



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 12:04 AM EDT

PDB ID : 7MB3
Title : SARS-CoV-2 Main Protease (Mpro) in Complex with Covalent Inhibitor SM145
Authors : Lockbaum, G.J.; Schiffer, C.A.
Deposited on : 2021-03-31
Resolution : 1.81 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 : 2.35.1
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

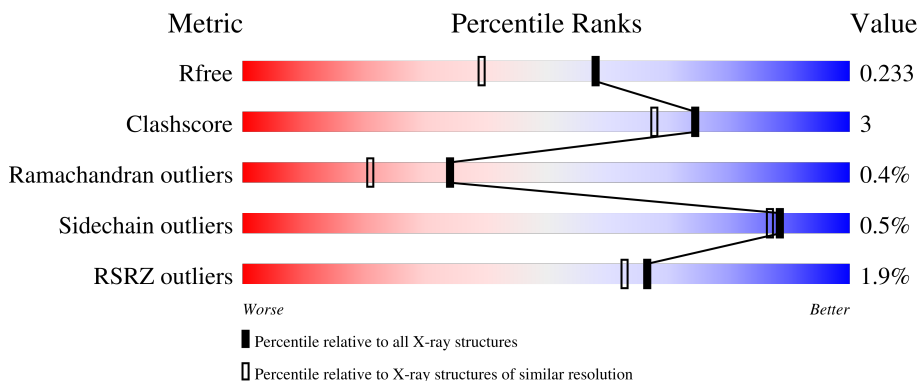
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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.



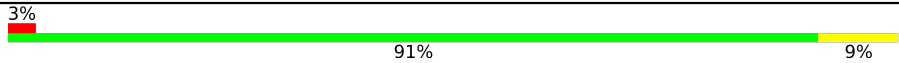
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	306	
1	B	306	
1	C	306	
1	D	306	
1	E	306	

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Mol	Chain	Length	Quality of chain
1	F	306	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '3%', a large green segment in the middle labeled '91%', and a small yellow segment on the right labeled '9%'.</p>

2 Entry composition i

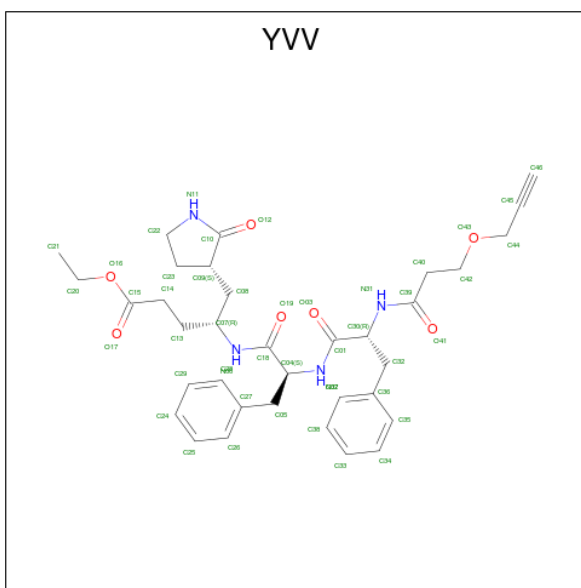
There are 3 unique types of molecules in this entry. The entry contains 28317 atoms, of which 13310 are hydrogens and 0 are deuteriums.

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 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	305	Total 4550	C 1468	H 2233	N 393	O 435	S 21	0	0	0
1	D	302	Total 4473	C 1445	H 2190	N 389	O 428	S 21	0	0	0
1	C	305	Total 4565	C 1474	H 2236	N 394	O 439	S 22	0	0	0
1	B	302	Total 4421	C 1436	H 2151	N 385	O 427	S 22	0	0	0
1	E	301	Total 4337	C 1418	H 2094	N 379	O 425	S 21	0	0	0
1	F	305	Total 4429	C 1447	H 2148	N 387	O 427	S 20	0	0	0

- Molecule 2 is N-{3-[(prop-2-yn-1-yl)oxy]propanoyl}-D-phenylalanyl-N-[(2R)-5-ethoxy-5-oxo-1-[(3S)-2-oxopyrrolidin-3-yl]pentan-2-yl]-L-phenylalaninamide (three-letter code: YVV) (formula: C₃₅H₄₄N₄O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			89	35	43	4	7		
2	D	1	Total	C	H	N	O	0	0
			89	35	43	4	7		
2	C	1	Total	C	H	N	O	0	0
			89	35	43	4	7		
2	B	1	Total	C	H	N	O	0	0
			89	35	43	4	7		
2	E	1	Total	C	H	N	O	0	0
			89	35	43	4	7		
2	F	1	Total	C	H	N	O	0	0
			89	35	43	4	7		

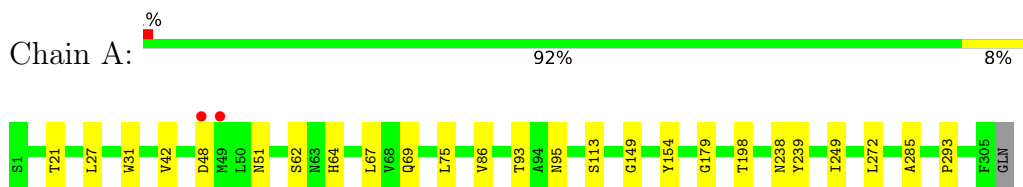
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total	O	0	0
			233	233		
3	D	173	Total	O	0	0
			173	173		
3	C	243	Total	O	0	0
			243	243		
3	B	145	Total	O	0	0
			145	145		
3	E	97	Total	O	0	0
			97	97		
3	F	117	Total	O	0	0
			117	117		

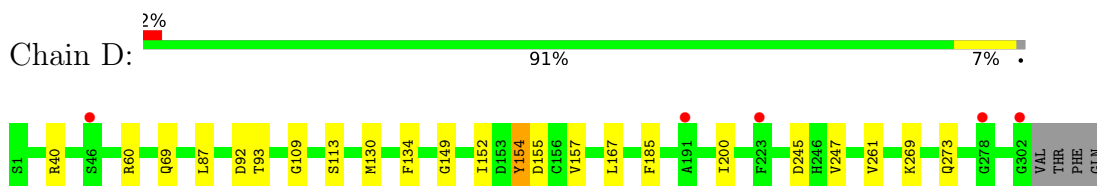
3 Residue-property plots [i](#)

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.

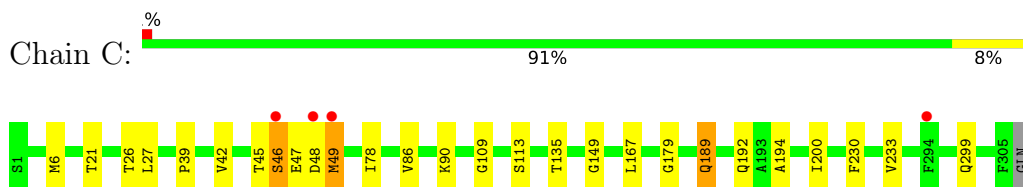
- Molecule 1: 3C-like proteinase



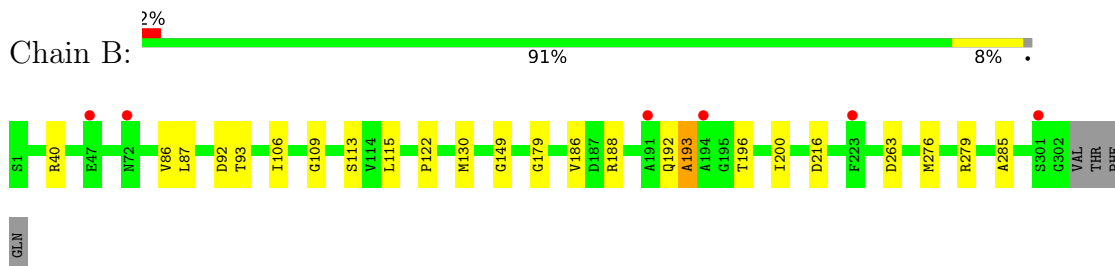
- Molecule 1: 3C-like proteinase



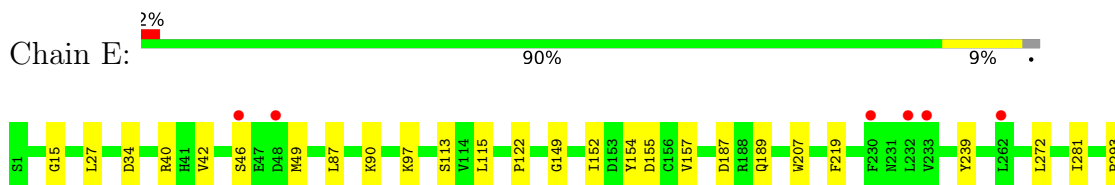
- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase

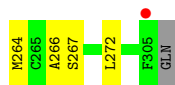
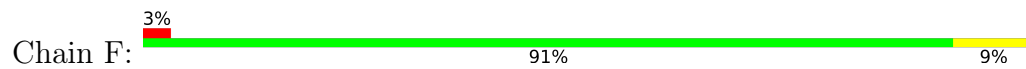


- Molecule 1: 3C-like proteinase





- Molecule 1: 3C-like proteinase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.55Å 67.32Å 117.89Å 92.00° 90.31° 118.95°	Depositor
Resolution (Å)	29.44 – 1.81 29.44 – 1.81	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.44-1.81) 92.1 (29.44-1.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.195 , 0.233 0.195 , 0.233	Depositor DCC
R_{free} test set	2023 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.002 for h+k,-h,l 0.002 for -k,h+k,l 0.003 for k,-h-k,l 0.003 for -h-k,h,l 0.127 for h,-h-k,-l 0.015 for -h-k,k,-l 0.010 for -h,-k,l 0.019 for k,h,-l 0.009 for -k,-h,-l 0.011 for -h,h+k,-l 0.011 for h+k,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28317	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: YVV

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	0.33	0/2369	0.56	0/3226
1	B	0.32	0/2321	0.55	0/3164
1	C	0.35	0/2382	0.58	0/3244
1	D	0.34	0/2334	0.55	0/3179
1	E	0.31	0/2294	0.53	0/3132
1	F	0.32	0/2334	0.53	0/3186
All	All	0.33	0/14034	0.55	0/19131

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 [i](#)

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	2317	2233	2233	12	0
1	B	2270	2151	2153	17	0
1	C	2329	2236	2236	17	0
1	D	2283	2190	2191	13	0
1	E	2243	2094	2094	14	0
1	F	2281	2148	2148	15	0
2	A	46	43	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	46	43	0	0	0
2	C	46	43	0	1	0
2	D	46	43	0	0	0
2	E	46	43	0	0	0
2	F	46	43	0	0	0
3	A	233	0	0	0	0
3	B	145	0	0	2	2
3	C	243	0	0	0	0
3	D	173	0	0	0	0
3	E	97	0	0	0	0
3	F	117	0	0	1	2
All	All	15007	13310	13055	87	2

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 3.

All (87) 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:B:188:ARG:NH2	3:B:501:HOH:O	1.85	0.86
1:C:45:THR:O	1:C:47:GLU:N	2.16	0.79
1:F:188:ARG:NH2	3:F:501:HOH:O	2.26	0.68
1:C:86:VAL:HG23	1:C:179:GLY:HA2	1.78	0.65
1:B:188:ARG:HG2	1:B:188:ARG:HH11	1.62	0.65
1:C:167:LEU:HD22	1:C:192:GLN:O	1.97	0.64
1:D:92:ASP:OD1	1:D:93:THR:HG23	1.96	0.64
1:B:106:ILE:HD11	1:B:130:MET:HE3	1.82	0.62
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.83	0.61
1:E:27:LEU:HD21	1:E:42:VAL:HB	1.82	0.60
1:C:46:SER:HA	1:C:49:MET:HE1	1.84	0.60
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.84	0.59
1:B:115:LEU:HD11	1:B:122:PRO:HB3	1.85	0.59
1:E:34:ASP:OD2	1:E:90:LYS:HE3	2.02	0.59
1:A:62:SER:OG	1:A:64:HIS:ND1	2.36	0.59
1:C:49:MET:CG	1:C:189:GLN:HG3	2.34	0.58
1:F:198:THR:CG2	1:F:240:GLU:HG2	2.36	0.55
1:A:51:ASN:O	1:A:51:ASN:OD1	2.25	0.54
1:D:247:VAL:HG13	1:D:261:VAL:HG11	1.88	0.54
1:F:198:THR:HG22	1:F:240:GLU:HG2	1.88	0.54
1:D:269:LYS:O	1:D:273:GLN:HG3	2.09	0.52
1:D:109:GLY:HA2	1:D:200:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:VAL:HG22	1:F:90:LYS:HD3	1.93	0.51
1:E:40:ARG:CB	1:E:87:LEU:HD13	2.40	0.51
1:C:45:THR:O	1:C:48:ASP:N	2.40	0.50
1:F:208:LEU:HD13	1:F:264:MET:HE2	1.94	0.50
1:C:135:THR:HG21	1:C:194:ALA:HB2	1.94	0.50
1:F:264:MET:HE3	1:F:267:SER:HB2	1.94	0.50
1:D:60:ARG:NH1	1:D:60:ARG:HG2	2.27	0.49
1:C:113:SER:O	1:C:149:GLY:HA2	2.13	0.49
1:F:22:CYS:SG	1:F:61:LYS:HD2	2.53	0.49
1:A:27:LEU:HD21	1:A:42:VAL:HB	1.96	0.48
1:F:109:GLY:HA2	1:F:200:ILE:HD13	1.95	0.48
1:F:17:MET:HG3	1:F:117:CYS:SG	2.54	0.48
1:F:115:LEU:HD11	1:F:122:PRO:HB3	1.96	0.47
1:D:152:ILE:CD1	1:D:157:VAL:HG22	2.45	0.47
1:F:86:VAL:HG13	1:F:179:GLY:HA2	1.97	0.47
1:F:169:THR:OG1	1:F:171:VAL:HG22	2.15	0.47
1:D:40:ARG:CB	1:D:87:LEU:HD13	2.44	0.47
1:E:46:SER:HA	1:E:49:MET:HE3	1.97	0.47
1:C:6:MET:SD	1:C:299:GLN:HG3	2.56	0.46
1:A:86:VAL:HG23	1:A:179:GLY:HA2	1.97	0.46
1:C:78:ILE:HD11	1:C:90:LYS:HG2	1.98	0.46
1:B:263:ASP:OD2	3:B:502:HOH:O	2.21	0.45
1:A:75:LEU:HD22	1:A:93:THR:CG2	2.47	0.45
1:C:109:GLY:HA2	1:C:200:ILE:HD13	1.99	0.45
1:C:21:THR:HG22	1:C:26:THR:HG23	2.00	0.44
1:E:239:TYR:CE1	1:E:272:LEU:HD21	2.53	0.44
1:D:154:TYR:O	1:D:155:ASP:CB	2.66	0.44
1:D:130:MET:SD	1:D:134:PHE:HA	2.58	0.44
1:B:40:ARG:HA	1:B:87:LEU:HD13	1.99	0.44
1:F:223:PHE:O	1:F:266:ALA:CB	2.66	0.44
1:B:186:VAL:HG23	1:B:188:ARG:HG3	1.99	0.43
1:A:21:THR:HB	1:A:67:LEU:HB3	1.99	0.43
1:E:293:PRO:O	1:E:297:VAL:HG23	2.19	0.43
1:D:247:VAL:HG13	1:D:261:VAL:CG1	2.49	0.43
1:A:31:TRP:CD2	1:A:95:ASN:HB2	2.54	0.43
1:D:60:ARG:HG2	1:D:60:ARG:HH11	1.84	0.42
1:E:113:SER:O	1:E:149:GLY:HA2	2.19	0.42
1:F:40:ARG:O	1:F:43:ILE:HG12	2.19	0.42
1:C:49:MET:HB2	2:C:401:YVV:C25	2.49	0.42
1:B:40:ARG:CB	1:B:87:LEU:HD13	2.49	0.42
1:E:15:GLY:O	1:E:97:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:MET:HB3	1:E:189:GLN:HG3	2.02	0.42
1:B:192:GLN:O	1:B:193:ALA:HB2	2.19	0.42
1:C:49:MET:HE2	1:C:49:MET:HB3	1.83	0.42
1:E:219:PHE:CD2	1:E:281:ILE:HD13	2.55	0.42
1:F:239:TYR:CE1	1:F:272:LEU:HD21	2.54	0.42
1:A:198:THR:HG22	1:A:238:ASN:OD1	2.20	0.42
1:A:249:ILE:HG22	1:A:293:PRO:HG2	2.01	0.42
1:D:167:LEU:HD11	1:D:185:PHE:CE1	2.55	0.42
1:B:188:ARG:HH11	1:B:188:ARG:CG	2.29	0.42
1:A:239:TYR:CZ	1:A:272:LEU:HD21	2.55	0.41
1:E:115:LEU:HD11	1:E:122:PRO:HB3	2.01	0.41
1:B:113:SER:O	1:B:149:GLY:HA2	2.20	0.41
1:A:285:ALA:HB3	1:B:285:ALA:HB3	2.01	0.41
1:E:207:TRP:CH2	1:E:281:ILE:HB	2.56	0.41
1:C:27:LEU:HD21	1:C:42:VAL:HB	2.03	0.41
1:E:152:ILE:CD1	1:E:157:VAL:HG22	2.51	0.41
1:A:113:SER:O	1:A:149:GLY:HA2	2.21	0.41
1:D:113:SER:O	1:D:149:GLY:HA2	2.20	0.41
1:C:230:PHE:O	1:C:233:VAL:CG1	2.69	0.41
1:B:188:ARG:HG2	1:B:188:ARG:NH1	2.34	0.40
1:C:27:LEU:HD13	1:C:39:PRO:HD2	2.03	0.40
1:E:187:ASP:OD1	1:E:187:ASP:N	2.53	0.40
1:B:92:ASP:OD1	1:B:93:THR:HG23	2.21	0.40
1:B:276:MET:HE2	1:B:279:ARG:O	2.21	0.40

All (2) 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:B:632:HOH:O	3:F:549:HOH:O[1_556]	1.99	0.21
3:B:635:HOH:O	3:F:612:HOH:O[1_456]	2.02	0.18

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	303/306 (99%)	293 (97%)	8 (3%)	2 (1%)	22	10
1	B	300/306 (98%)	288 (96%)	10 (3%)	2 (1%)	22	10
1	C	303/306 (99%)	296 (98%)	6 (2%)	1 (0%)	41	27
1	D	300/306 (98%)	291 (97%)	8 (3%)	1 (0%)	41	27
1	E	299/306 (98%)	294 (98%)	4 (1%)	1 (0%)	41	27
1	F	303/306 (99%)	296 (98%)	7 (2%)	0	100	100
All	All	1808/1836 (98%)	1758 (97%)	43 (2%)	7 (0%)	34	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	154	TYR
1	A	48	ASP
1	C	46	SER
1	B	196	THR
1	E	154	TYR
1	A	154	TYR
1	B	193	ALA

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	252/263 (96%)	251 (100%)	1 (0%)	91	89
1	B	242/263 (92%)	241 (100%)	1 (0%)	91	89
1	C	254/263 (97%)	252 (99%)	2 (1%)	81	77
1	D	246/263 (94%)	244 (99%)	2 (1%)	81	77
1	E	235/263 (89%)	234 (100%)	1 (0%)	91	89
1	F	240/263 (91%)	239 (100%)	1 (0%)	91	89
All	All	1469/1578 (93%)	1461 (100%)	8 (0%)	88	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	D	69	GLN
1	D	245	ASP
1	C	49	MET
1	C	189	GLN
1	B	216	ASP
1	E	155	ASP
1	F	1	SER

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

Mol	Chain	Res	Type
1	C	72	ASN
1	C	189	GLN

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](#)

6 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
2	YVV	D	401	1	48,48,48	4.71	21 (43%)	58,61,61	1.57	8 (13%)
2	YVV	E	401	1	48,48,48	4.79	25 (52%)	58,61,61	1.30	6 (10%)
2	YVV	A	401	1	48,48,48	4.66	22 (45%)	58,61,61	1.58	10 (17%)
2	YVV	B	401	1	48,48,48	4.76	23 (47%)	58,61,61	1.44	8 (13%)
2	YVV	C	401	1	48,48,48	4.65	23 (47%)	58,61,61	1.67	9 (15%)
2	YVV	F	401	1	48,48,48	4.78	24 (50%)	58,61,61	1.39	5 (8%)

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
2	YVV	D	401	1	-	8/46/56/56	0/3/3/3
2	YVV	E	401	1	-	8/46/56/56	0/3/3/3
2	YVV	A	401	1	-	7/46/56/56	0/3/3/3
2	YVV	B	401	1	-	11/46/56/56	0/3/3/3
2	YVV	C	401	1	-	9/46/56/56	0/3/3/3
2	YVV	F	401	1	-	8/46/56/56	0/3/3/3

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	YVV	C10-N11	18.37	1.53	1.33
2	F	401	YVV	C10-N11	18.28	1.53	1.33
2	B	401	YVV	C10-N11	17.89	1.52	1.33
2	D	401	YVV	C10-N11	17.86	1.52	1.33
2	A	401	YVV	C10-N11	17.83	1.52	1.33
2	C	401	YVV	C10-N11	17.74	1.52	1.33
2	A	401	YVV	C34-C35	7.28	1.54	1.38
2	B	401	YVV	C38-C37	7.27	1.54	1.38
2	E	401	YVV	C38-C37	7.27	1.54	1.38
2	E	401	YVV	C34-C35	7.24	1.54	1.38
2	C	401	YVV	C34-C35	7.24	1.54	1.38
2	B	401	YVV	C34-C35	7.22	1.54	1.38
2	F	401	YVV	C34-C35	7.19	1.54	1.38
2	D	401	YVV	C25-C26	7.17	1.54	1.38
2	D	401	YVV	C34-C35	7.16	1.54	1.38
2	D	401	YVV	C38-C37	7.15	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	YVV	C38-C37	7.15	1.54	1.38
2	F	401	YVV	C25-C26	7.14	1.54	1.38
2	C	401	YVV	C29-C28	7.14	1.53	1.38
2	B	401	YVV	C29-C28	7.11	1.53	1.38
2	E	401	YVV	C25-C26	7.09	1.53	1.38
2	E	401	YVV	C35-C36	7.09	1.54	1.38
2	F	401	YVV	C38-C37	7.08	1.53	1.38
2	B	401	YVV	C35-C36	7.07	1.54	1.38
2	C	401	YVV	C38-C37	7.07	1.53	1.38
2	A	401	YVV	C25-C26	7.00	1.53	1.38
2	F	401	YVV	C35-C36	6.98	1.53	1.38
2	F	401	YVV	C29-C28	6.94	1.53	1.38
2	B	401	YVV	C37-C36	6.92	1.53	1.38
2	D	401	YVV	C35-C36	6.91	1.53	1.38
2	E	401	YVV	C09-C10	-6.91	1.43	1.52
2	E	401	YVV	C29-C28	6.90	1.53	1.38
2	C	401	YVV	C37-C36	6.86	1.53	1.38
2	F	401	YVV	C28-C27	6.86	1.53	1.38
2	F	401	YVV	C37-C36	6.86	1.53	1.38
2	B	401	YVV	C25-C26	6.85	1.53	1.38
2	D	401	YVV	C37-C36	6.82	1.53	1.38
2	B	401	YVV	C26-C27	6.81	1.53	1.38
2	C	401	YVV	C35-C36	6.78	1.53	1.38
2	E	401	YVV	C37-C36	6.78	1.53	1.38
2	F	401	YVV	C26-C27	6.76	1.53	1.38
2	A	401	YVV	C29-C28	6.75	1.53	1.38
2	D	401	YVV	C28-C27	6.74	1.53	1.38
2	D	401	YVV	C29-C28	6.73	1.53	1.38
2	B	401	YVV	C09-C10	-6.71	1.44	1.52
2	E	401	YVV	C28-C27	6.70	1.53	1.38
2	E	401	YVV	C39-N31	6.68	1.48	1.34
2	B	401	YVV	C28-C27	6.67	1.53	1.38
2	D	401	YVV	C09-C10	-6.66	1.44	1.52
2	A	401	YVV	C28-C27	6.63	1.53	1.38
2	C	401	YVV	C28-C27	6.62	1.53	1.38
2	F	401	YVV	C09-C10	-6.62	1.44	1.52
2	A	401	YVV	C26-C27	6.61	1.53	1.38
2	E	401	YVV	C26-C27	6.61	1.53	1.38
2	E	401	YVV	C01-N02	6.59	1.48	1.34
2	C	401	YVV	C25-C26	6.57	1.52	1.38
2	A	401	YVV	C37-C36	6.55	1.53	1.38
2	A	401	YVV	C35-C36	6.54	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	YVV	C26-C27	6.52	1.52	1.38
2	A	401	YVV	C09-C10	-6.51	1.44	1.52
2	D	401	YVV	C26-C27	6.50	1.52	1.38
2	B	401	YVV	C39-N31	6.50	1.47	1.34
2	F	401	YVV	C39-N31	6.44	1.47	1.34
2	B	401	YVV	C18-N06	6.40	1.48	1.34
2	B	401	YVV	C01-N02	6.37	1.48	1.34
2	E	401	YVV	C18-N06	6.35	1.48	1.34
2	D	401	YVV	C39-N31	6.30	1.47	1.34
2	F	401	YVV	C01-N02	6.29	1.47	1.34
2	A	401	YVV	C39-N31	6.26	1.47	1.34
2	F	401	YVV	C18-N06	6.24	1.47	1.34
2	C	401	YVV	C39-N31	6.20	1.47	1.34
2	D	401	YVV	C18-N06	6.18	1.47	1.34
2	B	401	YVV	C38-C33	6.13	1.54	1.38
2	C	401	YVV	C18-N06	6.09	1.47	1.34
2	D	401	YVV	C01-N02	6.08	1.47	1.34
2	C	401	YVV	C09-C10	-6.08	1.44	1.52
2	D	401	YVV	C38-C33	6.07	1.54	1.38
2	A	401	YVV	C01-N02	6.06	1.47	1.34
2	F	401	YVV	C38-C33	6.05	1.54	1.38
2	E	401	YVV	C38-C33	6.00	1.53	1.38
2	E	401	YVV	C34-C33	5.98	1.53	1.38
2	C	401	YVV	C38-C33	5.98	1.53	1.38
2	B	401	YVV	C34-C33	5.95	1.53	1.38
2	F	401	YVV	C34-C33	5.92	1.53	1.38
2	A	401	YVV	C18-N06	5.92	1.47	1.34
2	F	401	YVV	C25-C24	5.91	1.53	1.38
2	D	401	YVV	C25-C24	5.91	1.53	1.38
2	D	401	YVV	C34-C33	5.91	1.53	1.38
2	E	401	YVV	C25-C24	5.90	1.53	1.38
2	A	401	YVV	C38-C33	5.89	1.53	1.38
2	B	401	YVV	C25-C24	5.87	1.53	1.38
2	B	401	YVV	C29-C24	5.83	1.53	1.38
2	F	401	YVV	C29-C24	5.82	1.53	1.38
2	A	401	YVV	C34-C33	5.80	1.53	1.38
2	C	401	YVV	C01-N02	5.79	1.46	1.34
2	E	401	YVV	C29-C24	5.77	1.53	1.38
2	A	401	YVV	C25-C24	5.77	1.53	1.38
2	C	401	YVV	C34-C33	5.76	1.53	1.38
2	D	401	YVV	C29-C24	5.72	1.53	1.38
2	C	401	YVV	C29-C24	5.70	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	YVV	C29-C24	5.56	1.52	1.38
2	C	401	YVV	C25-C24	5.50	1.52	1.38
2	F	401	YVV	C08-C09	3.92	1.62	1.53
2	C	401	YVV	C08-C09	3.89	1.62	1.53
2	B	401	YVV	C08-C09	3.74	1.62	1.53
2	A	401	YVV	C08-C09	3.69	1.62	1.53
2	D	401	YVV	C08-C09	3.69	1.62	1.53
2	C	401	YVV	O16-C15	3.23	1.42	1.33
2	D	401	YVV	O16-C15	3.22	1.42	1.33
2	A	401	YVV	O16-C15	3.10	1.42	1.33
2	B	401	YVV	O16-C15	3.03	1.42	1.33
2	E	401	YVV	O16-C15	2.90	1.41	1.33
2	F	401	YVV	O16-C15	2.89	1.41	1.33
2	C	401	YVV	O41-C39	-2.44	1.18	1.23
2	E	401	YVV	C40-C39	2.38	1.55	1.51
2	E	401	YVV	O41-C39	-2.38	1.18	1.23
2	E	401	YVV	O03-C01	-2.28	1.18	1.23
2	D	401	YVV	O41-C39	-2.25	1.18	1.23
2	F	401	YVV	O41-C39	-2.23	1.18	1.23
2	B	401	YVV	O41-C39	-2.19	1.18	1.23
2	C	401	YVV	C44-C45	2.19	1.54	1.46
2	A	401	YVV	C32-C36	2.16	1.56	1.51
2	F	401	YVV	O19-C18	-2.15	1.19	1.23
2	A	401	YVV	C44-C45	2.14	1.54	1.46
2	A	401	YVV	O41-C39	-2.14	1.18	1.23
2	E	401	YVV	C44-C45	2.14	1.54	1.46
2	B	401	YVV	O19-C18	-2.13	1.19	1.23
2	F	401	YVV	O03-C01	-2.12	1.19	1.23
2	B	401	YVV	O03-C01	-2.10	1.19	1.23
2	E	401	YVV	O19-C18	-2.10	1.19	1.23
2	F	401	YVV	C44-C45	2.08	1.54	1.46
2	F	401	YVV	C40-C39	2.08	1.55	1.51
2	E	401	YVV	O12-C10	-2.06	1.19	1.23
2	B	401	YVV	C44-C45	2.05	1.54	1.46
2	E	401	YVV	C32-C36	2.05	1.56	1.51
2	C	401	YVV	C04-N02	-2.02	1.41	1.45
2	C	401	YVV	O19-C18	-2.01	1.19	1.23
2	D	401	YVV	C44-C45	2.00	1.54	1.46

All (46) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	YVV	C13-C07-N06	-7.47	100.02	110.54
2	D	401	YVV	C13-C07-N06	-6.36	101.59	110.54
2	A	401	YVV	C13-C07-N06	-6.32	101.64	110.54
2	B	401	YVV	C13-C07-N06	-5.24	103.16	110.54
2	F	401	YVV	C13-C07-N06	-4.89	103.65	110.54
2	D	401	YVV	C05-C04-C18	-4.36	98.95	110.25
2	C	401	YVV	C05-C04-C18	-3.80	100.39	110.25
2	A	401	YVV	C05-C04-C18	-3.74	100.56	110.25
2	F	401	YVV	C08-C09-C10	-3.71	104.73	112.89
2	B	401	YVV	C05-C04-C18	-3.64	100.82	110.25
2	A	401	YVV	C08-C09-C10	-3.47	105.26	112.89
2	C	401	YVV	O16-C15-C14	3.35	122.41	111.91
2	E	401	YVV	C13-C07-N06	-3.31	105.89	110.54
2	E	401	YVV	C05-C04-C18	-3.18	102.00	110.25
2	E	401	YVV	C23-C09-C10	3.17	107.00	102.88
2	A	401	YVV	C22-N11-C10	-3.12	107.72	113.84
2	C	401	YVV	C22-N11-C10	-3.05	107.86	113.84
2	E	401	YVV	C22-N11-C10	-3.02	107.91	113.84
2	C	401	YVV	C08-C09-C10	-3.01	106.28	112.89
2	D	401	YVV	C22-N11-C10	-3.00	107.94	113.84
2	F	401	YVV	C05-C04-C18	-2.86	102.83	110.25
2	B	401	YVV	C22-N11-C10	-2.82	108.31	113.84
2	F	401	YVV	C22-N11-C10	-2.78	108.37	113.84
2	D	401	YVV	C08-C09-C10	-2.78	106.78	112.89
2	B	401	YVV	C08-C09-C10	-2.74	106.87	112.89
2	B	401	YVV	C08-C09-C23	-2.63	107.65	117.31
2	D	401	YVV	O16-C15-C14	2.59	120.03	111.91
2	D	401	YVV	C08-C09-C23	-2.56	107.90	117.31
2	A	401	YVV	C04-N02-C01	-2.50	116.31	121.67
2	E	401	YVV	O16-C15-C14	2.43	119.53	111.91
2	A	401	YVV	O16-C15-C14	2.42	119.52	111.91
2	B	401	YVV	O16-C15-C14	2.33	119.23	111.91
2	F	401	YVV	C08-C09-C23	-2.33	108.76	117.31
2	D	401	YVV	C04-N02-C01	-2.29	116.77	121.67
2	C	401	YVV	C08-C09-C23	-2.24	109.06	117.31
2	C	401	YVV	C36-C32-C30	-2.24	107.20	113.39
2	B	401	YVV	O12-C10-C09	-2.21	123.64	126.23
2	A	401	YVV	C08-C09-C23	-2.20	109.21	117.31
2	B	401	YVV	O03-C01-N02	-2.18	118.90	122.93
2	A	401	YVV	C30-C01-N02	2.17	121.45	116.70
2	A	401	YVV	O12-C10-C09	-2.13	123.73	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	YVV	C08-C07-C13	2.08	117.25	111.02
2	D	401	YVV	C28-C27-C26	2.05	121.38	118.17
2	A	401	YVV	C36-C32-C30	-2.03	107.77	113.39
2	C	401	YVV	C30-C01-N02	2.03	121.16	116.70
2	E	401	YVV	C05-C27-C28	-2.01	116.91	120.91

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	YVV	C39-C40-C42-O43
2	C	401	YVV	C39-C40-C42-O43
2	E	401	YVV	C39-C40-C42-O43
2	E	401	YVV	O43-C44-C45-C46
2	C	401	YVV	C21-C20-O16-C15
2	E	401	YVV	O17-C15-O16-C20
2	C	401	YVV	C14-C15-O16-C20
2	E	401	YVV	C14-C15-O16-C20
2	A	401	YVV	C14-C15-O16-C20
2	F	401	YVV	C14-C15-O16-C20
2	C	401	YVV	O17-C15-O16-C20
2	F	401	YVV	O17-C15-O16-C20
2	B	401	YVV	C07-C13-C14-C15
2	D	401	YVV	C14-C15-O16-C20
2	A	401	YVV	O17-C15-O16-C20
2	D	401	YVV	O17-C15-O16-C20
2	C	401	YVV	C45-C44-O43-C42
2	E	401	YVV	C04-C05-C27-C26
2	C	401	YVV	C04-C05-C27-C28
2	B	401	YVV	C04-C05-C27-C28
2	E	401	YVV	C04-C05-C27-C28
2	C	401	YVV	C04-C05-C27-C26
2	B	401	YVV	C04-C05-C27-C26
2	B	401	YVV	C14-C15-O16-C20
2	A	401	YVV	C04-C05-C27-C26
2	A	401	YVV	C04-C05-C27-C28
2	F	401	YVV	C04-C05-C27-C26
2	F	401	YVV	C04-C05-C27-C28
2	D	401	YVV	C04-C05-C27-C28
2	D	401	YVV	C04-C05-C27-C26
2	B	401	YVV	O17-C15-O16-C20
2	E	401	YVV	N31-C39-C40-C42

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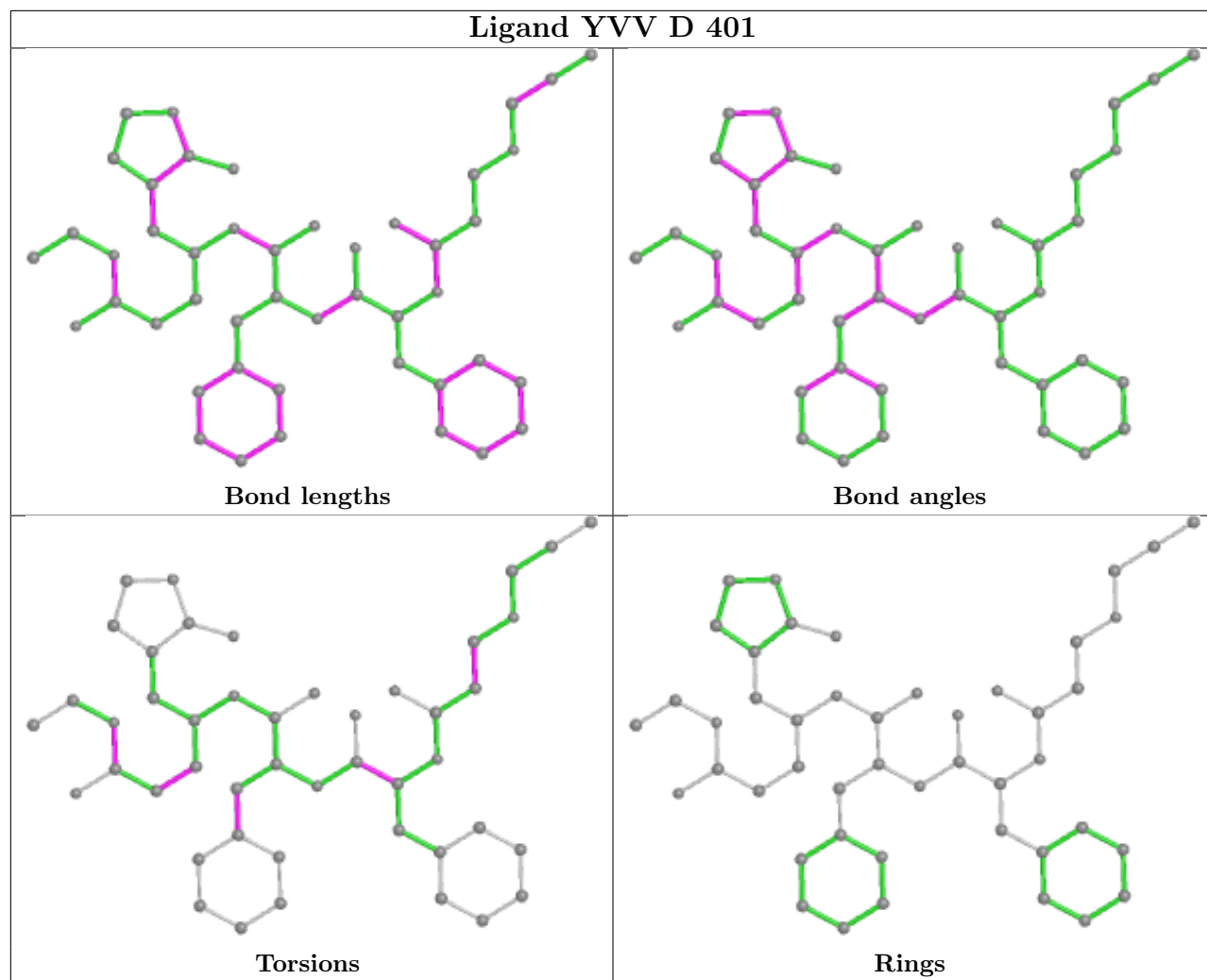
Mol	Chain	Res	Type	Atoms
2	B	401	YVV	C40-C42-O43-C44
2	D	401	YVV	O03-C01-C30-N31
2	F	401	YVV	C40-C42-O43-C44
2	A	401	YVV	C07-C13-C14-C15
2	E	401	YVV	C07-C13-C14-C15
2	C	401	YVV	C40-C42-O43-C44
2	D	401	YVV	N02-C01-C30-N31
2	B	401	YVV	C30-C32-C36-C37
2	B	401	YVV	C30-C32-C36-C35
2	B	401	YVV	O03-C01-C30-N31
2	D	401	YVV	C07-C13-C14-C15
2	F	401	YVV	O03-C01-C30-N31
2	B	401	YVV	N02-C01-C30-N31
2	F	401	YVV	N02-C01-C30-N31
2	A	401	YVV	C21-C20-O16-C15
2	A	401	YVV	O43-C44-C45-C46
2	C	401	YVV	O43-C44-C45-C46
2	B	401	YVV	O43-C44-C45-C46
2	F	401	YVV	O43-C44-C45-C46

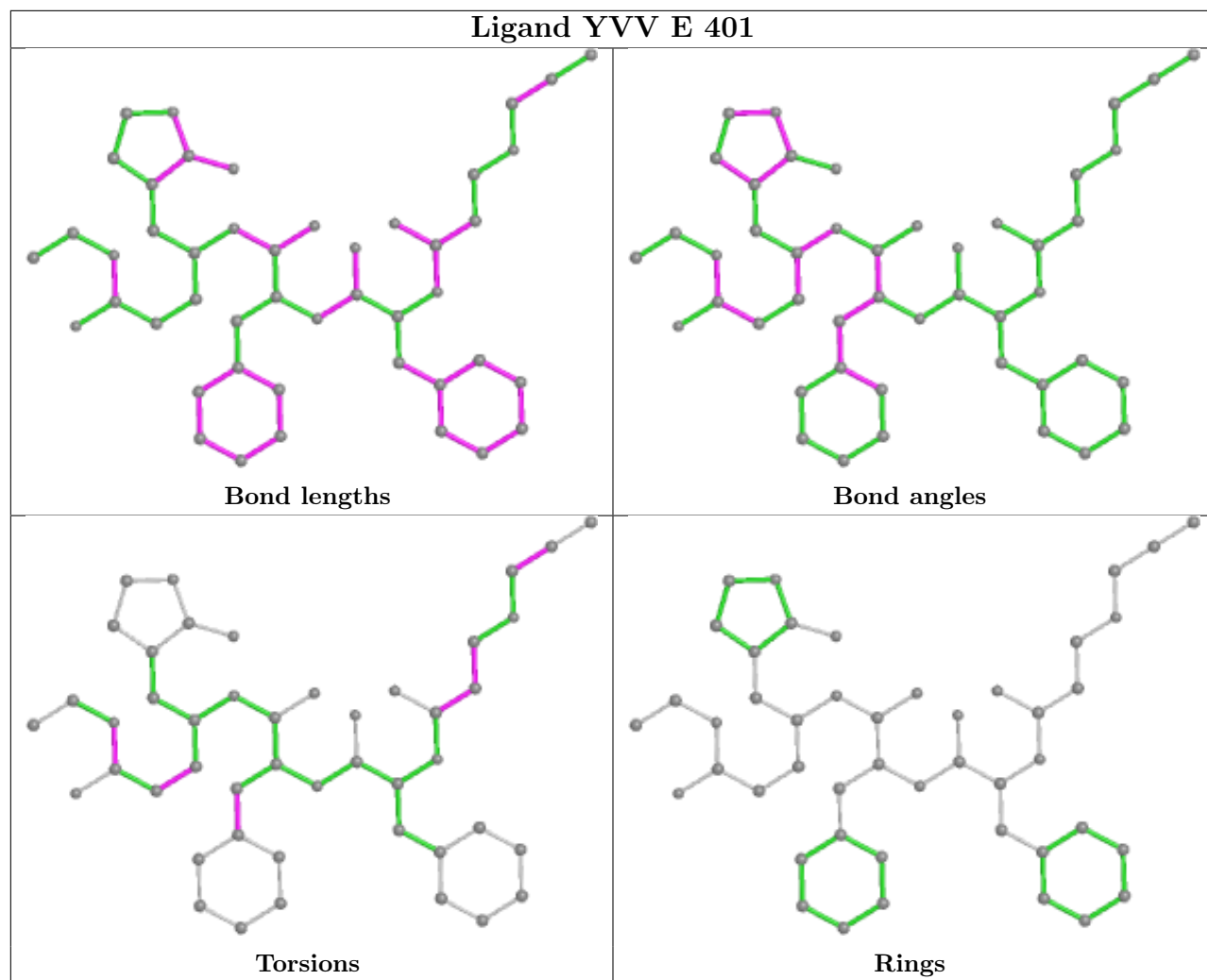
There are no ring outliers.

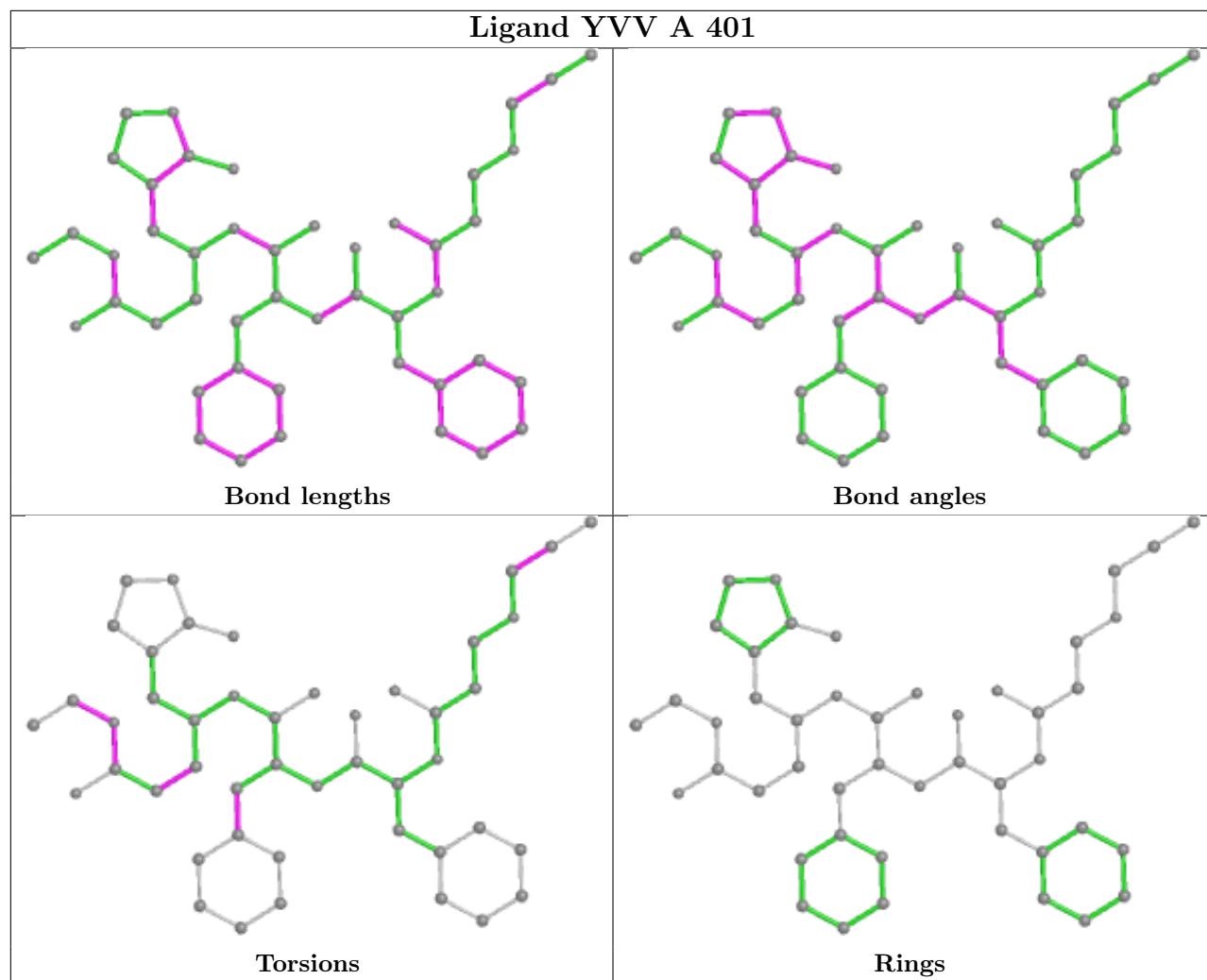
1 monomer is involved in 1 short contact:

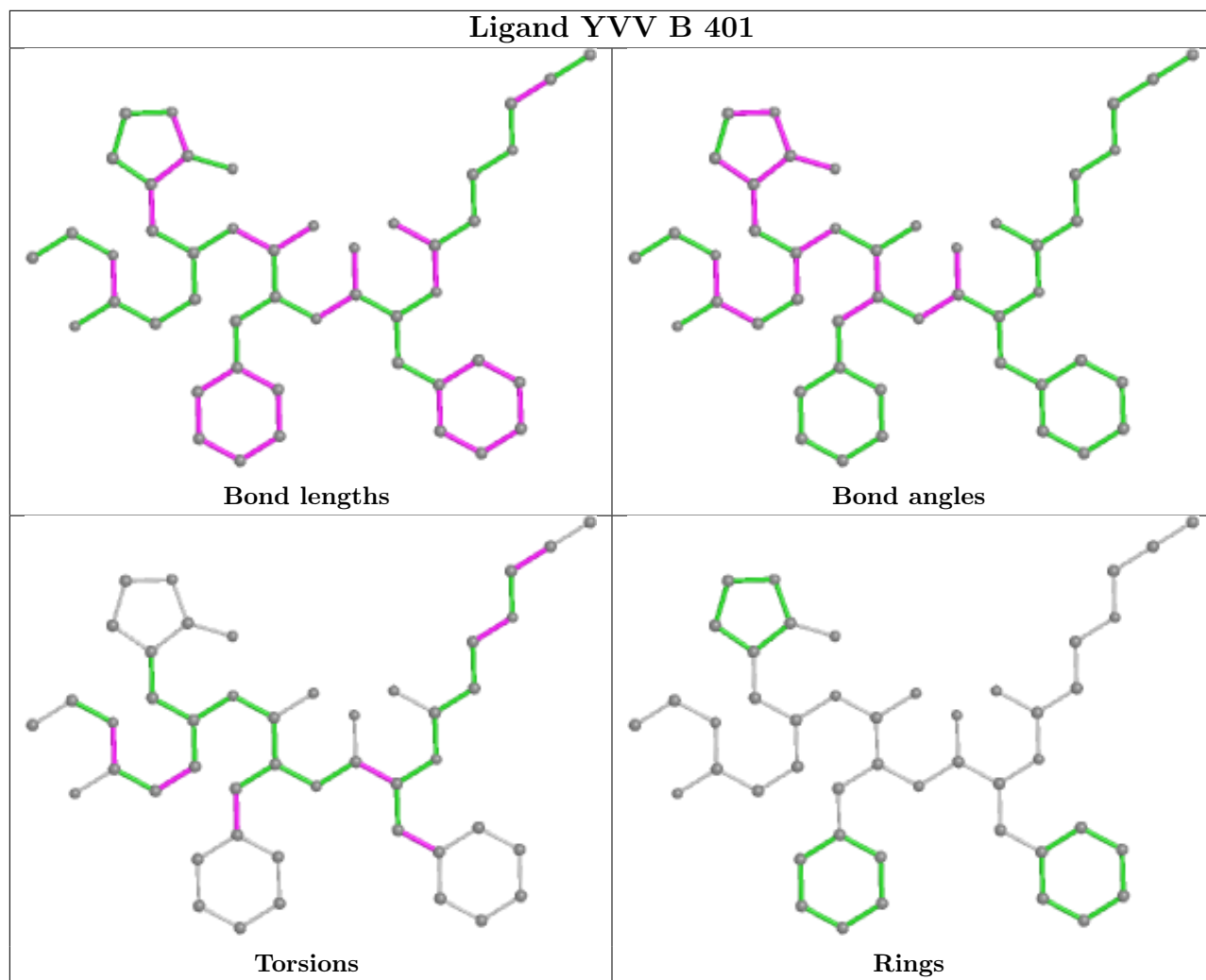
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	YVV	1	0

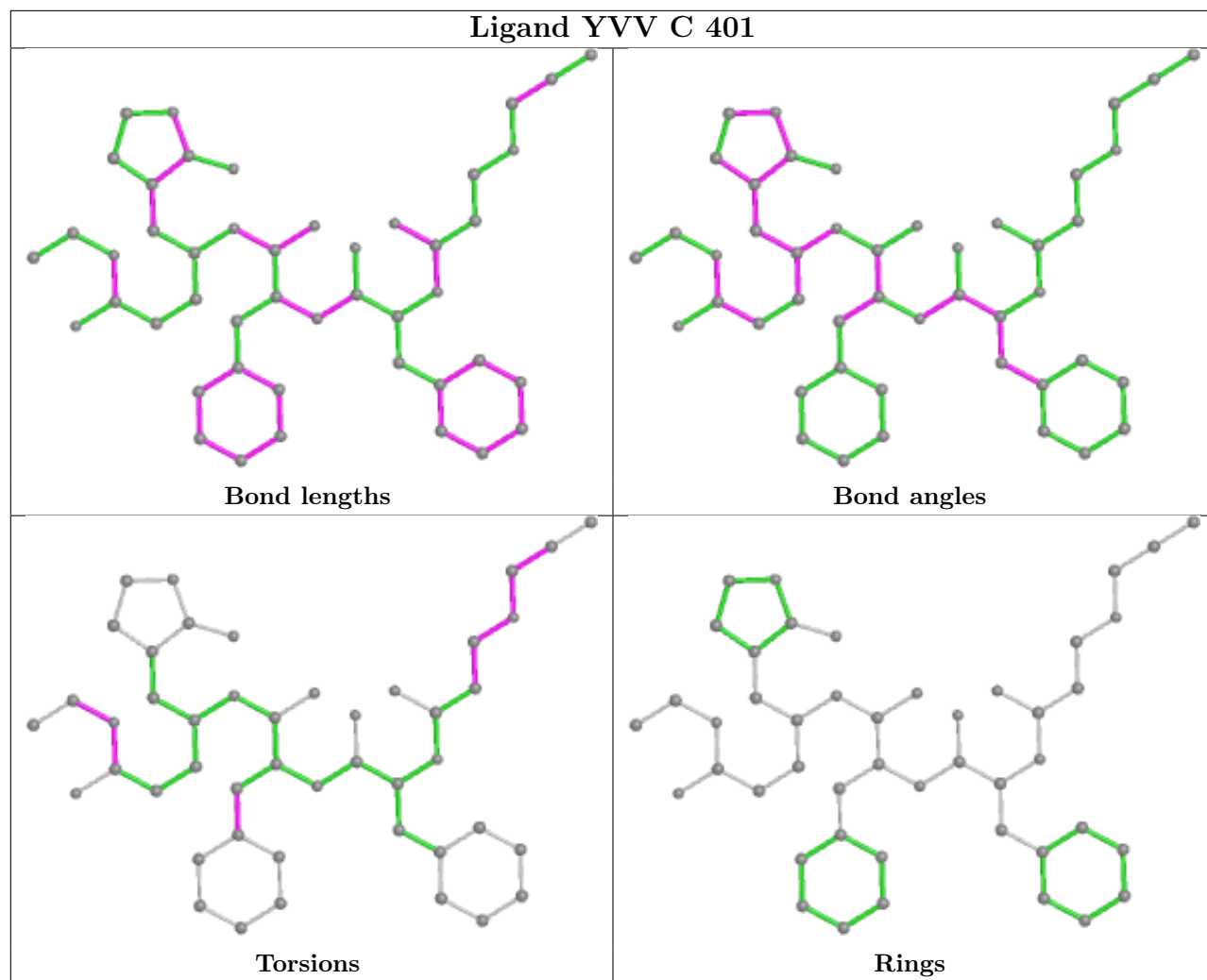
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

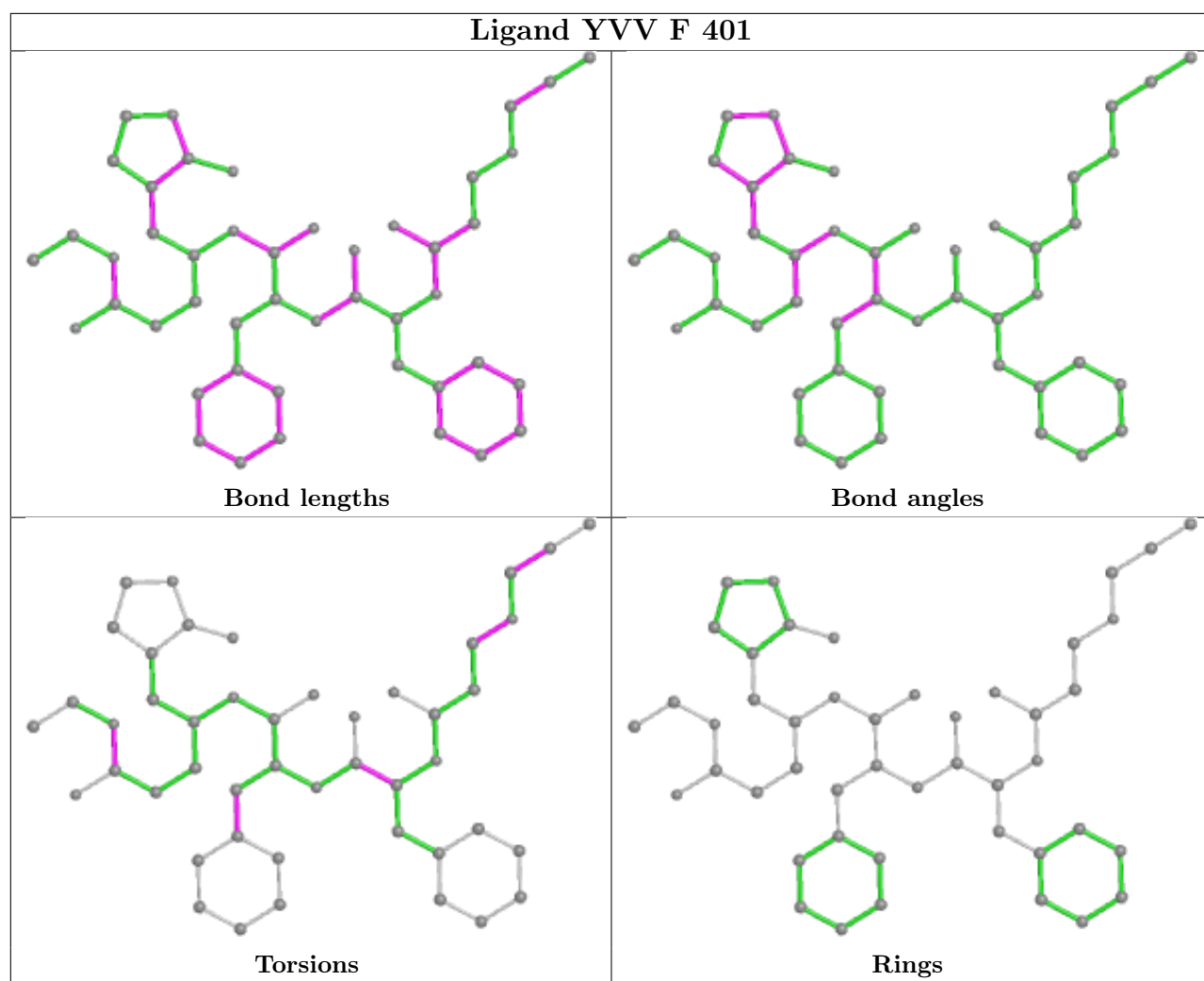












5.7 Other polymers [\(i\)](#)

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

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	305/306 (99%)	-0.47	2 (0%) 87 86	20, 30, 50, 91	0
1	B	302/306 (98%)	-0.32	6 (1%) 65 61	22, 34, 59, 86	0
1	C	305/306 (99%)	-0.40	4 (1%) 77 74	19, 28, 48, 106	0
1	D	302/306 (98%)	-0.37	5 (1%) 70 66	21, 32, 56, 89	0
1	E	301/306 (98%)	-0.05	7 (2%) 60 56	26, 44, 70, 103	0
1	F	305/306 (99%)	-0.13	10 (3%) 46 40	25, 40, 63, 102	0
All	All	1820/1836 (99%)	-0.29	34 (1%) 66 63	19, 34, 63, 106	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	ALA	6.8
1	C	49	MET	6.6
1	C	46	SER	5.6
1	D	278	GLY	4.5
1	E	301	SER	4.4
1	B	47	GLU	4.2
1	E	230	PHE	4.1
1	F	305	PHE	3.8
1	F	233	VAL	3.5
1	B	301	SER	3.5
1	E	232	LEU	3.4
1	F	46	SER	2.9
1	D	46	SER	2.9
1	E	262	LEU	2.9
1	D	191	ALA	2.9
1	F	223	PHE	2.8
1	A	49	MET	2.7
1	E	48	ASP	2.7
1	F	48	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	195	GLY	2.6
1	F	191	ALA	2.6
1	B	223	PHE	2.5
1	F	249	ILE	2.5
1	E	233	VAL	2.4
1	C	48	ASP	2.4
1	F	196	THR	2.3
1	B	72	ASN	2.2
1	D	302	GLY	2.2
1	A	48	ASP	2.2
1	D	223	PHE	2.2
1	E	46	SER	2.1
1	C	294	PHE	2.1
1	B	191	ALA	2.1
1	F	154	TYR	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.

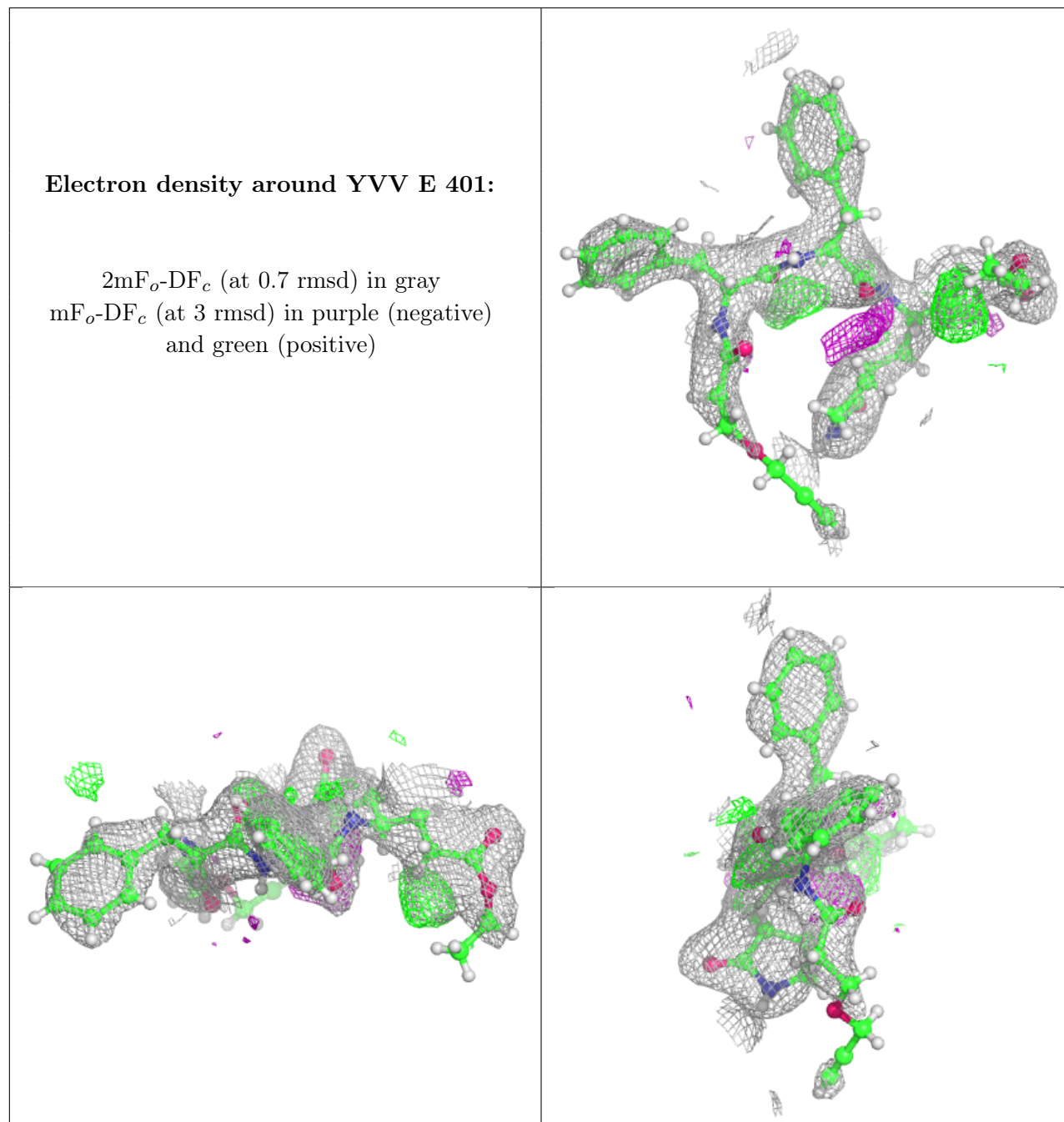
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	YVV	E	401	46/46	0.83	0.19	40,59,76,84	0
2	YVV	F	401	46/46	0.90	0.17	33,55,98,108	0
2	YVV	D	401	46/46	0.92	0.14	25,46,80,89	0
2	YVV	B	401	46/46	0.92	0.16	29,57,94,126	0
2	YVV	C	401	46/46	0.93	0.11	20,34,51,59	0
2	YVV	A	401	46/46	0.94	0.11	20,32,52,59	0

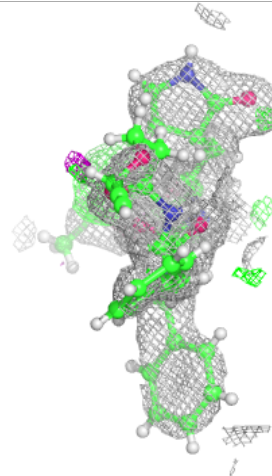
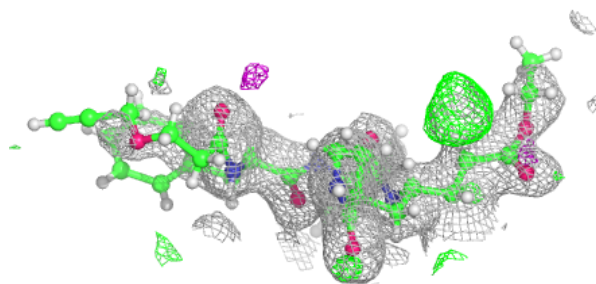
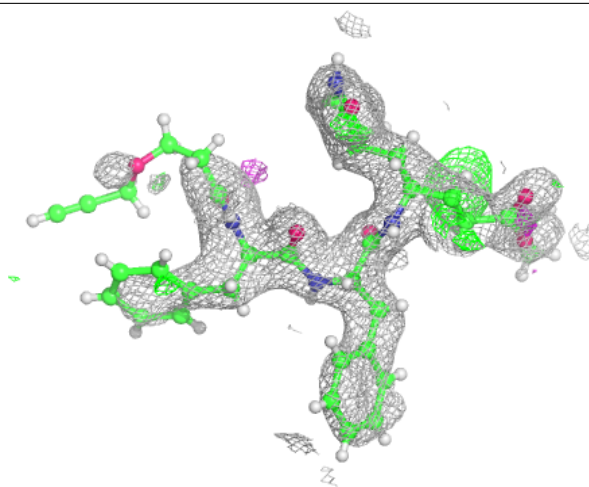
The following is a graphical depiction of the model fit to experimental electron density of all

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.



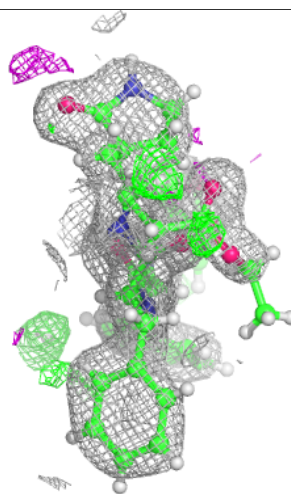
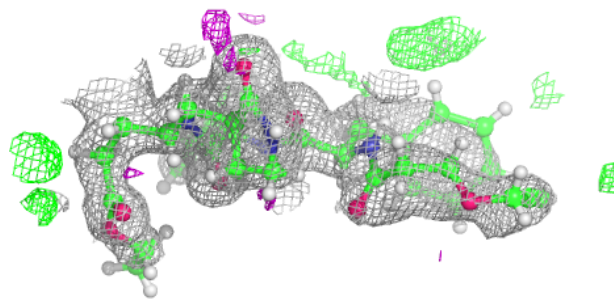
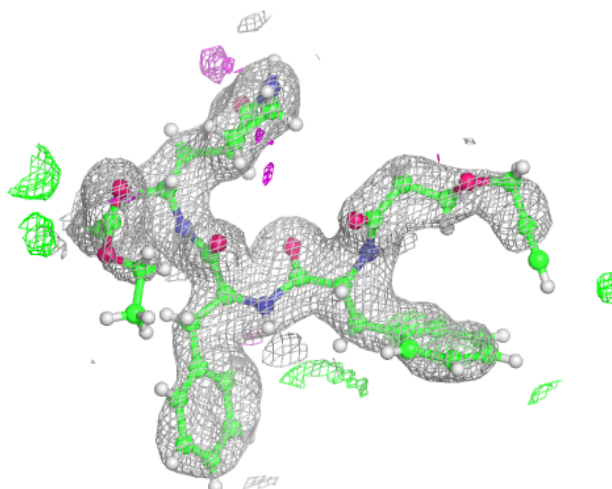
Electron density around YVV F 401:

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



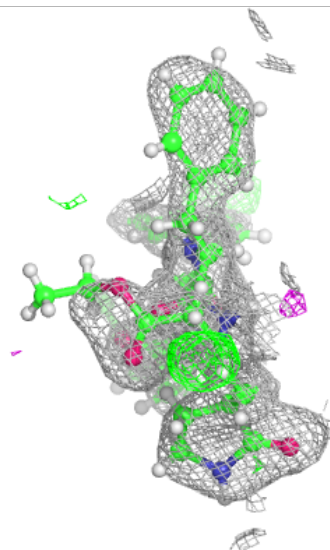
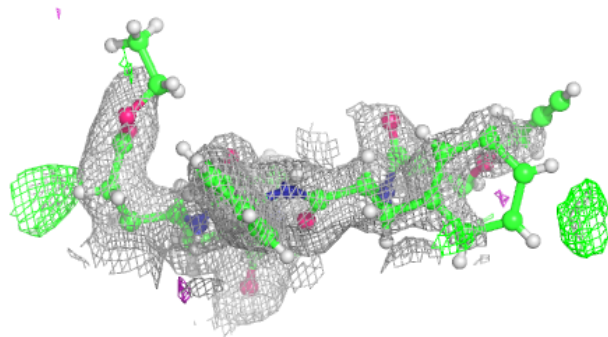
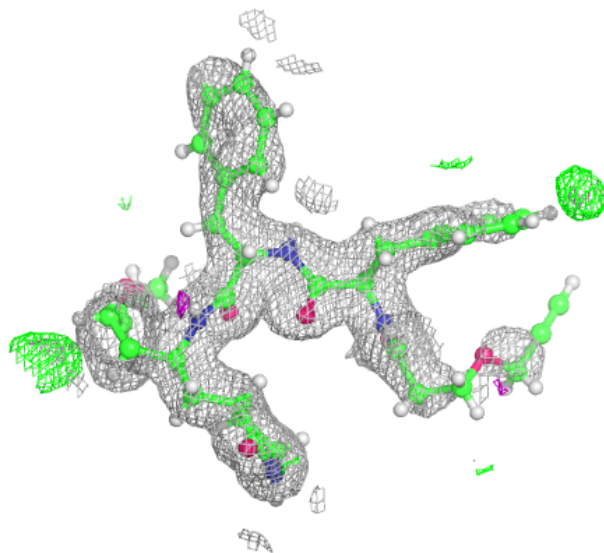
Electron density around YVV D 401:

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



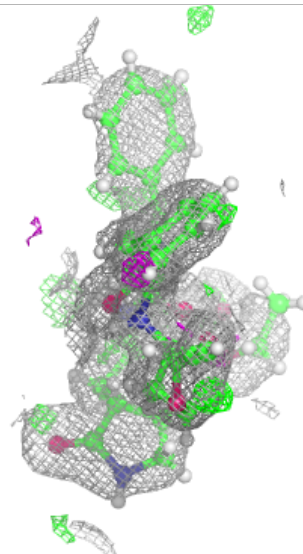
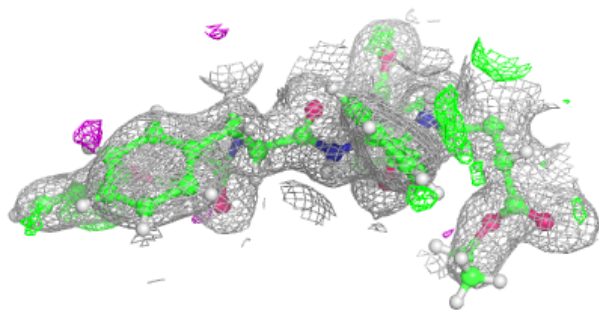
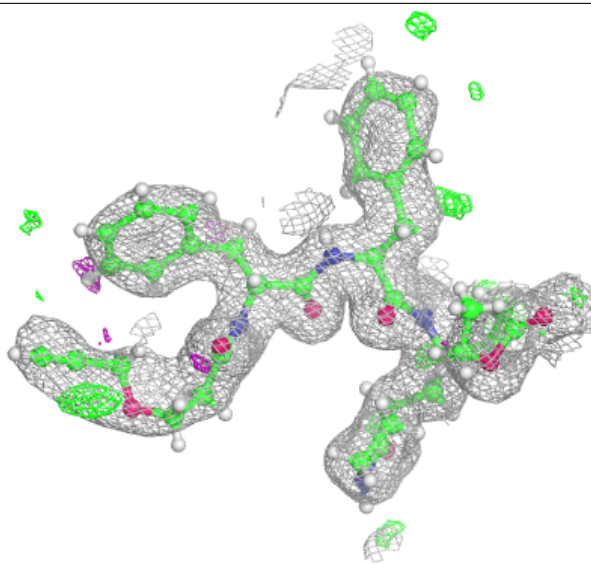
Electron density around YVV B 401:

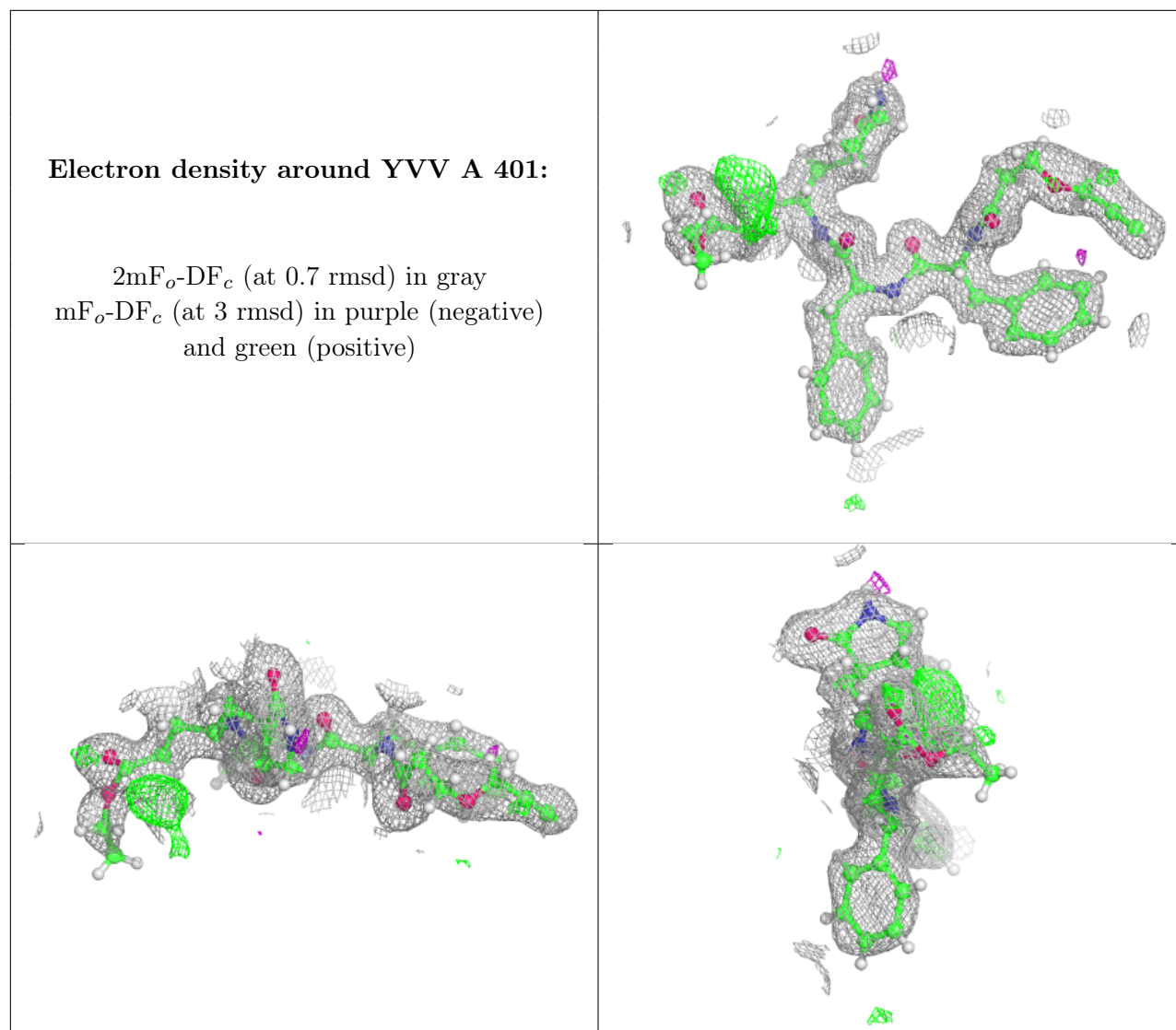
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around YVV C 401:

$2mF_o-DF_c$ (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.