Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 09:38 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)

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

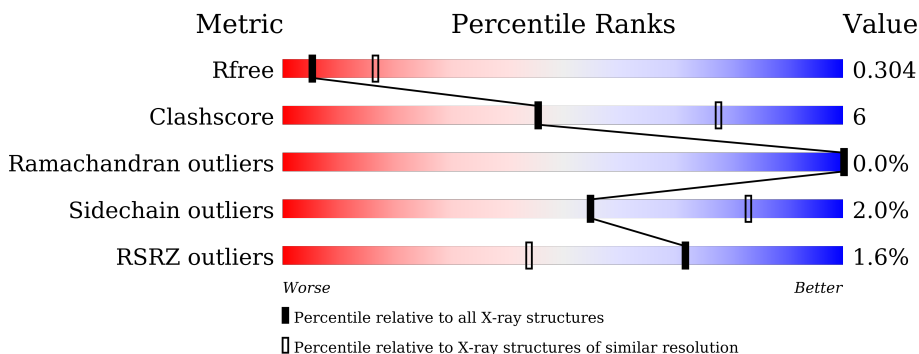|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 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	Percentile Ranks	Value
Rfree		0.304
Clashscore		6
Ramachandran outliers		0.0%
Sidechain outliers		2.0%
RSRZ outliers		1.6%

Worse — *Better*

▌Percentile relative to all X-ray structures

◻Percentile relative to X-ray structures of similar resolution

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 >=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	223	.% 80% 19%
1	D	223	2% 83% 16%
1	G	223	81% 18% •
1	J	223	.% 82% 17% •
2	B	214	84% 16%
2	E	214	86% 13%

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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 1679	C 1065	N 280	O 327	S 7	0	0	0
1	D	222	Total 1673	C 1062	N 279	O 326	S 6	0	0	0
1	G	221	Total 1667	C 1059	N 278	O 324	S 6	0	0	0
1	J	221	Total 1667	C 1059	N 278	O 324	S 6	0	0	0

- Molecule 2 is a protein called MW07 light chain.

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

- Molecule 3 is a protein called Spike protein S1.

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

- 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).
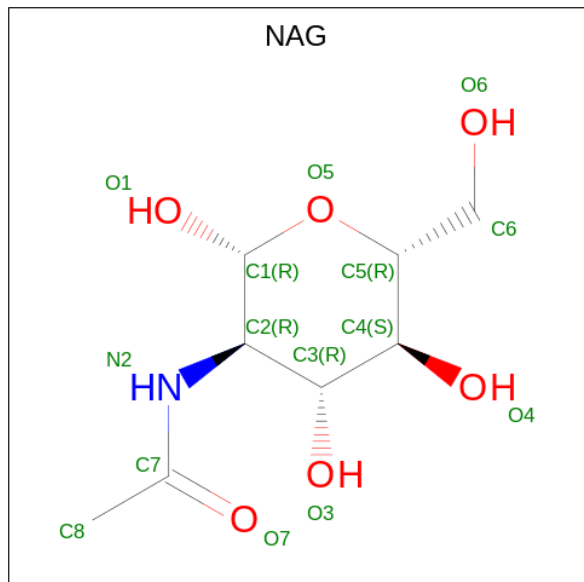
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

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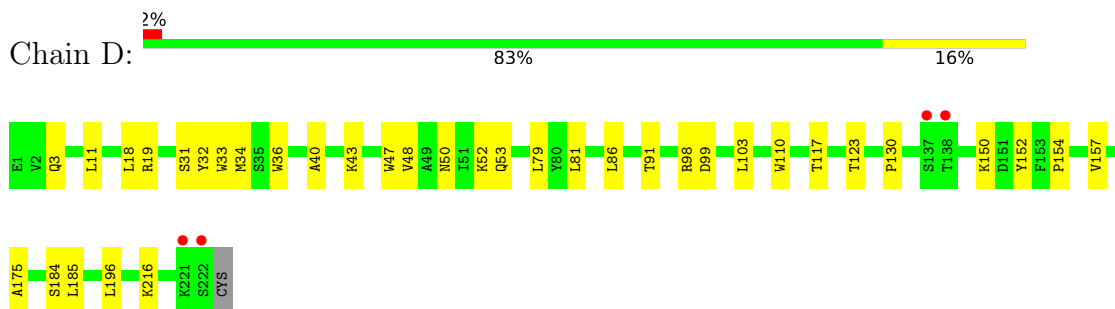| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	21	Total 21	O 21	0	0
5	H	13	Total 13	O 13	0	0
5	I	7	Total 7	O 7	0	0
5	J	19	Total 19	O 19	0	0
5	K	11	Total 11	O 11	0	0
5	L	5	Total 5	O 5	0	0

3 Residue-property plots ⓘ

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.
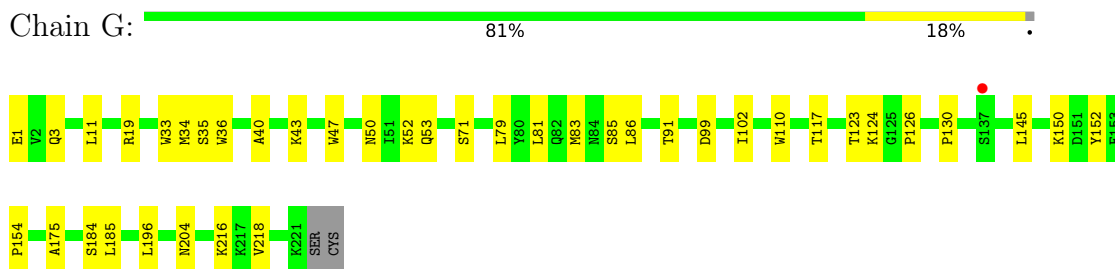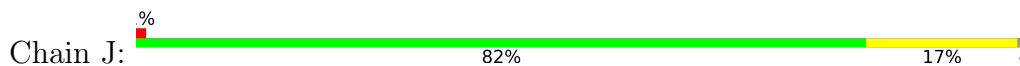
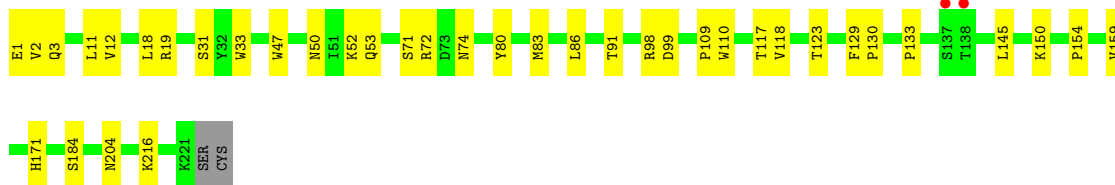• Molecule 1: MW07 heavy chain

Chain A:

• Molecule 1: MW07 heavy chain

Chain D:

• Molecule 1: MW07 heavy chain

Chain G:

• Molecule 1: MW07 heavy chain

Chain J:

E1 V2 Q3 L11 V12 L18 R19 S31 Y32 W33 W47 N50 I51 K52 Q53 S71 K72 D73 N74 Y80 M83 L86 T91 R98 D99 P109 W110 T117 V118 T123 F129 P130 P133 S137 T138 L145 K150 P154 V159

H171 S184 N204 K216 K221 SER CYS

• Molecule 2: MW07 light chain

Chain B:
84%   16%

D1 I2 Q3 S7 P8 S9 T20 R24 A25 S26 L33 Y36 Q37 L46 L47 L48 T53 L54 E55 S56 R61 D70 D82 Q89 T102 P120 A130 S131 V132 N137 N138 R142 K145 S176 Y186 Y192 T197 N210

E213 C214

• Molecule 2: MW07 light chain

Chain E:
86%   13%

D1 S7 P8 T20 I21 L33 Y36 Q37 L47 L48 T53 L54 V58 R61 D70 L73 D82 Q89 F98 T102 Q124 T129 K145 V146 Q147 S159 K169 S176 S177 T178 N210 E213 CYS

• Molecule 2: MW07 light chain

Chain H:
87%   13%

D1 S7 T20 R24 L33 Y36 Q37 L47 L48 T53 L54 E55 S56 G57 V58 R61 L73 D82 Q89 P95 R96 T97 F98 N137 N138 Q147 E161 S162 S176 N210 E213 C214

• Molecule 2: MW07 light chain

Chain K:
81%   17%

D1 I2 Q3 S7 P8 S9 S10 L11 S12 A13 T20 R24 A25 S26 L33 A34 W35 Y36 Q37 Q38 K39 K42 L47 L48 L54 R61 F71 Y86 Y87 C88 Q89 R96 T97 F98 G101 T102 K107 P113 P120 A130 S131 V132 F139

R142 K145 L154 K169 T197 H198 N210 E213 C214

• Molecule 3: Spike protein S1

Chain C:
3%
70%   15%   14%

ARG VAL GLN PRO THR GLU SER ILE VAL ARG PHE PRO ASN ILE THR ASN LEU C336 R346 N354 R357 D364 Y365 Y369 N370 S371 A372 F377 S383 P384 T385 K386 L387 D398 R403 G404 D405 E406 V407 R408 A411 Q414 I418 Y421 N422 Y423 K424

A435 N439 F456 L461 K462 E465 R466 D467 I468 Y473 F490 P491 S494 G502 Q506 P507 Y508 R509 A520 G526 PRO LYS LYS SER THR ASN LEU VAL LYS ASN LYS CYS VAL ASN PHE

• Molecule 3: Spike protein S1

4%

Chain F:

67% 18% 15%

ARG VAL GLN PRO THR GLU SER ILE VAL ARG PHE PRO ASN ILE THR ASN LEU C336 R357 Y365 L368 Y369 N370 S371 A372 T376 F377 K378 C379 Y380 G381 V382 S383 P384 T385 K386 L387 N388 T393 V401 E406 K417 I418 Y421 N422 T430 G431 C432 V433 I434

A435 N439 S443 Y449 F456 Y473 E484 F490 P491 L492 Q493 S494 Q498 N501 G502 Q506 R509 V512 L513 S514 F515 H519 A522 C525 GLY PRO LYS LYS SER THR ASN LEU VAL LYS ASN LYS CYS VAL ASN PHE

• Molecule 3: Spike protein S1

3%

Chain I:

66% 18% 15%

ARG VAL GLN PRO THR GLU SER ILE VAL ARG PHE PRO ASN ILE THR ASN LEU C336 I358 L368 S371 T376 F377 K378 C379 Y380 G381 V382 S383 P384 L387 T393 N394 V395 V401 I402 E406 V407 A411 Q414 K417 I418 Y421 N422 L425 T430

V433 T434 A435 Y449 Y453 F456 I472 Y473 Q474 P479 E484 N487 S494 G502 Q506 R509 V512 L513 S514 F515 H519 A522 T523 V524 CYS GLY PRO LYS LYS SER THR ASN LEU VAL LYS ASN LYS CYS VAL ASN PHE

• Molecule 3: Spike protein S1

3%

Chain L:

71% 14% 14%

ARG VAL GLN PRO THR GLU SER ILE VAL ARG PHE PRO ASN ILE THR ASN LEU C336 P337 F338 G339 E340 F347 Y365 Y369 A372 T376 F377 V382 S383 L387 F392 T393 S399 F400 V401 A411 P412 G413 Q414 K417 I418 M422 F429 V433 I434

A435 Y453 F456 Y473 Q474 P479 F490 P491 L492 G502 Q505 Q506 R509 V512 F515 E516 L517 L518 H519 G526 PRO LYS LYS SER THR ASN LEU VAL LYS ASN LYS CYS VAL ASN PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.13 (at 3.01Å)	Xtriage
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^2)	46.2	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 18.9	EDS
L-test for twinning[2]	$< \vert L \vert > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	19459	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage'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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \vert L \vert >$, $< L^2 >$ 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	0.30	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 ⓘ

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	17,19,21	0.45	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
4	NAG	C	601	3	14,14,15	0.42	0	17,19,21	0.63	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	L	601	3	-	1/6/23/26	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
4	NAG	C	601	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) 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

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

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG I 601

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG F 601

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 601

Bond lengths

Bond angles

Torsions

Rings
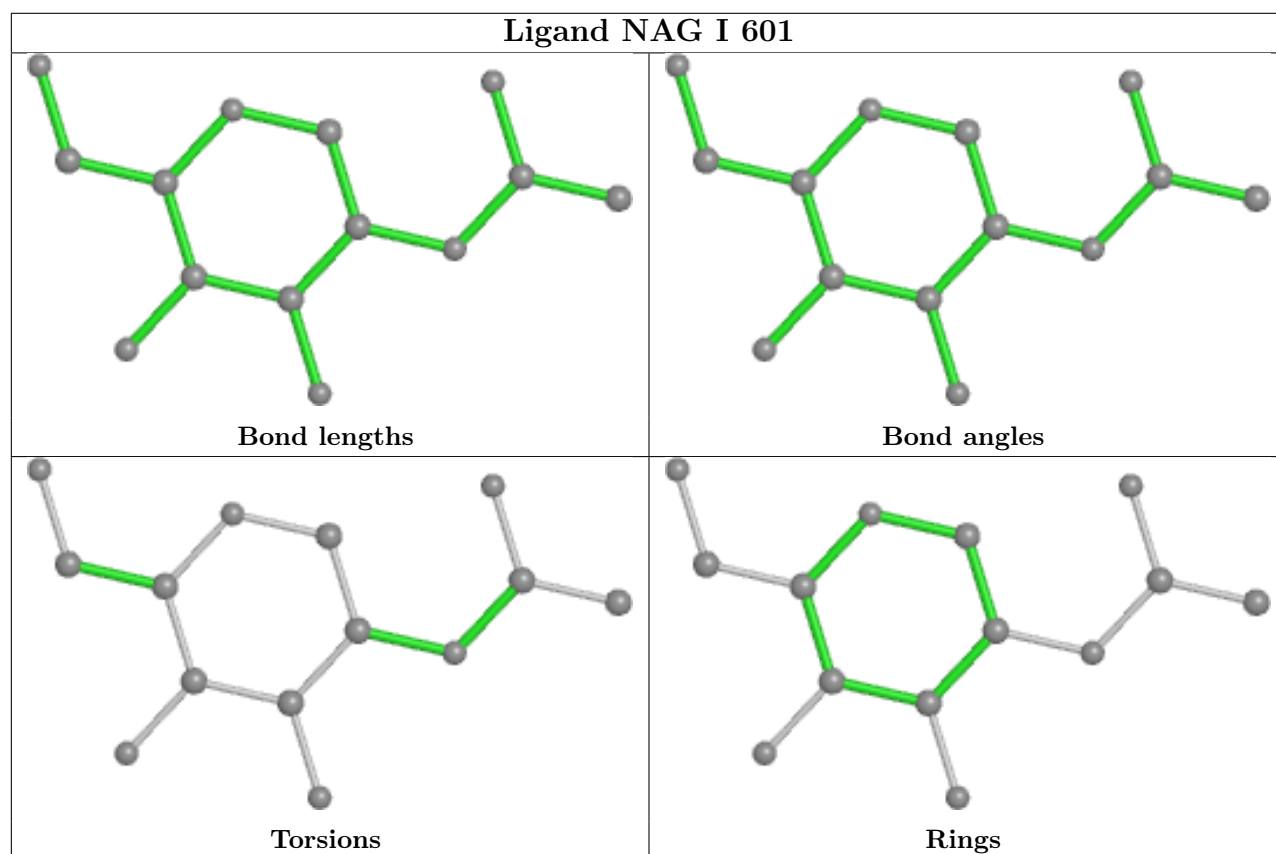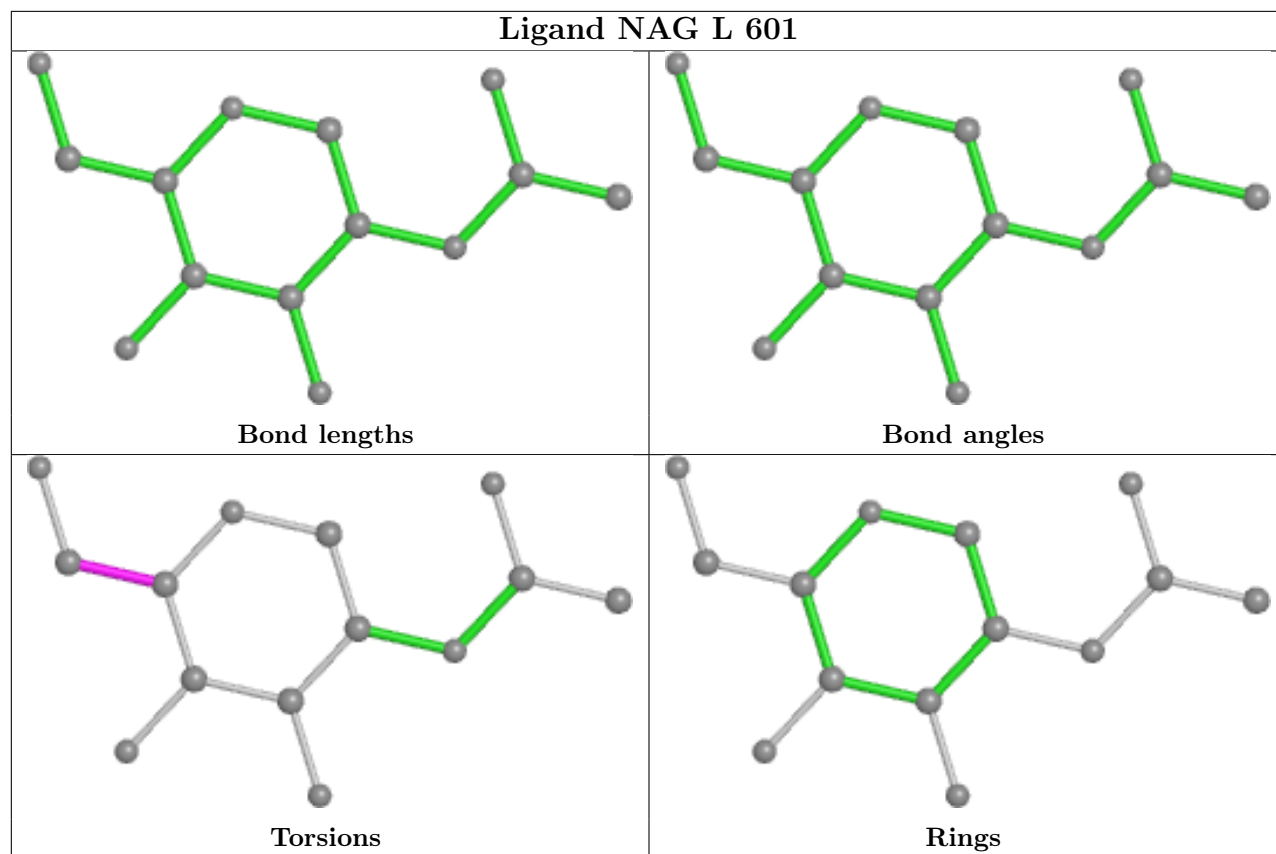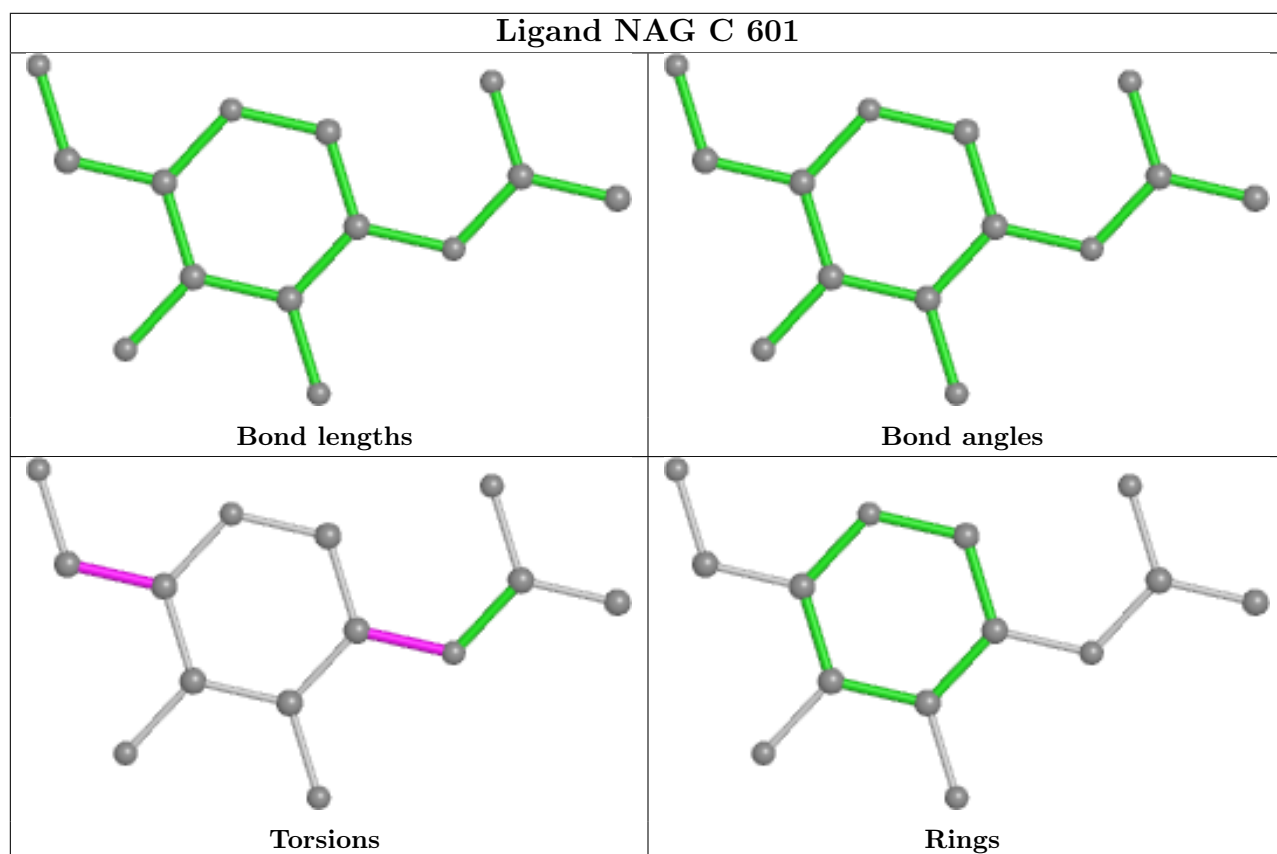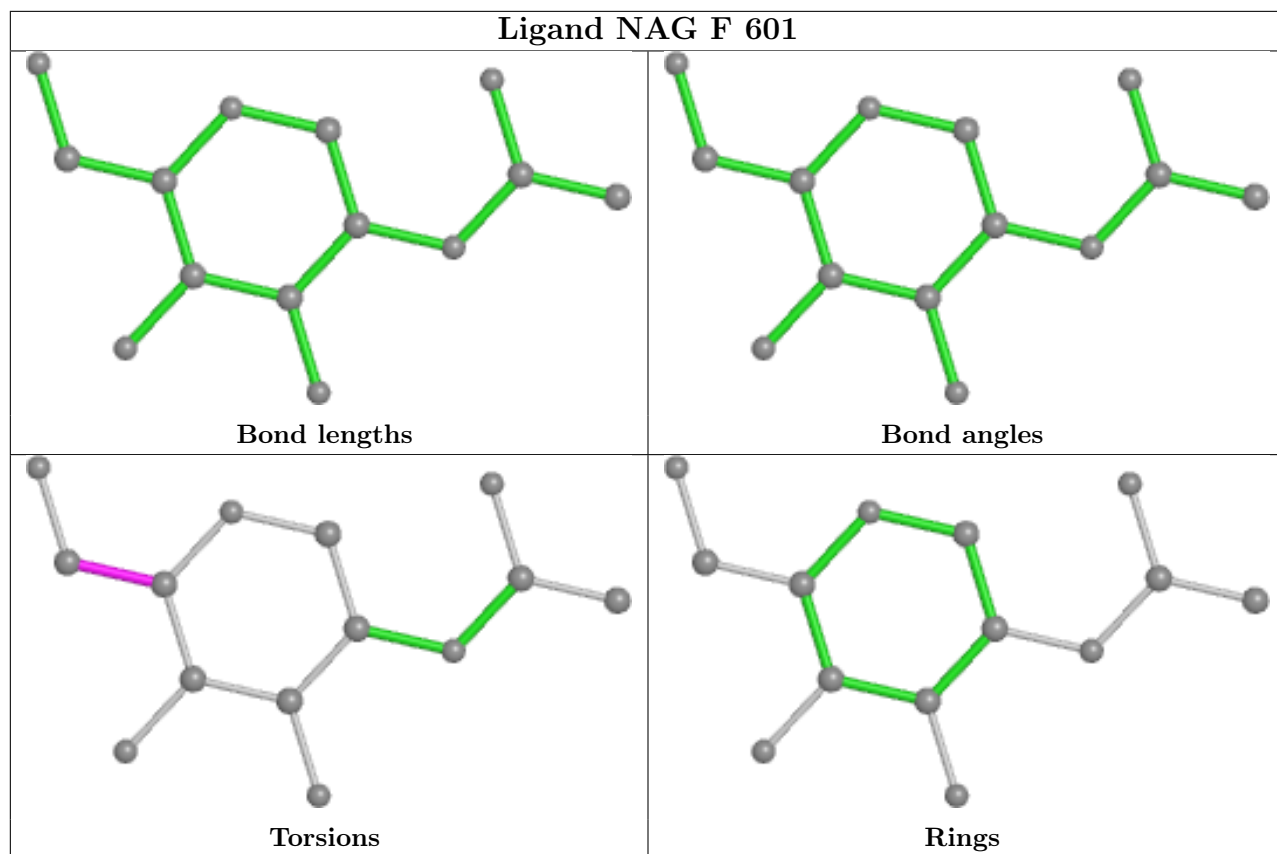
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	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 ⓘ

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

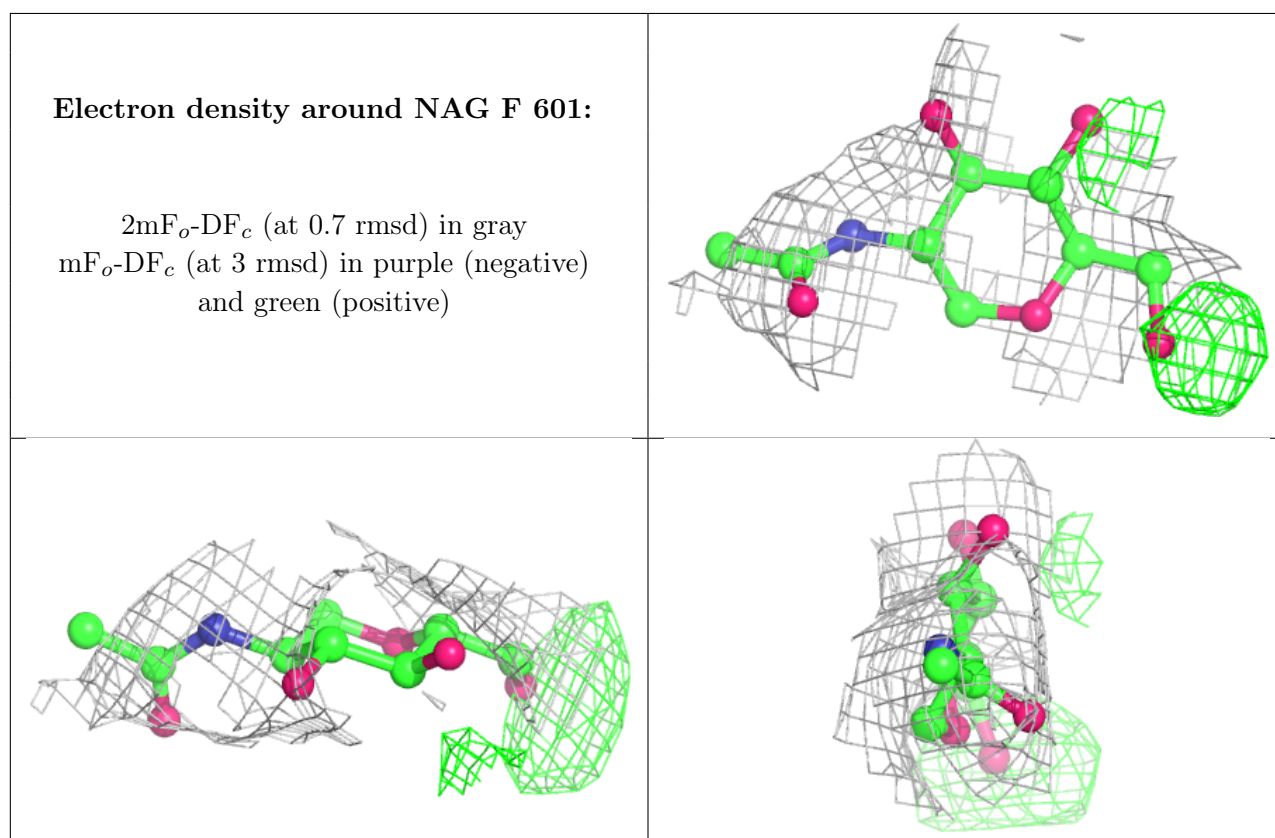## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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 F 601:

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

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)

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)
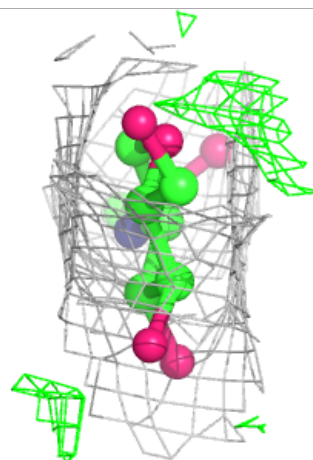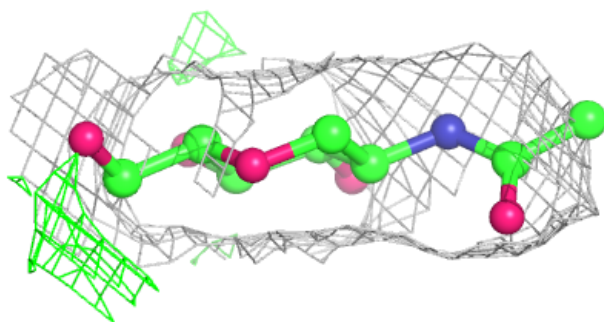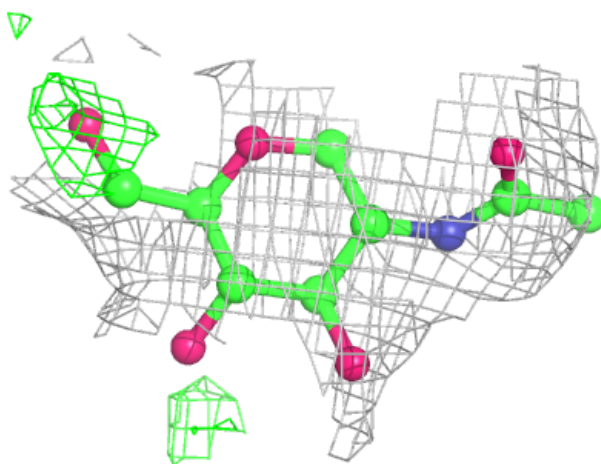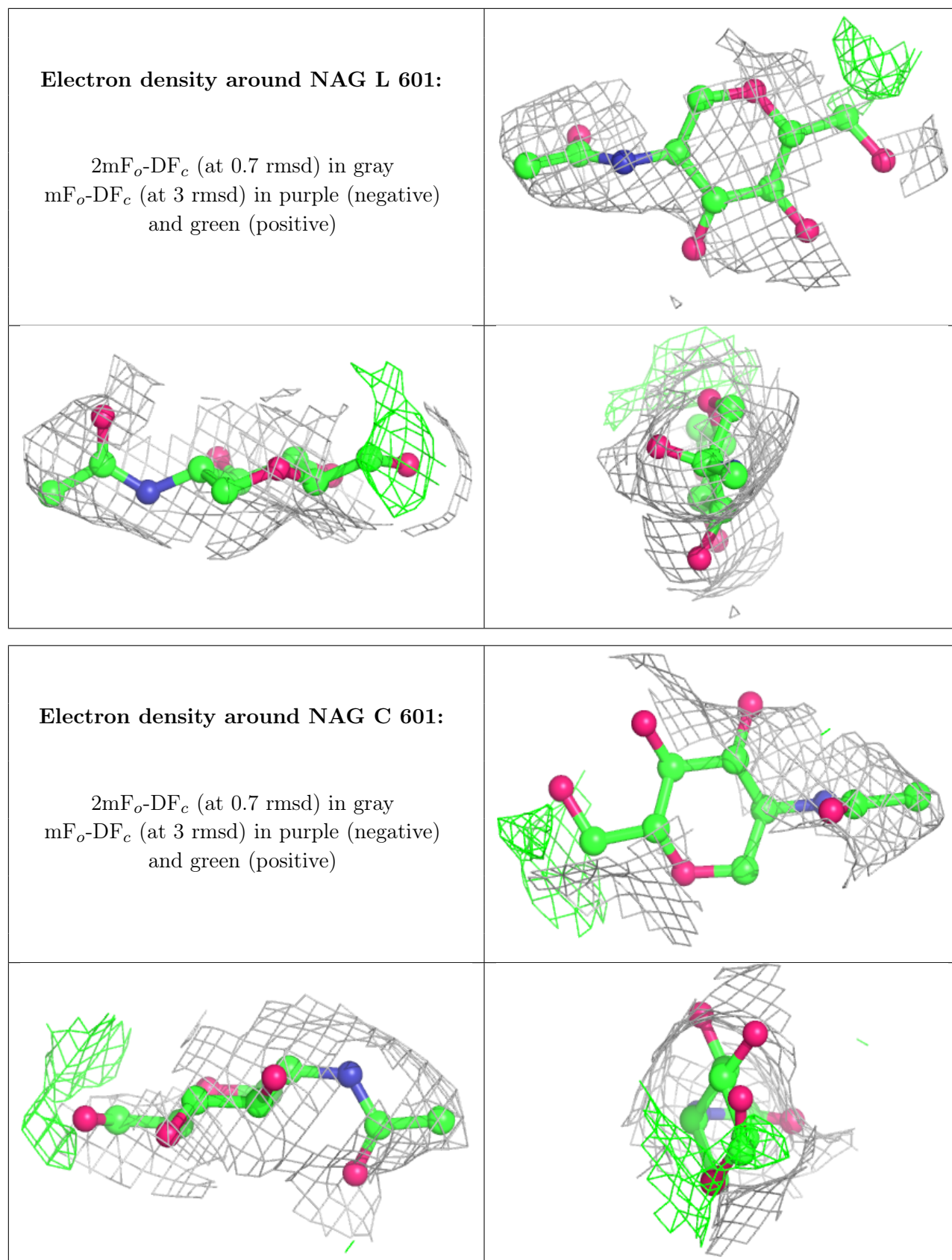
6.5 Other polymers (i)

There are no such residues in this entry.