



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:19 AM UTC

PDB ID : 9AWT / pdb_00009awt
Title : Structure of the A type blood alpha-D-galactosamine galactosaminidase from
Flavonifractor plautii in complex with GalN-pNP
Authors : Worrall, L.J.; Strynadka, N.C.J.
Deposited on : 2024-03-05
Resolution : 2.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

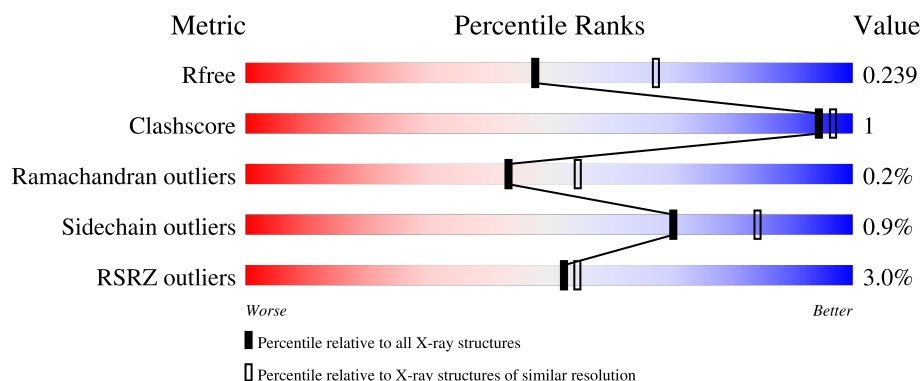
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	672	
1	B	672	
1	C	672	
1	D	672	
1	E	672	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27471 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 A type blood alpha-D-galactosamine galactosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5067	3200	832	1011	24			
1	B	654	Total	C	N	O	S	0	0	0
			5067	3200	832	1011	24			
1	C	654	Total	C	N	O	S	0	0	0
			5067	3200	832	1011	24			
1	D	654	Total	C	N	O	S	0	0	0
			5067	3200	832	1011	24			
1	E	654	Total	C	N	O	S	0	0	0
			5067	3200	832	1011	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	ALA	GLU	conflict	UNP P0DTR5
A	625	ALA	LYS	conflict	UNP P0DTR5
B	624	ALA	GLU	conflict	UNP P0DTR5
B	625	ALA	LYS	conflict	UNP P0DTR5
C	624	ALA	GLU	conflict	UNP P0DTR5
C	625	ALA	LYS	conflict	UNP P0DTR5
D	624	ALA	GLU	conflict	UNP P0DTR5
D	625	ALA	LYS	conflict	UNP P0DTR5
E	624	ALA	GLU	conflict	UNP P0DTR5
E	625	ALA	LYS	conflict	UNP P0DTR5

- 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	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0
3	E	1	Total 1	Cl 1	0	0

- Molecule 4 is COBALT (II) ION (CCD ID: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Co 1	0	0
4	B	1	Total 1	Co 1	0	0
4	C	1	Total 1	Co 1	0	0
4	D	1	Total 1	Co 1	0	0
4	E	1	Total 1	Co 1	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

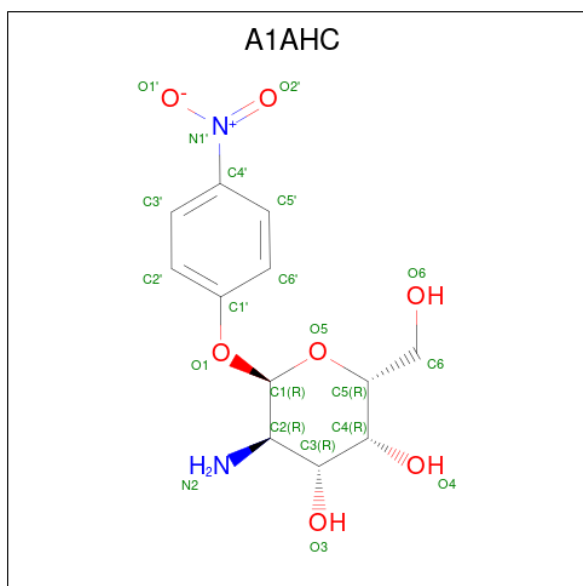
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		
5	E	1	Total	Mn	0	0
			1	1		

- Molecule 6 is 4-nitrophenyl 2-amino-2-deoxy- α -D-galactopyranoside (CCD ID: A1AHC) (formula: $C_{12}H_{16}N_2O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			21	12	2	7		
6	B	1	Total	C	N	O	0	0
			21	12	2	7		
6	C	1	Total	C	N	O	0	0
			21	12	2	7		
6	D	1	Total	C	N	O	0	0
			21	12	2	7		
6	E	1	Total	C	N	O	0	0
			21	12	2	7		

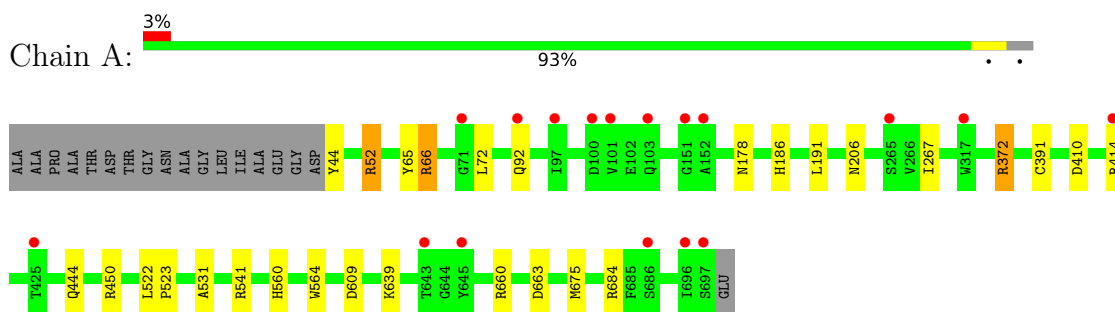
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	454	Total 454	O 454	0	0
7	B	469	Total 469	O 469	0	0
7	C	306	Total 306	O 306	0	0
7	D	419	Total 419	O 419	0	0
7	E	363	Total 363	O 363	0	0

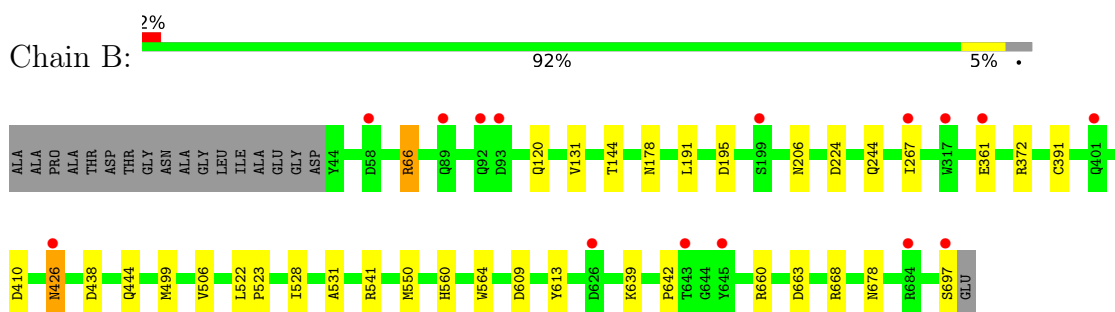
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

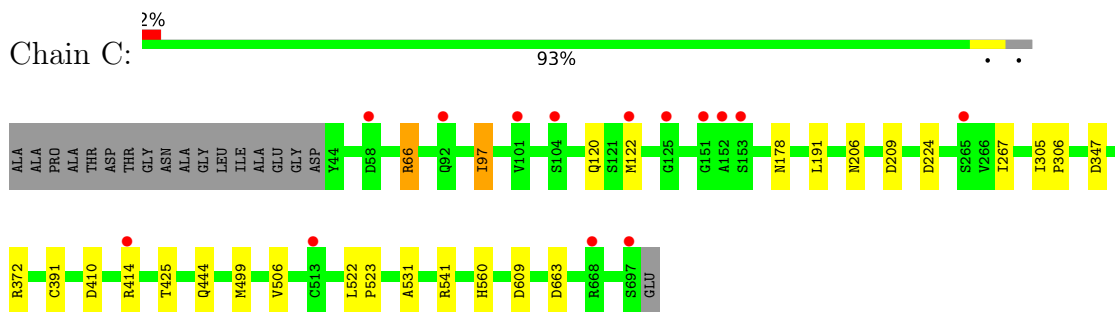
- Molecule 1: A type blood alpha-D-galactosamine galactosaminidase



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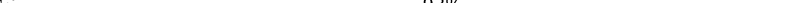
- Molecule 1: A type blood alpha-D-galactosamine galactosaminidase

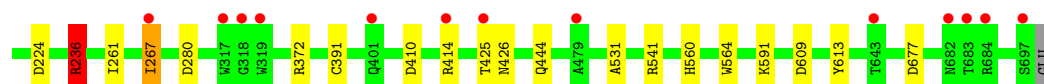


- Molecule 1: A type blood alpha-D-galactosamine galactosaminidase





- Chain E:  4% 93% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.68Å 166.57Å 133.21Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	46.39 – 2.30 46.39 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.39-2.30) 98.4 (46.39-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.207 , 0.234 0.214 , 0.239	Depositor DCC
R_{free} test set	9855 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27471	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, A1AHC, CO, ZN, CL

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	0.61	0/5200	0.99	5/7087 (0.1%)
1	B	0.62	0/5200	0.99	10/7087 (0.1%)
1	C	0.59	0/5200	0.97	7/7087 (0.1%)
1	D	0.59	0/5200	0.97	6/7087 (0.1%)
1	E	0.61	0/5200	0.99	10/7087 (0.1%)
All	All	0.60	0/26000	0.98	38/35435 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	C	0	2
1	D	0	1
1	E	0	2
All	All	0	10

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	236	ARG	NE-CZ-NH1	-11.35	110.15	121.50
1	E	236	ARG	NE-CZ-NH2	10.98	129.08	119.20
1	E	236	ARG	CD-NE-CZ	8.72	136.62	124.40
1	D	683	THR	CA-CB-OG1	8.25	121.97	109.60
1	D	425	THR	OG1-CB-CG2	6.64	122.57	109.30
1	B	609	ASP	CA-CB-CG	6.30	118.91	112.60
1	A	609	ASP	CA-CB-CG	5.87	118.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	209	ASP	CA-CB-CG	5.85	118.45	112.60
1	D	609	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	609	ASP	CA-CB-CG	5.81	118.41	112.60
1	E	609	ASP	CA-CB-CG	5.77	118.37	112.60
1	C	372	ARG	N-CA-CB	-5.75	101.66	110.12
1	E	372	ARG	N-CA-CB	-5.62	101.86	110.12
1	A	663	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	372	ARG	N-CA-CB	-5.51	102.02	110.12
1	B	668	ARG	CG-CD-NE	5.47	124.04	112.00
1	B	410	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	639	LYS	CG-CD-CE	5.42	123.75	111.30
1	A	675	MET	CG-SD-CE	5.40	112.79	100.90
1	B	438	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	66	ARG	N-CA-CB	-5.37	101.89	111.08
1	B	663	ASP	CA-CB-CG	5.36	117.96	112.60
1	D	410	ASP	CA-CB-CG	5.33	117.93	112.60
1	E	410	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	372	ARG	N-CA-CB	-5.32	102.30	110.12
1	D	372	ARG	N-CA-CB	-5.25	102.40	110.12
1	C	410	ASP	CA-CB-CG	5.20	117.80	112.60
1	E	677	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	209	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	426	ASN	CB-CA-C	5.15	117.41	108.91
1	C	663	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	347	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	195	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	425	THR	OG1-CB-CG2	5.12	119.55	109.30
1	A	410	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	425	THR	CA-CB-OG1	-5.04	102.05	109.60
1	E	280	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	347	ASP	CA-CB-CG	5.00	117.61	112.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	66	ARG	Sidechain
1	A	660	ARG	Sidechain
1	A	684	ARG	Sidechain
1	C	414	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	66	ARG	Sidechain
1	D	668	ARG	Sidechain
1	E	236	ARG	Sidechain
1	E	414	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5067	0	4764	12	0
1	B	5067	0	4764	15	0
1	C	5067	0	4764	8	0
1	D	5067	0	4764	16	0
1	E	5067	0	4764	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	21	0	0	0	0
6	B	21	0	0	0	0
6	C	21	0	0	0	0
6	D	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	21	0	0	0	0
7	A	454	0	0	5	0
7	B	469	0	0	7	0
7	C	306	0	0	0	0
7	D	419	0	0	4	0
7	E	363	0	0	4	0
All	All	27471	0	23820	64	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 1.

All (64) 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:E:97:ILE:HD11	1:E:120:GLN:HB2	1.64	0.79
1:E:236:ARG:HD2	7:E:904:HOH:O	1.82	0.79
1:D:178:ASN:HD22	1:D:206:ASN:HD21	1.37	0.72
1:E:178:ASN:HD22	1:E:206:ASN:HD21	1.39	0.71
1:B:178:ASN:HD22	1:B:206:ASN:HD21	1.38	0.70
1:C:178:ASN:HD22	1:C:206:ASN:HD21	1.38	0.69
1:A:178:ASN:HD22	1:A:206:ASN:HD21	1.39	0.68
1:B:191:LEU:HD13	1:B:541:ARG:HB3	1.80	0.64
1:B:361:GLU:HB3	7:B:1223:HOH:O	2.02	0.59
1:D:52:ARG:HG3	1:D:72:LEU:HD11	1.84	0.59
1:D:191:LEU:HD13	1:D:541:ARG:HB3	1.84	0.59
1:E:191:LEU:HD13	1:E:541:ARG:HB3	1.84	0.59
1:C:191:LEU:HD13	1:C:541:ARG:HB3	1.85	0.58
1:A:191:LEU:HD13	1:A:541:ARG:HB3	1.86	0.56
1:B:391:CYS:H	1:B:444:GLN:HE22	1.56	0.53
1:A:391:CYS:H	1:A:444:GLN:HE22	1.56	0.53
1:B:697:SER:HB3	7:B:1104:HOH:O	2.09	0.53
1:E:391:CYS:H	1:E:444:GLN:HE22	1.57	0.53
1:E:261:ILE:HG12	1:E:267:ILE:HD11	1.92	0.52
1:A:52:ARG:HG3	1:A:72:LEU:HD11	1.92	0.51
1:E:236:ARG:CD	7:E:904:HOH:O	2.50	0.51
1:D:391:CYS:H	1:D:444:GLN:HE22	1.57	0.51
1:C:391:CYS:H	1:C:444:GLN:HE22	1.58	0.50
1:B:66:ARG:NH1	1:B:224:ASP:O	2.46	0.48
1:D:66:ARG:NH1	1:D:224:ASP:O	2.47	0.48
1:E:66:ARG:NH1	1:E:224:ASP:O	2.45	0.47
1:A:92:GLN:HB2	7:A:803:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:LYS:HE2	7:D:1088:HOH:O	2.14	0.46
1:B:642:PRO:HB3	7:B:967:HOH:O	2.14	0.46
1:C:66:ARG:NH1	1:C:224:ASP:O	2.48	0.46
1:B:244:GLN:HB3	7:B:1234:HOH:O	2.17	0.45
1:E:591:LYS:HE3	7:E:975:HOH:O	2.17	0.44
1:D:541:ARG:HD3	1:D:613:TYR:CZ	2.52	0.44
1:A:92:GLN:N	7:A:803:HOH:O	2.40	0.43
1:A:372:ARG:HG3	7:A:1111:HOH:O	2.19	0.43
1:D:499:MET:HB3	1:D:506:VAL:HG21	2.01	0.43
1:D:72:LEU:HD23	1:D:72:LEU:HA	1.94	0.43
1:B:522:LEU:N	1:B:523:PRO:CD	2.82	0.43
1:E:94:PHE:HB2	7:E:1076:HOH:O	2.19	0.42
1:A:44:TYR:HA	7:A:1178:HOH:O	2.19	0.42
1:B:678:ASN:ND2	7:B:806:HOH:O	2.44	0.42
1:A:52:ARG:HB2	1:A:65:TYR:HB2	2.01	0.42
1:B:131:VAL:O	1:B:144:THR:HA	2.19	0.42
1:B:660:ARG:NH1	7:B:810:HOH:O	2.49	0.42
1:D:70:SER:HA	7:D:838:HOH:O	2.20	0.42
1:C:97:ILE:HD11	1:C:120:GLN:HB2	2.01	0.41
1:D:522:LEU:N	1:D:523:PRO:CD	2.83	0.41
1:C:522:LEU:N	1:C:523:PRO:CD	2.84	0.41
1:D:92:GLN:HB2	7:D:899:HOH:O	2.20	0.41
1:E:52:ARG:HG3	1:E:72:LEU:HD11	2.03	0.41
1:E:66:ARG:HB2	1:E:75:MET:HG2	2.02	0.41
1:A:450:ARG:HD3	7:A:951:HOH:O	2.20	0.41
1:B:499:MET:HB3	1:B:506:VAL:HG21	2.03	0.41
1:A:522:LEU:N	1:A:523:PRO:CD	2.84	0.41
1:B:528:ILE:CD1	1:B:550:MET:HG3	2.51	0.41
1:B:541:ARG:HD3	1:B:613:TYR:CZ	2.56	0.41
1:C:305:ILE:HA	1:C:306:PRO:HD3	1.96	0.40
1:D:678:ASN:HD22	1:D:678:ASN:C	2.29	0.40
1:A:186:HIS:HD2	7:B:987:HOH:O	2.03	0.40
1:C:499:MET:HB3	1:C:506:VAL:HG21	2.02	0.40
1:D:66:ARG:HB3	1:D:75:MET:HG2	2.04	0.40
1:E:541:ARG:HD3	1:E:613:TYR:CZ	2.56	0.40
1:D:44:TYR:HA	7:D:1037:HOH:O	2.21	0.40
1:D:131:VAL:O	1:D:144:THR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	652/672 (97%)	632 (97%)	19 (3%)	1 (0%)	43	55
1	B	652/672 (97%)	634 (97%)	17 (3%)	1 (0%)	43	55
1	C	652/672 (97%)	633 (97%)	18 (3%)	1 (0%)	43	55
1	D	652/672 (97%)	632 (97%)	19 (3%)	1 (0%)	43	55
1	E	652/672 (97%)	632 (97%)	19 (3%)	1 (0%)	43	55
All	All	3260/3360 (97%)	3163 (97%)	92 (3%)	5 (0%)	43	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	531	ALA
1	B	531	ALA
1	C	531	ALA
1	D	531	ALA
1	E	531	ALA

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	536/546 (98%)	531 (99%)	5 (1%)	70	84
1	B	536/546 (98%)	531 (99%)	5 (1%)	70	84
1	C	536/546 (98%)	532 (99%)	4 (1%)	76	87
1	D	536/546 (98%)	529 (99%)	7 (1%)	61	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	536/546 (98%)	532 (99%)	4 (1%)	76	87
All	All	2680/2730 (98%)	2655 (99%)	25 (1%)	70	84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	267	ILE
1	A	560	HIS
1	A	564	TRP
1	A	639	LYS
1	B	120	GLN
1	B	267	ILE
1	B	426	ASN
1	B	560	HIS
1	B	564	TRP
1	C	97	ILE
1	C	122	MET
1	C	267	ILE
1	C	560	HIS
1	D	66	ARG
1	D	95	SER
1	D	267	ILE
1	D	425	THR
1	D	560	HIS
1	D	683	THR
1	D	684	ARG
1	E	267	ILE
1	E	426	ASN
1	E	560	HIS
1	E	564	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	186	HIS
1	A	444	GLN
1	B	178	ASN
1	B	186	HIS
1	B	444	GLN

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Mol	Chain	Res	Type
1	B	678	ASN
1	C	178	ASN
1	C	186	HIS
1	C	444	GLN
1	D	178	ASN
1	D	186	HIS
1	D	444	GLN
1	D	678	ASN
1	E	178	ASN
1	E	444	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 20 are monoatomic - leaving 5 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	$\# Z > 2$
6	A1AHC	A	705	4	22,22,22	2.21	4 (18%)	29,31,31	1.19	3 (10%)
6	A1AHC	B	705	4	22,22,22	2.28	4 (18%)	29,31,31	1.65	7 (24%)
6	A1AHC	C	705	4	22,22,22	2.19	3 (13%)	29,31,31	1.67	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	A1AHC	D	705	4	22,22,22	2.19	3 (13%)	29,31,31	1.17	4 (13%)
6	A1AHC	E	705	4	22,22,22	2.35	3 (13%)	29,31,31	1.49	4 (13%)

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
6	A1AHC	A	705	4	-	2/8/30/30	0/2/2/2
6	A1AHC	B	705	4	-	4/8/30/30	0/2/2/2
6	A1AHC	C	705	4	-	2/8/30/30	0/2/2/2
6	A1AHC	D	705	4	-	2/8/30/30	0/2/2/2
6	A1AHC	E	705	4	-	2/8/30/30	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	705	A1AHC	O2'-N1'	9.58	1.39	1.22
6	D	705	A1AHC	O2'-N1'	8.76	1.37	1.22
6	C	705	A1AHC	O2'-N1'	8.68	1.37	1.22
6	B	705	A1AHC	O2'-N1'	8.37	1.37	1.22
6	A	705	A1AHC	O2'-N1'	8.26	1.37	1.22
6	A	705	A1AHC	C4'-N1'	-3.35	1.37	1.45
6	C	705	A1AHC	C4'-N1'	-3.26	1.37	1.45
6	B	705	A1AHC	O1-C1	3.17	1.46	1.41
6	B	705	A1AHC	C1-C2	3.00	1.58	1.52
6	B	705	A1AHC	C4'-N1'	-2.95	1.38	1.45
6	D	705	A1AHC	C4'-N1'	-2.92	1.38	1.45
6	E	705	A1AHC	O1-C1	2.79	1.45	1.41
6	A	705	A1AHC	O1-C1	2.65	1.45	1.41
6	D	705	A1AHC	C1-C2	2.58	1.57	1.52
6	C	705	A1AHC	O1-C1	2.21	1.44	1.41
6	A	705	A1AHC	C1-C2	2.09	1.56	1.52
6	E	705	A1AHC	C4'-N1'	-2.06	1.40	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	705	A1AHC	C1'-O1-C1	4.44	124.08	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	705	A1AHC	O1-C1-C2	4.05	113.13	107.35
6	E	705	A1AHC	O1-C1-C2	3.57	112.45	107.35
6	C	705	A1AHC	C4-C3-C2	-3.52	105.15	110.99
6	B	705	A1AHC	C5'-C4'-N1'	-3.45	116.33	119.34
6	B	705	A1AHC	C1'-O1-C1	3.37	122.57	117.82
6	E	705	A1AHC	O3-C3-C2	-3.21	104.46	110.22
6	B	705	A1AHC	O1-C1-C2	3.21	111.93	107.35
6	E	705	A1AHC	O3-C3-C4	3.10	117.68	110.38
6	B	705	A1AHC	O2'-N1'-C4'	-3.08	114.58	118.82
6	D	705	A1AHC	O1-C1-C2	2.99	111.62	107.35
6	C	705	A1AHC	O3-C3-C4	2.93	117.29	110.38
6	A	705	A1AHC	C1'-O1-C1	2.88	121.88	117.82
6	D	705	A1AHC	C1'-O1-C1	2.84	121.82	117.82
6	A	705	A1AHC	O1-C1-C2	2.62	111.09	107.35
6	E	705	A1AHC	C1'-O1-C1	2.54	121.40	117.82
6	B	705	A1AHC	C4-C3-C2	-2.48	106.87	110.99
6	D	705	A1AHC	C4-C3-C2	-2.44	106.94	110.99
6	D	705	A1AHC	O3-C3-C4	2.16	115.47	110.38
6	C	705	A1AHC	C6'-C5'-C4'	-2.08	117.32	120.08
6	B	705	A1AHC	O5-C1-O1	2.07	113.72	108.42
6	A	705	A1AHC	C5'-C4'-N1'	-2.04	117.56	119.34
6	B	705	A1AHC	C3'-C4'-N1'	2.02	121.11	119.34
6	C	705	A1AHC	C1-C2-N2	-2.01	106.57	110.20

There are no chirality outliers.

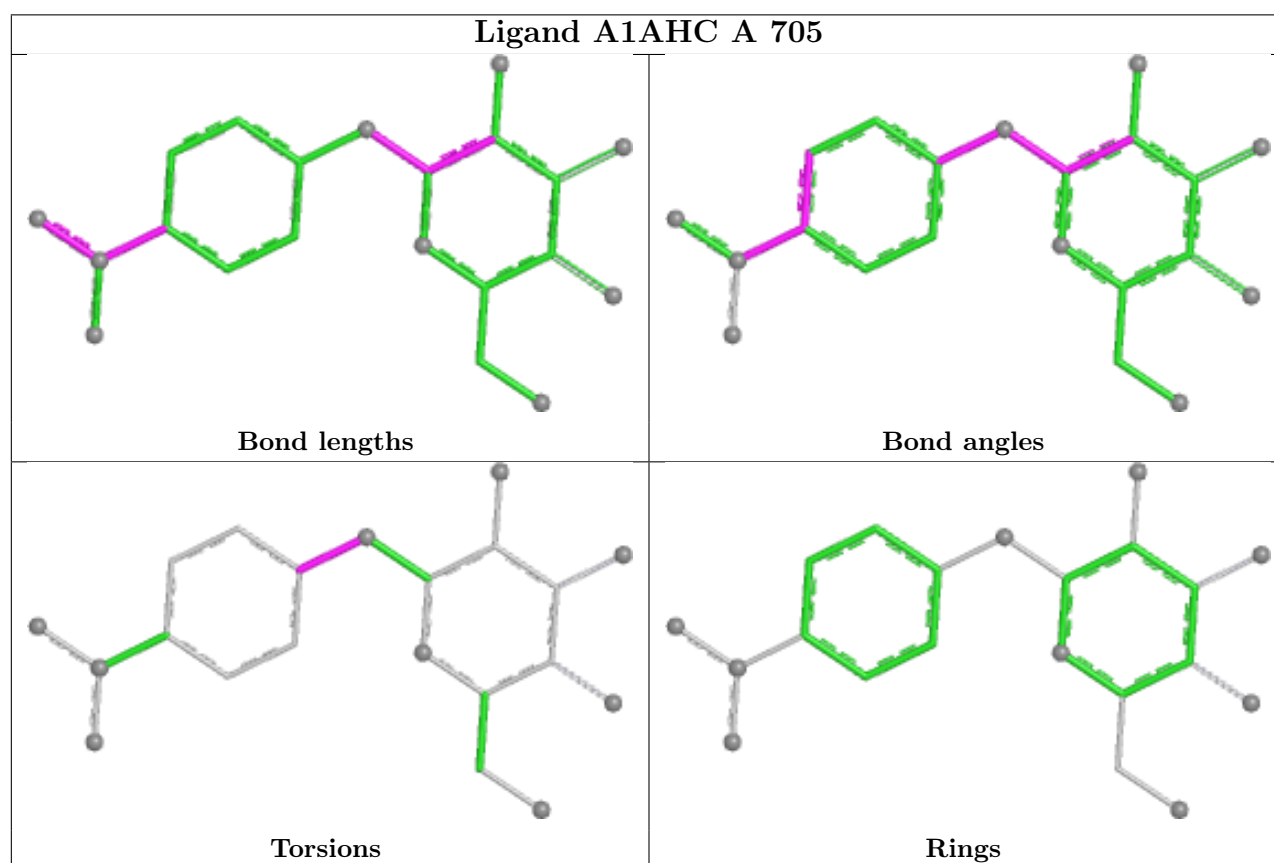
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	705	A1AHC	C3'-C4'-N1'-O2'
6	B	705	A1AHC	C5'-C4'-N1'-O2'
6	B	705	A1AHC	C2'-C1'-O1-C1
6	B	705	A1AHC	C6'-C1'-O1-C1
6	C	705	A1AHC	C2'-C1'-O1-C1
6	C	705	A1AHC	C6'-C1'-O1-C1
6	E	705	A1AHC	C6'-C1'-O1-C1
6	D	705	A1AHC	C6'-C1'-O1-C1
6	E	705	A1AHC	C2'-C1'-O1-C1
6	A	705	A1AHC	C2'-C1'-O1-C1
6	D	705	A1AHC	C2'-C1'-O1-C1
6	A	705	A1AHC	C6'-C1'-O1-C1

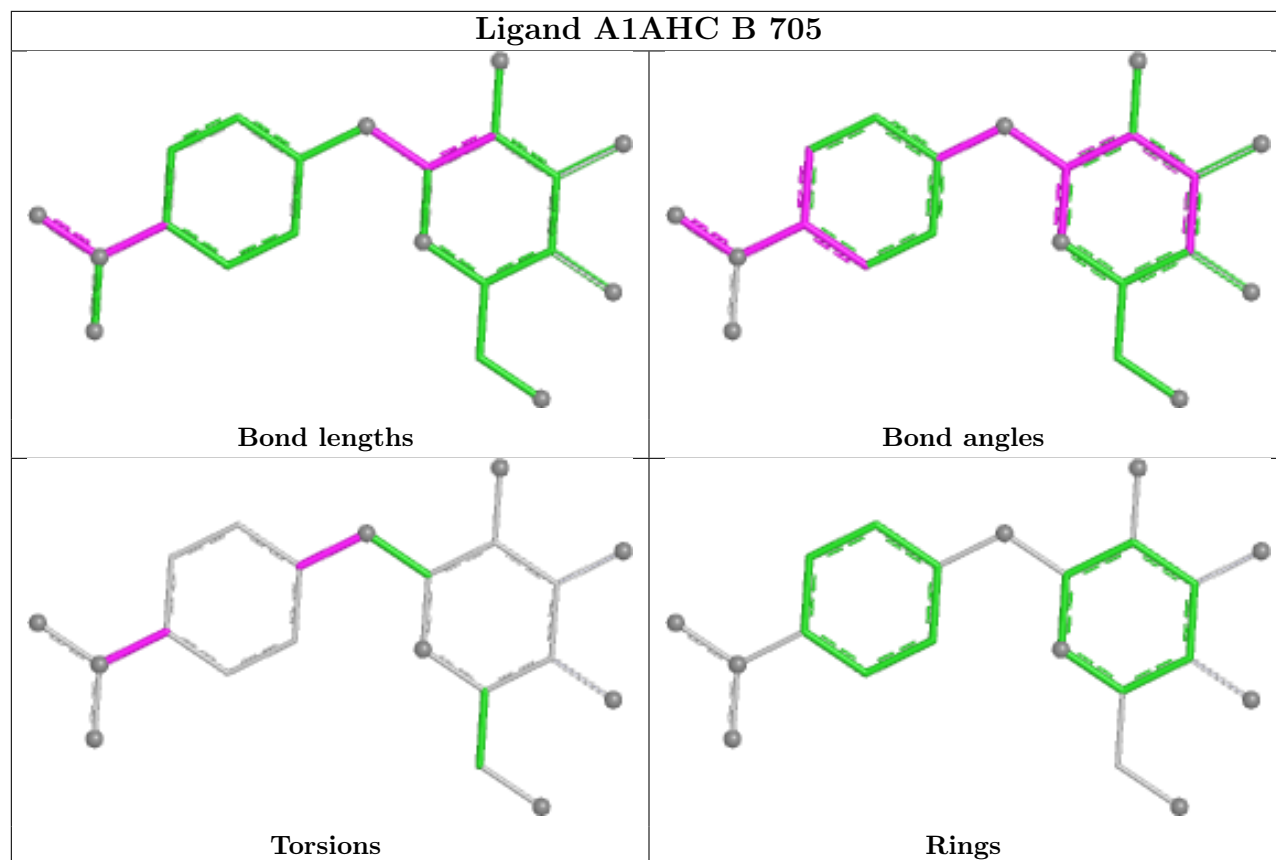
There are no ring outliers.

No monomer is involved in short contacts.

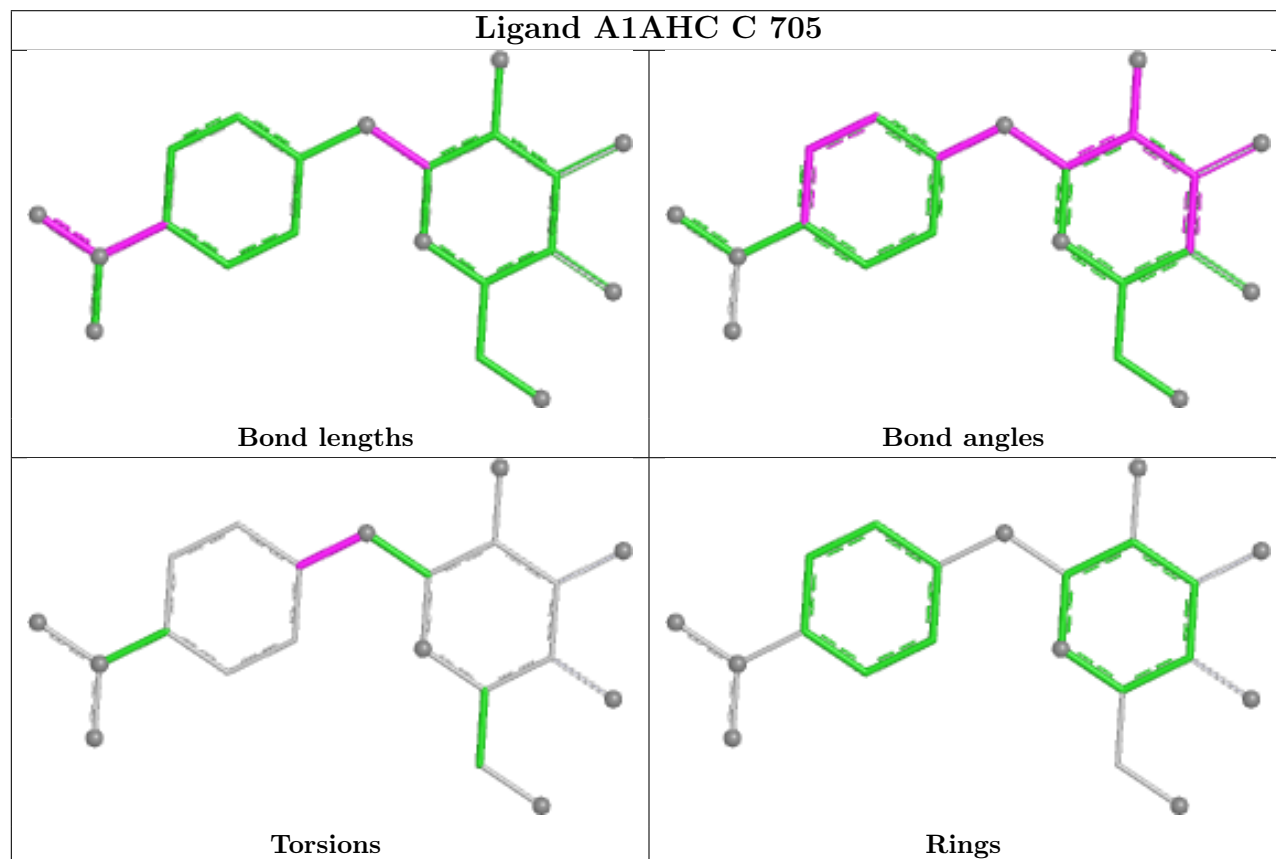
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



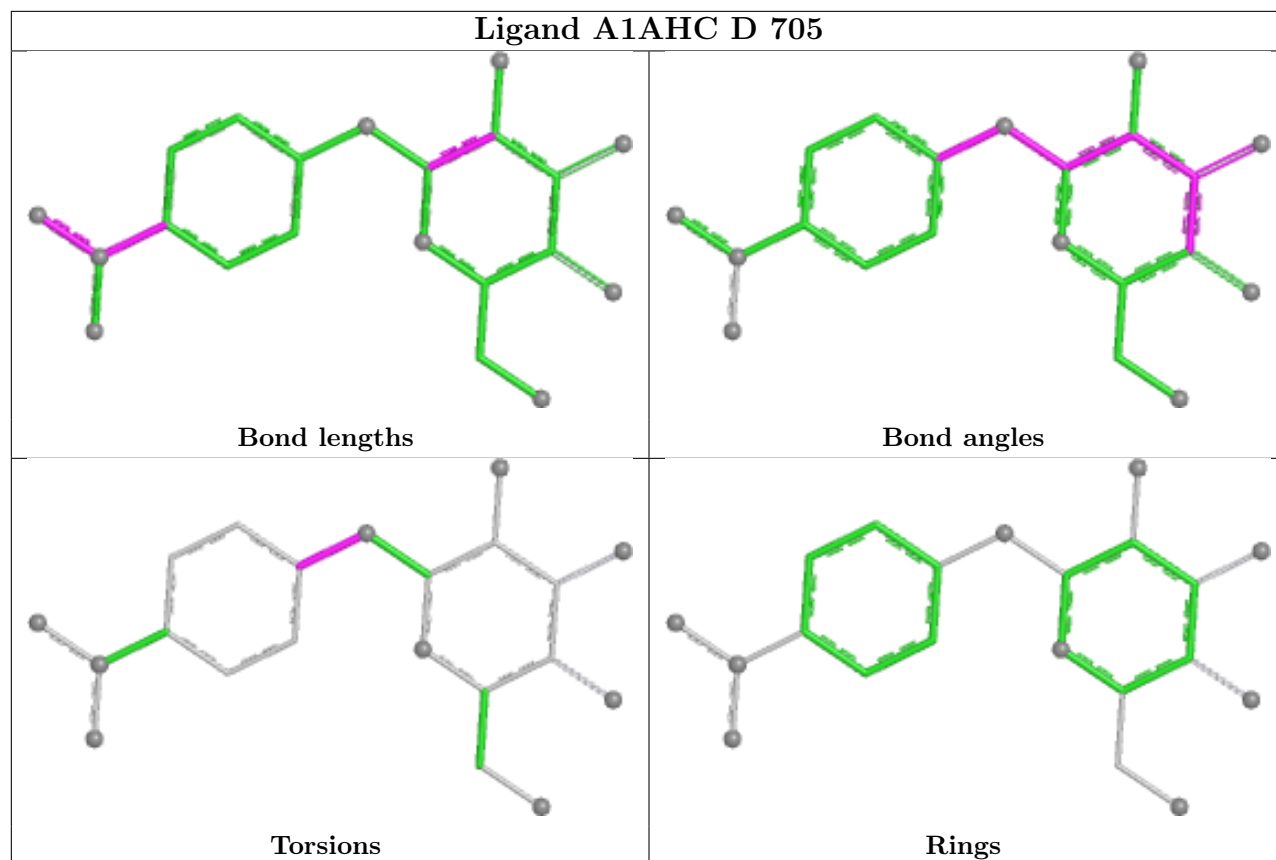
Ligand A1AHC B 705



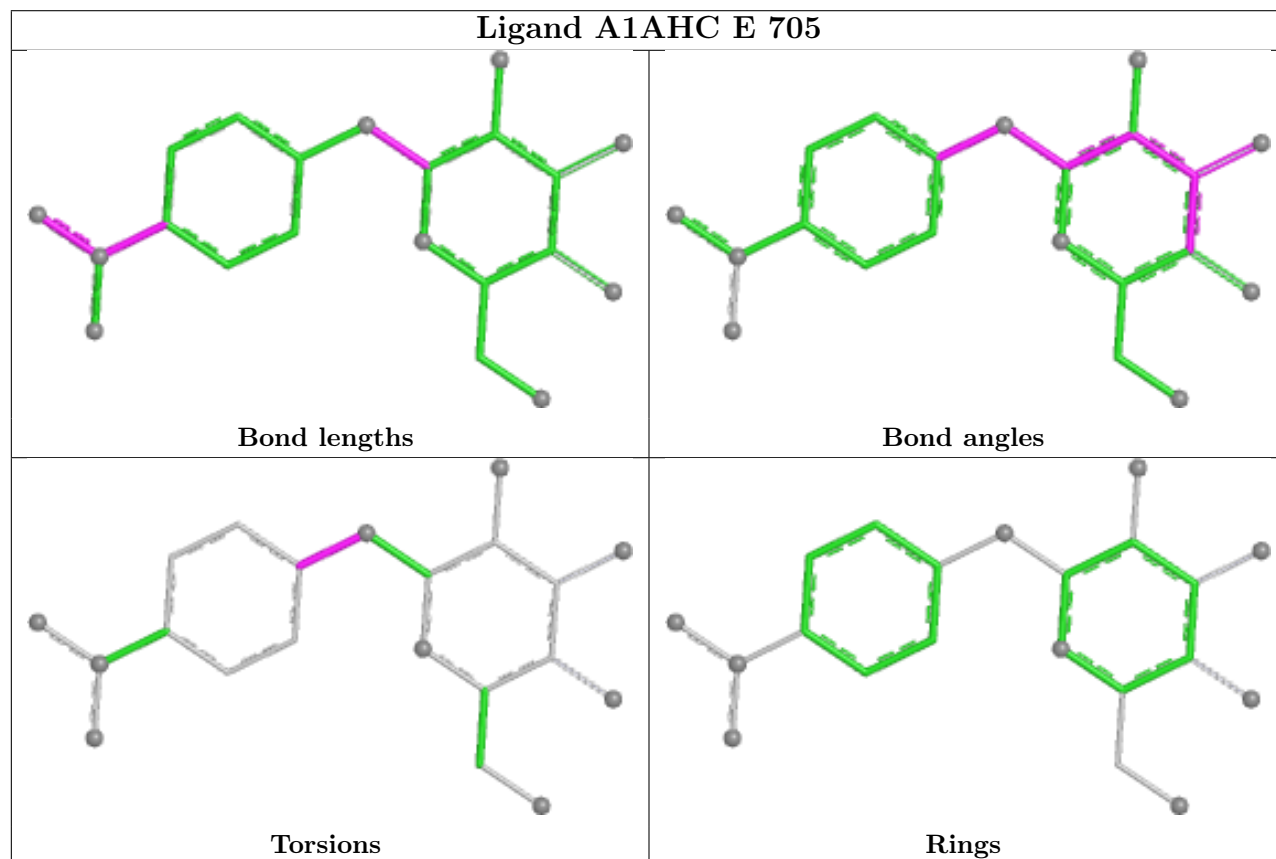
Ligand A1AHC C 705



Ligand A1AHC D 705



Ligand A1AHC E 705



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	654/672 (97%)	0.15	17 (2%) 57 59	22, 33, 59, 75	0
1	B	654/672 (97%)	0.06	15 (2%) 61 63	21, 31, 53, 79	0
1	C	654/672 (97%)	0.32	14 (2%) 63 65	25, 37, 65, 87	0
1	D	654/672 (97%)	0.38	23 (3%) 47 49	27, 38, 66, 91	0
1	E	654/672 (97%)	0.34	30 (4%) 37 39	24, 36, 66, 82	0
All	All	3270/3360 (97%)	0.25	99 (3%) 52 54	21, 35, 64, 91	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	317	TRP	4.9
1	E	267	ILE	4.2
1	C	697	SER	4.1
1	A	71	GLY	3.9
1	C	152	ALA	3.9
1	B	643	THR	3.7
1	B	697	SER	3.7
1	D	697	SER	3.7
1	C	265	SER	3.7
1	A	265	SER	3.6
1	E	425	THR	3.5
1	D	152	ALA	3.5
1	C	92	GLN	3.4
1	E	153	SER	3.4
1	E	97	ILE	3.3
1	E	44	TYR	3.3
1	E	683	THR	3.3
1	A	645	TYR	3.3
1	A	414	ARG	3.2
1	E	319	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	683	THR	3.2
1	B	626	ASP	3.1
1	D	265	SER	3.1
1	E	152	ALA	3.1
1	C	125	GLY	3.0
1	E	479	ALA	2.9
1	C	101	VAL	2.9
1	D	267	ILE	2.9
1	A	100	ASP	2.9
1	A	317	TRP	2.9
1	A	643	THR	2.9
1	D	643	THR	2.9
1	B	93	ASP	2.9
1	E	697	SER	2.8
1	A	425	THR	2.8
1	E	682	ASN	2.7
1	C	513	CYS	2.7
1	E	151	GLY	2.7
1	C	104	SER	2.7
1	D	684	ARG	2.7
1	E	72	LEU	2.7
1	D	92	GLN	2.7
1	C	414	ARG	2.6
1	B	645	TYR	2.6
1	E	318	GLY	2.6
1	B	92	GLN	2.6
1	C	122	MET	2.6
1	B	89	GLN	2.5
1	D	686	SER	2.5
1	E	92	GLN	2.5
1	B	199	SER	2.4
1	D	626	ASP	2.4
1	D	95	SER	2.4
1	B	684	ARG	2.4
1	D	263	ALA	2.4
1	A	97	ILE	2.4
1	C	151	GLY	2.3
1	D	425	THR	2.3
1	D	682	ASN	2.3
1	E	684	ARG	2.3
1	C	58	ASP	2.3
1	A	151	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	152	ALA	2.3
1	A	686	SER	2.3
1	D	104	SER	2.3
1	E	95	SER	2.3
1	E	69	GLY	2.3
1	D	319	TRP	2.3
1	D	475	ALA	2.3
1	D	584	THR	2.3
1	A	103	GLN	2.3
1	E	120	GLN	2.3
1	E	91	VAL	2.3
1	A	696	ILE	2.2
1	C	668	ARG	2.2
1	D	474	PRO	2.2
1	E	71	GLY	2.2
1	A	92	GLN	2.2
1	E	103	GLN	2.2
1	A	697	SER	2.2
1	B	267	ILE	2.2
1	E	81	LEU	2.2
1	B	401	GLN	2.2
1	E	414	ARG	2.1
1	A	101	VAL	2.1
1	B	361	GLU	2.1
1	D	264	GLY	2.1
1	C	153	SER	2.1
1	E	643	THR	2.1
1	E	105	THR	2.1
1	E	122	MET	2.1
1	D	317	TRP	2.1
1	D	73	ILE	2.1
1	E	98	SER	2.0
1	E	401	GLN	2.0
1	B	58	ASP	2.0
1	B	426	ASN	2.0
1	B	317	TRP	2.0
1	D	696	ILE	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

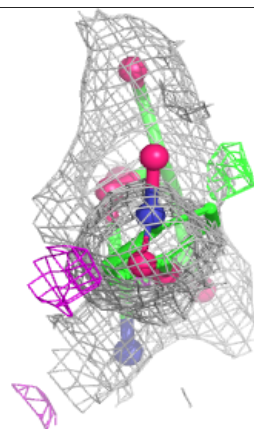
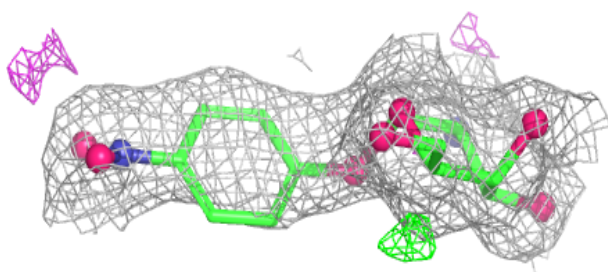
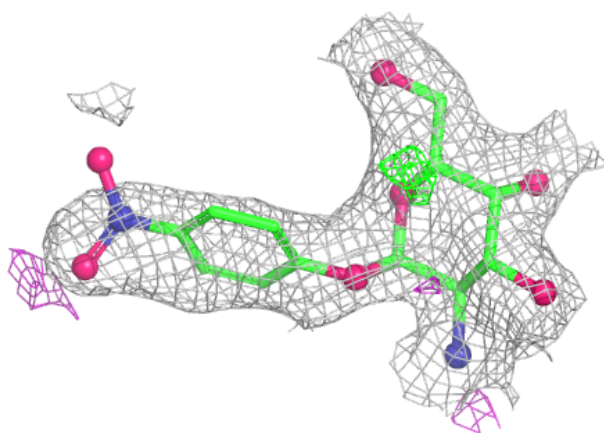
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	A1AHC	B	705	21/21	0.88	0.13	35,48,73,83	0
6	A1AHC	D	705	21/21	0.89	0.13	34,45,69,81	0
6	A1AHC	E	705	21/21	0.89	0.14	37,48,82,92	0
6	A1AHC	A	705	21/21	0.90	0.13	36,48,71,81	0
4	CO	D	703	1/1	0.92	0.11	66,66,66,66	0
6	A1AHC	C	705	21/21	0.92	0.11	34,43,68,81	0
4	CO	A	703	1/1	0.94	0.11	64,64,64,64	0
4	CO	C	703	1/1	0.95	0.09	68,68,68,68	0
4	CO	E	703	1/1	0.96	0.10	58,58,58,58	0
4	CO	B	703	1/1	0.97	0.10	61,61,61,61	0
5	MN	E	704	1/1	0.98	0.04	45,45,45,45	0
3	CL	B	702	1/1	0.98	0.07	26,26,26,26	0
3	CL	C	702	1/1	0.99	0.06	26,26,26,26	0
5	MN	A	704	1/1	0.99	0.03	45,45,45,45	0
5	MN	B	704	1/1	0.99	0.07	49,49,49,49	0
5	MN	C	704	1/1	0.99	0.05	46,46,46,46	0
5	MN	D	704	1/1	0.99	0.04	47,47,47,47	0
3	CL	D	702	1/1	0.99	0.05	28,28,28,28	0
3	CL	E	702	1/1	0.99	0.06	27,27,27,27	0
2	ZN	C	701	1/1	0.99	0.03	32,32,32,32	0
2	ZN	E	701	1/1	0.99	0.03	31,31,31,31	0
3	CL	A	702	1/1	0.99	0.04	25,25,25,25	0
2	ZN	A	701	1/1	0.99	0.05	30,30,30,30	0
2	ZN	D	701	1/1	1.00	0.02	31,31,31,31	0
2	ZN	B	701	1/1	1.00	0.01	27,27,27,27	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.

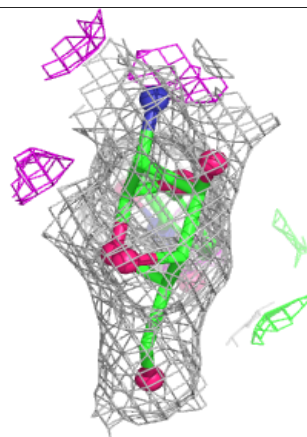
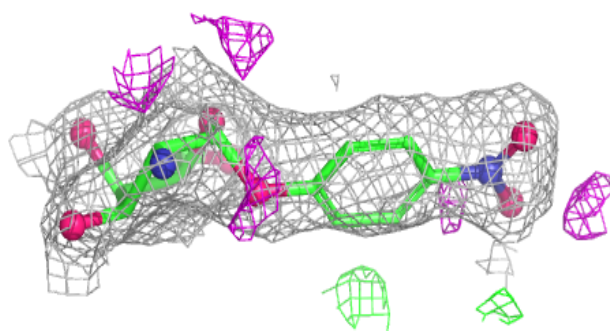
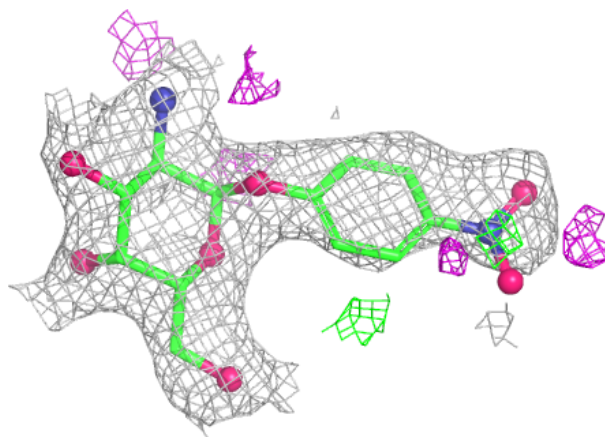
Electron density around A1AHC B 705:

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



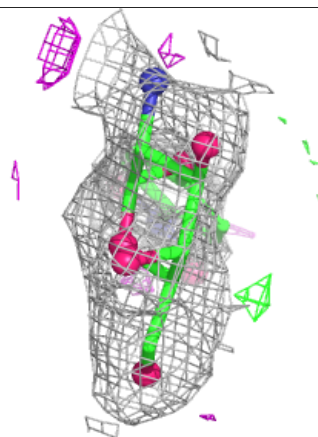
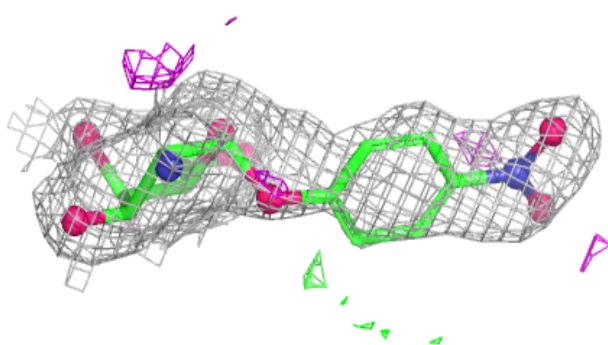
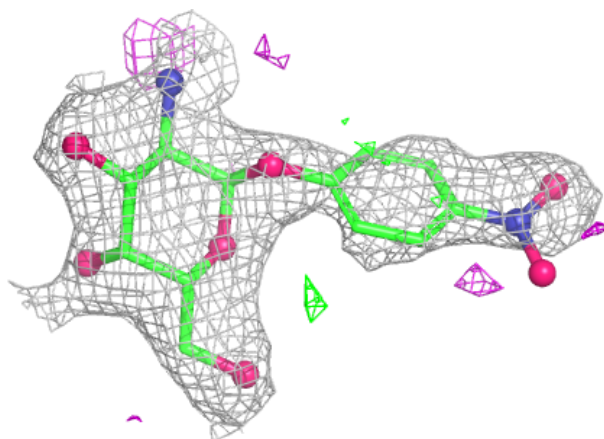
Electron density around A1AHC D 705:

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



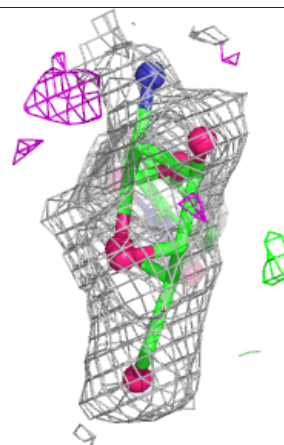
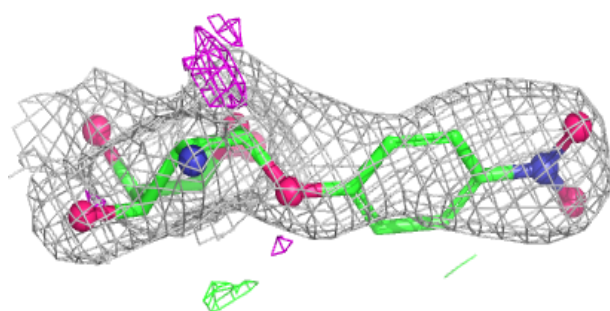
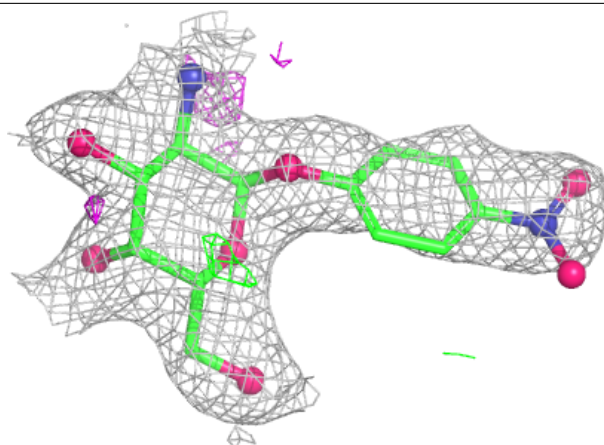
Electron density around A1AHC E 705:

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



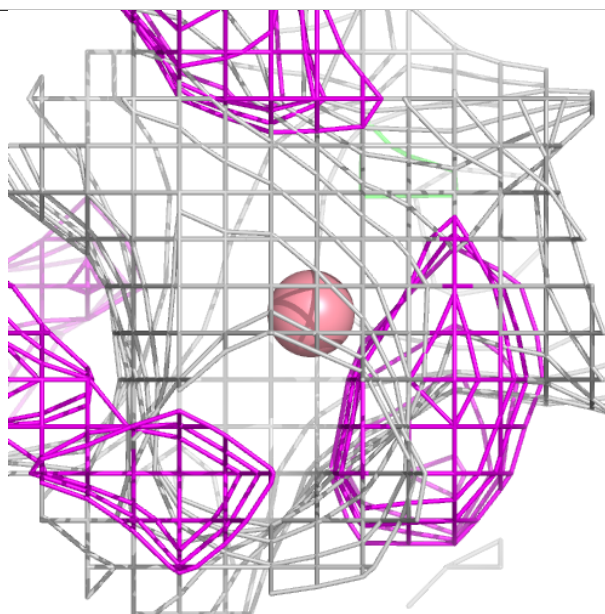
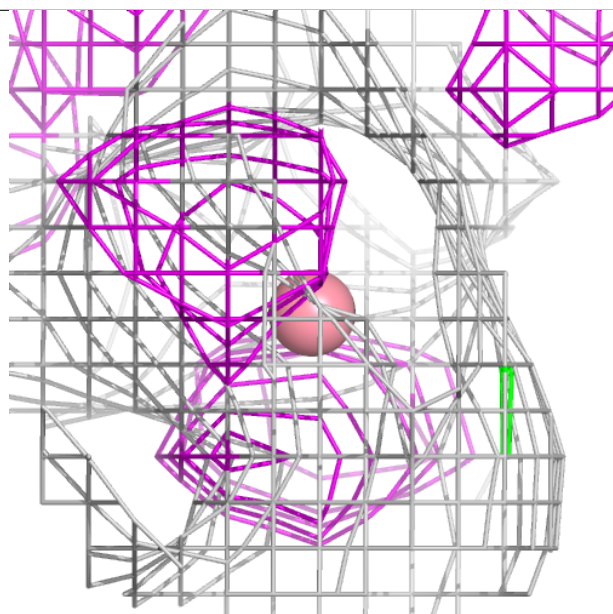
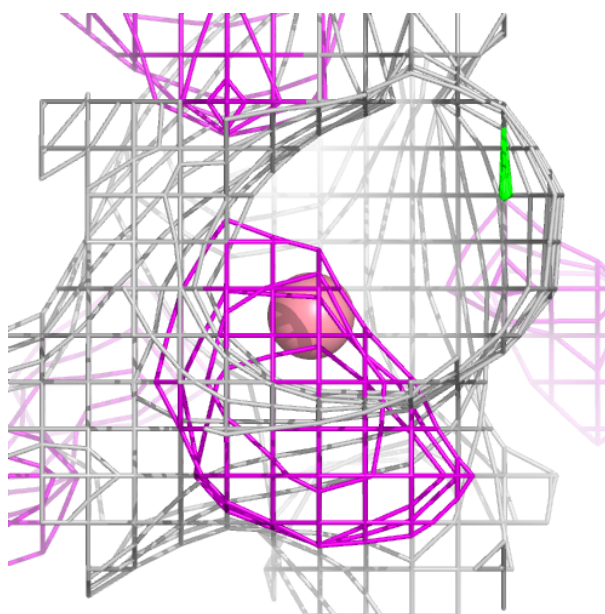
Electron density around A1AHC A 705:

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



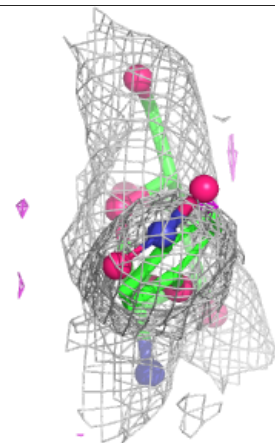
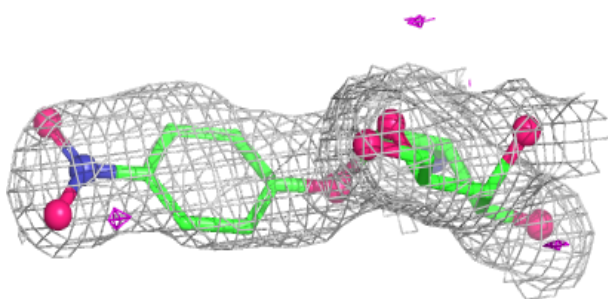
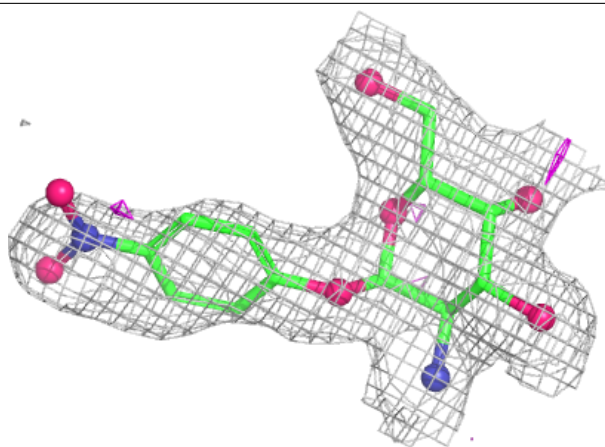
Electron density around CO D 703:

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



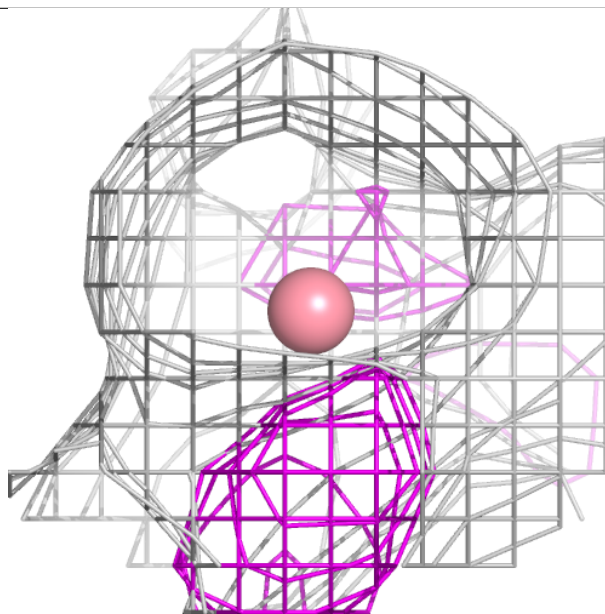
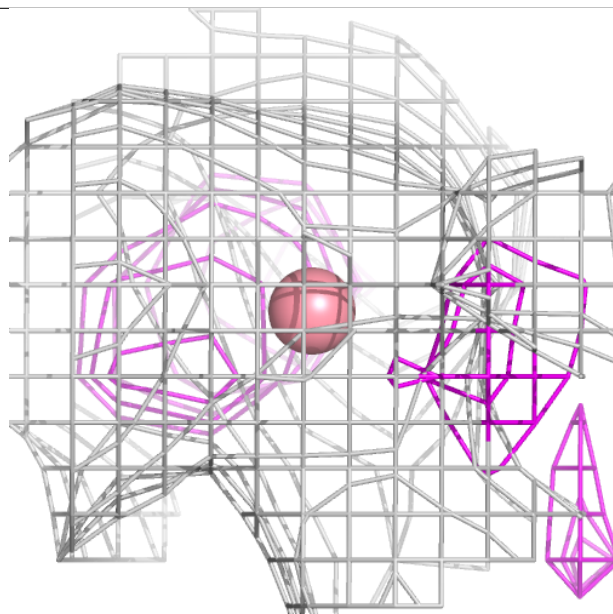
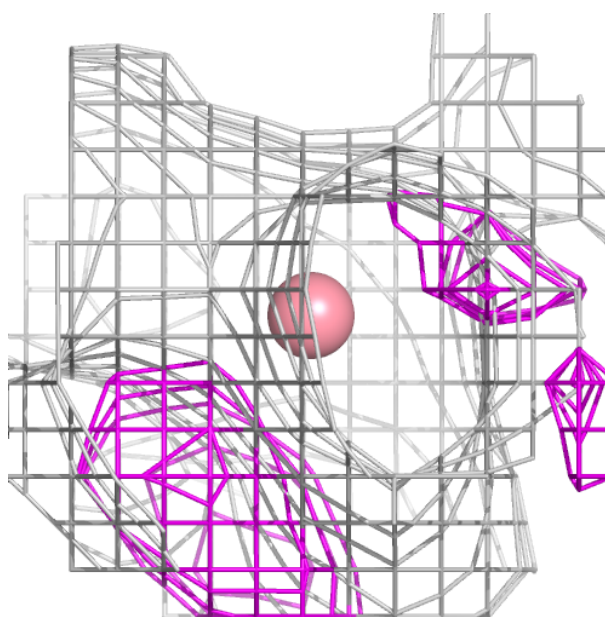
Electron density around A1AHC C 705:

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



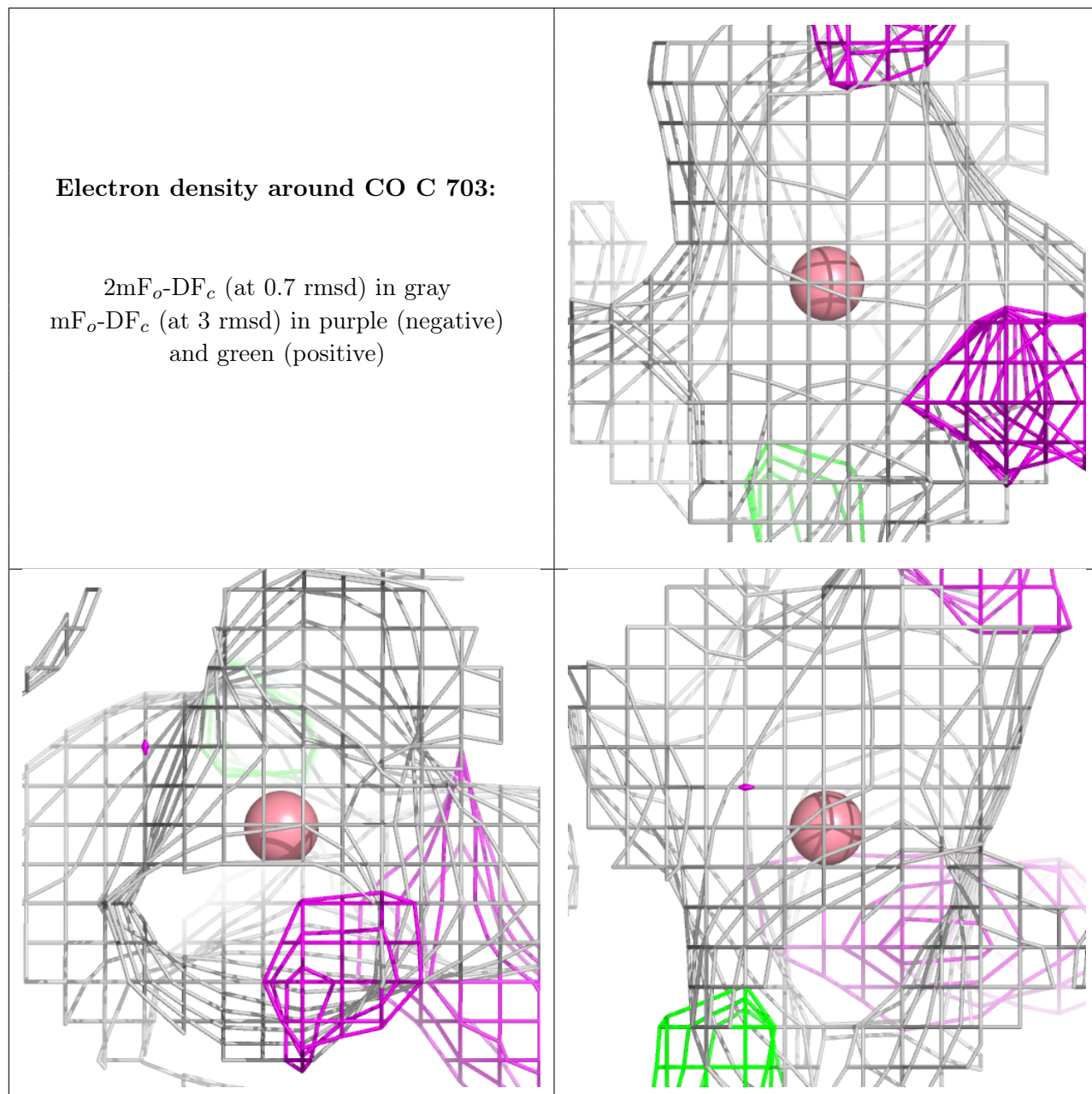
Electron density around CO A 703:

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



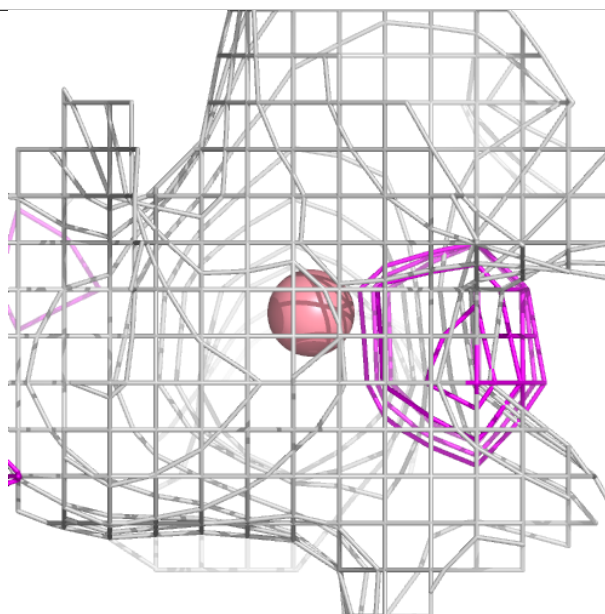
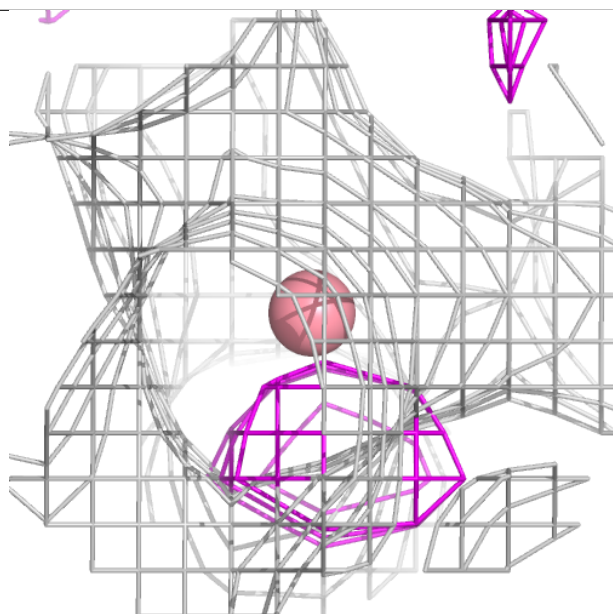
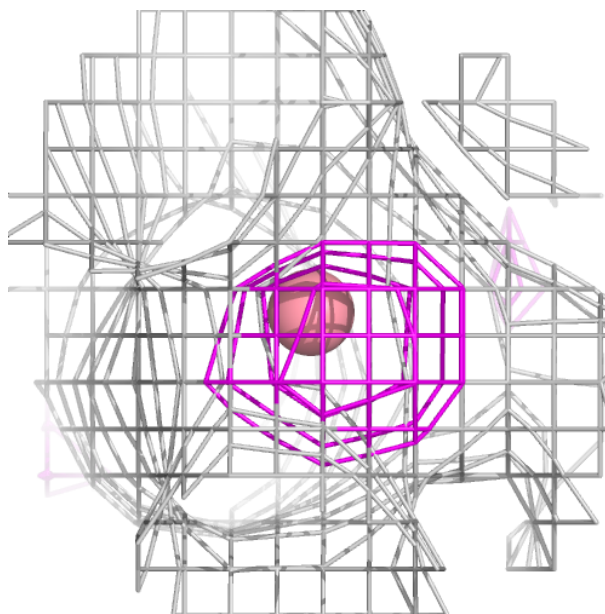
Electron density around CO C 703:

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



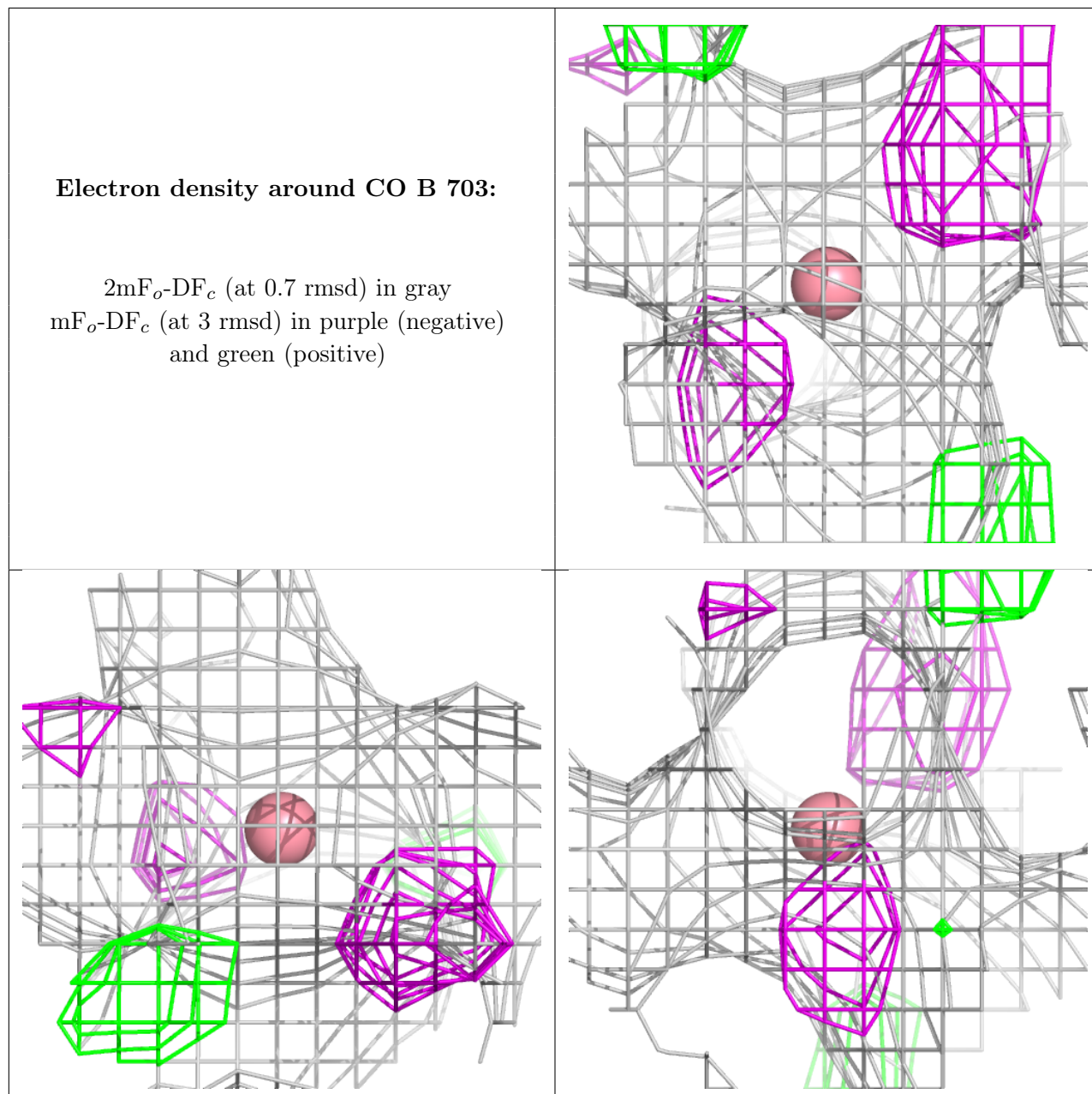
Electron density around CO E 703:

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



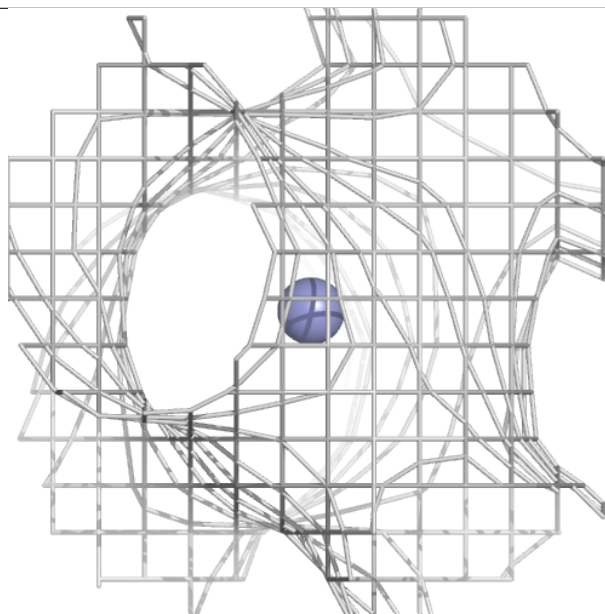
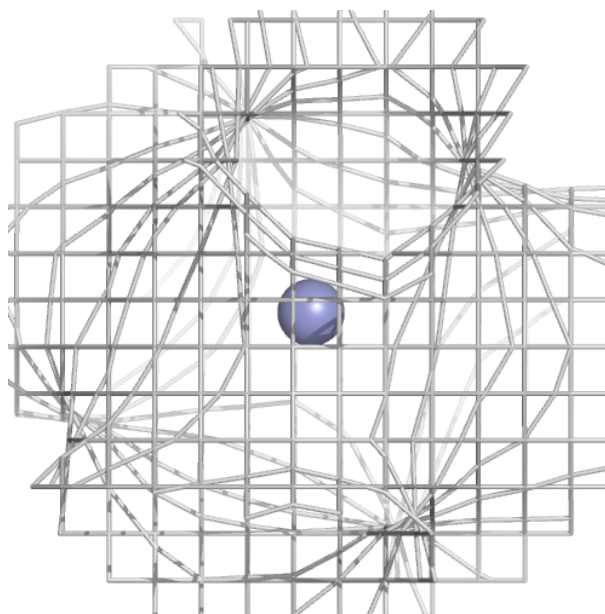
Electron density around CO B 703:

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



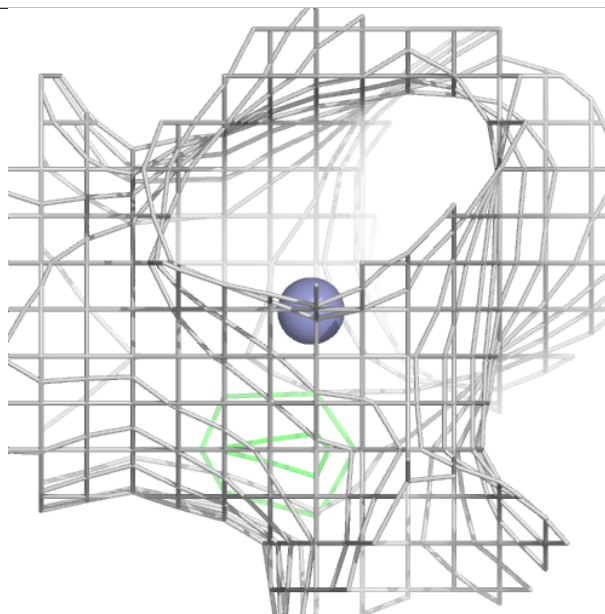
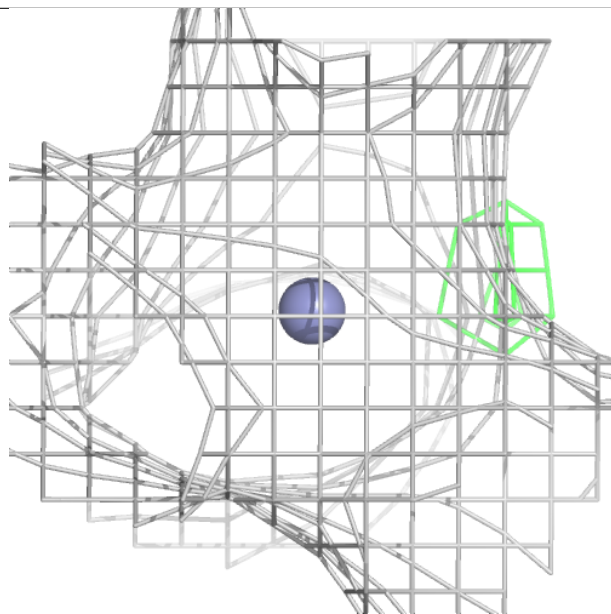
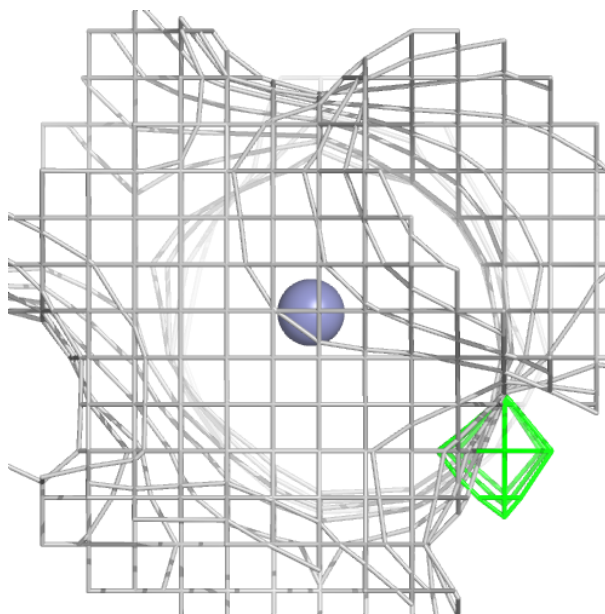
Electron density around ZN C 701:

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



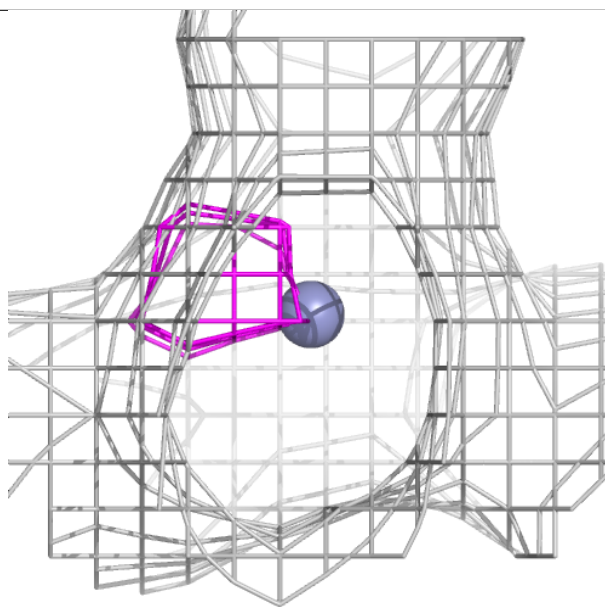
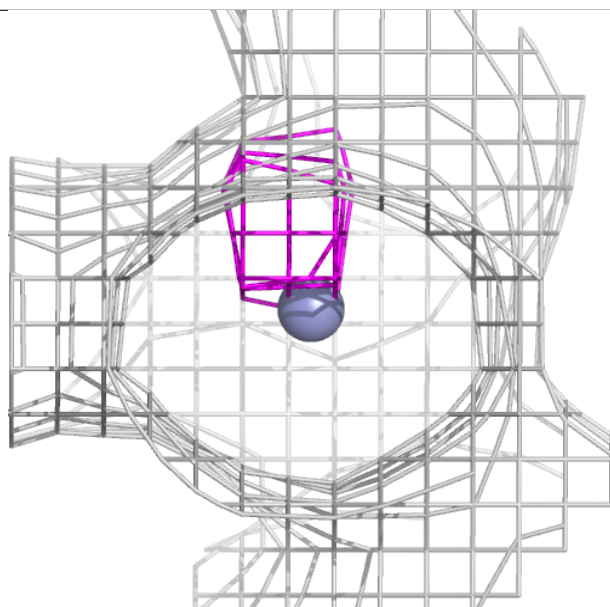
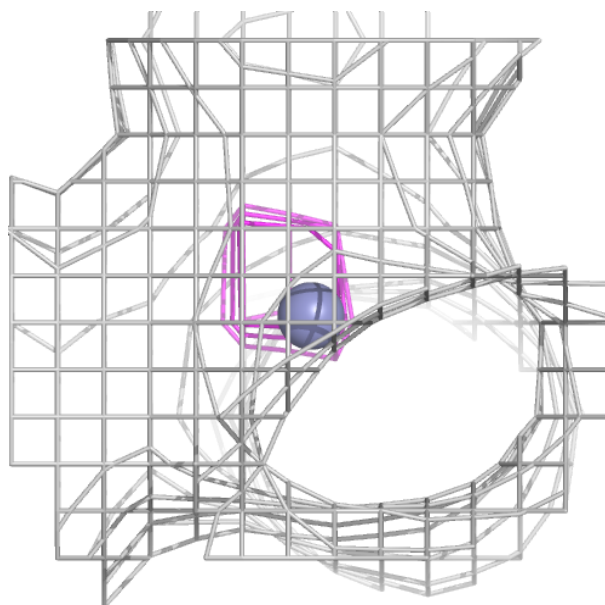
Electron density around ZN E 701:

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



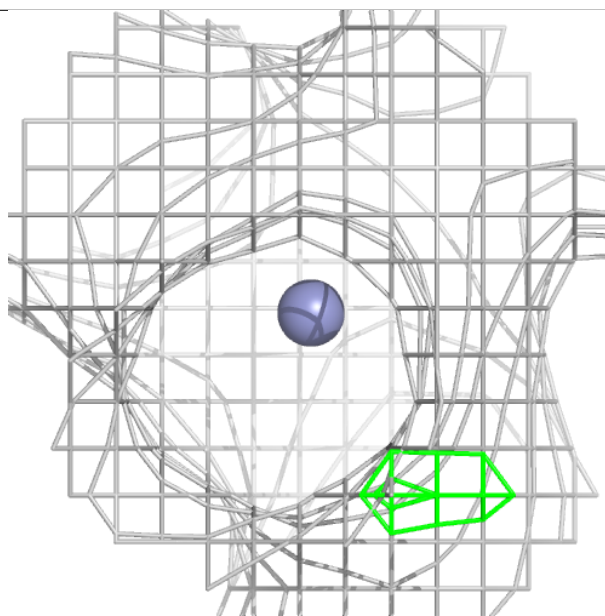
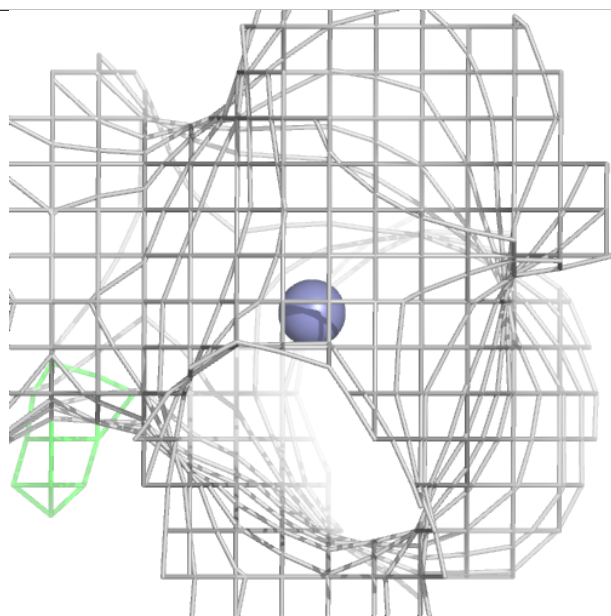
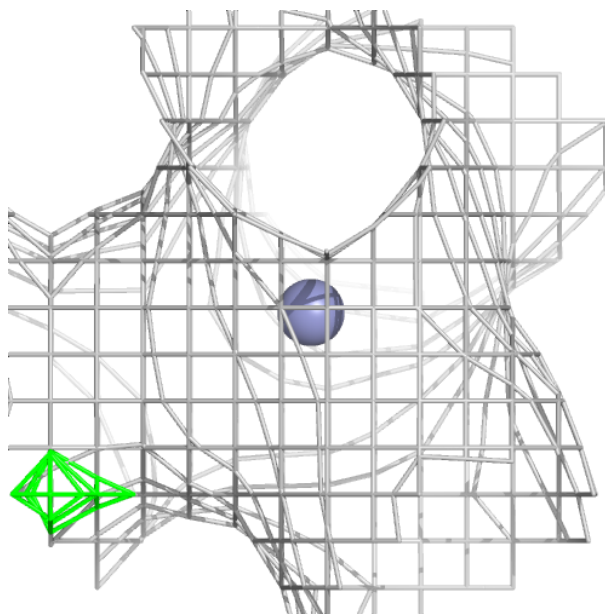
Electron density around ZN A 701:

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



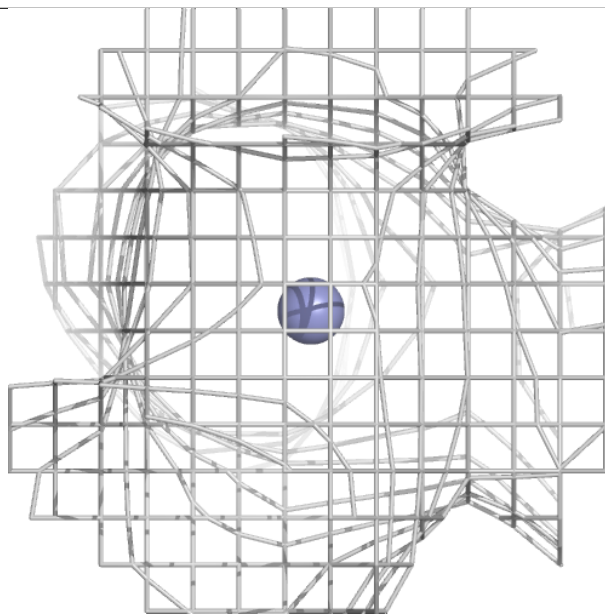
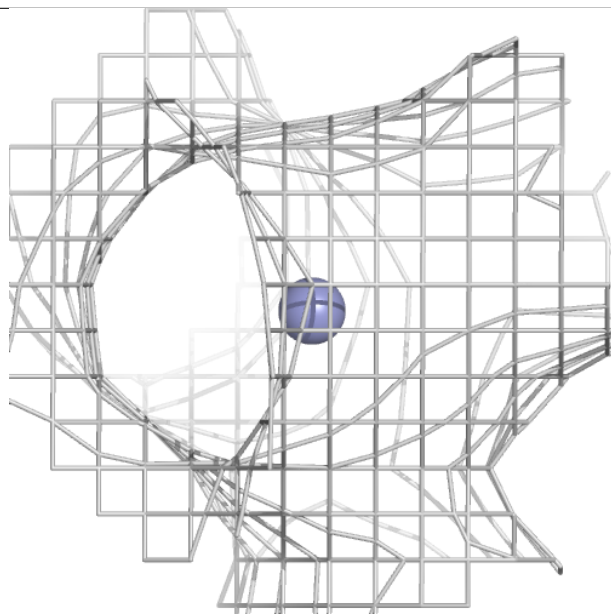
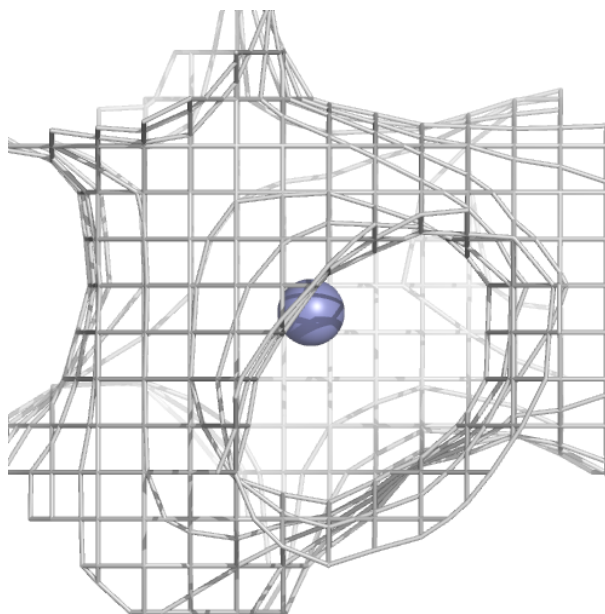
Electron density around ZN D 701:

$2mF_o-DF_c$ (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:

$2mF_o-DF_c$ (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.