



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:27 AM UTC

PDB ID : 7X2H / pdb_00007x2h
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	:	4-5-2 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

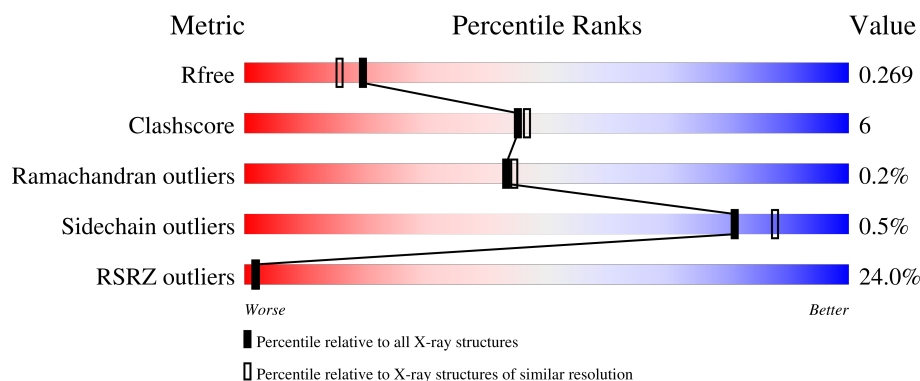
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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	
1	C	222	
2	B	214	
2	D	214	
3	E	195	

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Mol	Chain	Length	Quality of chain
3	F	195	79% 73%22% . .

2 Entry composition

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
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
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
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 (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

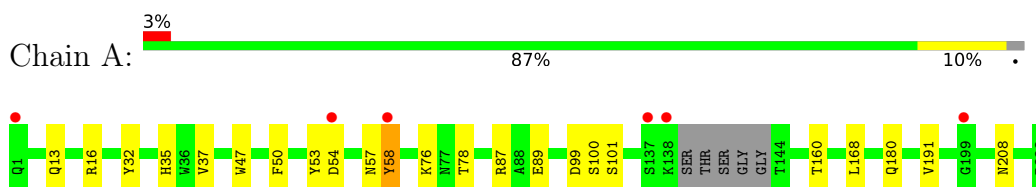
- Molecule 5 is water.

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

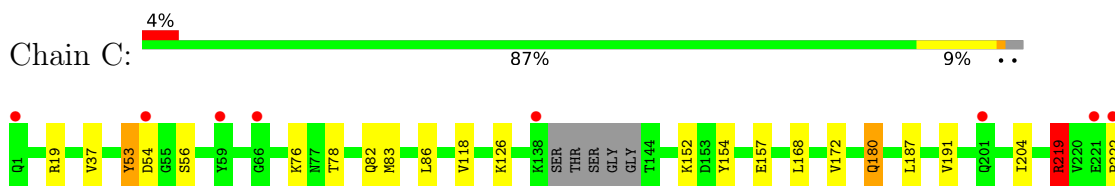
3 Residue-property plots [i](#)

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.

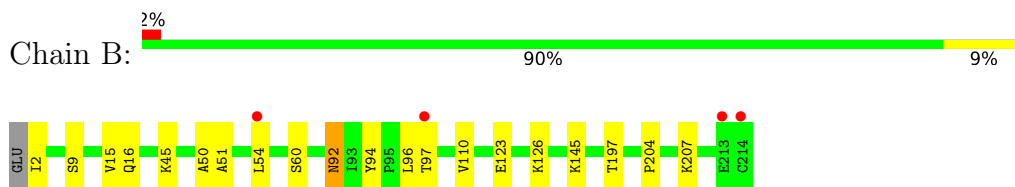
- Molecule 1: 6-2C H chain



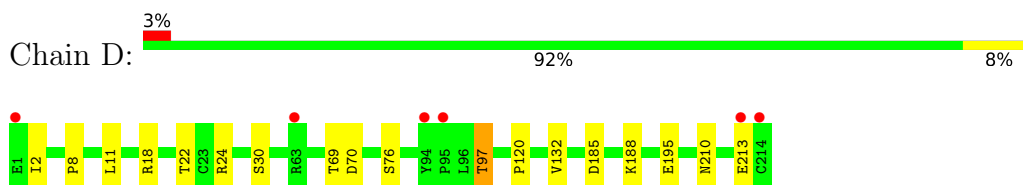
- Molecule 1: 6-2C H chain



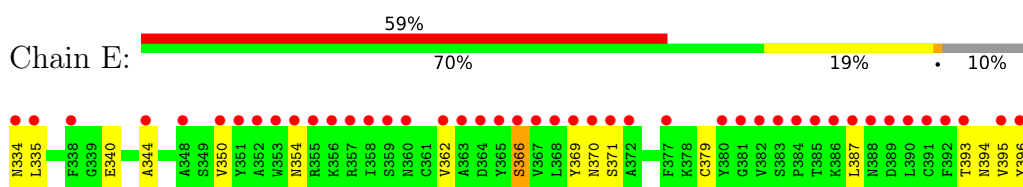
- Molecule 2: 6-2C L chain

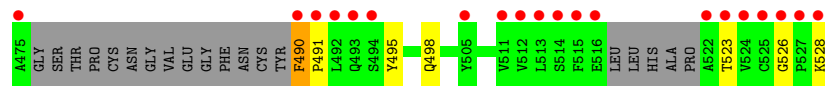
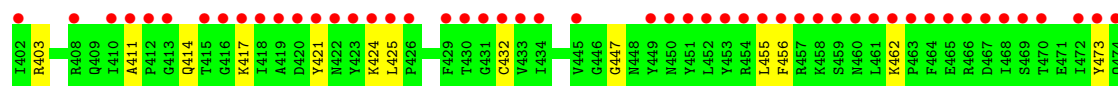


- Molecule 2: 6-2C L chain

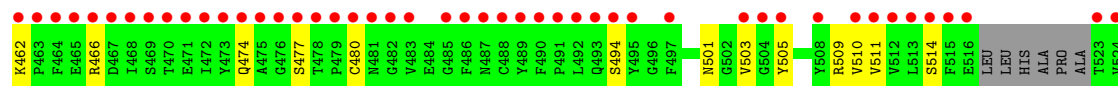
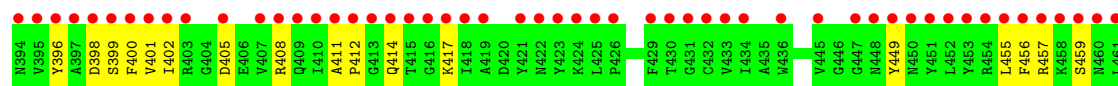
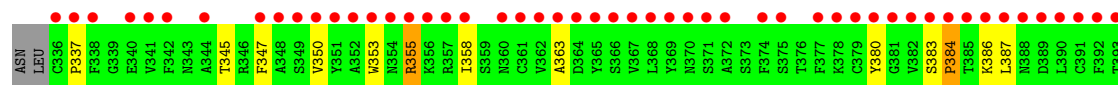
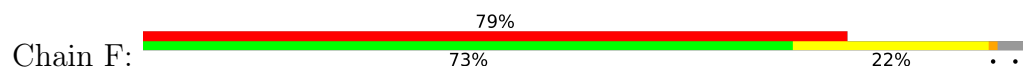


- Molecule 3: Spike protein S1





● 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) 99.2 (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)	Xtriage
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 (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

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	0.43	0/1713	0.67	1/2337 (0.0%)
1	C	0.40	0/1713	0.75	5/2337 (0.2%)
2	B	0.51	0/1675	0.75	1/2276 (0.0%)
2	D	0.48	0/1684	0.77	0/2288
3	E	0.40	0/1445	0.71	0/1961
3	F	0.48	0/1527	0.85	2/2074 (0.1%)
All	All	0.45	0/9757	0.75	9/13273 (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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	355	ARG	CB-CA-C	-10.18	89.20	109.35
1	C	222	PRO	N-CA-C	-6.65	95.48	112.10
1	C	53	TYR	CA-C-N	6.26	128.96	120.38
1	C	53	TYR	C-N-CA	6.26	128.96	120.38
1	C	180	GLN	CA-CB-CG	6.04	126.19	114.10
2	B	94	TYR	CB-CA-C	5.90	118.68	109.42
1	A	180	GLN	CA-CB-CG	-5.79	102.52	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	456	PHE	CA-CB-CG	5.54	119.34	113.80
1	C	219	ARG	NE-CZ-NH1	-5.15	116.35	121.50

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	14	0
2	B	1640	0	1608	14	0
2	D	1649	0	1617	11	0
3	E	1408	0	1341	25	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	3	0
5	C	104	0	0	1	0
5	D	126	0	0	0	0
5	E	11	0	0	0	0
5	F	2	0	0	2	0
All	All	10021	0	9195	110	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 (110) 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
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
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: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
2:B:207:LYS:NZ	5:B:305:HOH:O	2.33	0.51
3:E:455:LEU:HB3	3:E:456:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:SER:OG	2:D:195:GLU:OE2	2.30	0.50
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
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: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
3:E:369:TYR:C	3:E:371:SER:H	2.21	0.48
1:A:53:TYR:CZ	1:A:54:ASP:OD1	2.67	0.48
2:B:45:LYS:NZ	5:B:307:HOH:O	2.37	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
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
1:A:32:TYR:CE2	1:A:100:SER:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:ALA:O	2:B:51:ALA:HB3	2.18	0.43
2:D:185:ASP:HA	2:D:188:LYS:HZ3	1.82	0.43
1:C:83:MET:HB3	1:C:86:LEU:HD21	1.99	0.43
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
1:C:187:LEU:HD12	1:C:187:LEU:C	2.43	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
1:C:83:MET:HE1	1:C:118:VAL:HG21	2.01	0.42
3:E:395:VAL:C	3:E:396:TYR:HD1	2.26	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
1:C:154:TYR:OH	1:C:157:GLU:OE2	2.35	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

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	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
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%)	21	18
3	F	183/195 (94%)	171 (93%)	11 (6%)	1 (0%)	24	22
All	All	1202/1262 (95%)	1152 (96%)	48 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

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

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	187/190 (98%)	186 (100%)	1 (0%)	81	88
1	C	187/190 (98%)	186 (100%)	1 (0%)	81	88
2	B	187/188 (100%)	186 (100%)	1 (0%)	81	88
2	D	188/188 (100%)	187 (100%)	1 (0%)	81	88
3	E	153/168 (91%)	152 (99%)	1 (1%)	76	83
3	F	162/168 (96%)	162 (100%)	0	100	100
All	All	1064/1092 (97%)	1059 (100%)	5 (0%)	81	88

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

Mol	Chain	Res	Type
1	A	37	VAL
2	B	92	ASN
1	C	37	VAL
2	D	97	THR
3	E	366	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	201	GLN
2	B	38	GLN
2	B	92	ASN
2	B	189	HIS
1	C	3	GLN
1	C	180	GLN
1	C	201	GLN
2	D	37	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 oligosaccharides 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	F	601	3	14,14,15	0.26	0	17,19,21	0.62	0
4	NAG	E	601	3	14,14,15	0.27	0	17,19,21	0.62	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	E	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:

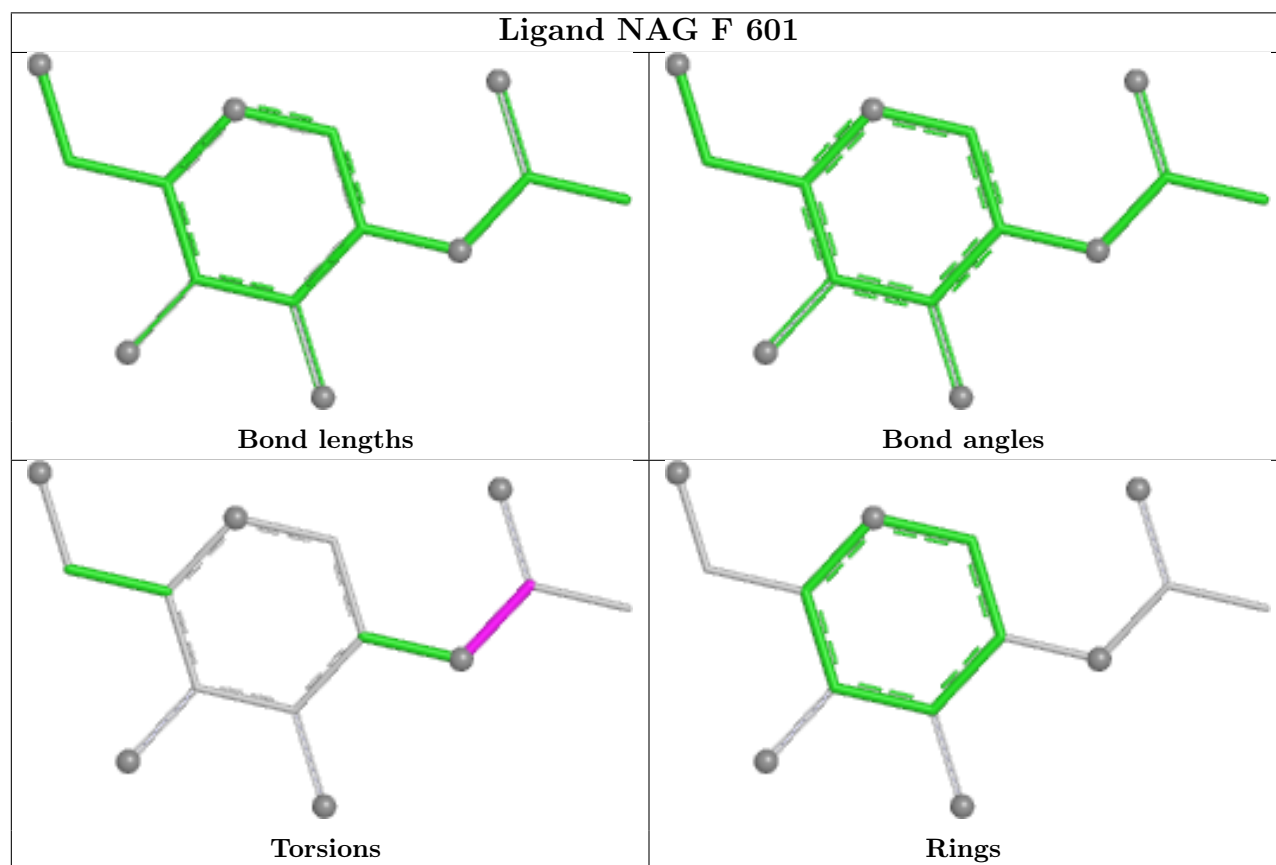
Mol	Chain	Res	Type	Atoms
4	F	601	NAG	C8-C7-N2-C2
4	F	601	NAG	O7-C7-N2-C2
4	E	601	NAG	C8-C7-N2-C2
4	E	601	NAG	O7-C7-N2-C2

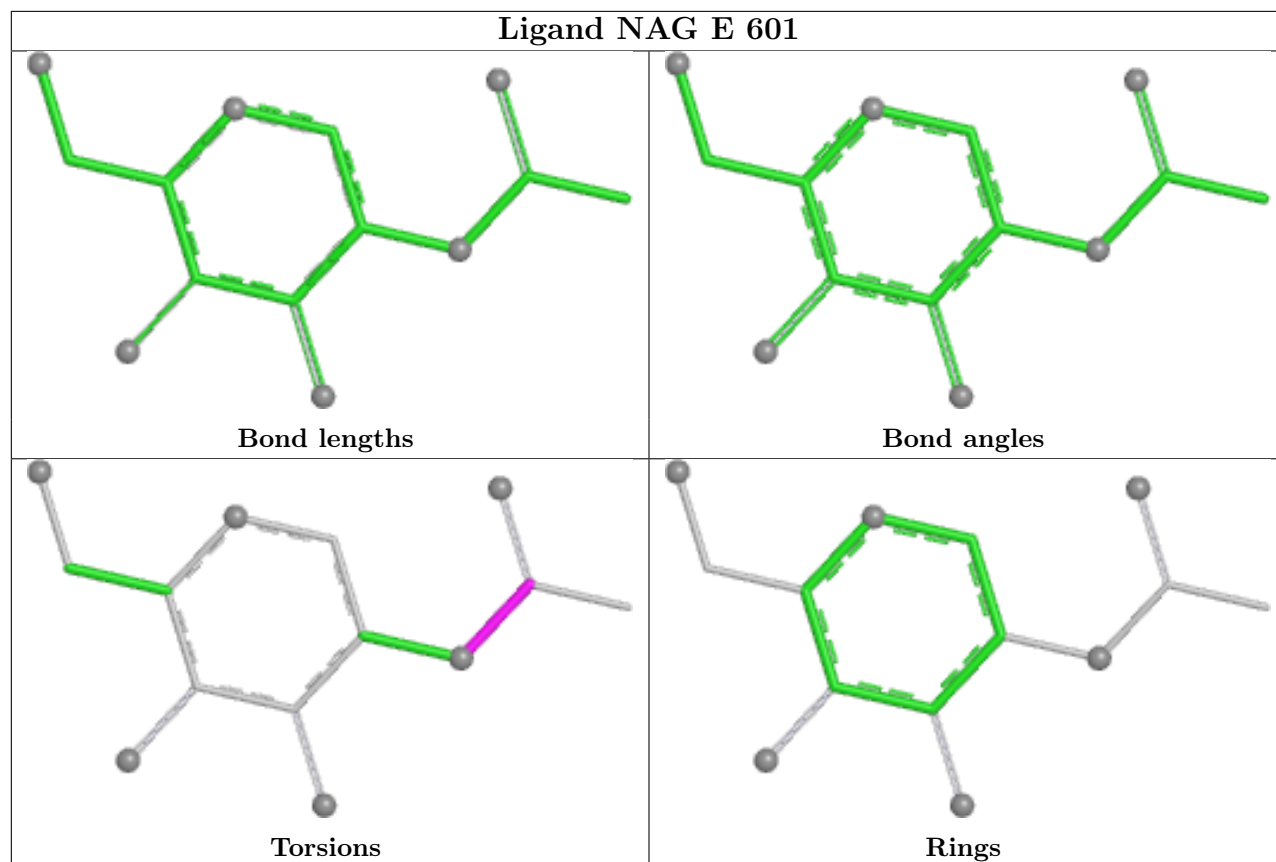
There are no ring outliers.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/222 (97%)	0.19	6 (2%) 55 57	24, 33, 48, 65	0
1	C	217/222 (97%)	0.28	8 (3%) 45 47	24, 33, 51, 67	0
2	B	213/214 (99%)	-0.01	4 (1%) 66 69	20, 29, 41, 69	0
2	D	214/214 (100%)	0.13	6 (2%) 55 57	22, 31, 45, 70	0
3	E	176/195 (90%)	2.52	115 (65%) 0 0	31, 72, 103, 119	0
3	F	187/195 (95%)	3.11	155 (82%) 0 0	30, 82, 123, 140	0
All	All	1224/1262 (96%)	0.94	294 (24%) 2 2	20, 36, 100, 140	0

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	392	PHE	9.7
3	E	456	PHE	8.9
3	F	365	TYR	8.7
3	F	390	LEU	7.3
3	E	472	ILE	7.2
3	F	413	GLY	7.0
3	E	369	TYR	6.4
3	F	475	ALA	6.2
3	F	368	LEU	6.0
3	E	421	TYR	6.0
3	F	369	TYR	5.9
3	E	475	ALA	5.7
3	E	473	TYR	5.7
3	E	455	LEU	5.7
3	F	515	PHE	5.7
3	F	389	ASP	5.6
3	E	522	ALA	5.5
3	F	363	ALA	5.3
3	F	489	TYR	5.3

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Mol	Chain	Res	Type	RSRZ
3	E	490	PHE	5.2
3	F	453	TYR	5.2
3	E	524	VAL	5.2
3	E	464	PHE	5.1
3	F	525	CYS	5.1
3	F	367	VAL	5.1
3	F	478	THR	5.0
3	F	476	GLY	5.0
3	F	350	VAL	4.9
3	F	486	PHE	4.9
3	F	481	ASN	4.9
3	F	461	LEU	4.8
3	E	390	LEU	4.8
3	F	384	PRO	4.7
3	F	458	LYS	4.7
3	F	396	TYR	4.7
3	F	418	ILE	4.7
3	F	393	THR	4.6
3	E	491	PRO	4.6
3	E	392	PHE	4.5
3	F	485	GLY	4.5
3	F	356	LYS	4.5
3	F	526	GLY	4.4
3	F	395	VAL	4.4
3	E	367	VAL	4.4
3	F	371	SER	4.4
3	F	483	VAL	4.3
3	E	463	PRO	4.3
3	F	468	ILE	4.3
3	F	472	ILE	4.3
3	F	466	ARG	4.2
3	E	387	LEU	4.2
3	E	417	LYS	4.1
3	F	387	LEU	4.1
3	E	416	GLY	4.0
3	E	523	THR	4.0
3	F	362	VAL	4.0
3	F	400	PHE	4.0
3	F	493	GLN	4.0
3	F	470	THR	3.9
3	F	523	THR	3.9
3	F	464	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
3	F	452	LEU	3.9
3	F	473	TYR	3.9
3	E	415	THR	3.9
3	F	524	VAL	3.9
3	F	492	LEU	3.9
3	F	429	PHE	3.8
3	E	526	GLY	3.8
3	F	455	LEU	3.8
3	F	353	TRP	3.8
3	F	482	GLY	3.8
3	F	391	CYS	3.8
3	E	452	LEU	3.8
3	F	490	PHE	3.8
3	F	528	LYS	3.8
3	E	395	VAL	3.8
3	E	410	ILE	3.7
3	E	418	ILE	3.7
3	E	527	PRO	3.7
3	E	468	ILE	3.7
3	E	382	VAL	3.7
3	F	456	PHE	3.7
3	E	351	TYR	3.7
1	A	1	GLN	3.7
3	E	492	LEU	3.6
3	F	382	VAL	3.6
3	E	457	ARG	3.6
3	E	515	PHE	3.6
3	E	344	ALA	3.6
3	E	461	LEU	3.6
3	F	380	TYR	3.6
3	E	528	LYS	3.6
3	F	503	VAL	3.6
3	E	423	TYR	3.6
3	F	449	TYR	3.6
3	F	344	ALA	3.6
2	D	214	CYS	3.6
3	E	396	TYR	3.6
3	F	385	THR	3.5
3	E	363	ALA	3.5
3	F	491	PRO	3.5
3	F	421	TYR	3.5
3	F	401	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
3	E	429	PHE	3.5
3	F	480	CYS	3.5
3	E	385	THR	3.5
3	F	477	SER	3.5
3	F	351	TYR	3.5
3	F	479	PRO	3.4
3	F	415	THR	3.4
3	F	388	ASN	3.4
3	F	358	ILE	3.4
3	F	459	SER	3.4
3	F	433	VAL	3.4
3	F	337	PRO	3.4
3	F	513	LEU	3.4
3	E	516	GLU	3.3
3	F	505	TYR	3.3
3	E	413	GLY	3.3
3	F	463	PRO	3.3
3	E	358	ILE	3.3
3	E	391	CYS	3.3
3	F	512	VAL	3.3
3	F	398	ASP	3.3
3	E	512	VAL	3.3
3	E	425	LEU	3.3
3	F	487	ASN	3.3
3	F	416	GLY	3.2
3	E	352	ALA	3.2
3	E	338	PHE	3.2
3	E	381	GLY	3.2
3	F	423	TYR	3.2
3	E	514	SER	3.2
3	F	430	THR	3.2
3	E	525	CYS	3.2
3	F	419	ALA	3.2
3	F	386	LYS	3.2
3	F	445	VAL	3.1
3	F	457	ARG	3.1
3	F	527	PRO	3.1
3	F	352	ALA	3.1
3	F	407	VAL	3.1
3	F	510	VAL	3.1
1	A	58	TYR	3.1
3	F	495	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
3	E	356	LYS	3.1
3	F	424	LYS	3.1
3	E	474	GLN	3.1
3	E	493	GLN	3.1
3	F	431	GLY	3.1
3	F	394	ASN	3.1
3	E	453	TYR	3.0
3	F	354	ASN	3.0
3	F	469	SER	3.0
3	E	372	ALA	3.0
3	F	366	SER	3.0
3	F	408	ARG	3.0
3	F	454	ARG	3.0
1	C	221	GLU	3.0
3	E	393	THR	3.0
1	C	222	PRO	3.0
3	F	357	ARG	2.9
3	E	458	LYS	2.9
3	E	398	ASP	2.9
3	F	342	PHE	2.9
3	F	494	SER	2.9
3	E	462	LYS	2.9
3	F	511	VAL	2.8
3	F	516	GLU	2.8
3	E	459	SER	2.8
3	F	411	ALA	2.8
3	E	424	LYS	2.8
3	E	454	ARG	2.8
1	A	54	ASP	2.8
3	E	354	ASN	2.8
3	E	366	SER	2.8
2	D	95	PRO	2.8
3	F	425	LEU	2.7
1	C	1	GLN	2.7
3	E	334	ASN	2.7
3	F	450	ASN	2.7
3	E	467	ASP	2.7
3	F	364	ASP	2.7
3	F	397	ALA	2.7
3	F	497	PHE	2.7
3	E	357	ARG	2.7
3	E	470	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	426	PRO	2.7
3	E	460	ASN	2.7
3	F	471	GLU	2.7
1	A	137	SER	2.7
2	B	213	GLU	2.6
3	E	359	SER	2.6
3	F	399	SER	2.6
1	A	138	LYS	2.6
3	F	402	ILE	2.6
2	D	1	GLU	2.6
3	F	436	TRP	2.6
3	E	411	ALA	2.6
3	F	448	ASN	2.6
3	E	449	TYR	2.6
3	F	361	CYS	2.6
3	E	431	GLY	2.6
3	E	388	ASN	2.6
3	F	412	PRO	2.6
3	F	426	PRO	2.6
3	E	377	PHE	2.6
3	E	420	ASP	2.6
3	F	338	PHE	2.6
3	F	355	ARG	2.6
3	E	434	ILE	2.6
3	F	336	CYS	2.6
3	E	408	ARG	2.6
3	E	445	VAL	2.5
3	F	488	CYS	2.5
3	E	430	THR	2.5
3	E	412	PRO	2.5
3	E	335	LEU	2.5
3	F	378	LYS	2.5
3	E	422	ASN	2.5
3	F	432	CYS	2.5
3	F	467	ASP	2.5
3	F	462	LYS	2.5
3	E	350	VAL	2.5
3	E	433	VAL	2.5
3	F	341	VAL	2.5
3	E	505	TYR	2.5
3	E	353	TRP	2.5
3	F	422	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	465	GLU	2.4
1	C	59	TYR	2.4
3	E	380	TYR	2.4
3	E	362	VAL	2.4
3	E	466	ARG	2.4
1	A	199	GLY	2.4
3	F	405	ASP	2.4
3	E	383	SER	2.4
3	F	410	ILE	2.4
3	E	371	SER	2.4
3	F	474	GLN	2.3
3	F	370	ASN	2.3
3	F	377	PHE	2.3
3	F	403	ARG	2.3
3	F	508	TYR	2.3
3	F	360	ASN	2.3
3	F	514	SER	2.3
3	F	434	ILE	2.3
2	D	213	GLU	2.3
3	E	494	SER	2.3
1	C	201	GLN	2.3
3	F	460	ASN	2.3
2	B	214	CYS	2.3
3	E	419	ALA	2.3
3	E	513	LEU	2.3
2	D	94	TYR	2.3
3	E	469	SER	2.2
3	E	384	PRO	2.2
3	E	511	VAL	2.2
3	E	360	ASN	2.2
3	E	348	ALA	2.2
3	F	504	GLY	2.2
3	E	368	LEU	2.2
2	D	63	ARG	2.2
3	F	347	PHE	2.2
1	C	54	ASP	2.2
3	F	409	GLN	2.2
3	F	349	SER	2.2
1	C	138	LYS	2.2
3	E	402	ILE	2.2
3	F	348	ALA	2.2
3	F	375	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	365	TYR	2.2
3	F	451	TYR	2.2
2	B	97	THR	2.2
3	F	374	PHE	2.1
3	F	414	GLN	2.1
3	E	451	TYR	2.1
1	C	66	GLY	2.1
3	F	372	ALA	2.1
2	B	54	LEU	2.1
3	E	432	CYS	2.1
3	F	383	SER	2.1
3	F	381	GLY	2.1
3	E	389	ASP	2.1
3	E	355	ARG	2.1
3	F	465	GLU	2.0
3	E	370	ASN	2.0
3	E	364	ASP	2.0
3	F	340	GLU	2.0
3	E	450	ASN	2.0
3	F	379	CYS	2.0
3	E	386	LYS	2.0
3	F	417	LYS	2.0
3	F	447	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

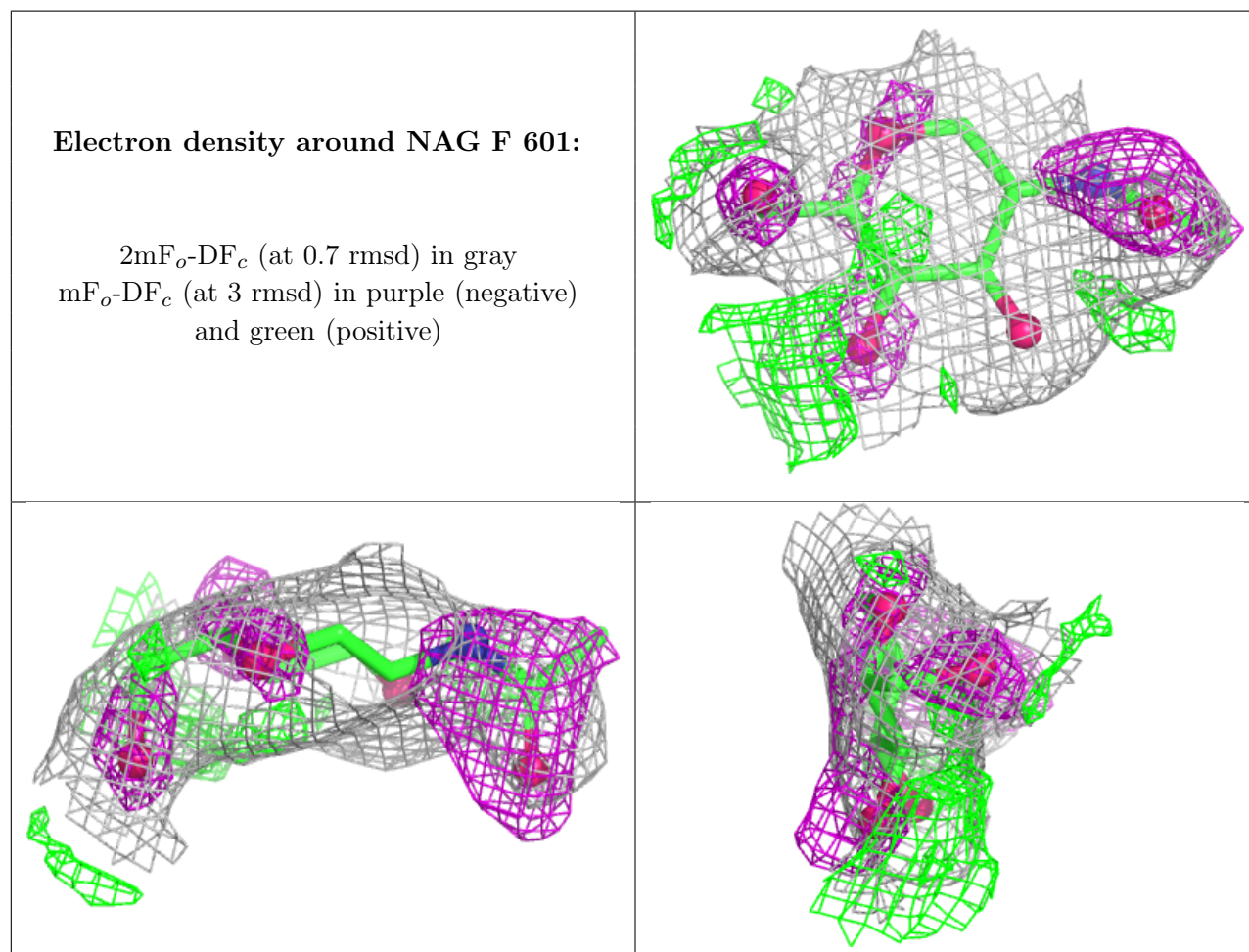
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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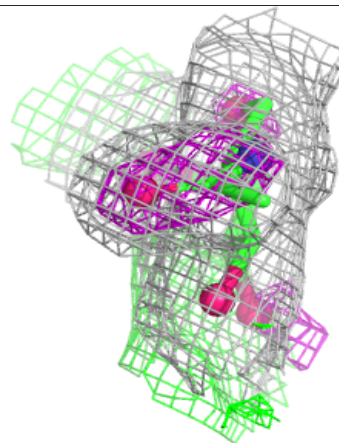
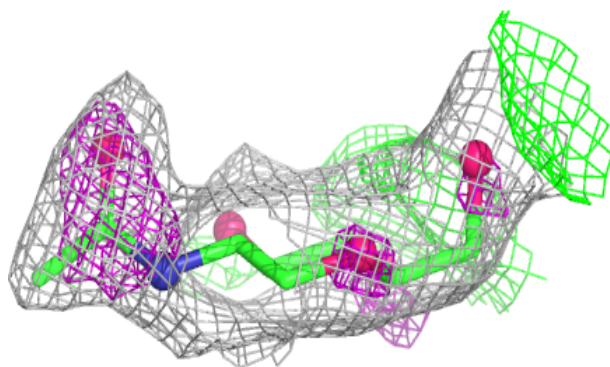
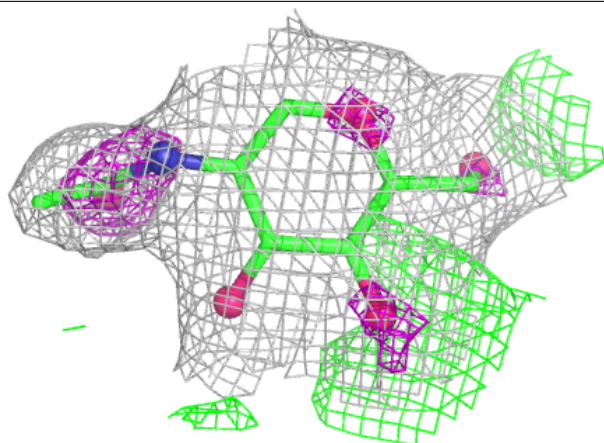
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	601	14/15	0.62	0.16	30,30,30,30	0
4	NAG	E	601	14/15	0.77	0.12	30,30,30,30	0

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.



Electron density around NAG E 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.