
5	K	11	0	0	0	0
5	L	5	0	0	1	0
All	All	19459	0	18683	242	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:TRP:HZ2	1:G:50:ASN:HB2	1.34	0.91
1:J:47:TRP:HZ2	1:J:50:ASN:HB2	1.36	0.90
1:D:47:TRP:HZ2	1:D:50:ASN:HB2	1.37	0.89
1:A:47:TRP:HZ2	1:A:50:ASN:HB2	1.41	0.83
1:J:91:THR:HG23	1:J:117:THR:HA	1.62	0.80
1:A:91:THR:HG23	1:A:117:THR:HA	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:LYS:HG3	2:K:169:LYS:HD3	1.70	0.74
2:B:210:ASN:HB2	2:B:213:GLU:HG3	1.71	0.73
1:A:134:SER:HB2	1:A:136:LYS:HD2	1.73	0.71
1:A:136:LYS:HE2	2:B:214:CYS:HB3	1.72	0.70
1:G:91:THR:HG23	1:G:117:THR:HA	1.73	0.69
2:B:36:TYR:HE2	2:B:89:GLN:HG2	1.55	0.69
3:F:519:HIS:HB3	3:I:519:HIS:HB3	1.74	0.69
2:H:61:ARG:NH2	2:H:82:ASP:OD1	2.27	0.68
1:G:123:THR:HG22	1:G:154:PRO:HD3	1.74	0.67
3:C:414:GLN:O	3:C:424:LYS:NZ	2.27	0.67
1:J:47:TRP:CZ2	1:J:50:ASN:HB2	2.25	0.66
1:J:83:MET:HB3	1:J:86:LEU:HD21	1.77	0.66
2:H:36:TYR:HE1	2:H:89:GLN:HG2	1.61	0.66
2:K:36:TYR:HE1	2:K:89:GLN:HG2	1.62	0.65
1:A:150:LYS:HA	1:A:184:SER:HB2	1.78	0.64
2:H:210:ASN:HB2	2:H:213:GLU:HG3	1.79	0.64
1:J:123:THR:HG22	1:J:154:PRO:HD3	1.80	0.63
2:B:48:LEU:HD23	2:B:54:LEU:HA	1.81	0.62
1:D:91:THR:HG23	1:D:117:THR:HA	1.81	0.62
2:E:21:ILE:HD11	2:E:73:LEU:HD23	1.80	0.62
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.82	0.61
2:K:48:LEU:HD23	2:K:54:LEU:HA	1.82	0.61
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.83	0.60
3:F:381:GLY:HA3	3:F:430:THR:HG22	1.82	0.60
1:G:3:GLN:HB3	1:G:110:TRP:CE3	2.36	0.60
2:E:36:TYR:HE2	2:E:89:GLN:HG2	1.67	0.59
1:D:123:THR:HG22	1:D:154:PRO:HD3	1.84	0.59
3:F:393:THR:HA	3:F:522:ALA:HA	1.85	0.59
1:G:130:PRO:HG3	1:G:216:LYS:HD2	1.85	0.59
2:H:147:GLN:NE2	5:H:301:HOH:O	2.35	0.59
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.85	0.59
3:I:381:GLY:HA3	3:I:430:THR:HG22	1.85	0.58
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.85	0.58
2:K:37:GLN:HB2	2:K:47:LEU:HD11	1.84	0.58
3:L:433:VAL:HG22	3:L:512:VAL:HG22	1.85	0.58
1:D:34:MET:HB3	1:D:79:LEU:HD22	1.86	0.57
1:A:47:TRP:CZ2	1:A:50:ASN:HB2	2.30	0.57
2:K:8:PRO:O	2:K:102:THR:OG1	2.15	0.57
2:H:137:ASN:ND2	2:H:138:ASN:OD1	2.38	0.57
1:J:150:LYS:HA	1:J:184:SER:HB2	1.87	0.57
2:K:210:ASN:ND2	2:K:213:GLU:OE2	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:LEU:HA	2:H:58:VAL:HG21	1.88	0.56
3:C:456:PHE:HB3	3:C:473:TYR:CG	2.41	0.55
1:G:47:TRP:CZ2	1:G:50:ASN:HB2	2.26	0.55
3:I:383:SER:HB2	3:I:387:LEU:HD13	1.89	0.55
3:F:380:TYR:O	3:F:430:THR:HA	2.07	0.55
2:B:36:TYR:CE2	2:B:89:GLN:HG2	2.40	0.55
2:H:48:LEU:HD23	2:H:54:LEU:HA	1.89	0.55
1:A:11:LEU:HD23	1:A:117:THR:HB	1.89	0.55
3:I:502:GLY:O	3:I:506:GLN:HG3	2.06	0.54
1:A:202:ILE:HG12	1:A:217:LYS:HG3	1.88	0.54
2:K:8:PRO:HG2	2:K:11:LEU:HB2	1.88	0.54
1:A:12:VAL:HG23	1:A:118:VAL:HG22	1.90	0.54
1:D:130:PRO:HG3	1:D:216:LYS:HD2	1.89	0.54
1:J:52:LYS:HG2	1:J:53:GLN:H	1.73	0.54
3:I:393:THR:HA	3:I:522:ALA:HA	1.90	0.53
3:I:380:TYR:O	3:I:430:THR:HA	2.09	0.53
2:K:3:GLN:HB2	2:K:26:SER:HB3	1.90	0.53
1:G:83:MET:HB3	1:G:86:LEU:HD21	1.89	0.53
2:H:210:ASN:HB2	2:H:213:GLU:CG	2.38	0.53
1:D:3:GLN:HB3	1:D:110:TRP:CE3	2.44	0.53
1:A:123:THR:HG22	1:A:154:PRO:HD3	1.90	0.53
1:G:150:LYS:HA	1:G:184:SER:HB2	1.90	0.53
1:A:207:HIS:CD2	1:A:209:PRO:HD2	2.43	0.52
3:F:418:ILE:HA	3:F:422:ASN:HD22	1.74	0.52
3:L:347:PHE:CE2	3:L:399:SER:HB2	2.44	0.52
2:E:53:THR:HG21	3:F:421:TYR:CZ	2.44	0.52
3:I:401:VAL:HG22	3:I:509:ARG:HG2	1.92	0.51
2:B:186:TYR:HA	2:B:192:TYR:OH	2.11	0.51
3:F:433:VAL:HG22	3:F:512:VAL:HG22	1.92	0.51
2:E:61:ARG:NH2	2:E:82:ASP:OD1	2.43	0.51
2:B:145:LYS:HB3	2:B:197:THR:HB	1.92	0.50
3:C:383:SER:HB2	3:C:387:LEU:HD22	1.92	0.50
1:J:130:PRO:HG3	1:J:216:LYS:HD2	1.93	0.50
2:B:53:THR:HG21	3:C:421:TYR:CZ	2.46	0.50
3:L:412:PRO:HG3	3:L:429:PHE:HB3	1.94	0.50
2:B:24:ARG:NH1	2:K:20:THR:O	2.45	0.50
1:J:11:LEU:HD23	1:J:117:THR:HB	1.93	0.49
3:I:376:THR:HB	3:I:435:ALA:HB3	1.94	0.49
3:L:383:SER:HB2	3:L:387:LEU:HD22	1.95	0.49
3:I:379:CYS:SG	3:I:384:PRO:HB3	2.53	0.49
3:I:433:VAL:HG22	3:I:512:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:113:PRO:HB3	2:K:139:PHE:CD2	2.47	0.49
2:H:96:ARG:NH2	3:I:487:ASN:OD1	2.45	0.49
3:L:502:GLY:O	3:L:506:GLN:HG3	2.13	0.49
3:F:502:GLY:O	3:F:506:GLN:HG3	2.12	0.49
1:J:2:VAL:HG21	1:J:98:ARG:NH2	2.27	0.49
2:E:47:LEU:HA	2:E:58:VAL:HG21	1.95	0.49
3:F:376:THR:HB	3:F:435:ALA:HB3	1.94	0.49
1:D:47:TRP:CZ2	1:D:50:ASN:HB2	2.29	0.49
1:J:33:TRP:HB2	1:J:99:ASP:HB3	1.95	0.48
3:L:411:ALA:HB3	3:L:414:GLN:HG3	1.94	0.48
1:D:33:TRP:HB2	1:D:99:ASP:HB3	1.95	0.48
3:L:401:VAL:HG22	3:L:509:ARG:HG2	1.94	0.48
3:C:439:ASN:HA	3:C:507:PRO:HG2	1.95	0.48
3:L:490:PHE:HE2	3:L:492:LEU:HB2	1.77	0.48
3:C:466:ARG:HH12	3:C:468:ILE:HD11	1.79	0.48
3:I:417:LYS:HD3	3:I:453:TYR:CD2	2.48	0.48
3:L:417:LYS:HD3	3:L:453:TYR:CD2	2.49	0.48
1:A:150:LYS:NZ	1:A:178:GLN:OE1	2.43	0.48
2:E:159:SER:HA	2:E:178:THR:O	2.14	0.48
1:J:3:GLN:HB3	1:J:110:TRP:CE3	2.49	0.48
3:C:411:ALA:HB3	3:C:414:GLN:HG3	1.95	0.48
2:K:120:PRO:HD3	2:K:132:VAL:HG22	1.95	0.48
1:D:150:LYS:HA	1:D:184:SER:HB2	1.95	0.47
1:A:33:TRP:HB2	1:A:99:ASP:HB3	1.95	0.47
3:C:466:ARG:NH1	3:C:468:ILE:HD11	2.29	0.47
1:D:40:ALA:HB3	1:D:43:LYS:HB2	1.96	0.47
1:G:47:TRP:CD2	2:H:96:ARG:HB2	2.48	0.47
2:K:39:LYS:HB2	2:K:42:LYS:HG2	1.96	0.47
2:B:9:SER:O	2:B:102:THR:HA	2.14	0.47
3:I:425:LEU:HD21	3:I:512:VAL:HG11	1.97	0.47
3:I:456:PHE:HB3	3:I:473:TYR:CD1	2.50	0.47
1:J:1:GLU:HG2	3:L:505:TYR:CG	2.50	0.47
1:J:12:VAL:HG23	1:J:118:VAL:HG22	1.96	0.47
3:L:392:PHE:HD1	3:L:517:LEU:HB2	1.80	0.47
2:K:120:PRO:HG2	2:K:130:ALA:HB1	1.97	0.47
3:F:383:SER:HB2	3:F:387:LEU:HD22	1.97	0.46
1:D:175:ALA:HA	1:D:185:LEU:HB3	1.97	0.46
1:D:36:TRP:O	1:D:48:VAL:HG22	2.15	0.46
2:B:120:PRO:HG2	2:B:130:ALA:HB1	1.98	0.46
1:D:52:LYS:HG2	1:D:53:GLN:H	1.80	0.46
3:F:498:GLN:HB2	3:F:501:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:365:TYR:CD2	3:F:388:ASN:HB3	2.49	0.46
1:A:32:TYR:HD1	1:A:100:LEU:HG	1.81	0.46
2:B:61:ARG:NH2	2:B:82:ASP:OD1	2.46	0.46
3:L:456:PHE:HB3	3:L:473:TYR:CG	2.51	0.46
1:A:1:GLU:O	1:A:26:GLY:HA3	2.16	0.46
2:H:1:ASP:HB2	2:H:95:PRO:HD2	1.98	0.46
3:I:472:ILE:HD12	3:I:484:GLU:HG2	1.97	0.46
2:K:35:TRP:CZ3	2:K:88:CYS:HB3	2.51	0.46
3:L:456:PHE:HB3	3:L:473:TYR:CD1	2.51	0.45
1:J:133:PRO:HD3	1:J:145:LEU:HB3	1.98	0.45
2:H:1:ASP:HB3	5:H:307:HOH:O	2.16	0.45
1:G:33:TRP:HB2	1:G:99:ASP:HB3	1.98	0.45
2:B:3:GLN:HB2	2:B:26:SER:HB3	1.97	0.45
3:F:439:ASN:OD1	3:F:443:SER:OG	2.33	0.45
3:F:456:PHE:HB3	3:F:473:TYR:CD1	2.51	0.45
1:G:126:PRO:HB3	1:G:152:TYR:HB3	1.99	0.45
3:I:411:ALA:HB3	3:I:414:GLN:HG3	1.98	0.45
2:K:96:ARG:NH1	5:L:701:HOH:O	2.41	0.45
3:L:376:THR:HB	3:L:435:ALA:HB3	1.98	0.45
1:G:36:TRP:NE1	1:G:81:LEU:HB2	2.32	0.45
1:D:18:LEU:HD12	1:D:18:LEU:HA	1.88	0.45
2:H:89:GLN:HB3	2:H:98:PHE:CE1	2.52	0.45
3:C:456:PHE:HB3	3:C:473:TYR:CD1	2.52	0.44
3:C:403:ARG:HE	3:C:405:ASP:HB2	1.82	0.44
3:F:449:TYR:HB3	3:F:494:SER:HB3	1.99	0.44
1:G:34:MET:HB3	1:G:79:LEU:HD22	1.99	0.44
3:C:490:PHE:CD1	3:C:491:PRO:HD2	2.52	0.44
1:D:11:LEU:HD23	1:D:117:THR:HB	1.99	0.44
3:C:354:ASN:O	3:C:398:ASP:HA	2.18	0.44
1:D:86:LEU:HA	1:D:86:LEU:HD23	1.79	0.44
3:I:418:ILE:HA	3:I:422:ASN:HD22	1.82	0.44
1:A:67:ARG:NH1	1:A:68:PHE:HE1	2.15	0.44
1:G:11:LEU:HD23	1:G:117:THR:HB	1.98	0.44
1:G:86:LEU:HD23	1:G:86:LEU:HA	1.85	0.44
2:E:145:LYS:HZ2	2:E:147:GLN:HG3	1.83	0.43
3:C:520:ALA:O	3:L:519:HIS:NE2	2.51	0.43
3:F:379:CYS:HB2	3:F:384:PRO:HB3	1.98	0.43
1:A:223:CYS:HB3	2:B:214:CYS:HA	2.00	0.43
2:E:210:ASN:ND2	2:E:213:GLU:OE1	2.49	0.43
1:A:34:MET:HB3	1:A:79:LEU:HD22	2.00	0.43
1:G:175:ALA:HA	1:G:185:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HB3	1:A:96:CYS:SG	2.59	0.43
2:K:13:ALA:O	2:K:107:LYS:N	2.46	0.43
2:E:48:LEU:HD23	2:E:54:LEU:HA	1.99	0.43
3:I:402:ILE:HD11	3:I:407:VAL:HA	2.01	0.43
3:I:406:GLU:HB3	3:I:418:ILE:HG13	2.01	0.43
3:F:368:LEU:O	3:F:371:SER:HB3	2.19	0.43
2:H:20:THR:HA	2:H:73:LEU:O	2.19	0.43
1:J:71:SER:OG	1:J:80:TYR:HB2	2.19	0.43
1:J:86:LEU:HD23	1:J:86:LEU:HA	1.73	0.43
2:B:36:TYR:CD1	2:B:46:LEU:HA	2.54	0.42
1:G:52:LYS:HG2	1:G:53:GLN:H	1.84	0.42
1:A:36:TRP:NE1	1:A:81:LEU:HB2	2.34	0.42
2:E:124:GLN:HG2	2:E:129:THR:O	2.20	0.42
2:K:39:LYS:HG3	2:K:42:LYS:HE3	2.00	0.42
2:K:145:LYS:HB3	2:K:197:THR:HB	2.00	0.42
3:F:490:PHE:CE2	3:F:492:LEU:HB2	2.54	0.42
1:G:35:SER:OG	1:G:99:ASP:OD2	2.37	0.42
1:A:123:THR:HA	1:A:153:PHE:HD2	1.84	0.42
2:B:120:PRO:HD3	2:B:132:VAL:HG22	2.00	0.42
2:E:8:PRO:O	2:E:102:THR:OG1	2.26	0.42
3:F:417:LYS:HE2	3:F:417:LYS:HB3	1.79	0.42
2:K:33:LEU:HD22	2:K:71:PHE:CG	2.55	0.42
3:C:461:LEU:HD22	3:C:465:GLU:HB3	2.01	0.42
3:C:462:LYS:HD2	3:C:462:LYS:H	1.85	0.42
1:J:72:ARG:HD3	1:J:74:ASN:OD1	2.20	0.42
2:E:7:SER:HA	2:E:8:PRO:HA	1.78	0.42
2:H:53:THR:HG21	3:I:421:TYR:CZ	2.55	0.42
1:A:33:TRP:CZ2	1:A:52:LYS:HG3	2.55	0.42
3:C:435:ALA:HA	3:C:509:ARG:O	2.20	0.42
1:G:196:LEU:HD23	1:G:196:LEU:HA	1.89	0.42
1:J:18:LEU:HD12	1:J:18:LEU:HA	1.91	0.42
1:J:109:PRO:HD2	1:J:110:TRP:CD1	2.54	0.42
1:A:207:HIS:ND1	1:A:210:SER:OG	2.29	0.42
2:B:56:SER:HB3	3:C:406:GLU:HG2	2.01	0.42
1:D:152:TYR:CE2	1:D:157:VAL:HG13	2.54	0.42
1:D:196:LEU:HD23	1:D:196:LEU:HA	1.90	0.42
2:K:36:TYR:CE1	2:K:89:GLN:HG2	2.48	0.42
1:A:172:THR:OG1	5:A:301:HOH:O	2.21	0.41
1:D:36:TRP:NE1	1:D:81:LEU:HB2	2.35	0.41
1:D:103:LEU:HD12	2:E:98:PHE:HZ	1.85	0.41
2:E:7:SER:HB3	2:H:24:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:GLU:HA	2:H:176:SER:O	2.20	0.41
3:L:393:THR:N	3:L:516:GLU:O	2.53	0.41
1:G:40:ALA:HB3	1:G:43:LYS:HB2	2.01	0.41
2:K:86:TYR:O	2:K:101:GLY:HA2	2.20	0.41
3:F:484:GLU:CD	3:F:490:PHE:HB2	2.41	0.41
1:G:102:ILE:H	1:G:102:ILE:HG13	1.68	0.41
3:L:418:ILE:HA	3:L:422:ASN:HD22	1.85	0.41
3:F:368:LEU:HD21	4:F:601:NAG:H83	2.02	0.41
1:G:145:LEU:HB2	1:G:218:VAL:HG11	2.03	0.41
1:D:32:TYR:CZ	1:D:98:ARG:HD2	2.56	0.41
3:F:401:VAL:HG22	3:F:509:ARG:HG2	2.02	0.41
3:I:474:GLN:OE1	3:I:479:PRO:HA	2.21	0.41
1:J:129:PHE:HA	1:J:130:PRO:HD3	1.95	0.41
2:K:113:PRO:HD3	2:K:198:HIS:ND1	2.35	0.41
1:D:36:TRP:CD1	1:D:81:LEU:HB2	2.56	0.41
2:E:20:THR:HA	2:E:73:LEU:O	2.21	0.41
3:F:406:GLU:HB3	3:F:418:ILE:HG13	2.03	0.41
2:H:56:SER:HB3	3:I:406:GLU:HG2	2.03	0.41
2:K:89:GLN:HB3	2:K:98:PHE:CD1	2.55	0.41
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.75	0.41
2:B:137:ASN:ND2	2:B:138:ASN:OD1	2.53	0.41
1:G:71:SER:O	1:G:79:LEU:HD12	2.21	0.41
3:I:368:LEU:O	3:I:371:SER:HB3	2.21	0.40
1:J:171:HIS:HA	5:J:315:HOH:O	2.20	0.40
2:B:20:THR:O	2:K:24:ARG:NH1	2.54	0.40
3:C:502:GLY:O	3:C:506:GLN:HG3	2.20	0.40
3:L:474:GLN:OE1	3:L:479:PRO:HA	2.21	0.40
3:C:418:ILE:HA	3:C:422:ASN:HD22	1.87	0.40
3:I:449:TYR:HB3	3:I:494:SER:OG	2.21	0.40
1:J:159:VAL:HA	1:J:204:ASN:O	2.20	0.40
1:A:109:PRO:HD2	1:A:110:TRP:CD1	2.56	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	221/223 (99%)	209 (95%)	12 (5%)	0	100	100
1	D	220/223 (99%)	208 (94%)	12 (6%)	0	100	100
1	G	219/223 (98%)	207 (94%)	12 (6%)	0	100	100
1	J	219/223 (98%)	207 (94%)	12 (6%)	0	100	100
2	B	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
2	E	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
2	H	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
2	K	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	29	68
3	C	189/223 (85%)	167 (88%)	22 (12%)	0	100	100
3	F	188/223 (84%)	168 (89%)	20 (11%)	0	100	100
3	I	187/223 (84%)	168 (90%)	19 (10%)	0	100	100
3	L	189/223 (85%)	169 (89%)	20 (11%)	0	100	100
All	All	2479/2640 (94%)	2317 (94%)	161 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	9	SER

### 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	187/187 (100%)	183 (98%)	4 (2%)	53	82
1	D	186/187 (100%)	184 (99%)	2 (1%)	73	90
1	G	185/187 (99%)	180 (97%)	5 (3%)	44	77
1	J	185/187 (99%)	183 (99%)	2 (1%)	73	90
2	B	187/187 (100%)	182 (97%)	5 (3%)	44	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	186/187 (100%)	182 (98%)	4 (2%)	52	81
2	H	187/187 (100%)	183 (98%)	4 (2%)	53	82
2	K	187/187 (100%)	181 (97%)	6 (3%)	39	74
3	C	164/196 (84%)	159 (97%)	5 (3%)	41	75
3	F	164/196 (84%)	162 (99%)	2 (1%)	71	90
3	I	163/196 (83%)	162 (99%)	1 (1%)	86	95
3	L	164/196 (84%)	162 (99%)	2 (1%)	71	90
All	All	2145/2280 (94%)	2103 (98%)	42 (2%)	55	83

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	31	SER
1	A	136	LYS
1	A	138	THR
2	B	7	SER
2	B	33	LEU
2	B	70	ASP
2	B	142	ARG
2	B	176	SER
3	C	346	ARG
3	C	357	ARG
3	C	377	PHE
3	C	408	ARG
3	C	494	SER
1	D	19	ARG
1	D	31	SER
2	E	7	SER
2	E	33	LEU
2	E	70	ASP
2	E	176	SER
3	F	357	ARG
3	F	377	PHE
1	G	1	GLU
1	G	19	ARG
1	G	85	SER
1	G	124	LYS
1	G	204	ASN
2	H	7	SER

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Mol	Chain	Res	Type
2	H	33	LEU
2	H	53	THR
2	H	162	SER
3	I	377	PHE
1	J	19	ARG
1	J	31	SER
2	K	7	SER
2	K	33	LEU
2	K	61	ARG
2	K	89	GLN
2	K	102	THR
2	K	142	ARG
3	L	377	PHE
3	L	519	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	79	GLN
2	B	89	GLN
3	C	501	ASN
3	C	519	HIS
2	E	79	GLN
2	E	147	GLN
2	E	155	GLN
3	F	501	ASN
1	G	171	HIS
2	H	137	ASN
2	H	147	GLN
3	I	501	ASN
2	K	79	GLN
3	L	501	ASN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	L	601	3	14,14,15	0.40	0	12,19,21	0.35	0
4	NAG	C	601	3	14,14,15	0.42	0	17,19,21	0.63	0
4	NAG	I	601	3	14,14,15	0.40	0	17,19,21	0.51	0
4	NAG	F	601	3	14,14,15	0.35	0	17,19,21	0.50	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
4	NAG	C	601	3	-	3/6/23/26	0/1/1/1
4	NAG	I	601	3	-	0/6/23/26	0/1/1/1
4	NAG	F	601	3	-	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 (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	601	NAG	O5-C5-C6-O6
4	F	601	NAG	C4-C5-C6-O6
4	C	601	NAG	O5-C5-C6-O6

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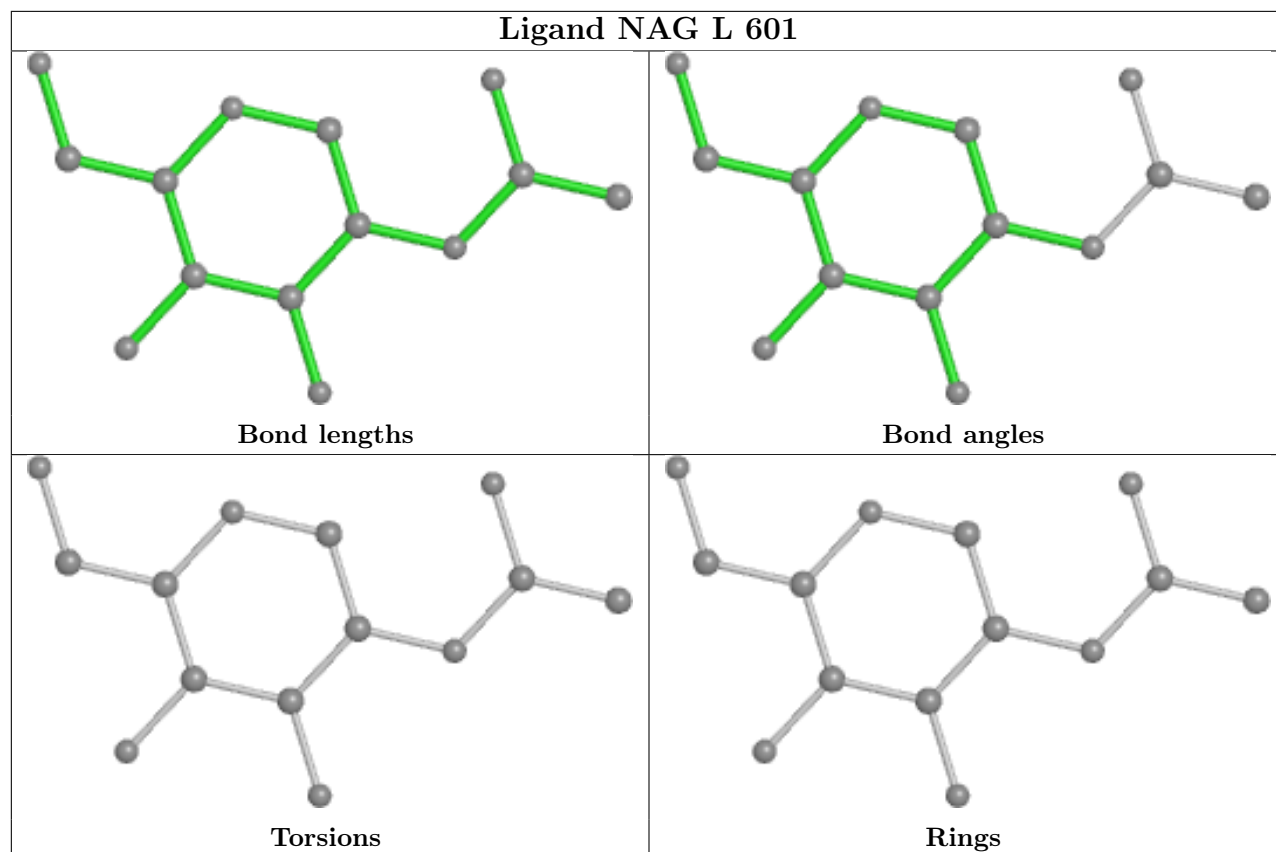
Mol	Chain	Res	Type	Atoms
4	C	601	NAG	C4-C5-C6-O6
4	C	601	NAG	C3-C2-N2-C7

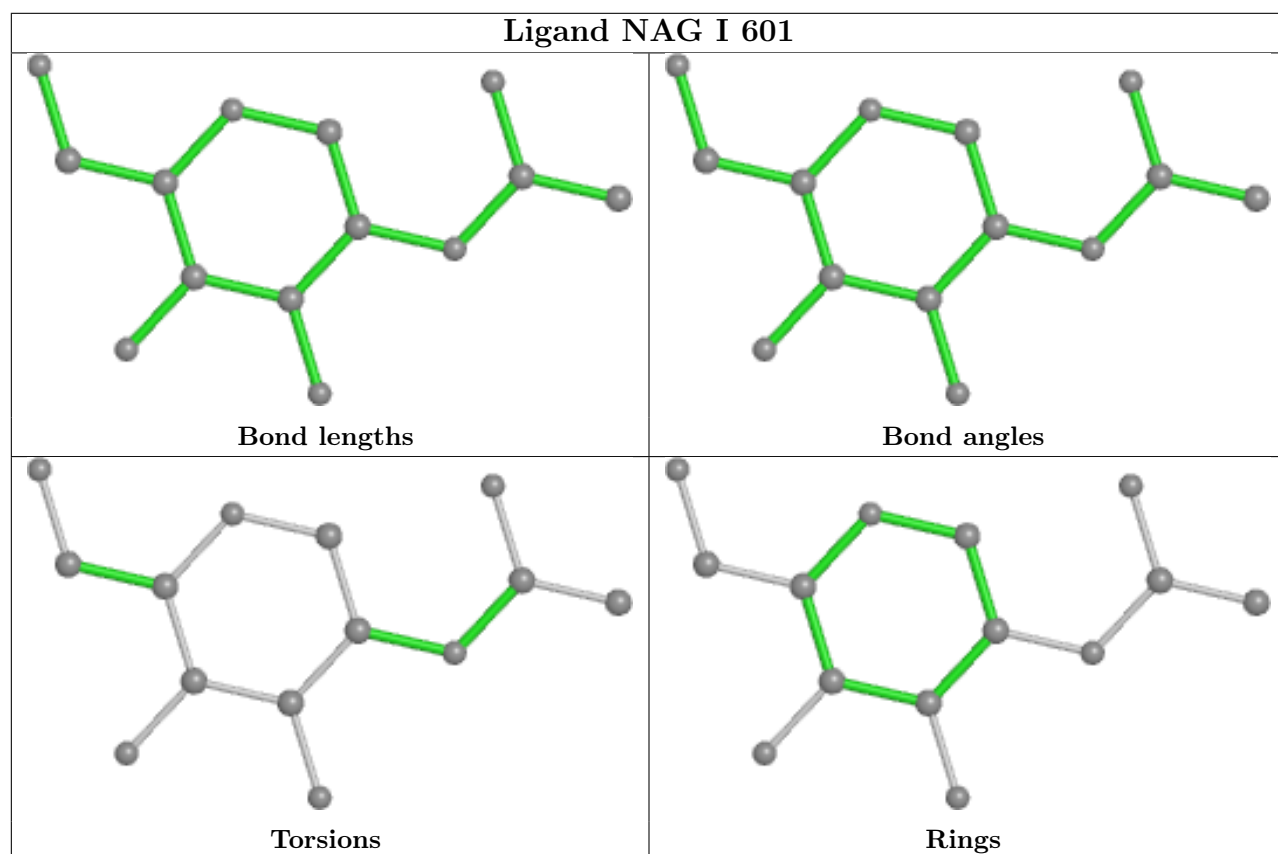
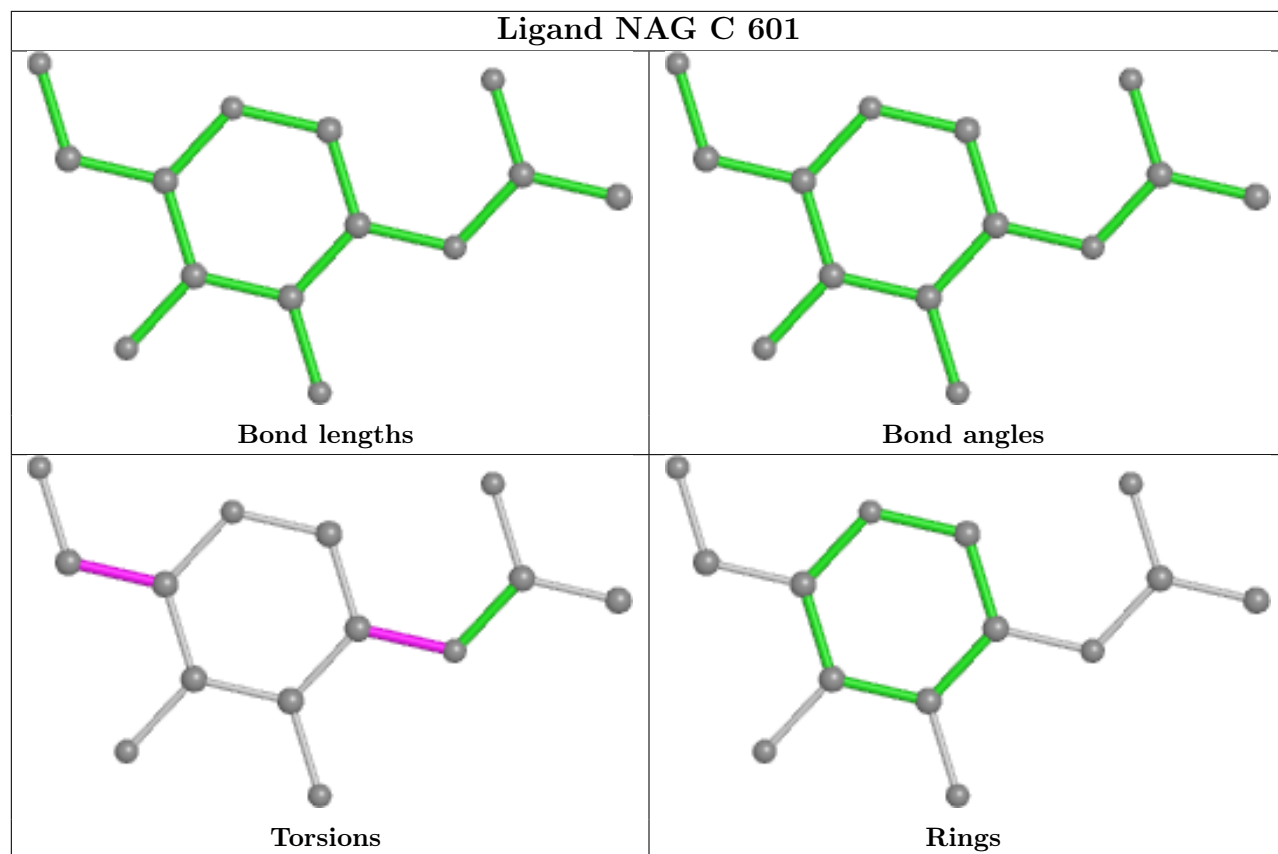
There are no ring outliers.

1 monomer is involved in 1 short contact:

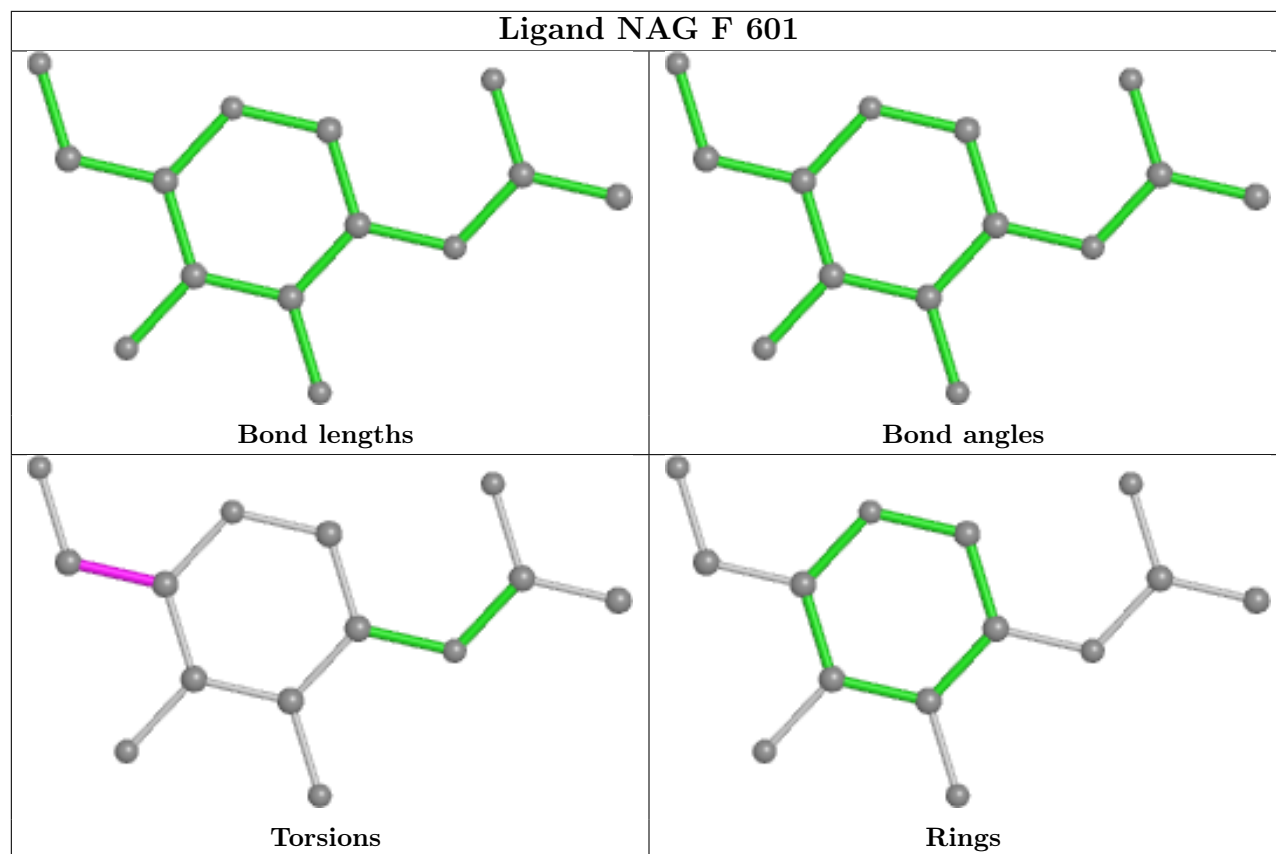
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	601	NAG	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	223/223 (100%)	-0.51	3 (1%) 77 51	19, 32, 72, 123	0
1	D	222/223 (99%)	-0.51	4 (1%) 68 40	19, 33, 73, 108	0
1	G	221/223 (99%)	-0.57	1 (0%) 91 75	19, 32, 66, 104	0
1	J	221/223 (99%)	-0.55	2 (0%) 84 63	18, 34, 70, 100	0
2	B	214/214 (100%)	-0.52	0 100 100	25, 40, 83, 103	0
2	E	213/214 (99%)	-0.54	0 100 100	25, 40, 78, 95	0
2	H	214/214 (100%)	-0.52	0 100 100	25, 39, 72, 94	0
2	K	214/214 (100%)	-0.47	1 (0%) 91 75	22, 39, 86, 105	0
3	C	191/223 (85%)	-0.21	7 (3%) 41 17	27, 54, 117, 140	0
3	F	190/223 (85%)	-0.10	8 (4%) 36 14	28, 58, 119, 133	0
3	I	189/223 (84%)	-0.05	6 (3%) 47 20	30, 60, 127, 133	0
3	L	191/223 (85%)	-0.18	7 (3%) 41 17	31, 55, 123, 128	0
All	All	2503/2640 (94%)	-0.41	39 (1%) 72 44	18, 42, 108, 140	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	137	SER	4.3
3	F	513	LEU	4.0
1	D	222	SER	4.0
3	I	515	PHE	3.8
3	L	365	TYR	3.6
3	C	370	ASN	3.5
3	I	358	ILE	3.3
3	I	513	LEU	3.2
3	I	381	GLY	3.2
1	A	137	SER	3.1
1	J	138	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	372	ALA	2.9
3	C	364	ASP	2.9
1	J	137	SER	2.9
3	F	514	SER	2.8
1	D	138	THR	2.8
3	F	372	ALA	2.7
3	F	515	PHE	2.6
1	A	223	CYS	2.5
3	C	371	SER	2.5
3	C	365	TYR	2.5
3	I	514	SER	2.5
3	L	369	TYR	2.5
3	L	372	ALA	2.4
1	G	137	SER	2.4
3	C	385	THR	2.4
1	A	222	SER	2.4
3	F	432	CYS	2.3
3	F	370	ASN	2.2
3	L	515	PHE	2.2
3	C	369	TYR	2.2
1	D	221	LYS	2.2
3	L	382	VAL	2.2
3	L	340	GLU	2.2
3	L	338	PHE	2.2
2	K	154	LEU	2.1
3	I	395	VAL	2.1
3	F	385	THR	2.1
3	F	381	GLY	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.

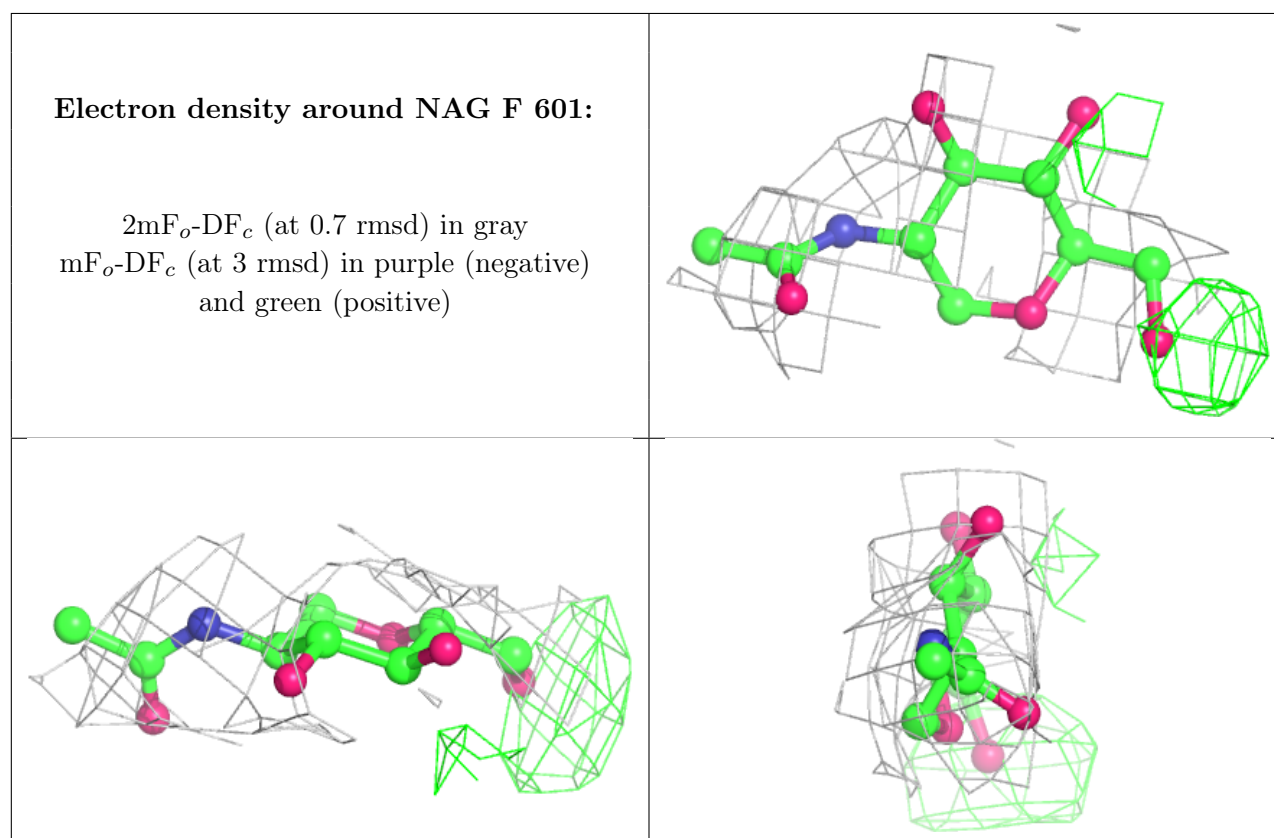
## 6.4 Ligands [i](#)

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<sup>th</sup> 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.

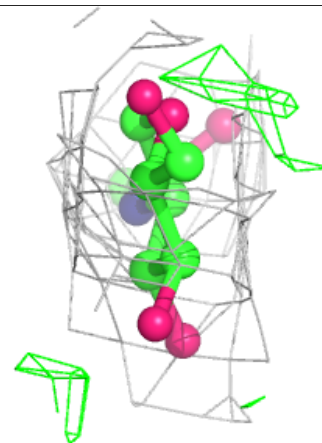
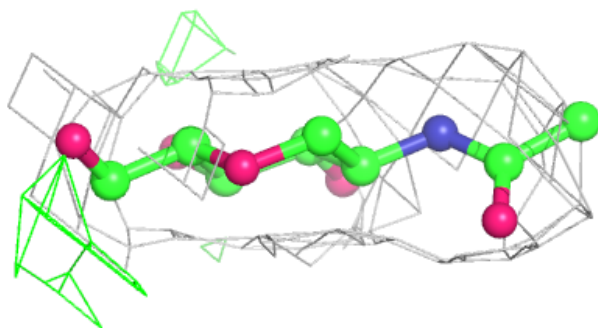
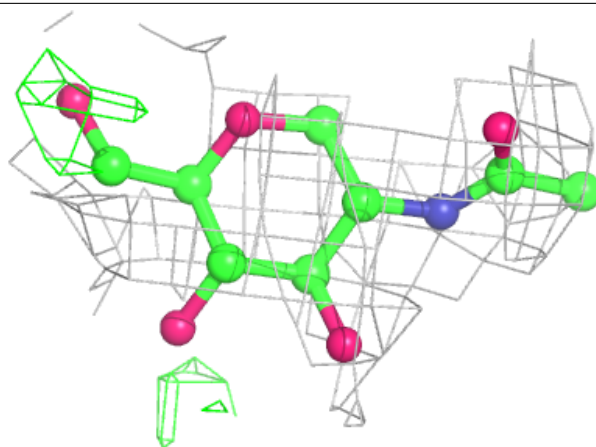
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	F	601	14/15	0.63	0.20	70,89,96,99	0
4	NAG	I	601	14/15	0.66	0.17	69,94,98,99	0
4	NAG	L	601	14/15	0.72	0.18	74,83,94,97	0
4	NAG	C	601	14/15	0.78	0.15	75,91,96,96	0

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.

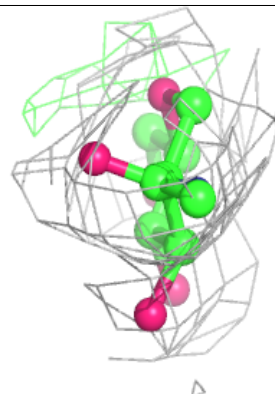
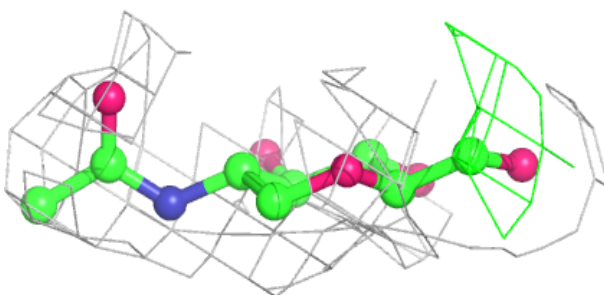
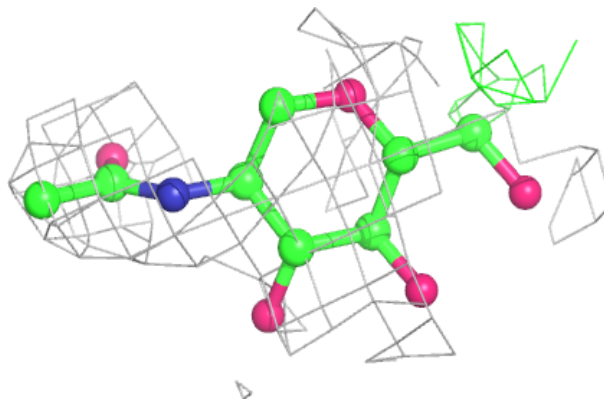


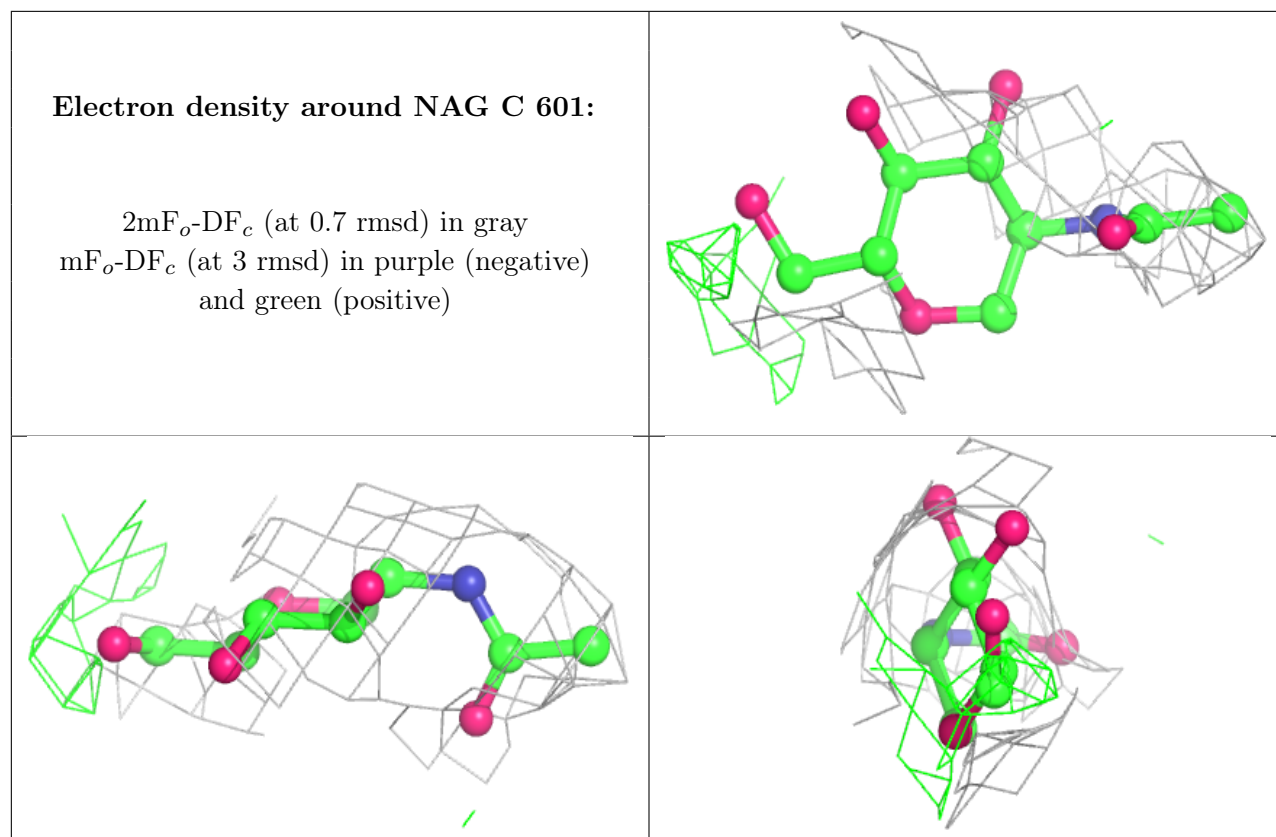
**Electron density around NAG I 601:**

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

**Electron density around NAG L 601:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.