



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:00 PM UTC

PDB ID : 9T7U / pdb_00009t7u
Title : Glyceraldehyde-3-phosphate dehydrogenase A (GAPDH)
Authors : Basle, A.; Pelicoli-Riboldi, G.; Waldron, K.
Deposited on : 2025-11-11
Resolution : 1.70 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

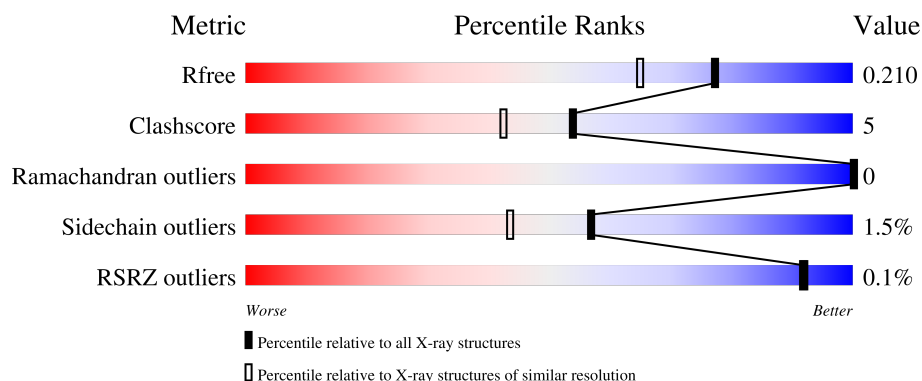
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	AAA	336	 89% 10% ..
1	BBB	336	 89% 10% ..
1	CCC	336	 89% 10% ..
1	DDD	336	 90% 8% ..

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACY	AAA	401	-	-	X	-
2	ACY	CCC	501	-	-	X	-
2	ACY	CCC	502	-	-	X	-
2	ACY	CCC	503	-	X	-	-

2 Entry composition [i](#)

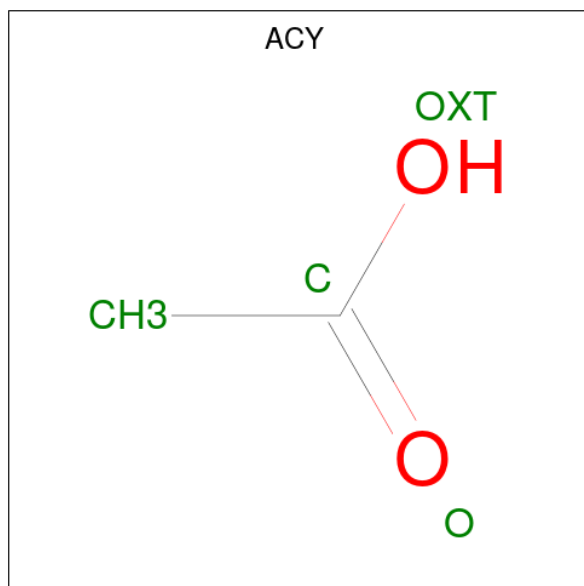
There are 6 unique types of molecules in this entry. The entry contains 10795 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde-3-phosphate dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	334	Total	C	N	O	S	0	0	0
			2529	1574	435	511	9			
1	BBB	334	Total	C	N	O	S	0	0	0
			2533	1577	436	511	9			
1	CCC	334	Total	C	N	O	S	0	0	0
			2529	1574	435	511	9			
1	DDD	332	Total	C	N	O	S	0	0	0
			2518	1568	433	508	9			

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0

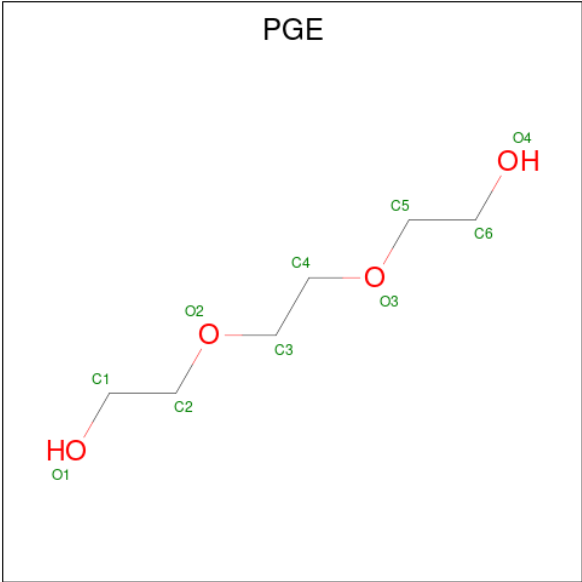
- Molecule 3 is COPPER (I) ION (CCD ID: CU1) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Cu 1 1	0	0
3	BBB	1	Total Cu 1 1	0	0
3	CCC	1	Total Cu 1 1	0	0
3	DDD	1	Total Cu 1 1	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	2	Total Na 2 2	0	0
4	BBB	2	Total Na 2 2	0	0
4	DDD	1	Total Na 1 1	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	DDD	1	Total	C	O	0	0
			10	6	4		

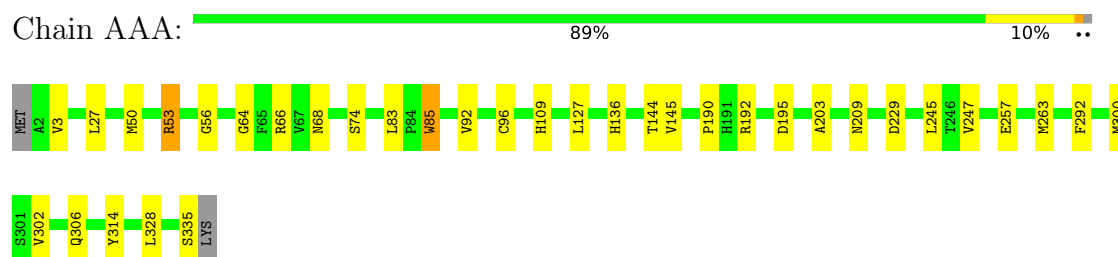
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	190	Total	O	0	0
			190	190		
6	BBB	165	Total	O	0	0
			165	165		
6	CCC	129	Total	O	0	0
			129	129		
6	DDD	147	Total	O	0	0
			147	147		

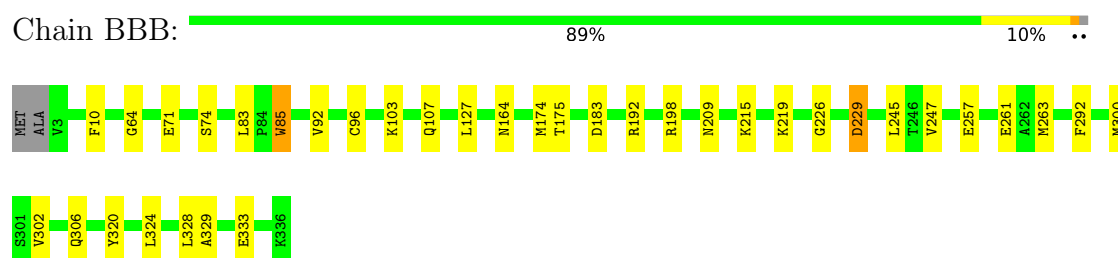
3 Residue-property plots [i](#)

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.

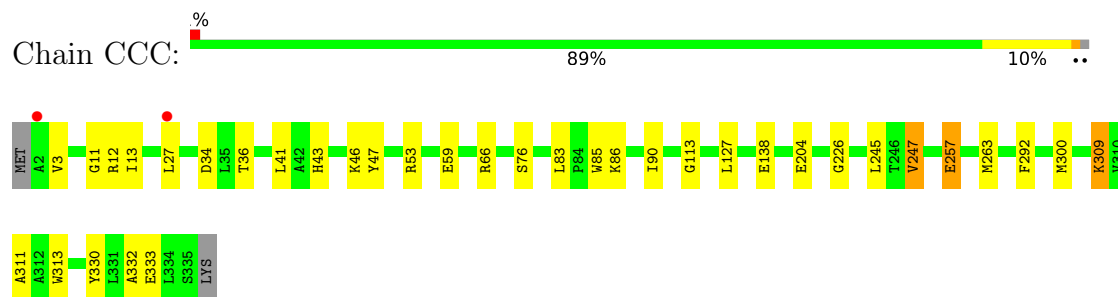
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



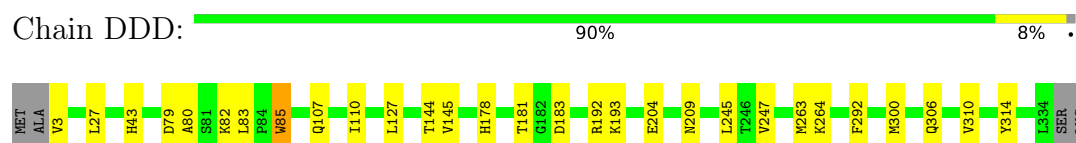
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.90Å 98.90Å 252.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.83 – 1.70 46.83 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.83-1.70) 100.0 (46.83-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.152 , 0.209 0.152 , 0.210	Depositor DCC
R_{free} test set	6948 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10795	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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: NA, ACY, PGE, CU1

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	AAA	1.07	3/2563 (0.1%)	1.22	6/3473 (0.2%)
1	BBB	1.02	0/2567	1.20	5/3477 (0.1%)
1	CCC	1.01	6/2563 (0.2%)	1.22	3/3473 (0.1%)
1	DDD	0.94	3/2552 (0.1%)	1.12	1/3458 (0.0%)
All	All	1.01	12/10245 (0.1%)	1.19	15/13881 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	192	ARG	CG-CD	6.04	1.70	1.52
1	AAA	136	HIS	CE1-NE2	6.02	1.38	1.32
1	CCC	204	GLU	CD-OE2	5.76	1.36	1.25
1	CCC	309	LYS	C-N	5.53	1.41	1.33
1	DDD	178	HIS	CG-ND1	5.35	1.44	1.38
1	DDD	204	GLU	CD-OE2	5.26	1.35	1.25
1	DDD	43	HIS	CE1-NE2	5.26	1.37	1.32
1	CCC	311	ALA	C-N	5.19	1.40	1.33
1	AAA	109	HIS	CG-ND1	5.16	1.44	1.38
1	CCC	313	TRP	C-N	5.14	1.40	1.33
1	CCC	43	HIS	CE1-NE2	5.12	1.37	1.32
1	CCC	257	GLU	CD-OE1	5.09	1.35	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	53	ARG	CB-CG-CD	6.88	127.13	111.30
1	AAA	195	ASP	CA-CB-CG	6.83	119.43	112.60
1	CCC	138	GLU	CB-CG-CD	6.17	123.09	112.60
1	BBB	257	GLU	CB-CG-CD	5.92	122.66	112.60
1	AAA	53	ARG	CB-CG-CD	-5.81	97.93	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	229	ASP	CA-C-N	-5.42	113.97	121.23
1	BBB	229	ASP	C-N-CA	-5.42	113.97	121.23
1	AAA	257	GLU	CB-CG-CD	5.28	121.57	112.60
1	BBB	96	CYS	CB-CA-C	-5.25	102.52	111.02
1	BBB	164	ASN	CA-CB-CG	-5.21	107.39	112.60
1	DDD	310	VAL	CA-C-O	-5.10	116.58	121.63
1	AAA	229	ASP	CA-C-N	-5.05	114.47	121.23
1	AAA	229	ASP	C-N-CA	-5.05	114.47	121.23
1	AAA	53	ARG	CG-CD-NE	5.03	123.06	112.00
1	CCC	247	VAL	O-C-N	5.03	128.70	123.02

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	AAA	2529	0	2504	18	0
1	BBB	2533	0	2512	25	0
1	CCC	2529	0	2504	38	0
1	DDD	2518	0	2494	20	0
2	AAA	12	0	9	3	0
2	CCC	16	0	13	9	0
2	DDD	8	0	7	1	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	1	0	0	0	0
4	AAA	2	0	0	0	0
4	BBB	2	0	0	0	0
4	DDD	1	0	0	0	0
5	DDD	10	0	14	1	0
6	AAA	190	0	0	2	0
6	BBB	165	0	0	5	0
6	CCC	129	0	0	1	0
6	DDD	147	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10795	0	10057	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (98) 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:CCC:3:VAL:HB	1:CCC:27:LEU:HD23	1.30	1.12
1:CCC:86:LYS:HG2	1:CCC:113:GLY:HA3	1.42	0.98
1:CCC:3:VAL:HB	1:CCC:27:LEU:CD2	1.94	0.96
1:CCC:85:TRP:CE3	1:CCC:90:ILE:CD1	2.55	0.89
1:DDD:79:ASP:O	1:DDD:82:LYS:HG2	1.73	0.88
1:BBB:215:LYS:HE3	1:BBB:229:ASP:OD1	1.73	0.85
1:CCC:11:GLY:HA3	2:CCC:504:ACY:H1	1.60	0.83
1:AAA:53:ARG:NH2	6:AAA:501:HOH:O	2.14	0.80
1:CCC:85:TRP:HA	1:CCC:90:ILE:HD12	1.63	0.79
1:CCC:86:LYS:HG2	1:CCC:113:GLY:CA	2.13	0.78
1:BBB:183:ASP:OD2	1:BBB:198:ARG:NH1	2.16	0.77
1:AAA:50:MET:O	2:AAA:401:ACY:H2	1.87	0.75
1:CCC:46:LYS:HE3	1:CCC:47:TYR:CE2	2.23	0.74
1:BBB:300:MET:HE1	1:CCC:226:GLY:O	1.87	0.73
1:AAA:335:SER:HA	6:AAA:640:HOH:O	1.89	0.71
2:CCC:501:ACY:O	2:CCC:502:ACY:H2	1.93	0.67
5:DDD:401:PGE:H62	6:DDD:509:HOH:O	1.94	0.67
1:BBB:192:ARG:HH21	1:DDD:192:ARG:NH2	1.93	0.66
1:CCC:85:TRP:CE3	1:CCC:90:ILE:HD11	2.29	0.66
1:AAA:64:GLY:HA2	1:AAA:74:SER:HB3	1.79	0.65
1:CCC:85:TRP:CE3	1:CCC:90:ILE:HD13	2.31	0.65
1:AAA:144:THR:HG23	1:AAA:145:VAL:HG23	1.79	0.64
1:CCC:34:ASP:O	1:CCC:76:SER:HA	1.97	0.64
2:DDD:402:ACY:H1	6:DDD:626:HOH:O	1.98	0.63
1:BBB:192:ARG:NH2	1:DDD:192:ARG:HH21	1.97	0.62
1:BBB:192:ARG:NH2	1:DDD:192:ARG:NH2	2.48	0.61
1:DDD:193:LYS:NZ	6:DDD:501:HOH:O	2.33	0.61
1:CCC:13:ILE:HG13	2:CCC:502:ACY:H1	1.82	0.61
1:BBB:175:THR:OG1	1:CCC:309:LYS:NZ	2.36	0.59
1:BBB:103:LYS:HE3	6:BBB:502:HOH:O	2.04	0.57
1:DDD:144:THR:HB	6:DDD:515:HOH:O	2.04	0.57
1:AAA:3:VAL:HB	1:AAA:27:LEU:HD23	1.86	0.56
1:CCC:13:ILE:CG1	2:CCC:502:ACY:H1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:85:TRP:CD2	1:CCC:90:ILE:HD13	2.41	0.56
1:CCC:13:ILE:HG12	2:CCC:501:ACY:H3	1.86	0.56
1:CCC:257:GLU:HG3	6:CCC:701:HOH:O	2.05	0.55
1:AAA:50:MET:O	2:AAA:401:ACY:CH3	2.53	0.55
1:CCC:13:ILE:H	2:CCC:501:ACY:CH3	2.19	0.55
1:BBB:215:LYS:CE	1:BBB:229:ASP:OD1	2.52	0.54
1:CCC:330:TYR:O	1:CCC:333:GLU:HG2	2.07	0.54
1:BBB:226:GLY:O	1:CCC:300:MET:HE1	2.08	0.53
1:CCC:83:LEU:HD13	1:CCC:85:TRP:CZ2	2.42	0.53
1:CCC:85:TRP:CA	1:CCC:90:ILE:HD12	2.36	0.53
1:CCC:36:THR:HG22	1:CCC:41:LEU:HD21	1.89	0.52
1:BBB:107:GLN:NE2	6:BBB:502:HOH:O	2.39	0.52
1:BBB:329:ALA:O	1:BBB:333:GLU:HG2	2.10	0.52
1:CCC:86:LYS:HE2	1:CCC:113:GLY:HA2	1.90	0.52
1:BBB:83:LEU:HD13	1:BBB:85:TRP:CZ2	2.45	0.52
1:CCC:13:ILE:H	2:CCC:501:ACY:H3	1.73	0.52
1:AAA:203:ALA:O	2:AAA:403:ACY:C	2.58	0.52
1:DDD:144:THR:HG23	1:DDD:145:VAL:HG23	1.92	0.52
1:AAA:263:MET:HG3	1:AAA:292:PHE:CZ	2.46	0.51
1:AAA:83:LEU:HD13	1:AAA:85:TRP:CZ2	2.46	0.51
1:BBB:245:LEU:HG	1:BBB:247:VAL:HG13	1.93	0.51
1:DDD:107:GLN:HA	1:DDD:110:ILE:HD12	1.92	0.51
1:DDD:83:LEU:HD13	1:DDD:85:TRP:CZ2	2.46	0.50
1:DDD:3:VAL:N	6:DDD:504:HOH:O	2.45	0.49
1:AAA:56:GLY:HA3	1:AAA:68:ASN:OD1	2.13	0.49
1:BBB:92:VAL:HG21	1:BBB:328:LEU:HD12	1.95	0.49
1:BBB:263:MET:HG3	1:BBB:292:PHE:CZ	2.48	0.48
1:BBB:300:MET:HE3	1:BBB:302:VAL:HG23	1.95	0.48
1:CCC:36:THR:CG2	1:CCC:41:LEU:HD21	2.43	0.48
1:CCC:245:LEU:HG	1:CCC:247:VAL:HG13	1.96	0.48
1:CCC:3:VAL:CB	1:CCC:27:LEU:CD2	2.80	0.48
1:DDD:263:MET:HG3	1:DDD:292:PHE:CZ	2.49	0.47
1:AAA:92:VAL:HG11	1:AAA:328:LEU:HD23	1.96	0.47
1:DDD:80:ALA:HA	1:DDD:83:LEU:HD12	1.96	0.47
1:CCC:85:TRP:CD2	1:CCC:90:ILE:CD1	2.97	0.46
1:BBB:300:MET:HE3	1:BBB:302:VAL:CG2	2.46	0.46
1:DDD:264:LYS:HD3	6:DDD:631:HOH:O	2.14	0.46
1:BBB:219:LYS:NZ	6:BBB:507:HOH:O	2.48	0.46
1:CCC:12:ARG:HB2	2:CCC:501:ACY:H1	1.98	0.45
1:BBB:261:GLU:HG2	6:BBB:660:HOH:O	2.15	0.45
1:CCC:36:THR:CG2	1:CCC:41:LEU:CD2	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:59:GLU:HG3	1:CCC:66:ARG:HB3	1.99	0.44
1:BBB:300:MET:O	1:BBB:306:GLN:HA	2.17	0.44
1:AAA:92:VAL:HG11	1:AAA:328:LEU:CD2	2.48	0.44
1:DDD:3:VAL:HB	1:DDD:27:LEU:HD23	2.00	0.44
1:DDD:263:MET:HG3	1:DDD:292:PHE:CE1	2.52	0.44
1:AAA:300:MET:HE3	1:AAA:302:VAL:CG2	2.48	0.43
1:AAA:263:MET:HG3	1:AAA:292:PHE:CE1	2.53	0.43
1:AAA:64:GLY:HA2	1:AAA:74:SER:CB	2.47	0.43
1:BBB:64:GLY:HA2	1:BBB:74:SER:HB3	1.99	0.43
1:CCC:263:MET:HG3	1:CCC:292:PHE:CZ	2.54	0.42
1:BBB:174:MET:HG2	1:BBB:175:THR:N	2.35	0.42
1:DDD:264:LYS:CD	6:DDD:631:HOH:O	2.68	0.42
1:CCC:3:VAL:HG21	1:CCC:332:ALA:HB1	2.01	0.42
1:CCC:12:ARG:N	2:CCC:501:ACY:H1	2.34	0.42
1:DDD:79:ASP:O	1:DDD:82:LYS:CG	2.55	0.42
1:AAA:245:LEU:HG	1:AAA:247:VAL:HG13	2.00	0.41
1:AAA:300:MET:O	1:AAA:306:GLN:HA	2.20	0.41
1:DDD:245:LEU:HG	1:DDD:247:VAL:HG13	2.01	0.41
1:DDD:300:MET:O	1:DDD:306:GLN:HA	2.20	0.41
1:CCC:263:MET:HG3	1:CCC:292:PHE:CE1	2.55	0.41
1:BBB:320:TYR:CE2	1:BBB:324:LEU:HD11	2.56	0.41
1:DDD:181:THR:OG1	1:DDD:183:ASP:OD1	2.36	0.41
1:CCC:85:TRP:HE3	1:CCC:90:ILE:CD1	2.25	0.41
1:BBB:71:GLU:HB2	6:BBB:641:HOH:O	2.20	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	AAA	332/336 (99%)	325 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	332/336 (99%)	323 (97%)	9 (3%)	0	100	100
1	CCC	332/336 (99%)	320 (96%)	12 (4%)	0	100	100
1	DDD	330/336 (98%)	318 (96%)	12 (4%)	0	100	100
All	All	1326/1344 (99%)	1286 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	272/274 (99%)	265 (97%)	7 (3%)	40	23
1	BBB	273/274 (100%)	269 (98%)	4 (2%)	57	43
1	CCC	272/274 (99%)	271 (100%)	1 (0%)	84	80
1	DDD	271/274 (99%)	267 (98%)	4 (2%)	57	43
All	All	1088/1096 (99%)	1072 (98%)	16 (2%)	57	43

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	66	ARG
1	AAA	85	TRP
1	AAA	96	CYS
1	AAA	127	LEU
1	AAA	190	PRO
1	AAA	209	ASN
1	AAA	314	TYR
1	BBB	10	PHE
1	BBB	85	TRP
1	BBB	127	LEU
1	BBB	209	ASN
1	CCC	127	LEU
1	DDD	85	TRP

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Mol	Chain	Res	Type
1	DDD	127	LEU
1	DDD	209	ASN
1	DDD	314	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	$\# Z > 2$
2	ACY	AAA	402	-	3,3,3	1.28	0	3,3,3	0.75	0
2	ACY	AAA	401	-	3,3,3	2.49	1 (33%)	3,3,3	1.04	0
2	ACY	CCC	503	-	3,3,3	3.13	2 (66%)	3,3,3	1.67	1 (33%)
2	ACY	CCC	504	-	3,3,3	1.33	0	3,3,3	0.99	0
2	ACY	CCC	501	-	3,3,3	2.06	1 (33%)	3,3,3	0.73	0
5	PGE	DDD	401	-	9,9,9	0.31	0	8,8,8	0.43	0
2	ACY	DDD	402	-	3,3,3	1.58	1 (33%)	3,3,3	1.88	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACY	AAA	403	-	3,3,3	2.79	2 (66%)	3,3,3	0.59	0
2	ACY	CCC	502	-	3,3,3	2.93	2 (66%)	3,3,3	1.42	0
2	ACY	DDD	403	-	3,3,3	1.97	1 (33%)	3,3,3	1.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	DDD	401	-	-	2/7/7/7	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	503	ACY	CH3-C	4.66	1.67	1.49
2	AAA	401	ACY	CH3-C	3.92	1.64	1.49
2	CCC	502	ACY	CH3-C	3.61	1.63	1.49
2	AAA	403	ACY	CH3-C	3.37	1.62	1.49
2	AAA	403	ACY	O-C	3.35	1.36	1.22
2	CCC	502	ACY	O-C	3.06	1.35	1.22
2	DDD	403	ACY	CH3-C	3.04	1.61	1.49
2	CCC	503	ACY	O-C	2.39	1.32	1.22
2	CCC	501	ACY	CH3-C	-2.37	1.39	1.49
2	DDD	402	ACY	OXT-C	2.31	1.41	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	402	ACY	O-C-CH3	-2.54	112.10	122.53
2	CCC	503	ACY	O-C-CH3	-2.10	113.92	122.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	DDD	401	PGE	C6-C5-O3-C4
5	DDD	401	PGE	O2-C3-C4-O3

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	401	ACY	2	0
2	CCC	504	ACY	1	0
2	CCC	501	ACY	6	0
5	DDD	401	PGE	1	0
2	DDD	402	ACY	1	0
2	AAA	403	ACY	1	0
2	CCC	502	ACY	3	0

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 [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	AAA	334/336 (99%)	-0.73	0 100 100	16, 23, 41, 54	0
1	BBB	334/336 (99%)	-0.65	0 100 100	17, 25, 45, 70	0
1	CCC	334/336 (99%)	-0.48	2 (0%) 85 88	16, 28, 58, 96	0
1	DDD	332/336 (98%)	-0.48	0 100 100	17, 28, 63, 91	0
All	All	1334/1344 (99%)	-0.58	2 (0%) 92 92	16, 26, 55, 96	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	2	ALA	2.2
1	CCC	27	LEU	2.0

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](#)

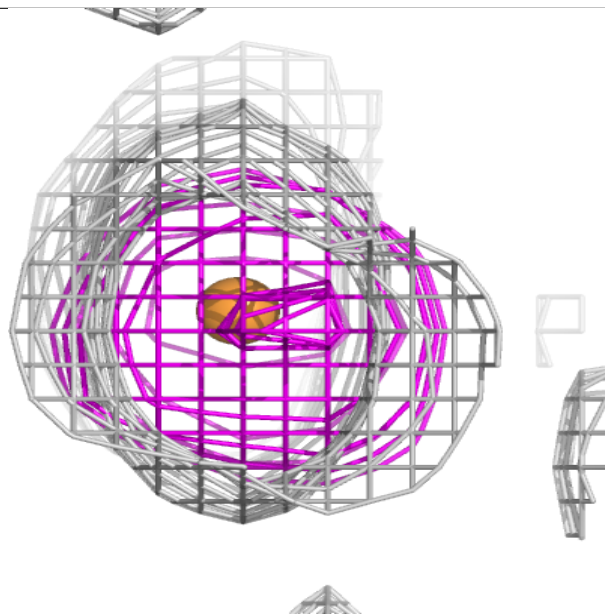
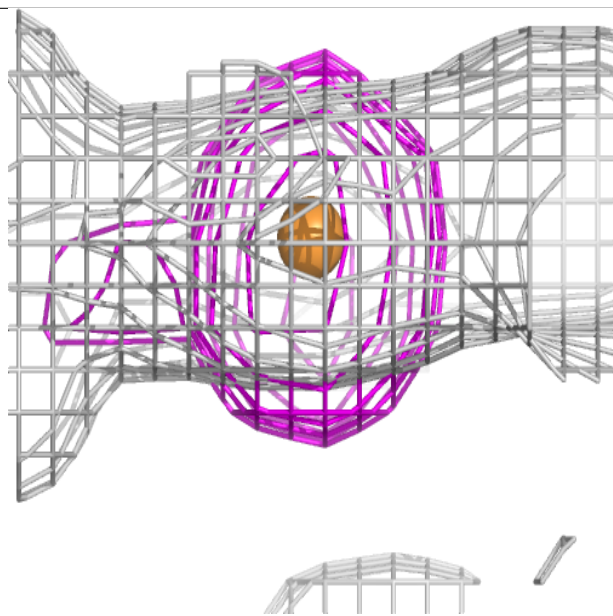
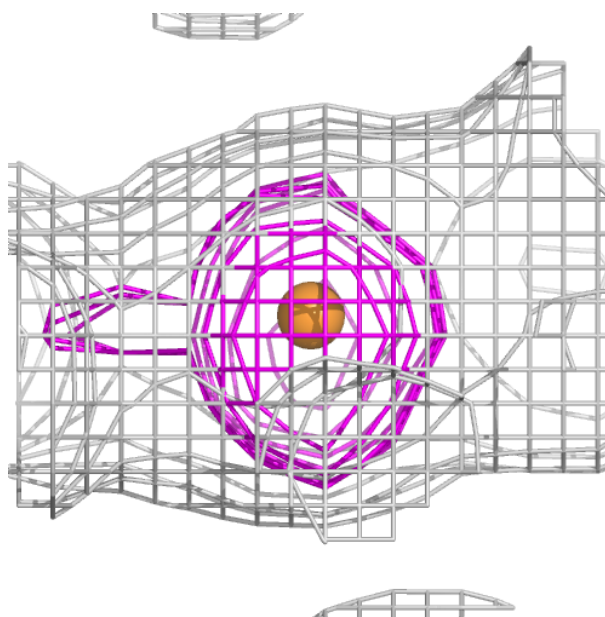
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACY	CCC	503	4/4	0.41	0.20	57,59,60,68	0
2	ACY	CCC	502	4/4	0.78	0.12	41,46,56,60	0
2	ACY	DDD	402	4/4	0.80	0.15	28,29,31,43	0
2	ACY	AAA	401	4/4	0.86	0.12	30,37,38,41	0
2	ACY	AAA	402	4/4	0.89	0.11	41,45,45,51	0
2	ACY	DDD	403	4/4	0.89	0.11	35,37,40,41	0
2	ACY	AAA	403	4/4	0.90	0.14	37,38,41,44	0
2	ACY	CCC	504	4/4	0.92	0.07	21,25,26,26	0
2	ACY	CCC	501	4/4	0.93	0.09	20,23,30,30	0
5	PGE	DDD	401	10/10	0.96	0.08	35,38,42,52	0
4	NA	AAA	406	1/1	0.98	0.05	38,38,38,38	0
3	CU1	DDD	404	1/1	0.99	0.10	34,34,34,34	0
4	NA	BBB	403	1/1	0.99	0.10	34,34,34,34	0
4	NA	DDD	405	1/1	0.99	0.05	39,39,39,39	0
4	NA	AAA	405	1/1	0.99	0.04	27,27,27,27	0
4	NA	BBB	402	1/1	1.00	0.03	29,29,29,29	0
3	CU1	AAA	404	1/1	1.00	0.10	32,32,32,32	0
3	CU1	BBB	401	1/1	1.00	0.13	35,35,35,35	0
3	CU1	CCC	505	1/1	1.00	0.09	35,35,35,35	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.

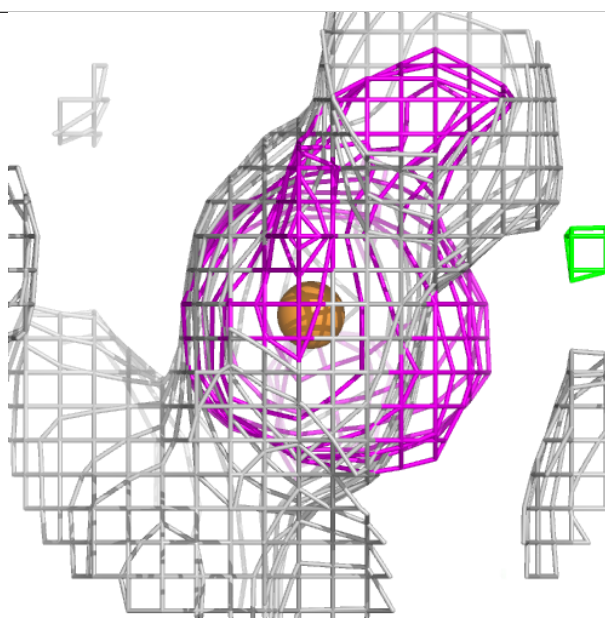
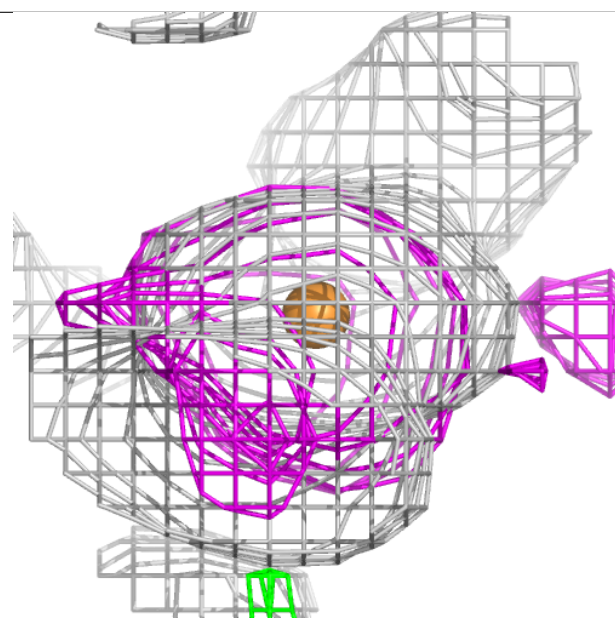
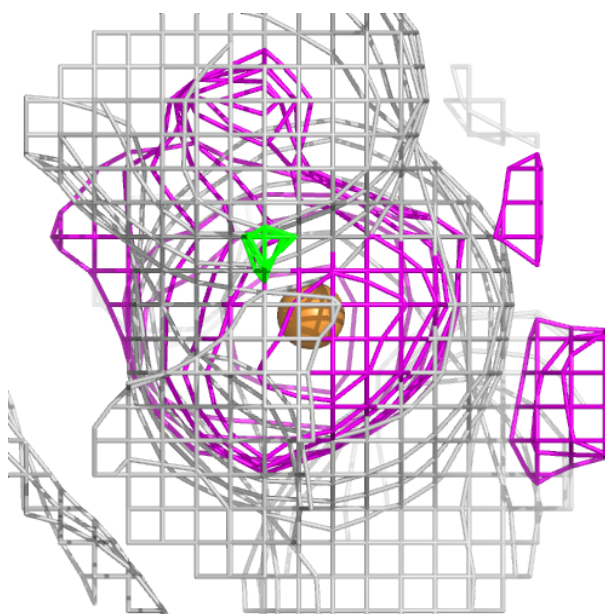
Electron density around CU1 DDD 404:

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



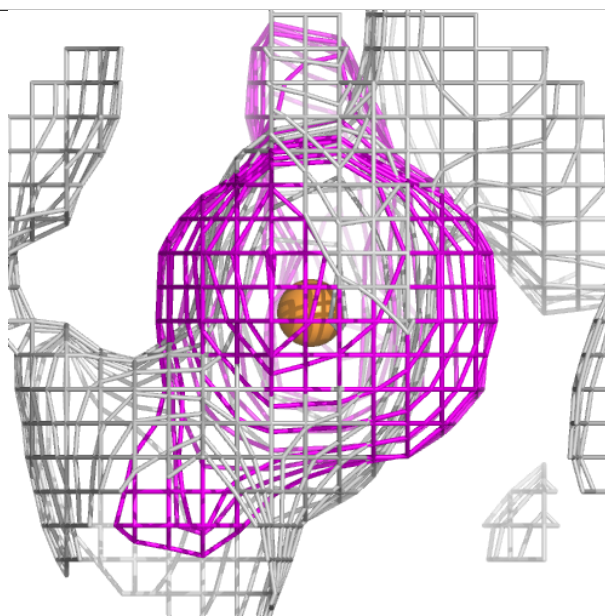
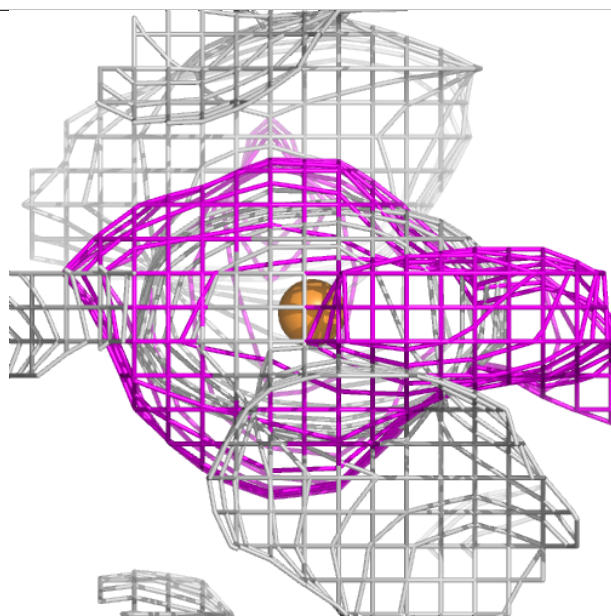
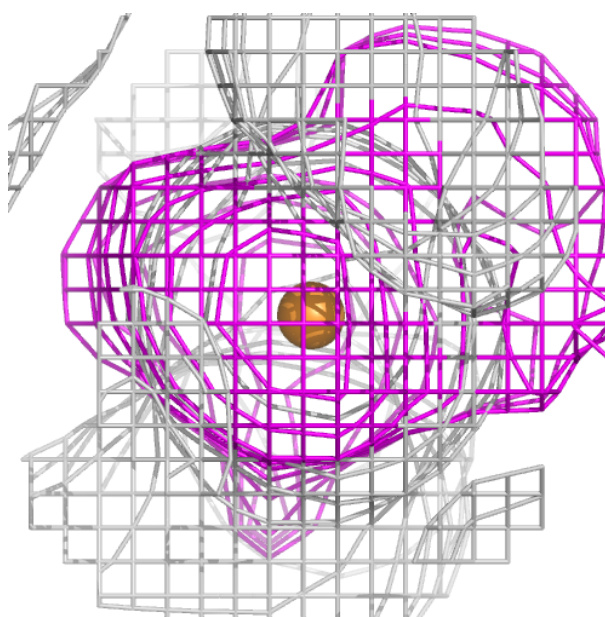
Electron density around CU1 AAA 404:

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and green (positive)



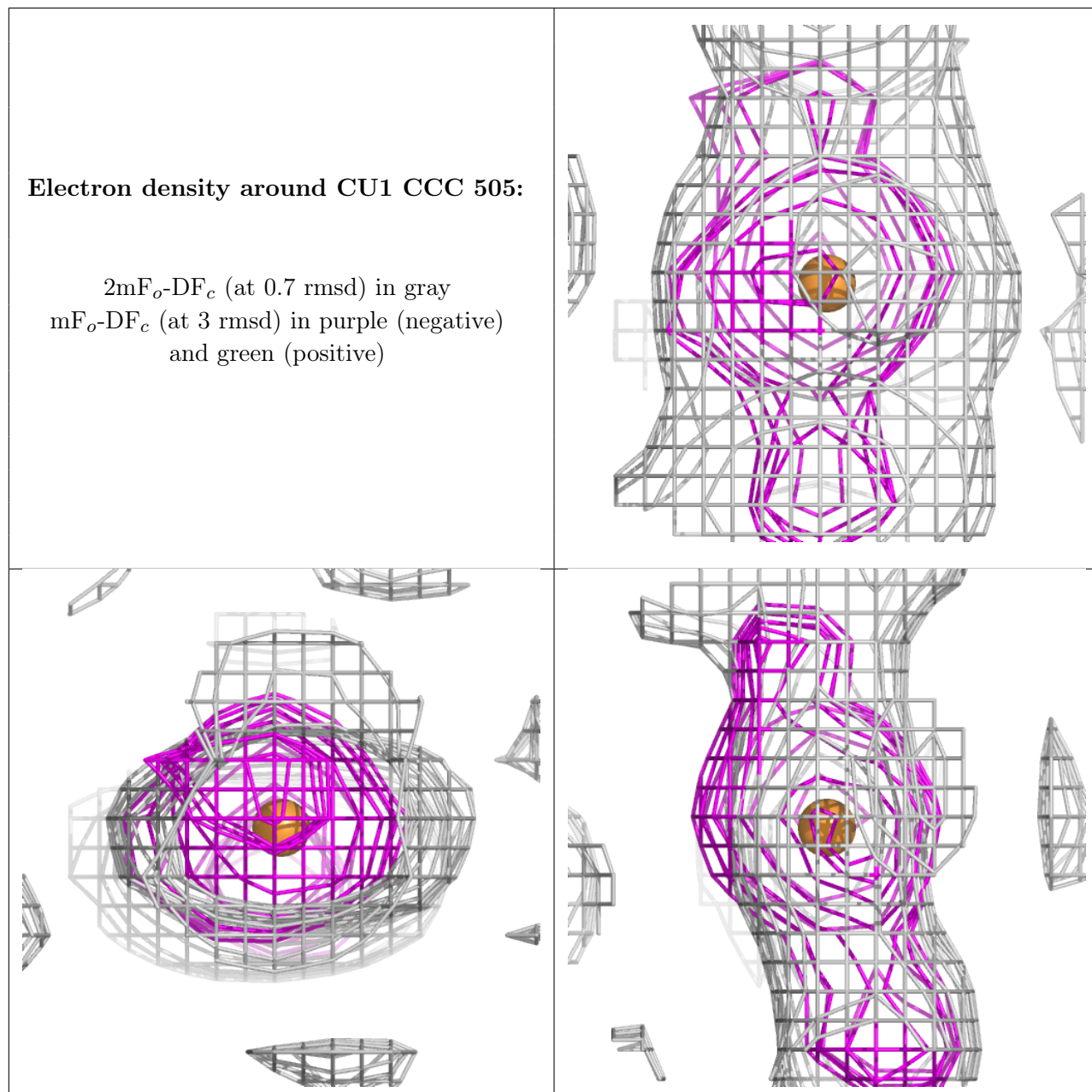
Electron density around CU1 BBB 401:

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



Electron density around CU1 CCC 505:

$2mF_o-DF_c$ (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.