



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:36 AM UTC

PDB ID : 5WI5 / pdb_00005wi5
Title : 2.0 Angstrom Resolution Crystal Structure of UDP-N-acetylglucosamine 1-carboxyvinyltransferase from *Streptococcus pneumoniae* in Complex with Uridine-diphosphate-2(n-acetylglucosaminyl) butyric acid, (2R)-2-(phosphonoxy) propanoic acid and Magnesium.
Authors : Minasov, G.; Shuvalova, L.; Dubrovskaya, I.; Kiryukhina, O.; Grimshaw, S.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2017-07-18
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12

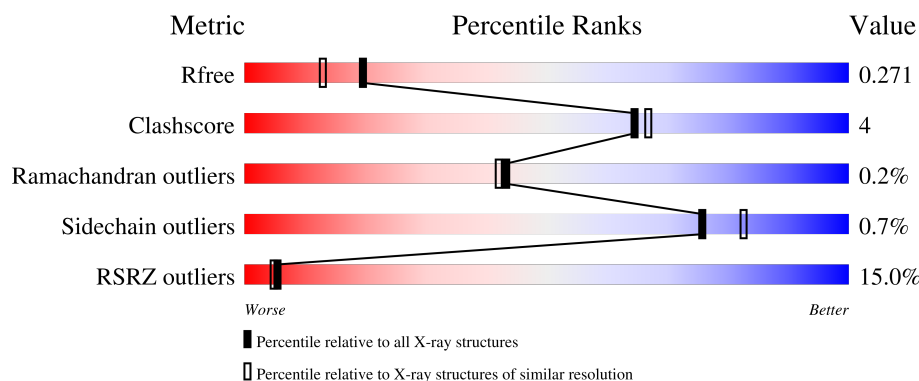
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	430	
1	B	430	
1	C	430	

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	430	25% 90% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13657 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.

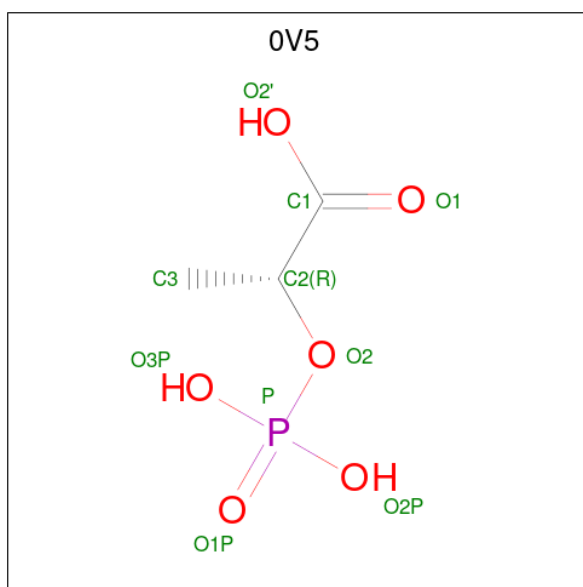
- Molecule 1 is a protein called UDP-N-acetylglucosamine 1-carboxyvinyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	8	0
			3242	2040	568	615	19			
1	B	422	Total	C	N	O	S	0	2	0
			3192	2009	560	605	18			
1	C	421	Total	C	N	O	S	0	1	0
			3178	2001	558	601	18			
1	D	422	Total	C	N	O	S	0	0	0
			3173	1998	556	601	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q97NQ4
A	-1	ASN	-	expression tag	UNP Q97NQ4
A	0	ALA	-	expression tag	UNP Q97NQ4
B	-2	SER	-	expression tag	UNP Q97NQ4
B	-1	ASN	-	expression tag	UNP Q97NQ4
B	0	ALA	-	expression tag	UNP Q97NQ4
C	-2	SER	-	expression tag	UNP Q97NQ4
C	-1	ASN	-	expression tag	UNP Q97NQ4
C	0	ALA	-	expression tag	UNP Q97NQ4
D	-2	SER	-	expression tag	UNP Q97NQ4
D	-1	ASN	-	expression tag	UNP Q97NQ4
D	0	ALA	-	expression tag	UNP Q97NQ4

- Molecule 2 is (2R)-2-(phosphonoxy)propanoic acid (CCD ID: 0V5) (formula: C₃H₇O₆P) (labeled as "Ligand of Interest" by depositor).

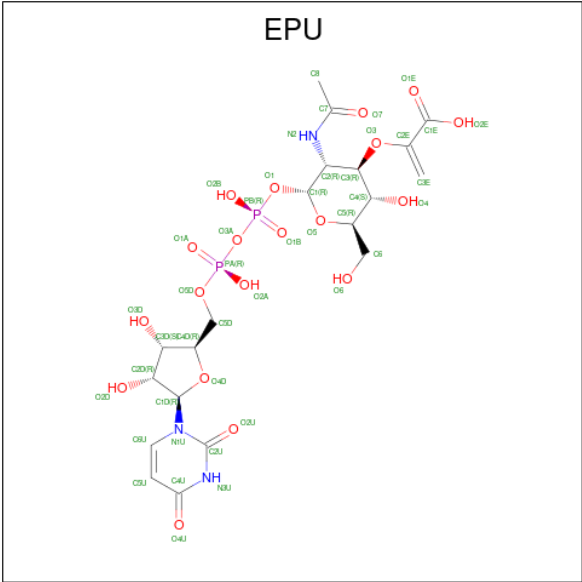


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	1	Total	C	O	P	0	0
			10	3	6	1		
2	C	1	Total	C	O	P	0	0
			10	3	6	1		
2	D	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is URIDINE-DIPHOSPHATE-2(N-ACETYLGUCOSAMINYL) BUTYRIC ACID (CCD ID: EPU) (formula: C₂₀H₂₉N₃O₁₉P₂) (labeled as "Ligand of Interest" by depositor).

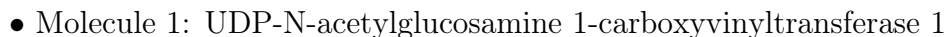
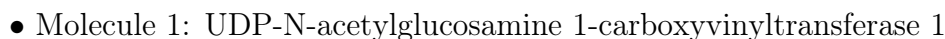


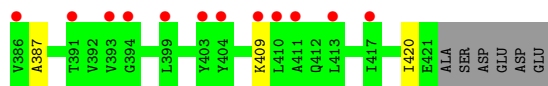
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
4	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
4	C	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
4	D	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

- Molecule 5 is water.

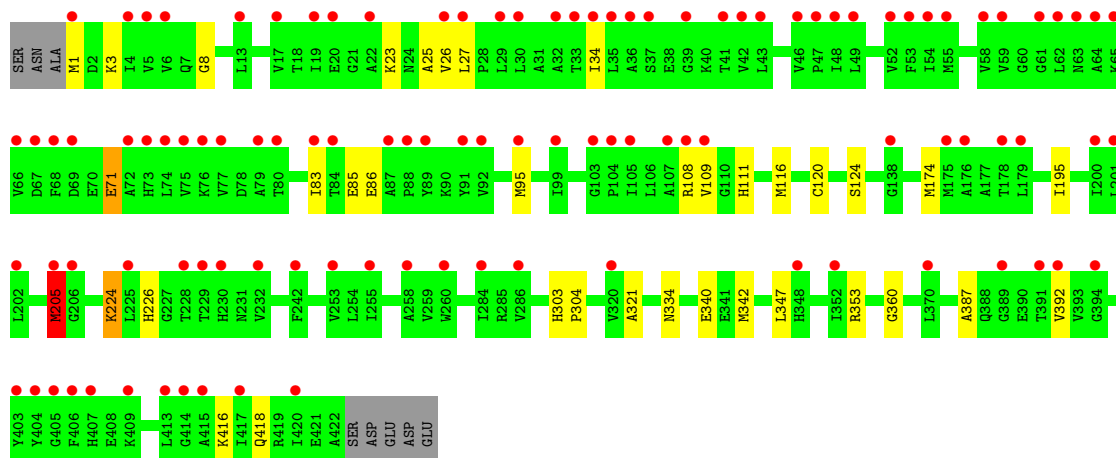
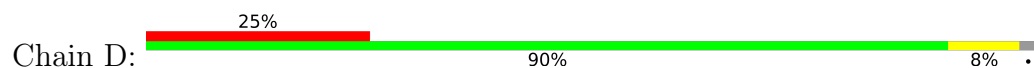
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	349	Total	O	0	10
			359	359		
5	B	167	Total	O	0	4
			171	171		
5	C	28	Total	O	0	0
			28	28		
5	D	93	Total	O	0	1
			94	94		

- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase 1





● Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.24Å 80.13Å 126.51Å 90.00° 95.76° 90.00°	Depositor
Resolution (Å)	29.29 – 2.00 29.29 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.29-2.00) 99.7 (29.29-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.222 , 0.266 0.228 , 0.271	Depositor DCC
R_{free} test set	5833 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13657	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPU, 0V5, MG

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	0.79	2/3286 (0.1%)	0.91	3/4446 (0.1%)
1	B	0.68	0/3236	0.90	5/4379 (0.1%)
1	C	0.62	0/3222	0.91	4/4360 (0.1%)
1	D	0.64	0/3216	0.91	5/4352 (0.1%)
All	All	0.69	2/12960 (0.0%)	0.91	17/17537 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	ARG	N-CA	6.87	1.52	1.46
1	A	125	ARG	CA-CB	5.72	1.57	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	86	GLU	N-CA-C	7.11	120.83	109.24
1	C	86	GLU	N-CA-C	6.83	120.37	109.24
1	B	86	GLU	N-CA-C	6.69	120.15	109.24
1	A	86	GLU	N-CA-C	6.55	119.92	109.24
1	A	85	GLU	N-CA-C	6.36	121.20	113.38
1	D	85	GLU	N-CA-C	6.30	121.12	113.38
1	D	205	MET	CG-SD-CE	-6.13	87.42	100.90
1	C	276	GLU	CA-CB-CG	5.86	125.83	114.10
1	B	10	ASP	N-CA-CB	-5.84	103.64	110.35
1	B	25	ALA	N-CA-C	-5.66	106.05	113.12
1	C	85	GLU	N-CA-C	5.64	120.32	113.38
1	B	85	GLU	N-CA-C	5.61	120.28	113.38
1	D	25	ALA	N-CA-C	-5.33	106.45	113.12
1	D	124	SER	N-CA-C	-5.32	101.99	109.96
1	C	25	ALA	N-CA-C	-5.03	106.83	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	HIS	N-CA-C	5.02	116.31	109.18
1	B	374	LEU	N-CA-C	5.01	117.14	111.02

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	3242	0	3315	18	0
1	B	3192	0	3270	23	0
1	C	3178	0	3260	45	0
1	D	3173	0	3259	22	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	C	10	0	5	0	0
2	D	10	0	4	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	44	0	26	0	0
4	B	44	0	26	0	0
4	C	44	0	26	1	0
4	D	44	0	26	1	0
5	A	359	0	0	1	0
5	B	171	0	0	1	0
5	C	28	0	0	0	0
5	D	94	0	0	3	0
All	All	13657	0	13225	102	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 (102) 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:250:GLY:HA2	1:B:288:SER:OG	1.78	0.84
1:C:276:GLU:HG2	1:C:278:ILE:HD11	1.61	0.82
1:C:276:GLU:CG	1:C:278:ILE:HD11	2.12	0.80
1:D:27:LEU:HD13	1:D:95:MET:HE3	1.65	0.77
1:B:345:MET:HE3	1:B:369:VAL:HG11	1.71	0.72
1:C:14:VAL:HG22	1:C:252:ASP:OD1	1.91	0.70
1:C:269:LYS:HE3	1:C:297:HIS:O	1.94	0.67
1:C:174:MET:HE2	1:C:198:LEU:HD23	1.78	0.65
1:C:119:GLY:HA2	1:D:340:GLU:HG2	1.79	0.65
1:C:342:MET:HE2	1:C:347:LEU:HD22	1.79	0.65
1:A:174[B]:MET:HE1	1:A:195:ILE:HG23	1.80	0.64
1:D:205:MET:HG3	1:D:226:HIS:O	1.98	0.64
1:C:278:ILE:HD12	1:C:278:ILE:N	2.13	0.63
1:B:26:VAL:HG23	1:B:232:VAL:HG11	1.79	0.63
1:B:342:MET:HE2	1:B:347:LEU:HD22	1.81	0.62
1:C:269:LYS:HG2	1:C:298:VAL:HG22	1.83	0.61
1:D:342:MET:HE2	1:D:347:LEU:HD22	1.83	0.61
1:C:34:ILE:HG23	1:C:83:ILE:HD13	1.84	0.59
1:C:99:ILE:HG22	1:C:99:ILE:O	2.01	0.59
1:D:174:MET:HE1	1:D:195:ILE:HG23	1.83	0.59
1:B:161:TYR:CE1	1:C:268:ALA:HB1	2.37	0.58
1:C:99:ILE:HD12	1:C:114:VAL:HG12	1.86	0.58
1:C:243:MET:HE1	1:C:267:ILE:CG1	2.34	0.58
1:C:269:LYS:CE	1:C:297:HIS:O	2.51	0.58
1:C:174:MET:CE	1:C:198:LEU:HD23	2.34	0.57
1:B:26:VAL:HG22	1:B:232:VAL:HG21	1.85	0.57
1:D:3:LYS:HE3	1:D:392:VAL:HG12	1.85	0.57
1:B:321:ALA:O	1:B:360:GLY:HA3	2.05	0.56
1:A:342:MET:HE2	1:A:347:LEU:HD22	1.86	0.56
1:B:248:MET:HG2	1:B:317:LEU:HA	1.88	0.56
1:D:34:ILE:HG23	1:D:83:ILE:HD13	1.87	0.56
1:C:420:ILE:HD12	1:C:420:ILE:N	2.21	0.56
1:C:276:GLU:HG3	1:C:278:ILE:HD11	1.89	0.55
1:C:321:ALA:O	1:C:360:GLY:HA3	2.06	0.55
1:B:159:HIS:HA	1:B:185:VAL:HG23	1.89	0.55
1:D:418:GLN:HA	5:D:629:HOH:O	2.07	0.55
1:A:321:ALA:O	1:A:360:GLY:HA3	2.06	0.55
1:C:134:LEU:HD23	1:C:137:MET:CE	2.37	0.55
1:A:248:MET:HG2	1:A:317:LEU:HA	1.89	0.54
1:D:3:LYS:HE3	1:D:392:VAL:CG1	2.38	0.54
1:B:183:VAL:HG22	1:B:220:THR:HG22	1.89	0.53
1:D:321:ALA:O	1:D:360:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:MET:HG2	1:C:317:LEU:HA	1.92	0.52
1:C:109:VAL:HG12	1:C:111:HIS:CD2	2.45	0.52
1:B:412:GLN:NE2	5:B:611:HOH:O	2.43	0.51
1:D:109:VAL:HG12	1:D:111:HIS:CD2	2.45	0.51
1:B:71:GLU:H	1:B:71:GLU:CD	2.18	0.51
1:A:109:VAL:HG12	1:A:111:HIS:CD2	2.46	0.50
1:C:344:ARG:NH2	1:C:344:ARG:HB3	2.27	0.50
1:C:276:GLU:HG2	1:C:278:ILE:CD1	2.37	0.50
1:C:205:MET:HG3	1:C:226:HIS:O	2.12	0.49
1:A:174[B]:MET:HE2	1:A:217:ILE:HD13	1.94	0.49
1:B:159:HIS:HA	1:B:185:VAL:CG2	2.44	0.48
1:D:8:GLY:HA3	1:D:387:ALA:O	2.15	0.47
1:C:243:MET:HE1	1:C:267:ILE:HG13	1.97	0.47
1:C:8:GLY:HA3	1:C:387:ALA:O	2.15	0.47
1:C:99:ILE:HD12	1:C:114:VAL:CG1	2.44	0.47
1:A:8:GLY:HA3	1:A:387:ALA:O	2.15	0.46
1:A:34:ILE:HD11	1:A:59:VAL:HG13	1.96	0.46
1:B:8:GLY:HA3	1:B:387:ALA:O	2.15	0.46
1:C:303:HIS:CG	1:C:304:PRO:HA	2.51	0.46
1:B:34:ILE:HD11	1:B:59:VAL:HG13	1.98	0.45
1:D:23:LYS:HE2	4:D:503:EPU:O1E	2.16	0.45
1:B:303:HIS:CG	1:B:304:PRO:HA	2.52	0.45
1:A:303:HIS:CG	1:A:304:PRO:HA	2.52	0.45
1:A:357:ARG:HE	1:C:352:ILE:HD11	1.81	0.45
1:C:137:MET:HE2	1:C:173:LEU:HD22	1.98	0.45
1:C:238:GLU:OE2	1:C:409:LYS:NZ	2.46	0.45
1:D:120:CYS:HA	2:D:501:OV5:C1	2.46	0.45
1:D:71:GLU:OE2	5:D:601:HOH:O	2.21	0.45
1:C:127:ILE:HD11	1:C:148:ILE:HD11	1.99	0.44
1:C:344:ARG:NE	1:D:116:MET:O	2.49	0.44
1:D:303:HIS:CG	1:D:304:PRO:HA	2.52	0.44
1:A:23:LYS:HE2	1:A:51:ASP:OD2	2.18	0.44
1:C:119:GLY:HA2	1:D:340:GLU:CG	2.48	0.44
1:D:34:ILE:O	1:D:108:ARG:HG3	2.18	0.44
1:C:134:LEU:HD23	1:C:137:MET:HE3	1.98	0.43
1:D:224:LYS:HD2	1:D:224:LYS:O	2.18	0.43
1:C:34:ILE:O	1:C:108:ARG:HG3	2.17	0.43
1:D:334:ASN:ND2	5:D:609:HOH:O	2.52	0.43
1:A:34:ILE:O	1:A:108:ARG:HG3	2.19	0.43
1:B:127:ILE:HD11	1:B:148:ILE:HD11	2.00	0.42
1:C:29:LEU:HD22	1:C:201:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:CG1	1:A:74[B]:LEU:HD11	2.49	0.42
1:C:348[B]:HIS:NE2	1:C:350:GLU:OE2	2.46	0.42
1:B:44:GLN:HG2	1:B:74:LEU:CD2	2.49	0.42
1:C:23:LYS:O	1:C:26:VAL:HG12	2.20	0.42
1:C:35:LEU:HB3	1:C:225:LEU:HD12	2.00	0.42
1:C:125:ARG:HA	4:C:503:EPU:O2D	2.20	0.42
1:A:357:ARG:NE	1:C:352:ILE:HD11	2.34	0.41
1:B:345:MET:HE3	1:B:369:VAL:CG1	2.47	0.41
1:A:29:LEU:HD22	1:A:201:LEU:HD22	2.02	0.41
1:A:23:LYS:O	1:A:26:VAL:HG12	2.21	0.41
1:B:34:ILE:O	1:B:108:ARG:HG3	2.21	0.41
1:B:338:HIS:HB3	1:B:376:ALA:HB1	2.03	0.41
1:A:7[A]:GLN:HB2	1:A:416:LYS:HD2	2.02	0.41
1:C:14:VAL:HG13	1:C:252:ASP:CG	2.46	0.41
1:C:14:VAL:HG13	1:C:252:ASP:OD1	2.21	0.41
1:B:250:GLY:CA	1:B:288:SER:OG	2.60	0.41
1:A:324:GLU:OE2	5:A:601:HOH:O	2.22	0.40
1:D:23:LYS:O	1:D:26:VAL:HG12	2.21	0.40
1:B:29:LEU:HD22	1:B:201:LEU:HD22	2.02	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	428/430 (100%)	415 (97%)	12 (3%)	1 (0%)	43	42
1	B	422/430 (98%)	408 (97%)	13 (3%)	1 (0%)	43	42
1	C	420/430 (98%)	408 (97%)	11 (3%)	1 (0%)	43	42
1	D	420/430 (98%)	408 (97%)	11 (3%)	1 (0%)	43	42
All	All	1690/1720 (98%)	1639 (97%)	47 (3%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	353	ARG
1	B	353	ARG
1	A	353	ARG
1	D	353	ARG

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	344/343 (100%)	343 (100%)	1 (0%)	86	91
1	B	338/343 (98%)	336 (99%)	2 (1%)	78	85
1	C	337/343 (98%)	336 (100%)	1 (0%)	86	91
1	D	336/343 (98%)	331 (98%)	5 (2%)	57	64
All	All	1355/1372 (99%)	1346 (99%)	9 (1%)	76	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	ARG
1	B	143	GLN
1	B	418	GLN
1	C	153	GLU
1	D	1	MET
1	D	71	GLU
1	D	205	MET
1	D	224	LYS
1	D	416	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	A	337	GLN

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Mol	Chain	Res	Type
1	A	398	HIS
1	B	226	HIS
1	B	337	GLN
1	C	73	HIS
1	C	334	ASN
1	D	337	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	0V5	A	501	1,3	8,9,9	1.03	0	11,13,13	1.23	1 (9%)
4	EPU	C	503	-	45,46,46	1.25	6 (13%)	63,69,69	1.51	9 (14%)
2	0V5	B	501	1,3	8,9,9	1.13	1 (12%)	11,13,13	0.95	0
2	0V5	D	501	1,3	8,9,9	0.89	0	11,13,13	1.10	0
4	EPU	A	503	-	45,46,46	1.23	5 (11%)	63,69,69	1.67	7 (11%)
4	EPU	D	503	-	45,46,46	1.40	5 (11%)	63,69,69	1.65	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	0V5	C	501	1,3	8,9,9	1.18	1 (12%)	11,13,13	0.98	0
4	EPU	B	503	-	45,46,46	1.22	5 (11%)	63,69,69	1.50	8 (12%)

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	0V5	A	501	1,3	-	4/9/9/9	-
4	EPU	C	503	-	-	5/32/71/71	0/3/3/3
2	0V5	B	501	1,3	-	1/9/9/9	-
2	0V5	D	501	1,3	-	0/9/9/9	-
4	EPU	A	503	-	-	8/32/71/71	0/3/3/3
4	EPU	D	503	-	-	6/32/71/71	0/3/3/3
2	0V5	C	501	1,3	-	4/9/9/9	-
4	EPU	B	503	-	-	9/32/71/71	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	EPU	PB-O3A	4.80	1.64	1.59
4	A	503	EPU	C2E-C1E	-3.87	1.45	1.49
4	D	503	EPU	O3-C2E	3.73	1.48	1.36
4	C	503	EPU	O3-C2E	3.58	1.47	1.36
4	B	503	EPU	C2E-C1E	-3.55	1.45	1.49
4	B	503	EPU	O3-C2E	3.42	1.47	1.36
4	C	503	EPU	PB-O3A	3.26	1.63	1.59
4	D	503	EPU	C2U-N1U	3.04	1.43	1.38
4	A	503	EPU	O3-C2E	2.92	1.45	1.36
4	D	503	EPU	PA-O3A	2.82	1.62	1.59
4	B	503	EPU	C5U-C4U	-2.72	1.37	1.43
4	B	503	EPU	C2U-N1U	2.63	1.42	1.38
4	A	503	EPU	C2U-N3U	-2.39	1.33	1.38
4	B	503	EPU	O2U-C2U	2.38	1.27	1.23
4	A	503	EPU	PA-O3A	2.35	1.62	1.59
4	C	503	EPU	C4U-N3U	-2.29	1.34	1.38
4	C	503	EPU	C2U-N1U	2.20	1.41	1.38
4	A	503	EPU	C4U-N3U	-2.19	1.34	1.38
4	D	503	EPU	C2U-N3U	-2.17	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	0V5	P-O2	2.15	1.63	1.59
2	B	501	0V5	O1-C1	2.15	1.28	1.22
4	C	503	EPU	C5U-C4U	-2.08	1.39	1.43
4	C	503	EPU	PA-O3A	2.03	1.61	1.59

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	EPU	O2E-C1E-C2E	5.92	124.01	113.91
4	A	503	EPU	O1E-C1E-C2E	-5.72	113.17	121.79
4	D	503	EPU	C4U-N3U-C2U	-4.56	120.95	126.61
4	C	503	EPU	O2E-C1E-C2E	4.55	121.67	113.91
4	B	503	EPU	C5U-C4U-N3U	4.42	121.00	114.80
4	C	503	EPU	C5U-C4U-N3U	4.32	120.86	114.80
4	C	503	EPU	C4U-N3U-C2U	-4.16	121.45	126.61
4	B	503	EPU	C4U-N3U-C2U	-4.15	121.46	126.61
4	B	503	EPU	O4U-C4U-C5U	-4.14	118.02	125.16
4	D	503	EPU	O2E-C1E-C2E	4.04	120.80	113.91
4	D	503	EPU	N3U-C2U-N1U	4.01	120.11	114.89
4	B	503	EPU	O2E-C1E-C2E	3.99	120.72	113.91
4	A	503	EPU	C5U-C4U-N3U	3.91	120.28	114.80
4	A	503	EPU	C4U-N3U-C2U	-3.72	122.00	126.61
4	D	503	EPU	C5U-C4U-N3U	3.59	119.83	114.80
4	D	503	EPU	O4U-C4U-C5U	-3.41	119.28	125.16
4	A	503	EPU	N3U-C2U-N1U	3.40	119.31	114.89
4	B	503	EPU	O1E-C1E-C2E	-3.32	116.79	121.79
4	C	503	EPU	N3U-C2U-N1U	3.22	119.08	114.89
4	C	503	EPU	O4U-C4U-C5U	-3.16	119.71	125.16
4	A	503	EPU	C2D-C1D-N1U	-2.94	105.06	113.25
4	C	503	EPU	O3A-PB-O1B	-2.92	101.93	110.70
4	D	503	EPU	O3-C3-C2	2.66	112.84	107.92
4	D	503	EPU	O2B-PB-O1B	2.58	124.43	112.44
4	B	503	EPU	N3U-C2U-N1U	2.56	118.22	114.89
4	A	503	EPU	O4U-C4U-C5U	-2.54	120.79	125.16
4	B	503	EPU	C3E-C2E-C1E	-2.50	118.11	122.73
4	D	503	EPU	C3-C2-N2	2.44	114.79	110.91
4	B	503	EPU	O3-C3-C2	2.40	112.36	107.92
2	A	501	0V5	O2'-C1-C2	2.40	122.71	113.96
4	C	503	EPU	O3-C3-C4	2.35	113.16	107.76
4	D	503	EPU	C1D-N1U-C2U	2.23	121.60	117.59
4	C	503	EPU	O1E-C1E-C2E	-2.22	118.45	121.79
4	C	503	EPU	O2B-PB-O1B	2.15	122.47	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	EPU	O4D-C1D-N1U	2.15	113.23	108.36
4	D	503	EPU	O2A-PA-O5D	2.12	117.17	107.57
4	D	503	EPU	C3E-C2E-C1E	-2.06	118.93	122.73
4	D	503	EPU	O3-C2E-C1E	2.05	120.69	115.59

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	EPU	C5D-O5D-PA-O1A
4	A	503	EPU	C5D-O5D-PA-O2A
4	A	503	EPU	C5D-O5D-PA-O3A
4	A	503	EPU	O1E-C1E-C2E-C3E
4	A	503	EPU	O2E-C1E-C2E-O3
4	A	503	EPU	O2E-C1E-C2E-C3E
4	B	503	EPU	C5D-O5D-PA-O1A
4	B	503	EPU	C5D-O5D-PA-O2A
4	B	503	EPU	C5D-O5D-PA-O3A
4	B	503	EPU	O1E-C1E-C2E-C3E
4	B	503	EPU	O2E-C1E-C2E-O3
4	B	503	EPU	O2E-C1E-C2E-C3E
4	C	503	EPU	C5D-O5D-PA-O2A
4	C	503	EPU	C5D-O5D-PA-O3A
4	D	503	EPU	C5D-O5D-PA-O2A
4	D	503	EPU	O1E-C1E-C2E-C3E
4	D	503	EPU	O2E-C1E-C2E-O3
4	D	503	EPU	O2E-C1E-C2E-C3E
2	B	501	0V5	C2-O2-P-O1P
4	A	503	EPU	O1E-C1E-C2E-O3
4	B	503	EPU	O1E-C1E-C2E-O3
4	D	503	EPU	O1E-C1E-C2E-O3
4	C	503	EPU	PB-O3A-PA-O1A
2	A	501	0V5	O2'-C1-C2-C3
2	C	501	0V5	O2'-C1-C2-C3
2	C	501	0V5	O2'-C1-C2-O2
4	C	503	EPU	C5D-O5D-PA-O1A
2	C	501	0V5	O1-C1-C2-C3
4	A	503	EPU	PB-O3A-PA-O1A
4	B	503	EPU	O4D-C4D-C5D-O5D
4	C	503	EPU	PB-O3A-PA-O2A
2	A	501	0V5	O2'-C1-C2-O2
2	A	501	0V5	C2-O2-P-O1P

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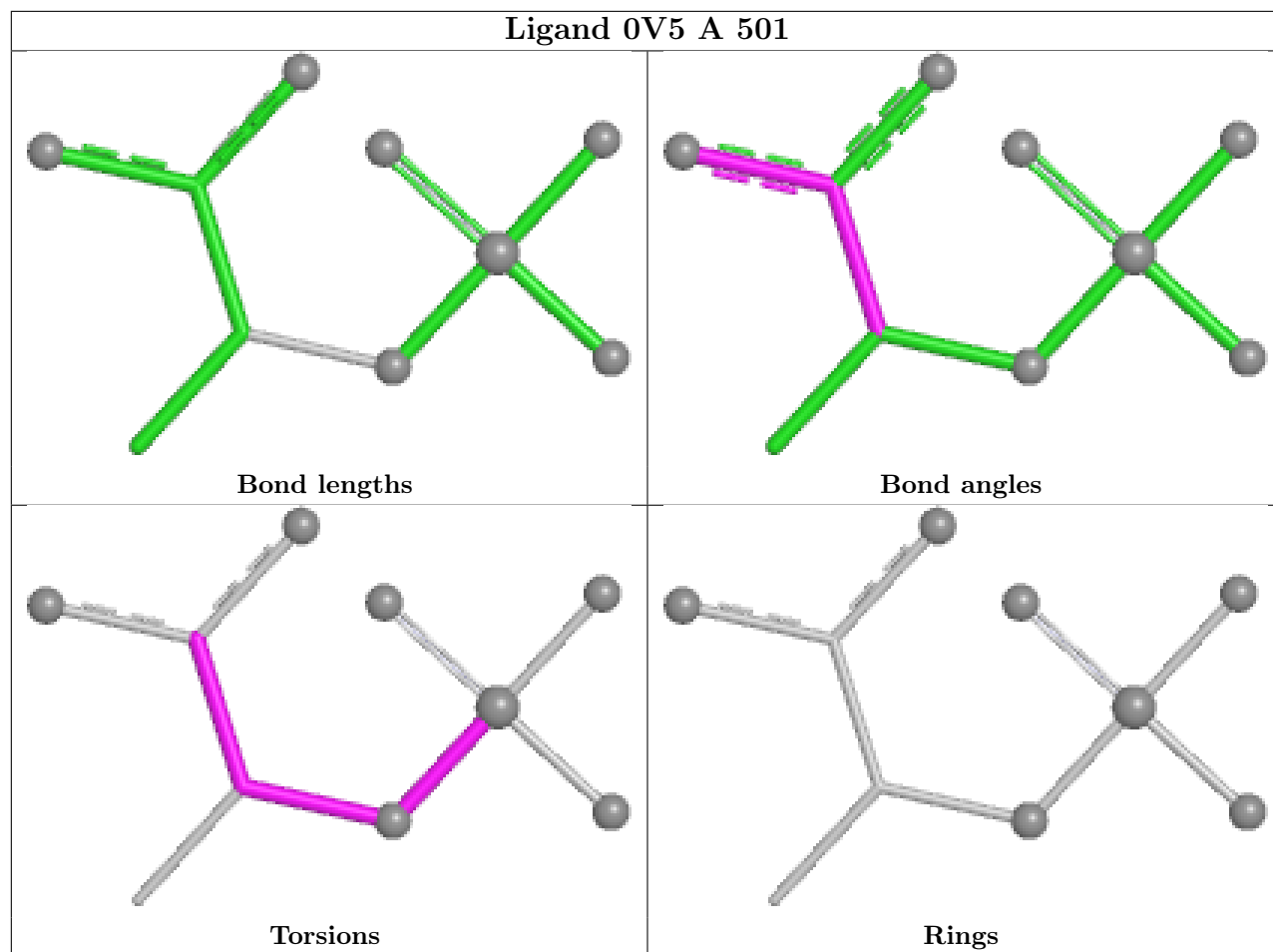
Mol	Chain	Res	Type	Atoms
2	A	501	0V5	C3-C2-O2-P
2	C	501	0V5	C3-C2-O2-P
4	B	503	EPU	PB-O3A-PA-O2A
4	D	503	EPU	PB-O3A-PA-O2A

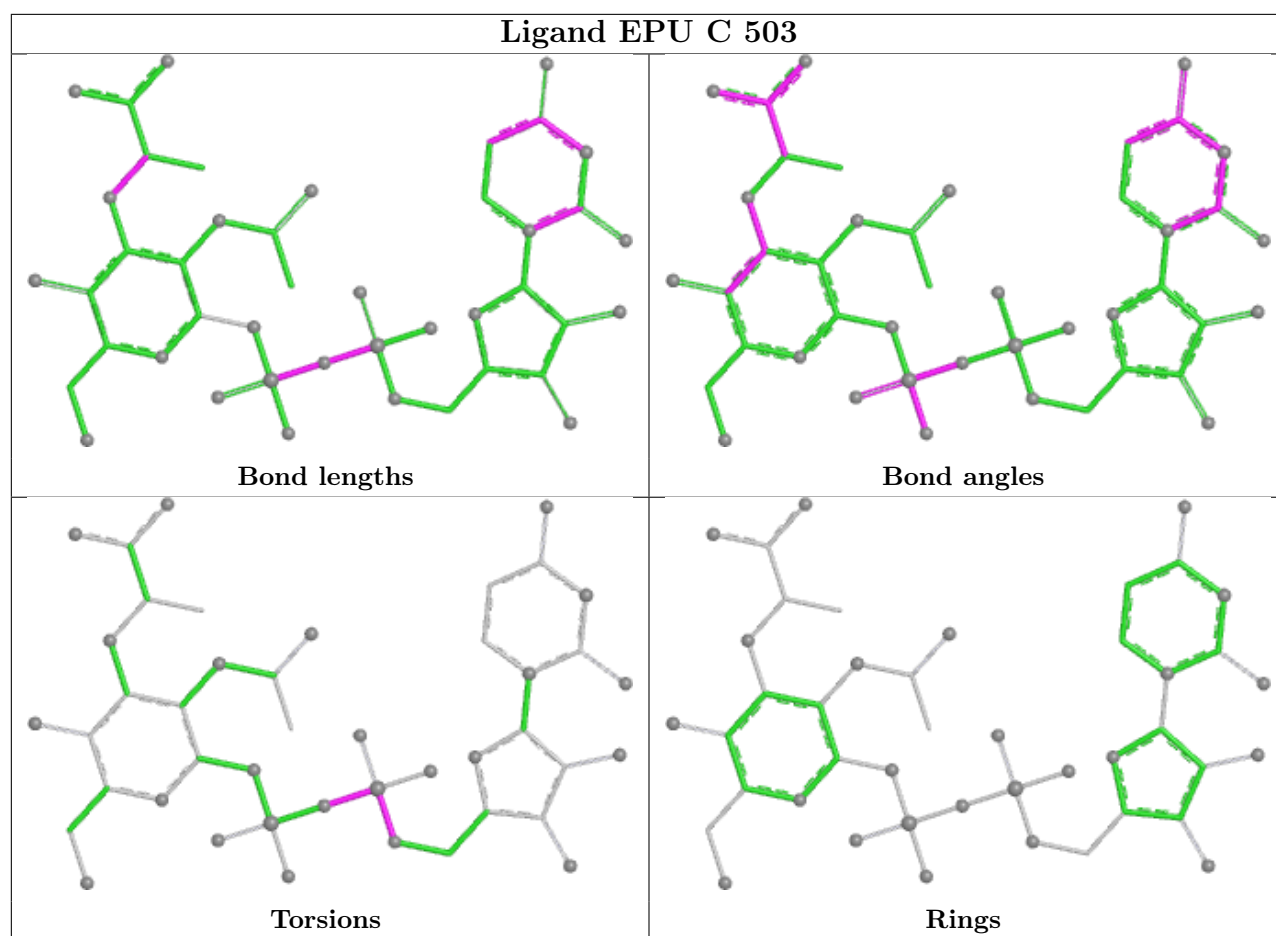
There are no ring outliers.

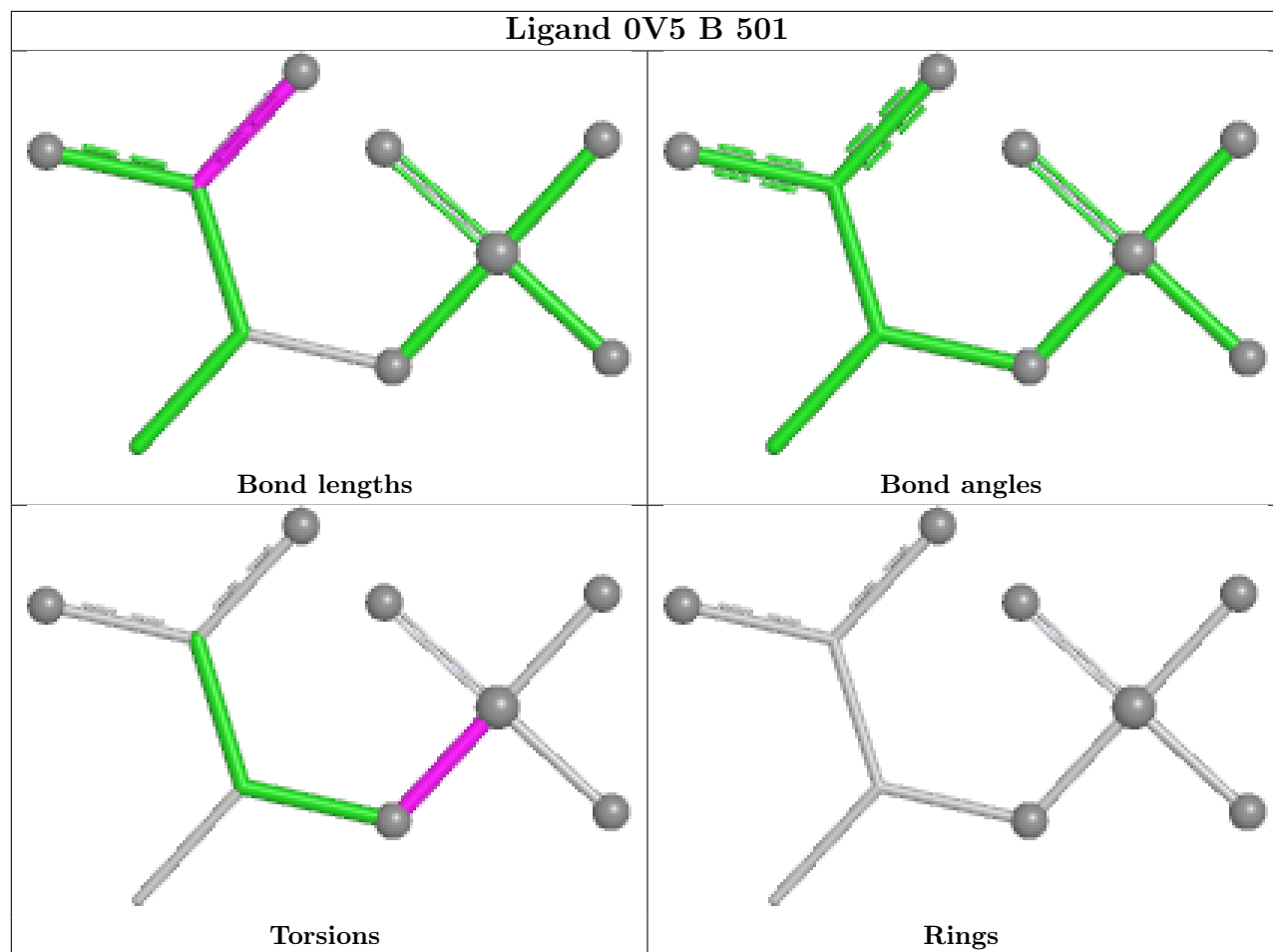
3 monomers are involved in 3 short contacts:

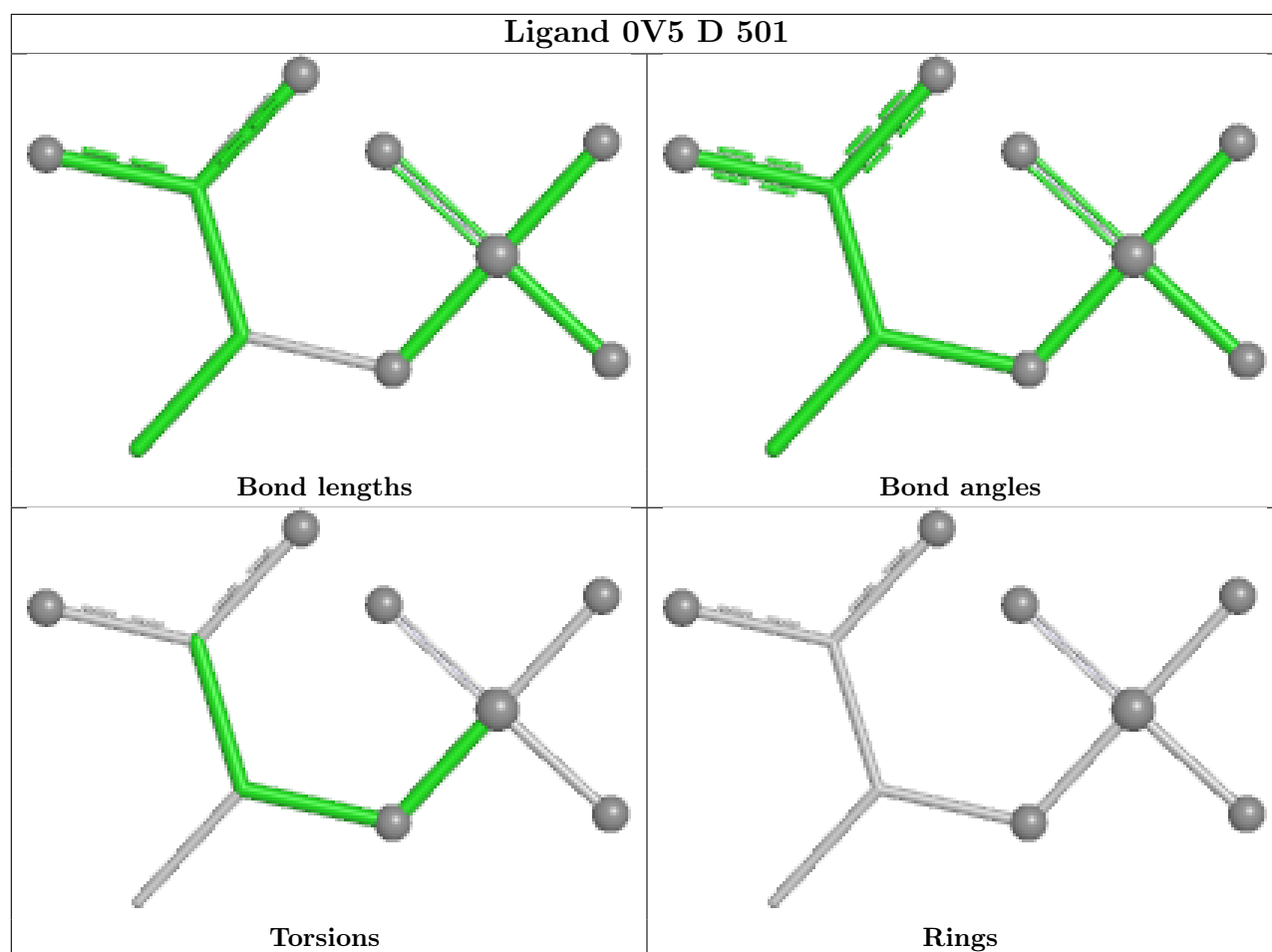
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	EPU	1	0
2	D	501	0V5	1	0
4	D	503	EPU	1	0

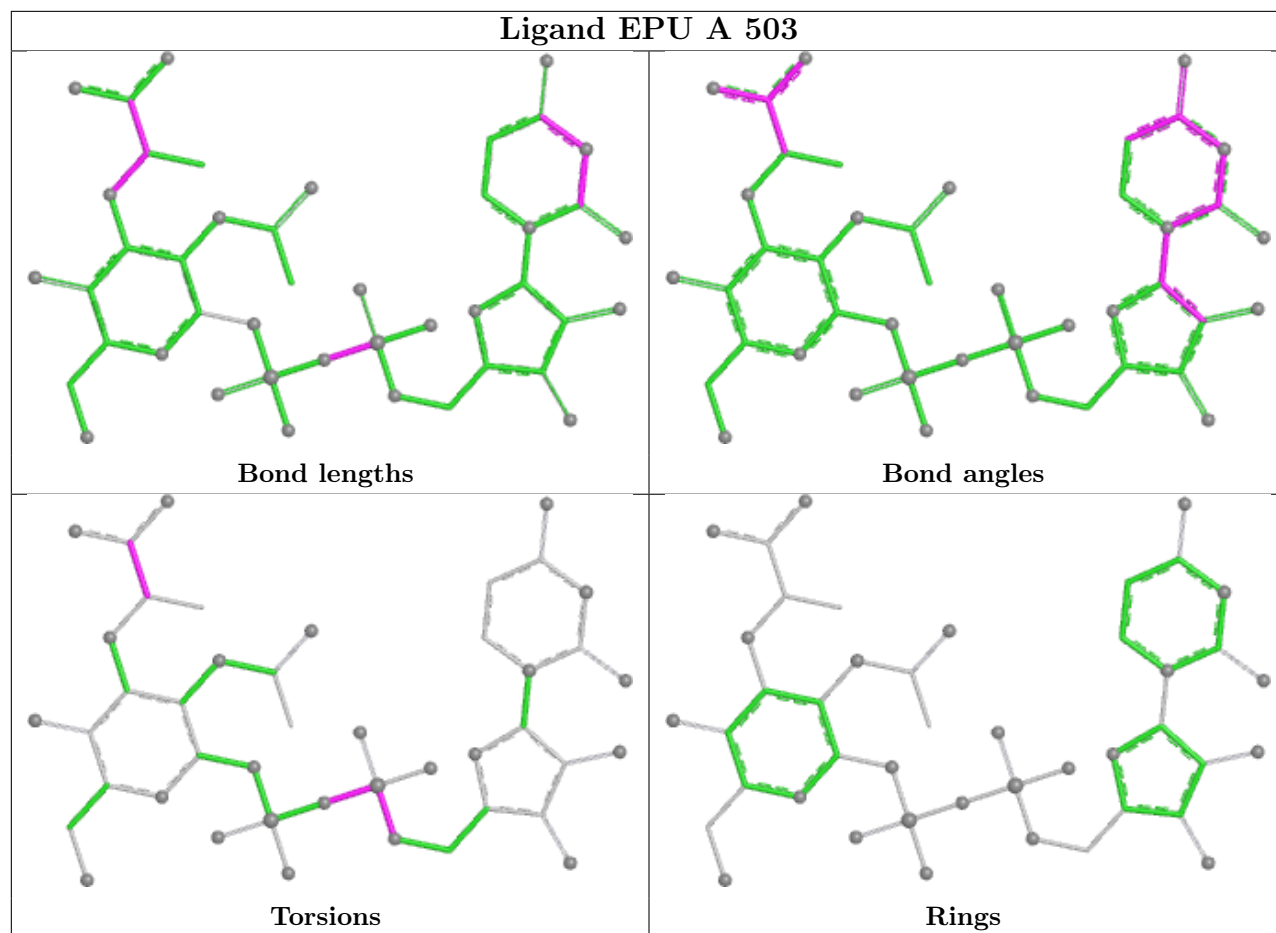
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

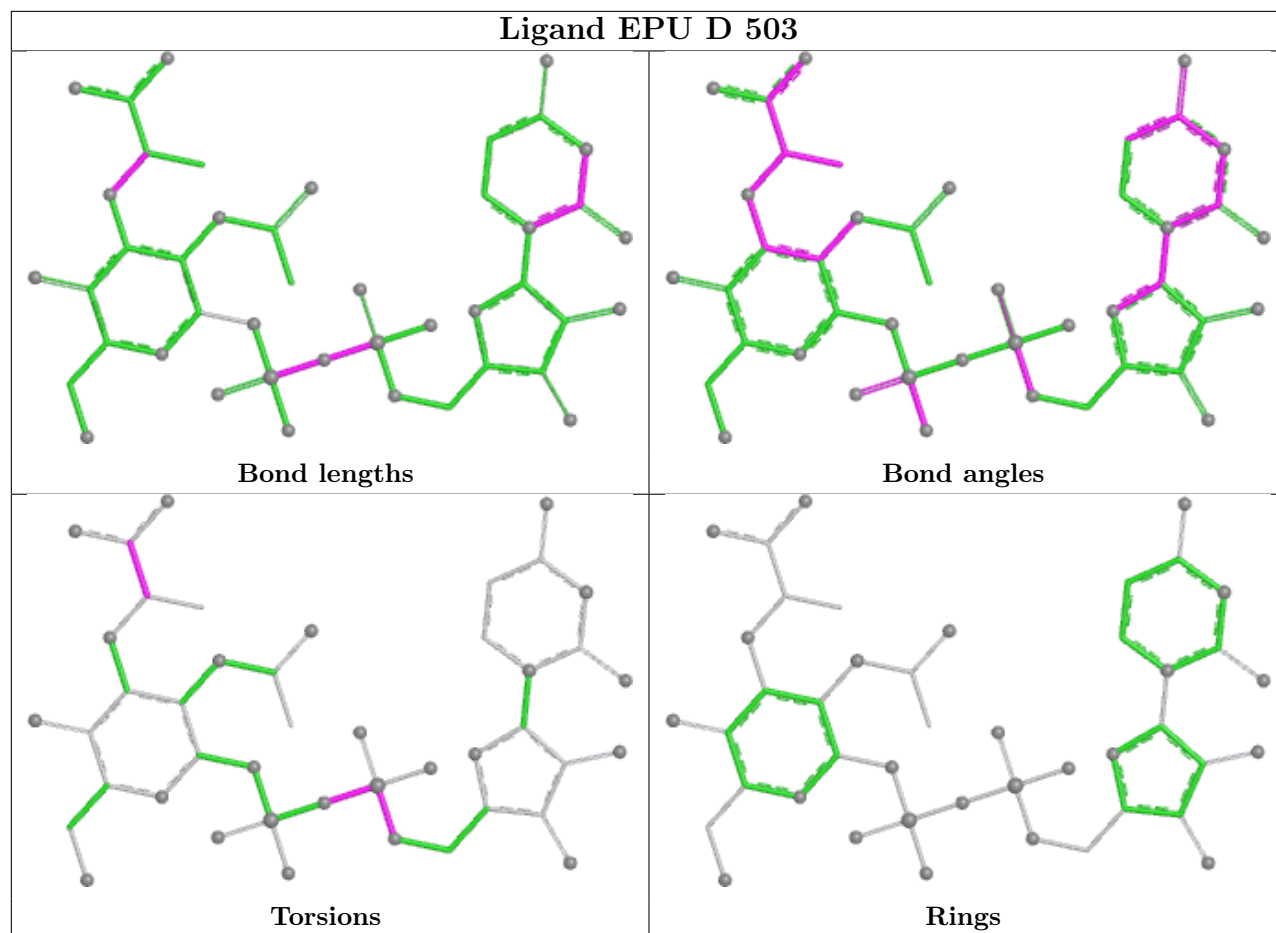


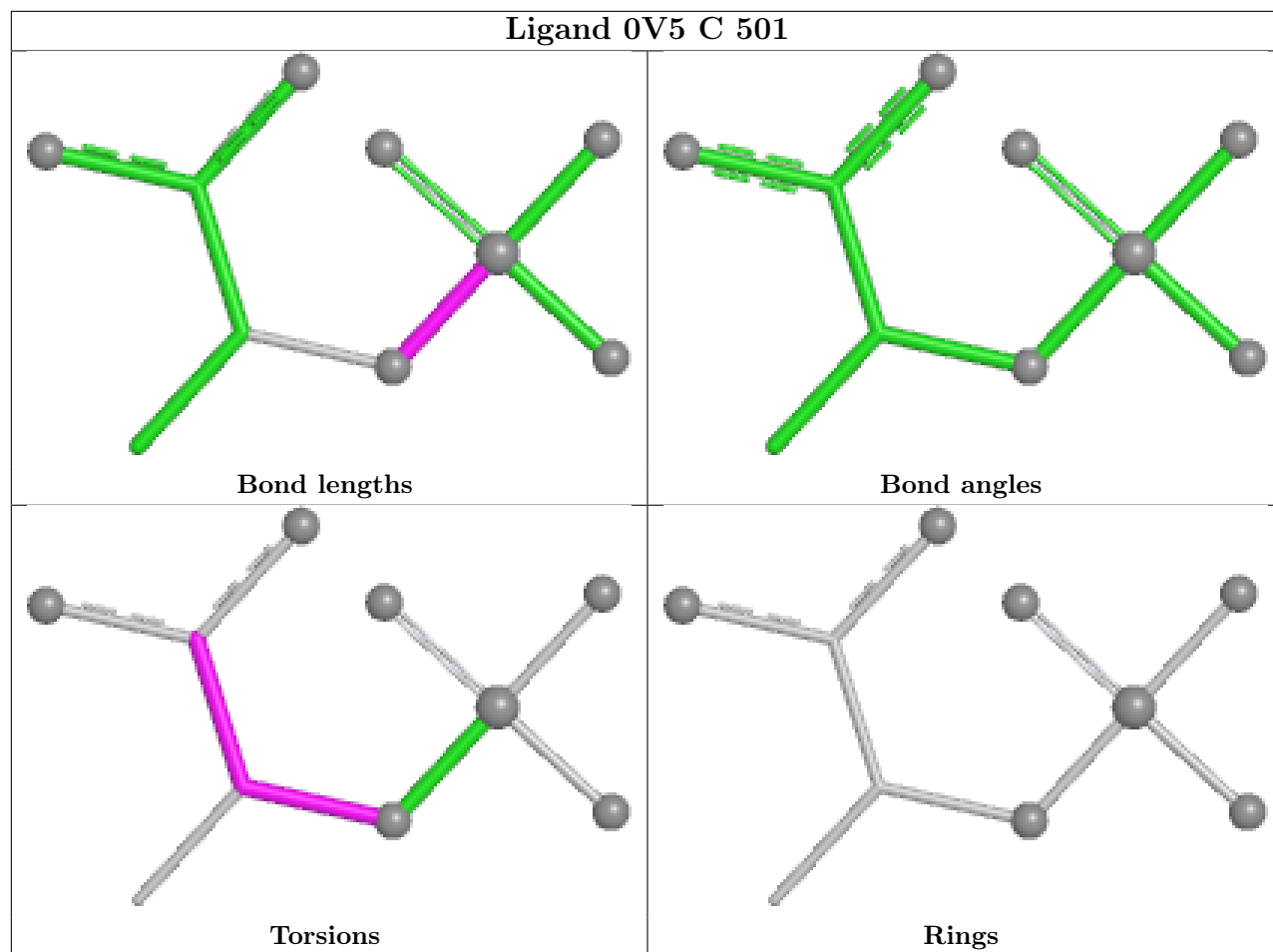


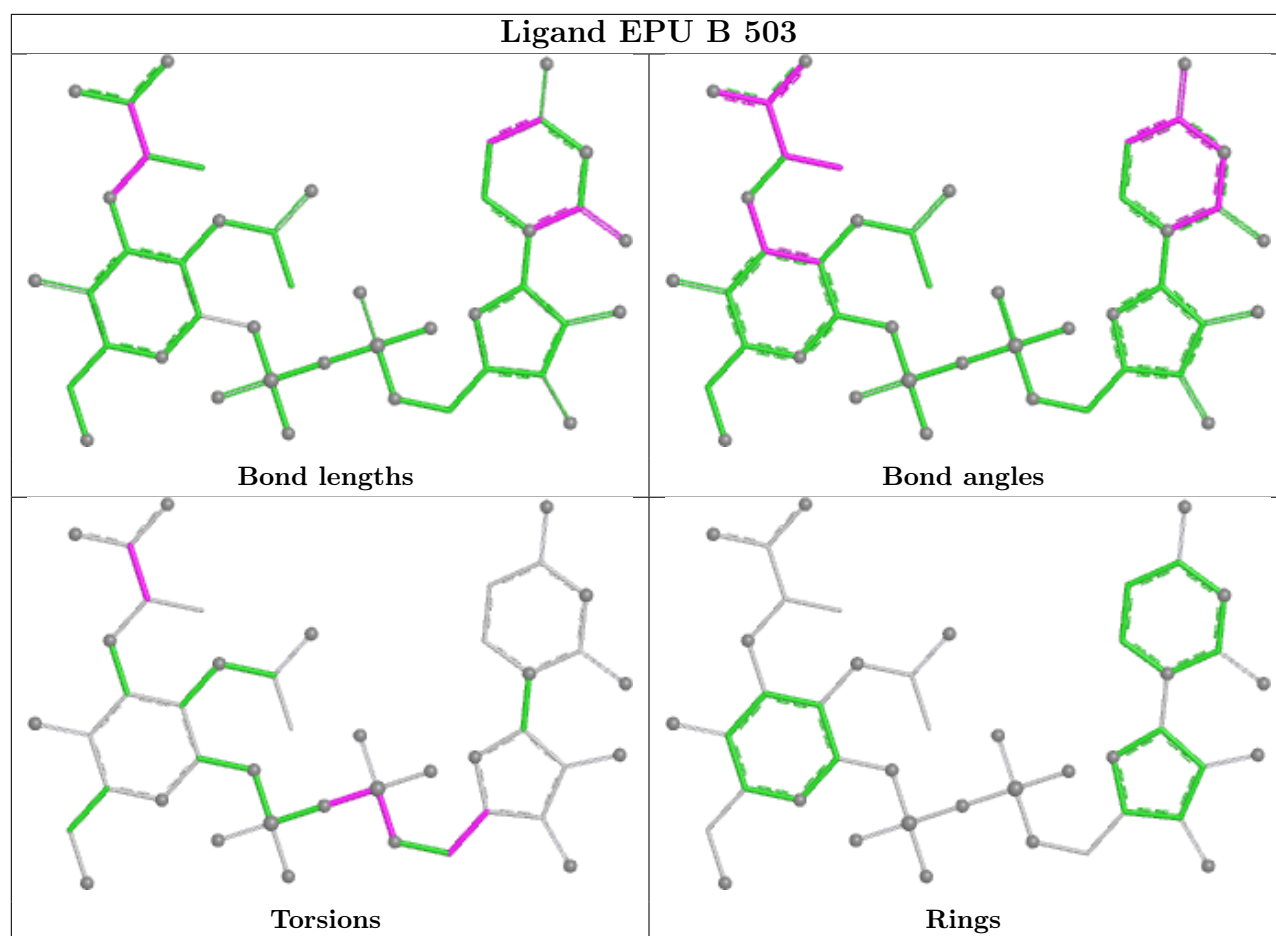












5.7 Other polymers [i](#)

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	422/430 (98%)	-0.34	1 (0%) 91 90	12, 26, 42, 81	8 (1%)
1	B	422/430 (98%)	0.61	20 (4%) 36 35	21, 43, 65, 112	2 (0%)
1	C	421/430 (97%)	1.69	126 (29%) 1 1	29, 72, 98, 121	1 (0%)
1	D	422/430 (98%)	1.49	106 (25%) 1 1	34, 60, 89, 104	0
All	All	1687/1720 (98%)	0.86	253 (14%) 5 5	12, 50, 90, 121	11 (0%)

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	77	VAL	6.0
1	D	66	VAL	5.4
1	D	79	ALA	4.8
1	C	36	ALA	4.6
1	D	53	PHE	4.6
1	D	42	VAL	4.4
1	D	39	GLY	4.3
1	C	277	VAL	4.3
1	B	161	TYR	4.0
1	C	13	LEU	3.9
1	D	73	HIS	3.9
1	D	74	LEU	3.9
1	D	17	VAL	3.9
1	D	34	ILE	3.9
1	C	253	VAL	3.9
1	C	255	ILE	3.8
1	D	30	LEU	3.8
1	D	41	THR	3.8
1	C	77	VAL	3.8
1	C	270	LEU	3.7
1	C	410	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	58	VAL	3.7
1	C	237	ILE	3.7
1	D	83	ILE	3.7
1	D	92	VAL	3.7
1	C	271	LEU	3.6
1	C	382	LEU	3.6
1	C	385	LEU	3.6
1	D	225	LEU	3.6
1	D	75	VAL	3.6
1	C	225	LEU	3.6
1	C	297	HIS	3.6
1	C	33	THR	3.5
1	D	68	PHE	3.5
1	D	91	TYR	3.5
1	D	229	THR	3.5
1	C	246	ALA	3.4
1	B	74	LEU	3.4
1	D	43	LEU	3.4
1	D	26	VAL	3.4
1	C	222	VAL	3.4
1	D	255	ILE	3.4
1	C	64	ALA	3.3
1	C	34	ILE	3.3
1	C	48	ILE	3.3
1	C	76	LYS	3.3
1	C	26	VAL	3.3
1	D	284	ILE	3.3
1	C	106	LEU	3.2
1	C	394	GLY	3.2
1	C	17	VAL	3.2
1	B	422	ALA	3.2
1	D	201	LEU	3.2
1	C	233	VAL	3.2
1	D	13	LEU	3.1
1	D	76	LYS	3.1
1	C	100	VAL	3.1
1	C	160	ILE	3.1
1	D	47	PRO	3.1
1	D	320	VAL	3.1
1	C	260	TRP	3.0
1	C	41	THR	3.0
1	C	91	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	404	TYR	3.0
1	D	64	ALA	3.0
1	C	198	LEU	3.0
1	C	141	ILE	3.0
1	D	352	ILE	3.0
1	D	228	THR	3.0
1	D	36	ALA	3.0
1	D	46	VAL	3.0
1	C	381	ILE	3.0
1	D	420	ILE	3.0
1	D	72	ALA	2.9
1	D	370	LEU	2.9
1	C	35	LEU	2.9
1	D	62	LEU	2.9
1	C	99	ILE	2.9
1	C	80	THR	2.9
1	D	65	LYS	2.9
1	C	62	LEU	2.8
1	C	370	LEU	2.8
1	C	399	LEU	2.8
1	C	101	VAL	2.8
1	B	255	ILE	2.8
1	D	48	ILE	2.8
1	C	79	ALA	2.8
1	C	42	VAL	2.8
1	C	284	ILE	2.8
1	C	379	ALA	2.8
1	D	58	VAL	2.8
1	D	286	VAL	2.8
1	C	27	LEU	2.8
1	B	277	VAL	2.8
1	D	258	ALA	2.7
1	D	403	TYR	2.7
1	D	413	LEU	2.7
1	D	88	PRO	2.7
1	C	286	VAL	2.7
1	C	219	ILE	2.7
1	C	212	ALA	2.7
1	D	33	THR	2.7
1	C	150	ALA	2.7
1	C	74	LEU	2.7
1	C	254	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	297	HIS	2.7
1	C	6	VAL	2.7
1	C	417	ILE	2.7
1	D	5	VAL	2.7
1	C	252	ASP	2.7
1	C	376	ALA	2.6
1	C	278	ILE	2.6
1	D	52	VAL	2.6
1	D	417	ILE	2.6
1	D	206	GLY	2.6
1	D	1	MET	2.6
1	D	415	ALA	2.6
1	C	275	VAL	2.6
1	C	39	GLY	2.6
1	C	378	ALA	2.6
1	C	155	LEU	2.6
1	C	37	SER	2.6
1	B	404	TYR	2.6
1	D	200	ILE	2.6
1	D	22	ALA	2.6
1	C	78	ASP	2.6
1	D	35	LEU	2.6
1	D	6	VAL	2.5
1	D	89	TYR	2.5
1	C	87	ALA	2.5
1	C	180	ALA	2.5
1	C	374	LEU	2.5
1	D	405	GLY	2.5
1	D	253	VAL	2.5
1	C	161	TYR	2.5
1	C	403	TYR	2.5
1	C	372	THR	2.5
1	C	391	THR	2.5
1	D	178	THR	2.5
1	B	254	LEU	2.5
1	D	27	LEU	2.5
1	C	320	VAL	2.4
1	D	20	GLU	2.4
1	D	37	SER	2.4
1	C	148	ILE	2.4
1	D	54	ILE	2.4
1	C	102	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	389	GLY	2.4
1	D	67	ASP	2.4
1	C	202	LEU	2.4
1	C	221	GLY	2.4
1	C	251	GLY	2.4
1	D	63	ASN	2.4
1	B	352	ILE	2.4
1	C	4	ILE	2.4
1	C	386	VAL	2.4
1	C	72	ALA	2.3
1	D	32	ALA	2.3
1	D	176	ALA	2.3
1	D	49	LEU	2.3
1	A	1	MET	2.3
1	C	174	MET	2.3
1	D	242	PHE	2.3
1	C	105	ILE	2.3
1	D	19	ILE	2.3
1	C	47	PRO	2.3
1	D	202	LEU	2.3
1	D	95	MET	2.3
1	B	278	ILE	2.3
1	B	284	ILE	2.3
1	C	195	ILE	2.3
1	D	348	HIS	2.3
1	C	183	VAL	2.3
1	C	104	PRO	2.3
1	D	414	GLY	2.3
1	C	217	ILE	2.3
1	C	184	THR	2.3
1	D	104	PRO	2.3
1	C	21	GLY	2.3
1	C	413	LEU	2.3
1	C	404	TYR	2.3
1	D	407	HIS	2.2
1	B	217	ILE	2.2
1	C	114	VAL	2.2
1	C	220	THR	2.2
1	C	176	ALA	2.2
1	D	103	GLY	2.2
1	C	173	LEU	2.2
1	C	348[A]	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	230	HIS	2.2
1	C	59	VAL	2.2
1	D	59	VAL	2.2
1	D	109	VAL	2.2
1	B	1	MET	2.2
1	C	67	ASP	2.2
1	D	61	GLY	2.2
1	C	207	ALA	2.2
1	C	258	ALA	2.2
1	D	87	ALA	2.2
1	C	29	LEU	2.2
1	C	293	LEU	2.2
1	D	108	ARG	2.2
1	D	69	ASP	2.2
1	B	17	VAL	2.2
1	D	392	VAL	2.2
1	C	179	LEU	2.2
1	C	288	SER	2.2
1	D	205	MET	2.2
1	D	406	PHE	2.1
1	C	66	VAL	2.1
1	D	394	GLY	2.1
1	C	316	ALA	2.1
1	C	1	MET	2.1
1	D	80	THR	2.1
1	C	267	ILE	2.1
1	B	233	VAL	2.1
1	B	253	VAL	2.1
1	C	409	LYS	2.1
1	D	29	LEU	2.1
1	D	84	THR	2.1
1	C	186	ILE	2.1
1	D	4	ILE	2.1
1	D	99	ILE	2.1
1	D	260	TRP	2.1
1	C	167	VAL	2.1
1	D	232	VAL	2.1
1	C	411	ALA	2.1
1	D	107	ALA	2.1
1	C	290	LEU	2.1
1	B	304	PRO	2.1
1	D	138	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	105	ILE	2.1
1	B	196	VAL	2.1
1	C	75	VAL	2.1
1	C	393	VAL	2.1
1	D	55	MET	2.0
1	B	271	LEU	2.0
1	C	131	LEU	2.0
1	C	339	LEU	2.0
1	C	181	ASP	2.0
1	C	373	ASP	2.0
1	D	391	THR	2.0
1	C	361	GLY	2.0
1	C	244	VAL	2.0
1	C	273	MET	2.0
1	D	175	MET	2.0
1	D	179	LEU	2.0
1	C	353	ARG	2.0
1	D	409	LYS	2.0
1	C	383	THR	2.0
1	B	414	GLY	2.0
1	C	123	GLY	2.0
1	C	206	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

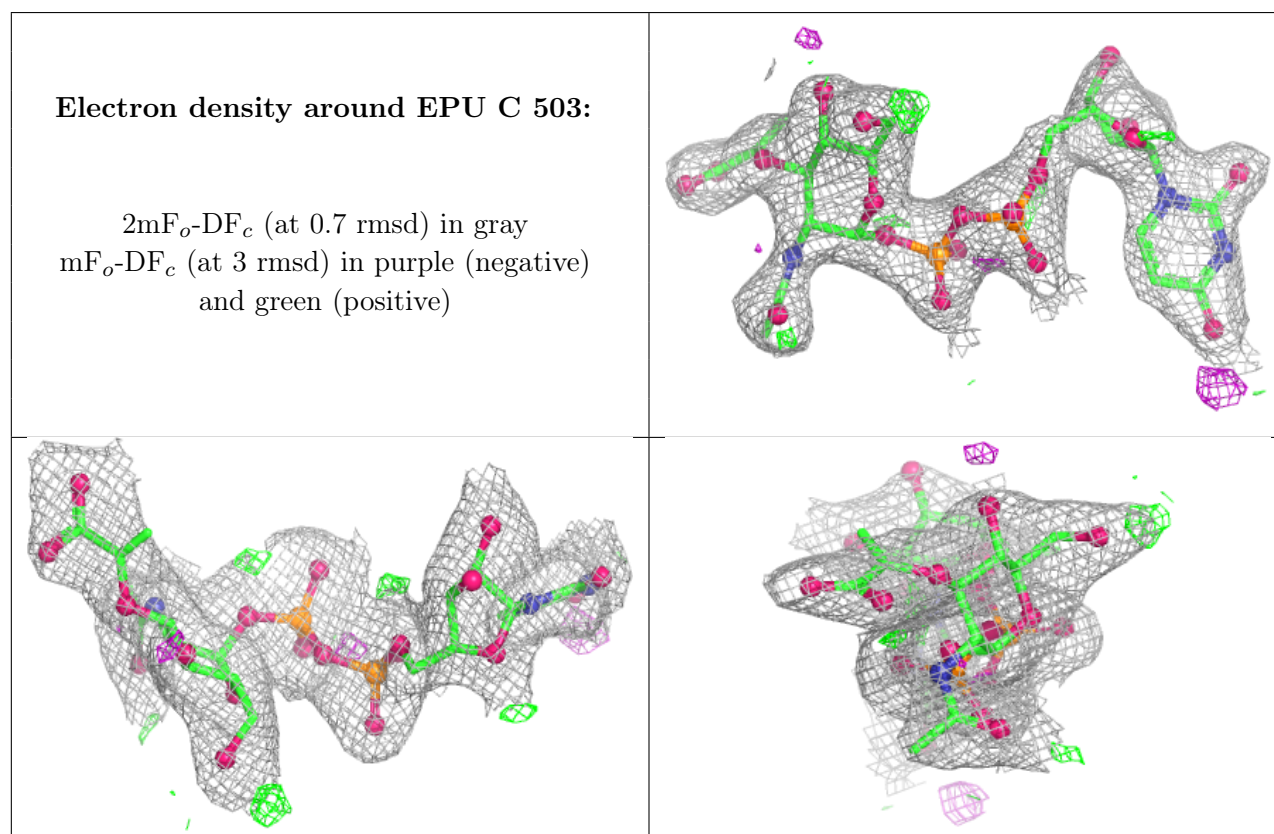
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EPU	C	503	44/44	0.90	0.11	40,52,69,76	0

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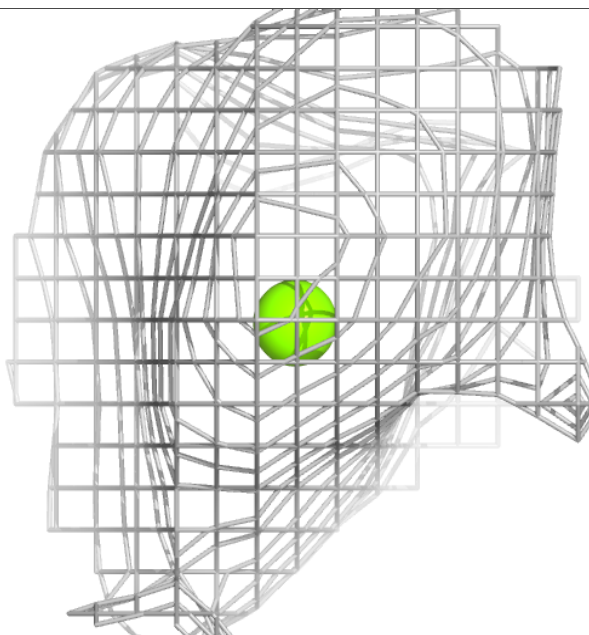
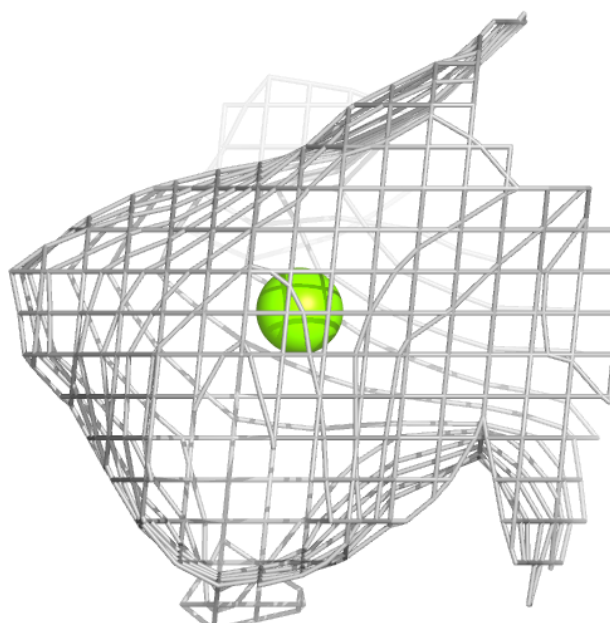
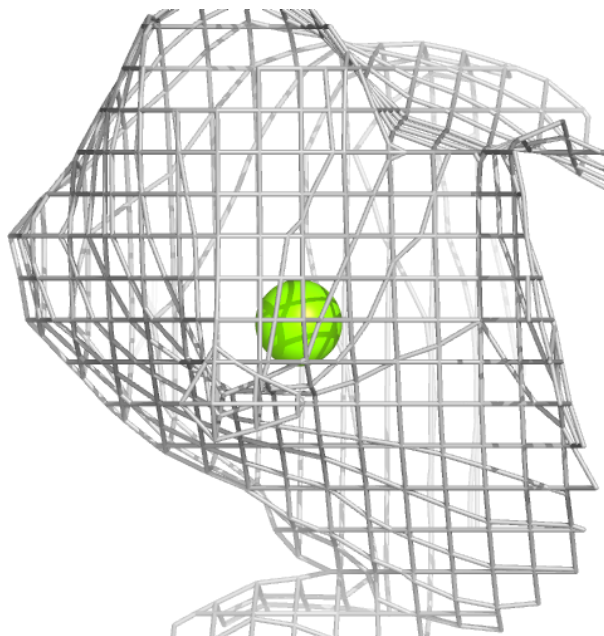
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	502	1/1	0.91	0.07	60,60,60,60	0
2	OV5	D	501	10/10	0.91	0.09	36,53,57,58	0
3	MG	D	502	1/1	0.93	0.07	59,59,59,59	0
2	OV5	C	501	10/10	0.93	0.08	37,54,57,64	0
4	EPU	D	503	44/44	0.94	0.09	29,43,51,60	0
4	EPU	B	503	44/44	0.96	0.07	28,37,44,46	0
3	MG	A	502	1/1	0.97	0.04	31,31,31,31	0
2	OV5	B	501	10/10	0.97	0.06	28,31,41,47	0
2	OV5	A	501	10/10	0.98	0.04	25,28,31,32	0
3	MG	B	502	1/1	0.98	0.03	35,35,35,35	0
4	EPU	A	503	44/44	0.98	0.05	18,24,33,40	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.



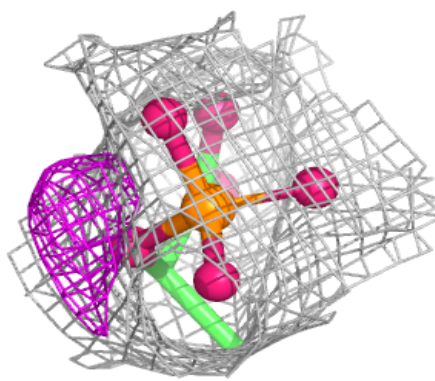
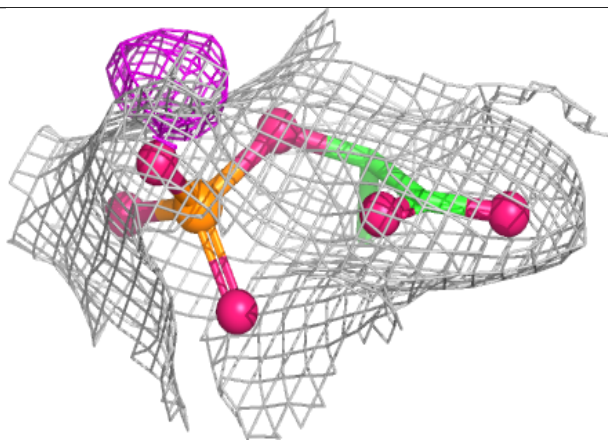
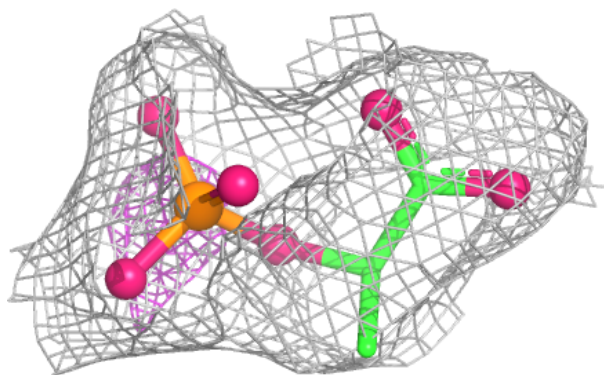
Electron density around MG C 502:

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



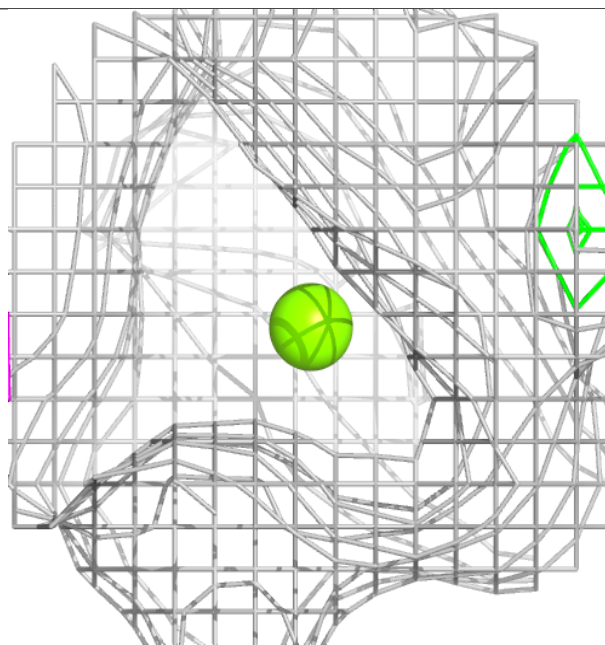
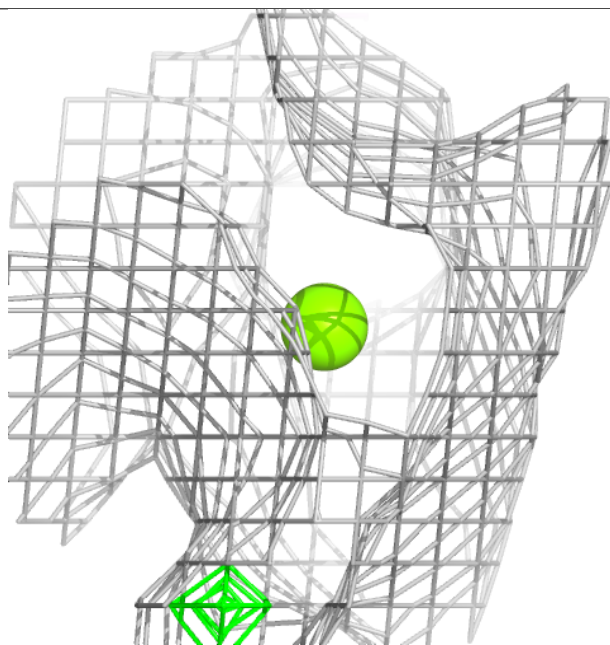
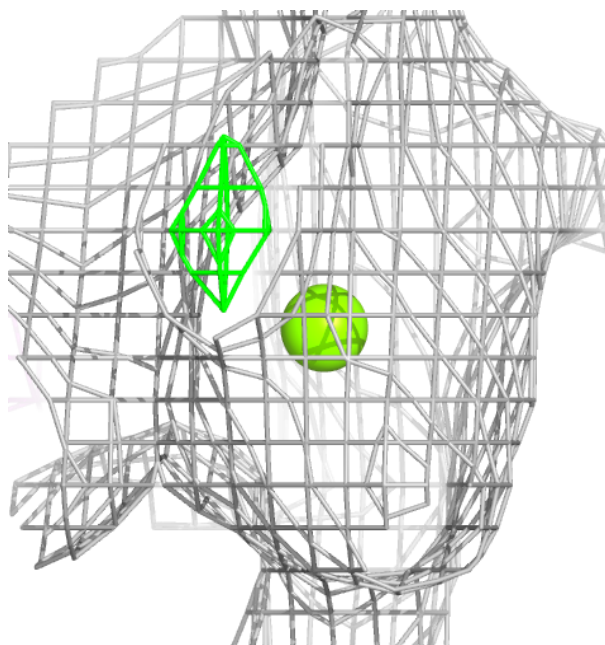
Electron density around 0V5 D 501:

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



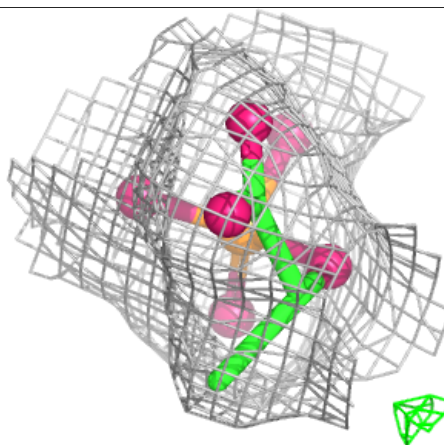
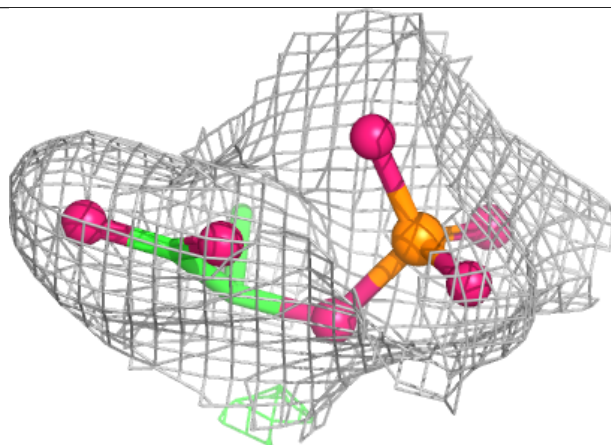
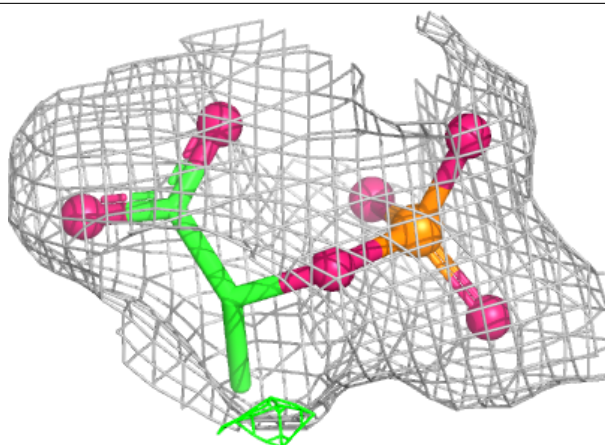
Electron density around MG D 502:

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

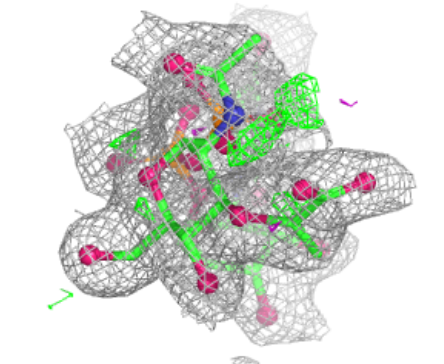
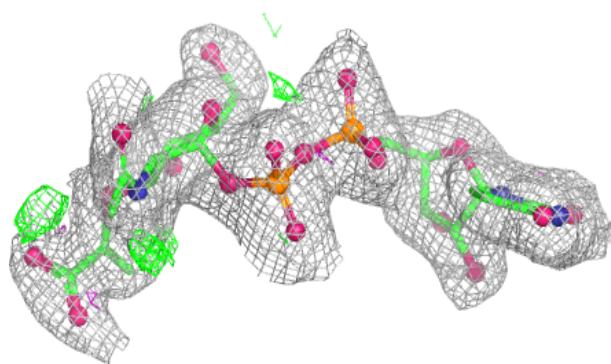
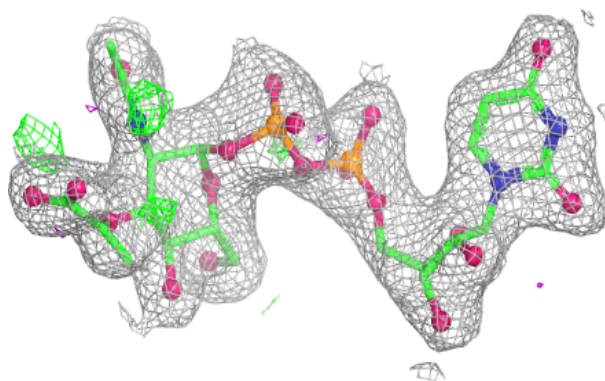


Electron density around 0V5 C 501:

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

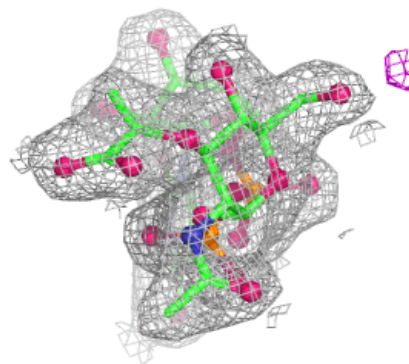
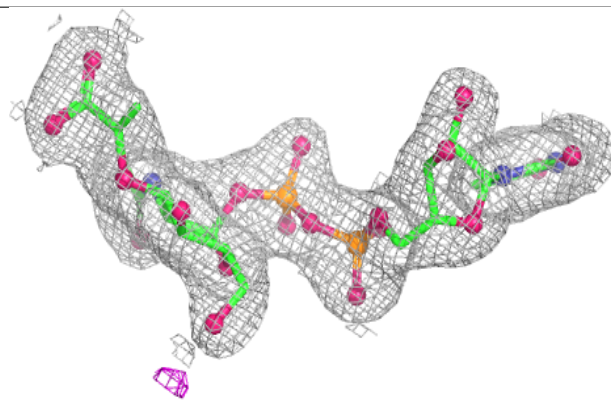
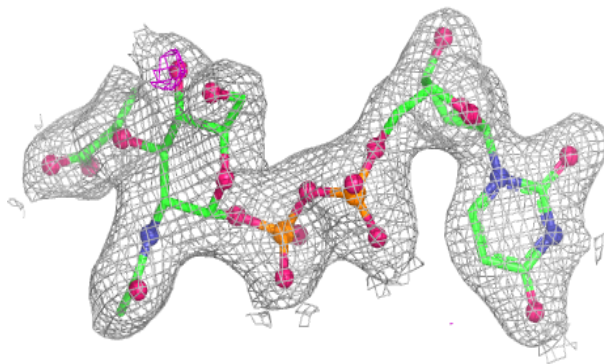
**Electron density around EPU D 503:**

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



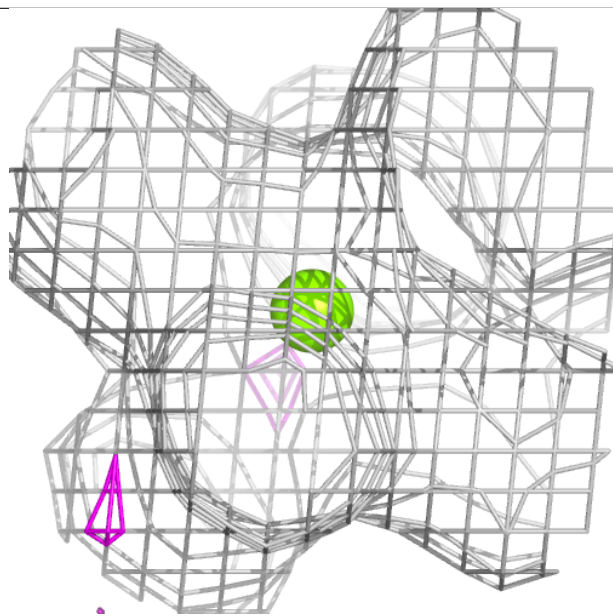
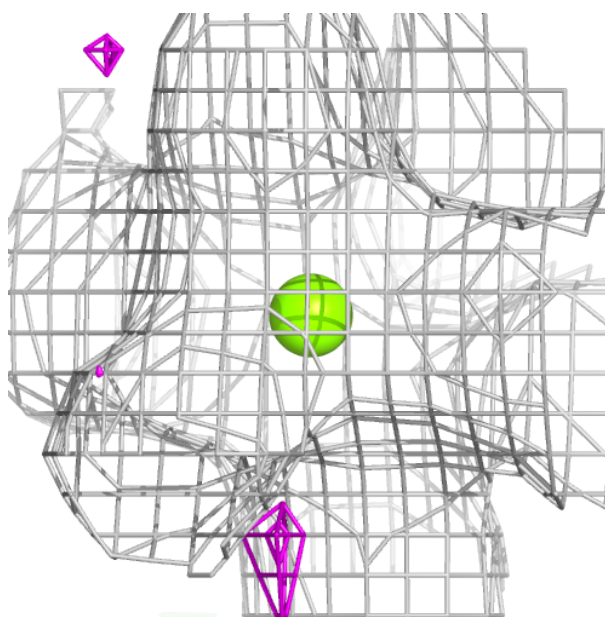
Electron density around EPU B 503:

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



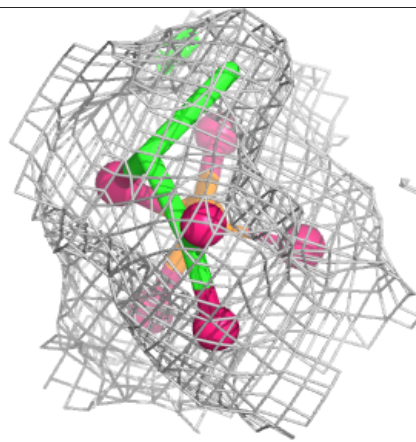
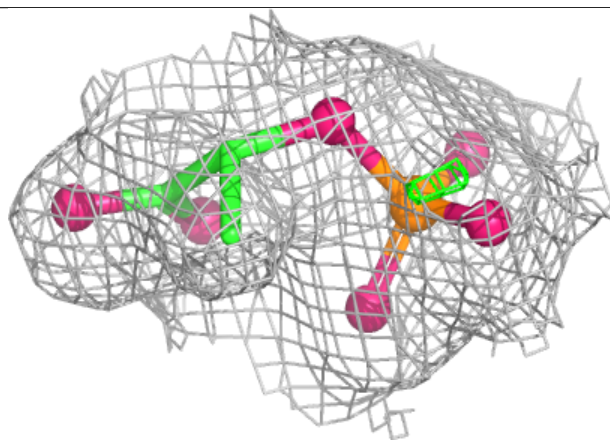
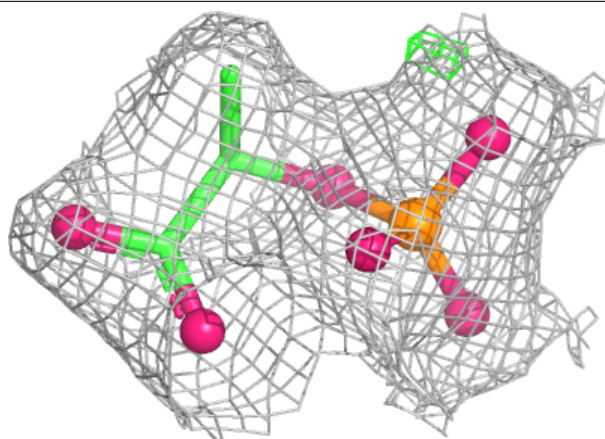
Electron density around MG A 502:

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



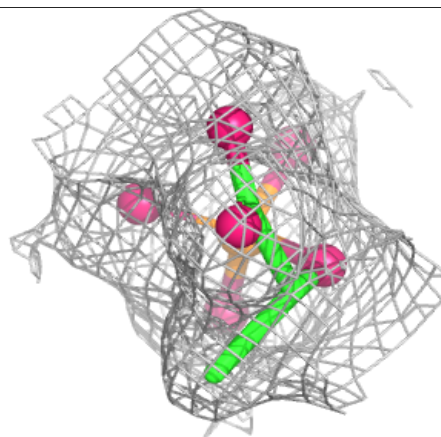
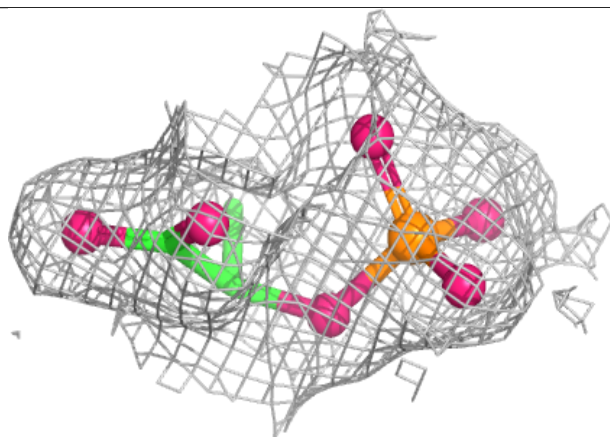
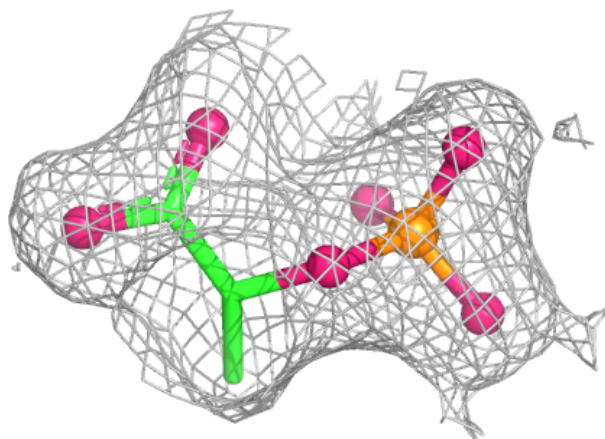
Electron density around 0V5 B 501:

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



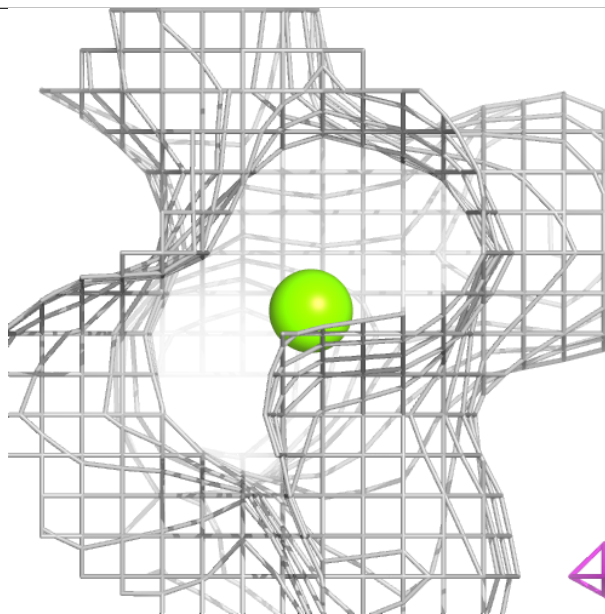
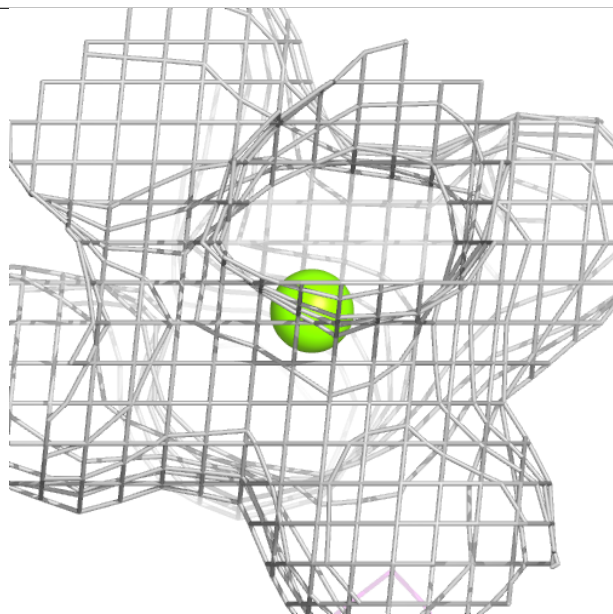
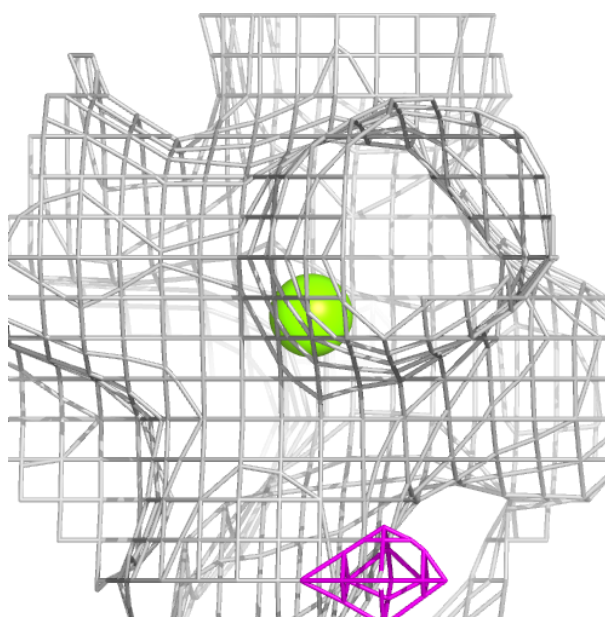
Electron density around 0V5 A 501:

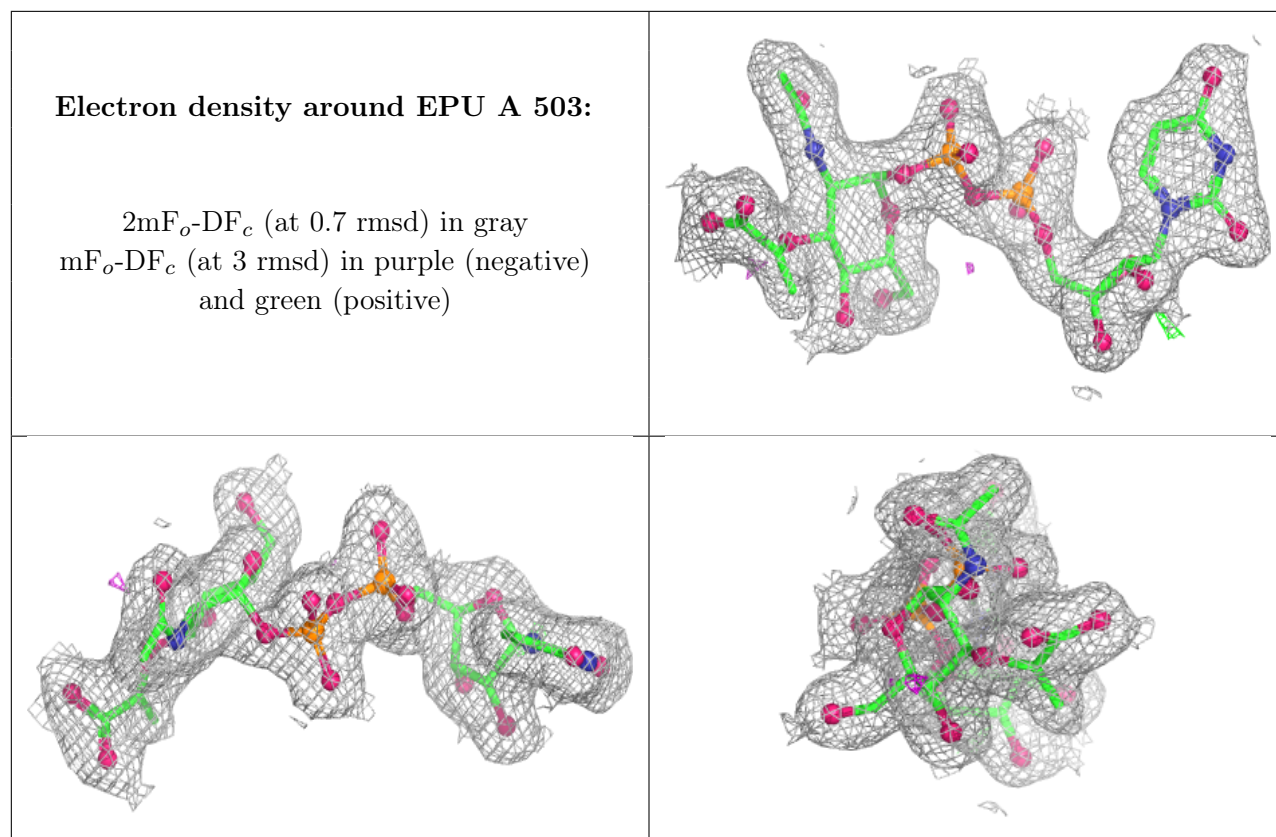
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 502:

$2mF_o-DF_c$ (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.