



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2025 – 04:16 PM EDT

PDB ID : 8SE1 / pdb_00008se1
Title : Structure of Full-length Human Protein Kinase C Beta 2 (PKCBII) in the Inactive Conformation
Authors : Cong, A.T.Q.; Witter, T.L.; Bruinsma, E.S.; Jayaraman, S.; Dugan, M.B.; Hawse, J.R.; Goetz, M.P.; Schellenberg, M.J.
Deposited on : 2023-04-07
Resolution : 3.32 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

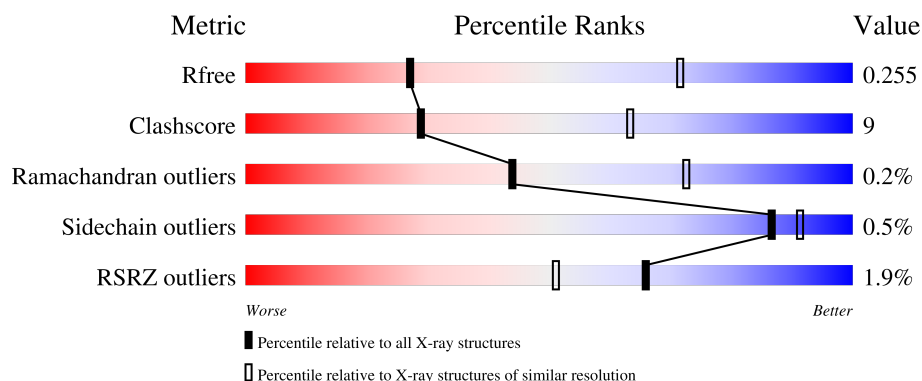
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

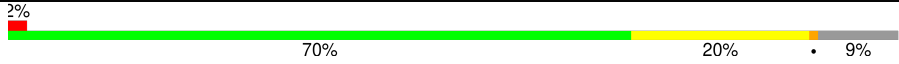

The reported resolution of this entry is 3.32 Å.

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}	164625	1066 (3.34-3.30)
Clashscore	180529	1111 (3.34-3.30)
Ramachandran outliers	177936	1109 (3.34-3.30)
Sidechain outliers	177891	1108 (3.34-3.30)
RSRZ outliers	164620	1066 (3.34-3.30)

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	674	
1	B	674	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10229 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 Protein kinase C beta type.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	610	Total	C	N	O	P	S	0	0	0
			4947	3159	843	902	3	40			
1	B	634	Total	C	N	O	P	S	0	0	0
			5134	3270	876	945	3	40			

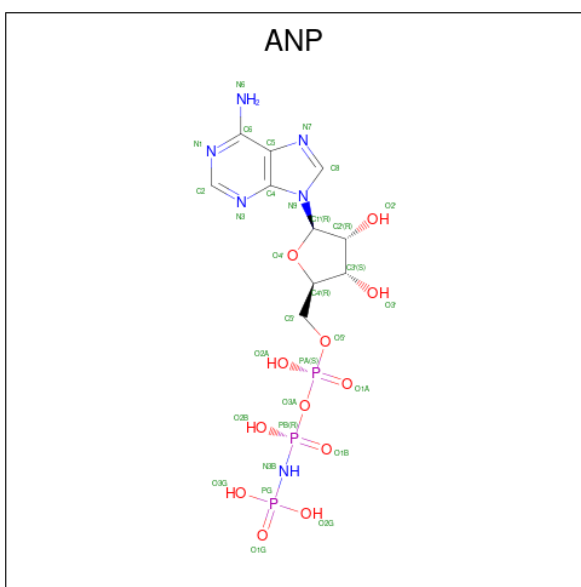
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P05771
A	1	ASN	-	expression tag	UNP P05771
B	0	SER	-	expression tag	UNP P05771
B	1	ASN	-	expression tag	UNP P05771

- 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	5	Total	Zn	0	0
			5	5		
2	B	5	Total	Zn	0	0
			5	5		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



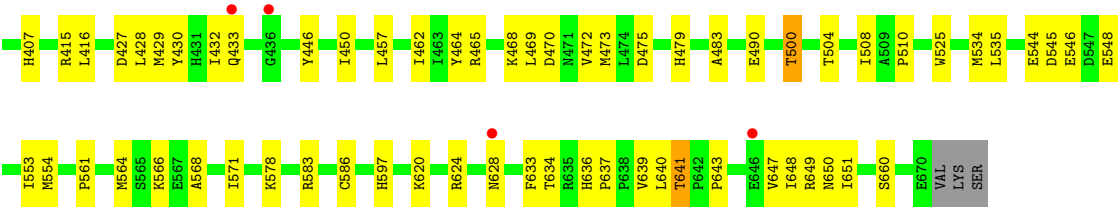
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0
4	B	3	Total Mg 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	34	Total O 34 34	0	0
5	B	36	Total O 36 36	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.56Å 89.10Å 160.71Å 90.00° 107.05° 90.00°	Depositor
Resolution (Å)	48.75 – 3.32 48.75 – 3.32	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.75-3.32) 98.0 (48.75-3.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.199 , 0.256 0.199 , 0.255	Depositor DCC
R_{free} test set	1288 reflections (3.62%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10229	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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: ANP, SEP, ZN, MG, TPO

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	0.23	2/5043 (0.0%)	0.39	0/6791
1	B	0.20	2/5230 (0.0%)	0.37	0/7040
All	All	0.21	4/10273 (0.0%)	0.38	0/13831

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	HIS	C-N	-10.06	1.20	1.33
1	B	155	HIS	C-N	-8.83	1.22	1.33
1	A	156	THR	C-N	6.08	1.41	1.33
1	B	156	THR	C-N	5.14	1.40	1.33

There are no bond angle outliers.

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	4947	0	4829	82	0
1	B	5134	0	5002	89	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	13	1	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	34	0	0	0	0
5	B	36	0	0	1	0
All	All	10229	0	9857	173	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 9.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LYS:HE3	1:B:415:ARG:HH22	1.30	0.94
1:B:415:ARG:NH2	1:B:641:TPO:O	2.10	0.85
1:B:374:LYS:HG2	1:B:415:ARG:NH1	1.93	0.82
1:A:186:MET:HE3	1:A:256:MET:HG2	1.63	0.79
1:A:114:PHE:HE1	1:A:381:ASP:HB3	1.53	0.74
1:B:367:LEU:HD21	1:B:624:ARG:HG2	1.72	0.71
1:A:354:GLY:HA3	1:A:372:ILE:O	1.92	0.70
1:B:387:THR:HG21	1:B:416:LEU:HD13	1.74	0.69
1:A:387:THR:HG21	1:A:416:LEU:HD13	1.74	0.69
1:B:393:VAL:HG22	1:B:462:ILE:HD13	1.76	0.68
1:B:415:ARG:NH1	5:B:802:HOH:O	2.27	0.68
1:A:566:LYS:NZ	1:A:567:GLU:OE2	2.27	0.68
1:B:165:GLN:HB2	1:B:176:LEU:HB3	1.76	0.68
1:B:374:LYS:CG	1:B:415:ARG:HH12	2.07	0.67
1:B:354:GLY:HA3	1:B:372:ILE:O	1.95	0.66
1:B:427:ASP:HA	1:B:473:MET:HA	1.78	0.66
1:B:374:LYS:CG	1:B:415:ARG:NH1	2.60	0.65
1:B:104:PHE:HE2	1:B:147:VAL:HG21	1.62	0.64
1:A:336:ARG:NH2	1:A:660:SEP:O2P	2.24	0.64
1:B:310:ILE:HG22	1:B:311:SER:H	1.62	0.64
1:A:446:TYR:HB2	1:A:534:MET:HE1	1.80	0.63
1:A:429:MET:O	1:A:433:GLN:HG2	1.97	0.63
1:B:468:LYS:HE3	1:B:470:ASP:HB2	1.79	0.63
1:A:110:SER:O	1:A:350:LYS:NZ	2.27	0.63
1:A:415:ARG:NH2	1:A:641:TPO:O	2.33	0.62
1:B:446:TYR:HB2	1:B:534:MET:HE1	1.81	0.61
1:B:620:LYS:O	1:B:628:ASN:ND2	2.30	0.61
1:B:465:ARG:NH1	1:B:500:TPO:O3P	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:HG22	1:A:244:ILE:HG12	1.83	0.60
1:B:90:ASP:HB3	1:B:148:PRO:HG3	1.82	0.60
1:A:105:LYS:HE2	1:A:133:ASP:OD2	2.01	0.59
1:A:232:LYS:N	1:A:235:ASP:OD2	2.31	0.59
1:B:355:LYS:NZ	1:B:639:VAL:O	2.36	0.59
1:B:199:LYS:HG3	1:B:241:SER:HB3	1.85	0.59
1:A:432:ILE:HD11	1:A:469:LEU:HD13	1.85	0.58
1:A:553:ILE:O	1:A:578:LYS:NZ	2.35	0.58
1:A:620:LYS:O	1:A:628:ASN:ND2	2.35	0.58
1:A:165:GLN:HB2	1:A:176:LEU:HB3	1.84	0.58
1:B:212:THR:HG22	1:B:227:PHE:CZ	2.39	0.58
1:B:235:ASP:HA	1:B:238:ARG:HD3	1.85	0.58
1:A:565:SER:OG	1:A:567:GLU:OE1	2.22	0.58
1:B:105:LYS:HE2	1:B:133:ASP:OD2	2.04	0.58
1:B:464:TYR:OH	1:B:483:ALA:O	2.20	0.57
1:B:371:LYS:NZ	1:B:390:GLU:OE2	2.22	0.56
1:A:464:TYR:OH	1:A:483:ALA:O	2.23	0.56
1:B:93:PRO:HG3	1:B:184:VAL:HG11	1.87	0.56
1:B:311:SER:O	1:B:650:ASN:ND2	2.37	0.56
1:B:349:GLY:HA2	1:B:633:PHE:CD2	2.41	0.56
1:B:246:ASP:OD2	1:B:248:ASP:OD2	2.24	0.56
1:A:427:ASP:HA	1:A:473:MET:HA	1.88	0.56
1:A:468:LYS:HE3	1:A:470:ASP:HB2	1.88	0.56
1:A:57:ILE:HG23	1:A:63:GLN:HB2	1.87	0.55
1:A:545:ASP:OD1	1:A:548:GLU:N	2.31	0.55
1:A:98:PRO:HG3	1:A:185:PRO:HB2	1.89	0.55
1:A:235:ASP:HA	1:A:238:ARG:HD2	1.89	0.55
1:B:374:LYS:HE3	1:B:415:ARG:NH2	2.12	0.55
1:A:647:VAL:O	1:A:651:ILE:HG23	2.06	0.54
1:A:212:THR:HG22	1:A:227:PHE:HZ	1.73	0.54
1:A:589:GLU:HB3	1:A:592:ARG:HE	1.73	0.54
1:B:309:LYS:O	1:B:312:GLN:NE2	2.41	0.54
1:A:162:ILE:HD12	1:A:244:ILE:HD11	1.90	0.53
1:A:179:ASP:HB3	1:A:222:GLU:HG3	1.90	0.52
1:A:265:GLU:O	1:A:269:ALA:CB	2.58	0.52
1:B:429:MET:O	1:B:433:GLN:HG2	2.10	0.52
1:B:637:PRO:HB2	1:B:639:VAL:HG13	1.92	0.52
1:B:561:PRO:HG2	1:B:564:MET:HG3	1.92	0.52
1:A:212:THR:HG22	1:A:227:PHE:CZ	2.44	0.52
1:A:579:HIS:HD2	1:A:580:PRO:HD2	1.75	0.51
1:B:104:PHE:CE2	1:B:147:VAL:HG21	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:THR:HG22	1:B:227:PHE:HZ	1.76	0.51
1:B:247:TRP:CZ2	1:B:249:LEU:HB2	2.46	0.50
1:B:648:ILE:O	1:B:651:ILE:HG12	2.12	0.50
1:B:47:PRO:HA	1:B:57:ILE:O	2.11	0.50
1:B:196:VAL:HG22	1:B:244:ILE:HG12	1.92	0.50
1:B:545:ASP:OD1	1:B:546:GLU:N	2.45	0.50
1:A:345:LEU:HD11	1:A:360:GLU:HB2	1.93	0.50
1:A:348:LEU:HD21	1:A:358:LEU:HB2	1.91	0.50
1:A:265:GLU:O	1:A:269:ALA:HB2	2.12	0.49
1:B:337:MET:HE3	1:B:407:HIS:CE1	2.47	0.49
1:A:353:PHE:HB2	1:A:373:LEU:HD22	1.94	0.49
1:B:35:LYS:HB3	1:B:85:SER:HA	1.94	0.49
1:A:52:HIS:NE2	1:A:81:PHE:O	2.46	0.48
1:A:560:TYR:HE2	1:A:573:LYS:HE3	1.78	0.48
1:B:37:HIS:HE1	1:B:70:CYS:SG	2.36	0.48
3:A:706:ANP:N3B	3:A:706:ANP:O1A	2.47	0.48
1:B:205:LYS:HB2	1:B:207:GLU:HG3	1.96	0.48
1:B:173:LEU:HB2	1:B:231:LEU:HD11	1.95	0.48
1:A:349:GLY:HA2	1:A:633:PHE:CD2	2.49	0.47
1:B:428:LEU:O	1:B:432:ILE:HG12	2.14	0.47
1:A:510:PRO:HD3	1:A:525:TRP:CE2	2.49	0.47
1:A:34:VAL:O	1:A:37:HIS:HB2	2.14	0.47
1:A:648:ILE:O	1:A:651:ILE:HG12	2.14	0.47
1:A:232:LYS:C	1:A:234:SER:H	2.22	0.47
1:A:93:PRO:HB3	1:A:159:ARG:HH12	1.79	0.47
1:B:168:ILE:HD12	1:B:267:GLN:HG3	1.97	0.47
3:B:706:ANP:N3B	3:B:706:ANP:O1A	2.48	0.47
1:B:553:ILE:O	1:B:578:LYS:NZ	2.37	0.47
1:A:100:SER:C	1:A:102:HIS:H	2.23	0.46
1:A:95:SER:OG	1:A:96:ASP:N	2.47	0.46
1:A:104:PHE:HB3	1:A:130:MET:HB3	1.97	0.46
1:B:374:LYS:HG3	1:B:415:ARG:HH12	1.78	0.46
1:A:394:LEU:HB3	1:A:406:LEU:HB2	1.98	0.46
1:B:427:ASP:OD1	1:B:427:ASP:N	2.44	0.46
1:A:101:LYS:O	1:A:103:LYS:N	2.40	0.46
1:B:504:THR:O	1:B:508:ILE:HG13	2.16	0.46
1:A:191:LEU:HD22	1:A:217:CYS:SG	2.56	0.46
1:A:372:ILE:HG12	1:A:417:TYR:CD2	2.52	0.45
1:B:194:PRO:HD2	1:B:215:ILE:O	2.17	0.45
1:B:392:ARG:NH2	1:B:490:GLU:OE1	2.49	0.45
1:A:35:LYS:HB3	1:A:85:SER:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLN:O	1:B:307:ARG:HG3	2.15	0.45
1:B:179:ASP:HB3	1:B:222:GLU:HG3	1.98	0.45
1:A:111:SER:OG	1:A:641:TPO:O1P	2.22	0.45
1:B:554:MET:HE3	1:B:554:MET:HB3	1.87	0.45
1:A:509:ALA:HB3	1:A:522:VAL:HG12	1.99	0.45
1:B:312:GLN:HA	1:B:649:ARG:HH22	1.82	0.45
1:B:372:ILE:HD13	1:B:640:LEU:HD21	1.99	0.45
1:A:535:LEU:HD13	1:A:568:ALA:HB1	1.98	0.45
1:B:348:LEU:HD21	1:B:358:LEU:HB2	1.98	0.45
1:B:475:ASP:OD1	1:B:479:HIS:N	2.45	0.45
1:B:535:LEU:HD13	1:B:568:ALA:HB1	1.99	0.45
1:B:42:ARG:HD2	1:B:119:GLY:HA3	1.99	0.44
1:B:399:LYS:NZ	1:B:404:THR:O	2.50	0.44
1:A:428:LEU:O	1:A:432:ILE:HG12	2.17	0.44
1:B:647:VAL:O	1:B:651:ILE:HG23	2.17	0.44
1:B:350:LYS:HG2	1:B:355:LYS:HG2	2.00	0.44
1:B:571:ILE:HB	1:B:597:HIS:CE1	2.52	0.44
1:B:450:ILE:HD11	1:B:472:VAL:HG11	1.99	0.44
1:A:179:ASP:OD2	1:A:181:LYS:HE2	2.18	0.44
1:A:258:SER:OG	1:A:283:GLY:HA3	2.18	0.43
1:A:429:MET:HE2	1:A:469:LEU:HB2	1.99	0.43
1:A:20:PHE:CE2	1:A:432:ILE:HD12	2.52	0.43
1:A:62:LYS:HD3	1:A:379:ILE:O	2.17	0.43
1:A:511:GLU:OE1	1:A:583:ARG:NH2	2.48	0.43
1:B:197:LYS:HE3	1:B:197:LYS:HB2	1.78	0.43
1:A:154:ASP:OD2	1:A:156:THR:OG1	2.28	0.43
1:A:411:GLN:HG2	1:A:660:SEP:O3P	2.18	0.43
1:B:27:ARG:HG2	1:B:123:TYR:CZ	2.54	0.43
1:B:510:PRO:HD3	1:B:525:TRP:CE2	2.54	0.43
1:B:583:ARG:HB3	1:B:586:CYS:SG	2.59	0.43
1:A:120:SER:HB2	1:A:140:HIS:HE1	1.84	0.43
1:A:75:HIS:HB2	1:A:78:CYS:SG	2.58	0.42
1:A:487:MET:HE3	1:A:487:MET:HB2	1.92	0.42
1:B:636:HIS:HB3	1:B:637:PRO:CD	2.49	0.42
1:A:93:PRO:HG3	1:A:184:VAL:HG11	1.99	0.42
1:B:93:PRO:CG	1:B:184:VAL:HG11	2.48	0.42
1:A:93:PRO:HD3	1:A:150:LEU:HD11	2.02	0.42
1:B:34:VAL:O	1:B:37:HIS:HB2	2.20	0.42
1:A:405:GLN:HB2	1:A:421:GLU:OE2	2.20	0.42
1:B:643:PRO:HG2	1:B:648:ILE:HG13	2.01	0.42
1:A:216:LYS:HE2	1:A:247:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:SER:OG	1:B:252:ARG:N	2.53	0.42
1:B:276:LYS:HG3	1:B:290:VAL:HG22	2.02	0.42
1:A:140:HIS:HB2	1:A:143:CYS:SG	2.61	0.41
1:A:431:HIS:O	1:A:435:VAL:HG23	2.20	0.41
1:A:33:GLU:HA	1:A:37:HIS:O	2.20	0.41
1:B:139:VAL:HG11	1:B:147:VAL:HG11	2.02	0.41
1:B:566:LYS:HE2	1:B:566:LYS:HB3	1.93	0.41
1:B:374:LYS:HG2	1:B:415:ARG:CZ	2.50	0.41
1:A:57:ILE:HG12	1:A:75:HIS:CD2	2.55	0.41
1:B:430:TYR:HA	1:B:433:GLN:HG3	2.03	0.41
1:B:427:ASP:HB3	1:B:473:MET:HG2	2.02	0.41
1:B:544:GLU:HG2	1:B:548:GLU:OE1	2.20	0.41
1:A:427:ASP:OD1	1:A:427:ASP:N	2.43	0.41
1:A:625:ASN:O	1:A:627:GLU:N	2.52	0.41
1:B:634:THR:C	1:B:636:HIS:H	2.29	0.41
1:B:432:ILE:HD11	1:B:469:LEU:HD13	2.02	0.41
1:B:232:LYS:N	1:B:235:ASP:OD2	2.44	0.40
1:A:571:ILE:HB	1:A:597:HIS:CE1	2.56	0.40
1:B:457:LEU:HD23	1:B:457:LEU:HA	1.90	0.40
1:A:98:PRO:CG	1:A:185:PRO:HB2	2.50	0.40
1:A:560:TYR:CD2	1:A:569:VAL:HG13	2.56	0.40
1:A:560:TYR:CE2	1:A:573:LYS:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	603/674 (90%)	551 (91%)	51 (8%)	1 (0%)	44	72
1	B	625/674 (93%)	573 (92%)	51 (8%)	1 (0%)	44	72
All	All	1228/1348 (91%)	1124 (92%)	102 (8%)	2 (0%)	44	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	PHE
1	B	253	ASN

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	540/594 (91%)	538 (100%)	2 (0%)	89	93
1	B	560/594 (94%)	557 (100%)	3 (0%)	86	91
All	All	1100/1188 (93%)	1095 (100%)	5 (0%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	SER
1	A	558	VAL
1	B	54	THR
1	B	307	ARG
1	B	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	A	431	HIS
1	A	491	ASN
1	A	556	HIS
1	A	579	HIS
1	B	63	GLN
1	B	167	HIS
1	B	312	GLN
1	B	407	HIS
1	B	433	GLN

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Mol	Chain	Res	Type
1	B	491	ASN
1	B	551	GLN
1	B	556	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	SEP	B	660	1	8,9,10	1.05	0	7,12,14	1.55	1 (14%)
1	SEP	A	660	1	8,9,10	1.00	0	7,12,14	1.24	1 (14%)
1	TPO	B	641	1	8,10,11	1.66	1 (12%)	10,14,16	2.00	1 (10%)
1	TPO	A	500	1	8,10,11	1.10	0	10,14,16	2.06	1 (10%)
1	TPO	B	500	1	8,10,11	1.62	1 (12%)	10,14,16	2.20	1 (10%)
1	TPO	A	641	1	8,10,11	1.66	1 (12%)	10,14,16	2.11	1 (10%)

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
1	SEP	B	660	1	-	5/6/8/10	-
1	SEP	A	660	1	-	3/6/8/10	-
1	TPO	B	641	1	-	1/9/11/13	-
1	TPO	A	500	1	-	2/9/11/13	-
1	TPO	B	500	1	-	2/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	641	1	-	0/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	500	TPO	P-O1P	3.51	1.61	1.50
1	A	641	TPO	P-O1P	3.46	1.61	1.50
1	B	641	TPO	P-O1P	3.43	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	500	TPO	P-OG1-CB	-6.51	105.65	123.33
1	A	641	TPO	P-OG1-CB	-6.00	107.01	123.33
1	A	500	TPO	P-OG1-CB	-5.92	107.25	123.33
1	B	641	TPO	P-OG1-CB	-5.68	107.90	123.33
1	B	660	SEP	OG-CB-CA	3.48	111.53	108.14
1	A	660	SEP	OG-CB-CA	2.46	110.54	108.14

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	660	SEP	N-CA-CB-OG
1	A	660	SEP	C-CA-CB-OG
1	B	660	SEP	N-CA-CB-OG
1	B	660	SEP	C-CA-CB-OG
1	B	660	SEP	CB-OG-P-O1P
1	B	660	SEP	CB-OG-P-O2P
1	B	660	SEP	CB-OG-P-O3P
1	A	660	SEP	CA-CB-OG-P
1	B	500	TPO	CB-OG1-P-O3P
1	A	500	TPO	C-CA-CB-CG2
1	B	500	TPO	C-CA-CB-CG2
1	B	641	TPO	O-C-CA-CB
1	A	500	TPO	CB-OG1-P-O1P

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	660	SEP	2	0
1	B	641	TPO	1	0
1	B	500	TPO	1	0
1	A	641	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 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	ANP	B	706	4	29,33,33	1.13	4 (13%)	31,52,52	0.86	1 (3%)
3	ANP	A	706	4	29,33,33	1.09	3 (10%)	31,52,52	0.88	2 (6%)

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	ANP	B	706	4	-	6/14/38/38	0/3/3/3
3	ANP	A	706	4	-	6/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	ANP	PG-N3B	2.62	1.70	1.63
3	B	706	ANP	PG-N3B	2.54	1.70	1.63
3	A	706	ANP	PG-O1G	2.47	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	706	ANP	PB-O3A	-2.46	1.56	1.59
3	B	706	ANP	PG-O1G	2.45	1.49	1.46
3	B	706	ANP	PB-O1B	2.27	1.49	1.46
3	A	706	ANP	PB-O3A	-2.09	1.56	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	706	ANP	C5-C6-N6	2.30	123.82	120.31
3	A	706	ANP	C5-C6-N6	2.28	123.78	120.31
3	A	706	ANP	O3G-PG-O1G	-2.02	108.37	113.45

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	706	ANP	PG-N3B-PB-O1B
3	A	706	ANP	PG-N3B-PB-O3A
3	B	706	ANP	PG-N3B-PB-O1B
3	B	706	ANP	PG-N3B-PB-O3A
3	A	706	ANP	O4'-C4'-C5'-O5'
3	B	706	ANP	O4'-C4'-C5'-O5'
3	A	706	ANP	C3'-C4'-C5'-O5'
3	B	706	ANP	C3'-C4'-C5'-O5'
3	A	706	ANP	PB-O3A-PA-O1A
3	B	706	ANP	PB-O3A-PA-O1A
3	A	706	ANP	PB-O3A-PA-O2A
3	B	706	ANP	PB-O3A-PA-O2A

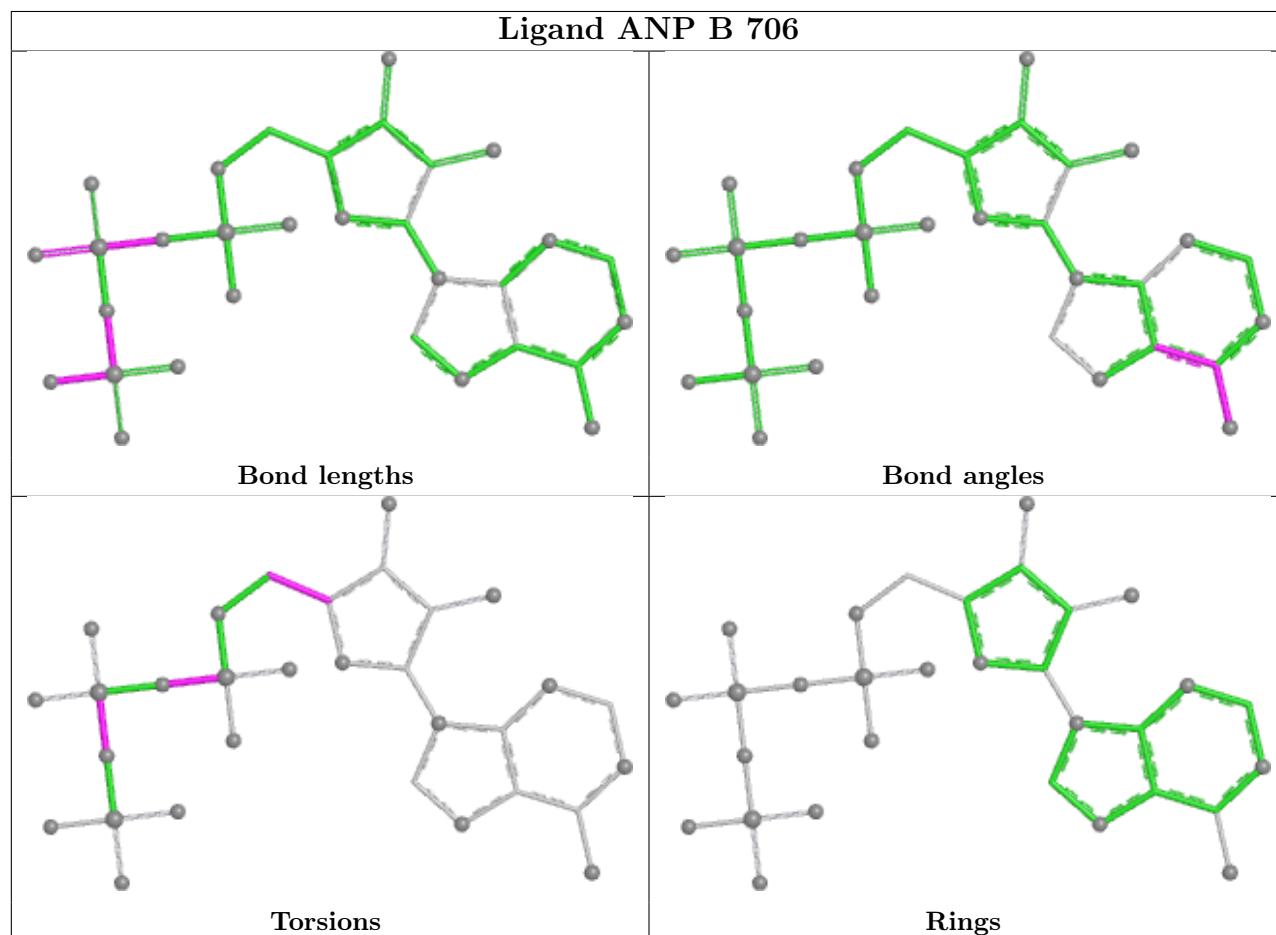
There are no ring outliers.

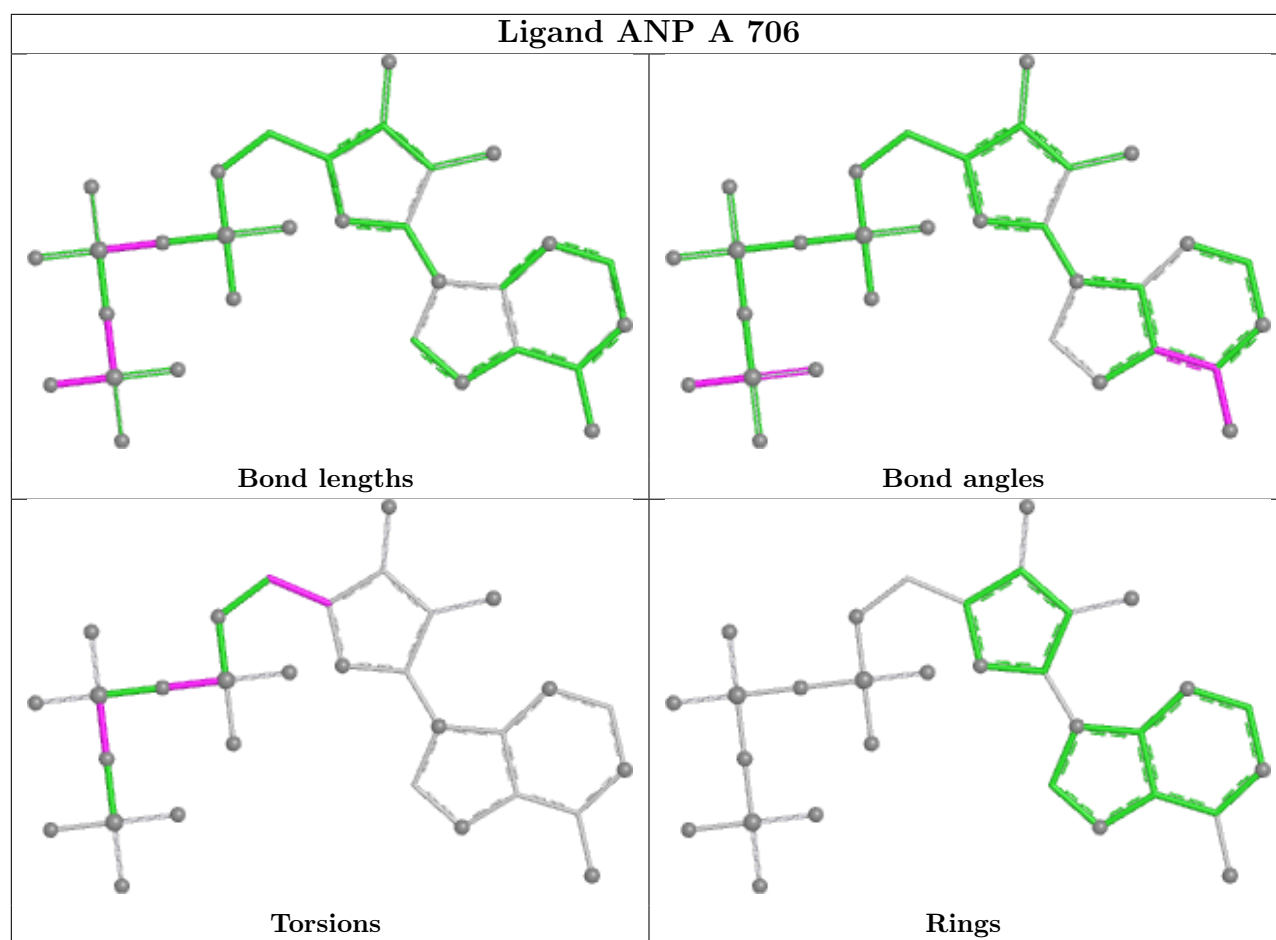
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	706	ANP	1	0
3	A	706	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	607/674 (90%)	0.12	12 (1%)	64 49	29, 65, 119, 191	0
1	B	631/674 (93%)	-0.01	12 (1%)	66 51	31, 52, 98, 163	0
All	All	1238/1348 (91%)	0.05	24 (1%)	66 51	29, 58, 110, 191	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	PRO	3.9
1	A	62	LYS	3.2
1	B	250	THR	3.1
1	A	60	PHE	3.0
1	A	249	LEU	2.9
1	B	312	GLN	2.8
1	A	414	ASP	2.8
1	B	436	GLY	2.8
1	A	189	ASN	2.6
1	A	208	SER	2.5
1	A	291	PRO	2.5
1	A	61	GLY	2.4
1	A	290	VAL	2.4
1	A	51	SER	2.3
1	B	433	GLN	2.3
1	B	19	ARG	2.3
1	B	251	SER	2.2
1	B	335	ASP	2.2
1	B	310	ILE	2.1
1	B	62	LYS	2.1
1	B	322	THR	2.1
1	B	646	GLU	2.1
1	A	93	PRO	2.1
1	B	628	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	B	641	11/12	0.87	0.10	60,65,75,77	0
1	TPO	A	641	11/12	0.90	0.10	70,78,88,89	0
1	SEP	B	660	10/11	0.92	0.10	46,52,58,58	0
1	SEP	A	660	10/11	0.95	0.08	41,47,54,56	0
1	TPO	A	500	11/12	0.96	0.08	37,40,43,44	0
1	TPO	B	500	11/12	0.96	0.09	28,34,41,46	0

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.

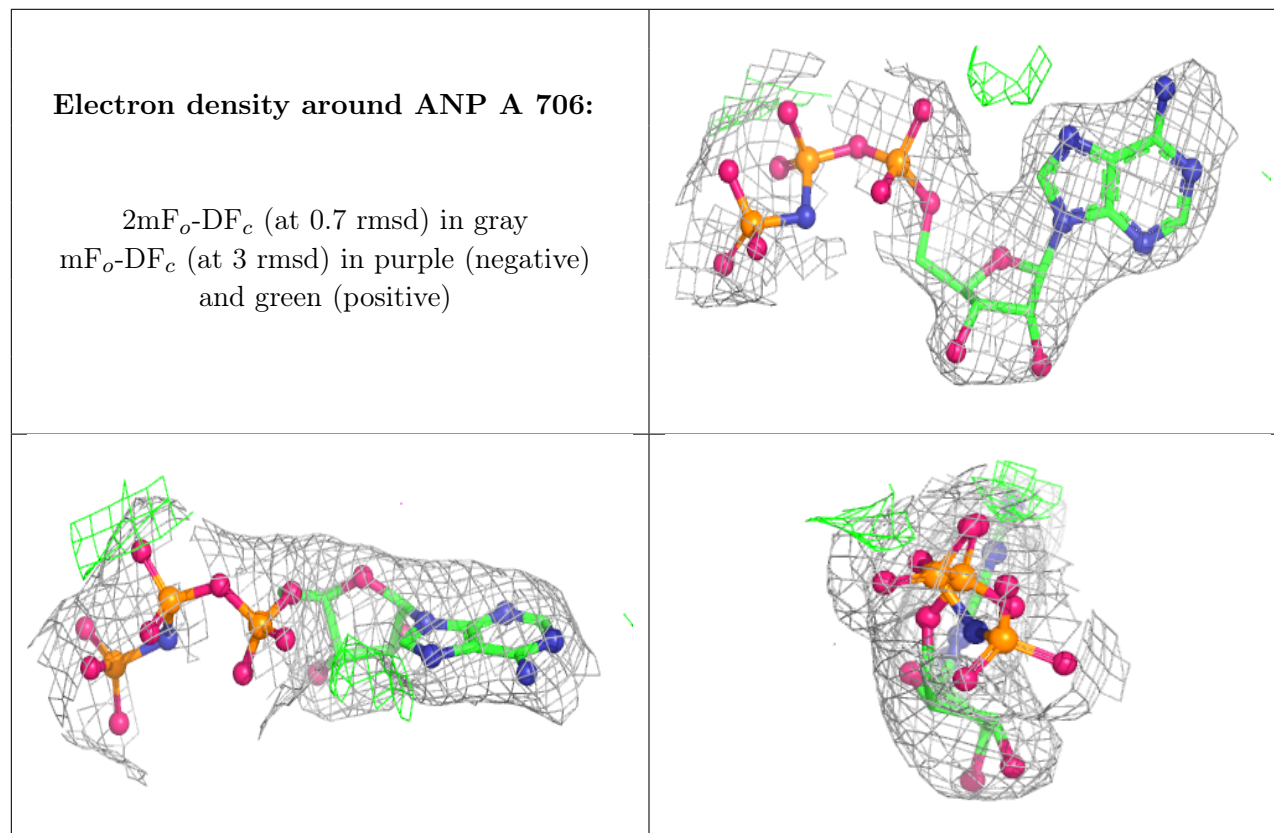
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ANP	A	706	31/31	0.97	0.07	32,36,41,42	0
3	ANP	B	706	31/31	0.97	0.07	29,40,44,45	0
4	MG	A	709	1/1	0.97	0.09	74,74,74,74	0
2	ZN	A	703	1/1	0.98	0.04	51,51,51,51	0
2	ZN	B	702	1/1	0.99	0.03	30,30,30,30	0
2	ZN	B	703	1/1	0.99	0.02	41,41,41,41	0
2	ZN	B	705	1/1	0.99	0.02	22,22,22,22	0
2	ZN	A	701	1/1	0.99	0.05	60,60,60,60	0
2	ZN	A	705	1/1	0.99	0.05	32,32,32,32	0
4	MG	A	707	1/1	0.99	0.03	29,29,29,29	0
4	MG	A	708	1/1	0.99	0.04	47,47,47,47	0
2	ZN	B	701	1/1	0.99	0.02	35,35,35,35	0
4	MG	B	707	1/1	0.99	0.04	23,23,23,23	0
4	MG	B	708	1/1	0.99	0.05	32,32,32,32	0
4	MG	B	709	1/1	0.99	0.05	33,33,33,33	0
2	ZN	A	702	1/1	1.00	0.04	50,50,50,50	0

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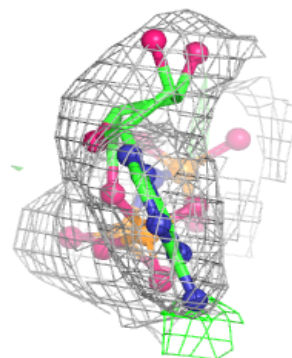
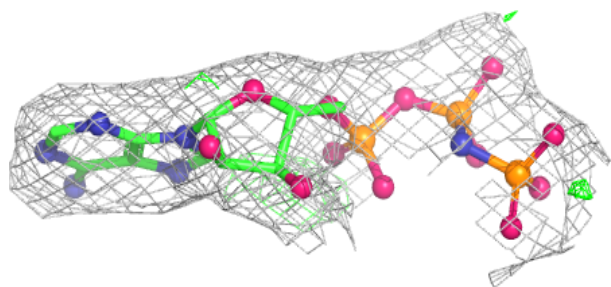
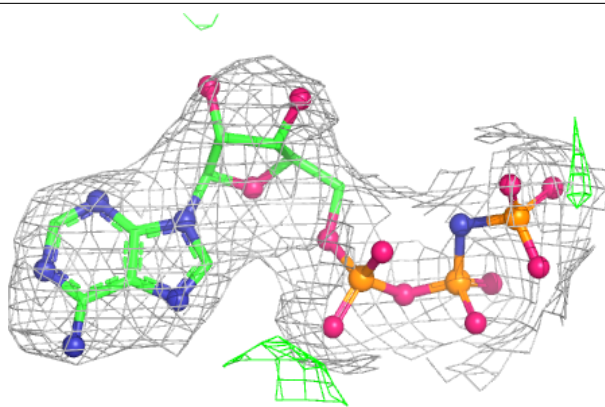
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	A	704	1/1	1.00	0.04	38,38,38,38	0
2	ZN	B	704	1/1	1.00	0.03	37,37,37,37	0

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.



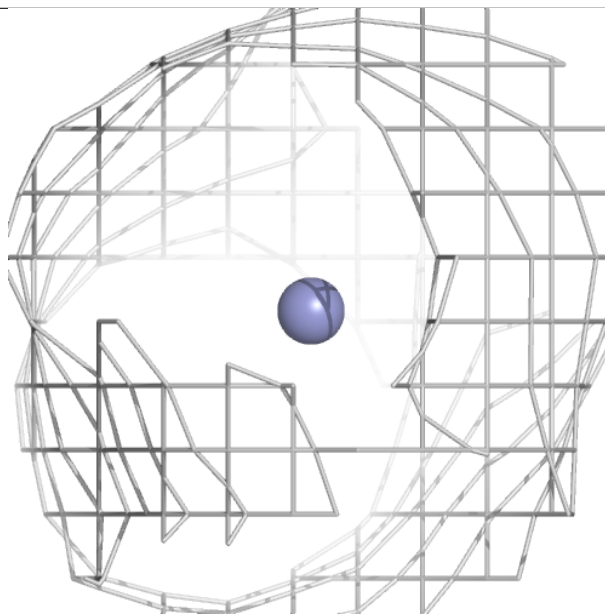
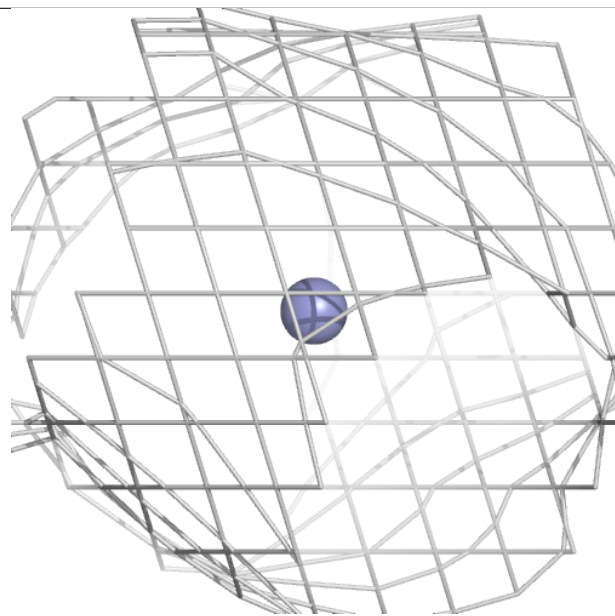
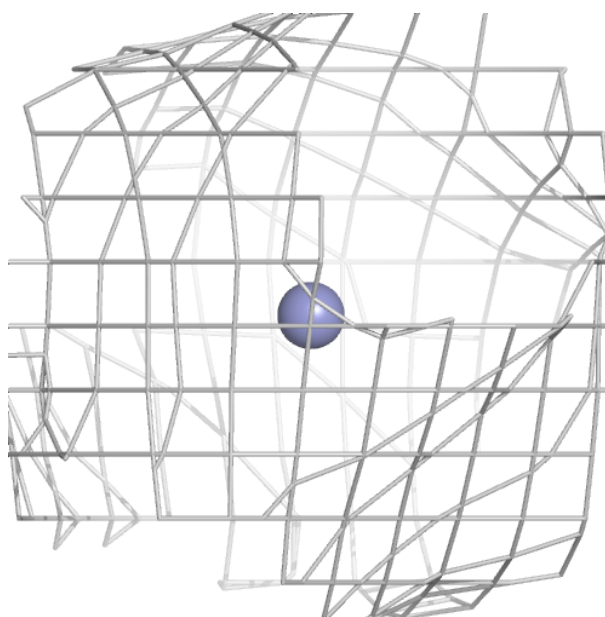
Electron density around ANP B 706:

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



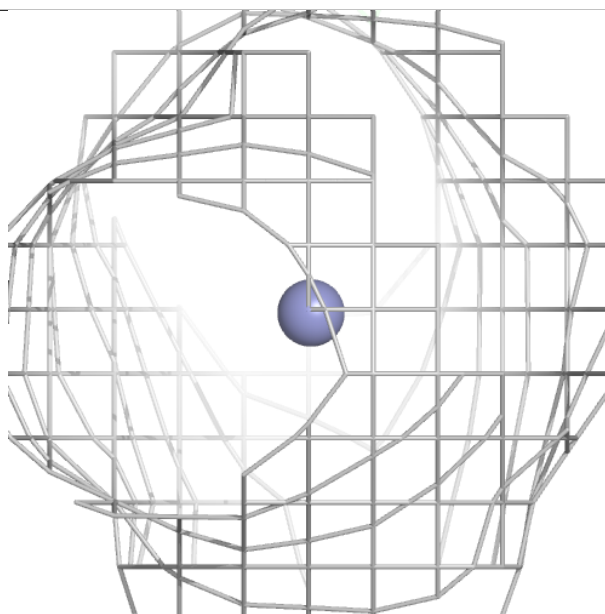
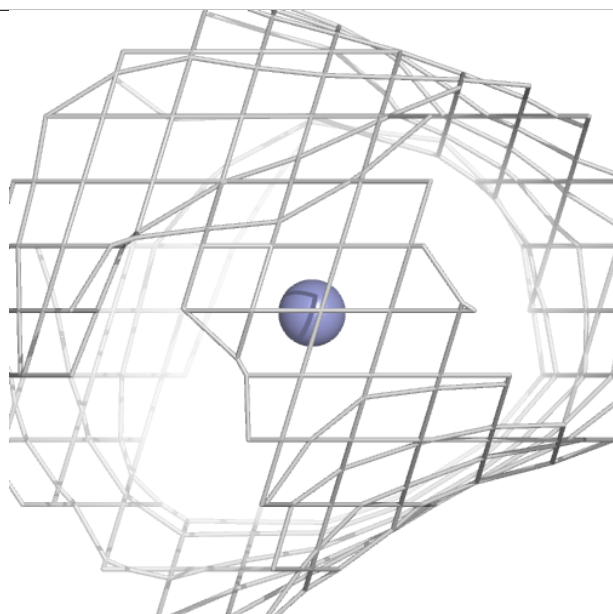
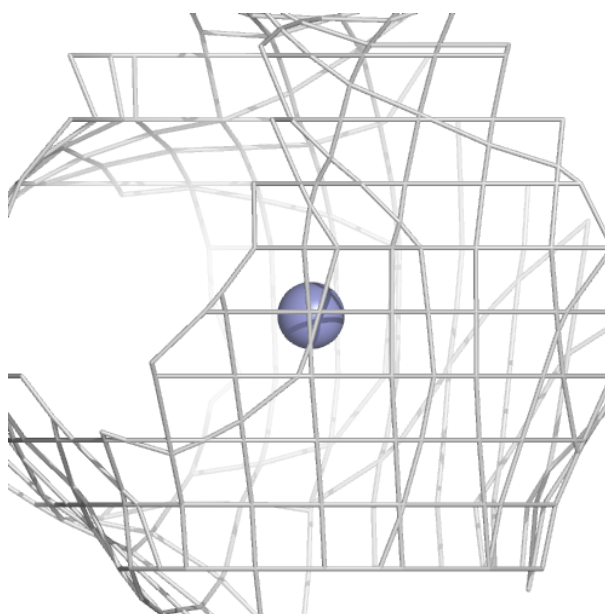
Electron density around ZN A 703:

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



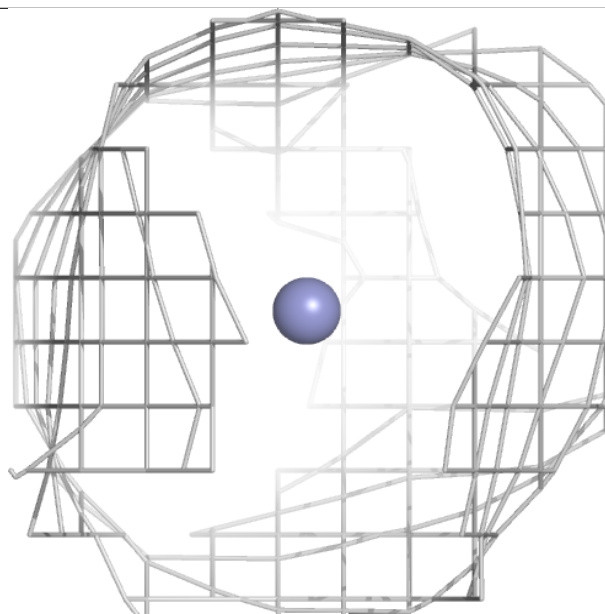
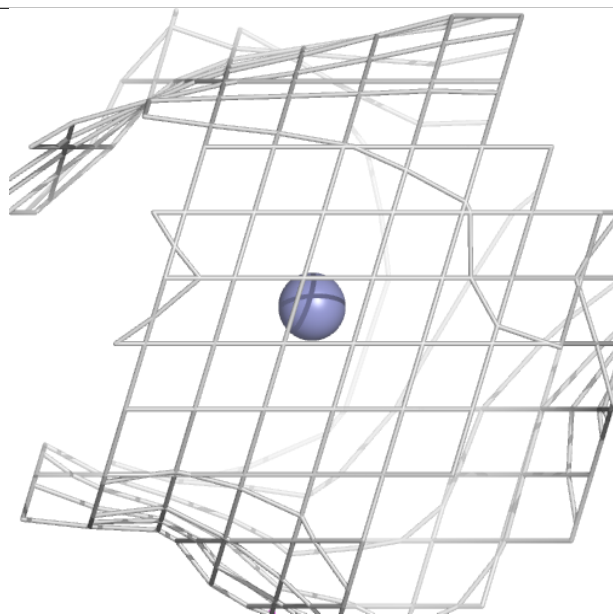
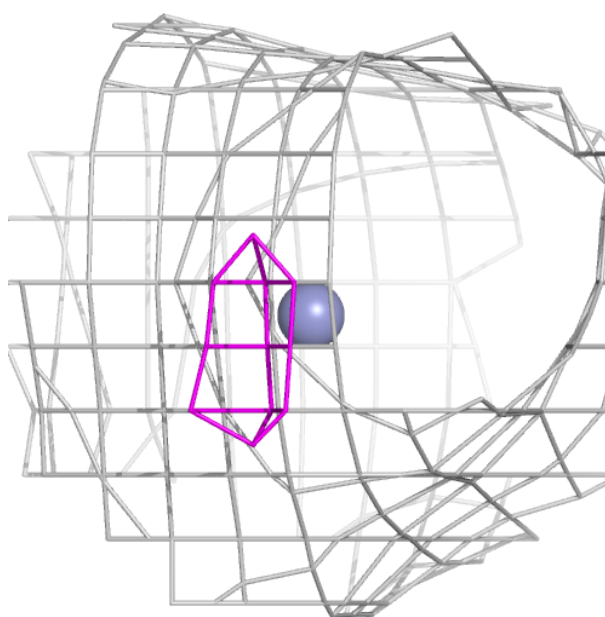
Electron density around ZN B 702:

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



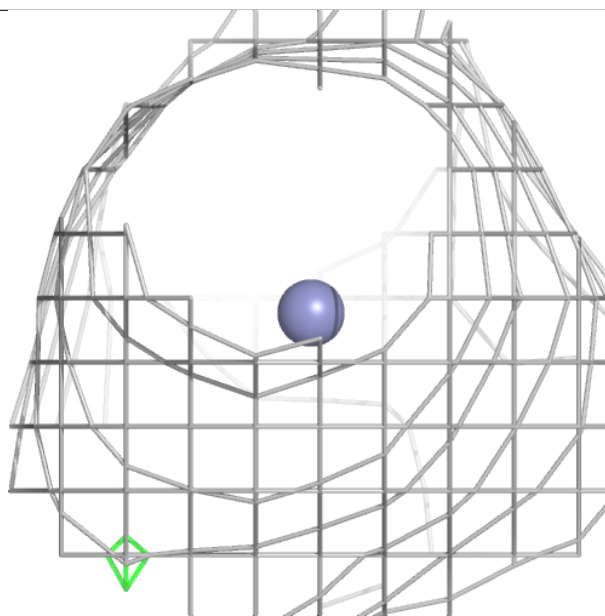
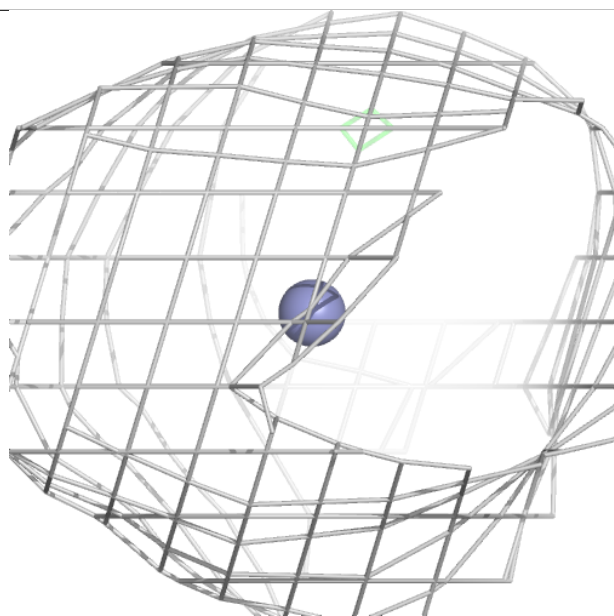
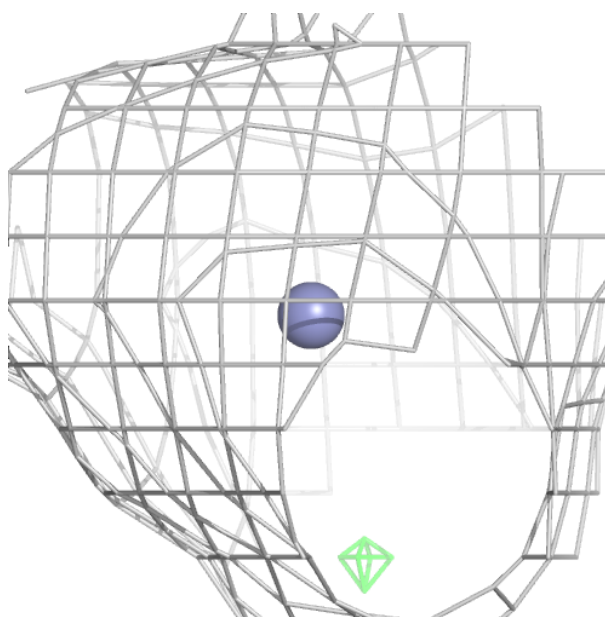
Electron density around ZN B 703:

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



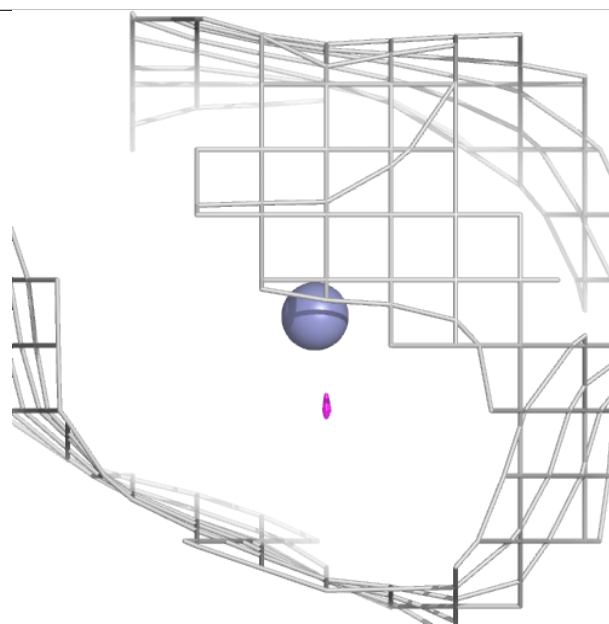
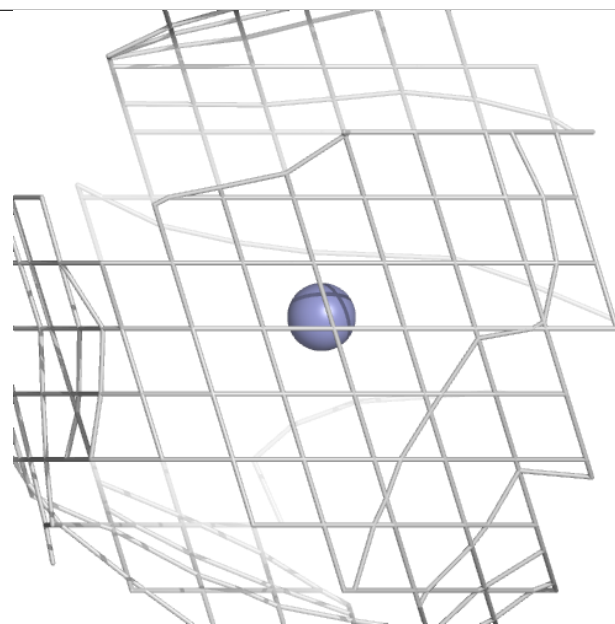
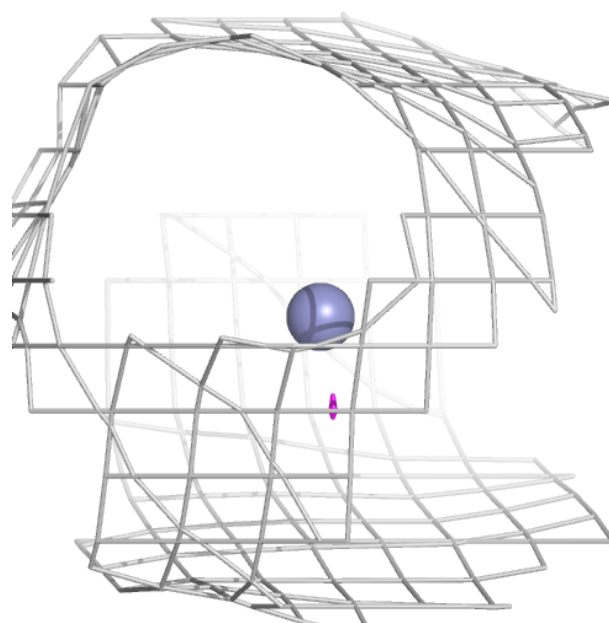
Electron density around ZN B 705:

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



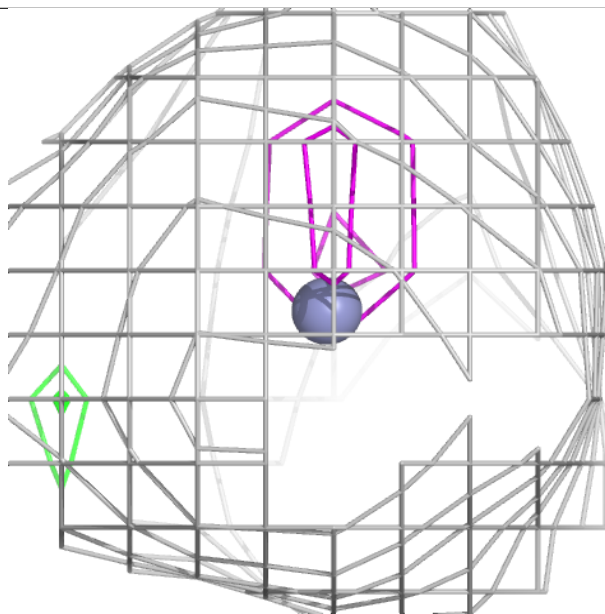
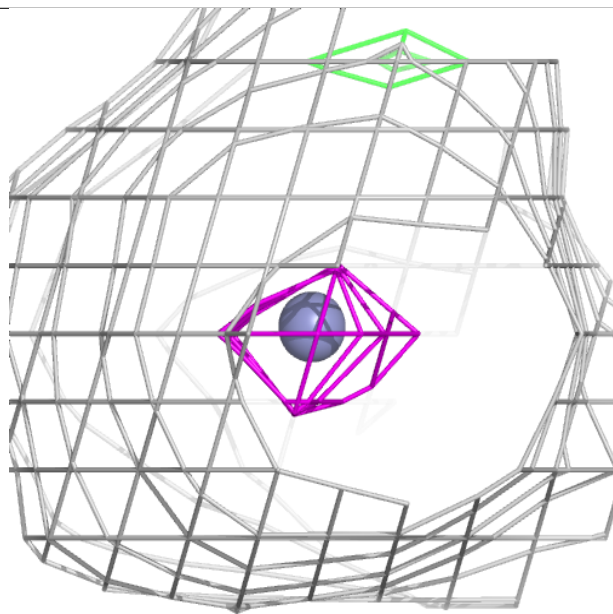
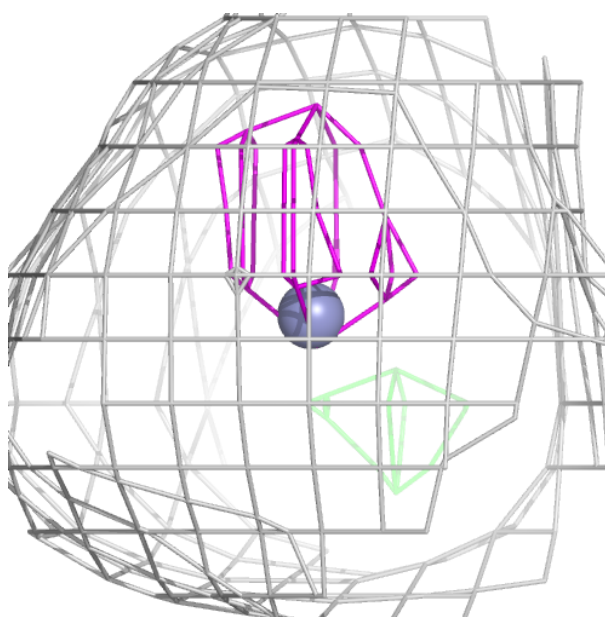
Electron density around ZN A 701:

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



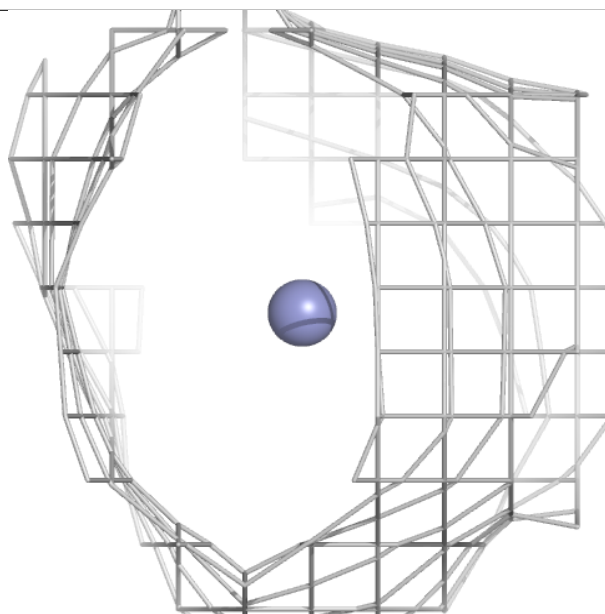
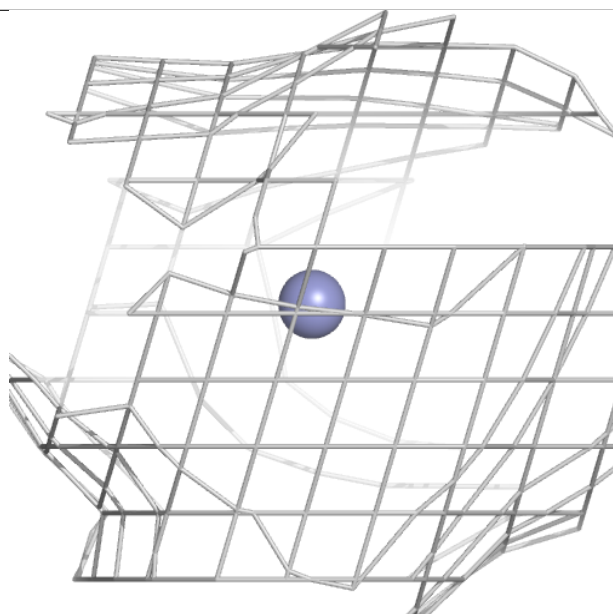
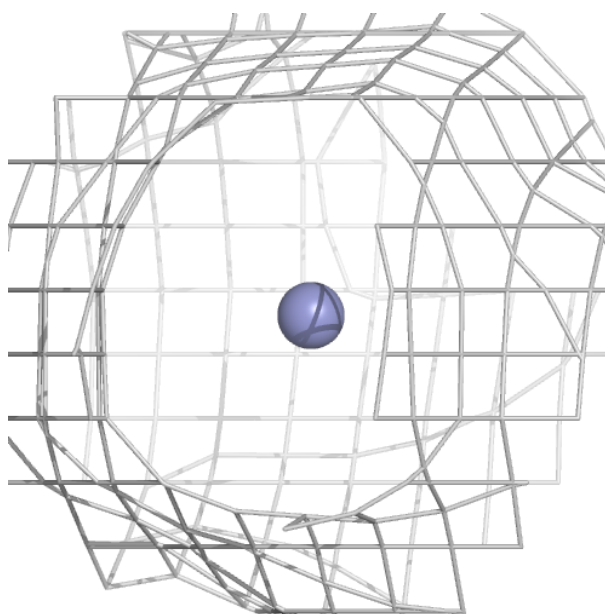
Electron density around ZN A 705:

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



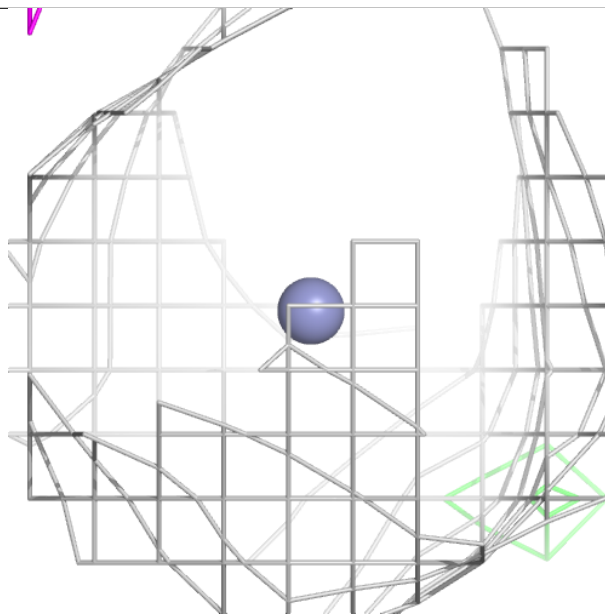
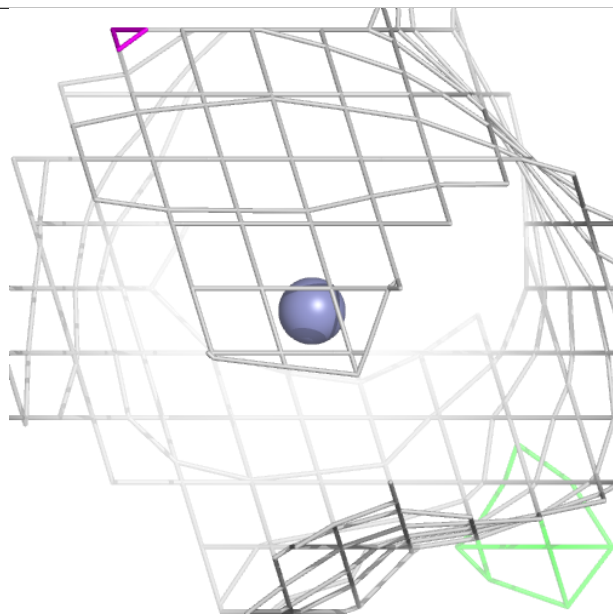
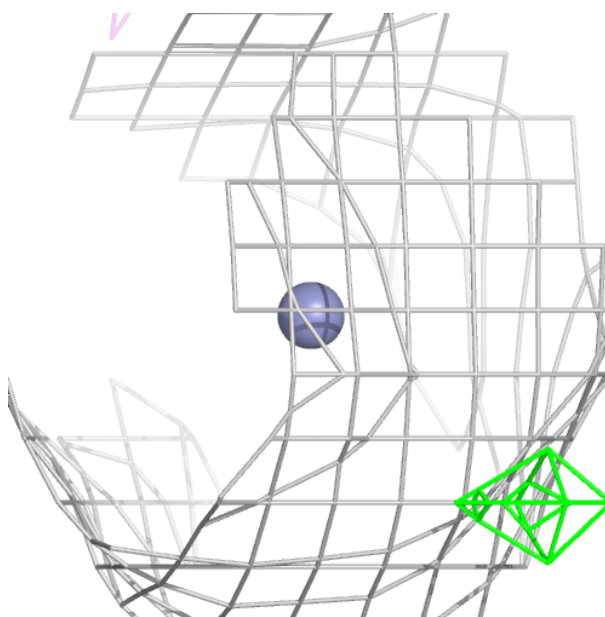
Electron density around ZN B 701:

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



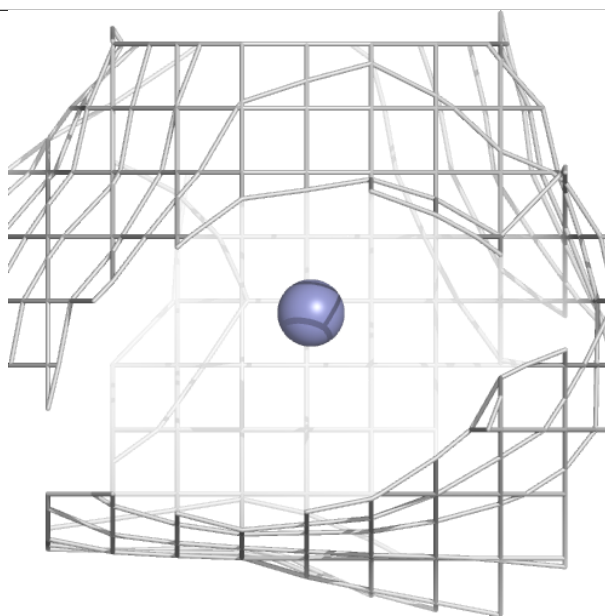
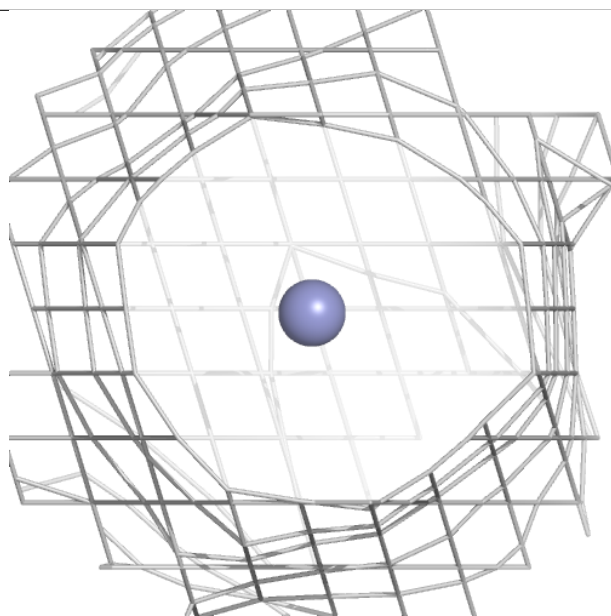
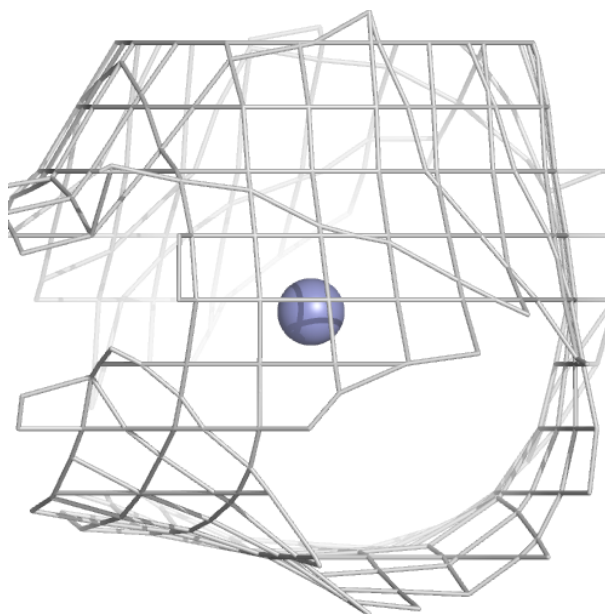
Electron density around ZN A 702:

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



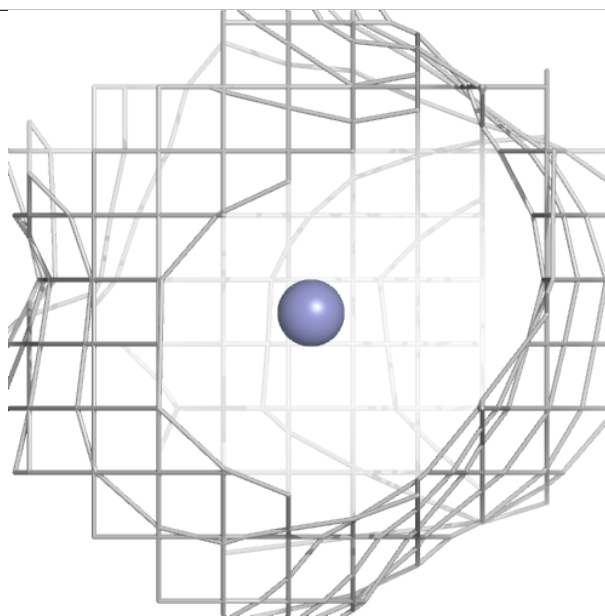
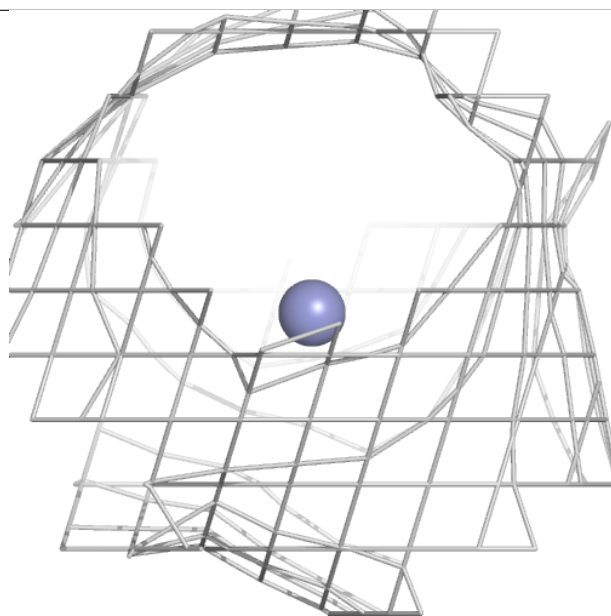
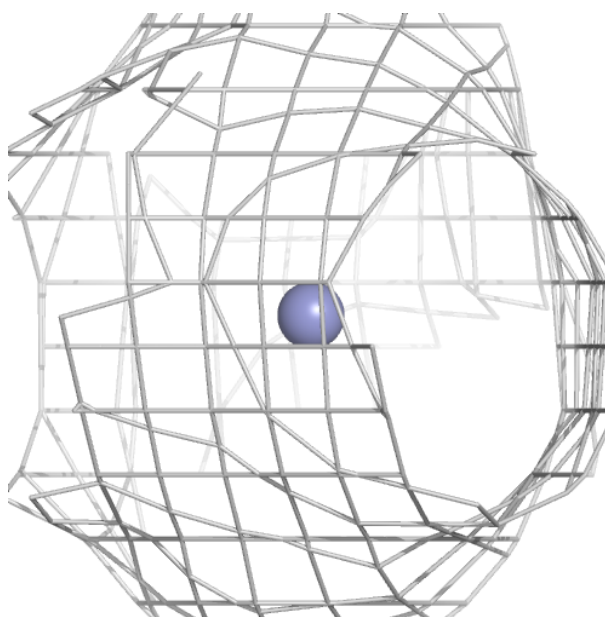
Electron density around ZN A 704:

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



Electron density around ZN B 704:

$2mF_o-DF_c$ (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.