



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2023 – 02:12 PM JST

PDB ID : 7X2H
Title : Crystal structure of SARS-CoV-2 spike receptor-binding domain bound with 6-2C Fab
Authors : Wang, X.; Wang, Z.
Deposited on : 2022-02-25
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

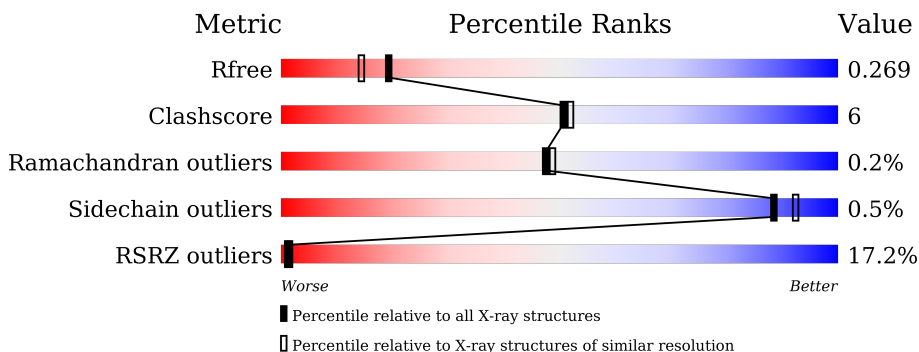
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	222	 3% (poor fit), 88% (0-1 outliers), 9% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
1	C	222	 4% (poor fit), 90% (0-1 outliers), 7% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
2	B	214	 0% (poor fit), 92% (0-1 outliers), 7% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
2	D	214	 6% (poor fit), 90% (0-1 outliers), 9% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
3	E	195	 42% (poor fit), 71% (0-1 outliers), 17% (2-3 outliers), 0% (4+ outliers), 10% (not modelled)
3	F	195	 51% (poor fit), 74% (0-1 outliers), 21% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10021 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 6-2C H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	Total	C	N	O	S	0	0	0
			1665	1057	282	320	6			
1	C	217	Total	C	N	O	S	0	0	0
			1665	1057	282	320	6			

- Molecule 2 is a protein called 6-2C L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	Total	C	N	O	S	0	0	0
			1640	1032	276	327	5			
2	D	214	Total	C	N	O	S	0	0	0
			1649	1037	277	330	5			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	176	Total	C	N	O	S	0	0	0
			1408	905	235	262	6			
3	F	187	Total	C	N	O	S	0	0	0
			1486	952	247	279	8			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

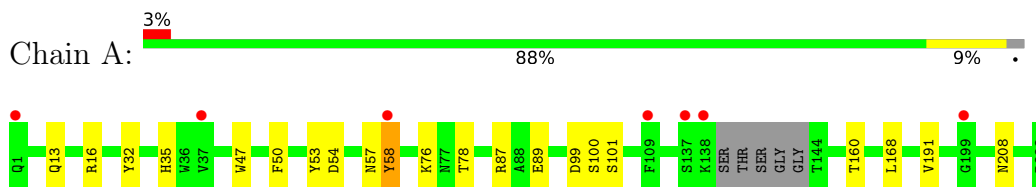
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	108	108	108	0	0
5	B	129	129	129	0	0
5	C	104	104	104	0	0
5	D	126	126	126	0	0
5	E	11	11	11	0	0
5	F	2	2	2	0	0

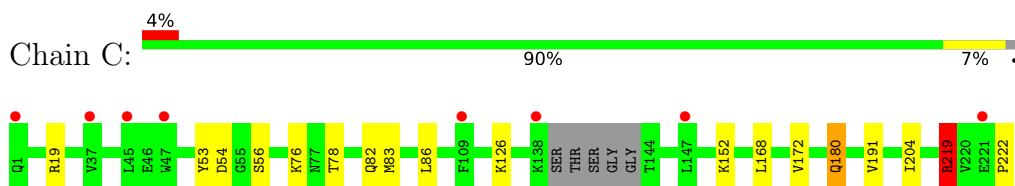
3 Residue-property plots [i](#)

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.

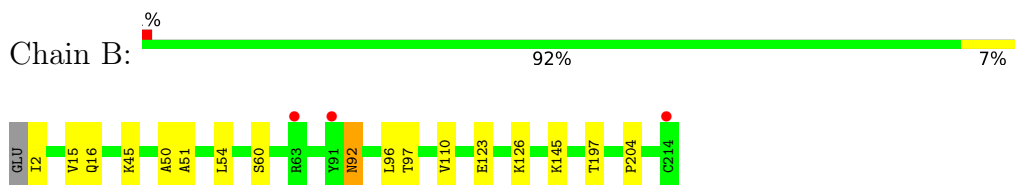
- Molecule 1: 6-2C H chain



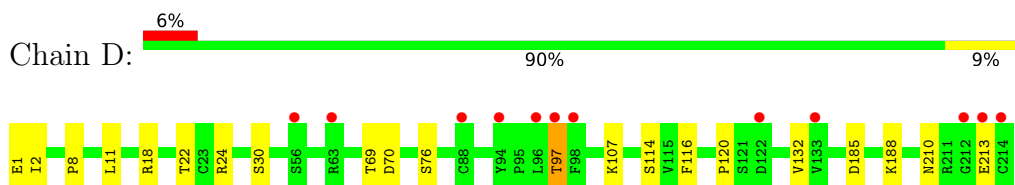
- Molecule 1: 6-2C H chain



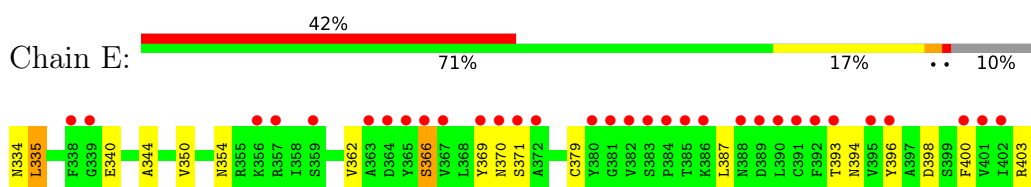
- Molecule 2: 6-2C L chain

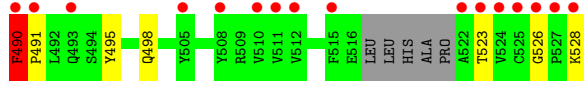
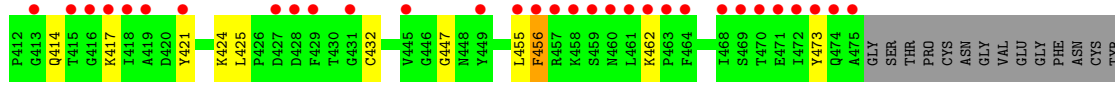


- Molecule 2: 6-2C L chain

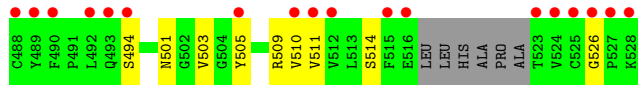
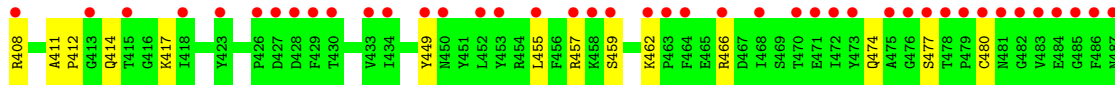
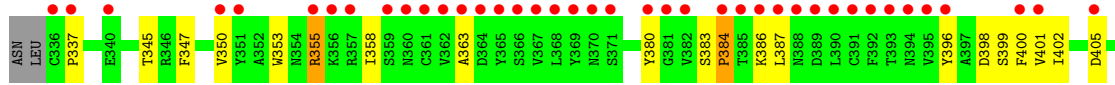
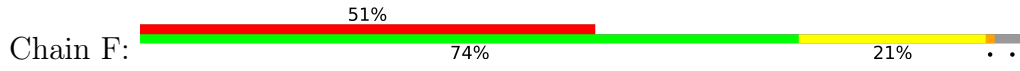


- Molecule 3: Spike protein S1





• Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	179.05Å 72.00Å 112.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.52 – 2.10 31.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.52-2.10) 99.3 (31.52-2.10)	Depositor EDS
R_{merge}	0.99	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.228 , 0.269 0.233 , 0.269	Depositor DCC
R_{free} test set	4093 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	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	0.93	EDS
Total number of atoms	10021	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/1713	0.69	0/2337
1	C	0.47	0/1713	0.73	4/2337 (0.2%)
2	B	0.51	0/1675	0.68	0/2276
2	D	0.49	0/1684	0.69	0/2288
3	E	0.40	0/1445	0.68	2/1961 (0.1%)
3	F	0.47	0/1527	0.74	1/2074 (0.0%)
All	All	0.48	0/9757	0.70	7/13273 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
3	E	0	1
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	355	ARG	CB-CA-C	-10.60	89.20	110.40
3	E	490	PHE	CB-CG-CD2	-8.47	114.87	120.80
1	C	219	ARG	NE-CZ-NH1	-7.90	116.35	120.30
3	E	335	LEU	CB-CG-CD2	-7.22	98.73	111.00
1	C	222	PRO	N-CA-C	-6.39	95.48	112.10
1	C	180	GLN	CA-CB-CG	5.81	126.19	113.40
1	C	219	ARG	NE-CZ-NH2	5.35	122.97	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	TYR	Sidechain
1	C	219	ARG	Sidechain
3	E	490	PHE	Sidechain

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	1665	0	1601	15	0
1	C	1665	0	1601	11	0
2	B	1640	0	1608	12	0
2	D	1649	0	1617	12	0
3	E	1408	0	1341	24	1
3	F	1486	0	1401	37	1
4	E	14	0	13	0	0
4	F	14	0	13	0	0
5	A	108	0	0	2	0
5	B	129	0	0	2	0
5	C	104	0	0	1	0
5	D	126	0	0	1	0
5	E	11	0	0	0	0
5	F	2	0	0	2	0
All	All	10021	0	9195	106	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:355:ARG:NH2	3:F:466:ARG:HD3	1.75	1.00
2:B:197:THR:HG22	2:B:204:PRO:HB3	1.60	0.82
3:F:417:LYS:HE3	3:F:455:LEU:HD13	1.62	0.82
3:F:355:ARG:HH21	3:F:466:ARG:HH11	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:SER:HB2	3:F:503:VAL:HG11	1.67	0.77
3:F:355:ARG:HH22	3:F:466:ARG:HD3	1.45	0.77
3:F:505:TYR:O	5:F:701:HOH:O	2.02	0.76
3:F:355:ARG:NH2	3:F:466:ARG:HH11	1.84	0.75
3:F:355:ARG:HH21	3:F:466:ARG:NH1	1.88	0.71
3:F:411:ALA:HB3	3:F:414:GLN:HG3	1.75	0.69
1:A:87:ARG:HD3	1:A:89:GLU:OE1	1.96	0.66
2:D:30:SER:CB	3:F:503:VAL:HG11	2.26	0.65
2:B:123:GLU:O	2:B:126:LYS:HG2	1.97	0.64
3:E:411:ALA:HB3	3:E:414:GLN:HG3	1.80	0.63
3:F:383:SER:HB3	3:F:386:LYS:HG2	1.81	0.63
3:E:393:THR:O	3:E:523:THR:OG1	2.13	0.61
3:E:334:ASN:O	3:E:362:VAL:HG12	2.02	0.59
3:E:394:ASN:HB3	3:E:396:TYR:HE1	1.69	0.58
2:D:69:THR:HG23	2:D:70:ASP:OD1	2.04	0.58
3:F:380:TYR:CD2	3:F:412:PRO:HG2	2.39	0.58
2:B:110:VAL:O	5:B:301:HOH:O	2.17	0.58
2:D:107:LYS:NZ	5:D:301:HOH:O	2.28	0.57
1:C:126:LYS:NZ	5:C:301:HOH:O	2.15	0.56
1:C:204:ILE:HG12	1:C:219:ARG:HG2	1.87	0.56
3:E:424:LYS:NZ	3:E:425:LEU:O	2.33	0.55
3:E:403:ARG:HG3	3:E:495:TYR:CE1	2.42	0.55
3:E:455:LEU:HB3	3:E:456:PHE:HD1	1.72	0.54
3:F:355:ARG:HH21	3:F:466:ARG:HD3	1.67	0.54
1:A:16:ARG:HH11	1:A:16:ARG:HG3	1.72	0.54
2:D:2:ILE:O	2:D:97:THR:HG21	2.08	0.54
3:F:474:GLN:OE1	3:F:477:SER:HA	2.08	0.54
3:E:490:PHE:CD1	3:E:491:PRO:HD2	2.43	0.53
3:F:417:LYS:HE3	3:F:455:LEU:CD1	2.34	0.53
2:B:145:LYS:HB3	2:B:197:THR:OG1	2.09	0.53
3:F:337:PRO:HD2	3:F:358:ILE:HD12	1.91	0.52
3:F:350:VAL:O	3:F:353:TRP:HD1	1.92	0.52
2:D:22:THR:HG21	2:D:24:ARG:NH2	2.23	0.52
2:D:114:SER:HG	2:D:116:PHE:HE1	1.58	0.52
2:D:210:ASN:O	2:D:213:GLU:HG2	2.09	0.52
3:F:353:TRP:CZ2	3:F:466:ARG:HB2	2.45	0.52
3:E:362:VAL:HG23	3:E:526:GLY:O	2.09	0.51
3:E:369:TYR:OH	3:E:387:LEU:HD23	2.11	0.51
3:E:455:LEU:HB3	3:E:456:PHE:CD1	2.46	0.51
1:A:58:TYR:HE2	5:A:397:HOH:O	1.94	0.50
3:F:405:ASP:O	3:F:408:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:396:TYR:HB3	3:F:514:SER:OG	2.11	0.50
2:B:2:ILE:O	2:B:97:THR:HG21	2.12	0.50
3:E:394:ASN:HB3	3:E:396:TYR:CE1	2.46	0.49
2:B:45:LYS:NZ	5:B:307:HOH:O	2.37	0.49
2:B:54:LEU:HD21	2:B:60:SER:HA	1.93	0.49
1:C:54:ASP:HB3	1:C:56:SER:H	1.77	0.49
3:F:347:PHE:CE2	3:F:509:ARG:HB3	2.48	0.49
1:A:57:ASN:O	1:A:58:TYR:HB3	2.13	0.49
3:F:398:ASP:O	3:F:511:VAL:HA	2.13	0.48
1:A:99:ASP:OD1	1:A:101:SER:HB3	2.13	0.48
1:A:53:TYR:CZ	1:A:54:ASP:OD1	2.67	0.48
3:F:384:PRO:O	3:F:387:LEU:HB2	2.13	0.48
3:F:457:ARG:HD3	3:F:459:SER:O	2.14	0.48
1:A:168:LEU:HD21	1:A:191:VAL:HG11	1.95	0.47
3:F:449:TYR:HD1	3:F:494:SER:CB	2.26	0.47
1:C:76:LYS:O	1:C:78:THR:HG23	2.14	0.47
3:E:421:TYR:CE2	3:E:456:PHE:HA	2.49	0.47
3:F:449:TYR:HD1	3:F:494:SER:HB3	1.80	0.47
3:F:474:GLN:HB3	3:F:480:CYS:SG	2.55	0.47
1:A:47:TRP:CD2	2:B:96:LEU:HB2	2.51	0.46
3:E:366:SER:HA	3:E:369:TYR:CD2	2.50	0.46
3:F:383:SER:HA	3:F:384:PRO:HD2	1.42	0.46
3:F:501:ASN:OD1	5:F:701:HOH:O	2.20	0.46
1:A:76:LYS:O	1:A:78:THR:HG23	2.15	0.46
3:E:340:GLU:O	3:E:344:ALA:HB2	2.16	0.46
1:A:47:TRP:CG	2:B:96:LEU:HB2	2.51	0.46
1:C:19:ARG:HD2	1:C:82:GLN:OE1	2.17	0.45
3:F:353:TRP:CE2	3:F:466:ARG:HD2	2.52	0.45
2:B:92:ASN:HD22	2:B:92:ASN:HA	1.56	0.44
2:D:185:ASP:HA	2:D:188:LYS:HZ3	1.82	0.44
3:E:354:ASN:O	3:E:398:ASP:HA	2.17	0.44
3:E:417:LYS:HE2	3:E:417:LYS:HB2	1.75	0.44
3:F:363:ALA:O	3:F:526:GLY:HA2	2.18	0.44
1:A:35:HIS:CE1	1:A:50:PHE:HB2	2.52	0.44
3:E:335:LEU:HD23	3:E:362:VAL:HG13	1.99	0.44
3:F:399:SER:HA	3:F:510:VAL:O	2.18	0.44
3:F:401:VAL:HG22	3:F:509:ARG:HG2	1.99	0.44
3:E:369:TYR:C	3:E:371:SER:H	2.21	0.44
1:A:32:TYR:CE2	1:A:100:SER:HB3	2.53	0.43
2:B:50:ALA:O	2:B:51:ALA:HB3	2.18	0.43
1:C:83:MET:HB3	1:C:86:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:350:VAL:HA	3:E:400:PHE:HB2	1.99	0.43
1:C:53:TYR:OH	3:F:345:THR:HG23	2.18	0.43
3:F:350:VAL:O	3:F:353:TRP:CD1	2.71	0.43
1:C:168:LEU:HD21	1:C:191:VAL:HG11	1.99	0.43
2:D:120:PRO:HD3	2:D:132:VAL:HG22	2.00	0.43
1:C:53:TYR:CG	1:C:54:ASP:N	2.87	0.42
2:D:18:ARG:HG3	2:D:76:SER:HA	2.00	0.42
3:F:400:PHE:CD1	3:F:402:ILE:HG23	2.55	0.42
1:C:172:VAL:HG22	1:C:191:VAL:HG22	2.01	0.41
3:F:462:LYS:HB3	3:F:462:LYS:HE3	1.86	0.41
1:A:160:THR:OG1	1:A:208:ASN:HB3	2.20	0.41
2:B:15:VAL:HG12	2:B:16:GLN:HG2	2.01	0.41
3:E:379:CYS:HA	3:E:432:CYS:HA	2.03	0.41
3:E:528:LYS:HD3	3:E:528:LYS:HA	1.81	0.41
1:A:13:GLN:HB2	1:A:16:ARG:HD2	2.03	0.41
3:E:462:LYS:HE3	3:E:462:LYS:HB3	1.86	0.41
3:E:447:GLY:HA2	3:E:498:GLN:HG2	2.03	0.41
1:A:208:ASN:OD1	5:A:301:HOH:O	2.22	0.40
1:C:152:LYS:HE2	1:C:180:GLN:HE22	1.86	0.40
2:D:8:PRO:HG2	2:D:11:LEU:HD23	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:473:TYR:OH	3:F:505:TYR:OH[1_556]	1.87	0.33

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	213/222 (96%)	208 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	213/222 (96%)	206 (97%)	7 (3%)	0	100	100
2	B	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
2	D	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
3	E	170/195 (87%)	159 (94%)	10 (6%)	1 (1%)	25	21
3	F	183/195 (94%)	171 (93%)	11 (6%)	1 (0%)	29	26
All	All	1202/1262 (95%)	1152 (96%)	48 (4%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	384	PRO
3	E	370	ASN

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	187/190 (98%)	187 (100%)	0	100	100
1	C	187/190 (98%)	187 (100%)	0	100	100
2	B	187/188 (100%)	186 (100%)	1 (0%)	88	92
2	D	188/188 (100%)	186 (99%)	2 (1%)	73	79
3	E	153/168 (91%)	151 (99%)	2 (1%)	69	75
3	F	162/168 (96%)	162 (100%)	0	100	100
All	All	1064/1092 (97%)	1059 (100%)	5 (0%)	88	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	92	ASN
2	D	1	GLU
2	D	97	THR
3	E	366	SER

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Mol	Chain	Res	Type
3	E	456	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	92	ASN
2	B	189	HIS
1	C	180	GLN
3	E	493	GLN
3	F	370	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	E	601	3	14,14,15	0.27	0	17,19,21	0.66	0
4	NAG	F	601	3	14,14,15	0.26	0	17,19,21	0.67	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	E	601	3	-	2/6/23/26	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.

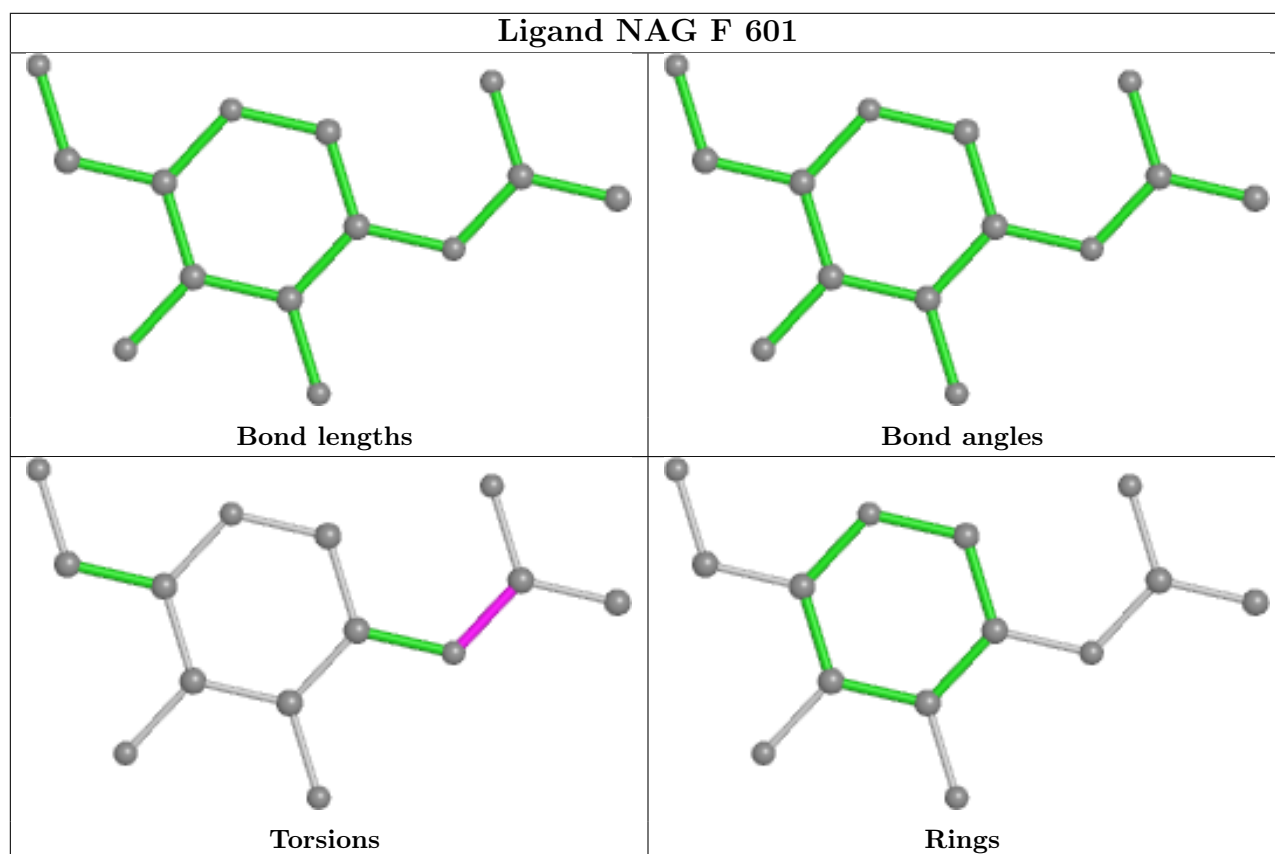
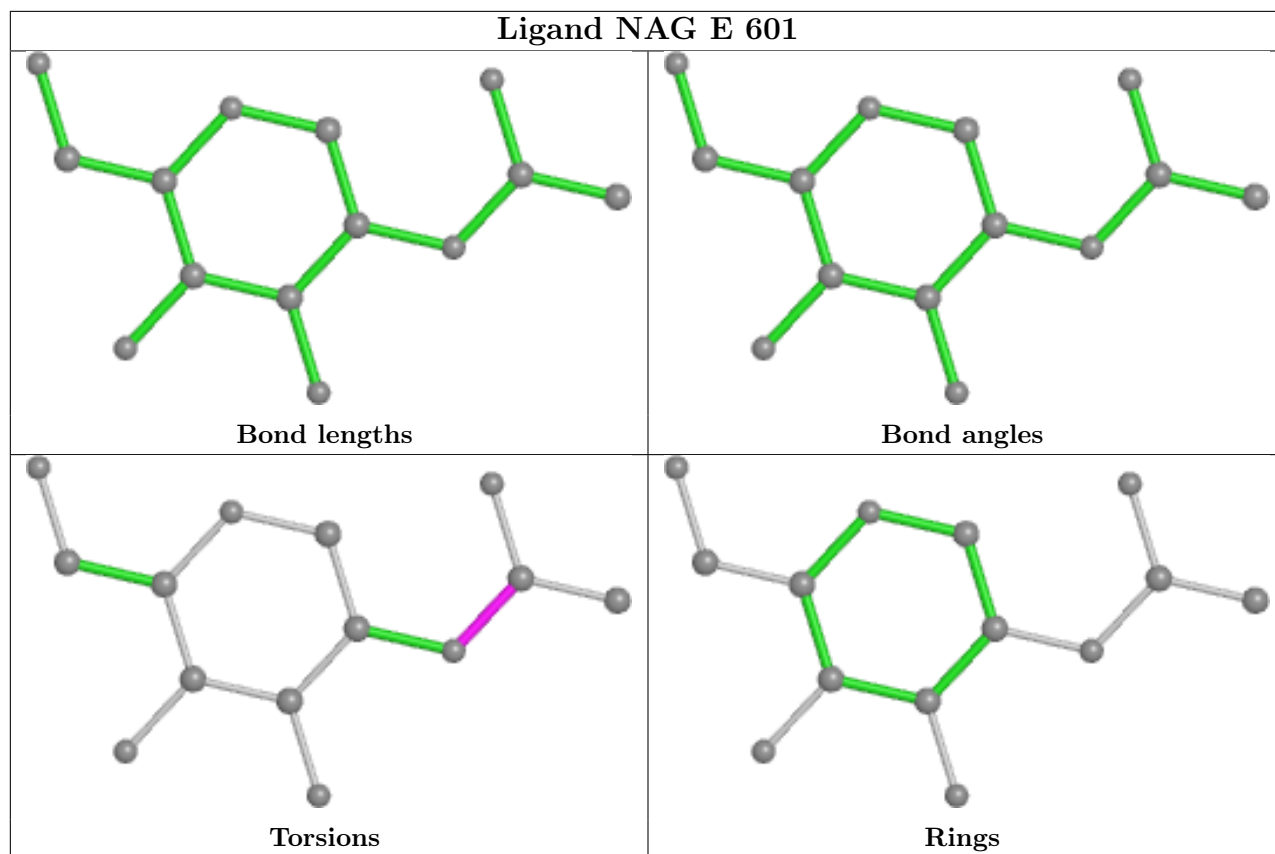
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	601	NAG	C8-C7-N2-C2
4	F	601	NAG	O7-C7-N2-C2
4	E	601	NAG	C8-C7-N2-C2
4	E	601	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	217/222 (97%)	0.09	7 (3%) 47 54	24, 33, 48, 65	0
1	C	217/222 (97%)	0.09	8 (3%) 41 48	24, 33, 51, 67	0
2	B	213/214 (99%)	-0.17	3 (1%) 75 78	20, 29, 41, 69	0
2	D	214/214 (100%)	0.09	12 (5%) 24 29	22, 31, 45, 70	0
3	E	176/195 (90%)	2.30	81 (46%) 0 0	31, 72, 103, 119	0
3	F	187/195 (95%)	3.00	100 (53%) 0 0	30, 82, 123, 140	0
All	All	1224/1262 (96%)	0.81	211 (17%) 1 1	20, 36, 100, 140	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	392	PHE	15.2
3	F	528	LYS	12.9
3	F	526	GLY	11.6
3	F	458	LYS	11.5
3	F	390	LEU	10.9
3	F	486	PHE	10.8
3	E	528	LYS	10.3
3	F	365	TYR	9.9
3	F	391	CYS	9.6
3	F	525	CYS	9.3
3	E	456	PHE	9.2
3	E	385	THR	8.9
3	E	369	TYR	8.9
3	F	479	PRO	8.7
3	F	477	SER	8.5
3	E	522	ALA	8.4
3	F	389	ASP	8.3
3	E	524	VAL	8.2
3	E	523	THR	8.0

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Mol	Chain	Res	Type	RSRZ
3	F	481	ASN	7.6
2	D	214	CYS	7.6
3	F	369	TYR	7.6
2	B	214	CYS	7.5
3	F	393	THR	7.4
3	F	413	GLY	7.2
3	E	527	PRO	7.2
3	F	475	ALA	7.2
3	F	366	SER	6.8
3	F	476	GLY	6.8
3	F	489	TYR	6.5
3	E	366	SER	6.5
3	F	523	THR	6.4
3	E	421	TYR	6.3
3	F	449	TYR	6.0
3	E	473	TYR	6.0
3	F	357	ARG	5.8
3	F	493	GLN	5.7
3	F	457	ARG	5.7
3	F	364	ASP	5.6
3	E	526	GLY	5.6
3	E	388	ASN	5.6
3	E	386	LYS	5.6
3	E	413	GLY	5.5
3	F	515	PHE	5.5
3	F	363	ALA	5.5
3	E	490	PHE	5.4
3	F	478	THR	5.4
3	F	516	GLU	5.3
3	F	367	VAL	5.2
3	F	524	VAL	5.1
3	F	394	ASN	5.1
3	F	482	GLY	5.0
3	F	370	ASN	5.0
3	F	466	ARG	5.0
3	E	428	ASP	4.9
3	E	383	SER	4.9
3	E	367	VAL	4.8
3	F	527	PRO	4.8
3	E	468	ILE	4.8
3	F	494	SER	4.8
3	E	370	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
3	E	391	CYS	4.7
3	E	474	GLN	4.6
3	F	453	TYR	4.6
3	E	475	ALA	4.4
3	F	360	ASN	4.4
3	F	471	GLU	4.4
3	F	361	CYS	4.4
3	F	371	SER	4.3
3	E	525	CYS	4.3
3	F	470	THR	4.3
3	E	471	GLU	4.3
3	E	457	ARG	4.2
3	F	472	ILE	4.2
3	E	469	SER	4.2
3	F	368	LEU	4.2
3	E	396	TYR	4.1
3	F	356	LYS	4.1
2	D	96	LEU	4.0
3	F	490	PHE	3.9
1	A	138	LYS	3.9
3	F	418	ILE	3.8
3	F	362	VAL	3.8
3	F	340	GLU	3.8
3	E	418	ILE	3.8
3	F	337	PRO	3.8
1	A	199	GLY	3.8
3	E	472	ILE	3.7
3	F	386	LYS	3.7
3	E	392	PHE	3.7
3	F	483	VAL	3.7
1	C	1	GLN	3.7
3	E	462	LYS	3.7
3	F	455	LEU	3.7
3	E	455	LEU	3.6
3	E	510	VAL	3.6
3	F	388	ASN	3.6
1	A	58	TYR	3.5
3	E	372	ALA	3.5
3	F	487	ASN	3.5
1	A	137	SER	3.5
3	F	385	THR	3.5
1	C	221	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
3	E	357	ARG	3.4
3	F	464	PHE	3.4
3	E	364	ASP	3.4
3	F	484	GLU	3.4
3	F	462	LYS	3.4
3	F	488	CYS	3.4
3	E	445	VAL	3.4
3	F	380	TYR	3.3
3	F	415	THR	3.3
3	E	401	VAL	3.3
3	E	410	ILE	3.3
3	E	458	LYS	3.2
3	F	396	TYR	3.2
3	E	491	PRO	3.2
3	E	505	TYR	3.2
3	F	382	VAL	3.2
3	F	359	SER	3.2
3	F	473	TYR	3.2
3	F	387	LEU	3.2
3	E	381	GLY	3.1
3	E	461	LEU	3.1
3	F	429	PHE	3.1
3	E	380	TYR	3.1
3	E	512	VAL	3.1
3	E	393	THR	3.1
3	F	350	VAL	3.1
3	F	355	ARG	3.1
3	F	428	ASP	3.1
3	E	382	VAL	3.1
3	F	459	SER	3.0
1	C	37	VAL	2.9
3	E	407	VAL	2.9
3	F	430	THR	2.9
3	E	493	GLN	2.9
3	E	459	SER	2.9
3	F	485	GLY	2.9
3	F	480	CYS	2.9
3	E	371	SER	2.9
3	F	384	PRO	2.9
3	F	400	PHE	2.8
3	E	384	PRO	2.8
1	C	45	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	F	452	LEU	2.8
3	E	415	THR	2.8
3	F	381	GLY	2.8
3	F	426	PRO	2.7
3	E	429	PHE	2.7
3	E	470	THR	2.7
3	E	363	ALA	2.7
2	D	94	TYR	2.7
1	C	109	PHE	2.7
3	E	463	PRO	2.7
3	F	408	ARG	2.7
3	F	505	TYR	2.6
3	F	511	VAL	2.6
3	E	390	LEU	2.6
1	A	1	GLN	2.6
3	F	463	PRO	2.6
1	C	47	TRP	2.6
3	F	395	VAL	2.6
3	F	401	VAL	2.5
2	D	213	GLU	2.5
3	F	423	TYR	2.5
1	C	138	LYS	2.5
2	D	56	SER	2.5
3	E	356	LYS	2.5
3	F	450	ASN	2.5
3	E	419	ALA	2.5
3	E	359	SER	2.4
3	E	389	ASP	2.4
3	F	512	VAL	2.4
3	E	431	GLY	2.4
3	F	492	LEU	2.4
3	E	395	VAL	2.4
3	E	508	TYR	2.4
3	F	510	VAL	2.4
3	F	336	CYS	2.3
3	F	434	ILE	2.3
2	B	91	TYR	2.3
3	F	351	TYR	2.3
3	E	416	GLY	2.3
3	F	468	ILE	2.3
3	F	405	ASP	2.3
3	E	460	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	417	LYS	2.3
2	D	98	PHE	2.2
3	E	427	ASP	2.2
2	D	63	ARG	2.2
2	B	63	ARG	2.2
2	D	97	THR	2.2
3	E	339	GLY	2.2
3	E	402	ILE	2.2
3	E	338	PHE	2.2
3	E	464	PHE	2.2
1	A	109	PHE	2.1
3	E	365	TYR	2.1
1	A	37	VAL	2.1
3	E	511	VAL	2.1
3	F	427	ASP	2.1
3	E	400	PHE	2.1
3	F	433	VAL	2.1
2	D	88	CYS	2.1
3	E	449	TYR	2.0
2	D	122	ASP	2.0
1	C	147	LEU	2.0
3	E	515	PHE	2.0
2	D	133	VAL	2.0
2	D	212	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](#)

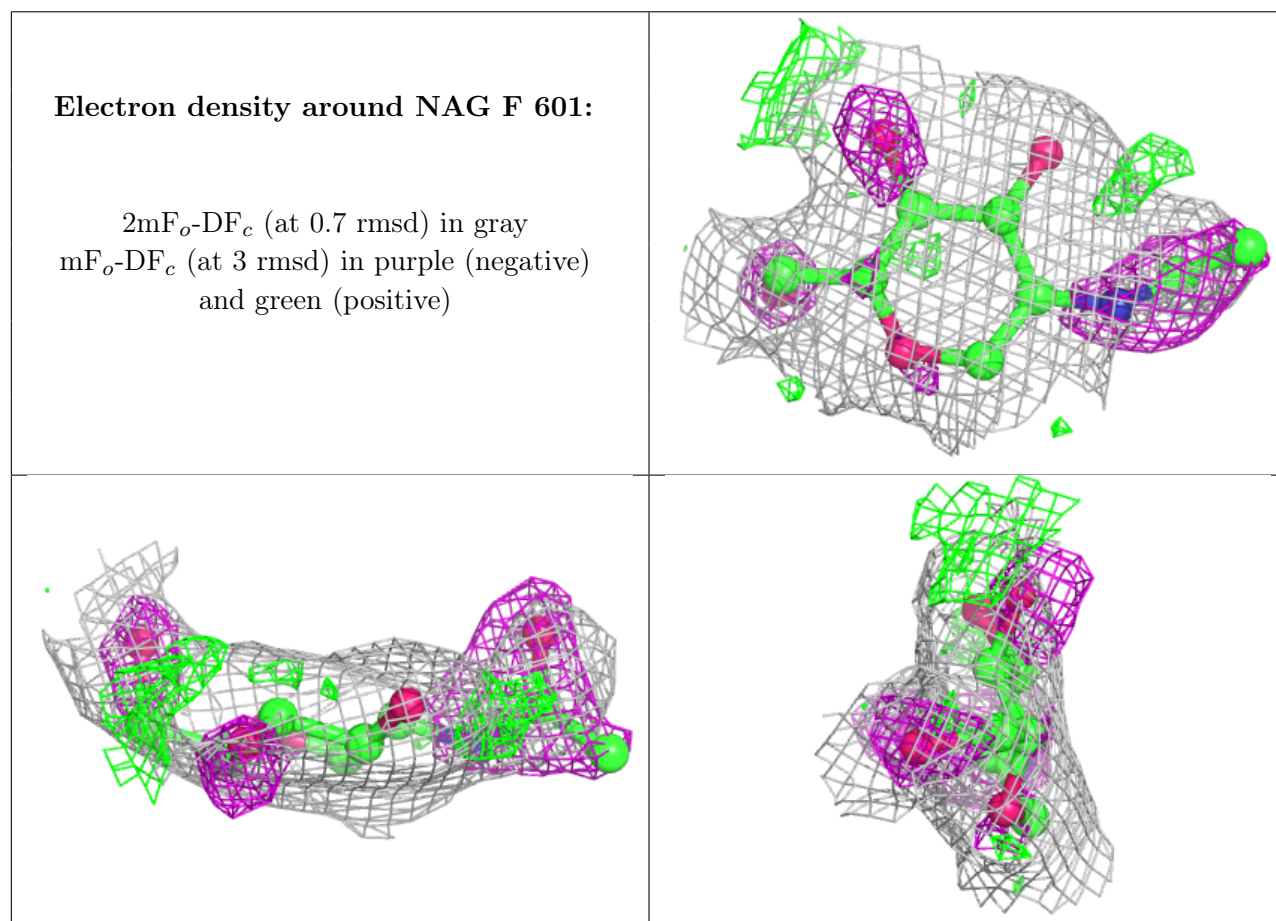
There are no monosaccharides in this entry.

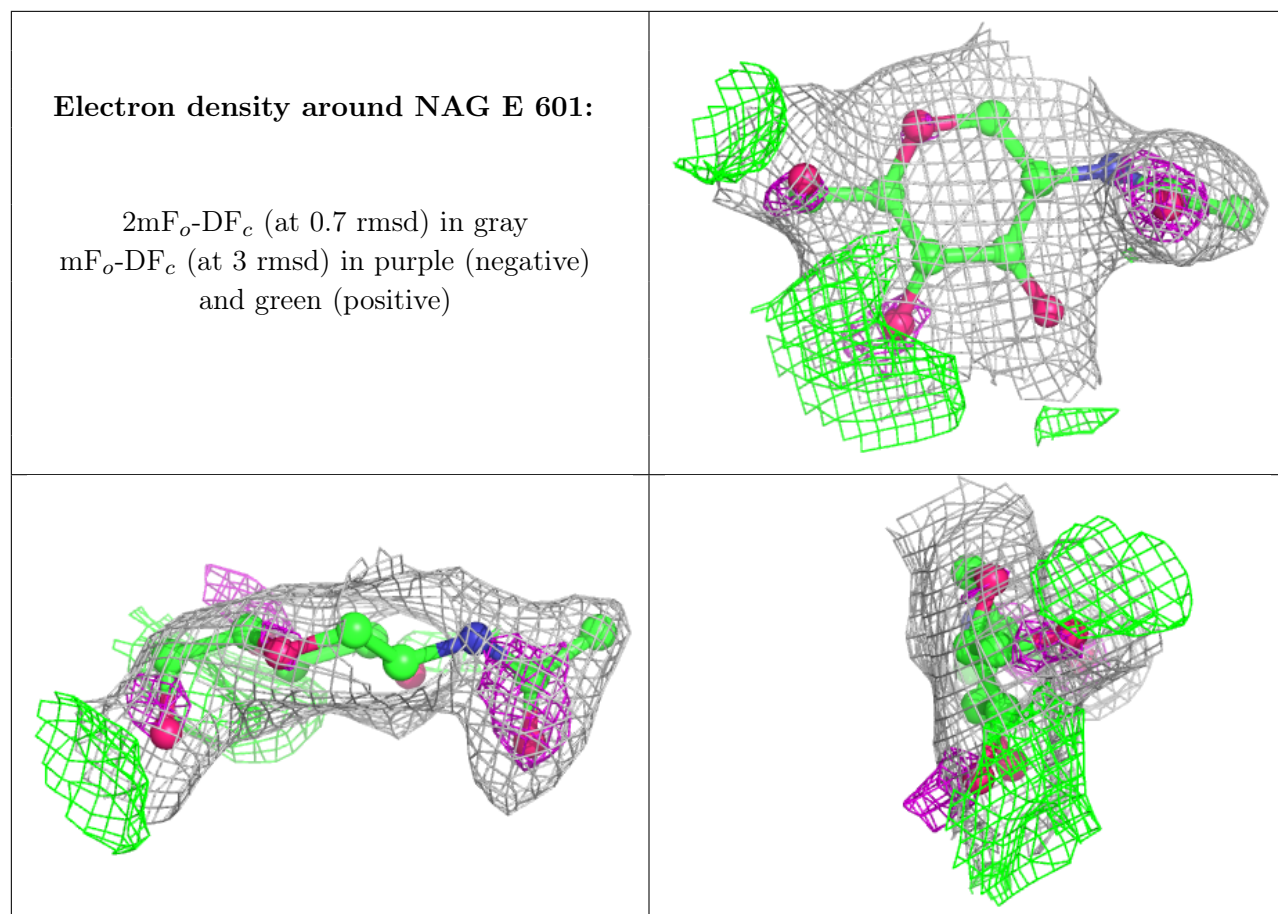
6.4 Ligands [i](#)

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, 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(\AA^2)	Q<0.9
4	NAG	F	601	14/15	0.75	0.29	30,30,30,30	0
4	NAG	E	601	14/15	0.87	0.20	30,30,30,30	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.