Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2022 – 07:11 pm BST

PDB ID	:	7P0H
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 following versions of software and data (see references ⓘ) were used in the production of this report:

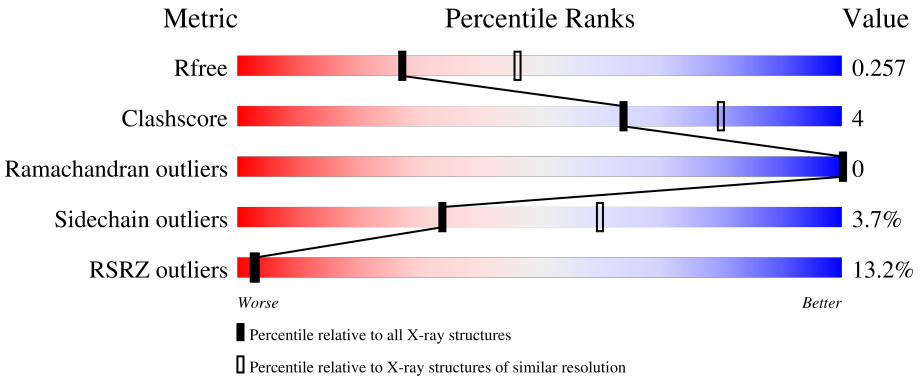
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	9% 81% 15%
1	B	427	17% 85% 11%
1	C	427	11% 84% 12%
1	D	427	13% 85% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	B	503	-	-	-	X
4	MG	D	503	-	-	-	X

2 Entry composition (i)

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.

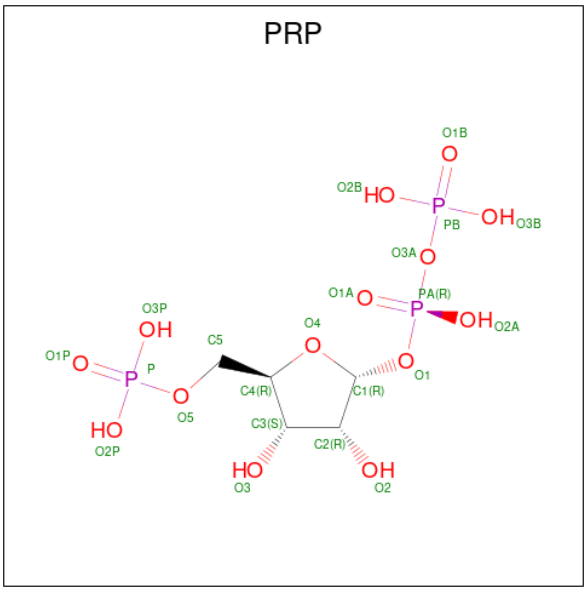
- Molecule 1 is a protein called Helicobacter pylori ComF fused to an artificial alphaREP crystallization helper (named B2).

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 (three-letter code: 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 (three-letter code: PRP) (formula: $C_5H_{13}O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

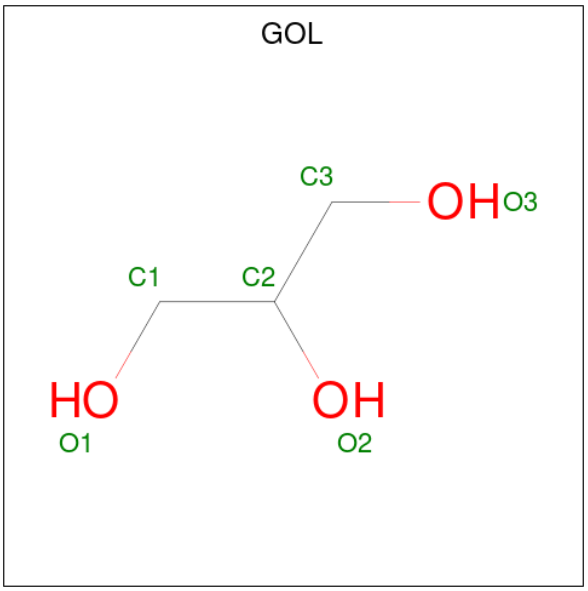


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 22 5 14 3	0	0
3	B	1	Total C O P 22 5 14 3	0	0
3	C	1	Total C O P 22 5 14 3	0	0
3	D	1	Total C O P 22 5 14 3	0	0

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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	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	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.

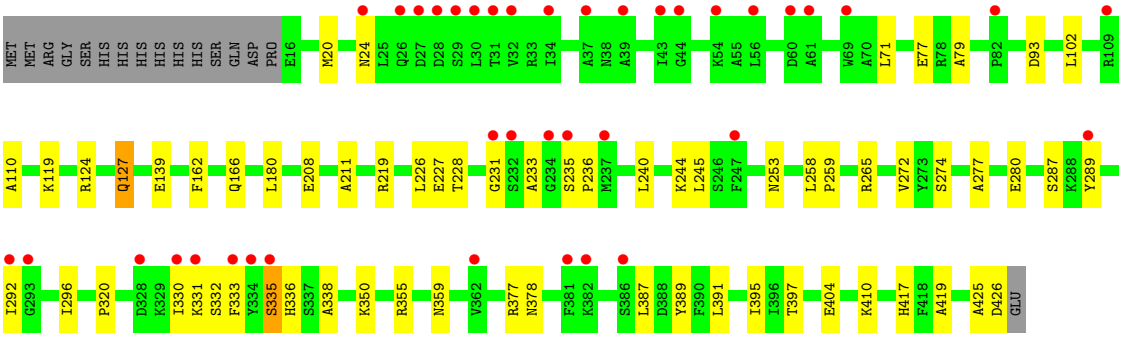
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	95	Total O 95 95	0	0
6	B	40	Total O 40 40	0	0
6	C	83	Total O 83 83	0	0
6	D	64	Total O 64 64	0	0

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.

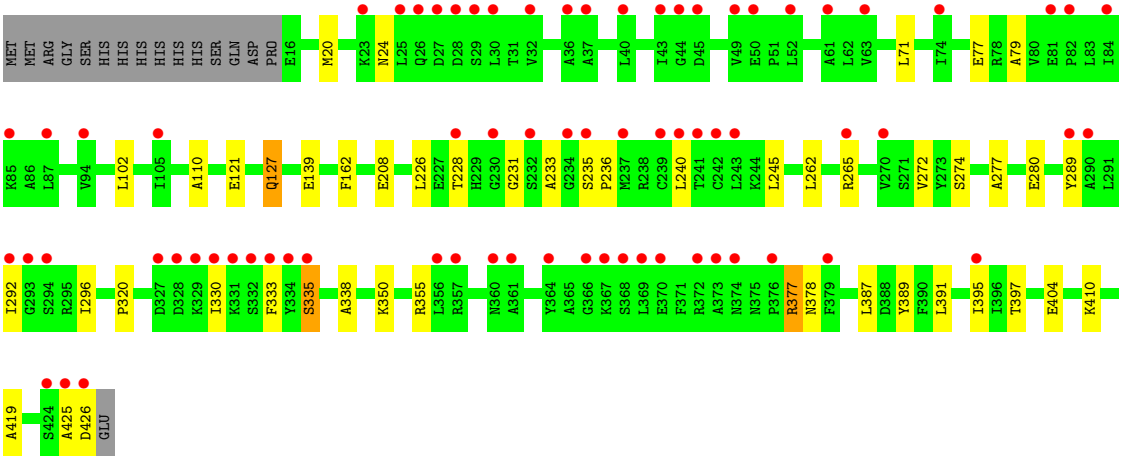
• Molecule 1: Helicobacter pylori ComF fused to an artificial alphaREP crystallization helper (named B2)

Chain A:



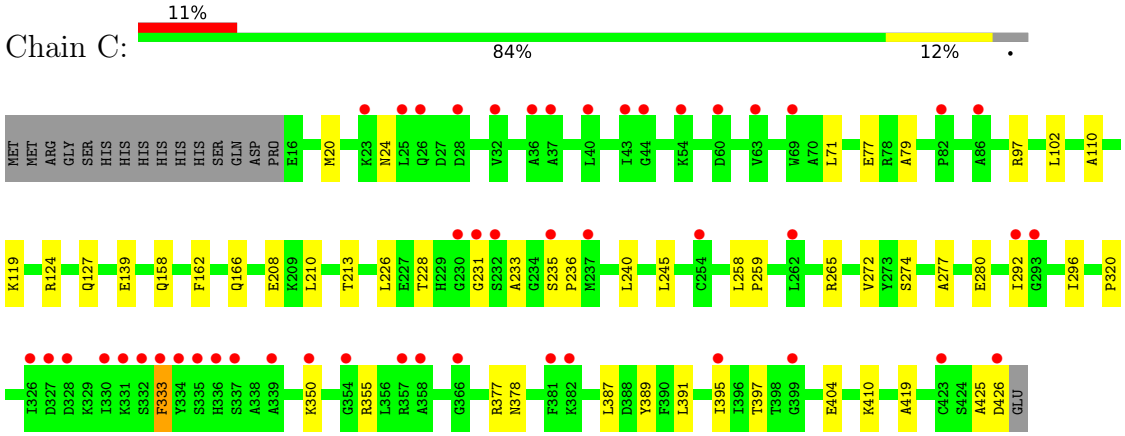
• Molecule 1: Helicobacter pylori ComF fused to an artificial alphaREP crystallization helper (named B2)

Chain B:



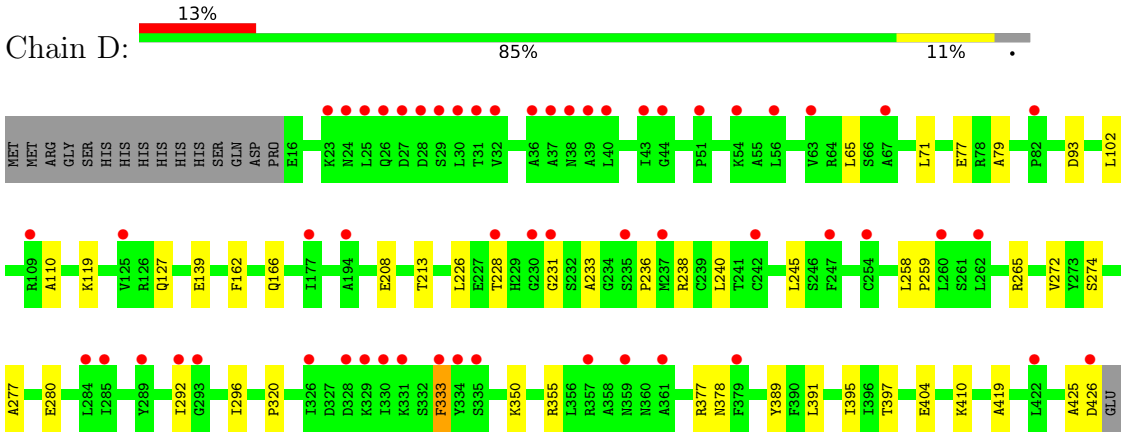
• Molecule 1: Helicobacter pylori ComF fused to an artificial alphaREP crystallization helper (named B2)

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.00%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	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.*

[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: MG, PRP, GOL, ZN

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	0.34	0/3212	0.53	0/4328
1	B	0.33	0/3212	0.52	0/4328
1	C	0.34	0/3212	0.53	0/4328
1	D	0.34	0/3212	0.53	0/4328
All	All	0.33	0/12848	0.53	0/17312

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	3168	0	3251	41	0
1	B	3168	0	3251	29	0
1	C	3168	0	3251	30	0
1	D	3168	0	3251	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	22	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	8	2	0
3	C	22	0	8	1	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	109	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 (109) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:320:PRO:HB3	1:B:350:LYS:HZ2	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:235:SER:OG	1:C:166:GLN:NE2	2.46	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:289:TYR:OH	3:A:502:PRP:O1B	2.29	0.45
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: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
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:B:320:PRO:HB3	1:B:350:LYS:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:377:ARG:H	1:B:377:ARG:HG2	1.75	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	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 (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	329/342 (96%)	317 (96%)	12 (4%)	35	61
1	B	329/342 (96%)	315 (96%)	14 (4%)	29	53
1	C	329/342 (96%)	317 (96%)	12 (4%)	35	61
1	D	329/342 (96%)	318 (97%)	11 (3%)	38	64
All	All	1316/1368 (96%)	1267 (96%)	49 (4%)	34	60

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	119	LYS
1	A	127	GLN
1	A	139	GLU
1	A	228	THR
1	A	333	PHE
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	121	GLU
1	B	127	GLN
1	B	139	GLU
1	B	228	THR
1	B	262	LEU
1	B	333	PHE
1	B	335	SER
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	119	LYS
1	C	127	GLN
1	C	139	GLU
1	C	228	THR
1	C	333	PHE
1	C	377	ARG

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Mol	Chain	Res	Type
1	C	378	ASN
1	C	387	LEU
1	C	391	LEU
1	C	404	GLU
1	C	410	LYS
1	D	77	GLU
1	D	119	LYS
1	D	127	GLN
1	D	139	GLU
1	D	228	THR
1	D	333	PHE
1	D	377	ARG
1	D	378	ASN
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	336	HIS
1	A	378	ASN
1	B	127	GLN
1	C	38	ASN
1	C	127	GLN
1	C	158	GLN
1	C	166	GLN
1	D	127	GLN

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 (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
3	PRP	A	502	4	19,22,22	0.74	0	33,35,35	1.01	3 (9%)
5	GOL	A	508	-	5,5,5	0.09	0	5,5,5	0.34	0
5	GOL	C	506	-	5,5,5	0.12	0	5,5,5	0.36	0
5	GOL	C	505	-	5,5,5	0.10	0	5,5,5	0.31	0
3	PRP	C	502	4	19,22,22	0.68	0	33,35,35	0.95	2 (6%)
5	GOL	A	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	A	506	-	5,5,5	0.10	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	C	507	-	5,5,5	0.05	0	5,5,5	0.31	0
5	GOL	A	509	-	5,5,5	0.09	0	5,5,5	0.36	0
3	PRP	B	502	4	19,22,22	0.70	0	33,35,35	0.91	1 (3%)
5	GOL	B	505	-	5,5,5	0.09	0	5,5,5	0.34	0
3	PRP	D	502	4	19,22,22	0.65	0	33,35,35	0.95	2 (6%)
5	GOL	D	504	-	5,5,5	0.07	0	5,5,5	0.23	0
5	GOL	A	505	-	5,5,5	0.11	0	5,5,5	0.29	0
5	GOL	A	504	-	5,5,5	0.14	0	5,5,5	0.24	0
5	GOL	D	505	-	5,5,5	0.05	0	5,5,5	0.33	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
3	PRP	A	502	4	-	8/16/33/33	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	508	-	-	0/4/4/4	-
5	GOL	C	506	-	-	1/4/4/4	-
5	GOL	C	505	-	-	0/4/4/4	-
3	PRP	C	502	4	-	8/16/33/33	0/1/1/1
5	GOL	A	507	-	-	0/4/4/4	-
5	GOL	C	504	-	-	0/4/4/4	-
5	GOL	A	506	-	-	0/4/4/4	-
5	GOL	B	504	-	-	0/4/4/4	-
5	GOL	C	507	-	-	1/4/4/4	-
5	GOL	A	509	-	-	0/4/4/4	-
3	PRP	B	502	4	-	2/16/33/33	0/1/1/1
5	GOL	B	505	-	-	1/4/4/4	-
3	PRP	D	502	4	-	3/16/33/33	0/1/1/1
5	GOL	D	504	-	-	0/4/4/4	-
5	GOL	A	505	-	-	0/4/4/4	-
5	GOL	A	504	-	-	0/4/4/4	-
5	GOL	D	505	-	-	2/4/4/4	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	PRP	PA-O1-C1	2.82	130.65	119.74
3	B	502	PRP	PA-O1-C1	2.75	130.38	119.74
3	D	502	PRP	PA-O1-C1	2.73	130.30	119.74
3	A	502	PRP	PA-O1-C1	2.71	130.23	119.74
3	A	502	PRP	O3B-PB-O3A	2.27	112.23	104.64
3	D	502	PRP	O1-C1-C2	2.26	110.54	106.72
3	C	502	PRP	O3B-PB-O3A	2.25	112.18	104.64
3	A	502	PRP	O1-C1-C2	2.18	110.41	106.72

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	PRP	C1-O1-PA-O2A
3	A	502	PRP	PA-O3A-PB-O2B
3	A	502	PRP	PA-O3A-PB-O3B
3	B	502	PRP	PA-O3A-PB-O2B
3	C	502	PRP	C1-O1-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	C	502	PRP	PA-O3A-PB-O2B
3	C	502	PRP	PA-O3A-PB-O3B
3	D	502	PRP	PA-O3A-PB-O2B
3	A	502	PRP	C1-O1-PA-O3A
3	C	502	PRP	C1-O1-PA-O3A
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	B	502	PRP	C1-O1-PA-O3A
3	D	502	PRP	C1-O1-PA-O3A
3	A	502	PRP	PB-O3A-PA-O1A
3	C	502	PRP	PB-O3A-PA-O1A
3	A	502	PRP	C1-O1-PA-O1A
3	C	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
3	A	502	PRP	PB-O3A-PA-O2A
3	C	502	PRP	PB-O3A-PA-O2A
5	B	505	GOL	O2-C2-C3-O3

There are no ring outliers.

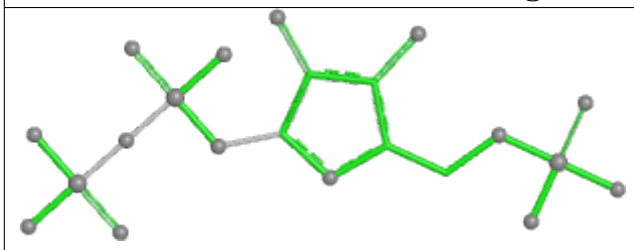
9 monomers are involved in 12 short contacts:

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

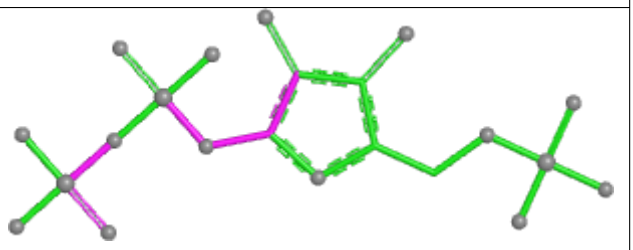
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

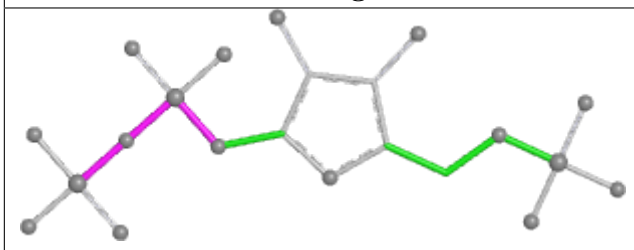
Ligand PRP A 502



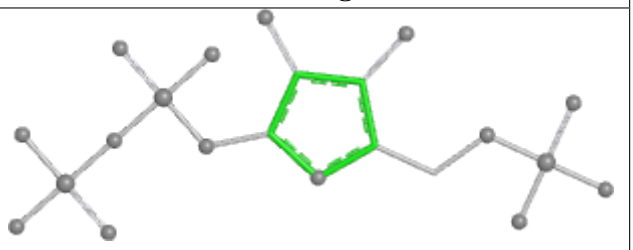
Bond lengths



Bond angles

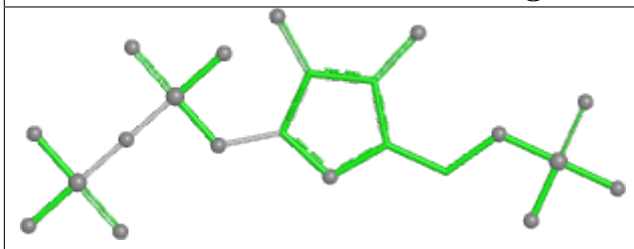


Torsions

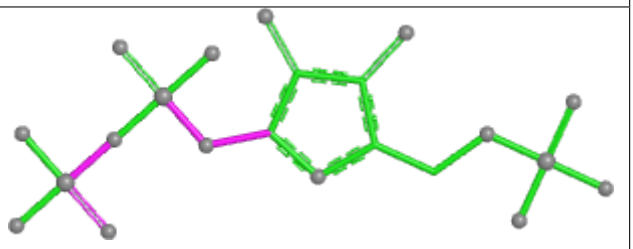


Rings

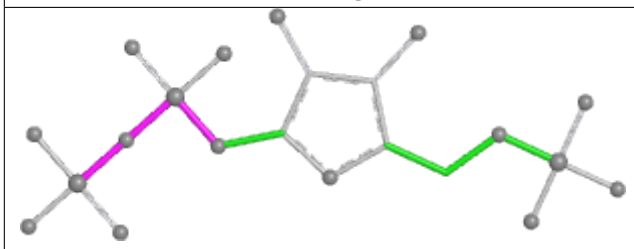
Ligand PRP C 502



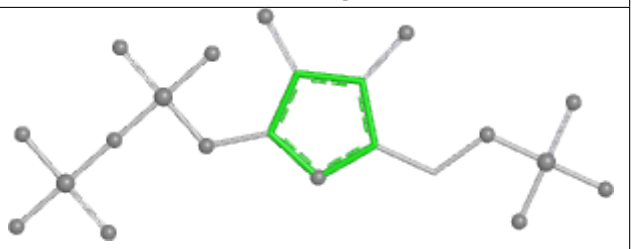
Bond lengths



Bond angles

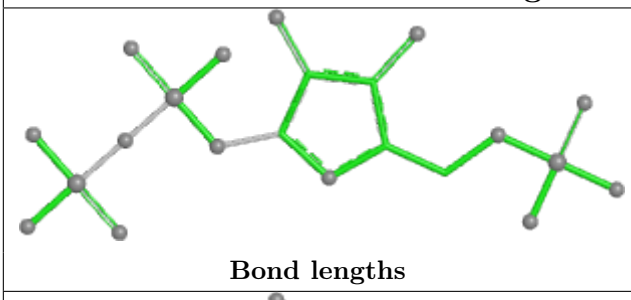


Torsions

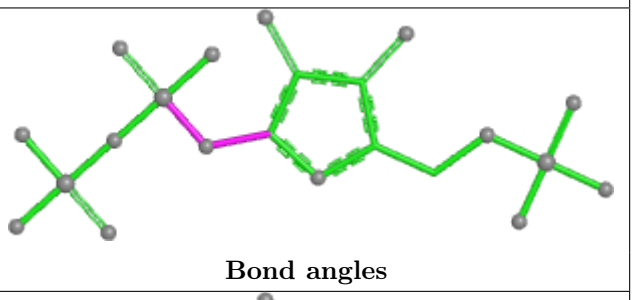


Rings

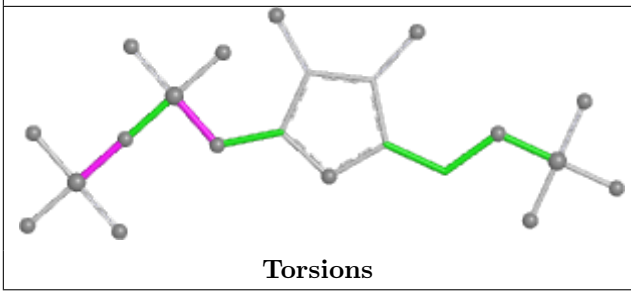
Ligand PRP B 502



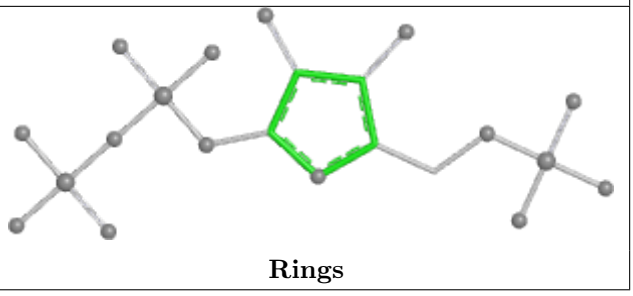
Bond lengths



Bond angles

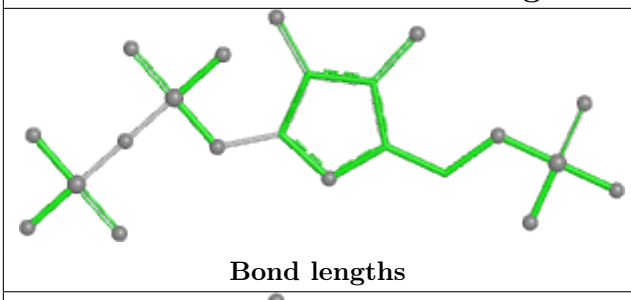


Torsions

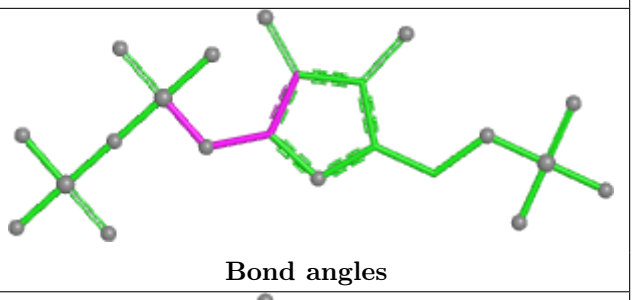


Rings

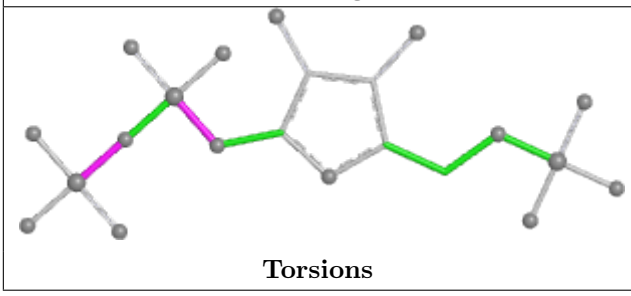
Ligand PRP D 502



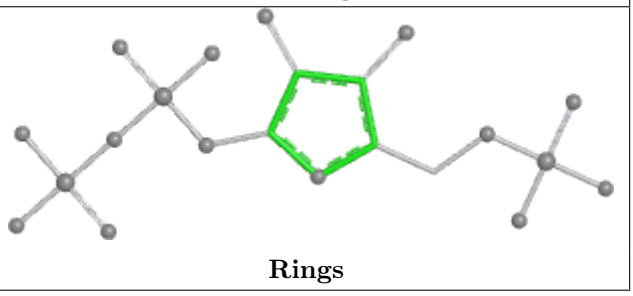
Bond lengths



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, 95^{th} 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%)	0.95	39 (9%) 8 8	39, 62, 89, 104	0
1	B	409/427 (95%)	1.21	73 (17%) 1 1	49, 71, 116, 135	0
1	C	409/427 (95%)	1.07	48 (11%) 4 4	42, 64, 99, 117	0
1	D	409/427 (95%)	1.12	56 (13%) 3 2	42, 68, 107, 121	0
All	All	1636/1708 (95%)	1.09	216 (13%) 3 3	39, 67, 103, 135	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	PHE	11.0
1	B	330	ILE	10.6
1	C	334	TYR	9.2
1	D	330	ILE	8.7
1	B	235	SER	8.6
1	B	373	ALA	7.7
1	D	30	LEU	7.5
1	A	333	PHE	7.5
1	A	235	SER	7.4
1	C	330	ILE	7.2
1	C	332	SER	7.1
1	C	235	SER	7.0
1	D	333	PHE	6.7
1	D	334	TYR	6.5
1	D	335	SER	6.3
1	D	361	ALA	6.0
1	C	335	SER	5.9
1	A	334	TYR	5.8
1	A	330	ILE	5.7
1	D	25	LEU	5.7
1	B	292	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	237	MET	5.6
1	A	293	GLY	5.6
1	B	369	LEU	5.5
1	B	43	ILE	5.5
1	B	366	GLY	5.5
1	B	331	LYS	5.4
1	D	235	SER	5.3
1	D	293	GLY	5.2
1	B	28	ASP	5.1
1	D	26	GLN	5.1
1	C	381	PHE	5.0
1	A	237	MET	4.8
1	B	335	SER	4.8
1	B	334	TYR	4.8
1	B	333	PHE	4.8
1	A	30	LEU	4.7
1	C	44	GLY	4.6
1	C	32	VAL	4.6
1	B	370	GLU	4.5
1	C	357	ARG	4.4
1	B	40	LEU	4.4
1	B	82	PRO	4.4
1	B	37	ALA	4.4
1	A	43	ILE	4.3
1	D	237	MET	4.3
1	D	292	ILE	4.3
1	A	335	SER	4.2
1	B	367	LYS	4.1
1	C	331	LYS	4.0
1	C	293	GLY	4.0
1	A	232	SER	3.9
1	B	426	ASP	3.9
1	D	247	PHE	3.9
1	A	292	ILE	3.9
1	B	26	GLN	3.9
1	D	289	TYR	3.8
1	D	331	LYS	3.8
1	D	82	PRO	3.7
1	B	52	LEU	3.7
1	C	292	ILE	3.7
1	A	61	ALA	3.6
1	C	25	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	31	THR	3.5
1	D	37	ALA	3.5
1	B	328	ASP	3.4
1	A	34	ILE	3.4
1	A	289	TYR	3.4
1	B	372	ARG	3.4
1	D	328	ASP	3.4
1	C	336	HIS	3.4
1	D	56	LEU	3.4
1	B	32	VAL	3.3
1	A	328	ASP	3.3
1	C	237	MET	3.3
1	D	29	SER	3.3
1	B	36	ALA	3.3
1	B	361	ALA	3.3
1	D	27	ASP	3.3
1	A	37	ALA	3.2
1	B	265	ARG	3.2
1	D	28	ASP	3.1
1	B	27	ASP	3.1
1	C	426	ASP	3.1
1	D	44	GLY	3.1
1	D	230	GLY	3.0
1	C	28	ASP	3.0
1	D	23	LYS	3.0
1	A	362	VAL	3.0
1	A	26	GLN	3.0
1	B	50	GLU	2.9
1	B	357	ARG	2.9
1	B	289	TYR	2.9
1	B	368	SER	2.9
1	A	32	VAL	2.9
1	B	332	SER	2.9
1	A	31	THR	2.8
1	C	43	ILE	2.8
1	A	231	GLY	2.8
1	B	230	GLY	2.8
1	A	56	LEU	2.8
1	A	27	ASP	2.8
1	B	327	ASP	2.8
1	B	85	LYS	2.7
1	A	109	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	328	ASP	2.7
1	C	423	CYS	2.7
1	C	358	ALA	2.7
1	A	28	ASP	2.7
1	D	39	ALA	2.7
1	C	23	LYS	2.6
1	D	54	LYS	2.6
1	A	69	TRP	2.6
1	B	23	LYS	2.6
1	C	36	ALA	2.6
1	B	294	SER	2.6
1	D	426	ASP	2.6
1	B	87	LEU	2.6
1	D	260	LEU	2.6
1	B	105	ILE	2.6
1	A	29	SER	2.6
1	C	337	SER	2.6
1	C	63	VAL	2.6
1	C	231	GLY	2.6
1	D	32	VAL	2.5
1	B	29	SER	2.5
1	D	125	VAL	2.5
1	B	374	ASN	2.5
1	B	234	GLY	2.5
1	C	86	ALA	2.5
1	C	339	ALA	2.5
1	A	24	ASN	2.5
1	D	38	ASN	2.5
1	B	364	TYR	2.5
1	D	40	LEU	2.5
1	C	232	SER	2.5
1	B	44	GLY	2.4
1	B	25	LEU	2.4
1	B	293	GLY	2.4
1	C	26	GLN	2.4
1	B	241	THR	2.4
1	D	43	ILE	2.4
1	A	82	PRO	2.4
1	A	331	LYS	2.4
1	B	63	VAL	2.4
1	D	359	ASN	2.4
1	A	234	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	60	ASP	2.3
1	D	67	ALA	2.3
1	B	30	LEU	2.3
1	C	69	TRP	2.3
1	B	94	VAL	2.3
1	C	60	ASP	2.3
1	D	51	PRO	2.3
1	D	254	CYS	2.3
1	D	379	PHE	2.3
1	D	357	ARG	2.3
1	C	54	LYS	2.3
1	C	230	GLY	2.3
1	C	354	GLY	2.3
1	C	399	GLY	2.2
1	B	232	SER	2.2
1	A	382	LYS	2.2
1	B	376	PRO	2.2
1	C	382	LYS	2.2
1	D	36	ALA	2.2
1	D	177	ILE	2.2
1	C	82	PRO	2.2
1	B	49	VAL	2.2
1	B	239	CYS	2.2
1	D	285	ILE	2.2
1	B	424	SER	2.2
1	C	254	CYS	2.2
1	D	262	LEU	2.2
1	A	386	SER	2.2
1	B	74	ILE	2.2
1	C	395	ILE	2.2
1	B	84	ILE	2.2
1	C	366	GLY	2.2
1	D	242	CYS	2.2
1	D	329	LYS	2.1
1	D	63	VAL	2.1
1	D	194	ALA	2.1
1	C	262	LEU	2.1
1	A	54	LYS	2.1
1	B	270	VAL	2.1
1	C	37	ALA	2.1
1	D	422	LEU	2.1
1	D	24	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	242	CYS	2.1
1	C	40	LEU	2.1
1	D	284	LEU	2.1
1	B	290	ALA	2.1
1	D	228	THR	2.1
1	A	381	PHE	2.1
1	B	243	LEU	2.1
1	B	61	ALA	2.1
1	D	109	ARG	2.1
1	B	360	ASN	2.1
1	B	45	ASP	2.1
1	D	231	GLY	2.1
1	B	356	LEU	2.0
1	A	44	GLY	2.0
1	C	327	ASP	2.0
1	A	39	ALA	2.0
1	B	81	GLU	2.0
1	B	228	THR	2.0
1	C	350	LYS	2.0
1	A	247	PHE	2.0
1	B	425	ALA	2.0
1	B	240	LEU	2.0
1	B	395	ILE	2.0
1	C	326	ILE	2.0
1	D	326	ILE	2.0
1	B	379	PHE	2.0
1	B	329	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

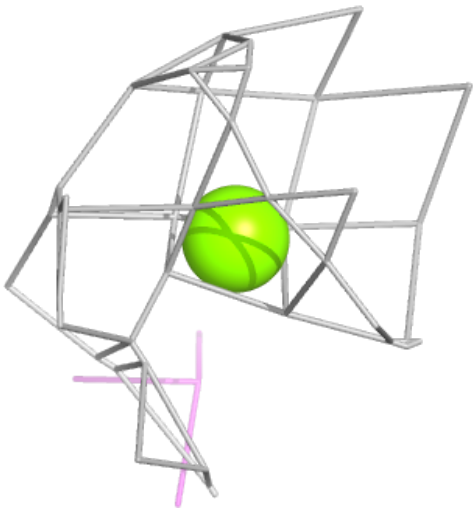
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

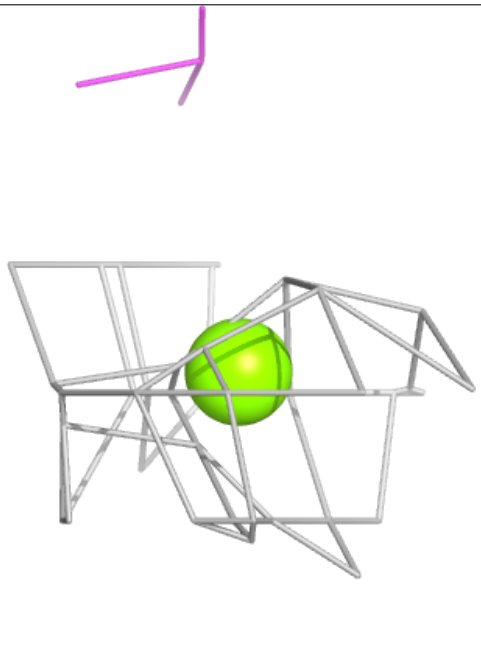
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	B	503	1/1	-0.36	1.11	113,113,113,113	0
4	MG	D	503	1/1	0.72	0.45	108,108,108,108	0
5	GOL	A	509	6/6	0.77	0.31	69,70,70,70	0
4	MG	C	503	1/1	0.80	0.23	102,102,102,102	0
5	GOL	B	505	6/6	0.82	0.28	89,89,89,89	0
5	GOL	A	508	6/6	0.83	0.26	73,73,73,73	0
5	GOL	A	504	6/6	0.85	0.25	56,57,57,57	0
3	PRP	C	502	22/22	0.85	0.25	88,94,103,103	0
5	GOL	A	507	6/6	0.86	0.27	76,77,77,77	0
5	GOL	C	506	6/6	0.86	0.24	66,66,66,66	0
3	PRP	B	502	22/22	0.88	0.22	101,106,113,114	0
5	GOL	B	504	6/6	0.88	0.27	76,76,76,76	0
5	GOL	C	504	6/6	0.89	0.29	52,52,52,52	0
3	PRP	A	502	22/22	0.90	0.25	59,67,82,82	0
5	GOL	D	505	6/6	0.90	0.33	83,83,83,83	0
5	GOL	C	507	6/6	0.91	0.24	77,77,77,77	0
5	GOL	A	506	6/6	0.92	0.32	47,47,48,48	0
5	GOL	D	504	6/6	0.92	0.24	70,70,70,70	0
3	PRP	D	502	22/22	0.92	0.19	93,97,104,104	0
4	MG	C	508	1/1	0.93	0.15	49,49,49,49	0
5	GOL	C	505	6/6	0.93	0.32	58,58,58,58	0
5	GOL	A	505	6/6	0.96	0.31	47,47,48,49	0
4	MG	D	506	1/1	0.97	0.18	41,41,41,41	0
4	MG	A	503	1/1	0.97	0.15	62,62,62,62	0
4	MG	A	510	1/1	0.97	0.10	57,57,57,57	0
4	MG	B	506	1/1	0.98	0.06	41,41,41,41	0
2	ZN	C	501	1/1	0.99	0.20	54,54,54,54	0
2	ZN	D	501	1/1	0.99	0.21	59,59,59,59	0
2	ZN	A	501	1/1	0.99	0.20	52,52,52,52	0
2	ZN	B	501	1/1	0.99	0.23	66,66,66,66	0

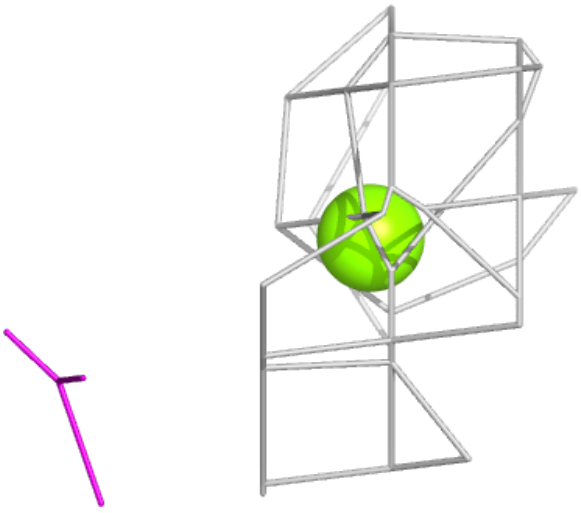
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

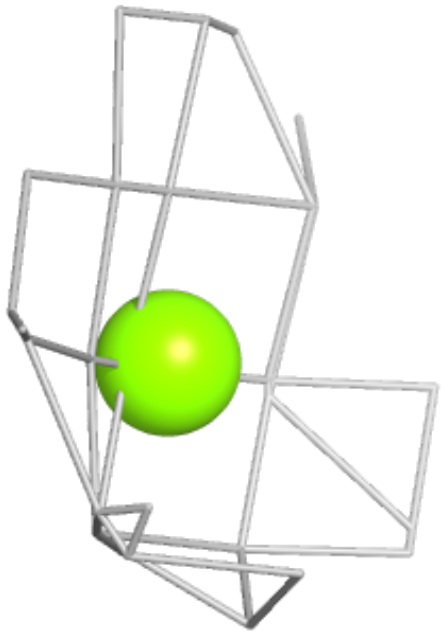


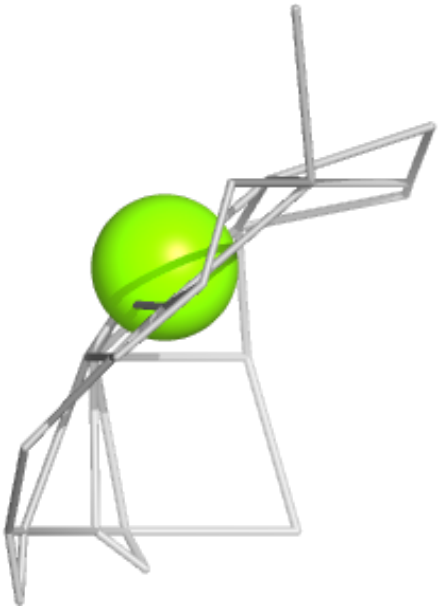


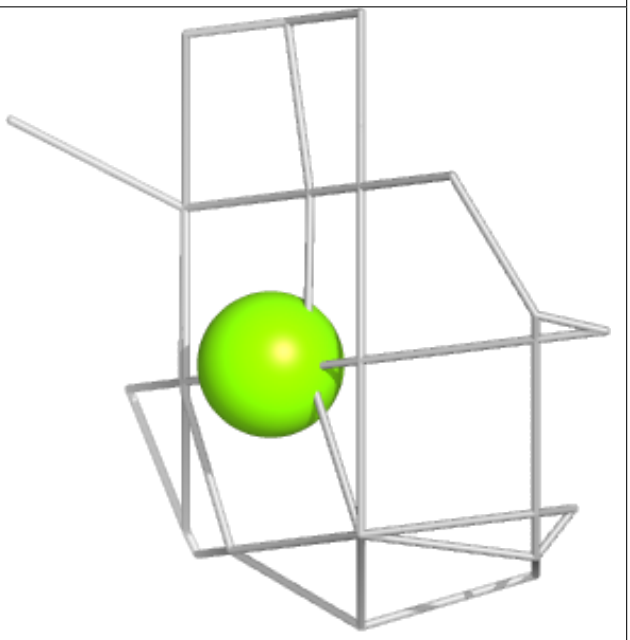


Electron density around MG D 503:

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

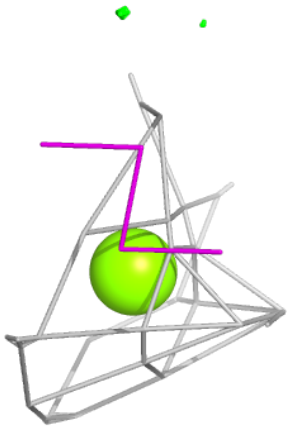


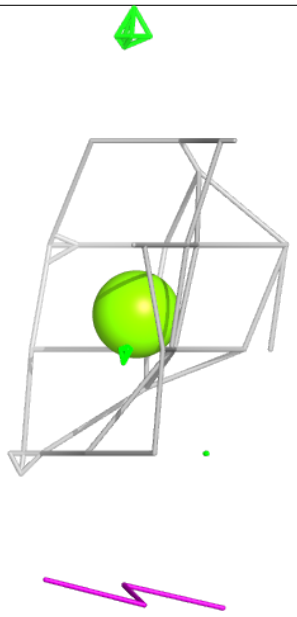


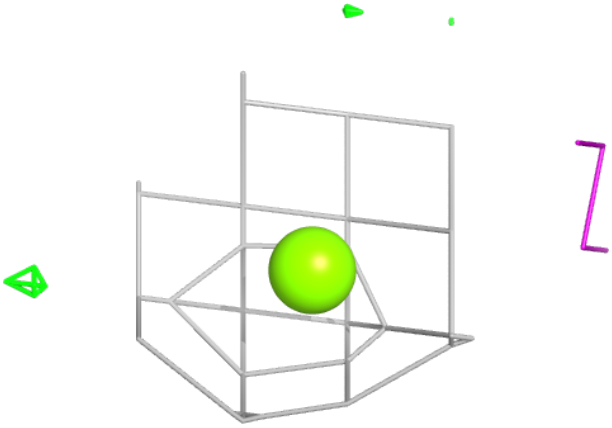


Electron density around MG C 503:

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

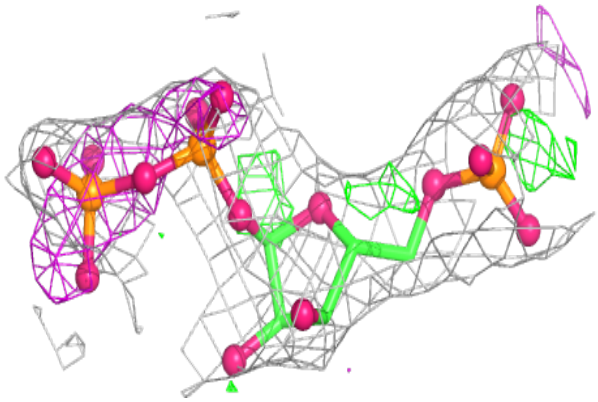


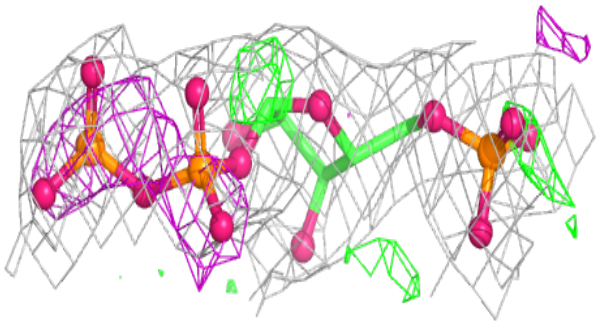


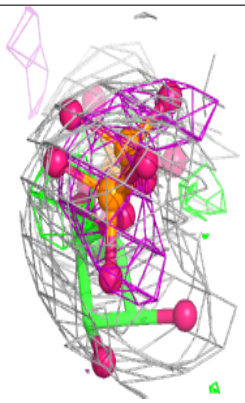


Electron density around PRP C 502:

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

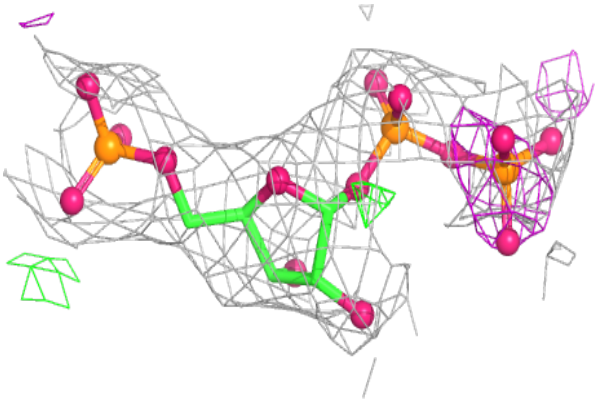


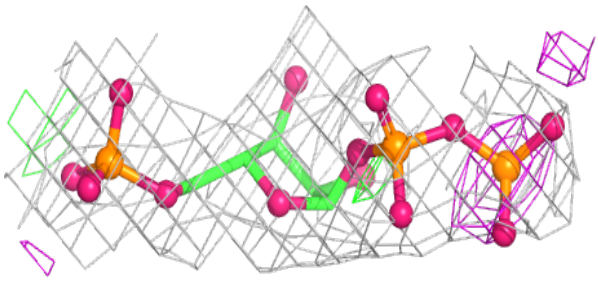


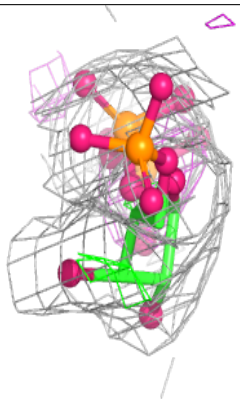


Electron density around PRP B 502:

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

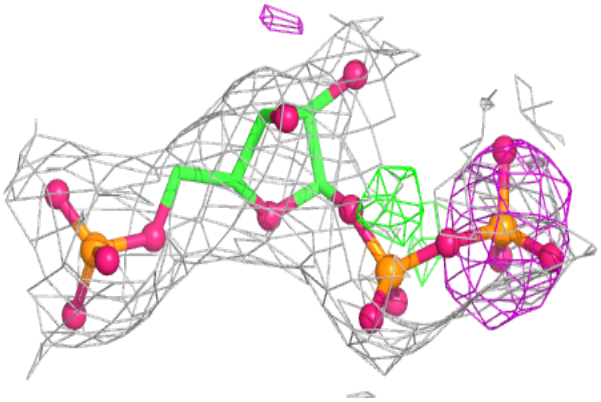


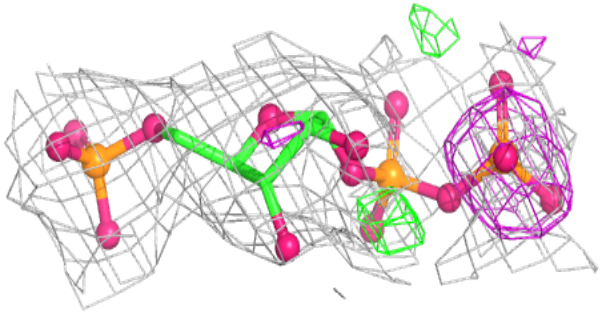


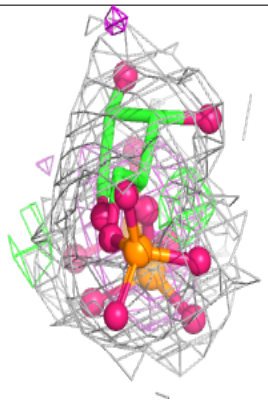


Electron density around PRP A 502:

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

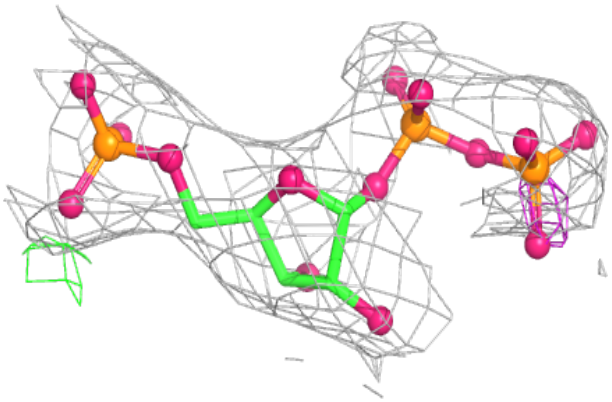


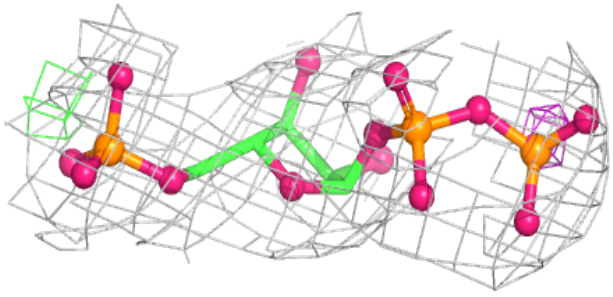


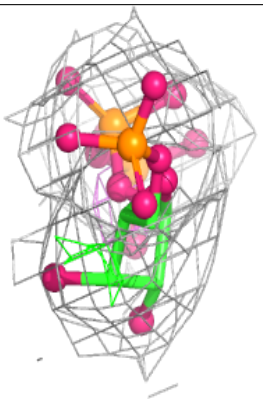


Electron density around PRP D 502:

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

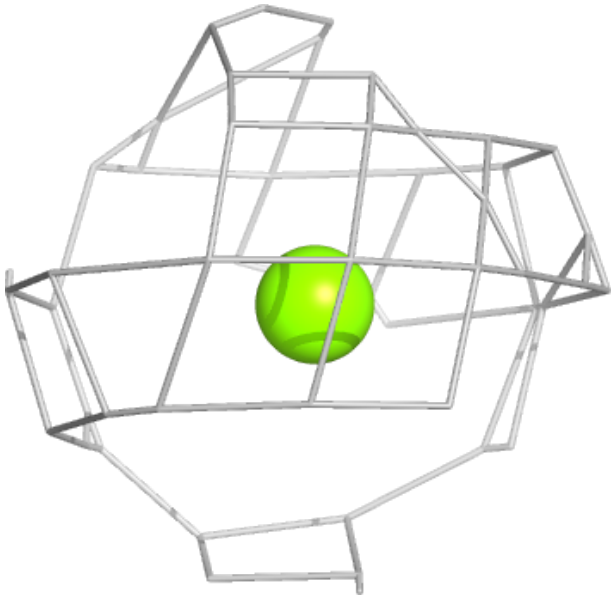


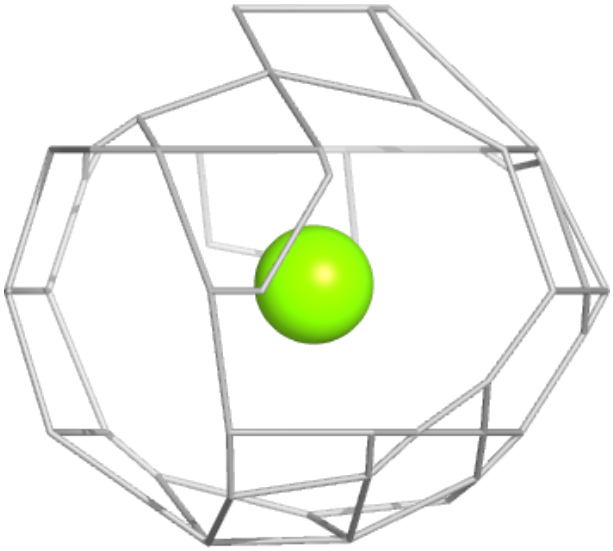


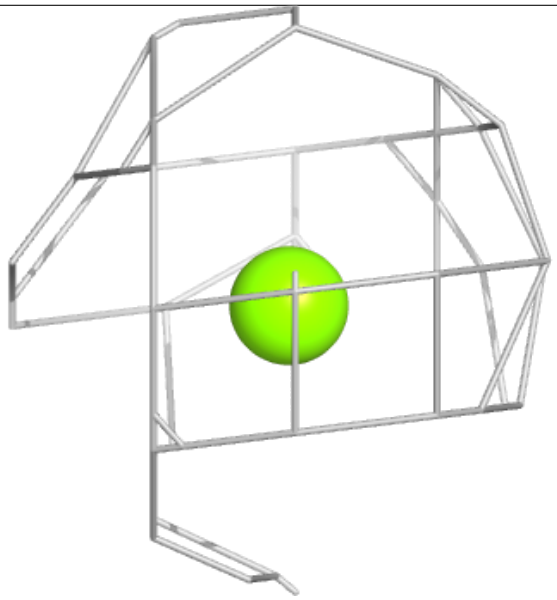


Electron density around MG C 508:

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

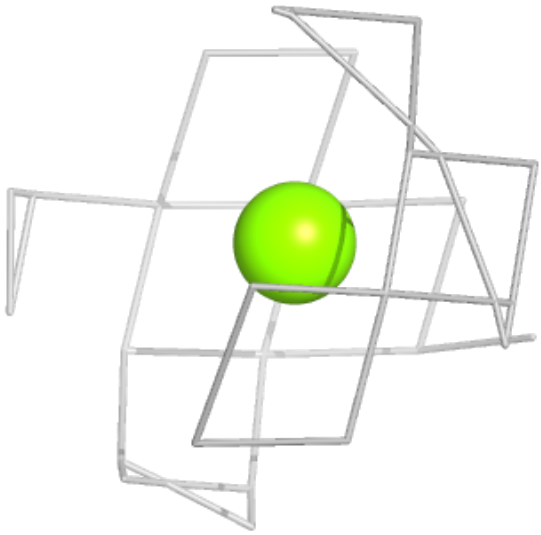


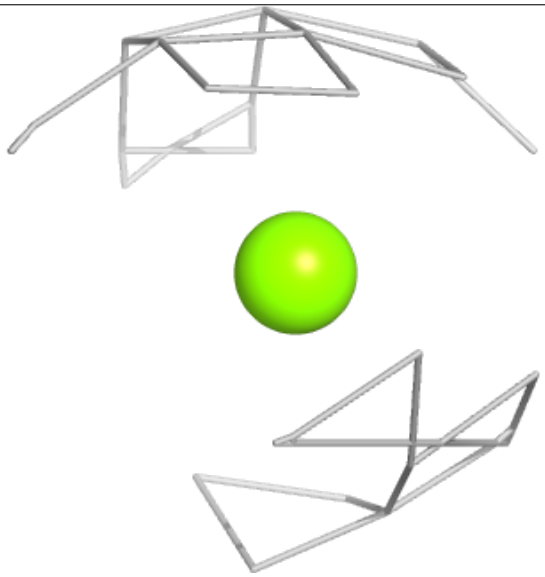


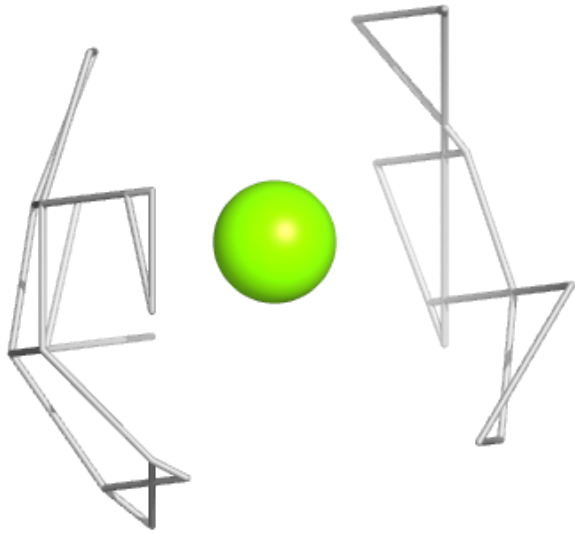


Electron density around MG D 506:

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

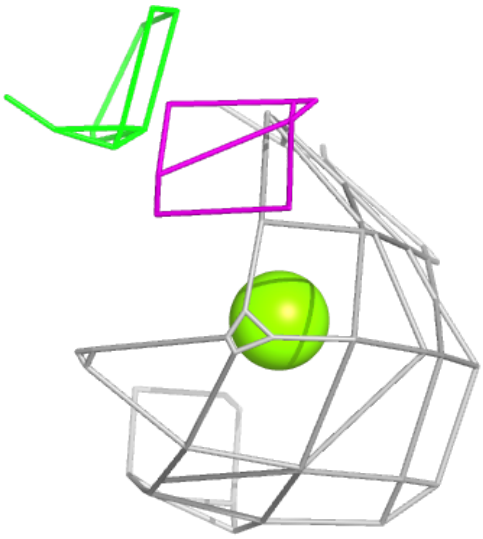


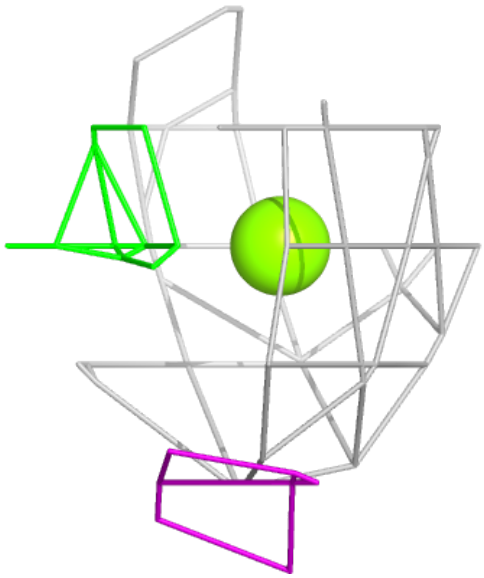


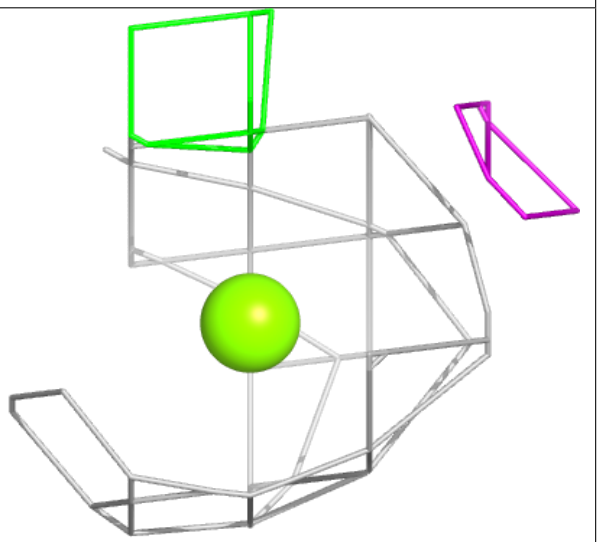


Electron density around MG A 503:

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

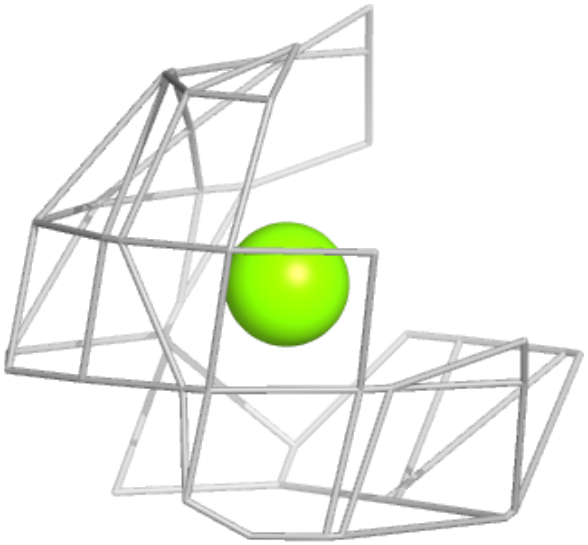


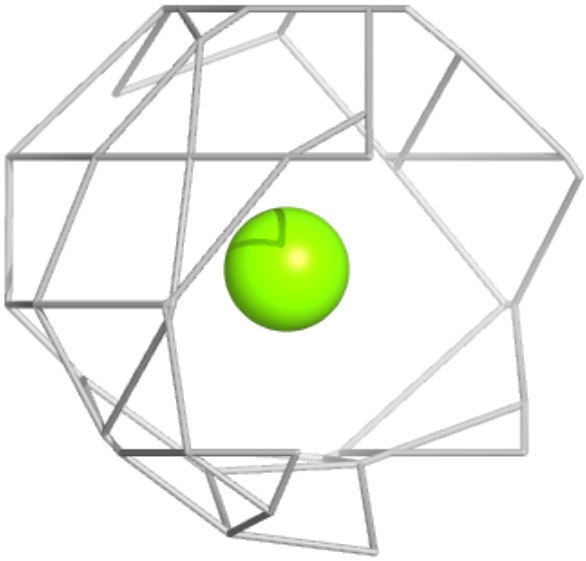


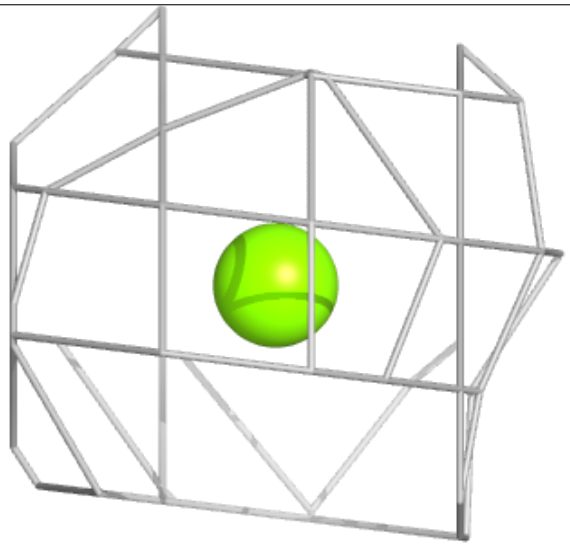


Electron density around MG A 510:

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

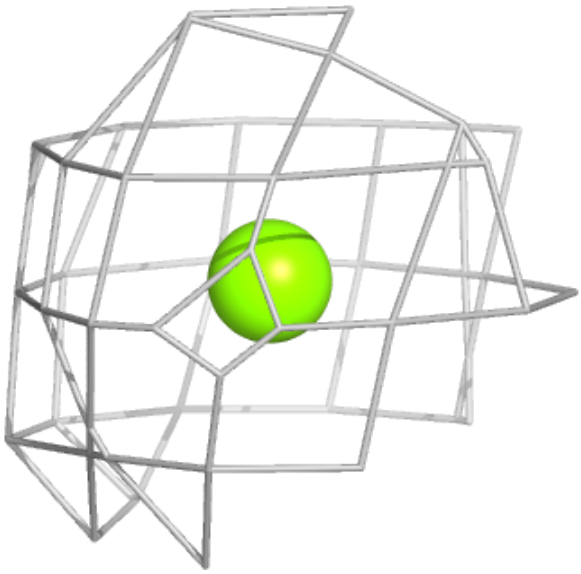


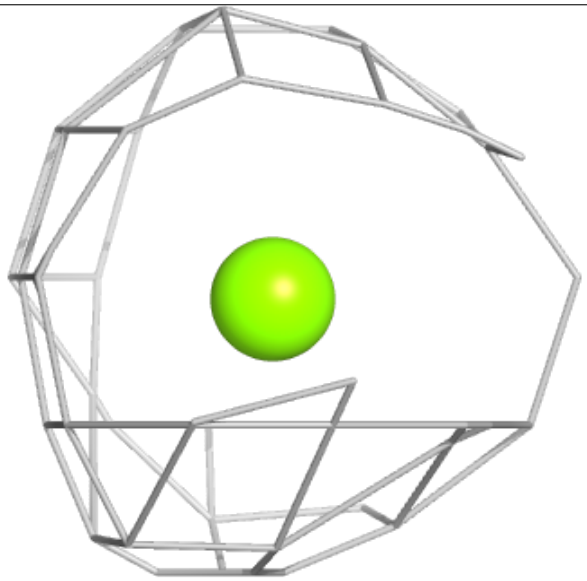


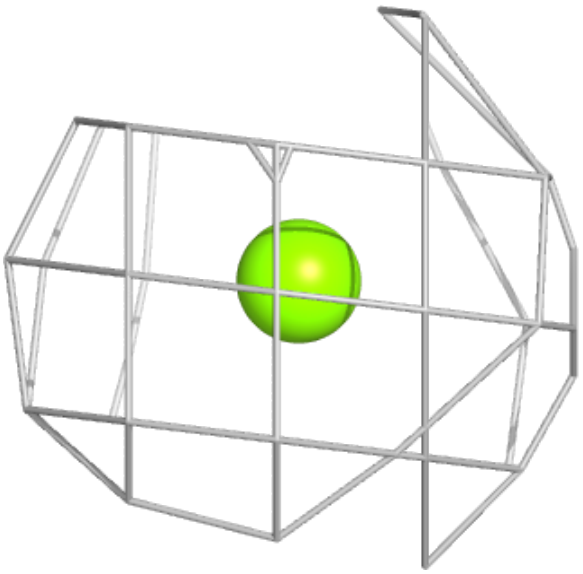


Electron density around MG B 506:

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

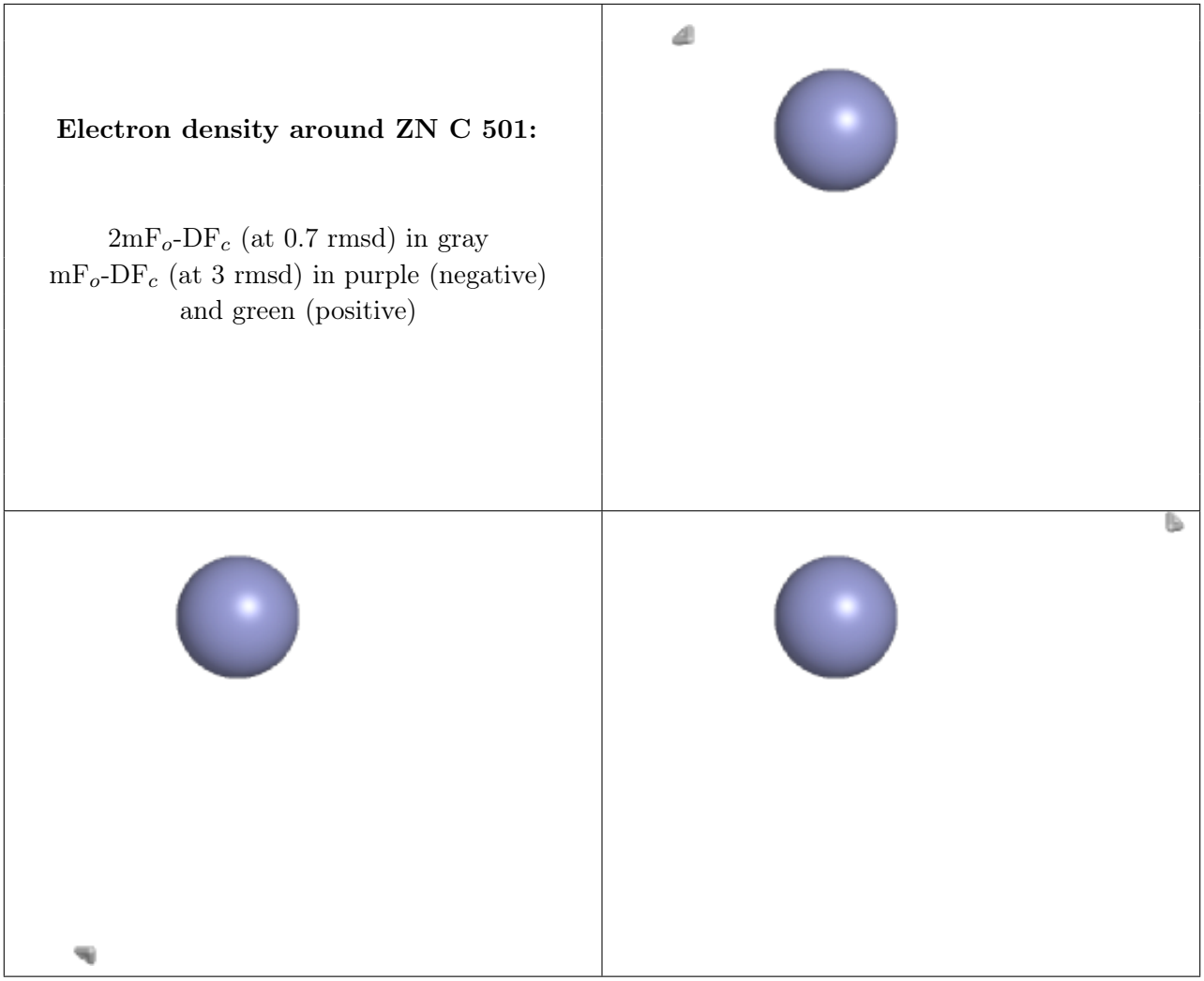






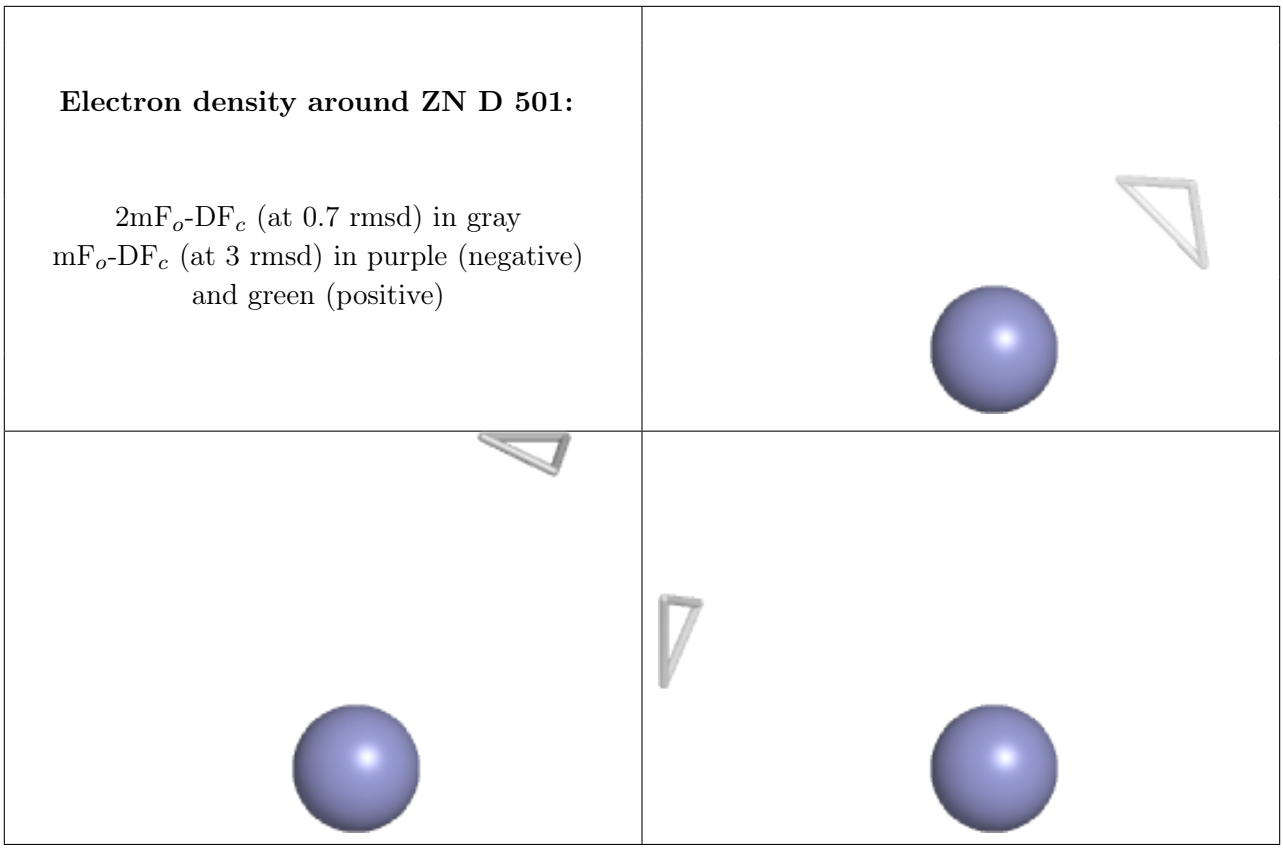
Electron density around ZN C 501:

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



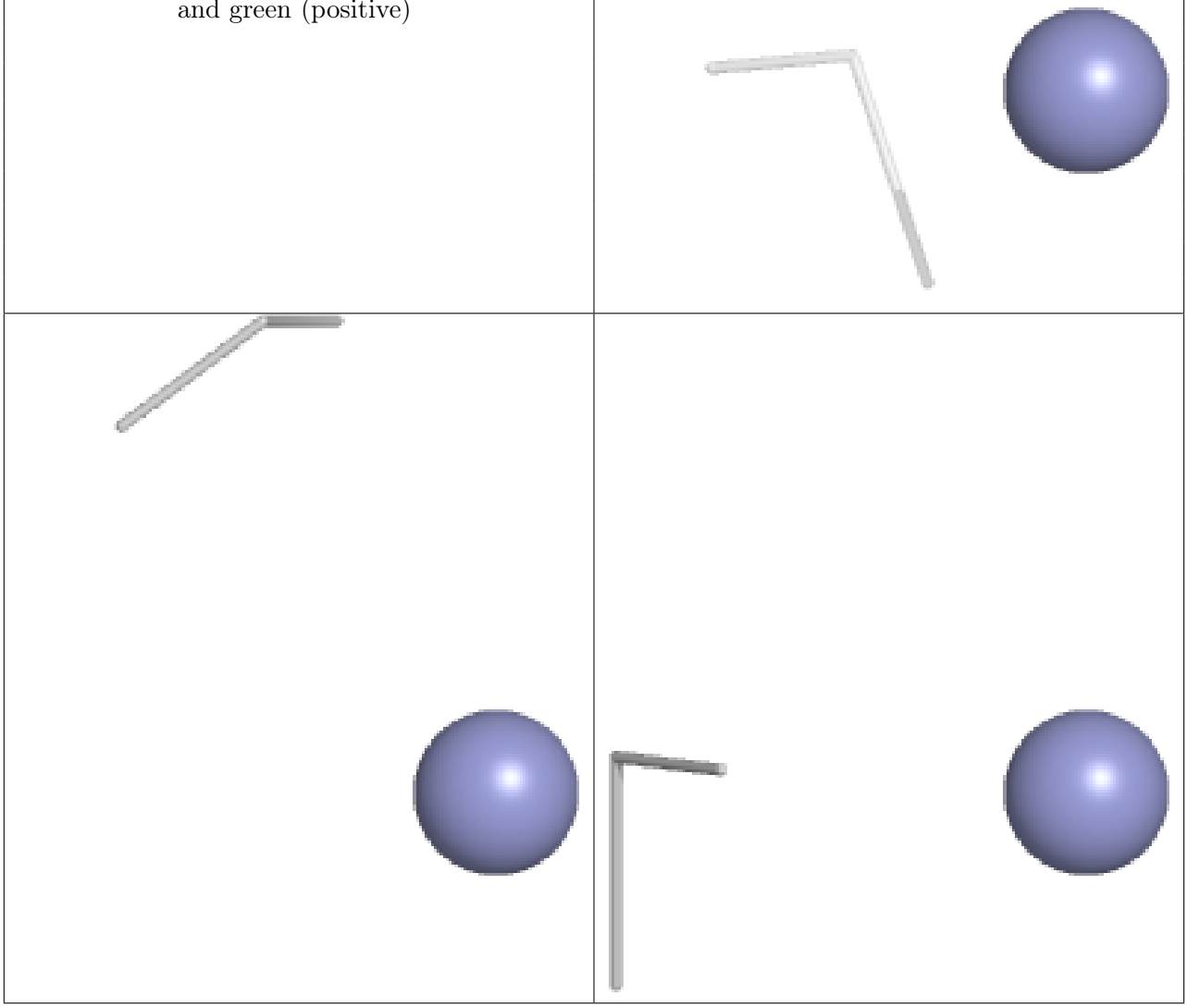
Electron density around ZN D 501:

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



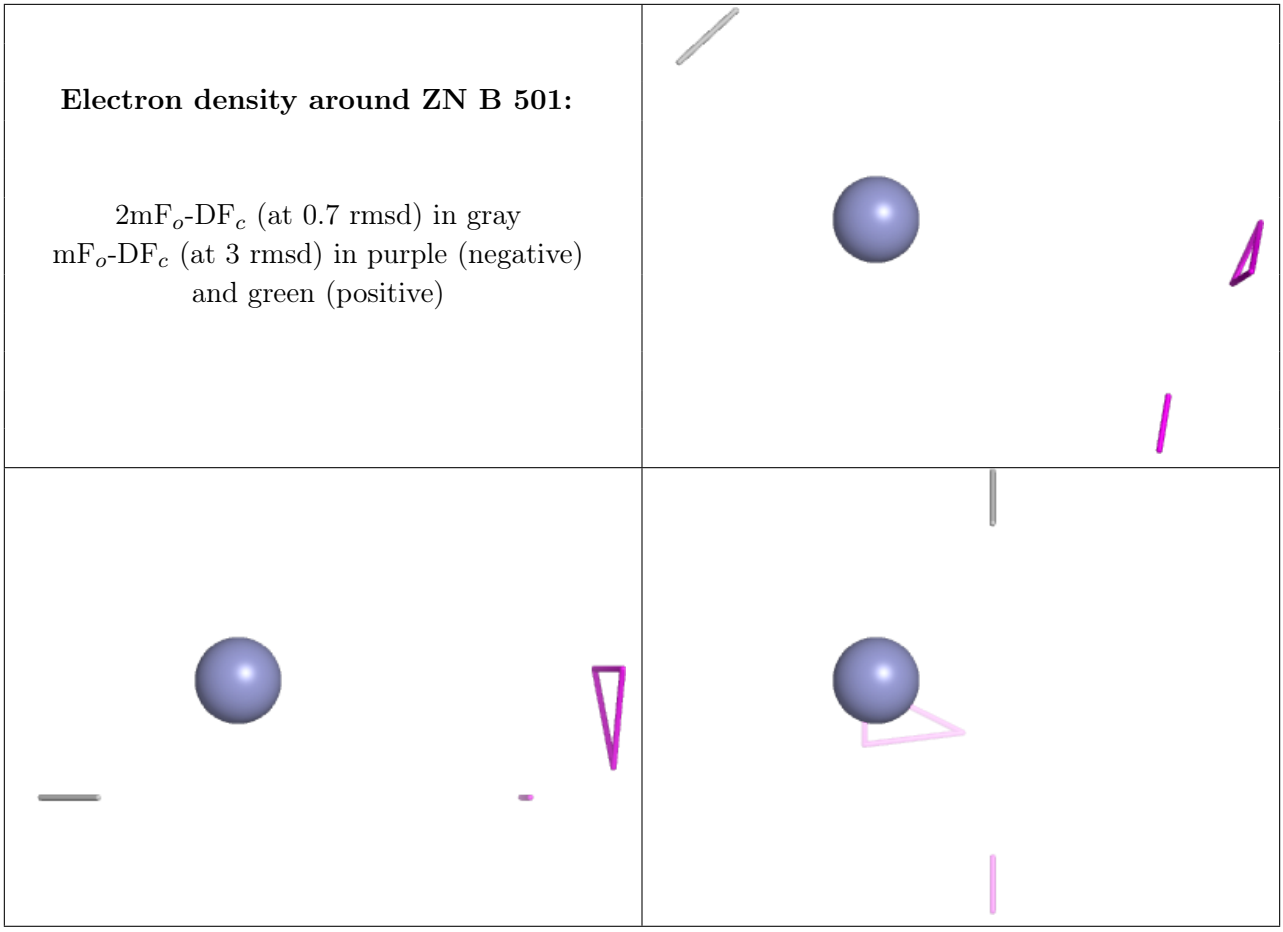
Electron density around ZN A 501:

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



Electron density around ZN 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)



6.5 Other polymers

There are no such residues in this entry.