Full wwPDB X-ray Structure Validation Report ⓘ

Nov 27, 2023 – 01:44 PM JST

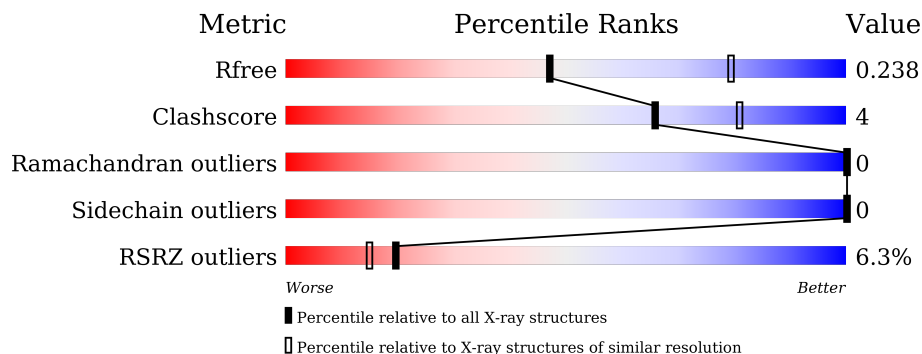|		
PDB ID	:	7Y0F
Title	:	Crystal structure of TMPRSS2 in complex with UK-371804
Authors	:	Wang, H.; Duan, Y.; Liu, X.; Sun, L.; Yang, H.
Deposited on	:	2022-06-04
Resolution	:	2.60 Å(reported)

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 2.60 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.238
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		6.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	146	8% / 79% / 9% / 12%
1	B	146	24% / 82% / • / 14%
2	C	249	87% / 10% / •
2	D	249	88% / 7% / 5%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 5724 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 Transmembrane protease serine 2 catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	0	0
			974	593	174	195	12			
1	B	126	Total	C	N	O	S	0	0	0
			912	563	158	178	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	ASP	SER	engineered mutation	UNP O15393
A	251	ASP	SER	engineered mutation	UNP O15393
A	252	ASP	ARG	engineered mutation	UNP O15393
A	253	ASP	GLN	engineered mutation	UNP O15393
A	254	LYS	SER	engineered mutation	UNP O15393
B	250	ASP	SER	engineered mutation	UNP O15393
B	251	ASP	SER	engineered mutation	UNP O15393
B	252	ASP	ARG	engineered mutation	UNP O15393
B	253	ASP	GLN	engineered mutation	UNP O15393
B	254	LYS	SER	engineered mutation	UNP O15393

- Molecule 2 is a protein called Transmembrane protease serine 2 catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	242	Total	C	N	O	S	0	0	0
			1867	1199	316	337	15			
2	D	237	Total	C	N	O	S	0	0	0
			1799	1155	303	326	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	493	GLU	-	expression tag	UNP O15393
C	494	PHE	-	expression tag	UNP O15393

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	495	VAL	-	expression tag	UNP O15393
C	496	GLU	-	expression tag	UNP O15393
C	497	HIS	-	expression tag	UNP O15393
C	498	HIS	-	expression tag	UNP O15393
C	499	HIS	-	expression tag	UNP O15393
C	500	HIS	-	expression tag	UNP O15393
C	501	HIS	-	expression tag	UNP O15393
C	502	HIS	-	expression tag	UNP O15393
C	503	HIS	-	expression tag	UNP O15393
C	504	HIS	-	expression tag	UNP O15393
D	493	GLU	-	expression tag	UNP O15393
D	494	PHE	-	expression tag	UNP O15393
D	495	VAL	-	expression tag	UNP O15393
D	496	GLU	-	expression tag	UNP O15393
D	497	HIS	-	expression tag	UNP O15393
D	498	HIS	-	expression tag	UNP O15393
D	499	HIS	-	expression tag	UNP O15393
D	500	HIS	-	expression tag	UNP O15393
D	501	HIS	-	expression tag	UNP O15393
D	502	HIS	-	expression tag	UNP O15393
D	503	HIS	-	expression tag	UNP O15393
D	504	HIS	-	expression tag	UNP O15393

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
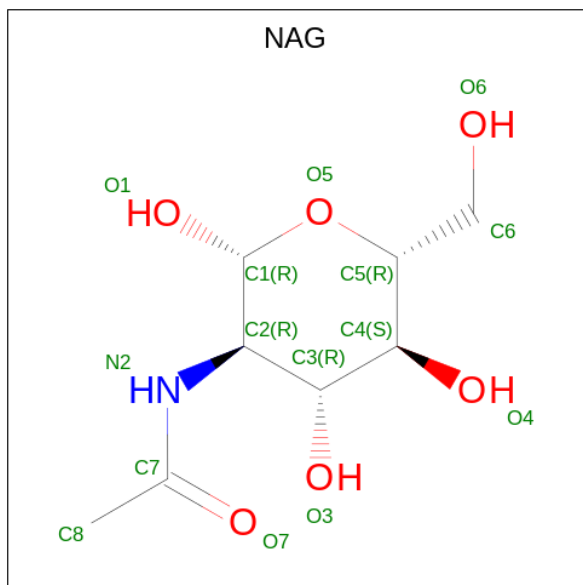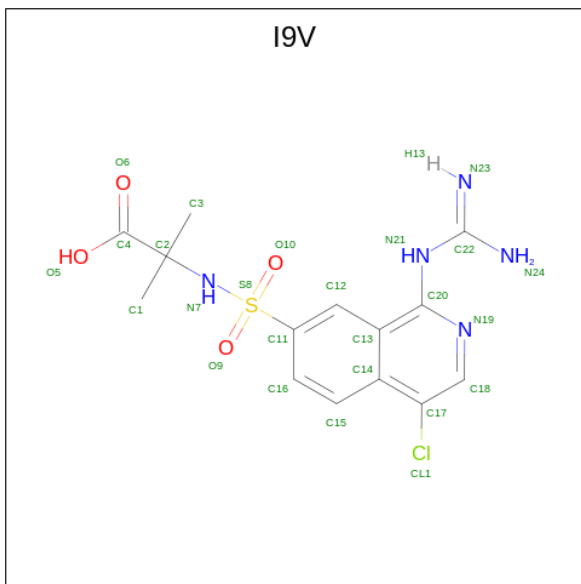
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	B	1	Total 1	Ca 1	0	0

- Molecule 5 is 2-[(1-carbamimidamido-4-chloranyl-isoquinolin-7-yl)sulfonylamino]-2-methyl-propanoic acid (three-letter code: I9V) (formula: $C_{14}H_{16}ClN_5O_4S$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total 25	C 14	Cl 1	N 5	O 4	S 1	0	0
5	D	1	Total 25	C 14	Cl 1	N 5	O 4	S 1	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total 12	O 12	0	0
6	C	34	Total 34	O 34	0	0
6	B	4	Total 4	O 4	0	0
6	D	42	Total 42	O 42	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
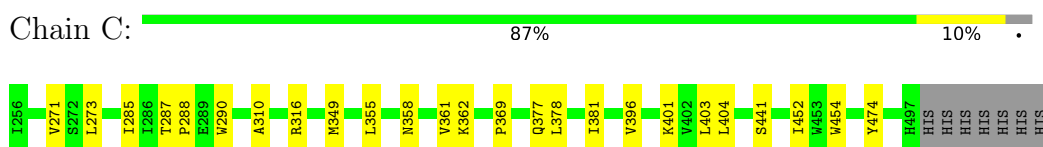
- Molecule 1: Transmembrane protease serine 2 catalytic chain
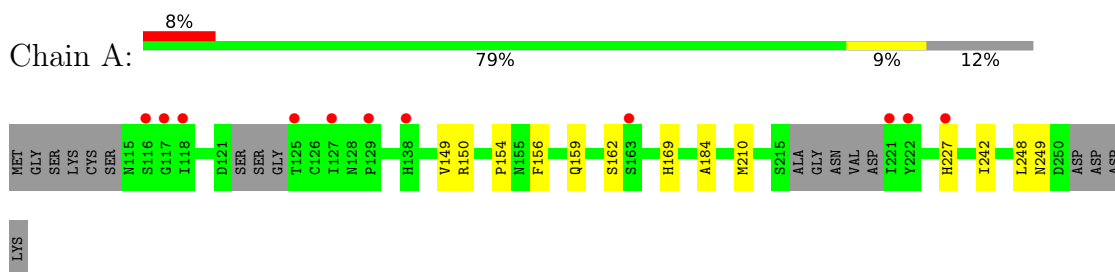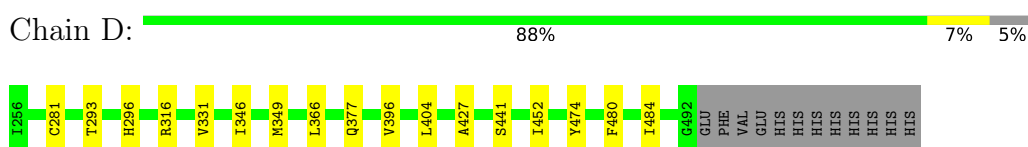
Chain A:

- Molecule 1: Transmembrane protease serine 2 catalytic chain

Chain B:
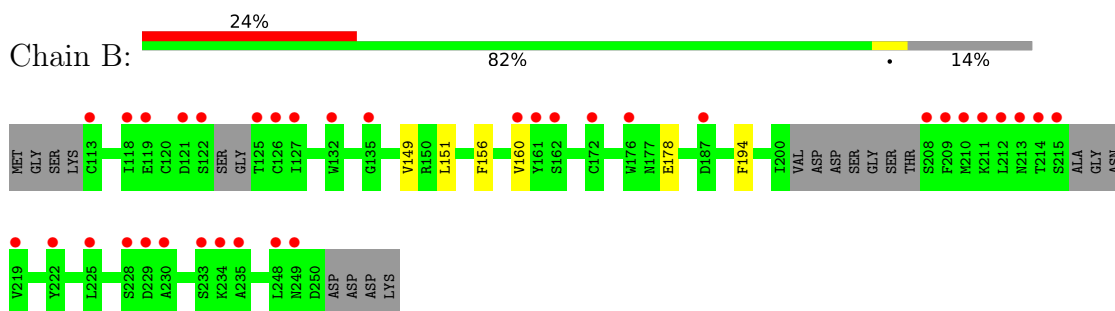
- Molecule 2: Transmembrane protease serine 2 catalytic chain

Chain C:

- Molecule 2: Transmembrane protease serine 2 catalytic chain

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.05Å　91.21Å　90.70Å 90.00°　100.44°　90.00°	Depositor
Resolution (Å)	47.25　–　2.60 47.25　–　2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.25-2.60) 98.7 (47.25-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.217　,　0.237 0.215　,　0.238	Depositor DCC
R_{free} test set	2010 reflections (8.56%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5724	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: I9V, NAG, CA

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	0/994	0.67	0/1345
1	B	0.46	0/930	0.67	0/1262
2	C	0.53	0/1923	0.72	0/2627
2	D	0.49	0/1853	0.67	0/2538
All	All	0.49	0/5700	0.69	0/7772

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	974	0	860	14	0
1	B	912	0	775	6	0
2	C	1867	0	1793	17	0
2	D	1799	0	1704	11	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	25	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	25	0	0	1	0
6	A	12	0	0	0	0
6	B	4	0	0	0	0
6	C	34	0	0	0	0
6	D	42	0	0	0	0
All	All	5724	0	5158	43	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 4.

All (43) 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:A:169:HIS:CD2	1:A:227:HIS:HE1	1.91	0.88
2:C:441:SER:OG	5:C:601:I9V:CL1	2.33	0.81
1:B:149:VAL:HG12	1:B:160:VAL:HG22	1.67	0.77
1:A:162:SER:HB2	1:A:227:HIS:NE2	2.00	0.76
1:A:248:LEU:HD12	1:A:249:ASN:OD1	1.90	0.72
1:B:178:GLU:HG3	1:B:194:PHE:CE2	2.28	0.68
1:A:169:HIS:CD2	1:A:227:HIS:CE1	2.81	0.62
2:C:378:LEU:HD11	2:C:401:LYS:HB3	1.86	0.58
2:C:287:THR:OG1	2:C:290:TRP:HB2	2.04	0.57
1:A:150:ARG:HD2	2:C:369:PRO:HG3	1.88	0.56
1:B:178:GLU:HG3	1:B:194:PHE:HE2	1.72	0.54
2:D:441:SER:OG	5:D:601:I9V:CL1	2.52	0.54
1:A:162:SER:CB	1:A:227:HIS:NE2	2.71	0.54
2:C:273:LEU:HD13	2:C:349:MET:HE3	1.90	0.53
2:C:271:VAL:CG2	2:C:285:ILE:HG13	2.40	0.52
2:D:296:HIS:CE1	2:D:441:SER:HB3	2.46	0.51
1:A:248:LEU:HD12	1:A:249:ASN:CG	2.31	0.50
2:D:331:VAL:HG22	2:D:349:MET:HG2	1.94	0.50
2:D:366:LEU:HD11	2:D:484:ILE:HG21	1.94	0.49
1:A:149:VAL:HG11	1:A:184:ALA:HB1	1.95	0.49
1:A:210:MET:SD	1:A:227:HIS:CD2	3.06	0.48
1:B:178:GLU:CG	1:B:194:PHE:CE2	2.96	0.47
2:D:316:ARG:HG2	2:D:396:VAL:HG12	1.96	0.47
2:D:427:ALA:HB3	2:D:474:TYR:CE1	2.50	0.47
1:A:242:ILE:HD11	2:C:288:PRO:HD3	1.96	0.46
2:C:381:ILE:HG21	2:C:474:TYR:OH	2.15	0.46
1:A:248:LEU:CD1	1:A:249:ASN:OD1	2.64	0.45
2:C:271:VAL:HG11	2:C:310:ALA:HB1	1.99	0.45

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:THR:HG21	2:D:349:MET:HE3	1.98	0.45
2:D:377:GLN:HB3	2:D:404:LEU:HD12	1.99	0.44
2:C:355:LEU:HD22	2:C:361:VAL:HG11	2.00	0.44
2:D:281:CYS:SG	2:D:441:SER:HB2	2.57	0.44
1:A:150:ARG:HG2	1:A:159:GLN:HB2	2.01	0.42
2:C:378:LEU:HA	2:C:403:LEU:HD23	2.00	0.42
1:B:156:PHE:HE1	2:D:452:ILE:HD13	1.85	0.42
2:D:346:ILE:HD13	2:D:480:PHE:CD2	2.54	0.42
2:C:316:ARG:HG2	2:C:396:VAL:HG12	2.01	0.41
1:B:151:LEU:HD13	1:B:156:PHE:HD2	1.85	0.41
2:C:377:GLN:HB3	2:C:404:LEU:HD12	2.02	0.41
1:A:156:PHE:HE1	2:C:452:ILE:HD13	1.84	0.41
2:C:271:VAL:HG23	2:C:285:ILE:HG13	2.02	0.41
1:A:154:PRO:HA	2:C:454:TRP:CZ2	2.56	0.41
2:C:358:ASN:O	2:C:362:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/146 (84%)	116 (95%)	6 (5%)	0	100	100
1	B	118/146 (81%)	115 (98%)	3 (2%)	0	100	100
2	C	240/249 (96%)	230 (96%)	10 (4%)	0	100	100
2	D	235/249 (94%)	224 (95%)	11 (5%)	0	100	100
All	All	715/790 (90%)	685 (96%)	30 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	107/127 (84%)	107 (100%)	0	100	100
1	B	93/127 (73%)	93 (100%)	0	100	100
2	C	198/210 (94%)	198 (100%)	0	100	100
2	D	187/210 (89%)	187 (100%)	0	100	100
All	All	585/674 (87%)	585 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	227	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	#$|Z| > 2$
5	I9V	C	601	-	26,26,26	3.14	10 (38%)	37,40,40	2.97	8 (21%)
5	I9V	D	601	-	26,26,26	3.13	11 (42%)	37,40,40	3.05	9 (24%)
3	NAG	B	601	1	14,14,15	0.38	0	17,19,21	1.04	1 (5%)
3	NAG	A	601	1	14,14,15	0.50	0	17,19,21	1.51	3 (17%)

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
5	I9V	C	601	-	-	8/22/22/22	0/2/2/2
5	I9V	D	601	-	-	10/22/22/22	0/2/2/2
3	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	601	1	-	3/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	I9V	C22-N21	-9.84	1.26	1.37
5	D	601	I9V	C22-N21	-9.77	1.26	1.37
5	C	601	I9V	S8-N7	7.07	1.72	1.61
5	D	601	I9V	S8-N7	6.76	1.71	1.61
5	D	601	I9V	C20-N21	5.72	1.46	1.36
5	C	601	I9V	C20-N21	5.66	1.46	1.36
5	C	601	I9V	C11-S8	3.60	1.82	1.76
5	D	601	I9V	C11-S8	3.58	1.82	1.76
5	C	601	I9V	C22-N23	3.33	1.45	1.32
5	D	601	I9V	C22-N23	3.32	1.45	1.32
5	C	601	I9V	O10-S8	3.07	1.47	1.43
5	D	601	I9V	O10-S8	2.97	1.46	1.43
5	C	601	I9V	C14-C13	-2.95	1.38	1.43
5	D	601	I9V	C14-C13	-2.94	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	I9V	O9-S8	2.92	1.46	1.43
5	C	601	I9V	O9-S8	2.76	1.46	1.43
5	D	601	I9V	C22-N24	2.66	1.45	1.34
5	C	601	I9V	C22-N24	2.60	1.45	1.34
5	C	601	I9V	C20-C13	-2.60	1.41	1.44
5	D	601	I9V	C20-C13	-2.54	1.41	1.44
5	D	601	I9V	C2-N7	-2.19	1.45	1.48

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	I9V	O10-S8-O9	-15.43	100.58	119.55
5	C	601	I9V	O10-S8-O9	-15.05	101.04	119.55
5	D	601	I9V	C12-C13-C20	-4.72	120.62	124.88
5	C	601	I9V	C12-C13-C20	-4.09	121.19	124.88
3	A	601	NAG	C3-C4-C5	3.85	117.10	110.24
5	C	601	I9V	C17-C18-N19	-3.46	119.87	122.84
5	C	601	I9V	C18-N19-C20	3.33	122.74	116.05
5	D	601	I9V	C18-N19-C20	3.30	122.67	116.05
5	D	601	I9V	O10-S8-C11	3.01	111.68	107.97
5	D	601	I9V	C17-C18-N19	-2.79	120.44	122.84
5	D	601	I9V	O10-S8-N7	2.75	113.58	107.32
5	D	601	I9V	O9-S8-C11	2.72	111.32	107.97
3	B	601	NAG	O5-C1-C2	-2.58	107.22	111.29
5	C	601	I9V	O10-S8-N7	2.56	113.16	107.32
3	A	601	NAG	C1-C2-N2	-2.35	106.47	110.49
5	D	601	I9V	C13-C20-N19	-2.31	119.44	121.35
5	D	601	I9V	C20-C13-C14	2.27	120.07	117.42
3	A	601	NAG	C4-C3-C2	2.21	114.25	111.02
5	C	601	I9V	O9-S8-N7	2.15	112.21	107.32
5	C	601	I9V	C15-C14-C17	-2.13	121.27	125.06
5	C	601	I9V	O9-S8-C11	2.03	110.46	107.97

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	601	I9V	N7-C2-C4-O5
5	C	601	I9V	N7-C2-C4-O6
5	D	601	I9V	N7-C2-C4-O5
5	D	601	I9V	N7-C2-C4-O6
3	A	601	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	601	NAG	O7-C7-N2-C2
5	D	601	I9V	C2-N7-S8-O9
3	B	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
5	C	601	I9V	C2-N7-S8-O9
5	C	601	I9V	C2-N7-S8-C11
5	C	601	I9V	C12-C11-S8-O9
5	C	601	I9V	C3-C2-C4-O5
5	C	601	I9V	C3-C2-C4-O6
5	D	601	I9V	C1-C2-C4-O6
5	D	601	I9V	C2-N7-S8-C11
5	C	601	I9V	C16-C11-S8-O9
5	D	601	I9V	C1-C2-C4-O5
5	D	601	I9V	C2-N7-S8-O10
5	D	601	I9V	C13-C20-N21-C22
5	D	601	I9V	C12-C11-S8-O9
5	D	601	I9V	C16-C11-S8-O9

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	I9V	1	0
5	D	601	I9V	1	0

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

Ligand I9V C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand I9V D 601
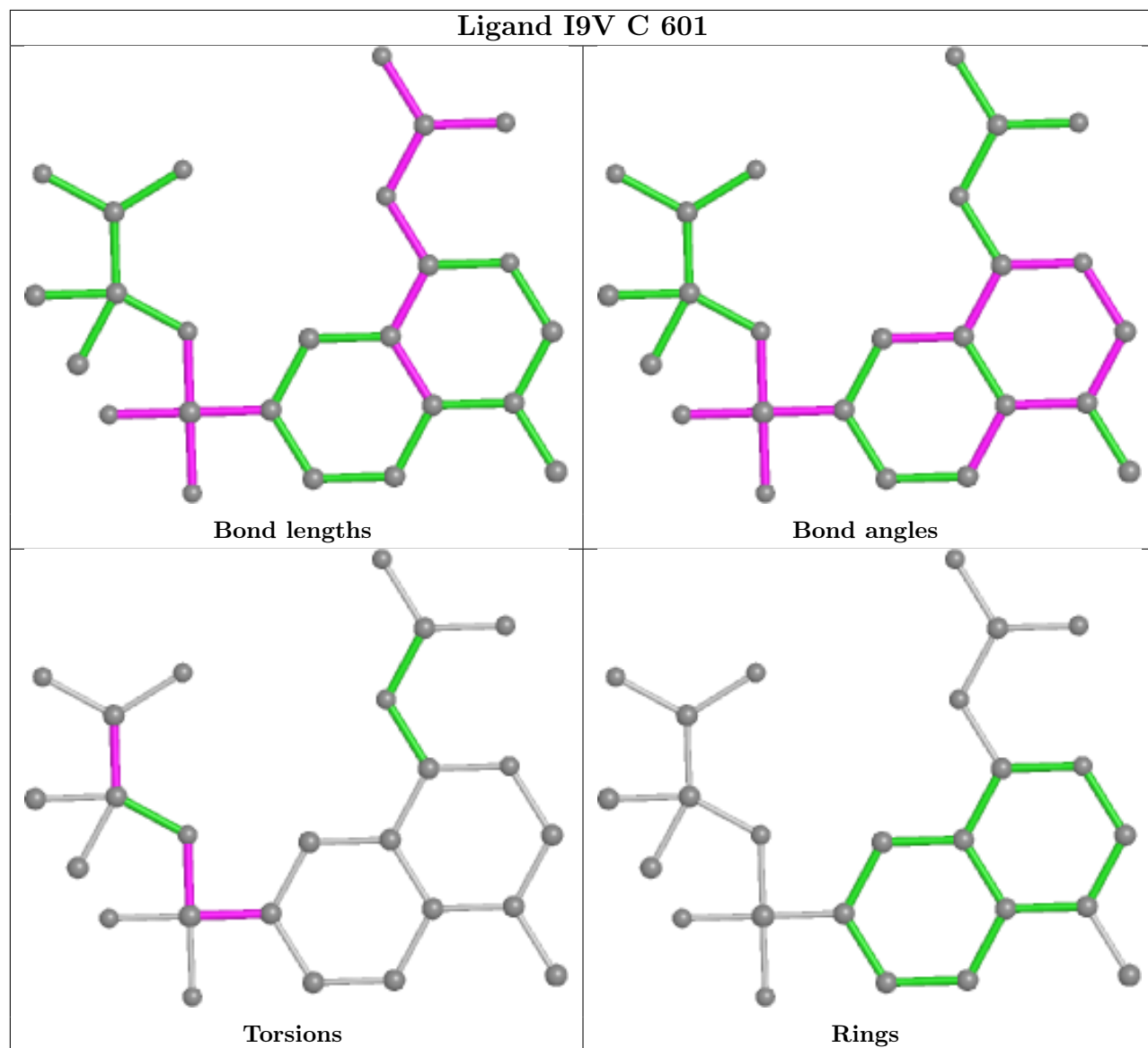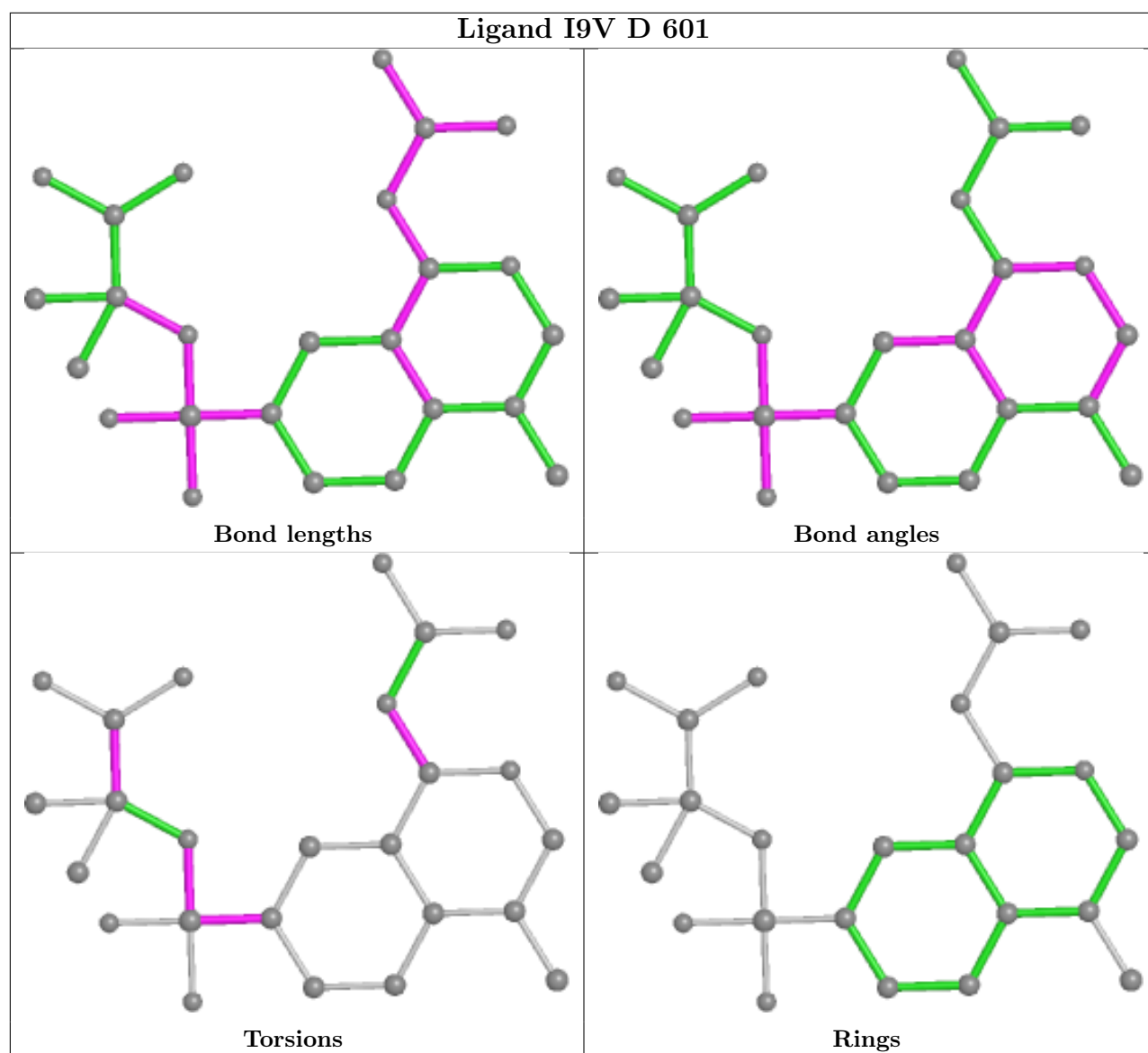
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	128/146 (87%)	0.52	11 (8%)	10	7	29, 45, 80, 100	0
1	B	126/146 (86%)	1.37	35 (27%)	0	0	39, 62, 89, 101	0
2	C	242/249 (97%)	0.03	0	100	100	26, 33, 51, 74	0
2	D	237/249 (95%)	0.05	0	100	100	25, 37, 53, 63	0
All	All	733/790 (92%)	0.35	46 (6%)	20	15	25, 39, 77, 101	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	GLY	5.7
1	A	129	PRO	5.2
1	B	176	TRP	4.9
1	B	212	LEU	4.6
1	B	235	ALA	4.5
1	B	126	CYS	4.3
1	B	162	SER	4.2
1	B	233	SER	4.2
1	B	121	ASP	3.8
1	A	221	ILE	3.8
1	A	138	HIS	3.7
1	B	229	ASP	3.7
1	B	125	THR	3.6
1	B	127	ILE	3.4
1	B	230	ALA	3.3
1	B	249	ASN	3.3
1	B	160	VAL	3.1
1	B	214	THR	3.0
1	B	228	SER	3.0
1	B	113	CYS	2.9
1	B	219	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	222	TYR	2.9
1	A	227	HIS	2.8
1	B	118	ILE	2.8
1	A	127	ILE	2.7
1	A	118	ILE	2.7
1	A	163	SER	2.6
1	A	222	TYR	2.5
1	B	135	GLY	2.4
1	B	132	TRP	2.4
1	B	248	LEU	2.4
1	A	125	THR	2.4
1	B	208	SER	2.4
1	B	225	LEU	2.4
1	B	215	SER	2.3
1	B	187	ASP	2.3
1	B	209	PHE	2.2
1	B	210	MET	2.1
1	B	172	CYS	2.1
1	B	122	SER	2.1
1	B	161	TYR	2.1
1	B	213	ASN	2.1
1	B	119	GLU	2.1
1	A	116	SER	2.0
1	B	234	LYS	2.0
1	B	211	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	NAG	A	601	14/15	0.70	0.22	61,78,84,85	0
3	NAG	B	601	14/15	0.78	0.35	79,88,94,95	0
4	CA	A	602	1/1	0.87	0.08	69,69,69,69	0
5	I9V	D	601	25/25	0.92	0.20	38,45,65,70	0
5	I9V	C	601	25/25	0.93	0.18	30,41,66,70	0
4	CA	B	602	1/1	0.94	0.13	61,61,61,61	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.
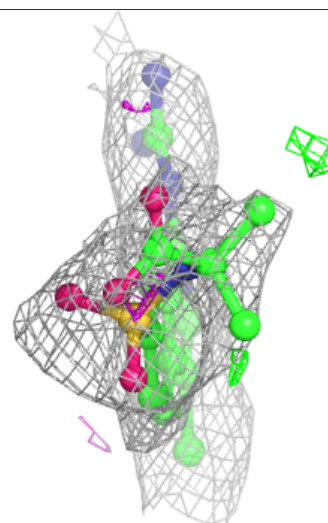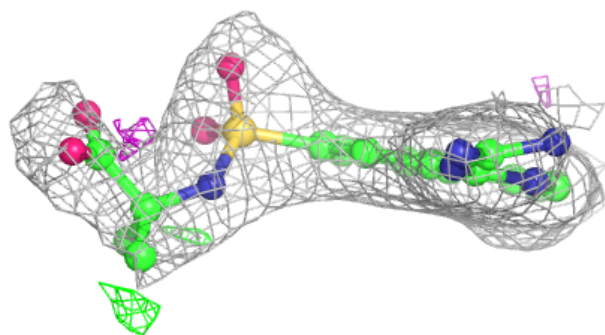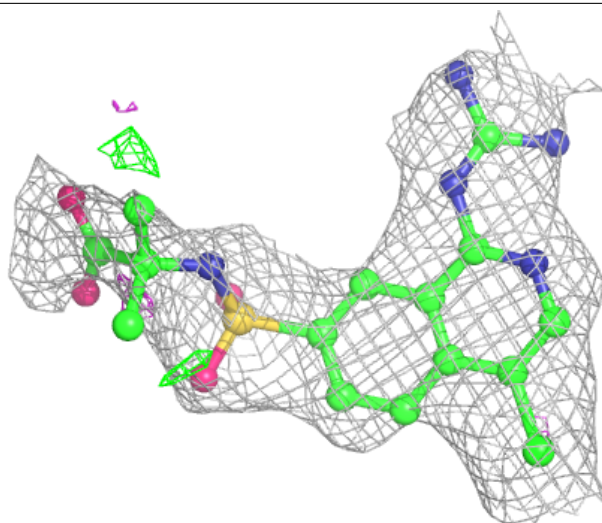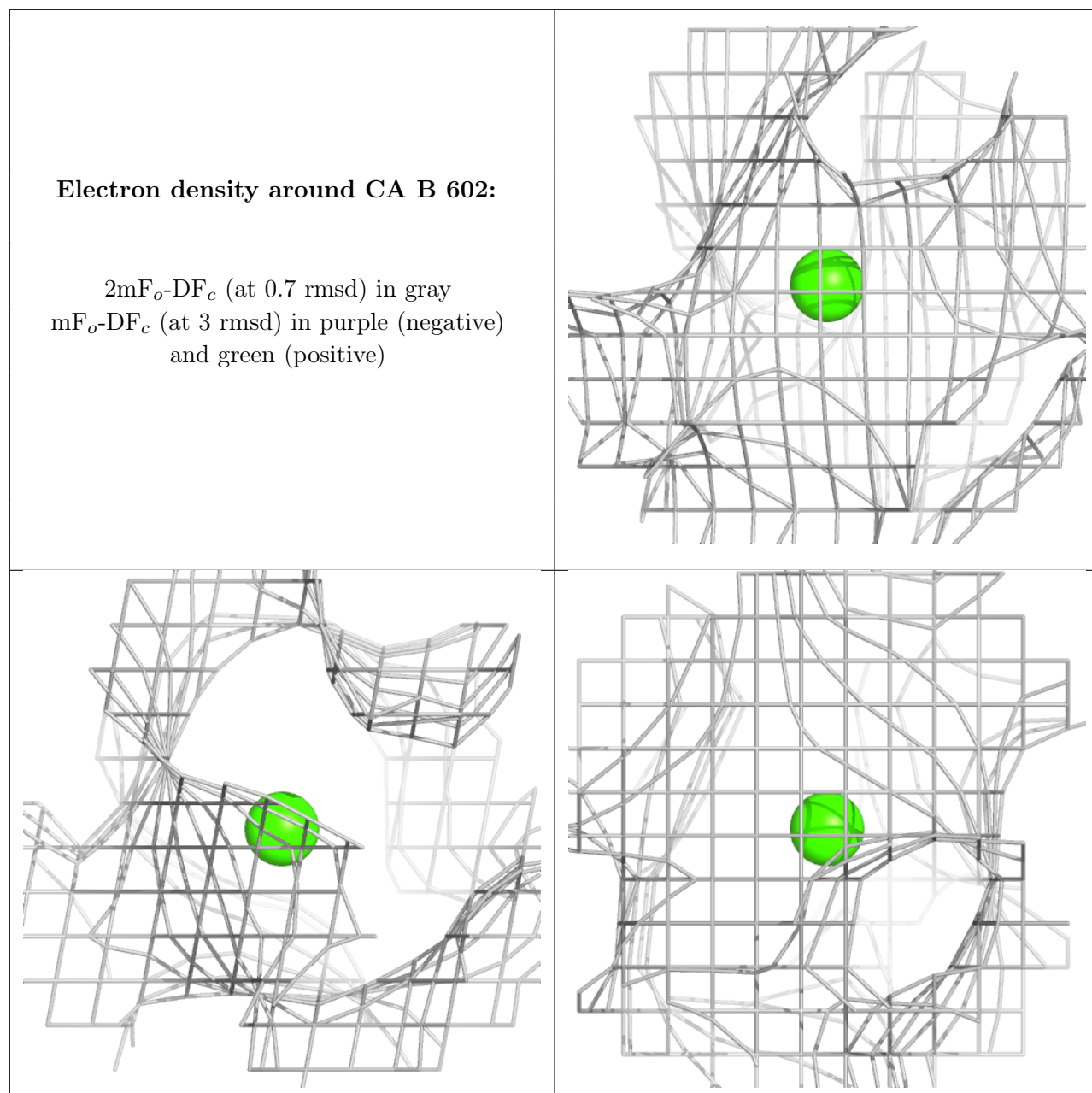

Electron density around CA A 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
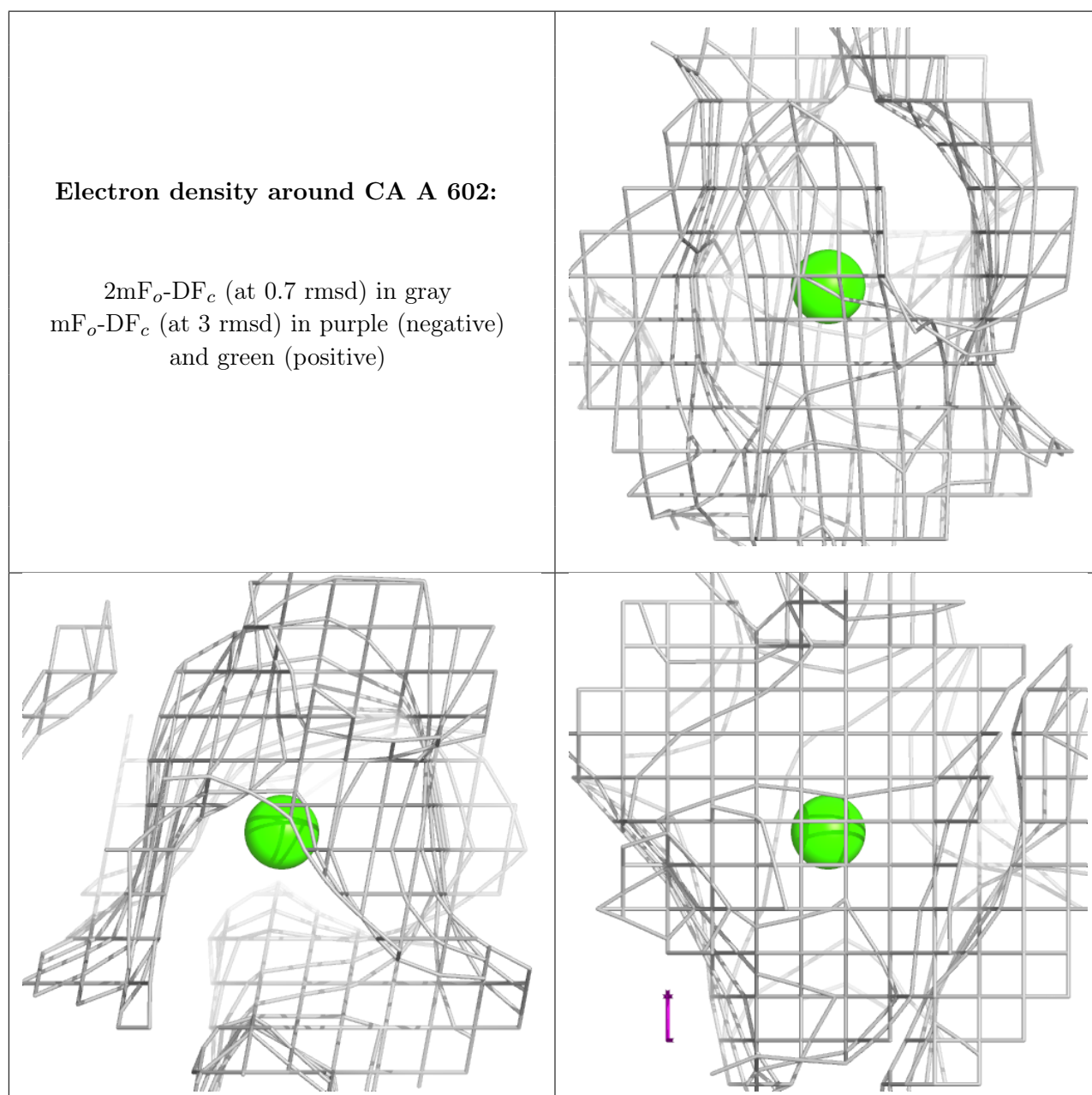
Electron density around I9V D 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
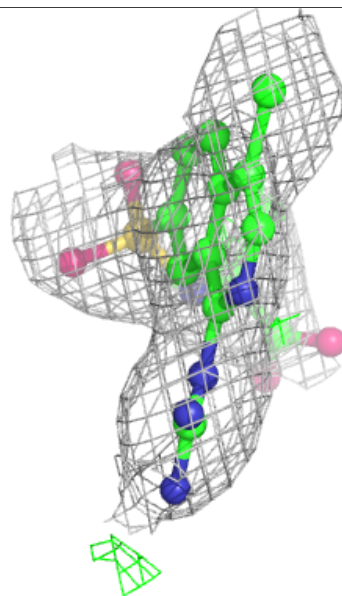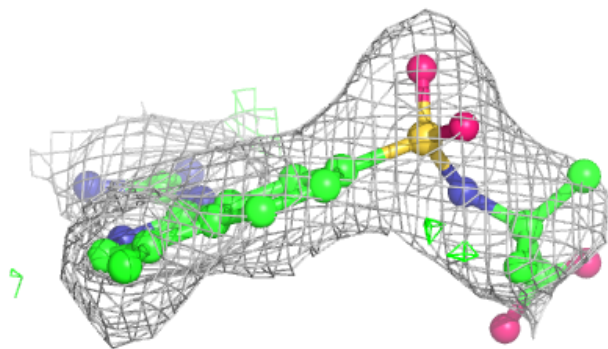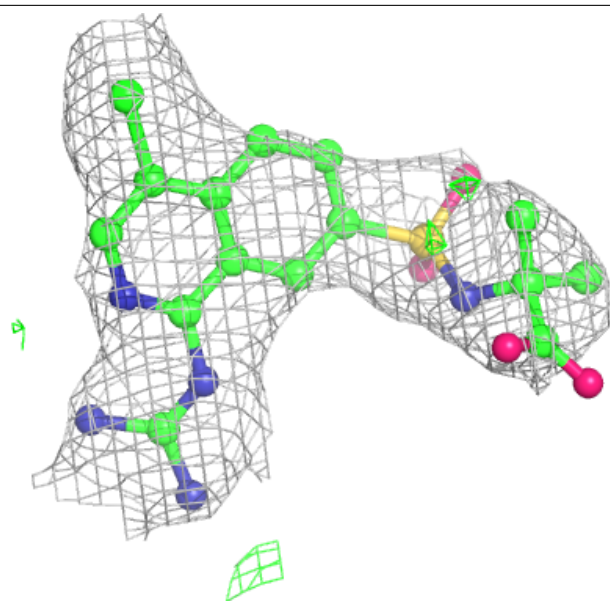
Electron density around I9V C 601:

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 CA B 602:

$2mF_o$-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 ⓘ

There are no such residues in this entry.