



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:03 PM UTC

PDB ID : 7DK2 / pdb_00007dk2
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

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

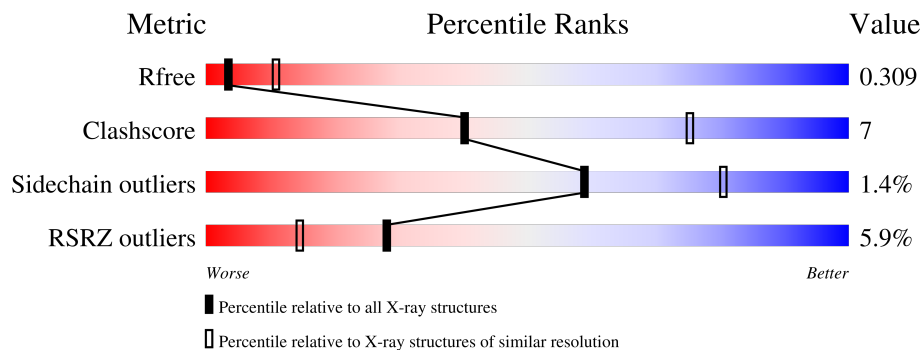
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	<p>4% 86% 13%</p>
2	K	214	<p>5% 80% 18%</p>
3	C	223	<p>6% 70% 15% 14%</p>
3	F	223	<p>10% 68% 17% 15%</p>
3	I	223	<p>13% 66% 18% 15%</p>
3	L	223	<p>7% 71% 14% 14%</p>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
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

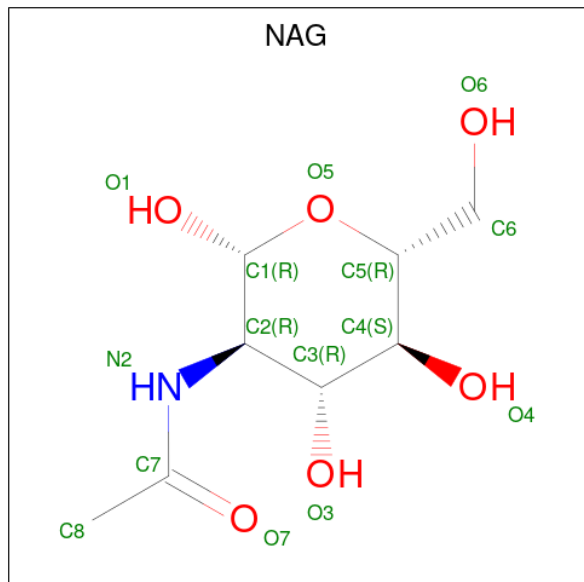
- Molecule 2 is a protein called MW07 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

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

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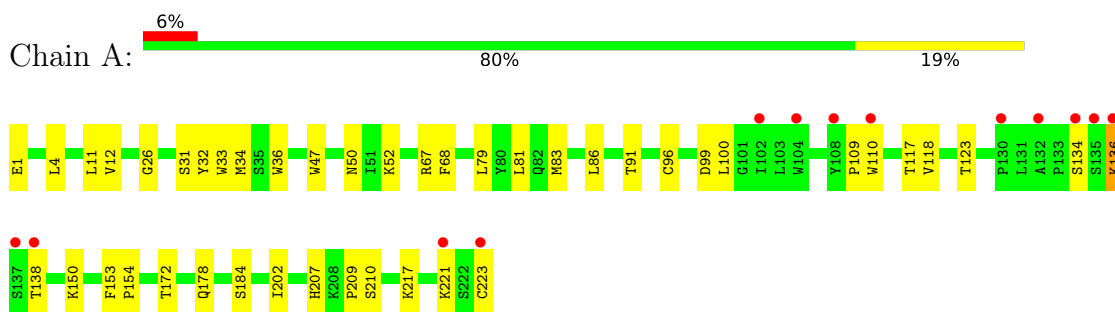
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	21	Total 21	O 21	0	0
5	H	13	Total 13	O 13	0	0
5	I	7	Total 7	O 7	0	0
5	J	19	Total 19	O 19	0	0
5	K	11	Total 11	O 11	0	0
5	L	5	Total 5	O 5	0	0

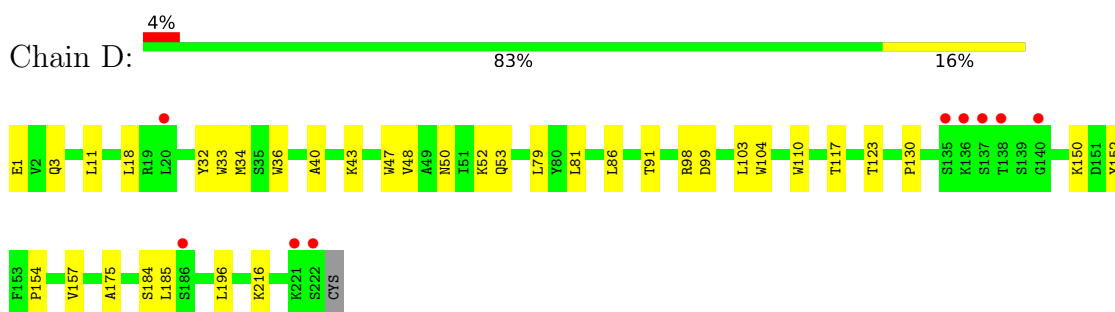
3 Residue-property plots [i](#)

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.

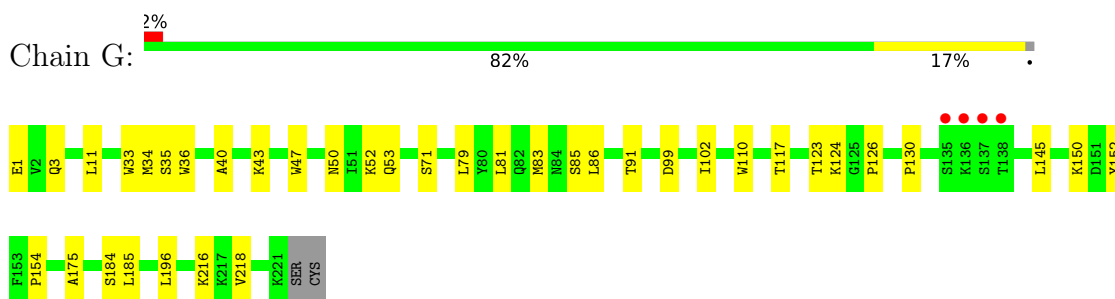
- Molecule 1: MW07 heavy chain



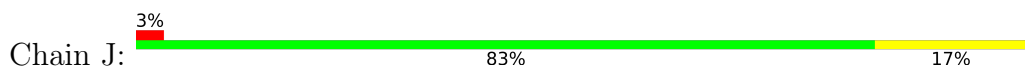
- Molecule 1: MW07 heavy chain

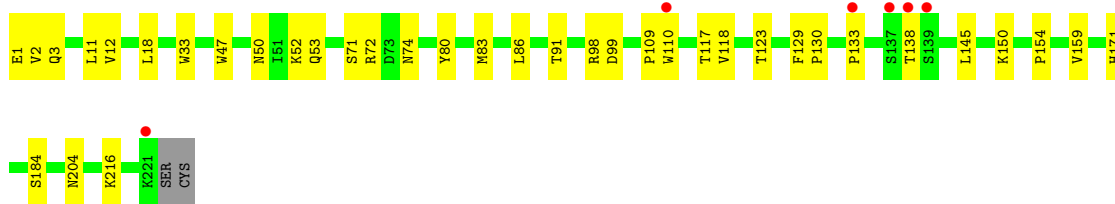


- Molecule 1: MW07 heavy chain

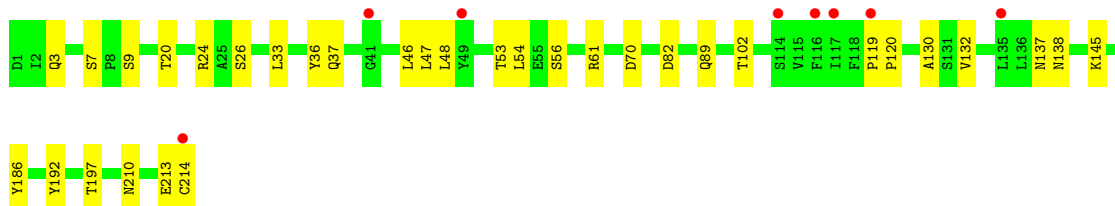
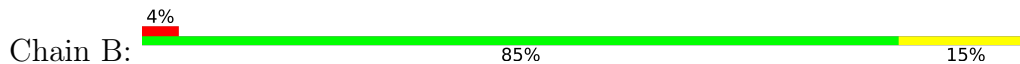


- Molecule 1: MW07 heavy chain

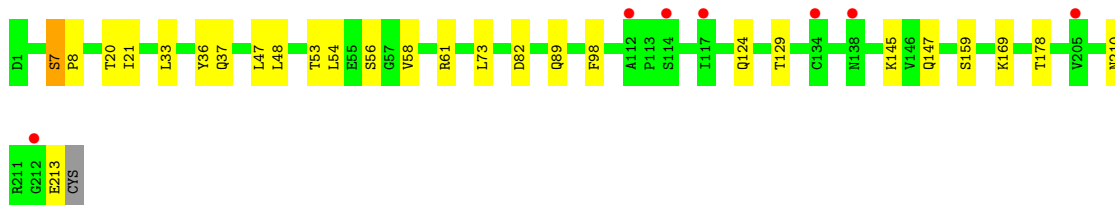
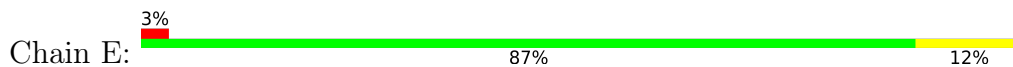




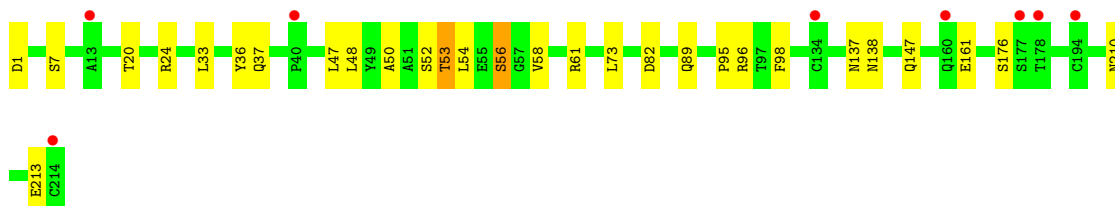
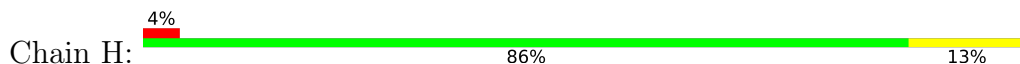
- Molecule 2: MW07 light chain



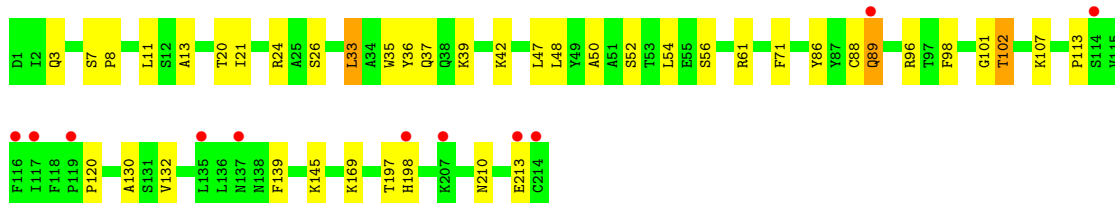
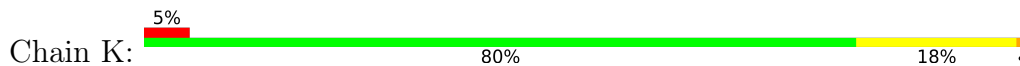
- Molecule 2: MW07 light chain



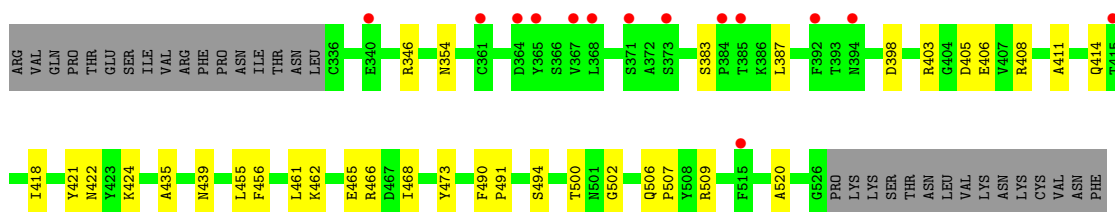
- Molecule 2: MW07 light chain



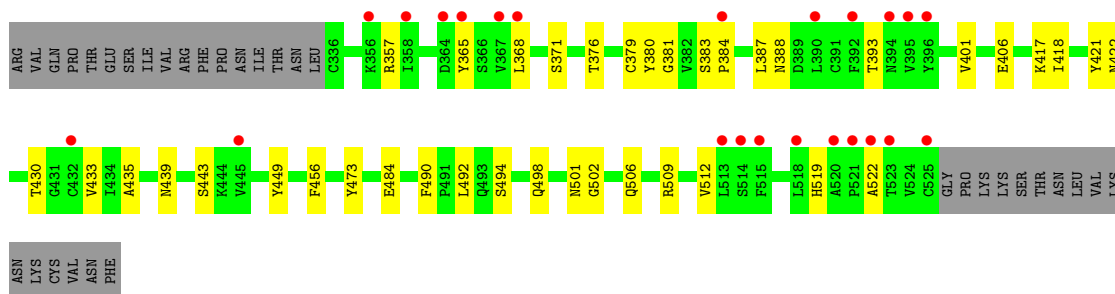
- Molecule 2: MW07 light chain



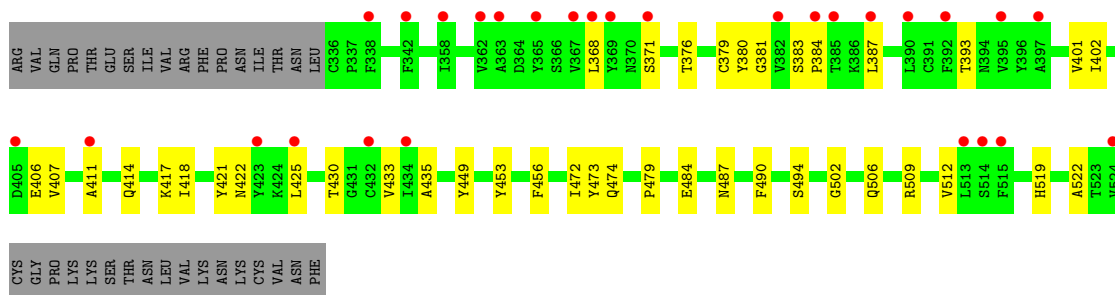
- Molecule 3: Spike protein S1



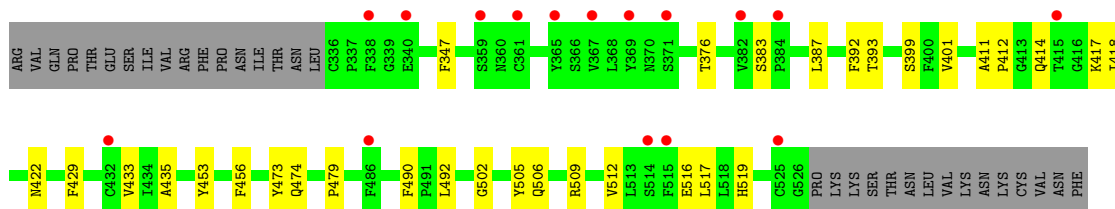
- Molecule 3: Spike protein S1



- 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, 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) 97.7 (46.47-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.258 , 0.304 0.267 , 0.309	Depositor DCC
R_{free} test set	3445 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 9.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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

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	0.20	0/1721	0.46	0/2343
1	D	0.19	0/1715	0.46	0/2335
1	G	0.20	0/1709	0.47	0/2327
1	J	0.20	0/1709	0.45	0/2327
2	B	0.19	0/1670	0.44	0/2266
2	E	0.20	0/1664	0.44	0/2258
2	H	0.20	0/1670	0.44	0/2266
2	K	0.19	0/1670	0.44	0/2266
3	C	0.15	0/1556	0.34	0/2117
3	F	0.15	0/1552	0.35	0/2112
3	I	0.15	0/1546	0.36	0/2104
3	L	0.15	0/1556	0.35	0/2117
All	All	0.18	0/19738	0.42	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	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1673	0	1643	23	0
1	G	1667	0	1638	23	0
1	J	1667	0	1638	23	0
2	B	1636	0	1591	21	0
2	E	1630	0	1587	17	0
2	H	1636	0	1592	20	0
2	K	1636	0	1592	26	0
3	C	1513	0	1428	19	0
3	F	1509	0	1425	23	0
3	I	1503	0	1422	25	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	249	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 7.

All (249) 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:A:221:LYS:HZ3	2:B:119:PRO:HD2	1.74	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
2:K:39:LYS:H	2:K:42:LYS:HZ2	1.58	0.51
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:484:GLU:CD	3:F:490:PHE:HB2	2.41	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
2:E:145:LYS:HZ2	2:E:147:GLN:HG3	1.82	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:D:98:ARG:HH21	1:D:104:TRP:CG	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:110:TRP:CD1	1:A:110:TRP:H	2.37	0.42
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
2:H:50:ALA:C	2:H:52:SER:H	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:K:50:ALA:C	2:K:52:SER:H	2.28	0.40
1:A:109:PRO:HD2	1:A:110:TRP:CD1	2.56	0.40
2:E:61:ARG:HH21	2:E:82:ASP:CG	2.27	0.40
3:I:484:GLU:CD	3:I:490:PHE:HB2	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/187 (100%)	184 (98%)	3 (2%)	55	79
1	D	186/187 (100%)	185 (100%)	1 (0%)	81	89
1	G	185/187 (99%)	182 (98%)	3 (2%)	55	79
1	J	185/187 (99%)	184 (100%)	1 (0%)	81	89
2	B	187/187 (100%)	184 (98%)	3 (2%)	55	79
2	E	186/187 (100%)	183 (98%)	3 (2%)	55	79
2	H	187/187 (100%)	183 (98%)	4 (2%)	47	75
2	K	187/187 (100%)	180 (96%)	7 (4%)	30	64
3	C	164/196 (84%)	159 (97%)	5 (3%)	36	69
3	F	164/196 (84%)	163 (99%)	1 (1%)	78	88
3	I	163/196 (83%)	163 (100%)	0	100	100
3	L	164/196 (84%)	164 (100%)	0	100	100
All	All	2145/2280 (94%)	2114 (99%)	31 (1%)	59	80

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	136	LYS
1	A	138	THR
2	B	7	SER
2	B	33	LEU
2	B	70	ASP
3	C	346	ARG

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Mol	Chain	Res	Type
3	C	408	ARG
3	C	455	LEU
3	C	494	SER
3	C	500	THR
1	D	1	GLU
2	E	7	SER
2	E	33	LEU
2	E	56	SER
3	F	357	ARG
1	G	1	GLU
1	G	85	SER
1	G	124	LYS
2	H	7	SER
2	H	33	LEU
2	H	53	THR
2	H	56	SER
1	J	138	THR
2	K	7	SER
2	K	21	ILE
2	K	33	LEU
2	K	56	SER
2	K	61	ARG
2	K	89	GLN
2	K	102	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
2	B	38	GLN
2	B	137	ASN
2	B	199	GLN
3	C	501	ASN
3	C	519	HIS
1	D	39	GLN
1	D	206	ASN
2	E	38	GLN
2	E	147	GLN
2	E	155	GLN
3	F	501	ASN
1	G	171	HIS
1	G	178	GLN

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Mol	Chain	Res	Type
2	H	38	GLN
2	H	137	ASN
2	H	147	GLN
2	H	152	ASN
3	I	498	GLN
3	I	501	ASN
1	J	39	GLN
1	J	206	ASN
2	K	38	GLN
2	K	199	GLN
3	L	501	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	F	601	3	14,14,15	0.35	0	17,19,21	0.52	0
4	NAG	I	601	3	14,14,15	0.41	0	17,19,21	0.53	0
4	NAG	L	601	3	14,14,15	0.40	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	601	3	14,14,15	0.44	0	17,19,21	0.65	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	F	601	3	-	2/6/23/26	0/1/1/1
4	NAG	I	601	3	-	0/6/23/26	0/1/1/1
4	NAG	L	601	3	-	1/6/23/26	0/1/1/1
4	NAG	C	601	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) 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
4	C	601	NAG	C4-C5-C6-O6
4	L	601	NAG	O5-C5-C6-O6
4	C	601	NAG	C3-C2-N2-C7
4	C	601	NAG	C1-C2-N2-C7

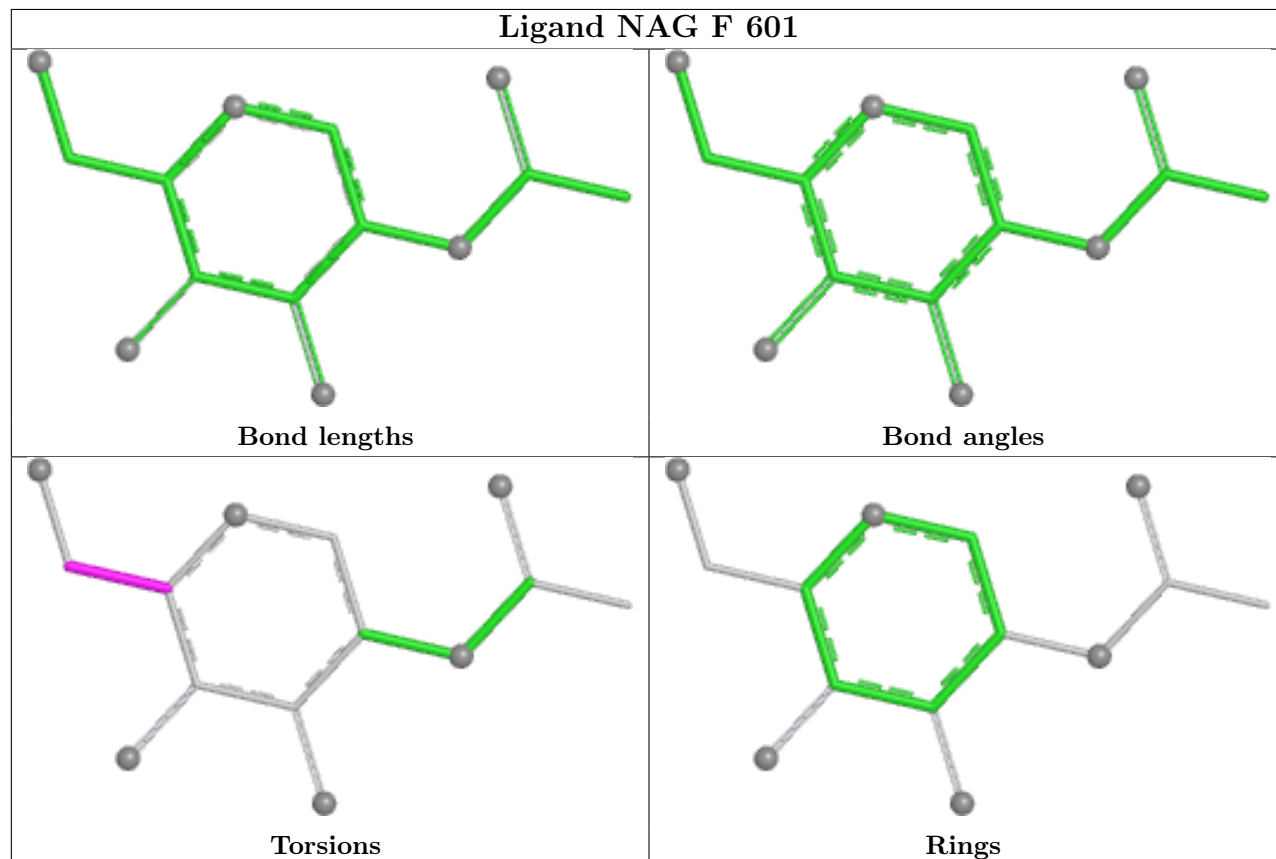
There are no ring outliers.

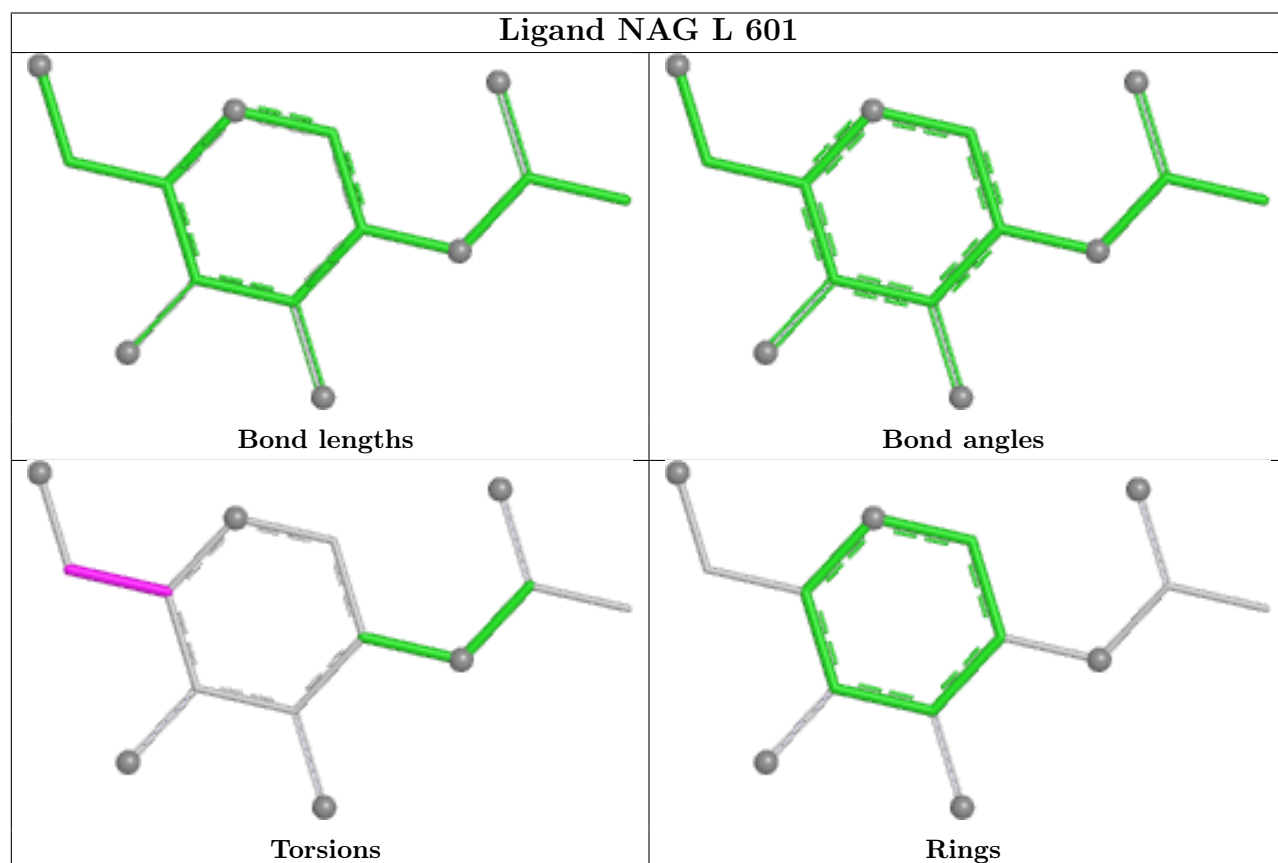
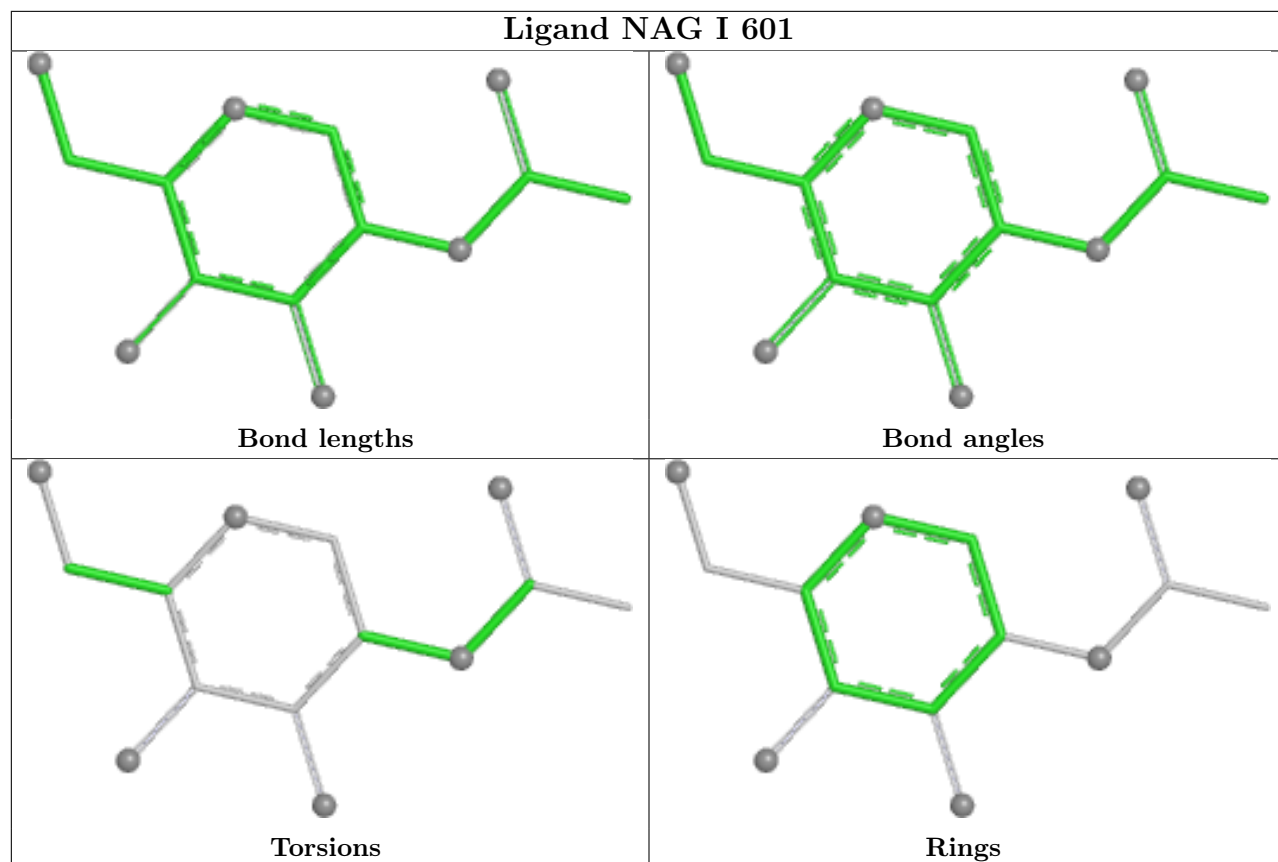
1 monomer is involved in 1 short contact:

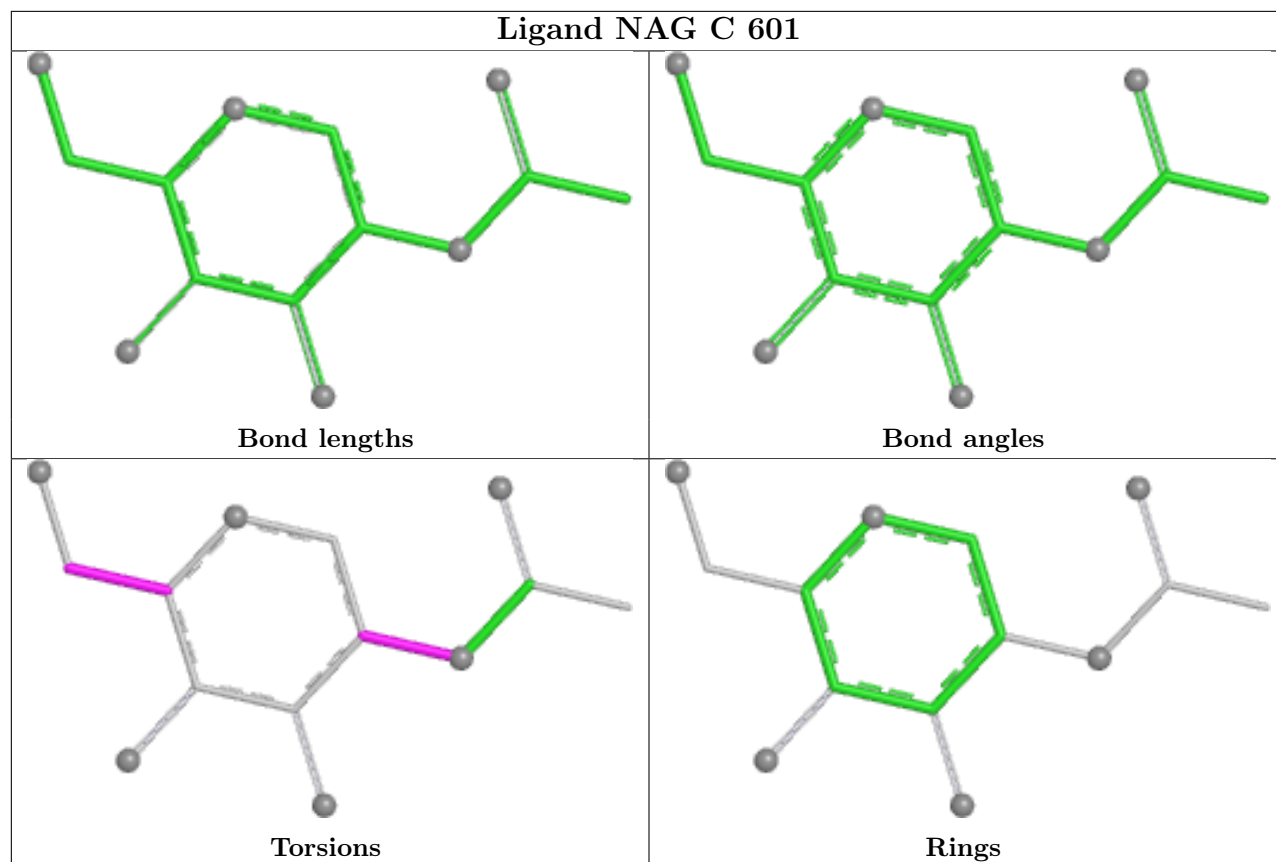
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	601	NAG	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	223/223 (100%)	0.32	13 (5%) 29 15	19, 32, 72, 123	0
1	D	222/223 (99%)	0.29	9 (4%) 41 23	19, 33, 73, 108	0
1	G	221/223 (99%)	0.27	4 (1%) 67 44	19, 32, 66, 104	0
1	J	221/223 (99%)	0.30	6 (2%) 56 33	18, 34, 70, 100	0
2	B	214/214 (100%)	0.53	8 (3%) 45 25	25, 40, 83, 103	0
2	E	213/214 (99%)	0.51	7 (3%) 49 28	25, 40, 78, 95	0
2	H	214/214 (100%)	0.43	8 (3%) 45 25	25, 39, 72, 94	0
2	K	214/214 (100%)	0.59	11 (5%) 33 17	22, 39, 86, 105	0
3	C	191/223 (85%)	0.81	14 (7%) 21 11	27, 54, 117, 140	0
3	F	190/223 (85%)	0.95	23 (12%) 8 5	28, 58, 119, 133	0
3	I	189/223 (84%)	1.05	28 (14%) 5 3	30, 60, 127, 133	0
3	L	191/223 (85%)	0.88	16 (8%) 17 9	31, 55, 123, 128	0
All	All	2503/2640 (94%)	0.56	147 (5%) 28 14	18, 42, 108, 140	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	SER	5.2
3	I	432	CYS	5.2
1	G	137	SER	4.8
3	I	513	LEU	4.8
3	F	513	LEU	4.6
3	I	515	PHE	4.5
3	C	515	PHE	4.3
2	H	134	CYS	4.2
3	F	515	PHE	4.2
1	D	137	SER	4.1
3	C	392	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
3	F	432	CYS	4.1
3	L	369	TYR	4.1
3	C	365	TYR	4.0
3	I	363	ALA	3.9
3	L	340	GLU	3.9
2	K	214	CYS	3.8
3	I	395	VAL	3.8
3	F	384	PRO	3.7
2	E	134	CYS	3.7
1	D	186	SER	3.6
3	C	368	LEU	3.6
2	K	135	LEU	3.6
3	L	365	TYR	3.6
3	I	368	LEU	3.5
3	C	384	PRO	3.5
1	D	222	SER	3.4
1	J	137	SER	3.4
3	I	384	PRO	3.4
1	J	221	LYS	3.4
3	L	338	PHE	3.3
3	I	358	ILE	3.3
3	F	514	SER	3.3
3	I	365	TYR	3.3
3	F	396	TYR	3.2
2	K	117	ILE	3.2
1	D	138	THR	3.2
2	B	49	TYR	3.2
1	A	221	LYS	3.1
1	D	221	LYS	3.1
2	H	177	SER	3.1
3	I	362	VAL	3.1
3	I	367	VAL	3.0
3	F	523	THR	3.0
1	J	110	TRP	2.9
2	E	112	ALA	2.9
3	C	364	ASP	2.9
3	I	405	ASP	2.9
3	F	368	LEU	2.9
1	G	138	THR	2.9
3	C	394	ASN	2.9
2	B	116	PHE	2.9
3	I	514	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	K	116	PHE	2.8
2	B	41	GLY	2.8
3	F	395	VAL	2.8
3	L	415	THR	2.8
3	F	392	PHE	2.7
3	C	367	VAL	2.7
3	L	371	SER	2.7
1	A	134	SER	2.7
3	C	371	SER	2.7
3	I	387	LEU	2.7
1	J	138	THR	2.7
1	G	136	LYS	2.6
1	D	136	LYS	2.6
3	L	367	VAL	2.6
2	E	117	ILE	2.6
3	C	415	THR	2.6
2	B	119	PRO	2.6
2	B	135	LEU	2.6
1	A	138	THR	2.6
2	K	137	ASN	2.5
3	I	411	ALA	2.5
2	K	114	SER	2.5
3	F	522	ALA	2.5
3	I	338	PHE	2.5
3	I	369	TYR	2.5
3	L	384	PRO	2.5
3	C	373	SER	2.5
3	I	524	VAL	2.5
2	E	114	SER	2.5
3	C	385	THR	2.5
3	L	514	SER	2.4
3	F	390	LEU	2.4
3	I	390	LEU	2.4
1	A	135	SER	2.4
2	B	114	SER	2.4
3	L	525	CYS	2.4
3	C	340	GLU	2.4
3	F	367	VAL	2.4
2	K	89	GLN	2.4
1	G	135	SER	2.4
2	B	214	CYS	2.4
3	F	525	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	I	392	PHE	2.4
3	L	359	SER	2.4
2	K	119	PRO	2.4
3	F	521	PRO	2.4
3	L	382	VAL	2.4
1	A	108	TYR	2.3
2	H	13	ALA	2.3
3	I	342	PHE	2.3
1	A	110	TRP	2.3
1	A	223	CYS	2.3
3	C	361	CYS	2.3
3	L	432	CYS	2.3
2	B	117	ILE	2.3
1	D	135	SER	2.3
1	J	133	PRO	2.2
1	A	132	ALA	2.2
3	I	425	LEU	2.2
3	L	486	PHE	2.2
1	J	139	SER	2.2
2	H	214	CYS	2.2
2	K	207	LYS	2.2
2	H	160	GLN	2.2
3	F	394	ASN	2.2
3	F	364	ASP	2.2
3	I	371	SER	2.1
2	K	213	GLU	2.1
1	D	140	GLY	2.1
2	E	138	ASN	2.1
3	L	515	PHE	2.1
2	E	205	VAL	2.1
3	F	518	LEU	2.1
3	I	423	TYR	2.1
3	I	397	ALA	2.1
2	H	40	PRO	2.1
1	A	102	ILE	2.1
3	L	361	CYS	2.1
2	E	212	GLY	2.1
3	F	445	VAL	2.1
3	I	382	VAL	2.1
3	F	358	ILE	2.1
2	K	198	HIS	2.1
1	D	20	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	I	434	ILE	2.0
1	A	104	TRP	2.0
2	H	178	THR	2.0
3	F	365	TYR	2.0
3	I	385	THR	2.0
2	H	194	CYS	2.0
1	A	136	LYS	2.0
3	F	520	ALA	2.0
1	A	130	PRO	2.0
3	F	356	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

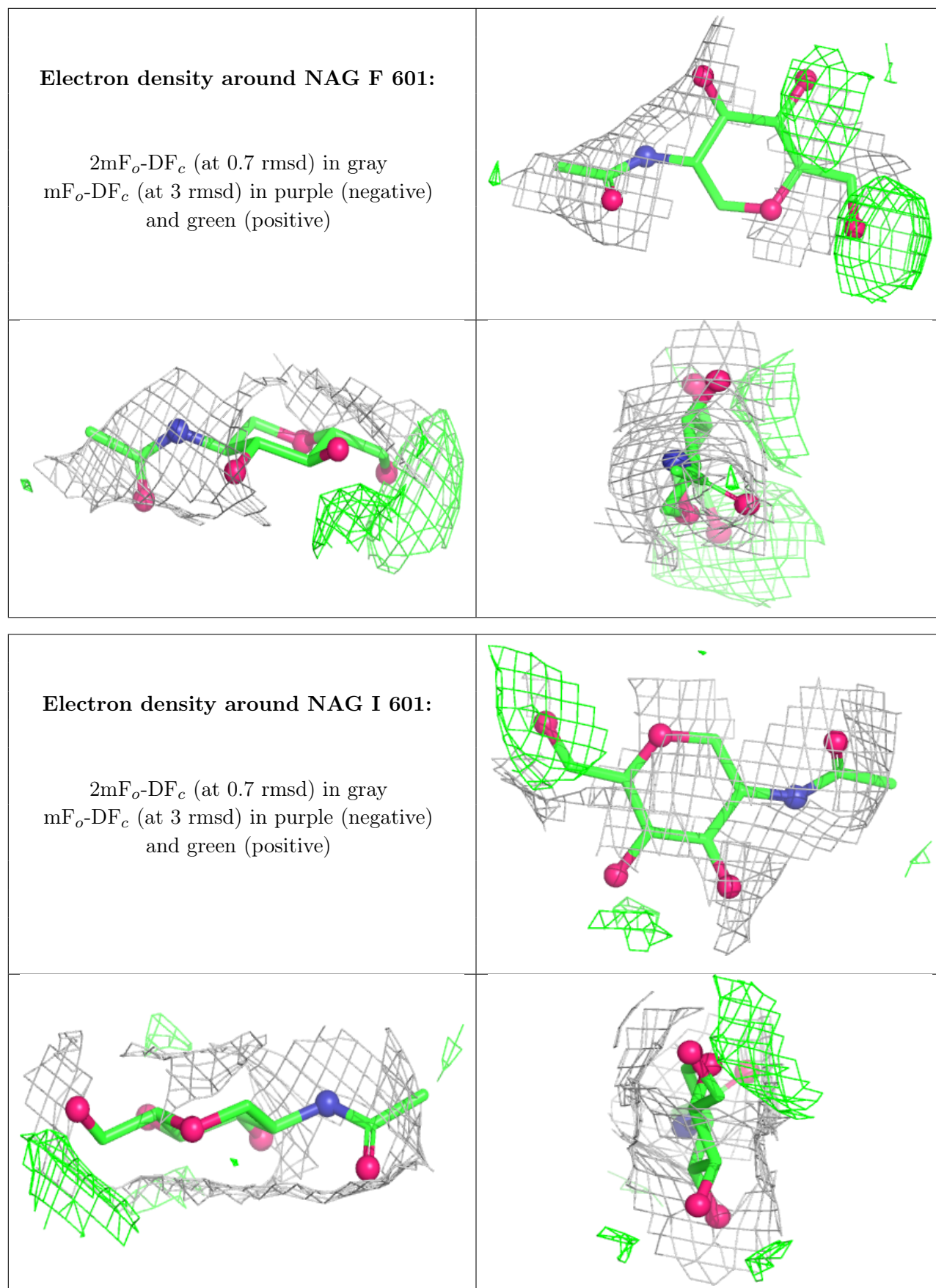
There are no oligosaccharides in this entry.

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.

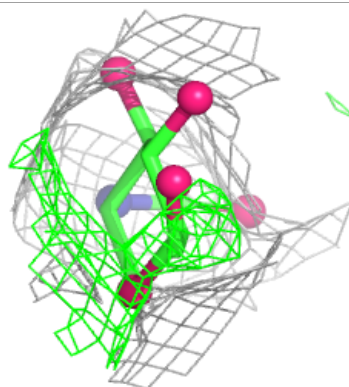
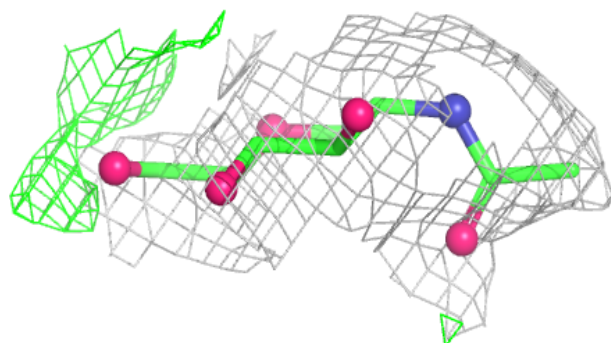
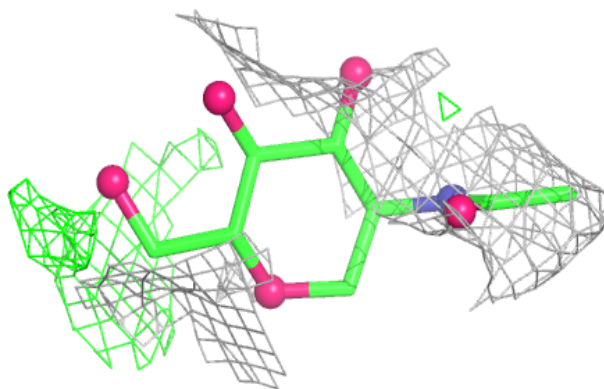
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	F	601	14/15	0.50	0.18	70,89,96,99	0
4	NAG	I	601	14/15	0.61	0.17	69,94,98,99	0
4	NAG	C	601	14/15	0.65	0.15	75,91,96,96	0
4	NAG	L	601	14/15	0.70	0.16	74,83,94,97	0

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.

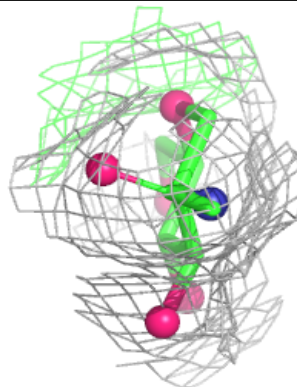
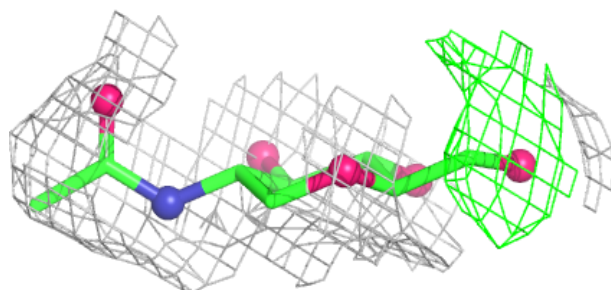
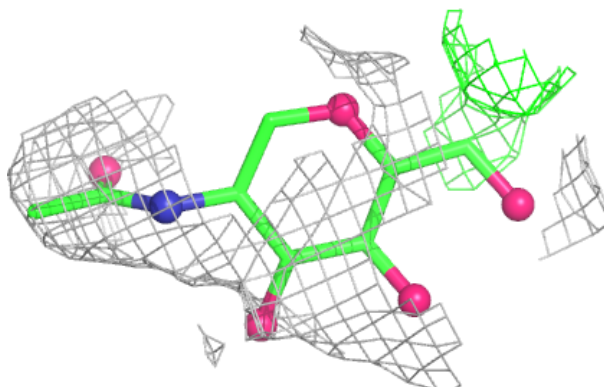


Electron density around NAG C 601:

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

**Electron density around NAG 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.