



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:12 PM UTC

PDB ID : 7P0H / pdb_00007p0h
Title : Crystal structure of Helicobacter pylori ComF fused to an artificial alphaREP crystallization helper(named B2)
Authors : Celma, L.; Walbott, H.; Legrand, P.; Quevillon-Cheruel, S.
Deposited on : 2021-06-29
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

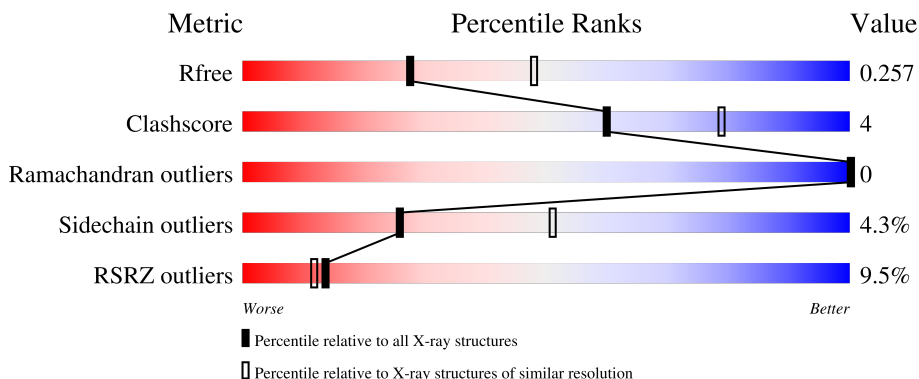
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	427	7% 80% 16% .
1	B	427	10% 85% 11% ..
1	C	427	11% 83% 13% .
1	D	427	8% 85% 11% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13138 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.

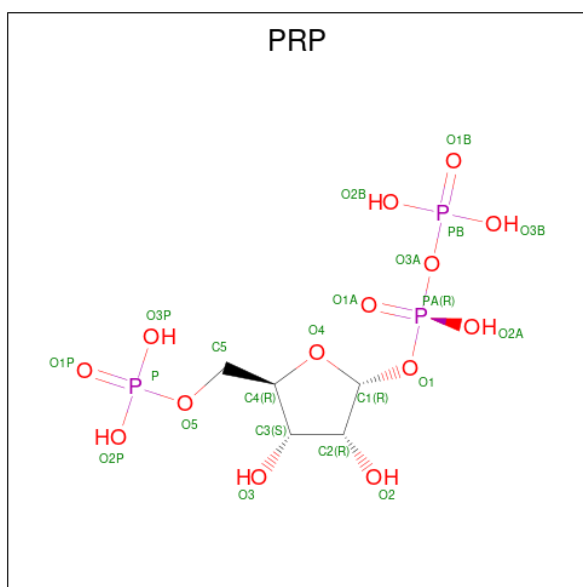
- Molecule 1 is a protein called *Helicobacter pylori* ComF fused to an artificial alphaREP crystallization helper (named B2).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	Se	0	0	0
			3168	2010	550	599	7	2			
1	B	411	Total	C	N	O	S	Se	0	0	0
			3168	2010	550	599	7	2			
1	C	411	Total	C	N	O	S	Se	0	0	0
			3168	2010	550	599	7	2			
1	D	411	Total	C	N	O	S	Se	0	0	0
			3168	2010	550	599	7	2			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose (CCD ID: PRP) (formula: C₅H₁₃O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			22	5	14	3		
3	B	1	Total	C	O	P	0	0
			22	5	14	3		
3	C	1	Total	C	O	P	0	0
			22	5	14	3		
3	D	1	Total	C	O	P	0	0
			22	5	14	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

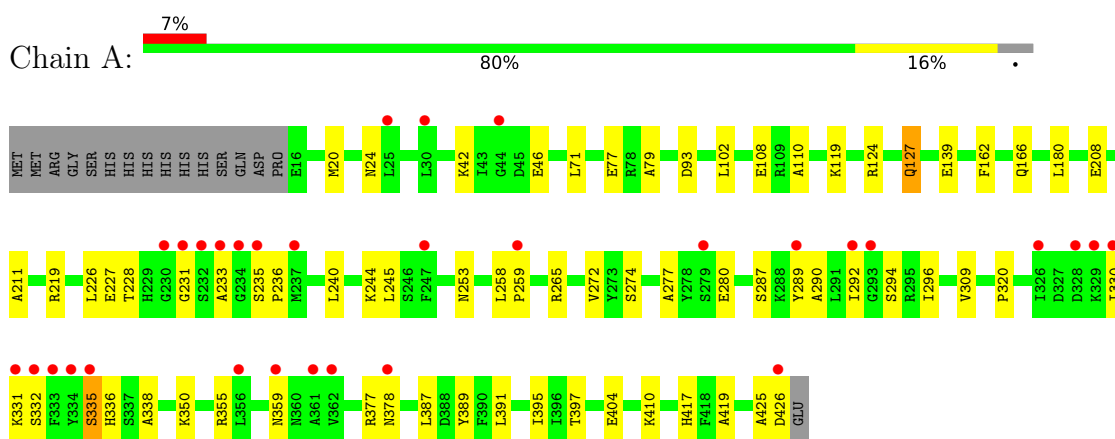
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	95	Total 95	O 95	0	0
6	B	40	Total 40	O 40	0	0
6	C	83	Total 83	O 83	0	0
6	D	64	Total 64	O 64	0	0

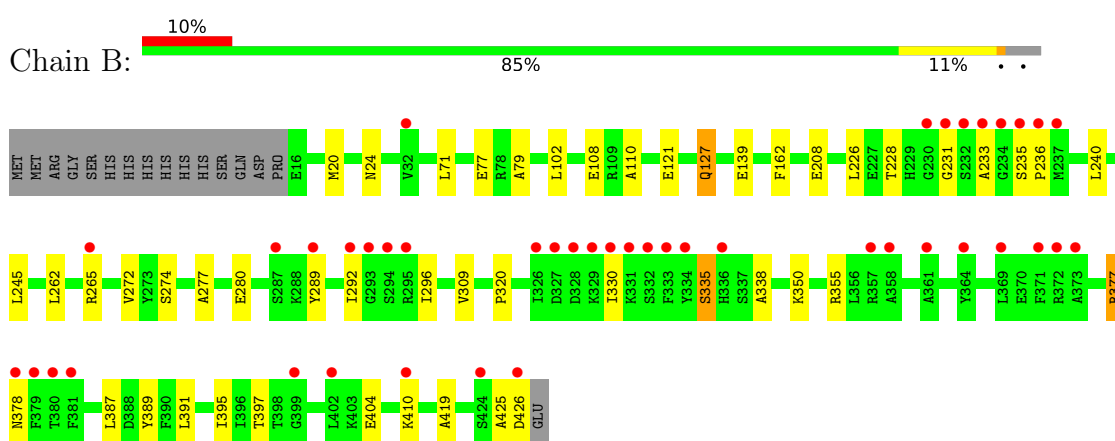
3 Residue-property plots [i](#)

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.

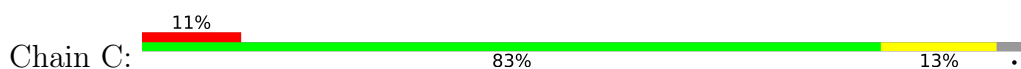
- Molecule 1: *Helicobacter pylori* ComF fused to an artificial alphaREP crystallization helper (named B2)

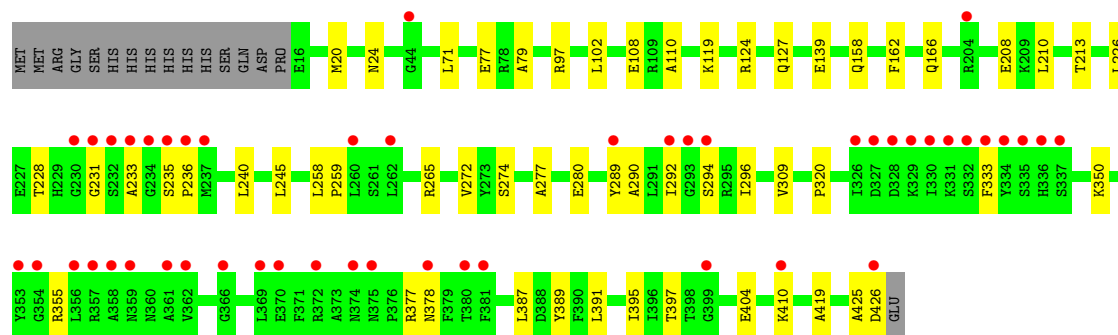


- Molecule 1: *Helicobacter pylori* ComF fused to an artificial alphaREP crystallization helper (named B2)

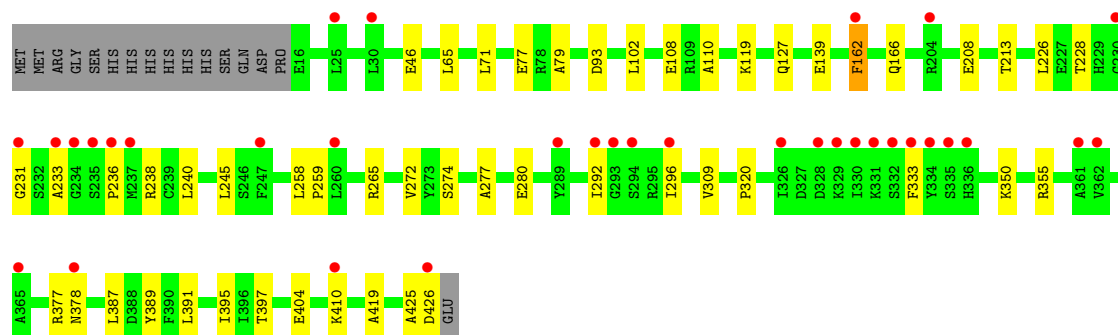
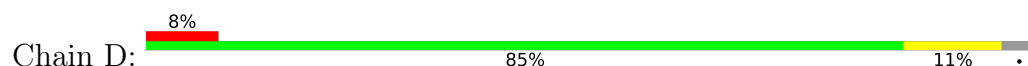


- Molecule 1: *Helicobacter pylori* ComF fused to an artificial alphaREP crystallization helper (named B2)





- Molecule 1: *Helicobacter pylori* ComF fused to an artificial alphaREP crystallization helper (named B2)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.88Å 87.98Å 122.79Å 80.23° 76.44° 76.39°	Depositor
Resolution (Å)	46.47 – 2.50 46.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	80.2 (46.47-2.50) 80.2 (46.47-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.221 , 0.245 0.229 , 0.257	Depositor DCC
R_{free} test set	3156 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13138	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: GOL, ZN, MG, PRP

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	0.66	0/3212	1.06	0/4328
1	B	0.65	0/3212	1.05	0/4328
1	C	0.66	0/3212	1.05	0/4328
1	D	0.65	0/3212	1.05	1/4328 (0.0%)
All	All	0.65	0/12848	1.05	1/17312 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	PHE	CA-CB-CG	5.16	118.96	113.80

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	3168	0	3251	42	0
1	B	3168	0	3251	29	0
1	C	3168	0	3251	32	0
1	D	3168	0	3251	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	22	0	8	2	0
3	B	22	0	8	2	0
3	C	22	0	8	2	0
3	D	22	0	8	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	36	0	48	3	0
5	B	12	0	16	0	0
5	C	24	0	32	2	0
5	D	12	0	16	1	0
6	A	95	0	0	0	0
6	B	40	0	0	0	0
6	C	83	0	0	0	0
6	D	64	0	0	0	0
All	All	13138	0	13148	112	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 (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:HB2	1:A:336:HIS:HD2	1.27	0.97
1:A:292:ILE:HD12	1:C:162:PHE:HB3	1.73	0.70
1:B:162:PHE:HB3	1:D:292:ILE:HD12	1.74	0.70
1:D:240:LEU:HD12	1:D:296:ILE:HD11	1.75	0.68
1:B:292:ILE:HD12	1:D:162:PHE:HB3	1.75	0.68
1:A:240:LEU:HD12	1:A:296:ILE:HD11	1.76	0.67
1:C:240:LEU:HD12	1:C:296:ILE:HD11	1.78	0.64
1:B:240:LEU:HD12	1:B:296:ILE:HD11	1.79	0.64
1:C:320:PRO:HB3	1:C:350:LYS:NZ	2.13	0.63
1:A:332:SER:HB2	1:A:336:HIS:CD2	2.19	0.63
1:A:320:PRO:HB3	1:A:350:LYS:NZ	2.15	0.61
1:D:320:PRO:HB3	1:D:350:LYS:NZ	2.16	0.61
1:B:320:PRO:HB3	1:B:350:LYS:NZ	2.15	0.60
1:A:330:ILE:CD1	1:C:97:ARG:HE	2.14	0.60
1:B:127:GLN:HE22	1:D:333:PHE:HE2	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:THR:O	1:B:426:ASP:HB3	2.04	0.58
1:A:397:THR:O	1:A:426:ASP:HB3	2.04	0.58
1:C:397:THR:O	1:C:426:ASP:HB3	2.03	0.57
1:A:277:ALA:HB3	1:A:280:GLU:HG3	1.87	0.57
1:D:397:THR:O	1:D:426:ASP:HB3	2.04	0.57
1:C:277:ALA:HB3	1:C:280:GLU:HG3	1.87	0.56
1:D:277:ALA:HB3	1:D:280:GLU:HG3	1.86	0.56
1:A:227:GLU:HB3	1:A:244:LYS:HG2	1.87	0.56
1:B:127:GLN:NE2	1:D:333:PHE:HE2	2.03	0.56
1:B:277:ALA:HB3	1:B:280:GLU:HG3	1.88	0.55
1:D:272:VAL:HG22	1:D:419:ALA:HB3	1.88	0.55
1:B:272:VAL:HG22	1:B:419:ALA:HB3	1.88	0.55
1:A:162:PHE:HB3	1:C:292:ILE:HD12	1.89	0.55
1:B:265:ARG:HH22	1:B:274:SER:HB3	1.71	0.55
1:C:272:VAL:HG22	1:C:419:ALA:HB3	1.89	0.54
1:A:272:VAL:HG22	1:A:419:ALA:HB3	1.88	0.54
1:B:320:PRO:HB3	1:B:350:LYS:HZ2	1.71	0.54
1:C:265:ARG:HH12	1:C:274:SER:HB3	1.73	0.53
1:A:287:SER:OG	1:C:158:GLN:NE2	2.36	0.53
1:A:265:ARG:HH22	1:A:274:SER:HB3	1.72	0.53
1:A:331:LYS:HA	1:C:124:ARG:HD2	1.91	0.52
1:B:395:ILE:HD11	1:B:425:ALA:HB2	1.92	0.52
1:D:265:ARG:HH12	1:D:274:SER:HB3	1.75	0.52
1:D:395:ILE:HD11	1:D:425:ALA:HB2	1.92	0.51
1:A:320:PRO:HB3	1:A:350:LYS:HZ2	1.75	0.51
1:A:359:ASN:HB2	1:A:378:ASN:HB2	1.93	0.50
1:B:208:GLU:HA	1:B:226:LEU:HD11	1.93	0.50
1:C:208:GLU:HA	1:C:226:LEU:HD11	1.93	0.50
1:A:180:LEU:O	5:A:509:GOL:O3	2.29	0.50
1:A:208:GLU:HA	1:A:226:LEU:HD11	1.93	0.50
1:D:213:THR:HG1	5:D:505:GOL:HO2	1.58	0.50
1:A:330:ILE:HD12	1:C:97:ARG:HE	1.77	0.49
1:C:320:PRO:HB3	1:C:350:LYS:HZ2	1.77	0.49
1:C:320:PRO:HB3	1:C:350:LYS:HZ3	1.77	0.49
1:A:395:ILE:HD11	1:A:425:ALA:HB2	1.94	0.49
1:D:320:PRO:HB3	1:D:350:LYS:HZ3	1.77	0.49
1:B:330:ILE:HD13	1:D:65:LEU:HD13	1.94	0.49
1:A:335:SER:HB3	1:A:338:ALA:HB3	1.95	0.49
1:D:208:GLU:HA	1:D:226:LEU:HD11	1.94	0.49
1:A:289:TYR:OH	3:A:502:PRP:O1B	2.29	0.48
1:A:235:SER:OG	1:C:166:GLN:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HD11	1:C:97:ARG:HG2	1.96	0.48
1:D:355:ARG:NH1	1:D:389:TYR:OH	2.47	0.48
1:B:231:GLY:HA3	1:B:245:LEU:HD11	1.96	0.47
1:B:335:SER:HB3	1:B:338:ALA:HB3	1.97	0.47
1:C:355:ARG:NH1	1:C:389:TYR:OH	2.48	0.47
1:B:235:SER:HB2	1:D:166:GLN:NE2	2.29	0.47
1:B:355:ARG:NH1	1:B:389:TYR:OH	2.48	0.47
1:C:395:ILE:HD11	1:C:425:ALA:HB2	1.96	0.47
1:A:355:ARG:NH1	1:A:389:TYR:OH	2.48	0.46
1:B:289:TYR:OH	3:B:502:PRP:O3B	2.29	0.46
1:D:231:GLY:HA3	1:D:245:LEU:HD11	1.97	0.46
1:C:395:ILE:HG23	3:C:502:PRP:H2	1.98	0.46
1:A:166:GLN:NE2	1:C:235:SER:OG	2.49	0.46
1:C:231:GLY:HA3	1:C:245:LEU:HD11	1.98	0.45
1:A:231:GLY:HA3	1:A:245:LEU:HD11	1.98	0.45
1:A:211:ALA:O	1:A:219:ARG:NH1	2.49	0.45
1:B:330:ILE:HG12	1:D:93:ASP:HB3	1.98	0.45
1:C:258:LEU:HA	1:C:259:PRO:HD3	1.90	0.45
1:B:102:LEU:HD22	1:B:110:ALA:HB2	1.98	0.45
1:C:102:LEU:HD22	1:C:110:ALA:HB2	1.98	0.45
1:D:320:PRO:HB3	1:D:350:LYS:HZ2	1.82	0.44
1:A:253:ASN:HB3	5:A:507:GOL:H31	1.98	0.44
1:D:233:ALA:O	1:D:236:PRO:HD3	2.18	0.44
1:C:233:ALA:O	1:C:236:PRO:HD3	2.18	0.44
1:C:213:THR:OG1	5:C:507:GOL:O2	2.29	0.44
1:D:102:LEU:HD22	1:D:110:ALA:HB2	2.00	0.44
1:A:320:PRO:HB3	1:A:350:LYS:HZ3	1.83	0.44
1:C:290:ALA:O	1:C:294:SER:OG	2.33	0.43
1:C:289:TYR:OH	3:C:502:PRP:O1B	2.32	0.43
1:A:102:LEU:HD22	1:A:110:ALA:HB2	1.99	0.43
1:B:233:ALA:O	1:B:236:PRO:HD3	2.17	0.43
1:A:395:ILE:HG23	3:A:502:PRP:H2	2.00	0.43
1:D:395:ILE:HG23	3:D:502:PRP:H2	1.99	0.43
1:A:258:LEU:HA	1:A:259:PRO:HD3	1.89	0.43
1:A:240:LEU:HD11	1:A:292:ILE:HG22	2.01	0.43
1:D:258:LEU:HA	1:D:259:PRO:HD3	1.90	0.43
1:B:71:LEU:HD22	1:B:79:ALA:HB2	2.01	0.43
1:A:93:ASP:OD1	1:A:124:ARG:NH2	2.51	0.42
1:B:20:MSE:HE2	1:B:24:ASN:HD21	1.85	0.42
1:C:20:MSE:HE2	1:C:24:ASN:HD21	1.83	0.42
1:C:71:LEU:HD22	1:C:79:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:HD11	1:B:292:ILE:HG22	2.02	0.42
1:D:236:PRO:HG2	1:D:238:ARG:HH11	1.85	0.41
1:A:71:LEU:HD22	1:A:79:ALA:HB2	2.02	0.41
1:A:233:ALA:O	1:A:236:PRO:HD3	2.19	0.41
1:A:290:ALA:O	1:A:294:SER:OG	2.30	0.41
1:C:210:LEU:CD1	5:C:507:GOL:H32	2.51	0.41
1:A:20:MSE:HE2	1:A:24:ASN:HD21	1.85	0.41
1:A:127:GLN:HE22	1:C:333:PHE:HE2	1.68	0.41
1:D:71:LEU:HD22	1:D:79:ALA:HB2	2.03	0.41
1:A:265:ARG:HH22	1:A:274:SER:CB	2.33	0.41
1:A:417:HIS:HA	5:A:504:GOL:H11	2.02	0.40
1:B:395:ILE:HG23	3:B:502:PRP:H2	2.02	0.40
1:B:265:ARG:HH22	1:B:274:SER:CB	2.32	0.40
1:B:320:PRO:HB3	1:B:350:LYS:HZ3	1.87	0.40
1:B:377:ARG:H	1:B:377:ARG:HG2	1.75	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	409/427 (96%)	398 (97%)	11 (3%)	0	100	100
1	B	409/427 (96%)	400 (98%)	9 (2%)	0	100	100
1	C	409/427 (96%)	398 (97%)	11 (3%)	0	100	100
1	D	409/427 (96%)	398 (97%)	11 (3%)	0	100	100
All	All	1636/1708 (96%)	1594 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/342 (96%)	314 (95%)	15 (5%)	24	48
1	B	329/342 (96%)	314 (95%)	15 (5%)	24	48
1	C	329/342 (96%)	316 (96%)	13 (4%)	28	54
1	D	329/342 (96%)	315 (96%)	14 (4%)	26	51
All	All	1316/1368 (96%)	1259 (96%)	57 (4%)	26	51

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	46	GLU
1	A	77	GLU
1	A	108	GLU
1	A	119	LYS
1	A	127	GLN
1	A	139	GLU
1	A	228	THR
1	A	309	VAL
1	A	335	SER
1	A	377	ARG
1	A	387	LEU
1	A	391	LEU
1	A	404	GLU
1	A	410	LYS
1	B	77	GLU
1	B	108	GLU
1	B	121	GLU
1	B	127	GLN
1	B	139	GLU
1	B	228	THR
1	B	262	LEU
1	B	309	VAL
1	B	335	SER

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Mol	Chain	Res	Type
1	B	377	ARG
1	B	378	ASN
1	B	387	LEU
1	B	391	LEU
1	B	404	GLU
1	B	410	LYS
1	C	77	GLU
1	C	108	GLU
1	C	119	LYS
1	C	127	GLN
1	C	139	GLU
1	C	228	THR
1	C	309	VAL
1	C	377	ARG
1	C	378	ASN
1	C	387	LEU
1	C	391	LEU
1	C	404	GLU
1	C	410	LYS
1	D	46	GLU
1	D	77	GLU
1	D	108	GLU
1	D	119	LYS
1	D	127	GLN
1	D	139	GLU
1	D	228	THR
1	D	309	VAL
1	D	377	ARG
1	D	378	ASN
1	D	387	LEU
1	D	391	LEU
1	D	404	GLU
1	D	410	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	38	ASN
1	A	104	GLN
1	A	166	GLN
1	A	336	HIS

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Mol	Chain	Res	Type
1	A	378	ASN
1	B	24	ASN
1	B	38	ASN
1	B	104	GLN
1	B	253	ASN
1	B	336	HIS
1	C	24	ASN
1	C	38	ASN
1	C	104	GLN
1	C	158	GLN
1	C	166	GLN
1	C	253	ASN
1	C	336	HIS
1	D	24	ASN
1	D	38	ASN
1	D	104	GLN
1	D	253	ASN
1	D	336	HIS

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 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	A	508	-	5,5,5	0.09	0	5,5,5	0.34	0
5	GOL	A	505	-	5,5,5	0.11	0	5,5,5	0.28	0
5	GOL	C	505	-	5,5,5	0.10	0	5,5,5	0.30	0
5	GOL	C	506	-	5,5,5	0.12	0	5,5,5	0.36	0
5	GOL	D	505	-	5,5,5	0.05	0	5,5,5	0.33	0
5	GOL	A	506	-	5,5,5	0.10	0	5,5,5	0.36	0
3	PRP	C	502	4	20,22,22	0.64	0	32,35,35	0.90	2 (6%)
3	PRP	B	502	4	20,22,22	0.66	0	32,35,35	0.89	1 (3%)
5	GOL	A	509	-	5,5,5	0.09	0	5,5,5	0.36	0
5	GOL	B	504	-	5,5,5	0.08	0	5,5,5	0.31	0
5	GOL	B	505	-	5,5,5	0.10	0	5,5,5	0.34	0
3	PRP	A	502	4	20,22,22	0.71	0	32,35,35	0.98	3 (9%)
5	GOL	C	507	-	5,5,5	0.05	0	5,5,5	0.31	0
5	GOL	C	504	-	5,5,5	0.15	0	5,5,5	0.40	0
5	GOL	D	504	-	5,5,5	0.08	0	5,5,5	0.23	0
3	PRP	D	502	4	20,22,22	0.63	0	32,35,35	0.96	3 (9%)
5	GOL	A	507	-	5,5,5	0.06	0	5,5,5	0.31	0
5	GOL	A	504	-	5,5,5	0.14	0	5,5,5	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	508	-	-	0/4/4/4	-
5	GOL	A	505	-	-	0/4/4/4	-
5	GOL	C	505	-	-	0/4/4/4	-
5	GOL	C	506	-	-	1/4/4/4	-
5	GOL	D	505	-	-	2/4/4/4	-
5	GOL	A	506	-	-	0/4/4/4	-
3	PRP	C	502	4	-	7/16/33/33	0/1/1/1
3	PRP	B	502	4	-	4/16/33/33	0/1/1/1
5	GOL	A	509	-	-	0/4/4/4	-
5	GOL	B	504	-	-	0/4/4/4	-
5	GOL	B	505	-	-	1/4/4/4	-
3	PRP	A	502	4	-	7/16/33/33	0/1/1/1
5	GOL	C	507	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	504	-	-	0/4/4/4	-
5	GOL	D	504	-	-	0/4/4/4	-
3	PRP	D	502	4	-	5/16/33/33	0/1/1/1
5	GOL	A	507	-	-	0/4/4/4	-
5	GOL	A	504	-	-	0/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	PRP	O1-C1-C2	2.40	110.54	106.65
3	A	502	PRP	O1-C1-C2	2.32	110.41	106.65
3	C	502	PRP	PA-O1-C1	2.32	130.65	121.21
3	A	502	PRP	O3B-PB-O3A	2.27	112.23	104.64
3	B	502	PRP	PA-O1-C1	2.25	130.38	121.21
3	C	502	PRP	O3B-PB-O3A	2.25	112.18	104.64
3	D	502	PRP	PA-O1-C1	2.23	130.30	121.21
3	A	502	PRP	PA-O1-C1	2.21	130.23	121.21
3	D	502	PRP	O5-P-O1P	2.06	112.00	106.44

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	PRP	C1-O1-PA-O2A
3	A	502	PRP	C1-O1-PA-O3A
3	A	502	PRP	PA-O3A-PB-O2B
3	A	502	PRP	PA-O3A-PB-O3B
3	B	502	PRP	C1-O1-PA-O3A
3	B	502	PRP	PA-O3A-PB-O2B
3	C	502	PRP	C1-O1-PA-O2A
3	C	502	PRP	C1-O1-PA-O3A
3	C	502	PRP	PA-O3A-PB-O2B
3	C	502	PRP	PA-O3A-PB-O3B
3	D	502	PRP	C1-O1-PA-O1A
3	D	502	PRP	C1-O1-PA-O3A
3	D	502	PRP	PA-O3A-PB-O2B
5	C	506	GOL	C1-C2-C3-O3
5	C	507	GOL	O1-C1-C2-C3
5	D	505	GOL	O1-C1-C2-C3
3	A	502	PRP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	502	PRP	PB-O3A-PA-O1A
3	B	502	PRP	C1-O1-PA-O1A
5	D	505	GOL	O1-C1-C2-O2
3	A	502	PRP	PA-O3A-PB-O1B
3	C	502	PRP	PA-O3A-PB-O1B
3	D	502	PRP	PA-O3A-PB-O1B
5	B	505	GOL	O2-C2-C3-O3
3	A	502	PRP	PB-O3A-PA-O2A
3	C	502	PRP	PB-O3A-PA-O2A
3	B	502	PRP	PB-O3A-PA-O2A
3	D	502	PRP	PB-O3A-PA-O2A

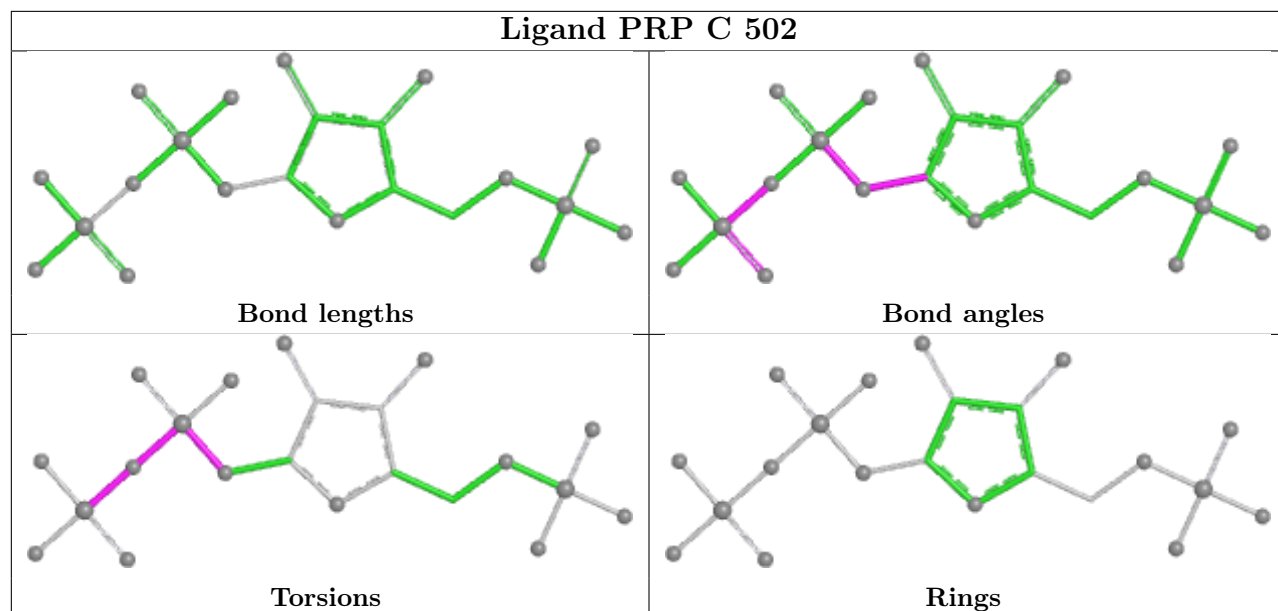
There are no ring outliers.

9 monomers are involved in 13 short contacts:

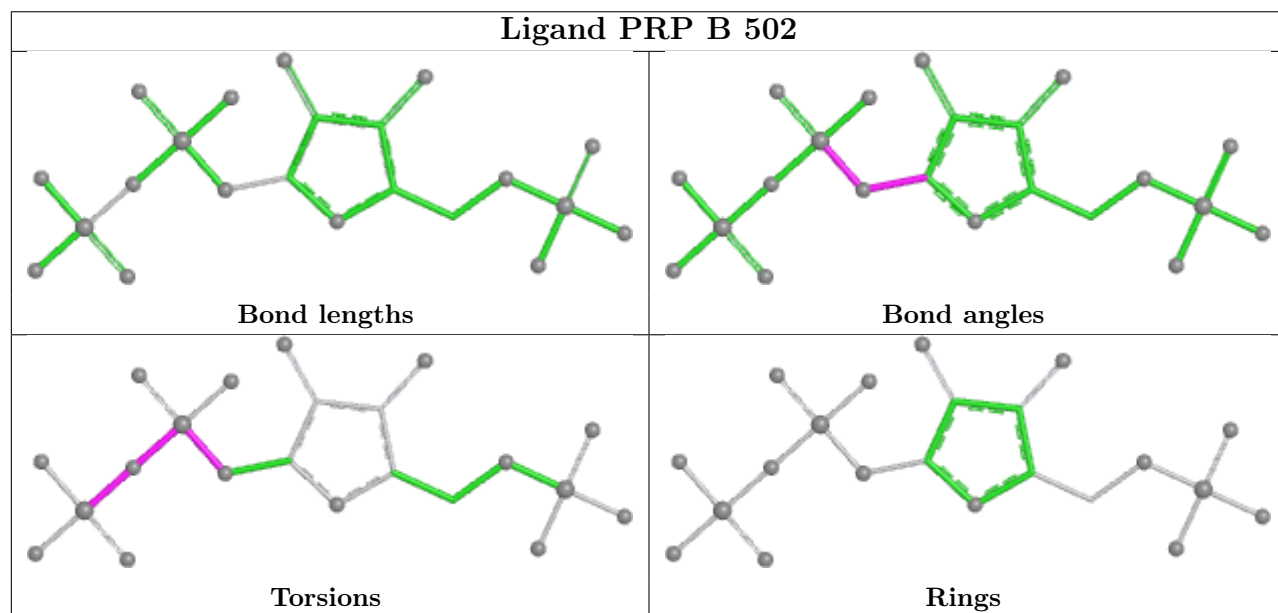
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	505	GOL	1	0
3	C	502	PRP	2	0
3	B	502	PRP	2	0
5	A	509	GOL	1	0
3	A	502	PRP	2	0
5	C	507	GOL	2	0
3	D	502	PRP	1	0
5	A	507	GOL	1	0
5	A	504	GOL	1	0

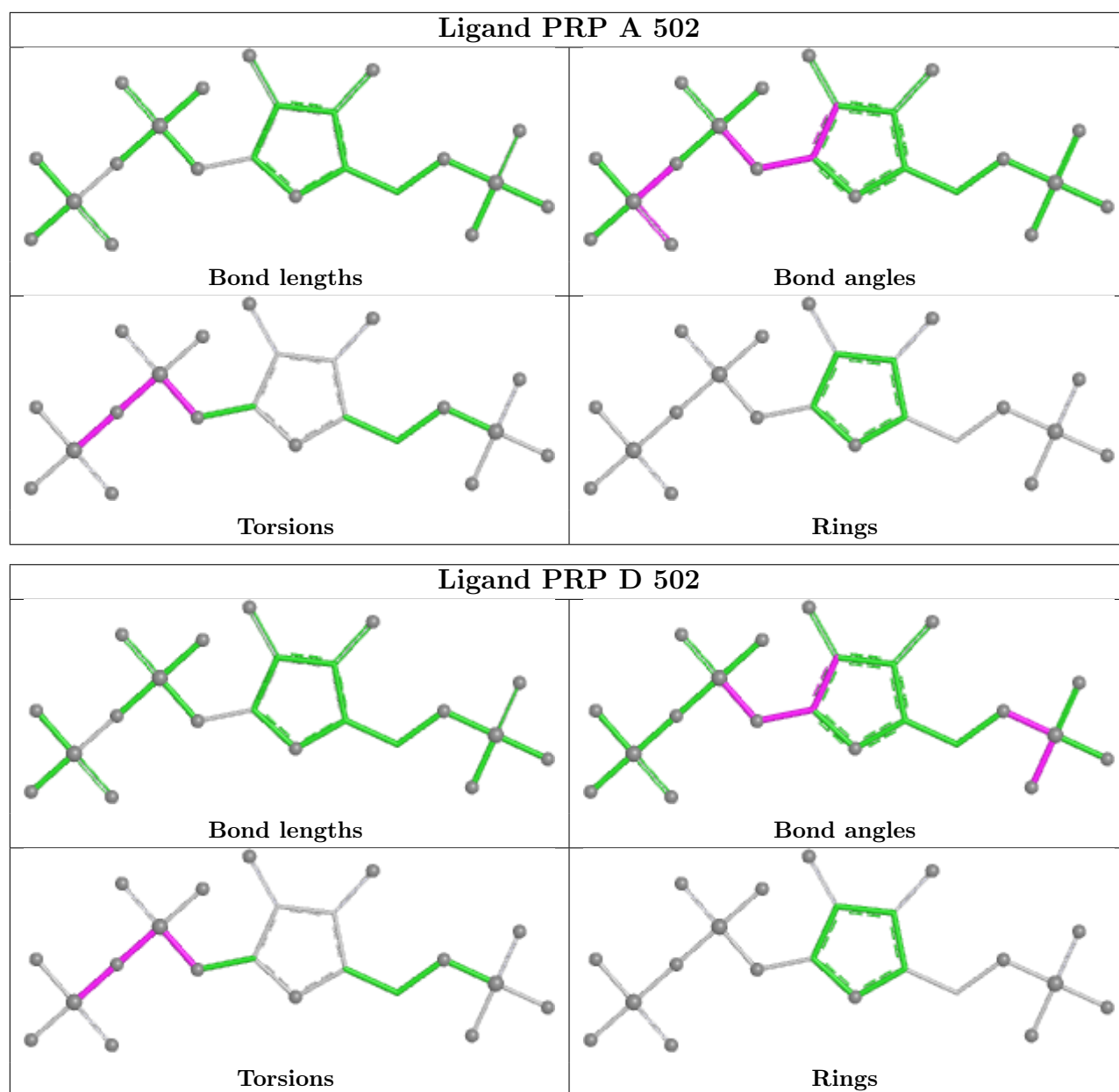
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand PRP C 502



Ligand PRP B 502





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	409/427 (95%)	0.60	31 (7%) 20 17	39, 62, 89, 104	0
1	B	409/427 (95%)	0.87	43 (10%) 11 10	49, 71, 116, 135	0
1	C	409/427 (95%)	0.78	48 (11%) 9 7	42, 64, 99, 117	0
1	D	409/427 (95%)	0.78	34 (8%) 17 15	42, 68, 107, 121	0
All	All	1636/1708 (95%)	0.75	156 (9%) 14 12	39, 67, 103, 135	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	361	ALA	7.1
1	C	333	PHE	6.7
1	D	330	ILE	6.5
1	C	330	ILE	6.4
1	D	331	LYS	6.3
1	B	235	SER	6.2
1	D	293	GLY	6.0
1	A	333	PHE	6.0
1	D	333	PHE	6.0
1	A	292	ILE	5.6
1	D	292	ILE	5.6
1	C	235	SER	5.6
1	C	331	LYS	5.5
1	B	292	ILE	5.1
1	A	235	SER	5.1
1	C	292	ILE	5.1
1	A	237	MET	5.0
1	B	333	PHE	4.9
1	B	361	ALA	4.8
1	B	331	LYS	4.8
1	B	330	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	289	TYR	4.6
1	B	334	TYR	4.6
1	B	237	MET	4.5
1	B	336	HIS	4.5
1	A	331	LYS	4.5
1	D	237	MET	4.5
1	D	334	TYR	4.4
1	A	330	ILE	4.4
1	C	329	LYS	4.4
1	A	230	GLY	4.4
1	D	230	GLY	4.4
1	C	336	HIS	4.3
1	A	293	GLY	4.2
1	C	44	GLY	4.2
1	A	334	TYR	4.2
1	C	293	GLY	4.1
1	A	231	GLY	4.1
1	C	334	TYR	4.0
1	B	234	GLY	4.0
1	D	30	LEU	3.8
1	A	361	ALA	3.7
1	B	289	TYR	3.7
1	D	329	LYS	3.7
1	A	362	VAL	3.6
1	C	362	VAL	3.6
1	A	232	SER	3.6
1	C	335	SER	3.6
1	D	235	SER	3.6
1	A	234	GLY	3.6
1	A	328	ASP	3.6
1	A	289	TYR	3.5
1	B	293	GLY	3.5
1	C	237	MET	3.4
1	B	369	LEU	3.4
1	C	357	ARG	3.4
1	B	329	LYS	3.4
1	B	233	ALA	3.4
1	B	232	SER	3.4
1	C	381	PHE	3.3
1	D	260	LEU	3.3
1	B	230	GLY	3.3
1	D	247	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	372	ARG	3.2
1	D	336	HIS	3.2
1	D	362	VAL	3.2
1	C	234	GLY	3.2
1	B	380	THR	3.2
1	D	335	SER	3.1
1	C	231	GLY	3.1
1	B	373	ALA	3.0
1	B	231	GLY	3.0
1	D	231	GLY	3.0
1	D	25	LEU	2.9
1	B	294	SER	2.9
1	C	289	TYR	2.9
1	C	232	SER	2.9
1	B	326	ILE	2.9
1	A	329	LYS	2.9
1	C	358	ALA	2.9
1	C	230	GLY	2.9
1	B	332	SER	2.8
1	C	326	ILE	2.8
1	B	424	SER	2.8
1	B	236	PRO	2.8
1	B	426	ASP	2.8
1	B	372	ARG	2.8
1	C	332	SER	2.8
1	C	426	ASP	2.8
1	C	262	LEU	2.7
1	B	295	ARG	2.7
1	C	359	ASN	2.6
1	C	233	ALA	2.6
1	C	353	TYR	2.6
1	D	236	PRO	2.6
1	C	354	GLY	2.6
1	D	328	ASP	2.6
1	A	359	ASN	2.6
1	C	361	ALA	2.6
1	A	44	GLY	2.6
1	B	381	PHE	2.6
1	C	356	LEU	2.6
1	C	369	LEU	2.5
1	D	332	SER	2.5
1	B	328	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	265	ARG	2.5
1	B	399	GLY	2.5
1	C	378	ASN	2.5
1	C	260	LEU	2.4
1	B	379	PHE	2.4
1	C	375	ASN	2.4
1	B	410	LYS	2.4
1	C	327	ASP	2.4
1	D	378	ASN	2.4
1	C	410	LYS	2.4
1	C	366	GLY	2.4
1	B	364	TYR	2.4
1	A	247	PHE	2.4
1	B	32	VAL	2.4
1	B	327	ASP	2.4
1	A	233	ALA	2.4
1	C	294	SER	2.3
1	A	426	ASP	2.3
1	A	378	ASN	2.3
1	B	358	ALA	2.3
1	C	236	PRO	2.3
1	D	234	GLY	2.3
1	D	162	PHE	2.3
1	A	259	PRO	2.3
1	B	357	ARG	2.3
1	A	326	ILE	2.3
1	D	204	ARG	2.3
1	B	402	LEU	2.3
1	D	326	ILE	2.3
1	B	287	SER	2.2
1	D	294	SER	2.2
1	D	410	LYS	2.2
1	C	380	THR	2.2
1	D	296	ILE	2.2
1	A	335	SER	2.2
1	C	337	SER	2.2
1	C	328	ASP	2.2
1	C	204	ARG	2.2
1	D	233	ALA	2.1
1	D	426	ASP	2.1
1	B	371	PHE	2.1
1	A	30	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	365	ALA	2.1
1	A	25	LEU	2.1
1	B	378	ASN	2.1
1	A	356	LEU	2.0
1	C	370	GLU	2.0
1	C	399	GLY	2.0
1	A	279	SER	2.0
1	C	374	ASN	2.0
1	A	332	SER	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	MG	B	503	1/1	0.25	0.21	113,113,113,113	0
4	MG	C	503	1/1	0.53	0.19	102,102,102,102	0
4	MG	D	503	1/1	0.73	0.17	108,108,108,108	0
5	GOL	B	505	6/6	0.79	0.19	89,89,89,89	0
4	MG	A	503	1/1	0.84	0.09	62,62,62,62	0
5	GOL	A	507	6/6	0.85	0.16	76,77,77,77	0
3	PRP	B	502	22/22	0.85	0.13	101,106,113,114	0
5	GOL	A	504	6/6	0.86	0.14	56,57,57,57	0
5	GOL	A	508	6/6	0.87	0.15	73,73,73,73	0
3	PRP	C	502	22/22	0.87	0.14	88,94,103,103	0
5	GOL	B	504	6/6	0.88	0.15	76,76,76,76	0
5	GOL	D	505	6/6	0.88	0.16	83,83,83,83	0
5	GOL	A	509	6/6	0.89	0.20	69,70,70,70	0
5	GOL	C	506	6/6	0.89	0.14	66,66,66,66	0

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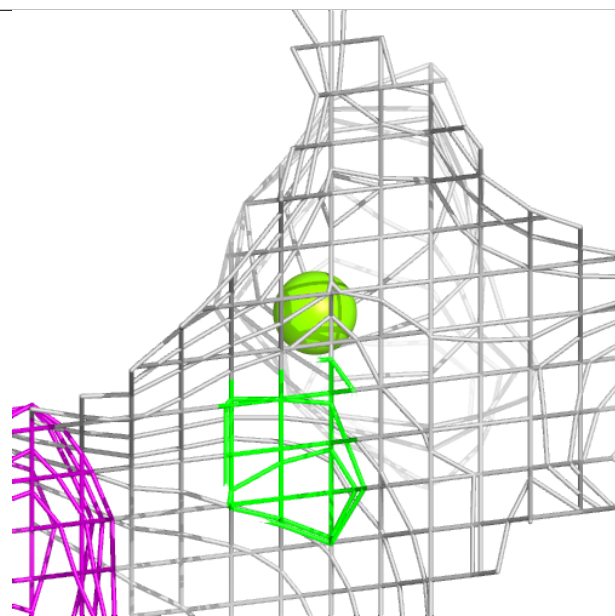
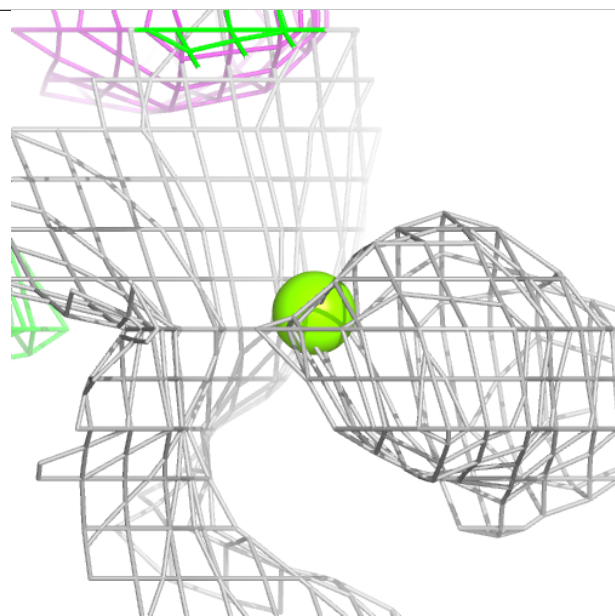
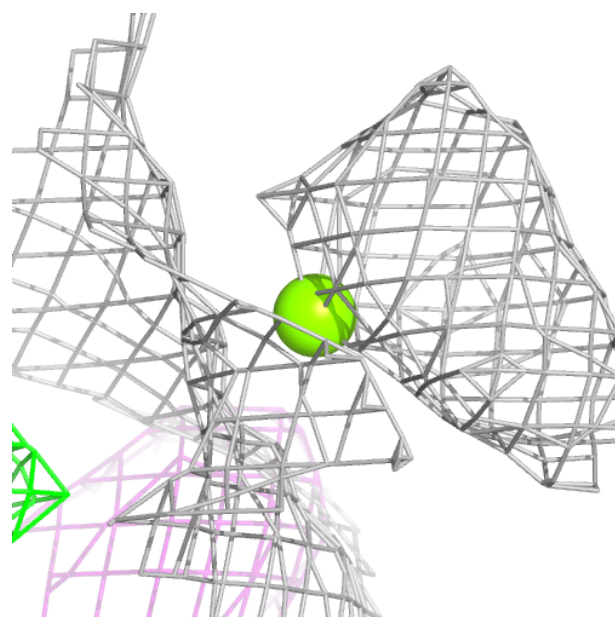
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PRP	D	502	22/22	0.89	0.12	93,97,104,104	0
3	PRP	A	502	22/22	0.90	0.12	59,67,82,82	0
5	GOL	D	504	6/6	0.91	0.12	70,70,70,70	0
5	GOL	C	507	6/6	0.91	0.13	77,77,77,77	0
5	GOL	C	504	6/6	0.92	0.14	52,52,52,52	0
5	GOL	A	506	6/6	0.93	0.12	47,47,48,48	0
5	GOL	C	505	6/6	0.93	0.12	58,58,58,58	0
5	GOL	A	505	6/6	0.94	0.14	47,47,48,49	0
4	MG	C	508	1/1	0.95	0.14	49,49,49,49	0
4	MG	D	506	1/1	0.95	0.12	41,41,41,41	0
4	MG	A	510	1/1	0.97	0.07	57,57,57,57	0
2	ZN	A	501	1/1	0.99	0.03	52,52,52,52	0
4	MG	B	506	1/1	0.99	0.03	41,41,41,41	0
2	ZN	D	501	1/1	1.00	0.04	59,59,59,59	0
2	ZN	B	501	1/1	1.00	0.05	66,66,66,66	0
2	ZN	C	501	1/1	1.00	0.04	54,54,54,54	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.

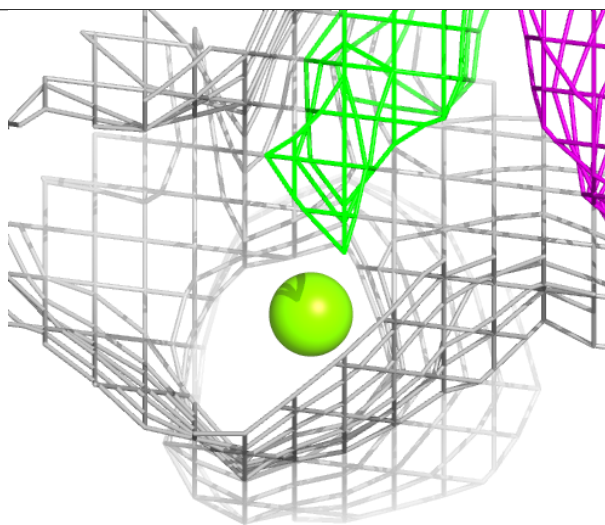
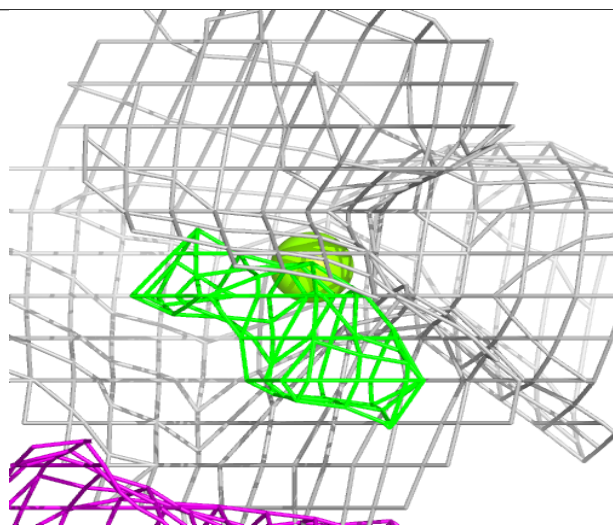
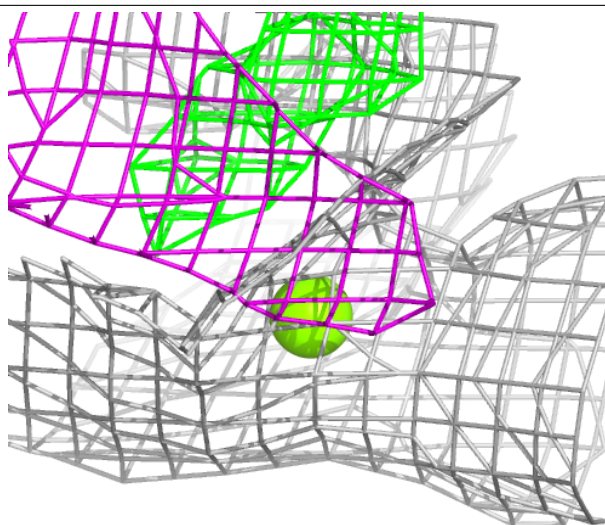
Electron density around MG B 503:

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



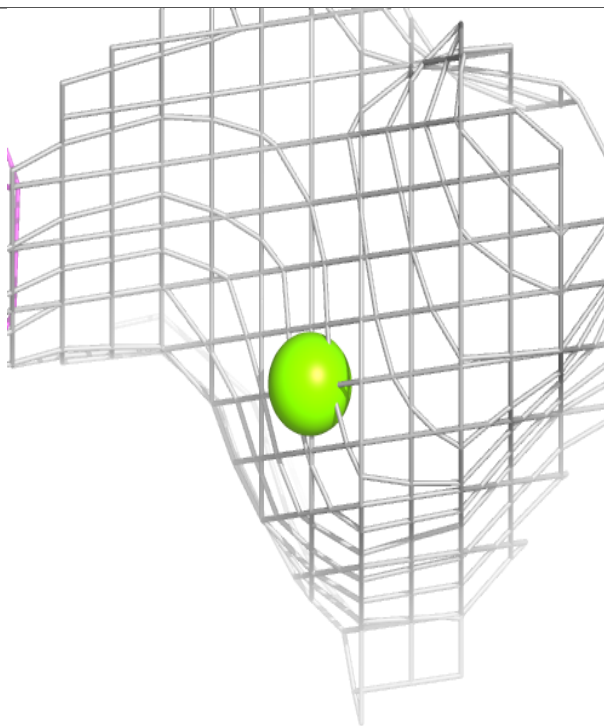
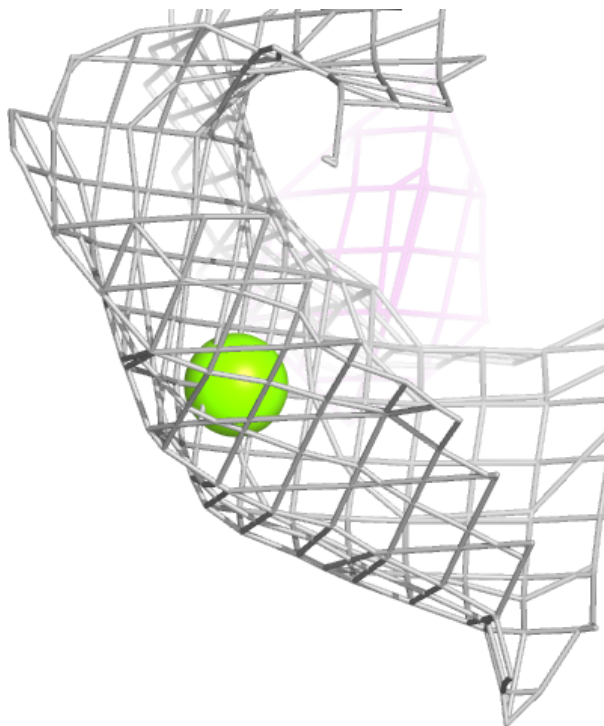
Electron density around MG C 503:

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



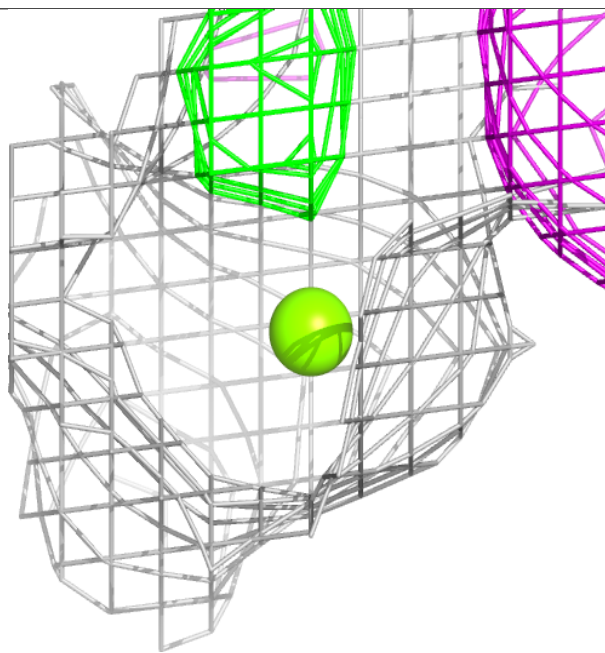
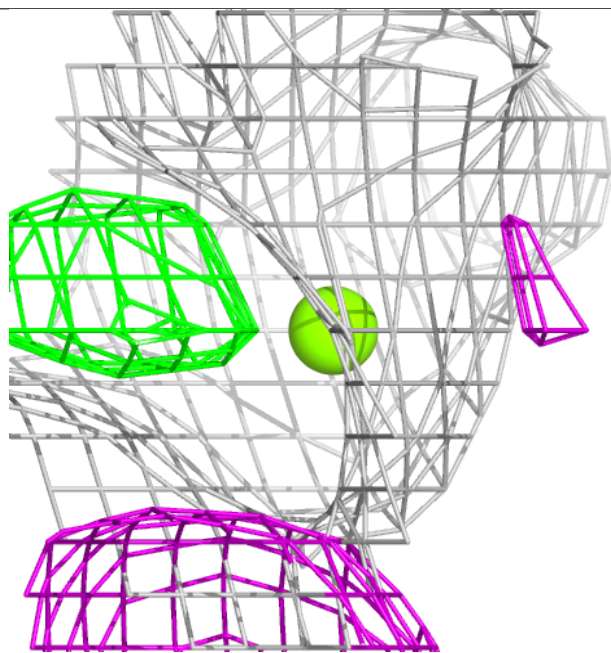
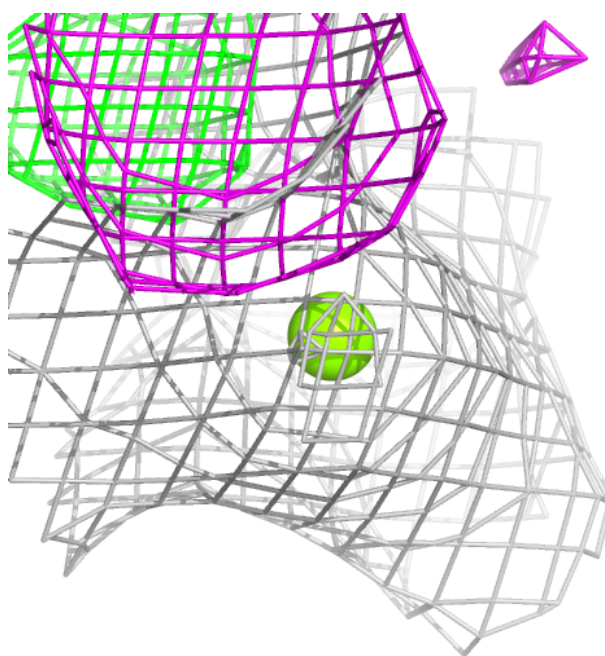
Electron density around MG D 503:

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



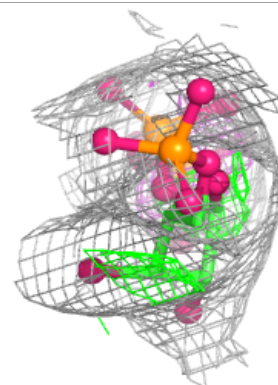
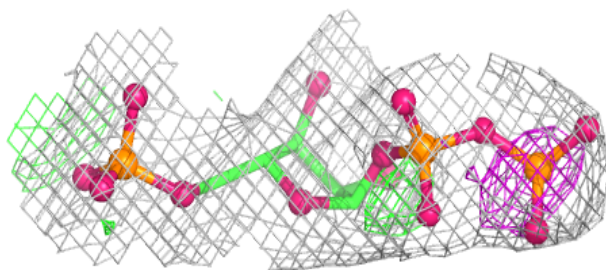
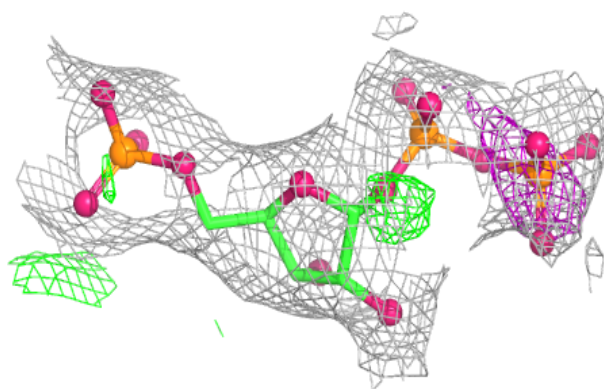
Electron density around MG A 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

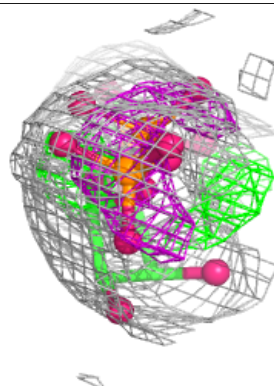
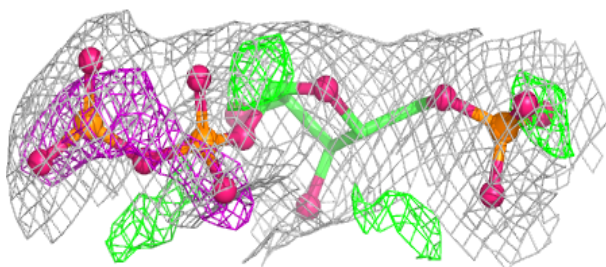
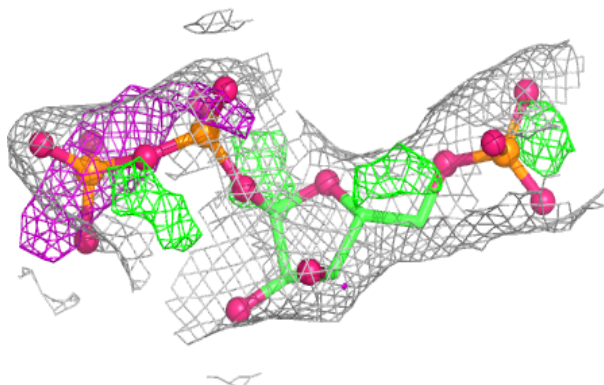


Electron density around PRP B 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

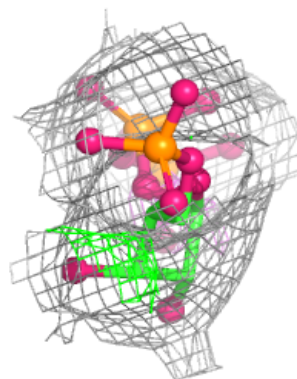
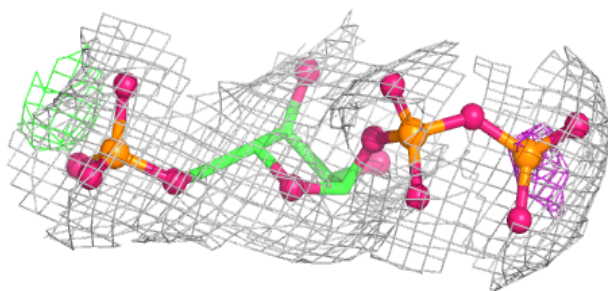
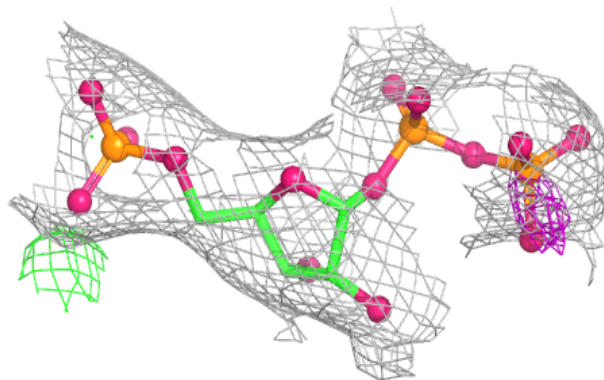
**Electron density around PRP C 502:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

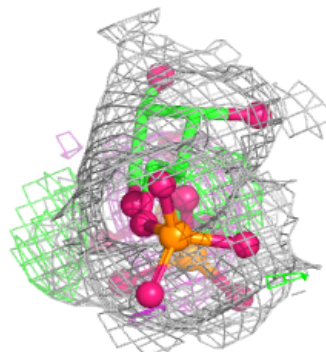
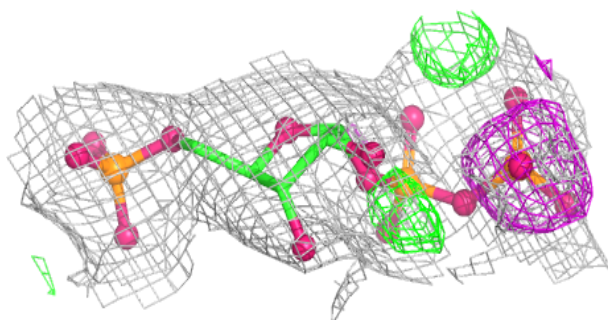
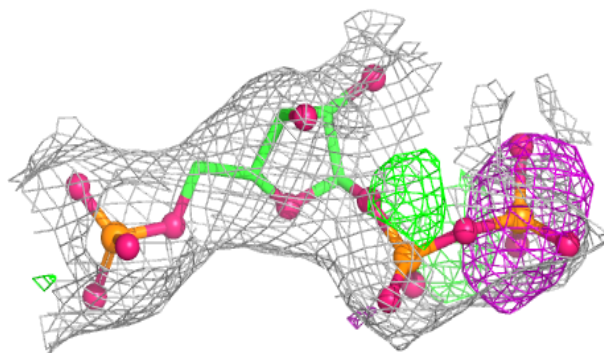


Electron density around PRP D 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

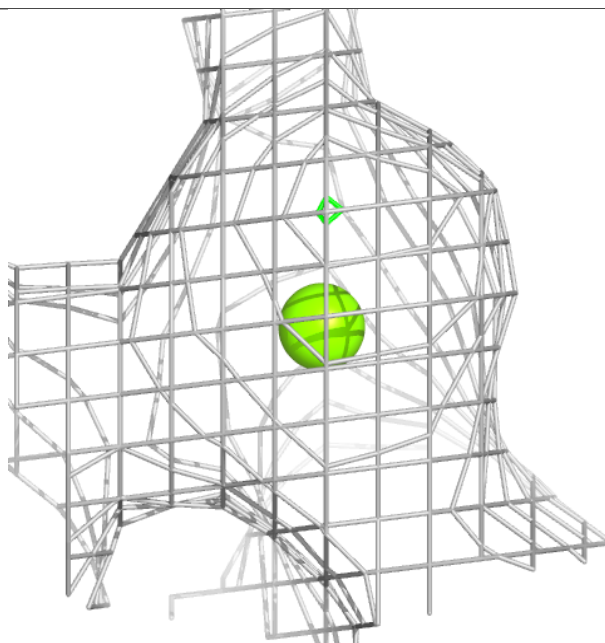
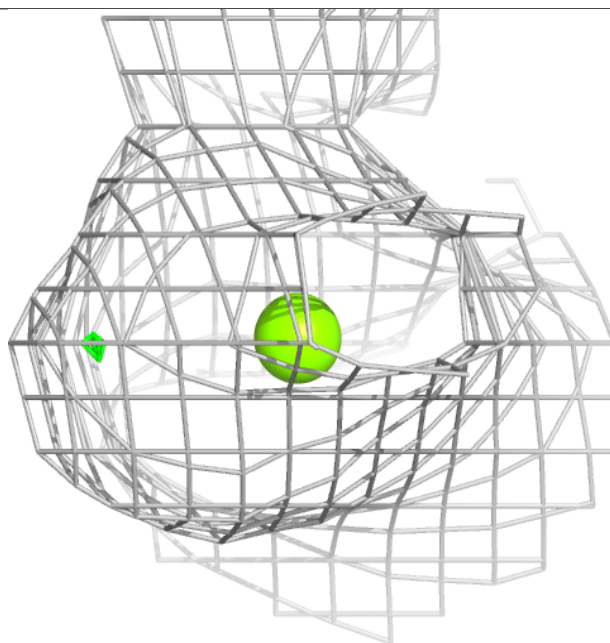
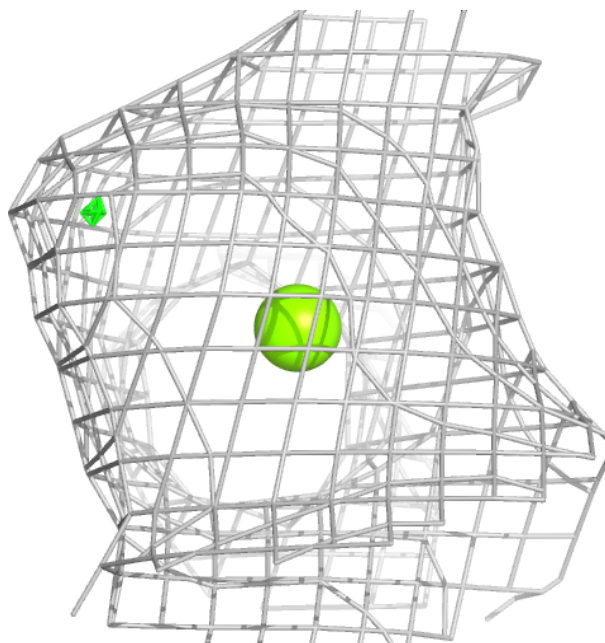
**Electron density around PRP A 502:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



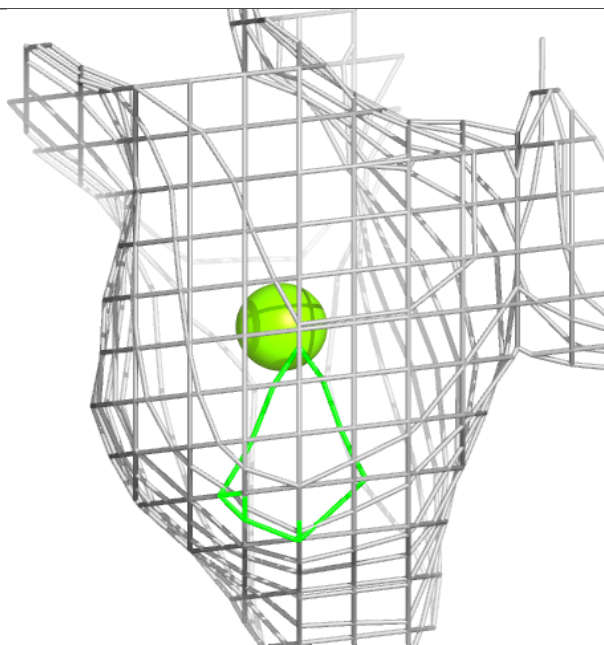
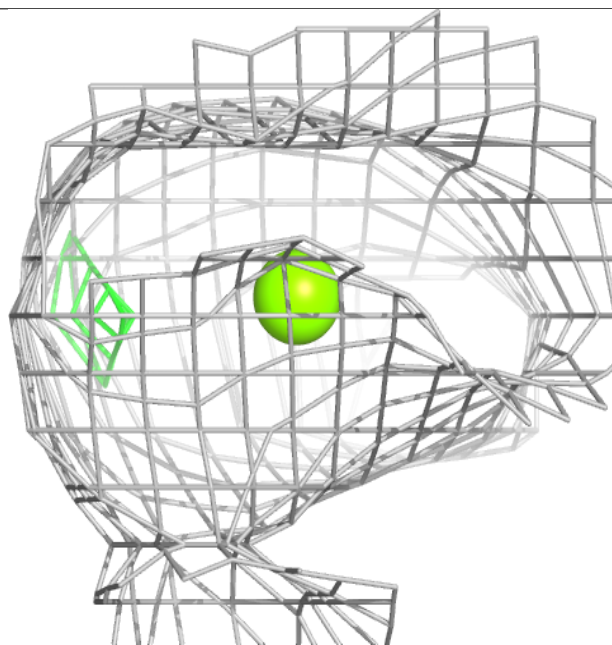
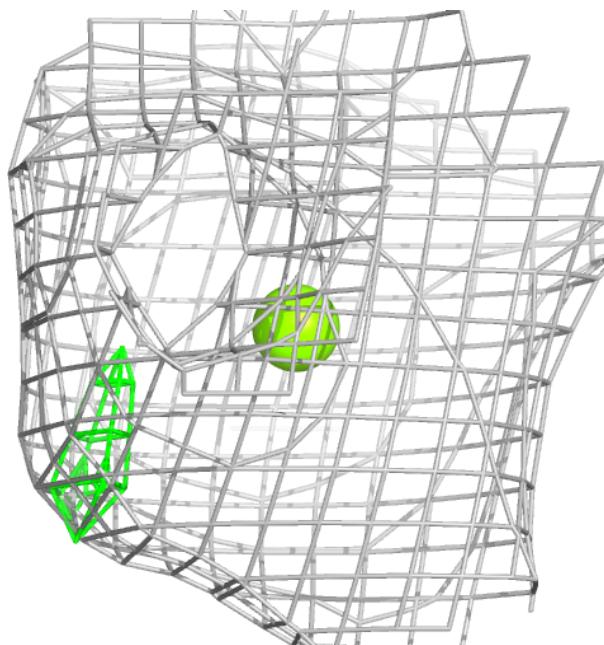
Electron density around MG C 508:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



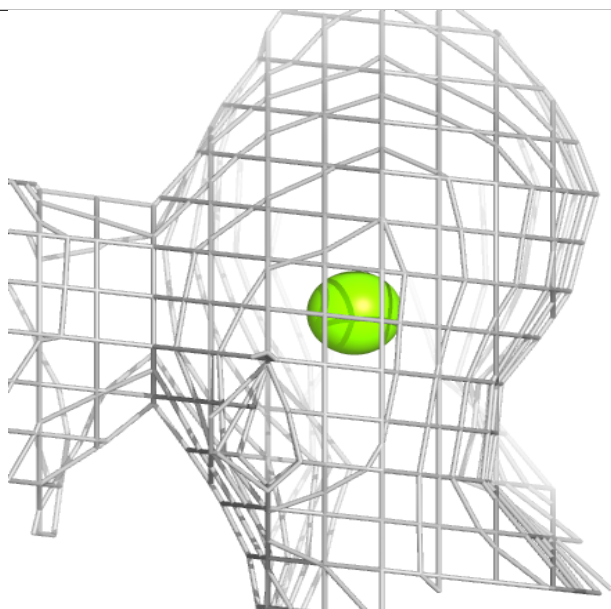
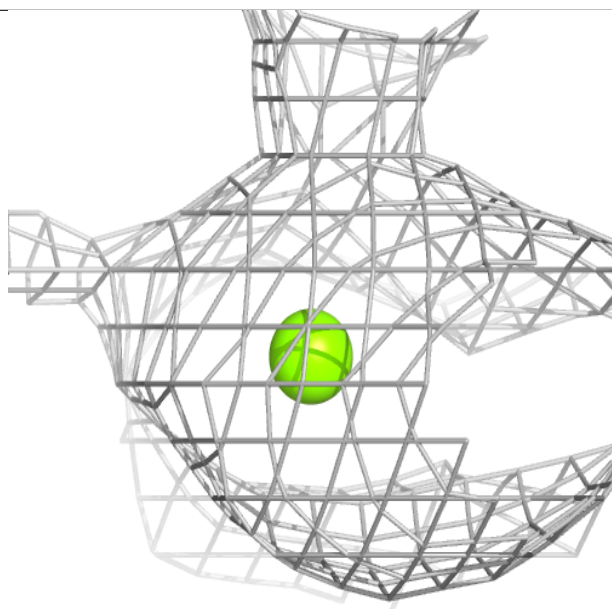
Electron density around MG D 506:

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and green (positive)



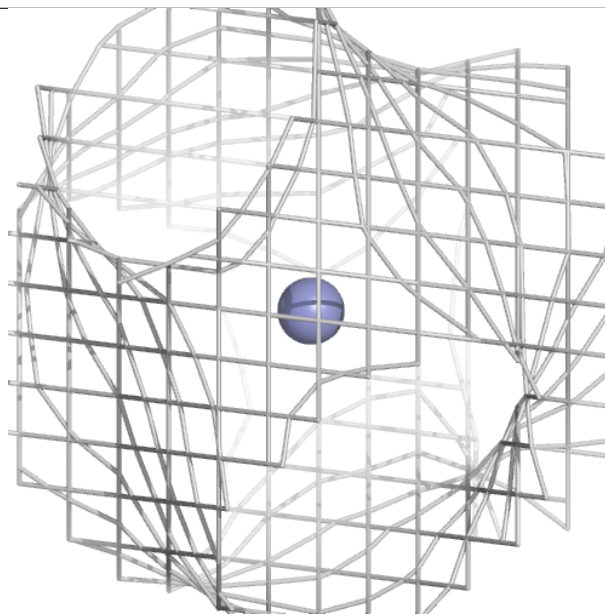
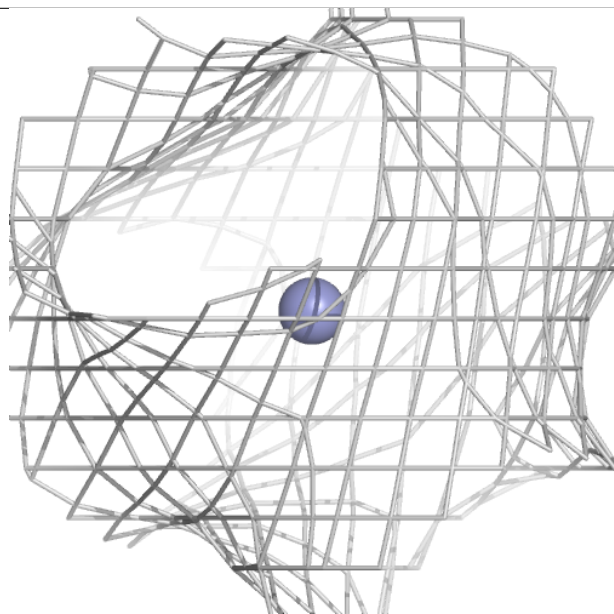
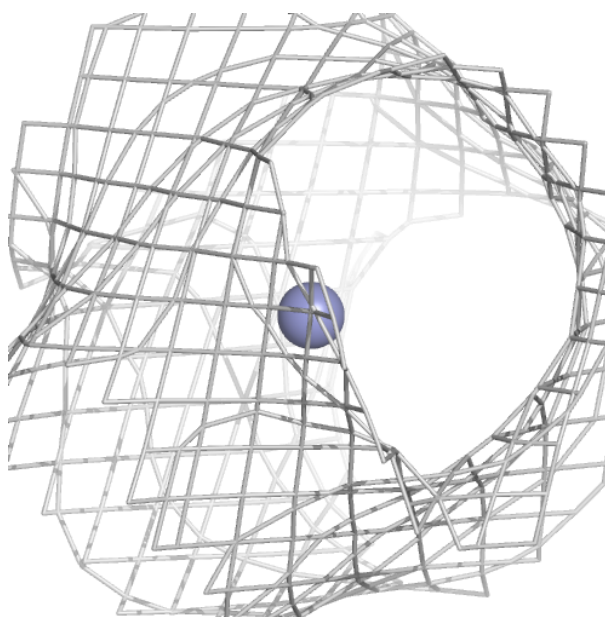
Electron density around MG A 510:

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and green (positive)



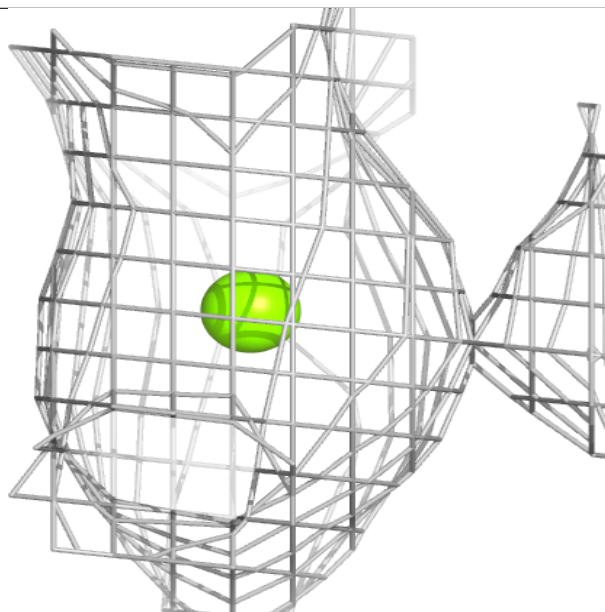
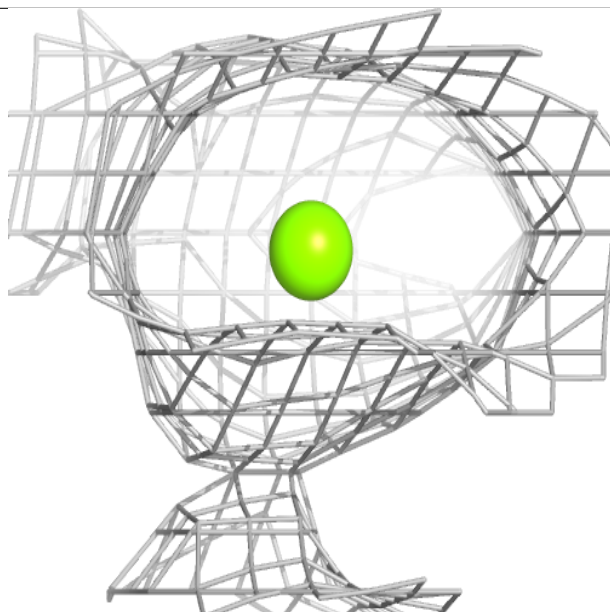
Electron density around ZN A 501:

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



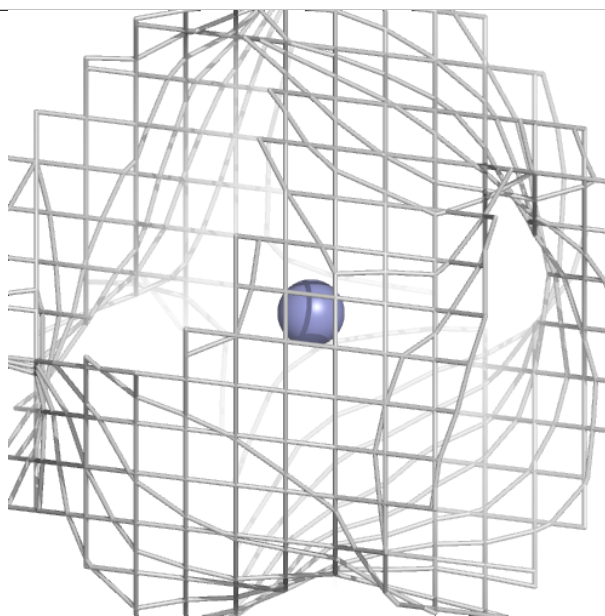
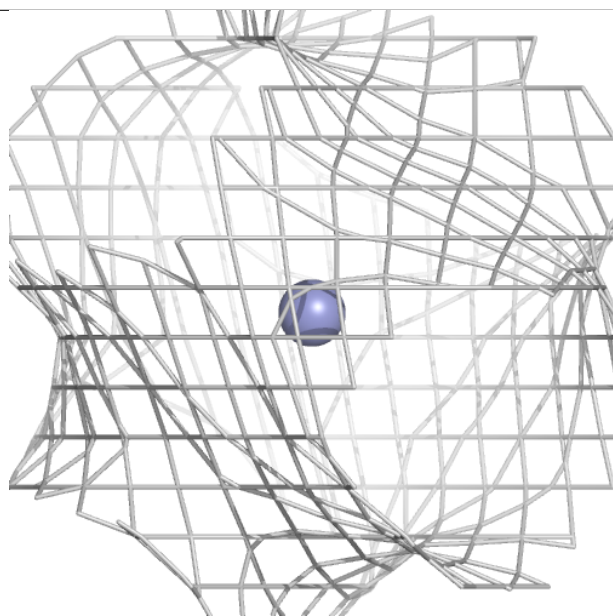
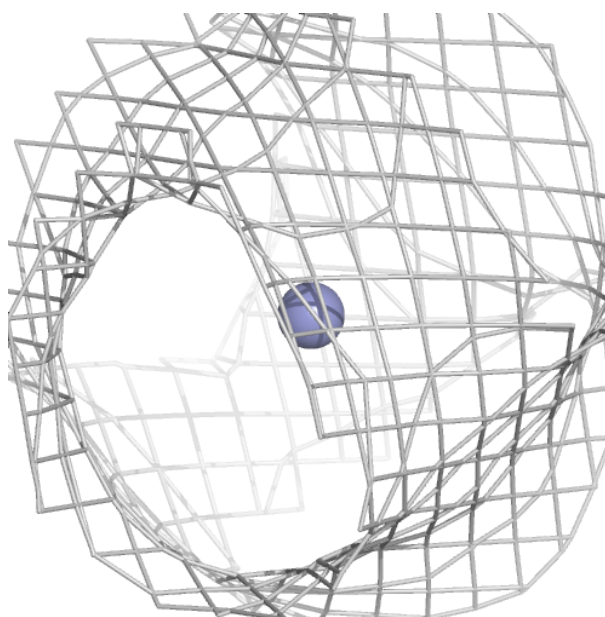
Electron density around MG B 506:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



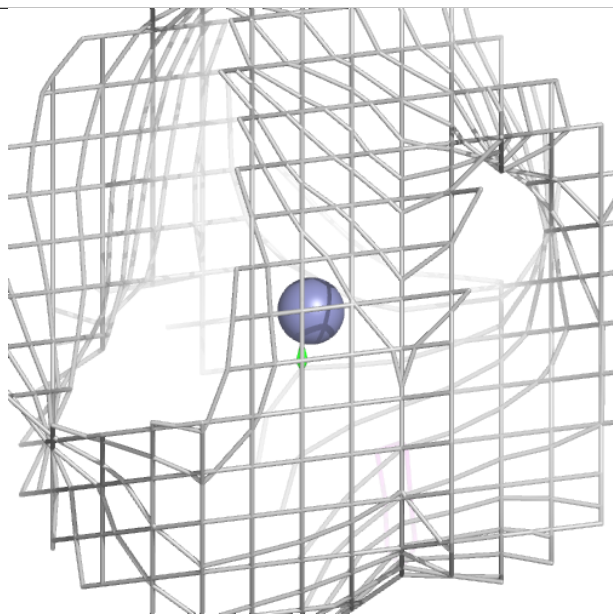
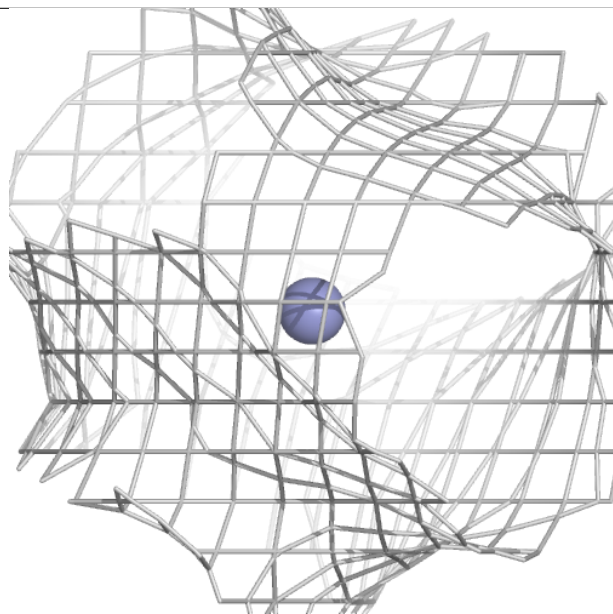
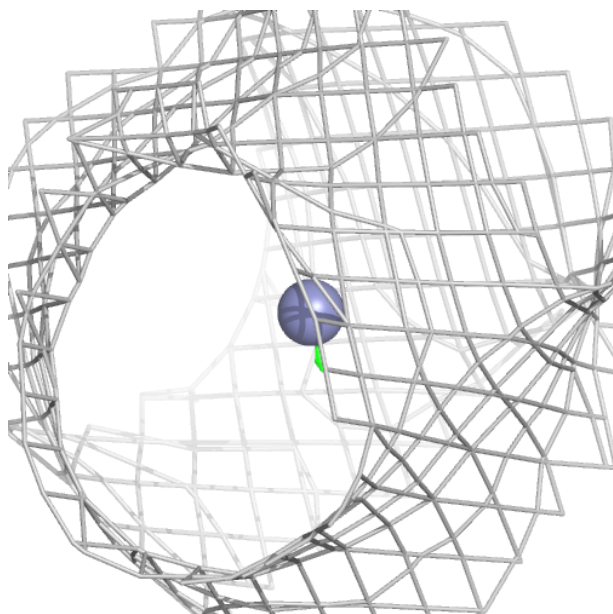
Electron density around ZN D 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



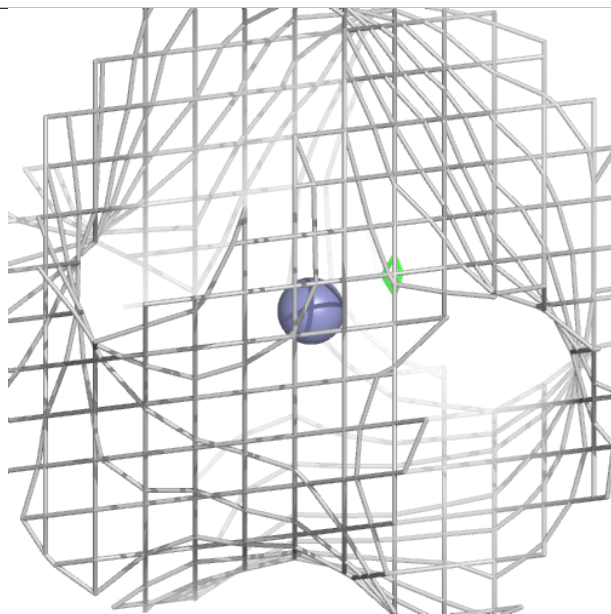
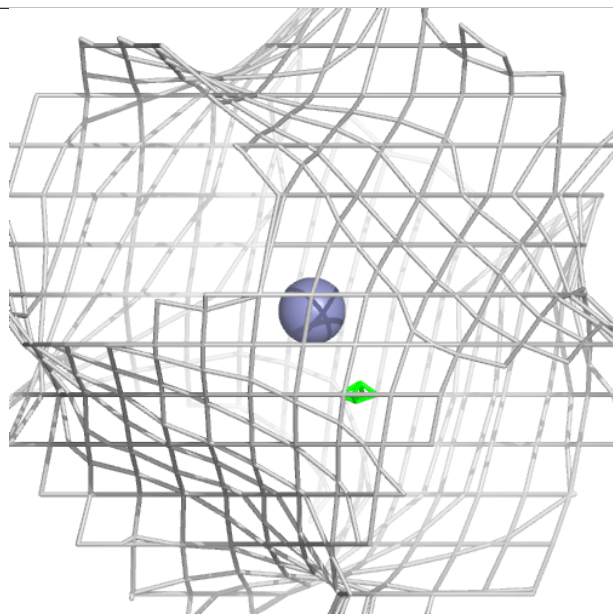
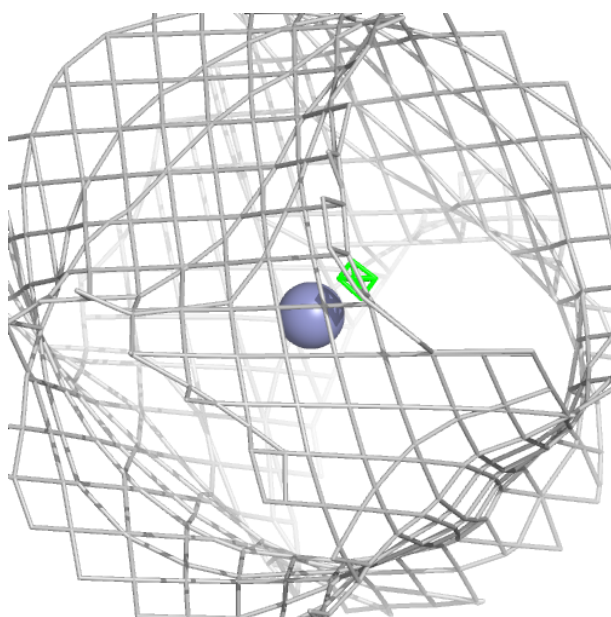
Electron density around ZN B 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.