Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 09:47 PM JST

PDB ID	:	6AKR
Title	:	Crystal structure of the PDE4D catalytic domain in complex with osthole
Authors	:	Wang, S.; Huo, Y.W.; Xie, Y.
Deposited on	:	2018-09-03
Resolution	:	2.33 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 (i) 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 (i)) were used in the production of this report:

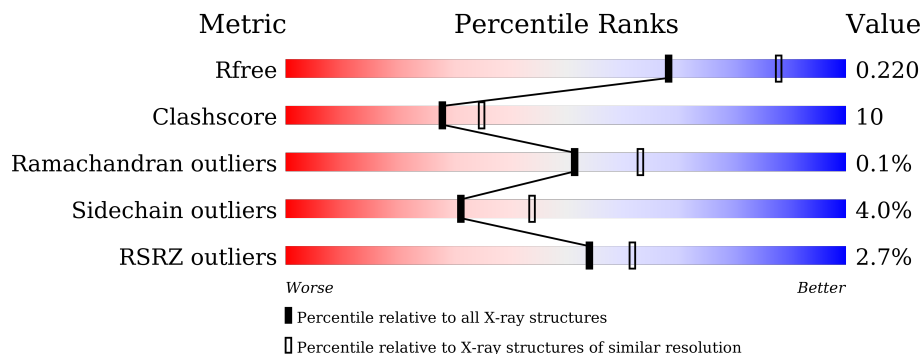|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.33 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	Percentile Ranks	Value
Rfree		0.220
Clashscore		10
Ramachandran outliers		0.1%
Sidechain outliers		4.0%
RSRZ outliers		2.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 <=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	364	.% 77% 12% • 11%
1	B	364	4% 74% 15% • 10%
1	C	364	2% 66% 22% • 11%
1	D	364	3% 68% 19% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	A0O	B	703	-	-	-	X
3	A0O	D	703	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11094 atoms, of which 64 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

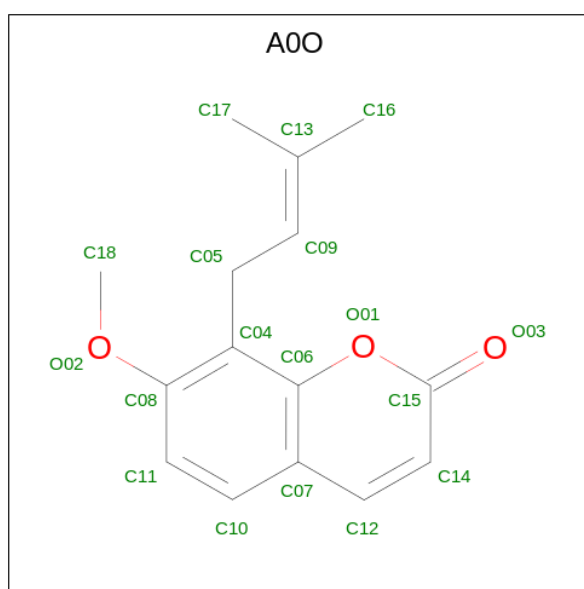| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2631	1664	450	503	14			
1	B	329	Total	C	N	O	S	0	0	0
			2662	1685	454	509	14			
1	C	325	Total	C	N	O	S	0	0	0
			2631	1664	449	504	14			
1	D	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	GLY	-	expression tag	UNP Q08499
A	314	SER	-	expression tag	UNP Q08499
A	315	HIS	-	expression tag	UNP Q08499
A	316	MET	-	expression tag	UNP Q08499
B	313	GLY	-	expression tag	UNP Q08499
B	314	SER	-	expression tag	UNP Q08499
B	315	HIS	-	expression tag	UNP Q08499
B	316	MET	-	expression tag	UNP Q08499
C	313	GLY	-	expression tag	UNP Q08499
C	314	SER	-	expression tag	UNP Q08499
C	315	HIS	-	expression tag	UNP Q08499
C	316	MET	-	expression tag	UNP Q08499
D	313	GLY	-	expression tag	UNP Q08499
D	314	SER	-	expression tag	UNP Q08499
D	315	HIS	-	expression tag	UNP Q08499
D	316	MET	-	expression tag	UNP Q08499

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

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

- Molecule 3 is 7-methoxy-8-(3-methylbut-2-enyl)chromen-2-one (three-letter code: A0O) (formula: $C_{15}H_{16}O_3$) (labeled as "Ligand of Interest" by depositor).

A0O

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 34	C 15	H 16	O 3	0	0
3	B	1	Total 34	C 15	H 16	O 3	0	0
3	C	1	Total 34	C 15	H 16	O 3	0	0
3	D	1	Total 34	C 15	H 16	O 3	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	131	Total 131	O 131	0	0

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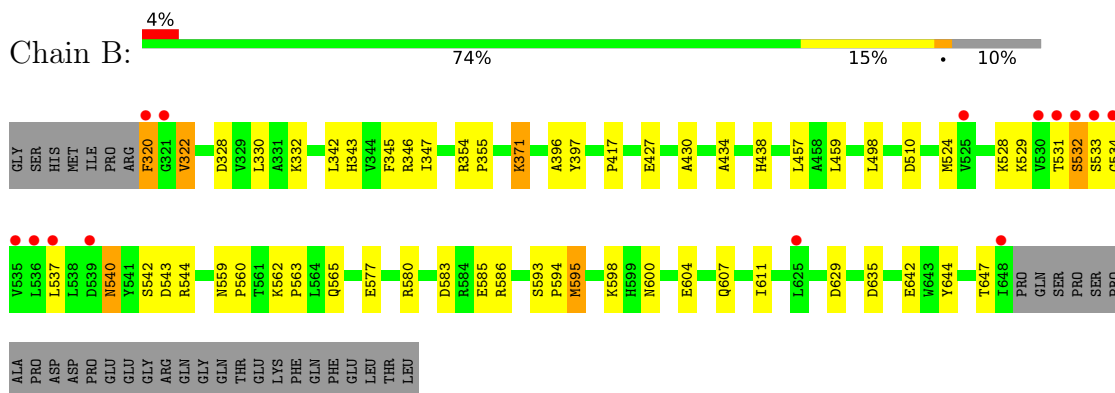| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	111	Total 111	O 111	0	0
4	C	73	Total 73	O 73	0	0
4	D	89	Total 89	O 89	0	0

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.
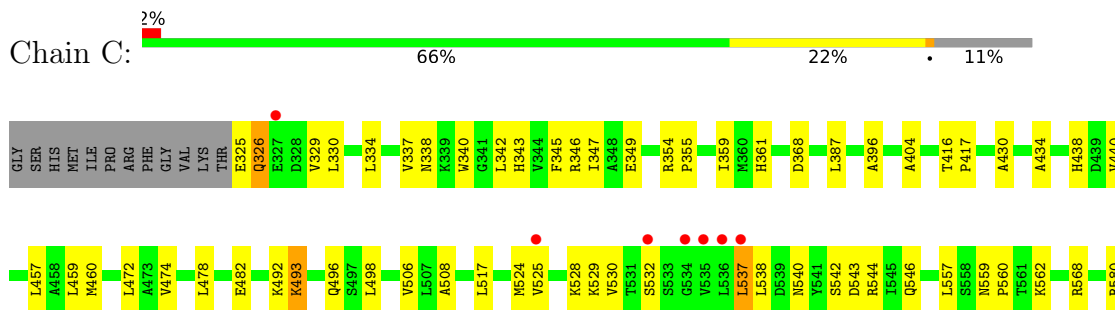
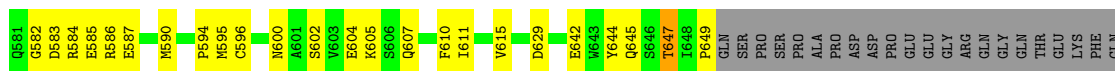• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D
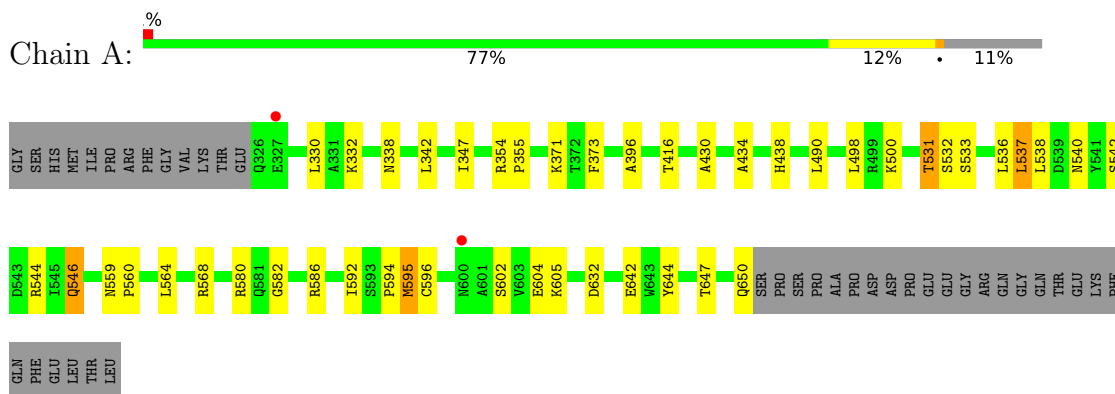
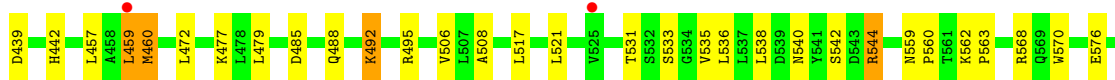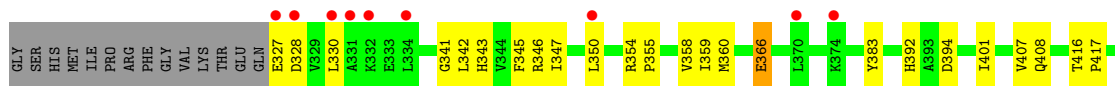• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Q581 G582 D583 R584 E585 R586 E587 M590 P594 M595 C596 N600 A601 S602 V603 E604 K605 S606 Q607 F610 I611 V615 D629 E642 W643 Y644 Q645 S646 T647 I648 P649 GLN SER PRO SER PRO ALA PRO ASP ASP PRO GLU GLU GLY ARG GLN GLY GLN THR GLU LYS PHE GLN

PHE GLU LEU THR LEU

• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain D:

GLY SER HIS MET ILE PRO ARG PHE GLY VAL LYS THR GLU GLN E327 D328 V329 L330 A331 K332 E333 L334 G341 L342 H343 V344 F345 R346 I347 L350 R354 P355 V358 I359 M360 E366 L370 K374 Y383 H392 A393 D394 I401 V407 Q408 T416 P417

D439 H442 L457 A458 L459 M460 L472 K477 L478 L479 D485 Q488 K492 R495 V506 L507 A508 L517 L521 V525 T531 S532 S533 G534 V535 L536 L537 L538 D539 N540 Y541 S542 D543 R544 N559 P560 T561 K562 P563 R568 Q569 W570 E576

R580 D583 R584 E585 R586 E587 R588 P594 M595 N600 E604 Q607 H616 P617 L625 V626 H627 P628 D629 R641 E642 W643 T647 I648 P649 Q650 SER PRO SER PRO ALA PRO ASP ASP PRO GLU GLU GLY ARG GLN GLY GLN THR GLU LYS PHE GLN PHE GLU LEU THR

LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.77Å 111.43Å 159.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.64 – 2.33 48.64 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.64-2.33) 95.3 (48.64-2.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.187 , 0.220 0.188 , 0.220	Depositor DCC
R_{free} test set	2000 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11094	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A0O

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	0.43	0/2685	0.54	0/3648
1	B	0.40	0/2716	0.52	0/3688
1	C	0.37	0/2685	0.53	0/3648
1	D	0.39	0/2676	0.53	0/3636
All	All	0.40	0/10762	0.53	0/14620

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2631	0	2586	42	0
1	B	2662	0	2618	49	0
1	C	2631	0	2584	54	1
1	D	2622	0	2578	65	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	18	16	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	16	0	1	0
3	C	18	16	0	1	0
3	D	18	16	0	3	0
4	A	131	0	0	7	0
4	B	111	0	0	5	0
4	C	73	0	0	5	0
4	D	89	0	0	2	0
All	All	11030	64	10366	208	1

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 10.

All (208) 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:604:GLU:HG2	1:A:647:THR:HG23	1.15	1.11
1:B:371:LYS:HB2	1:B:371:LYS:NZ	1.71	1.04
1:B:371:LYS:HB2	1:B:371:LYS:HZ3	1.25	0.98
1:D:595:MET:HG2	3:D:703:A0O:C17	1.92	0.98
1:A:396:ALA:HB2	1:A:580:ARG:HH22	1.31	0.95
1:C:329:VAL:HG23	4:C:805:HOH:O	1.67	0.94
1:C:326:GLN:HA	4:C:805:HOH:O	1.64	0.94
1:C:604:GLU:HG2	1:C:647:THR:HG23	1.50	0.94
1:D:492:LYS:HA	1:D:492:LYS:HE3	1.51	0.92
1:D:460:MET:O	1:D:460:MET:HE3	1.70	0.91
1:C:644:TYR:O	1:C:647:THR:HG22	1.73	0.89
1:A:604:GLU:CG	1:A:647:THR:HG23	2.06	0.82
1:D:343:HIS:HD2	1:D:346:ARG:H	1.29	0.81
1:D:604:GLU:HG2	1:D:647:THR:HG22	1.60	0.80
1:A:531:THR:CG2	1:A:533:SER:H	1.95	0.79
1:A:644:TYR:O	1:A:647:THR:HG22	1.84	0.78
1:D:343:HIS:CD2	1:D:346:ARG:H	2.03	0.77
1:A:604:GLU:HG2	1:A:647:THR:CG2	2.07	0.74
1:C:529:LYS:HD3	1:C:537:LEU:HD12	1.70	0.73
1:A:531:THR:HG22	1:A:533:SER:H	1.52	0.73
1:A:650:GLN:OE1	4:A:801:HOH:O	2.05	0.73
1:B:531:THR:OG1	1:B:537:LEU:HD12	1.90	0.71
1:A:586:ARG:HH11	1:A:592:ILE:HD11	1.54	0.71
1:D:559:ASN:HB2	1:D:560:PRO:HD3	1.73	0.71
1:A:396:ALA:HB2	1:A:580:ARG:NH2	2.04	0.70
1:D:492:LYS:HA	1:D:492:LYS:CE	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:GLU:CG	1:C:647:THR:HG23	2.22	0.69
1:B:644:TYR:O	1:B:647:THR:HG22	1.92	0.68
1:B:531:THR:O	1:B:533:SER:N	2.26	0.68
1:D:576:GLU:OE2	1:D:580:ARG:NH2	2.26	0.67
1:D:459:LEU:HD12	1:D:459:LEU:O	1.94	0.67
1:A:371:LYS:NZ	4:A:803:HOH:O	2.28	0.66
1:B:371:LYS:HB2	1:B:371:LYS:HZ2	1.60	0.66
1:A:632:ASP:OD2	1:B:371:LYS:HG3	1.96	0.66
1:D:583:ASP:OD1	1:D:586:ARG:NH2	2.29	0.65
1:B:417:PRO:HD2	1:B:629:ASP:OD2	1.97	0.65
1:B:635:ASP:OD2	4:B:801:HOH:O	2.14	0.65
1:B:531:THR:O	1:B:534:GLY:N	2.30	0.64
1:D:616:HIS:HB3	1:D:617:PRO:HD3	1.78	0.64
1:C:325:GLU:N	4:C:803:HOH:O	2.31	0.64
1:A:531:THR:HG23	1:A:532:SER:N	2.13	0.64
1:A:644:TYR:HA	1:A:647:THR:HG22	1.80	0.64
1:A:586:ARG:NH1	1:A:592:ILE:HD11	2.12	0.63
1:A:544:ARG:NH2	4:A:802:HOH:O	2.25	0.63
1:C:583:ASP:OD1	1:C:586:ARG:NH2	2.32	0.63
1:C:559:ASN:HB2	1:C:560:PRO:HD3	1.82	0.62
1:A:586:ARG:NH1	1:A:592:ILE:CD1	2.63	0.62
1:C:460:MET:O	1:C:460:MET:HE3	1.98	0.62
1:B:342:LEU:HD11	1:B:347:ILE:HD11	1.82	0.61
1:C:540:ASN:O	1:C:544:ARG:HG3	2.01	0.61
1:D:492:LYS:HE3	1:D:495:ARG:NH2	2.16	0.60
1:B:537:LEU:HA	4:B:826:HOH:O	2.02	0.59
1:D:366:GLU:HA	1:D:366:GLU:OE1	2.02	0.59
1:A:559:ASN:HB2	1:A:560:PRO:HD3	1.83	0.59
1:D:508:ALA:HB1	1:D:517:LEU:HD11	1.85	0.59
1:D:540:ASN:O	1:D:544:ARG:HG3	2.02	0.59
1:B:427:GLU:OE1	1:B:544:ARG:NH1	2.36	0.59
1:A:531:THR:HG22	1:A:533:SER:N	2.18	0.58
1:C:342:LEU:HD11	1:C:347:ILE:HD11	1.86	0.58
1:D:531:THR:HG23	1:D:533:SER:H	1.68	0.58
1:D:594:PRO:O	1:D:595:MET:HB2	2.03	0.58
1:D:604:GLU:HG2	1:D:647:THR:CG2	2.32	0.58
1:C:525:VAL:O	1:C:528:LYS:HB2	2.04	0.58
1:B:343:HIS:HE1	1:B:345:PHE:HB2	1.68	0.58
1:C:540:ASN:ND2	1:C:542:SER:HB2	2.18	0.57
1:D:346:ARG:NH2	1:D:350:LEU:HD21	2.20	0.57
1:D:531:THR:HG21	1:D:535:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:647:THR:HG22	1:D:647:THR:O	2.05	0.56
1:B:322:VAL:HG21	1:C:361:HIS:ND1	2.20	0.56
1:D:568:ARG:HD3	1:D:643:TRP:CH2	2.40	0.56
1:B:595:MET:HG2	3:B:703:A0O:C17	2.36	0.55
1:C:537:LEU:HD22	1:C:538:LEU:N	2.22	0.55
1:B:459:LEU:HD12	4:B:816:HOH:O	2.06	0.55
1:D:648:ILE:O	1:D:650:GLN:NE2	2.39	0.55
1:A:531:THR:CG2	1:A:532:SER:N	2.70	0.55
1:C:430:ALA:HB2	1:C:498:LEU:HD12	1.90	0.54
1:C:417:PRO:HD2	1:C:629:ASP:CG	2.28	0.54
1:D:492:LYS:NZ	1:D:495:ARG:HH12	2.06	0.54
1:B:559:ASN:HB2	1:B:560:PRO:HD3	1.90	0.54
1:B:604:GLU:HG2	1:B:647:THR:HG23	1.90	0.54
1:B:343:HIS:CE1	1:B:345:PHE:HB2	2.43	0.53
1:A:537:LEU:O	1:A:538:LEU:HD23	2.09	0.53
1:B:328:ASP:OD2	1:B:332:LYS:NZ	2.42	0.52
1:D:460:MET:HE3	1:D:460:MET:C	2.30	0.52
1:C:396:ALA:H	1:C:580:ARG:HH12	1.55	0.52
1:D:568:ARG:HD3	1:D:643:TRP:CZ3	2.44	0.52
1:D:417:PRO:HD2	1:D:629:ASP:CG	2.30	0.52
1:D:492:LYS:CE	1:D:492:LYS:CA	2.85	0.52
1:C:345:PHE:O	1:C:349:GLU:HG3	2.10	0.52
1:C:438:HIS:O	4:C:801:HOH:O	2.19	0.51
1:B:342:LEU:HD11	1:B:347:ILE:CD1	2.40	0.51
1:B:354:ARG:N	1:B:355:PRO:CD	2.74	0.51
1:B:430:ALA:HB2	1:B:498:LEU:HD12	1.92	0.50
1:D:354:ARG:N	1:D:355:PRO:CD	2.74	0.50
1:A:354:ARG:N	1:A:355:PRO:CD	2.75	0.50
1:D:540:ASN:ND2	1:D:540:ASN:H	2.08	0.50
1:D:604:GLU:HB2	4:D:810:HOH:O	2.12	0.50
1:C:417:PRO:HD2	1:C:629:ASP:OD2	2.12	0.50
1:A:430:ALA:HB2	1:A:498:LEU:HD12	1.94	0.49
1:D:472:LEU:HD21	1:D:506:VAL:HB	1.94	0.49
1:A:644:TYR:HA	1:A:647:THR:CG2	2.42	0.49
1:C:540:ASN:OD1	1:C:540:ASN:N	2.41	0.49
1:B:371:LYS:HZ2	1:B:371:LYS:CB	2.23	0.49
1:B:531:THR:CG2	1:B:532:SER:N	2.76	0.49
1:B:594:PRO:O	1:B:595:MET:HB2	2.11	0.48
1:D:531:THR:HG22	1:D:535:VAL:H	1.78	0.48
1:D:358:VAL:HG23	1:D:359:ILE:N	2.29	0.48
1:B:417:PRO:CD	1:B:629:ASP:OD2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:ASP:OD1	1:B:598:LYS:HE2	2.14	0.47
1:D:342:LEU:HD11	1:D:347:ILE:HD11	1.96	0.47
1:B:371:LYS:NZ	1:B:371:LYS:CB	2.51	0.47
1:B:644:TYR:C	1:B:647:THR:HG22	2.35	0.47
1:C:387:LEU:HD12	1:C:440:VAL:HG21	1.97	0.47
1:C:645:GLN:C	1:C:647:THR:H	2.17	0.47
1:D:392:HIS:HB3	1:D:394:ASP:OD1	2.14	0.47
1:B:607:GLN:O	1:B:611:ILE:HG13	2.15	0.47
1:C:524:MET:CE	1:C:543:ASP:HA	2.44	0.47
1:D:460:MET:HE2	1:D:460:MET:HB3	1.50	0.47
1:C:594:PRO:O	1:C:595:MET:HB2	2.14	0.47
1:C:604:GLU:CG	1:C:647:THR:CG2	2.93	0.47
1:B:540:ASN:ND2	1:B:540:ASN:H	2.13	0.47
1:B:565:GLN:H	1:B:565:GLN:CD	2.18	0.46
1:D:459:LEU:HD12	1:D:459:LEU:C	2.36	0.46
1:A:531:THR:HG23	1:A:533:SER:H	1.74	0.46
1:A:564:LEU:O	1:A:568:ARG:HG3	2.16	0.46
1:A:644:TYR:C	1:A:647:THR:HG22	2.36	0.46
1:D:531:THR:CG2	1:D:535:VAL:HG22	2.46	0.46
1:B:427:GLU:OE2	1:B:544:ARG:HD3	2.16	0.45
1:D:477:LYS:HG3	4:D:852:HOH:O	2.17	0.45
1:A:332:LYS:HA	4:A:873:HOH:O	2.16	0.45
1:C:474:VAL:O	1:C:478:LEU:HG	2.16	0.45
1:A:605:LYS:HE3	1:A:605:LYS:HB2	1.81	0.45
1:C:585:GLU:HG2	1:C:590:MET:HE2	1.99	0.45
1:A:650:GLN:HG2	1:C:568:ARG:HH12	1.82	0.45
1:C:359:ILE:HD12	1:C:404:ALA:HB1	1.98	0.45
1:C:605:LYS:HE3	1:C:605:LYS:HB2	1.64	0.45
1:B:396:ALA:H	1:B:580:ARG:HH12	1.65	0.44
1:B:562:LYS:O	1:B:563:PRO:C	2.55	0.44
1:A:500:LYS:NZ	4:A:809:HOH:O	2.43	0.44
1:B:644:TYR:HA	1:B:647:THR:HG22	1.99	0.44
1:C:343:HIS:CE1	1:C:345:PHE:HB2	2.52	0.44
1:C:611:ILE:HA	1:C:615:VAL:HB	2.00	0.44
1:A:644:TYR:CA	1:A:647:THR:HG22	2.45	0.44
1:B:434:ALA:O	1:B:438:HIS:HB3	2.18	0.44
1:D:607:GLN:HE22	3:D:703:A0O:C15	2.30	0.44
1:A:594:PRO:O	1:A:595:MET:HB2	2.18	0.44
1:B:510:ASP:OD1	4:B:802:HOH:O	2.21	0.43
1:D:343:HIS:NE2	1:D:345:PHE:HB2	2.32	0.43
1:D:627:HIS:HA	1:D:628:PRO:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:PHE:HB3	1:A:490:LEU:HD11	2.00	0.43
1:C:346:ARG:HD2	1:C:346:ARG:HA	1.78	0.43
1:D:342:LEU:HD21	1:D:347:ILE:HD12	2.00	0.43
1:A:540:ASN:O	1:A:544:ARG:HG3	2.18	0.43
1:C:492:LYS:O	1:C:496:GLN:HG3	2.19	0.43
1:C:334:LEU:O	1:C:337:VAL:HB	2.18	0.43
1:C:607:GLN:O	1:C:611:ILE:HG13	2.19	0.43
1:C:368:ASP:HA	4:C:850:HOH:O	2.18	0.43
1:D:341:GLY:O	1:D:342:LEU:C	2.56	0.43
1:D:536:LEU:HD12	1:D:536:LEU:HA	1.72	0.42
1:B:585:GLU:OE2	1:B:593:SER:OG	2.33	0.42
1:C:340:TRP:CE2	1:C:562:LYS:HE2	2.54	0.42
1:C:542:SER:O	1:C:546:GLN:HB2	2.20	0.42
1:C:582:GLY:HA3	1:C:596:CYS:O	2.20	0.42
1:A:542:SER:O	1:A:546:GLN:HB2	2.19	0.42
1:A:586:ARG:HH11	1:A:592:ILE:CD1	2.24	0.42
1:D:492:LYS:HZ1	1:D:495:ARG:HH12	1.66	0.42
1:D:562:LYS:HB3	1:D:563:PRO:HD2	2.01	0.42
1:B:397:TYR:HB3	1:B:577:GLU:OE1	2.20	0.42
1:C:434:ALA:O	1:C:438:HIS:HB3	2.20	0.42
1:D:383:TYR:CD2	1:D:383:TYR:C	2.93	0.42
1:D:439:ASP:O	1:D:442:HIS:HB2	2.19	0.42
1:A:580:ARG:NH1	4:A:807:HOH:O	2.39	0.42
1:D:485:ASP:O	1:D:488:GLN:NE2	2.36	0.42
1:C:354:ARG:N	1:C:355:PRO:CD	2.83	0.42
1:B:320:PHE:N	1:B:320:PHE:CD2	2.89	0.41
1:D:342:LEU:HD22	1:D:408:GLN:HG3	2.00	0.41
3:C:703:A0O:O01	3:C:703:A0O:C09	2.68	0.41
1:D:401:ILE:HG22	1:D:570:TRP:HH2	1.85	0.41
1:C:493:LYS:O	1:C:493:LYS:HG2	2.20	0.41
1:D:383:TYR:CE1	1:D:479:LEU:HD23	2.56	0.41
1:B:594:PRO:O	1:B:595:MET:CB	2.68	0.41
1:C:508:ALA:HB1	1:C:517:LEU:HD11	2.03	0.41
1:D:366:GLU:OE1	1:D:366:GLU:CA	2.66	0.41
1:A:434:ALA:O	1:A:438:HIS:HB3	2.20	0.41
1:A:582:GLY:HA3	1:A:596:CYS:O	2.20	0.41
1:C:557:LEU:HD22	1:C:610:PHE:HZ	1.86	0.41
1:D:517:LEU:HD23	1:D:517:LEU:HA	1.90	0.41
1:B:354:ARG:HH11	1:B:354:ARG:HD3	1.73	0.41
1:B:565:GLN:OE1	1:B:565:GLN:N	2.47	0.41
1:C:584:ARG:O	1:C:587:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:MET:SD	1:D:407:VAL:HG11	2.61	0.41
1:D:607:GLN:NE2	3:D:703:A0O:O03	2.54	0.41
1:B:524:MET:HE1	1:B:543:ASP:HA	2.03	0.41
1:D:521:LEU:HD11	1:D:625:LEU:HD22	2.03	0.40
1:A:342:LEU:HD11	1:A:347:ILE:HD11	2.03	0.40
1:B:528:LYS:C	1:B:529:LYS:HG3	2.41	0.40
1:B:586:ARG:NH1	4:B:813:HOH:O	2.54	0.40
1:C:334:LEU:HD23	1:C:347:ILE:HD13	2.03	0.40
1:C:459:LEU:HD23	1:C:459:LEU:O	2.21	0.40
1:C:472:LEU:HD21	1:C:506:VAL:HB	2.03	0.40
1:D:531:THR:HG21	1:D:535:VAL:CG2	2.51	0.40
1:D:641:ARG:HD2	1:D:642:GLU:OE2	2.21	0.40
1:C:460:MET:HE2	1:C:460:MET:HB3	1.84	0.40
1:D:538:LEU:HB3	1:D:544:ARG:HG2	2.02	0.40
1:D:531:THR:HG22	1:D:535:VAL:N	2.37	0.40
1:D:588:ARG:HH11	1:D:588:ARG:HD3	1.76	0.40
1:A:338:ASN:HB2	4:A:839:HOH:O	2.20	0.40
1:C:337:VAL:HG13	1:C:338:ASN:OD1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:GLU:OE1	1:D:492:LYS:NZ[3_444]	1.96	0.24

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	323/364 (89%)	317 (98%)	6 (2%)	0	100	100
1	B	327/364 (90%)	314 (96%)	12 (4%)	1 (0%)	41	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	323/364 (89%)	312 (97%)	11 (3%)	0	100	100
1	D	322/364 (88%)	305 (95%)	17 (5%)	0	100	100
All	All	1295/1456 (89%)	1248 (96%)	46 (4%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	532	SER

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	297/331 (90%)	288 (97%)	9 (3%)	41	56
1	B	300/331 (91%)	289 (96%)	11 (4%)	34	47
1	C	297/331 (90%)	284 (96%)	13 (4%)	28	39
1	D	296/331 (89%)	281 (95%)	15 (5%)	24	33
All	All	1190/1324 (90%)	1142 (96%)	48 (4%)	31	44

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	LEU
1	A	416	THR
1	A	531	THR
1	A	536	LEU
1	A	537	LEU
1	A	546	GLN
1	A	595	MET
1	A	602	SER
1	A	642	GLU
1	B	320	PHE
1	B	322	VAL

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Mol	Chain	Res	Type
1	B	330	LEU
1	B	346	ARG
1	B	371	LYS
1	B	457	LEU
1	B	540	ASN
1	B	542	SER
1	B	595	MET
1	B	600	ASN
1	B	642	GLU
1	C	326	GLN
1	C	330	LEU
1	C	416	THR
1	C	457	LEU
1	C	493	LYS
1	C	530	VAL
1	C	532	SER
1	C	537	LEU
1	C	600	ASN
1	C	602	SER
1	C	642	GLU
1	C	647	THR
1	C	649	PRO
1	D	327	GLU
1	D	328	ASP
1	D	330	LEU
1	D	366	GLU
1	D	416	THR
1	D	457	LEU
1	D	459	LEU
1	D	460	MET
1	D	492	LYS
1	D	542	SER
1	D	544	ARG
1	D	584	ARG
1	D	595	MET
1	D	600	ASN
1	D	642	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	343	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	A0O	D	703	-	19,19,19	1.77	4 (21%)	26,26,26	3.30	11 (42%)
3	A0O	C	703	-	19,19,19	1.69	3 (15%)	26,26,26	3.93	11 (42%)
3	A0O	A	703	-	19,19,19	1.69	3 (15%)	26,26,26	3.13	13 (50%)
3	A0O	B	703	-	19,19,19	1.81	4 (21%)	26,26,26	3.70	12 (46%)

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	A0O	D	703	-	-	2/7/7/7	0/2/2/2
3	A0O	C	703	-	-	6/7/7/7	0/2/2/2
3	A0O	A	703	-	-	1/7/7/7	0/2/2/2
3	A0O	B	703	-	-	5/7/7/7	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	A0O	O01-C06	4.59	1.45	1.38
3	D	703	A0O	O01-C06	4.39	1.45	1.38
3	A	703	A0O	O01-C06	4.33	1.45	1.38
3	B	703	A0O	O01-C15	4.23	1.45	1.38
3	D	703	A0O	O01-C15	4.17	1.45	1.38
3	C	703	A0O	O01-C06	3.92	1.44	1.38
3	C	703	A0O	O01-C15	3.75	1.44	1.38
3	A	703	A0O	O01-C15	3.22	1.43	1.38
3	D	703	A0O	C14-C12	-2.85	1.29	1.34
3	A	703	A0O	C14-C12	-2.81	1.29	1.34
3	B	703	A0O	C14-C12	-2.67	1.30	1.34
3	C	703	A0O	C14-C12	-2.63	1.30	1.34
3	D	703	A0O	C09-C13	2.36	1.39	1.32
3	B	703	A0O	C05-C04	-2.27	1.49	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	A0O	C06-O01-C15	-14.31	109.76	121.99
3	B	703	A0O	C06-O01-C15	-13.09	110.81	121.99
3	A	703	A0O	C06-O01-C15	-9.64	113.75	121.99
3	D	703	A0O	C06-O01-C15	-8.95	114.34	121.99
3	C	703	A0O	C05-C09-C13	-7.78	118.13	127.59
3	B	703	A0O	C05-C09-C13	-7.60	118.34	127.59
3	D	703	A0O	O02-C08-C04	6.72	122.47	115.35
3	D	703	A0O	C05-C09-C13	-6.65	119.50	127.59
3	A	703	A0O	C05-C09-C13	-6.13	120.13	127.59
3	C	703	A0O	O02-C08-C04	5.96	121.66	115.35
3	A	703	A0O	O02-C08-C04	5.20	120.86	115.35
3	C	703	A0O	C18-O02-C08	4.87	124.88	117.53
3	B	703	A0O	O01-C15-O03	4.61	122.32	116.44
3	D	703	A0O	O03-C15-C14	-4.56	117.52	126.00
3	A	703	A0O	O03-C15-C14	-4.18	118.22	126.00
3	B	703	A0O	O03-C15-C14	-4.08	118.42	126.00
3	B	703	A0O	O02-C08-C04	4.06	119.65	115.35
3	D	703	A0O	O02-C08-C11	-4.04	117.44	124.37
3	D	703	A0O	C06-C07-C12	3.83	121.30	117.52
3	B	703	A0O	C08-C04-C06	3.68	121.03	116.63
3	C	703	A0O	O01-C15-O03	3.66	121.11	116.44
3	A	703	A0O	O01-C15-O03	3.38	120.75	116.44
3	C	703	A0O	O03-C15-C14	-3.36	119.76	126.00
3	D	703	A0O	O01-C15-O03	3.32	120.67	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	A0O	O01-C06-C04	3.25	119.65	115.96
3	A	703	A0O	C06-C07-C12	3.15	120.62	117.52
3	D	703	A0O	O01-C15-C14	3.08	121.81	117.12
3	A	703	A0O	C08-C04-C06	2.94	120.15	116.63
3	A	703	A0O	O02-C08-C11	-2.91	119.38	124.37
3	D	703	A0O	C04-C05-C09	2.88	116.72	112.17
3	C	703	A0O	O02-C08-C11	-2.85	119.48	124.37
3	A	703	A0O	C18-O02-C08	2.85	121.83	117.53
3	B	703	A0O	C18-O02-C08	2.71	121.61	117.53
3	C	703	A0O	C06-C07-C12	2.70	120.18	117.52
3	C	703	A0O	C08-C04-C06	2.56	119.70	116.63
3	A	703	A0O	O01-C15-C14	2.56	121.02	117.12
3	B	703	A0O	C12-C14-C15	-2.54	118.14	121.43
3	C	703	A0O	C12-C14-C15	-2.49	118.22	121.43
3	B	703	A0O	C06-C07-C12	2.43	119.92	117.52
3	D	703	A0O	C10-C07-C12	-2.42	117.50	122.44
3	D	703	A0O	O01-C06-C04	2.40	118.68	115.96
3	B	703	A0O	C04-C05-C09	-2.34	108.47	112.17
3	A	703	A0O	O01-C06-C04	2.22	118.48	115.96
3	C	703	A0O	C05-C04-C06	-2.21	117.46	121.37
3	B	703	A0O	C16-C13-C17	2.20	119.45	114.60
3	A	703	A0O	C05-C04-C06	-2.06	117.74	121.37
3	A	703	A0O	C10-C07-C12	-2.05	118.25	122.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	703	A0O	C04-C08-O02-C18
3	B	703	A0O	C05-C09-C13-C17
3	C	703	A0O	C05-C09-C13-C17
3	D	703	A0O	C05-C09-C13-C16
3	C	703	A0O	C11-C08-O02-C18
3	A	703	A0O	C05-C09-C13-C17
3	D	703	A0O	C05-C09-C13-C17
3	C	703	A0O	C06-C04-C05-C09
3	B	703	A0O	C06-C04-C05-C09
3	C	703	A0O	C08-C04-C05-C09
3	B	703	A0O	C11-C08-O02-C18
3	B	703	A0O	C08-C04-C05-C09
3	B	703	A0O	C04-C08-O02-C18
3	C	703	A0O	C05-C09-C13-C16

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	703	A0O	3	0
3	C	703	A0O	1	0
3	B	703	A0O	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A0O D 703

Bond lengths

Bond angles

Torsions

Rings

Ligand A0O C 703

Bond lengths

Bond angles

Torsions

Rings

Ligand A0O A 703

Bond lengths

Bond angles

Torsions

Rings

Ligand A0O B 703

Bond lengths

Bond angles

Torsions

Rings
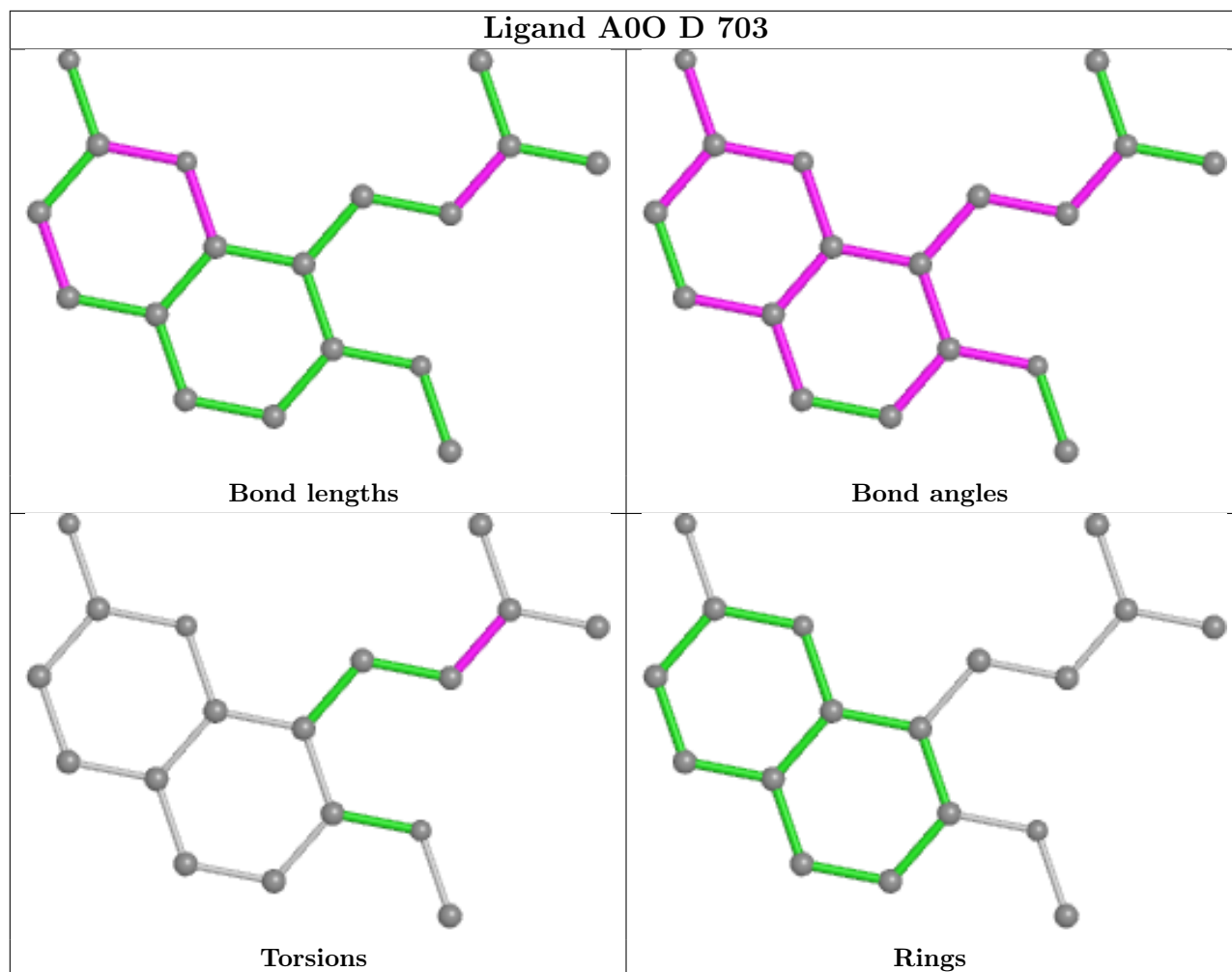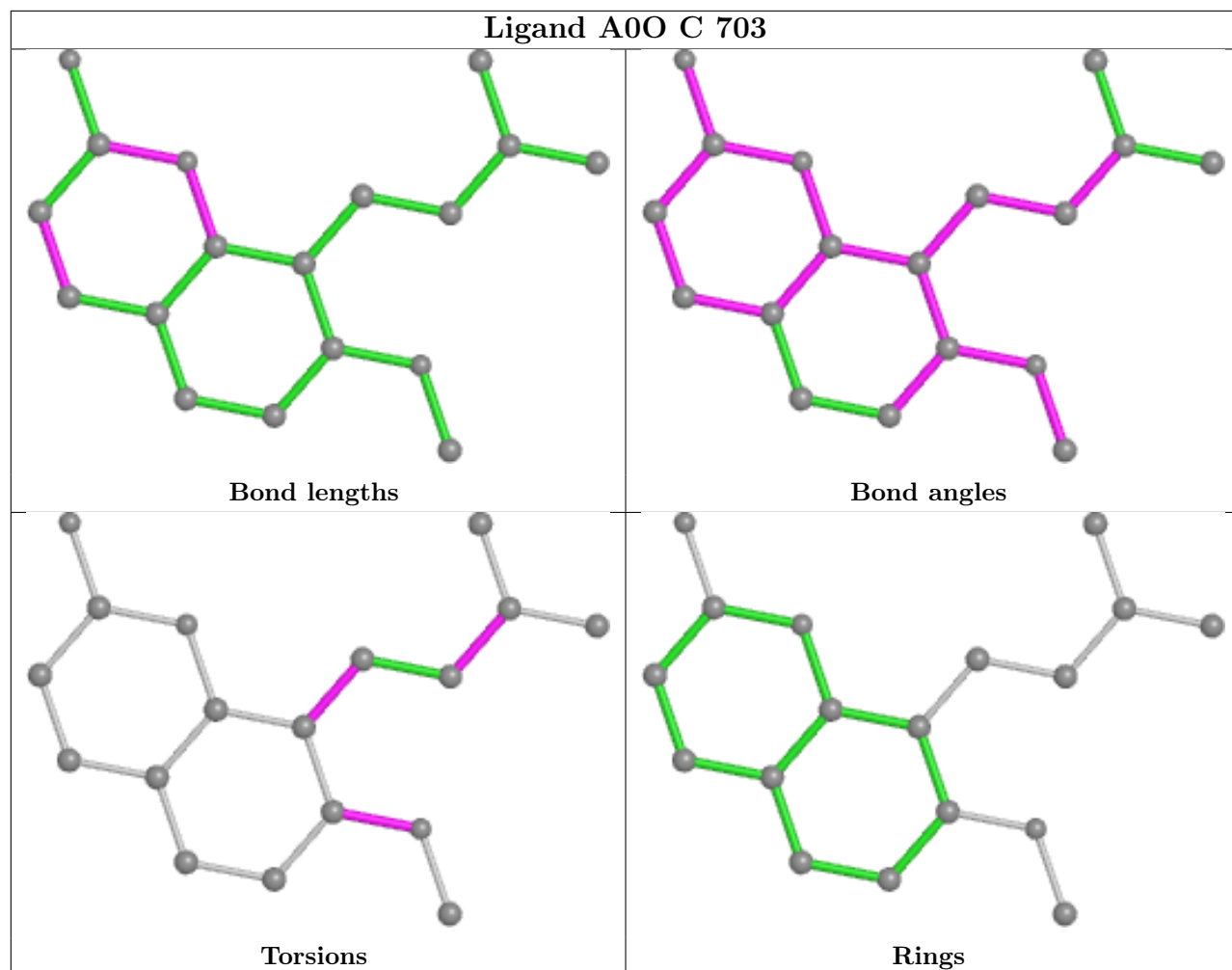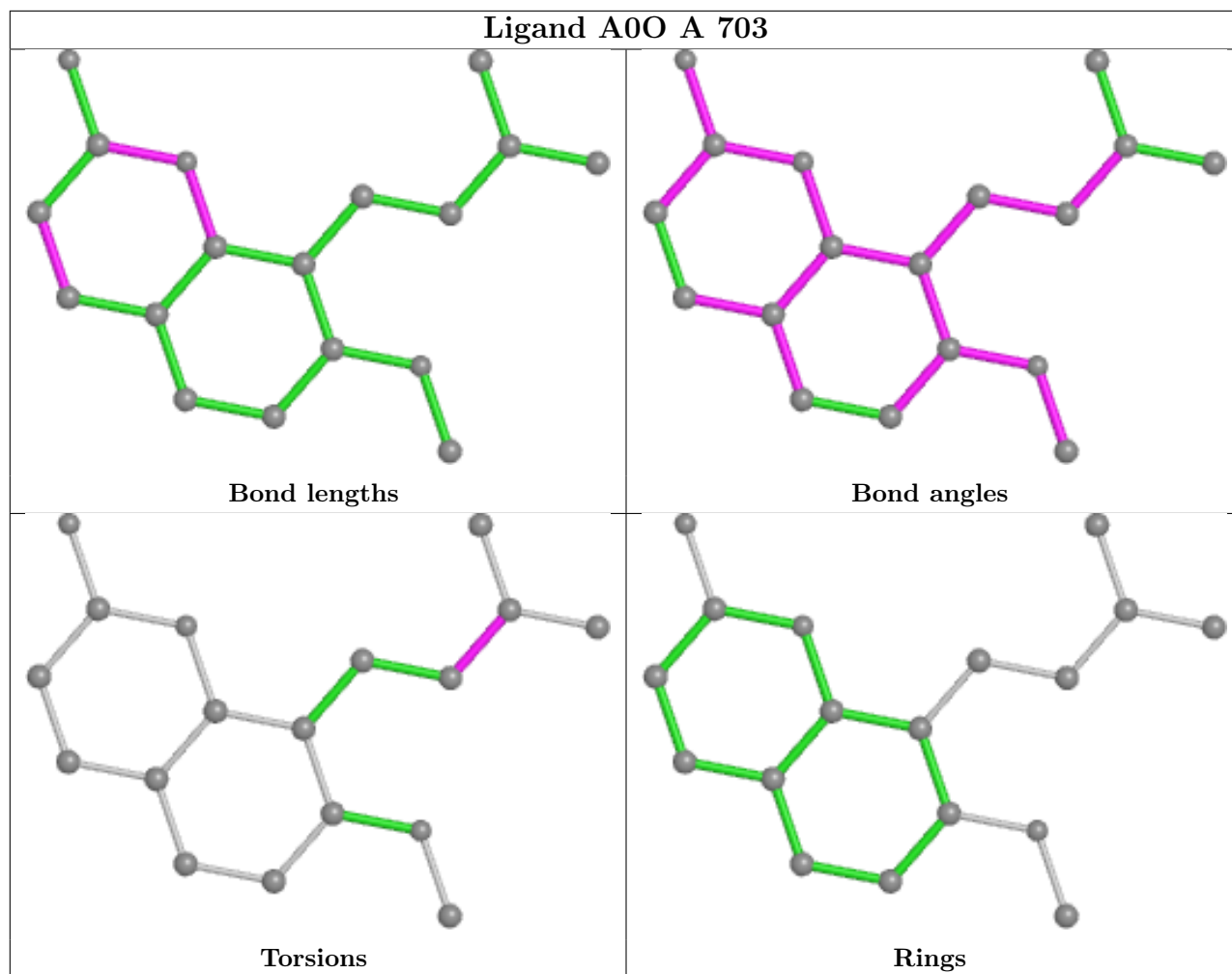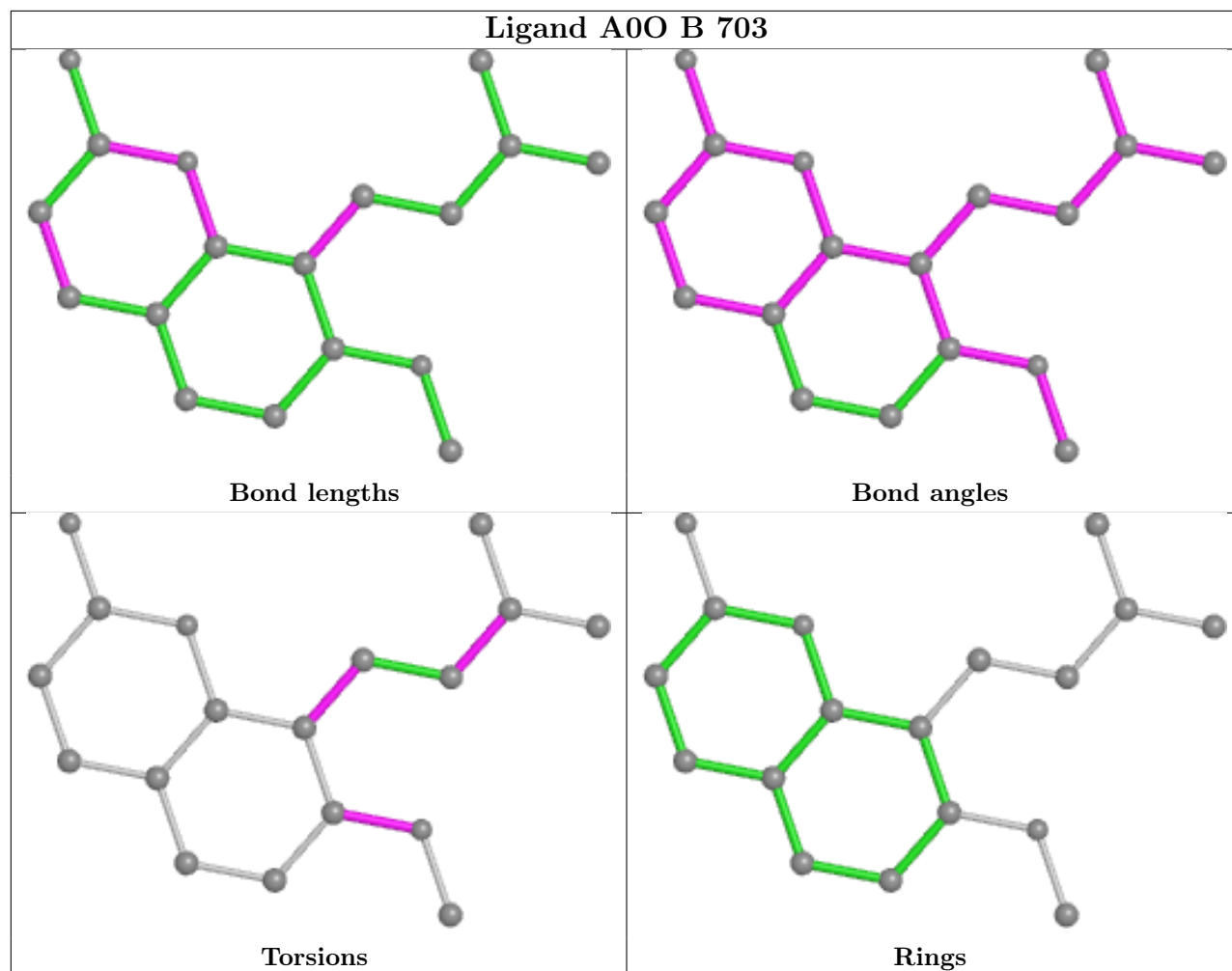
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	325/364 (89%)	-0.24	2 (0%)	89	92	8, 19, 36, 61	0
1	B	329/364 (90%)	0.08	14 (4%)	35	42	10, 24, 47, 80	0
1	C	325/364 (89%)	0.03	7 (2%)	62	69	14, 30, 54, 73	0
1	D	324/364 (89%)	0.15	12 (3%)	41	48	12, 32, 47, 70	0
All	All	1303/1456 (89%)	0.01	35 (2%)	54	62	8, 27, 47, 80	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	327	GLU	5.4
1	C	525	VAL	5.3
1	B	321	GLY	4.9
1	B	533	SER	4.7
1	B	532	SER	4.6
1	B	535	VAL	3.9
1	D	334	LEU	3.9
1	A	327	GLU	3.7
1	D	330	LEU	3.3
1	C	536	LEU	3.3
1	C	532	SER	3.3
1	B	320	PHE	3.3
1	B	539	ASP	3.0
1	B	531	THR	3.0
1	D	332	LYS	2.8
1	B	537	LEU	2.8
1	C	327	GLU	2.8
1	D	370	LEU	2.7
1	C	535	VAL	2.7
1	C	537	LEU	2.7
1	D	525	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	648	ILE	2.6
1	B	625	LEU	2.5
1	D	374	LYS	2.4
1	B	534	GLY	2.4
1	B	536	LEU	2.3
1	C	534	GLY	2.3
1	A	600	ASN	2.2
1	D	328	ASP	2.2
1	D	331	ALA	2.2
1	D	350	LEU	2.2
1	D	625	LEU	2.1
1	B	530	VAL	2.1
1	B	525	VAL	2.0
1	D	459	LEU	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 monosaccharides 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, 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	A0O	D	703	18/18	0.64	0.43	35,44,58,58	0
3	A0O	B	703	18/18	0.75	0.41	35,48,60,60	0
3	A0O	C	703	18/18	0.79	0.31	33,42,50,50	0
2	ZN	C	702	1/1	0.88	0.05	62,62,62,62	0
2	ZN	D	702	1/1	0.91	0.08	70,70,70,70	0
2	ZN	B	702	1/1	0.92	0.07	59,59,59,59	0
2	ZN	A	702	1/1	0.92	0.05	57,57,57,57	0
3	A0O	A	703	18/18	0.93	0.28	26,36,44,44	0
2	ZN	D	701	1/1	0.98	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	701	1/1	1.00	0.11	20,20,20,20	0
2	ZN	C	701	1/1	1.00	0.08	25,25,25,25	0
2	ZN	B	701	1/1	1.00	0.11	22,22,22,22	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 A0O D 703:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
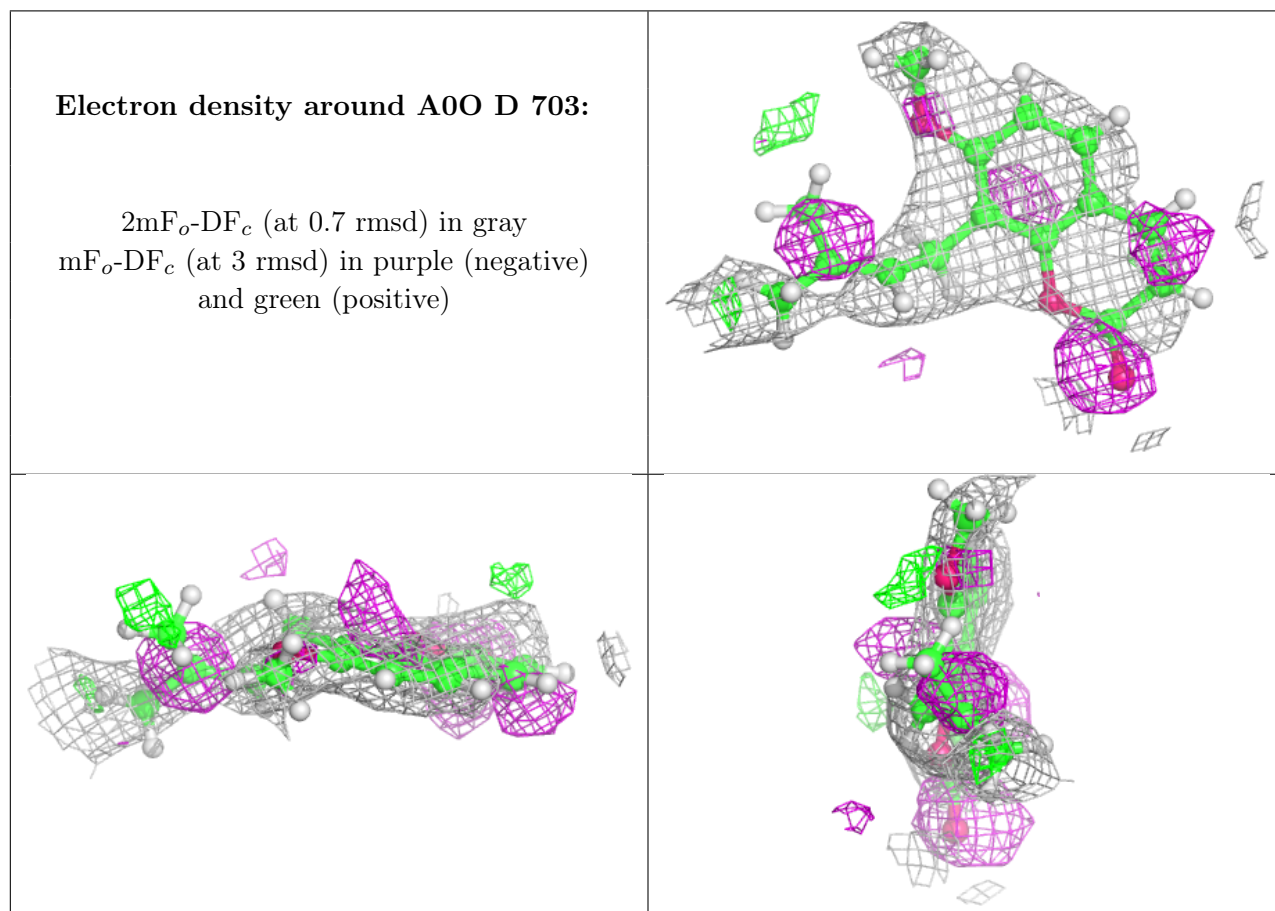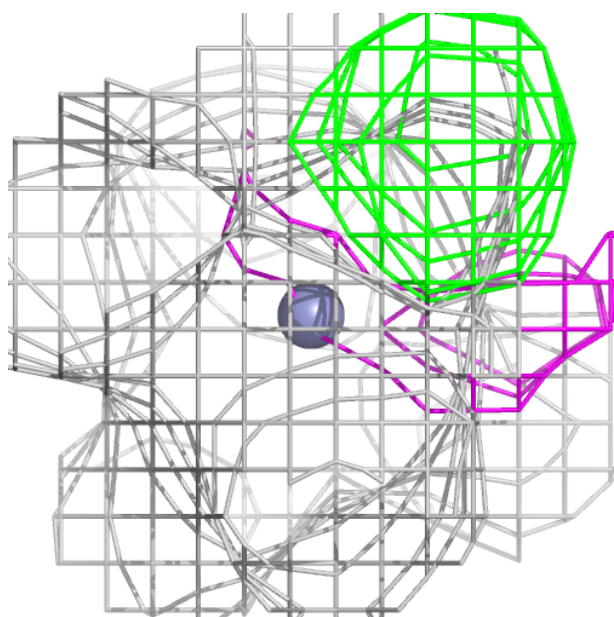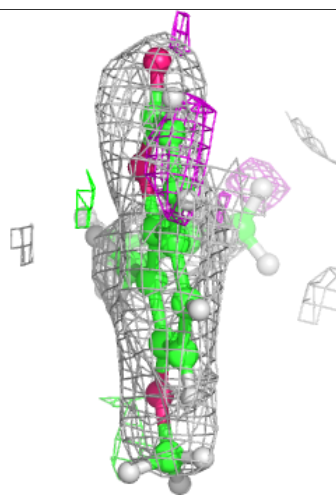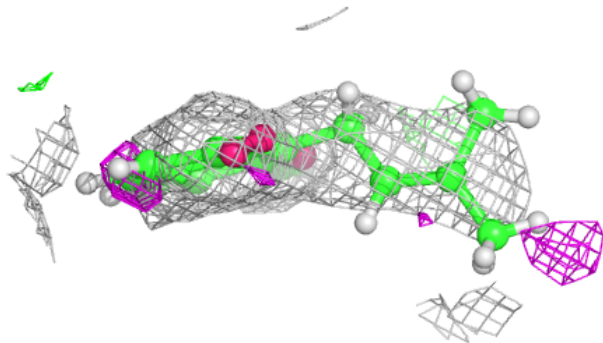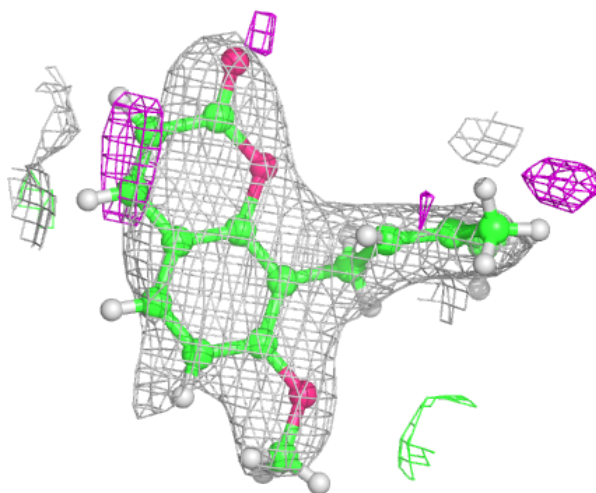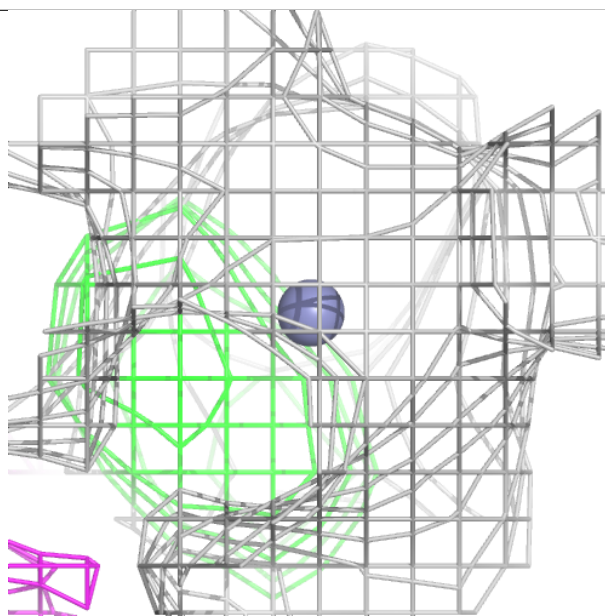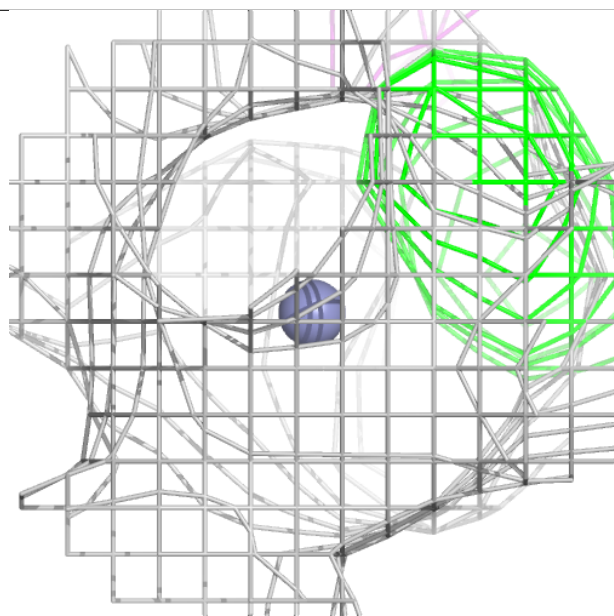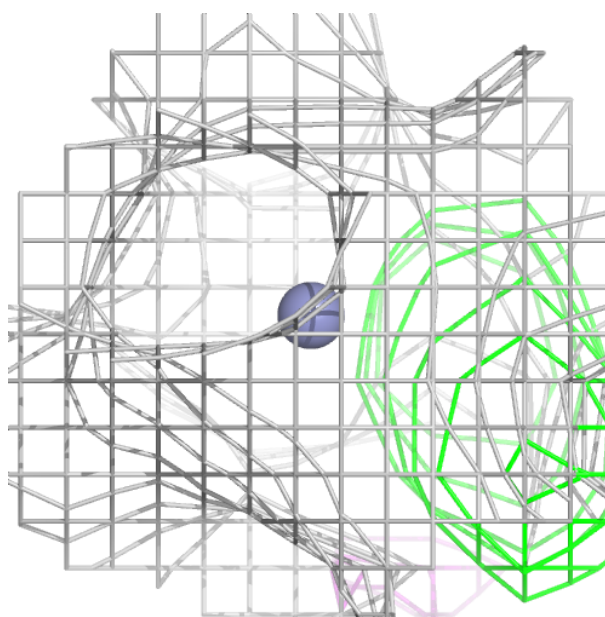
Electron density around A0O B 703:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
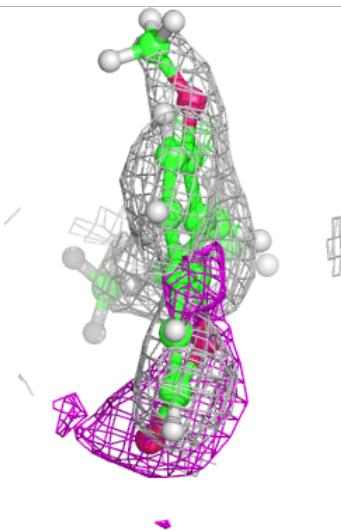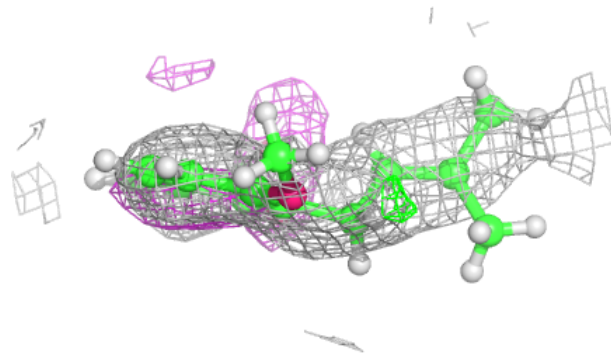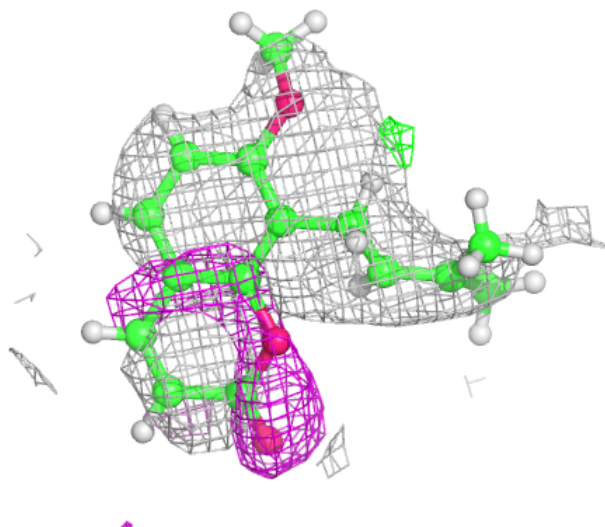
Electron density around A0O C 703:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
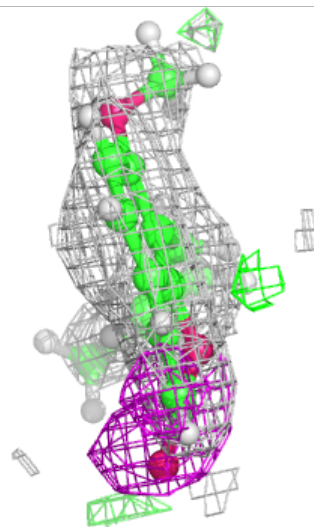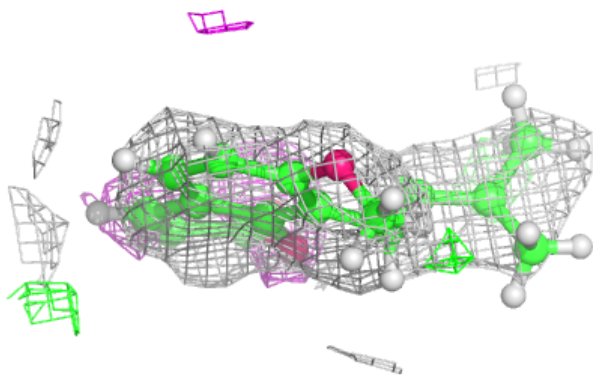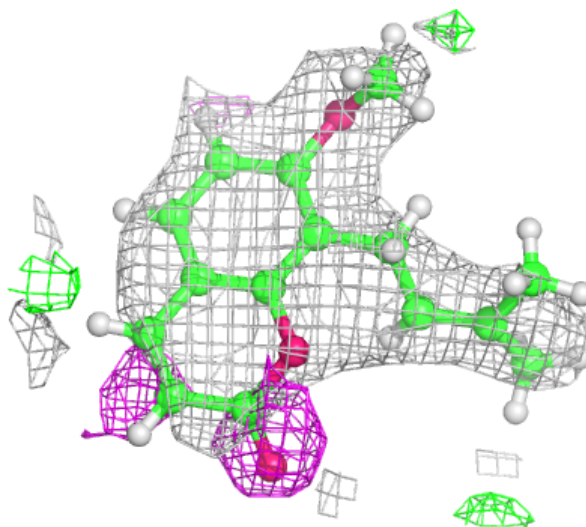
Electron density around ZN C 702:

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

Full wwPDB X-ray Structure Validation Report
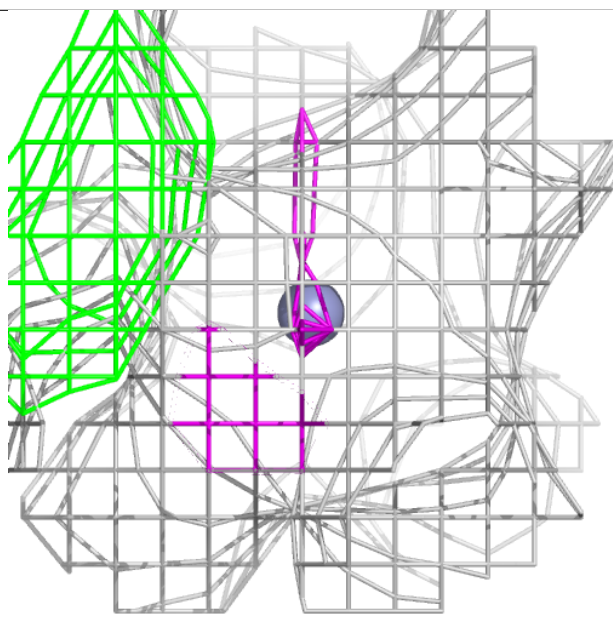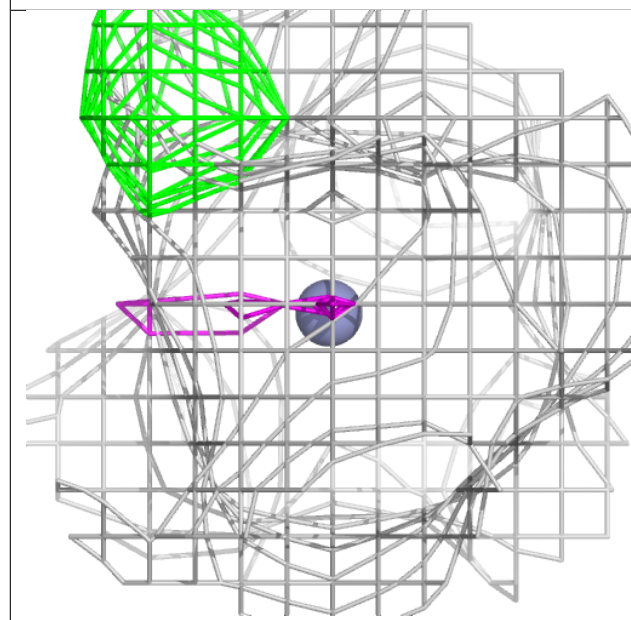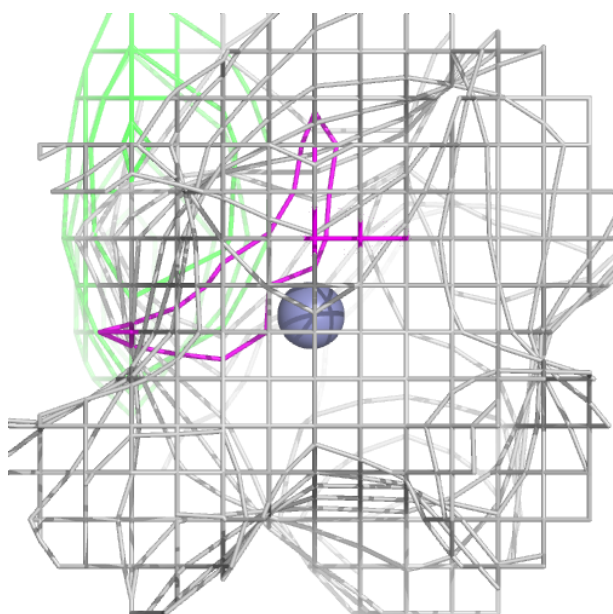
Electron density around ZN D 702:

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and green (positive)
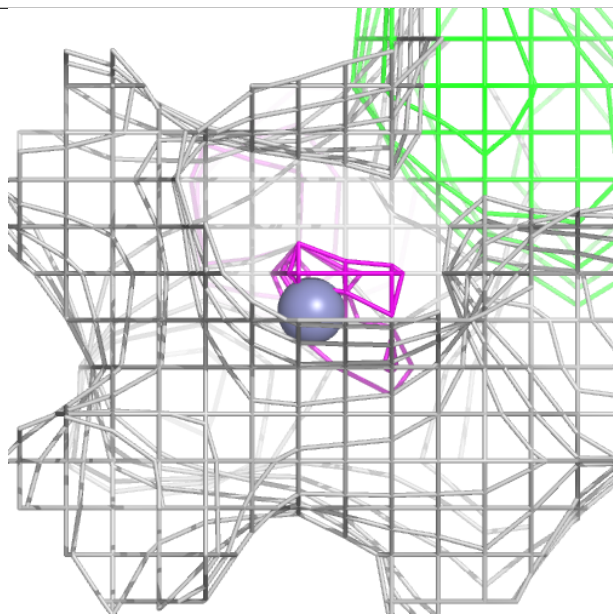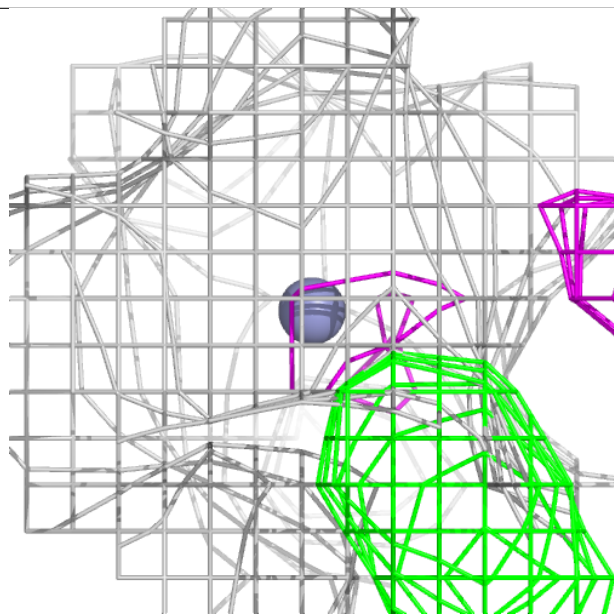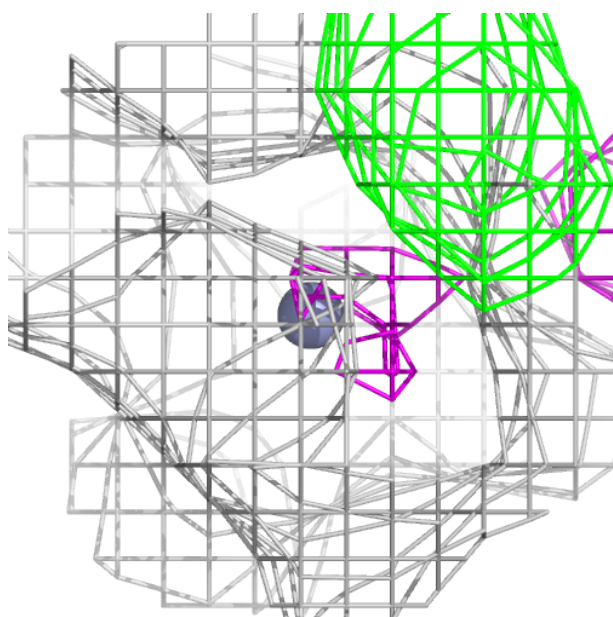
Electron density around ZN B 702:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
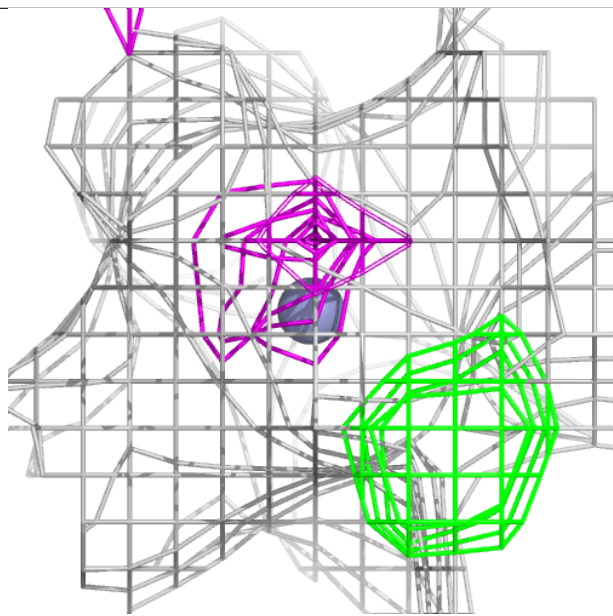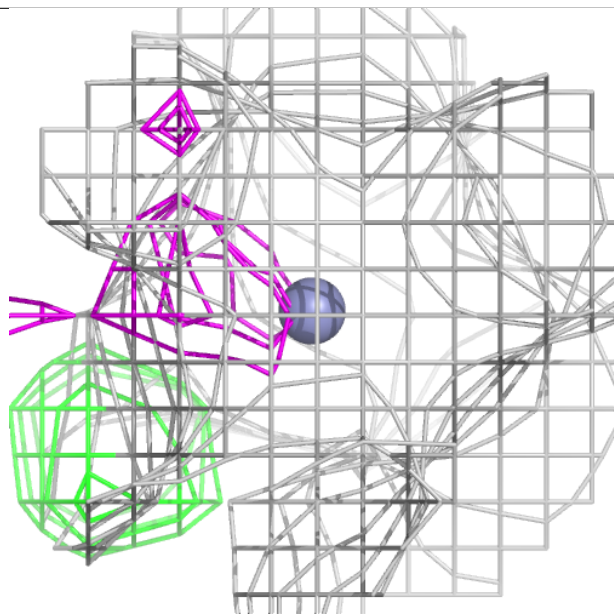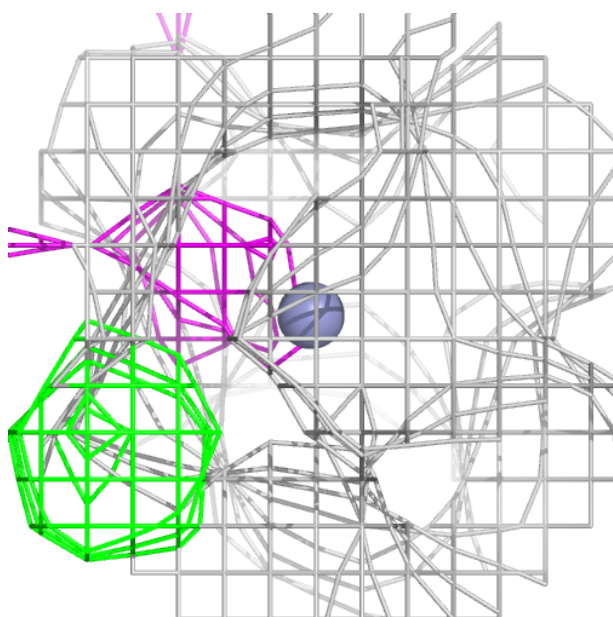
Electron density around ZN A 702:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
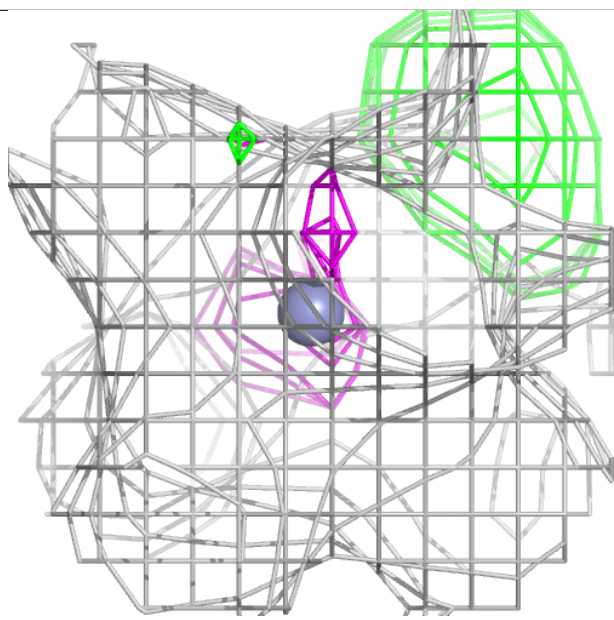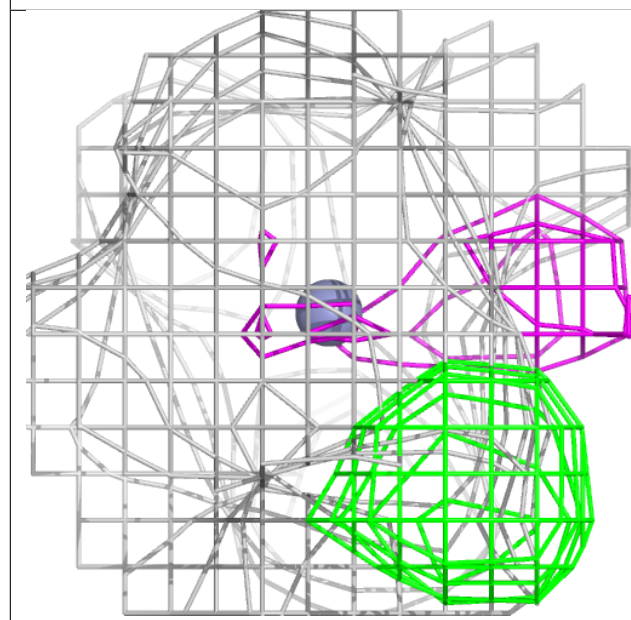
Electron density around A0O A 703:

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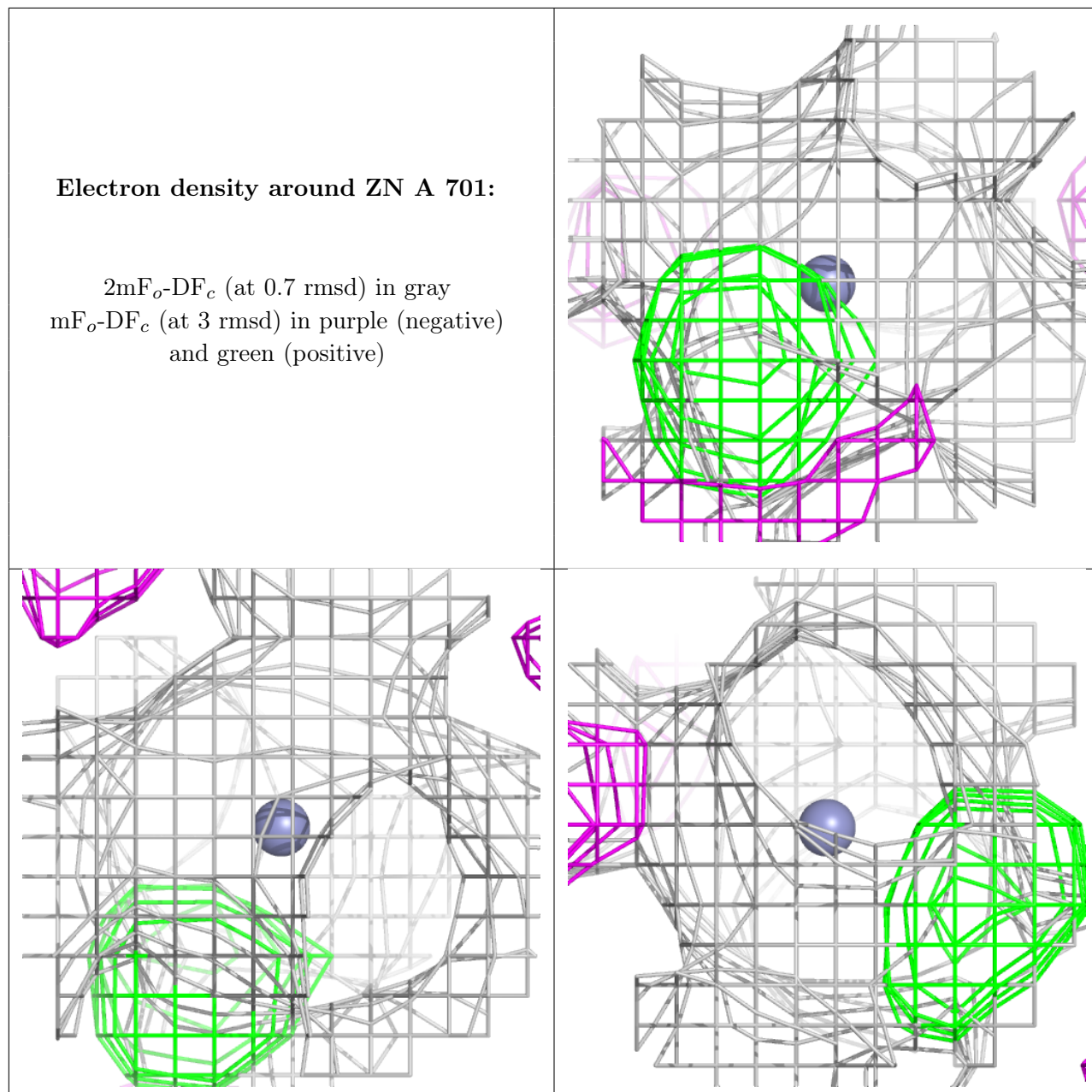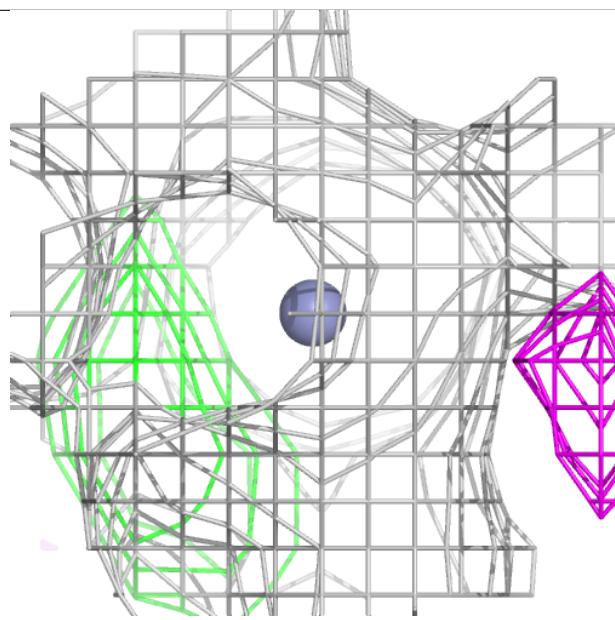mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Full wwPDB X-ray Structure Validation Report

Electron density around ZN D 701:

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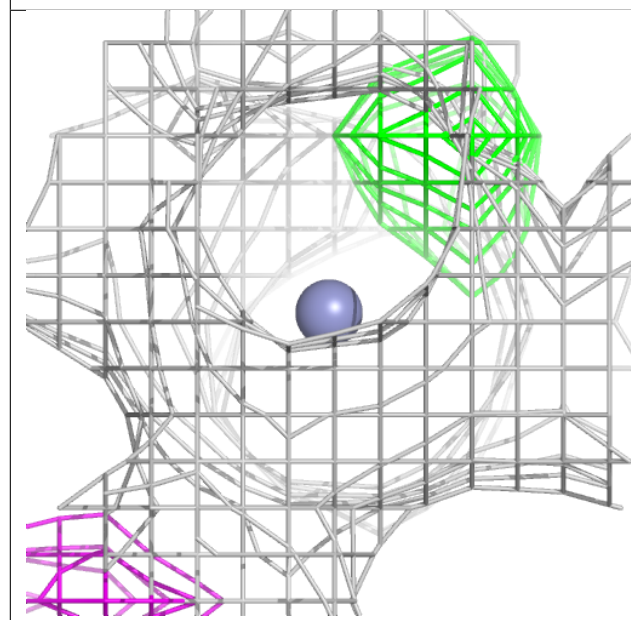$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
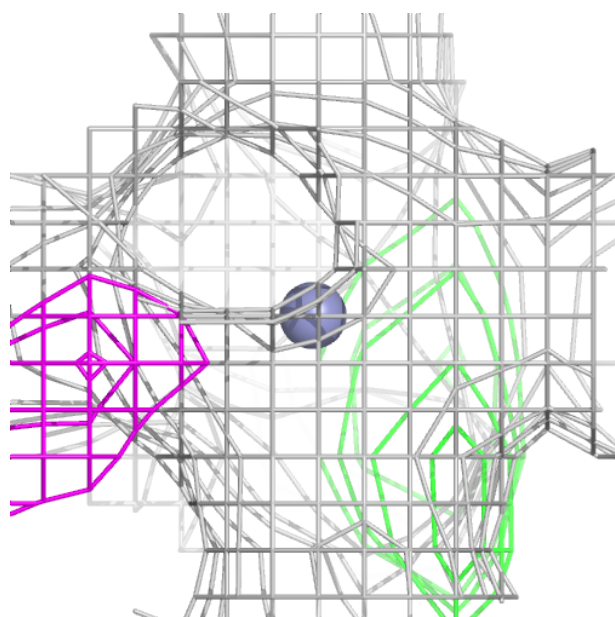and green (positive)

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 C 701:
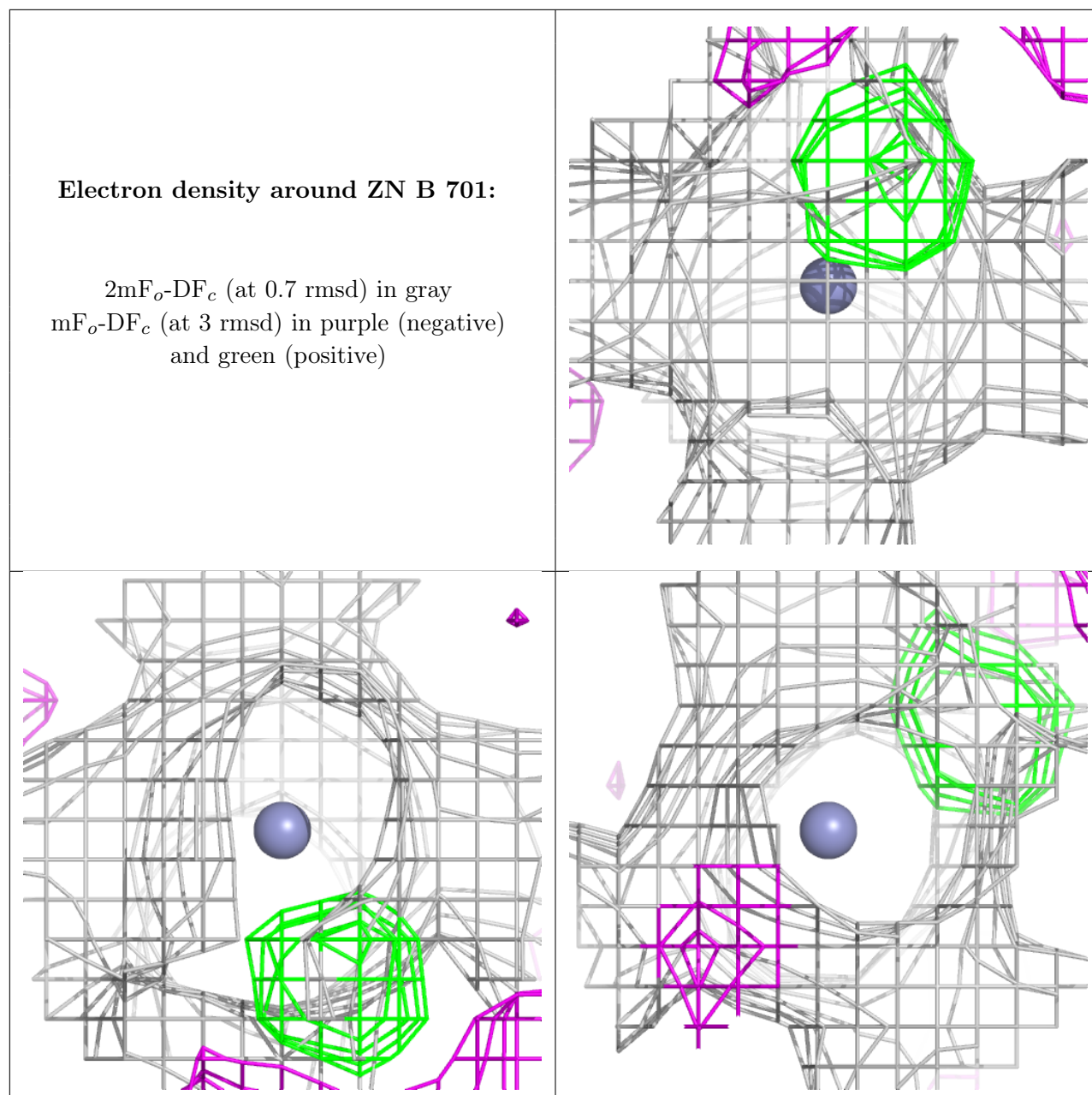
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ZN B 701:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.