WORLDWIDE wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 07:54 PM EDT

PDB ID	:	7REC
Title	:	Structure of Thr354Asn, Glu355Gln, Thr412Asn, Ile414Met, Ile464His, and Phe467Met mutant human CaMKII alpha hub bound to 5-HDC
Authors	:	McSpadden, E.D.; Chi, C.C.; Gee, C.L.; Kuriyan, J.
Deposited on	:	2021-07-12
Resolution	:	2.20 Å(reported)

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

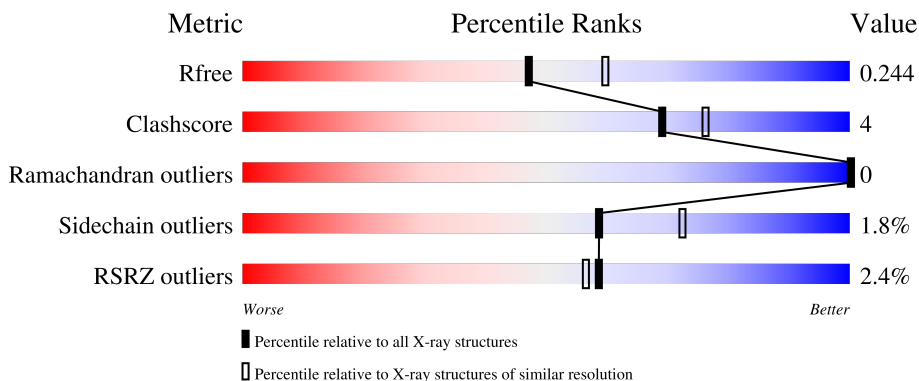|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.
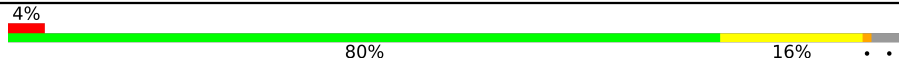
Metric	Percentile Ranks	Value
Rfree		0.244
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.8%
RSRZ outliers		2.4%

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	135	% 92% 6% ·
1	B	135	3% 88% 9% ·
1	C	135	3% 83% 11% 6%
1	D	135	% 87% 7% 5%
1	E	135	3% 77% 15% · 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	135	4% 80% 16% · ·
1	G	135	% 85% 8% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7511 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 Calcium/calmodulin-dependent protein kinase type II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	126	Total	C	N	O	S	0	0	0
			1019	639	186	186	8			
1	D	128	Total	C	N	O	S	0	1	0
			1041	653	190	190	8			
1	A	132	Total	C	N	O	S	0	0	0
			1073	672	198	195	8			
1	B	131	Total	C	N	O	S	0	0	0
			1062	666	195	194	7			
1	C	127	Total	C	N	O	S	0	0	0
			1028	645	188	187	8			
1	E	125	Total	C	N	O	S	0	2	0
			1024	644	186	186	8			
1	F	130	Total	C	N	O	S	0	0	0
			1056	666	192	190	8			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	341	GLY	-	expression tag	UNP Q9UQM7
G	342	PRO	-	expression tag	UNP Q9UQM7
G	343	HIS	-	expression tag	UNP Q9UQM7
G	344	MET	-	expression tag	UNP Q9UQM7
G	354	ASN	THR	engineered mutation	UNP Q9UQM7
G	355	GLN	GLU	engineered mutation	UNP Q9UQM7
G	412	ASN	THR	engineered mutation	UNP Q9UQM7
G	414	MET	ILE	engineered mutation	UNP Q9UQM7
G	464	HIS	ILE	engineered mutation	UNP Q9UQM7
G	467	MET	PHE	engineered mutation	UNP Q9UQM7
D	341	GLY	-	expression tag	UNP Q9UQM7
D	342	PRO	-	expression tag	UNP Q9UQM7
D	343	HIS	-	expression tag	UNP Q9UQM7
D	344	MET	-	expression tag	UNP Q9UQM7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	354	ASN	THR	engineered mutation	UNP Q9UQM7
D	355	GLN	GLU	engineered mutation	UNP Q9UQM7
D	412	ASN	THR	engineered mutation	UNP Q9UQM7
D	414	MET	ILE	engineered mutation	UNP Q9UQM7
D	464	HIS	ILE	engineered mutation	UNP Q9UQM7
D	467	MET	PHE	engineered mutation	UNP Q9UQM7
A	341	GLY	-	expression tag	UNP Q9UQM7
A	342	PRO	-	expression tag	UNP Q9UQM7
A	343	HIS	-	expression tag	UNP Q9UQM7
A	344	MET	-	expression tag	UNP Q9UQM7
A	354	ASN	THR	engineered mutation	UNP Q9UQM7
A	355	GLN	GLU	engineered mutation	UNP Q9UQM7
A	412	ASN	THR	engineered mutation	UNP Q9UQM7
A	414	MET	ILE	engineered mutation	UNP Q9UQM7
A	464	HIS	ILE	engineered mutation	UNP Q9UQM7
A	467	MET	PHE	engineered mutation	UNP Q9UQM7
B	341	GLY	-	expression tag	UNP Q9UQM7
B	342	PRO	-	expression tag	UNP Q9UQM7
B	343	HIS	-	expression tag	UNP Q9UQM7
B	344	MET	-	expression tag	UNP Q9UQM7
B	354	ASN	THR	engineered mutation	UNP Q9UQM7
B	355	GLN	GLU	engineered mutation	UNP Q9UQM7
B	412	ASN	THR	engineered mutation	UNP Q9UQM7
B	414	MET	ILE	engineered mutation	UNP Q9UQM7
B	464	HIS	ILE	engineered mutation	UNP Q9UQM7
B	467	MET	PHE	engineered mutation	UNP Q9UQM7
C	341	GLY	-	expression tag	UNP Q9UQM7
C	342	PRO	-	expression tag	UNP Q9UQM7
C	343	HIS	-	expression tag	UNP Q9UQM7
C	344	MET	-	expression tag	UNP Q9UQM7
C	354	ASN	THR	engineered mutation	UNP Q9UQM7
C	355	GLN	GLU	engineered mutation	UNP Q9UQM7
C	412	ASN	THR	engineered mutation	UNP Q9UQM7
C	414	MET	ILE	engineered mutation	UNP Q9UQM7
C	464	HIS	ILE	engineered mutation	UNP Q9UQM7
C	467	MET	PHE	engineered mutation	UNP Q9UQM7
E	341	GLY	-	expression tag	UNP Q9UQM7
E	342	PRO	-	expression tag	UNP Q9UQM7
E	343	HIS	-	expression tag	UNP Q9UQM7
E	344	MET	-	expression tag	UNP Q9UQM7
E	354	ASN	THR	engineered mutation	UNP Q9UQM7
E	355	GLN	GLU	engineered mutation	UNP Q9UQM7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	412	ASN	THR	engineered mutation	UNP Q9UQM7
E	414	MET	ILE	engineered mutation	UNP Q9UQM7
E	464	HIS	ILE	engineered mutation	UNP Q9UQM7
E	467	MET	PHE	engineered mutation	UNP Q9UQM7
F	341	GLY	-	expression tag	UNP Q9UQM7
F	342	PRO	-	expression tag	UNP Q9UQM7
F	343	HIS	-	expression tag	UNP Q9UQM7
F	344	MET	-	expression tag	UNP Q9UQM7
F	354	ASN	THR	engineered mutation	UNP Q9UQM7
F	355	GLN	GLU	engineered mutation	UNP Q9UQM7
F	412	ASN	THR	engineered mutation	UNP Q9UQM7
F	414	MET	ILE	engineered mutation	UNP Q9UQM7
F	464	HIS	ILE	engineered mutation	UNP Q9UQM7
F	467	MET	PHE	engineered mutation	UNP Q9UQM7

- Molecule 2 is 5-hydroxydiclofenac (three-letter code: 7ZV) (formula: $C_{14}H_{11}Cl_2NO_3$) (labeled as "Ligand of Interest" by depositor).
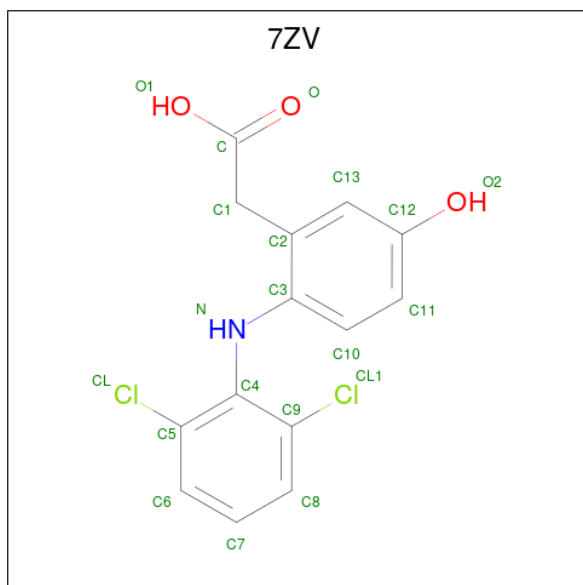
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	Cl	N	O	0	0
			20	14	2	1	3		
2	D	1	Total	C	Cl	N	O	0	0
			20	14	2	1	3		
2	B	1	Total	C	Cl	N	O	0	0
			20	14	2	1	3		
2	C	1	Total	C	Cl	N	O	0	0
			20	14	2	1	3		

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	Cl	N	O	0	0
			20	14	2	1	3		
2	F	1	Total	C	Cl	N	O	0	0
			20	14	2	1	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

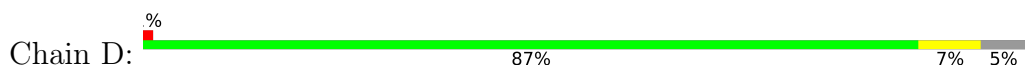| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	16	Total	O	0	0
			16	16		
4	D	16	Total	O	0	0
			16	16		
4	A	13	Total	O	0	0
			13	13		
4	B	14	Total	O	0	0
			14	14		
4	C	14	Total	O	0	0
			14	14		
4	E	7	Total	O	0	0
			7	7		
4	F	7	Total	O	0	0
			7	7		

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.
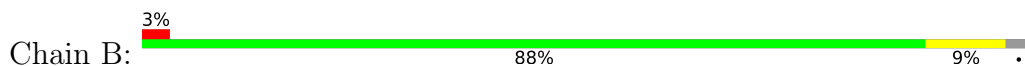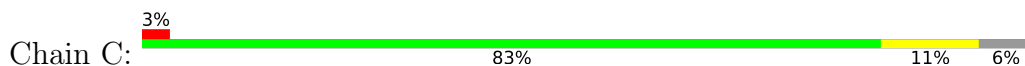
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha
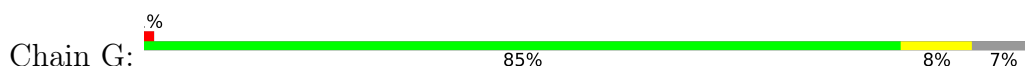
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha
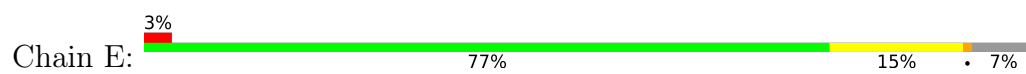

- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha
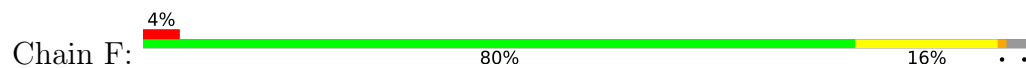

- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain E:

• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain F:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	101.43Å 182.96Å 106.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.48 – 2.20 91.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (91.48-2.20) 89.7 (91.48-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.67 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.209 , 0.244 0.209 , 0.244	Depositor DCC
R_{free} test set	1701 reflections (3.36%)	wwPDB-VP
Wilson B-factor (Å^2)	54.1	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.0	EDS
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7511	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: 7ZV, NA

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	0.25	0/1102	0.43	0/1489
1	B	0.25	0/1090	0.43	0/1474
1	C	0.25	0/1054	0.42	0/1422
1	D	0.25	0/1068	0.43	0/1443
1	E	0.26	0/1049	0.46	0/1415
1	F	0.25	0/1085	0.43	0/1466
1	G	0.25	0/1045	0.45	0/1410
All	All	0.25	0/7493	0.44	0/10119

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	1073	0	1025	8	0
1	B	1062	0	1018	9	0
1	C	1028	0	984	9	0
1	D	1041	0	996	5	0
1	E	1024	0	986	11	0
1	F	1056	0	1012	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1019	0	973	8	0
2	B	20	0	0	0	0
2	C	20	0	0	2	0
2	D	20	0	0	0	0
2	E	20	0	0	1	0
2	F	20	0	0	0	0
2	G	20	0	0	2	0
3	C	1	0	0	0	0
4	A	13	0	0	0	0
4	B	14	0	0	0	0
4	C	14	0	0	0	0
4	D	16	0	0	0	0
4	E	7	0	0	0	0
4	F	7	0	0	0	0
4	G	16	0	0	0	0
All	All	7511	0	6994	54	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 (54) 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:E:433:ARG:NH2	2:E:500:7ZV:CL	2.49	0.83
1:A:422:MET:HG2	1:B:456:HIS:HB2	1.70	0.74
1:E:414:MET:HG2	1:E:417:PRO:HG3	1.75	0.69
1:B:405:ARG:HA	1:B:408:LYS:HD3	1.78	0.65
1:F:343:HIS:HA	1:F:346:ARG:HG3	1.78	0.64
1:A:438:LEU:HD21	1:F:401:ASN:HD22	1.64	0.63
1:E:374:ASP:OD2	1:E:458:ARG:NH2	2.27	0.62
1:B:356:GLN:HB2	1:B:372:MET:HE1	1.82	0.60
1:G:348:GLN:OE1	1:G:352:LYS:NZ	2.38	0.56
1:A:456:HIS:HB2	1:B:422:MET:HG2	1.87	0.55
1:E:344:MET:O	1:E:348:GLN:NE2	2.39	0.55
1:D:378:THR:HB	1:D:388:LEU:HD11	1.92	0.52
1:E:378:THR:HB	1:E:388:LEU:HD11	1.93	0.51
1:F:357:LEU:O	1:F:361:ILE:HG12	2.10	0.51
1:E:422:MET:HG2	1:F:456:HIS:HB2	1.92	0.51
1:A:408:LYS:HB3	1:A:438:LEU:HD12	1.93	0.51
1:C:367:GLU:O	1:C:371:LYS:HG3	2.11	0.51
1:C:443:ILE:HG21	1:C:445:ARG:HH11	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ARG:HH22	1:B:457:ARG:NH2	2.10	0.50
1:G:369:TYR:OH	2:G:500:7ZV:O	2.28	0.49
1:G:469:ARG:NH2	2:G:500:7ZV:O1	2.45	0.48
1:F:361:ILE:HD13	1:F:399:PHE:HZ	1.79	0.48
1:G:348:GLN:O	1:G:352:LYS:HG2	2.13	0.48
1:F:413:THR:HB	1:F:434:ILE:HG22	1.95	0.48
1:F:433:ARG:NH1	1:F:451:GLU:OE2	2.42	0.48
1:C:433:ARG:NH2	2:C:501:7ZV:CL	2.84	0.47
1:F:402:LEU:HD21	1:F:475:VAL:HG11	1.97	0.47
1:E:456:HIS:HB2	1:F:422:MET:HG2	1.97	0.47
1:C:461:LYS:HA	1:C:461:LYS:HD2	1.74	0.46
1:C:408:LYS:HE2	1:C:409:PRO:HD2	1.98	0.45
1:C:349:GLU:O	1:C:353:VAL:HG23	2.15	0.45
1:B:401:ASN:HB2	1:E:444:PRO:HG3	1.99	0.45
1:G:368:SER:O	1:G:372:MET:HG3	2.18	0.44
1:B:366:PHE:CZ	1:B:396:ARG:HB2	2.51	0.44
1:A:456:HIS:CE1	1:B:422:MET:HA	2.51	0.44
1:F:467:MET:HE1	1:F:469:ARG:HH11	1.82	0.44
1:D:396:ARG:O	1:D:400:GLU:HG3	2.18	0.44
1:F:414:MET:HG3	1:F:431:TYR:CD1	2.52	0.43
1:E:464:HIS:CE1	1:E:467:MET:HB3	2.53	0.43
1:F:342:PRO:HB2	1:F:343:HIS:H	1.62	0.43
1:G:346:ARG:O	1:G:350:ILE:HG12	2.19	0.43
1:A:456:HIS:CG	1:B:422:MET:HG2	2.53	0.43
1:E:383:GLU:HB3	1:E:398:TYR:OH	2.19	0.42
1:D:458:ARG:O	1:D:461:LYS:HG2	2.19	0.42
1:A:378:THR:HB	1:A:388:LEU:HD11	2.02	0.42
1:C:389:VAL:HG11	1:C:394:PHE:CB	2.50	0.42
1:C:445:ARG:HA	1:C:445:ARG:HD3	1.89	0.41
1:E:414:MET:HG3	1:E:431:TYR:CD1	2.55	0.41
1:A:414:MET:HG3	1:A:431:TYR:CD2	2.55	0.41
1:G:346:ARG:HB3	1:G:421:LEU:HD13	2.02	0.41
1:G:422:MET:HG2	1:D:456:HIS:HB2	2.03	0.41
1:C:453:ARG:HH22	2:C:501:7ZV:C	2.34	0.41
1:D:415:LEU:HD23	1:D:415:LEU:HA	1.91	0.40
1:F:464:HIS:CE1	1:F:467:MET:HB3	2.56	0.40

There are no symmetry-related clashes.

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	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
1	B	129/135 (96%)	124 (96%)	5 (4%)	0	100	100
1	C	123/135 (91%)	119 (97%)	4 (3%)	0	100	100
1	D	125/135 (93%)	120 (96%)	5 (4%)	0	100	100
1	E	123/135 (91%)	121 (98%)	2 (2%)	0	100	100
1	F	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
1	G	122/135 (90%)	118 (97%)	4 (3%)	0	100	100
All	All	878/945 (93%)	851 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	115/117 (98%)	115 (100%)	0	100	100
1	B	114/117 (97%)	113 (99%)	1 (1%)	78	88
1	C	110/117 (94%)	108 (98%)	2 (2%)	59	72
1	D	112/117 (96%)	110 (98%)	2 (2%)	59	72
1	E	109/117 (93%)	104 (95%)	5 (5%)	27	34
1	F	113/117 (97%)	110 (97%)	3 (3%)	44	57
1	G	109/117 (93%)	108 (99%)	1 (1%)	78	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	782/819 (96%)	768 (98%)	14 (2%)	59 72

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	425	GLU
1	D	392	LEU
1	D	438	LEU
1	B	404	SER
1	C	344	MET
1	C	426	SER
1	E	346	ARG
1	E	348	GLN
1	E	393	ASP
1	E	396	ARG
1	E	408	LYS
1	F	344	MET
1	F	425	GLU
1	F	456	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	#$|Z| > 2$
2	7ZV	E	500	-	21,21,21	1.14	3 (14%)	29,29,29	1.18	3 (10%)
2	7ZV	C	501	-	21,21,21	1.14	3 (14%)	29,29,29	1.06	2 (6%)
2	7ZV	B	500	-	21,21,21	1.16	3 (14%)	29,29,29	1.04	2 (6%)
2	7ZV	D	500	-	21,21,21	1.15	3 (14%)	29,29,29	0.99	2 (6%)
2	7ZV	G	500	-	21,21,21	1.15	3 (14%)	29,29,29	1.01	2 (6%)
2	7ZV	F	500	-	21,21,21	1.16	3 (14%)	29,29,29	1.04	1 (3%)

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	7ZV	E	500	-	-	0/8/8/8	0/2/2/2
2	7ZV	C	501	-	-	0/8/8/8	0/2/2/2
2	7ZV	B	500	-	-	0/8/8/8	0/2/2/2
2	7ZV	D	500	-	-	0/8/8/8	0/2/2/2
2	7ZV	G	500	-	-	0/8/8/8	0/2/2/2
2	7ZV	F	500	-	-	1/8/8/8	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	7ZV	C3-N	2.33	1.46	1.39
2	F	500	7ZV	C5-CL	2.31	1.79	1.73
2	E	500	7ZV	C9-CL1	2.29	1.79	1.73
2	B	500	7ZV	C5-CL	2.27	1.79	1.73
2	C	501	7ZV	C9-CL1	2.26	1.79	1.73
2	D	500	7ZV	C9-CL1	2.26	1.79	1.73
2	G	500	7ZV	C9-CL1	2.26	1.79	1.73
2	G	500	7ZV	C3-N	2.26	1.46	1.39
2	F	500	7ZV	C9-CL1	2.25	1.79	1.73
2	F	500	7ZV	C3-N	2.25	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	7ZV	C5-CL	2.23	1.78	1.73
2	D	500	7ZV	C5-CL	2.21	1.78	1.73
2	B	500	7ZV	C9-CL1	2.20	1.78	1.73
2	G	500	7ZV	C5-CL	2.19	1.78	1.73
2	E	500	7ZV	C5-CL	2.16	1.78	1.73
2	D	500	7ZV	C3-N	2.15	1.45	1.39
2	C	501	7ZV	C3-N	2.15	1.45	1.39
2	E	500	7ZV	C3-N	2.06	1.45	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	500	7ZV	C5-C4-C9	2.79	120.47	116.14
2	C	501	7ZV	C5-C4-C9	2.73	120.37	116.14
2	E	500	7ZV	C5-C4-N	-2.56	118.72	122.04
2	D	500	7ZV	C5-C4-C9	2.50	120.01	116.14
2	B	500	7ZV	C13-C2-C3	2.46	120.63	118.54
2	G	500	7ZV	C5-C4-C9	2.44	119.93	116.14
2	E	500	7ZV	C13-C2-C3	2.44	120.61	118.54
2	F	500	7ZV	C5-C4-C9	2.43	119.92	116.14
2	B	500	7ZV	C5-C4-C9	2.42	119.89	116.14
2	C	501	7ZV	C5-C4-N	-2.20	119.18	122.04
2	G	500	7ZV	C13-C2-C3	2.12	120.34	118.54
2	D	500	7ZV	C5-C4-N	-2.01	119.43	122.04

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	500	7ZV	O-C-C1-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	500	7ZV	1	0
2	C	501	7ZV	2	0
2	G	500	7ZV	2	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
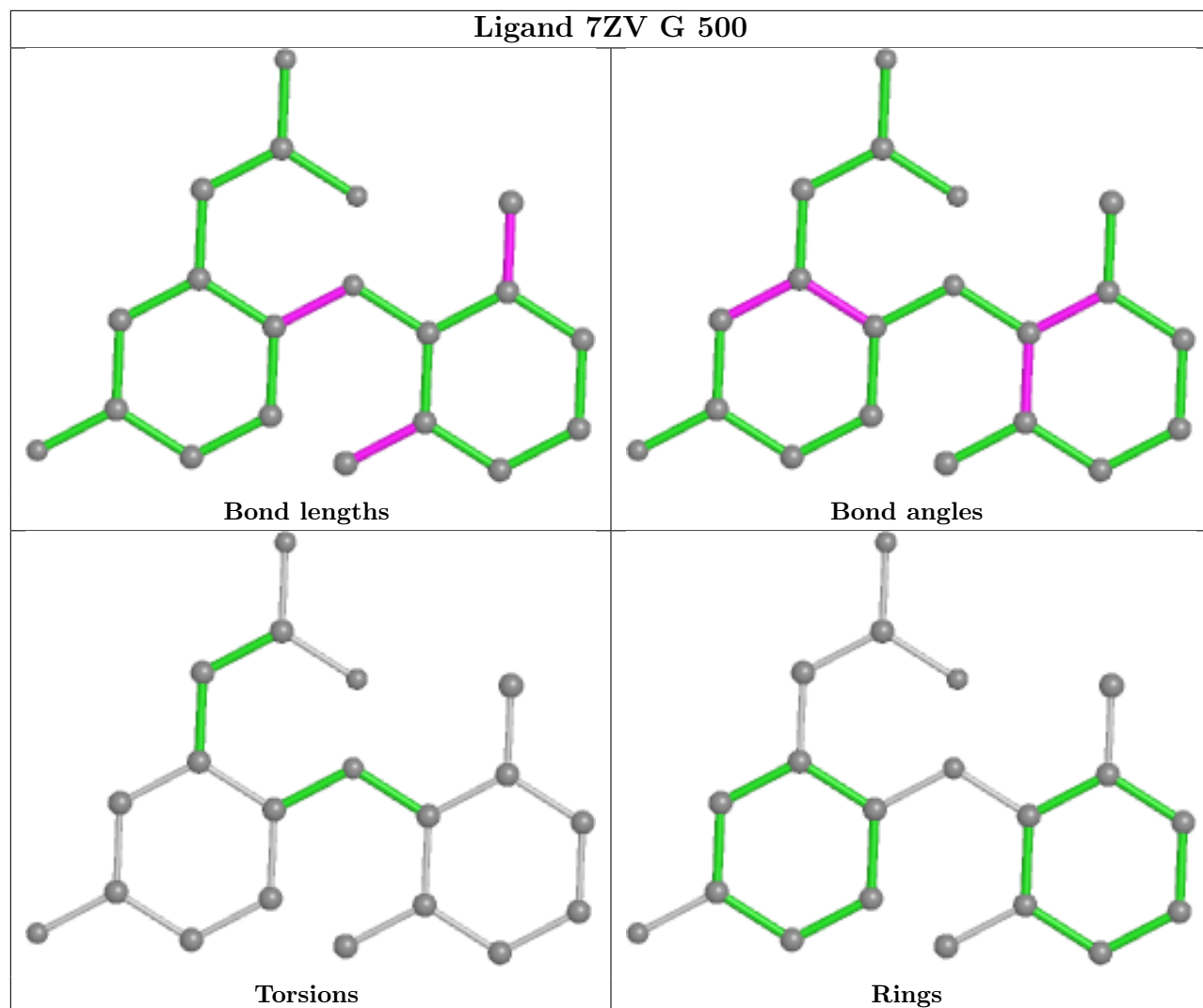
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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 7ZV E 500

Bond lengths

Bond angles

Torsions

Rings

Ligand 7ZV C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 7ZV B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand 7ZV D 500

Bond lengths

Bond angles

Torsions

Rings

Ligand 7ZV G 500

Bond lengths

Bond angles

Torsions

Rings

Ligand 7ZV F 500

Bond lengths

Bond angles

Torsions

Rings
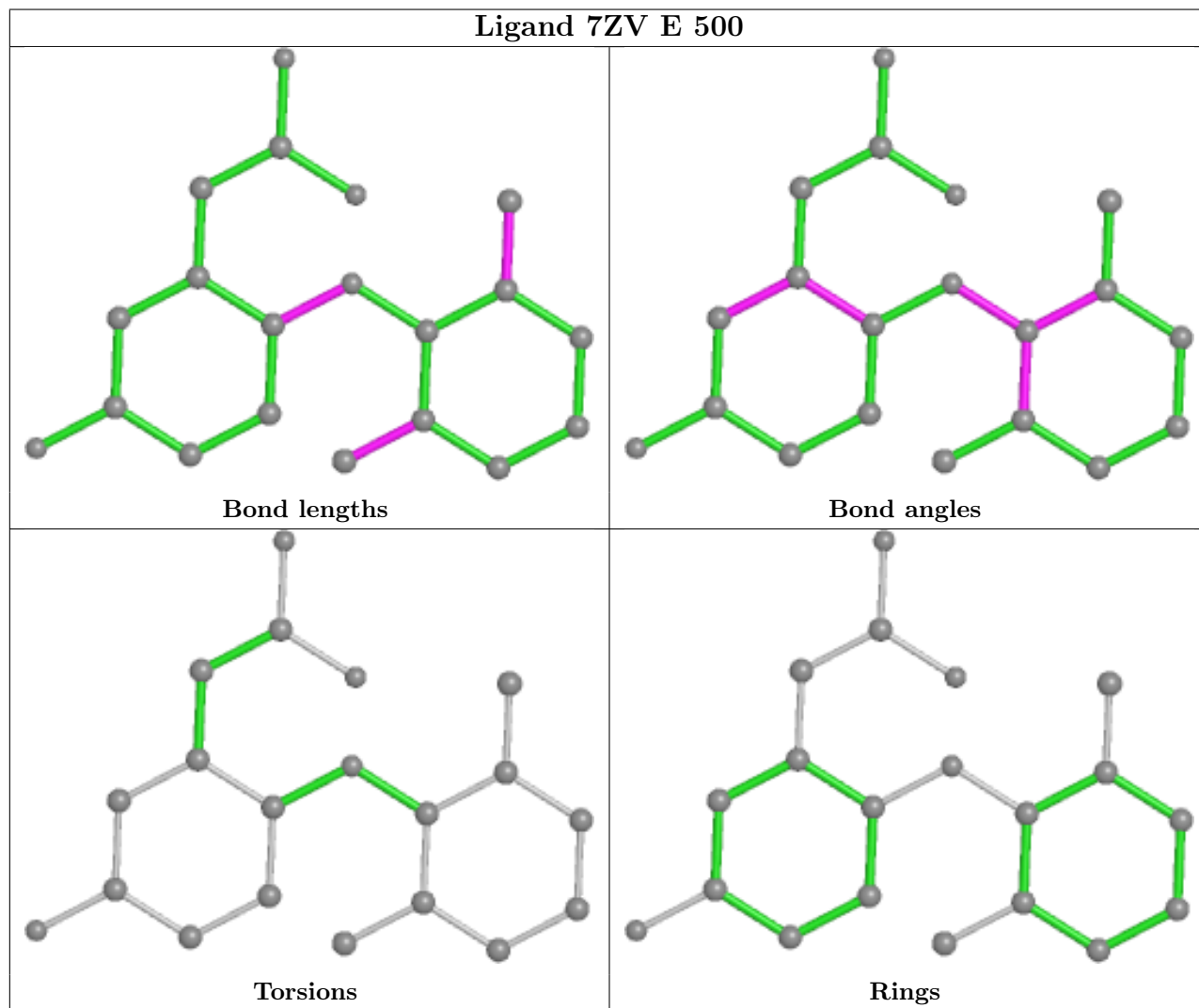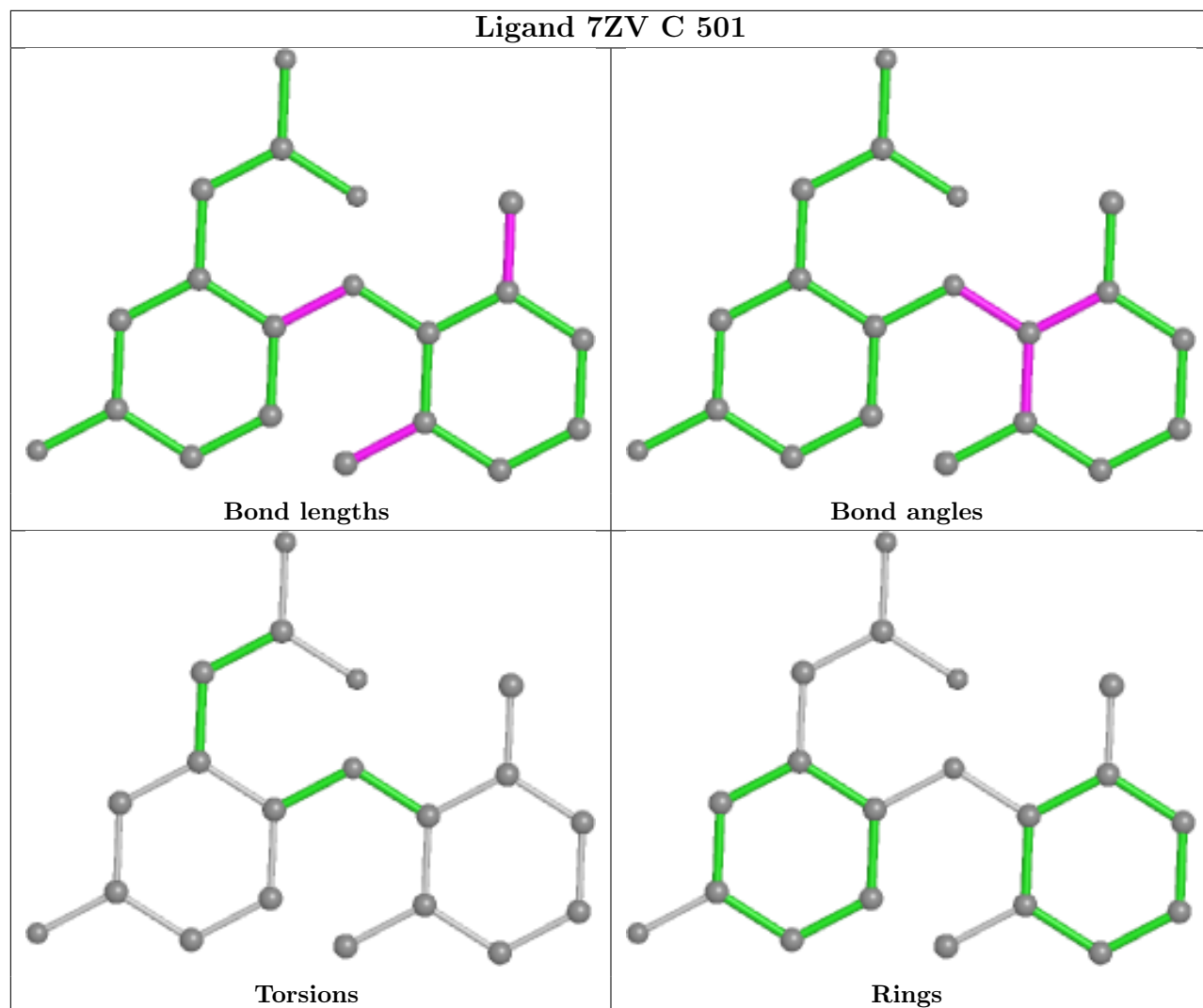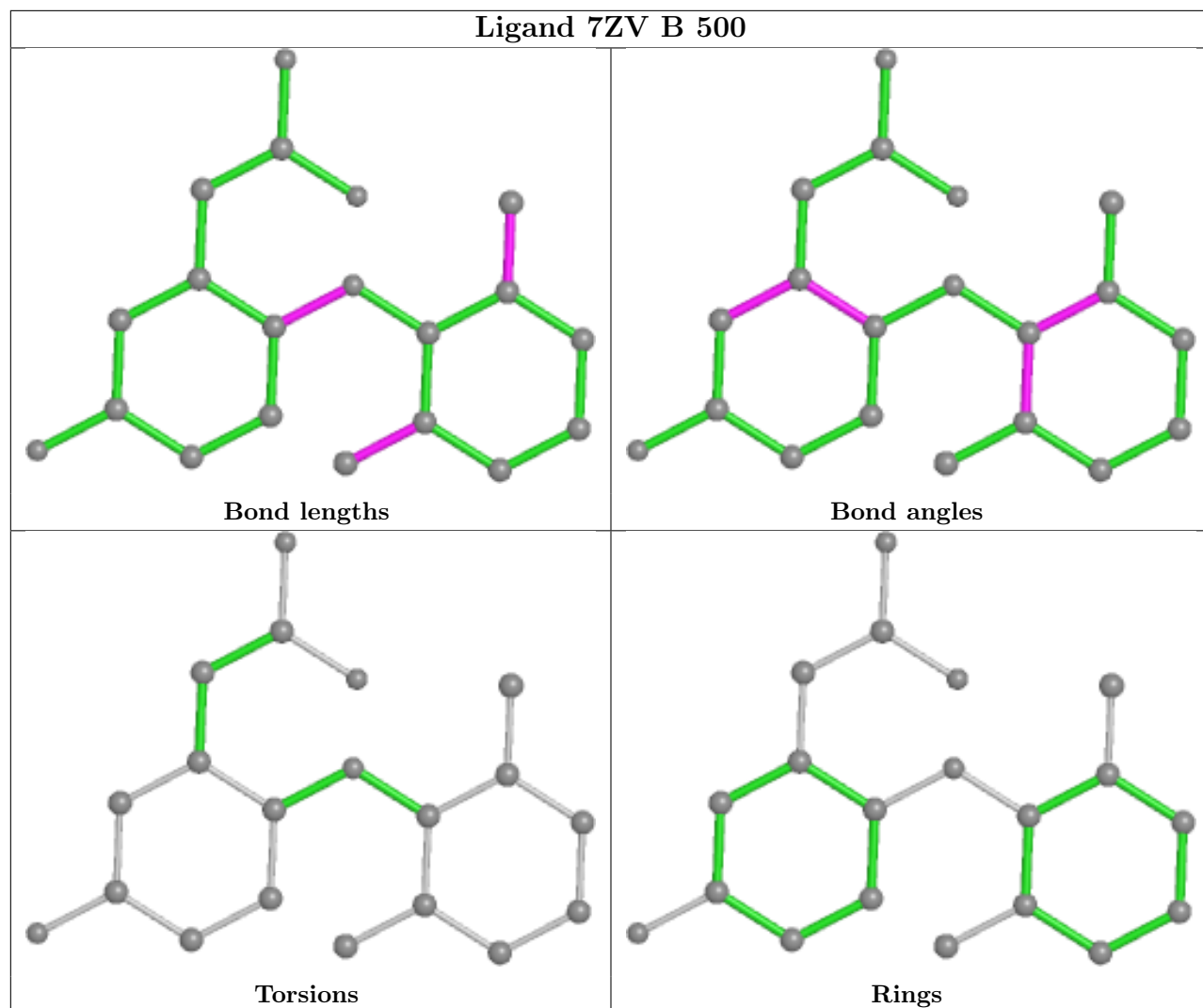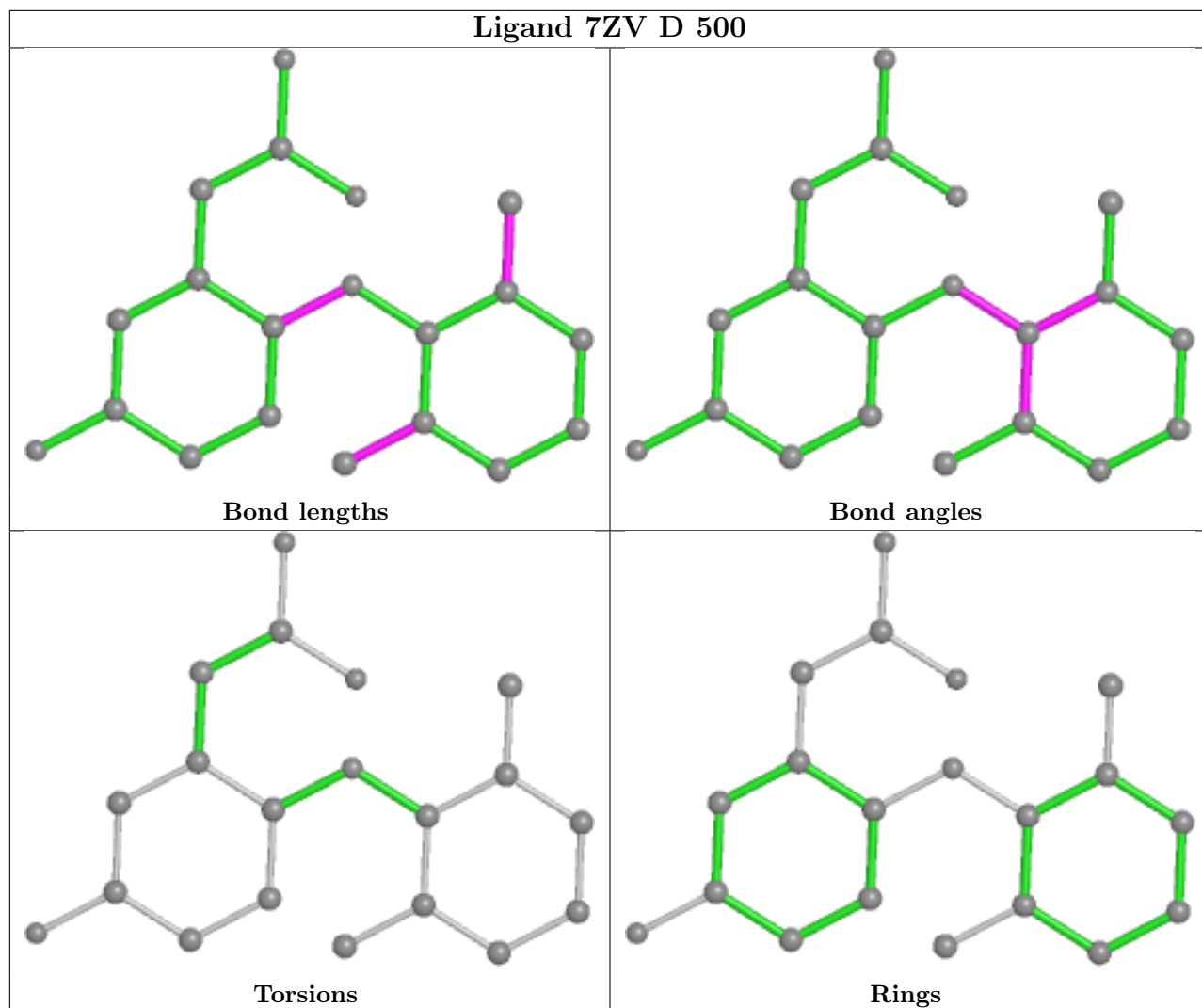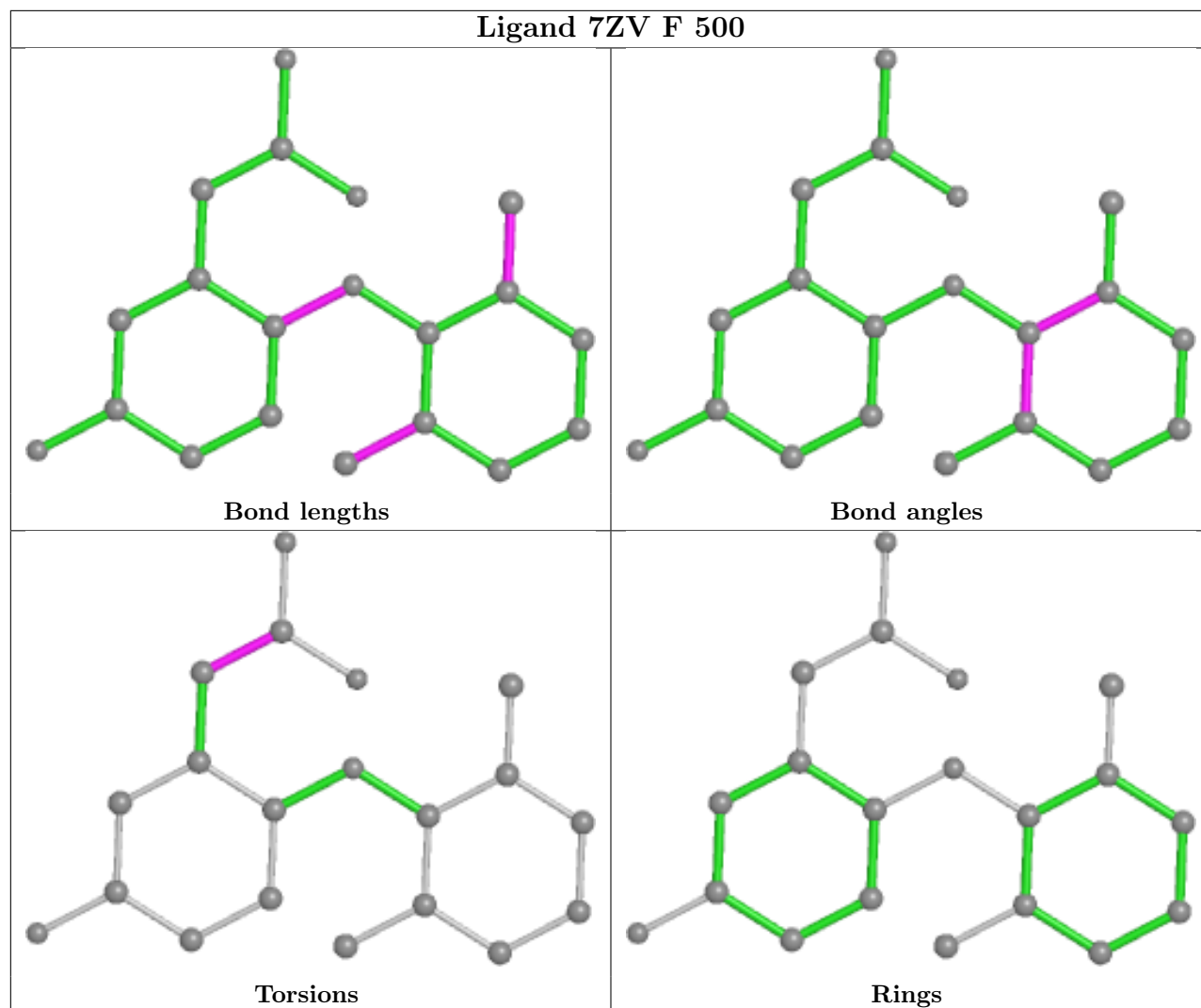
5.7 Other polymers ⓘ

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	132/135 (97%)	0.18	2 (1%)	73	72	52, 80, 135, 169	0
1	B	131/135 (97%)	0.28	4 (3%)	49	47	50, 86, 128, 182	0
1	C	127/135 (94%)	0.21	4 (3%)	49	47	46, 76, 133, 164	0
1	D	128/135 (94%)	0.01	1 (0%)	86	85	42, 69, 108, 157	0
1	E	125/135 (92%)	0.17	4 (3%)	47	45	46, 78, 119, 143	0
1	F	130/135 (96%)	0.33	5 (3%)	40	38	47, 89, 138, 167	0
1	G	126/135 (93%)	0.06	2 (1%)	72	70	42, 72, 136, 159	0
All	All	899/945 (95%)	0.18	22 (2%)	59	56	42, 78, 133, 182	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	344	MET	6.1
1	E	402	LEU	5.5
1	C	343	HIS	4.5
1	G	440	ALA	3.5
1	B	345	VAL	3.0
1	F	343	HIS	2.9
1	C	440	ALA	2.8
1	B	459	ASP	2.8
1	F	345	VAL	2.6
1	B	440	ALA	2.6
1	G	438	LEU	2.5
1	C	345	VAL	2.5
1	D	414	MET	2.4
1	E	345	VAL	2.4
1	F	461	LYS	2.3
1	A	403	TRP	2.3
1	F	460	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	407	SER	2.2
1	F	425	GLU	2.2
1	B	371	LYS	2.1
1	C	425	GLU	2.1
1	E	409	PRO	2.1

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
2	7ZV	E	500	20/20	0.82	0.24	65,70,97,102	0
2	7ZV	G	500	20/20	0.90	0.13	58,70,85,92	0
2	7ZV	B	500	20/20	0.92	0.13	58,71,82,92	0
2	7ZV	F	500	20/20	0.92	0.14	55,60,92,104	0
3	NA	C	502	1/1	0.92	0.29	79,79,79,79	0
2	7ZV	C	501	20/20	0.93	0.15	61,69,91,97	0
2	7ZV	D	500	20/20	0.94	0.10	54,63,69,72	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 7ZV E 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
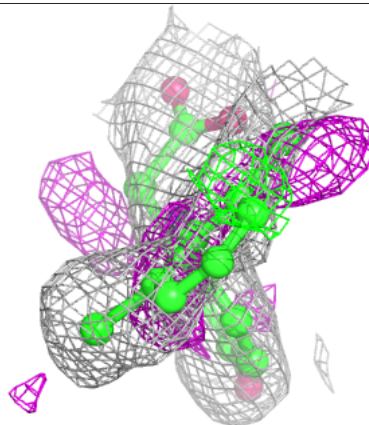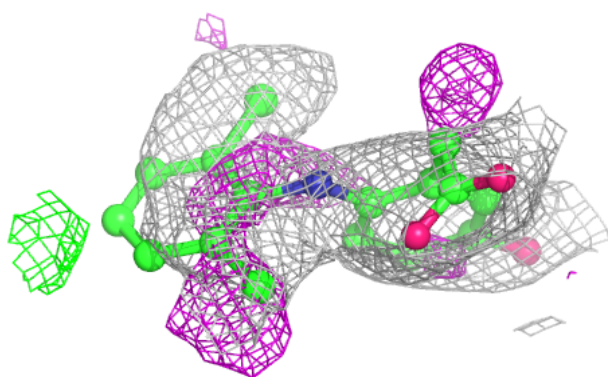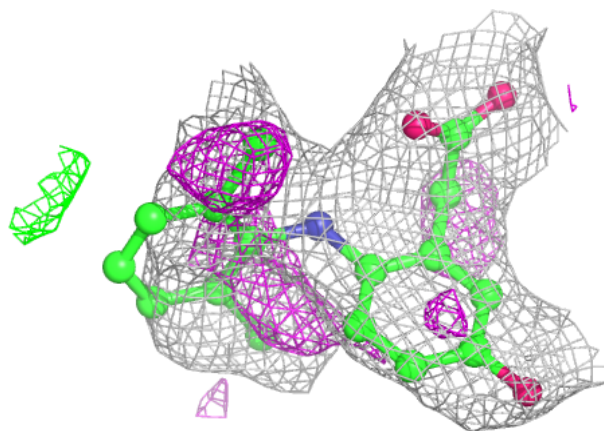
Electron density around 7ZV G 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
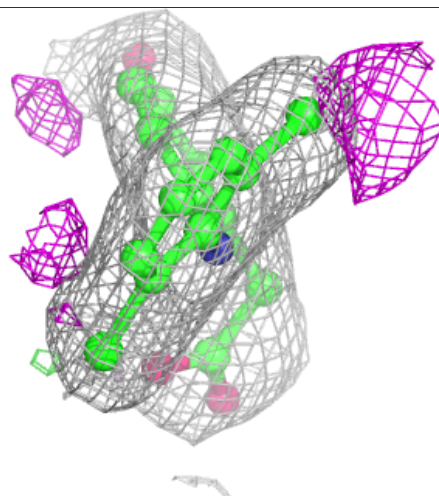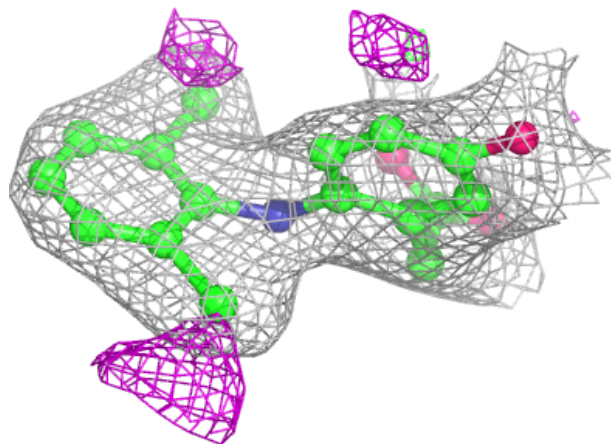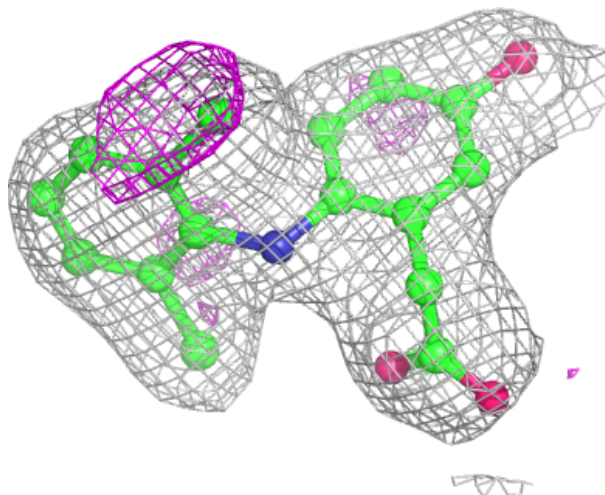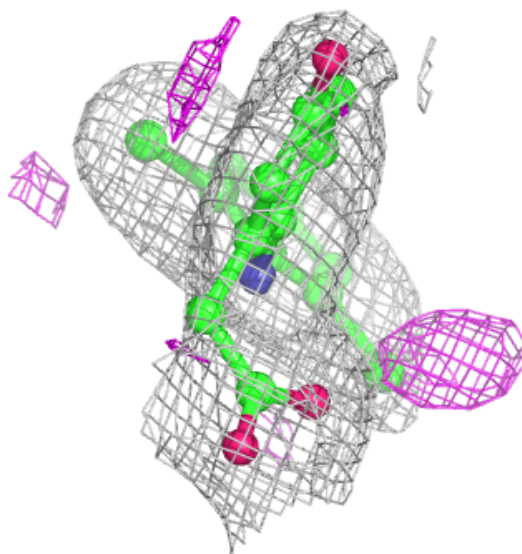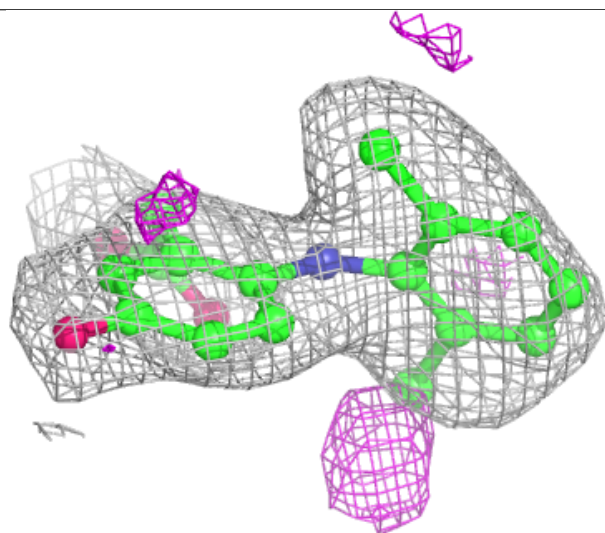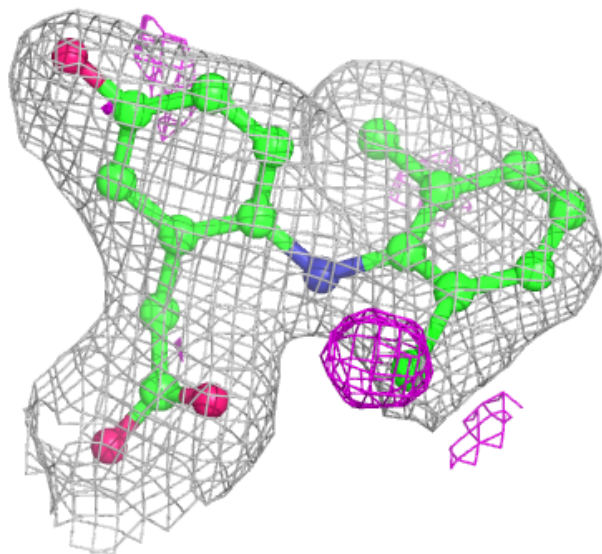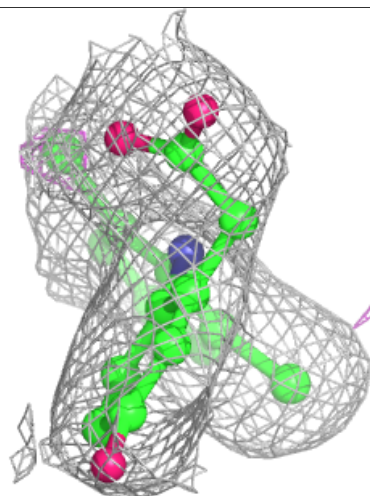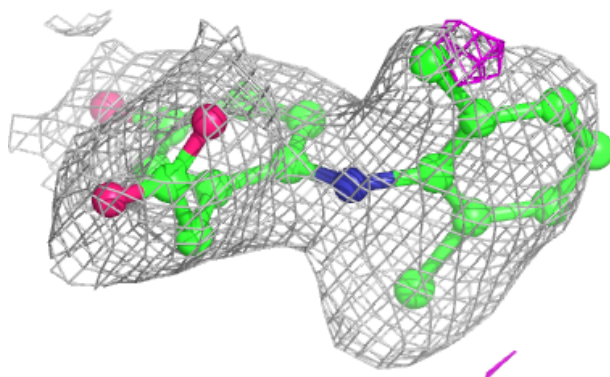$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
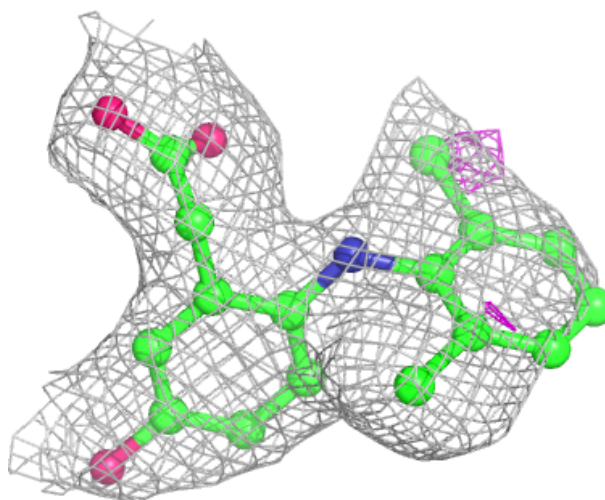and green (positive)
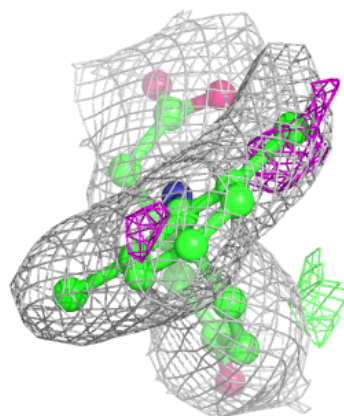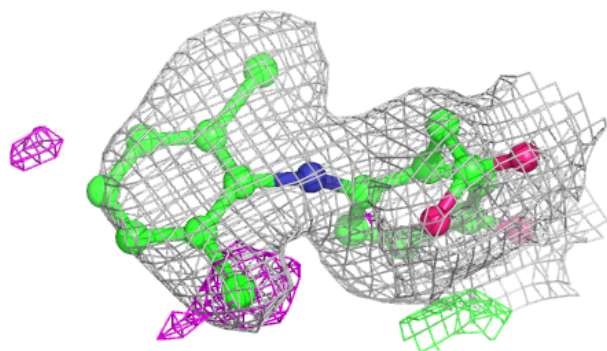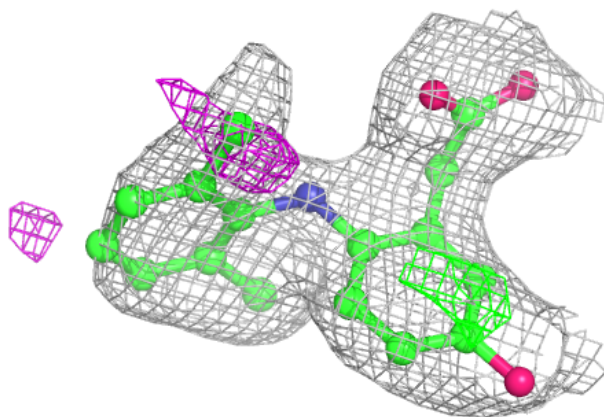
Electron density around 7ZV B 500:

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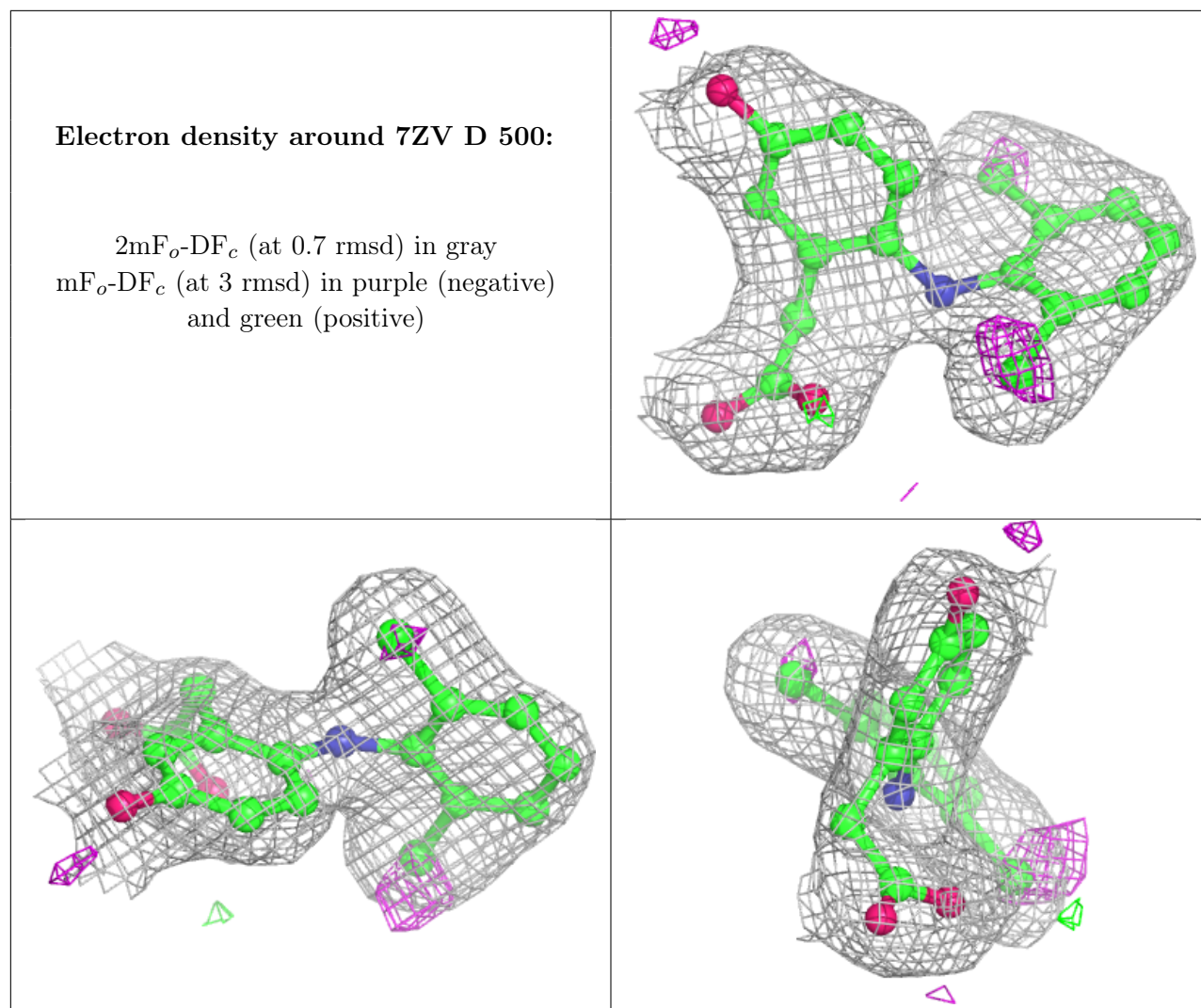and green (positive)

Electron density around 7ZV F 500:

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

Electron density around 7ZV C 501:

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

Electron density around 7ZV D 500:

$2mF_o$-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.