



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2026 – 12:11 PM JST

PDB ID : 20ZQ / pdb\_000020zq  
Title : Crystal structure of rice HPPD  
Authors : Chen, L.; Ran, T.; Wang, W.W.; Zhang, B.L.  
Deposited on : 2025-12-03  
Resolution : 1.90 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](mailto: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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
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

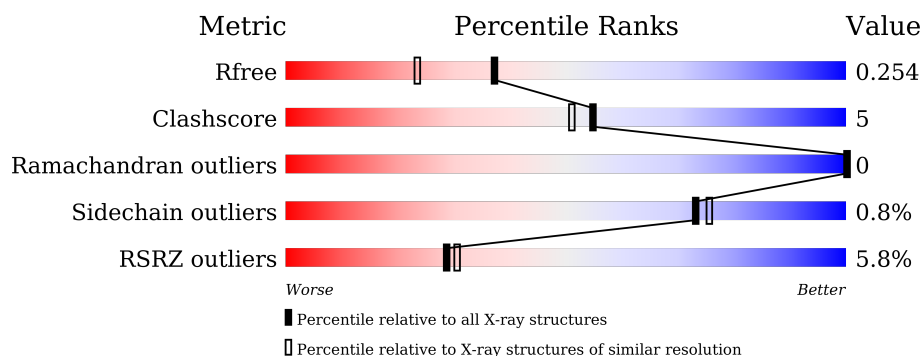
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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  $\geq 3$ , 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	454	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	B	454	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>7%</div> </div> </div>
1	C	454	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>11%</div> </div> </div>
1	D	454	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13261 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 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	2	0
			3112	1962	559	583	8			
1	B	423	Total	C	N	O	S	0	1	0
			3188	2008	575	597	8			
1	C	402	Total	C	N	O	S	0	0	0
			3024	1911	538	567	8			
1	D	406	Total	C	N	O	S	0	0	0
			3060	1933	548	571	8			

There are 32 discrepancies between the modelled and reference sequences:

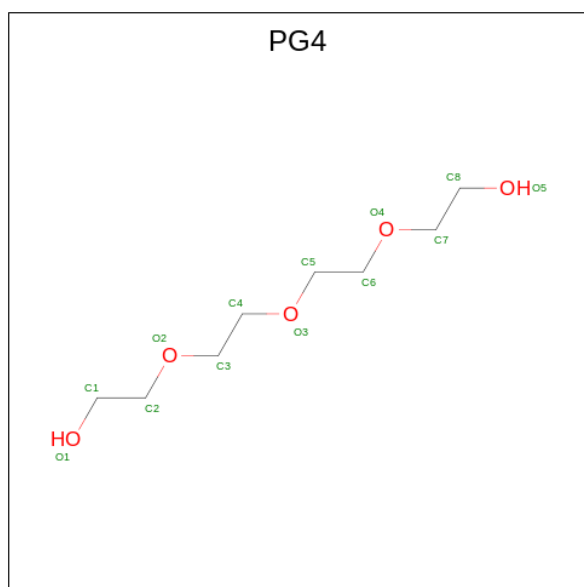
Chain	Residue	Modelled	Actual	Comment	Reference
A	447	LEU	-	expression tag	UNP A0A0E0G1W2
A	448	GLU	-	expression tag	UNP A0A0E0G1W2
A	449	HIS	-	expression tag	UNP A0A0E0G1W2
A	450	HIS	-	expression tag	UNP A0A0E0G1W2
A	451	HIS	-	expression tag	UNP A0A0E0G1W2
A	452	HIS	-	expression tag	UNP A0A0E0G1W2
A	453	HIS	-	expression tag	UNP A0A0E0G1W2
A	454	HIS	-	expression tag	UNP A0A0E0G1W2
B	447	LEU	-	expression tag	UNP A0A0E0G1W2
B	448	GLU	-	expression tag	UNP A0A0E0G1W2
B	449	HIS	-	expression tag	UNP A0A0E0G1W2
B	450	HIS	-	expression tag	UNP A0A0E0G1W2
B	451	HIS	-	expression tag	UNP A0A0E0G1W2
B	452	HIS	-	expression tag	UNP A0A0E0G1W2
B	453	HIS	-	expression tag	UNP A0A0E0G1W2
B	454	HIS	-	expression tag	UNP A0A0E0G1W2
C	447	LEU	-	expression tag	UNP A0A0E0G1W2
C	448	GLU	-	expression tag	UNP A0A0E0G1W2
C	449	HIS	-	expression tag	UNP A0A0E0G1W2
C	450	HIS	-	expression tag	UNP A0A0E0G1W2
C	451	HIS	-	expression tag	UNP A0A0E0G1W2

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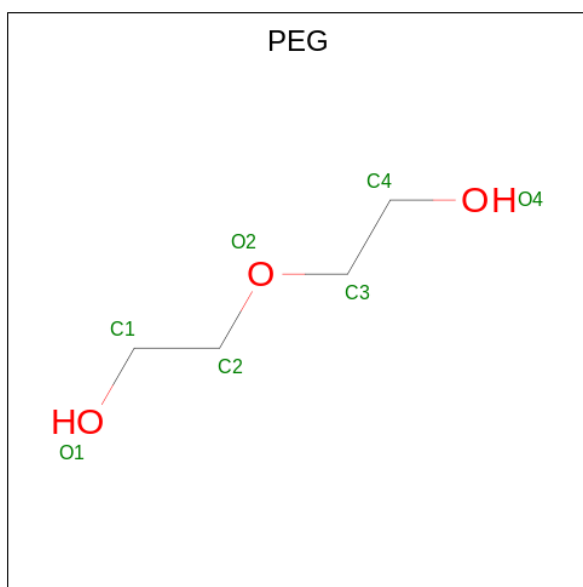
Chain	Residue	Modelled	Actual	Comment	Reference
C	452	HIS	-	expression tag	UNP A0A0E0G1W2
C	453	HIS	-	expression tag	UNP A0A0E0G1W2
C	454	HIS	-	expression tag	UNP A0A0E0G1W2
D	447	LEU	-	expression tag	UNP A0A0E0G1W2
D	448	GLU	-	expression tag	UNP A0A0E0G1W2
D	449	HIS	-	expression tag	UNP A0A0E0G1W2
D	450	HIS	-	expression tag	UNP A0A0E0G1W2
D	451	HIS	-	expression tag	UNP A0A0E0G1W2
D	452	HIS	-	expression tag	UNP A0A0E0G1W2
D	453	HIS	-	expression tag	UNP A0A0E0G1W2
D	454	HIS	-	expression tag	UNP A0A0E0G1W2

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ) (labeled as "Ligand of Interest" by depositor).



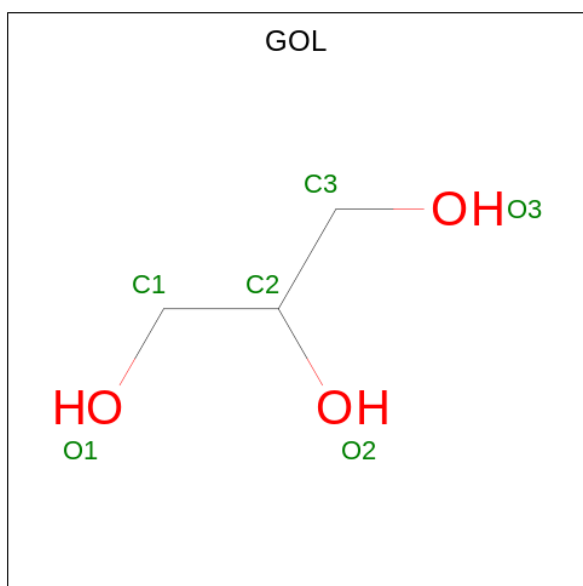
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

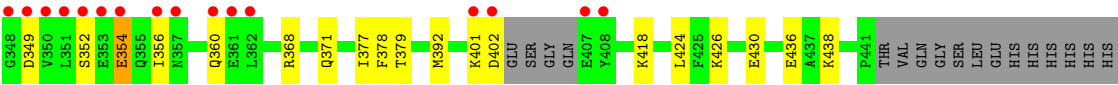
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

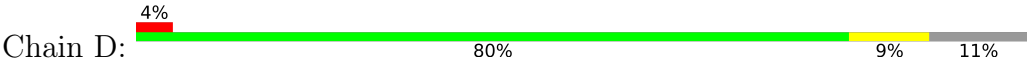
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	274	Total 274	O 274	0	0
6	B	218	Total 218	O 218	0	0
6	C	145	Total 145	O 145	0	0
6	D	177	Total 177	O 177	0	0





• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.06Å 93.44Å 113.96Å 90.00° 109.85° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-1.90) 98.0 (20.00-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.199 , 0.243 0.214 , 0.254	Depositor DCC
$R_{free}$ test set	6229 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13261	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2684e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, ZN, PEG, PG4

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	0.41	0/3186	0.65	0/4319
1	B	0.42	0/3266	0.66	0/4429
1	C	0.39	0/3096	0.62	1/4200 (0.0%)
1	D	0.42	0/3133	0.64	1/4247 (0.0%)
All	All	0.41	0/12681	0.64	2/17195 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	341	ASP	N-CA-C	-5.93	104.82	111.28
1	C	57	ALA	N-CA-C	-5.51	106.56	113.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	130	ARG	Sidechain
1	B	344	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	345	ARG	Sidechain
1	D	346	ARG	Sidechain

## 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	3112	0	2984	31	0
1	B	3188	0	3056	29	0
1	C	3024	0	2905	35	0
1	D	3060	0	2944	24	0
2	A	26	0	36	2	0
2	D	13	0	18	1	0
3	A	7	0	10	0	0
3	D	7	0	10	0	0
4	A	6	0	8	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	274	0	0	8	0
6	B	218	0	0	3	0
6	C	145	0	0	4	0
6	D	177	0	0	3	0
All	All	13261	0	11971	118	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 5.

All (118) 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:D:320:MET:HE1	1:D:392:MET:HE3	1.51	0.90
1:B:400:GLU:HG3	1:B:410:LYS:HD3	1.54	0.88
1:A:108:ASP:OD1	1:A:109:HIS:N	2.18	0.77
1:A:155:ARG:NH2	6:A:602:HOH:O	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:PHE:CE1	1:B:323:ARG:HG3	2.26	0.70
1:C:34:PHE:CZ	1:C:246:GLU:HG2	2.29	0.68
1:B:210:ASN:OD1	1:B:213:ALA:HB2	1.96	0.65
1:C:252:ALA:HB2	1:C:282:VAL:HG21	1.80	0.64
1:C:340:TYR:CZ	1:C:360:GLN:HA	2.32	0.64
1:B:68:PHE:CZ	1:B:323:ARG:HG3	2.33	0.63
1:D:344:ARG:HG3	1:D:356:ILE:HG21	1.82	0.61
1:B:225:VAL:HG21	1:B:305:HIS:CE1	2.37	0.59
1:C:356:ILE:H	1:C:356:ILE:HD12	1.67	0.59
1:A:127:GLY:HA2	1:A:130[B]:ARG:HH12	1.67	0.59
1:C:231:LEU:HD11	1:C:265:VAL:HG12	1.85	0.59
1:C:340:TYR:O	1:C:344:ARG:HG3	2.02	0.58
1:A:127:GLY:HA2	1:A:130[B]:ARG:NH1	2.19	0.58
1:C:246:GLU:OE2	1:C:249:GLU:HB3	2.04	0.58
1:D:33:ARG:NH1	6:D:607:HOH:O	2.37	0.57
1:A:104:PRO:HB3	1:A:124:PHE:HZ	1.70	0.56
1:B:378:PHE:CG	1:B:424:LEU:HD13	2.42	0.55
1:D:86:ALA:HB2	1:D:115:ALA:O	2.07	0.55
1:B:85:SER:HB2	1:B:115:ALA:HB1	1.88	0.54
1:B:111:VAL:HG23	1:B:115:ALA:HB3	1.90	0.54
1:A:378:PHE:CG	1:A:424:LEU:HD13	2.43	0.53
1:B:163:ARG:NH1	6:B:608:HOH:O	2.42	0.53
1:A:286:LYS:HG3	6:A:814:HOH:O	2.10	0.52
1:D:378:PHE:CG	1:D:424:LEU:HD13	2.44	0.52
1:A:225:VAL:HG21	1:A:305:HIS:CE1	2.44	0.52
1:C:352:SER:O	1:C:356:ILE:HD12	2.09	0.51
1:D:225:VAL:HG21	1:D:305:HIS:CE1	2.46	0.51
1:C:401:LYS:HD3	1:C:402:ASP:N	2.26	0.51
1:B:350:VAL:HG11	1:B:373:VAL:HG21	1.92	0.51
1:C:136:HIS:NE2	1:C:185:ASP:OD2	2.31	0.51
1:D:371:GLN:NE2	6:D:603:HOH:O	2.31	0.50
1:C:70:LEU:HA	1:C:320:MET:HE2	1.92	0.50
1:B:246:GLU:OE2	1:B:249:GLU:HB2	2.12	0.50
2:A:502:PG4:H22	1:D:299:GLY:HA3	1.94	0.49
1:B:56:CYS:HB3	6:B:774:HOH:O	2.12	0.49
1:A:376:GLN:NE2	6:A:610:HOH:O	2.35	0.49
1:A:56:CYS:HB3	6:A:803:HOH:O	2.12	0.49
1:D:400:GLU:OE2	1:D:410:LYS:NZ	2.27	0.49
1:A:70:LEU:HD23	1:A:320:MET:HE3	1.94	0.48
1:D:231:LEU:HD11	1:D:265:VAL:HG12	1.95	0.48
1:A:318:ARG:HH21	1:A:358:GLU:HG2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:LEU:HD22	1:D:362:LEU:HD12	1.95	0.48
1:B:55:TRP:CE3	1:B:129:ALA:HA	2.49	0.48
1:B:231:LEU:HD11	1:B:265:VAL:HB	1.94	0.48
1:A:68:PHE:CZ	1:A:323:ARG:HG3	2.49	0.47
1:B:111:VAL:CG2	1:B:115:ALA:HB3	2.44	0.47
1:C:287:ARG:NH1	1:C:287:ARG:HG2	2.28	0.47
1:C:371:GLN:O	6:C:601:HOH:O	2.20	0.47
1:C:320:MET:HE1	1:C:392:MET:HE2	1.96	0.47
1:D:334:PRO:HB3	1:D:363:GLY:HA2	1.97	0.47
1:D:352:SER:OG	1:D:355:GLN:HG3	2.14	0.46
1:A:246:GLU:OE2	1:A:249:GLU:HB2	2.16	0.46
1:C:82:THR:CG2	1:C:206:GLU:HG3	2.46	0.46
1:A:130[B]:ARG:NH1	1:A:130[B]:ARG:HB3	2.31	0.46
1:D:428:ILE:O	1:D:432:GLU:HG3	2.16	0.46
1:B:313:VAL:HB	1:B:394:GLN:HB2	1.97	0.45
1:C:68:PHE:CE2	1:C:323:ARG:HB3	2.51	0.45
1:C:84:ASN:HD21	1:C:87:HIS:CE1	2.34	0.45
1:A:33:ARG:NH2	1:B:422[A]:SER:HB2	2.32	0.45
1:A:106:GLY:HA2	2:A:502:PG4:H31	1.98	0.45
1:A:80:LEU:HD22	2:D:501:PG4:H72	1.98	0.45
1:B:318:ARG:HH21	1:B:358:GLU:HG2	1.82	0.45
1:B:223:HIS:HB3	1:B:275:LEU:HB2	1.99	0.44
1:C:418:LYS:NZ	6:C:613:HOH:O	2.48	0.44
1:C:354:GLU:H	1:C:354:GLU:HG3	1.58	0.44
1:C:36:ARG:HD2	6:C:602:HOH:O	2.16	0.44
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.82	0.44
1:A:138:LEU:HA	6:A:608:HOH:O	2.17	0.44
1:A:219:ARG:HA	1:A:219:ARG:HD3	1.84	0.44
1:B:219:ARG:HD3	1:B:219:ARG:HA	1.83	0.44
1:C:259:GLU:HB2	6:C:674:HOH:O	2.18	0.44
1:C:262:LEU:HD12	1:C:262:LEU:C	2.43	0.44
1:A:334:PRO:HB3	1:A:363:GLY:HA2	2.00	0.43
1:D:140:VAL:HG21	1:D:306:ILE:HD11	2.00	0.43
1:D:262:LEU:C	1:D:262:LEU:HD12	2.43	0.43
1:B:444:GLN:O	1:B:448:GLU:HG3	2.19	0.43
1:B:326:MET:HE3	1:B:326:MET:HB3	1.85	0.43
1:C:438:LYS:HB3	1:C:438:LYS:HE2	1.80	0.43
1:C:287:ARG:HH22	1:C:436:GLU:CD	2.23	0.43
1:D:313:VAL:HB	1:D:394:GLN:HB2	2.01	0.43
1:B:338:ASN:N	1:B:338:ASN:OD1	2.45	0.43
1:B:155:ARG:HG2	1:B:155:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.90	0.42
4:A:504:GOL:H11	6:A:714:HOH:O	2.19	0.42
1:C:331:PHE:HA	1:C:379:THR:HA	2.01	0.42
1:A:130[B]:ARG:NH2	6:A:627:HOH:O	2.51	0.42
1:B:444:GLN:HB2	6:B:651:HOH:O	2.19	0.42
1:C:152:ASP:OD1	1:C:155:ARG:NH2	2.52	0.42
1:A:259:GLU:HG2	1:A:286:LYS:HD3	2.02	0.42
1:D:432:GLU:O	1:D:436:GLU:HG3	2.20	0.42
1:D:378:PHE:CD1	1:D:424:LEU:HD13	2.54	0.42
1:B:155:ARG:HG2	1:B:155:ARG:HH11	1.84	0.42
1:D:378:PHE:CD2	1:D:424:LEU:HD13	2.55	0.42
1:B:316:THR:CG2	1:B:320:MET:HE3	2.50	0.42
1:D:418:LYS:NZ	6:D:606:HOH:O	2.37	0.42
1:C:378:PHE:CD1	1:C:424:LEU:HD13	2.55	0.41
1:C:426:LYS:O	1:C:430:GLU:HG2	2.19	0.41
1:C:219:ARG:HD3	1:C:219:ARG:HA	1.79	0.41
1:C:377:ILE:HG22	1:C:392:MET:HB2	2.02	0.41
1:A:140:VAL:HG21	1:A:306:ILE:HD11	2.01	0.41
1:C:287:ARG:HG2	1:C:287:ARG:HH11	1.85	0.41
1:D:309:ALA:HA	1:D:393:ILE:O	2.20	0.41
1:A:378:PHE:CD1	1:A:424:LEU:HD13	2.55	0.41
1:A:57:ALA:HB3	1:D:57:ALA:CB	2.51	0.41
1:C:332:LEU:HD12	1:C:378:PHE:HB2	2.02	0.41
1:A:337:PRO:O	6:A:601:HOH:O	2.22	0.41
1:C:99:PHE:HB3	1:C:101:PHE:CE1	2.56	0.41
1:C:218:LEU:HD21	1:C:392:MET:HE2	2.02	0.41
1:C:349:ASP:CG	1:C:368:ARG:HH12	2.28	0.41
1:D:317:LEU:HD23	1:D:317:LEU:HA	1.91	0.41
1:A:223:HIS:HB3	1:A:275:LEU:HB2	2.02	0.40
1:A:410:LYS:NZ	4:A:504:GOL:H32	2.36	0.40
1:B:140:VAL:HG21	1:B:306:ILE:HD11	2.02	0.40
1:B:316:THR:HG22	1:B:320:MET:HE3	2.04	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	408/454 (90%)	401 (98%)	7 (2%)	0	100	100
1	B	420/454 (92%)	412 (98%)	8 (2%)	0	100	100
1	C	396/454 (87%)	390 (98%)	6 (2%)	0	100	100
1	D	400/454 (88%)	394 (98%)	6 (2%)	0	100	100
All	All	1624/1816 (89%)	1597 (98%)	27 (2%)	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	309/337 (92%)	308 (100%)	1 (0%)	86	88
1	B	317/337 (94%)	312 (98%)	5 (2%)	55	54
1	C	301/337 (89%)	300 (100%)	1 (0%)	86	88
1	D	304/337 (90%)	301 (99%)	3 (1%)	68	70
All	All	1231/1348 (91%)	1221 (99%)	10 (1%)	73	75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	SER
1	B	198	ASP
1	B	345	ARG
1	B	368	ARG
1	B	401	LYS
1	B	442	THR
1	C	354	GLU
1	D	195	ASP

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Mol	Chain	Res	Type
1	D	282	VAL
1	D	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	338	ASN
1	B	371	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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PEG	D	502	-	6,6,6	0.24	0	5,5,5	0.07	0
4	GOL	A	504	-	5,5,5	1.05	0	5,5,5	0.83	0
2	PG4	A	502	-	12,12,12	0.18	0	11,11,11	0.60	0
2	PG4	A	501	-	12,12,12	0.19	0	11,11,11	0.61	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	A	503	-	6,6,6	0.26	0	5,5,5	0.11	0
2	PG4	D	501	-	12,12,12	0.22	0	11,11,11	0.30	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	PEG	D	502	-	-	0/4/4/4	-
4	GOL	A	504	-	-	2/4/4/4	-
2	PG4	A	502	-	-	5/10/10/10	-
2	PG4	A	501	-	-	2/10/10/10	-
3	PEG	A	503	-	-	2/4/4/4	-
2	PG4	D	501	-	-	2/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

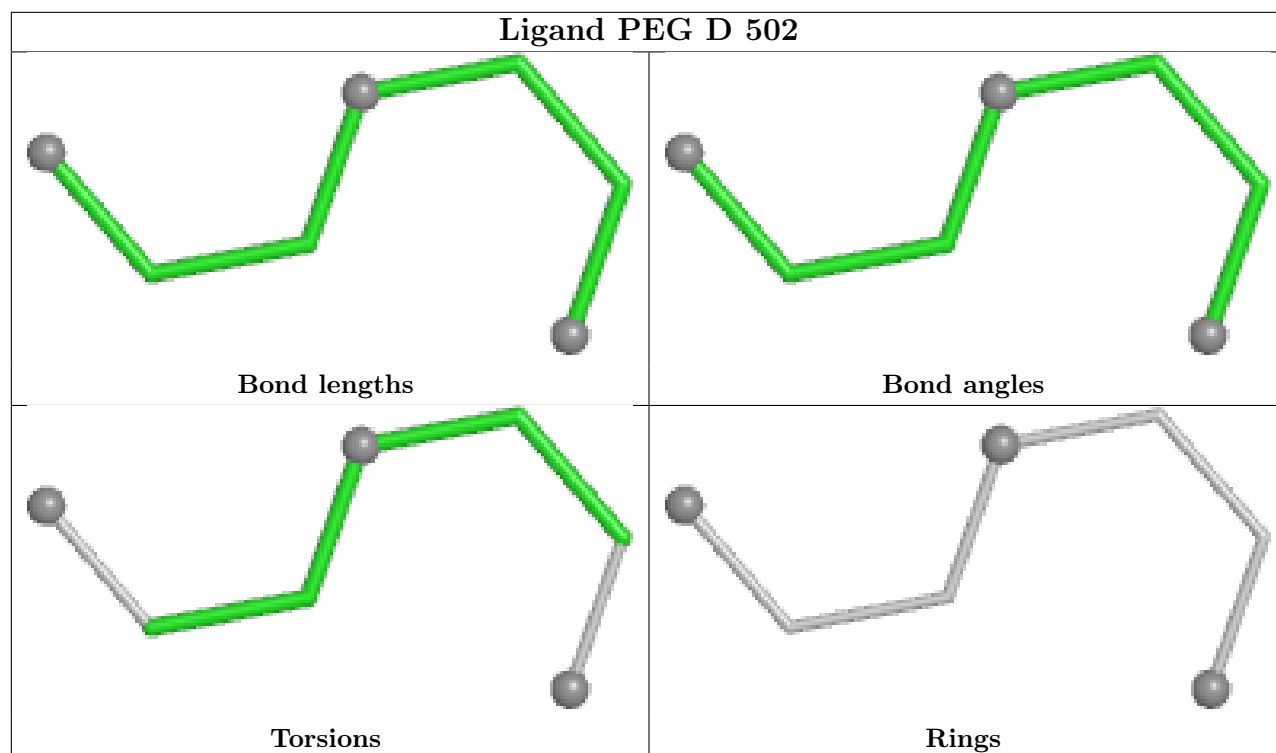
Mol	Chain	Res	Type	Atoms
4	A	504	GOL	O1-C1-C2-C3
2	A	502	PG4	O3-C5-C6-O4
2	A	502	PG4	O1-C1-C2-O2
2	A	502	PG4	O2-C3-C4-O3
4	A	504	GOL	O1-C1-C2-O2
3	A	503	PEG	O2-C3-C4-O4
2	D	501	PG4	O3-C5-C6-O4
2	A	501	PG4	O4-C7-C8-O5
3	A	503	PEG	C1-C2-O2-C3
2	A	502	PG4	C1-C2-O2-C3
2	A	502	PG4	C6-C5-O3-C4
2	A	501	PG4	O3-C5-C6-O4
2	D	501	PG4	C4-C3-O2-C2

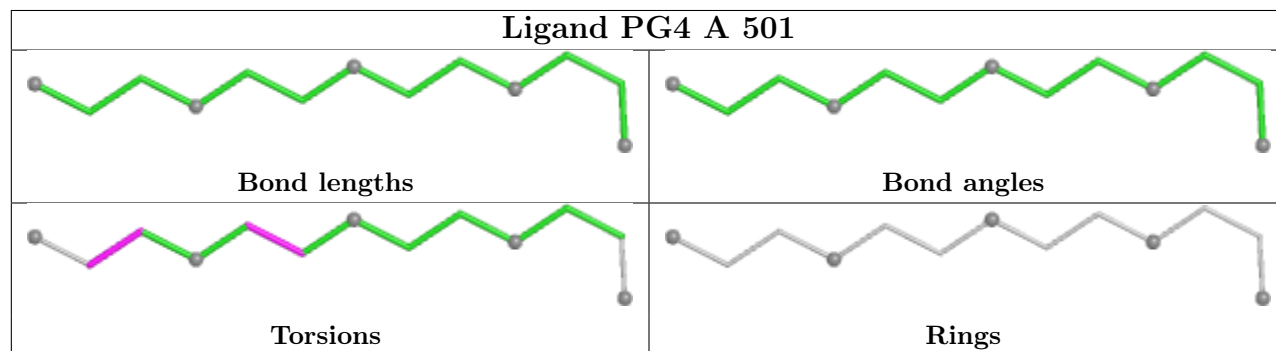
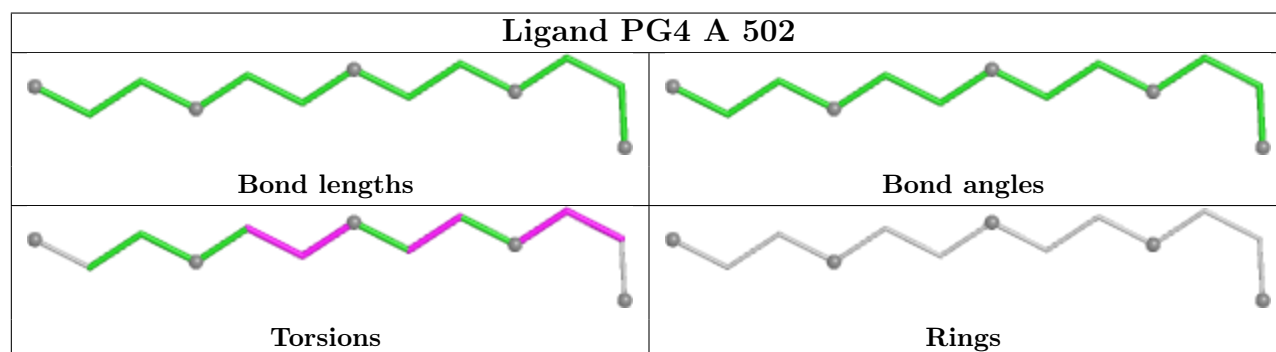
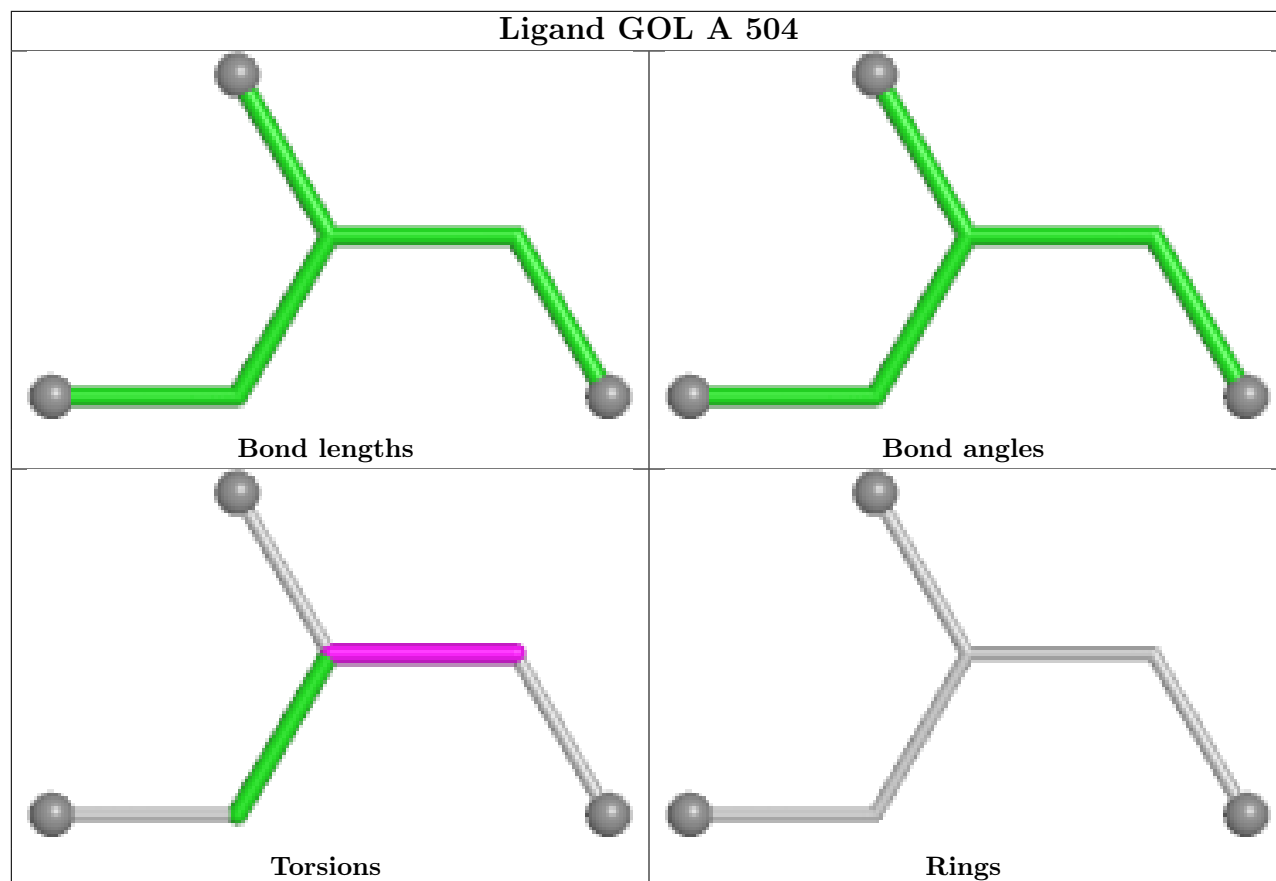
There are no ring outliers.

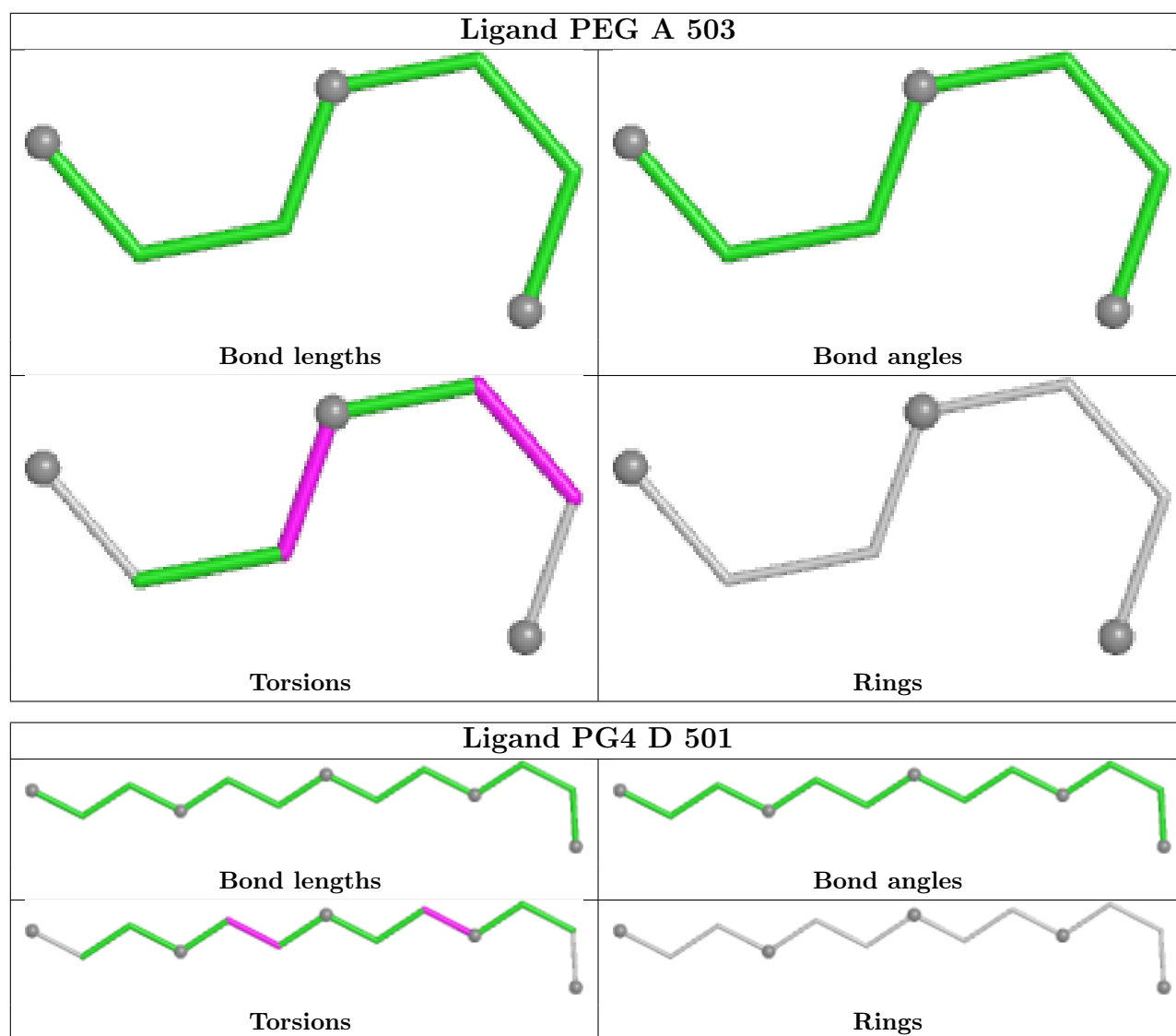
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	GOL	2	0
2	A	502	PG4	2	0
2	D	501	PG4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	412/454 (90%)	-0.22	9 (2%) 62 66	9, 19, 35, 71	2 (0%)
1	B	423/454 (93%)	0.10	31 (7%) 21 22	9, 22, 51, 69	1 (0%)
1	C	402/454 (88%)	0.40	36 (8%) 15 16	15, 26, 56, 67	0
1	D	406/454 (89%)	0.10	20 (4%) 35 37	14, 22, 51, 63	0
All	All	1643/1816 (90%)	0.09	96 (5%) 29 30	9, 22, 51, 71	3 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	GLY	5.6
1	B	408	TYR	5.5
1	A	23	ASN	5.3
1	D	26	PHE	4.5
1	B	447	LEU	4.5
1	B	110	GLY	4.3
1	B	109	HIS	4.3
1	B	108	ASP	4.2
1	B	111	VAL	4.0
1	D	107	GLY	3.6
1	B	113	ALA	3.5
1	C	197	ALA	3.4
1	A	209	SER	3.4
1	B	106	GLY	3.3
1	D	115	ALA	3.3
1	B	442	THR	3.3
1	C	209	SER	3.3
1	B	24	ALA	3.3
1	C	340	TYR	3.2
1	C	68	PHE	3.2
1	C	353	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	210	ASN	3.1
1	C	341	ASP	3.1
1	C	361	GLU	3.1
1	D	211	PRO	3.1
1	C	356	ILE	3.0
1	D	350	VAL	3.0
1	A	211	PRO	3.0
1	B	68	PHE	3.0
1	D	209	SER	3.0
1	B	197	ALA	3.0
1	B	450	HIS	3.0
1	C	351	LEU	2.9
1	C	350	VAL	2.9
1	C	352	SER	2.9
1	A	24	ALA	2.9
1	C	196	GLY	2.9
1	D	116	ALA	2.8
1	A	402	ASP	2.8
1	B	114	ASP	2.8
1	B	401	LYS	2.8
1	B	449	HIS	2.8
1	C	198	ASP	2.8
1	C	348	GLY	2.7
1	D	196	GLY	2.7
1	C	362	LEU	2.7
1	B	209	SER	2.7
1	D	37	ALA	2.7
1	A	408	TYR	2.7
1	B	196	GLY	2.7
1	C	360	GLN	2.7
1	D	345	ARG	2.7
1	C	116	ALA	2.6
1	B	112	GLY	2.6
1	D	197	ALA	2.6
1	C	402	ASP	2.6
1	B	444	GLN	2.5
1	B	115	ALA	2.5
1	C	35	VAL	2.5
1	C	115	ALA	2.5
1	A	407	GLU	2.4
1	D	354	GLU	2.4
1	C	185	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	402	ASP	2.4
1	C	338	ASN	2.4
1	C	357	ASN	2.4
1	C	349	ASP	2.4
1	C	354	GLU	2.4
1	B	451	HIS	2.4
1	C	401	LYS	2.3
1	B	198	ASP	2.3
1	D	410	LYS	2.3
1	D	406	GLN	2.3
1	B	211	PRO	2.3
1	D	198	ASP	2.3
1	B	443	VAL	2.2
1	D	357	ASN	2.2
1	C	210	ASN	2.2
1	C	344	ARG	2.2
1	C	345	ARG	2.2
1	B	407	GLU	2.2
1	B	195	ASP	2.2
1	D	210	ASN	2.2
1	C	407	GLU	2.1
1	C	408	TYR	2.1
1	C	285	THR	2.1
1	D	117	THR	2.1
1	A	286	LYS	2.1
1	C	211	PRO	2.1
1	C	347	ALA	2.1
1	B	116	ALA	2.1
1	D	195	ASP	2.1
1	B	410	LYS	2.0
1	C	339	TYR	2.0
1	A	210	ASN	2.0
1	C	336	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

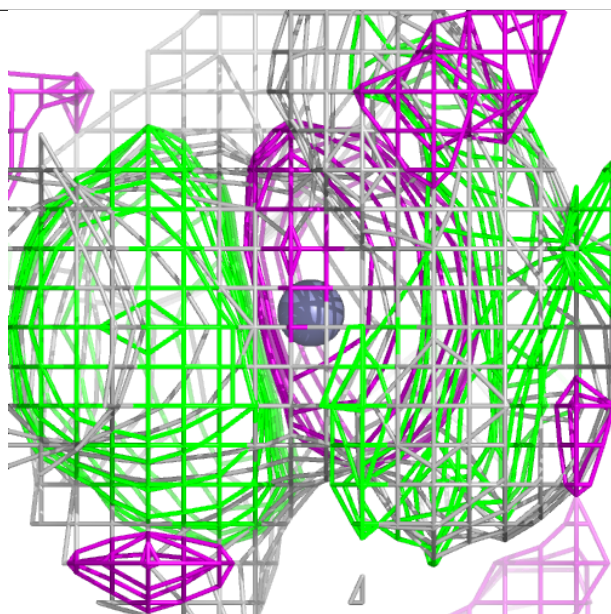
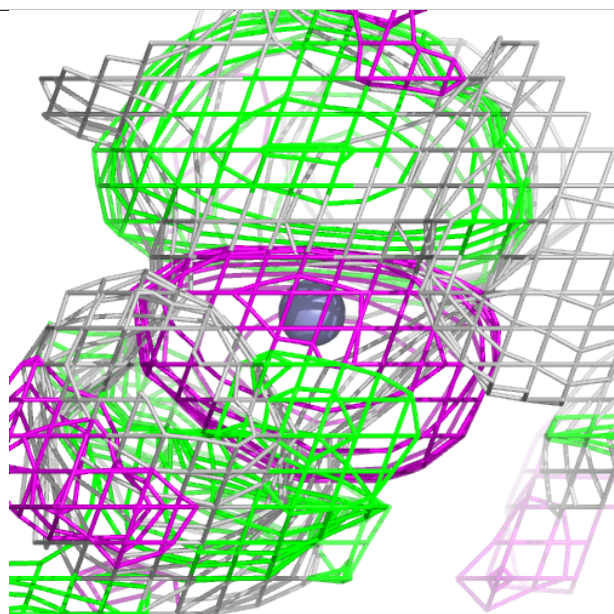
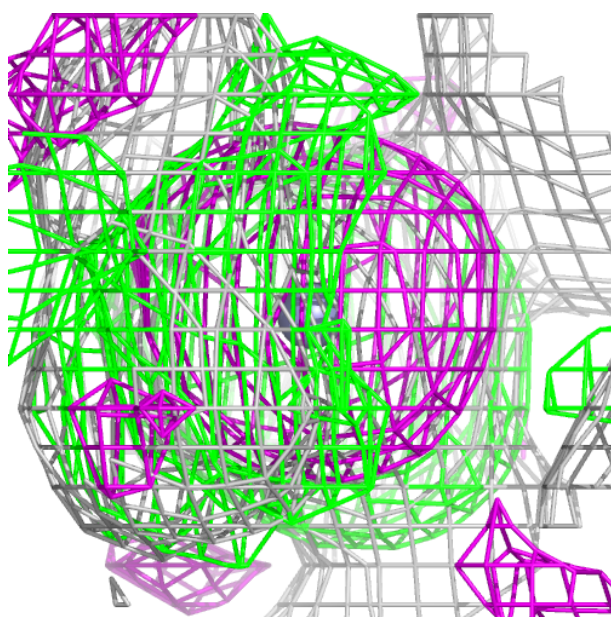
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	ZN	D	503	1/1	0.40	0.28	16,16,16,16	0
5	ZN	B	501	1/1	0.47	0.29	17,17,17,17	0
5	ZN	A	505	1/1	0.51	0.33	14,14,14,14	0
5	ZN	C	501	1/1	0.66	0.15	20,20,20,20	0
4	GOL	A	504	6/6	0.67	0.19	36,39,45,59	0
2	PG4	D	501	13/13	0.87	0.11	27,32,35,36	0
3	PEG	A	503	7/7	0.88	0.13	31,32,42,42	0
2	PG4	A	502	13/13	0.88	0.10	27,29,35,37	0
3	PEG	D	502	7/7	0.90	0.11	24,27,32,33	0
2	PG4	A	501	13/13	0.93	0.08	19,25,28,30	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.



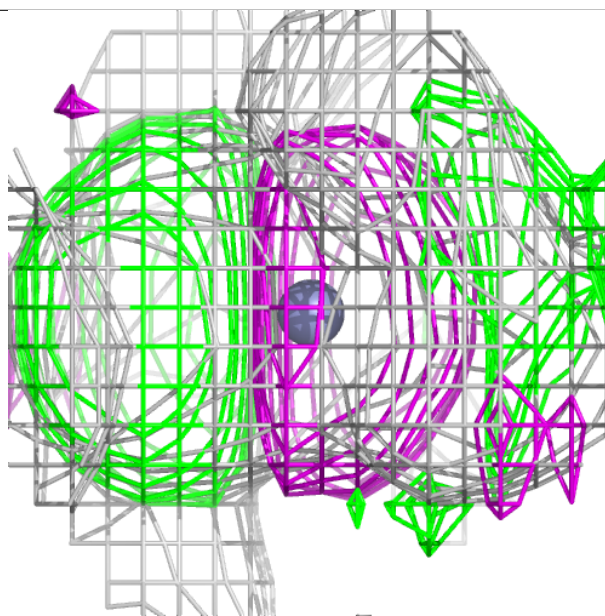
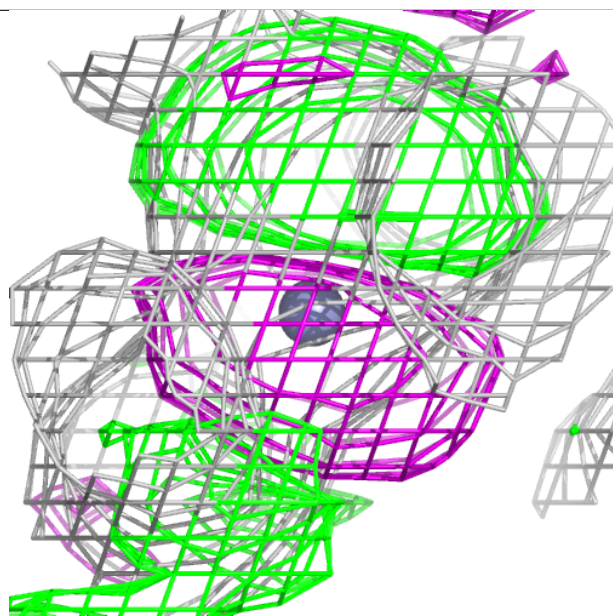
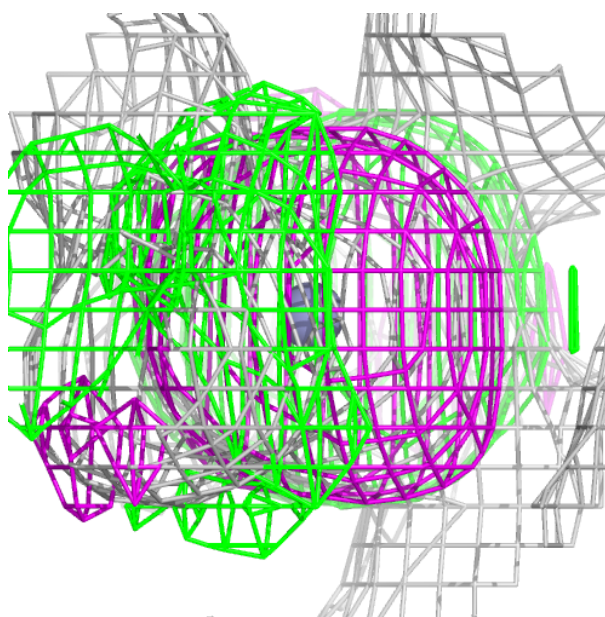
**Electron density around ZN D 503:**

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



**Electron density around ZN B 501:**

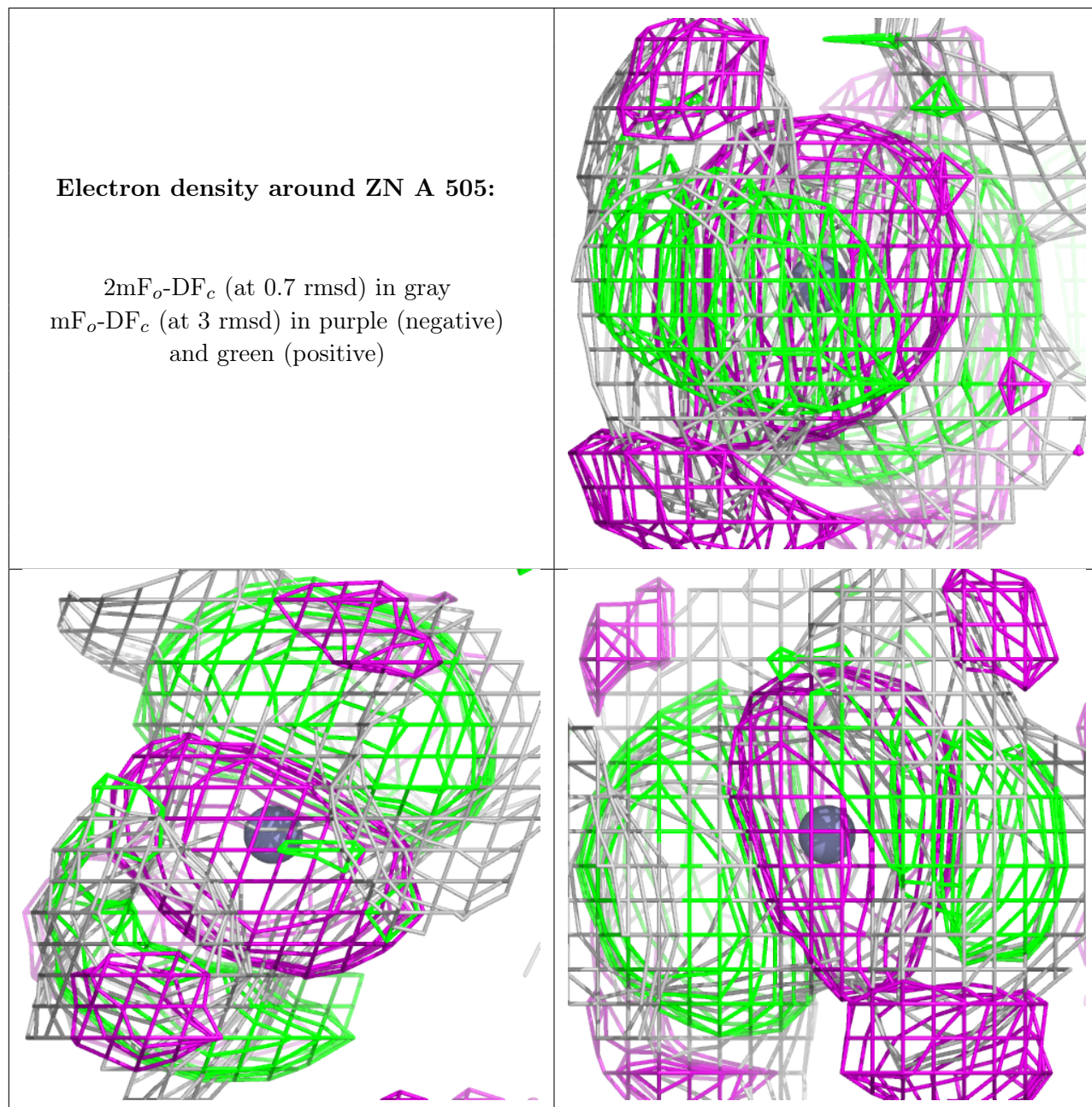
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





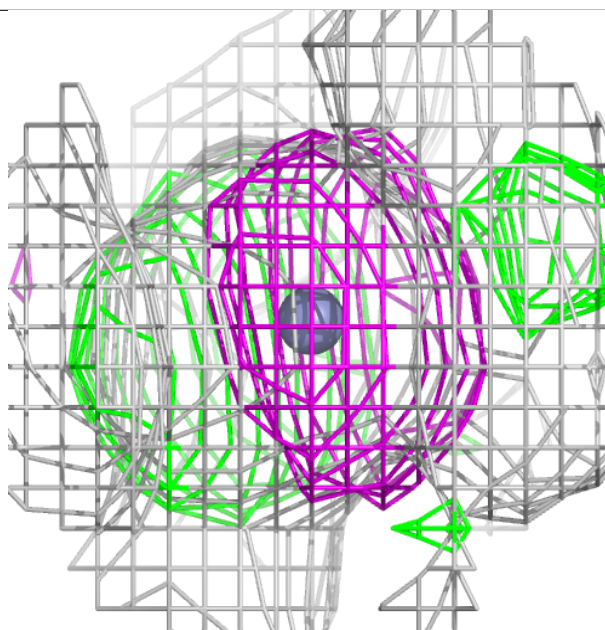
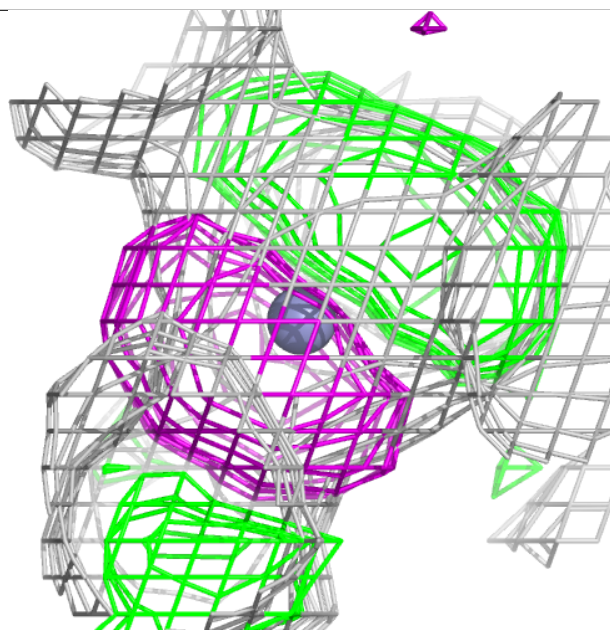
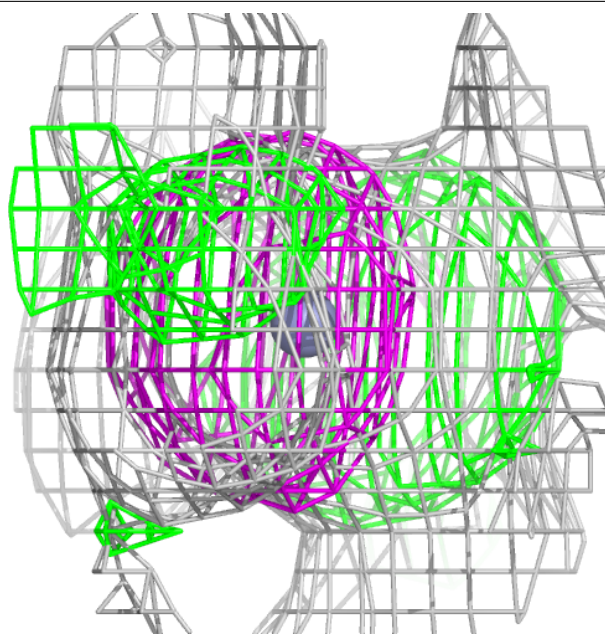
**Electron density around ZN A 505:**

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



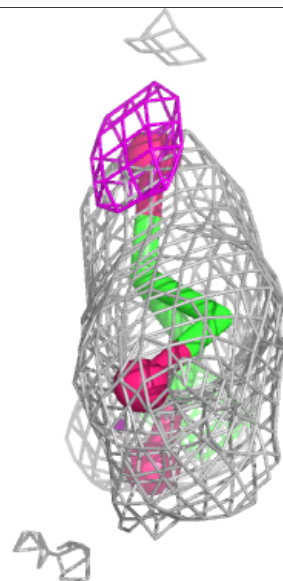
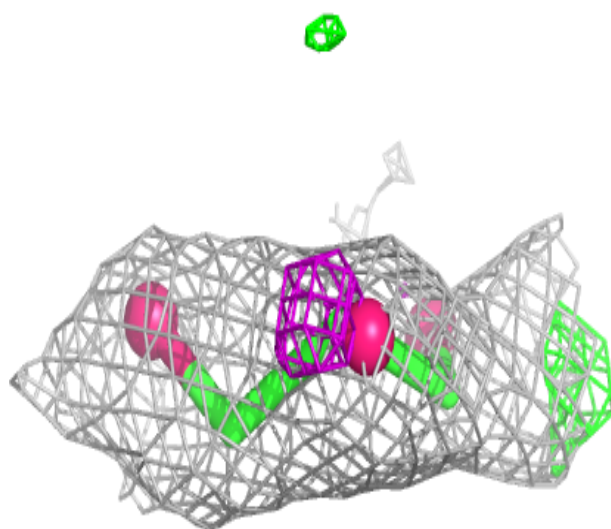
**Electron density around ZN C 501:**

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



**Electron density around GOL A 504:**

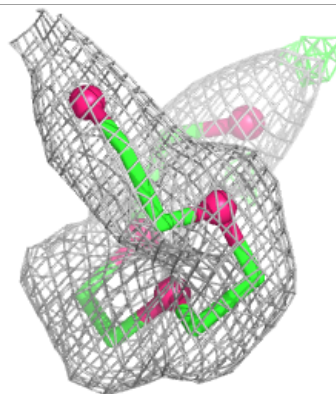
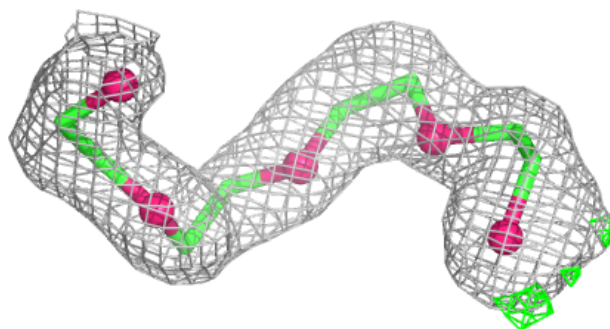
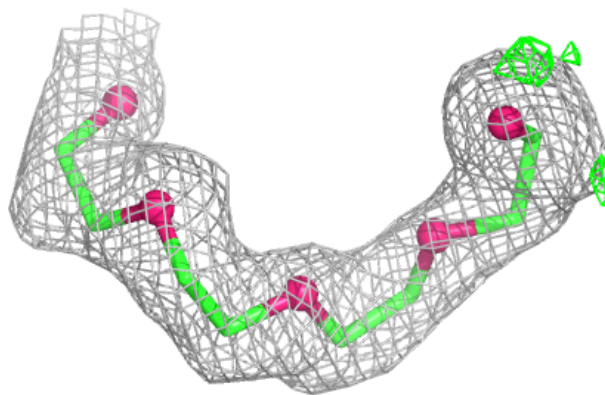
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



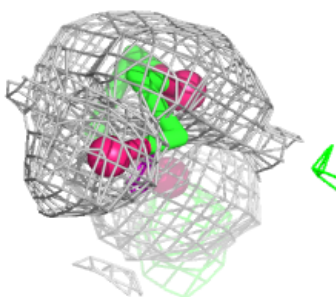
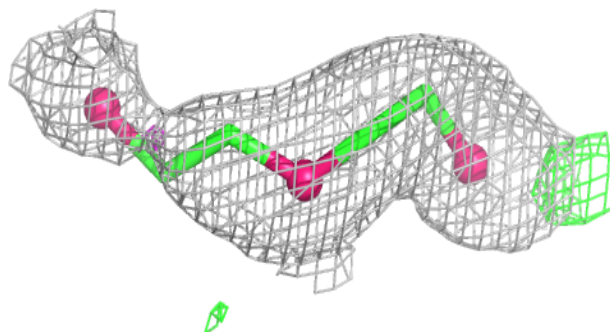
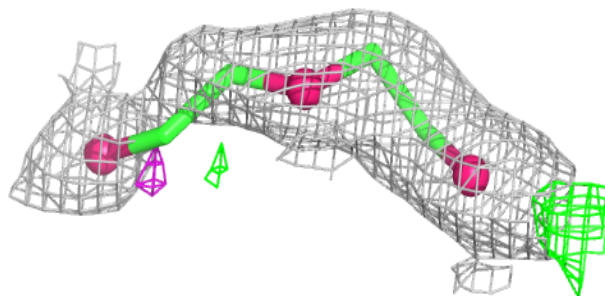


**Electron density around PG4 D 501:**

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

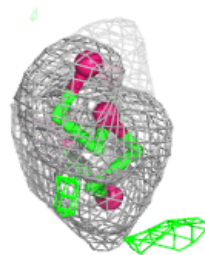
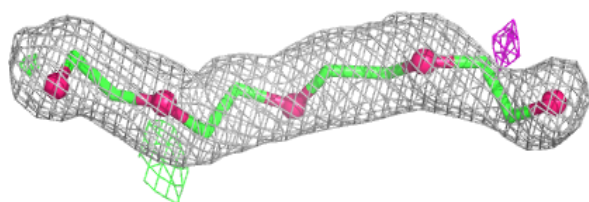
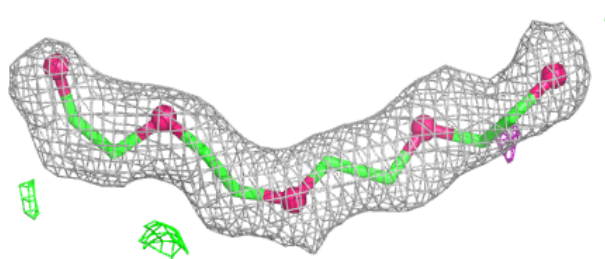
**Electron density around PEG A 503:**

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



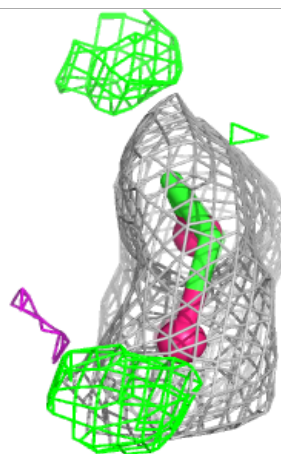
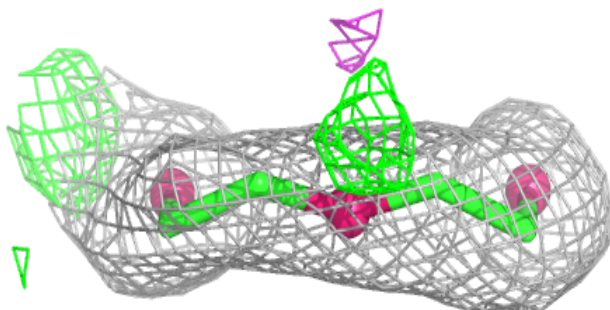
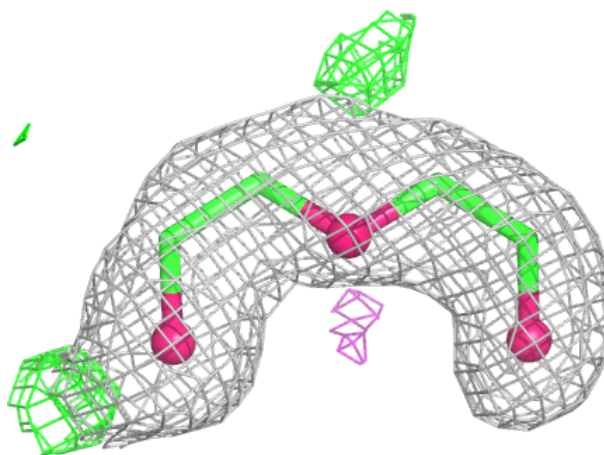
**Electron density around PG4 A 502:**

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



**Electron density around PEG D 502:**

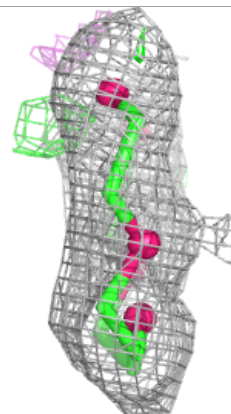
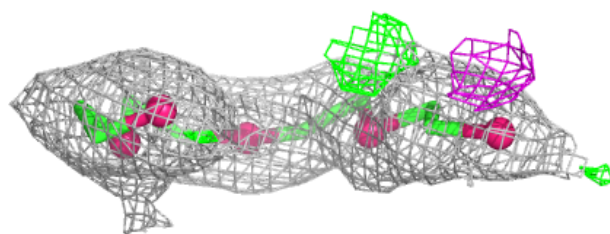
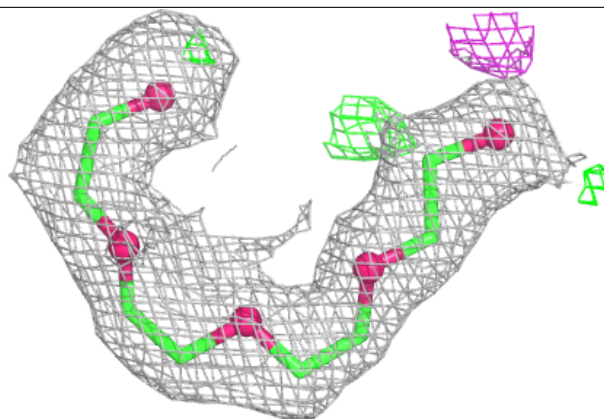
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PG4 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.