



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:22 PM UTC

PDB ID : 8ABQ / pdb_00008abq
Title : Structure of the SNX1-SNX5 complex, Pt derivative
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Deposited on : 2022-07-04
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

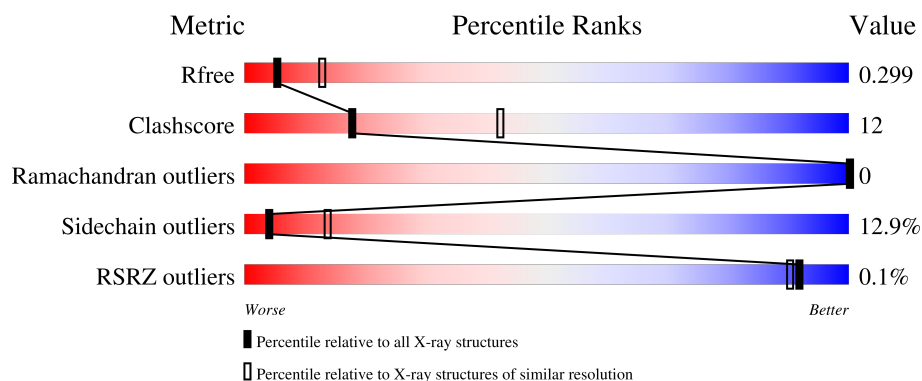
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	222	
1	B	222	
2	C	210	
2	D	210	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6660 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 Sorting nexin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1820	1154	320	343	3			
1	B	216	Total	C	N	O	S	0	0	0
			1812	1150	319	340	3			

- Molecule 2 is a protein called Sorting nexin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	182	Total	C	N	O	S	0	0	0
			1508	951	263	286	8			
2	D	182	Total	C	N	O	S	0	0	0
			1508	951	263	286	8			

- Molecule 3 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Pt	0	0
			3	3		
3	B	2	Total	Pt	0	0
			2	2		
3	D	3	Total	Pt	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		

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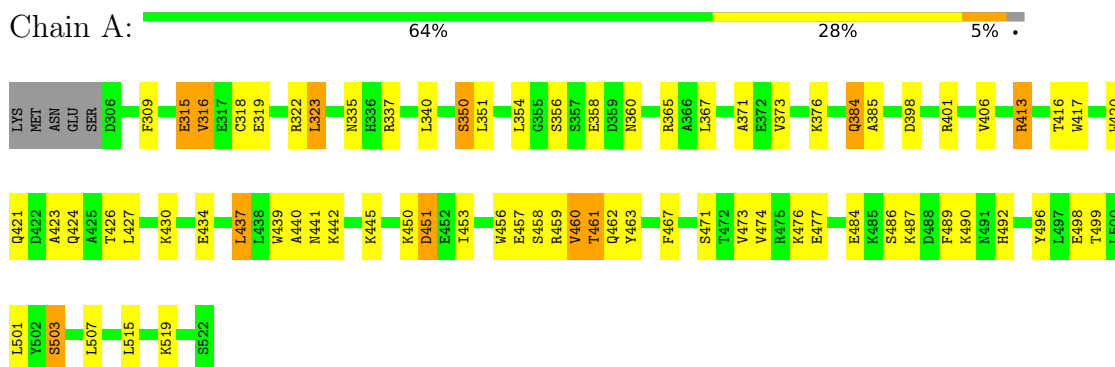
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	O	0	0
			1	1		

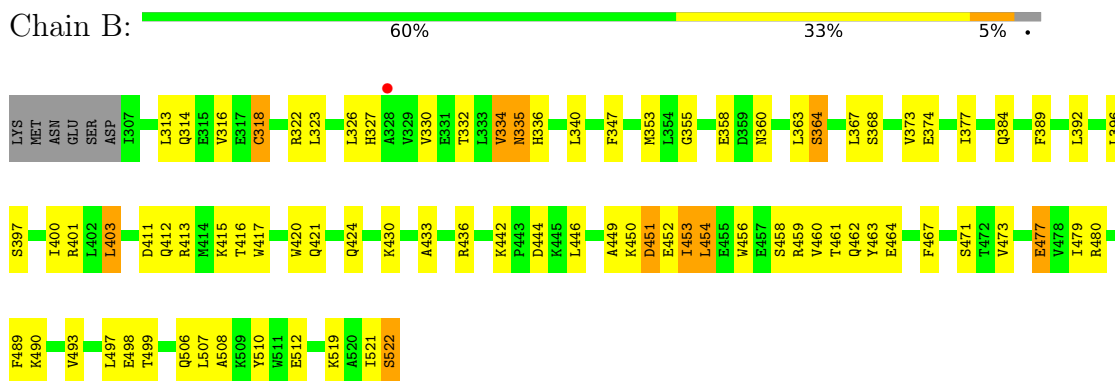
3 Residue-property plots

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.

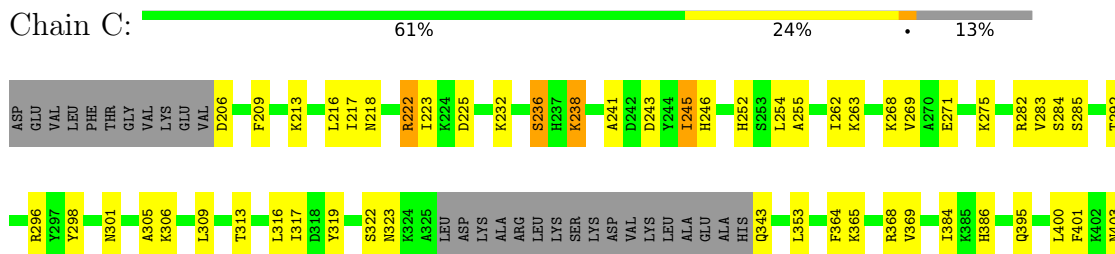
• Molecule 1: Sorting nexin-1



• Molecule 1: Sorting nexin-1



• Molecule 2: Sorting nexin-5





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	52.69Å 51.47Å 192.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.47 – 2.81 51.47 – 2.81	Depositor EDS
% Data completeness (in resolution range)	81.5 (51.47-2.81) 82.9 (51.47-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18-3855-000	Depositor
R, R_{free}	0.252 , 0.305 0.250 , 0.299	Depositor DCC
R_{free} test set	1049 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l 0.029 for -k,-h,-l 0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	4 of 20925 reflections (0.019%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6660	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.57% 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: PT

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	0.11	0/1851	0.25	0/2490
1	B	0.10	0/1843	0.26	0/2479
2	C	0.10	0/1527	0.26	0/2041
2	D	0.11	0/1527	0.28	0/2041
All	All	0.11	0/6748	0.26	0/9051

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 [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	1820	0	1820	54	0
1	B	1812	0	1817	52	0
2	C	1508	0	1527	26	0
2	D	1508	0	1527	55	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	D	3	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
All	All	6660	0	6691	164	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 12.

All (164) 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:398:ASP:HB3	1:A:401:ARG:HH11	1.51	0.75
1:A:315:GLU:O	1:A:319:GLU:N	2.20	0.73
1:B:451:ASP:OD1	1:B:451:ASP:N	2.23	0.72
1:A:365:ARG:HG3	2:D:289:LEU:HD21	1.74	0.70
1:A:456:TRP:HA	1:A:459:ARG:HB2	1.74	0.70
2:D:282:ARG:NH1	2:D:286:ASP:OD2	2.27	0.67
1:A:451:ASP:N	1:A:451:ASP:OD1	2.30	0.64
1:A:434:GLU:OE1	1:A:450:LYS:NZ	2.31	0.64
2:D:312:ARG:NE	2:D:354:SER:OG	2.29	0.63
1:B:358:GLU:OE2	2:D:368:ARG:NH1	2.27	0.63
1:A:501:LEU:HD21	2:C:395:GLN:HE22	1.64	0.62
1:A:337:ARG:HG2	1:A:385:ALA:HB2	1.81	0.62
1:A:484:GLU:HA	1:A:487:LYS:HE3	1.81	0.62
1:A:365:ARG:HA	2:D:289:LEU:HD11	1.82	0.61
1:B:456:TRP:HA	1:B:459:ARG:HB2	1.81	0.61
2:C:217:ILE:HA	2:C:306:LYS:HZ1	1.66	0.60
1:A:340:LEU:HD13	2:C:236:SER:HB2	1.84	0.59
1:A:496:TYR:O	1:A:499:THR:OG1	2.21	0.59
1:A:384:GLN:NE2	1:A:503:SER:OG	2.36	0.58
2:D:312:ARG:HG3	2:D:354:SER:HA	1.85	0.58
2:C:255:ALA:HB1	2:C:263:LYS:HG3	1.85	0.58
1:B:477:GLU:HG3	1:B:480:ARG:HH12	1.67	0.58
1:A:473:VAL:HA	1:A:476:LYS:HD3	1.86	0.58
2:C:292:THR:O	2:C:296:ARG:N	2.30	0.58
1:B:442:LYS:NZ	1:B:444:ASP:OD1	2.37	0.58
1:A:423:ALA:HB2	1:A:463:TYR:HD1	1.69	0.57
1:B:316:VAL:HG13	1:B:403:LEU:HD12	1.86	0.56
2:C:206:ASP:HB3	2:C:209:PHE:HE2	1.71	0.56
1:B:326:LEU:HD23	2:D:250:CYS:HB2	1.88	0.56
2:C:365:LYS:HE2	2:C:369:VAL:HG21	1.87	0.55
2:D:319:TYR:CD2	2:D:346:CYS:HB2	2.41	0.55
2:C:243:ASP:HA	2:C:246:HIS:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:LYS:O	2:D:353:LEU:HB2	2.06	0.55
1:B:430:LYS:NZ	1:B:452:GLU:OE1	2.40	0.54
2:D:308:LEU:HD23	2:D:357:ALA:HA	1.90	0.53
1:A:315:GLU:OE2	1:A:316:VAL:N	2.36	0.53
1:B:420:TRP:C	1:B:420:TRP:CD1	2.86	0.53
1:A:356:SER:O	2:D:282:ARG:NH2	2.40	0.52
2:D:248:ALA:HA	2:D:251:LEU:HB2	1.89	0.52
2:D:206:ASP:HB2	2:D:312:ARG:HH22	1.75	0.52
2:D:362:ILE:HG22	2:D:366:ARG:HG2	1.91	0.52
1:B:490:LYS:HE3	2:D:265:TYR:HE1	1.73	0.52
1:A:420:TRP:O	1:A:424:GLN:HG3	2.09	0.52
1:B:522:SER:O	1:B:522:SER:OG	2.25	0.52
2:D:379:MET:HE3	2:D:382:LEU:HD12	1.92	0.52
1:B:327:HIS:CE1	1:B:397:SER:HB3	2.45	0.51
2:D:245:ILE:HD13	2:D:277:ARG:HD3	1.92	0.51
2:D:393:LEU:O	2:D:396:SER:OG	2.28	0.51
1:B:360:ASN:HD22	1:B:363:LEU:H	1.58	0.50
2:D:305:ALA:HA	2:D:308:LEU:HD13	1.93	0.50
2:D:346:CYS:O	2:D:350:PHE:N	2.43	0.50
1:A:499:THR:O	1:A:503:SER:OG	2.26	0.50
1:A:358:GLU:OE1	1:A:360:ASN:N	2.45	0.49
1:B:314:GLN:O	1:B:318:CYS:N	2.42	0.49
2:D:352:GLN:N	2:D:352:GLN:OE1	2.46	0.49
1:A:456:TRP:O	1:A:460:VAL:HG13	2.13	0.49
2:D:352:GLN:O	2:D:356:SER:OG	2.20	0.49
1:A:354:LEU:HD11	2:C:223:ILE:HG12	1.95	0.48
1:A:323:LEU:HD22	2:C:254:LEU:HD11	1.94	0.48
1:B:334:VAL:HG11	1:B:389:PHE:HB2	1.95	0.48
2:C:217:ILE:HD12	2:C:218:ASN:N	2.28	0.48
1:A:318:CYS:HB3	1:A:322:ARG:CZ	2.44	0.48
1:A:440:ALA:HB3	1:A:442:LYS:NZ	2.29	0.48
2:D:312:ARG:HE	2:D:354:SER:HG	1.56	0.48
1:A:467:PHE:O	1:A:471:SER:OG	2.27	0.47
1:B:358:GLU:OE2	2:D:219:TYR:OH	2.27	0.47
2:D:391:VAL:O	2:D:395:GLN:HB2	2.15	0.47
2:C:301:ASN:HB3	2:C:364:PHE:CZ	2.50	0.47
1:B:413:ARG:NH1	1:B:471:SER:OG	2.44	0.47
1:B:498:GLU:HG2	2:D:398:ILE:HD13	1.96	0.47
2:D:213:LYS:O	2:D:217:ILE:HG12	2.15	0.47
1:A:490:LYS:NZ	2:C:401:PHE:O	2.42	0.47
2:D:378:GLU:HA	2:D:381:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:VAL:HA	1:A:477:GLU:HB2	1.97	0.46
2:C:232:LYS:O	2:C:236:SER:OG	2.28	0.46
2:D:378:GLU:O	2:D:382:LEU:HG	2.16	0.46
1:A:309:PHE:CE2	1:A:471:SER:HB3	2.51	0.46
1:A:437:LEU:HD13	1:A:445:LYS:HB3	1.96	0.46
1:B:411:ASP:O	1:B:415:LYS:N	2.48	0.46
1:A:427:LEU:HD22	1:A:460:VAL:HG11	1.97	0.46
2:C:309:LEU:O	2:C:313:THR:HG23	2.16	0.46
1:A:401:ARG:HE	1:A:401:ARG:HB3	1.61	0.46
2:D:358:LYS:O	2:D:362:ILE:HD12	2.16	0.45
1:B:364:SER:HA	1:B:367:LEU:HB2	1.98	0.45
2:D:373:ARG:O	2:D:377:ILE:HG12	2.16	0.45
1:A:309:PHE:HE2	1:A:471:SER:HB3	1.80	0.45
1:A:319:GLU:HG3	1:A:323:LEU:HD23	1.98	0.45
2:C:213:LYS:HB2	2:C:309:LEU:HD13	1.98	0.45
1:B:358:GLU:HG2	2:D:219:TYR:HE1	1.81	0.45
1:B:450:LYS:HA	1:B:450:LYS:HD2	1.72	0.45
1:B:490:LYS:HE2	2:D:404:ASN:ND2	2.31	0.45
2:D:209:PHE:HZ	2:D:354:SER:O	1.99	0.45
2:D:315:ALA:HA	2:D:318:ASP:HB3	1.99	0.45
1:B:347:PHE:CD2	1:B:374:GLU:HG2	2.51	0.45
1:A:373:VAL:HA	1:A:376:LYS:HE3	1.98	0.45
1:B:323:LEU:HB3	1:B:400:ILE:HD11	1.98	0.45
1:B:420:TRP:CE2	1:B:464:GLU:HG2	2.52	0.45
1:B:347:PHE:HD2	1:B:374:GLU:HG2	1.80	0.45
1:B:460:VAL:O	1:B:464:GLU:HG3	2.17	0.45
1:A:309:PHE:HB3	1:A:413:ARG:HH11	1.81	0.44
1:A:318:CYS:HB3	1:A:322:ARG:NH1	2.31	0.44
1:A:350:SER:HB2	2:C:225:ASP:OD1	2.18	0.44
2:C:319:TYR:O	2:C:323:ASN:HB2	2.17	0.44
2:D:272:LEU:HD21	2:D:394:LEU:HD12	1.99	0.44
1:B:373:VAL:O	1:B:377:ILE:HG12	2.17	0.44
1:B:506:GLN:NE2	1:B:510:TYR:OH	2.51	0.44
2:C:238:LYS:HD2	2:C:241:ALA:HB3	2.00	0.44
2:C:268:LYS:HD2	2:C:268:LYS:HA	1.81	0.44
1:A:519:LYS:HA	1:A:519:LYS:HD2	1.64	0.44
1:B:412:GLN:O	1:B:416:THR:HG23	2.18	0.44
1:A:413:ARG:O	1:A:416:THR:OG1	2.32	0.44
1:B:521:ILE:HB	2:D:373:ARG:HD2	1.99	0.44
1:B:420:TRP:CZ2	1:B:464:GLU:HG2	2.52	0.44
1:B:459:ARG:NH1	1:B:463:TYR:OH	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:TRP:O	1:B:421:GLN:HB2	2.18	0.44
1:B:461:THR:HA	1:B:464:GLU:HB2	2.00	0.44
2:D:296:ARG:HD3	2:D:296:ARG:HA	1.75	0.44
1:A:445:LYS:HA	1:A:445:LYS:HD2	1.82	0.43
2:D:260:THR:O	2:D:264:LYS:HG3	2.18	0.43
1:B:433:ALA:HA	1:B:436:ARG:HG2	2.00	0.43
2:D:358:LYS:O	2:D:361:LEU:N	2.49	0.43
1:A:439:TRP:HA	1:A:439:TRP:CE3	2.54	0.43
2:C:301:ASN:O	2:C:305:ALA:N	2.43	0.43
2:C:271:GLU:O	2:C:275:LYS:HG3	2.18	0.42
1:B:355:GLY:O	1:B:358:GLU:HB2	2.19	0.42
2:D:291:LEU:HD12	2:D:379:MET:SD	2.59	0.42
1:A:351:LEU:HB2	1:A:371:ALA:HB2	2.01	0.42
1:A:458:SER:O	1:A:462:GLN:N	2.50	0.42
2:D:245:ILE:HD12	2:D:245:ILE:HA	1.82	0.42
1:A:490:LYS:HB3	1:A:490:LYS:HE3	1.85	0.42
2:C:245:ILE:HD12	2:C:245:ILE:HA	1.93	0.42
1:B:403:LEU:HD13	1:B:403:LEU:HA	1.84	0.42
1:A:457:GLU:O	1:A:461:THR:OG1	2.33	0.41
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.87	0.41
1:B:519:LYS:HG3	2:D:377:ILE:HD12	2.02	0.41
1:A:423:ALA:HB1	1:A:460:VAL:HG12	2.01	0.41
1:A:430:LYS:HB3	1:A:453:ILE:HG12	2.01	0.41
1:B:335:ASN:OD1	1:B:335:ASN:N	2.47	0.41
1:B:322:ARG:HB3	2:D:254:LEU:HD12	2.02	0.41
1:B:454:LEU:HD23	1:B:454:LEU:HA	1.88	0.41
1:A:356:SER:C	2:D:282:ARG:HH22	2.28	0.41
2:C:222:ARG:HH21	2:C:225:ASP:HB2	1.85	0.41
1:B:336:HIS:ND1	2:D:243:ASP:OD1	2.50	0.41
2:D:314:LYS:O	2:D:317:ILE:HG13	2.21	0.41
1:B:449:ALA:O	1:B:453:ILE:HG22	2.20	0.41
1:B:489:PHE:O	1:B:493:VAL:HG12	2.21	0.41
2:C:282:ARG:HD2	2:C:386:HIS:CE1	2.56	0.41
2:C:298:TYR:OH	2:C:368:ARG:HA	2.21	0.41
2:D:349:LYS:HG3	2:D:353:LEU:HD13	2.03	0.41
2:D:393:LEU:HD23	2:D:393:LEU:HA	1.92	0.41
2:D:401:PHE:O	2:D:404:ASN:ND2	2.54	0.41
1:B:322:ARG:HD2	1:B:322:ARG:N	2.36	0.41
1:B:392:LEU:HD12	1:B:392:LEU:HA	1.93	0.41
1:A:503:SER:O	1:A:507:LEU:HB2	2.21	0.40
2:D:296:ARG:O	2:D:300:LEU:HD22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:LYS:HE3	2:D:265:TYR:CE1	2.54	0.40
1:A:417:TRP:CZ3	1:A:421:GLN:HG3	2.56	0.40
1:A:423:ALA:HB2	1:A:463:TYR:CD1	2.53	0.40
1:B:353:MET:SD	2:D:222:ARG:NH2	2.95	0.40
2:D:291:LEU:O	2:D:295:LEU:HD12	2.21	0.40
1:A:323:LEU:HD13	1:A:323:LEU:HA	1.97	0.40
1:B:420:TRP:NE1	1:B:424:GLN:OE1	2.47	0.40
1:B:508:ALA:O	1:B:512:GLU:HG3	2.21	0.40
2:D:267:LEU:HD12	2:D:268:LYS:HG2	2.04	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	215/222 (97%)	209 (97%)	6 (3%)	0	100	100
1	B	214/222 (96%)	212 (99%)	2 (1%)	0	100	100
2	C	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
2	D	178/210 (85%)	167 (94%)	11 (6%)	0	100	100
All	All	785/864 (91%)	763 (97%)	22 (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	193/198 (98%)	173 (90%)	20 (10%)	7	21
1	B	192/198 (97%)	165 (86%)	27 (14%)	3	11
2	C	167/191 (87%)	148 (89%)	19 (11%)	5	18
2	D	167/191 (87%)	140 (84%)	27 (16%)	2	8
All	All	719/778 (92%)	626 (87%)	93 (13%)	4	14

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	GLU
1	A	316	VAL
1	A	323	LEU
1	A	335	ASN
1	A	350	SER
1	A	384	GLN
1	A	406	VAL
1	A	413	ARG
1	A	426	THR
1	A	437	LEU
1	A	441	ASN
1	A	451	ASP
1	A	460	VAL
1	A	461	THR
1	A	486	SER
1	A	489	PHE
1	A	492	HIS
1	A	498	GLU
1	A	503	SER
1	A	515	LEU
2	C	216	LEU
2	C	222	ARG
2	C	236	SER
2	C	238	LYS
2	C	245	ILE
2	C	252	HIS
2	C	262	ILE
2	C	269	VAL
2	C	283	VAL
2	C	284	SER
2	C	285	SER
2	C	316	LEU
2	C	317	ILE

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Mol	Chain	Res	Type
2	C	322	SER
2	C	343	GLN
2	C	353	LEU
2	C	384	ILE
2	C	400	LEU
2	C	403	ASN
1	B	313	LEU
1	B	318	CYS
1	B	330	VAL
1	B	332	THR
1	B	334	VAL
1	B	335	ASN
1	B	340	LEU
1	B	364	SER
1	B	368	SER
1	B	384	GLN
1	B	396	LEU
1	B	401	ARG
1	B	403	LEU
1	B	446	LEU
1	B	451	ASP
1	B	453	ILE
1	B	454	LEU
1	B	458	SER
1	B	462	GLN
1	B	467	PHE
1	B	473	VAL
1	B	477	GLU
1	B	479	ILE
1	B	497	LEU
1	B	499	THR
1	B	507	LEU
1	B	522	SER
2	D	216	LEU
2	D	218	ASN
2	D	220	TYR
2	D	226	SER
2	D	231	ASP
2	D	234	THR
2	D	245	ILE
2	D	251	LEU
2	D	253	SER

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Mol	Chain	Res	Type
2	D	254	LEU
2	D	260	THR
2	D	267	LEU
2	D	274	GLU
2	D	276	LEU
2	D	278	LYS
2	D	283	VAL
2	D	291	LEU
2	D	293	GLU
2	D	300	LEU
2	D	317	ILE
2	D	322	SER
2	D	346	CYS
2	D	347	CYS
2	D	352	GLN
2	D	354	SER
2	D	361	LEU
2	D	368	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	A	379	GLN
1	A	381	HIS
1	A	384	GLN
1	A	412	GLN
1	A	418	GLN
1	A	428	GLN
1	A	505	GLN
2	C	211	GLN
2	C	239	ASN
2	C	321	ASN
2	C	323	ASN
2	C	348	GLN
2	C	386	HIS
2	C	395	GLN
2	C	403	ASN
1	B	327	HIS
1	B	379	GLN
1	B	447	GLN
1	B	505	GLN

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Mol	Chain	Res	Type
1	B	506	GLN
2	D	218	ASN
2	D	252	HIS
2	D	301	ASN
2	D	321	ASN
2	D	363	ASN
2	D	375	ASN
2	D	386	HIS
2	D	390	ASN
2	D	395	GLN
2	D	404	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	217/222 (97%)	-1.62	0 100 100	36, 65, 96, 116	0
1	B	216/222 (97%)	-1.58	1 (0%) 87 82	39, 66, 102, 115	0
2	C	182/210 (86%)	-1.48	0 100 100	36, 76, 96, 117	0
2	D	182/210 (86%)	-1.46	0 100 100	33, 74, 107, 123	0
All	All	797/864 (92%)	-1.54	1 (0%) 92 90	33, 69, 102, 123	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	328	ALA	3.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PT	A	602	1/1	0.98	0.04	203,203,203,203	0

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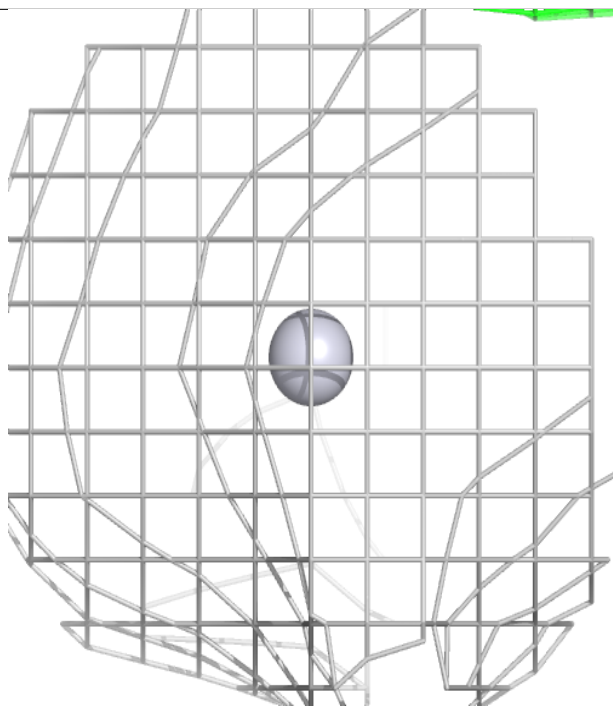
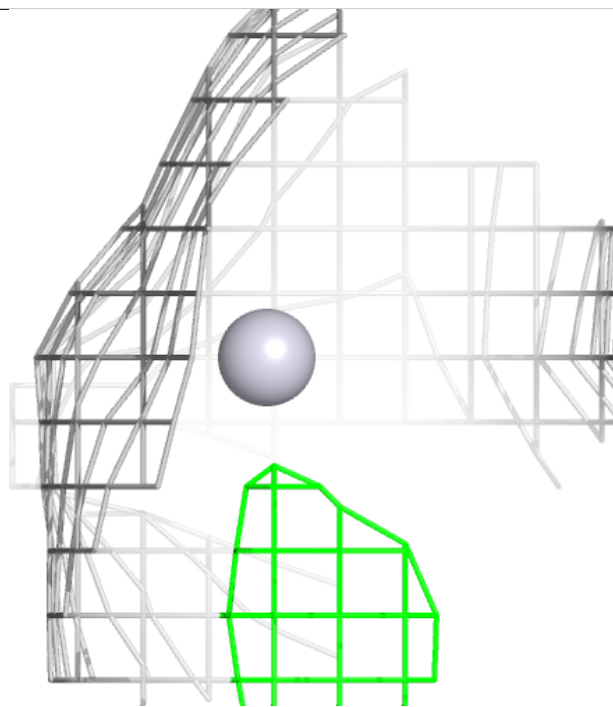
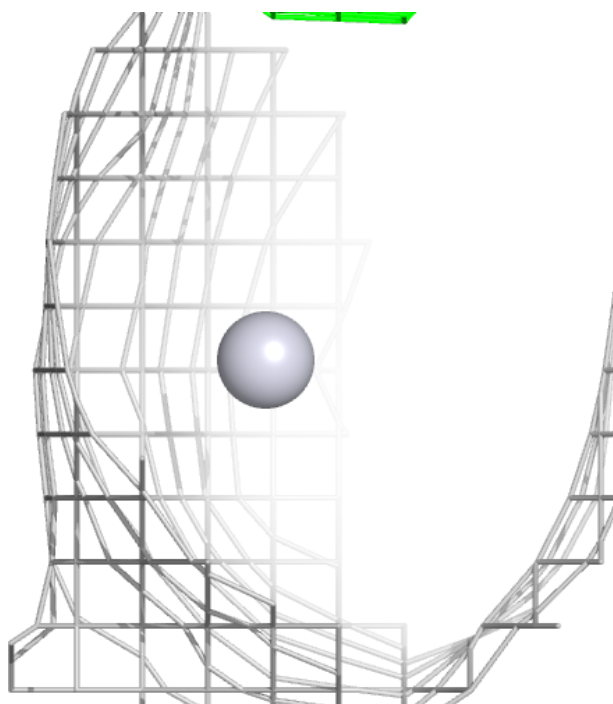
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PT	D	503	1/1	0.98	0.03	231,231,231,231	0
3	PT	A	603	1/1	0.99	0.03	152,152,152,152	0
3	PT	B	601	1/1	0.99	0.03	191,191,191,191	0
3	PT	D	501	1/1	0.99	0.05	178,178,178,178	0
3	PT	A	601	1/1	0.99	0.03	146,146,146,146	0
3	PT	D	502	1/1	1.00	0.02	126,126,126,126	0
3	PT	B	602	1/1	1.00	0.02	137,137,137,137	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.

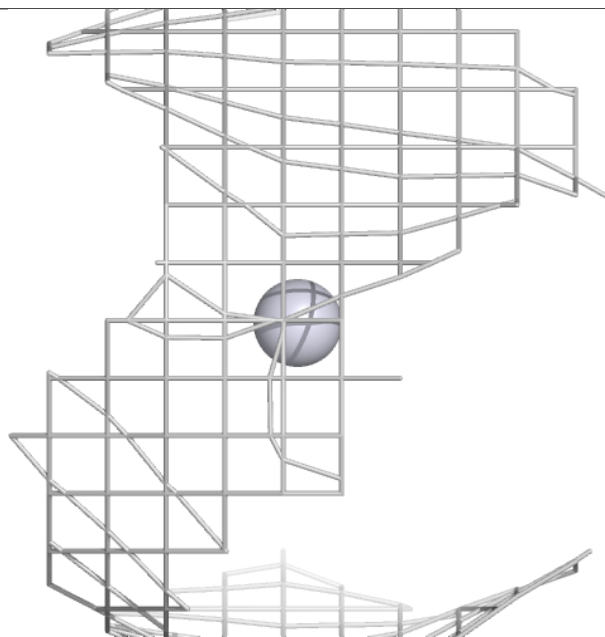
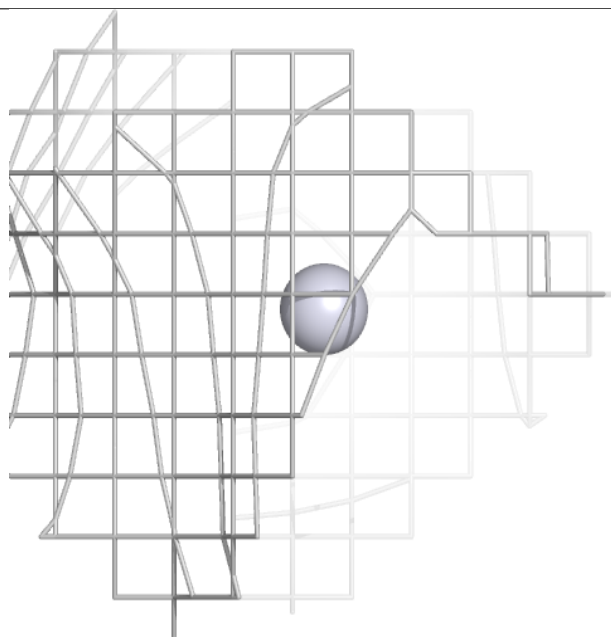
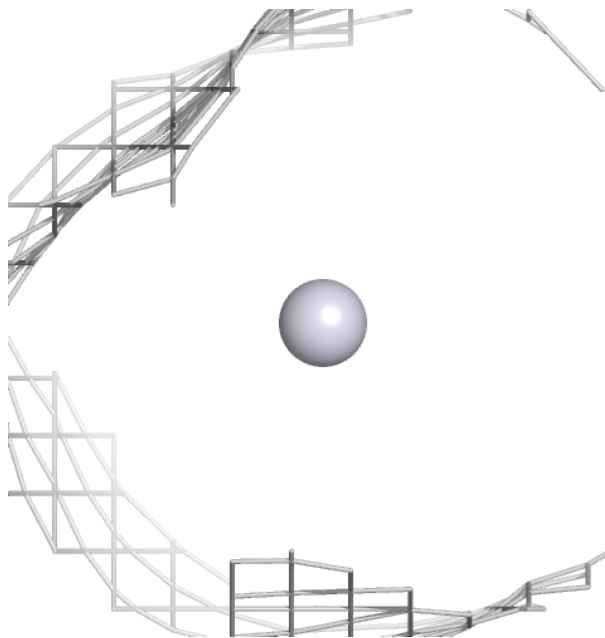
Electron density around PT A 602:

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



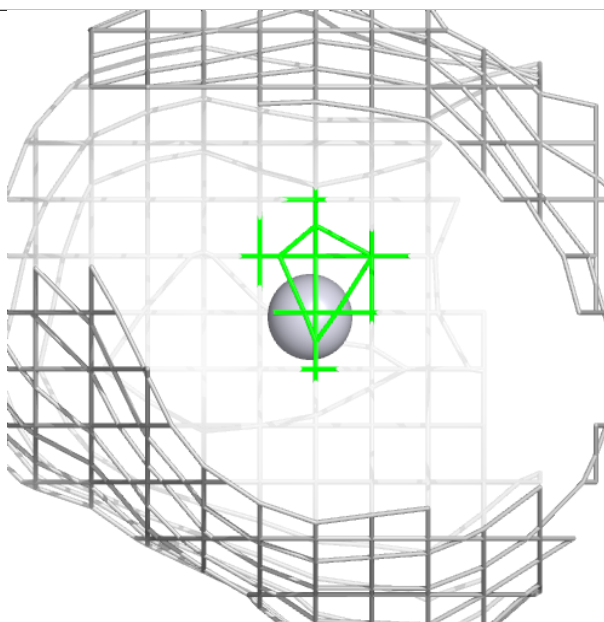
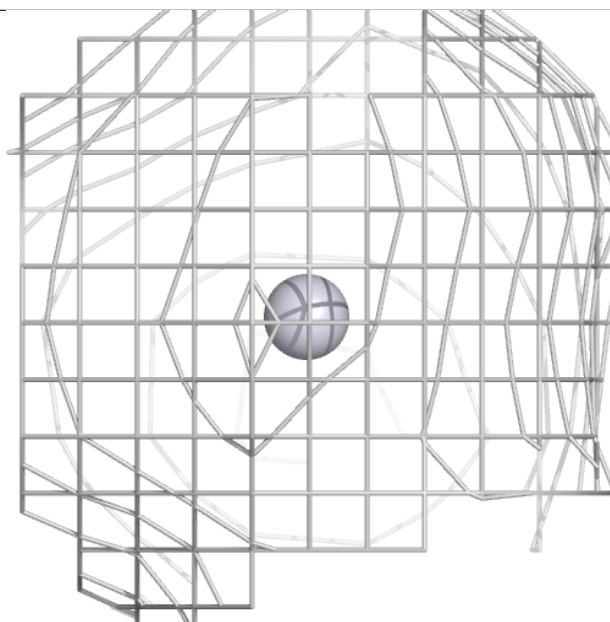
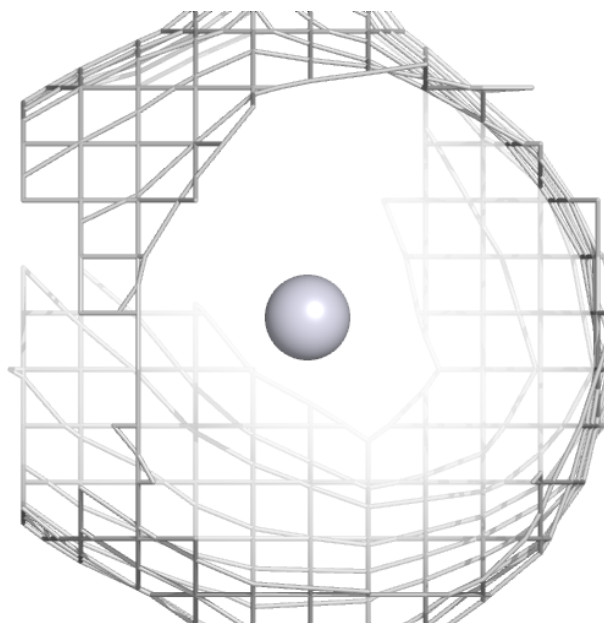
Electron density around PT D 503:

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



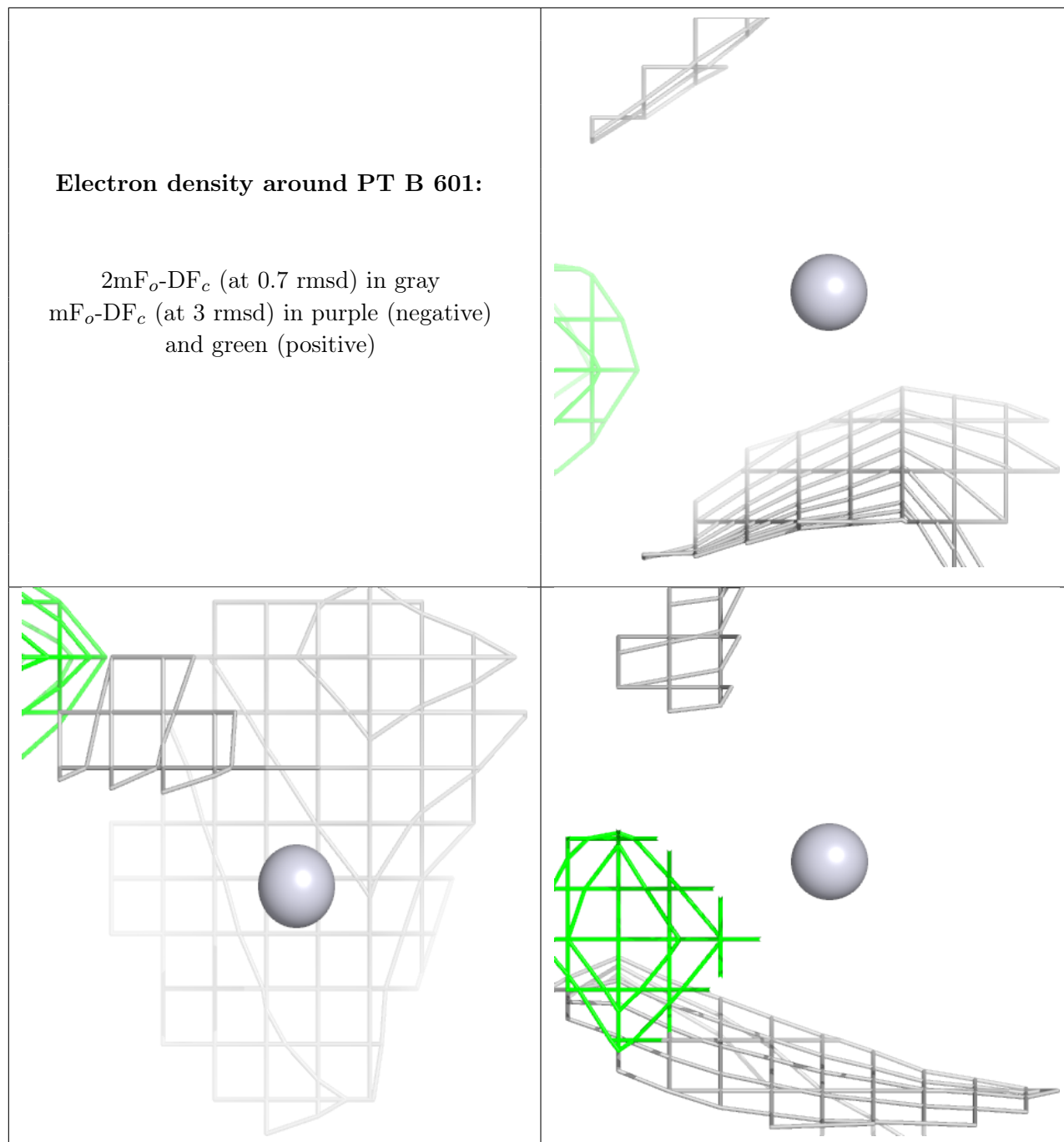
Electron density around PT A 603:

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



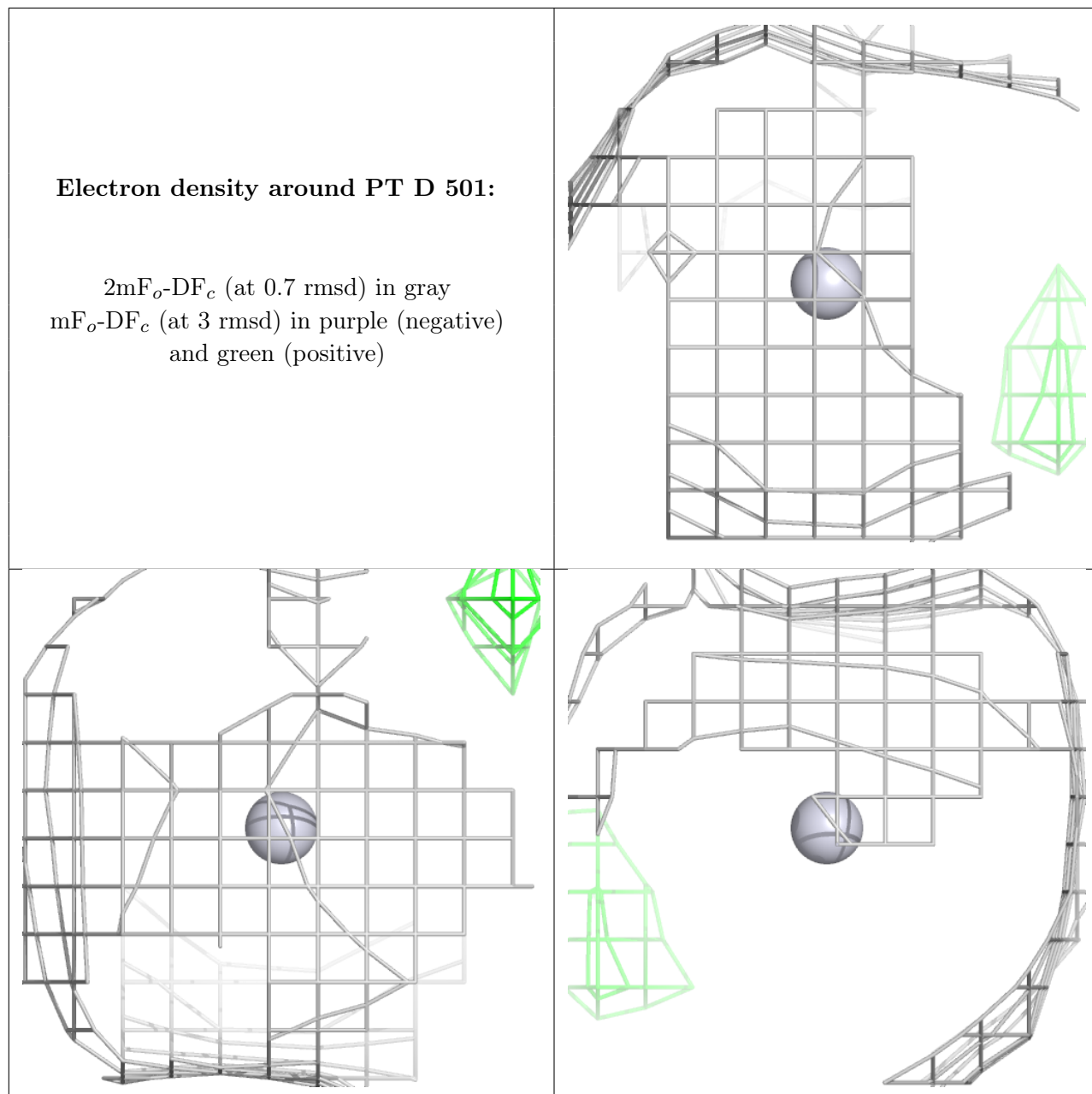
Electron density around PT B 601:

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



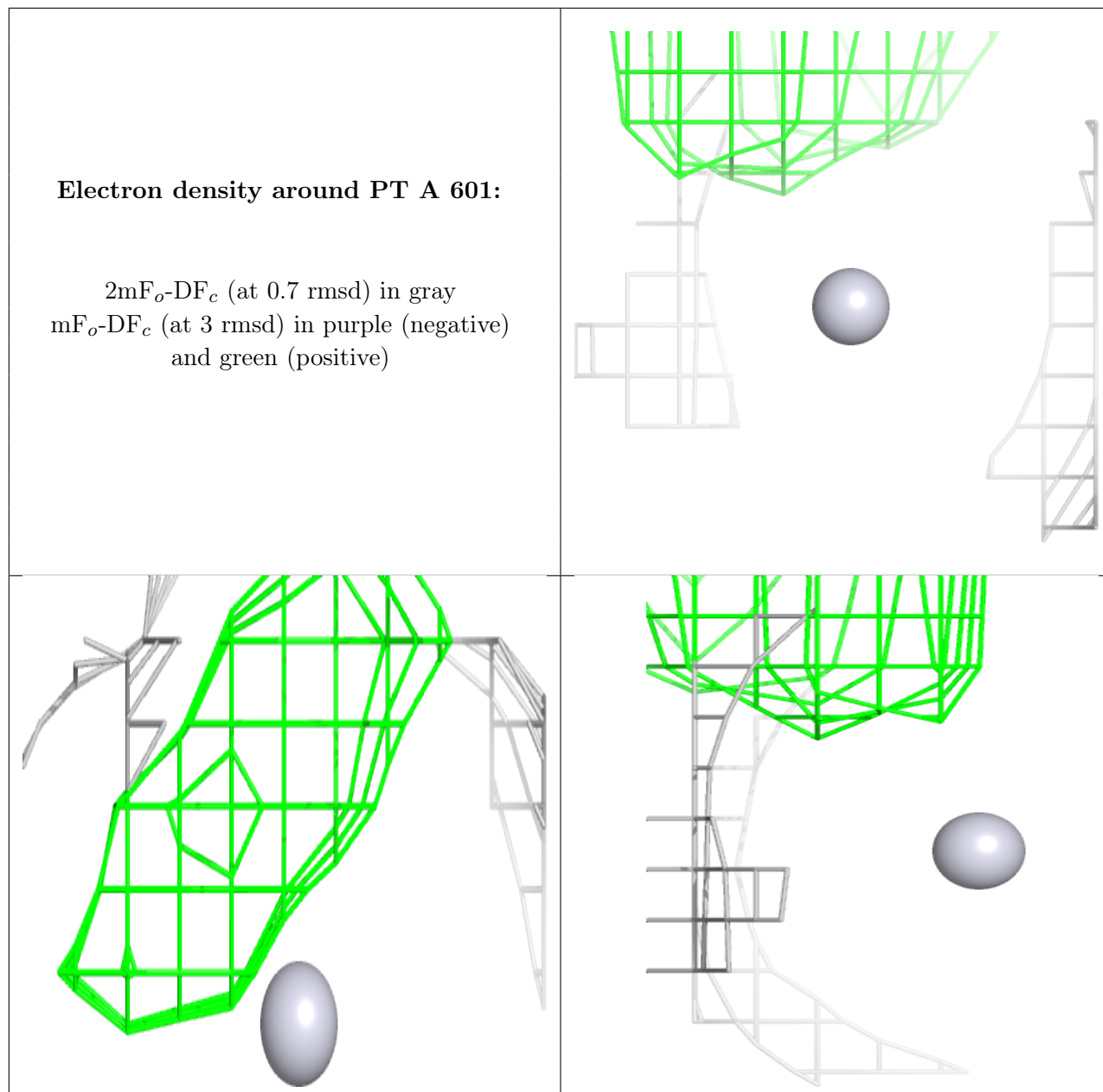
Electron density around PT D 501:

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



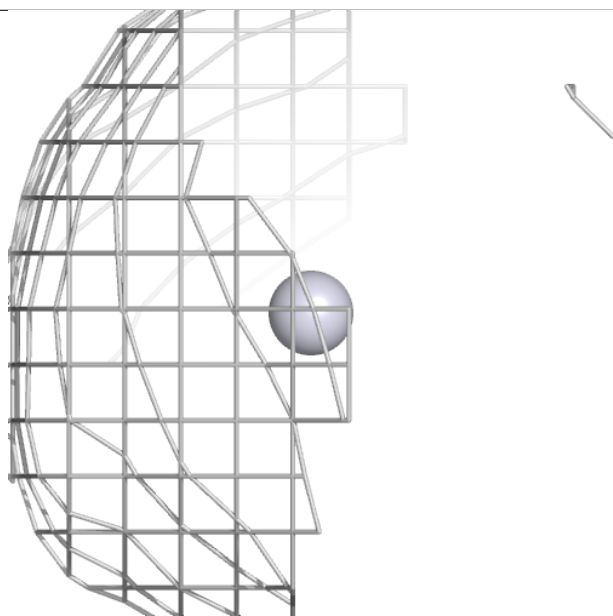
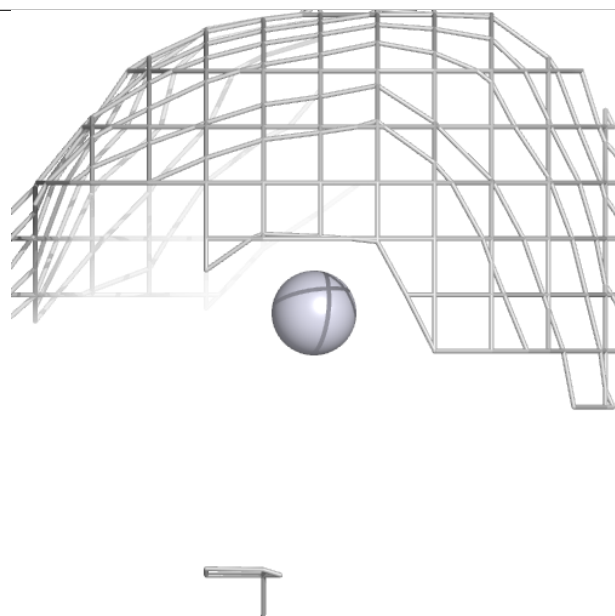
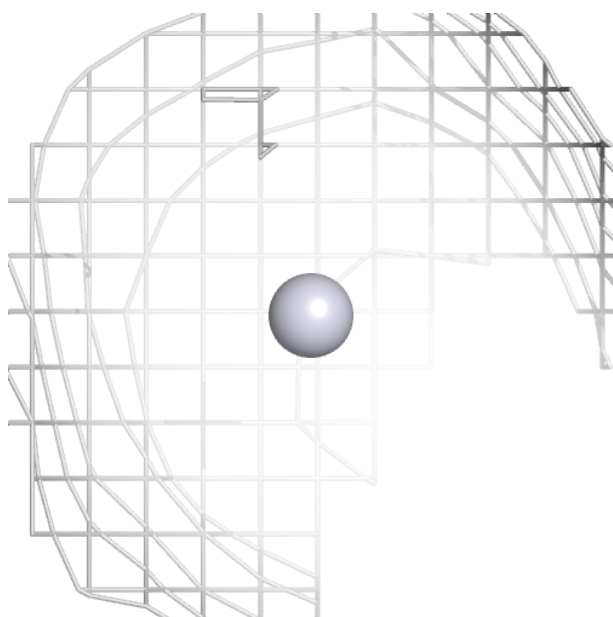
Electron density around PT A 601:

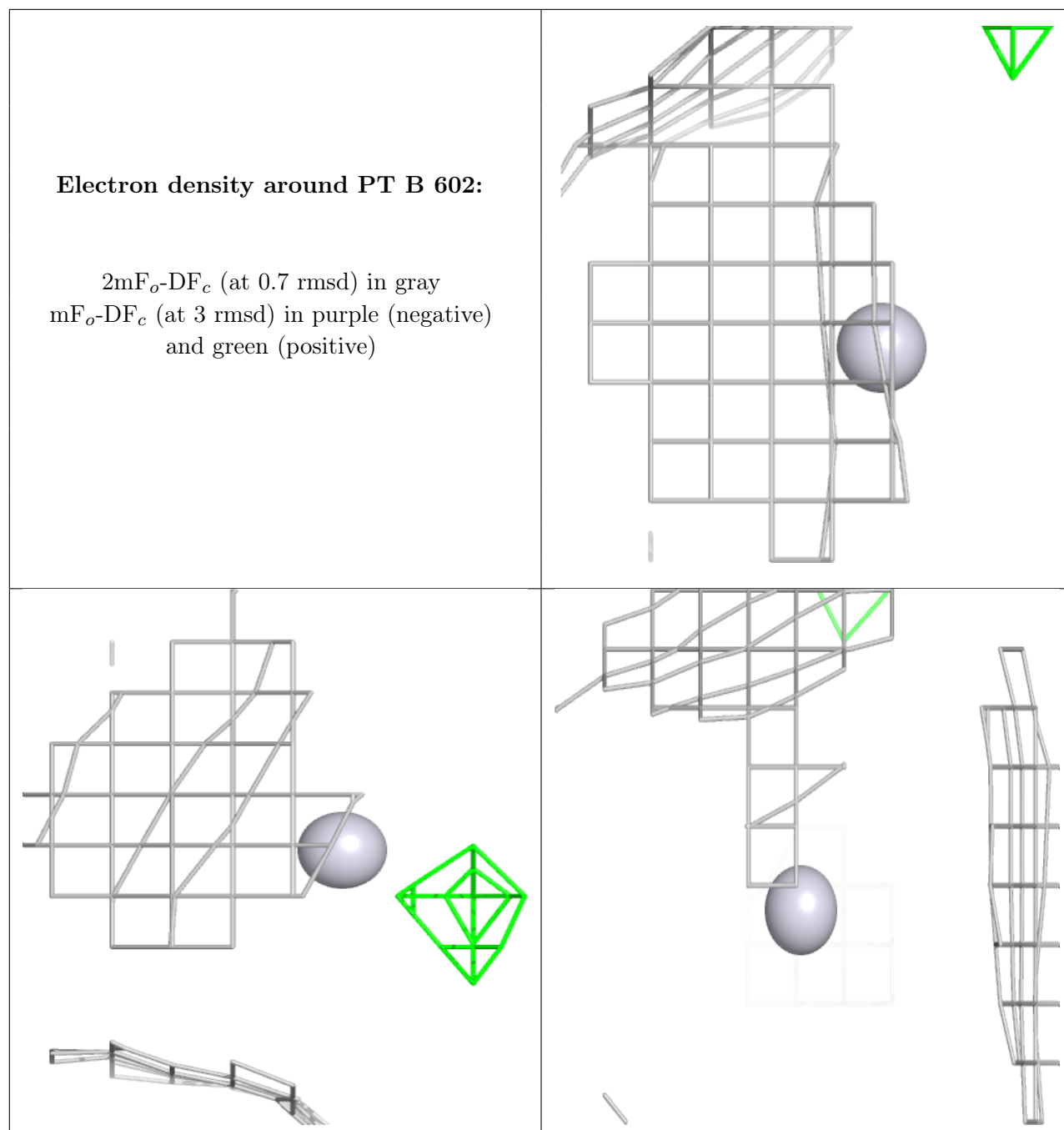
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PT 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.